Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 02:24 PM JST

PDB ID	:	7EWK
EMDB ID	:	EMD-31350
Title	:	Barley photosystem I-LHCI-Lhca6 supercomplex
Authors	:	Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on	:	2021-05-25
Resolution	:	3.88 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

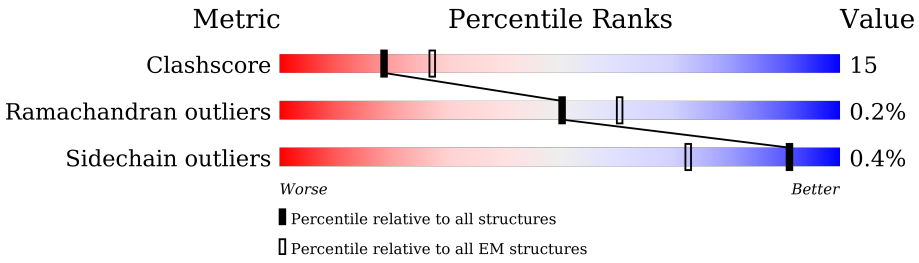
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	72% 28%
2	B	733	72% 27%
3	C	81	65% 35%
4	D	142	68% 32%
5	E	68	6% 75% 25%
6	F	158	65% 34%
7	H	61	25% 79% 21%
8	I	30	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	42	5% 64% 31% 5%
10	K	84	18% 73% 26%
11	L	146	12% 75% 25%
12	1	193	5% 62% 38%
13	3	222	14% 65% 34%
14	4	197	70% 30%
15	6	211	71% 28%

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
16	CL0	A	801	X	-	-	-
17	CLA	1	504	X	-	-	-
17	CLA	1	506	X	-	-	-
17	CLA	1	507	X	-	-	-
17	CLA	1	508	X	-	-	-
17	CLA	1	509	X	-	-	-
17	CLA	1	510	X	-	-	-
17	CLA	1	511	X	-	-	-
17	CLA	1	513	X	-	-	-
17	CLA	1	515	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	316	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	305	X	-	-	-
17	CLA	4	306	X	-	-	-
17	CLA	4	307	X	-	-	-
17	CLA	4	308	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	311	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	315	X	-	-	-
17	CLA	4	317	X	-	-	-
17	CLA	6	504	X	-	-	-
17	CLA	6	506	X	-	-	-
17	CLA	6	507	X	-	-	-
17	CLA	6	508	X	-	-	-
17	CLA	6	509	X	-	-	-
17	CLA	6	510	X	-	-	-
17	CLA	6	511	X	-	-	-
17	CLA	6	514	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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	852	X	-	-	-
17	CLA	A	853	X	-	-	-
17	CLA	B	801	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	812	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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	843	X	-	-	-
17	CLA	F	802	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	205	X	-	-	-
17	CLA	L	302	X	-	-	-
17	CLA	L	303	X	-	-	-
17	CLA	L	304	X	-	-	-
24	LUT	1	502	X	-	-	-
25	CHL	1	512	X	-	-	-
25	CHL	1	514	X	-	-	-
25	CHL	1	517	X	-	-	-
25	CHL	3	313	X	-	-	-
25	CHL	4	313	X	-	-	-
25	CHL	4	314	X	-	-	-
25	CHL	4	316	X	-	-	-
25	CHL	6	512	X	-	-	-
25	CHL	6	513	X	-	-	-
25	CHL	6	515	X	-	-	-
25	CHL	6	517	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 32765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5798	3797	987	996	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5840	3832	991	1003	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			613	377	105	119	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1112	714	195	200	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			540	341	99	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1188	768	203	216	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			447	298	73	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	30	Total	C	N	O	S	0	0
			235	163	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			332	225	51	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			576	361	101	110	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	146	Total	C	N	O	0	0
			1090	720	174	196		

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	193	Total	C	N	O	S	0	0
			1484	965	248	269	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	222	Total	C	N	O	S	0	0
			1672	1097	272	298	5		

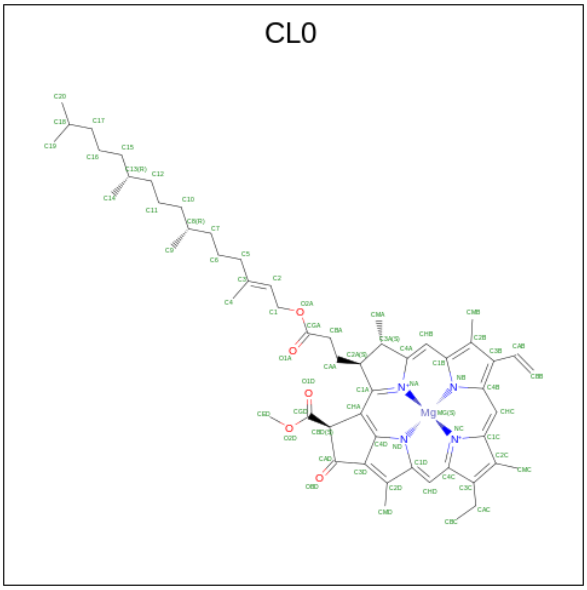
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	197	Total	C	N	O	S	0	0
			1529	991	253	282	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca6.

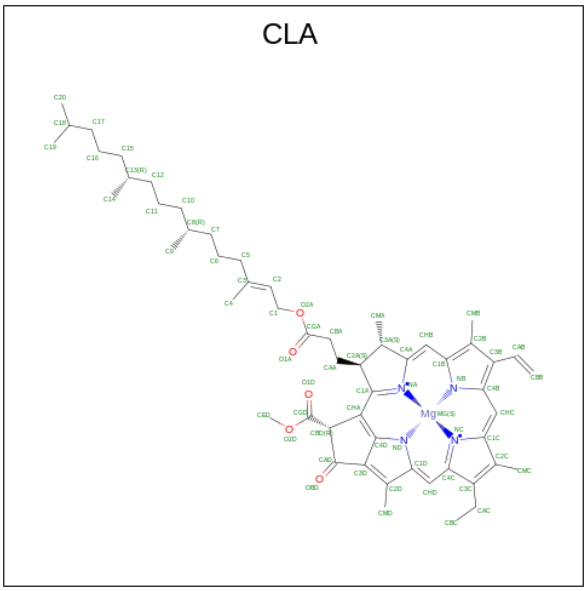
Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	211	Total	C	N	O	S	0	0
			1655	1088	274	285	8		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

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



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
17	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

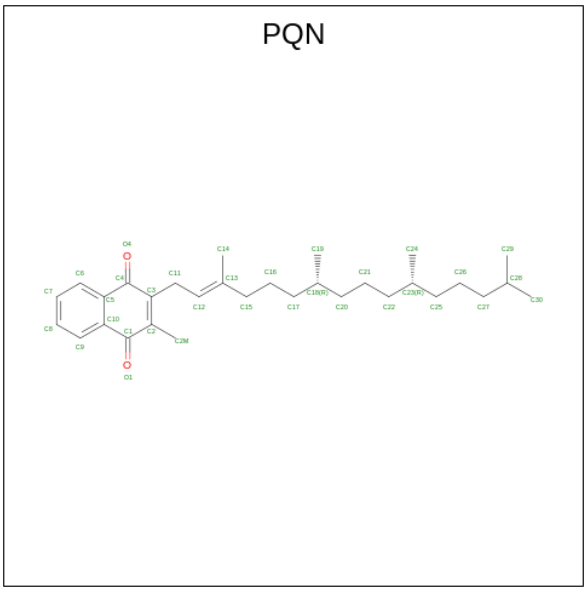
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

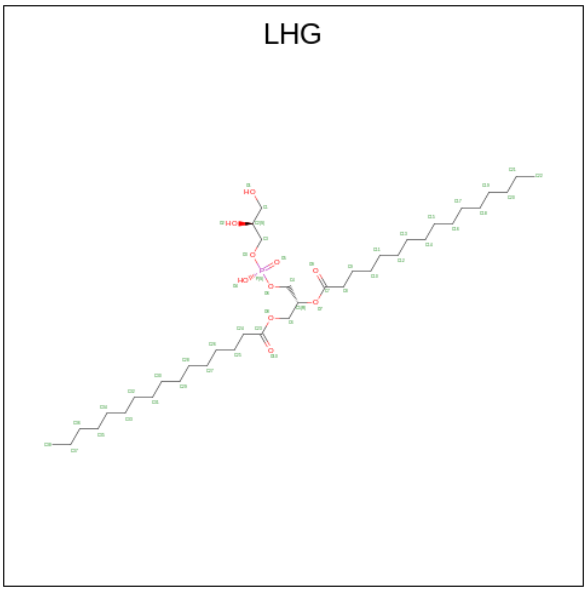
Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			14	12	2	
18	B	1	Total	C	O	0
			16	14	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



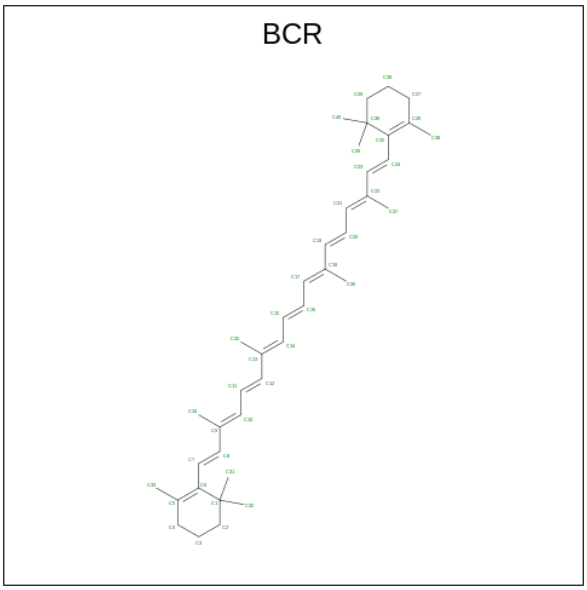
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			40	29	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O P 25 15 9 1	0
19	B	1	Total C O P 38 27 10 1	0
19	1	1	Total C O P 49 38 10 1	0
19	6	1	Total C O P 35 24 10 1	0

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



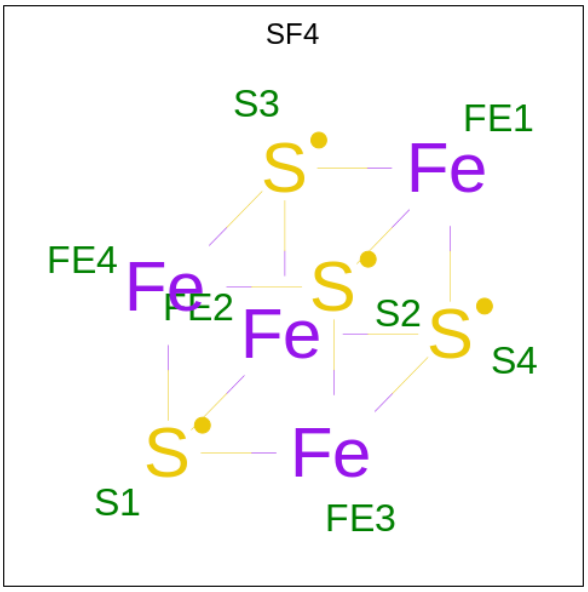
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

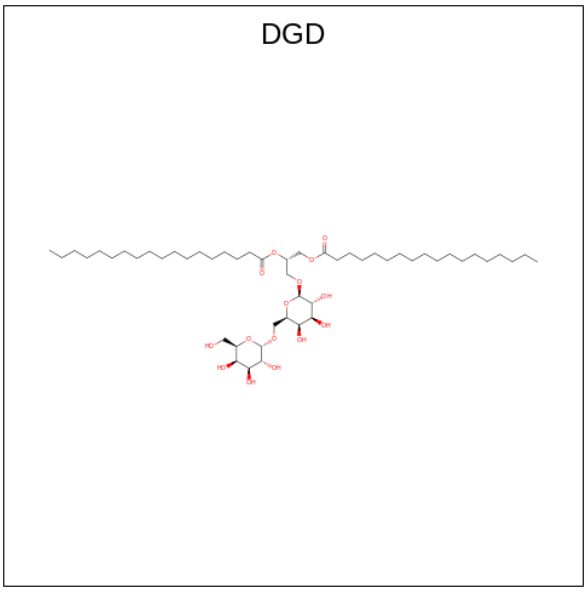
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 39 39	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	1	1	Total C 11 11	0
20	3	1	Total C 40 40	0
20	4	1	Total C 40 40	0
20	6	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



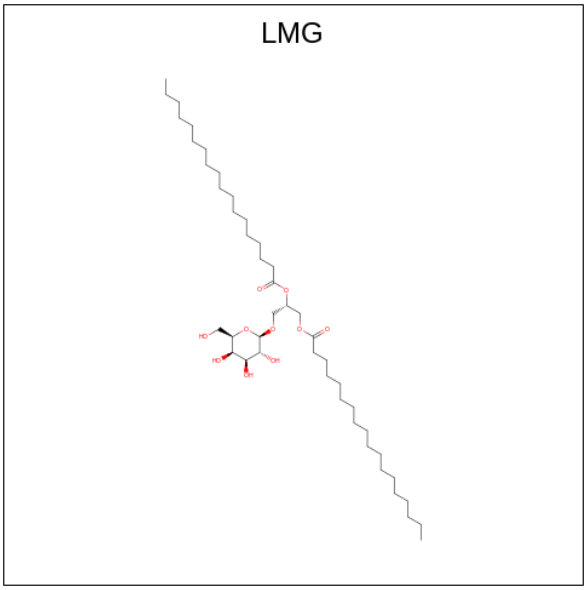
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0
21	C	1	Total Fe S 8 4 4	0

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



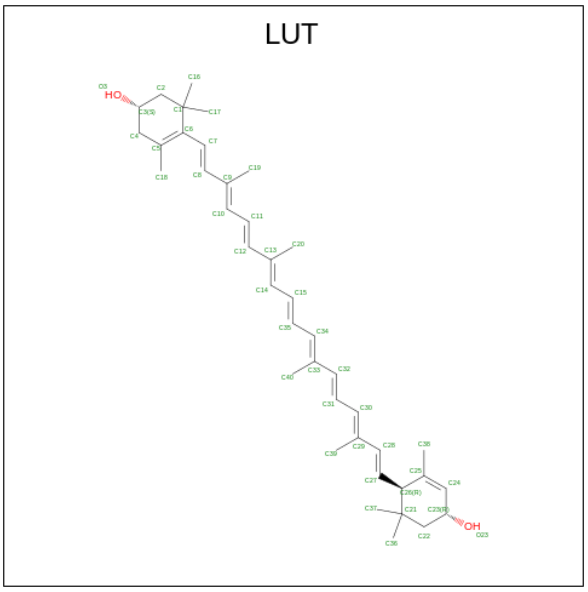
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total 52	C 37	O 15	0
22	J	1	Total 66	C 51	O 15	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



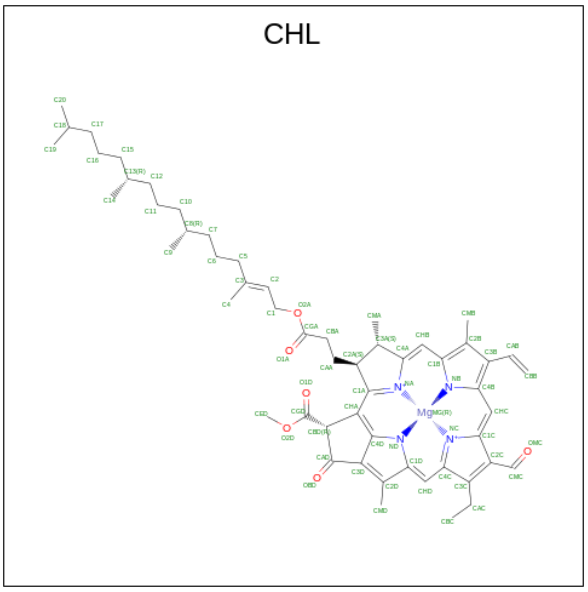
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total 30	C 20	O 10	0
23	4	1	Total 18	C 10	O 8	0

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



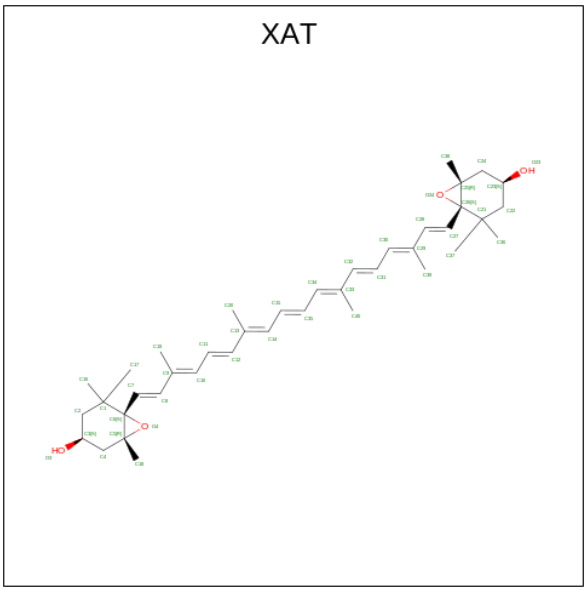
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	1	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	4	1	Total	C	O	0
			42	40	2	
24	6	1	Total	C	O	0
			42	40	2	

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 26 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: $C_{40}H_{56}O_4$).



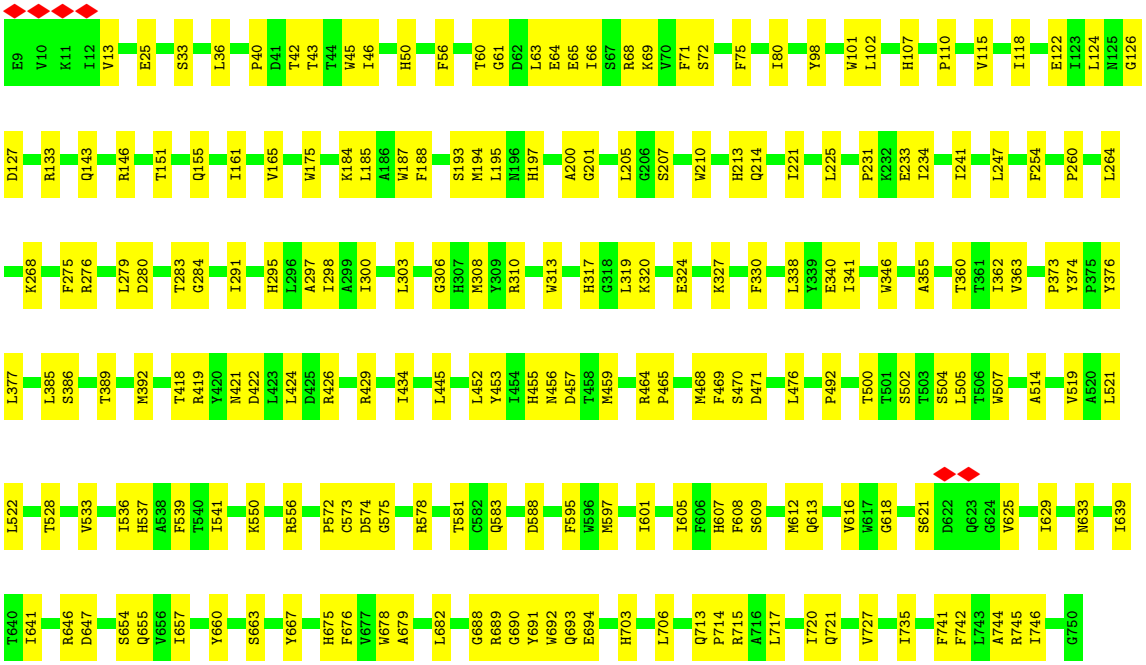
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			44	40	4	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

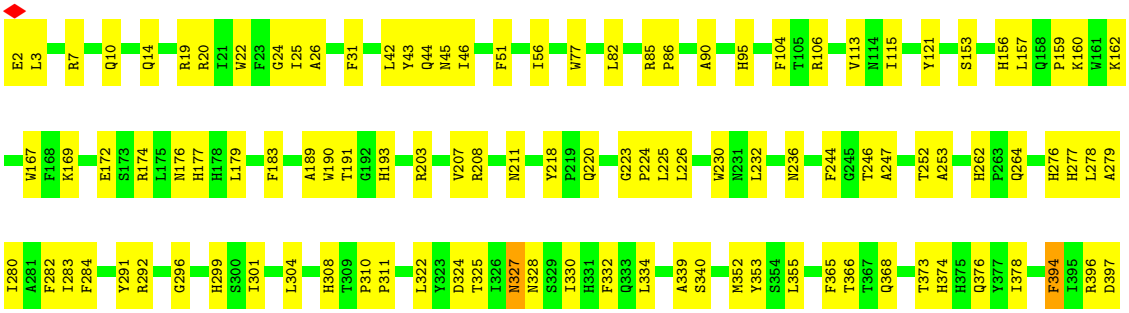
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



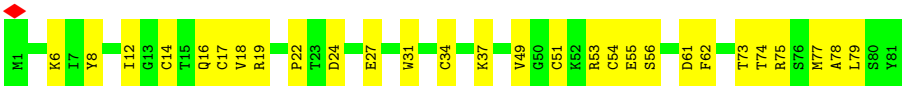
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



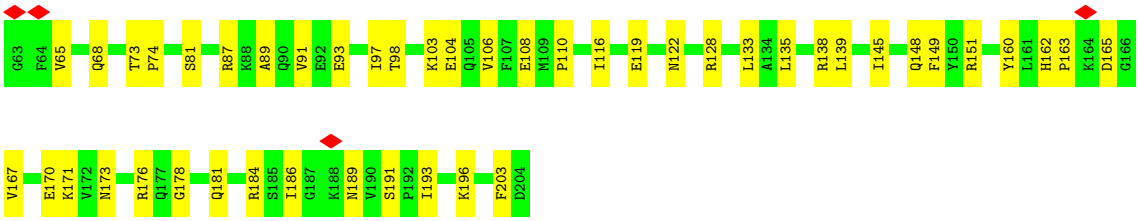
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



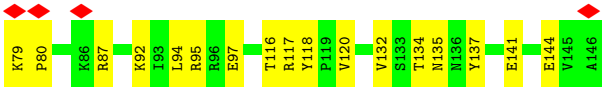
• Molecule 4: Photosystem I reaction center subunit D

Chain D:



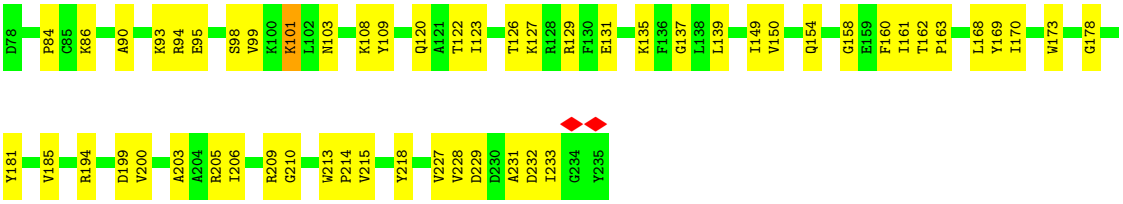
• Molecule 5: Photosystem I reaction center subunit E

Chain E:



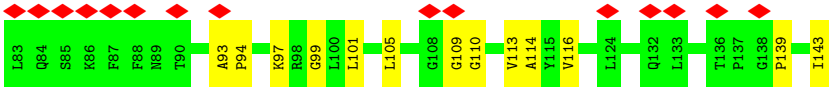
• Molecule 6: Photosystem I reaction center subunit F

Chain F:

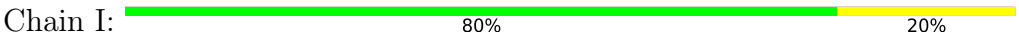


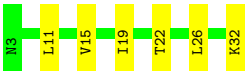
• Molecule 7: Photosystem I reaction center subunit H

Chain H:

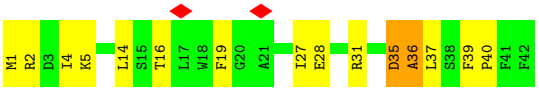


• Molecule 8: Photosystem I reaction center subunit VIII

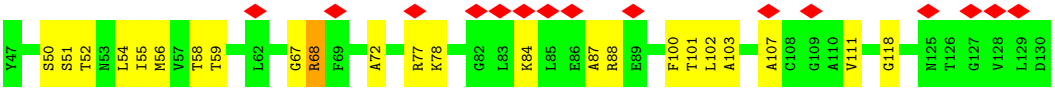




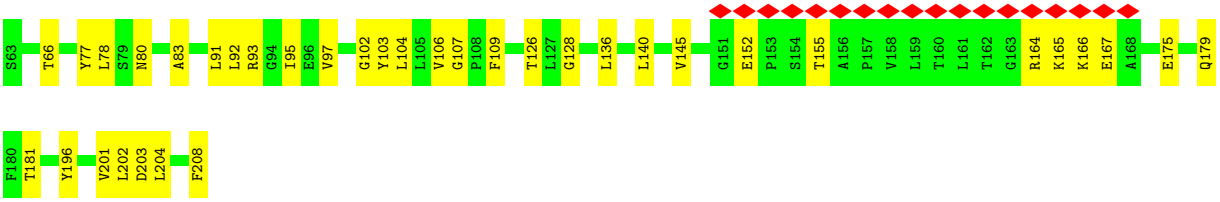
• Molecule 9: Photosystem I reaction center subunit IX



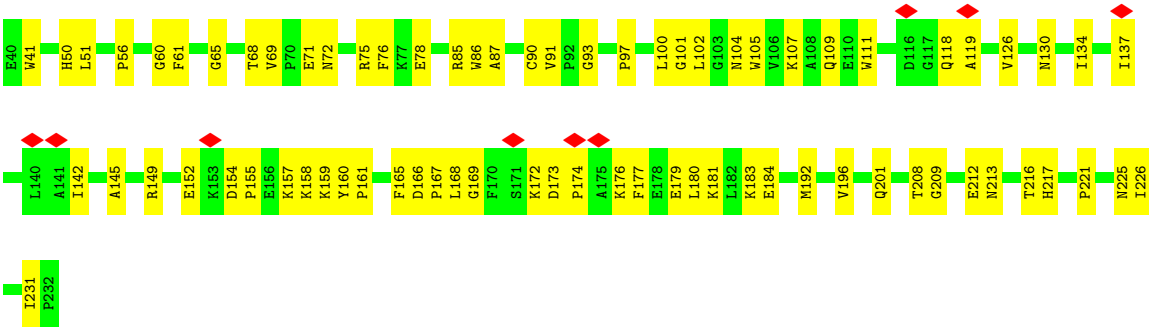
• Molecule 10: Photosystem I reaction center subunit K



• Molecule 11: Photosystem I reaction center subunit L

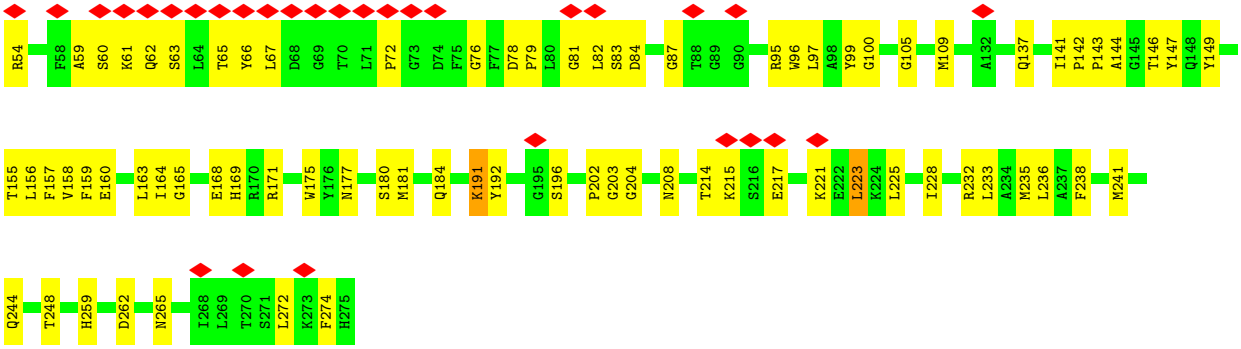


• Molecule 12: Chlorophyll a-b binding protein Lhca1



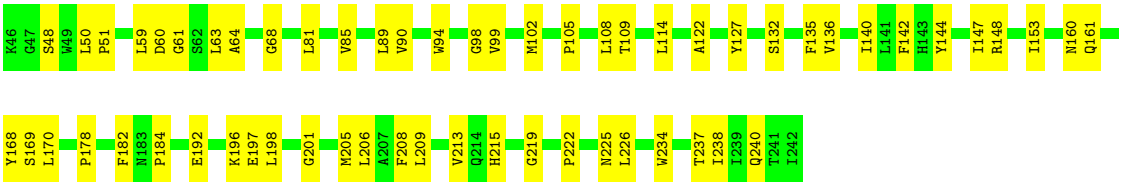
• Molecule 13: Chlorophyll a-b binding protein Lhca3

Chain 3:



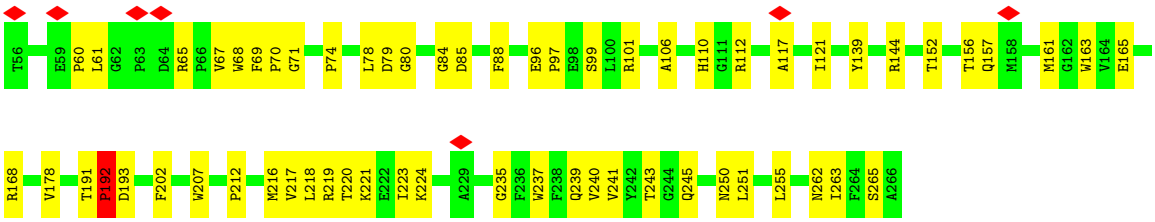
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



• Molecule 15: Chlorophyll a-b binding protein Lhca6

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.561	Depositor
Minimum map value	-1.733	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

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: DGD, LUT, CL0, LHG, SF4, PQN, BCR, CHL, CLA, XAT, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/5993	0.43	0/8178
2	B	0.36	3/6052 (0.0%)	0.43	1/8267 (0.0%)
3	C	0.30	0/624	0.46	0/844
4	D	0.27	0/1141	0.47	0/1540
5	E	0.30	0/553	0.47	0/751
6	F	0.26	0/1214	0.45	0/1643
7	H	0.26	0/460	0.45	0/623
8	I	0.27	0/241	0.41	0/327
9	J	0.26	0/342	0.45	0/465
10	K	0.26	0/581	0.51	0/786
11	L	0.27	0/1122	0.46	0/1537
12	1	0.28	0/1535	0.45	0/2097
13	3	0.30	0/1727	0.48	0/2353
14	4	0.27	0/1577	0.44	0/2153
15	6	0.27	0/1723	0.48	2/2358 (0.1%)
All	All	0.31	3/24885 (0.0%)	0.45	3/33922 (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
9	J	0	1
12	1	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	TRP	CB-CG	-10.12	1.32	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	TRP	C-O	-6.31	1.11	1.23
2	B	657	TRP	CG-CD1	-6.28	1.27	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	657	TRP	CB-CA-C	-5.93	98.55	110.40
15	6	192	PRO	N-CA-C	5.69	126.89	112.10
15	6	192	PRO	C-N-CA	-5.19	108.73	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1	231	ILE	Peptide
9	J	35	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5798	0	5613	173	0
2	B	5840	0	5580	173	0
3	C	613	0	607	27	0
4	D	1112	0	1113	40	0
5	E	540	0	539	12	0
6	F	1188	0	1178	39	0
7	H	447	0	472	9	0
8	I	235	0	261	6	0
9	J	332	0	335	17	0
10	K	576	0	584	17	0
11	L	1090	0	1075	30	0
12	1	1484	0	1410	62	0
13	3	1672	0	1575	69	0
14	4	1529	0	1448	47	0
15	6	1655	0	1530	54	0
16	A	61	0	62	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	1	474	0	373	27	0
17	3	543	0	404	28	0
17	4	525	0	424	23	0
17	6	447	0	371	25	0
17	A	2028	0	1626	85	0
17	B	1921	0	1521	85	0
17	F	41	0	29	0	0
17	J	83	0	59	1	0
17	K	162	0	112	3	0
17	L	145	0	118	7	0
18	A	14	0	7	2	0
18	B	16	0	10	7	0
19	1	49	0	74	7	0
19	6	35	0	40	1	0
19	A	65	0	77	2	0
19	B	38	0	46	1	0
20	1	11	0	16	1	0
20	3	40	0	56	3	0
20	4	40	0	56	5	0
20	6	40	0	56	4	0
20	A	280	0	392	23	0
20	B	239	0	333	13	0
20	F	80	0	112	2	0
20	I	80	0	112	5	0
20	J	40	0	56	3	0
20	K	40	0	56	1	0
20	L	80	0	112	3	0
21	B	8	0	0	0	0
21	C	16	0	0	1	0
22	B	52	0	62	2	0
22	J	66	0	96	2	0
23	4	18	0	12	0	0
23	J	30	0	30	1	0
24	1	84	0	111	12	0
24	3	84	0	112	11	0
24	4	42	0	56	9	0
24	6	42	0	56	6	0
25	1	137	0	91	6	0
25	3	46	0	31	1	0
25	4	141	0	97	3	0
25	6	183	0	121	8	0
26	4	44	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	6	44	0	56	9	0
All	All	32765	0	31017	927	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (927) 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)
2:B:700:LEU:HB2	18:B:844:PQN:H6	1.62	0.81
3:C:54:CYS:SG	3:C:55:GLU:N	2.61	0.72
6:F:215:VAL:O	6:F:218:TYR:HB3	1.89	0.72
1:A:175:TRP:HB2	17:A:810:CLA:HMC3	1.72	0.71
12:1:90:CYS:CB	24:1:502:LUT:H392	2.21	0.70
15:6:67:VAL:HG22	15:6:69:PHE:H	1.57	0.69
15:6:207:TRP:HA	15:6:212:PRO:HG3	1.75	0.69
1:A:69:LYS:NZ	17:A:810:CLA:OBD	2.26	0.69
2:B:174:ARG:HE	17:B:826:CLA:HMD1	1.58	0.69
1:A:197:HIS:O	1:A:201:GLY:N	2.24	0.69
15:6:161:MET:HG2	17:6:514:CLA:HMC3	1.75	0.68
17:1:509:CLA:H11	17:1:515:CLA:CAD	2.23	0.68
2:B:700:LEU:HB2	18:B:844:PQN:C6	2.23	0.68
2:B:299:HIS:HD2	2:B:304:LEU:HD21	1.59	0.67
13:3:168:GLU:OE2	13:3:171:ARG:NE	2.27	0.67
14:4:51:PRO:HB2	15:6:178:VAL:HG22	1.76	0.67
2:B:311:PRO:HB2	19:B:852:LHG:HC12	1.77	0.66
15:6:168:ARG:NH2	17:6:514:CLA:O1D	2.27	0.66
3:C:73:THR:HG22	3:C:74:THR:H	1.59	0.66
1:A:453:TYR:HB3	1:A:641:ILE:HD11	1.78	0.66
1:A:33:SER:HB3	1:A:36:LEU:HB2	1.78	0.66
1:A:210:TRP:NE1	1:A:214:GLN:OE1	2.29	0.66
19:1:516:LHG:H151	19:1:516:LHG:H271	1.78	0.66
12:1:69:VAL:HB	12:1:72:ASN:HB2	1.79	0.65
14:4:144:TYR:OH	14:4:148:ARG:NH1	2.29	0.65
1:A:13:VAL:HG22	1:A:184:LYS:HD3	1.78	0.65
12:1:152:GLU:O	12:1:158:LYS:NZ	2.29	0.65
14:4:234:TRP:O	14:4:240:GLN:NE2	2.29	0.65
17:4:309:CLA:H3A	25:4:316:CHL:HBC2	1.78	0.65
13:3:225:LEU:O	13:3:228:ILE:HG22	1.97	0.65
14:4:98:GLY:O	14:4:102:MET:HG2	1.97	0.65
2:B:90:ALA:HA	2:B:113:VAL:HG12	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:203:ASP:HB2	11:L:208:PHE:HZ	1.63	0.64
2:B:353:TYR:HA	2:B:368:GLN:HE21	1.62	0.64
14:4:226:LEU:HD11	24:4:302:LUT:H163	1.78	0.64
3:C:61:ASP:HA	5:E:135:ASN:HD22	1.62	0.64
11:L:104:LEU:HD11	17:L:303:CLA:HMB3	1.78	0.64
15:6:262:ASN:H	15:6:265:SER:HG	1.43	0.64
2:B:352:MET:O	2:B:368:GLN:NE2	2.30	0.64
2:B:683:GLU:OE2	4:D:87:ARG:N	2.31	0.64
13:3:164:ILE:HG21	17:3:314:CLA:HMC3	1.80	0.64
1:A:426:ARG:HG2	1:A:429:ARG:HH21	1.62	0.64
5:E:116:THR:HG22	5:E:118:TYR:H	1.63	0.64
12:1:201:GLN:OE1	12:1:213:ASN:ND2	2.31	0.64
1:A:655:GLN:OE1	1:A:745:ARG:NH1	2.31	0.64
2:B:582:TRP:CH2	17:B:803:CLA:HAB	2.33	0.64
15:6:192:PRO:O	15:6:193:ASP:C	2.30	0.64
1:A:194:MET:HB2	17:A:812:CLA:HBC2	1.80	0.63
17:B:835:CLA:HBD	17:B:835:CLA:HBA1	1.79	0.63
2:B:654:HIS:NE2	17:B:804:CLA:NA	2.45	0.63
12:1:142:ILE:HD11	17:1:515:CLA:HMB3	1.80	0.63
1:A:193:SER:O	1:A:197:HIS:ND1	2.30	0.63
17:A:809:CLA:H2A	17:A:809:CLA:O2D	1.99	0.63
2:B:397:ASP:OD1	4:D:196:LYS:NZ	2.31	0.63
1:A:42:THR:HG22	1:A:713:GLN:HB2	1.81	0.63
2:B:700:LEU:CB	18:B:844:PQN:H6	2.28	0.63
15:6:112:ARG:NH1	25:6:513:CHL:OBD	2.32	0.63
1:A:578:ARG:HH11	1:A:581:THR:HG21	1.64	0.63
17:A:828:CLA:CBA	17:A:828:CLA:O1A	2.46	0.63
2:B:481:THR:O	2:B:487:ASN:ND2	2.31	0.62
2:B:169:LYS:NZ	2:B:327:ASN:O	2.29	0.62
11:L:140:LEU:HB3	11:L:181:THR:HG22	1.80	0.62
1:A:717:LEU:HD23	1:A:721:GLN:HG2	1.82	0.62
13:3:177:ASN:ND2	15:6:71:GLY:O	2.32	0.62
13:3:137:GLN:HG2	13:3:144:ALA:HB1	1.81	0.62
24:1:502:LUT:H28	24:1:502:LUT:H361	1.82	0.62
1:A:241:ILE:HD11	17:A:814:CLA:HMA3	1.81	0.62
26:6:502:XAT:H193	25:6:512:CHL:HMB1	1.82	0.62
1:A:573:CYS:SG	1:A:575:GLY:N	2.71	0.62
17:A:806:CLA:HMA1	17:A:807:CLA:HMB3	1.81	0.61
9:J:28:GLU:OE1	9:J:31:ARG:NH2	2.32	0.61
12:1:109:GLN:HG2	17:1:515:CLA:HAC2	1.81	0.61
19:1:516:LHG:H342	14:4:140:ILE:HD13	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:180:LEU:HD23	12:1:183:LYS:HD2	1.82	0.61
10:K:67:GLY:O	10:K:77:ARG:NH1	2.29	0.61
11:L:126:THR:HG21	11:L:196:TYR:HB2	1.83	0.61
1:A:706:LEU:HD21	17:B:833:CLA:H3A	1.83	0.61
2:B:529:THR:O	2:B:533:ILE:HG12	2.00	0.61
17:B:805:CLA:HMB1	17:B:805:CLA:HBB1	1.83	0.61
17:B:821:CLA:HMC2	17:B:826:CLA:H18	1.83	0.61
15:6:157:GLN:HG2	25:6:515:CHL:HMA3	1.82	0.61
2:B:334:LEU:HB2	17:B:807:CLA:HMD3	1.82	0.61
2:B:2:GLU:HB2	2:B:7:ARG:HH11	1.65	0.60
1:A:13:VAL:HA	13:3:87:GLY:HA3	1.83	0.60
17:4:307:CLA:HHD	17:4:312:CLA:HBB2	1.83	0.60
17:B:832:CLA:HBC1	20:B:848:BCR:H21C	1.83	0.60
1:A:127:ASP:OD2	6:F:108:LYS:NZ	2.31	0.60
2:B:310:PRO:HG3	17:B:843:CLA:HBD	1.83	0.60
12:1:165:PHE:HD2	17:1:504:CLA:HMD1	1.65	0.60
13:3:191:LYS:HE3	13:3:192:TYR:CZ	2.37	0.60
1:A:533:VAL:HG11	1:A:607:HIS:CG	2.37	0.60
20:A:851:BCR:H313	9:J:31:ARG:HD3	1.82	0.60
14:4:144:TYR:CZ	14:4:148:ARG:HD2	2.37	0.59
17:B:803:CLA:HMB1	17:B:803:CLA:HBB1	1.83	0.59
1:A:421:ASN:OD1	1:A:422:ASP:N	2.35	0.59
2:B:56:ILE:HG21	17:B:808:CLA:HMD2	1.85	0.59
13:3:214:THR:HG23	13:3:215:LYS:H	1.65	0.59
14:4:206:LEU:HD22	17:4:306:CLA:HAB	1.83	0.59
1:A:72:SER:OG	17:A:810:CLA:HHD	2.03	0.59
2:B:299:HIS:CD2	2:B:304:LEU:HD21	2.37	0.59
17:B:834:CLA:HAB	17:B:835:CLA:HMB2	1.84	0.59
25:1:512:CHL:HHC	25:1:512:CHL:HBB1	1.85	0.59
15:6:139:TYR:CG	15:6:240:VAL:HG11	2.38	0.59
15:6:239:GLN:O	15:6:243:THR:N	2.35	0.59
1:A:536:ILE:HD12	16:A:801:CL0:H63	1.84	0.59
15:6:262:ASN:N	15:6:265:SER:OG	2.31	0.59
2:B:174:ARG:HB2	17:B:815:CLA:HBC2	1.84	0.58
1:A:155:GLN:N	1:A:155:GLN:OE1	2.36	0.58
1:A:330:PHE:O	1:A:426:ARG:NH2	2.37	0.58
17:6:506:CLA:H11	17:6:511:CLA:HED2	1.85	0.58
2:B:654:HIS:NE2	17:B:804:CLA:C1A	2.67	0.58
15:6:237:TRP:O	15:6:241:VAL:HG23	2.04	0.58
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.36	0.58
25:1:514:CHL:HHC	25:1:514:CHL:HBB1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:SER:OG	17:A:827:CLA:HHB	2.03	0.58
17:B:808:CLA:H12	17:B:831:CLA:H12	1.84	0.58
1:A:60:THR:HG22	1:A:61:GLY:H	1.68	0.58
1:A:522:LEU:HD21	1:A:616:VAL:HA	1.86	0.58
2:B:355:LEU:HB2	17:B:819:CLA:HED1	1.85	0.58
17:4:305:CLA:HED2	17:4:305:CLA:H2A	1.85	0.58
6:F:150:VAL:HG12	6:F:160:PHE:HB2	1.85	0.57
17:1:505:CLA:HBB1	17:1:505:CLA:HMB1	1.85	0.57
17:3:308:CLA:HMB1	17:3:308:CLA:HBB1	1.86	0.57
12:1:154:ASP:HB3	12:1:157:LYS:H	1.69	0.57
17:A:807:CLA:HMC3	17:A:808:CLA:HMD2	1.85	0.57
20:A:850:BCR:H372	2:B:438:VAL:HG21	1.86	0.57
2:B:10:GLN:NE2	2:B:14:GLN:OE1	2.36	0.57
3:C:61:ASP:OD2	5:E:95:ARG:NH1	2.37	0.57
1:A:25:GLU:HB2	17:A:810:CLA:HBA1	1.86	0.57
1:A:689:ARG:NH2	2:B:565:GLY:O	2.38	0.57
17:A:821:CLA:HED2	17:A:821:CLA:H2A	1.85	0.57
11:L:77:TYR:HD2	11:L:78:LEU:HD12	1.69	0.57
12:1:160:TYR:HE2	17:1:504:CLA:HMA3	1.70	0.57
13:3:62:GLN:O	13:3:65:THR:OG1	2.22	0.57
15:6:117:ALA:HB1	26:6:502:XAT:H161	1.87	0.57
2:B:717:TYR:CE1	17:B:804:CLA:HED1	2.39	0.57
10:K:72:ALA:HA	10:K:84:LYS:HZ3	1.69	0.57
9:J:1:MET:HG3	9:J:5:LYS:HE2	1.86	0.57
1:A:717:LEU:N	18:A:842:PQN:O4	2.37	0.57
2:B:51:PHE:HB3	2:B:153:SER:HB2	1.85	0.57
17:A:839:CLA:HBB2	6:F:178:GLY:HA3	1.86	0.56
24:3:301:LUT:H30	17:3:304:CLA:HBB1	1.86	0.56
2:B:366:THR:HG22	2:B:729:THR:HG23	1.85	0.56
2:B:19:ARG:HA	2:B:22:TRP:HD1	1.70	0.56
3:C:24:ASP:OD2	4:D:162:HIS:ND1	2.37	0.56
13:3:147:TYR:HB3	13:3:149:TYR:CZ	2.41	0.56
13:3:156:LEU:HD11	17:3:315:CLA:HMD3	1.86	0.56
13:3:184:GLN:NE2	15:6:67:VAL:O	2.35	0.56
2:B:279:ALA:O	2:B:283:ILE:HG12	2.06	0.56
15:6:224:LYS:NZ	19:6:516:LHG:O5	2.33	0.56
1:A:618:GLY:HA2	1:A:629:ILE:HG12	1.88	0.56
17:A:820:CLA:HMB2	17:A:824:CLA:HMA3	1.87	0.56
17:B:826:CLA:HBB1	17:B:826:CLA:HMB1	1.88	0.56
17:A:825:CLA:HBB1	17:A:825:CLA:HMB1	1.87	0.56
2:B:223:GLY:HA2	2:B:226:LEU:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:THR:HG21	2:B:609:PHE:HB2	1.86	0.56
11:L:175:GLU:O	11:L:179:GLN:HG2	2.06	0.56
5:E:97:GLU:N	5:E:97:GLU:OE1	2.36	0.56
15:6:106:ALA:O	15:6:110:HIS:ND1	2.39	0.55
14:4:206:LEU:HD21	17:4:306:CLA:H101	1.88	0.55
1:A:691:TYR:CE1	2:B:536:LYS:HD2	2.41	0.55
3:C:27:GLU:HG3	4:D:176:ARG:HH11	1.72	0.55
14:4:144:TYR:CE2	20:4:301:BCR:H12C	2.41	0.55
1:A:146:ARG:HH21	1:A:376:TYR:HE2	1.54	0.55
17:A:853:CLA:HBB1	17:A:853:CLA:HMB1	1.88	0.55
22:B:851:DGD:O5D	22:B:851:DGD:O4D	2.22	0.55
4:D:106:VAL:HG12	4:D:116:ILE:HG22	1.87	0.55
20:I:102:BCR:H403	11:L:136:LEU:HD12	1.88	0.55
13:3:54:ARG:NH2	13:3:67:LEU:O	2.39	0.55
1:A:313:TRP:NE1	17:A:819:CLA:O1A	2.39	0.55
1:A:445:LEU:HB3	1:A:539:PHE:HB2	1.87	0.55
1:A:675:HIS:NE2	16:A:801:CL0:NA	2.55	0.55
1:A:340:GLU:HB3	1:A:419:ARG:HH11	1.71	0.55
14:4:160:ASN:HB3	14:4:170:LEU:HD22	1.88	0.55
2:B:85:ARG:HB3	2:B:115:ILE:HD12	1.89	0.55
2:B:582:TRP:HH2	17:B:803:CLA:HAB	1.72	0.55
2:B:733:PHE:HD2	7:H:139:PRO:HG2	1.71	0.55
3:C:14:CYS:O	3:C:16:GLN:NE2	2.40	0.55
14:4:237:THR:N	14:4:240:GLN:OE1	2.39	0.55
14:4:213:VAL:HG21	17:4:306:CLA:HAC2	1.89	0.55
15:6:239:GLN:OE1	15:6:250:ASN:ND2	2.39	0.55
17:B:808:CLA:HMA2	17:B:808:CLA:H42	1.89	0.55
10:K:101:THR:HG23	10:K:103:ALA:H	1.72	0.55
17:A:832:CLA:C3B	17:A:833:CLA:HMB2	2.37	0.54
14:4:208:PHE:CD2	26:4:303:XAT:H12	2.41	0.54
24:6:501:LUT:H362	17:6:506:CLA:HMB3	1.88	0.54
1:A:200:ALA:HB2	1:A:306:GLY:HA3	1.89	0.54
17:A:802:CLA:HBB1	17:A:802:CLA:HMB1	1.88	0.54
2:B:203:ARG:NH2	2:B:253:ALA:O	2.37	0.54
2:B:207:VAL:HA	2:B:211:ASN:HD21	1.72	0.54
4:D:87:ARG:O	4:D:91:VAL:HG22	2.07	0.54
1:A:56:PHE:HB3	1:A:66:ILE:HG22	1.89	0.54
4:D:171:LYS:O	4:D:176:ARG:NH2	2.33	0.54
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.42	0.54
13:3:157:PHE:CD2	17:3:312:CLA:HAA2	2.42	0.54
14:4:89:LEU:HD22	14:4:198:LEU:HD21	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PRO:HB3	17:A:852:CLA:HMC3	1.90	0.54
8:I:26:LEU:HD21	11:L:145:VAL:HG13	1.89	0.54
12:1:134:ILE:HA	12:1:137:ILE:HG22	1.89	0.54
15:6:96:GLU:OE2	15:6:99:SER:N	2.38	0.54
1:A:75:PHE:CZ	17:A:809:CLA:HBB1	2.43	0.54
2:B:279:ALA:HA	17:B:818:CLA:HMC3	1.89	0.54
2:B:426:SER:HB3	17:B:801:CLA:HBA1	1.89	0.54
2:B:167:TRP:HH2	17:B:813:CLA:HMB3	1.72	0.54
2:B:176:ASN:ND2	2:B:291:TYR:O	2.41	0.54
2:B:330:ILE:HG21	17:B:807:CLA:HAC1	1.88	0.54
3:C:77:MET:HB3	3:C:79:LEU:HG	1.89	0.54
1:A:264:LEU:HD23	17:K:203:CLA:HMD2	1.89	0.54
20:A:846:BCR:H362	20:A:847:BCR:H21C	1.90	0.54
17:B:818:CLA:CHD	17:B:819:CLA:HBB2	2.38	0.54
17:B:807:CLA:HMB1	17:B:807:CLA:HBB1	1.90	0.54
15:6:144:ARG:HH11	17:6:509:CLA:H2A	1.71	0.54
2:B:43:TYR:HE1	2:B:330:ILE:HD11	1.72	0.53
12:1:166:ASP:N	12:1:167:PRO:HD3	2.24	0.53
2:B:304:LEU:O	2:B:308:HIS:ND1	2.42	0.53
2:B:438:VAL:HG12	17:B:835:CLA:HAC1	1.91	0.53
17:3:309:CLA:HBB1	17:3:309:CLA:HMB1	1.89	0.53
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.26	0.53
2:B:506:ASN:OD1	2:B:508:LEU:N	2.35	0.53
17:B:810:CLA:O1A	17:B:829:CLA:HBD	2.09	0.53
8:I:11:LEU:HA	8:I:15:VAL:HG22	1.90	0.53
11:L:203:ASP:HB2	11:L:208:PHE:CZ	2.44	0.53
1:A:660:TYR:OH	2:B:441:ASP:OD1	2.21	0.53
6:F:194:ARG:NH2	23:J:105:LMG:O3	2.40	0.53
12:1:177:PHE:HE1	17:1:504:CLA:HED1	1.72	0.53
17:3:306:CLA:HMB2	17:3:311:CLA:HAC2	1.91	0.53
14:4:226:LEU:HG	24:4:302:LUT:H22	1.90	0.53
1:A:213:HIS:HB2	17:A:813:CLA:CHC	2.39	0.53
14:4:142:PHE:CE2	25:4:316:CHL:HMB3	2.43	0.53
14:4:209:LEU:HD13	17:4:308:CLA:HBB2	1.91	0.53
1:A:64:GLU:OE2	1:A:68:ARG:NH2	2.42	0.53
1:A:283:THR:OG1	1:A:376:TYR:N	2.41	0.53
17:A:803:CLA:HBA2	17:A:810:CLA:H2	1.90	0.53
17:A:818:CLA:CAC	20:A:847:BCR:H352	2.39	0.53
10:K:67:GLY:HA2	10:K:72:ALA:HB3	1.91	0.53
14:4:60:ASP:OD1	14:4:61:GLY:N	2.41	0.53
17:A:820:CLA:HMB1	17:A:820:CLA:HBB1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:OE1	1:A:340:GLU:N	2.42	0.52
1:A:572:PRO:HD3	1:A:720:ILE:HD11	1.91	0.52
2:B:700:LEU:HG	18:B:844:PQN:O4	2.09	0.52
17:B:806:CLA:HHC	17:B:808:CLA:OBD	2.09	0.52
6:F:227:VAL:HG12	6:F:228:VAL:H	1.74	0.52
1:A:392:MET:HG3	1:A:601:ILE:HD12	1.90	0.52
17:6:504:CLA:O1D	17:6:504:CLA:H2A	2.09	0.52
1:A:225:LEU:HD21	1:A:231:PRO:HG3	1.91	0.52
1:A:373:PRO:HG2	1:A:374:TYR:CD1	2.44	0.52
1:A:455:HIS:HB2	17:A:833:CLA:C1C	2.39	0.52
17:B:827:CLA:HMB2	17:B:840:CLA:H3A	1.92	0.52
4:D:178:GLY:CA	4:D:181:GLN:HE22	2.22	0.52
12:1:56:PRO:HG3	12:1:181:LYS:HE2	1.92	0.52
17:B:801:CLA:H3A	17:B:801:CLA:CGA	2.39	0.52
1:A:470:SER:OG	1:A:471:ASP:N	2.43	0.52
1:A:575:GLY:HA2	2:B:562:PRO:HD3	1.91	0.52
7:H:114:ALA:HB2	8:I:11:LEU:HD11	1.92	0.52
13:3:159:PHE:CG	17:6:511:CLA:HBA1	2.45	0.52
1:A:703:HIS:CE1	17:A:852:CLA:HAC1	2.45	0.52
12:1:104:ASN:OD1	12:1:105:TRP:N	2.43	0.52
12:1:93:GLY:O	24:1:502:LUT:H24	2.09	0.52
17:4:306:CLA:NC	17:4:306:CLA:H52	2.25	0.52
1:A:65:GLU:OE1	1:A:65:GLU:N	2.31	0.52
2:B:658:ALA:HB3	17:B:805:CLA:HBB2	1.92	0.52
13:3:165:GLY:O	13:3:169:HIS:ND1	2.39	0.52
1:A:735:ILE:HG21	17:A:827:CLA:HMC2	1.92	0.51
20:A:854:BCR:H403	10:K:107:ALA:HB1	1.91	0.51
10:K:50:SER:OG	10:K:51:SER:N	2.42	0.51
12:1:183:LYS:HG2	17:1:510:CLA:OBD	2.10	0.51
19:1:516:LHG:H132	25:1:517:CHL:HBB1	1.92	0.51
15:6:262:ASN:N	15:6:265:SER:HG	2.06	0.51
2:B:339:ALA:HB2	20:B:849:BCR:H372	1.92	0.51
3:C:14:CYS:SG	3:C:16:GLN:HG2	2.50	0.51
11:L:152:GLU:N	11:L:152:GLU:OE1	2.44	0.51
13:3:233:LEU:HD22	17:3:310:CLA:HHD	1.91	0.51
12:1:168:LEU:O	12:1:172:LYS:NZ	2.43	0.51
12:1:173:ASP:HB2	12:1:176:LYS:HB3	1.92	0.51
13:3:259:HIS:ND1	17:3:306:CLA:HMA2	2.25	0.51
12:1:87:ALA:O	12:1:91:VAL:HG23	2.09	0.51
13:3:163:LEU:HB3	20:3:303:BCR:H363	1.92	0.51
17:4:307:CLA:HMB1	17:4:307:CLA:HBB1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:808:CLA:HED1	17:B:831:CLA:H43	1.92	0.51
19:1:516:LHG:H162	19:1:516:LHG:H302	1.92	0.51
13:3:244:GLN:O	13:3:248:THR:N	2.31	0.51
17:6:506:CLA:HMA1	17:6:511:CLA:HBC3	1.92	0.51
1:A:279:LEU:HD11	1:A:521:LEU:HD12	1.92	0.51
2:B:432:HIS:HD2	22:J:104:DGD:HAF2	1.76	0.51
13:3:63:SER:HB2	13:3:67:LEU:HD12	1.92	0.51
15:6:70:PRO:HD2	25:6:517:CHL:O1D	2.11	0.51
1:A:161:ILE:O	1:A:165:VAL:HG23	2.10	0.51
1:A:195:LEU:HD12	1:A:319:LEU:HD11	1.93	0.51
6:F:158:GLY:O	9:J:39:PHE:N	2.44	0.51
20:3:303:BCR:C20	17:3:315:CLA:H3A	2.41	0.51
13:3:181:MET:HG3	25:3:313:CHL:HMC	1.93	0.51
1:A:418:THR:HG23	1:A:419:ARG:HG2	1.93	0.51
1:A:688:GLY:HA3	2:B:569:ASP:HB2	1.93	0.51
17:A:838:CLA:H42	20:A:849:BCR:H363	1.92	0.51
2:B:85:ARG:HG3	7:H:143:ILE:HA	1.93	0.51
1:A:452:LEU:HD22	1:A:469:PHE:HE2	1.76	0.51
2:B:431:PHE:HZ	20:F:801:BCR:H372	1.76	0.50
12:1:100:LEU:O	12:1:102:LEU:N	2.44	0.50
13:3:83:SER:HB2	13:3:97:LEU:HD11	1.93	0.50
10:K:118:GLY:HA3	17:K:202:CLA:HBC3	1.93	0.50
3:C:61:ASP:OD1	3:C:62:PHE:N	2.40	0.50
6:F:173:TRP:CD2	6:F:210:GLY:HA3	2.46	0.50
12:1:75:ARG:HG3	25:1:514:CHL:HED1	1.91	0.50
3:C:54:CYS:HB3	21:C:101:SF4:S4	2.52	0.50
15:6:163:TRP:HH2	20:6:503:BCR:H321	1.76	0.50
1:A:133:ARG:NH1	6:F:109:TYR:OH	2.45	0.50
1:A:601:ILE:O	1:A:605:ILE:HG12	2.11	0.50
1:A:456:ASN:ND2	1:A:639:ILE:HB	2.26	0.50
17:A:852:CLA:H93	9:J:14:LEU:HD11	1.93	0.50
2:B:225:LEU:HA	2:B:230:TRP:CD1	2.47	0.50
4:D:110:PRO:HD3	4:D:135:LEU:HD12	1.92	0.50
2:B:3:LEU:HA	8:I:32:LYS:HB3	1.93	0.50
17:B:810:CLA:HMC3	17:B:811:CLA:C3D	2.42	0.50
6:F:84:PRO:HG3	6:F:139:LEU:HD23	1.93	0.50
13:3:147:TYR:HB3	13:3:149:TYR:CE2	2.47	0.50
13:3:196:SER:N	13:3:202:PRO:O	2.45	0.50
1:A:392:MET:HG2	1:A:605:ILE:HD11	1.93	0.50
1:A:434:ILE:HG23	17:A:838:CLA:HBB2	1.94	0.50
16:A:801:CL0:H13	17:B:803:CLA:OBD	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:62:GLN:HB3	13:3:81:GLY:HA3	1.93	0.49
15:6:152:THR:O	15:6:156:THR:HG23	2.11	0.49
1:A:595:PHE:CZ	1:A:727:VAL:HG23	2.47	0.49
2:B:179:LEU:HD21	17:B:821:CLA:HAB	1.94	0.49
2:B:324:ASP:OD1	2:B:328:ASN:ND2	2.45	0.49
2:B:700:LEU:H	18:B:844:PQN:H6	1.77	0.49
6:F:206:ILE:HD13	6:F:209:ARG:HH12	1.77	0.49
13:3:65:THR:OG1	13:3:84:ASP:OD1	2.21	0.49
14:4:108:LEU:HB3	14:4:114:LEU:HD12	1.94	0.49
2:B:449:PRO:O	2:B:452:GLN:NE2	2.45	0.49
2:B:654:HIS:CE1	17:B:804:CLA:ND	2.80	0.49
4:D:108:GLU:O	4:D:138:ARG:NH1	2.45	0.49
12:1:196:VAL:HG12	17:1:506:CLA:HAC1	1.93	0.49
15:6:216:MET:O	15:6:220:THR:OG1	2.24	0.49
1:A:207:SER:OG	1:A:295:HIS:O	2.27	0.49
2:B:25:ILE:HD13	20:I:102:BCR:HC21	1.95	0.49
6:F:228:VAL:HG11	6:F:231:ALA:HB3	1.93	0.49
12:1:177:PHE:CE2	12:1:181:LYS:HD2	2.47	0.49
13:3:156:LEU:HD21	17:3:315:CLA:C1D	2.42	0.49
13:3:262:ASP:O	13:3:265:ASN:ND2	2.45	0.49
4:D:108:GLU:HG3	4:D:138:ARG:NH1	2.27	0.49
6:F:232:ASP:OD1	6:F:233:ILE:N	2.46	0.49
14:4:178:PRO:HB2	14:4:182:PHE:CD1	2.48	0.49
1:A:310:ARG:N	1:A:317:HIS:O	2.37	0.49
17:B:821:CLA:HMB2	17:B:826:CLA:HMA3	1.95	0.49
24:1:501:LUT:H21	17:1:506:CLA:HMB3	1.94	0.49
13:3:259:HIS:CD2	13:3:265:ASN:HD22	2.31	0.49
17:A:805:CLA:O1D	17:A:805:CLA:H2A	2.13	0.49
17:A:830:CLA:C4D	19:A:845:LHG:HC92	2.43	0.49
2:B:86:PRO:HB3	2:B:121:TYR:CE2	2.48	0.49
12:1:111:TRP:NE1	12:1:119:ALA:HA	2.27	0.49
13:3:141:ILE:HG22	13:3:143:PRO:HG2	1.95	0.49
1:A:504:SER:H	1:A:507:TRP:HE1	1.61	0.49
2:B:2:GLU:HG3	2:B:7:ARG:HA	1.94	0.49
11:L:201:VAL:HG12	11:L:202:LEU:HD12	1.95	0.49
13:3:204:GLY:O	13:3:208:ASN:N	2.46	0.49
2:B:43:TYR:CE1	2:B:330:ILE:HD11	2.47	0.48
2:B:193:HIS:HB2	17:B:816:CLA:CHC	2.43	0.48
17:B:827:CLA:CAD	17:B:838:CLA:HBB1	2.43	0.48
4:D:149:PHE:CE2	4:D:162:HIS:HB2	2.48	0.48
6:F:126:THR:OG1	6:F:129:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:ARG:HH21	2:B:551:LYS:HD2	1.77	0.48
4:D:139:LEU:HD22	4:D:145:ILE:HD11	1.95	0.48
5:E:132:VAL:HG12	5:E:134:THR:H	1.78	0.48
6:F:90:ALA:O	6:F:94:ARG:HG2	2.14	0.48
12:1:160:TYR:HB3	17:1:504:CLA:HED3	1.95	0.48
1:A:187:TRP:CZ2	17:A:809:CLA:HMA1	2.48	0.48
1:A:456:ASN:HD22	1:A:639:ILE:HB	1.77	0.48
1:A:689:ARG:N	2:B:568:CYS:SG	2.87	0.48
2:B:502:ASN:OD1	2:B:503:GLU:N	2.47	0.48
12:1:65:GLY:O	12:1:68:THR:HG23	2.13	0.48
12:1:169:GLY:O	12:1:172:LYS:N	2.45	0.48
17:4:306:CLA:CHB	17:4:311:CLA:HMD3	2.43	0.48
15:6:65:ARG:HH12	15:6:85:ASP:CG	2.17	0.48
15:6:84:GLY:HA3	15:6:223:ILE:HD13	1.95	0.48
1:A:279:LEU:HG	1:A:505:LEU:HD23	1.94	0.48
17:B:821:CLA:HBB1	17:B:826:CLA:H62	1.95	0.48
12:1:41:TRP:NE1	12:1:60:GLY:O	2.46	0.48
1:A:197:HIS:CD2	17:A:812:CLA:HAB	2.49	0.48
1:A:429:ARG:O	4:D:81:SER:HB3	2.13	0.48
2:B:20:ARG:O	2:B:24:GLY:N	2.45	0.48
2:B:498:LEU:HA	2:B:501:VAL:HG22	1.95	0.48
14:4:59:LEU:HD12	14:4:68:GLY:HA2	1.96	0.48
1:A:573:CYS:SG	1:A:574:ASP:N	2.87	0.48
2:B:42:LEU:O	2:B:46:ILE:HG12	2.14	0.48
13:3:67:LEU:HD22	17:3:307:CLA:HED2	1.95	0.48
17:4:308:CLA:H2A	17:4:308:CLA:HED2	1.96	0.48
1:A:107:HIS:O	1:A:107:HIS:ND1	2.46	0.48
1:A:280:ASP:O	1:A:284:GLY:N	2.41	0.48
1:A:682:LEU:HB2	17:B:801:CLA:HMC3	1.96	0.48
2:B:376:GLN:HE22	17:B:827:CLA:HMD1	1.78	0.48
17:B:842:CLA:HBC1	20:B:850:BCR:H24C	1.96	0.48
6:F:129:ARG:HD3	9:J:35:ASP:OD2	2.14	0.48
12:1:179:GLU:O	12:1:183:LYS:HG3	2.14	0.48
1:A:300:ILE:HD12	20:A:854:BCR:H352	1.96	0.47
15:6:117:ALA:HB2	26:6:502:XAT:H10	1.96	0.47
2:B:322:LEU:HA	2:B:325:THR:HG22	1.96	0.47
2:B:675:ILE:HD11	20:B:850:BCR:H282	1.96	0.47
19:1:516:LHG:H242	25:1:517:CHL:C1C	2.44	0.47
14:4:184:PRO:HD2	24:4:302:LUT:H23	1.95	0.47
15:6:202:PHE:O	24:6:501:LUT:H42	2.14	0.47
12:1:61:PHE:N	17:1:507:CLA:OBD	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:501:LUT:H15	24:1:501:LUT:H201	1.69	0.47
24:3:302:LUT:H32	17:3:307:CLA:HAB	1.96	0.47
1:A:418:THR:OG1	1:A:419:ARG:NH2	2.47	0.47
1:A:421:ASN:ND2	1:A:424:LEU:H	2.13	0.47
2:B:593:TYR:CZ	17:B:838:CLA:HBC3	2.50	0.47
13:3:155:THR:HA	13:3:158:VAL:HG12	1.96	0.47
14:4:48:SER:C	14:4:50:LEU:H	2.17	0.47
20:4:301:BCR:H15C	20:4:301:BCR:H351	1.72	0.47
17:A:838:CLA:HBB1	17:A:838:CLA:HMB1	1.95	0.47
2:B:410:ARG:NH1	17:B:832:CLA:O1D	2.48	0.47
6:F:206:ILE:HA	6:F:209:ARG:HH12	1.79	0.47
20:F:803:BCR:H11C	20:F:803:BCR:H341	1.64	0.47
13:3:76:GLY:N	17:3:307:CLA:OBD	2.47	0.47
24:4:302:LUT:H35	24:4:302:LUT:H401	1.76	0.47
17:6:505:CLA:HMD2	17:6:510:CLA:C1D	2.44	0.47
1:A:507:TRP:CZ2	17:A:826:CLA:HMC3	2.48	0.47
8:I:19:ILE:HA	8:I:22:THR:HG22	1.97	0.47
17:1:506:CLA:HMB2	17:1:511:CLA:HMD3	1.97	0.47
1:A:360:THR:HA	1:A:363:VAL:HG22	1.96	0.47
1:A:457:ASP:OD1	2:B:635:TYR:OH	2.27	0.47
17:A:804:CLA:H152	20:A:846:BCR:H323	1.96	0.47
17:A:815:CLA:HBC2	17:3:312:CLA:HBB2	1.96	0.47
17:B:810:CLA:C1A	17:B:810:CLA:CGA	2.93	0.47
20:B:850:BCR:H20C	20:B:850:BCR:H361	1.74	0.47
10:K:55:ILE:O	10:K:59:THR:HG23	2.14	0.47
12:1:86:TRP:HB2	24:1:502:LUT:H402	1.95	0.47
15:6:243:THR:OG1	15:6:245:GLN:OE1	2.20	0.47
17:A:826:CLA:H12	20:A:849:BCR:H15C	1.96	0.47
17:A:837:CLA:H41	17:A:837:CLA:H62	1.75	0.47
2:B:700:LEU:N	18:B:844:PQN:H6	2.30	0.47
6:F:86:LYS:HE2	6:F:137:GLY:H	1.79	0.47
11:L:80:ASN:HB3	17:L:302:CLA:HAC1	1.97	0.47
17:3:315:CLA:HMB1	17:3:315:CLA:HBB1	1.96	0.47
15:6:139:TYR:CZ	25:6:512:CHL:HMA2	2.50	0.47
1:A:115:VAL:HG11	1:A:124:LEU:HB2	1.95	0.47
17:B:832:CLA:HMB2	17:B:833:CLA:C2D	2.45	0.47
15:6:144:ARG:NH1	17:6:509:CLA:H2A	2.29	0.47
2:B:44:GLN:NE2	2:B:162:LYS:HE2	2.30	0.47
2:B:223:GLY:N	2:B:224:PRO:HD2	2.30	0.47
20:I:101:BCR:H351	20:I:101:BCR:H15C	1.68	0.47
26:4:303:XAT:H35	26:4:303:XAT:H401	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ALA:HB1	20:A:849:BCR:H343	1.97	0.46
1:A:362:ILE:HD12	1:A:392:MET:SD	2.54	0.46
17:A:839:CLA:HED2	2:B:420:SER:HB2	1.96	0.46
2:B:555:TYR:HE1	2:B:572:ALA:HB3	1.80	0.46
4:D:149:PHE:CZ	4:D:162:HIS:HB2	2.49	0.46
13:3:66:TYR:OH	13:3:78:ASP:OD2	2.25	0.46
24:3:301:LUT:H31	24:3:301:LUT:H391	1.72	0.46
14:4:105:PRO:O	14:4:109:THR:HG23	2.15	0.46
2:B:582:TRP:HE1	17:B:801:CLA:C1D	2.27	0.46
17:1:510:CLA:HED2	17:1:510:CLA:H2A	1.98	0.46
24:3:301:LUT:H35	24:3:301:LUT:H401	1.67	0.46
1:A:550:LYS:NZ	2:B:673:GLU:OE1	2.47	0.46
2:B:77:TRP:CZ3	2:B:121:TYR:HB3	2.50	0.46
6:F:154:GLN:HE22	6:F:161:ILE:HG21	1.80	0.46
14:4:201:GLY:O	14:4:205:MET:HG3	2.14	0.46
1:A:275:PHE:HD1	17:A:817:CLA:HMB2	1.80	0.46
17:A:812:CLA:HMB1	17:A:812:CLA:HBB1	1.98	0.46
17:A:818:CLA:HBB1	17:A:818:CLA:HMB1	1.96	0.46
11:L:83:ALA:HB2	17:L:303:CLA:HMD1	1.98	0.46
17:L:304:CLA:HMB1	17:L:304:CLA:HBB1	1.98	0.46
17:3:314:CLA:CHB	17:3:316:CLA:HBB1	2.46	0.46
14:4:142:PHE:CD1	17:4:315:CLA:HMC3	2.50	0.46
24:6:501:LUT:H15	24:6:501:LUT:H201	1.67	0.46
1:A:291:ILE:HD11	17:A:818:CLA:H2A	1.97	0.46
1:A:597:MET:HB3	1:A:597:MET:HE3	1.74	0.46
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.50	0.46
20:B:847:BCR:H24C	20:B:847:BCR:H371	1.56	0.46
5:E:144:GLU:OE1	5:E:144:GLU:N	2.45	0.46
9:J:1:MET:O	9:J:4:ILE:HG22	2.15	0.46
14:4:142:PHE:CG	17:4:315:CLA:HMC3	2.51	0.46
15:6:192:PRO:O	15:6:193:ASP:O	2.34	0.46
15:6:219:ARG:O	15:6:223:ILE:HG22	2.16	0.46
2:B:547:MET:HE2	2:B:570:ILE:HD13	1.98	0.46
18:B:844:PQN:H2M1	18:B:844:PQN:H111	1.70	0.46
9:J:40:PRO:HG2	22:J:104:DGD:HD61	1.97	0.46
11:L:93:ARG:O	11:L:97:VAL:HG23	2.15	0.46
12:1:155:PRO:O	12:1:159:LYS:NZ	2.49	0.46
1:A:126:GLY:HA3	1:A:663:SER:HB2	1.98	0.46
17:B:835:CLA:HBA2	9:J:36:ALA:HB3	1.98	0.46
20:B:850:BCR:H15C	20:B:850:BCR:H351	1.85	0.46
26:6:502:XAT:H192	25:6:512:CHL:HAB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ARG:HB3	3:C:49:VAL:HG13	1.98	0.46
4:D:73:THR:OG1	4:D:74:PRO:HD2	2.16	0.46
20:J:103:BCR:H24C	20:J:103:BCR:H371	1.78	0.46
12:1:85:ARG:HH21	12:1:184:GLU:CD	2.19	0.46
1:A:40:PRO:HB3	1:A:45:TRP:CE3	2.51	0.46
1:A:324:GLU:N	1:A:324:GLU:OE1	2.49	0.46
1:A:385:LEU:O	1:A:389:THR:HG22	2.16	0.46
16:A:801:CL0:H41	16:A:801:CL0:H49	1.78	0.46
2:B:654:HIS:HE1	17:B:804:CLA:ND	2.14	0.46
3:C:51:CYS:SG	3:C:53:ARG:NE	2.88	0.46
4:D:173:ASN:HB3	4:D:176:ARG:HH21	1.81	0.46
11:L:92:LEU:HA	11:L:95:ILE:HG22	1.97	0.46
13:3:157:PHE:O	13:3:160:GLU:HG3	2.15	0.46
20:6:503:BCR:H24C	20:6:503:BCR:H402	1.64	0.46
2:B:636:ASN:HB2	2:B:637:PRO:HD2	1.97	0.46
9:J:2:ARG:HA	9:J:5:LYS:HD2	1.98	0.46
11:L:203:ASP:OD1	11:L:203:ASP:N	2.48	0.46
12:1:51:LEU:HD23	12:1:51:LEU:HA	1.79	0.46
13:3:63:SER:HB3	13:3:78:ASP:O	2.16	0.45
17:A:839:CLA:H12	17:B:834:CLA:CGD	2.46	0.45
2:B:424:TRP:HZ3	17:B:840:CLA:HAC1	1.82	0.45
12:1:160:TYR:CE1	12:1:181:LYS:HE3	2.51	0.45
1:A:247:LEU:HD13	1:A:254:PHE:CE2	2.51	0.45
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.78	0.45
1:A:654:SER:O	1:A:657:ILE:HG22	2.17	0.45
17:A:830:CLA:HMA2	11:L:66:THR:HG21	1.98	0.45
2:B:365:PHE:HB3	2:B:602:TRP:CH2	2.52	0.45
2:B:373:THR:HG23	2:B:591:THR:HG21	1.98	0.45
6:F:194:ARG:HH21	6:F:199:ASP:HA	1.81	0.45
12:1:104:ASN:HB3	12:1:107:LYS:HG2	1.99	0.45
12:1:145:ALA:HB1	12:1:149:ARG:CZ	2.46	0.45
25:1:514:CHL:HBB1	25:1:514:CHL:CHC	2.46	0.45
14:4:197:GLU:HB2	17:4:304:CLA:C1B	2.46	0.45
17:A:803:CLA:HBA2	17:A:810:CLA:H51	1.99	0.45
2:B:332:PHE:CE2	20:B:849:BCR:H292	2.52	0.45
2:B:612:SER:O	2:B:612:SER:OG	2.25	0.45
3:C:17:CYS:SG	3:C:18:VAL:N	2.89	0.45
4:D:162:HIS:HB3	4:D:163:PRO:HD3	1.98	0.45
4:D:184:ARG:HH12	4:D:189:ASN:HA	1.82	0.45
1:A:578:ARG:HE	3:C:49:VAL:HG11	1.81	0.45
17:A:808:CLA:H2A	17:A:808:CLA:O1D	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:157:PHE:CE2	17:3:312:CLA:HMA2	2.51	0.45
1:A:741:PHE:CD1	16:A:801:CL0:H27	2.51	0.45
17:A:853:CLA:H2A	17:A:853:CLA:O2D	2.16	0.45
4:D:65:VAL:HB	4:D:165:ASP:HA	1.98	0.45
11:L:91:LEU:HB2	11:L:179:GLN:HB3	1.99	0.45
11:L:104:LEU:HG	17:L:304:CLA:HBC2	1.99	0.45
15:6:97:PRO:O	15:6:101:ARG:HG2	2.16	0.45
17:B:807:CLA:H2A	17:B:807:CLA:O1D	2.16	0.45
6:F:168:LEU:HD23	6:F:168:LEU:HA	1.80	0.45
14:4:215:HIS:O	14:4:219:GLY:N	2.49	0.45
24:6:501:LUT:H191	24:6:501:LUT:H11	1.78	0.45
17:A:807:CLA:H2A	17:A:807:CLA:O2D	2.15	0.45
20:A:850:BCR:H24C	20:A:850:BCR:H371	1.77	0.45
20:A:851:BCR:H341	20:A:851:BCR:H11C	1.72	0.45
2:B:177:HIS:CG	17:B:815:CLA:HMC2	2.52	0.45
2:B:276:HIS:HB2	17:B:819:CLA:CHB	2.46	0.45
2:B:301:ILE:HG23	17:B:821:CLA:HED2	1.98	0.45
2:B:477:LEU:HD12	2:B:477:LEU:H	1.82	0.45
12:1:50:HIS:CE1	12:1:68:THR:HG22	2.52	0.45
15:6:263:ILE:HD12	17:6:506:CLA:H42	1.99	0.45
24:6:501:LUT:H383	17:6:506:CLA:C2B	2.47	0.45
1:A:583:GLN:HA	1:A:588:ASP:OD2	2.16	0.45
1:A:621:SER:OG	1:A:625:VAL:N	2.49	0.45
17:A:803:CLA:HMA2	17:A:810:CLA:HMD2	1.99	0.45
20:A:854:BCR:H351	20:A:854:BCR:H15C	1.70	0.45
17:B:816:CLA:HBB1	17:B:816:CLA:HMB1	1.99	0.45
4:D:104:GLU:N	4:D:104:GLU:OE1	2.48	0.45
13:3:60:SER:OG	13:3:61:LYS:N	2.49	0.45
24:3:301:LUT:H11	24:3:301:LUT:H191	1.76	0.45
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.78	0.45
17:A:826:CLA:H2	17:A:826:CLA:H62	1.76	0.45
2:B:374:HIS:O	2:B:378:ILE:HG12	2.17	0.45
6:F:181:TYR:O	6:F:185:VAL:HG22	2.17	0.45
12:1:118:GLN:NE2	12:1:126:VAL:O	2.50	0.45
12:1:160:TYR:CZ	12:1:181:LYS:HE3	2.52	0.45
1:A:320:LYS:NZ	1:A:340:GLU:OE2	2.48	0.44
1:A:502:SER:HB3	1:A:507:TRP:HD1	1.80	0.44
1:A:641:ILE:HD12	1:A:641:ILE:H	1.81	0.44
1:A:675:HIS:O	1:A:678:TRP:CB	2.66	0.44
17:A:836:CLA:HBA2	17:A:837:CLA:HAA2	1.99	0.44
2:B:498:LEU:HA	2:B:498:LEU:HD12	1.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ILE:HD13	2:B:590:VAL:HG22	1.98	0.44
2:B:725:LEU:O	2:B:729:THR:HG22	2.15	0.44
20:B:849:BCR:H351	20:B:849:BCR:H15C	1.74	0.44
14:4:48:SER:O	14:4:50:LEU:N	2.50	0.44
1:A:205:LEU:HD23	1:A:303:LEU:HD11	1.99	0.44
1:A:260:PRO:HB3	1:A:268:LYS:HG3	1.99	0.44
1:A:504:SER:OG	1:A:505:LEU:N	2.50	0.44
1:A:667:TYR:HB3	1:A:744:ALA:HB2	1.97	0.44
17:A:834:CLA:O1D	17:A:834:CLA:H2A	2.17	0.44
2:B:276:HIS:O	2:B:280:ILE:HG12	2.17	0.44
2:B:692:ARG:NH1	11:L:155:THR:OG1	2.29	0.44
4:D:178:GLY:HA3	4:D:181:GLN:HE22	1.81	0.44
6:F:169:TYR:HA	6:F:213:TRP:HZ2	1.82	0.44
20:I:102:BCR:H20C	20:I:102:BCR:H361	1.84	0.44
17:4:317:CLA:O2D	17:4:317:CLA:H2A	2.17	0.44
17:A:839:CLA:H202	17:A:852:CLA:H61	1.98	0.44
2:B:82:LEU:HD23	2:B:82:LEU:HA	1.75	0.44
17:B:828:CLA:H2A	17:B:828:CLA:O1D	2.17	0.44
4:D:160:TYR:CE1	4:D:163:PRO:HD2	2.53	0.44
12:1:69:VAL:HG12	12:1:71:GLU:HG3	1.99	0.44
13:3:82:LEU:H	13:3:82:LEU:HD12	1.82	0.44
14:4:81:LEU:O	14:4:85:VAL:HG23	2.17	0.44
1:A:197:HIS:HB3	17:A:812:CLA:HAB	2.00	0.44
2:B:299:HIS:HE1	17:B:823:CLA:NA	2.15	0.44
17:B:806:CLA:HMC3	17:B:808:CLA:HED2	1.99	0.44
7:H:101:LEU:O	7:H:105:LEU:HG	2.17	0.44
10:K:107:ALA:O	10:K:111:VAL:HG23	2.18	0.44
12:1:90:CYS:CB	24:1:502:LUT:C39	2.93	0.44
2:B:460:ALA:HB2	17:B:839:CLA:HED2	1.99	0.44
17:B:808:CLA:HBB1	17:B:808:CLA:HMB1	2.00	0.44
10:K:101:THR:OG1	10:K:102:LEU:N	2.49	0.44
1:A:609:SER:OG	1:A:613:GLN:OE1	2.33	0.44
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.99	0.44
6:F:162:THR:OG1	6:F:163:PRO:HD3	2.17	0.44
1:A:476:LEU:HB2	1:A:528:THR:HG23	1.99	0.44
2:B:244:PHE:N	2:B:264:GLN:OE1	2.44	0.44
17:B:835:CLA:O1D	9:J:35:ASP:HA	2.18	0.44
3:C:12:ILE:HA	3:C:34:CYS:SG	2.58	0.44
7:H:97:LYS:NZ	7:H:99:GLY:H	2.15	0.44
12:1:157:LYS:HD2	12:1:161:PRO:O	2.17	0.44
14:4:168:TYR:O	14:4:168:TYR:CG	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:PHE:O	1:A:679:ALA:HB3	2.17	0.44
17:A:830:CLA:HBB2	17:A:838:CLA:HAB	2.00	0.44
2:B:334:LEU:HD13	17:B:807:CLA:C2D	2.48	0.44
2:B:596:TRP:O	2:B:600:THR:HG23	2.18	0.44
4:D:89:ALA:HA	4:D:93:GLU:O	2.18	0.44
7:H:110:GLY:HA2	8:I:15:VAL:HG11	2.00	0.44
24:1:501:LUT:H32	17:1:504:CLA:CHC	2.48	0.44
24:4:302:LUT:H391	24:4:302:LUT:H31	1.71	0.44
25:6:513:CHL:HHC	25:6:513:CHL:HBB1	2.00	0.44
2:B:159:PRO:O	2:B:160:LYS:HB2	2.18	0.44
2:B:167:TRP:CZ2	17:B:813:CLA:HHB	2.53	0.44
4:D:68:GLN:OE1	4:D:148:GLN:NE2	2.51	0.44
20:L:305:BCR:H24C	20:L:305:BCR:H371	1.72	0.44
12:1:130:ASN:O	12:1:134:ILE:HG12	2.17	0.44
13:3:217:GLU:O	13:3:221:LYS:HG2	2.16	0.44
15:6:60:PRO:O	15:6:65:ARG:HB2	2.17	0.44
2:B:86:PRO:HB3	2:B:121:TYR:CD2	2.53	0.43
20:B:848:BCR:H15C	20:B:848:BCR:H351	1.68	0.43
17:A:808:CLA:CAB	17:B:835:CLA:HMD2	2.48	0.43
14:4:122:ALA:O	14:4:127:TYR:OH	2.22	0.43
17:6:505:CLA:H41	17:6:505:CLA:H61	1.85	0.43
17:6:510:CLA:H91	17:6:510:CLA:H112	1.83	0.43
1:A:646:ARG:HA	2:B:632:ILE:HD12	2.00	0.43
2:B:51:PHE:HE2	2:B:156:HIS:HD2	1.66	0.43
2:B:396:ARG:HB3	4:D:196:LYS:NZ	2.34	0.43
2:B:401:GLU:HA	2:B:404:GLU:HG2	2.00	0.43
11:L:166:LYS:HA	11:L:166:LYS:HD2	1.87	0.43
24:1:501:LUT:H11	24:1:501:LUT:H191	1.74	0.43
20:3:303:BCR:H15C	20:3:303:BCR:H351	1.80	0.43
24:4:302:LUT:H32	17:4:304:CLA:CAB	2.49	0.43
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.88	0.43
2:B:561:GLY:O	2:B:567:THR:OG1	2.32	0.43
11:L:103:TYR:OH	17:L:304:CLA:OBD	2.29	0.43
13:3:241:MET:HA	13:3:244:GLN:OE1	2.18	0.43
15:6:235:GLY:O	15:6:239:GLN:HG3	2.19	0.43
1:A:276:ARG:O	1:A:500:THR:OG1	2.22	0.43
2:B:208:ARG:C	17:B:816:CLA:HMD1	2.38	0.43
4:D:165:ASP:OD2	4:D:167:VAL:HB	2.18	0.43
7:H:93:ALA:HB3	7:H:94:PRO:HD3	2.01	0.43
10:K:68:ARG:HE	17:K:201:CLA:HMD2	1.82	0.43
12:1:226:ILE:HG12	17:1:506:CLA:HBD	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:851:BCR:H15C	20:A:851:BCR:H351	1.75	0.43
15:6:251:LEU:O	15:6:255:LEU:HG	2.18	0.43
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.89	0.43
1:A:363:VAL:HA	17:A:825:CLA:HED2	2.01	0.43
17:A:825:CLA:CHB	17:A:838:CLA:HAA2	2.49	0.43
20:A:854:BCR:H402	10:K:111:VAL:HG21	2.00	0.43
6:F:170:ILE:O	6:F:173:TRP:HB3	2.19	0.43
13:3:232:ARG:O	13:3:236:LEU:HG	2.18	0.43
14:4:132:SER:O	14:4:136:VAL:HG13	2.19	0.43
1:A:741:PHE:CD1	16:A:801:CL0:CMD	3.02	0.43
2:B:282:PHE:CZ	17:B:818:CLA:HBB2	2.53	0.43
7:H:113:VAL:HA	7:H:116:VAL:HG12	2.00	0.43
14:4:161:GLN:HA	14:4:169:SER:HB3	2.01	0.43
1:A:46:ILE:HD11	17:A:852:CLA:HMB3	2.01	0.43
17:A:852:CLA:H62	9:J:14:LEU:HD21	2.00	0.43
17:B:825:CLA:HAB	17:B:832:CLA:HMD2	1.99	0.43
20:J:103:BCR:H341	20:J:103:BCR:H11C	1.79	0.43
13:3:78:ASP:HA	24:3:302:LUT:O23	2.19	0.43
13:3:96:TRP:CE2	17:3:314:CLA:HED1	2.54	0.43
13:3:146:THR:OG1	13:3:147:TYR:N	2.52	0.43
17:4:307:CLA:H62	17:4:307:CLA:H41	1.86	0.43
15:6:79:ASP:OD1	15:6:80:GLY:N	2.51	0.43
2:B:609:PHE:O	2:B:613:SER:OG	2.34	0.43
2:B:651:LEU:HD23	2:B:651:LEU:HA	1.82	0.43
6:F:98:SER:O	6:F:101:LYS:HG3	2.19	0.43
12:1:78:GLU:HA	12:1:159:LYS:HG2	2.01	0.43
13:3:105:GLY:O	13:3:109:MET:HG3	2.19	0.43
20:6:503:BCR:H361	20:6:503:BCR:H21C	2.01	0.43
20:A:846:BCR:H20C	20:A:846:BCR:H361	1.78	0.42
2:B:455:ILE:HD12	2:B:517:PHE:CE2	2.54	0.42
2:B:481:THR:HA	2:B:486:PHE:CD2	2.54	0.42
3:C:75:ARG:HH12	4:D:151:ARG:CZ	2.32	0.42
6:F:131:GLU:O	6:F:135:LYS:HG3	2.19	0.42
24:3:301:LUT:H15	24:3:301:LUT:H201	1.91	0.42
26:4:303:XAT:H15	26:4:303:XAT:H201	1.80	0.42
15:6:117:ALA:CB	26:6:502:XAT:H10	2.49	0.42
1:A:101:TRP:NE1	1:A:110:PRO:HG3	2.34	0.42
1:A:221:ILE:HG13	1:A:234:ILE:HG21	2.00	0.42
1:A:308:MET:HG2	17:A:821:CLA:CAC	2.49	0.42
1:A:327:LYS:H	17:A:843:CLA:HAC1	1.83	0.42
17:A:838:CLA:H2A	17:A:838:CLA:O2D	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:TRP:CH2	17:B:813:CLA:HMB3	2.53	0.42
17:B:840:CLA:H2A	17:B:840:CLA:O1D	2.19	0.42
12:1:104:ASN:HD22	12:1:107:LYS:NZ	2.17	0.42
13:3:235:MET:HB3	24:3:302:LUT:H402	2.01	0.42
15:6:221:LYS:HG2	17:6:510:CLA:OBD	2.19	0.42
17:6:508:CLA:HMB1	17:6:508:CLA:HBB1	2.01	0.42
1:A:143:GLN:HB3	1:A:374:TYR:HB3	2.00	0.42
2:B:31:PHE:CE2	2:B:45:ASN:HB3	2.54	0.42
2:B:169:LYS:NZ	2:B:328:ASN:HA	2.34	0.42
2:B:340:SER:OG	17:B:826:CLA:H2	2.19	0.42
2:B:519:VAL:HG11	2:B:593:TYR:HB2	2.00	0.42
3:C:78:ALA:O	4:D:128:ARG:NH1	2.52	0.42
13:3:156:LEU:HD11	17:3:315:CLA:CMD	2.50	0.42
1:A:75:PHE:HZ	17:A:809:CLA:HBB1	1.84	0.42
2:B:292:ARG:HD2	2:B:296:GLY:HA2	2.00	0.42
2:B:689:ASN:OD1	2:B:689:ASN:N	2.53	0.42
9:J:19:PHE:HE1	17:J:101:CLA:HMC3	1.84	0.42
11:L:107:GLY:HA2	17:L:304:CLA:HMA3	2.01	0.42
11:L:204:LEU:HD12	11:L:204:LEU:HA	1.91	0.42
12:1:177:PHE:CE1	17:1:504:CLA:HED1	2.54	0.42
12:1:208:THR:OG1	12:1:209:GLY:N	2.52	0.42
17:B:834:CLA:H2A	17:B:834:CLA:O1D	2.19	0.42
6:F:200:VAL:HA	6:F:203:ALA:HB3	2.01	0.42
12:1:134:ILE:HD13	17:1:515:CLA:HMD3	2.00	0.42
24:1:501:LUT:C32	17:1:504:CLA:HMC2	2.49	0.42
13:3:142:PRO:N	13:3:143:PRO:HD2	2.34	0.42
15:6:96:GLU:CD	15:6:99:SER:H	2.22	0.42
26:6:502:XAT:H391	26:6:502:XAT:H31	1.77	0.42
20:A:846:BCR:H351	20:A:846:BCR:H15C	1.71	0.42
2:B:183:PHE:CE2	17:B:821:CLA:HBB2	2.54	0.42
6:F:228:VAL:HG12	6:F:229:ASP:N	2.35	0.42
12:1:154:ASP:CB	12:1:157:LYS:H	2.33	0.42
13:3:156:LEU:HD11	17:3:315:CLA:C2D	2.50	0.42
15:6:218:LEU:HD23	15:6:218:LEU:HA	1.91	0.42
17:6:510:CLA:HBA1	17:6:510:CLA:H3A	1.90	0.42
1:A:122:GLU:HG2	6:F:122:THR:HG21	2.02	0.42
1:A:233:GLU:OE2	1:A:233:GLU:N	2.46	0.42
2:B:220:GLN:O	2:B:224:PRO:HD3	2.20	0.42
7:H:109:GLY:O	7:H:113:VAL:HG12	2.20	0.42
20:1:503:BCR:H381	17:1:509:CLA:H12	2.02	0.42
2:B:95:HIS:CE1	17:B:811:CLA:HMB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:ASN:O	2:B:490:ARG:NH2	2.53	0.42
2:B:519:VAL:HG11	2:B:593:TYR:CG	2.55	0.42
17:B:818:CLA:H92	17:B:818:CLA:H62	1.84	0.42
13:3:202:PRO:HG2	17:3:304:CLA:OBD	2.20	0.42
13:3:238:PHE:CE2	24:3:302:LUT:H14	2.54	0.42
15:6:224:LYS:HZ3	17:6:510:CLA:C3D	2.32	0.42
1:A:98:TYR:CE2	1:A:102:LEU:HD11	2.55	0.42
1:A:102:LEU:HD13	1:A:151:THR:HA	2.02	0.42
1:A:151:THR:HG21	1:A:221:ILE:HD11	2.02	0.42
1:A:197:HIS:HD2	17:A:812:CLA:HAB	1.83	0.42
1:A:338:LEU:HA	1:A:341:ILE:HD13	2.01	0.42
20:A:851:BCR:H24C	20:A:851:BCR:H371	1.87	0.42
2:B:394:PHE:HD1	2:B:394:PHE:HA	1.71	0.42
2:B:594:TRP:HB2	17:B:838:CLA:HMC1	2.01	0.42
2:B:674:LEU:HD12	2:B:674:LEU:HA	1.85	0.42
20:B:845:BCR:H15C	20:B:845:BCR:H351	1.88	0.42
4:D:98:THR:HG23	4:D:122:ASN:O	2.19	0.42
12:1:76:PHE:O	17:1:507:CLA:HMB3	2.19	0.42
13:3:165:GLY:C	13:3:169:HIS:HD1	2.23	0.42
20:4:301:BCR:H341	20:4:301:BCR:H11C	1.79	0.42
1:A:118:ILE:HD11	9:J:27:ILE:HB	2.02	0.42
1:A:693:GLN:HB3	2:B:546:LEU:HD22	2.02	0.42
17:A:827:CLA:O1D	17:A:828:CLA:HHB	2.20	0.42
17:A:829:CLA:H62	17:A:829:CLA:H41	1.97	0.42
2:B:527:LEU:HD23	2:B:527:LEU:HA	1.88	0.42
17:B:804:CLA:HAA2	17:B:804:CLA:O2D	2.18	0.42
3:C:6:LYS:HE3	4:D:203:PHE:HD1	1.84	0.42
4:D:191:SER:OG	4:D:193:ILE:HG22	2.20	0.42
5:E:92:LYS:HD2	5:E:92:LYS:HA	1.79	0.42
17:A:804:CLA:H161	17:A:804:CLA:H202	1.77	0.41
20:A:848:BCR:H15C	20:A:848:BCR:H351	1.84	0.41
3:C:31:TRP:O	3:C:37:LYS:NZ	2.47	0.41
11:L:164:ARG:NH2	11:L:166:LYS:HA	2.35	0.41
12:1:226:ILE:HD11	17:1:506:CLA:H11	2.01	0.41
24:1:501:LUT:H35	24:1:501:LUT:H401	1.75	0.41
13:3:159:PHE:CD1	17:6:511:CLA:HBA1	2.55	0.41
17:3:311:CLA:H3A	17:3:311:CLA:CGA	2.50	0.41
15:6:217:VAL:HG13	17:6:510:CLA:HED1	2.02	0.41
24:6:501:LUT:H383	17:6:506:CLA:C3B	2.50	0.41
25:6:512:CHL:HHC	25:6:512:CHL:HBB1	2.01	0.41
1:A:146:ARG:NH1	1:A:225:LEU:HD13	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD22	1:A:469:PHE:CE2	2.53	0.41
1:A:465:PRO:HA	1:A:468:MET:HG3	2.02	0.41
2:B:26:ALA:HB2	22:B:851:DGD:HA22	2.02	0.41
2:B:189:ALA:HB1	17:B:816:CLA:HAB	2.02	0.41
2:B:236:ASN:O	2:B:252:THR:N	2.54	0.41
2:B:246:THR:OG1	2:B:247:ALA:N	2.53	0.41
2:B:416:GLU:OE1	2:B:416:GLU:N	2.45	0.41
4:D:103:LYS:HD3	4:D:103:LYS:HA	1.82	0.41
5:E:79:LYS:N	5:E:80:PRO:HD2	2.35	0.41
6:F:95:GLU:O	6:F:99:VAL:HG22	2.21	0.41
10:K:54:LEU:O	10:K:58:THR:HG22	2.19	0.41
14:4:192:GLU:HG2	14:4:196:LYS:HE3	2.01	0.41
14:4:237:THR:OG1	14:4:238:ILE:N	2.53	0.41
2:B:439:HIS:NE2	2:B:453:ILE:HG13	2.35	0.41
20:B:848:BCR:H24C	20:B:848:BCR:H371	1.91	0.41
6:F:139:LEU:HD12	6:F:149:ILE:HG13	2.03	0.41
10:K:78:LYS:HD3	10:K:78:LYS:HA	1.93	0.41
11:L:109:PHE:CE1	11:L:128:GLY:HA3	2.55	0.41
20:L:305:BCR:H351	20:L:305:BCR:H15C	1.75	0.41
13:3:95:ARG:HG3	13:3:175:TRP:HH2	1.84	0.41
1:A:43:THR:HG22	1:A:715:ARG:HB2	2.02	0.41
1:A:80:ILE:HD12	20:J:103:BCR:HC31	2.01	0.41
1:A:556:ARG:HD2	1:A:556:ARG:HA	1.83	0.41
2:B:172:GLU:H	2:B:172:GLU:CD	2.23	0.41
2:B:615:TYR:O	2:B:618:GLY:N	2.49	0.41
20:B:849:BCR:H11C	20:B:849:BCR:H341	1.78	0.41
3:C:53:ARG:HA	3:C:56:SER:HB3	2.01	0.41
6:F:90:ALA:HA	6:F:93:LYS:HG2	2.02	0.41
6:F:99:VAL:O	6:F:103:ASN:ND2	2.53	0.41
6:F:206:ILE:HG23	6:F:209:ARG:HH22	1.85	0.41
20:I:102:BCR:H351	20:I:102:BCR:H15C	1.73	0.41
24:3:302:LUT:H15	24:3:302:LUT:H201	1.87	0.41
20:4:301:BCR:H24C	20:4:301:BCR:H371	1.87	0.41
24:4:302:LUT:H15	24:4:302:LUT:H201	1.72	0.41
17:4:306:CLA:H51	17:4:306:CLA:H11	1.79	0.41
17:4:310:CLA:H2A	17:4:310:CLA:O2D	2.20	0.41
1:A:71:PHE:HD2	1:A:188:PHE:CE1	2.38	0.41
1:A:742:PHE:O	1:A:746:ILE:HG22	2.20	0.41
13:3:203:GLY:N	17:3:304:CLA:OBD	2.54	0.41
17:3:305:CLA:H61	17:3:305:CLA:H41	1.79	0.41
14:4:90:VAL:O	14:4:94:TRP:HD1	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:165:GLU:OE1	15:6:168:ARG:NE	2.40	0.41
1:A:537:HIS:CD2	17:A:836:CLA:HAB	2.55	0.41
2:B:190:TRP:HZ2	17:B:820:CLA:HED2	1.86	0.41
2:B:276:HIS:HB2	17:B:819:CLA:C1B	2.51	0.41
2:B:451:LYS:HE3	9:J:35:ASP:HB3	2.02	0.41
4:D:104:GLU:OE2	4:D:119:GLU:N	2.54	0.41
5:E:87:ARG:HD3	5:E:87:ARG:HA	1.76	0.41
19:1:516:LHG:H241	20:4:301:BCR:HC21	2.01	0.41
13:3:272:LEU:HB3	13:3:274:PHE:CE2	2.55	0.41
1:A:210:TRP:CZ2	17:A:818:CLA:O1D	2.73	0.41
1:A:605:ILE:HG22	1:A:742:PHE:CZ	2.56	0.41
20:A:848:BCR:H11C	20:A:848:BCR:H341	1.73	0.41
2:B:680:TRP:HE1	2:B:684:ARG:NH1	2.18	0.41
6:F:205:ARG:O	6:F:209:ARG:NH1	2.54	0.41
10:K:77:ARG:HA	10:K:87:ALA:HA	2.02	0.41
12:1:97:PRO:HB3	17:1:509:CLA:O1D	2.20	0.41
12:1:174:PRO:O	12:1:177:PHE:HB3	2.20	0.41
12:1:212:GLU:O	12:1:216:THR:HG23	2.20	0.41
13:3:79:PRO:HD2	24:3:302:LUT:O23	2.20	0.41
17:4:306:CLA:H41	17:4:306:CLA:H61	1.80	0.41
26:6:502:XAT:H35	26:6:502:XAT:H401	1.79	0.41
17:A:813:CLA:H3A	20:A:846:BCR:C33	2.50	0.41
17:A:839:CLA:HMA2	17:B:833:CLA:HMB3	2.03	0.41
17:A:843:CLA:H3A	17:A:843:CLA:HBA1	1.76	0.41
2:B:574:ASP:O	2:B:577:TYR:HB3	2.21	0.41
3:C:8:TYR:HE2	4:D:186:ILE:HG13	1.86	0.41
11:L:102:GLY:O	11:L:106:VAL:HG23	2.20	0.41
13:3:59:ALA:HB2	13:3:76:GLY:O	2.20	0.41
15:6:78:LEU:HD13	15:6:78:LEU:HA	1.96	0.41
1:A:56:PHE:CD2	17:A:804:CLA:HMC2	2.56	0.41
1:A:346:TRP:HB3	17:A:804:CLA:HAC1	2.02	0.41
1:A:633:ASN:ND2	1:A:647:ASP:OD1	2.54	0.41
1:A:692:TRP:CE2	18:A:842:PQN:H2M3	2.56	0.41
1:A:721:GLN:HE21	19:A:844:LHG:HC92	1.85	0.41
17:A:803:CLA:H2	17:A:803:CLA:H61	1.76	0.41
2:B:218:TYR:OH	2:B:232:LEU:O	2.21	0.41
2:B:451:LYS:HB3	2:B:451:LYS:HE2	1.90	0.41
2:B:457:PRO:O	2:B:461:GLN:HG3	2.21	0.41
17:B:813:CLA:HBA1	17:B:813:CLA:H3A	1.79	0.41
5:E:120:VAL:HG12	5:E:137:TYR:O	2.21	0.41
6:F:120:GLN:HA	6:F:123:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:52:THR:O	10:K:56:MET:HG2	2.21	0.41
10:K:68:ARG:HA	10:K:100:PHE:CZ	2.56	0.41
11:L:165:LYS:HA	11:L:165:LYS:HD2	1.82	0.41
11:L:166:LYS:NZ	11:L:167:GLU:HB3	2.36	0.41
12:1:161:PRO:HG2	17:1:504:CLA:OBD	2.21	0.41
19:1:516:LHG:HC82	19:1:516:LHG:H111	1.79	0.41
13:3:72:PRO:HB3	13:3:221:LYS:NZ	2.35	0.41
13:3:159:PHE:HB2	17:6:511:CLA:HAA2	2.03	0.41
13:3:180:SER:OG	15:6:71:GLY:HA2	2.21	0.41
20:6:503:BCR:H382	20:6:503:BCR:H23C	2.03	0.41
20:A:851:BCR:H403	9:J:16:THR:HG21	2.01	0.41
2:B:104:PHE:O	2:B:106:ARG:HG2	2.21	0.41
5:E:94:LEU:HD22	5:E:141:GLU:HA	2.02	0.41
5:E:116:THR:HG22	5:E:117:ARG:N	2.36	0.41
12:1:192:MET:CB	24:1:502:LUT:H202	2.51	0.41
14:4:99:VAL:HG21	24:4:302:LUT:H10	2.03	0.41
26:6:502:XAT:H15	26:6:502:XAT:H201	1.61	0.41
1:A:492:PRO:HG2	1:A:502:SER:HA	2.03	0.40
20:A:849:BCR:H11C	20:A:849:BCR:H341	1.93	0.40
3:C:19:ARG:NH2	4:D:170:GLU:OE2	2.55	0.40
4:D:97:ILE:HD13	4:D:135:LEU:HD22	2.04	0.40
20:K:204:BCR:H11C	20:K:204:BCR:H341	1.82	0.40
12:1:145:ALA:HB1	12:1:149:ARG:NE	2.36	0.40
12:1:226:ILE:HG12	17:1:506:CLA:CBD	2.51	0.40
17:1:505:CLA:HBA1	17:1:505:CLA:HMA2	2.03	0.40
13:3:259:HIS:CE1	17:3:306:CLA:HMA2	2.56	0.40
14:4:64:ALA:O	17:4:307:CLA:HED1	2.21	0.40
14:4:198:LEU:HD23	14:4:198:LEU:HA	1.92	0.40
1:A:46:ILE:HD12	17:A:853:CLA:HBD	2.02	0.40
1:A:297:ALA:HB1	17:A:816:CLA:HBC2	2.03	0.40
1:A:690:GLY:O	1:A:694:GLU:HG3	2.22	0.40
17:A:833:CLA:H2A	17:A:833:CLA:HED3	2.03	0.40
2:B:649:MET:O	2:B:652:PHE:HB3	2.21	0.40
3:C:24:ASP:HB2	4:D:133:LEU:HD22	2.03	0.40
6:F:127:LYS:O	6:F:131:GLU:HG2	2.21	0.40
20:L:301:BCR:H24C	20:L:301:BCR:H371	1.88	0.40
13:3:223:LEU:HD12	13:3:223:LEU:HA	1.76	0.40
14:4:153:ILE:HD13	14:4:153:ILE:HA	1.93	0.40
1:A:374:TYR:HB2	1:A:377:LEU:HD22	2.02	0.40
1:A:502:SER:HB3	1:A:507:TRP:CD1	2.55	0.40
1:A:522:LEU:HD23	1:A:616:VAL:HG13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:THR:HG22	3:C:74:THR:N	2.33	0.40
9:J:35:ASP:O	9:J:37:LEU:N	2.54	0.40
14:4:222:PRO:HA	14:4:225:ASN:ND2	2.37	0.40
1:A:298:ILE:HD11	17:A:817:CLA:C3C	2.52	0.40
1:A:514:ALA:HB2	1:A:519:VAL:HG12	2.04	0.40
1:A:541:ILE:HG21	17:A:838:CLA:HED1	2.03	0.40
1:A:608:PHE:O	1:A:612:MET:HG2	2.21	0.40
2:B:183:PHE:HB3	2:B:284:PHE:CD2	2.56	0.40
3:C:22:PRO:O	4:D:133:LEU:HD23	2.22	0.40
4:D:163:PRO:C	4:D:165:ASP:H	2.24	0.40
13:3:95:ARG:HH12	13:3:99:TYR:HD1	1.67	0.40
13:3:100:GLY:HA2	17:3:314:CLA:HED3	2.03	0.40
13:3:142:PRO:HG2	17:3:312:CLA:HMB3	2.03	0.40
14:4:135:PHE:HB2	25:4:313:CHL:HBC1	2.03	0.40
24:4:302:LUT:C14	17:4:305:CLA:HBB1	2.52	0.40
17:4:307:CLA:CGA	17:4:307:CLA:H3A	2.51	0.40
15:6:61:LEU:HD11	15:6:74:PRO:HG2	2.03	0.40
15:6:121:ILE:HG13	26:6:502:XAT:H163	2.02	0.40
17:6:505:CLA:O2A	17:6:505:CLA:H2A	2.18	0.40
1:A:45:TRP:HE3	1:A:46:ILE:HG22	1.86	0.40
1:A:46:ILE:O	1:A:50:HIS:ND1	2.54	0.40
1:A:63:LEU:HD23	1:A:63:LEU:H	1.85	0.40
1:A:459:MET:CE	1:A:464:ARG:HH21	2.34	0.40
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.56	0.40
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.98	0.40
2:B:407:VAL:O	2:B:411:MET:HG2	2.22	0.40
2:B:623:TYR:O	2:B:627:ASN:HB2	2.22	0.40
11:L:164:ARG:HH21	11:L:166:LYS:HA	1.87	0.40
12:1:165:PHE:CE2	17:1:513:CLA:HBA2	2.57	0.40
14:4:63:LEU:HD12	14:4:63:LEU:H	1.85	0.40
14:4:147:ILE:HD12	14:4:147:ILE:HA	1.97	0.40
15:6:68:TRP:CD2	15:6:88:PHE:HD1	2.40	0.40
15:6:239:GLN:HG2	17:6:506:CLA:C4D	2.52	0.40
17:6:511:CLA:H3A	17:6:511:CLA:HBA2	1.60	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	740/742 (100%)	684 (92%)	56 (8%)	0	100 100
2	B	731/733 (100%)	680 (93%)	51 (7%)	0	100 100
3	C	79/81 (98%)	68 (86%)	11 (14%)	0	100 100
4	D	140/142 (99%)	125 (89%)	15 (11%)	0	100 100
5	E	66/68 (97%)	61 (92%)	5 (8%)	0	100 100
6	F	156/158 (99%)	148 (95%)	8 (5%)	0	100 100
7	H	59/61 (97%)	56 (95%)	3 (5%)	0	100 100
8	I	28/30 (93%)	28 (100%)	0	0	100 100
9	J	40/42 (95%)	38 (95%)	1 (2%)	1 (2%)	5 36
10	K	82/84 (98%)	75 (92%)	7 (8%)	0	100 100
11	L	144/146 (99%)	134 (93%)	10 (7%)	0	100 100
12	1	191/193 (99%)	171 (90%)	18 (9%)	2 (1%)	15 52
13	3	220/222 (99%)	193 (88%)	27 (12%)	0	100 100
14	4	195/197 (99%)	183 (94%)	12 (6%)	0	100 100
15	6	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	15 52
All	All	3080/3110 (99%)	2834 (92%)	241 (8%)	5 (0%)	50 79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	6	191	THR
15	6	192	PRO
9	J	36	ALA
12	1	101	GLY
12	1	221	PRO

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	588/600 (98%)	588 (100%)	0	100 100
2	B	589/600 (98%)	587 (100%)	2 (0%)	92 95
3	C	71/71 (100%)	71 (100%)	0	100 100
4	D	118/119 (99%)	118 (100%)	0	100 100
5	E	58/59 (98%)	58 (100%)	0	100 100
6	F	115/127 (91%)	114 (99%)	1 (1%)	78 87
7	H	47/49 (96%)	47 (100%)	0	100 100
8	I	27/27 (100%)	27 (100%)	0	100 100
9	J	34/36 (94%)	34 (100%)	0	100 100
10	K	56/61 (92%)	54 (96%)	2 (4%)	35 61
11	L	110/115 (96%)	110 (100%)	0	100 100
12	1	147/155 (95%)	145 (99%)	2 (1%)	67 81
13	3	159/176 (90%)	157 (99%)	2 (1%)	69 81
14	4	156/164 (95%)	156 (100%)	0	100 100
15	6	162/172 (94%)	162 (100%)	0	100 100
All	All	2437/2531 (96%)	2428 (100%)	9 (0%)	91 94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	327	ASN
2	B	394	PHE
6	F	101	LYS
10	K	68	ARG
10	K	88	ARG
12	1	217	HIS
12	1	225	ASN
13	3	191	LYS
13	3	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	GLN
2	B	368	GLN
2	B	432	HIS
3	C	16	GLN
4	D	68	GLN
4	D	148	GLN
4	D	181	GLN
5	E	135	ASN
13	3	255	ASN
13	3	265	ASN
15	6	250	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

196 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	A	833	-	41,49,73	1.82	8 (19%)	47,84,113	1.62	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	834	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	7 (13%)
17	CLA	B	837	-	42,50,73	1.84	6 (14%)	48,85,113	1.58	6 (12%)
17	CLA	1	508	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	6 (7%)
17	CLA	B	806	-	41,49,73	1.81	6 (14%)	47,84,113	1.62	7 (14%)
17	CLA	A	802	-	39,48,73	1.87	7 (17%)	45,82,113	1.76	8 (17%)
17	CLA	1	506	-	55,63,73	1.61	6 (10%)	64,101,113	1.42	9 (14%)
19	LHG	1	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	4 (7%)
17	CLA	A	813	-	42,50,73	1.83	7 (16%)	48,85,113	1.57	7 (14%)
17	CLA	J	102	-	42,50,73	1.84	5 (11%)	48,85,113	1.60	6 (12%)
17	CLA	K	202	-	45,53,73	1.78	5 (11%)	52,89,113	1.57	9 (17%)
17	CLA	L	303	-	60,68,73	1.51	6 (10%)	70,107,113	1.43	7 (10%)
20	BCR	B	850	-	40,40,41	0.76	0	54,54,56	2.08	15 (27%)
25	CHL	1	514	-	47,55,74	2.42	16 (34%)	50,91,114	2.77	20 (40%)
17	CLA	A	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.66	9 (15%)
17	CLA	B	828	-	41,49,73	1.81	8 (19%)	47,84,113	1.74	7 (14%)
17	CLA	B	841	-	41,49,73	1.80	7 (17%)	47,84,113	1.69	7 (14%)
23	LMG	J	105	-	30,30,55	1.20	2 (6%)	38,38,63	1.22	3 (7%)
17	CLA	A	825	-	41,49,73	1.78	6 (14%)	47,84,113	1.71	8 (17%)
17	CLA	6	508	-	40,48,73	1.84	6 (15%)	46,83,113	1.73	8 (17%)
20	BCR	L	305	-	41,41,41	0.71	0	56,56,56	2.18	18 (32%)
17	CLA	A	828	-	43,51,73	1.78	7 (16%)	48,85,113	1.61	6 (12%)
17	CLA	3	306	-	41,49,73	1.86	6 (14%)	47,84,113	1.69	8 (17%)
17	CLA	A	840	-	41,49,73	1.80	6 (14%)	47,84,113	1.70	7 (14%)
17	CLA	A	824	-	56,64,73	1.55	7 (12%)	65,102,113	1.45	9 (13%)
17	CLA	A	853	-	45,53,73	1.74	7 (15%)	52,89,113	1.66	8 (15%)
17	CLA	A	827	-	41,49,73	1.80	8 (19%)	47,84,113	1.64	10 (21%)
17	CLA	B	804	-	43,50,73	2.36	9 (20%)	46,83,113	2.07	9 (19%)
17	CLA	B	810	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
17	CLA	1	505	-	46,54,73	1.65	6 (13%)	53,90,113	1.54	8 (15%)
17	CLA	3	308	-	42,50,73	1.81	5 (11%)	48,85,113	1.69	6 (12%)
19	LHG	A	845	-	24,24,48	0.96	1 (4%)	26,29,54	1.26	3 (11%)
17	CLA	A	832	-	43,51,73	1.80	6 (13%)	49,86,113	1.56	8 (16%)
17	CLA	B	836	-	59,66,73	1.68	7 (11%)	64,103,113	1.42	8 (12%)
17	CLA	4	308	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	7 (14%)
24	LUT	1	502	-	42,43,43	2.39	1 (2%)	51,60,60	1.81	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CHL	4	313	-	47,55,74	2.39	16 (34%)	50,91,114	2.74	20 (40%)
17	CLA	B	843	19	37,46,73	1.89	5 (13%)	44,80,113	1.67	7 (15%)
17	CLA	B	830	-	38,47,73	1.93	8 (21%)	48,81,113	1.81	10 (20%)
17	CLA	6	514	-	39,48,73	1.83	6 (15%)	45,82,113	1.74	8 (17%)
20	BCR	F	803	-	41,41,41	0.76	0	56,56,56	2.16	18 (32%)
17	CLA	6	511	-	50,58,73	1.70	6 (12%)	58,95,113	1.53	8 (13%)
17	CLA	A	804	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	6 (7%)
17	CLA	6	507	-	51,59,73	1.66	7 (13%)	59,96,113	1.53	8 (13%)
17	CLA	K	205	-	37,47,73	1.97	6 (16%)	42,81,113	1.63	7 (16%)
20	BCR	B	845	-	41,41,41	0.75	0	56,56,56	2.15	19 (33%)
20	BCR	I	102	-	41,41,41	0.70	0	56,56,56	2.15	16 (28%)
17	CLA	A	810	17	55,63,73	1.61	8 (14%)	64,101,113	1.45	8 (12%)
20	BCR	J	103	-	41,41,41	0.77	1 (2%)	56,56,56	2.11	17 (30%)
25	CHL	3	313	-	47,54,74	2.40	15 (31%)	45,89,114	2.89	19 (42%)
24	LUT	3	302	-	42,43,43	0.77	0	51,60,60	1.85	16 (31%)
17	CLA	3	311	-	48,56,73	1.72	6 (12%)	55,92,113	1.54	7 (12%)
17	CLA	B	819	-	41,49,73	1.83	6 (14%)	47,84,113	1.63	8 (17%)
17	CLA	L	304	-	45,53,73	1.76	6 (13%)	52,89,113	1.60	6 (11%)
17	CLA	4	310	-	42,50,73	1.84	6 (14%)	48,85,113	1.61	7 (14%)
21	SF4	B	802	-	0,12,12	-	-	-		
17	CLA	1	509	-	50,58,73	1.50	6 (12%)	58,95,113	2.06	16 (27%)
17	CLA	B	840	-	41,49,73	1.81	7 (17%)	47,84,113	1.72	9 (19%)
20	BCR	6	503	-	41,41,41	0.71	0	56,56,56	3.61	30 (53%)
17	CLA	B	839	-	41,49,73	1.81	5 (12%)	47,84,113	1.72	8 (17%)
17	CLA	A	823	-	42,50,73	1.83	7 (16%)	52,85,113	1.74	9 (17%)
17	CLA	3	307	13	39,48,73	1.90	5 (12%)	45,82,113	1.71	8 (17%)
17	CLA	A	843	-	49,57,73	1.75	6 (12%)	61,94,113	1.67	8 (13%)
17	CLA	B	833	-	43,51,73	1.77	6 (13%)	49,86,113	1.55	6 (12%)
25	CHL	1	512	-	47,55,74	2.44	16 (34%)	50,91,114	2.79	22 (44%)
17	CLA	3	316	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
20	BCR	4	301	-	41,41,41	0.72	0	56,56,56	1.85	14 (25%)
17	CLA	B	809	-	52,60,73	1.66	8 (15%)	60,97,113	1.47	8 (13%)
16	CL0	A	801	-	61,69,73	1.64	10 (16%)	70,107,113	2.21	16 (22%)
21	SF4	C	102	-	0,12,12	-	-	-		
17	CLA	A	808	1	41,49,73	1.85	7 (17%)	47,84,113	1.67	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	I	101	-	41,41,41	0.80	1 (2%)	56,56,56	2.29	21 (37%)
17	CLA	F	802	-	41,49,73	1.86	6 (14%)	47,84,113	1.63	7 (14%)
19	LHG	6	516	-	34,34,48	1.08	2 (5%)	37,40,54	1.14	3 (8%)
17	CLA	B	814	-	43,51,73	1.77	7 (16%)	49,86,113	1.61	6 (12%)
17	CLA	4	315	14	41,49,73	1.85	6 (14%)	47,84,113	1.70	10 (21%)
17	CLA	B	821	-	55,63,73	1.60	7 (12%)	64,101,113	1.47	7 (10%)
17	CLA	4	306	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
17	CLA	A	811	-	41,49,73	1.83	8 (19%)	47,84,113	1.64	8 (17%)
20	BCR	B	847	-	41,41,41	0.74	0	56,56,56	2.24	18 (32%)
17	CLA	4	317	-	50,58,73	1.68	6 (12%)	58,95,113	1.51	9 (15%)
17	CLA	6	504	-	40,47,73	2.26	8 (20%)	49,81,113	1.74	9 (18%)
20	BCR	F	801	-	41,41,41	0.74	0	56,56,56	2.22	21 (37%)
17	CLA	1	515	-	39,48,73	1.93	7 (17%)	45,82,113	1.74	8 (17%)
17	CLA	B	831	-	56,64,73	1.59	7 (12%)	65,102,113	1.49	7 (10%)
17	CLA	B	834	-	43,51,73	1.77	6 (13%)	49,86,113	1.65	7 (14%)
17	CLA	1	504	-	41,49,73	1.84	7 (17%)	47,84,113	1.73	9 (19%)
17	CLA	A	805	-	46,54,73	1.73	6 (13%)	53,90,113	1.57	6 (11%)
17	CLA	A	807	-	42,50,73	1.81	6 (14%)	48,85,113	1.66	7 (14%)
17	CLA	4	311	-	46,54,73	1.78	7 (15%)	53,90,113	1.54	8 (15%)
17	CLA	4	312	-	41,49,73	1.82	6 (14%)	47,84,113	1.65	7 (14%)
17	CLA	A	852	-	57,65,73	1.57	7 (12%)	66,103,113	1.43	7 (10%)
17	CLA	K	203	-	41,49,73	1.80	6 (14%)	47,84,113	1.71	8 (17%)
20	BCR	A	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.19	18 (32%)
20	BCR	1	503	-	10,11,41	0.69	0	15,16,56	1.94	4 (26%)
17	CLA	B	826	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	8 (10%)
17	CLA	B	832	-	39,48,73	1.86	7 (17%)	45,82,113	1.76	8 (17%)
17	CLA	1	511	-	38,47,73	2.06	8 (21%)	46,80,113	1.72	10 (21%)
26	XAT	6	502	-	39,47,47	0.91	0	54,74,74	2.89	22 (40%)
17	CLA	B	813	-	54,62,73	1.68	6 (11%)	67,100,113	1.51	10 (14%)
17	CLA	3	304	-	40,46,73	2.85	9 (22%)	47,79,113	1.57	8 (17%)
19	LHG	A	844	-	39,39,48	1.00	2 (5%)	42,45,54	1.23	4 (9%)
17	CLA	6	509	-	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
20	BCR	K	204	-	41,41,41	0.70	0	56,56,56	2.09	18 (32%)
17	CLA	B	815	-	43,51,73	1.78	6 (13%)	49,86,113	1.51	6 (12%)
20	BCR	A	848	-	41,41,41	0.80	1 (2%)	56,56,56	2.15	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	818	-	55,63,73	1.58	6 (10%)	64,101,113	1.46	7 (10%)
17	CLA	3	310	-	41,49,73	1.89	6 (14%)	47,84,113	1.65	7 (14%)
25	CHL	6	517	15	47,55,74	2.27	15 (31%)	50,91,114	2.81	19 (38%)
17	CLA	A	826	-	64,72,73	1.52	8 (12%)	79,112,113	1.50	9 (11%)
17	CLA	6	506	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
17	CLA	A	838	-	52,60,73	1.60	7 (13%)	60,97,113	1.57	8 (13%)
17	CLA	A	829	-	58,66,73	1.60	8 (13%)	67,104,113	1.46	7 (10%)
17	CLA	A	816	-	60,68,73	1.55	6 (10%)	70,107,113	1.41	6 (8%)
20	BCR	B	848	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	16 (28%)
17	CLA	3	305	-	52,60,73	1.70	6 (11%)	60,97,113	1.52	10 (16%)
17	CLA	A	837	-	55,63,73	1.57	6 (10%)	64,101,113	1.54	10 (15%)
17	CLA	B	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
17	CLA	A	821	-	42,50,73	1.76	7 (16%)	48,85,113	1.64	6 (12%)
17	CLA	A	803	17	52,60,73	1.65	6 (11%)	60,97,113	1.55	9 (15%)
17	CLA	4	307	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	8 (11%)
17	CLA	A	841	-	41,49,73	1.83	8 (19%)	47,84,113	1.66	8 (17%)
17	CLA	B	812	-	39,48,73	1.86	7 (17%)	45,82,113	1.77	8 (17%)
17	CLA	6	510	-	60,68,73	1.54	6 (10%)	70,107,113	1.38	6 (8%)
25	CHL	6	512	-	47,55,74	2.43	16 (34%)	50,91,114	2.76	19 (38%)
17	CLA	B	816	-	39,46,73	1.83	7 (17%)	44,79,113	1.62	5 (11%)
17	CLA	A	835	1	41,50,73	1.88	7 (17%)	49,85,113	1.54	7 (14%)
17	CLA	B	807	-	41,49,73	1.80	6 (14%)	47,84,113	1.69	9 (19%)
17	CLA	B	811	2	51,59,73	1.69	7 (13%)	59,96,113	1.52	10 (16%)
17	CLA	K	201	-	38,45,73	1.91	7 (18%)	43,78,113	1.64	7 (16%)
23	LMG	4	318	-	18,18,55	1.60	2 (11%)	22,23,63	1.61	2 (9%)
24	LUT	6	501	-	42,43,43	0.78	0	51,60,60	1.89	13 (25%)
17	CLA	A	814	-	42,50,73	1.81	7 (16%)	48,85,113	1.59	6 (12%)
22	DGD	J	104	-	67,67,67	0.84	2 (2%)	81,81,81	0.88	3 (3%)
17	CLA	A	815	-	45,53,73	1.81	6 (13%)	52,89,113	1.56	6 (11%)
17	CLA	4	305	-	50,58,73	1.71	6 (12%)	58,95,113	1.50	8 (13%)
24	LUT	1	501	-	42,43,43	0.80	0	51,60,60	1.97	13 (25%)
17	CLA	A	817	-	39,47,73	1.86	7 (17%)	42,81,113	1.73	8 (19%)
17	CLA	1	513	-	52,60,73	1.68	6 (11%)	60,97,113	1.51	8 (13%)
26	XAT	4	303	-	39,47,47	0.88	0	54,74,74	2.72	20 (37%)
17	CLA	3	309	-	50,58,73	1.67	5 (10%)	58,95,113	1.60	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LUT	3	301	-	42,43,43	0.79	0	51,60,60	2.00	11 (21%)
22	DGD	B	851	-	53,53,67	0.93	2 (3%)	67,67,81	1.06	3 (4%)
17	CLA	B	838	-	39,48,73	1.83	7 (17%)	45,82,113	1.71	8 (17%)
17	CLA	4	304	-	38,47,73	1.90	7 (18%)	48,81,113	1.93	10 (20%)
20	BCR	A	849	-	41,41,41	0.74	0	56,56,56	2.06	16 (28%)
20	BCR	A	850	-	41,41,41	0.81	2 (4%)	56,56,56	2.33	20 (35%)
21	SF4	C	101	-	0,12,12	-	-	-		
17	CLA	B	808	-	54,62,73	1.58	6 (11%)	62,99,113	1.51	8 (12%)
17	CLA	3	315	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	7 (13%)
18	PQN	A	842	-	15,15,34	1.44	2 (13%)	22,22,45	0.87	2 (9%)
19	LHG	B	852	17	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
17	CLA	A	822	-	41,49,73	1.82	7 (17%)	47,84,113	1.70	7 (14%)
17	CLA	B	824	-	42,50,73	1.81	7 (16%)	48,85,113	1.62	6 (12%)
17	CLA	B	817	-	43,51,73	1.77	7 (16%)	49,86,113	1.57	6 (12%)
17	CLA	A	831	-	56,64,73	1.56	6 (10%)	65,102,113	1.46	7 (10%)
17	CLA	A	812	-	37,47,73	1.85	7 (18%)	41,80,113	1.75	8 (19%)
17	CLA	B	842	-	41,49,73	1.83	8 (19%)	47,84,113	1.69	8 (17%)
17	CLA	B	823	-	41,49,73	1.84	8 (19%)	47,84,113	1.66	7 (14%)
17	CLA	B	829	-	50,58,73	1.64	6 (12%)	58,95,113	1.60	10 (17%)
20	BCR	A	854	-	41,41,41	0.70	0	56,56,56	2.26	19 (33%)
24	LUT	4	302	-	42,43,43	0.76	0	51,60,60	1.90	13 (25%)
25	CHL	4	314	-	51,59,74	2.14	15 (29%)	55,96,114	2.75	20 (36%)
17	CLA	B	827	-	41,48,73	1.96	8 (19%)	45,82,113	1.70	8 (17%)
17	CLA	A	836	-	51,59,73	1.65	6 (11%)	59,96,113	1.52	6 (10%)
17	CLA	B	822	-	41,49,73	1.85	6 (14%)	47,84,113	1.62	8 (17%)
17	CLA	B	835	-	45,53,73	1.74	7 (15%)	52,89,113	1.63	9 (17%)
20	BCR	B	849	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	16 (28%)
20	BCR	A	851	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
25	CHL	6	513	-	48,56,74	2.31	16 (33%)	51,92,114	2.77	22 (43%)
17	CLA	A	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
17	CLA	A	818	-	40,47,73	2.03	7 (17%)	44,81,113	2.14	12 (27%)
17	CLA	L	302	-	40,48,73	1.93	6 (15%)	50,83,113	1.88	9 (18%)
20	BCR	L	301	-	41,41,41	0.75	1 (2%)	56,56,56	2.04	17 (30%)
17	CLA	B	805	-	37,46,73	1.83	7 (18%)	40,79,113	1.88	7 (17%)
17	CLA	B	801	-	64,72,73	1.50	8 (12%)	79,112,113	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	3	303	-	41,41,41	0.79	1 (2%)	56,56,56	2.00	18 (32%)
20	BCR	B	846	-	41,41,41	0.73	0	56,56,56	1.96	14 (25%)
17	CLA	A	819	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	7 (13%)
17	CLA	B	825	-	42,50,73	1.79	7 (16%)	48,85,113	1.59	6 (12%)
17	CLA	J	101	-	41,49,73	1.93	7 (17%)	51,84,113	1.55	6 (11%)
17	CLA	4	309	-	50,58,73	1.66	6 (12%)	58,95,113	1.54	7 (12%)
20	BCR	A	847	-	41,41,41	0.76	0	56,56,56	1.90	17 (30%)
25	CHL	6	515	-	40,49,74	2.39	14 (35%)	42,83,114	2.99	19 (45%)
17	CLA	3	312	13	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
17	CLA	B	803	-	40,49,73	1.73	6 (15%)	44,83,113	1.64	6 (13%)
17	CLA	3	314	-	39,48,73	1.84	6 (15%)	45,82,113	1.84	8 (17%)
17	CLA	A	806	-	41,49,73	1.81	7 (17%)	47,84,113	1.70	9 (19%)
25	CHL	1	517	-	43,51,74	2.37	15 (34%)	45,86,114	2.90	19 (42%)
25	CHL	4	316	-	43,51,74	2.30	14 (32%)	45,86,114	2.85	19 (42%)
17	CLA	A	830	-	50,58,73	1.69	8 (16%)	58,95,113	1.51	8 (13%)
17	CLA	A	820	-	41,49,73	1.78	6 (14%)	47,84,113	1.71	7 (14%)
17	CLA	6	505	-	52,60,73	1.66	7 (13%)	60,97,113	1.51	6 (10%)
18	PQN	B	844	-	17,17,34	2.13	2 (11%)	21,24,45	1.20	3 (14%)
17	CLA	1	510	-	46,54,73	1.76	7 (15%)	53,90,113	1.49	6 (11%)
17	CLA	1	507	12	40,48,73	1.88	7 (17%)	50,83,113	1.74	10 (20%)

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	A	833	-	1/1/10/20	4/8/86/115	-
17	CLA	A	834	-	1/1/11/20	5/13/91/115	-
17	CLA	B	837	-	1/1/10/20	3/10/88/115	-
17	CLA	1	508	-	1/1/15/20	17/37/115/115	-
17	CLA	B	806	-	1/1/10/20	2/8/86/115	-
17	CLA	A	802	-	1/1/9/20	4/8/82/115	-
17	CLA	1	506	-	1/1/13/20	10/25/103/115	-
19	LHG	1	516	-	-	12/53/53/53	-
17	CLA	A	813	-	1/1/10/20	4/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	J	102	-	1/1/10/20	4/10/88/115	-
17	CLA	K	202	-	1/1/11/20	8/13/91/115	-
17	CLA	L	303	-	1/1/14/20	12/31/109/115	-
25	CHL	1	514	-	3/3/16/26	7/17/115/137	-
20	BCR	B	850	-	-	2/27/61/63	0/2/2/2
17	CLA	A	809	-	1/1/12/20	4/19/97/115	-
17	CLA	B	828	-	1/1/10/20	4/8/86/115	-
17	CLA	B	841	-	1/1/10/20	3/8/86/115	-
23	LMG	J	105	-	-	5/25/45/70	0/1/1/1
17	CLA	A	825	-	1/1/10/20	0/8/86/115	-
17	CLA	6	508	-	1/1/10/20	2/6/84/115	-
20	BCR	L	305	-	-	2/29/63/63	0/2/2/2
17	CLA	A	828	-	1/1/10/20	5/10/88/115	-
17	CLA	3	306	-	1/1/10/20	3/8/86/115	-
17	CLA	A	840	-	1/1/10/20	1/8/86/115	-
17	CLA	A	824	-	1/1/13/20	9/27/105/115	-
17	CLA	A	853	-	1/1/11/20	8/13/91/115	-
17	CLA	A	827	-	1/1/10/20	1/8/86/115	-
17	CLA	B	804	-	1/1/9/20	4/10/84/115	-
17	CLA	B	810	-	1/1/15/20	10/37/115/115	-
17	CLA	3	308	-	1/1/10/20	5/10/88/115	-
17	CLA	1	505	-	-	5/15/93/115	-
19	LHG	A	845	-	-	10/28/28/53	-
17	CLA	A	832	-	1/1/10/20	6/11/89/115	-
17	CLA	B	836	-	1/1/12/20	11/29/103/115	-
17	CLA	4	308	-	1/1/10/20	4/8/86/115	-
24	LUT	1	502	-	1/1/12/27	9/29/67/67	0/2/2/2
25	CHL	4	313	-	3/3/16/26	5/17/115/137	-
17	CLA	B	843	19	1/1/9/20	0/2/80/115	-
17	CLA	B	830	-	1/1/9/20	3/8/80/115	-
17	CLA	6	514	-	1/1/9/20	2/8/82/115	-
20	BCR	F	803	-	-	2/29/63/63	0/2/2/2
17	CLA	6	511	-	1/1/12/20	7/19/97/115	-
17	CLA	A	804	-	1/1/15/20	16/37/115/115	-
17	CLA	6	507	-	1/1/12/20	8/21/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	K	205	-	1/1/9/20	0/6/80/115	-
25	CHL	3	313	-	3/3/15/26	11/17/111/137	-
20	BCR	B	845	-	-	7/29/63/63	0/2/2/2
17	CLA	A	810	17	1/1/13/20	10/25/103/115	-
20	BCR	I	102	-	-	8/29/63/63	0/2/2/2
20	BCR	J	103	-	-	2/29/63/63	0/2/2/2
24	LUT	3	302	-	-	6/29/67/67	0/2/2/2
17	CLA	3	311	-	1/1/11/20	8/17/95/115	-
17	CLA	B	819	-	1/1/10/20	2/8/86/115	-
17	CLA	L	304	-	1/1/11/20	6/13/91/115	-
17	CLA	4	310	-	1/1/10/20	3/10/88/115	-
21	SF4	B	802	-	-	-	0/6/5/5
17	CLA	1	509	-	1/1/12/20	8/19/97/115	-
17	CLA	B	840	-	1/1/10/20	4/8/86/115	-
20	BCR	6	503	-	-	7/29/63/63	0/2/2/2
17	CLA	B	839	-	1/1/10/20	4/8/86/115	-
17	CLA	A	823	-	1/1/10/20	3/11/87/115	-
17	CLA	3	307	13	-	3/8/82/115	-
17	CLA	A	843	-	1/1/12/20	9/19/95/115	-
17	CLA	B	833	-	1/1/10/20	3/11/89/115	-
25	CHL	1	512	-	3/3/16/26	3/17/115/137	-
17	CLA	3	316	-	1/1/11/20	7/15/93/115	-
20	BCR	4	301	-	-	6/29/63/63	0/2/2/2
17	CLA	B	809	-	1/1/12/20	3/22/100/115	-
16	CL0	A	801	-	3/3/18/25	5/33/125/135	-
21	SF4	C	102	-	-	-	0/6/5/5
17	CLA	A	808	1	1/1/10/20	4/8/86/115	-
20	BCR	I	101	-	-	6/29/63/63	0/2/2/2
17	CLA	F	802	-	1/1/10/20	2/8/86/115	-
19	LHG	6	516	-	-	6/39/39/53	-
17	CLA	B	814	-	1/1/10/20	4/11/89/115	-
17	CLA	4	315	14	1/1/10/20	2/8/86/115	-
17	CLA	B	821	-	1/1/13/20	8/25/103/115	-
17	CLA	4	306	-	1/1/15/20	16/37/115/115	-
17	CLA	A	811	-	1/1/10/20	4/8/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	B	847	-	-	6/29/63/63	0/2/2/2
17	CLA	4	317	-	1/1/12/20	7/19/97/115	-
17	CLA	6	504	-	1/1/10/20	3/8/84/115	-
20	BCR	F	801	-	-	2/29/63/63	0/2/2/2
17	CLA	1	515	-	1/1/9/20	3/8/82/115	-
17	CLA	B	831	-	1/1/13/20	5/27/105/115	-
17	CLA	B	834	-	1/1/10/20	3/11/89/115	-
17	CLA	1	504	-	1/1/10/20	5/8/86/115	-
17	CLA	A	805	-	1/1/11/20	4/15/93/115	-
17	CLA	A	807	-	1/1/10/20	2/10/88/115	-
17	CLA	4	311	-	1/1/11/20	4/15/93/115	-
17	CLA	4	312	-	1/1/10/20	3/8/86/115	-
17	CLA	A	852	-	1/1/13/20	9/28/106/115	-
17	CLA	K	203	-	1/1/10/20	4/8/86/115	-
20	BCR	A	846	-	-	4/29/63/63	0/2/2/2
20	BCR	1	503	-	-	1/1/19/63	0/1/1/2
17	CLA	B	826	-	1/1/15/20	11/37/115/115	-
17	CLA	B	832	-	1/1/9/20	2/8/82/115	-
17	CLA	1	511	-	1/1/8/20	2/8/79/115	-
26	XAT	6	502	-	-	6/31/93/93	0/4/4/4
17	CLA	B	813	-	1/1/13/20	10/25/101/115	-
17	CLA	3	304	-	1/1/10/20	0/6/84/115	-
19	LHG	A	844	-	-	8/44/44/53	-
17	CLA	6	509	-	1/1/12/20	6/19/97/115	-
20	BCR	K	204	-	-	9/29/63/63	0/2/2/2
17	CLA	B	815	-	1/1/10/20	4/11/89/115	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	B	818	-	1/1/13/20	9/25/103/115	-
17	CLA	3	310	-	1/1/10/20	3/8/86/115	-
25	CHL	6	517	15	3/3/16/26	3/17/115/137	-
17	CLA	A	826	-	1/1/15/20	18/37/113/115	-
17	CLA	6	506	-	1/1/15/20	19/37/115/115	-
17	CLA	A	838	-	1/1/12/20	4/22/100/115	-
17	CLA	A	829	-	1/1/13/20	13/29/107/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	816	-	1/1/14/20	11/31/109/115	-
20	BCR	B	848	-	-	0/29/63/63	0/2/2/2
17	CLA	3	305	-	1/1/12/20	7/22/100/115	-
17	CLA	A	837	-	1/1/13/20	11/25/103/115	-
17	CLA	B	820	-	1/1/12/20	11/19/97/115	-
17	CLA	A	821	-	1/1/10/20	5/10/88/115	-
17	CLA	A	803	17	1/1/12/20	5/22/100/115	-
17	CLA	4	307	-	1/1/14/20	12/31/109/115	-
17	CLA	A	841	-	1/1/10/20	2/8/86/115	-
17	CLA	B	812	-	1/1/9/20	4/8/82/115	-
17	CLA	6	510	-	1/1/14/20	11/31/109/115	-
25	CHL	6	512	-	3/3/16/26	5/17/115/137	-
17	CLA	B	816	-	1/1/8/20	1/4/78/115	-
17	CLA	A	835	1	1/1/10/20	2/7/85/115	-
17	CLA	B	807	-	1/1/10/20	2/8/86/115	-
17	CLA	B	811	2	1/1/12/20	6/21/99/115	-
17	CLA	K	201	-	1/1/8/20	0/2/76/115	-
23	LMG	4	318	-	-	11/11/28/70	0/1/1/1
24	LUT	6	501	-	-	4/29/67/67	0/2/2/2
17	CLA	A	814	-	1/1/10/20	5/10/88/115	-
22	DGD	J	104	-	-	14/55/95/95	0/2/2/2
17	CLA	A	815	-	1/1/11/20	7/13/91/115	-
17	CLA	4	305	-	1/1/12/20	6/19/97/115	-
24	LUT	1	501	-	-	2/29/67/67	0/2/2/2
17	CLA	A	817	-	1/1/9/20	0/2/82/115	-
17	CLA	1	513	-	1/1/12/20	5/22/100/115	-
26	XAT	4	303	-	-	2/31/93/93	0/4/4/4
17	CLA	3	309	-	1/1/12/20	5/19/97/115	-
24	LUT	3	301	-	-	6/29/67/67	0/2/2/2
22	DGD	B	851	-	-	9/41/81/95	0/2/2/2
17	CLA	B	838	-	1/1/9/20	5/8/82/115	-
17	CLA	4	304	-	1/1/9/20	3/8/80/115	-
20	BCR	A	849	-	-	7/29/63/63	0/2/2/2
20	BCR	A	850	-	-	6/29/63/63	0/2/2/2
21	SF4	C	101	-	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	808	-	1/1/12/20	6/23/101/115	-
17	CLA	3	315	-	-	8/13/91/115	-
19	LHG	B	852	17	-	13/42/42/53	-
18	PQN	A	842	-	-	-	0/2/2/2
17	CLA	A	822	-	1/1/10/20	1/8/86/115	-
17	CLA	B	824	-	1/1/10/20	4/10/88/115	-
17	CLA	B	817	-	1/1/10/20	5/11/89/115	-
17	CLA	A	831	-	1/1/13/20	7/27/105/115	-
17	CLA	A	812	-	1/1/8/20	3/5/79/115	-
17	CLA	B	842	-	1/1/10/20	0/8/86/115	-
17	CLA	B	823	-	1/1/10/20	2/8/86/115	-
17	CLA	B	829	-	1/1/12/20	9/19/97/115	-
25	CHL	4	314	-	3/3/17/26	4/21/119/137	-
20	BCR	A	854	-	-	4/29/63/63	0/2/2/2
24	LUT	4	302	-	-	2/29/67/67	0/2/2/2
17	CLA	B	827	-	1/1/9/20	1/8/82/115	-
17	CLA	A	836	-	1/1/12/20	6/21/99/115	-
17	CLA	B	822	-	1/1/10/20	0/8/86/115	-
17	CLA	B	835	-	1/1/11/20	8/13/91/115	-
20	BCR	B	849	-	-	0/29/63/63	0/2/2/2
20	BCR	A	851	-	-	4/29/63/63	0/2/2/2
25	CHL	6	513	-	3/3/16/26	5/18/116/137	-
17	CLA	A	839	-	1/1/15/20	16/37/115/115	-
17	CLA	A	818	-	1/1/9/20	4/6/80/115	-
17	CLA	L	302	-	1/1/10/20	2/8/84/115	-
20	BCR	L	301	-	-	2/29/63/63	0/2/2/2
17	CLA	B	805	-	1/1/8/20	0/2/78/115	-
17	CLA	B	801	-	1/1/15/20	13/37/113/115	-
20	BCR	3	303	-	-	7/29/63/63	0/2/2/2
20	BCR	B	846	-	-	7/29/63/63	0/2/2/2
17	CLA	A	819	-	1/1/11/20	5/13/91/115	-
17	CLA	B	825	-	1/1/10/20	3/10/88/115	-
17	CLA	J	101	-	1/1/10/20	6/10/86/115	-
17	CLA	4	309	-	1/1/12/20	7/19/97/115	-
20	BCR	A	847	-	-	0/29/63/63	0/2/2/2
25	CHL	6	515	-	3/3/14/26	4/10/104/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	312	13	1/1/14/20	12/31/109/115	-
17	CLA	B	803	-	1/1/10/20	3/10/88/115	-
17	CLA	3	314	-	1/1/9/20	2/8/82/115	-
17	CLA	A	806	-	1/1/10/20	1/8/86/115	-
25	CHL	1	517	-	3/3/15/26	5/12/110/137	-
25	CHL	4	316	-	3/3/15/26	3/12/110/137	-
17	CLA	A	830	-	1/1/12/20	6/19/97/115	-
17	CLA	A	820	-	1/1/10/20	3/8/86/115	-
17	CLA	6	505	-	-	8/22/100/115	-
18	PQN	B	844	-	-	0/3/23/43	0/2/2/2
17	CLA	1	510	-	1/1/11/20	7/15/93/115	-
17	CLA	1	507	12	1/1/10/20	4/8/84/115	-

All (1113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	502	LUT	C24-C25	14.61	1.51	1.33
17	3	304	CLA	C3B-C4B	9.98	1.49	1.43
17	6	504	CLA	C3B-C4B	8.58	1.49	1.39
17	3	304	CLA	C2B-C1B	8.49	1.49	1.39
17	B	804	CLA	CHB-C4A	8.43	1.41	1.34
17	J	101	CLA	C4B-NB	7.86	1.42	1.35
17	3	310	CLA	C4B-NB	7.71	1.42	1.35
17	1	515	CLA	C4B-NB	7.70	1.42	1.35
17	6	509	CLA	C4B-NB	7.69	1.42	1.35
17	A	829	CLA	C4B-NB	7.64	1.42	1.35
17	4	305	CLA	C4B-NB	7.63	1.42	1.35
17	4	311	CLA	C4B-NB	7.62	1.42	1.35
17	1	510	CLA	C4B-NB	7.61	1.42	1.35
17	A	835	CLA	C4B-NB	7.60	1.42	1.35
17	K	205	CLA	C4B-NB	7.56	1.42	1.35
17	F	802	CLA	C4B-NB	7.55	1.41	1.35
17	4	310	CLA	C4B-NB	7.54	1.41	1.35
17	1	513	CLA	C4B-NB	7.54	1.41	1.35
17	6	511	CLA	C4B-NB	7.54	1.41	1.35
17	J	102	CLA	C4B-NB	7.52	1.41	1.35
17	B	837	CLA	C4B-NB	7.52	1.41	1.35
17	A	815	CLA	C4B-NB	7.52	1.41	1.35
17	3	306	CLA	C4B-NB	7.51	1.41	1.35
17	A	818	CLA	CHB-C4A	7.50	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	822	CLA	C4B-NB	7.50	1.41	1.35
17	L	302	CLA	C4B-NB	7.48	1.41	1.35
16	A	801	CL0	MG-NA	7.46	2.24	2.06
17	A	813	CLA	C4B-NB	7.45	1.41	1.35
17	3	305	CLA	C4B-NB	7.45	1.41	1.35
17	6	505	CLA	C4B-NB	7.44	1.41	1.35
17	B	813	CLA	C4B-NB	7.42	1.41	1.35
17	4	315	CLA	C4B-NB	7.42	1.41	1.35
17	A	816	CLA	C4B-NB	7.40	1.41	1.35
17	K	201	CLA	C4B-NB	7.39	1.41	1.35
17	A	843	CLA	C4B-NB	7.39	1.41	1.35
17	3	308	CLA	C4B-NB	7.39	1.41	1.35
17	3	307	CLA	C4B-NB	7.38	1.41	1.35
17	A	808	CLA	C4B-NB	7.36	1.41	1.35
17	A	822	CLA	C4B-NB	7.36	1.41	1.35
17	A	811	CLA	C4B-NB	7.34	1.41	1.35
17	K	202	CLA	C4B-NB	7.34	1.41	1.35
17	A	817	CLA	C4B-NB	7.34	1.41	1.35
17	B	811	CLA	C4B-NB	7.34	1.41	1.35
17	1	504	CLA	C4B-NB	7.34	1.41	1.35
17	A	807	CLA	C4B-NB	7.34	1.41	1.35
17	1	511	CLA	C4B-NB	7.33	1.41	1.35
17	L	304	CLA	C4B-NB	7.32	1.41	1.35
17	3	311	CLA	C4B-NB	7.32	1.41	1.35
17	A	832	CLA	C4B-NB	7.32	1.41	1.35
17	3	316	CLA	C4B-NB	7.32	1.41	1.35
17	B	823	CLA	C4B-NB	7.32	1.41	1.35
17	A	802	CLA	C4B-NB	7.31	1.41	1.35
17	3	315	CLA	C4B-NB	7.31	1.41	1.35
17	1	506	CLA	C4B-NB	7.31	1.41	1.35
17	3	312	CLA	C4B-NB	7.31	1.41	1.35
17	B	826	CLA	C4B-NB	7.29	1.41	1.35
17	B	824	CLA	C4B-NB	7.29	1.41	1.35
17	A	803	CLA	C4B-NB	7.29	1.41	1.35
17	B	836	CLA	C4B-NB	7.28	1.41	1.35
17	4	317	CLA	C4B-NB	7.27	1.41	1.35
17	4	306	CLA	C4B-NB	7.27	1.41	1.35
17	A	810	CLA	C4B-NB	7.26	1.41	1.35
17	A	814	CLA	C4B-NB	7.26	1.41	1.35
17	B	814	CLA	C4B-NB	7.26	1.41	1.35
17	1	508	CLA	C4B-NB	7.26	1.41	1.35
17	6	510	CLA	C4B-NB	7.26	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	C4B-NB	7.25	1.41	1.35
17	3	309	CLA	C4B-NB	7.24	1.41	1.35
17	3	304	CLA	C4B-NB	7.24	1.41	1.35
17	A	830	CLA	C4B-NB	7.24	1.41	1.35
17	A	839	CLA	C4B-NB	7.23	1.41	1.35
17	4	308	CLA	C4B-NB	7.23	1.41	1.35
17	A	809	CLA	C4B-NB	7.23	1.41	1.35
17	A	841	CLA	C4B-NB	7.23	1.41	1.35
17	B	809	CLA	C4B-NB	7.23	1.41	1.35
17	A	826	CLA	C4B-NB	7.22	1.41	1.35
17	A	819	CLA	C4B-NB	7.21	1.41	1.35
17	4	312	CLA	C4B-NB	7.21	1.41	1.35
17	A	805	CLA	C4B-NB	7.21	1.41	1.35
17	B	843	CLA	C4B-NB	7.21	1.41	1.35
17	6	507	CLA	C4B-NB	7.20	1.41	1.35
17	B	825	CLA	C4B-NB	7.19	1.41	1.35
17	6	508	CLA	C4B-NB	7.19	1.41	1.35
18	B	844	PQN	C3-C2	7.19	1.48	1.35
17	B	815	CLA	C4B-NB	7.19	1.41	1.35
17	4	307	CLA	C4B-NB	7.19	1.41	1.35
17	6	506	CLA	C4B-NB	7.18	1.41	1.35
17	B	819	CLA	C4B-NB	7.18	1.41	1.35
17	A	823	CLA	C4B-NB	7.17	1.41	1.35
17	B	831	CLA	C4B-NB	7.16	1.41	1.35
17	A	828	CLA	C4B-NB	7.15	1.41	1.35
17	A	806	CLA	C4B-NB	7.15	1.41	1.35
17	A	840	CLA	C4B-NB	7.14	1.41	1.35
17	B	821	CLA	C4B-NB	7.14	1.41	1.35
17	B	842	CLA	C4B-NB	7.14	1.41	1.35
17	B	827	CLA	C4B-NB	7.14	1.41	1.35
17	B	816	CLA	C4B-NB	7.13	1.41	1.35
17	B	840	CLA	C4B-NB	7.13	1.41	1.35
17	B	839	CLA	C4B-NB	7.13	1.41	1.35
17	B	817	CLA	C4B-NB	7.13	1.41	1.35
17	B	832	CLA	C4B-NB	7.12	1.41	1.35
17	B	830	CLA	C4B-NB	7.12	1.41	1.35
17	A	833	CLA	C4B-NB	7.11	1.41	1.35
17	A	853	CLA	C4B-NB	7.11	1.41	1.35
17	B	833	CLA	C4B-NB	7.11	1.41	1.35
17	3	314	CLA	C4B-NB	7.10	1.41	1.35
17	A	831	CLA	C4B-NB	7.10	1.41	1.35
17	A	852	CLA	C4B-NB	7.10	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	806	CLA	C4B-NB	7.09	1.41	1.35
17	B	810	CLA	C4B-NB	7.09	1.41	1.35
17	B	812	CLA	C4B-NB	7.09	1.41	1.35
17	B	818	CLA	C4B-NB	7.08	1.41	1.35
17	B	807	CLA	C4B-NB	7.08	1.41	1.35
17	K	203	CLA	C4B-NB	7.06	1.41	1.35
17	B	841	CLA	C4B-NB	7.06	1.41	1.35
17	L	303	CLA	C4B-NB	7.05	1.41	1.35
17	1	507	CLA	C4B-NB	7.05	1.41	1.35
17	B	801	CLA	C4B-NB	7.04	1.41	1.35
17	A	836	CLA	C4B-NB	7.02	1.41	1.35
17	A	812	CLA	C4B-NB	7.02	1.41	1.35
17	A	834	CLA	C4B-NB	7.01	1.41	1.35
17	A	837	CLA	C4B-NB	7.01	1.41	1.35
17	4	304	CLA	C4B-NB	7.01	1.41	1.35
17	4	309	CLA	C4B-NB	7.00	1.41	1.35
17	A	825	CLA	C4B-NB	6.99	1.41	1.35
17	A	838	CLA	C4B-NB	6.99	1.41	1.35
17	A	824	CLA	C4B-NB	6.98	1.41	1.35
17	B	820	CLA	C4B-NB	6.97	1.41	1.35
17	6	504	CLA	C4B-NB	6.95	1.41	1.35
17	B	835	CLA	C4B-NB	6.94	1.41	1.35
17	6	514	CLA	C4B-NB	6.94	1.41	1.35
17	A	827	CLA	C4B-NB	6.93	1.41	1.35
17	A	820	CLA	C4B-NB	6.92	1.41	1.35
17	B	838	CLA	C4B-NB	6.92	1.41	1.35
17	B	829	CLA	C4B-NB	6.92	1.41	1.35
17	B	808	CLA	C4B-NB	6.89	1.41	1.35
17	B	828	CLA	C4B-NB	6.88	1.41	1.35
17	A	821	CLA	C4B-NB	6.88	1.41	1.35
17	A	804	CLA	C4B-NB	6.76	1.41	1.35
17	B	805	CLA	C4B-NB	6.75	1.41	1.35
17	B	803	CLA	C4B-NB	6.70	1.41	1.35
17	1	509	CLA	MG-NA	6.47	2.21	2.06
17	1	505	CLA	C4B-NB	6.38	1.40	1.35
17	A	818	CLA	MG-NA	6.33	2.21	2.06
17	B	804	CLA	MG-NA	6.18	2.21	2.06
25	3	313	CHL	C4D-C3D	-5.81	1.33	1.45
25	1	514	CHL	C3B-C2B	5.38	1.47	1.40
23	4	318	LMG	O7-C10	5.37	1.45	1.33
25	1	512	CHL	C3B-C2B	5.33	1.47	1.40
25	1	512	CHL	CHC-C1C	5.29	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	512	CHL	CHC-C1C	5.28	1.48	1.35
25	4	316	CHL	O2D-CGD	5.27	1.46	1.33
17	B	804	CLA	C2B-C1B	5.25	1.45	1.39
25	4	313	CHL	CHC-C1C	5.25	1.48	1.35
25	4	313	CHL	C3B-C2B	5.22	1.47	1.40
25	6	512	CHL	C3B-C2B	5.17	1.47	1.40
25	1	514	CHL	CHC-C1C	5.16	1.48	1.35
25	1	512	CHL	O2D-CGD	5.13	1.45	1.33
25	6	515	CHL	O2D-CGD	5.12	1.45	1.33
25	6	512	CHL	O2D-CGD	5.11	1.45	1.33
25	4	314	CHL	O2D-CGD	5.11	1.45	1.33
25	1	514	CHL	O2D-CGD	5.10	1.45	1.33
25	4	313	CHL	O2D-CGD	5.10	1.45	1.33
25	1	517	CHL	CHC-C1C	5.10	1.48	1.35
25	3	313	CHL	O2D-CGD	5.09	1.45	1.33
17	B	836	CLA	CHB-C4A	5.06	1.38	1.34
25	6	513	CHL	O2D-CGD	5.05	1.45	1.33
25	3	313	CHL	CHC-C1C	5.04	1.47	1.35
25	6	517	CHL	CHC-C1C	5.02	1.47	1.35
25	6	513	CHL	CHC-C1C	5.01	1.47	1.35
25	6	512	CHL	CHD-C1D	4.96	1.48	1.38
25	1	517	CHL	O2D-CGD	4.96	1.45	1.33
25	3	313	CHL	C3D-C2D	4.96	1.47	1.36
25	6	515	CHL	CHC-C1C	4.92	1.47	1.35
25	6	513	CHL	C3B-C2B	4.91	1.47	1.40
25	1	514	CHL	CHD-C1D	4.90	1.47	1.38
25	1	512	CHL	C2C-C3C	4.89	1.47	1.36
25	6	512	CHL	C2C-C3C	4.88	1.47	1.36
25	1	514	CHL	C3D-C4D	-4.88	1.33	1.44
25	1	512	CHL	CHD-C1D	4.85	1.47	1.38
17	1	511	CLA	CHB-C4A	4.85	1.38	1.34
25	6	517	CHL	O2D-CGD	4.84	1.45	1.33
25	6	515	CHL	C3B-C2B	4.84	1.47	1.40
25	6	512	CHL	C3D-C4D	-4.82	1.33	1.44
25	1	512	CHL	C3D-C4D	-4.81	1.33	1.44
25	4	316	CHL	CHC-C1C	4.79	1.47	1.35
25	1	517	CHL	C3D-C4D	-4.78	1.33	1.44
25	1	514	CHL	C2C-C3C	4.78	1.47	1.36
25	3	313	CHL	C3B-C2B	4.77	1.47	1.40
25	4	313	CHL	C3D-C4D	-4.75	1.33	1.44
25	1	517	CHL	C2C-C3C	4.75	1.46	1.36
25	6	513	CHL	C3D-C4D	-4.75	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	313	CHL	C2C-C3C	4.73	1.46	1.36
25	1	517	CHL	C3B-C2B	4.71	1.46	1.40
25	4	316	CHL	C3D-C4D	-4.69	1.33	1.44
25	4	314	CHL	C3D-C4D	-4.68	1.33	1.44
17	B	827	CLA	CHB-C4A	4.67	1.38	1.34
25	6	517	CHL	C3D-C4D	-4.66	1.33	1.44
25	6	515	CHL	C3D-C4D	-4.65	1.33	1.44
25	6	517	CHL	C3B-C2B	4.64	1.46	1.40
18	A	842	PQN	C10-C5	4.63	1.48	1.40
25	6	515	CHL	C2C-C3C	4.63	1.46	1.36
25	1	517	CHL	CHD-C1D	4.63	1.47	1.38
25	4	313	CHL	CHD-C1D	4.61	1.47	1.38
25	4	314	CHL	CHC-C1C	4.61	1.46	1.35
25	4	316	CHL	C3B-C2B	4.58	1.46	1.40
25	6	513	CHL	C2C-C3C	4.58	1.46	1.36
25	3	313	CHL	C2C-C3C	4.57	1.46	1.36
25	6	515	CHL	CHD-C1D	4.57	1.47	1.38
25	6	517	CHL	C2C-C3C	4.56	1.46	1.36
25	6	513	CHL	CHD-C1D	4.56	1.47	1.38
18	B	844	PQN	C10-C5	4.56	1.48	1.40
17	B	804	CLA	C3B-C4B	4.56	1.46	1.43
25	4	316	CHL	CHD-C1D	4.53	1.47	1.38
25	4	316	CHL	C2C-C3C	4.51	1.46	1.36
25	3	313	CHL	CHD-C1D	4.44	1.47	1.38
25	6	517	CHL	CHD-C1D	4.43	1.47	1.38
25	6	512	CHL	CHD-C4C	4.40	1.49	1.39
25	4	314	CHL	CHD-C1D	4.35	1.46	1.38
25	1	512	CHL	CHD-C4C	4.33	1.49	1.39
25	1	514	CHL	CHD-C4C	4.32	1.49	1.39
25	4	314	CHL	C2C-C3C	4.31	1.46	1.36
25	4	314	CHL	C3B-C2B	4.28	1.46	1.40
25	6	513	CHL	O2A-CGA	4.28	1.45	1.33
22	J	104	DGD	O2G-C1B	4.26	1.46	1.34
16	A	801	CL0	C2A-C1A	-4.26	1.50	1.53
23	J	105	LMG	O8-C28	4.25	1.45	1.33
25	1	517	CHL	CHD-C4C	4.24	1.48	1.39
19	6	516	LHG	O8-C23	4.18	1.45	1.33
25	4	314	CHL	O2A-CGA	4.18	1.45	1.33
22	B	851	DGD	O1G-C1A	4.18	1.45	1.33
25	4	313	CHL	CHD-C4C	4.18	1.48	1.39
19	1	516	LHG	O8-C23	4.14	1.45	1.33
19	B	852	LHG	O8-C23	4.14	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	104	DGD	O1G-C1A	4.14	1.45	1.33
25	6	515	CHL	CHD-C4C	4.12	1.48	1.39
19	A	844	LHG	O8-C23	4.11	1.45	1.33
19	B	852	LHG	O7-C7	4.10	1.45	1.34
19	1	516	LHG	O7-C7	4.07	1.45	1.34
25	6	517	CHL	CHD-C4C	4.06	1.48	1.39
25	6	512	CHL	O2A-CGA	4.05	1.45	1.33
17	3	307	CLA	C1D-ND	4.04	1.42	1.37
25	4	313	CHL	O2A-CGA	4.04	1.45	1.33
25	6	513	CHL	CHD-C4C	4.04	1.48	1.39
25	4	316	CHL	CHD-C4C	4.03	1.48	1.39
25	3	313	CHL	O2A-CGA	4.03	1.45	1.33
17	L	302	CLA	C1D-ND	4.02	1.42	1.37
25	1	514	CHL	O2A-CGA	4.01	1.45	1.33
17	K	205	CLA	C1D-ND	4.01	1.42	1.37
23	J	105	LMG	O7-C10	4.01	1.45	1.34
17	J	101	CLA	C1D-ND	4.00	1.42	1.37
19	A	845	LHG	O7-C7	4.00	1.45	1.34
25	1	512	CHL	O2A-CGA	3.99	1.45	1.33
25	4	314	CHL	CHD-C4C	3.98	1.48	1.39
25	6	517	CHL	O2A-CGA	3.98	1.45	1.33
17	1	513	CLA	C1D-ND	3.98	1.42	1.37
17	4	310	CLA	C1D-ND	3.98	1.42	1.37
22	B	851	DGD	O2G-C1B	3.97	1.45	1.34
17	3	308	CLA	C1D-ND	3.94	1.42	1.37
25	3	313	CHL	CHD-C4C	3.94	1.48	1.39
17	K	201	CLA	C1D-ND	3.93	1.42	1.37
19	A	844	LHG	O7-C7	3.93	1.45	1.34
19	6	516	LHG	O7-C7	3.92	1.45	1.34
17	J	102	CLA	C1D-ND	3.92	1.42	1.37
17	K	202	CLA	C1D-ND	3.91	1.42	1.37
17	3	305	CLA	C1D-ND	3.91	1.42	1.37
17	4	308	CLA	C1D-ND	3.88	1.42	1.37
17	3	316	CLA	C1D-ND	3.88	1.42	1.37
17	6	506	CLA	C1D-ND	3.88	1.42	1.37
17	A	817	CLA	C1D-ND	3.87	1.42	1.37
17	A	843	CLA	C1D-ND	3.87	1.42	1.37
17	3	309	CLA	C1D-ND	3.87	1.42	1.37
17	1	515	CLA	C1D-ND	3.87	1.42	1.37
17	3	312	CLA	C1D-ND	3.85	1.42	1.37
17	A	836	CLA	C1D-ND	3.84	1.42	1.37
17	3	310	CLA	C1D-ND	3.83	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	C1D-ND	3.83	1.42	1.37
17	6	510	CLA	C1D-ND	3.82	1.42	1.37
17	6	509	CLA	C1D-ND	3.81	1.42	1.37
17	B	843	CLA	C1D-ND	3.80	1.42	1.37
17	3	311	CLA	C1D-ND	3.80	1.42	1.37
17	4	312	CLA	C1D-ND	3.80	1.42	1.37
17	B	839	CLA	C1D-ND	3.79	1.42	1.37
17	K	203	CLA	C1D-ND	3.79	1.42	1.37
17	3	304	CLA	C1D-ND	3.79	1.42	1.37
17	3	315	CLA	C1D-ND	3.79	1.42	1.37
17	4	315	CLA	C1D-ND	3.78	1.42	1.37
17	A	809	CLA	C1D-ND	3.77	1.42	1.37
17	1	511	CLA	C1D-ND	3.77	1.42	1.37
17	B	813	CLA	C1D-ND	3.77	1.42	1.37
17	4	305	CLA	C1D-ND	3.77	1.42	1.37
17	A	835	CLA	C1D-ND	3.76	1.42	1.37
17	B	823	CLA	C1D-ND	3.76	1.42	1.37
17	1	507	CLA	CAB-C3B	-3.76	1.43	1.51
17	6	511	CLA	C1D-ND	3.75	1.42	1.37
17	6	514	CLA	C1D-ND	3.75	1.42	1.37
17	4	309	CLA	C1D-ND	3.74	1.42	1.37
17	A	807	CLA	C1D-ND	3.74	1.42	1.37
17	4	317	CLA	C1D-ND	3.74	1.42	1.37
17	B	815	CLA	C1D-ND	3.73	1.42	1.37
25	1	512	CHL	OBD-CAD	3.73	1.28	1.22
17	L	304	CLA	C1D-ND	3.73	1.42	1.37
17	6	508	CLA	C1D-ND	3.73	1.42	1.37
17	A	808	CLA	C1D-ND	3.72	1.42	1.37
17	A	806	CLA	C1D-ND	3.72	1.42	1.37
17	F	802	CLA	C1D-ND	3.72	1.42	1.37
17	B	811	CLA	C1D-ND	3.72	1.42	1.37
17	B	807	CLA	C1D-ND	3.72	1.42	1.37
17	A	839	CLA	C1D-ND	3.71	1.42	1.37
25	4	313	CHL	OBD-CAD	3.71	1.28	1.22
17	B	808	CLA	C1D-ND	3.71	1.42	1.37
17	B	822	CLA	C1D-ND	3.71	1.42	1.37
17	6	504	CLA	C4B-CHC	-3.71	1.36	1.43
17	A	802	CLA	C1D-ND	3.71	1.42	1.37
17	4	311	CLA	C1D-ND	3.70	1.42	1.37
17	A	841	CLA	C1D-ND	3.70	1.42	1.37
17	A	815	CLA	C1D-ND	3.70	1.42	1.37
17	1	506	CLA	C1D-ND	3.70	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	304	CLA	C1D-ND	3.69	1.42	1.37
17	B	824	CLA	C1D-ND	3.69	1.42	1.37
17	A	804	CLA	C1D-ND	3.69	1.42	1.37
17	A	813	CLA	C1D-ND	3.69	1.42	1.37
17	B	830	CLA	CAB-C3B	-3.69	1.44	1.51
17	3	304	CLA	C3C-C4C	3.69	1.46	1.40
17	A	826	CLA	CAB-C3B	-3.68	1.44	1.51
17	4	306	CLA	C1D-ND	3.68	1.42	1.37
17	B	836	CLA	C1D-ND	3.68	1.42	1.37
17	B	819	CLA	C1D-ND	3.68	1.42	1.37
17	1	508	CLA	C1D-ND	3.68	1.42	1.37
17	B	835	CLA	C1D-ND	3.68	1.42	1.37
17	A	816	CLA	C1D-ND	3.67	1.42	1.37
17	4	307	CLA	C1D-ND	3.67	1.42	1.37
17	B	806	CLA	C1D-ND	3.67	1.42	1.37
25	6	515	CHL	OBD-CAD	3.67	1.28	1.22
17	A	821	CLA	C1D-ND	3.66	1.42	1.37
17	1	505	CLA	C1D-ND	3.66	1.42	1.37
17	B	830	CLA	C1D-ND	3.66	1.42	1.37
17	A	832	CLA	C1D-ND	3.66	1.42	1.37
17	B	837	CLA	C1D-ND	3.65	1.42	1.37
17	A	829	CLA	C1D-ND	3.65	1.42	1.37
17	A	814	CLA	C1D-ND	3.65	1.42	1.37
17	A	811	CLA	C1D-ND	3.65	1.42	1.37
17	A	828	CLA	C1D-ND	3.65	1.42	1.37
17	B	832	CLA	C1D-ND	3.64	1.42	1.37
17	B	840	CLA	C1D-ND	3.64	1.42	1.37
17	B	810	CLA	C1D-ND	3.63	1.42	1.37
17	3	314	CLA	C1D-ND	3.63	1.42	1.37
17	B	828	CLA	C1D-ND	3.63	1.42	1.37
17	A	823	CLA	C1D-ND	3.63	1.42	1.37
25	4	316	CHL	OBD-CAD	3.63	1.28	1.22
17	B	812	CLA	C1D-ND	3.63	1.42	1.37
17	A	853	CLA	C1D-ND	3.62	1.42	1.37
17	A	810	CLA	C1D-ND	3.62	1.42	1.37
17	A	826	CLA	C1D-ND	3.62	1.42	1.37
17	L	303	CLA	C1D-ND	3.62	1.42	1.37
25	6	513	CHL	OBD-CAD	3.62	1.28	1.22
17	B	801	CLA	C1D-ND	3.62	1.42	1.37
17	A	840	CLA	C1D-ND	3.61	1.42	1.37
17	A	852	CLA	C1D-ND	3.61	1.42	1.37
17	6	507	CLA	C1D-ND	3.61	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	838	CLA	C1D-ND	3.61	1.42	1.37
17	A	803	CLA	C1D-ND	3.61	1.42	1.37
17	6	505	CLA	C1D-ND	3.61	1.42	1.37
25	4	314	CHL	OBD-CAD	3.61	1.28	1.22
17	B	809	CLA	C1D-ND	3.60	1.42	1.37
17	B	814	CLA	C1D-ND	3.60	1.42	1.37
17	B	801	CLA	CAB-C3B	-3.59	1.44	1.51
25	1	517	CHL	OBD-CAD	3.59	1.28	1.22
17	B	817	CLA	C1D-ND	3.59	1.42	1.37
23	4	318	LMG	O7-C8	-3.59	1.42	1.46
17	B	813	CLA	CAB-C3B	-3.58	1.44	1.51
17	B	818	CLA	C1D-ND	3.58	1.42	1.37
17	B	825	CLA	C1D-ND	3.58	1.42	1.37
17	B	804	CLA	MG-ND	-3.58	1.98	2.05
25	1	514	CHL	OBD-CAD	3.58	1.28	1.22
17	B	833	CLA	C1D-ND	3.57	1.42	1.37
17	B	820	CLA	C1D-ND	3.57	1.42	1.37
17	A	837	CLA	C1D-ND	3.57	1.42	1.37
17	B	826	CLA	C1D-ND	3.57	1.42	1.37
25	6	517	CHL	OBD-CAD	3.57	1.28	1.22
17	B	804	CLA	C2A-C1A	-3.57	1.50	1.53
25	6	512	CHL	OBD-CAD	3.57	1.28	1.22
17	A	825	CLA	C1D-ND	3.56	1.42	1.37
17	B	842	CLA	C1D-ND	3.56	1.42	1.37
17	A	824	CLA	C1D-ND	3.55	1.42	1.37
17	1	507	CLA	C1D-ND	3.55	1.42	1.37
17	A	820	CLA	C1D-ND	3.54	1.42	1.37
17	B	821	CLA	C1D-ND	3.54	1.42	1.37
17	1	510	CLA	C1D-ND	3.53	1.42	1.37
17	A	805	CLA	C1D-ND	3.53	1.42	1.37
17	B	831	CLA	C1D-ND	3.52	1.42	1.37
17	6	504	CLA	C1D-ND	3.52	1.42	1.37
17	B	841	CLA	C1D-ND	3.52	1.42	1.37
17	A	834	CLA	C1D-ND	3.52	1.42	1.37
17	A	819	CLA	C1D-ND	3.52	1.42	1.37
17	1	504	CLA	C1D-ND	3.51	1.42	1.37
17	A	830	CLA	C1D-ND	3.50	1.42	1.37
17	B	827	CLA	C1D-ND	3.50	1.42	1.37
17	A	822	CLA	C1D-ND	3.50	1.42	1.37
17	B	838	CLA	C1D-ND	3.48	1.42	1.37
17	4	304	CLA	CAB-C3B	-3.46	1.44	1.51
16	A	801	CL0	C1D-ND	-3.46	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	302	CLA	CAB-C3B	-3.46	1.44	1.51
17	A	833	CLA	C1D-ND	3.46	1.42	1.37
17	B	834	CLA	C1D-ND	3.46	1.42	1.37
17	A	818	CLA	MG-ND	-3.45	1.98	2.05
17	A	812	CLA	C1D-ND	3.43	1.42	1.37
17	A	831	CLA	C1D-ND	3.42	1.42	1.37
17	B	829	CLA	C1D-ND	3.42	1.42	1.37
17	A	823	CLA	CAB-C3B	-3.41	1.44	1.51
17	B	816	CLA	C1D-ND	3.38	1.41	1.37
17	B	805	CLA	C1D-ND	3.38	1.41	1.37
17	1	509	CLA	CBB-CAB	3.36	1.51	1.29
17	1	509	CLA	MG-ND	-3.36	1.99	2.05
17	A	818	CLA	CBB-CAB	3.35	1.51	1.29
17	A	843	CLA	CAB-C3B	-3.35	1.44	1.51
17	1	513	CLA	CHC-C1C	3.32	1.43	1.35
17	B	804	CLA	CBB-CAB	3.30	1.51	1.29
17	1	505	CLA	C4D-ND	-3.30	1.33	1.37
17	3	312	CLA	CHC-C1C	3.28	1.43	1.35
17	B	805	CLA	C4D-ND	-3.28	1.33	1.37
17	3	304	CLA	C3B-CAB	-3.27	1.43	1.48
17	A	837	CLA	C4D-ND	-3.26	1.33	1.37
25	6	512	CHL	C1D-C2D	3.26	1.51	1.45
17	B	838	CLA	C4D-ND	-3.26	1.33	1.37
17	A	827	CLA	C1D-ND	3.25	1.41	1.37
17	A	804	CLA	C4D-ND	-3.25	1.33	1.37
17	J	101	CLA	CAB-C3B	-3.25	1.44	1.51
17	B	828	CLA	C4D-ND	-3.25	1.33	1.37
17	B	835	CLA	C4D-ND	-3.24	1.33	1.37
17	4	306	CLA	CHC-C1C	3.24	1.43	1.35
17	1	504	CLA	CHC-C1C	3.23	1.43	1.35
17	B	808	CLA	C4D-ND	-3.22	1.33	1.37
25	1	512	CHL	C3D-C2D	3.22	1.47	1.39
17	A	828	CLA	C4D-ND	-3.22	1.33	1.37
17	A	823	CLA	CHC-C1C	3.21	1.43	1.35
17	3	314	CLA	C4D-ND	-3.21	1.33	1.37
17	A	813	CLA	CHC-C1C	3.21	1.43	1.35
25	4	313	CHL	C3D-C2D	3.21	1.47	1.39
17	3	304	CLA	C4D-ND	-3.20	1.33	1.37
17	B	822	CLA	C4D-ND	-3.20	1.33	1.37
17	B	821	CLA	C4D-ND	-3.19	1.33	1.37
17	B	821	CLA	CHC-C1C	3.19	1.43	1.35
17	A	812	CLA	C4D-ND	-3.19	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	827	CLA	C4D-ND	-3.19	1.33	1.37
17	B	827	CLA	CHC-C1C	3.19	1.43	1.35
17	B	834	CLA	C4D-ND	-3.19	1.33	1.37
17	A	839	CLA	CHC-C1C	3.18	1.43	1.35
17	B	834	CLA	CHC-C1C	3.18	1.43	1.35
17	4	307	CLA	CHC-C1C	3.18	1.43	1.35
25	6	512	CHL	C3D-C2D	3.18	1.47	1.39
17	1	510	CLA	C4D-ND	-3.18	1.33	1.37
17	A	814	CLA	C4D-ND	-3.18	1.33	1.37
17	B	814	CLA	CHC-C1C	3.18	1.43	1.35
17	A	803	CLA	CHC-C1C	3.18	1.43	1.35
17	4	304	CLA	CHC-C1C	3.18	1.43	1.35
17	B	819	CLA	C4D-ND	-3.17	1.33	1.37
17	B	803	CLA	C2D-C1D	3.17	1.48	1.42
17	B	809	CLA	C4D-ND	-3.17	1.33	1.37
25	1	514	CHL	C3D-C2D	3.16	1.47	1.39
17	A	833	CLA	C4D-ND	-3.15	1.33	1.37
17	A	843	CLA	CHC-C1C	3.15	1.43	1.35
17	B	810	CLA	C4D-ND	-3.15	1.33	1.37
17	3	316	CLA	CHC-C1C	3.15	1.43	1.35
17	B	825	CLA	C4D-ND	-3.15	1.33	1.37
17	A	834	CLA	C4D-ND	-3.14	1.33	1.37
17	A	826	CLA	CHC-C1C	3.14	1.43	1.35
17	A	825	CLA	C4D-ND	-3.14	1.33	1.37
17	A	820	CLA	C4D-ND	-3.14	1.33	1.37
17	A	841	CLA	C4D-ND	-3.14	1.33	1.37
17	A	806	CLA	CHC-C1C	3.14	1.43	1.35
17	A	830	CLA	C4D-ND	-3.14	1.33	1.37
17	B	815	CLA	C4D-ND	-3.13	1.33	1.37
17	3	305	CLA	CHC-C1C	3.13	1.43	1.35
17	A	831	CLA	CHC-C1C	3.13	1.43	1.35
17	K	201	CLA	CHC-C1C	3.13	1.43	1.35
17	6	504	CLA	CHC-C1C	3.13	1.43	1.35
17	A	837	CLA	CHC-C1C	3.13	1.43	1.35
17	A	805	CLA	C4D-ND	-3.13	1.33	1.37
17	A	835	CLA	C4D-ND	-3.13	1.33	1.37
17	B	818	CLA	CHC-C1C	3.13	1.43	1.35
17	B	838	CLA	CHC-C1C	3.13	1.43	1.35
17	A	821	CLA	C4D-ND	-3.13	1.33	1.37
17	B	832	CLA	C4D-ND	-3.13	1.33	1.37
17	4	317	CLA	CHC-C1C	3.13	1.43	1.35
17	B	841	CLA	CHC-C1C	3.12	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	CHC-C1C	3.12	1.43	1.35
17	B	808	CLA	CHC-C1C	3.12	1.43	1.35
17	A	814	CLA	CHC-C1C	3.12	1.43	1.35
17	K	202	CLA	CHC-C1C	3.12	1.43	1.35
17	A	826	CLA	C4D-ND	-3.12	1.33	1.37
17	B	840	CLA	C4D-ND	-3.12	1.33	1.37
17	B	812	CLA	C4D-ND	-3.12	1.33	1.37
17	1	507	CLA	C4D-ND	-3.12	1.33	1.37
17	B	816	CLA	CHC-C1C	3.12	1.43	1.35
17	B	837	CLA	CHC-C1C	3.12	1.43	1.35
17	3	304	CLA	CHC-C1C	3.12	1.43	1.35
17	3	315	CLA	C4D-ND	-3.12	1.33	1.37
17	A	824	CLA	C4D-ND	-3.11	1.33	1.37
17	B	831	CLA	C4D-ND	-3.11	1.33	1.37
17	6	505	CLA	C4D-ND	-3.11	1.33	1.37
17	1	508	CLA	CHC-C1C	3.11	1.42	1.35
17	6	509	CLA	CHC-C1C	3.11	1.42	1.35
25	1	512	CHL	C1D-C2D	3.11	1.51	1.45
17	A	810	CLA	CHC-C1C	3.11	1.42	1.35
17	3	307	CLA	CHC-C1C	3.11	1.42	1.35
17	A	828	CLA	CHC-C1C	3.11	1.42	1.35
17	A	813	CLA	C4D-ND	-3.10	1.33	1.37
17	A	819	CLA	C4D-ND	-3.10	1.33	1.37
17	A	833	CLA	CHC-C1C	3.10	1.42	1.35
17	3	308	CLA	CHC-C1C	3.10	1.42	1.35
17	4	317	CLA	C4D-ND	-3.10	1.33	1.37
17	6	511	CLA	CHC-C1C	3.10	1.42	1.35
17	A	808	CLA	CHC-C1C	3.10	1.42	1.35
17	B	839	CLA	CHC-C1C	3.10	1.42	1.35
17	6	510	CLA	C4D-ND	-3.10	1.33	1.37
25	1	517	CHL	C3D-C2D	3.10	1.47	1.39
17	B	825	CLA	CHC-C1C	3.10	1.42	1.35
17	J	102	CLA	CHC-C1C	3.10	1.42	1.35
17	B	816	CLA	C4D-ND	-3.10	1.33	1.37
17	A	815	CLA	CHC-C1C	3.10	1.42	1.35
17	1	511	CLA	CHC-C1C	3.10	1.42	1.35
17	A	807	CLA	CHC-C1C	3.10	1.42	1.35
17	A	822	CLA	C4D-ND	-3.10	1.33	1.37
17	A	831	CLA	C4D-ND	-3.10	1.33	1.37
17	A	819	CLA	CHC-C1C	3.09	1.42	1.35
17	B	806	CLA	C4D-ND	-3.09	1.33	1.37
17	4	311	CLA	CHC-C1C	3.09	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	506	CLA	CHC-C1C	3.09	1.42	1.35
17	B	803	CLA	CHC-C1C	3.09	1.42	1.35
17	3	314	CLA	CHC-C1C	3.09	1.42	1.35
25	4	313	CHL	C1D-C2D	3.09	1.51	1.45
17	6	507	CLA	CHC-C1C	3.09	1.42	1.35
17	B	815	CLA	CHC-C1C	3.09	1.42	1.35
17	B	819	CLA	CHC-C1C	3.09	1.42	1.35
17	B	833	CLA	CHC-C1C	3.09	1.42	1.35
17	A	830	CLA	CHC-C1C	3.09	1.42	1.35
17	A	832	CLA	CHC-C1C	3.09	1.42	1.35
17	1	505	CLA	CHC-C1C	3.08	1.42	1.35
17	B	804	CLA	C1C-NC	-3.08	1.33	1.37
17	4	305	CLA	CHC-C1C	3.08	1.42	1.35
17	B	841	CLA	C4D-ND	-3.08	1.33	1.37
17	L	304	CLA	CHC-C1C	3.08	1.42	1.35
17	B	830	CLA	CHC-C1C	3.08	1.42	1.35
17	A	805	CLA	CHC-C1C	3.08	1.42	1.35
17	A	803	CLA	C4D-ND	-3.08	1.33	1.37
17	B	806	CLA	CHC-C1C	3.08	1.42	1.35
17	B	801	CLA	C4D-ND	-3.08	1.33	1.37
17	A	822	CLA	CHC-C1C	3.08	1.42	1.35
17	A	825	CLA	CHC-C1C	3.08	1.42	1.35
17	B	836	CLA	CHC-C1C	3.08	1.42	1.35
17	6	507	CLA	C4D-ND	-3.08	1.33	1.37
17	3	309	CLA	CHC-C1C	3.08	1.42	1.35
17	A	853	CLA	C4D-ND	-3.07	1.33	1.37
17	4	306	CLA	C4D-ND	-3.07	1.33	1.37
17	B	818	CLA	C4D-ND	-3.07	1.33	1.37
17	3	316	CLA	C4D-ND	-3.07	1.33	1.37
17	6	505	CLA	CHC-C1C	3.07	1.42	1.35
17	6	506	CLA	CHC-C1C	3.07	1.42	1.35
25	6	513	CHL	C3D-C2D	3.07	1.47	1.39
17	B	842	CLA	C4D-ND	-3.07	1.33	1.37
17	3	307	CLA	C4D-ND	-3.07	1.33	1.37
17	6	510	CLA	CHC-C1C	3.07	1.42	1.35
17	A	834	CLA	CHC-C1C	3.07	1.42	1.35
25	6	513	CHL	C1D-C2D	3.06	1.51	1.45
17	6	508	CLA	CHC-C1C	3.06	1.42	1.35
17	3	311	CLA	CHC-C1C	3.06	1.42	1.35
17	4	307	CLA	C4D-ND	-3.06	1.33	1.37
17	A	816	CLA	CHC-C1C	3.06	1.42	1.35
17	4	312	CLA	CHC-C1C	3.06	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	806	CLA	C4D-ND	-3.06	1.33	1.37
17	A	815	CLA	C4D-ND	-3.06	1.33	1.37
17	4	308	CLA	CHC-C1C	3.06	1.42	1.35
17	3	306	CLA	CHC-C1C	3.06	1.42	1.35
17	J	101	CLA	CHC-C1C	3.06	1.42	1.35
17	K	203	CLA	CHC-C1C	3.06	1.42	1.35
17	A	802	CLA	CHC-C1C	3.06	1.42	1.35
17	A	836	CLA	CHC-C1C	3.06	1.42	1.35
17	L	304	CLA	C4D-ND	-3.05	1.33	1.37
17	A	823	CLA	C4D-ND	-3.05	1.33	1.37
25	1	517	CHL	C1D-C2D	3.05	1.51	1.45
17	A	838	CLA	C4D-ND	-3.05	1.33	1.37
17	1	507	CLA	CHC-C1C	3.05	1.42	1.35
17	6	514	CLA	C4D-ND	-3.05	1.33	1.37
17	1	510	CLA	CHC-C1C	3.05	1.42	1.35
17	4	315	CLA	CHC-C1C	3.05	1.42	1.35
17	B	823	CLA	CHC-C1C	3.05	1.42	1.35
17	B	840	CLA	CHC-C1C	3.05	1.42	1.35
17	B	823	CLA	C4D-ND	-3.05	1.33	1.37
17	A	827	CLA	CHC-C1C	3.05	1.42	1.35
17	B	820	CLA	CHC-C1C	3.05	1.42	1.35
17	B	817	CLA	CHC-C1C	3.05	1.42	1.35
25	3	313	CHL	C1D-C2D	3.04	1.51	1.45
17	B	830	CLA	C4D-ND	-3.04	1.33	1.37
17	4	308	CLA	C4D-ND	-3.04	1.33	1.37
17	B	813	CLA	CHC-C1C	3.04	1.42	1.35
17	A	853	CLA	CHC-C1C	3.04	1.42	1.35
17	A	802	CLA	C4D-ND	-3.04	1.33	1.37
17	A	810	CLA	C4D-ND	-3.04	1.33	1.37
17	K	205	CLA	CHC-C1C	3.04	1.42	1.35
17	B	829	CLA	C4D-ND	-3.04	1.33	1.37
17	J	101	CLA	C4D-ND	-3.04	1.33	1.37
17	B	817	CLA	C4D-ND	-3.04	1.33	1.37
17	1	506	CLA	C4D-ND	-3.04	1.33	1.37
17	F	802	CLA	CHC-C1C	3.04	1.42	1.35
17	J	102	CLA	C4D-ND	-3.04	1.33	1.37
17	B	843	CLA	CHC-C1C	3.04	1.42	1.35
17	A	811	CLA	C4D-ND	-3.04	1.33	1.37
17	A	811	CLA	CHC-C1C	3.03	1.42	1.35
17	4	304	CLA	C4D-ND	-3.03	1.33	1.37
17	A	817	CLA	CHC-C1C	3.03	1.42	1.35
17	B	835	CLA	CHC-C1C	3.03	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	810	CLA	CHC-C1C	3.03	1.42	1.35
17	B	807	CLA	C4D-ND	-3.03	1.33	1.37
17	L	303	CLA	C4D-ND	-3.03	1.33	1.37
17	B	826	CLA	CHC-C1C	3.03	1.42	1.35
17	B	803	CLA	C4D-ND	-3.03	1.33	1.37
17	4	315	CLA	C4D-ND	-3.02	1.33	1.37
17	B	822	CLA	CHC-C1C	3.02	1.42	1.35
17	A	824	CLA	CHC-C1C	3.02	1.42	1.35
17	B	828	CLA	CHC-C1C	3.02	1.42	1.35
17	A	808	CLA	C4D-ND	-3.02	1.33	1.37
25	1	512	CHL	MG-NA	-3.02	1.99	2.06
17	A	812	CLA	CHC-C1C	3.02	1.42	1.35
17	L	303	CLA	CHC-C1C	3.02	1.42	1.35
17	A	829	CLA	C4D-ND	-3.02	1.33	1.37
17	A	840	CLA	C4D-ND	-3.02	1.33	1.37
17	A	852	CLA	C4D-ND	-3.02	1.33	1.37
17	B	829	CLA	CHC-C1C	3.01	1.42	1.35
17	B	811	CLA	C4D-ND	-3.01	1.33	1.37
17	6	508	CLA	C4D-ND	-3.01	1.33	1.37
17	6	514	CLA	CHC-C1C	3.01	1.42	1.35
17	K	203	CLA	C4D-ND	-3.01	1.33	1.37
17	B	842	CLA	CHC-C1C	3.01	1.42	1.35
17	A	820	CLA	CHC-C1C	3.01	1.42	1.35
17	A	804	CLA	CHC-C1C	3.01	1.42	1.35
17	A	835	CLA	CHC-C1C	3.01	1.42	1.35
17	3	309	CLA	C4D-ND	-3.00	1.33	1.37
17	B	836	CLA	C4D-ND	-3.00	1.33	1.37
17	3	310	CLA	CHC-C1C	3.00	1.42	1.35
17	3	315	CLA	CHC-C1C	3.00	1.42	1.35
17	B	824	CLA	C4D-ND	-3.00	1.33	1.37
17	A	840	CLA	CHC-C1C	3.00	1.42	1.35
17	B	801	CLA	CHC-C1C	3.00	1.42	1.35
25	1	514	CHL	C1D-C2D	3.00	1.51	1.45
17	A	836	CLA	C4D-ND	-2.99	1.33	1.37
17	6	506	CLA	C4D-ND	-2.99	1.33	1.37
25	6	517	CHL	C3D-C2D	2.99	1.47	1.39
17	F	802	CLA	C4D-ND	-2.99	1.33	1.37
17	B	814	CLA	C4D-ND	-2.99	1.33	1.37
17	B	833	CLA	C4D-ND	-2.99	1.33	1.37
17	3	311	CLA	C4D-ND	-2.99	1.33	1.37
17	4	310	CLA	C4D-ND	-2.99	1.33	1.37
17	B	832	CLA	CHC-C1C	2.98	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	CHC-C1C	2.98	1.42	1.35
17	4	305	CLA	C4D-ND	-2.98	1.33	1.37
17	A	838	CLA	CHC-C1C	2.98	1.42	1.35
17	1	515	CLA	CHC-C1C	2.98	1.42	1.35
17	B	812	CLA	CHC-C1C	2.98	1.42	1.35
25	6	512	CHL	MG-NA	-2.98	1.99	2.06
17	B	824	CLA	CHC-C1C	2.98	1.42	1.35
17	B	839	CLA	C4D-ND	-2.98	1.33	1.37
17	B	843	CLA	C4D-ND	-2.97	1.33	1.37
17	4	309	CLA	CHC-C1C	2.97	1.42	1.35
17	B	837	CLA	C4D-ND	-2.97	1.33	1.37
17	L	302	CLA	CHC-C1C	2.97	1.42	1.35
17	A	841	CLA	CHC-C1C	2.97	1.42	1.35
25	4	316	CHL	C3D-C2D	2.97	1.47	1.39
17	B	813	CLA	C4D-ND	-2.97	1.33	1.37
17	B	809	CLA	CHC-C1C	2.97	1.42	1.35
25	6	517	CHL	C1D-C2D	2.96	1.51	1.45
17	A	809	CLA	CHC-C1C	2.96	1.42	1.35
17	4	310	CLA	CHC-C1C	2.96	1.42	1.35
17	A	821	CLA	CHC-C1C	2.95	1.42	1.35
17	6	511	CLA	C4D-ND	-2.95	1.33	1.37
25	6	515	CHL	C1D-C2D	2.94	1.51	1.45
17	A	832	CLA	C4D-ND	-2.94	1.33	1.37
17	B	811	CLA	CHC-C1C	2.94	1.42	1.35
17	1	508	CLA	C4D-ND	-2.94	1.33	1.37
17	1	509	CLA	C1C-NC	-2.94	1.33	1.37
17	A	843	CLA	C4D-ND	-2.94	1.33	1.37
17	6	504	CLA	C4D-ND	-2.93	1.33	1.37
17	B	820	CLA	C4D-ND	-2.93	1.33	1.37
17	A	829	CLA	CHC-C1C	2.93	1.42	1.35
17	K	201	CLA	C4D-ND	-2.93	1.33	1.37
17	3	312	CLA	C4D-ND	-2.93	1.33	1.37
17	A	852	CLA	CHC-C1C	2.93	1.42	1.35
17	B	831	CLA	CHC-C1C	2.93	1.42	1.35
17	4	312	CLA	C4D-ND	-2.93	1.33	1.37
17	A	817	CLA	C4D-ND	-2.92	1.33	1.37
17	4	309	CLA	C4D-ND	-2.92	1.33	1.37
17	A	839	CLA	C4D-ND	-2.91	1.33	1.37
17	K	202	CLA	C4D-ND	-2.91	1.33	1.37
17	A	818	CLA	C1C-NC	-2.91	1.33	1.37
25	6	515	CHL	C3D-C2D	2.90	1.47	1.39
25	4	314	CHL	C1D-C2D	2.90	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	816	CLA	C4D-ND	-2.90	1.33	1.37
17	6	509	CLA	C4D-ND	-2.90	1.33	1.37
25	1	514	CHL	MG-NA	-2.90	1.99	2.06
17	1	515	CLA	C4D-ND	-2.90	1.33	1.37
25	4	316	CHL	C1D-C2D	2.89	1.51	1.45
17	A	807	CLA	C4D-ND	-2.89	1.33	1.37
17	B	826	CLA	C4D-ND	-2.88	1.33	1.37
17	4	311	CLA	C4D-ND	-2.88	1.33	1.37
17	3	310	CLA	C4D-ND	-2.86	1.33	1.37
17	3	306	CLA	C4D-ND	-2.86	1.33	1.37
17	B	831	CLA	CMB-C2B	-2.85	1.45	1.51
25	4	313	CHL	MG-NA	-2.84	1.99	2.06
17	1	504	CLA	C4D-ND	-2.83	1.33	1.37
17	3	308	CLA	C4D-ND	-2.83	1.33	1.37
17	A	809	CLA	C4D-ND	-2.83	1.33	1.37
17	1	511	CLA	C4D-ND	-2.82	1.33	1.37
17	K	205	CLA	C4D-ND	-2.81	1.33	1.37
25	4	314	CHL	C3D-C2D	2.78	1.46	1.39
17	L	302	CLA	C4D-ND	-2.78	1.33	1.37
17	A	827	CLA	C4D-ND	-2.77	1.33	1.37
17	A	829	CLA	CMB-C2B	-2.76	1.45	1.51
17	1	513	CLA	C4D-ND	-2.74	1.33	1.37
16	A	801	CL0	MG-NC	2.73	2.12	2.06
25	1	517	CHL	MG-NA	-2.72	1.99	2.06
17	B	804	CLA	CHC-C1C	2.72	1.41	1.35
25	3	313	CHL	CAD-CBD	-2.69	1.50	1.54
17	A	818	CLA	CHC-C1C	2.69	1.41	1.35
17	B	842	CLA	CMB-C2B	-2.68	1.46	1.51
16	A	801	CL0	CHC-C1C	2.67	1.41	1.35
25	1	512	CHL	C4B-CHC	2.67	1.48	1.41
17	3	305	CLA	C4D-ND	-2.66	1.34	1.37
16	A	801	CL0	C1C-NC	-2.64	1.33	1.37
17	A	817	CLA	CMB-C2B	-2.64	1.46	1.51
25	3	313	CHL	MG-NA	-2.63	2.00	2.06
17	1	509	CLA	CHC-C1C	2.63	1.41	1.35
16	A	801	CL0	C4C-C3C	2.62	1.49	1.45
17	A	830	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	833	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	841	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	819	CLA	CMB-C2B	-2.61	1.46	1.51
17	B	828	CLA	CMB-C2B	-2.61	1.46	1.51
17	3	314	CLA	CMB-C2B	-2.61	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	832	CLA	CMB-C2B	-2.60	1.46	1.51
25	4	313	CHL	C4B-CHC	2.59	1.48	1.41
17	A	810	CLA	CMB-C2B	-2.59	1.46	1.51
17	B	811	CLA	CMB-C2B	-2.59	1.46	1.51
17	A	852	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	808	CLA	CMB-C2B	-2.58	1.46	1.51
17	B	824	CLA	CMB-C2B	-2.58	1.46	1.51
17	B	829	CLA	CMB-C2B	-2.58	1.46	1.51
17	1	507	CLA	CMB-C2B	-2.57	1.46	1.51
17	B	830	CLA	CMB-C2B	-2.57	1.46	1.51
17	B	813	CLA	CMB-C2B	-2.57	1.46	1.51
17	B	819	CLA	CMB-C2B	-2.56	1.46	1.51
25	6	512	CHL	C4C-C3C	2.56	1.49	1.45
17	B	838	CLA	CMB-C2B	-2.56	1.46	1.51
17	A	816	CLA	CMB-C2B	-2.56	1.46	1.51
17	1	511	CLA	CMB-C2B	-2.55	1.46	1.51
17	B	833	CLA	CMB-C2B	-2.55	1.46	1.51
17	A	832	CLA	CMB-C2B	-2.55	1.46	1.51
17	A	807	CLA	CMB-C2B	-2.55	1.46	1.51
17	B	821	CLA	CMB-C2B	-2.55	1.46	1.51
17	B	809	CLA	CMB-C2B	-2.54	1.46	1.51
17	B	837	CLA	CMB-C2B	-2.54	1.46	1.51
17	B	841	CLA	CMB-C2B	-2.54	1.46	1.51
17	A	820	CLA	CMB-C2B	-2.54	1.46	1.51
17	A	824	CLA	CMB-C2B	-2.54	1.46	1.51
17	A	834	CLA	CMB-C2B	-2.54	1.46	1.51
18	A	842	PQN	C3-C2	2.53	1.48	1.35
17	A	815	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	835	CLA	CMB-C2B	-2.53	1.46	1.51
25	6	513	CHL	MG-NA	-2.52	2.00	2.06
25	1	514	CHL	C4B-CHC	2.52	1.48	1.41
25	6	512	CHL	C4B-CHC	2.52	1.48	1.41
17	B	827	CLA	CMB-C2B	-2.52	1.46	1.51
17	A	804	CLA	CMB-C2B	-2.51	1.46	1.51
17	3	306	CLA	CMB-C2B	-2.51	1.46	1.51
17	B	820	CLA	CMB-C2B	-2.51	1.46	1.51
17	A	836	CLA	CMB-C2B	-2.50	1.46	1.51
17	A	828	CLA	CMB-C2B	-2.50	1.46	1.51
17	K	201	CLA	CMB-C2B	-2.50	1.46	1.51
17	B	839	CLA	CMB-C2B	-2.50	1.46	1.51
17	A	811	CLA	CMB-C2B	-2.50	1.46	1.51
17	6	506	CLA	CMB-C2B	-2.50	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	836	CLA	CMB-C2B	-2.50	1.46	1.51
17	B	812	CLA	CMB-C2B	-2.49	1.46	1.51
17	B	825	CLA	CMB-C2B	-2.49	1.46	1.51
17	B	810	CLA	CMB-C2B	-2.49	1.46	1.51
17	A	803	CLA	CMB-C2B	-2.49	1.46	1.51
17	A	826	CLA	CMB-C2B	-2.49	1.46	1.51
17	B	823	CLA	CMB-C2B	-2.49	1.46	1.51
17	J	101	CLA	CMB-C2B	-2.49	1.46	1.51
25	4	316	CHL	MG-NA	-2.49	2.00	2.06
17	A	814	CLA	CMB-C2B	-2.48	1.46	1.51
17	B	807	CLA	CMB-C2B	-2.48	1.46	1.51
17	A	821	CLA	CMB-C2B	-2.48	1.46	1.51
17	1	504	CLA	CMB-C2B	-2.48	1.46	1.51
17	B	822	CLA	CMB-C2B	-2.48	1.46	1.51
17	A	839	CLA	CMB-C2B	-2.47	1.46	1.51
17	A	827	CLA	CMB-C2B	-2.47	1.46	1.51
17	A	806	CLA	CMB-C2B	-2.47	1.46	1.51
17	B	803	CLA	CMB-C2B	-2.47	1.46	1.51
17	4	309	CLA	CMB-C2B	-2.47	1.46	1.51
17	A	809	CLA	CMB-C2B	-2.47	1.46	1.51
17	B	818	CLA	CMB-C2B	-2.47	1.46	1.51
17	1	505	CLA	CMB-C2B	-2.47	1.46	1.51
17	L	302	CLA	CMB-C2B	-2.47	1.46	1.51
17	4	310	CLA	CMB-C2B	-2.46	1.46	1.51
17	4	308	CLA	CMB-C2B	-2.46	1.46	1.51
17	A	805	CLA	CMB-C2B	-2.46	1.46	1.51
17	K	205	CLA	CMB-C2B	-2.46	1.46	1.51
17	1	506	CLA	CMB-C2B	-2.46	1.46	1.51
25	6	517	CHL	MG-NA	-2.46	2.00	2.06
17	1	510	CLA	CMB-C2B	-2.46	1.46	1.51
17	3	310	CLA	CMB-C2B	-2.46	1.46	1.51
17	4	311	CLA	CMB-C2B	-2.46	1.46	1.51
17	B	814	CLA	CMB-C2B	-2.46	1.46	1.51
17	4	317	CLA	CMB-C2B	-2.45	1.46	1.51
17	F	802	CLA	CMB-C2B	-2.45	1.46	1.51
17	A	837	CLA	CMB-C2B	-2.45	1.46	1.51
17	4	315	CLA	CMB-C2B	-2.45	1.46	1.51
17	B	806	CLA	CMB-C2B	-2.45	1.46	1.51
25	1	512	CHL	C1B-CHB	2.44	1.47	1.41
25	1	517	CHL	C4B-CHC	2.44	1.47	1.41
17	3	308	CLA	CMB-C2B	-2.44	1.46	1.51
17	A	822	CLA	CMB-C2B	-2.44	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	316	CLA	CMB-C2B	-2.44	1.46	1.51
20	I	101	BCR	C30-C25	-2.44	1.50	1.53
17	B	817	CLA	CMB-C2B	-2.44	1.46	1.51
17	J	102	CLA	CMB-C2B	-2.44	1.46	1.51
17	A	812	CLA	CMB-C2B	-2.44	1.46	1.51
17	B	801	CLA	CMB-C2B	-2.44	1.46	1.51
17	A	813	CLA	CMB-C2B	-2.44	1.46	1.51
17	6	509	CLA	CMB-C2B	-2.43	1.46	1.51
25	1	514	CHL	C4C-C3C	2.43	1.49	1.45
17	4	312	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	843	CLA	CMB-C2B	-2.43	1.46	1.51
17	3	309	CLA	CMB-C2B	-2.43	1.46	1.51
17	A	853	CLA	CMB-C2B	-2.43	1.46	1.51
17	A	823	CLA	CMB-C2B	-2.43	1.46	1.51
17	6	510	CLA	CMB-C2B	-2.43	1.46	1.51
17	6	511	CLA	CMB-C2B	-2.43	1.46	1.51
17	A	802	CLA	CMB-C2B	-2.43	1.46	1.51
17	1	508	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	805	CLA	CMB-C2B	-2.43	1.46	1.51
17	4	305	CLA	CMB-C2B	-2.43	1.46	1.51
17	A	825	CLA	CMB-C2B	-2.43	1.46	1.51
17	4	306	CLA	CMB-C2B	-2.43	1.46	1.51
17	A	831	CLA	CMB-C2B	-2.42	1.46	1.51
17	A	838	CLA	CMB-C2B	-2.42	1.46	1.51
17	K	202	CLA	CMB-C2B	-2.42	1.46	1.51
17	6	508	CLA	CMB-C2B	-2.42	1.46	1.51
17	6	514	CLA	CMB-C2B	-2.42	1.46	1.51
17	B	835	CLA	CMB-C2B	-2.42	1.46	1.51
17	6	505	CLA	CMB-C2B	-2.42	1.46	1.51
17	B	816	CLA	CMB-C2B	-2.41	1.46	1.51
17	3	307	CLA	CMB-C2B	-2.41	1.46	1.51
25	6	515	CHL	MG-NA	-2.41	2.00	2.06
25	1	514	CHL	C1B-CHB	2.41	1.47	1.41
17	3	305	CLA	CMB-C2B	-2.41	1.46	1.51
17	3	311	CLA	CMB-C2B	-2.40	1.46	1.51
25	6	515	CHL	C4C-C3C	2.40	1.49	1.45
25	6	513	CHL	C4B-CHC	2.40	1.47	1.41
17	B	815	CLA	CMB-C2B	-2.40	1.46	1.51
17	4	307	CLA	CMB-C2B	-2.40	1.46	1.51
17	L	303	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	840	CLA	CMB-C2B	-2.39	1.46	1.51
25	4	313	CHL	C1B-CHB	2.39	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	CLA	CMB-C2B	-2.39	1.46	1.51
17	4	304	CLA	CMB-C2B	-2.39	1.46	1.51
25	1	512	CHL	C4C-C3C	2.39	1.49	1.45
16	A	801	CL0	C1D-C2D	2.38	1.50	1.45
17	B	808	CLA	CMB-C2B	-2.38	1.46	1.51
25	1	517	CHL	C1B-CHB	2.38	1.47	1.41
25	1	512	CHL	C1D-ND	-2.38	1.34	1.37
17	B	834	CLA	CMB-C2B	-2.38	1.46	1.51
25	6	512	CHL	C1B-CHB	2.38	1.47	1.41
17	K	203	CLA	CMB-C2B	-2.38	1.46	1.51
25	3	313	CHL	C4B-CHC	2.37	1.47	1.41
17	6	507	CLA	CMB-C2B	-2.37	1.46	1.51
17	B	831	CLA	CMD-C2D	-2.37	1.45	1.50
17	B	826	CLA	CMB-C2B	-2.37	1.46	1.51
17	A	843	CLA	CMB-C2B	-2.37	1.46	1.51
17	1	515	CLA	CMB-C2B	-2.37	1.46	1.51
25	1	517	CHL	C4C-C3C	2.36	1.49	1.45
17	L	304	CLA	CMB-C2B	-2.36	1.46	1.51
17	3	315	CLA	CMB-C2B	-2.36	1.46	1.51
25	4	314	CHL	C4C-C3C	2.36	1.49	1.45
17	3	312	CLA	CMB-C2B	-2.34	1.46	1.51
25	4	313	CHL	C1D-ND	-2.34	1.34	1.37
16	A	801	CL0	O2A-CGA	-2.33	1.31	1.42
25	4	316	CHL	C4C-C3C	2.33	1.49	1.45
17	K	203	CLA	CMD-C2D	-2.32	1.45	1.50
20	A	850	BCR	C1-C6	-2.32	1.50	1.53
17	B	828	CLA	CMC-C2C	-2.32	1.45	1.50
17	1	513	CLA	CMB-C2B	-2.31	1.46	1.51
25	1	514	CHL	C1D-ND	-2.31	1.34	1.37
25	6	517	CHL	C4B-CHC	2.30	1.47	1.41
17	1	510	CLA	CMD-C2D	-2.29	1.45	1.50
17	4	311	CLA	CMD-C2D	-2.29	1.46	1.50
17	1	511	CLA	C3B-C2B	-2.29	1.37	1.40
25	6	512	CHL	C1D-ND	-2.28	1.35	1.37
25	6	513	CHL	C4C-C3C	2.28	1.49	1.45
25	4	313	CHL	C4C-C3C	2.28	1.49	1.45
17	6	504	CLA	CMB-C2B	-2.27	1.46	1.51
25	6	513	CHL	C1B-CHB	2.27	1.47	1.41
17	A	833	CLA	C3B-C2B	-2.27	1.37	1.40
17	A	827	CLA	C3B-C2B	-2.27	1.37	1.40
25	6	515	CHL	C4B-CHC	2.26	1.47	1.41
25	6	517	CHL	C4C-C3C	2.25	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	816	CLA	CMD-C2D	-2.23	1.46	1.50
17	B	805	CLA	CMC-C2C	-2.22	1.46	1.50
17	A	816	CLA	CMD-C2D	-2.21	1.46	1.50
17	A	830	CLA	CMD-C2D	-2.21	1.46	1.50
16	A	801	CL0	CHB-C4A	2.20	1.36	1.34
25	4	314	CHL	MG-NA	-2.20	2.01	2.06
17	1	504	CLA	CMD-C2D	-2.20	1.46	1.50
25	4	316	CHL	C1B-CHB	2.19	1.47	1.41
25	3	313	CHL	C1B-CHB	2.19	1.47	1.41
17	B	830	CLA	CMD-C2D	-2.19	1.46	1.50
17	B	842	CLA	C3B-C2B	-2.19	1.37	1.40
17	A	833	CLA	CMD-C2D	-2.19	1.46	1.50
17	B	809	CLA	C3B-C2B	-2.17	1.37	1.40
17	B	807	CLA	CMD-C2D	-2.17	1.46	1.50
17	4	304	CLA	CMD-C2D	-2.16	1.46	1.50
17	6	505	CLA	CMD-C2D	-2.16	1.46	1.50
25	6	515	CHL	C1B-CHB	2.16	1.47	1.41
17	A	852	CLA	CMC-C2C	-2.15	1.46	1.50
17	3	310	CLA	CMD-C2D	-2.15	1.46	1.50
17	A	810	CLA	CMD-C2D	-2.15	1.46	1.50
17	B	842	CLA	CMD-C2D	-2.15	1.46	1.50
17	A	829	CLA	C3B-C2B	-2.14	1.37	1.40
17	A	804	CLA	CMD-C2D	-2.14	1.46	1.50
17	B	811	CLA	C3B-C2B	-2.14	1.37	1.40
25	4	316	CHL	C4B-CHC	2.14	1.46	1.41
17	6	511	CLA	CMD-C2D	-2.14	1.46	1.50
17	6	507	CLA	CMD-C2D	-2.13	1.46	1.50
17	A	802	CLA	CMD-C2D	-2.13	1.46	1.50
17	A	840	CLA	CMD-C2D	-2.13	1.46	1.50
25	4	314	CHL	C1B-CHB	2.13	1.46	1.41
17	1	508	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	825	CLA	CMD-C2D	-2.12	1.46	1.50
17	3	314	CLA	CMD-C2D	-2.12	1.46	1.50
17	B	817	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	812	CLA	CMD-C2D	-2.12	1.46	1.50
25	1	517	CHL	C1D-ND	-2.12	1.35	1.37
17	B	812	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	803	CLA	CMD-C2D	-2.12	1.46	1.50
17	3	305	CLA	C3B-C2B	-2.12	1.37	1.40
17	A	826	CLA	CMD-C2D	-2.11	1.46	1.50
17	K	201	CLA	CBD-CAD	2.11	1.56	1.51
17	B	805	CLA	CMD-C2D	-2.11	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	838	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	826	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	810	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	821	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	825	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	827	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	832	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	838	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	841	CLA	CMD-C2D	-2.10	1.46	1.50
17	3	311	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	829	CLA	CMD-C2D	-2.10	1.46	1.50
17	4	315	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	818	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	833	CLA	CMD-C2D	-2.10	1.46	1.50
17	L	303	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	806	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	828	CLA	CMD-C2D	-2.10	1.46	1.50
17	A	828	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	812	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	841	CLA	CMC-C2C	-2.10	1.46	1.50
20	B	849	BCR	C30-C25	-2.09	1.50	1.53
17	A	828	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	835	CLA	CMD-C2D	-2.09	1.46	1.50
17	6	514	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	827	CLA	CMD-C2D	-2.09	1.46	1.50
17	1	511	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	829	CLA	CMC-C2C	-2.09	1.46	1.50
17	B	834	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	840	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	823	CLA	CMD-C2D	-2.09	1.46	1.50
17	1	505	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	810	CLA	CMC-C2C	-2.09	1.46	1.50
17	A	829	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	822	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	839	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	808	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	801	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	801	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	817	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	841	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	807	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	824	CLA	CMD-C2D	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	848	BCR	C30-C25	-2.08	1.50	1.53
17	1	507	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	827	CLA	C3B-CAB	-2.08	1.43	1.47
17	4	308	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	837	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	836	CLA	CMD-C2D	-2.08	1.46	1.50
17	4	307	CLA	CMD-C2D	-2.08	1.46	1.50
25	3	313	CHL	C1D-ND	-2.08	1.35	1.37
17	A	830	CLA	C3B-C2B	-2.08	1.37	1.40
17	A	806	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	826	CLA	CMC-C2C	-2.07	1.46	1.50
17	B	821	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	852	CLA	CMD-C2D	-2.07	1.46	1.50
25	6	513	CHL	C1D-ND	-2.07	1.35	1.37
17	B	820	CLA	CMD-C2D	-2.07	1.46	1.50
17	4	305	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	819	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	823	CLA	C3B-C2B	-2.07	1.37	1.40
17	B	803	CLA	CMC-C2C	-2.07	1.46	1.50
17	A	837	CLA	CMD-C2D	-2.06	1.46	1.50
17	1	510	CLA	CMC-C2C	-2.06	1.46	1.50
17	A	805	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	831	CLA	CMD-C2D	-2.06	1.46	1.50
17	6	510	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	815	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	819	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	824	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	810	CLA	CMC-C2C	-2.06	1.46	1.50
17	J	101	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	813	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	820	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	820	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	804	CLA	CMC-C2C	-2.05	1.46	1.50
25	6	517	CHL	C1B-CHB	2.05	1.46	1.41
20	L	301	BCR	C1-C6	-2.05	1.50	1.53
17	A	834	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	841	CLA	CMC-C2C	-2.05	1.46	1.50
20	A	850	BCR	C30-C25	-2.05	1.50	1.53
17	3	315	CLA	CMD-C2D	-2.05	1.46	1.50
17	6	505	CLA	CMC-C2C	-2.05	1.46	1.50
17	B	809	CLA	CMD-C2D	-2.05	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	C3B-C2B	-2.05	1.37	1.40
17	A	821	CLA	CMC-C2C	-2.05	1.46	1.50
17	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
17	4	317	CLA	CMD-C2D	-2.05	1.46	1.50
25	4	314	CHL	C4B-CHC	2.04	1.46	1.41
17	A	814	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	853	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	818	CLA	C1A-CHA	2.04	1.51	1.43
17	4	306	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	802	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	816	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	814	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	811	CLA	C3B-C2B	-2.04	1.37	1.40
17	A	824	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	811	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	835	CLA	C3B-C2B	-2.04	1.37	1.40
17	A	806	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	824	CLA	C3B-C2B	-2.04	1.37	1.40
17	B	815	CLA	CMD-C2D	-2.04	1.46	1.50
17	6	507	CLA	CMC-C2C	-2.04	1.46	1.50
17	A	808	CLA	C3B-C2B	-2.04	1.37	1.40
17	A	811	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	840	CLA	CMC-C2C	-2.04	1.46	1.50
17	3	316	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
17	L	304	CLA	CMD-C2D	-2.03	1.46	1.50
17	F	802	CLA	CMD-C2D	-2.03	1.46	1.50
17	A	813	CLA	CMD-C2D	-2.03	1.46	1.50
17	4	309	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	846	BCR	C1-C6	-2.03	1.51	1.53
17	B	836	CLA	C3B-C2B	-2.03	1.37	1.40
17	3	312	CLA	CMD-C2D	-2.03	1.46	1.50
17	A	809	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	831	CLA	CMC-C2C	-2.03	1.46	1.50
17	1	509	CLA	MG-NC	2.03	2.11	2.06
20	J	103	BCR	C1-C6	-2.03	1.51	1.53
17	6	506	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	808	CLA	CMD-C2D	-2.02	1.46	1.50
20	B	848	BCR	C30-C25	-2.02	1.51	1.53
20	3	303	BCR	C30-C25	-2.02	1.51	1.53
17	A	841	CLA	C3B-C2B	-2.02	1.37	1.40
17	6	508	CLA	CMD-C2D	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	811	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	822	CLA	CMC-C2C	-2.02	1.46	1.50
17	A	830	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	821	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	822	CLA	CMD-C2D	-2.02	1.46	1.50
17	4	311	CLA	C3B-C2B	-2.02	1.37	1.40
17	B	823	CLA	CMC-C2C	-2.02	1.46	1.50
17	3	315	CLA	CMC-C2C	-2.02	1.46	1.50
17	4	312	CLA	CMD-C2D	-2.02	1.46	1.50
17	3	304	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	825	CLA	CMC-C2C	-2.02	1.46	1.50
17	A	834	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	812	CLA	CMC-C2C	-2.01	1.46	1.50
17	A	835	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	830	CLA	CMC-C2C	-2.01	1.46	1.50
17	A	833	CLA	C3B-CAB	-2.01	1.43	1.47
17	B	828	CLA	C3B-C2B	-2.01	1.37	1.40
17	K	205	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	306	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	838	CLA	CMC-C2C	-2.01	1.46	1.50
17	1	513	CLA	CMD-C2D	-2.01	1.46	1.50
17	A	853	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	823	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	515	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	809	CLA	CMC-C2C	-2.01	1.46	1.50
17	1	506	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	827	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	832	CLA	CMC-C2C	-2.01	1.46	1.50
17	K	201	CLA	CMD-C2D	-2.01	1.46	1.50
17	A	814	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	835	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	842	CLA	CMC-C2C	-2.01	1.46	1.50
17	6	504	CLA	CMD-C2D	-2.00	1.46	1.50
17	B	814	CLA	CMC-C2C	-2.00	1.46	1.50
17	A	838	CLA	CMC-C2C	-2.00	1.46	1.50
17	1	504	CLA	MG-ND	-2.00	2.01	2.05
17	A	817	CLA	CMC-C2C	-2.00	1.46	1.50
17	1	515	CLA	CMD-C2D	-2.00	1.46	1.50
17	A	810	CLA	C3B-C2B	-2.00	1.37	1.40

All (1884) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	503	BCR	C40-C30-C25	-12.39	90.20	110.30
16	A	801	CL0	C4A-NA-C1A	10.83	111.58	106.71
17	B	804	CLA	C4A-NA-C1A	9.99	111.20	106.71
20	6	503	BCR	C20-C21-C22	-9.47	113.80	127.31
17	1	509	CLA	C4A-NA-C1A	8.63	110.58	106.71
25	3	313	CHL	CMD-C2D-C1D	8.58	139.84	124.71
17	A	818	CLA	C4A-NA-C1A	8.55	110.55	106.71
25	6	515	CHL	CMD-C2D-C1D	8.39	139.50	124.71
25	4	314	CHL	CMD-C2D-C1D	8.32	139.37	124.71
20	6	503	BCR	C40-C30-C39	-8.28	83.12	108.53
25	6	517	CHL	CMD-C2D-C1D	8.23	139.23	124.71
25	4	316	CHL	CMD-C2D-C1D	8.20	139.16	124.71
25	6	512	CHL	CMD-C2D-C1D	8.20	139.16	124.71
26	6	502	XAT	O4-C5-C4	8.19	119.53	113.38
25	6	513	CHL	CMD-C2D-C1D	8.11	139.01	124.71
25	1	512	CHL	CMD-C2D-C1D	8.09	138.98	124.71
25	4	313	CHL	CMD-C2D-C1D	8.09	138.98	124.71
25	1	517	CHL	CMD-C2D-C1D	8.07	138.93	124.71
25	1	514	CHL	CMD-C2D-C1D	8.05	138.90	124.71
25	6	512	CHL	CHD-C1D-ND	-7.86	117.23	124.45
20	A	850	BCR	C7-C8-C9	-7.71	114.58	126.23
25	4	313	CHL	CHD-C1D-ND	-7.69	117.39	124.45
25	1	512	CHL	CHD-C1D-ND	-7.66	117.42	124.45
25	1	514	CHL	CHD-C1D-ND	-7.57	117.49	124.45
20	6	503	BCR	C24-C23-C22	-7.57	114.80	126.23
25	6	517	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
25	4	314	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
20	A	854	BCR	C16-C17-C18	-7.30	116.89	127.31
25	1	517	CHL	CHD-C1D-ND	-7.23	117.81	124.45
25	3	313	CHL	CHD-C1D-ND	-7.16	117.88	124.45
25	6	515	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
20	K	204	BCR	C16-C17-C18	-7.14	117.12	127.31
25	1	517	CHL	C2C-C3C-C4C	-7.13	101.40	106.49
25	1	514	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
24	1	502	LUT	C21-C26-C27	7.11	121.69	112.70
25	6	512	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
25	4	316	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
25	6	513	CHL	CHD-C1D-ND	-7.08	117.94	124.45
26	4	303	XAT	C18-C5-C6	-7.07	110.42	122.26
17	A	807	CLA	C4A-NA-C1A	7.04	109.87	106.71
17	B	830	CLA	C4A-NA-C1A	7.03	109.87	106.71
17	B	828	CLA	C4A-NA-C1A	7.01	109.86	106.71
17	B	839	CLA	C4A-NA-C1A	7.01	109.86	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	313	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
17	6	504	CLA	C4A-NA-C1A	6.99	109.85	106.71
17	6	505	CLA	C4A-NA-C1A	6.99	109.85	106.71
17	A	809	CLA	C4A-NA-C1A	6.98	109.84	106.71
25	1	512	CHL	C2C-C3C-C4C	-6.98	101.52	106.49
25	6	513	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
17	B	810	CLA	C4A-NA-C1A	6.95	109.83	106.71
17	3	306	CLA	C4A-NA-C1A	6.89	109.81	106.71
17	3	314	CLA	C4A-NA-C1A	6.88	109.80	106.71
17	B	805	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	1	515	CLA	C4A-NA-C1A	6.86	109.79	106.71
26	6	502	XAT	C18-C5-C6	-6.83	110.81	122.26
25	3	313	CHL	C2C-C3C-C4C	-6.82	101.63	106.49
26	4	303	XAT	O24-C25-C24	6.82	118.50	113.38
17	B	832	CLA	C4A-NA-C1A	6.80	109.77	106.71
17	A	822	CLA	C4A-NA-C1A	6.80	109.76	106.71
17	B	826	CLA	C4A-NA-C1A	6.80	109.76	106.71
26	6	502	XAT	C38-C25-C26	-6.78	110.89	122.26
17	A	814	CLA	C4A-NA-C1A	6.78	109.75	106.71
17	A	852	CLA	C4A-NA-C1A	6.77	109.75	106.71
17	B	814	CLA	C4A-NA-C1A	6.77	109.75	106.71
17	L	303	CLA	C4A-NA-C1A	6.77	109.75	106.71
17	B	841	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	6	517	CHL	CHD-C1D-ND	-6.75	118.25	124.45
17	A	840	CLA	C4A-NA-C1A	6.73	109.73	106.71
17	4	310	CLA	C4A-NA-C1A	6.72	109.73	106.71
17	A	810	CLA	C4A-NA-C1A	6.70	109.72	106.71
17	A	816	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	4	303	XAT	C38-C25-C26	-6.69	111.04	122.26
17	L	302	CLA	C4A-NA-C1A	6.69	109.72	106.71
20	I	101	BCR	C11-C10-C9	-6.69	117.77	127.31
17	A	808	CLA	C4A-NA-C1A	6.67	109.70	106.71
17	1	504	CLA	C4A-NA-C1A	6.66	109.70	106.71
17	6	511	CLA	C4A-NA-C1A	6.66	109.70	106.71
17	B	824	CLA	C4A-NA-C1A	6.65	109.70	106.71
17	B	822	CLA	C4A-NA-C1A	6.65	109.70	106.71
17	B	809	CLA	C4A-NA-C1A	6.64	109.69	106.71
17	B	813	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	6	515	CHL	CHD-C1D-ND	-6.64	118.36	124.45
17	B	840	CLA	C4A-NA-C1A	6.63	109.69	106.71
17	B	820	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	3	309	CLA	C4A-NA-C1A	6.62	109.68	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	829	CLA	C4A-NA-C1A	6.61	109.68	106.71
17	A	821	CLA	C4A-NA-C1A	6.58	109.67	106.71
17	B	812	CLA	C4A-NA-C1A	6.58	109.67	106.71
17	B	816	CLA	C4A-NA-C1A	6.58	109.66	106.71
26	6	502	XAT	O24-C25-C24	6.58	118.32	113.38
17	J	102	CLA	C4A-NA-C1A	6.58	109.66	106.71
17	A	820	CLA	C4A-NA-C1A	6.57	109.66	106.71
17	A	838	CLA	C4A-NA-C1A	6.57	109.66	106.71
17	B	823	CLA	C4A-NA-C1A	6.56	109.66	106.71
17	3	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
17	A	841	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	A	824	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	4	314	CHL	CHD-C1D-ND	-6.53	118.45	124.45
17	B	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	B	837	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	3	310	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	A	817	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	K	201	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	A	839	CLA	C4A-NA-C1A	6.51	109.63	106.71
17	B	838	CLA	C4A-NA-C1A	6.51	109.63	106.71
17	1	507	CLA	C4A-NA-C1A	6.49	109.62	106.71
17	L	304	CLA	C4A-NA-C1A	6.48	109.62	106.71
17	A	811	CLA	C4A-NA-C1A	6.48	109.62	106.71
17	6	514	CLA	C4A-NA-C1A	6.47	109.61	106.71
20	B	847	BCR	C7-C8-C9	-6.47	116.47	126.23
17	3	308	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	A	828	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	3	315	CLA	C4A-NA-C1A	6.44	109.60	106.71
17	B	842	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	1	510	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	A	853	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	A	802	CLA	C4A-NA-C1A	6.42	109.59	106.71
17	B	817	CLA	C4A-NA-C1A	6.41	109.59	106.71
17	B	825	CLA	C4A-NA-C1A	6.41	109.59	106.71
17	A	803	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	A	819	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	B	847	BCR	C24-C23-C22	-6.40	116.57	126.23
17	K	202	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	4	317	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	A	833	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	A	804	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	A	805	CLA	C4A-NA-C1A	6.39	109.58	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	203	CLA	C4A-NA-C1A	6.38	109.58	106.71
17	B	834	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	A	806	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	B	835	CLA	C4A-NA-C1A	6.36	109.57	106.71
20	L	301	BCR	C7-C8-C9	-6.36	116.63	126.23
17	B	801	CLA	C4A-NA-C1A	6.35	109.56	106.71
17	3	304	CLA	C4A-NA-C1A	6.35	109.56	106.71
17	3	307	CLA	C4A-NA-C1A	6.34	109.56	106.71
17	B	818	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	4	312	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	A	815	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	F	802	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	4	304	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	4	308	CLA	C4A-NA-C1A	6.31	109.54	106.71
17	B	811	CLA	C4A-NA-C1A	6.30	109.54	106.71
17	4	305	CLA	C4A-NA-C1A	6.30	109.54	106.71
17	A	825	CLA	C4A-NA-C1A	6.29	109.53	106.71
17	6	510	CLA	C4A-NA-C1A	6.29	109.53	106.71
25	4	316	CHL	CHD-C1D-ND	-6.28	118.69	124.45
17	B	843	CLA	C4A-NA-C1A	6.28	109.53	106.71
20	A	854	BCR	C15-C14-C13	-6.27	118.36	127.31
17	J	101	CLA	C4A-NA-C1A	6.27	109.53	106.71
26	6	502	XAT	C15-C14-C13	-6.26	118.37	127.31
17	B	833	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	4	311	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	6	506	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	B	819	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	6	508	CLA	C4A-NA-C1A	6.24	109.51	106.71
17	B	836	CLA	C4A-NA-C1A	6.23	109.51	106.71
20	6	503	BCR	C15-C16-C17	-6.22	110.73	123.47
17	6	509	CLA	C4A-NA-C1A	6.21	109.50	106.71
17	3	312	CLA	C4A-NA-C1A	6.21	109.50	106.71
17	1	511	CLA	C4A-NA-C1A	6.18	109.48	106.71
17	A	834	CLA	C4A-NA-C1A	6.17	109.48	106.71
17	A	826	CLA	C4A-NA-C1A	6.15	109.47	106.71
17	1	508	CLA	C4A-NA-C1A	6.15	109.47	106.71
17	B	831	CLA	C4A-NA-C1A	6.14	109.47	106.71
17	A	823	CLA	C4A-NA-C1A	6.13	109.46	106.71
17	A	836	CLA	C4A-NA-C1A	6.12	109.46	106.71
20	F	803	BCR	C11-C10-C9	-6.12	118.57	127.31
17	4	307	CLA	C4A-NA-C1A	6.12	109.46	106.71
17	A	832	CLA	C4A-NA-C1A	6.11	109.45	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	835	CLA	C4A-NA-C1A	6.09	109.44	106.71
20	A	846	BCR	C16-C17-C18	-6.08	118.63	127.31
16	A	801	CL0	CMD-C2D-C1D	6.07	135.41	124.71
17	A	843	CLA	C4A-NA-C1A	6.07	109.43	106.71
17	K	205	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	A	837	CLA	C4A-NA-C1A	6.04	109.42	106.71
17	B	829	CLA	C4A-NA-C1A	6.04	109.42	106.71
17	4	315	CLA	C4A-NA-C1A	6.04	109.42	106.71
20	F	801	BCR	C16-C17-C18	-6.03	118.70	127.31
17	A	831	CLA	C4A-NA-C1A	6.03	109.42	106.71
17	B	806	CLA	C4A-NA-C1A	6.02	109.41	106.71
17	A	812	CLA	C4A-NA-C1A	6.01	109.41	106.71
17	A	830	CLA	C4A-NA-C1A	6.00	109.41	106.71
17	B	807	CLA	C4A-NA-C1A	6.00	109.40	106.71
17	1	513	CLA	C4A-NA-C1A	5.99	109.40	106.71
17	B	821	CLA	C4A-NA-C1A	5.98	109.39	106.71
17	4	306	CLA	C4A-NA-C1A	5.97	109.39	106.71
17	3	316	CLA	C4A-NA-C1A	5.95	109.38	106.71
20	L	305	BCR	C20-C21-C22	-5.93	118.84	127.31
20	I	101	BCR	C7-C8-C9	-5.93	117.27	126.23
17	6	507	CLA	C4A-NA-C1A	5.93	109.37	106.71
20	B	850	BCR	C16-C17-C18	-5.93	118.85	127.31
20	B	846	BCR	C7-C8-C9	-5.90	117.31	126.23
20	6	503	BCR	C40-C30-C29	-5.90	85.30	108.91
20	F	801	BCR	C24-C23-C22	-5.89	117.33	126.23
17	3	305	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	1	517	CHL	O2D-CGD-CBD	5.83	121.63	111.27
17	1	506	CLA	C4A-NA-C1A	5.83	109.33	106.71
20	A	850	BCR	C20-C21-C22	-5.76	119.09	127.31
17	B	815	CLA	C4A-NA-C1A	5.75	109.29	106.71
24	3	301	LUT	C35-C34-C33	-5.75	119.11	127.31
17	A	813	CLA	C4A-NA-C1A	5.73	109.28	106.71
20	I	101	BCR	C15-C14-C13	-5.73	119.14	127.31
16	A	801	CL0	C1B-C2B-C3B	-5.71	101.61	106.92
17	B	827	CLA	C4A-NA-C1A	5.69	109.27	106.71
20	B	848	BCR	C15-C14-C13	-5.69	119.19	127.31
17	4	309	CLA	C4A-NA-C1A	5.65	109.24	106.71
24	6	501	LUT	C15-C14-C13	-5.62	119.29	127.31
25	1	512	CHL	C1B-CHB-C4A	-5.61	119.01	130.12
20	I	102	BCR	C7-C8-C9	-5.56	117.83	126.23
17	B	803	CLA	C4A-NA-C1A	5.53	109.19	106.71
17	1	509	CLA	CMD-C2D-C1D	5.53	134.45	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	827	CLA	C4A-NA-C1A	5.52	109.19	106.71
20	A	846	BCR	C20-C21-C22	-5.50	119.46	127.31
20	L	305	BCR	C16-C17-C18	-5.49	119.47	127.31
23	4	318	LMG	O7-C10-O9	-5.47	118.61	125.57
17	A	818	CLA	CMD-C2D-C1D	5.46	134.33	124.71
25	1	512	CHL	O2D-CGD-CBD	5.44	120.94	111.27
20	6	503	BCR	C39-C30-C25	5.42	119.09	110.30
17	1	509	CLA	O2A-C1-C2	5.39	122.79	108.64
24	1	501	LUT	C11-C10-C9	-5.37	119.64	127.31
20	6	503	BCR	C30-C25-C26	-5.37	115.05	122.61
20	L	301	BCR	C15-C14-C13	-5.37	119.65	127.31
25	6	517	CHL	O2D-CGD-CBD	5.34	120.75	111.27
24	3	301	LUT	C31-C30-C29	-5.33	119.71	127.31
20	A	846	BCR	C15-C14-C13	-5.32	119.72	127.31
20	J	103	BCR	C28-C27-C26	-5.31	104.60	114.08
24	4	302	LUT	C31-C30-C29	-5.28	119.77	127.31
25	6	513	CHL	O2D-CGD-CBD	5.26	120.62	111.27
20	A	846	BCR	C38-C26-C25	-5.26	118.62	124.53
26	4	303	XAT	O4-C5-C18	5.23	121.32	115.06
26	4	303	XAT	O4-C5-C4	5.23	117.31	113.38
20	B	845	BCR	C20-C21-C22	-5.20	119.89	127.31
25	1	514	CHL	C1B-CHB-C4A	-5.19	119.85	130.12
25	6	512	CHL	O2D-CGD-CBD	5.16	120.44	111.27
20	3	303	BCR	C15-C14-C13	-5.15	119.96	127.31
24	3	302	LUT	C35-C34-C33	-5.14	119.98	127.31
24	1	501	LUT	C15-C14-C13	-5.13	119.98	127.31
20	B	850	BCR	C20-C21-C22	-5.13	119.99	127.31
20	A	849	BCR	C16-C17-C18	-5.12	120.01	127.31
20	3	303	BCR	C7-C8-C9	-5.11	118.52	126.23
20	A	849	BCR	C20-C21-C22	-5.10	120.03	127.31
20	A	848	BCR	C11-C10-C9	-5.09	120.05	127.31
25	4	313	CHL	O2D-CGD-CBD	5.08	120.29	111.27
20	B	845	BCR	C24-C23-C22	-5.07	118.57	126.23
20	B	847	BCR	C16-C17-C18	-5.06	120.09	127.31
25	3	313	CHL	C1D-C2D-C3D	-5.03	99.59	106.94
24	4	302	LUT	C15-C14-C13	-5.02	120.14	127.31
20	A	851	BCR	C7-C8-C9	-5.01	118.67	126.23
20	F	803	BCR	C7-C8-C9	-5.00	118.68	126.23
20	A	851	BCR	C11-C10-C9	-4.98	120.20	127.31
20	A	854	BCR	C11-C10-C9	-4.98	120.21	127.31
20	B	849	BCR	C24-C23-C22	-4.94	118.77	126.23
20	B	845	BCR	C16-C17-C18	-4.93	120.27	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	302	LUT	C35-C34-C33	-4.93	120.27	127.31
20	I	102	BCR	C15-C14-C13	-4.93	120.28	127.31
25	4	314	CHL	C3C-C4C-NC	4.91	116.08	110.57
25	3	313	CHL	O2D-CGD-CBD	4.86	119.61	111.49
25	6	515	CHL	O2D-CGD-CBD	4.84	119.87	111.27
20	B	849	BCR	C15-C14-C13	-4.83	120.41	127.31
20	F	801	BCR	C28-C27-C26	-4.81	105.49	114.08
20	4	301	BCR	C15-C14-C13	-4.80	120.46	127.31
20	A	850	BCR	C16-C17-C18	-4.80	120.46	127.31
26	6	502	XAT	O24-C25-C38	4.79	120.79	115.06
25	1	514	CHL	O2D-CGD-CBD	4.77	119.74	111.27
17	4	304	CLA	CAB-C3B-C4B	-4.74	121.18	128.46
25	6	517	CHL	C3C-C4C-NC	4.74	115.89	110.57
24	1	502	LUT	C21-C26-C25	4.72	119.88	111.42
24	3	301	LUT	C11-C10-C9	-4.71	120.59	127.31
25	6	517	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
24	1	501	LUT	C7-C8-C9	-4.67	119.17	126.23
20	A	849	BCR	C24-C23-C22	-4.66	119.19	126.23
20	A	854	BCR	C28-C27-C26	-4.66	105.76	114.08
20	F	803	BCR	C15-C14-C13	-4.64	120.69	127.31
26	4	303	XAT	C26-C27-C28	-4.63	116.21	125.99
17	A	843	CLA	CAB-C3B-C4B	-4.62	121.37	128.46
25	4	316	CHL	O2D-CGD-CBD	4.59	119.43	111.27
25	1	514	CHL	C4A-NA-C1A	4.59	108.77	106.71
24	3	301	LUT	C7-C8-C9	-4.58	119.31	126.23
20	A	851	BCR	C15-C14-C13	-4.58	120.78	127.31
17	B	801	CLA	CAB-C3B-C4B	-4.57	121.44	128.46
25	4	316	CHL	C3C-C4C-NC	4.57	115.69	110.57
17	B	804	CLA	CMD-C2D-C1D	4.56	132.75	124.71
17	L	302	CLA	CAB-C3B-C4B	-4.56	121.45	128.46
20	L	305	BCR	C24-C23-C22	-4.56	119.34	126.23
20	1	503	BCR	C38-C26-C25	-4.56	119.41	124.53
17	A	826	CLA	CAB-C3B-C4B	-4.55	121.47	128.46
25	4	314	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
20	I	102	BCR	C28-C27-C26	-4.54	105.97	114.08
20	A	848	BCR	C16-C17-C18	-4.52	120.85	127.31
20	A	846	BCR	C33-C5-C6	-4.52	119.45	124.53
17	B	829	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
20	4	301	BCR	C33-C5-C6	-4.51	119.46	124.53
20	F	801	BCR	C20-C21-C22	-4.51	120.87	127.31
20	A	849	BCR	C15-C14-C13	-4.50	120.89	127.31
25	4	316	CHL	C3D-C2D-C1D	-4.50	99.69	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	847	BCR	C15-C14-C13	-4.50	120.89	127.31
17	1	505	CLA	C4A-NA-C1A	4.49	108.72	106.71
25	1	517	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
17	B	805	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
25	6	513	CHL	C3D-C2D-C1D	-4.48	99.71	105.83
19	A	844	LHG	O7-C7-C8	4.48	121.16	111.50
25	6	515	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
26	6	502	XAT	C31-C30-C29	-4.48	120.92	127.31
20	L	305	BCR	C33-C5-C6	-4.48	119.50	124.53
20	B	845	BCR	C11-C10-C9	-4.47	120.93	127.31
25	3	313	CHL	C3C-C4C-NC	4.47	115.59	110.57
20	L	301	BCR	C33-C5-C6	-4.47	119.51	124.53
25	6	515	CHL	C3C-C4C-NC	4.44	115.55	110.57
25	4	313	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
20	B	845	BCR	C15-C14-C13	-4.42	121.01	127.31
25	1	517	CHL	C1B-CHB-C4A	-4.41	121.38	130.12
20	A	848	BCR	C24-C23-C22	-4.41	119.58	126.23
17	1	505	CLA	CMB-C2B-C1B	-4.40	121.69	128.46
17	3	314	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
17	3	308	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
20	L	305	BCR	C15-C14-C13	-4.40	121.04	127.31
20	A	847	BCR	C16-C17-C18	-4.39	121.05	127.31
20	L	305	BCR	C11-C10-C9	-4.37	121.07	127.31
26	4	303	XAT	O24-C25-C38	4.36	120.28	115.06
20	J	103	BCR	C20-C21-C22	-4.36	121.09	127.31
20	J	103	BCR	C24-C23-C22	-4.34	119.67	126.23
20	A	851	BCR	C3-C4-C5	-4.34	106.33	114.08
17	A	823	CLA	CAB-C3B-C4B	-4.33	121.81	128.46
16	A	801	CL0	CHD-C1D-ND	-4.33	120.48	124.45
24	1	501	LUT	C35-C34-C33	-4.30	121.18	127.31
25	6	513	CHL	C3C-C4C-NC	4.30	115.39	110.57
20	A	848	BCR	C20-C21-C22	-4.30	121.18	127.31
20	B	846	BCR	C33-C5-C6	-4.29	119.71	124.53
20	B	849	BCR	C11-C10-C9	-4.27	121.22	127.31
17	A	853	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
20	I	102	BCR	C16-C17-C18	-4.27	121.22	127.31
25	1	512	CHL	C3D-C2D-C1D	-4.26	100.02	105.83
20	6	503	BCR	C36-C18-C19	4.26	124.78	118.08
20	F	803	BCR	C16-C17-C18	-4.26	121.24	127.31
17	4	304	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
25	3	313	CHL	C1B-CHB-C4A	-4.25	121.70	130.12
17	A	825	CLA	CMB-C2B-C1B	-4.23	121.96	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	514	CHL	C3D-C2D-C1D	-4.23	100.06	105.83
20	4	301	BCR	C11-C10-C9	-4.23	121.27	127.31
19	B	852	LHG	O7-C7-C8	4.23	120.62	111.50
20	B	850	BCR	C24-C23-C22	-4.23	119.85	126.23
17	3	309	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
25	6	512	CHL	C3D-C2D-C1D	-4.22	100.08	105.83
26	6	502	XAT	C35-C34-C33	-4.21	121.30	127.31
17	4	307	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
20	J	103	BCR	C11-C10-C9	-4.21	121.30	127.31
17	A	820	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
22	B	851	DGD	O2G-C1B-C2B	4.20	120.55	111.50
17	B	826	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	4	303	XAT	C35-C34-C33	-4.19	121.34	127.31
24	6	501	LUT	C11-C10-C9	-4.18	121.34	127.31
17	A	843	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
20	I	102	BCR	C20-C21-C22	-4.17	121.35	127.31
19	A	845	LHG	O7-C7-C8	4.17	120.49	111.50
20	A	848	BCR	C15-C14-C13	-4.17	121.36	127.31
25	1	517	CHL	C3C-C4C-NC	4.16	115.24	110.57
17	A	823	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
20	B	845	BCR	C33-C5-C6	-4.15	119.87	124.53
19	1	516	LHG	O7-C7-C8	4.14	120.42	111.50
17	B	830	CLA	CAB-C3B-C4B	-4.13	122.12	128.46
17	B	816	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
17	A	837	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
17	A	812	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
20	A	850	BCR	C24-C23-C22	-4.11	120.02	126.23
17	A	831	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
17	B	807	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
17	A	829	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
17	B	831	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
17	A	838	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
25	6	513	CHL	C1B-CHB-C4A	-4.09	122.02	130.12
26	4	303	XAT	C15-C14-C13	-4.09	121.48	127.31
25	4	313	CHL	C3C-C4C-NC	4.09	115.15	110.57
17	3	312	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
17	B	808	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
17	L	304	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
20	B	849	BCR	C38-C26-C25	-4.06	119.97	124.53
25	4	314	CHL	C3B-C4B-NB	4.05	114.45	109.21
17	3	315	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	6	502	XAT	O4-C5-C18	4.05	119.91	115.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	303	XAT	C6-C7-C8	-4.04	117.44	125.99
17	A	821	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
17	B	821	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
17	B	827	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
20	A	848	BCR	C28-C27-C26	-4.03	106.88	114.08
20	6	503	BCR	C3-C4-C5	-4.03	106.88	114.08
17	A	836	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
20	K	204	BCR	C16-C15-C14	-4.02	115.25	123.47
26	6	502	XAT	C6-C7-C8	-4.02	117.50	125.99
25	6	512	CHL	C1B-CHB-C4A	-4.01	122.17	130.12
17	1	513	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
23	J	105	LMG	O7-C10-C11	3.99	120.11	111.50
17	B	834	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
25	4	314	CHL	O2D-CGD-CBD	3.98	118.35	111.27
17	K	203	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
17	A	813	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	4	313	CHL	C1B-CHB-C4A	-3.96	122.27	130.12
20	A	847	BCR	C11-C10-C9	-3.96	121.66	127.31
17	B	801	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
17	6	508	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
17	A	839	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
17	L	302	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
25	4	314	CHL	CHD-C4C-C3C	-3.95	119.03	124.84
25	4	314	CHL	C2D-C1D-ND	3.94	113.01	110.10
17	6	509	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	4	316	CHL	CAC-C3C-C4C	3.94	129.92	124.81
17	B	818	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
25	4	314	CHL	C1D-ND-C4D	-3.93	103.54	106.33
25	1	514	CHL	C3C-C4C-NC	3.93	114.98	110.57
20	I	102	BCR	C3-C4-C5	-3.92	107.08	114.08
17	A	804	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	4	314	CHL	CAC-C3C-C4C	3.92	129.89	124.81
20	A	851	BCR	C16-C17-C18	-3.91	121.73	127.31
17	A	802	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
20	A	851	BCR	C28-C27-C26	-3.90	107.11	114.08
17	4	309	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
20	B	850	BCR	C8-C7-C6	-3.89	121.03	126.28
17	A	826	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
20	B	845	BCR	C7-C8-C9	-3.85	120.41	126.23
25	1	512	CHL	C3C-C4C-NC	3.85	114.89	110.57
17	B	832	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
17	4	306	CLA	CMB-C2B-C1B	-3.84	122.56	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	801	BCR	C33-C5-C6	-3.84	120.21	124.53
17	B	803	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
17	A	817	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	6	516	LHG	O7-C7-C8	3.83	119.76	111.50
17	B	814	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	6	515	CHL	C1B-CHB-C4A	-3.83	122.54	130.12
17	1	505	CLA	CMB-C2B-C3B	3.82	131.83	124.68
25	3	313	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
17	6	507	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
25	1	514	CHL	CAC-C3C-C4C	3.81	129.76	124.81
20	A	850	BCR	C15-C14-C13	-3.81	121.87	127.31
17	A	809	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
20	6	503	BCR	C29-C30-C25	3.80	116.33	110.48
17	A	806	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
17	6	514	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
20	I	101	BCR	C24-C23-C22	-3.79	120.50	126.23
25	4	316	CHL	C1B-CHB-C4A	-3.79	122.61	130.12
25	6	517	CHL	CHD-C4C-C3C	-3.78	119.29	124.84
20	A	849	BCR	C33-C5-C6	-3.77	120.29	124.53
20	A	848	BCR	C7-C8-C9	-3.77	120.54	126.23
25	6	513	CHL	CAC-C3C-C4C	3.77	129.70	124.81
17	A	824	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
20	6	503	BCR	C19-C18-C17	-3.77	113.16	118.94
17	B	835	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
20	K	204	BCR	C11-C10-C9	-3.76	121.94	127.31
17	6	506	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
17	A	837	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
20	A	849	BCR	C28-C27-C26	-3.75	107.38	114.08
20	I	102	BCR	C38-C26-C25	-3.75	120.32	124.53
20	B	849	BCR	C20-C21-C22	-3.74	121.97	127.31
17	3	308	CLA	CMB-C2B-C3B	3.74	131.67	124.68
25	6	512	CHL	C3C-C4C-NC	3.74	114.76	110.57
17	3	305	CLA	C1B-CHB-C4A	-3.73	122.73	130.12
25	6	517	CHL	C1B-CHB-C4A	-3.73	122.73	130.12
17	A	818	CLA	CHD-C1D-ND	-3.73	121.03	124.45
17	1	508	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
20	K	204	BCR	C33-C5-C6	-3.73	120.34	124.53
20	B	850	BCR	C33-C5-C6	-3.73	120.34	124.53
26	6	502	XAT	C26-C27-C28	-3.72	118.13	125.99
17	B	805	CLA	CMB-C2B-C3B	3.72	131.63	124.68
17	3	307	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
20	I	101	BCR	C3-C4-C5	-3.72	107.44	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	201	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	6	515	CHL	CAC-C3C-C4C	3.71	129.62	124.81
17	B	812	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
17	B	806	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
24	3	302	LUT	C10-C11-C12	-3.69	111.69	123.22
20	B	846	BCR	C24-C23-C22	-3.69	120.66	126.23
17	1	515	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
17	B	829	CLA	CMB-C2B-C3B	3.68	131.57	124.68
17	3	305	CLA	C2A-C1A-CHA	3.68	130.30	123.86
17	A	840	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
17	A	843	CLA	CAB-C3B-C2B	3.68	131.90	124.69
17	B	843	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
20	F	803	BCR	C33-C5-C6	-3.68	120.40	124.53
20	B	848	BCR	C33-C5-C6	-3.67	120.40	124.53
17	B	825	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	6	512	CHL	CAC-C3C-C4C	3.67	129.57	124.81
17	L	302	CLA	CAB-C3B-C2B	3.67	131.87	124.69
17	6	510	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
25	1	512	CHL	C4A-NA-C1A	3.67	108.35	106.71
20	A	851	BCR	C33-C5-C6	-3.66	120.42	124.53
17	A	825	CLA	CMB-C2B-C3B	3.64	131.49	124.68
16	A	801	CL0	C1-C2-C3	-3.64	119.75	126.04
20	A	851	BCR	C20-C21-C22	-3.63	122.13	127.31
17	4	304	CLA	CAB-C3B-C2B	3.62	131.78	124.69
17	A	830	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
17	A	834	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
24	6	501	LUT	C35-C34-C33	-3.62	122.15	127.31
25	6	517	CHL	C2D-C1D-ND	3.61	112.76	110.10
17	B	841	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
20	F	801	BCR	C3-C4-C5	-3.60	107.64	114.08
17	B	840	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
17	3	309	CLA	CMB-C2B-C3B	3.59	131.40	124.68
20	L	305	BCR	C7-C8-C9	-3.59	120.81	126.23
20	3	303	BCR	C33-C5-C6	-3.59	120.49	124.53
20	B	849	BCR	C7-C8-C9	-3.59	120.81	126.23
17	A	853	CLA	CMB-C2B-C3B	3.59	131.40	124.68
17	J	101	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
20	3	303	BCR	C11-C10-C9	-3.59	122.19	127.31
17	B	820	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
20	K	204	BCR	C3-C4-C5	-3.58	107.68	114.08
17	4	307	CLA	CMB-C2B-C3B	3.58	131.38	124.68
17	3	314	CLA	CMB-C2B-C3B	3.58	131.37	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	847	BCR	C34-C9-C10	-3.58	117.91	122.92
17	3	312	CLA	CMB-C2B-C3B	3.58	131.37	124.68
17	4	309	CLA	C1B-CHB-C4A	-3.58	123.04	130.12
20	6	503	BCR	C39-C30-C29	3.58	123.21	108.91
17	1	507	CLA	CAB-C3B-C4B	-3.57	122.97	128.46
20	3	303	BCR	C16-C17-C18	-3.57	122.21	127.31
17	B	838	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
16	A	801	CL0	CAB-C3B-C4B	-3.56	122.99	128.46
25	4	314	CHL	C3D-C4D-ND	3.56	116.00	110.24
17	B	813	CLA	CAB-C3B-C4B	-3.56	122.99	128.46
17	A	803	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
17	A	831	CLA	CMB-C2B-C3B	3.55	131.33	124.68
20	A	854	BCR	C29-C30-C25	3.55	115.95	110.48
20	6	503	BCR	C23-C22-C21	3.55	124.39	118.94
17	4	317	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
20	A	847	BCR	C33-C5-C6	-3.54	120.55	124.53
17	A	828	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
22	B	851	DGD	C2G-O2G-C1B	-3.54	109.08	117.79
17	B	807	CLA	CMB-C2B-C3B	3.54	131.29	124.68
17	B	816	CLA	CMB-C2B-C3B	3.54	131.29	124.68
17	A	807	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
17	B	828	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
17	4	315	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
20	A	850	BCR	C34-C9-C10	-3.51	118.00	122.92
17	A	802	CLA	CMB-C2B-C3B	3.51	131.25	124.68
17	B	826	CLA	CMB-C2B-C3B	3.51	131.24	124.68
17	1	504	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
17	4	308	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
24	4	302	LUT	C18-C5-C6	-3.51	120.59	124.53
17	B	833	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	4	316	CHL	CHD-C4C-C3C	-3.50	119.70	124.84
17	A	812	CLA	CBD-CHA-C1A	3.49	131.76	128.06
17	A	816	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
17	B	839	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
17	A	838	CLA	CMB-C2B-C3B	3.49	131.21	124.68
17	4	312	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
20	4	301	BCR	C28-C27-C26	-3.49	107.85	114.08
17	A	815	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
17	4	309	CLA	CMB-C2B-C3B	3.48	131.19	124.68
20	B	848	BCR	C20-C21-C22	-3.48	122.34	127.31
17	L	303	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
17	B	815	CLA	CMB-C2B-C1B	-3.47	123.12	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	846	BCR	C24-C23-C22	-3.47	120.99	126.23
20	B	848	BCR	C38-C26-C25	-3.47	120.63	124.53
17	A	837	CLA	CMB-C2B-C3B	3.47	131.17	124.68
17	4	305	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	4	308	CLA	CAA-C2A-C3A	-3.47	108.01	116.10
17	B	801	CLA	CAB-C3B-C2B	3.47	131.47	124.69
20	A	849	BCR	C38-C26-C25	-3.46	120.64	124.53
17	4	304	CLA	CMB-C2B-C3B	3.46	131.47	124.69
17	A	812	CLA	CMB-C2B-C3B	3.46	131.15	124.68
17	1	506	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
17	B	834	CLA	CMB-C2B-C3B	3.46	131.14	124.68
17	A	836	CLA	CMB-C2B-C3B	3.45	131.14	124.68
17	B	808	CLA	CMB-C2B-C3B	3.45	131.13	124.68
17	B	805	CLA	CBD-CHA-C1A	3.45	132.29	128.62
25	6	517	CHL	CAC-C3C-C4C	3.45	129.29	124.81
20	B	846	BCR	C34-C9-C10	-3.45	118.09	122.92
17	A	820	CLA	CMB-C2B-C3B	3.45	131.13	124.68
20	B	849	BCR	C33-C5-C6	-3.45	120.66	124.53
17	L	304	CLA	CMB-C2B-C3B	3.45	131.13	124.68
24	6	501	LUT	C15-C35-C34	-3.44	116.42	123.47
17	B	803	CLA	CMB-C2B-C3B	3.44	131.12	124.68
17	B	817	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
17	J	102	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
17	3	306	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
20	I	101	BCR	C30-C25-C26	-3.44	117.77	122.61
24	1	502	LUT	C7-C8-C9	-3.44	121.04	126.23
17	B	830	CLA	CBD-CHA-C1A	3.43	132.55	128.50
20	B	847	BCR	C37-C22-C21	-3.43	118.11	122.92
17	6	511	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
17	3	315	CLA	CMB-C2B-C3B	3.42	131.08	124.68
17	A	832	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
20	6	503	BCR	C37-C22-C21	-3.42	118.13	122.92
20	J	103	BCR	C16-C17-C18	-3.42	122.43	127.31
17	1	505	CLA	C1B-CHB-C4A	-3.42	123.34	130.12
17	B	842	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	A	809	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	1	510	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	A	805	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
20	6	503	BCR	C16-C15-C14	3.41	130.47	123.47
17	1	507	CLA	CAA-C2A-C3A	-3.41	108.14	116.10
17	A	843	CLA	CMB-C2B-C3B	3.41	131.36	124.69
25	1	512	CHL	CAC-C3C-C4C	3.40	129.23	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	801	BCR	C27-C26-C25	-3.40	117.79	122.73
17	1	513	CLA	CMB-C2B-C3B	3.40	131.04	124.68
24	3	301	LUT	C18-C5-C6	-3.40	120.71	124.53
17	A	819	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
20	K	204	BCR	C7-C8-C9	-3.39	121.11	126.23
20	J	103	BCR	C15-C14-C13	-3.39	122.47	127.31
17	A	813	CLA	CMB-C2B-C3B	3.39	131.03	124.68
25	6	515	CHL	C3B-C4B-NB	3.39	113.59	109.21
17	K	203	CLA	CMB-C2B-C3B	3.39	131.02	124.68
17	6	504	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
25	6	517	CHL	C3B-C4B-NB	3.39	113.59	109.21
17	B	823	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
17	A	827	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
20	F	801	BCR	C16-C15-C14	-3.38	116.55	123.47
17	B	827	CLA	CMB-C2B-C3B	3.38	131.00	124.68
17	A	808	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
17	A	821	CLA	CMB-C2B-C3B	3.38	130.99	124.68
17	1	509	CLA	O2D-CGD-CBD	3.37	117.26	111.27
17	1	515	CLA	CBD-CHA-C1A	3.37	132.47	128.50
20	I	102	BCR	C33-C5-C6	-3.36	120.75	124.53
20	B	850	BCR	C3-C4-C5	-3.36	108.07	114.08
17	A	823	CLA	CMB-C2B-C3B	3.36	131.27	124.69
17	B	821	CLA	CMB-C2B-C3B	3.36	130.97	124.68
17	6	508	CLA	CAA-C2A-C3A	-3.36	108.26	116.10
20	B	848	BCR	C23-C24-C25	-3.36	117.77	127.20
25	4	316	CHL	C3B-C4B-NB	3.35	113.55	109.21
20	F	803	BCR	C38-C26-C25	-3.35	120.76	124.53
17	6	508	CLA	CMB-C2B-C3B	3.35	130.95	124.68
17	B	810	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
20	A	851	BCR	C38-C26-C25	-3.35	120.77	124.53
17	A	823	CLA	CAB-C3B-C2B	3.35	131.24	124.69
20	B	850	BCR	C10-C11-C12	-3.35	116.32	124.67
25	1	517	CHL	CAC-C3C-C4C	3.35	129.15	124.81
17	A	819	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
17	A	835	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
17	B	840	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
20	L	301	BCR	C38-C26-C25	-3.34	120.78	124.53
17	1	511	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
20	B	848	BCR	C8-C7-C6	-3.33	117.84	127.20
17	A	822	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	B	819	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	A	802	CLA	CBD-CHA-C1A	3.33	132.43	128.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	848	BCR	C28-C27-C26	-3.33	108.13	114.08
17	B	818	CLA	CMB-C2B-C3B	3.32	130.89	124.68
17	4	310	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
17	A	804	CLA	CMB-C2B-C3B	3.31	130.88	124.68
17	A	818	CLA	O2D-CGD-CBD	3.31	117.16	111.27
17	K	202	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
17	1	511	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
24	3	302	LUT	C15-C14-C13	-3.30	122.60	127.31
22	J	104	DGD	O2G-C1B-C2B	3.30	118.62	111.50
17	A	826	CLA	CAB-C3B-C2B	3.30	131.15	124.69
20	B	846	BCR	C16-C17-C18	-3.29	122.61	127.31
25	6	512	CHL	C3D-C4D-ND	3.29	115.56	110.24
20	B	846	BCR	C15-C14-C13	-3.29	122.62	127.31
20	B	848	BCR	C16-C17-C18	-3.29	122.62	127.31
20	A	847	BCR	C38-C26-C25	-3.29	120.84	124.53
17	6	505	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
20	3	303	BCR	C21-C20-C19	-3.28	112.97	123.22
20	J	103	BCR	C7-C8-C9	-3.28	121.28	126.23
17	4	311	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
20	L	305	BCR	C28-C27-C26	-3.28	108.23	114.08
20	K	204	BCR	C38-C26-C25	-3.27	120.85	124.53
17	A	811	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
20	B	847	BCR	C33-C5-C6	-3.27	120.86	124.53
17	A	839	CLA	CMB-C2B-C3B	3.27	130.79	124.68
20	B	849	BCR	C3-C4-C5	-3.26	108.25	114.08
24	6	501	LUT	C21-C26-C27	-3.26	108.58	112.70
17	A	810	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	6	513	CHL	CHD-C4C-C3C	-3.26	120.05	124.84
25	4	316	CHL	C2D-C1D-ND	3.26	112.51	110.10
19	A	844	LHG	C5-O7-C7	-3.26	109.77	117.79
17	B	822	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
17	L	302	CLA	CMB-C2B-C3B	3.26	131.07	124.69
20	I	101	BCR	C16-C17-C18	-3.26	122.66	127.31
25	6	515	CHL	CHD-C4C-C3C	-3.26	120.05	124.84
25	4	313	CHL	C4A-NA-C1A	3.26	108.17	106.71
20	B	850	BCR	C15-C14-C13	-3.26	122.66	127.31
17	A	809	CLA	O2D-CGD-CBD	3.26	117.05	111.27
25	3	313	CHL	C2D-C1D-ND	3.26	112.50	110.10
17	3	311	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
26	4	303	XAT	C18-C5-C4	3.25	117.94	114.28
17	A	838	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
20	F	801	BCR	C29-C30-C25	3.25	115.49	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	205	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
20	B	845	BCR	C28-C27-C26	-3.25	108.27	114.08
20	J	103	BCR	C33-C5-C6	-3.24	120.89	124.53
17	A	829	CLA	CMB-C2B-C3B	3.24	130.73	124.68
17	B	824	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
20	A	848	BCR	C33-C5-C6	-3.23	120.90	124.53
20	F	803	BCR	C23-C24-C25	-3.22	118.15	127.20
20	I	101	BCR	C20-C21-C22	-3.22	122.71	127.31
17	B	835	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	6	513	CHL	C3D-C4D-ND	3.22	115.45	110.24
17	6	514	CLA	CMB-C2B-C3B	3.22	130.70	124.68
17	B	836	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
17	3	316	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
25	3	313	CHL	C3B-C4B-NB	3.22	113.37	109.21
26	6	502	XAT	C24-C23-C22	-3.22	104.56	110.77
20	A	846	BCR	C20-C19-C18	-3.22	117.38	126.42
20	B	848	BCR	C3-C4-C5	-3.22	108.33	114.08
20	J	103	BCR	C38-C26-C25	-3.21	120.92	124.53
17	B	830	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
17	B	814	CLA	CMB-C2B-C3B	3.21	130.69	124.68
20	B	847	BCR	C38-C26-C25	-3.21	120.92	124.53
20	J	103	BCR	C38-C26-C27	3.21	119.78	113.62
17	A	826	CLA	CMB-C2B-C3B	3.21	130.97	124.69
17	F	802	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
17	6	507	CLA	CMB-C2B-C3B	3.20	130.67	124.68
17	B	828	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
17	4	311	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	3	301	LUT	C35-C15-C14	-3.20	116.92	123.47
20	J	103	BCR	C3-C4-C5	-3.20	108.36	114.08
20	A	847	BCR	C7-C8-C9	-3.20	121.41	126.23
20	A	850	BCR	C20-C19-C18	-3.19	117.44	126.42
20	K	204	BCR	C24-C23-C22	-3.19	121.42	126.23
17	B	807	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
17	3	307	CLA	CMB-C2B-C3B	3.18	130.64	124.68
17	4	306	CLA	CMB-C2B-C3B	3.18	130.63	124.68
17	A	841	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
17	B	837	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
20	3	303	BCR	C15-C16-C17	-3.18	116.96	123.47
20	A	854	BCR	C11-C12-C13	-3.18	117.48	126.42
24	1	501	LUT	C18-C5-C6	-3.18	120.96	124.53
17	B	810	CLA	C1-C2-C3	-3.18	120.55	126.04
17	A	805	CLA	O2D-CGD-O1D	-3.18	117.63	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	301	BCR	C28-C27-C26	-3.17	108.41	114.08
17	A	822	CLA	CAA-C2A-C3A	-3.17	108.69	116.10
25	6	517	CHL	C3D-C4D-ND	3.17	115.37	110.24
20	4	301	BCR	C16-C17-C18	-3.17	122.78	127.31
17	B	826	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
17	A	809	CLA	C1-C2-C3	-3.17	121.62	126.75
17	A	806	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
24	3	302	LUT	C18-C5-C6	-3.16	120.98	124.53
17	6	509	CLA	CMB-C2B-C3B	3.16	130.59	124.68
20	A	850	BCR	C8-C9-C10	3.16	123.79	118.94
20	F	803	BCR	C28-C27-C26	-3.16	108.44	114.08
20	B	847	BCR	C8-C9-C10	3.16	123.78	118.94
20	B	848	BCR	C11-C10-C9	-3.15	122.81	127.31
17	4	310	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
17	A	814	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
17	A	803	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	4	313	CHL	C3D-C4D-ND	3.15	115.33	110.24
24	1	501	LUT	C22-C23-C24	-3.14	108.16	111.74
17	A	840	CLA	CMB-C2B-C3B	3.14	130.55	124.68
20	L	305	BCR	C38-C26-C25	-3.14	121.00	124.53
20	B	847	BCR	C23-C22-C21	3.14	123.75	118.94
17	1	504	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
20	K	204	BCR	C28-C27-C26	-3.13	108.48	114.08
20	B	848	BCR	C15-C16-C17	-3.13	117.06	123.47
17	A	806	CLA	CMB-C2B-C3B	3.13	130.53	124.68
17	B	832	CLA	CMB-C2B-C3B	3.13	130.53	124.68
17	1	507	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
17	6	510	CLA	CMB-C2B-C3B	3.12	130.52	124.68
25	6	515	CHL	CBD-CHA-C1A	3.12	132.18	128.50
25	1	512	CHL	C3D-C4D-ND	3.12	115.28	110.24
17	A	827	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
20	A	854	BCR	C3-C4-C5	-3.12	108.51	114.08
17	B	811	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
17	K	201	CLA	CMB-C2B-C3B	3.11	130.50	124.68
17	B	812	CLA	CMB-C2B-C3B	3.11	130.50	124.68
17	K	202	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
17	B	840	CLA	CMB-C2B-C3B	3.11	130.50	124.68
17	B	843	CLA	CMB-C2B-C3B	3.11	130.49	124.68
17	B	801	CLA	CMB-C2B-C3B	3.11	130.77	124.69
23	J	105	LMG	O8-C28-C29	3.11	119.53	111.38
17	6	504	CLA	CMB-C2B-C3B	3.11	130.62	124.93
25	1	517	CHL	C3D-C4D-ND	3.11	115.26	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	303	BCR	C28-C27-C26	-3.10	108.53	114.08
17	B	842	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
17	B	827	CLA	C2A-C3A-C4A	-3.10	102.84	106.26
20	B	846	BCR	C8-C9-C10	3.10	123.70	118.94
20	B	846	BCR	C20-C21-C22	-3.10	122.89	127.31
17	A	824	CLA	CMB-C2B-C3B	3.10	130.47	124.68
25	6	515	CHL	C2D-C1D-ND	3.10	112.39	110.10
17	B	831	CLA	CMB-C2B-C3B	3.09	130.47	124.68
24	6	501	LUT	C7-C8-C9	-3.09	121.56	126.23
17	1	508	CLA	CMB-C2B-C3B	3.09	130.46	124.68
17	B	806	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	L	301	BCR	C34-C9-C10	-3.09	118.59	122.92
17	B	804	CLA	C4B-NB-C1B	3.09	109.15	106.32
25	4	313	CHL	CAC-C3C-C4C	3.09	128.82	124.81
17	A	808	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
18	B	844	PQN	C2M-C2-C3	-3.09	119.36	124.40
17	3	310	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
25	6	513	CHL	C2D-C1D-ND	3.08	112.37	110.10
17	4	307	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
17	6	506	CLA	CMB-C2B-C3B	3.07	130.43	124.68
17	A	853	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	1	517	CHL	O2D-CGD-O1D	-3.07	117.83	123.84
20	F	803	BCR	C38-C26-C27	3.07	119.51	113.62
17	A	834	CLA	CMB-C2B-C3B	3.07	130.42	124.68
17	B	803	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
20	I	101	BCR	C15-C16-C17	-3.07	117.19	123.47
17	A	827	CLA	CMB-C2B-C3B	3.07	130.42	124.68
17	A	804	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
17	B	809	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
20	B	849	BCR	C15-C16-C17	-3.06	117.20	123.47
20	B	846	BCR	C28-C27-C26	-3.06	108.61	114.08
17	3	306	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
17	L	302	CLA	CAA-C2A-C3A	-3.06	108.95	116.10
25	6	513	CHL	C3B-C4B-NB	3.06	113.17	109.21
24	1	502	LUT	C22-C23-C24	-3.06	108.26	111.74
17	F	802	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
17	B	834	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
20	A	848	BCR	C33-C5-C4	3.05	119.47	113.62
17	1	515	CLA	CMB-C2B-C3B	3.05	130.38	124.68
20	B	848	BCR	C33-C5-C4	3.05	119.47	113.62
17	1	509	CLA	CHD-C1D-ND	-3.04	121.66	124.45
17	B	841	CLA	CMB-C2B-C3B	3.04	130.36	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	803	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
17	B	812	CLA	CBD-CHA-C1A	3.04	132.08	128.50
17	B	830	CLA	CAB-C3B-C2B	3.04	130.63	124.69
17	A	834	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	1	505	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
20	A	847	BCR	C28-C27-C26	-3.03	108.67	114.08
20	I	101	BCR	C38-C26-C27	3.03	119.43	113.62
17	B	833	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
17	1	505	CLA	C2A-C1A-CHA	3.03	129.15	123.86
17	B	831	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
17	A	817	CLA	CMB-C2B-C3B	3.03	130.34	124.68
17	3	307	CLA	CBD-CHA-C1A	3.02	132.06	128.50
17	A	807	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	B	825	CLA	CMB-C2B-C3B	3.02	130.33	124.68
24	3	302	LUT	C35-C15-C14	-3.02	117.29	123.47
20	F	803	BCR	C20-C21-C22	-3.02	123.00	127.31
25	4	316	CHL	C3D-C4D-ND	3.02	115.12	110.24
17	1	506	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
20	B	847	BCR	C33-C5-C4	3.01	119.40	113.62
25	6	515	CHL	C3D-C4D-ND	3.01	115.11	110.24
20	B	850	BCR	C28-C27-C26	-3.01	108.71	114.08
17	B	812	CLA	C2A-C1A-CHA	3.01	127.37	122.71
17	4	317	CLA	CMB-C2B-C3B	3.00	130.30	124.68
20	4	301	BCR	C38-C26-C25	-3.00	121.16	124.53
17	B	815	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	1	517	CHL	CHD-C4C-C3C	-3.00	120.43	124.84
17	4	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	6	512	CHL	C4A-NA-C1A	3.00	108.05	106.71
17	A	818	CLA	C2A-C3A-C4A	-3.00	102.95	106.26
17	B	838	CLA	CMB-C2B-C3B	3.00	130.29	124.68
17	3	310	CLA	CAA-C2A-C3A	-2.99	109.11	116.10
20	A	850	BCR	C38-C26-C25	-2.99	121.17	124.53
17	L	303	CLA	CMB-C2B-C3B	2.99	130.28	124.68
24	6	501	LUT	C18-C5-C6	-2.99	121.17	124.53
17	4	317	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
17	A	811	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
17	B	820	CLA	CMB-C2B-C3B	2.99	130.26	124.68
24	3	302	LUT	C8-C7-C6	-2.98	118.82	127.20
25	6	512	CHL	CMD-C2D-C3D	-2.98	120.76	127.61
17	3	314	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
17	3	311	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	6	515	CHL	CMD-C2D-C3D	-2.97	120.78	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	847	BCR	C15-C14-C13	-2.97	123.07	127.31
17	B	827	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
20	A	847	BCR	C23-C24-C25	-2.97	118.87	127.20
19	A	845	LHG	C5-O7-C7	-2.97	110.49	117.79
17	A	817	CLA	CAA-C2A-C3A	-2.97	109.17	116.10
20	J	103	BCR	C33-C5-C4	2.97	119.31	113.62
20	B	846	BCR	C3-C4-C5	-2.96	108.79	114.08
20	B	847	BCR	C28-C27-C26	-2.96	108.80	114.08
25	6	517	CHL	C1D-ND-C4D	-2.95	104.24	106.33
24	3	302	LUT	C21-C26-C27	-2.95	108.97	112.70
17	B	839	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
17	1	504	CLA	CHB-C4A-NA	2.94	128.58	124.51
17	B	812	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	B	839	CLA	CAA-C2A-C3A	-2.94	109.24	116.10
17	B	841	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	A	830	CLA	CMB-C2B-C3B	2.94	130.18	124.68
17	4	308	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	6	502	XAT	C11-C10-C9	-2.94	123.12	127.31
17	4	312	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	1	514	CHL	C3D-C4D-ND	2.93	114.98	110.24
17	6	504	CLA	CAA-C2A-C3A	-2.93	109.26	116.10
20	A	849	BCR	C38-C26-C27	2.93	119.25	113.62
20	I	102	BCR	C38-C26-C27	2.93	119.25	113.62
25	4	313	CHL	CHD-C4C-C3C	-2.93	120.53	124.84
17	4	315	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	A	807	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	1	506	CLA	CMB-C2B-C3B	2.92	130.15	124.68
20	A	847	BCR	C33-C5-C4	2.92	119.23	113.62
17	4	312	CLA	CMB-C2B-C3B	2.92	130.15	124.68
17	A	835	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
17	4	304	CLA	CBD-CHA-C1A	2.92	131.94	128.50
17	B	809	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	A	850	BCR	C1-C6-C5	-2.92	118.51	122.61
20	B	850	BCR	C8-C9-C10	-2.92	118.32	124.81
17	B	813	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
17	A	830	CLA	C1-C2-C3	-2.91	122.04	126.75
17	3	310	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
17	A	828	CLA	CMB-C2B-C3B	2.91	130.13	124.68
17	A	835	CLA	CMB-C2B-C3B	2.91	130.13	124.68
17	B	817	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	A	851	BCR	C24-C23-C22	-2.91	121.83	126.23
20	A	848	BCR	C3-C4-C5	-2.91	108.88	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	832	CLA	CBD-CHA-C1A	2.91	131.93	128.50
25	1	517	CHL	C4A-NA-C1A	2.91	108.01	106.71
17	B	813	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
20	A	850	BCR	C33-C5-C4	2.90	119.19	113.62
17	3	314	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
17	A	839	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	A	822	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	A	823	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	3	302	LUT	C7-C8-C9	-2.90	121.86	126.23
17	J	102	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	L	301	BCR	C24-C23-C22	-2.90	121.86	126.23
17	B	823	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
17	B	832	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
20	L	301	BCR	C15-C16-C17	-2.89	117.55	123.47
20	B	848	BCR	C38-C26-C27	2.89	119.17	113.62
17	1	511	CLA	C3A-C4A-CHB	-2.89	120.37	123.91
17	A	805	CLA	CMB-C2B-C3B	2.89	130.08	124.68
25	4	314	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
25	6	512	CHL	CMB-C2B-C3B	2.88	130.06	124.68
17	6	507	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	3	309	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
17	6	511	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	B	839	CLA	CMB-C2B-C3B	2.88	130.06	124.68
20	I	101	BCR	C27-C26-C25	-2.88	118.56	122.73
17	B	823	CLA	CAA-C2A-C3A	-2.88	109.39	116.10
17	4	306	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	4	308	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	1	512	CHL	CMD-C2D-C3D	-2.87	121.00	127.61
17	L	304	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	B	849	BCR	C33-C5-C4	2.87	119.13	113.62
20	1	503	BCR	C40-C30-C25	-2.87	105.64	110.30
17	3	316	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	1	517	CHL	C3B-C4B-NB	2.87	112.92	109.21
17	1	504	CLA	CMB-C2B-C3B	2.87	130.04	124.68
20	3	303	BCR	C23-C24-C25	-2.87	119.15	127.20
17	B	835	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	1	512	CHL	CMB-C2B-C3B	2.86	130.04	124.68
17	B	833	CLA	CMB-C2B-C3B	2.86	130.03	124.68
17	J	101	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	1	511	CLA	CBD-CHA-C1A	2.86	131.87	128.50
17	4	311	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	1	514	CHL	CMD-C2D-C3D	-2.86	121.05	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	309	CLA	C1-C2-C3	-2.85	122.13	126.75
17	F	802	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
20	A	850	BCR	C28-C27-C26	-2.85	108.98	114.08
17	6	509	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	4	314	CHL	CHB-C4A-NA	2.85	128.46	124.51
24	4	302	LUT	C22-C23-C24	2.85	114.99	111.74
20	6	503	BCR	C27-C26-C25	-2.85	118.59	122.73
17	B	818	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	B	845	BCR	C38-C26-C27	2.85	119.08	113.62
17	6	508	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	B	817	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	B	826	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	3	309	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
20	K	204	BCR	C15-C14-C13	-2.84	123.26	127.31
17	A	833	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	3	307	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	6	504	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	B	824	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	L	302	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	A	815	CLA	CMB-C2B-C3B	2.84	129.98	124.68
17	A	816	CLA	CMB-C2B-C3B	2.84	129.98	124.68
17	A	832	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	1	508	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	3	305	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	B	837	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	3	312	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	1	507	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	4	311	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	A	840	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	1	517	CHL	C2D-C1D-ND	2.83	112.19	110.10
17	3	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	4	303	XAT	C31-C30-C29	-2.83	123.28	127.31
17	A	852	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
20	A	847	BCR	C38-C26-C27	2.83	119.04	113.62
20	6	503	BCR	C7-C8-C9	-2.82	121.97	126.23
17	B	828	CLA	CMB-C2B-C3B	2.82	129.96	124.68
20	A	846	BCR	C38-C26-C27	2.82	119.04	113.62
20	A	847	BCR	C8-C7-C6	-2.82	119.28	127.20
20	B	850	BCR	C16-C15-C14	-2.82	117.70	123.47
17	A	814	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	B	810	CLA	CMB-C2B-C3B	2.82	129.95	124.68
17	A	828	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	802	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	4	316	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
17	B	840	CLA	CAA-C2A-C3A	-2.81	109.54	116.10
17	B	836	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	A	802	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	1	510	CLA	CMB-C2B-C3B	2.81	129.94	124.68
24	4	302	LUT	C21-C26-C27	-2.81	109.15	112.70
24	3	302	LUT	C19-C9-C8	2.81	122.50	118.08
17	A	843	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	3	314	CLA	CHB-C4A-NA	2.80	128.39	124.51
20	B	846	BCR	C33-C5-C4	2.80	119.00	113.62
17	K	205	CLA	CMB-C2B-C3B	2.80	129.92	124.68
17	B	819	CLA	CMB-C2B-C3B	2.80	129.92	124.68
17	B	820	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	A	846	BCR	C8-C7-C6	-2.80	119.35	127.20
17	A	841	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	A	831	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	1	509	CLA	C2D-C1D-ND	2.80	112.16	110.10
24	3	301	LUT	C18-C5-C4	2.79	119.53	114.36
17	1	510	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	6	514	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	A	809	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	A	802	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
20	A	854	BCR	C36-C18-C17	-2.79	119.02	122.92
17	B	820	CLA	C1-C2-C3	-2.79	122.24	126.75
17	L	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
20	A	851	BCR	C33-C5-C4	2.78	118.96	113.62
17	B	843	CLA	CBD-CHA-C1A	2.78	131.88	127.43
17	1	511	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	6	517	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
17	L	302	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	4	313	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
17	A	819	CLA	CHB-C4A-NA	2.78	128.35	124.51
17	B	819	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
17	B	813	CLA	CAB-C3B-C2B	2.77	130.12	124.69
17	6	514	CLA	CBD-CHA-C1A	2.77	131.77	128.50
17	A	852	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
17	4	315	CLA	CAA-C2A-C3A	-2.77	109.64	116.10
17	B	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	B	823	CLA	CMB-C2B-C3B	2.77	129.85	124.68
17	J	102	CLA	CMB-C2B-C3B	2.77	129.85	124.68
17	B	801	CLA	O2D-CGD-O1D	-2.76	118.44	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	316	CLA	CMB-C2B-C3B	2.76	129.84	124.68
20	4	301	BCR	C24-C23-C22	-2.76	122.06	126.23
17	3	311	CLA	CMB-C2B-C3B	2.76	129.84	124.68
17	B	838	CLA	CBD-CHA-C1A	2.76	131.75	128.50
20	L	301	BCR	C20-C21-C22	-2.75	123.38	127.31
25	6	513	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
24	4	302	LUT	C31-C32-C33	-2.75	118.68	126.42
17	B	829	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
17	A	825	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
17	B	811	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
20	F	801	BCR	C38-C26-C27	2.74	118.89	113.62
20	A	847	BCR	C3-C4-C5	-2.74	109.18	114.08
17	A	835	CLA	CBD-CHA-C1A	2.74	131.82	127.43
17	A	843	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
17	4	305	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	A	810	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	3	305	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
17	6	506	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	4	303	XAT	C38-C25-C24	2.74	117.36	114.28
17	F	802	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
17	A	819	CLA	CMB-C2B-C3B	2.73	129.79	124.68
17	1	509	CLA	C1D-ND-C4D	-2.73	104.39	106.33
17	4	315	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	A	837	CLA	O2D-CGD-CBD	2.73	116.12	111.27
20	F	803	BCR	C24-C23-C22	-2.73	122.11	126.23
26	4	303	XAT	C10-C11-C12	-2.73	114.70	123.22
20	F	803	BCR	C3-C4-C5	-2.73	109.20	114.08
25	6	517	CHL	CMD-C2D-C3D	-2.73	121.34	127.61
17	A	820	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
17	B	815	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
17	A	807	CLA	CHB-C4A-NA	2.72	128.28	124.51
17	B	808	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
20	L	305	BCR	C20-C19-C18	-2.72	118.77	126.42
17	A	832	CLA	CMB-C2B-C3B	2.72	129.77	124.68
17	A	833	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
17	B	810	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	1	517	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
17	A	822	CLA	CMB-C2B-C3B	2.72	129.76	124.68
17	3	310	CLA	CMB-C2B-C3B	2.72	129.76	124.68
16	A	801	CL0	C2D-C1D-ND	2.72	112.11	110.10
20	A	854	BCR	C7-C8-C9	-2.72	122.13	126.23
17	B	830	CLA	O2D-CGD-O1D	-2.72	118.53	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	809	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	4	303	XAT	C4-C3-C2	-2.72	105.53	110.77
17	B	803	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
25	6	512	CHL	C3B-C4B-NB	2.72	112.72	109.21
20	F	801	BCR	C10-C11-C12	-2.72	114.74	123.22
17	B	842	CLA	CMB-C2B-C3B	2.71	129.75	124.68
17	A	803	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
17	1	506	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
20	J	103	BCR	C8-C7-C6	-2.71	119.58	127.20
17	A	833	CLA	CAA-C2A-C3A	-2.71	109.77	116.10
25	6	513	CHL	O2A-CGA-CBA	2.71	120.42	111.91
20	A	848	BCR	C38-C26-C27	2.71	118.82	113.62
26	4	303	XAT	C24-C23-C22	-2.71	105.54	110.77
20	A	848	BCR	C8-C7-C6	-2.71	119.59	127.20
20	6	503	BCR	C10-C11-C12	-2.71	114.77	123.22
17	3	306	CLA	CAA-C2A-C3A	-2.71	109.78	116.10
17	4	305	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
17	3	312	CLA	CHB-C4A-NA	2.71	128.25	124.51
25	4	314	CHL	C1-C2-C3	-2.70	122.38	126.75
17	1	511	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
25	4	313	CHL	C3B-C4B-NB	2.70	112.70	109.21
20	3	303	BCR	C36-C18-C19	2.70	122.33	118.08
17	3	304	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
17	A	806	CLA	CAA-C2A-C3A	-2.70	109.80	116.10
17	B	814	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
20	B	849	BCR	C8-C7-C6	-2.69	119.64	127.20
17	K	203	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
17	3	314	CLA	CBD-CHA-C1A	2.69	131.67	128.50
25	4	313	CHL	C2D-C1D-ND	2.69	112.09	110.10
17	1	515	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	B	819	CLA	CAA-C2A-C3A	-2.69	109.82	116.10
17	4	310	CLA	CMB-C2B-C3B	2.69	129.71	124.68
17	3	309	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	A	826	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
16	A	801	CL0	O2D-CGD-O1D	-2.69	117.98	124.09
17	6	505	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	3	303	BCR	C24-C23-C22	-2.69	122.17	126.23
17	B	825	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	A	830	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	6	503	BCR	C21-C20-C19	2.69	131.60	123.22
20	B	847	BCR	C3-C4-C5	-2.68	109.28	114.08
17	A	810	CLA	CMB-C2B-C3B	2.68	129.70	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	850	BCR	C38-C26-C27	2.68	118.77	113.62
17	B	812	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	6	511	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	B	834	CLA	CHB-C4A-NA	2.68	128.22	124.51
20	A	850	BCR	C3-C4-C5	-2.68	109.29	114.08
17	B	822	CLA	CMB-C2B-C3B	2.68	129.69	124.68
25	3	313	CHL	C4A-NA-C1A	2.68	107.91	106.71
25	6	513	CHL	C4A-NA-C1A	2.68	107.91	106.71
17	6	514	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	4	313	CHL	CMB-C2B-C3B	2.67	129.68	124.68
17	A	841	CLA	CAA-C2A-C3A	-2.67	109.86	116.10
19	1	516	LHG	C5-O7-C7	-2.67	111.21	117.79
20	A	847	BCR	C20-C21-C22	-2.67	123.50	127.31
20	6	503	BCR	C4-C5-C6	-2.67	118.85	122.73
17	3	305	CLA	CMB-C2B-C3B	2.67	129.67	124.68
17	3	315	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	1	502	LUT	C38-C25-C24	-2.67	117.85	123.56
20	F	801	BCR	C33-C5-C4	2.67	118.74	113.62
17	B	821	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	A	853	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	B	839	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	B	836	CLA	CMB-C2B-C3B	2.67	129.67	124.68
20	A	850	BCR	C4-C5-C6	-2.67	118.86	122.73
20	L	301	BCR	C8-C9-C10	2.67	123.03	118.94
17	1	513	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
20	B	845	BCR	C33-C5-C4	2.66	118.73	113.62
20	A	854	BCR	C27-C26-C25	-2.66	118.87	122.73
24	4	302	LUT	C7-C8-C9	-2.66	122.22	126.23
24	6	501	LUT	C18-C5-C4	2.66	119.28	114.36
17	A	811	CLA	CMB-C2B-C3B	2.66	129.65	124.68
25	6	515	CHL	CMB-C2B-C3B	2.65	129.64	124.68
17	A	815	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	3	301	LUT	C15-C14-C13	-2.65	123.53	127.31
25	6	512	CHL	CHD-C1D-C2D	2.65	131.04	125.48
25	1	514	CHL	C3B-C4B-NB	2.65	112.64	109.21
17	3	311	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
20	I	102	BCR	C10-C11-C12	-2.65	114.96	123.22
20	I	102	BCR	C29-C30-C25	2.64	114.55	110.48
17	B	810	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
17	A	805	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	1	513	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	1	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	302	LUT	C8-C9-C10	-2.64	114.89	118.94
17	6	505	CLA	CMB-C2B-C3B	2.64	129.61	124.68
17	A	836	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
20	I	101	BCR	C28-C27-C26	-2.63	109.37	114.08
16	A	801	CL0	CMB-C2B-C3B	2.63	129.85	124.69
24	3	302	LUT	C18-C5-C4	2.63	119.23	114.36
24	3	302	LUT	C30-C31-C32	-2.63	115.00	123.22
17	A	816	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	B	838	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	B	806	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	3	306	CLA	O2D-CGD-CBD	2.63	115.93	111.27
17	6	504	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
20	I	101	BCR	C34-C9-C10	-2.62	119.25	122.92
25	4	314	CHL	C2A-C1A-CHA	-2.62	119.27	123.86
17	A	808	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	B	841	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
17	B	828	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	A	825	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
20	B	846	BCR	C38-C26-C25	-2.62	121.59	124.53
26	6	502	XAT	C15-C35-C34	-2.62	118.11	123.47
25	1	514	CHL	CMB-C2B-C3B	2.62	129.57	124.68
17	A	814	CLA	CMB-C2B-C3B	2.62	129.57	124.68
19	1	516	LHG	O8-C23-C24	2.62	120.11	111.91
17	A	816	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	B	824	CLA	CMB-C2B-C3B	2.61	129.57	124.68
17	B	837	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	A	840	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	B	809	CLA	CMB-C2B-C3B	2.61	129.56	124.68
17	1	507	CLA	CAB-C3B-C2B	2.61	129.80	124.69
25	3	313	CHL	C1D-ND-C4D	-2.61	104.48	106.33
16	A	801	CL0	CMD-C2D-C3D	-2.61	121.61	127.61
24	6	501	LUT	C8-C7-C6	-2.61	119.88	127.20
20	F	803	BCR	C11-C12-C13	-2.61	119.09	126.42
19	A	844	LHG	O8-C23-C24	2.61	120.09	111.91
17	1	504	CLA	O2D-CGD-CBD	2.61	115.90	111.27
17	A	803	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	4	314	CHL	O2A-CGA-CBA	2.61	120.08	111.91
17	A	840	CLA	CAA-C2A-C3A	-2.60	110.02	116.10
20	F	801	BCR	C8-C7-C6	-2.60	119.90	127.20
20	B	849	BCR	C16-C17-C18	-2.60	123.60	127.31
24	1	502	LUT	C31-C32-C33	-2.60	119.12	126.42
17	K	202	CLA	CMB-C2B-C3B	2.60	129.54	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	833	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
25	6	513	CHL	CMB-C2B-C3B	2.59	129.53	124.68
17	A	831	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
17	L	303	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	4	316	CHL	C1D-ND-C4D	-2.59	104.49	106.33
17	A	825	CLA	CHB-C4A-NA	2.59	128.10	124.51
17	6	508	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
20	6	503	BCR	C11-C10-C9	-2.59	123.61	127.31
17	3	314	CLA	CHD-C1D-ND	-2.59	122.07	124.45
17	A	827	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
19	B	852	LHG	C5-O7-C7	-2.59	111.42	117.79
17	A	829	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	6	507	CLA	C1-C2-C3	-2.59	121.57	126.04
17	B	834	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
25	1	514	CHL	CHD-C1D-C2D	2.59	130.90	125.48
17	A	815	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	B	804	CLA	CHD-C1D-ND	-2.58	122.08	124.45
17	A	853	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
20	B	846	BCR	C10-C11-C12	-2.58	115.16	123.22
17	A	830	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	B	813	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
20	4	301	BCR	C7-C8-C9	-2.58	122.34	126.23
17	A	841	CLA	CMB-C2B-C3B	2.58	129.50	124.68
17	6	510	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
16	A	801	CL0	C6-C5-C3	-2.57	106.70	113.45
17	A	834	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	F	803	BCR	C33-C5-C4	2.57	118.56	113.62
17	3	308	CLA	CHB-C4A-NA	2.57	128.07	124.51
17	A	802	CLA	C2A-C1A-CHA	2.57	126.70	122.71
17	3	310	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	1	501	LUT	C19-C9-C10	-2.57	119.32	122.92
17	B	809	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
20	4	301	BCR	C20-C21-C22	-2.57	123.64	127.31
17	B	835	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
17	A	821	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	4	315	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	6	502	XAT	C27-C28-C29	-2.56	121.55	125.53
17	B	830	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	4	305	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	A	810	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	B	845	BCR	C38-C26-C25	-2.56	121.66	124.53
20	L	301	BCR	C16-C17-C18	-2.56	123.66	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
17	4	309	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
20	I	102	BCR	C23-C24-C25	-2.56	120.02	127.20
25	4	316	CHL	C1C-C2C-C3C	-2.56	105.09	107.11
17	4	304	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	L	305	BCR	C33-C5-C4	2.55	118.52	113.62
25	1	512	CHL	CHD-C4C-C3C	-2.55	121.09	124.84
25	4	314	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
17	1	505	CLA	O2D-CGD-CBD	2.55	115.80	111.27
20	A	850	BCR	C10-C11-C12	-2.55	115.26	123.22
17	A	824	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
20	6	503	BCR	C2-C1-C6	2.55	114.40	110.48
17	B	804	CLA	C2D-C1D-ND	2.55	111.98	110.10
17	B	814	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	A	833	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	B	827	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
20	A	849	BCR	C11-C10-C9	-2.54	123.68	127.31
17	B	810	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	A	818	CLA	C2D-C1D-ND	2.54	111.98	110.10
17	3	306	CLA	CHB-C4A-NA	2.54	128.03	124.51
20	A	849	BCR	C3-C4-C5	-2.54	109.54	114.08
17	A	818	CLA	CMB-C2B-C3B	2.54	129.44	124.68
20	B	848	BCR	C24-C23-C22	-2.54	122.39	126.23
25	1	512	CHL	CHD-C1D-C2D	2.54	130.81	125.48
17	A	826	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	6	505	CLA	CHB-C4A-NA	2.54	128.03	124.51
17	B	819	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	A	847	BCR	C24-C23-C22	-2.54	122.40	126.23
20	6	503	BCR	C38-C26-C27	2.54	118.49	113.62
17	B	838	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	L	301	BCR	C11-C10-C9	-2.54	123.69	127.31
17	4	307	CLA	C1-C2-C3	-2.53	121.66	126.04
17	A	839	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	6	517	CHL	CMB-C2B-C3B	2.53	129.41	124.68
17	B	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	6	513	CHL	C1D-ND-C4D	-2.53	104.54	106.33
17	K	205	CLA	CBD-CHA-C1A	2.53	131.48	128.50
17	K	202	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	A	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	A	811	CLA	CAA-C2A-C3A	-2.53	110.20	116.10
17	4	304	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	A	836	CLA	CHB-C4A-NA	2.53	128.00	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	820	CLA	CHB-C4A-NA	2.53	128.00	124.51
26	6	502	XAT	C20-C13-C14	-2.52	119.39	122.92
20	A	854	BCR	C33-C5-C6	-2.52	121.69	124.53
17	B	808	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	B	840	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
17	B	806	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
17	B	840	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	A	808	CLA	CMB-C2B-C3B	2.52	129.40	124.68
20	A	849	BCR	C8-C7-C6	-2.52	120.13	127.20
17	B	830	CLA	CMB-C2B-C3B	2.52	129.62	124.69
17	A	813	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
20	3	303	BCR	C38-C26-C27	2.52	118.45	113.62
17	4	312	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	A	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
20	I	101	BCR	C33-C5-C6	-2.51	121.70	124.53
17	K	205	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
17	A	828	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	3	313	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
20	A	846	BCR	C7-C8-C9	-2.51	122.44	126.23
17	J	101	CLA	CMB-C2B-C3B	2.51	129.61	124.69
17	3	312	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
17	B	817	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	6	511	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	L	301	BCR	C33-C5-C4	2.51	118.43	113.62
17	B	828	CLA	CAA-C2A-C3A	-2.51	110.25	116.10
24	1	501	LUT	C20-C13-C14	-2.51	119.41	122.92
18	B	844	PQN	C2M-C2-C1	2.51	120.42	116.27
17	A	852	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B	822	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
20	A	851	BCR	C38-C26-C27	2.51	118.43	113.62
17	A	829	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
24	6	501	LUT	C30-C31-C32	-2.50	115.40	123.22
17	K	205	CLA	O2D-CGD-O1D	-2.50	118.40	124.09
20	F	803	BCR	C34-C9-C10	-2.50	119.42	122.92
17	B	815	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	B	841	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	A	826	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	I	102	BCR	C24-C23-C22	-2.50	122.46	126.23
20	A	849	BCR	C20-C19-C18	-2.50	119.39	126.42
17	B	837	CLA	CMB-C2B-C3B	2.50	129.35	124.68
20	B	847	BCR	C10-C11-C12	-2.50	115.42	123.22
17	B	805	CLA	C1B-CHB-C4A	-2.50	125.17	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	6	509	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
25	6	513	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
17	A	820	CLA	CAA-C2A-C3A	-2.49	110.28	116.10
17	6	511	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
17	B	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
17	B	835	CLA	CHB-C4A-NA	2.49	127.95	124.51
20	A	850	BCR	C16-C15-C14	-2.49	118.38	123.47
17	1	507	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	6	506	CLA	CHB-C4A-NA	2.48	127.95	124.51
25	1	512	CHL	O2D-CGD-O1D	-2.48	118.98	123.84
17	A	816	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
17	B	823	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	B	829	CLA	C1-C2-C3	-2.48	122.74	126.75
20	A	849	BCR	C7-C8-C9	-2.48	122.49	126.23
16	A	801	CL0	CAB-C3B-C2B	2.48	129.54	124.69
17	1	505	CLA	CHA-C1A-NA	-2.48	120.73	126.40
19	B	852	LHG	O8-C23-C24	2.48	119.68	111.91
17	B	835	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	B	842	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	B	843	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	6	502	XAT	C38-C25-C24	2.47	117.06	114.28
23	J	105	LMG	C8-O7-C10	-2.47	111.71	117.79
20	A	847	BCR	C16-C15-C14	-2.47	118.42	123.47
17	A	823	CLA	CHB-C4A-NA	2.47	127.92	124.51
17	B	821	CLA	CHB-C4A-NA	2.47	127.92	124.51
17	B	816	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	6	515	CHL	C1D-ND-C4D	-2.46	104.58	106.33
25	3	313	CHL	CMB-C2B-C3B	2.46	129.29	124.68
17	B	832	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	4	315	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
20	L	301	BCR	C38-C26-C27	2.46	118.34	113.62
17	J	102	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	4	307	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	1	509	CLA	O2A-CGA-CBA	2.46	119.63	111.91
17	B	819	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	L	304	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
20	A	854	BCR	C35-C13-C14	-2.45	119.49	122.92
22	B	851	DGD	O1G-C1A-C2A	2.45	119.61	111.91
22	J	104	DGD	O1G-C1A-C2A	2.45	119.61	111.91
17	4	317	CLA	C1-C2-C3	-2.45	122.78	126.75
19	6	516	LHG	O8-C23-C24	2.45	119.60	111.91
17	A	832	CLA	C1B-CHB-C4A	-2.45	125.26	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	854	BCR	C20-C21-C22	-2.45	123.81	127.31
17	6	509	CLA	CHB-C4A-NA	2.45	127.90	124.51
17	6	509	CLA	C1-C2-C3	-2.45	122.79	126.75
17	B	828	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
17	B	806	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
17	A	818	CLA	C1D-ND-C4D	-2.45	104.60	106.33
19	6	516	LHG	C5-O7-C7	-2.44	111.77	117.79
20	B	845	BCR	C30-C25-C26	-2.44	119.17	122.61
17	3	306	CLA	CMB-C2B-C3B	2.44	129.25	124.68
20	1	503	BCR	C40-C30-C29	2.44	118.68	108.91
20	A	848	BCR	C27-C26-C25	-2.44	119.19	122.73
20	A	848	BCR	C11-C12-C13	-2.44	119.56	126.42
17	A	820	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	1	507	CLA	CMB-C2B-C3B	2.44	129.47	124.69
20	B	850	BCR	C37-C22-C21	-2.44	119.50	122.92
17	B	822	CLA	CAA-C2A-C3A	-2.44	110.40	116.10
17	A	806	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	A	814	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	K	203	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	A	811	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	A	838	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	3	309	CLA	CHD-C1D-ND	-2.44	122.22	124.45
25	6	513	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
17	B	842	CLA	CAA-C2A-C3A	-2.43	110.42	116.10
17	6	510	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
17	1	506	CLA	C1-C2-C3	-2.43	121.84	126.04
20	B	849	BCR	C38-C26-C27	2.43	118.28	113.62
17	3	307	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
17	B	821	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
25	4	313	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
24	1	501	LUT	C37-C21-C26	-2.42	105.87	109.55
25	3	313	CHL	CAC-C3C-C4C	2.42	127.95	124.81
17	K	203	CLA	CAA-C2A-C3A	-2.42	110.44	116.10
17	A	817	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	4	312	CLA	CAA-C2A-C3A	-2.42	110.45	116.10
17	A	831	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	B	811	CLA	CMB-C2B-C3B	2.42	129.20	124.68
17	L	302	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	B	804	CLA	CHA-C4D-ND	2.42	137.55	132.50
17	K	201	CLA	CHB-C4A-NA	2.42	127.85	124.51
20	A	846	BCR	C15-C16-C17	-2.41	118.53	123.47
25	6	512	CHL	CHD-C4C-C3C	-2.41	121.29	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	515	CLA	C2A-C1A-CHA	2.41	126.45	122.71
17	A	821	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	A	804	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
17	3	316	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	B	822	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	B	833	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
20	6	503	BCR	C33-C5-C4	2.41	118.24	113.62
20	3	303	BCR	C10-C11-C12	-2.41	115.71	123.22
17	A	824	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	3	308	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
20	A	846	BCR	C23-C24-C25	-2.40	120.45	127.20
20	A	851	BCR	C2-C1-C6	2.40	114.18	110.48
20	B	845	BCR	C27-C26-C25	-2.40	119.24	122.73
17	4	317	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
17	B	831	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	A	801	CL0	CHA-C4D-ND	2.40	137.52	132.50
20	6	503	BCR	C35-C13-C12	2.40	121.86	118.08
17	A	839	CLA	C1-C2-C3	-2.40	121.89	126.04
20	B	845	BCR	C3-C4-C5	-2.40	109.79	114.08
25	4	313	CHL	CHD-C1D-C2D	2.40	130.51	125.48
20	B	847	BCR	C38-C26-C27	2.40	118.22	113.62
17	A	803	CLA	C1-C2-C3	-2.40	121.90	126.04
17	B	812	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
20	B	850	BCR	C33-C5-C4	2.39	118.22	113.62
17	A	837	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	A	846	BCR	C11-C10-C9	-2.39	123.89	127.31
17	6	506	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	B	823	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	B	813	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	4	310	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	1	512	CHL	C3B-C4B-NB	2.39	112.30	109.21
17	B	824	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	K	204	BCR	C36-C18-C17	-2.39	119.58	122.92
17	A	834	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
17	B	806	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	B	809	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	4	314	CHL	CMB-C2B-C3B	2.38	129.14	124.68
17	3	315	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	B	826	CLA	O2D-CGD-CBD	2.38	115.50	111.27
17	A	827	CLA	C2D-C1D-ND	-2.38	108.35	110.10
20	A	846	BCR	C37-C22-C21	-2.38	119.59	122.92
17	3	315	CLA	C1B-CHB-C4A	-2.38	125.40	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	805	CLA	C2A-C1A-CHA	2.38	126.40	122.71
20	I	102	BCR	C15-C16-C17	-2.38	118.60	123.47
17	B	831	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	F	801	BCR	C39-C30-C25	-2.38	106.44	110.30
20	J	103	BCR	C27-C26-C25	-2.38	119.28	122.73
17	B	801	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
17	B	818	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
20	6	503	BCR	C20-C19-C18	2.38	133.09	126.42
17	K	201	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
17	A	806	CLA	CMA-C3A-C2A	-2.37	110.56	116.10
17	4	307	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	A	819	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	1	515	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	B	850	BCR	C20-C19-C18	-2.37	119.76	126.42
17	B	801	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	B	833	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	B	811	CLA	CHB-C4A-NA	2.37	127.78	124.51
17	B	825	CLA	CHB-C4A-NA	2.37	127.78	124.51
20	A	848	BCR	C16-C15-C14	-2.36	118.63	123.47
17	4	310	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	A	850	BCR	C30-C25-C26	-2.36	119.29	122.61
17	A	806	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	4	312	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	B	838	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	B	826	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	1	501	LUT	C40-C33-C34	-2.36	119.62	122.92
17	4	306	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	3	313	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
20	A	850	BCR	C33-C5-C6	-2.35	121.89	124.53
17	6	514	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	B	845	BCR	C8-C7-C6	-2.35	120.60	127.20
17	A	813	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	A	815	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	F	801	BCR	C35-C13-C12	2.35	121.78	118.08
17	A	802	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	A	813	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	A	817	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	B	842	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	1	514	CHL	CHD-C4C-C3C	-2.34	121.40	124.84
26	6	502	XAT	C11-C12-C13	-2.34	119.84	126.42
25	4	314	CHL	C5-C3-C4	2.34	119.77	114.60
24	6	501	LUT	C22-C23-C24	2.34	114.40	111.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	848	BCR	C7-C8-C9	-2.34	122.70	126.23
17	4	308	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	A	839	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	4	306	CLA	C1-C2-C3	-2.34	122.00	126.04
17	3	304	CLA	O2D-CGD-CBD	2.34	115.42	111.27
17	A	837	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
17	B	837	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
17	A	820	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
17	4	305	CLA	C1-C2-C3	-2.33	122.97	126.75
17	4	315	CLA	CMA-C3A-C2A	-2.33	110.65	116.10
17	A	838	CLA	O2D-CGD-CBD	2.33	115.42	111.27
24	3	301	LUT	C31-C32-C33	-2.33	119.86	126.42
17	L	304	CLA	CHB-C4A-NA	2.33	127.74	124.51
17	1	508	CLA	CHB-C4A-NA	2.33	127.74	124.51
17	1	509	CLA	CHA-C4D-ND	2.33	137.38	132.50
20	I	101	BCR	C11-C12-C13	-2.33	119.87	126.42
17	A	828	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	K	204	BCR	C20-C21-C22	-2.33	123.98	127.31
17	4	317	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	F	803	BCR	C35-C13-C14	-2.33	119.66	122.92
17	4	308	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	J	101	CLA	CHB-C4A-NA	2.33	127.73	124.51
17	1	507	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	K	201	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
17	B	832	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	A	803	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
17	1	504	CLA	CBA-CAA-C2A	2.33	118.65	113.47
20	L	305	BCR	C36-C18-C17	-2.33	119.67	122.92
17	A	837	CLA	CHB-C4A-NA	2.32	127.73	124.51
17	A	807	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
26	6	502	XAT	C4-C3-C2	-2.32	106.29	110.77
17	A	809	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	A	846	BCR	C33-C5-C4	2.32	118.08	113.62
17	A	821	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	B	848	BCR	C21-C20-C19	-2.32	115.98	123.22
17	6	511	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
20	3	303	BCR	C38-C26-C25	-2.32	121.92	124.53
20	4	301	BCR	C8-C7-C6	-2.32	120.69	127.20
17	6	507	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	B	844	PQN	C11-C3-C4	2.32	120.98	118.50
17	B	807	CLA	CHB-C4A-NA	2.32	127.71	124.51
17	B	811	CLA	C1B-CHB-C4A	-2.31	125.53	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	829	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
17	A	812	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	6	508	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	B	843	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	4	304	CLA	C2A-C1A-CHA	2.31	126.30	122.71
20	A	854	BCR	C33-C5-C4	2.31	118.06	113.62
20	L	301	BCR	C23-C24-C25	-2.31	120.72	127.20
17	A	836	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
20	B	847	BCR	C36-C18-C17	-2.31	119.69	122.92
17	A	804	CLA	CHB-C4A-NA	2.31	127.70	124.51
17	A	805	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
20	A	854	BCR	C24-C23-C22	-2.30	122.75	126.23
25	6	512	CHL	O2D-CGD-O1D	-2.30	119.33	123.84
20	I	101	BCR	C38-C26-C25	-2.30	121.94	124.53
25	6	515	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
17	B	836	CLA	C3A-C4A-CHB	-2.30	120.09	124.24
17	4	311	CLA	O2D-CGD-CBD	2.30	115.36	111.27
17	3	316	CLA	CHB-C4A-NA	2.30	127.70	124.51
17	B	838	CLA	C2A-C1A-CHA	2.30	126.28	122.71
17	1	511	CLA	O2D-CGD-CBD	2.30	115.36	111.27
17	A	825	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	6	501	LUT	C31-C30-C29	-2.30	124.03	127.31
20	I	101	BCR	C21-C20-C19	-2.30	116.04	123.22
17	A	841	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	1	510	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	4	306	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	K	202	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	3	307	CLA	C2A-C1A-CHA	2.30	126.27	122.71
17	J	102	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	A	810	CLA	CHD-C1D-ND	-2.29	122.34	124.45
17	B	843	CLA	CAA-C2A-C3A	-2.29	110.75	116.10
17	1	504	CLA	CAA-C2A-C1A	2.29	117.22	112.14
17	B	803	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	4	301	BCR	C15-C16-C17	-2.29	118.78	123.47
17	B	831	CLA	C2D-C1D-ND	-2.29	108.42	110.10
17	B	836	CLA	CHD-C1D-ND	-2.29	122.35	124.45
17	3	304	CLA	CHC-C1C-C2C	-2.29	124.33	129.77
17	A	840	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
17	1	515	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
17	A	822	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
20	K	204	BCR	C38-C26-C27	2.28	118.00	113.62
17	B	836	CLA	CHB-C4A-NA	2.28	127.83	124.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	820	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
17	3	305	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	3	305	CLA	CHA-C1A-NA	-2.28	121.18	126.40
20	A	854	BCR	C19-C18-C17	2.28	122.44	118.94
25	6	512	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
17	3	307	CLA	CHB-C4A-NA	2.28	127.66	124.51
23	4	318	LMG	C7-O1-C1	-2.28	109.29	113.74
17	B	804	CLA	C1D-ND-C4D	-2.27	104.72	106.33
17	1	509	CLA	CMA-C3A-C4A	2.27	117.88	111.77
20	3	303	BCR	C37-C22-C23	2.27	121.66	118.08
20	F	801	BCR	C20-C19-C18	-2.27	120.04	126.42
20	L	305	BCR	C3-C4-C5	-2.27	110.03	114.08
17	B	830	CLA	C2A-C1A-CHA	2.27	126.23	122.71
17	B	808	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
20	B	845	BCR	C37-C22-C21	-2.27	119.75	122.92
20	A	846	BCR	C10-C11-C12	-2.27	116.14	123.22
17	A	829	CLA	CHB-C4A-NA	2.27	127.64	124.51
17	B	825	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
17	B	829	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
17	B	822	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
20	I	102	BCR	C33-C5-C4	2.26	117.97	113.62
17	A	808	CLA	CAA-C2A-C3A	-2.26	110.81	116.10
17	A	823	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
17	A	830	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	A	838	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	3	313	CHL	O1D-CGD-CBD	-2.26	120.30	124.51
20	I	102	BCR	C34-C9-C8	2.26	121.64	118.08
20	A	848	BCR	C38-C26-C25	-2.26	121.99	124.53
20	A	849	BCR	C10-C11-C12	-2.26	116.17	123.22
17	6	514	CLA	C2A-C1A-CHA	2.26	126.21	122.71
25	1	514	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
20	K	204	BCR	C33-C5-C4	2.25	117.95	113.62
17	B	841	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
17	J	101	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
17	F	802	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	1	512	CHL	C2D-C1D-ND	2.25	111.77	110.10
17	A	833	CLA	CMB-C2B-C3B	2.25	128.90	124.68
24	1	501	LUT	C11-C12-C13	-2.25	120.08	126.42
17	K	203	CLA	C2D-C1D-ND	-2.25	108.44	110.10
17	A	810	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
17	4	311	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	A	839	CLA	O2A-CGA-O1A	-2.25	117.91	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	801	BCR	C7-C8-C9	-2.25	122.83	126.23
17	4	305	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
17	6	504	CLA	C4B-CHC-C1C	-2.25	126.17	129.64
17	6	507	CLA	CHB-C4A-NA	2.25	127.62	124.51
24	1	501	LUT	C31-C30-C29	-2.25	124.10	127.31
24	4	302	LUT	C16-C1-C6	-2.25	106.65	110.30
18	A	842	PQN	C11-C3-C4	2.25	120.00	116.27
20	A	854	BCR	C8-C7-C6	-2.25	120.89	127.20
17	A	838	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
20	A	851	BCR	C23-C24-C25	-2.25	120.89	127.20
17	A	812	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	B	813	CLA	CMB-C2B-C3B	2.24	129.08	124.69
17	3	311	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	A	824	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
20	J	103	BCR	C23-C24-C25	-2.24	120.91	127.20
17	B	817	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
17	6	505	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	4	302	LUT	C10-C11-C12	-2.24	116.24	123.22
17	A	832	CLA	CBA-CAA-C2A	-2.23	109.30	114.02
17	A	833	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	6	515	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
17	6	509	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
20	F	801	BCR	C15-C14-C13	-2.23	124.13	127.31
17	1	513	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
17	A	852	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
20	A	846	BCR	C36-C18-C17	-2.23	119.80	122.92
17	A	852	CLA	CMB-C2B-C3B	2.23	128.84	124.68
17	4	306	CLA	CHB-C4A-NA	2.23	127.59	124.51
17	1	508	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
20	A	848	BCR	C23-C24-C25	-2.23	120.95	127.20
17	L	303	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
17	4	317	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
20	1	503	BCR	C39-C30-C25	-2.23	106.69	110.30
17	B	814	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
22	J	104	DGD	C6D-O5D-C1E	-2.22	109.41	113.74
17	A	808	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	K	202	CLA	O2D-CGD-CBD	2.22	115.20	111.27
20	B	849	BCR	C36-C18-C19	2.22	121.57	118.08
17	B	816	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
25	1	517	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
17	B	811	CLA	CAC-C3C-C4C	2.21	127.68	124.81
17	1	511	CLA	CHB-C4A-NA	2.21	127.72	124.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	304	CLA	C4C-C3C-C2C	-2.21	106.44	108.89
17	A	818	CLA	CHA-C4D-ND	2.21	137.12	132.50
17	1	513	CLA	CHD-C1D-ND	-2.21	122.42	124.45
17	3	310	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	A	811	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
17	4	310	CLA	O2D-CGD-CBD	2.21	115.19	111.27
17	B	815	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	K	203	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
17	B	807	CLA	CMA-C3A-C2A	-2.20	110.95	116.10
17	B	839	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
17	B	839	CLA	CMA-C3A-C2A	-2.20	110.96	116.10
17	A	814	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
25	6	512	CHL	C2D-C1D-ND	2.20	111.73	110.10
17	A	818	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
25	4	316	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
20	I	101	BCR	C2-C1-C6	2.20	113.86	110.48
17	4	315	CLA	CHD-C1D-ND	-2.20	122.44	124.45
17	B	807	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
17	1	509	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
17	A	827	CLA	O2D-CGD-CBD	2.19	115.17	111.27
24	4	302	LUT	C11-C10-C9	-2.19	124.18	127.31
17	B	836	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
20	K	204	BCR	C20-C19-C18	-2.19	120.25	126.42
17	B	829	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	4	316	CHL	CED-O2D-CGD	2.19	120.89	115.94
17	A	818	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
25	4	316	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
17	1	506	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	4	313	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
17	A	839	CLA	CHD-C1D-ND	-2.19	122.44	124.45
17	A	807	CLA	O2D-CGD-CBD	2.19	115.16	111.27
25	1	517	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
24	3	302	LUT	C39-C29-C28	2.19	121.52	118.08
20	B	845	BCR	C36-C18-C17	-2.19	119.86	122.92
20	L	305	BCR	C37-C22-C21	-2.19	119.86	122.92
24	3	301	LUT	C8-C7-C6	-2.19	121.06	127.20
20	6	503	BCR	C12-C13-C14	-2.19	115.59	118.94
26	4	303	XAT	C5-C4-C3	-2.18	108.43	112.75
26	4	303	XAT	C19-C9-C8	2.18	121.52	118.08
20	L	305	BCR	C34-C9-C10	-2.18	119.86	122.92
17	1	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
20	A	851	BCR	C31-C1-C6	-2.18	106.76	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	504	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
20	L	301	BCR	C3-C4-C5	-2.18	110.18	114.08
17	B	804	CLA	C3B-C2B-C1B	-2.18	104.92	109.86
17	4	311	CLA	C2D-C1D-ND	-2.18	108.50	110.10
17	B	830	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
17	A	827	CLA	CHB-C4A-NA	2.18	127.52	124.51
17	A	835	CLA	CHB-C4A-NA	2.17	127.52	124.51
20	B	850	BCR	C36-C18-C17	-2.17	119.88	122.92
17	B	832	CLA	C2A-C1A-CHA	2.17	126.08	122.71
17	3	315	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	A	843	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	6	502	XAT	C31-C32-C33	-2.17	120.33	126.42
17	B	809	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
17	6	504	CLA	C3B-C4B-NB	-2.17	107.78	110.36
24	3	302	LUT	C31-C30-C29	-2.17	124.22	127.31
20	A	848	BCR	C21-C20-C19	-2.16	116.47	123.22
17	A	808	CLA	CHD-C1D-ND	-2.16	122.47	124.45
20	A	848	BCR	C15-C16-C17	-2.16	119.04	123.47
16	A	801	CL0	C1-O2A-CGA	2.16	121.54	112.41
20	A	849	BCR	C33-C5-C4	2.16	117.77	113.62
26	6	502	XAT	O4-C5-C6	-2.16	57.17	58.96
25	6	517	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
17	B	818	CLA	CHD-C1D-ND	-2.16	122.47	124.45
17	A	852	CLA	C1-C2-C3	-2.16	122.31	126.04
25	1	517	CHL	CHD-C1D-C2D	2.16	130.00	125.48
25	1	512	CHL	O1D-CGD-CBD	-2.16	120.07	124.48
17	A	837	CLA	C1-C2-C3	-2.16	122.31	126.04
24	1	502	LUT	C40-C33-C34	-2.16	119.90	122.92
20	K	204	BCR	C37-C22-C23	2.15	121.47	118.08
17	K	201	CLA	CHD-C1D-ND	-2.15	122.47	124.45
25	6	517	CHL	O2A-CGA-CBA	2.15	120.74	112.23
20	B	849	BCR	C21-C20-C19	-2.15	116.50	123.22
17	A	824	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	1	509	CLA	CAC-C3C-C4C	2.15	127.60	124.81
17	A	803	CLA	CHD-C1D-ND	-2.15	122.48	124.45
20	A	850	BCR	C37-C22-C21	-2.15	119.91	122.92
18	A	842	PQN	C2M-C2-C1	2.15	119.83	116.27
20	F	801	BCR	C11-C10-C9	-2.15	124.24	127.31
17	B	821	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	6	511	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	4	302	LUT	C8-C7-C6	-2.15	121.17	127.20
20	F	801	BCR	C36-C18-C17	-2.15	119.92	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	304	CLA	CMA-C3A-C2A	-2.15	111.09	116.10
20	A	848	BCR	C4-C5-C6	-2.14	119.62	122.73
20	3	303	BCR	C27-C26-C25	-2.14	119.62	122.73
17	4	315	CLA	C2D-C1D-ND	-2.14	108.53	110.10
17	K	205	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	B	811	CLA	CHD-C1D-ND	-2.13	122.49	124.45
20	J	103	BCR	C29-C30-C25	2.13	113.77	110.48
17	3	306	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
17	A	832	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	6	504	CLA	O1D-CGD-CBD	2.13	128.85	124.48
17	3	312	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
17	3	304	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	A	851	BCR	C29-C30-C25	2.13	113.76	110.48
25	1	514	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
17	B	807	CLA	CAA-C2A-C3A	-2.13	111.14	116.10
20	B	847	BCR	C1-C6-C5	-2.13	119.62	122.61
20	L	305	BCR	C38-C26-C27	2.13	117.70	113.62
17	B	829	CLA	CHD-C1D-ND	-2.12	122.50	124.45
20	B	845	BCR	C20-C19-C18	-2.12	120.45	126.42
20	F	803	BCR	C21-C20-C19	-2.12	116.59	123.22
20	3	303	BCR	C8-C7-C6	-2.12	121.25	127.20
25	4	313	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
25	1	517	CHL	C1D-ND-C4D	-2.12	104.83	106.33
17	B	835	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
17	6	510	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	4	303	XAT	C35-C15-C14	-2.12	119.14	123.47
17	A	834	CLA	CHD-C1D-ND	-2.12	122.51	124.45
17	1	509	CLA	CMB-C2B-C3B	2.11	128.63	124.68
20	A	851	BCR	C11-C12-C13	-2.11	120.48	126.42
17	A	826	CLA	C1-C2-C3	-2.11	122.39	126.04
24	1	502	LUT	C11-C12-C13	-2.11	120.48	126.42
20	L	305	BCR	C8-C7-C6	-2.11	121.27	127.20
24	6	501	LUT	C10-C11-C12	-2.11	116.63	123.22
20	A	851	BCR	C15-C16-C17	-2.11	119.15	123.47
24	3	301	LUT	C3-C4-C5	-2.11	107.65	111.85
17	1	506	CLA	CHD-C1D-ND	-2.11	122.52	124.45
20	4	301	BCR	C35-C13-C14	-2.11	119.97	122.92
25	6	515	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
17	1	509	CLA	CHA-C1A-NA	-2.10	121.58	126.40
20	A	846	BCR	C34-C9-C8	2.10	121.39	118.08
17	A	817	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	3	316	CLA	CHD-C1D-ND	-2.10	122.52	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	503	BCR	C28-C29-C30	-2.10	107.08	114.60
20	K	204	BCR	C23-C24-C25	-2.10	121.30	127.20
17	B	804	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	1	509	CLA	C1-O2A-CGA	2.10	121.95	116.44
17	A	817	CLA	CMA-C3A-C2A	-2.10	111.20	116.10
25	4	316	CHL	CMB-C2B-C3B	2.10	128.60	124.68
17	A	829	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
17	A	841	CLA	CMA-C3A-C2A	-2.10	111.20	116.10
17	A	824	CLA	O1D-CGD-CBD	2.10	128.77	124.48
17	B	807	CLA	CHD-C1D-ND	-2.09	122.53	124.45
16	A	801	CL0	C3D-C2D-C1D	-2.09	102.97	105.83
20	A	851	BCR	C34-C9-C10	-2.09	119.99	122.92
24	3	302	LUT	C20-C13-C12	2.09	121.37	118.08
17	A	813	CLA	CHD-C1D-ND	-2.09	122.53	124.45
17	A	811	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
17	3	305	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
20	6	503	BCR	C24-C25-C26	2.09	126.52	121.46
17	A	835	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
17	1	509	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
24	1	501	LUT	C39-C29-C28	2.09	121.37	118.08
20	I	101	BCR	C36-C18-C19	2.09	121.36	118.08
20	A	849	BCR	C23-C24-C25	-2.08	121.35	127.20
25	1	512	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
20	A	847	BCR	C21-C20-C19	-2.08	116.72	123.22
17	1	506	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
17	A	824	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	6	512	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
17	A	853	CLA	O2D-CGD-CBD	2.08	114.97	111.27
25	4	313	CHL	O2A-CGA-CBA	2.08	120.45	112.23
20	B	849	BCR	C11-C12-C13	-2.08	120.58	126.42
20	L	301	BCR	C21-C20-C19	-2.08	116.74	123.22
17	B	813	CLA	C1-C2-C3	-2.08	122.45	126.04
17	A	827	CLA	CHD-C1D-ND	-2.08	122.55	124.45
17	4	307	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
16	A	801	CL0	C4-C3-C5	2.07	118.76	115.27
20	F	803	BCR	C27-C26-C25	-2.07	119.72	122.73
17	B	808	CLA	CBA-CAA-C2A	-2.07	110.56	114.28
20	B	847	BCR	C4-C5-C6	-2.07	119.72	122.73
26	4	303	XAT	C11-C10-C9	-2.07	124.35	127.31
20	K	204	BCR	C35-C13-C12	2.07	121.34	118.08
17	6	509	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	4	301	BCR	C33-C5-C4	2.07	117.59	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	823	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	B	827	CLA	CHB-C4A-NA	2.07	127.50	124.34
17	A	809	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
20	A	847	BCR	C10-C11-C12	-2.07	116.77	123.22
24	4	302	LUT	C15-C35-C34	-2.06	119.25	123.47
17	6	508	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	F	801	BCR	C34-C9-C8	2.06	121.33	118.08
17	B	840	CLA	O2D-CGD-CBD	2.06	114.93	111.27
25	1	514	CHL	O2A-CGA-CBA	2.06	120.38	112.23
17	B	809	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	K	202	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
20	B	846	BCR	C29-C30-C25	2.06	113.66	110.48
17	B	819	CLA	CMA-C3A-C2A	-2.06	111.29	116.10
17	B	840	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	A	844	LHG	O7-C7-O9	-2.06	118.72	123.70
25	6	513	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
17	B	842	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	B	811	CLA	C2D-C1D-ND	-2.06	108.59	110.10
24	3	302	LUT	C3-C4-C5	-2.05	107.76	111.85
17	1	511	CLA	C2A-C1A-CHA	2.05	125.90	122.71
17	A	837	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	B	834	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	A	853	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	A	833	CLA	CMA-C3A-C2A	-2.05	111.31	116.10
25	1	512	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
17	3	311	CLA	O2D-CGD-CBD	2.05	114.91	111.27
20	A	854	BCR	C37-C22-C23	2.05	121.31	118.08
25	1	514	CHL	C1C-C2C-C3C	-2.05	105.49	107.11
25	6	513	CHL	O1D-CGD-CBD	-2.05	120.29	124.48
17	4	309	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	A	812	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	B	835	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	6	517	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
17	B	826	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
17	B	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
17	B	811	CLA	C1-C2-C3	-2.04	122.51	126.04
25	3	313	CHL	CMD-C2D-C3D	-2.04	120.57	126.12
20	B	845	BCR	C35-C13-C14	-2.04	120.06	122.92
17	A	827	CLA	CMA-C3A-C2A	-2.04	111.33	116.10
17	A	819	CLA	O2D-CGD-CBD	2.04	114.89	111.27
25	3	313	CHL	O2A-CGA-CBA	2.04	120.29	112.23
24	1	502	LUT	C19-C9-C10	-2.04	120.07	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	810	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
19	1	516	LHG	O7-C7-O9	-2.03	118.78	123.70
17	A	812	CLA	C2A-C1A-CHA	2.03	125.86	122.71
20	3	303	BCR	C34-C9-C8	2.03	121.28	118.08
17	K	202	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	A	825	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	3	305	CLA	CAA-C2A-C1A	2.03	118.63	111.97
20	J	103	BCR	C4-C5-C6	-2.03	119.78	122.73
17	A	830	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	4	301	BCR	C3-C4-C5	-2.03	110.45	114.08
17	6	507	CLA	C2D-C1D-ND	-2.03	108.61	110.10
20	L	305	BCR	C35-C13-C14	-2.03	120.08	122.92
17	3	304	CLA	C1C-NC-C4C	2.02	107.61	106.71
25	1	514	CHL	C2D-C1D-ND	2.02	111.59	110.10
17	A	832	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	I	101	BCR	C33-C5-C4	2.02	117.50	113.62
17	4	305	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	A	845	LHG	O7-C7-O9	-2.02	118.82	123.70
25	1	512	CHL	C4D-CHA-C1A	-2.02	118.80	121.25
17	B	808	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	1	507	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	B	820	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	I	101	BCR	C35-C13-C14	-2.01	120.11	122.92
17	L	303	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
20	A	854	BCR	C16-C15-C14	-2.01	119.36	123.47
17	A	831	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
17	4	317	CLA	O2D-CGD-CBD	2.00	114.83	111.27
25	1	512	CHL	O2A-CGA-CBA	2.00	120.15	112.23
26	6	502	XAT	C18-C5-C4	2.00	116.53	114.28
17	B	829	CLA	C3C-C4C-NC	-2.00	108.32	110.57
17	A	818	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
25	6	513	CHL	CHD-C1D-C2D	2.00	129.68	125.48
17	B	813	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	A	806	CLA	O2D-CGD-CBD	2.00	114.82	111.27
17	B	822	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (170) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	ND
16	A	801	CL0	NC
16	A	801	CL0	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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
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	852	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	A	853	CLA	ND
17	B	801	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	812	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
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	B	843	CLA	ND
17	F	802	CLA	ND
17	J	101	CLA	ND
17	J	102	CLA	ND
17	K	201	CLA	ND
17	K	202	CLA	ND
17	K	203	CLA	ND
17	K	205	CLA	ND
17	L	302	CLA	ND
17	L	303	CLA	ND
17	L	304	CLA	ND
17	1	504	CLA	ND
17	1	506	CLA	ND
17	1	507	CLA	ND
17	1	508	CLA	ND
17	1	509	CLA	ND
17	1	510	CLA	ND
17	1	511	CLA	ND
17	1	513	CLA	ND
17	1	515	CLA	ND
17	3	304	CLA	ND
17	3	305	CLA	ND
17	3	306	CLA	ND
17	3	308	CLA	ND
17	3	309	CLA	ND
17	3	310	CLA	ND
17	3	311	CLA	ND
17	3	312	CLA	ND
17	3	314	CLA	ND
17	3	316	CLA	ND
17	4	304	CLA	ND
17	4	305	CLA	ND
17	4	306	CLA	ND
17	4	307	CLA	ND
17	4	308	CLA	ND
17	4	309	CLA	ND
17	4	310	CLA	ND
17	4	311	CLA	ND
17	4	312	CLA	ND
17	4	315	CLA	ND
17	4	317	CLA	ND
17	6	504	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	6	506	CLA	ND
17	6	507	CLA	ND
17	6	508	CLA	ND
17	6	509	CLA	ND
17	6	510	CLA	ND
17	6	511	CLA	ND
17	6	514	CLA	ND
24	1	502	LUT	C26
25	1	512	CHL	ND
25	1	512	CHL	NC
25	1	512	CHL	NA
25	1	514	CHL	ND
25	1	514	CHL	NC
25	1	514	CHL	NA
25	1	517	CHL	ND
25	1	517	CHL	NC
25	1	517	CHL	NA
25	3	313	CHL	ND
25	3	313	CHL	NC
25	3	313	CHL	NA
25	4	313	CHL	ND
25	4	313	CHL	NC
25	4	313	CHL	NA
25	4	314	CHL	ND
25	4	314	CHL	NC
25	4	314	CHL	NA
25	4	316	CHL	ND
25	4	316	CHL	NC
25	4	316	CHL	NA
25	6	512	CHL	ND
25	6	512	CHL	NC
25	6	512	CHL	NA
25	6	513	CHL	ND
25	6	513	CHL	NC
25	6	513	CHL	NA
25	6	515	CHL	ND
25	6	515	CHL	NC
25	6	515	CHL	NA
25	6	517	CHL	ND
25	6	517	CHL	NC
25	6	517	CHL	NA

All (1040) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	801	CL0	C1A-C2A-CAA-CBA
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	802	CLA	CAD-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CBD-CGD-O2D-CED
17	A	807	CLA	CBD-CGD-O2D-CED
17	A	808	CLA	CAD-CBD-CGD-O1D
17	A	808	CLA	CAD-CBD-CGD-O2D
17	A	809	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	C1A-C2A-CAA-CBA
17	A	810	CLA	C3A-C2A-CAA-CBA
17	A	810	CLA	C2A-CAA-CBA-CGA
17	A	811	CLA	CHA-CBD-CGD-O1D
17	A	811	CLA	CHA-CBD-CGD-O2D
17	A	811	CLA	CAD-CBD-CGD-O1D
17	A	812	CLA	CHA-CBD-CGD-O2D
17	A	812	CLA	CAD-CBD-CGD-O2D
17	A	813	CLA	C3A-C2A-CAA-CBA
17	A	815	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CBD-CGD-O2D-CED
17	A	819	CLA	CHA-CBD-CGD-O1D
17	A	819	CLA	CHA-CBD-CGD-O2D
17	A	819	CLA	CAD-CBD-CGD-O1D
17	A	820	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	826	CLA	C1A-C2A-CAA-CBA
17	A	826	CLA	CHA-CBD-CGD-O1D
17	A	826	CLA	CHA-CBD-CGD-O2D
17	A	826	CLA	CAD-CBD-CGD-O1D
17	A	826	CLA	CAD-CBD-CGD-O2D
17	A	828	CLA	CHA-CBD-CGD-O1D
17	A	828	CLA	CHA-CBD-CGD-O2D
17	A	830	CLA	CHA-CBD-CGD-O1D
17	A	830	CLA	CHA-CBD-CGD-O2D
17	A	831	CLA	O1A-CGA-O2A-C1
17	A	831	CLA	CHA-CBD-CGD-O1D
17	A	831	CLA	CHA-CBD-CGD-O2D
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	832	CLA	CAD-CBD-CGD-O1D
17	A	832	CLA	CBD-CGD-O2D-CED
17	A	834	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	834	CLA	CAD-CBD-CGD-O2D
17	A	839	CLA	CHA-CBD-CGD-O1D
17	A	839	CLA	CHA-CBD-CGD-O2D
17	A	839	CLA	C11-C12-C13-C14
17	A	843	CLA	CBD-CGD-O2D-CED
17	A	852	CLA	CBD-CGD-O2D-CED
17	A	853	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	CHA-CBD-CGD-O1D
17	B	801	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	CHA-CBD-CGD-O2D
17	B	806	CLA	CHA-CBD-CGD-O1D
17	B	806	CLA	CHA-CBD-CGD-O2D
17	B	807	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CAD-CBD-CGD-O2D
17	B	811	CLA	C2A-CAA-CBA-CGA
17	B	811	CLA	C4-C3-C5-C6
17	B	812	CLA	CAD-CBD-CGD-O1D
17	B	812	CLA	CAD-CBD-CGD-O2D
17	B	813	CLA	CBD-CGD-O2D-CED
17	B	813	CLA	O1D-CGD-O2D-CED
17	B	813	CLA	C4-C3-C5-C6
17	B	814	CLA	CHA-CBD-CGD-O1D
17	B	814	CLA	CHA-CBD-CGD-O2D
17	B	814	CLA	CAD-CBD-CGD-O1D
17	B	818	CLA	CHA-CBD-CGD-O1D
17	B	818	CLA	CHA-CBD-CGD-O2D
17	B	820	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	CBD-CGD-O2D-CED
17	B	828	CLA	CAD-CBD-CGD-O1D
17	B	828	CLA	CAD-CBD-CGD-O2D
17	B	829	CLA	C3A-C2A-CAA-CBA
17	B	835	CLA	C1A-C2A-CAA-CBA
17	B	836	CLA	C1A-C2A-CAA-CBA
17	B	836	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	CBD-CGD-O2D-CED
17	B	838	CLA	CHA-CBD-CGD-O1D
17	B	838	CLA	CHA-CBD-CGD-O2D
17	B	838	CLA	CAD-CBD-CGD-O1D
17	B	840	CLA	CAD-CBD-CGD-O1D
17	F	802	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	J	101	CLA	CAD-CBD-CGD-O1D
17	J	102	CLA	C1A-C2A-CAA-CBA
17	J	102	CLA	C3A-C2A-CAA-CBA
17	K	202	CLA	CHA-CBD-CGD-O1D
17	K	202	CLA	CHA-CBD-CGD-O2D
17	K	203	CLA	CBD-CGD-O2D-CED
17	L	302	CLA	CBD-CGD-O2D-CED
17	L	303	CLA	CHA-CBD-CGD-O1D
17	L	303	CLA	CHA-CBD-CGD-O2D
17	1	504	CLA	C3A-C2A-CAA-CBA
17	1	506	CLA	C1A-C2A-CAA-CBA
17	1	507	CLA	CBD-CGD-O2D-CED
17	1	509	CLA	CHA-CBD-CGD-O1D
17	1	509	CLA	CHA-CBD-CGD-O2D
17	1	510	CLA	CBD-CGD-O2D-CED
17	1	513	CLA	CBD-CGD-O2D-CED
17	3	305	CLA	C2A-CAA-CBA-CGA
17	3	305	CLA	CBD-CGD-O2D-CED
17	3	305	CLA	C4-C3-C5-C6
17	3	308	CLA	C1A-C2A-CAA-CBA
17	3	308	CLA	C3A-C2A-CAA-CBA
17	3	308	CLA	CBD-CGD-O2D-CED
17	3	309	CLA	C2A-CAA-CBA-CGA
17	3	311	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	C1A-C2A-CAA-CBA
17	3	312	CLA	C3A-C2A-CAA-CBA
17	3	312	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	O1D-CGD-O2D-CED
17	3	314	CLA	CBD-CGD-O2D-CED
17	3	315	CLA	CBA-CGA-O2A-C1
17	3	316	CLA	CBD-CGD-O2D-CED
17	4	304	CLA	CBD-CGD-O2D-CED
17	4	306	CLA	CBD-CGD-O2D-CED
17	4	308	CLA	CHA-CBD-CGD-O1D
17	4	308	CLA	CHA-CBD-CGD-O2D
17	4	309	CLA	C1A-C2A-CAA-CBA
17	4	309	CLA	CBD-CGD-O2D-CED
17	4	311	CLA	CBD-CGD-O2D-CED
17	4	315	CLA	CBD-CGD-O2D-CED
17	4	317	CLA	C1A-C2A-CAA-CBA
17	4	317	CLA	C3A-C2A-CAA-CBA
17	4	317	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	6	505	CLA	C1A-C2A-CAA-CBA
17	6	506	CLA	CHA-CBD-CGD-O1D
17	6	506	CLA	CHA-CBD-CGD-O2D
17	6	506	CLA	C11-C12-C13-C14
17	6	507	CLA	C1A-C2A-CAA-CBA
17	6	507	CLA	C3A-C2A-CAA-CBA
17	6	507	CLA	CBD-CGD-O2D-CED
17	6	508	CLA	CBD-CGD-O2D-CED
17	6	509	CLA	CBD-CGD-O2D-CED
17	6	510	CLA	C1A-C2A-CAA-CBA
17	6	510	CLA	C3A-C2A-CAA-CBA
17	6	510	CLA	CBD-CGD-O2D-CED
17	6	511	CLA	C1A-C2A-CAA-CBA
17	6	511	CLA	C3A-C2A-CAA-CBA
17	6	511	CLA	CBD-CGD-O2D-CED
17	6	514	CLA	CBD-CGD-O2D-CED
19	A	844	LHG	C4-O6-P-O3
19	A	845	LHG	C4-O6-P-O4
19	B	852	LHG	C3-O3-P-O4
19	B	852	LHG	C3-O3-P-O5
19	B	852	LHG	C3-O3-P-O6
19	B	852	LHG	C4-O6-P-O4
19	B	852	LHG	C4-O6-P-O5
19	1	516	LHG	C4-O6-P-O5
19	6	516	LHG	C4-O6-P-O3
19	6	516	LHG	C4-O6-P-O5
20	A	848	BCR	C23-C24-C25-C30
20	A	849	BCR	C21-C22-C23-C24
20	A	849	BCR	C37-C22-C23-C24
20	A	850	BCR	C1-C6-C7-C8
20	A	850	BCR	C5-C6-C7-C8
20	A	851	BCR	C1-C6-C7-C8
20	A	854	BCR	C17-C18-C19-C20
20	A	854	BCR	C36-C18-C19-C20
20	B	845	BCR	C7-C8-C9-C10
20	B	845	BCR	C7-C8-C9-C34
20	B	846	BCR	C21-C22-C23-C24
20	B	846	BCR	C37-C22-C23-C24
20	B	847	BCR	C7-C8-C9-C34
20	B	850	BCR	C21-C22-C23-C24
20	I	102	BCR	C21-C22-C23-C24
20	I	102	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	K	204	BCR	C1-C6-C7-C8
20	K	204	BCR	C7-C8-C9-C34
20	L	305	BCR	C23-C24-C25-C30
20	3	303	BCR	C7-C8-C9-C10
20	3	303	BCR	C7-C8-C9-C34
20	3	303	BCR	C23-C24-C25-C30
20	4	301	BCR	C7-C8-C9-C10
20	4	301	BCR	C7-C8-C9-C34
20	4	301	BCR	C23-C24-C25-C30
20	6	503	BCR	C13-C14-C15-C16
20	6	503	BCR	C23-C24-C25-C26
20	6	503	BCR	C23-C24-C25-C30
22	J	104	DGD	C2E-C1E-O5D-C6D
22	J	104	DGD	O6E-C1E-O5D-C6D
23	4	318	LMG	O6-C1-O1-C7
23	4	318	LMG	C7-C8-O7-C10
23	4	318	LMG	C9-C8-O7-C10
23	4	318	LMG	O9-C10-O7-C8
24	1	502	LUT	C21-C26-C27-C28
24	1	502	LUT	C27-C28-C29-C30
24	1	502	LUT	C27-C28-C29-C39
24	1	502	LUT	C31-C32-C33-C40
24	3	302	LUT	C7-C8-C9-C10
24	3	302	LUT	C7-C8-C9-C19
24	3	302	LUT	C11-C12-C13-C14
24	3	302	LUT	C11-C12-C13-C20
24	6	501	LUT	C1-C6-C7-C8
25	1	517	CHL	C1A-C2A-CAA-CBA
25	1	517	CHL	C3A-C2A-CAA-CBA
25	4	314	CHL	CBD-CGD-O2D-CED
26	6	502	XAT	O4-C6-C7-C8
26	6	502	XAT	C7-C8-C9-C10
26	6	502	XAT	C7-C8-C9-C19
26	6	502	XAT	C11-C12-C13-C14
26	6	502	XAT	C11-C12-C13-C20
17	A	810	CLA	O1D-CGD-O2D-CED
17	A	852	CLA	O1D-CGD-O2D-CED
17	F	802	CLA	O1D-CGD-O2D-CED
17	J	101	CLA	O1D-CGD-O2D-CED
17	K	203	CLA	O1D-CGD-O2D-CED
17	3	307	CLA	O1D-CGD-O2D-CED
17	3	310	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	311	CLA	O1D-CGD-O2D-CED
17	3	314	CLA	O1D-CGD-O2D-CED
17	4	317	CLA	O1D-CGD-O2D-CED
17	6	514	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
17	B	815	CLA	O1D-CGD-O2D-CED
17	L	302	CLA	O1D-CGD-O2D-CED
17	1	506	CLA	O1D-CGD-O2D-CED
17	1	509	CLA	O1D-CGD-O2D-CED
17	1	513	CLA	O1D-CGD-O2D-CED
17	3	305	CLA	O1D-CGD-O2D-CED
17	4	309	CLA	O1D-CGD-O2D-CED
17	6	505	CLA	O1D-CGD-O2D-CED
17	6	509	CLA	O1D-CGD-O2D-CED
17	6	510	CLA	O1D-CGD-O2D-CED
25	4	314	CHL	O1D-CGD-O2D-CED
17	A	802	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	CBD-CGD-O2D-CED
17	A	834	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CBD-CGD-O2D-CED
17	B	808	CLA	CBD-CGD-O2D-CED
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	819	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	CBD-CGD-O2D-CED
17	B	821	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	CBD-CGD-O2D-CED
17	B	833	CLA	CBD-CGD-O2D-CED
17	B	835	CLA	CBD-CGD-O2D-CED
17	B	839	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	CBD-CGD-O2D-CED
17	J	102	CLA	CBD-CGD-O2D-CED
17	1	504	CLA	CBD-CGD-O2D-CED
17	1	506	CLA	CBD-CGD-O2D-CED
17	1	509	CLA	CBD-CGD-O2D-CED
17	1	511	CLA	CBD-CGD-O2D-CED
17	1	515	CLA	CBD-CGD-O2D-CED
17	3	307	CLA	CBD-CGD-O2D-CED
17	3	309	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	315	CLA	CBD-CGD-O2D-CED
17	4	305	CLA	CBD-CGD-O2D-CED
17	4	308	CLA	CBD-CGD-O2D-CED
17	4	310	CLA	CBD-CGD-O2D-CED
17	4	317	CLA	CBD-CGD-O2D-CED
17	6	504	CLA	CBD-CGD-O2D-CED
17	6	505	CLA	CBD-CGD-O2D-CED
17	6	506	CLA	CBD-CGD-O2D-CED
25	1	514	CHL	CBD-CGD-O2D-CED
25	3	313	CHL	CBD-CGD-O2D-CED
25	6	513	CHL	CBD-CGD-O2D-CED
17	A	804	CLA	O1A-CGA-O2A-C1
17	1	509	CLA	O1A-CGA-O2A-C1
17	1	513	CLA	O1A-CGA-O2A-C1
17	4	306	CLA	O1A-CGA-O2A-C1
17	B	819	CLA	O1D-CGD-O2D-CED
17	B	839	CLA	O1D-CGD-O2D-CED
17	1	511	CLA	O1D-CGD-O2D-CED
17	3	309	CLA	O1D-CGD-O2D-CED
17	3	315	CLA	O1D-CGD-O2D-CED
17	6	506	CLA	O1D-CGD-O2D-CED
17	A	805	CLA	O1D-CGD-O2D-CED
17	A	807	CLA	O1D-CGD-O2D-CED
17	A	820	CLA	O1D-CGD-O2D-CED
17	A	832	CLA	O1D-CGD-O2D-CED
17	A	843	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	O1D-CGD-O2D-CED
17	4	304	CLA	O1D-CGD-O2D-CED
17	4	306	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	CBA-CGA-O2A-C1
17	1	509	CLA	CBA-CGA-O2A-C1
17	A	808	CLA	CBD-CGD-O2D-CED
17	A	818	CLA	CBD-CGD-O2D-CED
17	A	833	CLA	CBD-CGD-O2D-CED
17	A	836	CLA	CBD-CGD-O2D-CED
17	A	853	CLA	CBD-CGD-O2D-CED
17	B	825	CLA	CBD-CGD-O2D-CED
17	B	829	CLA	CBD-CGD-O2D-CED
17	K	202	CLA	CBD-CGD-O2D-CED
25	4	313	CHL	CBD-CGD-O2D-CED
17	6	506	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	809	CLA	O1D-CGD-O2D-CED
17	A	815	CLA	O1D-CGD-O2D-CED
17	6	508	CLA	O1D-CGD-O2D-CED
17	B	824	CLA	O1D-CGD-O2D-CED
17	1	507	CLA	O1D-CGD-O2D-CED
17	3	308	CLA	O1D-CGD-O2D-CED
17	4	311	CLA	O1D-CGD-O2D-CED
17	4	315	CLA	O1D-CGD-O2D-CED
17	6	507	CLA	O1D-CGD-O2D-CED
17	6	511	CLA	O1D-CGD-O2D-CED
17	B	841	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	O1D-CGD-O2D-CED
17	1	510	CLA	O1D-CGD-O2D-CED
17	3	316	CLA	O1D-CGD-O2D-CED
17	4	305	CLA	O1D-CGD-O2D-CED
17	4	310	CLA	O1D-CGD-O2D-CED
17	3	316	CLA	CBA-CGA-O2A-C1
17	3	316	CLA	O1A-CGA-O2A-C1
17	A	852	CLA	C3-C5-C6-C7
17	B	818	CLA	C3-C5-C6-C7
17	1	508	CLA	C3-C5-C6-C7
17	3	312	CLA	C3-C5-C6-C7
17	A	816	CLA	CBA-CGA-O2A-C1
17	1	513	CLA	CBA-CGA-O2A-C1
17	3	312	CLA	CBA-CGA-O2A-C1
17	4	306	CLA	CBA-CGA-O2A-C1
17	6	507	CLA	CBA-CGA-O2A-C1
17	1	515	CLA	O1D-CGD-O2D-CED
25	3	313	CHL	O1D-CGD-O2D-CED
25	6	512	CHL	CBD-CGD-O2D-CED
17	L	303	CLA	O1A-CGA-O2A-C1
17	3	315	CLA	O1A-CGA-O2A-C1
25	1	514	CHL	CBA-CGA-O2A-C1
17	A	810	CLA	C4-C3-C5-C6
17	4	306	CLA	C4-C3-C5-C6
17	B	813	CLA	C2-C3-C5-C6
17	3	305	CLA	C2-C3-C5-C6
17	B	828	CLA	CBD-CGD-O2D-CED
17	6	509	CLA	C2A-CAA-CBA-CGA
25	1	514	CHL	C2A-CAA-CBA-CGA
25	6	512	CHL	C2A-CAA-CBA-CGA
17	B	820	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	816	CLA	C3-C5-C6-C7
17	A	839	CLA	C3-C5-C6-C7
17	B	801	CLA	C3-C5-C6-C7
17	L	303	CLA	C3-C5-C6-C7
17	6	506	CLA	CBA-CGA-O2A-C1
17	A	841	CLA	CBD-CGD-O2D-CED
17	B	817	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	O1D-CGD-O2D-CED
17	A	834	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	O1D-CGD-O2D-CED
17	B	808	CLA	O1D-CGD-O2D-CED
17	J	102	CLA	O1D-CGD-O2D-CED
17	1	504	CLA	O1D-CGD-O2D-CED
17	4	308	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	O1A-CGA-O2A-C1
17	6	507	CLA	O1A-CGA-O2A-C1
17	B	821	CLA	O1D-CGD-O2D-CED
17	B	835	CLA	O1D-CGD-O2D-CED
24	1	502	LUT	C29-C30-C31-C32
17	A	828	CLA	CBD-CGD-O2D-CED
17	B	810	CLA	CBD-CGD-O2D-CED
17	1	505	CLA	CBD-CGD-O2D-CED
25	1	517	CHL	CBD-CGD-O2D-CED
17	B	820	CLA	O1D-CGD-O2D-CED
17	B	813	CLA	C3-C5-C6-C7
17	B	820	CLA	CBA-CGA-O2A-C1
17	L	303	CLA	CBA-CGA-O2A-C1
17	6	511	CLA	CBA-CGA-O2A-C1
17	3	312	CLA	O1A-CGA-O2A-C1
17	A	802	CLA	O1D-CGD-O2D-CED
17	6	504	CLA	O1D-CGD-O2D-CED
17	B	834	CLA	CBD-CGD-O2D-CED
25	6	513	CHL	O1D-CGD-O2D-CED
17	A	838	CLA	C3-C5-C6-C7
17	1	513	CLA	C3-C5-C6-C7
25	1	514	CHL	O1A-CGA-O2A-C1
17	B	829	CLA	C2A-CAA-CBA-CGA
25	3	313	CHL	C2A-CAA-CBA-CGA
17	B	833	CLA	O1D-CGD-O2D-CED
17	A	837	CLA	CBA-CGA-O2A-C1
17	A	808	CLA	O1D-CGD-O2D-CED
17	A	818	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	836	CLA	O1D-CGD-O2D-CED
25	1	514	CHL	O1D-CGD-O2D-CED
17	6	511	CLA	O1A-CGA-O2A-C1
23	J	105	LMG	C11-C10-O7-C8
17	A	837	CLA	O1A-CGA-O2A-C1
17	A	829	CLA	CBA-CGA-O2A-C1
17	B	831	CLA	CBA-CGA-O2A-C1
17	1	506	CLA	CBA-CGA-O2A-C1
17	3	309	CLA	CBA-CGA-O2A-C1
17	6	509	CLA	CBA-CGA-O2A-C1
17	A	814	CLA	CBD-CGD-O2D-CED
17	3	306	CLA	CBD-CGD-O2D-CED
16	A	801	CL0	CAA-CBA-CGA-O2A
17	4	306	CLA	C8-C10-C11-C12
23	4	318	LMG	C2-C1-O1-C7
17	A	826	CLA	CBA-CGA-O2A-C1
17	B	831	CLA	O1A-CGA-O2A-C1
17	A	810	CLA	C2-C3-C5-C6
17	A	824	CLA	C6-C7-C8-C9
17	A	829	CLA	C6-C7-C8-C9
17	1	508	CLA	C11-C10-C8-C9
17	6	506	CLA	C11-C10-C8-C9
17	A	853	CLA	O1D-CGD-O2D-CED
17	K	202	CLA	O1D-CGD-O2D-CED
17	B	840	CLA	CBD-CGD-O2D-CED
17	A	824	CLA	C2A-CAA-CBA-CGA
17	3	312	CLA	C2A-CAA-CBA-CGA
17	3	315	CLA	C2A-CAA-CBA-CGA
20	A	846	BCR	C37-C22-C23-C24
20	A	848	BCR	C7-C8-C9-C34
20	A	854	BCR	C7-C8-C9-C34
20	B	850	BCR	C37-C22-C23-C24
20	F	801	BCR	C37-C22-C23-C24
20	I	101	BCR	C7-C8-C9-C34
20	I	102	BCR	C7-C8-C9-C34
20	K	204	BCR	C37-C22-C23-C24
20	3	303	BCR	C37-C22-C23-C24
24	1	501	LUT	C7-C8-C9-C19
26	4	303	XAT	C7-C8-C9-C19
20	A	846	BCR	C21-C22-C23-C24
20	A	848	BCR	C7-C8-C9-C10
20	F	801	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	I	101	BCR	C7-C8-C9-C10
20	I	102	BCR	C7-C8-C9-C10
20	K	204	BCR	C21-C22-C23-C24
24	1	501	LUT	C7-C8-C9-C10
17	A	829	CLA	O1A-CGA-O2A-C1
17	1	506	CLA	O1A-CGA-O2A-C1
17	A	804	CLA	C15-C16-C17-C18
17	A	839	CLA	C5-C6-C7-C8
17	A	833	CLA	O1D-CGD-O2D-CED
17	B	829	CLA	O1D-CGD-O2D-CED
25	6	517	CHL	CBA-CGA-O2A-C1
17	B	825	CLA	O1D-CGD-O2D-CED
17	B	829	CLA	CBA-CGA-O2A-C1
17	A	804	CLA	C8-C10-C11-C12
17	1	508	CLA	C13-C15-C16-C17
19	1	516	LHG	C7-C8-C9-C10
17	A	804	CLA	C5-C6-C7-C8
17	A	804	CLA	C13-C15-C16-C17
17	A	810	CLA	C5-C6-C7-C8
17	A	815	CLA	C2C-C3C-CAC-CBC
25	4	316	CHL	CBD-CGD-O2D-CED
17	L	303	CLA	C8-C10-C11-C12
17	4	307	CLA	C8-C10-C11-C12
25	4	313	CHL	O1D-CGD-O2D-CED
23	J	105	LMG	O9-C10-O7-C8
17	B	826	CLA	C5-C6-C7-C8
17	A	832	CLA	C2A-CAA-CBA-CGA
17	B	833	CLA	C2A-CAA-CBA-CGA
17	L	303	CLA	C5-C6-C7-C8
17	4	306	CLA	C11-C12-C13-C15
17	B	808	CLA	C3-C5-C6-C7
20	I	101	BCR	C9-C10-C11-C12
25	6	515	CHL	CBD-CGD-O2D-CED
17	3	316	CLA	C2A-CAA-CBA-CGA
17	4	309	CLA	C2A-CAA-CBA-CGA
17	3	309	CLA	O1A-CGA-O2A-C1
17	6	509	CLA	O1A-CGA-O2A-C1
17	6	506	CLA	C8-C10-C11-C12
17	B	841	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	C3-C5-C6-C7
17	6	506	CLA	C10-C11-C12-C13
17	A	826	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	829	CLA	O1A-CGA-O2A-C1
17	A	839	CLA	C13-C15-C16-C17
19	A	844	LHG	C3-O3-P-O6
19	A	845	LHG	C3-O3-P-O6
19	A	845	LHG	C4-O6-P-O3
19	B	852	LHG	C4-O6-P-O3
19	1	516	LHG	C4-O6-P-O3
17	A	810	CLA	CBA-CGA-O2A-C1
17	B	826	CLA	C10-C11-C12-C13
25	6	512	CHL	O1D-CGD-O2D-CED
17	4	306	CLA	C2-C3-C5-C6
17	A	804	CLA	C2A-CAA-CBA-CGA
17	B	820	CLA	C2A-CAA-CBA-CGA
25	1	512	CHL	C2A-CAA-CBA-CGA
25	4	313	CHL	C2A-CAA-CBA-CGA
17	B	810	CLA	C16-C17-C18-C20
17	B	813	CLA	CBA-CGA-O2A-C1
17	1	508	CLA	CBA-CGA-O2A-C1
19	B	852	LHG	C7-C8-C9-C10
17	B	828	CLA	O1D-CGD-O2D-CED
17	B	836	CLA	C3-C5-C6-C7
17	6	510	CLA	C3-C5-C6-C7
17	L	303	CLA	C11-C12-C13-C14
17	1	506	CLA	C6-C7-C8-C9
22	J	104	DGD	CBB-CCB-CDB-CEB
17	A	841	CLA	O1D-CGD-O2D-CED
22	J	104	DGD	C7B-C8B-C9B-CAB
17	B	817	CLA	O1D-CGD-O2D-CED
19	B	852	LHG	O2-C2-C3-O3
17	B	826	CLA	C3-C5-C6-C7
17	1	508	CLA	C8-C10-C11-C12
17	A	810	CLA	O1A-CGA-O2A-C1
17	A	826	CLA	C4-C3-C5-C6
17	A	824	CLA	C2-C3-C5-C6
17	A	826	CLA	C14-C13-C15-C16
17	A	815	CLA	C4C-C3C-CAC-CBC
17	4	305	CLA	C2A-CAA-CBA-CGA
20	B	845	BCR	C37-C22-C23-C24
20	B	845	BCR	C21-C22-C23-C24
24	1	502	LUT	C31-C32-C33-C34
17	L	304	CLA	CBD-CGD-O2D-CED
17	B	821	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	L	303	CLA	C11-C12-C13-C15
22	J	104	DGD	O6D-C1D-O3G-C3G
17	B	810	CLA	C15-C16-C17-C18
17	1	510	CLA	CBA-CGA-O2A-C1
25	6	512	CHL	CBA-CGA-O2A-C1
17	4	312	CLA	CBD-CGD-O2D-CED
17	A	828	CLA	O1D-CGD-O2D-CED
25	1	517	CHL	O1D-CGD-O2D-CED
17	A	804	CLA	C3A-C2A-CAA-CBA
17	A	812	CLA	CBD-CGD-O2D-CED
17	A	826	CLA	C3A-C2A-CAA-CBA
17	A	853	CLA	C3A-C2A-CAA-CBA
17	1	506	CLA	C3A-C2A-CAA-CBA
17	3	315	CLA	C3A-C2A-CAA-CBA
17	3	316	CLA	C3A-C2A-CAA-CBA
17	6	505	CLA	C3A-C2A-CAA-CBA
17	A	837	CLA	C6-C7-C8-C9
17	B	810	CLA	O1D-CGD-O2D-CED
17	A	824	CLA	C4-C3-C5-C6
22	J	104	DGD	C2B-C1B-O2G-C2G
17	B	813	CLA	O1A-CGA-O2A-C1
17	A	826	CLA	C16-C17-C18-C19
17	A	839	CLA	C16-C17-C18-C20
17	B	836	CLA	CAA-CBA-CGA-O2A
25	6	517	CHL	O1A-CGA-O2A-C1
17	1	508	CLA	O1A-CGA-O2A-C1
22	J	104	DGD	O1B-C1B-O2G-C2G
17	1	509	CLA	C2-C1-O2A-CGA
17	6	506	CLA	C3-C5-C6-C7
20	A	848	BCR	C23-C24-C25-C26
20	A	849	BCR	C1-C6-C7-C8
20	A	849	BCR	C5-C6-C7-C8
20	A	849	BCR	C23-C24-C25-C26
20	A	849	BCR	C23-C24-C25-C30
20	A	851	BCR	C5-C6-C7-C8
20	A	851	BCR	C23-C24-C25-C26
20	A	851	BCR	C23-C24-C25-C30
20	I	101	BCR	C23-C24-C25-C26
20	I	102	BCR	C23-C24-C25-C26
20	I	102	BCR	C23-C24-C25-C30
20	K	204	BCR	C5-C6-C7-C8
20	K	204	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	K	204	BCR	C23-C24-C25-C30
20	L	305	BCR	C23-C24-C25-C26
20	3	303	BCR	C23-C24-C25-C26
20	4	301	BCR	C1-C6-C7-C8
20	4	301	BCR	C5-C6-C7-C8
20	4	301	BCR	C23-C24-C25-C26
24	3	301	LUT	C1-C6-C7-C8
24	3	301	LUT	C5-C6-C7-C8
24	6	501	LUT	C5-C6-C7-C8
17	A	824	CLA	C11-C10-C8-C9
17	B	834	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	C12-C13-C15-C16
17	A	826	CLA	C2-C3-C5-C6
17	1	508	CLA	C16-C17-C18-C20
17	A	809	CLA	CBA-CGA-O2A-C1
17	A	816	CLA	C2A-CAA-CBA-CGA
17	4	306	CLA	C2A-CAA-CBA-CGA
19	1	516	LHG	C28-C29-C30-C31
22	B	851	DGD	C5A-C6A-C7A-C8A
17	1	505	CLA	O1D-CGD-O2D-CED
17	B	810	CLA	C16-C17-C18-C19
17	A	803	CLA	C4-C3-C5-C6
17	A	804	CLA	C14-C13-C15-C16
17	4	306	CLA	C11-C12-C13-C14
19	1	516	LHG	C16-C17-C18-C19
17	6	506	CLA	C2A-CAA-CBA-CGA
19	B	852	LHG	C23-C24-C25-C26
24	3	301	LUT	C27-C28-C29-C39
25	4	316	CHL	O1D-CGD-O2D-CED
20	K	204	BCR	C7-C8-C9-C10
17	A	830	CLA	C1A-C2A-CAA-CBA
17	A	831	CLA	C1A-C2A-CAA-CBA
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	L	303	CLA	C1A-C2A-CAA-CBA
17	3	315	CLA	C1A-C2A-CAA-CBA
17	3	316	CLA	C1A-C2A-CAA-CBA
17	6	509	CLA	C1A-C2A-CAA-CBA
25	3	313	CHL	C1A-C2A-CAA-CBA
25	4	314	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	508	CLA	C16-C17-C18-C19
17	6	506	CLA	C5-C6-C7-C8
17	3	306	CLA	O1D-CGD-O2D-CED
19	A	844	LHG	C7-C8-C9-C10
17	B	821	CLA	C6-C7-C8-C9
17	1	506	CLA	C6-C7-C8-C10
17	A	830	CLA	CBA-CGA-O2A-C1
22	J	104	DGD	O6E-C5E-C6E-O5E
17	J	101	CLA	C3A-C2A-CAA-CBA
22	J	104	DGD	O6D-C5D-C6D-O5D
17	A	809	CLA	O1A-CGA-O2A-C1
23	4	318	LMG	C8-C7-O1-C1
17	A	814	CLA	O1D-CGD-O2D-CED
22	B	851	DGD	C4B-C5B-C6B-C7B
22	J	104	DGD	CFA-CGA-CHA-CIA
17	B	840	CLA	O1D-CGD-O2D-CED
17	4	307	CLA	C11-C12-C13-C15
17	3	311	CLA	CBA-CGA-O2A-C1
17	1	508	CLA	C5-C6-C7-C8
17	A	843	CLA	C2-C1-O2A-CGA
17	B	836	CLA	C8-C10-C11-C12
25	6	515	CHL	O1D-CGD-O2D-CED
17	A	803	CLA	C3-C5-C6-C7
17	A	830	CLA	O1A-CGA-O2A-C1
17	A	803	CLA	C2-C3-C5-C6
17	A	824	CLA	C6-C7-C8-C10
17	A	826	CLA	C11-C10-C8-C7
17	A	829	CLA	C6-C7-C8-C10
17	A	831	CLA	C6-C7-C8-C10
17	B	801	CLA	C12-C13-C15-C16
17	B	810	CLA	C6-C7-C8-C10
17	B	826	CLA	C12-C13-C15-C16
17	6	506	CLA	C12-C13-C15-C16
16	A	801	CL0	C3-C5-C6-C7
17	A	826	CLA	C11-C10-C8-C9
17	A	831	CLA	C6-C7-C8-C9
17	B	810	CLA	C6-C7-C8-C9
17	B	826	CLA	C14-C13-C15-C16
17	4	306	CLA	C14-C13-C15-C16
17	6	506	CLA	C14-C13-C15-C16
17	6	510	CLA	C6-C7-C8-C9
17	3	311	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	516	LHG	C24-C23-O8-C6
17	1	508	CLA	C15-C16-C17-C18
17	4	307	CLA	C4-C3-C5-C6
25	4	313	CHL	CBA-CGA-O2A-C1
17	B	821	CLA	C3A-C2A-CAA-CBA
25	3	313	CHL	CBA-CGA-O2A-C1
17	L	304	CLA	O1D-CGD-O2D-CED
22	B	851	DGD	O1G-C1G-C2G-C3G
23	4	318	LMG	O1-C7-C8-C9
23	4	318	LMG	C8-C9-O8-C28
17	4	312	CLA	O1D-CGD-O2D-CED
25	3	313	CHL	C3C-C2C-CMC-OMC
25	6	515	CHL	C3C-C2C-CMC-OMC
17	A	826	CLA	C3-C5-C6-C7
19	A	845	LHG	O6-C4-C5-O7
17	4	307	CLA	C11-C12-C13-C14
17	3	311	CLA	O2A-C1-C2-C3
17	A	839	CLA	CBA-CGA-O2A-C1
17	A	843	CLA	CBA-CGA-O2A-C1
17	A	839	CLA	C16-C17-C18-C19
17	A	826	CLA	C2-C1-O2A-CGA
17	1	506	CLA	C2-C1-O2A-CGA
17	B	801	CLA	C14-C13-C15-C16
17	A	826	CLA	C16-C17-C18-C20
20	A	846	BCR	C23-C24-C25-C26
20	A	846	BCR	C23-C24-C25-C30
20	I	101	BCR	C23-C24-C25-C30
20	I	102	BCR	C1-C6-C7-C8
20	I	102	BCR	C5-C6-C7-C8
20	J	103	BCR	C23-C24-C25-C26
20	J	103	BCR	C23-C24-C25-C30
24	4	302	LUT	C1-C6-C7-C8
24	4	302	LUT	C5-C6-C7-C8
17	B	838	CLA	C2C-C3C-CAC-CBC
24	6	501	LUT	C11-C12-C13-C20
17	B	808	CLA	CAA-CBA-CGA-O2A
17	A	828	CLA	C1A-C2A-CAA-CBA
17	B	816	CLA	C1A-C2A-CAA-CBA
17	1	504	CLA	C1A-C2A-CAA-CBA
20	B	847	BCR	C7-C8-C9-C10
26	4	303	XAT	C7-C8-C9-C10
17	B	808	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	845	LHG	O6-C4-C5-C6
17	A	829	CLA	C11-C10-C8-C7
17	A	839	CLA	C11-C12-C13-C15
17	A	839	CLA	C12-C13-C15-C16
17	B	826	CLA	C6-C7-C8-C10
17	1	508	CLA	C6-C7-C8-C10
17	1	508	CLA	C11-C10-C8-C7
17	4	306	CLA	C12-C13-C15-C16
17	6	506	CLA	C11-C10-C8-C7
17	6	510	CLA	C6-C7-C8-C10
26	6	502	XAT	C9-C10-C11-C12
17	A	837	CLA	C6-C7-C8-C10
25	6	512	CHL	O1A-CGA-O2A-C1
25	1	512	CHL	CBA-CGA-O2A-C1
17	4	309	CLA	CBA-CGA-O2A-C1
25	1	514	CHL	CAA-CBA-CGA-O2A
17	A	811	CLA	CAD-CBD-CGD-O2D
17	A	819	CLA	CAD-CBD-CGD-O2D
17	A	820	CLA	CAD-CBD-CGD-O2D
17	A	829	CLA	CAD-CBD-CGD-O2D
17	B	829	CLA	CAD-CBD-CGD-O2D
17	B	838	CLA	CAD-CBD-CGD-O2D
17	B	840	CLA	CAD-CBD-CGD-O2D
17	B	841	CLA	CAD-CBD-CGD-O2D
17	J	101	CLA	CAD-CBD-CGD-O2D
17	1	504	CLA	CAD-CBD-CGD-O2D
17	1	507	CLA	CAD-CBD-CGD-O2D
17	3	308	CLA	CAD-CBD-CGD-O2D
22	J	104	DGD	C1G-C2G-O2G-C1B
25	4	316	CHL	CAD-CBD-CGD-O2D
23	4	318	LMG	C7-C8-C9-O8
19	1	516	LHG	O6-C4-C5-O7
17	A	829	CLA	C2A-CAA-CBA-CGA
17	A	814	CLA	CHA-CBD-CGD-O1D
17	A	814	CLA	CHA-CBD-CGD-O2D
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	843	CLA	CHA-CBD-CGD-O1D
17	A	843	CLA	CHA-CBD-CGD-O2D
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	811	CLA	CHA-CBD-CGD-O1D
17	B	811	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	817	CLA	CHA-CBD-CGD-O1D
17	B	817	CLA	CHA-CBD-CGD-O2D
17	B	823	CLA	CHA-CBD-CGD-O1D
17	B	823	CLA	CHA-CBD-CGD-O2D
17	B	826	CLA	CHA-CBD-CGD-O1D
17	B	826	CLA	CHA-CBD-CGD-O2D
17	B	832	CLA	CHA-CBD-CGD-O1D
17	B	832	CLA	CHA-CBD-CGD-O2D
17	L	304	CLA	CHA-CBD-CGD-O1D
17	L	304	CLA	CHA-CBD-CGD-O2D
17	1	507	CLA	CHA-CBD-CGD-O1D
17	1	508	CLA	CHA-CBD-CGD-O1D
17	1	508	CLA	CHA-CBD-CGD-O2D
17	1	510	CLA	CHA-CBD-CGD-O1D
17	1	510	CLA	CHA-CBD-CGD-O2D
17	4	307	CLA	CHA-CBD-CGD-O1D
19	1	516	LHG	O10-C23-O8-C6
22	B	851	DGD	O1G-C1G-C2G-O2G
17	A	839	CLA	O1A-CGA-O2A-C1
25	6	513	CHL	CAA-CBA-CGA-O2A
17	B	810	CLA	C4-C3-C5-C6
17	A	843	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	C11-C10-C8-C9
17	A	829	CLA	C10-C11-C12-C13
17	4	309	CLA	O1A-CGA-O2A-C1
17	4	307	CLA	C5-C6-C7-C8
17	1	510	CLA	C2A-CAA-CBA-CGA
20	3	303	BCR	C21-C22-C23-C24
17	A	803	CLA	C1A-C2A-CAA-CBA
17	A	852	CLA	C1A-C2A-CAA-CBA
17	B	804	CLA	CAD-CBD-CGD-O2D
17	1	509	CLA	C1A-C2A-CAA-CBA
17	3	311	CLA	C1A-C2A-CAA-CBA
19	1	516	LHG	C3-O3-P-O6
19	B	852	LHG	C2-C3-O3-P
17	1	510	CLA	O1A-CGA-O2A-C1
19	A	844	LHG	C3-O3-P-O4
19	A	844	LHG	C4-O6-P-O4
19	A	845	LHG	C3-O3-P-O5
19	A	845	LHG	C4-O6-P-O5
19	1	516	LHG	C4-O6-P-O4
19	1	516	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	815	CLA	C2A-CAA-CBA-CGA
17	A	802	CLA	CAD-CBD-CGD-O1D
17	A	804	CLA	CAD-CBD-CGD-O1D
17	A	805	CLA	CAD-CBD-CGD-O1D
17	A	806	CLA	CAD-CBD-CGD-O1D
17	A	823	CLA	CAD-CBD-CGD-O1D
17	A	830	CLA	CAD-CBD-CGD-O1D
17	B	834	CLA	CAD-CBD-CGD-O1D
17	6	504	CLA	CAD-CBD-CGD-O1D
17	6	505	CLA	CAD-CBD-CGD-O1D
17	6	507	CLA	C2-C3-C5-C6
23	J	105	LMG	C13-C14-C15-C16
19	B	852	LHG	C24-C23-O8-C6
16	A	801	CL0	C2-C1-O2A-CGA
17	6	510	CLA	C11-C12-C13-C15
17	A	829	CLA	C4-C3-C5-C6
17	A	804	CLA	C6-C7-C8-C10
17	A	816	CLA	C11-C10-C8-C7
17	A	839	CLA	C11-C10-C8-C7
17	B	824	CLA	C3A-C2A-CAA-CBA
17	B	826	CLA	C11-C10-C8-C7
17	4	307	CLA	C6-C7-C8-C10
24	3	301	LUT	C25-C26-C27-C28
17	B	836	CLA	C3A-C2A-CAA-CBA
25	3	313	CHL	C1C-C2C-CMC-OMC
25	6	515	CHL	C1C-C2C-CMC-OMC
23	4	318	LMG	O1-C7-C8-O7
23	4	318	LMG	O7-C8-C9-O8
17	B	821	CLA	C2C-C3C-CAC-CBC
17	A	837	CLA	C4-C3-C5-C6
17	B	810	CLA	C2-C3-C5-C6
17	A	804	CLA	C6-C7-C8-C9
17	A	839	CLA	C14-C13-C15-C16
17	B	826	CLA	C6-C7-C8-C9
17	1	508	CLA	C6-C7-C8-C9
17	B	808	CLA	CBA-CGA-O2A-C1
20	6	503	BCR	C18-C19-C20-C21
17	B	801	CLA	C16-C17-C18-C19
17	A	839	CLA	C2A-CAA-CBA-CGA
17	B	818	CLA	C2A-CAA-CBA-CGA
19	6	516	LHG	O9-C7-O7-C5
17	B	801	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	824	CLA	C2-C1-O2A-CGA
20	K	204	BCR	C19-C20-C21-C22
17	B	801	CLA	O1A-CGA-O2A-C1
24	1	502	LUT	C1-C6-C7-C8
24	1	502	LUT	C5-C6-C7-C8
24	3	302	LUT	C1-C6-C7-C8
19	6	516	LHG	C8-C7-O7-C5
17	A	838	CLA	O1D-CGD-O2D-CED
20	1	503	BCR	C23-C24-C25-C26
19	6	516	LHG	C3-O3-P-O6
25	3	313	CHL	CAD-CBD-CGD-O2D
22	J	104	DGD	O1G-C1G-C2G-C3G
17	A	852	CLA	C4-C3-C5-C6
25	3	313	CHL	O1A-CGA-O2A-C1
17	A	839	CLA	C11-C10-C8-C9
17	4	307	CLA	C6-C7-C8-C9
17	1	506	CLA	C5-C6-C7-C8
17	4	307	CLA	C10-C11-C12-C13
20	A	848	BCR	C11-C12-C13-C35
20	A	854	BCR	C7-C8-C9-C10
17	A	824	CLA	C11-C10-C8-C7
17	4	307	CLA	C2-C3-C5-C6
19	B	852	LHG	O10-C23-O8-C6
17	A	838	CLA	CBD-CGD-O2D-CED
17	6	511	CLA	C2A-CAA-CBA-CGA
20	B	845	BCR	C9-C10-C11-C12
20	B	845	BCR	C13-C14-C15-C16
22	B	851	DGD	O6D-C5D-C6D-O5D
17	4	306	CLA	C10-C11-C12-C13
17	B	818	CLA	C2-C1-O2A-CGA
17	6	510	CLA	C11-C12-C13-C14
19	A	844	LHG	C24-C25-C26-C27
22	J	104	DGD	CCA-CDA-CEA-CFA
17	B	818	CLA	C5-C6-C7-C8
17	A	837	CLA	C2A-CAA-CBA-CGA
19	B	852	LHG	C25-C26-C27-C28
17	B	813	CLA	C3A-C2A-CAA-CBA
17	B	835	CLA	C3A-C2A-CAA-CBA
17	K	202	CLA	C4C-C3C-CAC-CBC
19	A	844	LHG	C26-C27-C28-C29
19	1	516	LHG	C13-C14-C15-C16
20	A	850	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	850	BCR	C16-C17-C18-C36
20	B	846	BCR	C11-C10-C9-C34
20	B	847	BCR	C11-C10-C9-C34
20	B	847	BCR	C20-C21-C22-C37
20	F	803	BCR	C35-C13-C14-C15
20	L	301	BCR	C11-C10-C9-C34
24	3	301	LUT	C21-C26-C27-C28
25	4	313	CHL	O1A-CGA-O2A-C1
17	B	813	CLA	C1A-C2A-CAA-CBA
17	A	853	CLA	CAA-CBA-CGA-O1A
17	1	505	CLA	C2A-CAA-CBA-CGA
22	J	104	DGD	C4D-C5D-C6D-O5D
20	A	850	BCR	C11-C10-C9-C8
20	A	850	BCR	C16-C17-C18-C19
20	B	846	BCR	C11-C10-C9-C8
20	B	847	BCR	C11-C10-C9-C8
20	B	847	BCR	C20-C21-C22-C23
20	F	803	BCR	C12-C13-C14-C15
20	L	301	BCR	C11-C10-C9-C8
17	4	305	CLA	CBA-CGA-O2A-C1
20	A	849	BCR	C19-C20-C21-C22
17	4	305	CLA	O1A-CGA-O2A-C1
17	3	312	CLA	C4-C3-C5-C6
17	4	317	CLA	C2-C1-O2A-CGA
17	B	836	CLA	CBA-CGA-O2A-C1
17	A	853	CLA	CAA-CBA-CGA-O2A
17	A	837	CLA	C3-C5-C6-C7
17	6	507	CLA	C4-C3-C5-C6
20	B	846	BCR	C23-C24-C25-C30
20	3	303	BCR	C1-C6-C7-C8
20	6	503	BCR	C1-C6-C7-C8
17	A	815	CLA	CAA-CBA-CGA-O2A
20	6	503	BCR	C15-C16-C17-C18
17	A	813	CLA	C1A-C2A-CAA-CBA
17	A	814	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	C16-C17-C18-C20
17	A	852	CLA	C2-C3-C5-C6
17	B	810	CLA	C8-C10-C11-C12
25	1	512	CHL	O1A-CGA-O2A-C1
17	A	819	CLA	C2A-CAA-CBA-CGA
17	A	815	CLA	CAA-CBA-CGA-O1A
19	A	845	LHG	C5-C6-O8-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	831	CLA	C4-C3-C5-C6
17	6	510	CLA	C4-C3-C5-C6
19	A	844	LHG	C25-C26-C27-C28
17	B	813	CLA	C6-C7-C8-C10
17	A	829	CLA	O1D-CGD-O2D-CED
17	A	835	CLA	CAA-CBA-CGA-O2A
17	A	829	CLA	C2-C3-C5-C6
17	A	837	CLA	C2-C3-C5-C6
17	3	312	CLA	C2-C3-C5-C6
17	A	829	CLA	C11-C10-C8-C9
17	B	826	CLA	C11-C10-C8-C9
17	B	836	CLA	C11-C10-C8-C9
17	4	306	CLA	C6-C7-C8-C9
22	B	851	DGD	C2B-C3B-C4B-C5B
17	A	837	CLA	C3A-C2A-CAA-CBA
17	A	852	CLA	C3A-C2A-CAA-CBA
17	4	309	CLA	C3A-C2A-CAA-CBA
17	A	805	CLA	CBA-CGA-O2A-C1
17	A	829	CLA	CBD-CGD-O2D-CED
17	A	803	CLA	CAD-CBD-CGD-O2D
17	A	815	CLA	CAD-CBD-CGD-O2D
17	A	816	CLA	CAD-CBD-CGD-O2D
17	A	821	CLA	CAD-CBD-CGD-O2D
17	A	822	CLA	CAD-CBD-CGD-O2D
17	A	824	CLA	CAD-CBD-CGD-O2D
17	A	840	CLA	CAD-CBD-CGD-O2D
17	A	853	CLA	CAD-CBD-CGD-O2D
17	B	803	CLA	CAD-CBD-CGD-O2D
17	B	814	CLA	CAD-CBD-CGD-O2D
17	B	815	CLA	CAD-CBD-CGD-O2D
17	B	820	CLA	CAD-CBD-CGD-O2D
17	B	821	CLA	CAD-CBD-CGD-O2D
17	B	824	CLA	CAD-CBD-CGD-O2D
17	B	827	CLA	CAD-CBD-CGD-O2D
17	B	831	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	B	837	CLA	CAD-CBD-CGD-O2D
17	B	839	CLA	CAD-CBD-CGD-O2D
17	3	307	CLA	CAD-CBD-CGD-O2D
17	3	310	CLA	CAD-CBD-CGD-O2D
17	4	312	CLA	CAD-CBD-CGD-O2D
17	6	510	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	1	517	CHL	CAD-CBD-CGD-O2D
25	6	517	CHL	CAD-CBD-CGD-O2D
17	A	836	CLA	C2A-CAA-CBA-CGA
17	L	304	CLA	CAA-CBA-CGA-O2A
17	B	820	CLA	CAA-CBA-CGA-O2A
17	B	809	CLA	C4-C3-C5-C6
17	B	818	CLA	C4-C3-C5-C6
17	6	505	CLA	C4-C3-C5-C6
20	A	848	BCR	C11-C12-C13-C14
24	1	502	LUT	C7-C8-C9-C10
24	3	301	LUT	C27-C28-C29-C30
17	L	304	CLA	CAA-CBA-CGA-O1A
17	6	505	CLA	CAA-CBA-CGA-O2A
17	A	843	CLA	O2A-C1-C2-C3
17	B	829	CLA	O2A-C1-C2-C3
17	1	508	CLA	O2A-C1-C2-C3
17	3	312	CLA	O2A-C1-C2-C3
25	4	314	CHL	O2A-C1-C2-C3
17	3	311	CLA	CAA-CBA-CGA-O2A
17	K	202	CLA	C2C-C3C-CAC-CBC
17	A	813	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	833	CLA	CHA-CBD-CGD-O1D
17	A	833	CLA	CHA-CBD-CGD-O2D
17	A	834	CLA	CHA-CBD-CGD-O2D
17	A	836	CLA	CHA-CBD-CGD-O1D
17	A	838	CLA	CHA-CBD-CGD-O2D
17	A	853	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	830	CLA	CHA-CBD-CGD-O2D
17	B	835	CLA	CHA-CBD-CGD-O1D
17	B	835	CLA	CHA-CBD-CGD-O2D
17	B	839	CLA	CHA-CBD-CGD-O1D
17	K	203	CLA	CHA-CBD-CGD-O1D
17	K	203	CLA	CHA-CBD-CGD-O2D
17	1	505	CLA	CHA-CBD-CGD-O1D
17	1	505	CLA	CHA-CBD-CGD-O2D
17	3	306	CLA	CHA-CBD-CGD-O1D
17	4	305	CLA	CHA-CBD-CGD-O2D
17	4	307	CLA	CHA-CBD-CGD-O2D
17	4	310	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	4	311	CLA	CHA-CBD-CGD-O1D
17	4	311	CLA	CHA-CBD-CGD-O2D
25	6	513	CHL	CHA-CBD-CGD-O1D
25	6	513	CHL	CHA-CBD-CGD-O2D
17	B	818	CLA	C2-C3-C5-C6
22	B	851	DGD	O2G-C2G-C3G-O3G
17	A	804	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	CAA-CBA-CGA-O2A
25	3	313	CHL	CAA-CBA-CGA-O2A
17	B	801	CLA	C2A-CAA-CBA-CGA
17	4	306	CLA	C15-C16-C17-C18
17	3	312	CLA	C8-C10-C11-C12
17	B	801	CLA	C6-C7-C8-C9
17	A	835	CLA	CAA-CBA-CGA-O1A
17	L	303	CLA	C2A-CAA-CBA-CGA
17	6	505	CLA	CAA-CBA-CGA-O1A
17	1	508	CLA	C4-C3-C5-C6
17	B	820	CLA	CAA-CBA-CGA-O1A
17	A	837	CLA	C1A-C2A-CAA-CBA
17	3	305	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C2-C1-O2A-CGA
17	4	306	CLA	C2-C1-O2A-CGA
20	B	845	BCR	C15-C16-C17-C18
17	A	826	CLA	C8-C10-C11-C12
23	J	105	LMG	O7-C10-C11-C12
17	B	811	CLA	CAA-CBA-CGA-O1A
19	6	516	LHG	C3-O3-P-O5
22	B	851	DGD	C2A-C3A-C4A-C5A
17	K	202	CLA	CAA-CBA-CGA-O2A
20	B	846	BCR	C1-C6-C7-C8
20	B	846	BCR	C23-C24-C25-C26
20	6	503	BCR	C5-C6-C7-C8
24	3	302	LUT	C5-C6-C7-C8
17	6	506	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	CAA-CBA-CGA-O2A
17	3	315	CLA	CAA-CBA-CGA-O2A
17	K	202	CLA	CAA-CBA-CGA-O1A
17	A	813	CLA	CAD-CBD-CGD-O1D
17	A	836	CLA	CAD-CBD-CGD-O1D
17	A	836	CLA	C2-C3-C5-C6
17	A	837	CLA	CAD-CBD-CGD-O1D
17	B	825	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	515	CLA	CAD-CBD-CGD-O1D
17	4	304	CLA	CAD-CBD-CGD-O1D
17	4	307	CLA	CAD-CBD-CGD-O1D
17	4	317	CLA	CAD-CBD-CGD-O1D
17	A	804	CLA	CAA-CBA-CGA-O1A
25	1	514	CHL	CAA-CBA-CGA-O1A
17	B	801	CLA	CAA-CBA-CGA-O2A
17	B	818	CLA	CAA-CBA-CGA-O2A
17	B	836	CLA	C6-C7-C8-C9
17	L	303	CLA	C11-C10-C8-C9
17	A	816	CLA	CAA-CBA-CGA-O2A
17	A	852	CLA	CAA-CBA-CGA-O2A
25	3	313	CHL	CAA-CBA-CGA-O1A
17	6	506	CLA	C11-C12-C13-C15
17	3	311	CLA	CAA-CBA-CGA-O1A
23	J	105	LMG	O9-C10-C11-C12
17	B	835	CLA	CAA-CBA-CGA-O2A
19	A	845	LHG	O7-C7-C8-C9
20	I	101	BCR	C21-C22-C23-C24
24	6	501	LUT	C11-C12-C13-C14
17	A	816	CLA	CAA-CBA-CGA-O1A
22	B	851	DGD	O2G-C1B-C2B-C3B
17	B	801	CLA	CAA-CBA-CGA-O1A
17	A	843	CLA	CAA-CBA-CGA-O2A
17	3	305	CLA	CAA-CBA-CGA-O2A
17	A	852	CLA	CAA-CBA-CGA-O1A
19	A	845	LHG	O9-C7-C8-C9
17	A	827	CLA	C2C-C3C-CAC-CBC
17	6	506	CLA	CAA-CBA-CGA-O1A
17	B	804	CLA	CAA-CBA-CGA-O1A
17	B	835	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

169 monomers are involved in 416 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	833	CLA	3	0
17	A	834	CLA	1	0
17	B	806	CLA	2	0
17	A	802	CLA	1	0
17	1	506	CLA	6	0
19	1	516	LHG	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	813	CLA	2	0
17	K	202	CLA	1	0
17	L	303	CLA	2	0
20	B	850	BCR	4	0
25	1	514	CHL	3	0
17	A	809	CLA	4	0
17	B	828	CLA	1	0
23	J	105	LMG	1	0
17	A	825	CLA	3	0
17	6	508	CLA	1	0
20	L	305	BCR	2	0
17	A	828	CLA	2	0
17	3	306	CLA	3	0
17	A	824	CLA	1	0
17	A	853	CLA	3	0
17	A	827	CLA	3	0
17	B	804	CLA	6	0
17	B	810	CLA	3	0
17	1	505	CLA	2	0
17	3	308	CLA	1	0
19	A	845	LHG	1	0
17	A	832	CLA	1	0
17	4	308	CLA	2	0
24	1	502	LUT	6	0
25	4	313	CHL	1	0
17	B	843	CLA	1	0
17	6	514	CLA	2	0
20	F	803	BCR	1	0
17	6	511	CLA	6	0
17	A	804	CLA	4	0
20	B	845	BCR	1	0
20	I	102	BCR	4	0
17	A	810	CLA	7	0
20	J	103	BCR	3	0
25	3	313	CHL	1	0
24	3	302	LUT	6	0
17	3	311	CLA	2	0
17	B	819	CLA	4	0
17	L	304	CLA	4	0
17	4	310	CLA	1	0
17	1	509	CLA	3	0
17	B	840	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	6	503	BCR	4	0
17	B	839	CLA	1	0
17	3	307	CLA	3	0
17	A	843	CLA	2	0
17	B	833	CLA	3	0
25	1	512	CHL	1	0
17	3	316	CLA	1	0
20	4	301	BCR	5	0
16	A	801	CL0	6	0
17	A	808	CLA	3	0
20	I	101	BCR	1	0
19	6	516	LHG	1	0
17	4	315	CLA	2	0
17	B	821	CLA	6	0
17	4	306	CLA	7	0
20	B	847	BCR	1	0
17	4	317	CLA	1	0
17	6	504	CLA	1	0
20	F	801	BCR	1	0
17	1	515	CLA	4	0
17	B	831	CLA	2	0
17	B	834	CLA	3	0
17	1	504	CLA	8	0
17	A	805	CLA	1	0
17	A	807	CLA	3	0
17	4	311	CLA	1	0
17	4	312	CLA	1	0
17	A	852	CLA	6	0
17	K	203	CLA	1	0
20	A	846	BCR	5	0
20	1	503	BCR	1	0
17	B	826	CLA	6	0
17	B	832	CLA	4	0
17	1	511	CLA	1	0
26	6	502	XAT	9	0
17	B	813	CLA	4	0
17	3	304	CLA	3	0
19	A	844	LHG	1	0
17	6	509	CLA	2	0
20	K	204	BCR	1	0
17	B	815	CLA	2	0
20	A	848	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	818	CLA	4	0
17	3	310	CLA	1	0
25	6	517	CHL	1	0
17	A	826	CLA	3	0
17	6	506	CLA	7	0
17	A	838	CLA	7	0
17	A	829	CLA	1	0
17	A	816	CLA	1	0
20	B	848	BCR	3	0
17	3	305	CLA	1	0
17	A	837	CLA	2	0
17	B	820	CLA	1	0
17	A	821	CLA	2	0
17	A	803	CLA	4	0
17	4	307	CLA	5	0
17	6	510	CLA	6	0
25	6	512	CHL	4	0
17	B	816	CLA	4	0
17	B	807	CLA	5	0
17	B	811	CLA	2	0
17	K	201	CLA	1	0
24	6	501	LUT	6	0
17	A	814	CLA	1	0
22	J	104	DGD	2	0
17	A	815	CLA	1	0
17	4	305	CLA	2	0
24	1	501	LUT	6	0
17	A	817	CLA	2	0
17	1	513	CLA	1	0
26	4	303	XAT	3	0
17	3	309	CLA	1	0
24	3	301	LUT	5	0
22	B	851	DGD	2	0
17	B	838	CLA	3	0
17	4	304	CLA	2	0
20	A	849	BCR	4	0
20	A	850	BCR	2	0
21	C	101	SF4	1	0
17	B	808	CLA	7	0
17	3	315	CLA	6	0
18	A	842	PQN	2	0
19	B	852	LHG	1	0

Continued on next page...

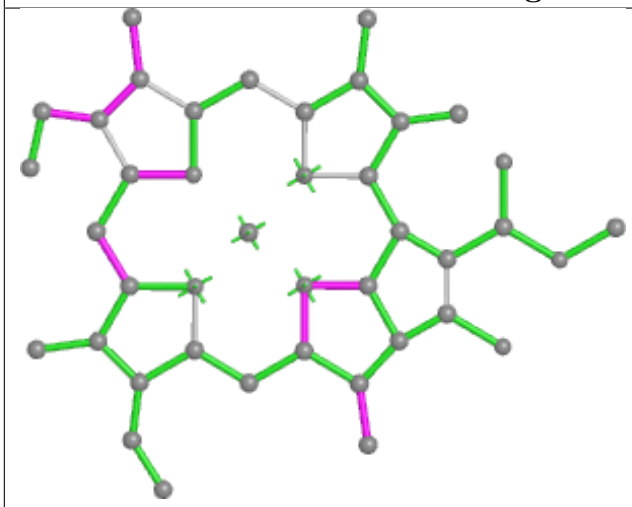
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	812	CLA	5	0
17	B	842	CLA	1	0
17	B	823	CLA	1	0
17	B	829	CLA	1	0
20	A	854	BCR	4	0
24	4	302	LUT	9	0
17	B	827	CLA	3	0
17	A	836	CLA	2	0
17	B	835	CLA	6	0
20	B	849	BCR	4	0
20	A	851	BCR	5	0
25	6	513	CHL	2	0
17	A	839	CLA	5	0
17	A	818	CLA	4	0
17	L	302	CLA	1	0
20	L	301	BCR	1	0
17	B	805	CLA	2	0
17	B	801	CLA	4	0
20	3	303	BCR	3	0
17	A	819	CLA	1	0
17	B	825	CLA	1	0
17	J	101	CLA	1	0
17	4	309	CLA	1	0
20	A	847	BCR	2	0
25	6	515	CHL	1	0
17	3	312	CLA	4	0
17	B	803	CLA	4	0
17	3	314	CLA	4	0
17	A	806	CLA	1	0
25	1	517	CHL	2	0
25	4	316	CHL	2	0
17	A	830	CLA	3	0
17	A	820	CLA	2	0
17	6	505	CLA	3	0
18	B	844	PQN	7	0
17	1	510	CLA	2	0
17	1	507	CLA	2	0

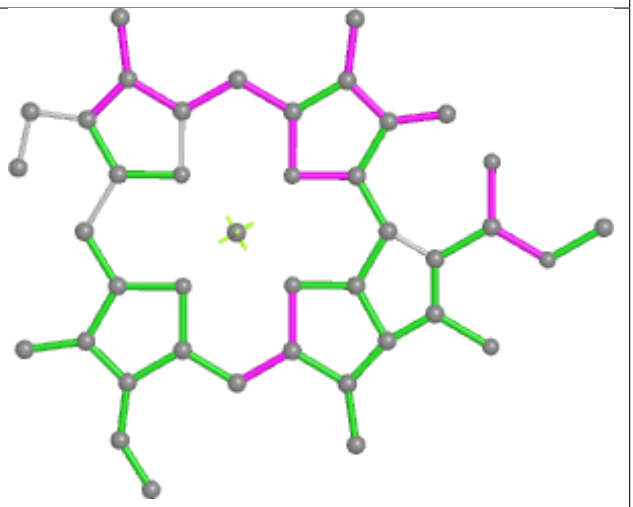
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

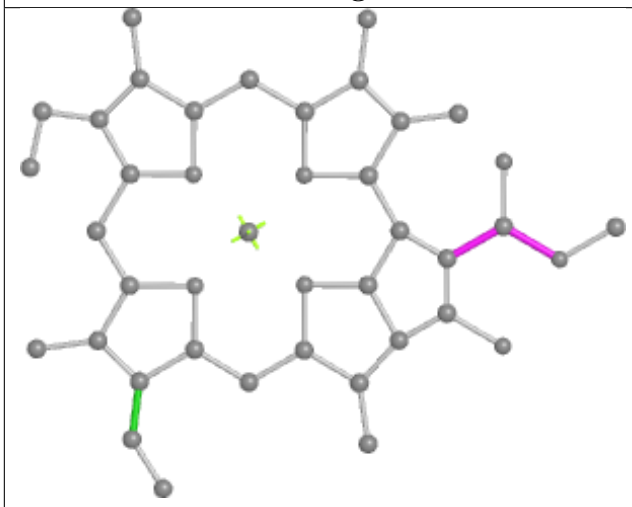
Ligand CLA A 833



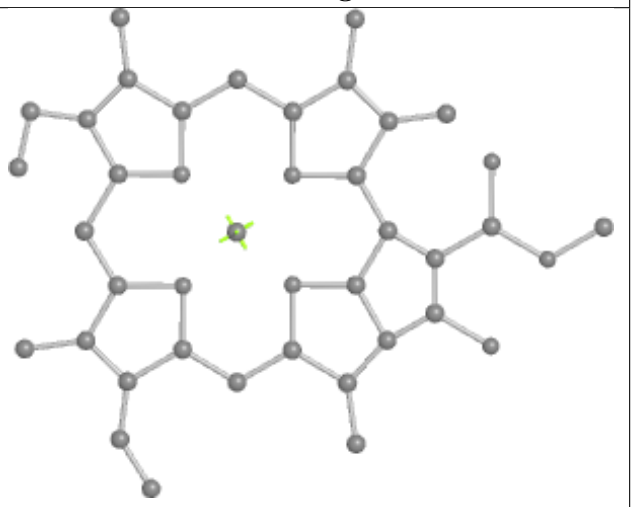
Bond lengths



Bond angles

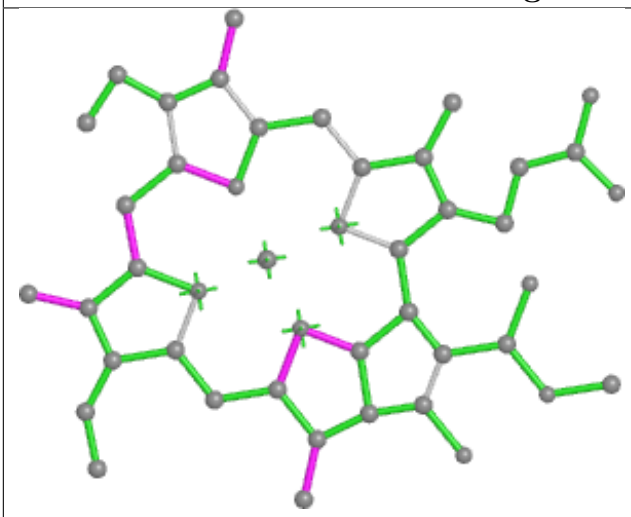


Torsions

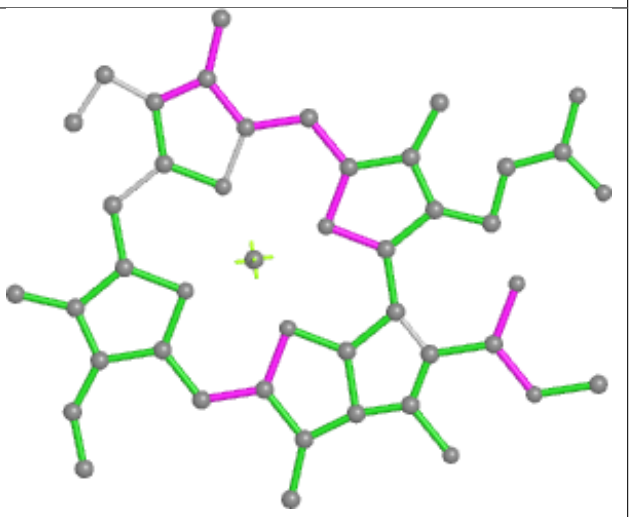


Rings

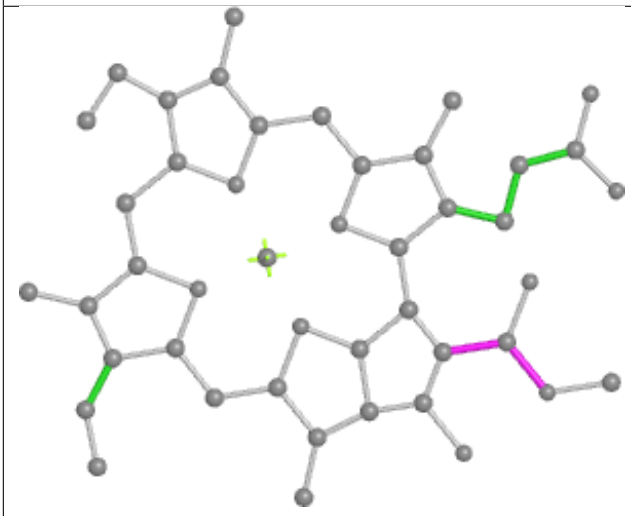
Ligand CLA A 834



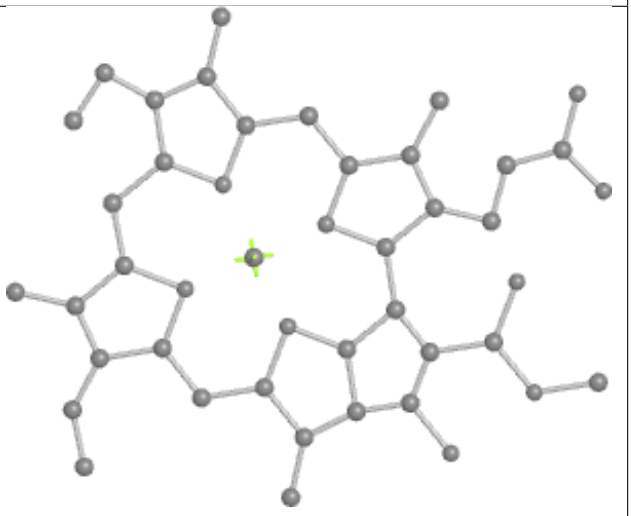
Bond lengths



Bond angles

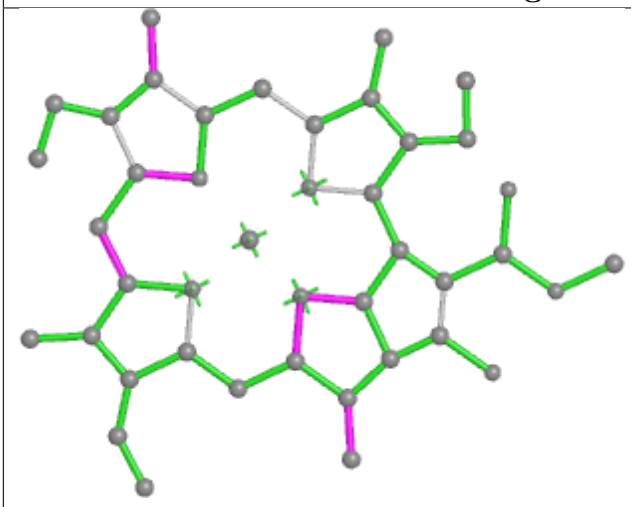


Torsions

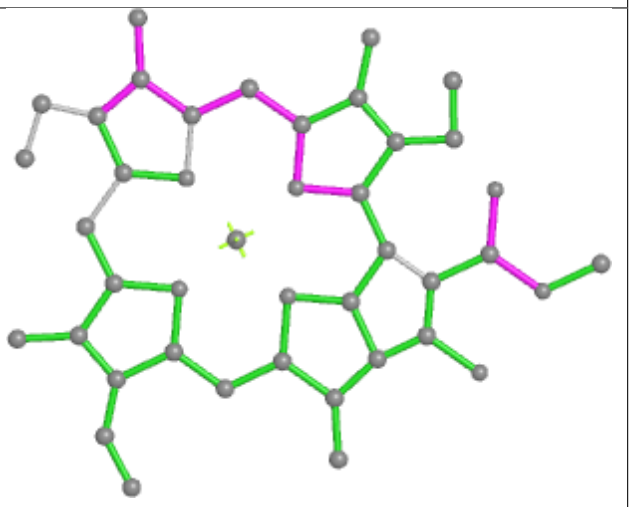


Rings

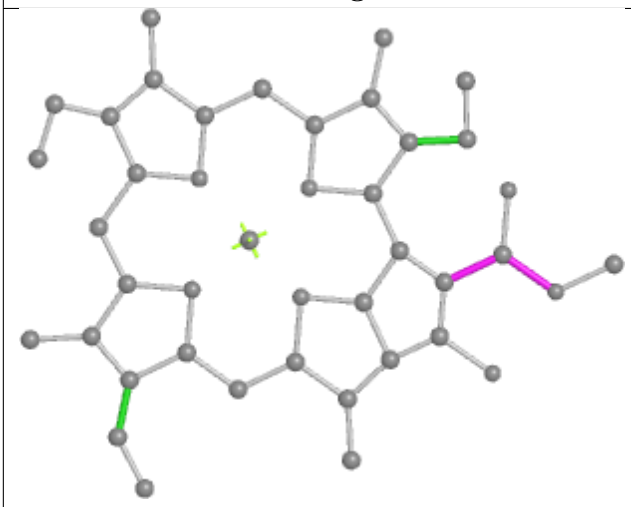
Ligand CLA B 837



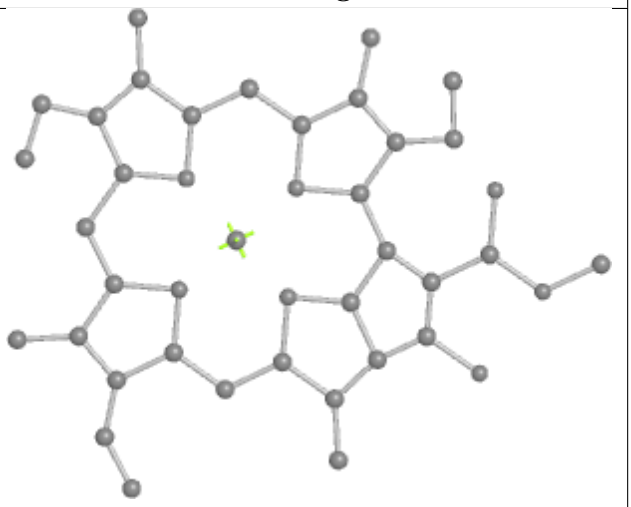
Bond lengths



Bond angles

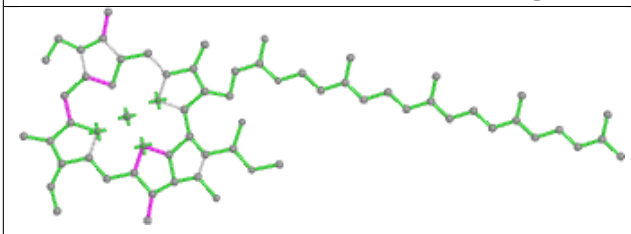


Torsions

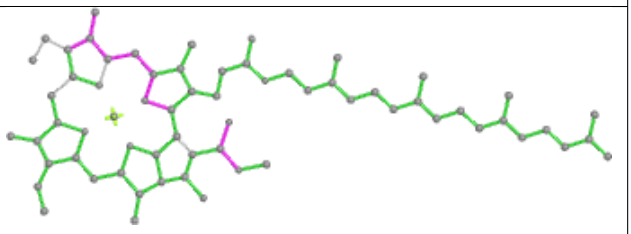


Rings

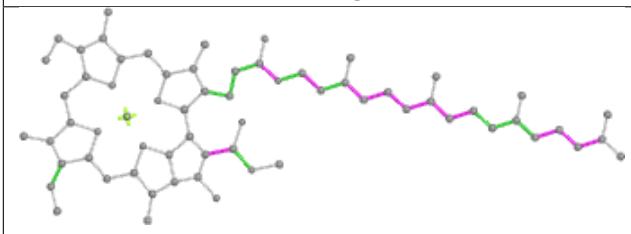
Ligand CLA 1 508



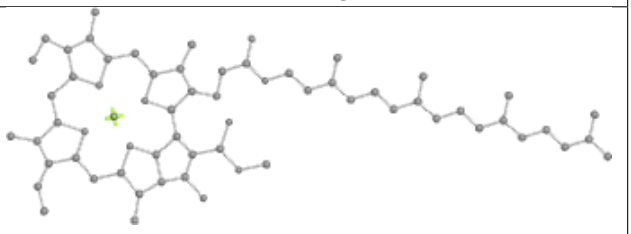
Bond lengths



Bond angles

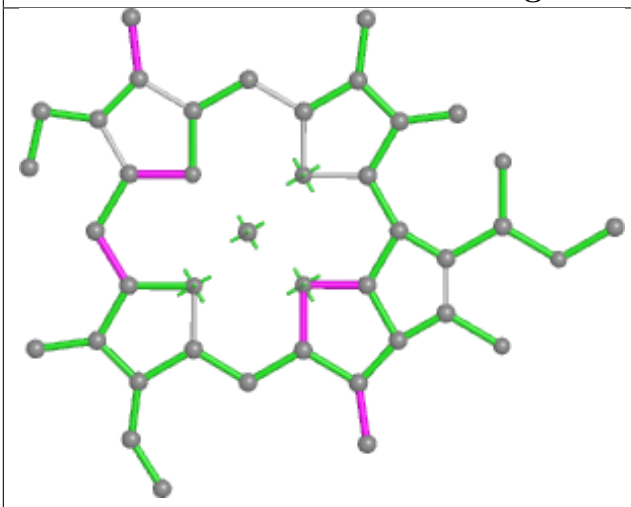


Torsions

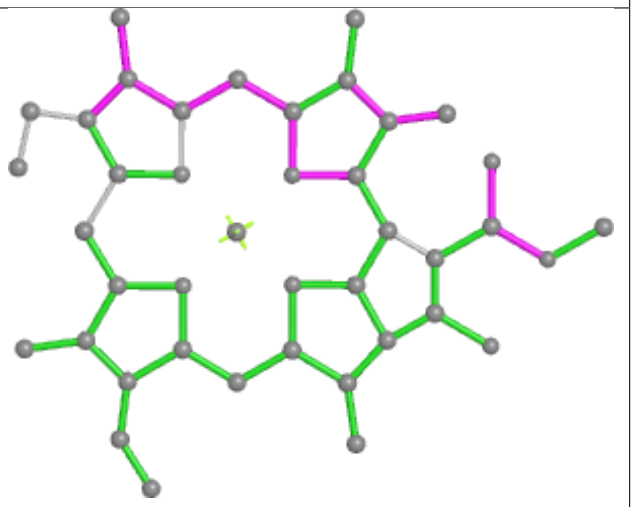


Rings

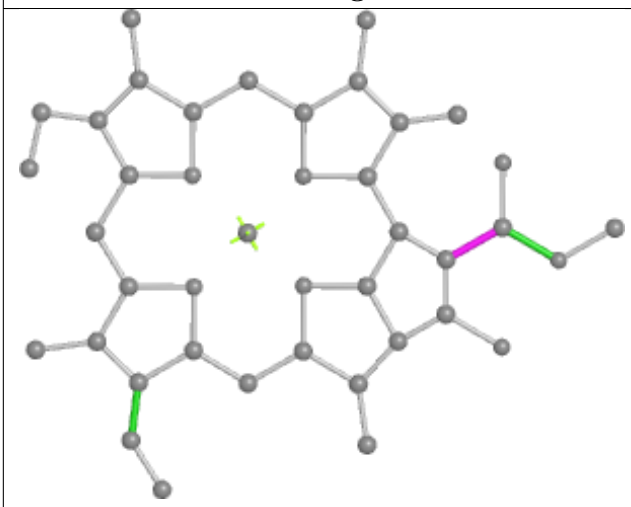
Ligand CLA B 806



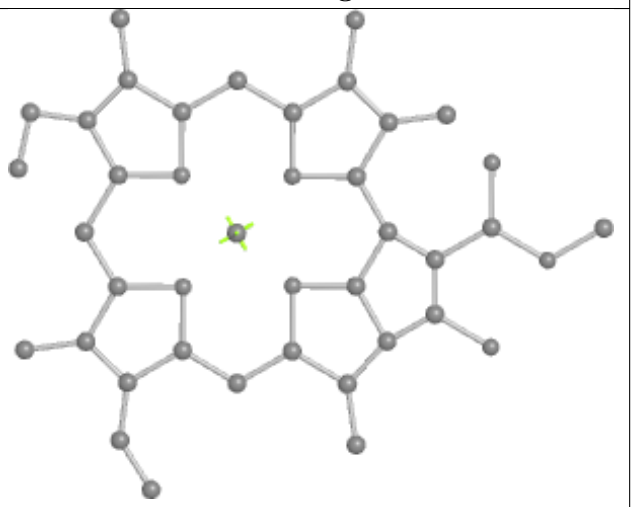
Bond lengths



Bond angles

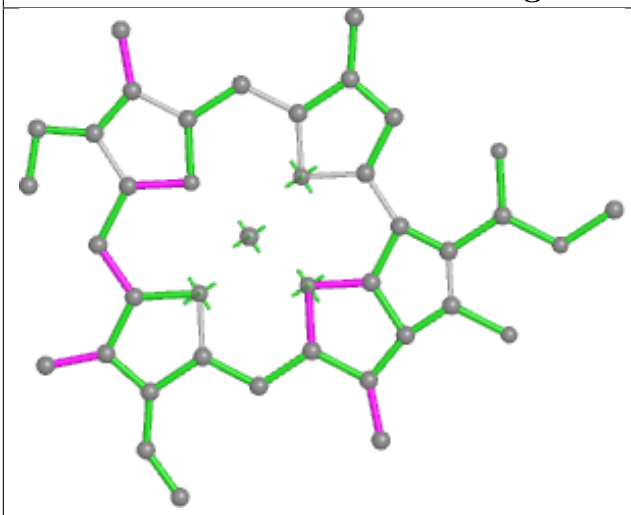


Torsions

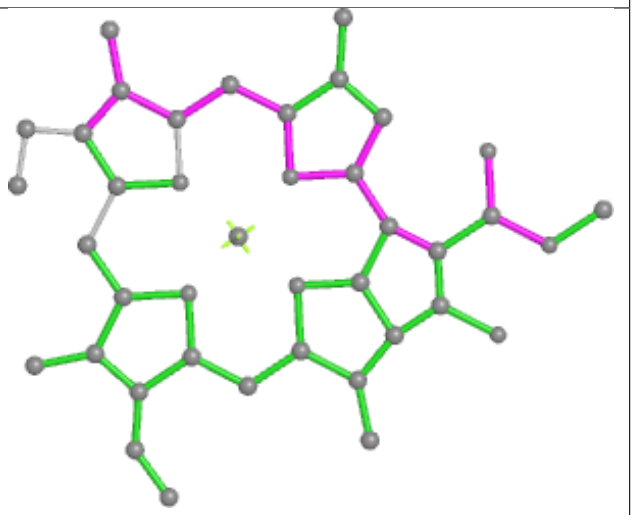


Rings

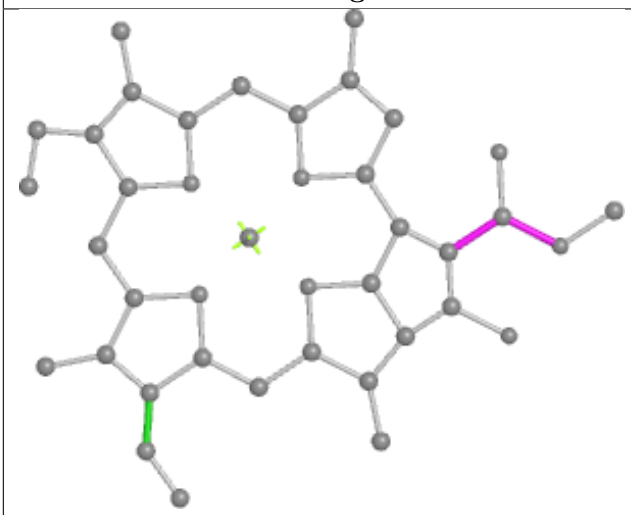
Ligand CLA A 802



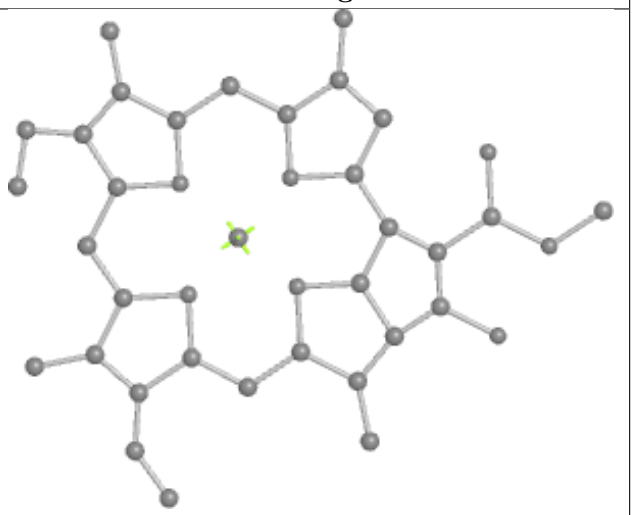
Bond lengths



Bond angles

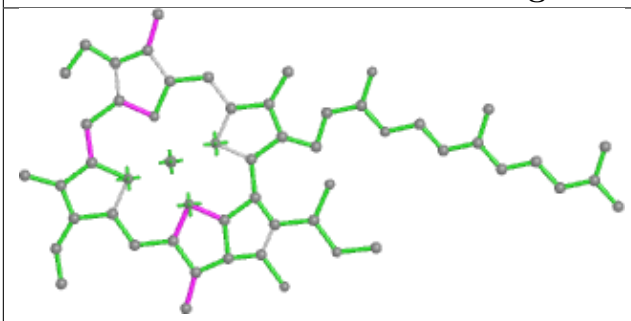


Torsions

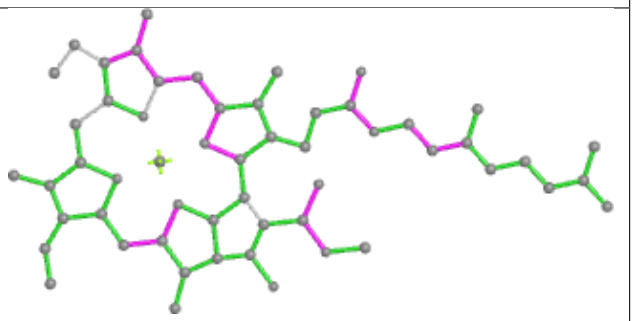


Rings

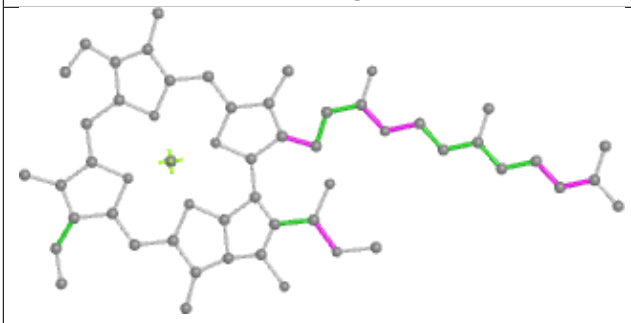
Ligand CLA 1 506



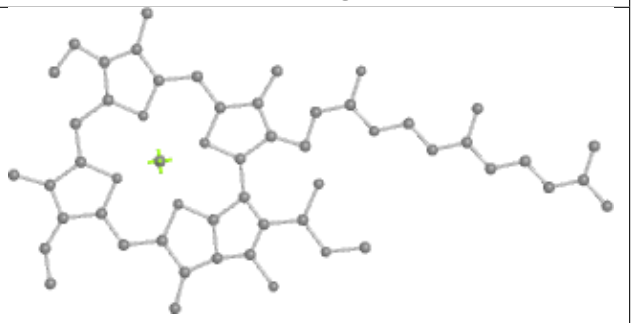
Bond lengths



Bond angles

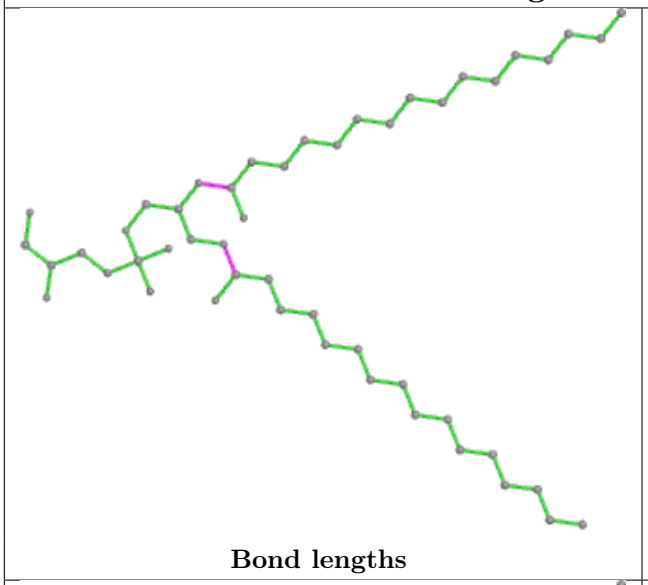


Torsions

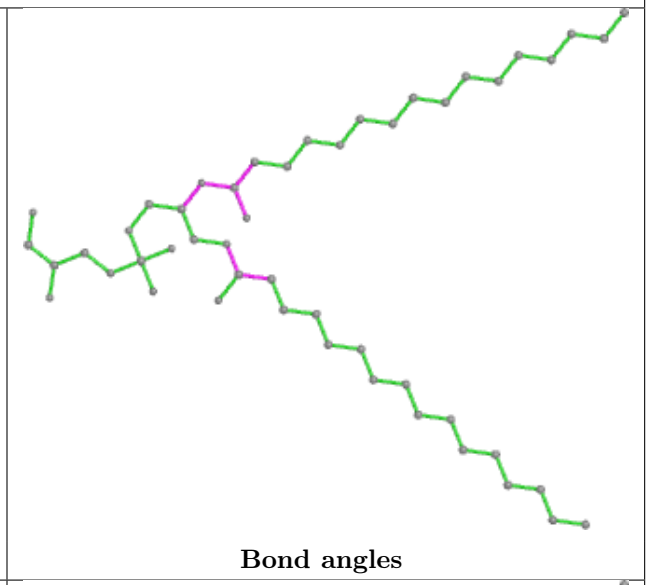


Rings

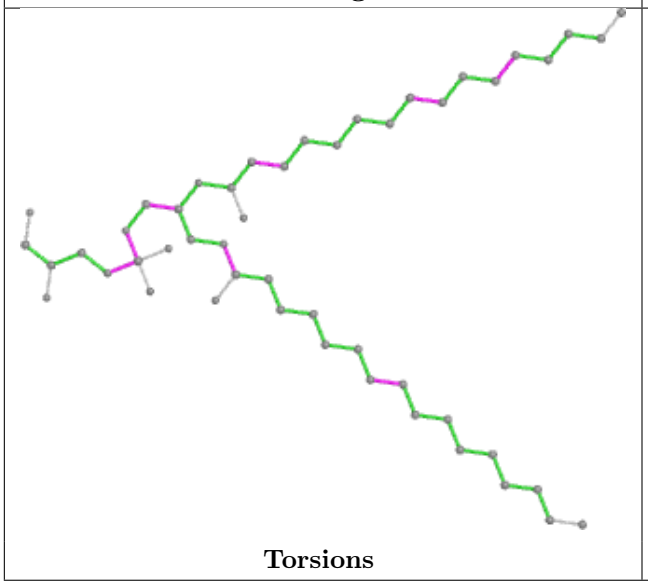
Ligand LHG 1 516



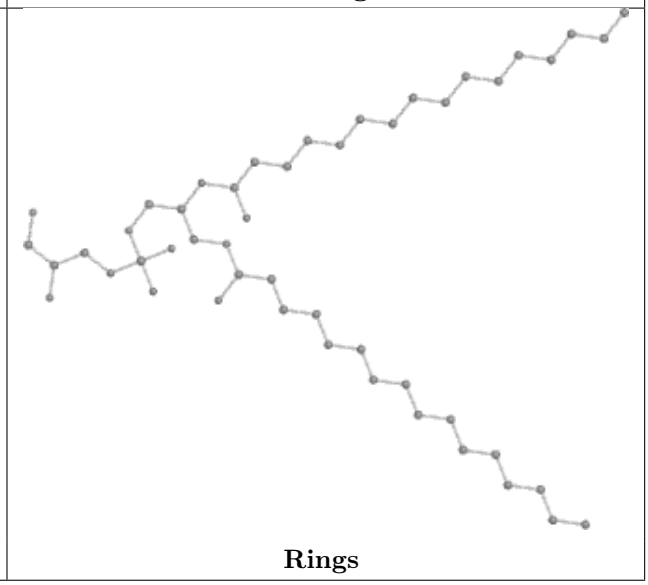
Bond lengths



Bond angles

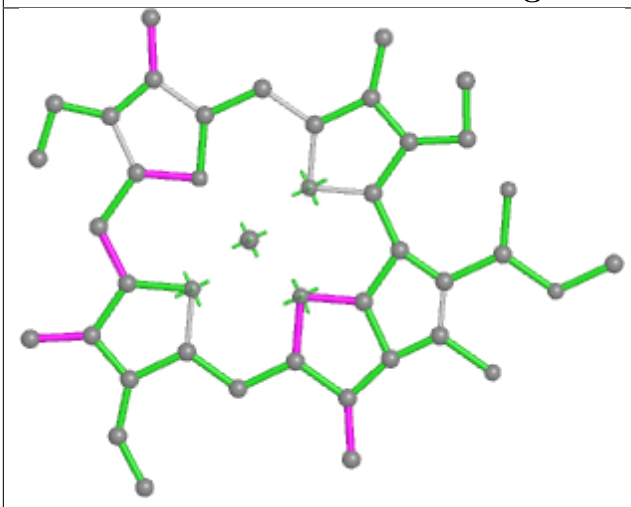


Torsions

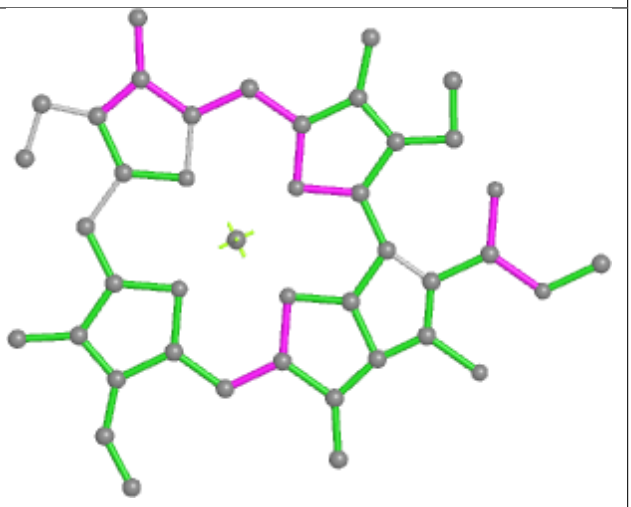


Rings

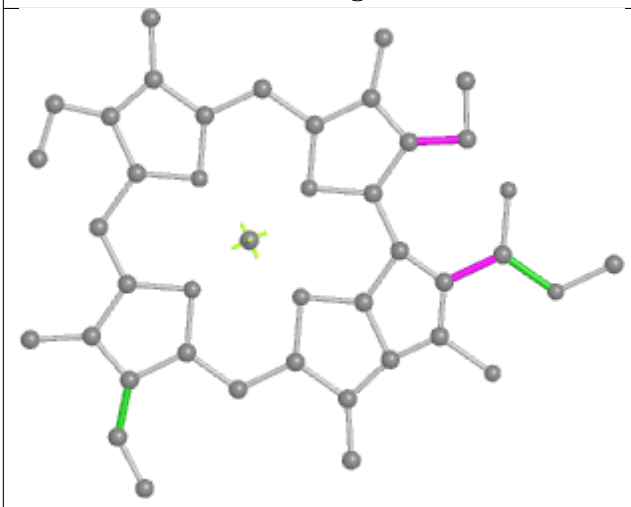
Ligand CLA A 813



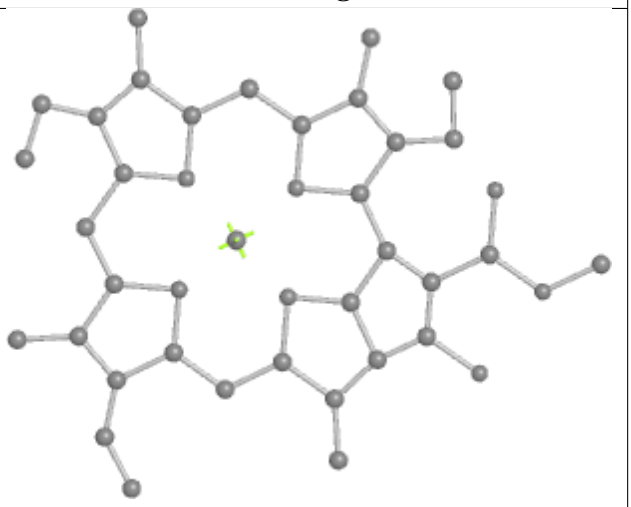
Bond lengths



Bond angles

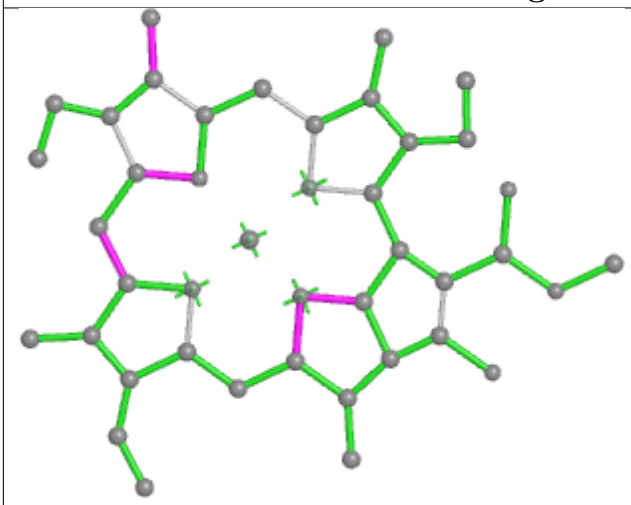


Torsions

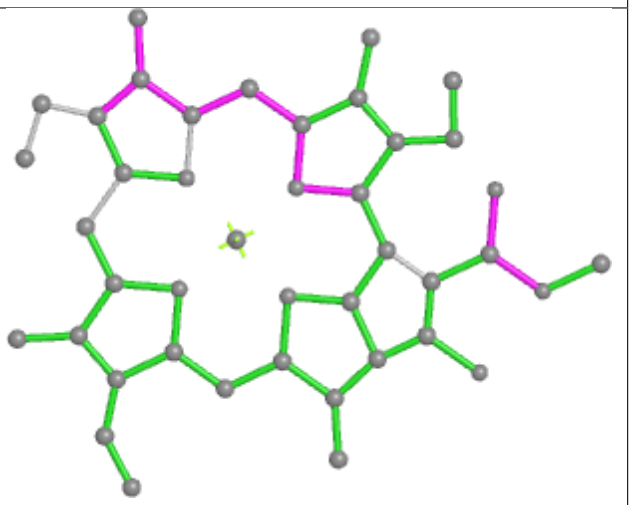


Rings

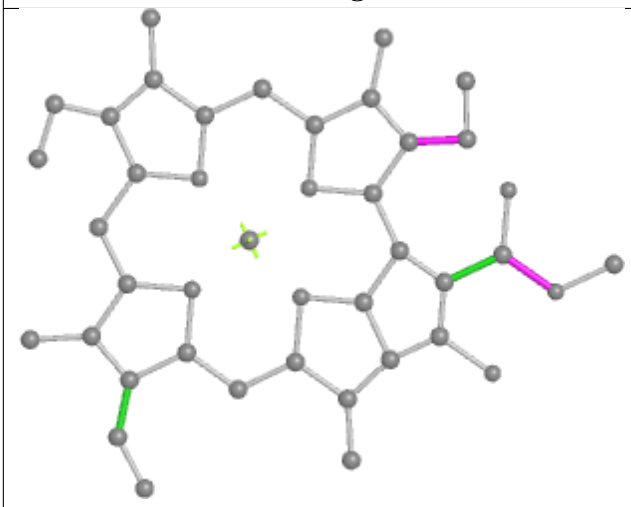
Ligand CLA J 102



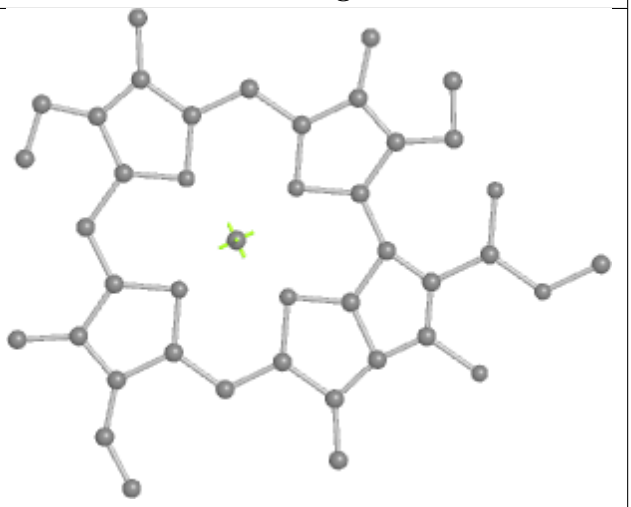
Bond lengths



Bond angles

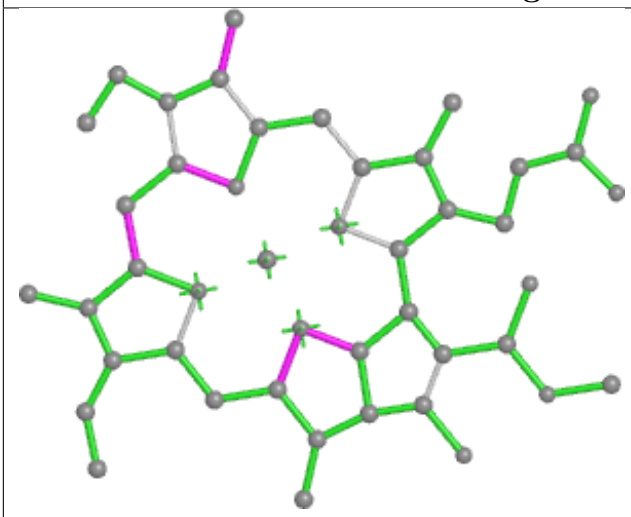


Torsions

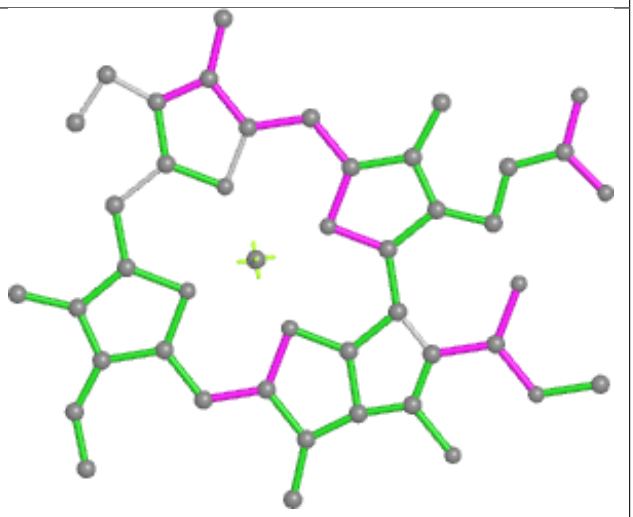


Rings

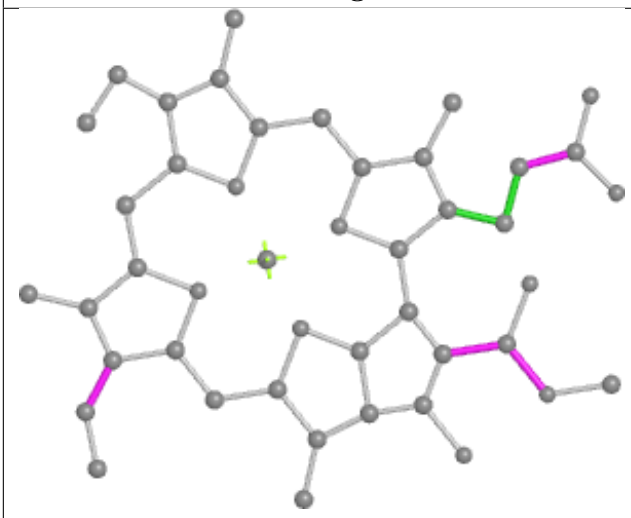
Ligand CLA K 202



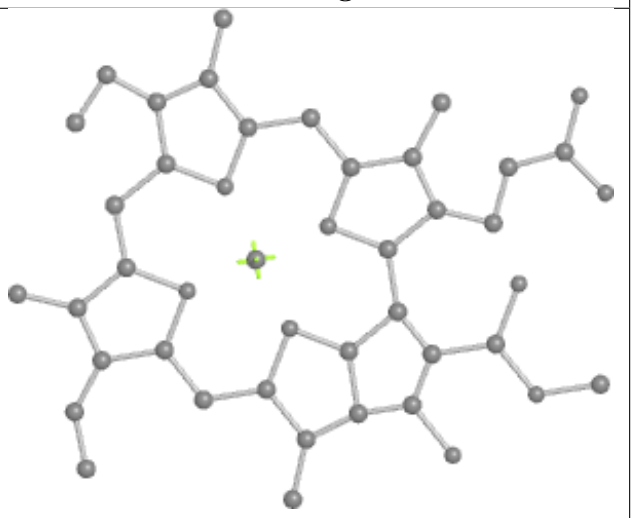
Bond lengths



Bond angles

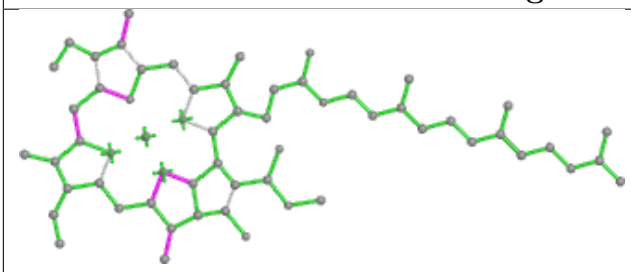


Torsions

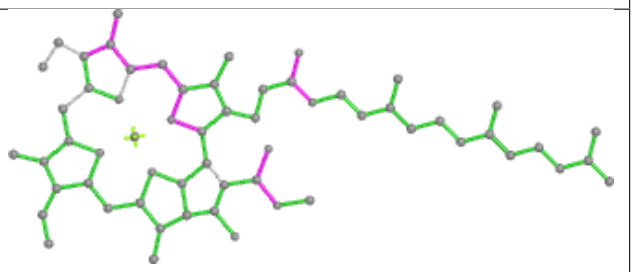


Rings

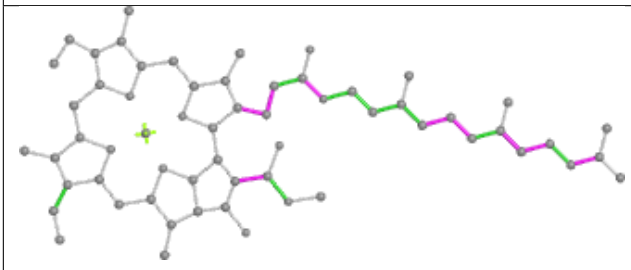
Ligand CLA L 303



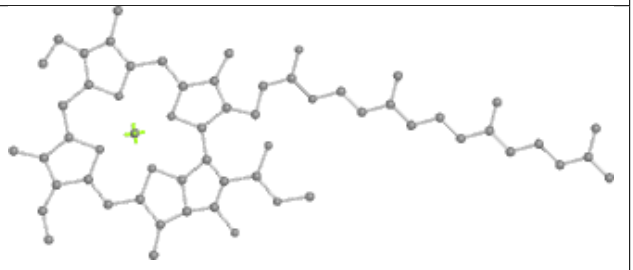
Bond lengths



Bond angles

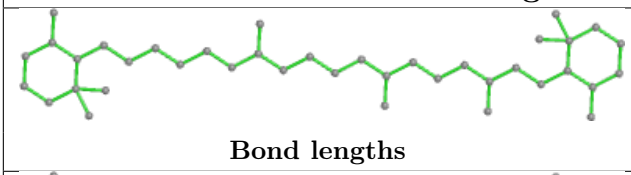


Torsions

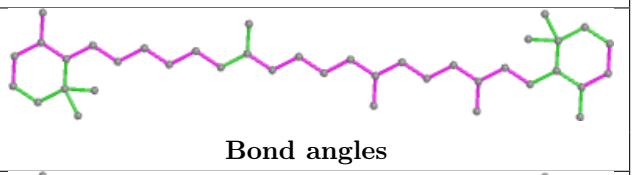


Rings

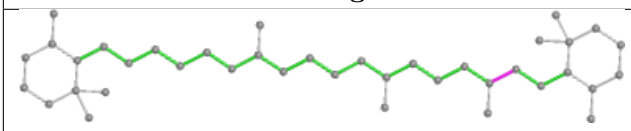
Ligand BCR B 850



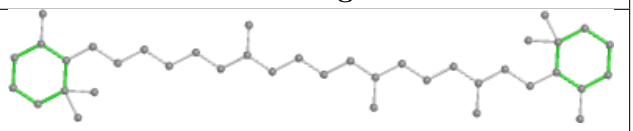
Bond lengths



Bond angles

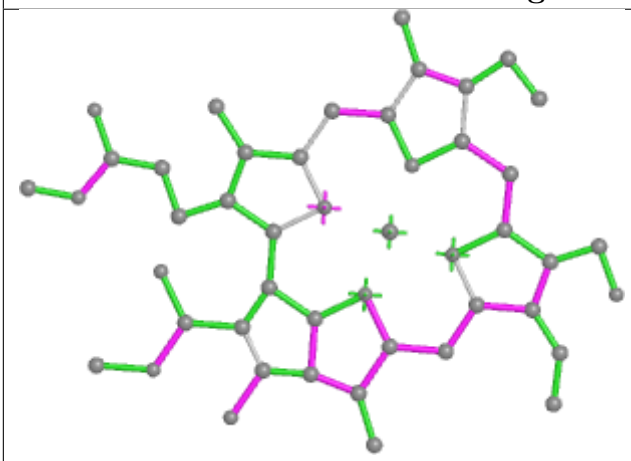


Torsions

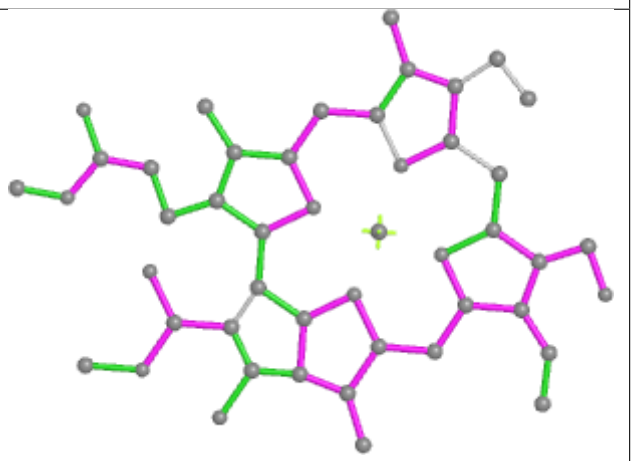


Rings

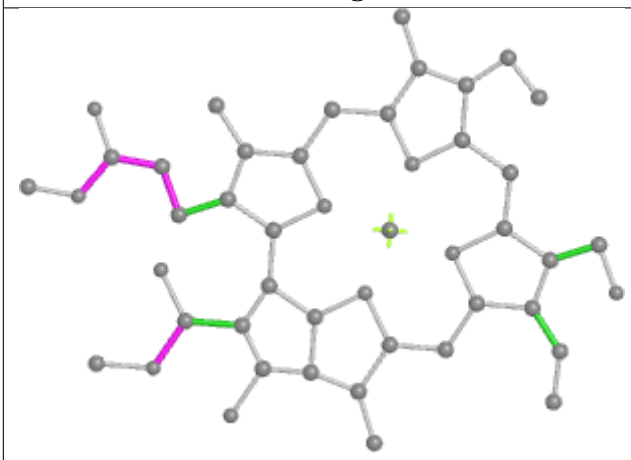
Ligand CHL 1 514



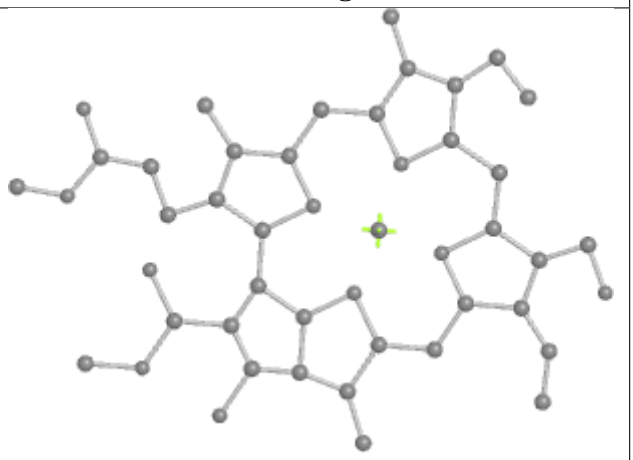
Bond lengths



Bond angles

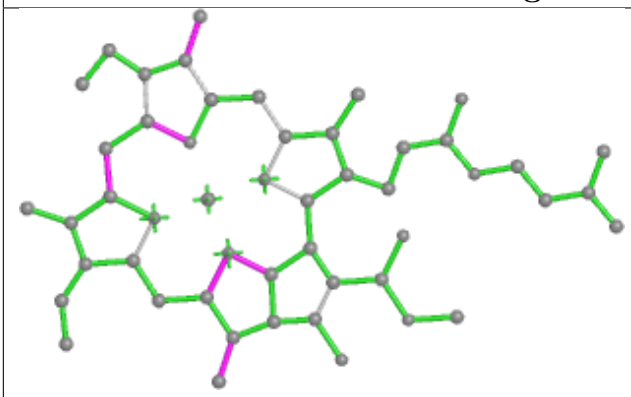


Torsions

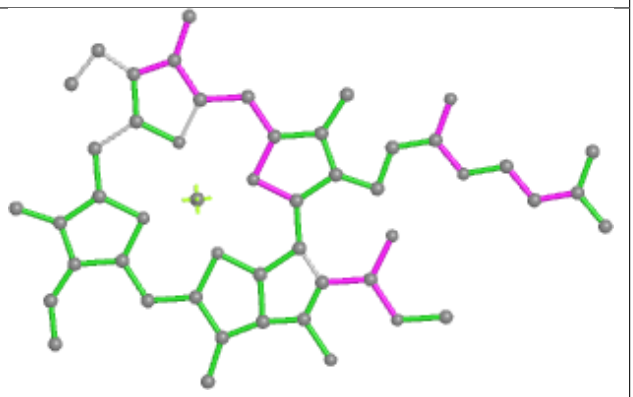


Rings

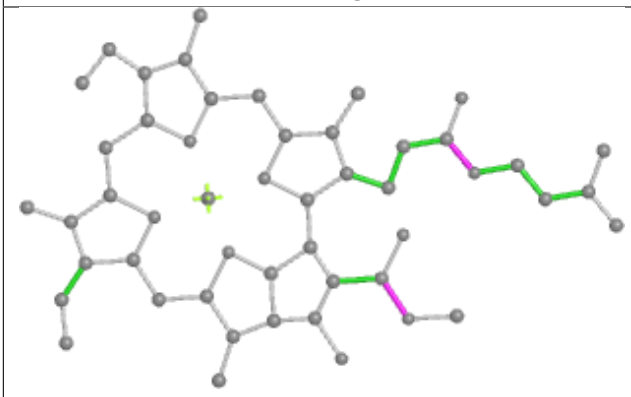
Ligand CLA A 809



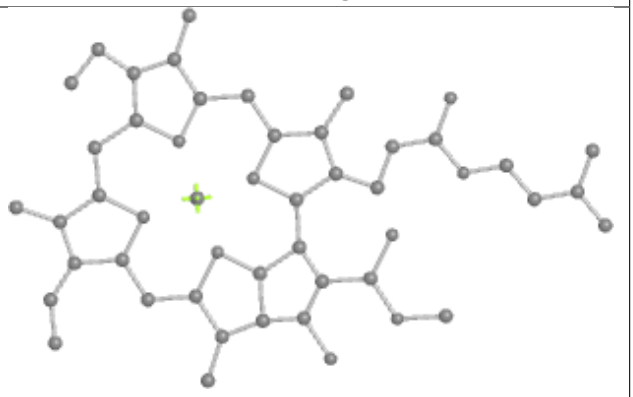
Bond lengths



Bond angles

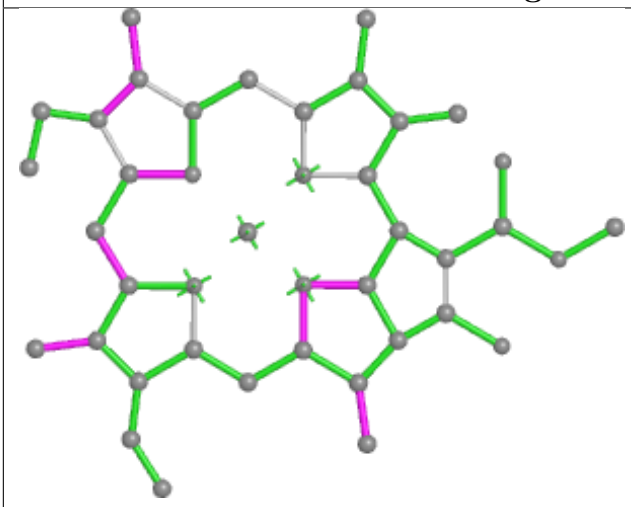


Torsions

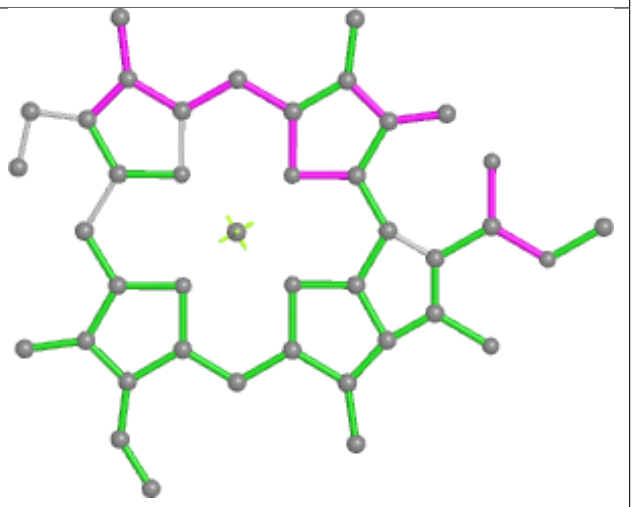


Rings

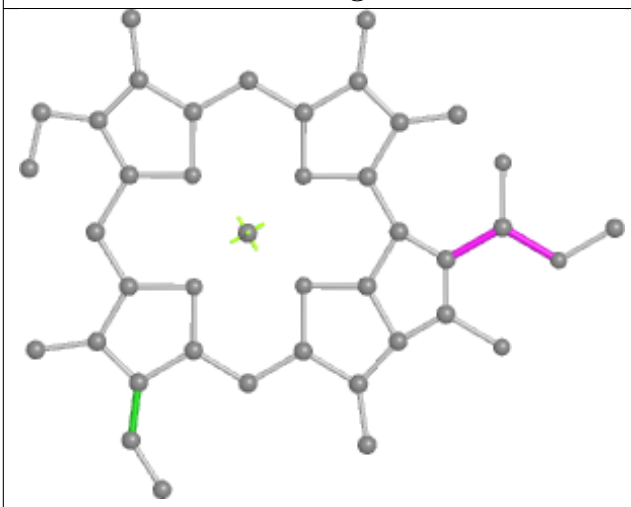
Ligand CLA B 828



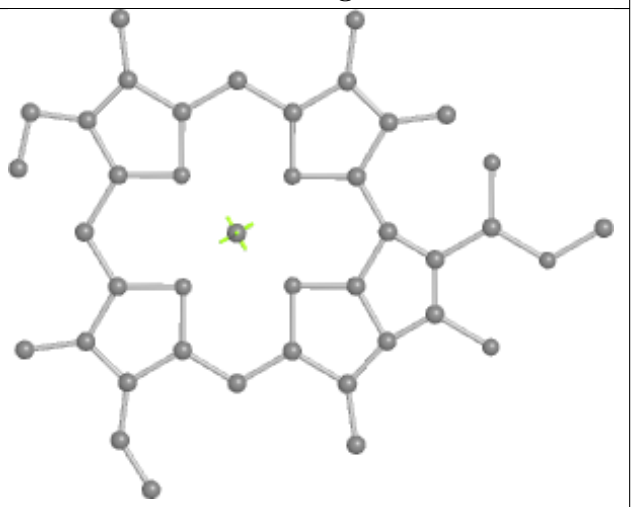
Bond lengths



Bond angles

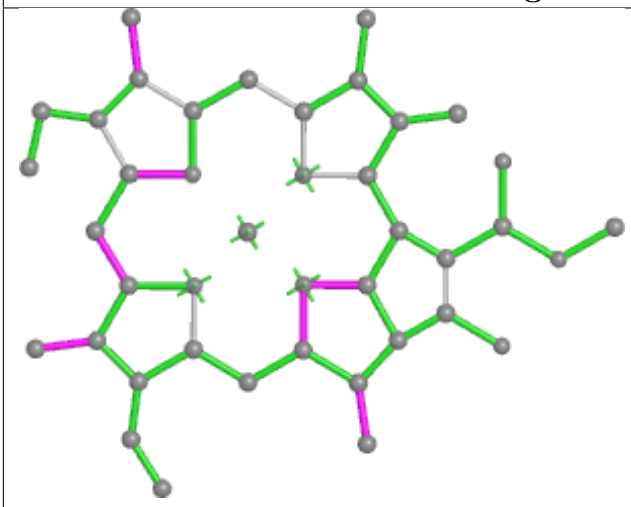


Torsions

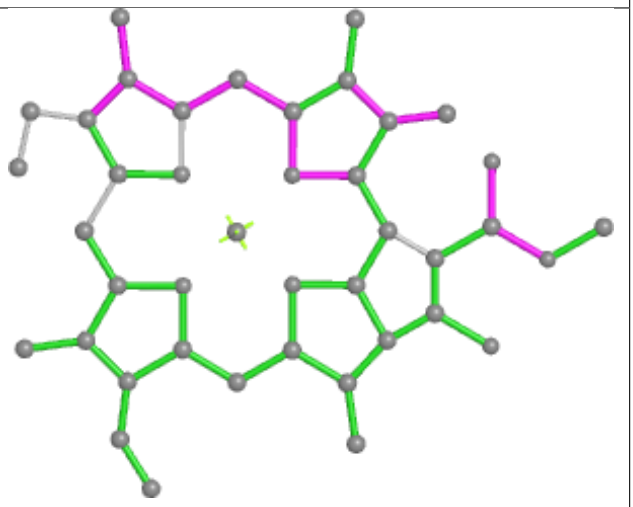


Rings

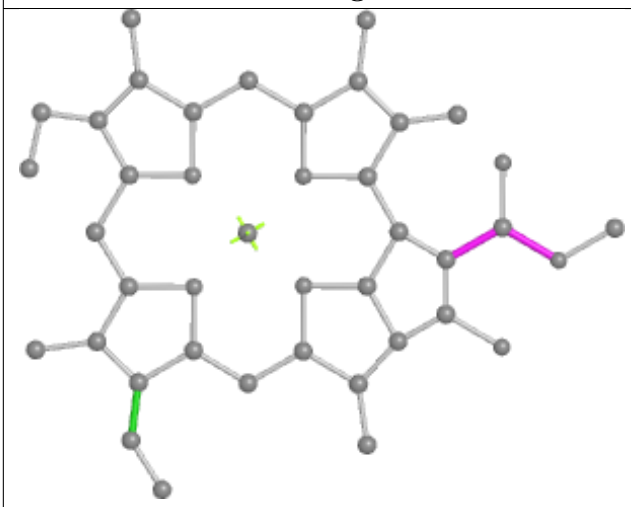
Ligand CLA B 841



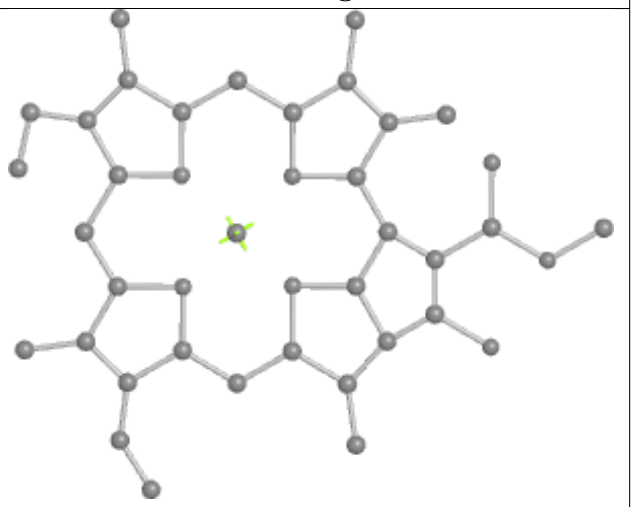
Bond lengths



Bond angles

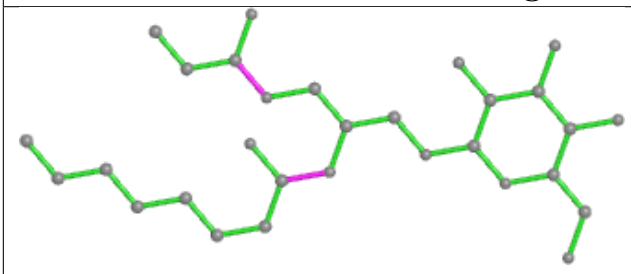


Torsions

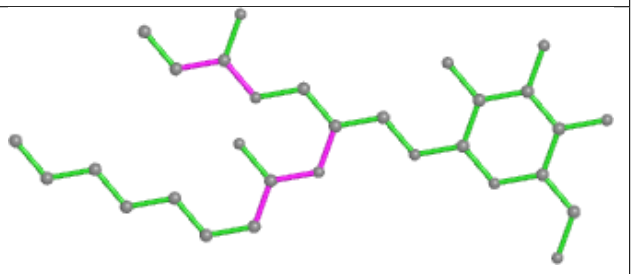


Rings

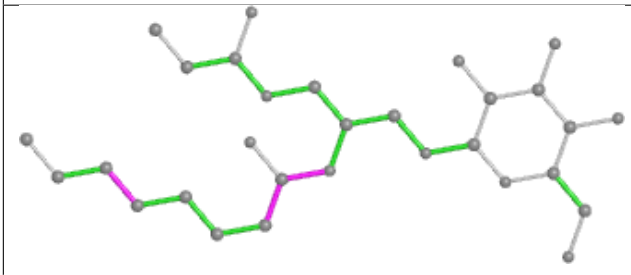
Ligand LMG J 105



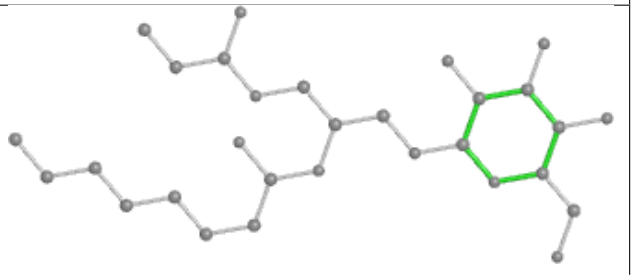
Bond lengths



Bond angles

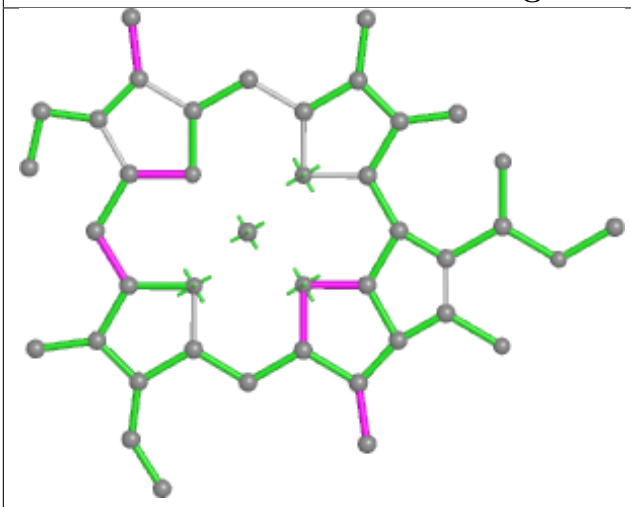


Torsions

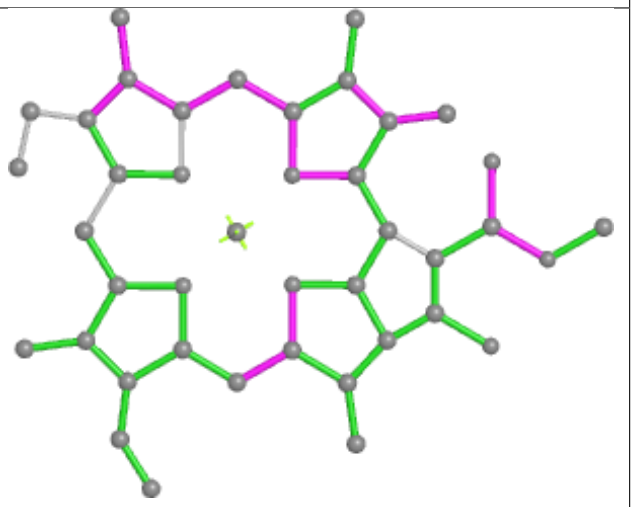


Rings

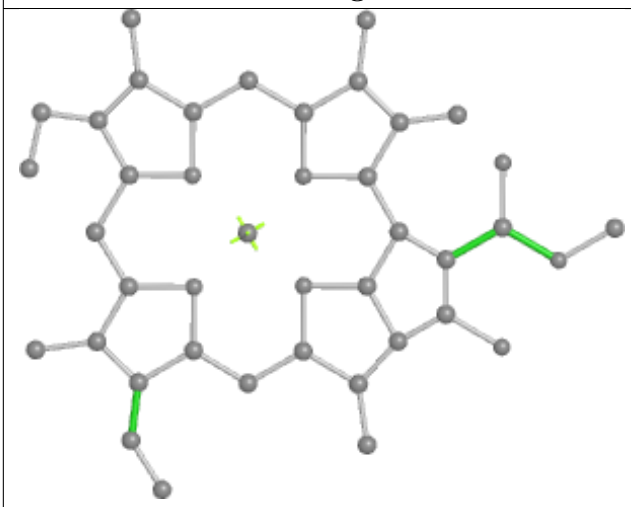
Ligand CLA A 825



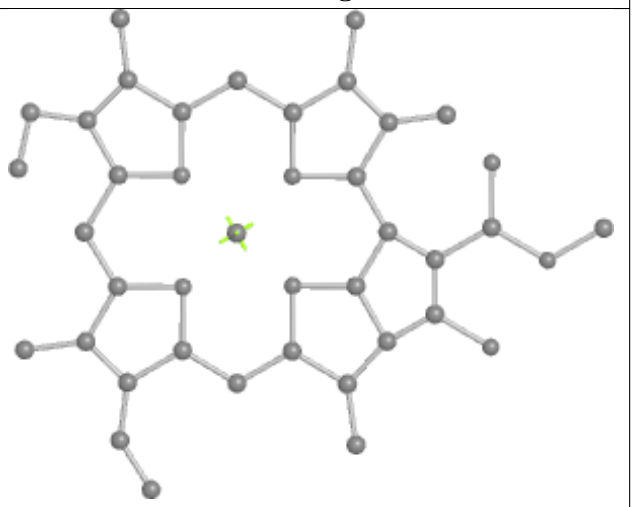
Bond lengths



Bond angles

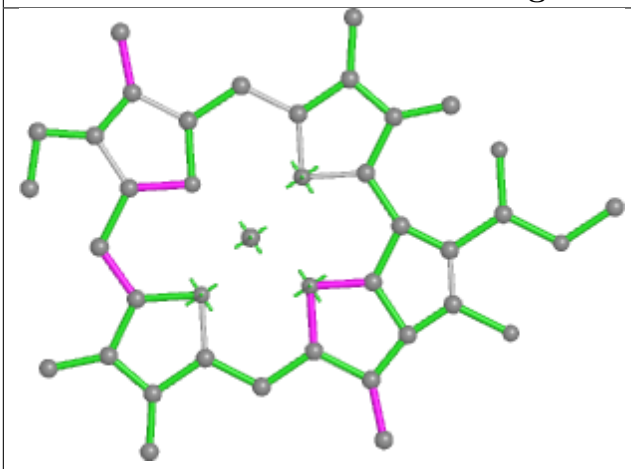


Torsions

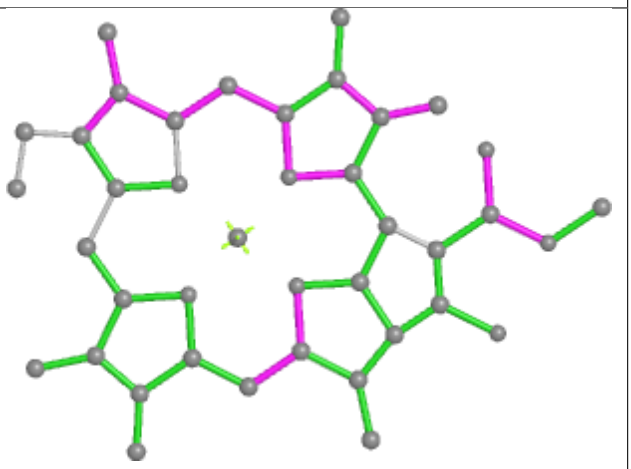


Rings

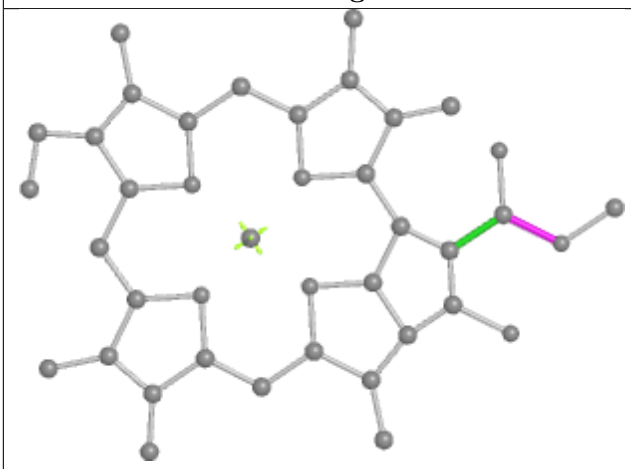
Ligand CLA 6 508



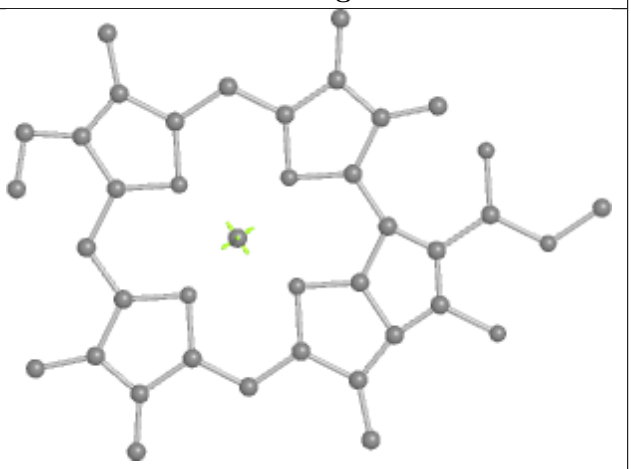
Bond lengths



Bond angles

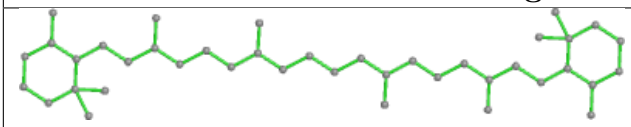


Torsions

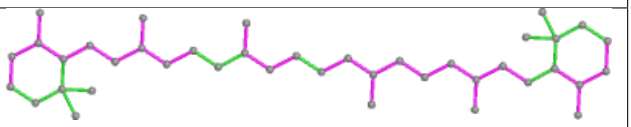


Rings

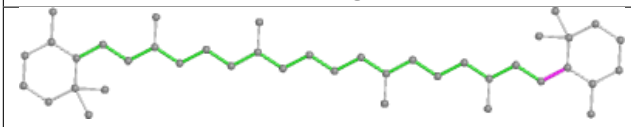
Ligand BCR L 305



Bond lengths



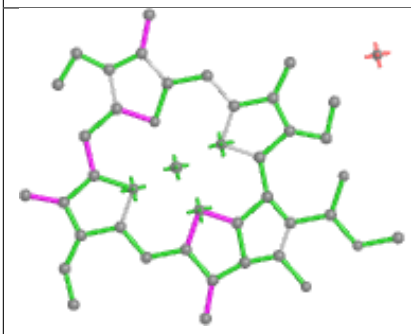
Bond angles



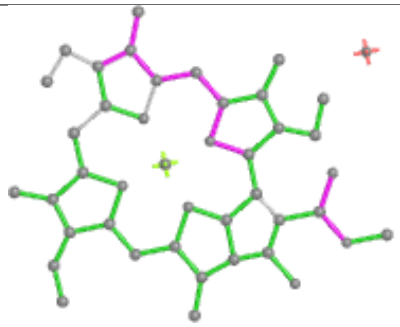
Torsions

Rings

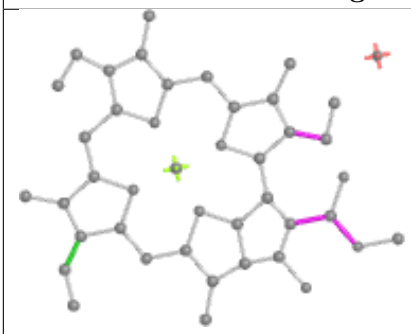
Ligand CLA A 828



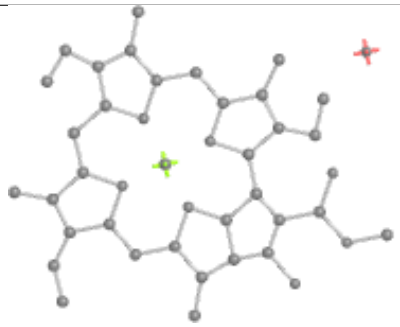
Bond lengths



Bond angles

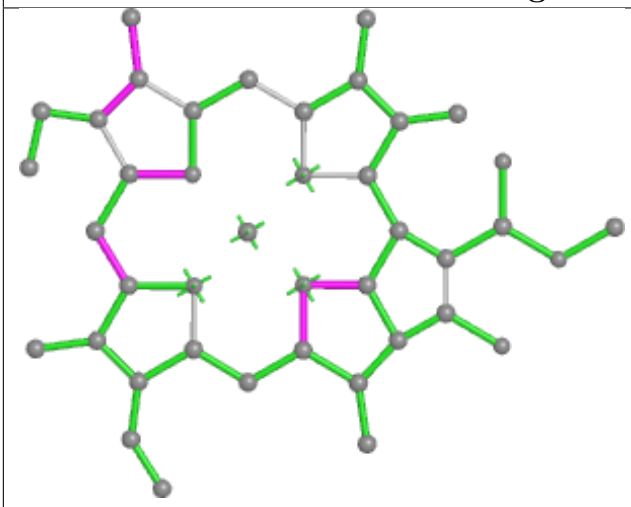


Torsions

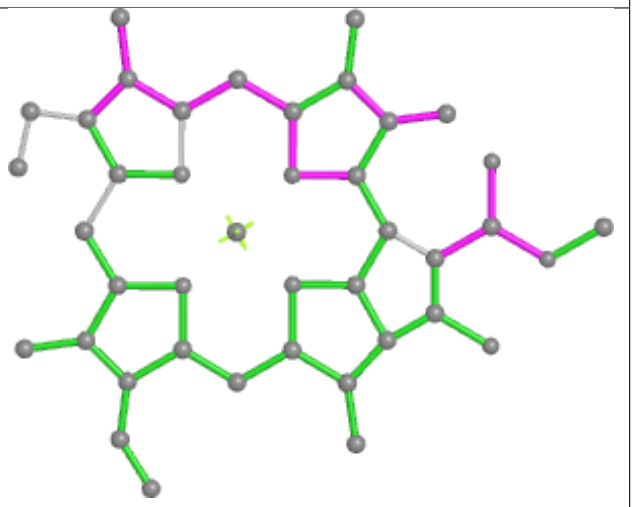


Rings

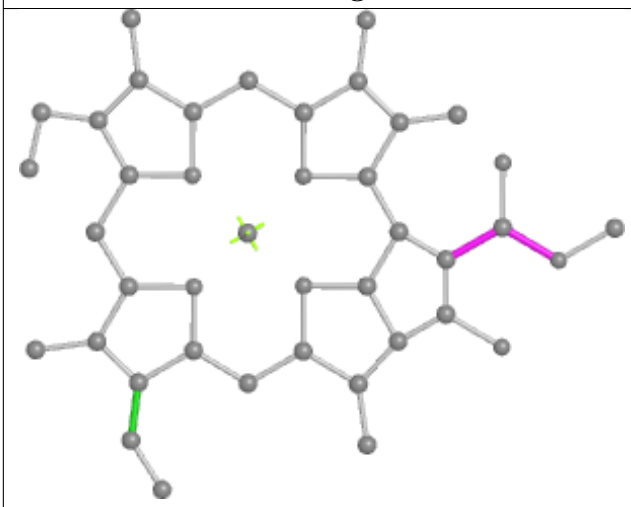
Ligand CLA 3 306



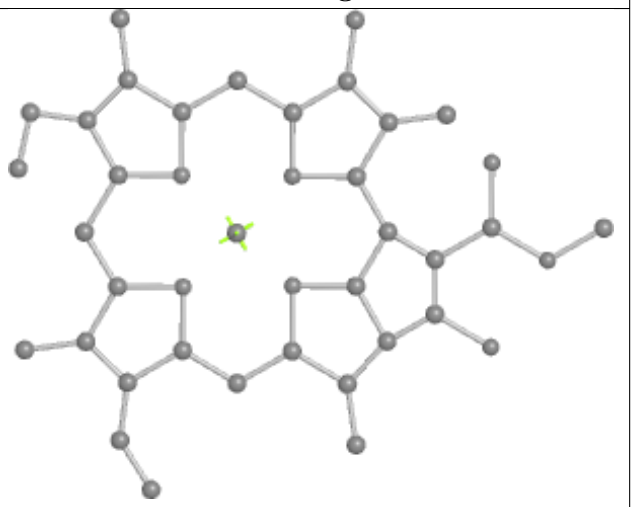
Bond lengths



Bond angles

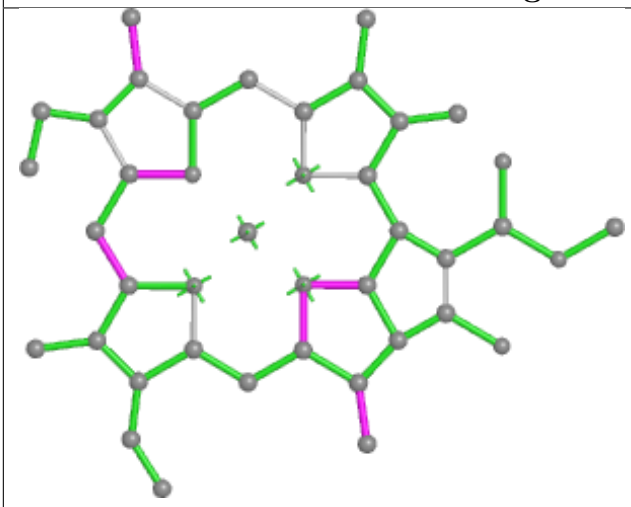


Torsions

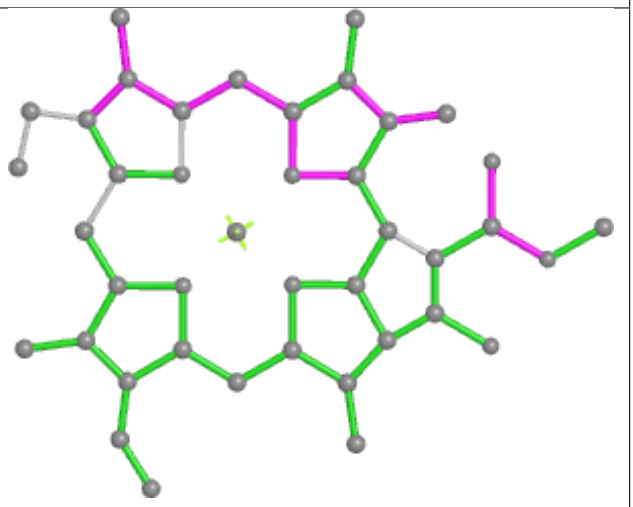


Rings

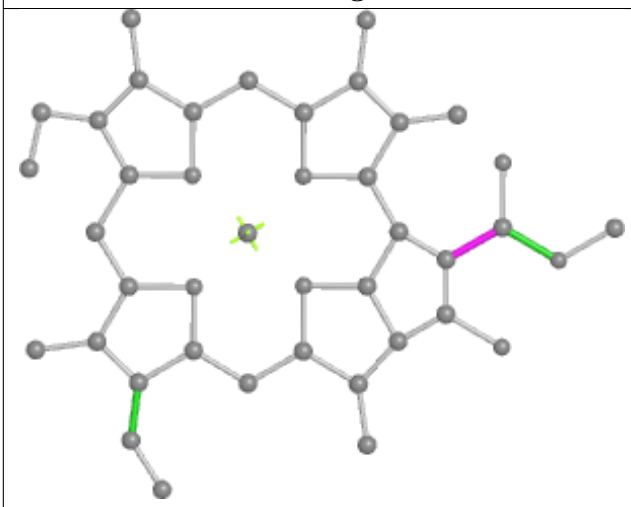
Ligand CLA A 840



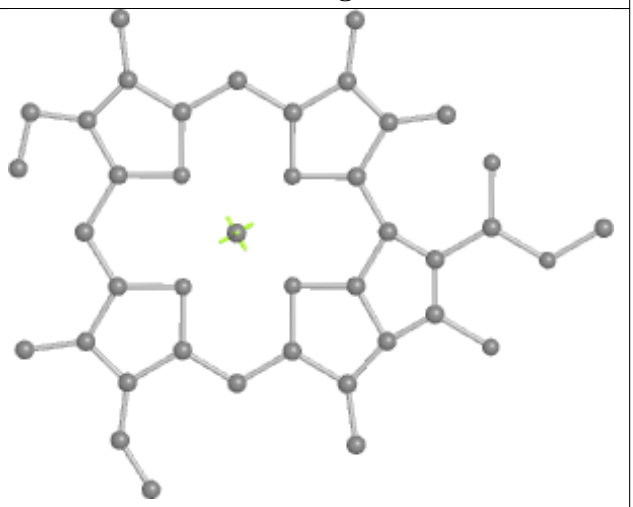
Bond lengths



Bond angles

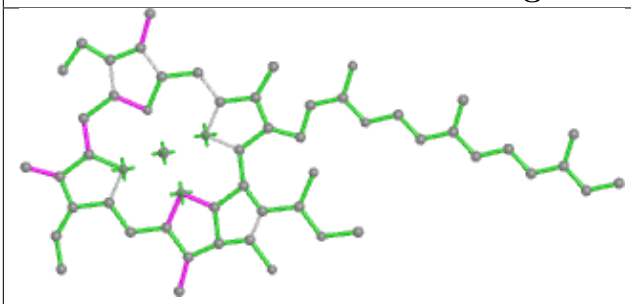


Torsions

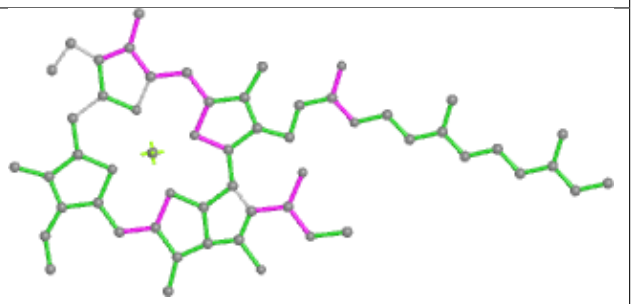


Rings

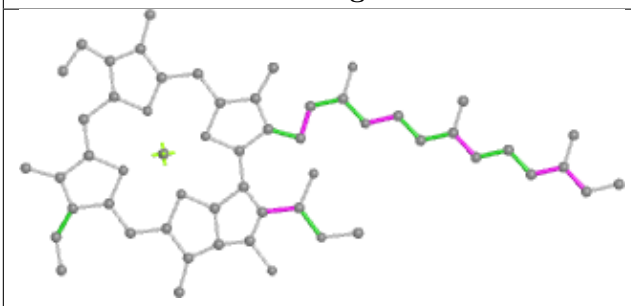
Ligand CLA A 824



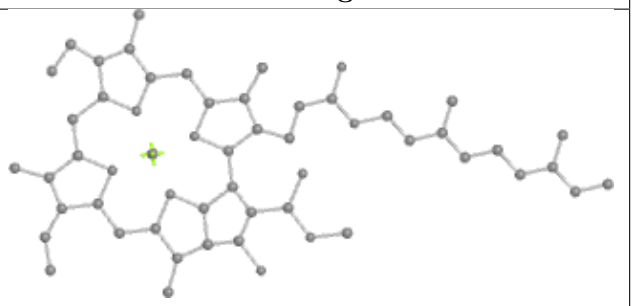
Bond lengths



Bond angles

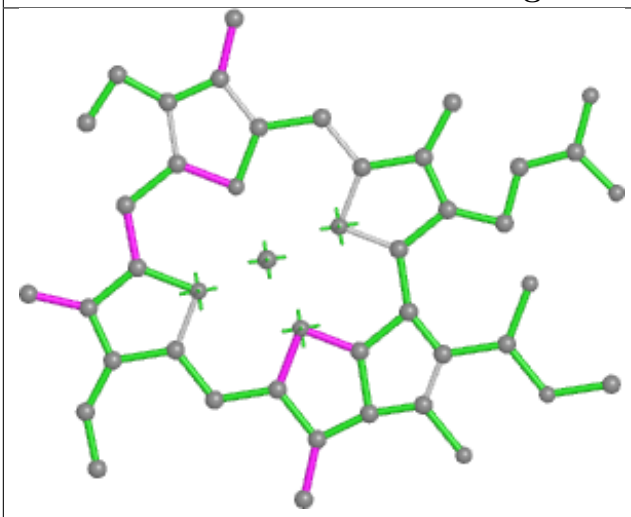


Torsions

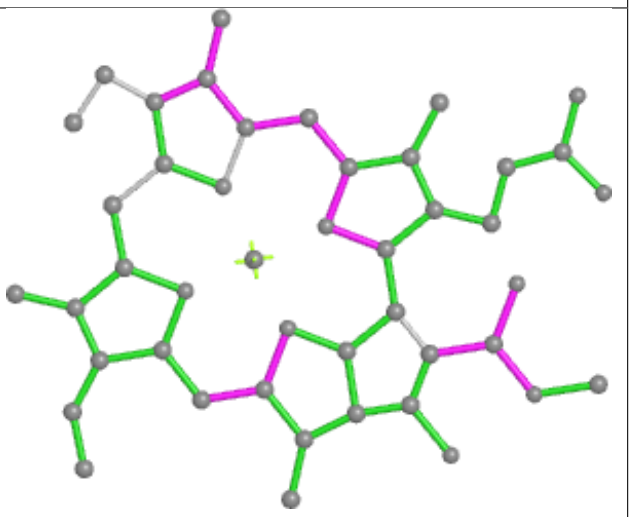


Rings

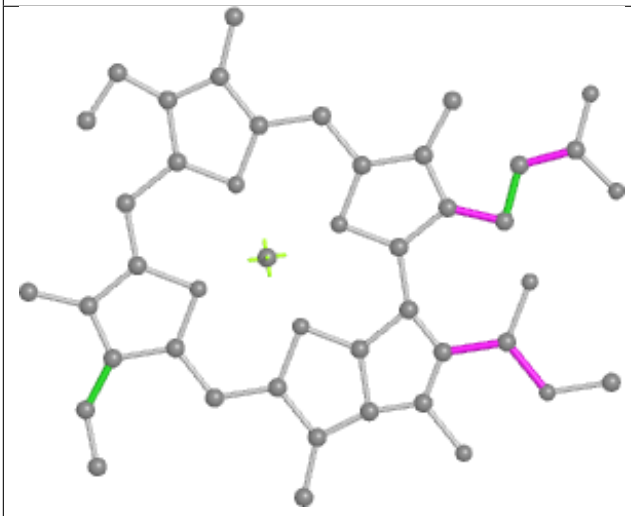
Ligand CLA A 853



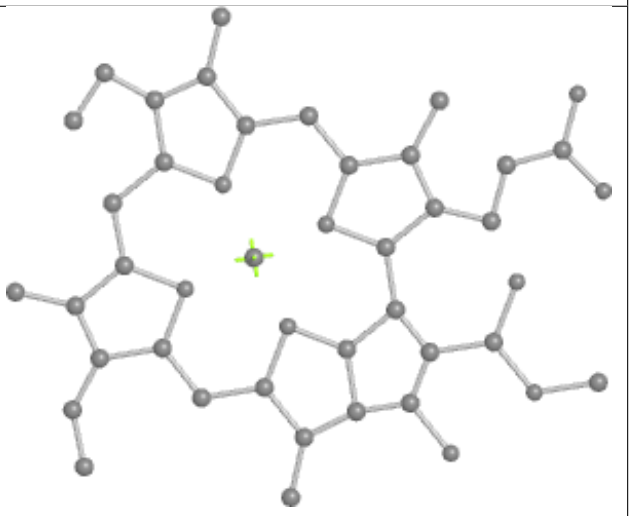
Bond lengths



Bond angles

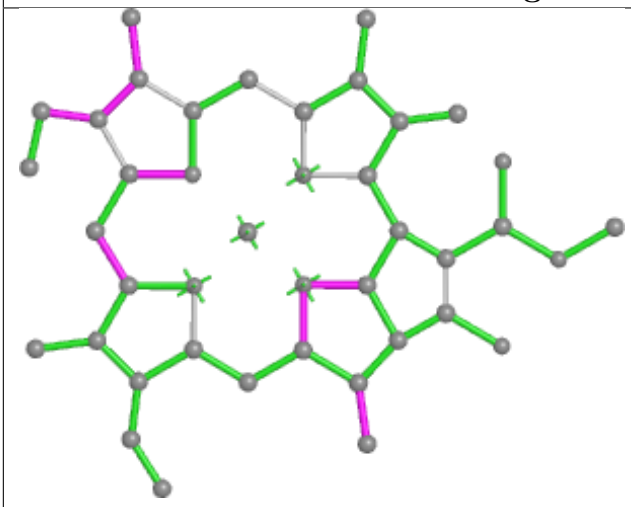


Torsions

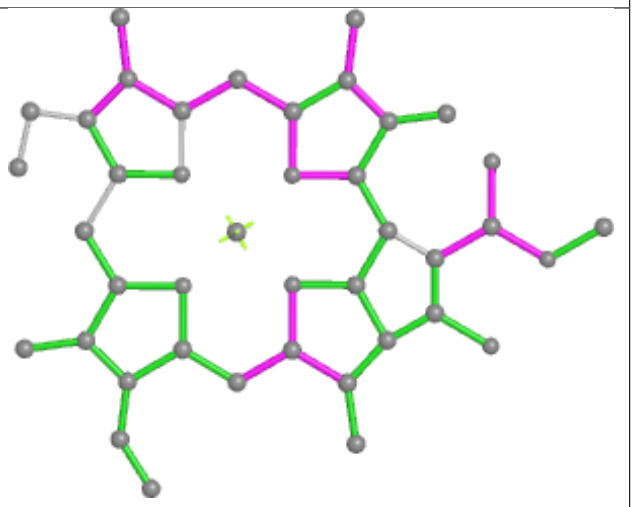


Rings

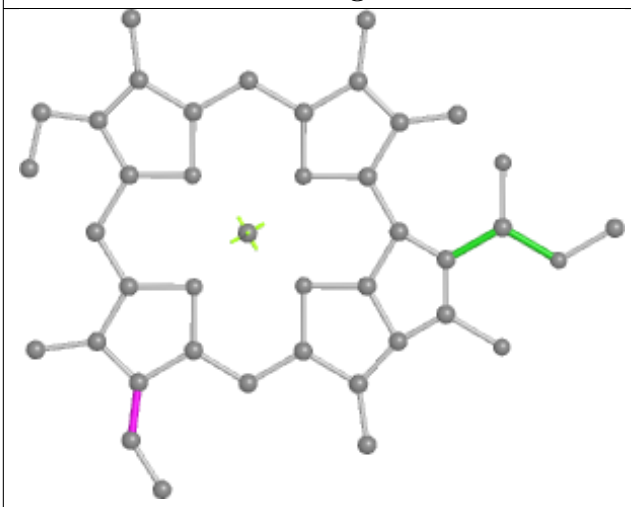
Ligand CLA A 827



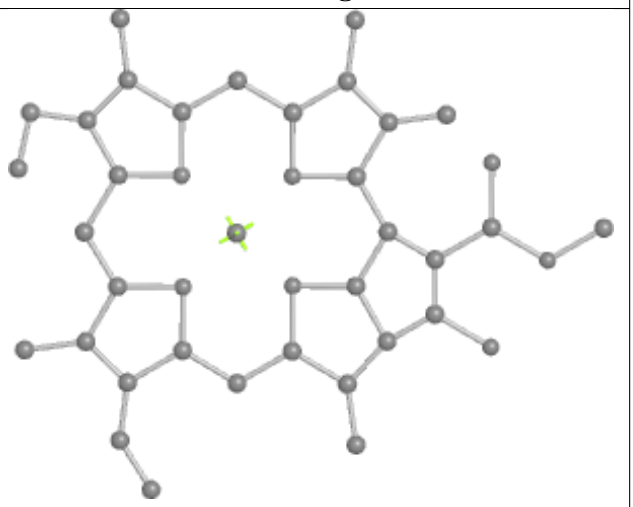
Bond lengths



Bond angles

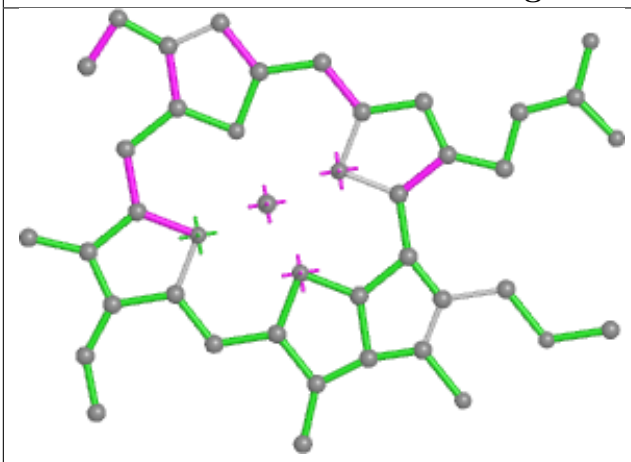


Torsions

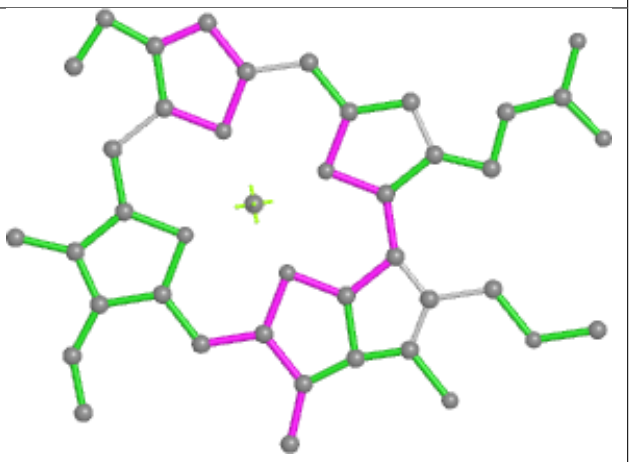


Rings

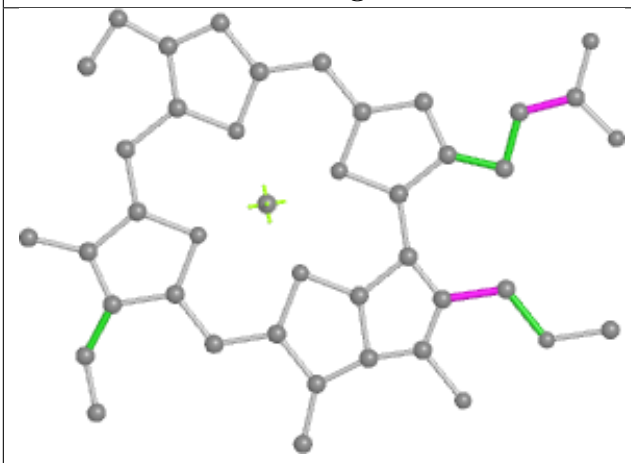
Ligand CLA B 804



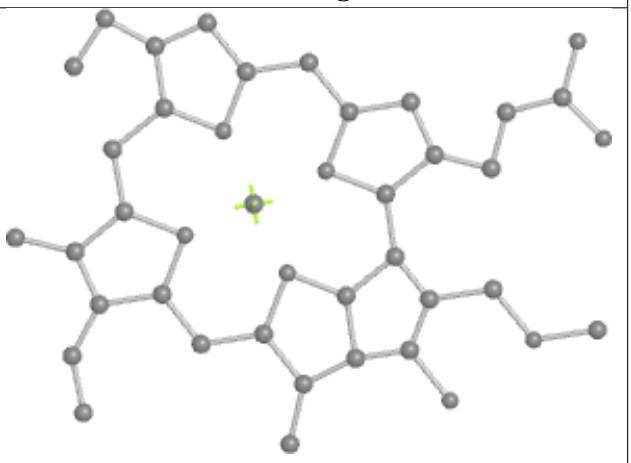
Bond lengths



Bond angles

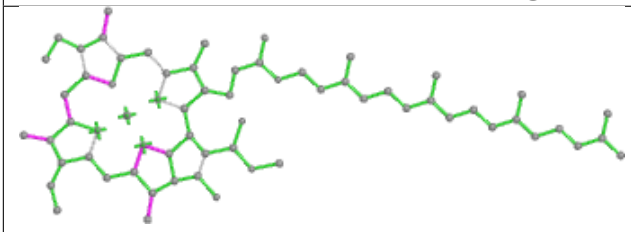


Torsions

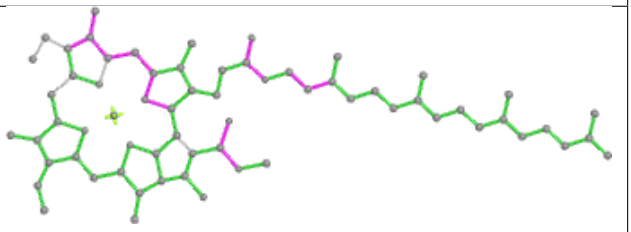


Rings

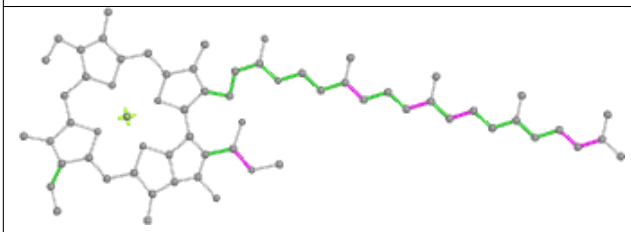
Ligand CLA B 810



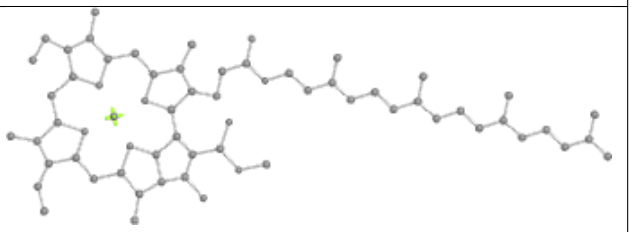
Bond lengths



Bond angles

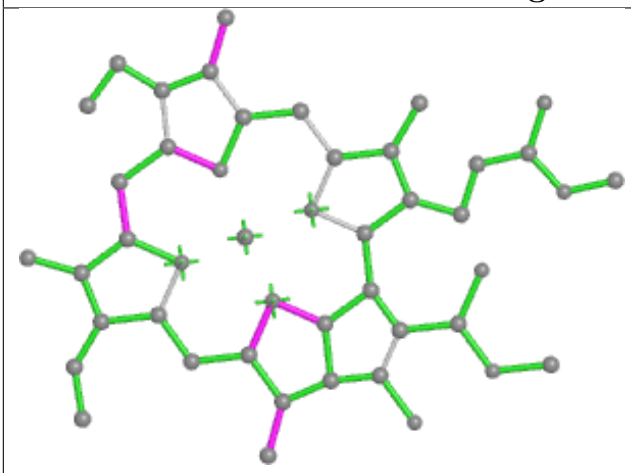


Torsions

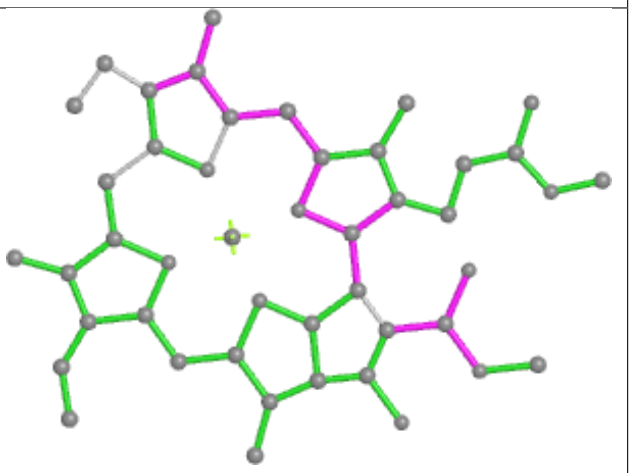


Rings

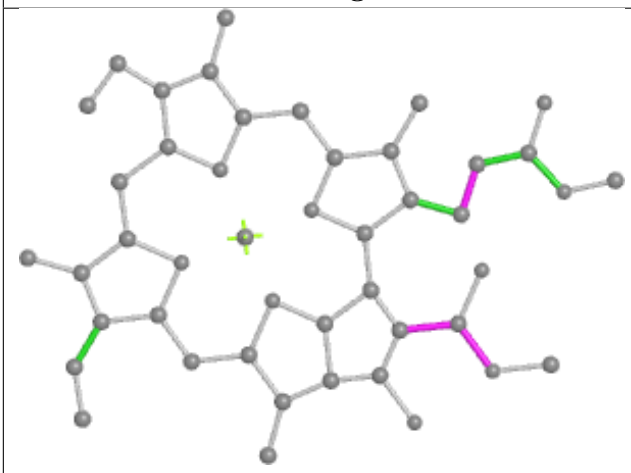
Ligand CLA 1 505



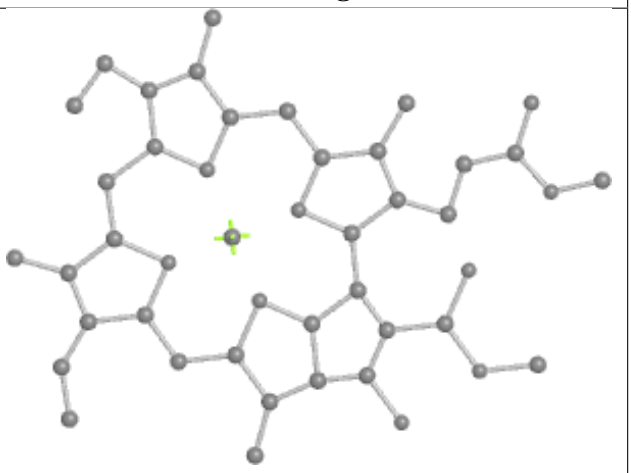
Bond lengths



Bond angles

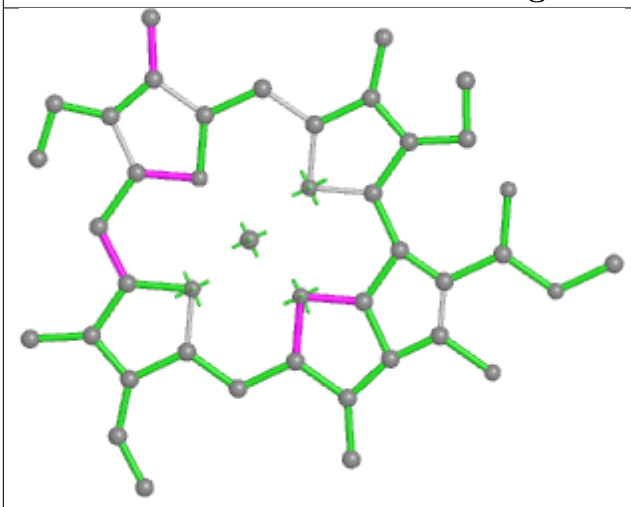


Torsions

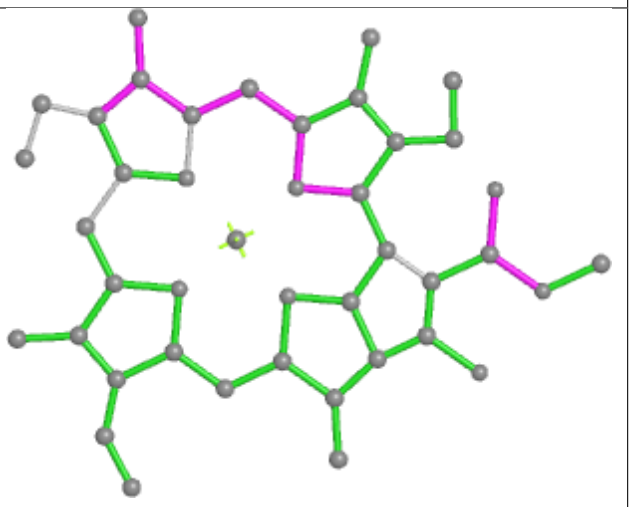


Rings

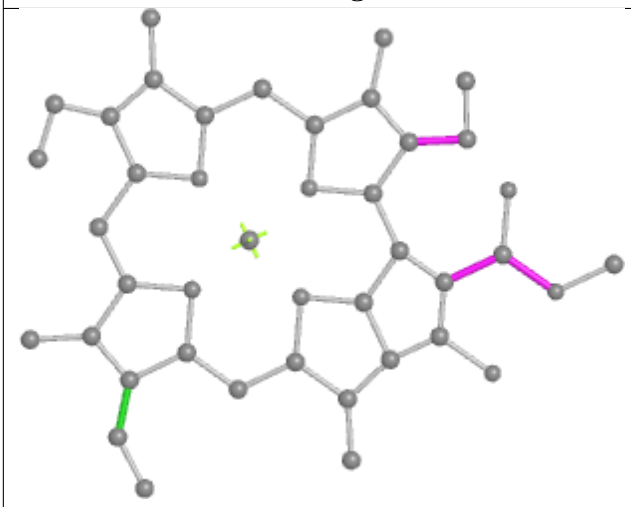
Ligand CLA 3 308



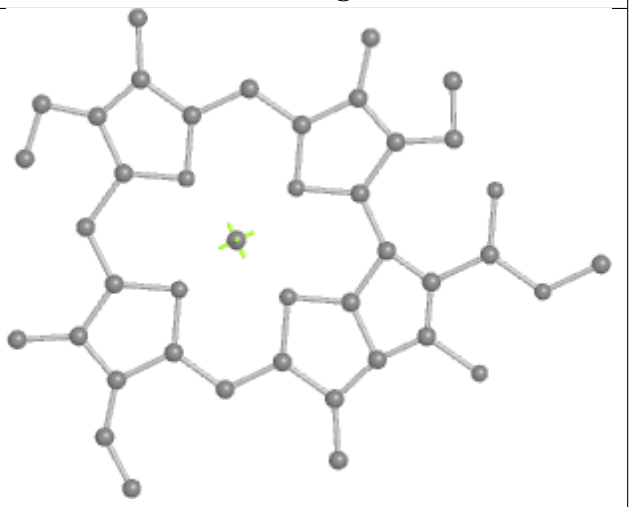
Bond lengths



Bond angles

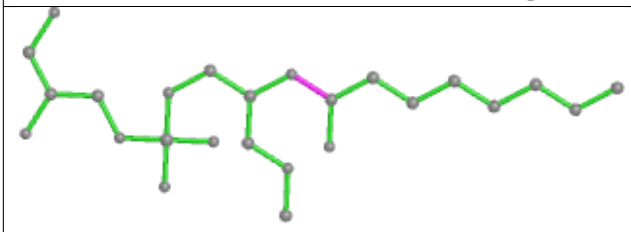


Torsions

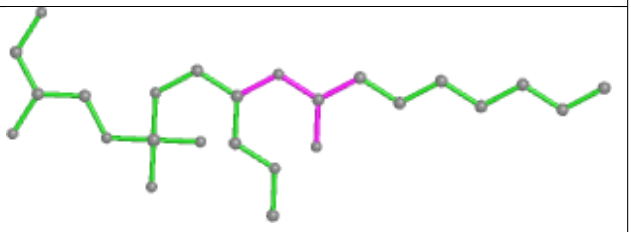


Rings

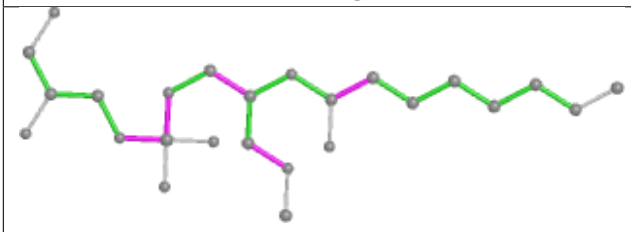
Ligand LHG A 845



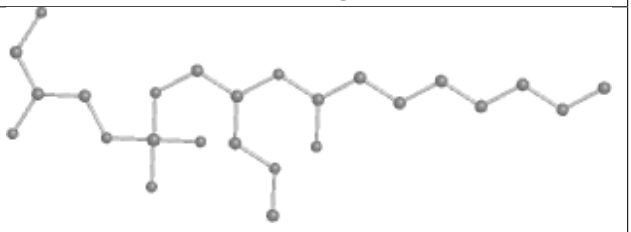
Bond lengths



Bond angles

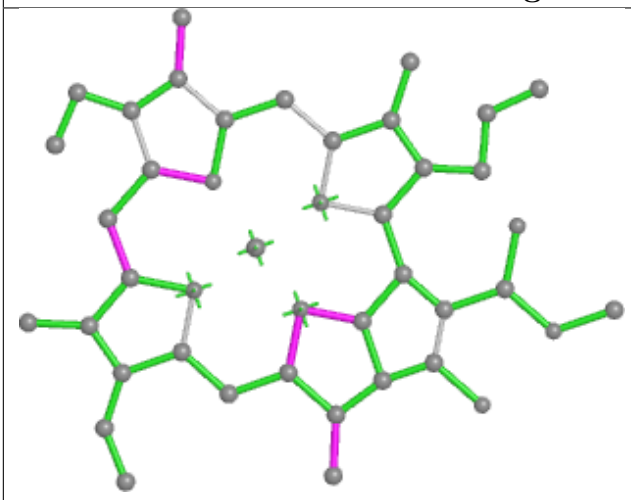


Torsions

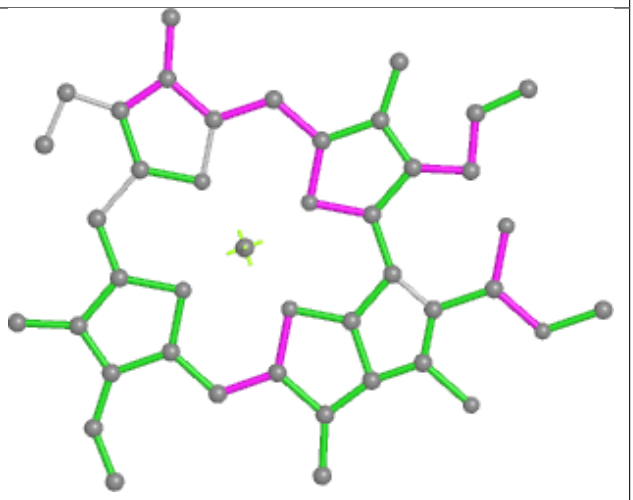


Rings

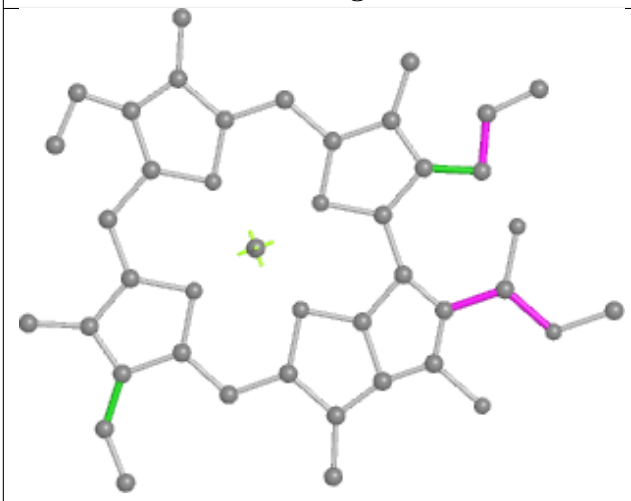
Ligand CLA A 832



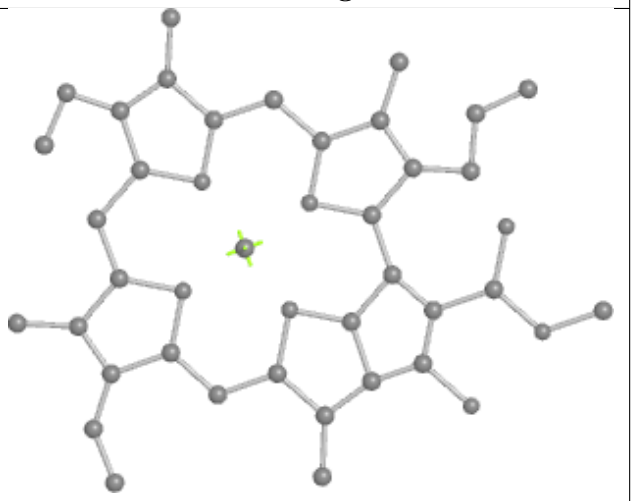
Bond lengths



Bond angles

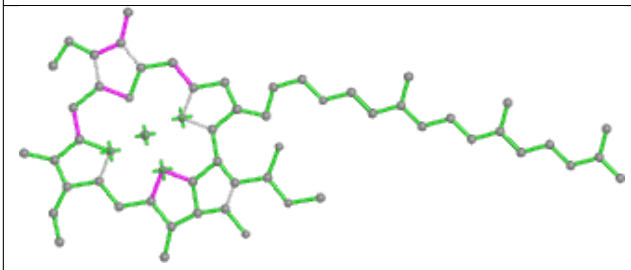


Torsions

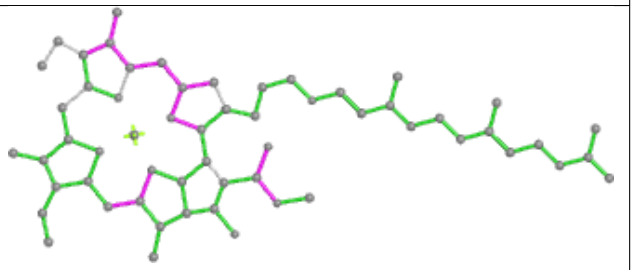


Rings

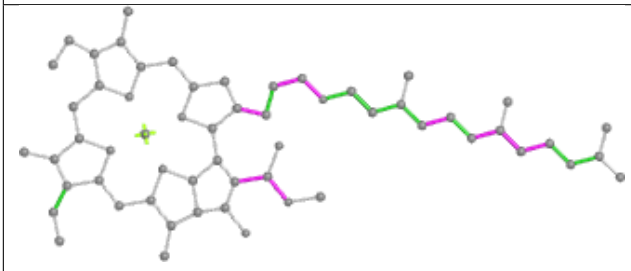
Ligand CLA B 836



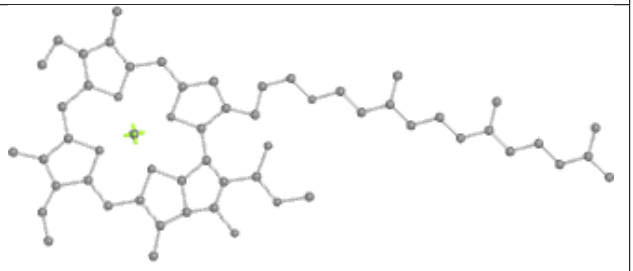
Bond lengths



Bond angles

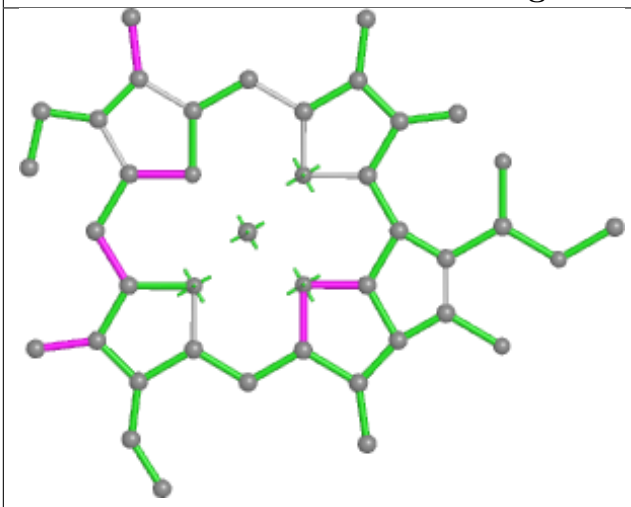


Torsions

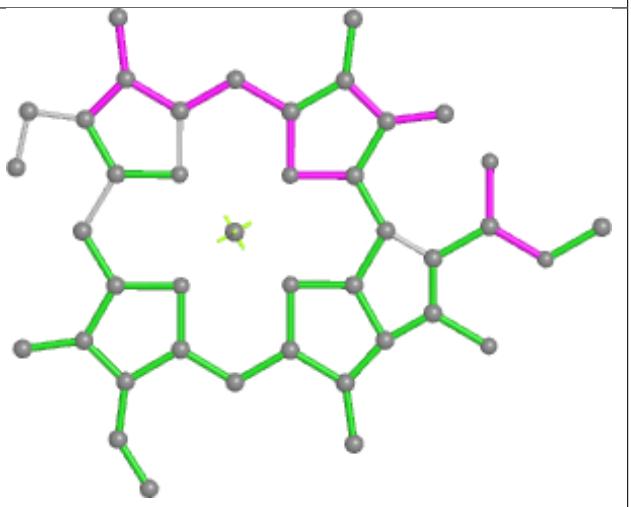


Rings

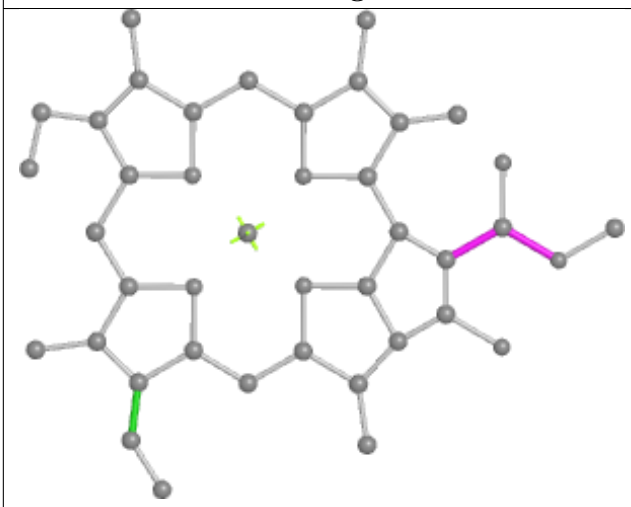
Ligand CLA 4 308



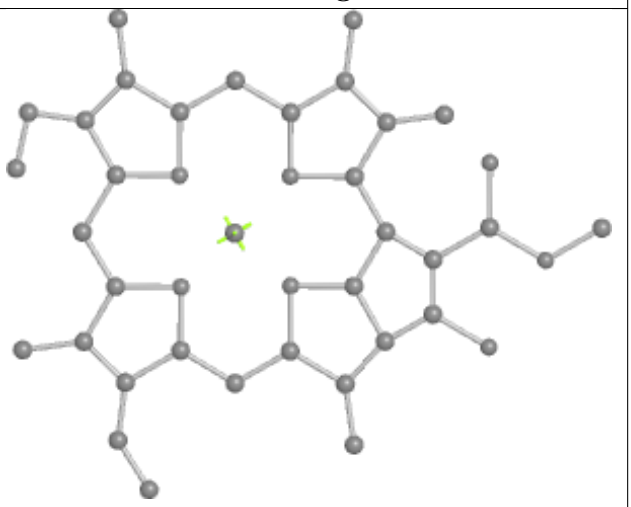
Bond lengths



Bond angles

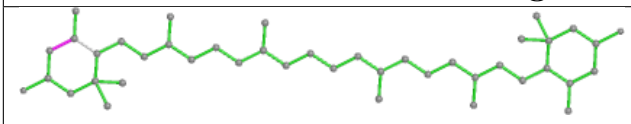


Torsions

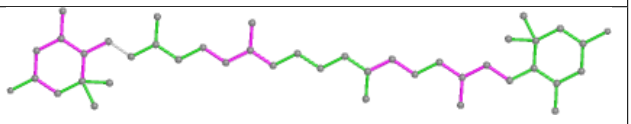


Rings

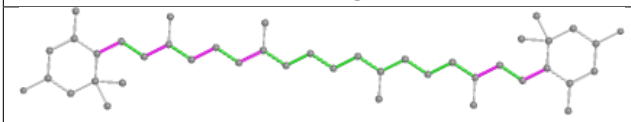
Ligand LUT 1 502



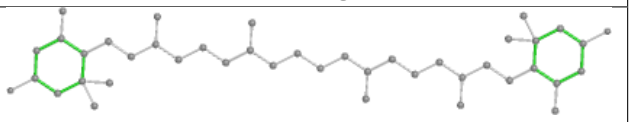
Bond lengths



Bond angles

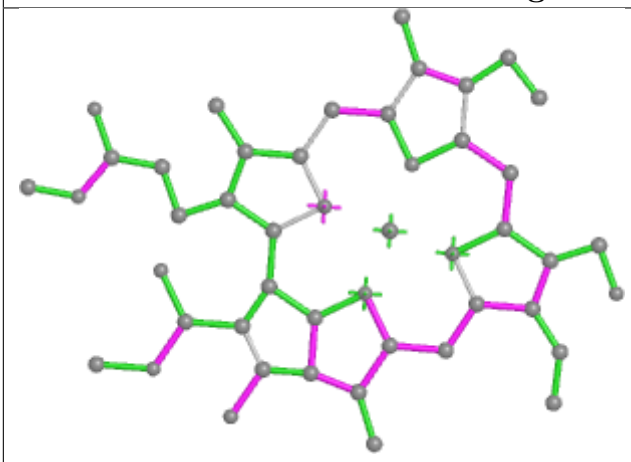


Torsions

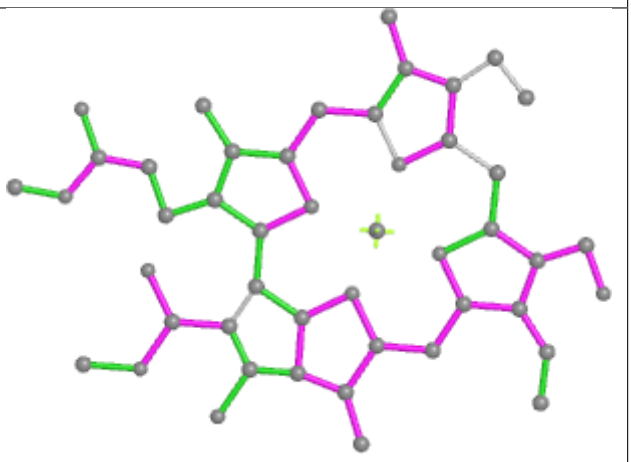


Rings

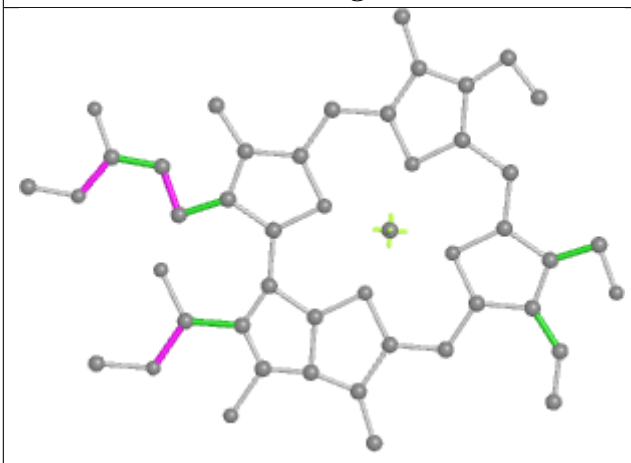
Ligand CHL 4 313



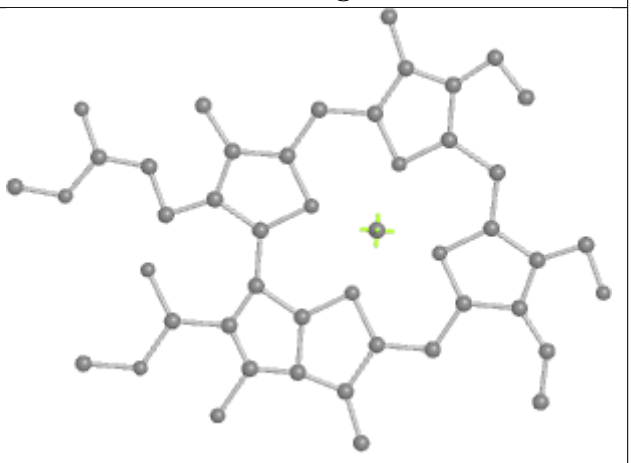
Bond lengths



Bond angles

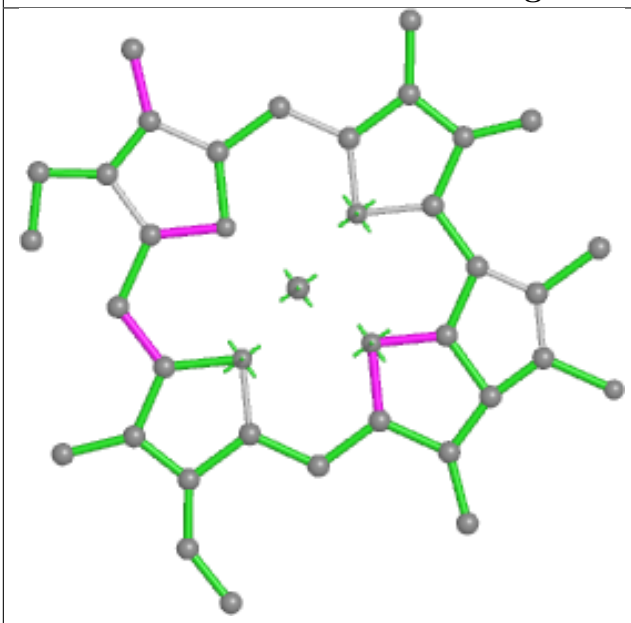


Torsions

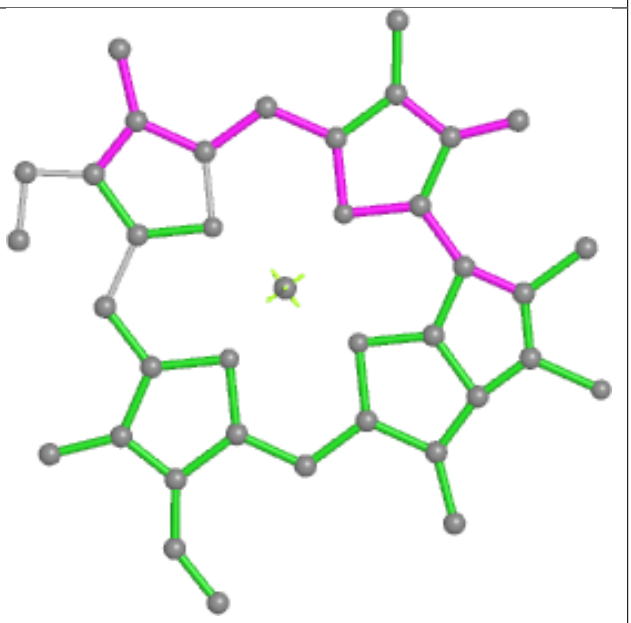


Rings

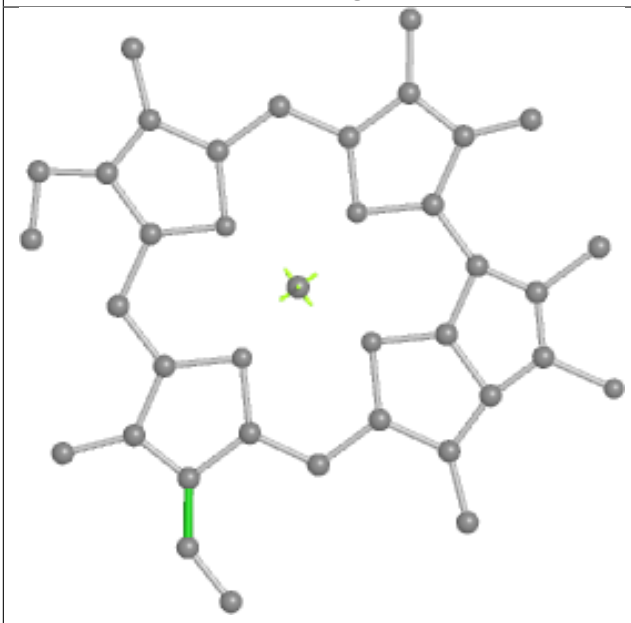
Ligand CLA B 843



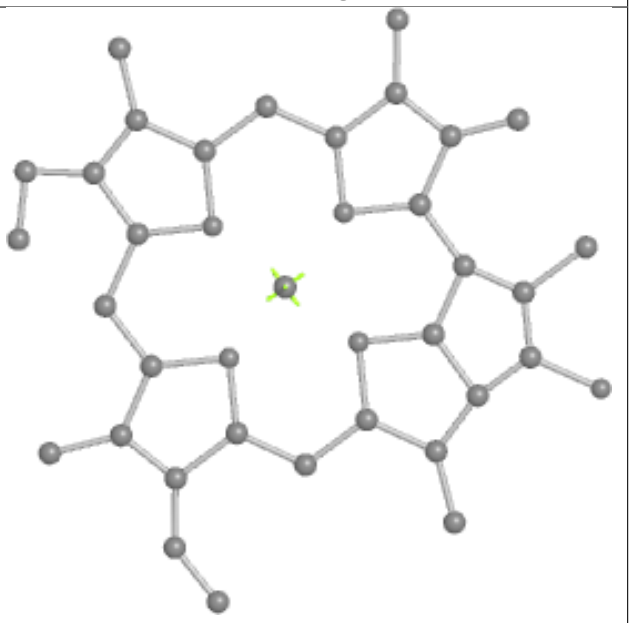
Bond lengths



Bond angles

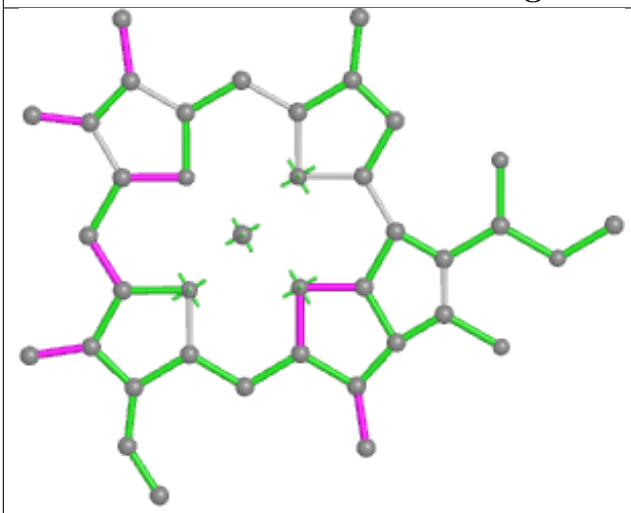


Torsions

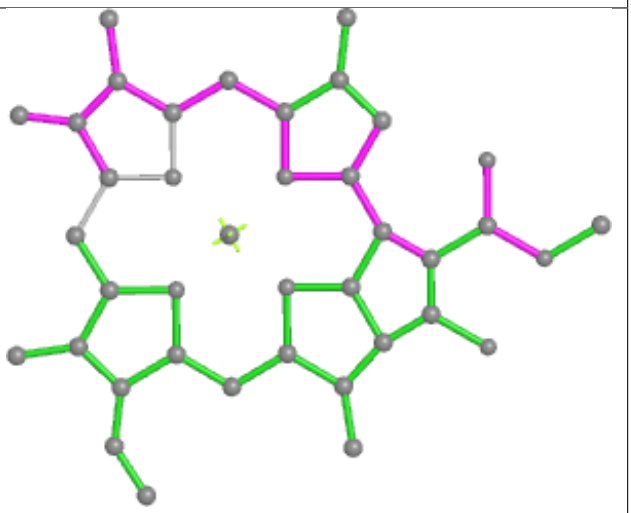


Rings

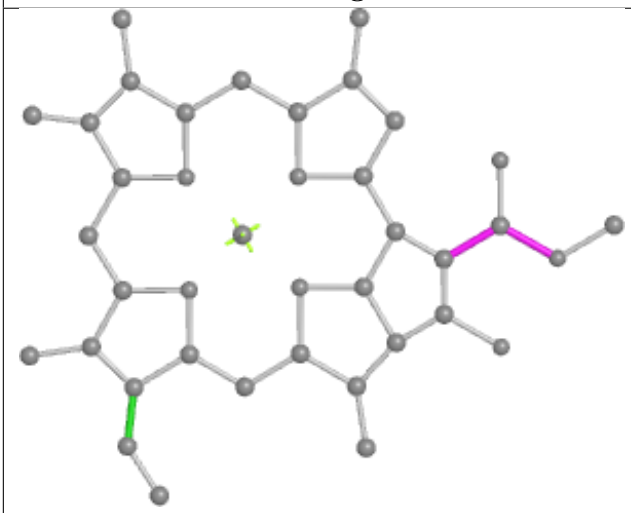
Ligand CLA B 830



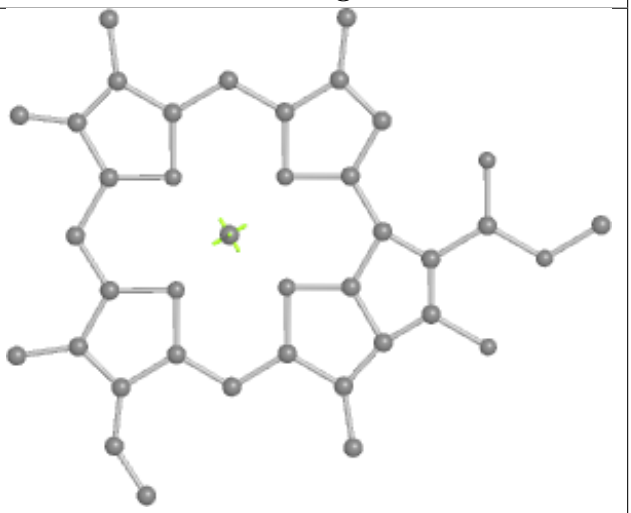
Bond lengths



Bond angles

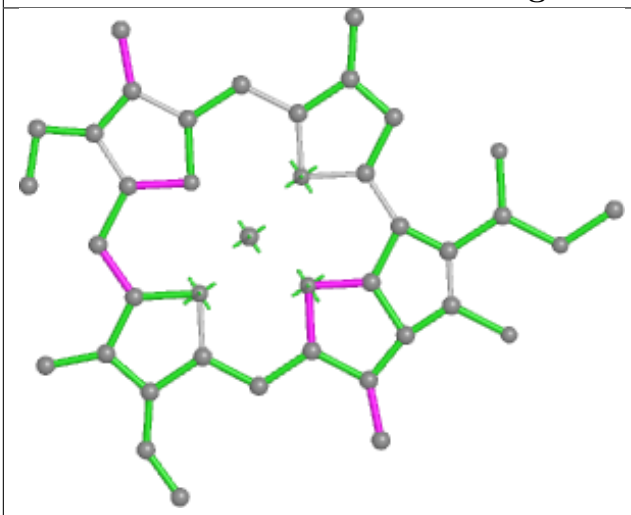


Torsions

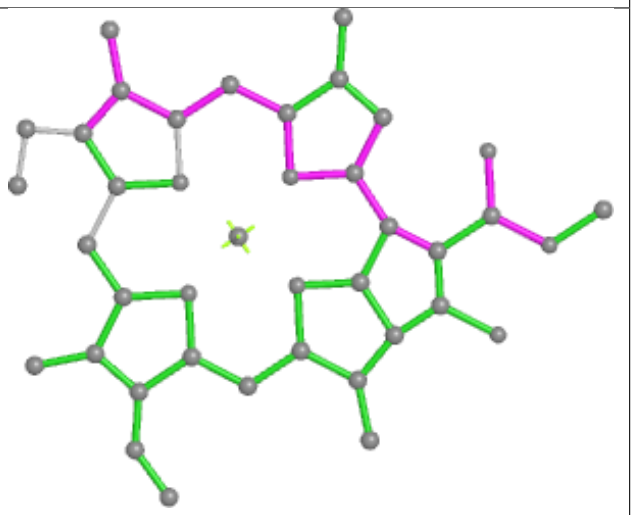


Rings

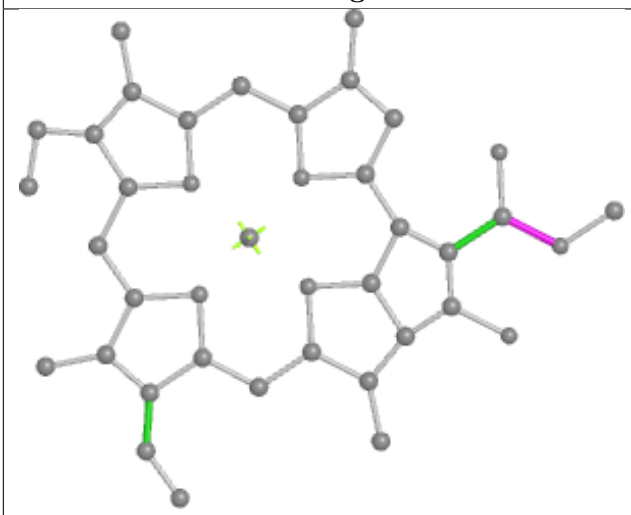
Ligand CLA 6 514



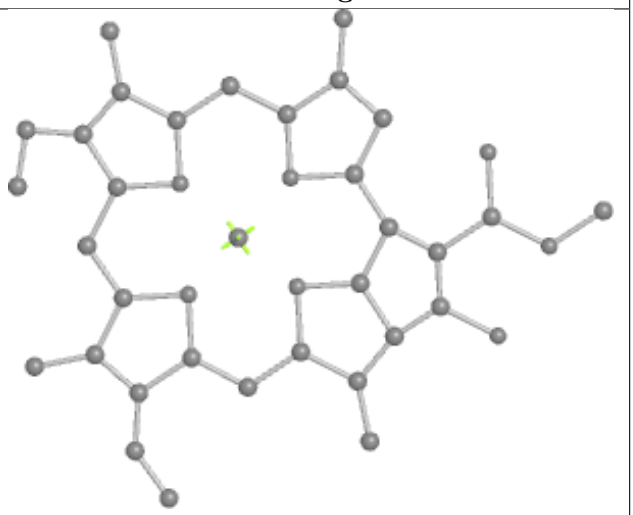
Bond lengths



Bond angles

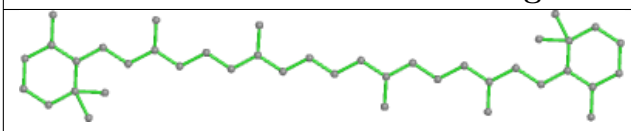


Torsions

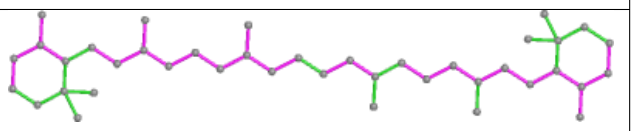


Rings

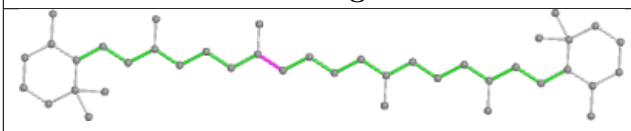
Ligand BCR F 803



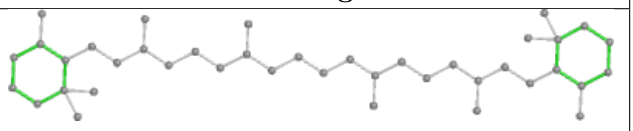
Bond lengths



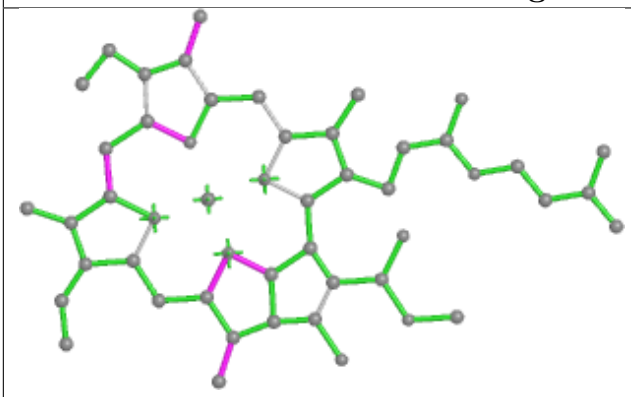
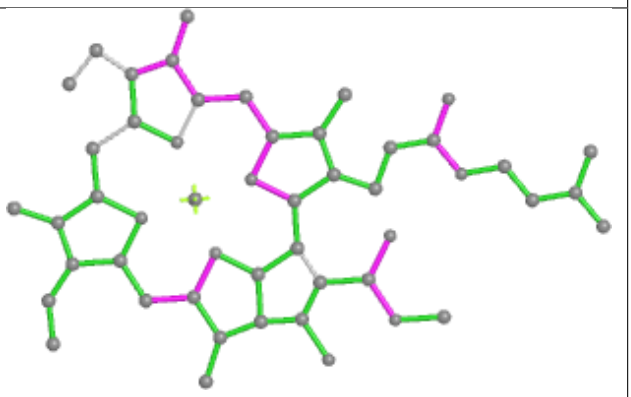
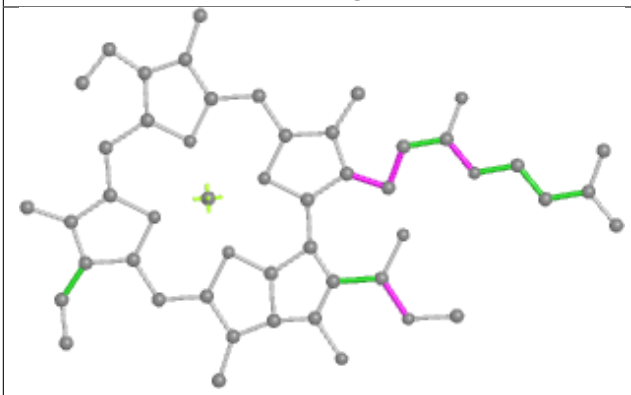
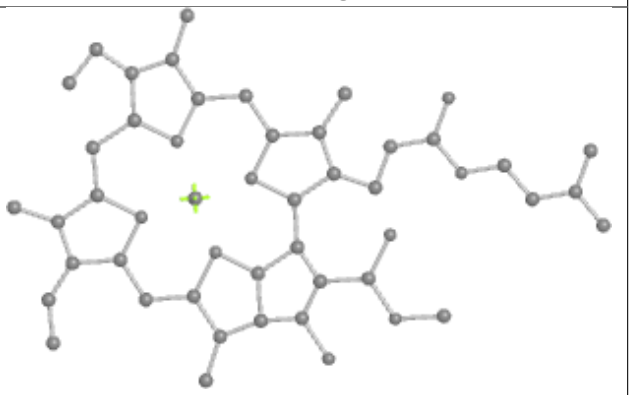
Bond angles

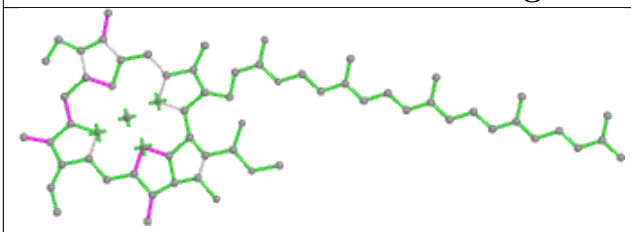
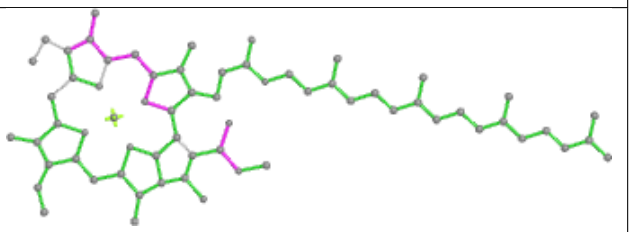
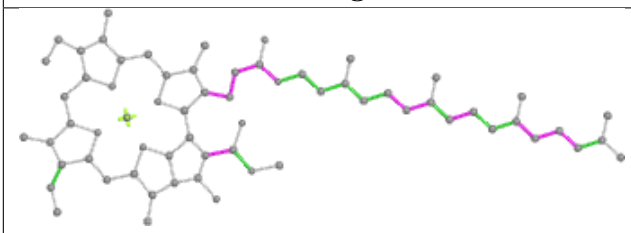
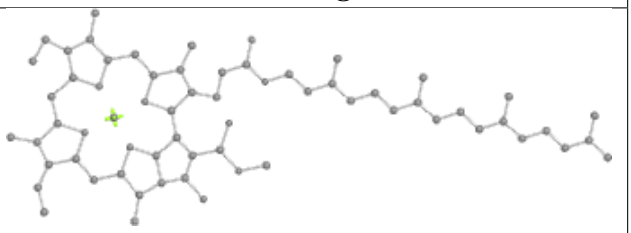


Torsions

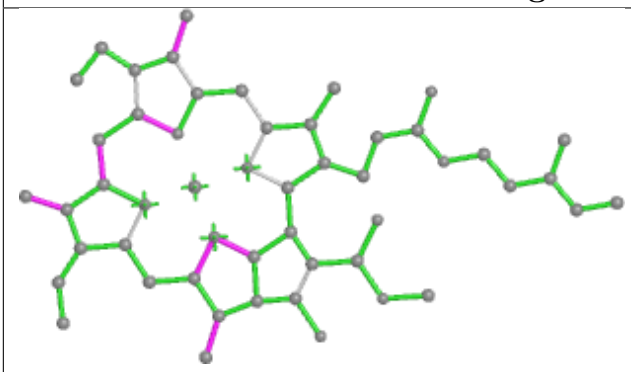


Rings

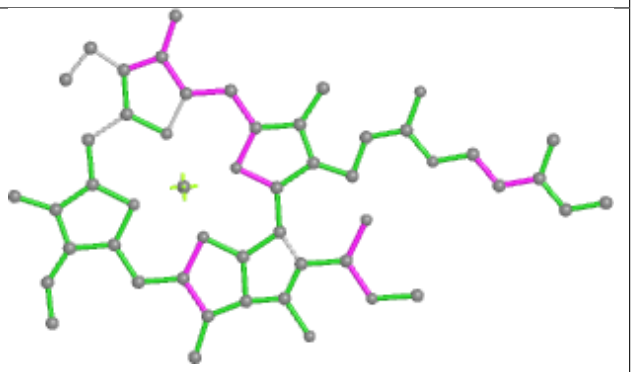
Ligand CLA 6 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

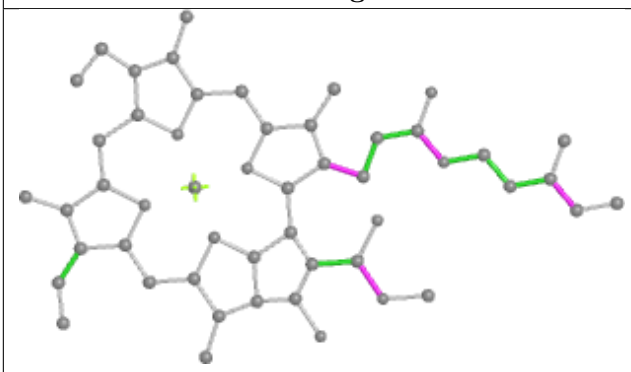
Ligand CLA 6 507



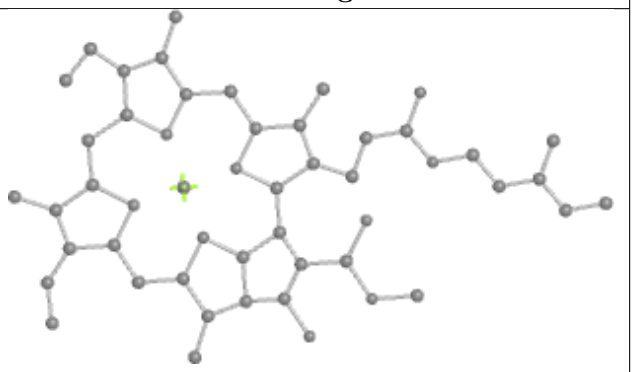
Bond lengths



Bond angles

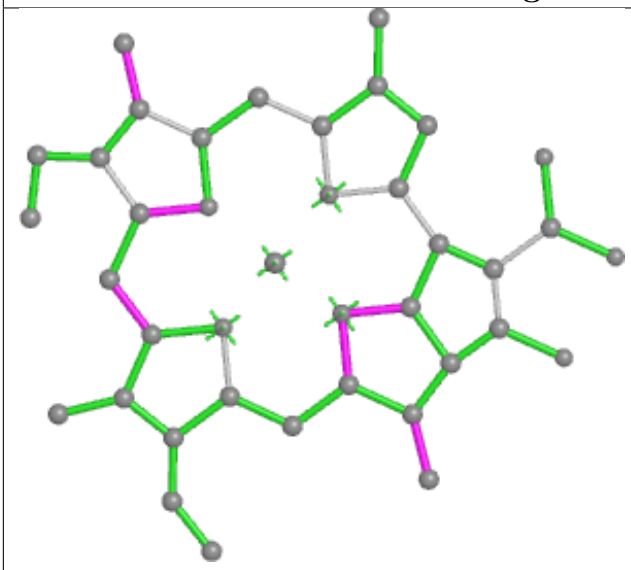


Torsions

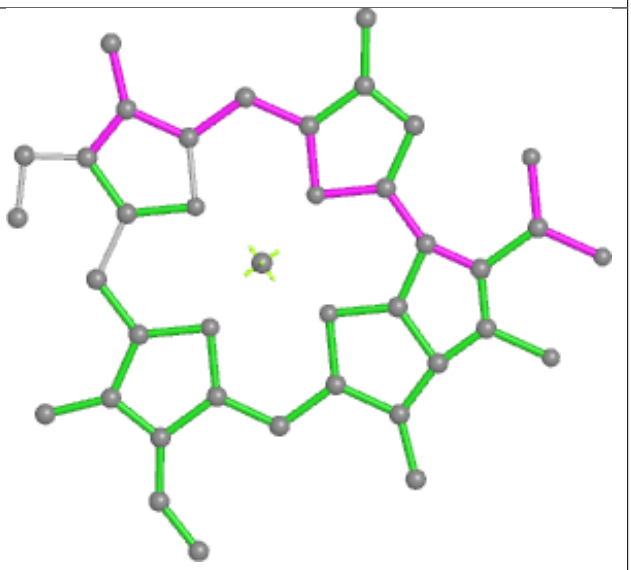


Rings

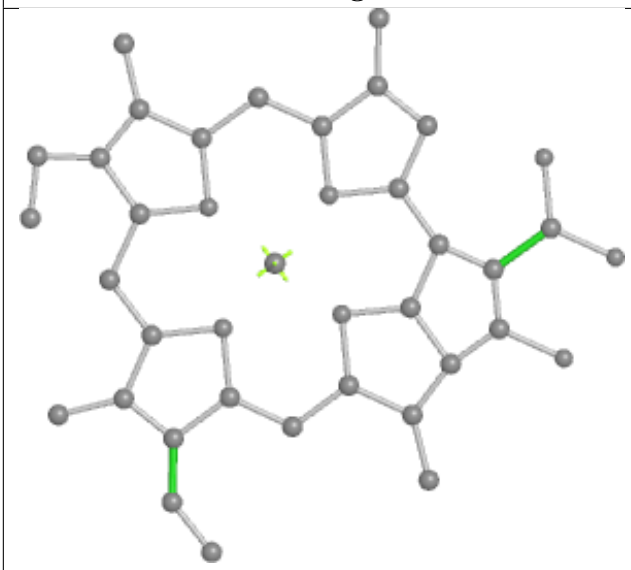
Ligand CLA K 205



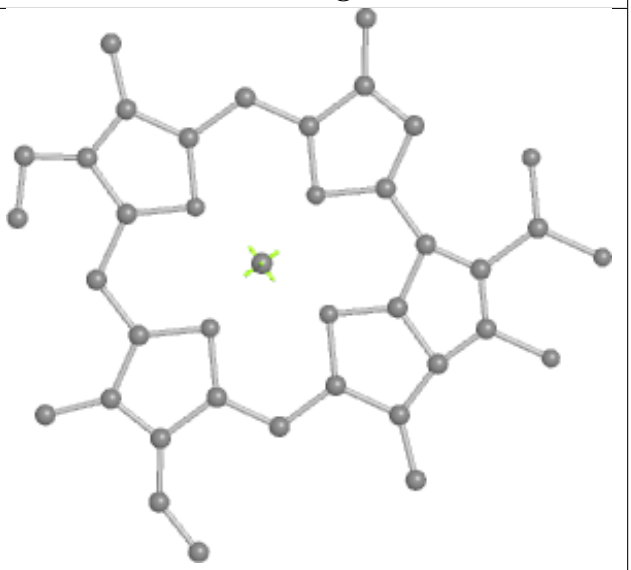
Bond lengths



Bond angles



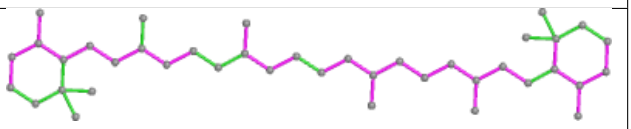
Torsions



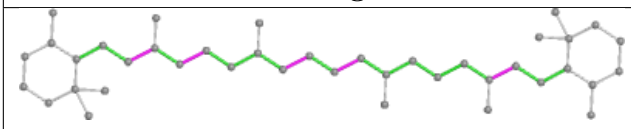
Rings

Ligand BCR B 845

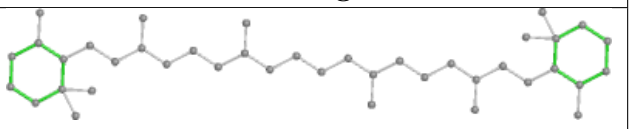
Bond lengths



Bond angles

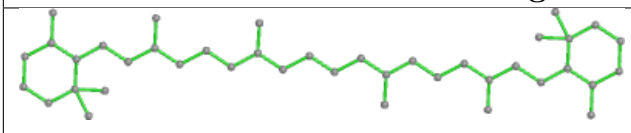


Torsions

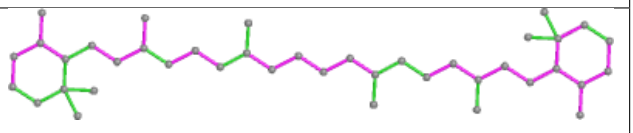


Rings

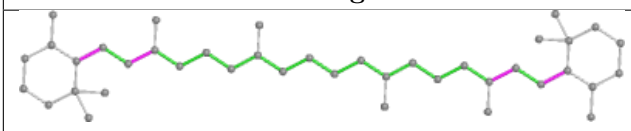
Ligand BCR I 102



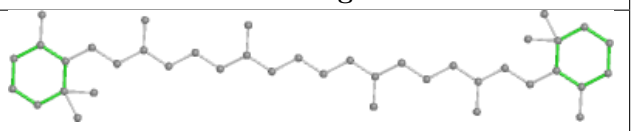
Bond lengths



Bond angles

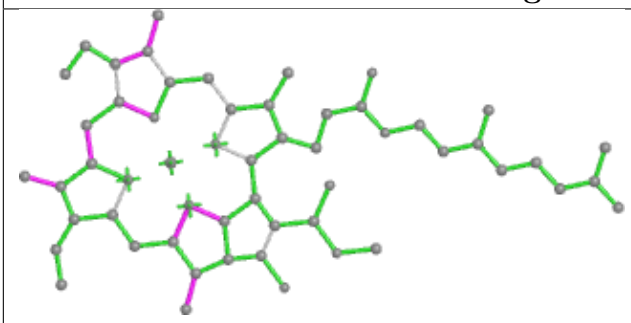


Torsions

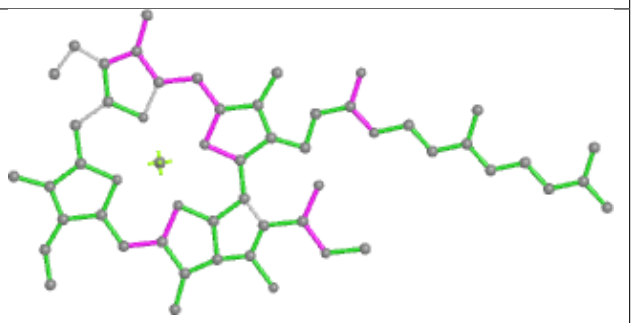


Rings

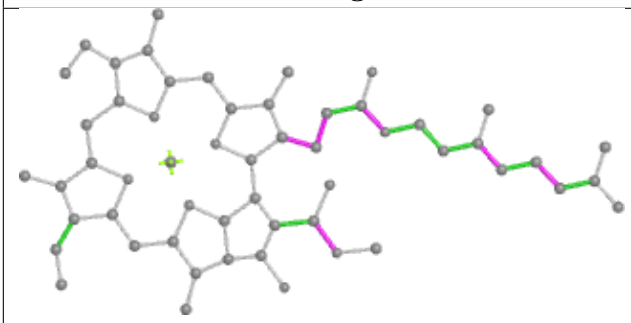
Ligand CLA A 810



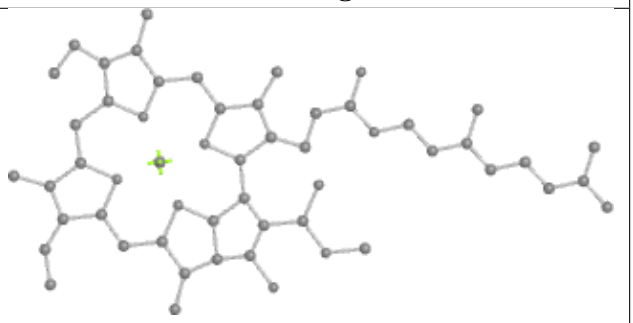
Bond lengths



Bond angles

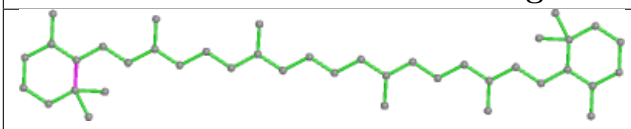


Torsions

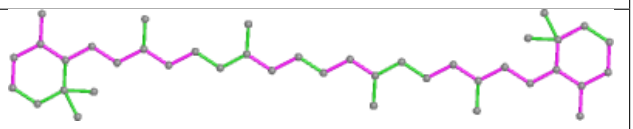


Rings

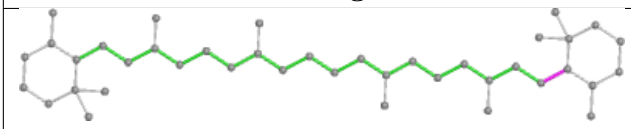
Ligand BCR J 103



Bond lengths



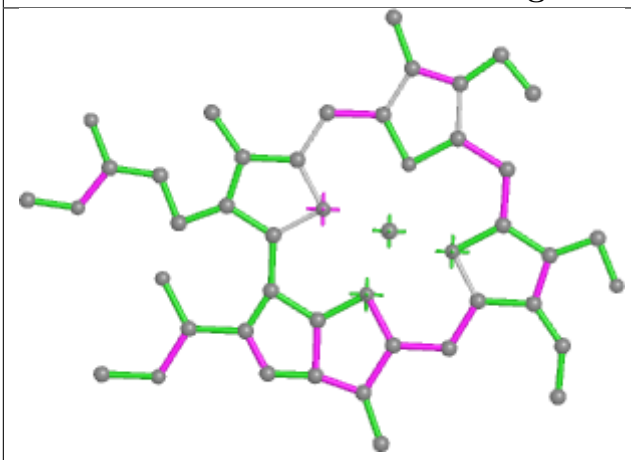
Bond angles



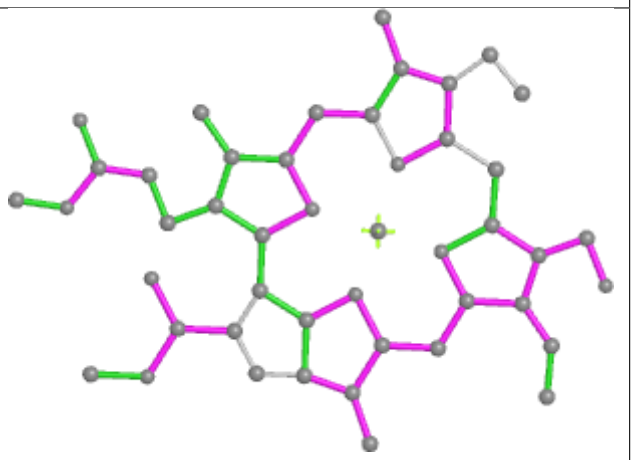
Torsions

Rings

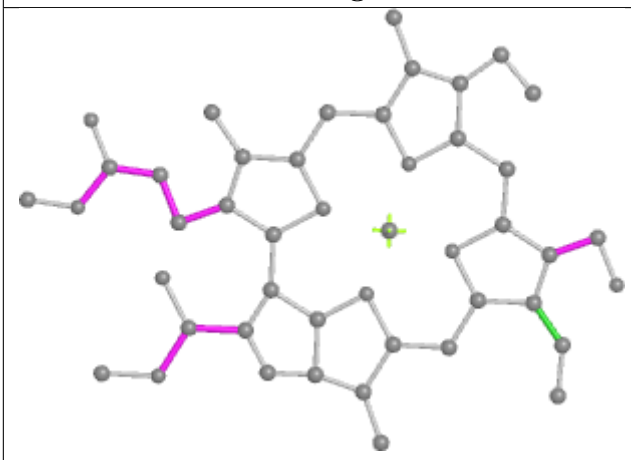
Ligand CHL 3 313



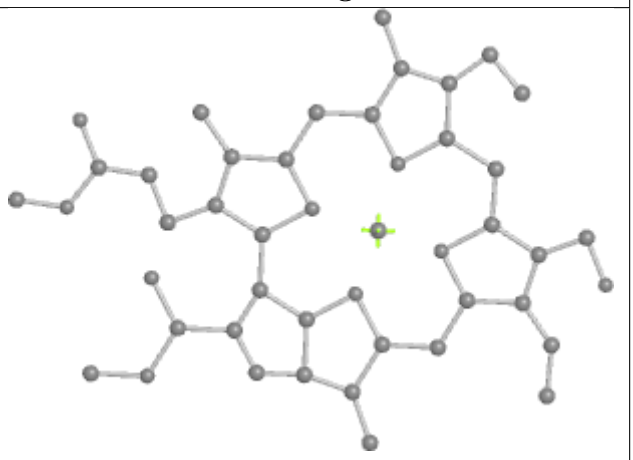
Bond lengths



Bond angles

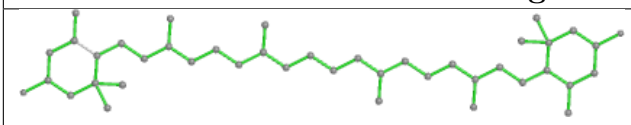


Torsions

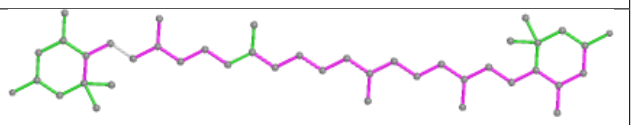


Rings

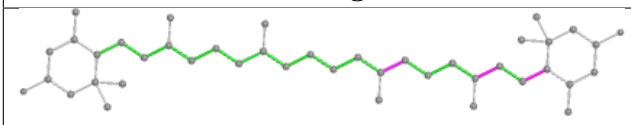
Ligand LUT 3 302



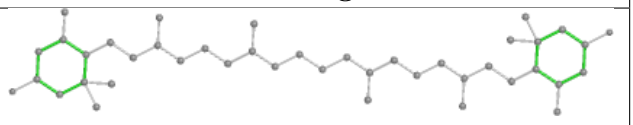
Bond lengths



Bond angles

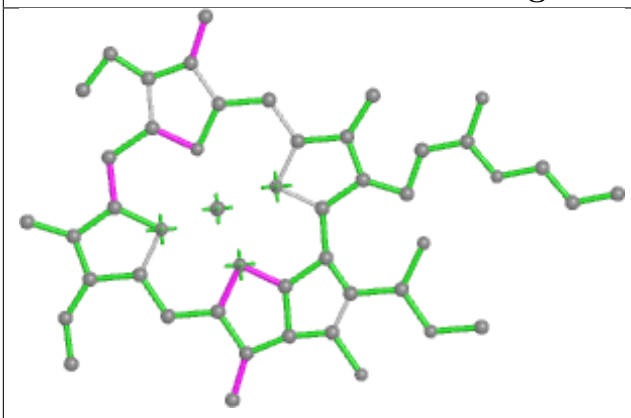


Torsions

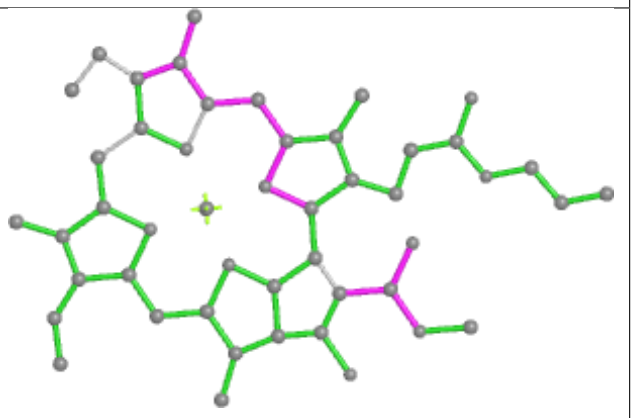


Rings

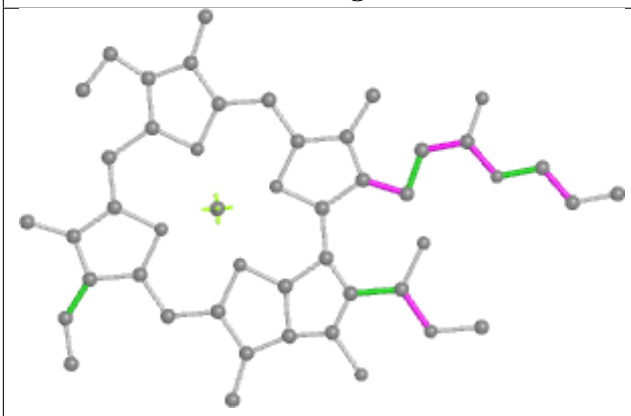
Ligand CLA 3 311



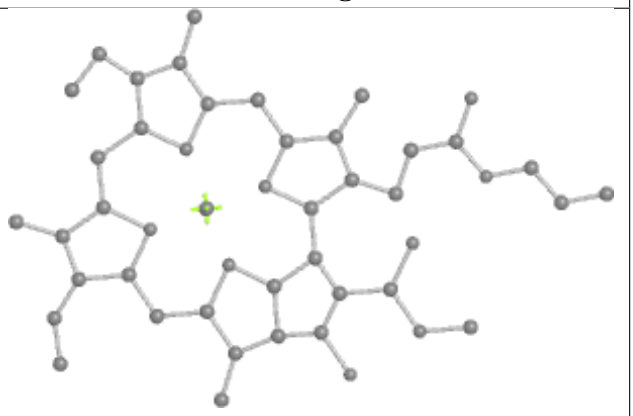
Bond lengths



Bond angles

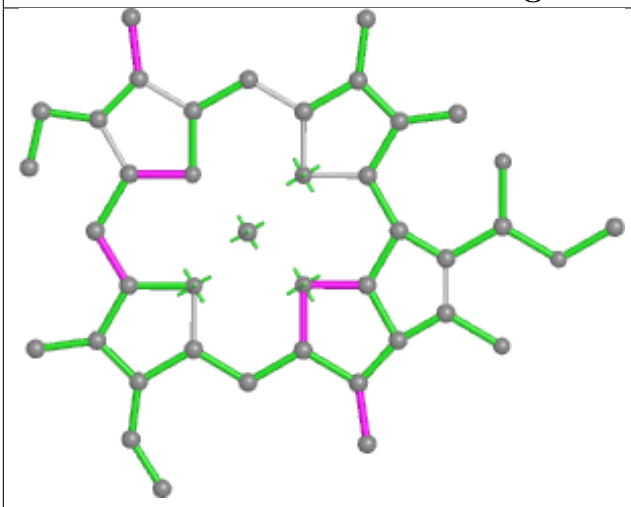


Torsions

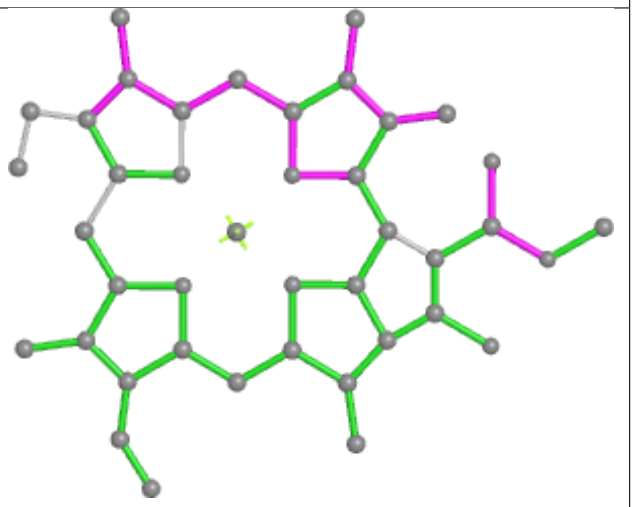


Rings

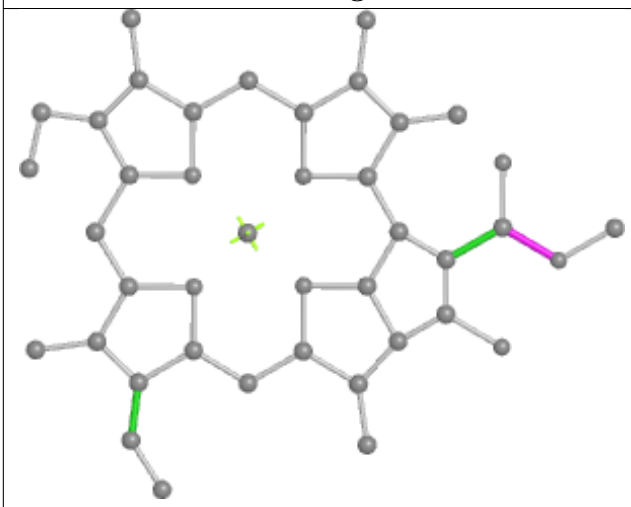
Ligand CLA B 819



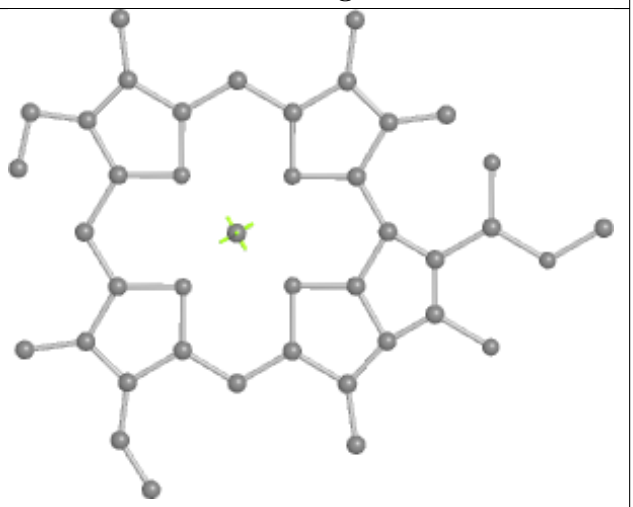
Bond lengths



Bond angles

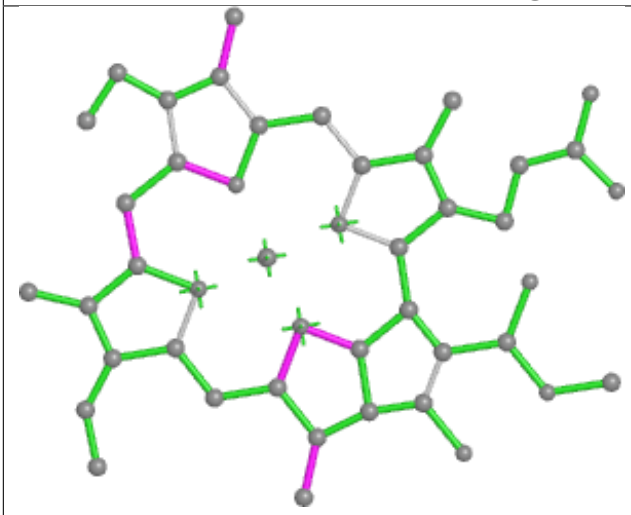


Torsions

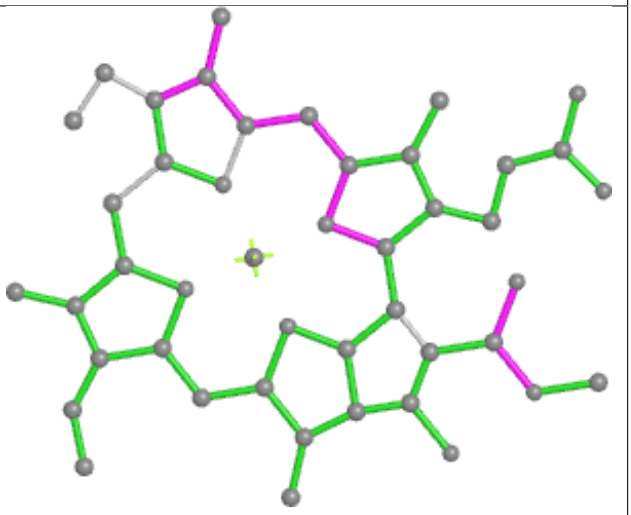


Rings

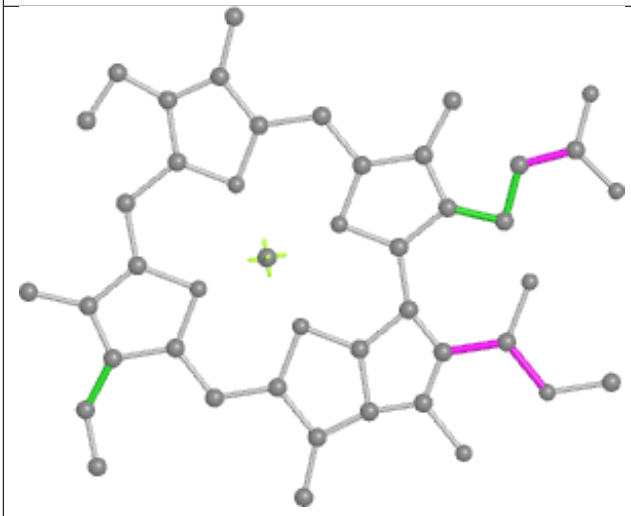
Ligand CLA L 304



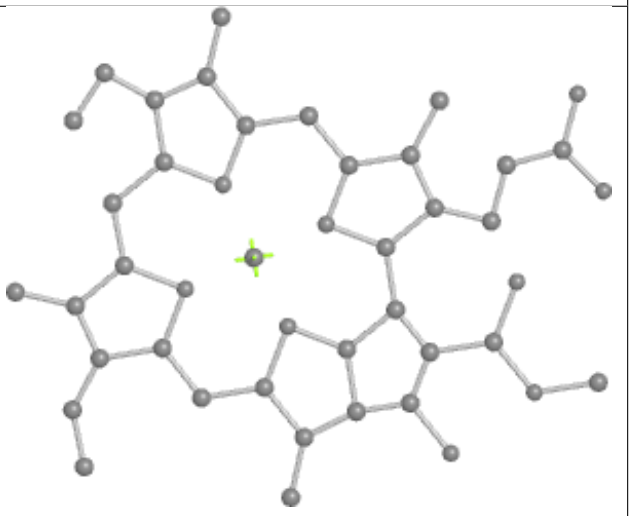
Bond lengths



Bond angles

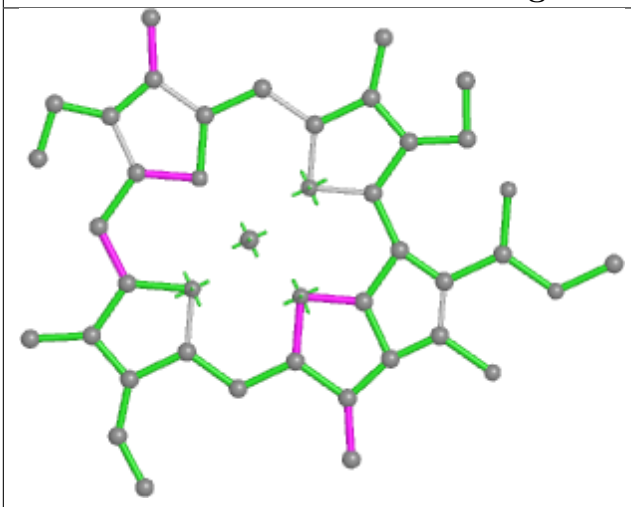


Torsions

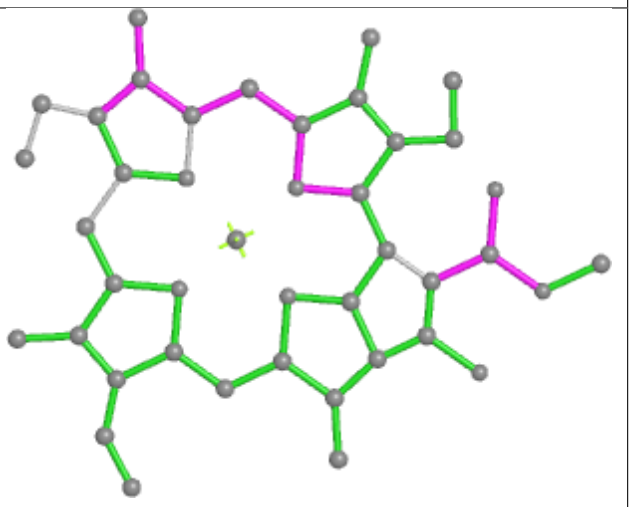


Rings

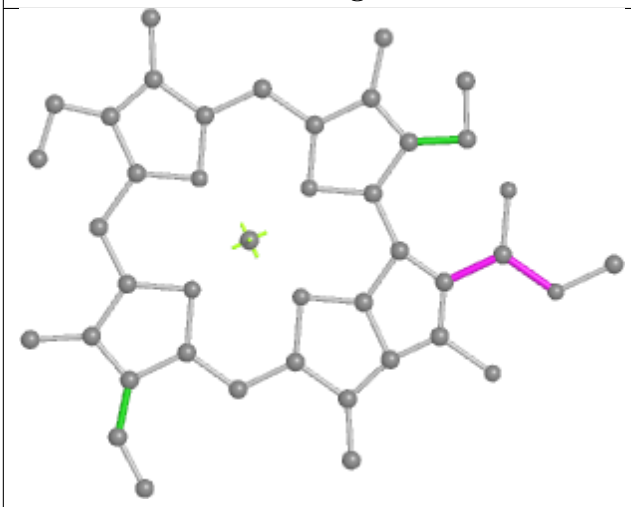
Ligand CLA 4 310



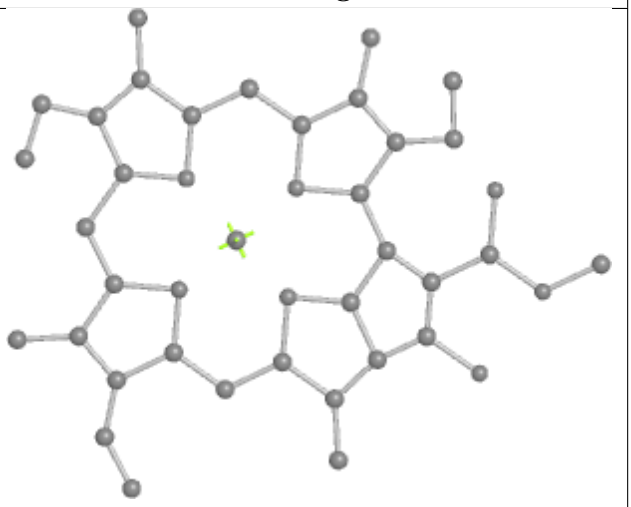
Bond lengths



Bond angles

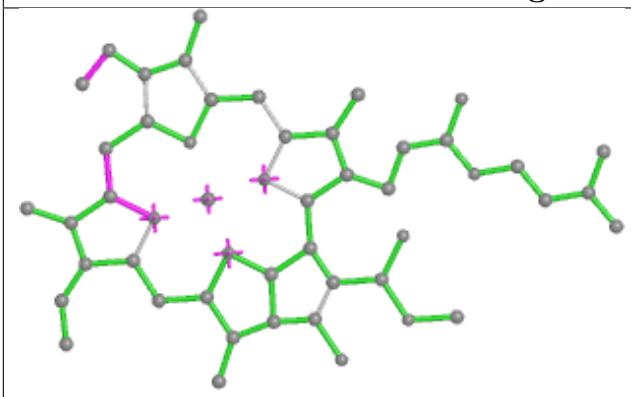


Torsions

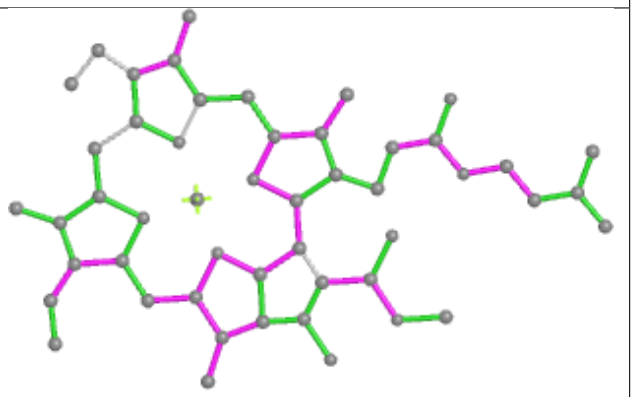


Rings

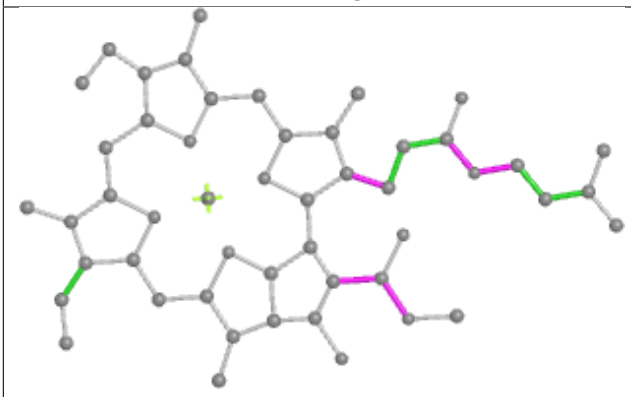
Ligand CLA 1 509



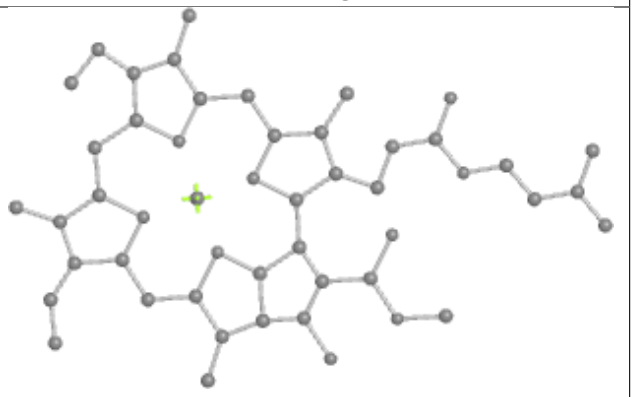
Bond lengths



Bond angles

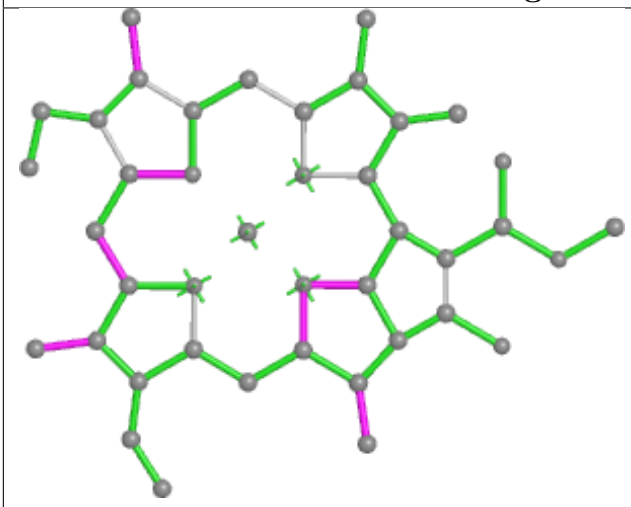


Torsions

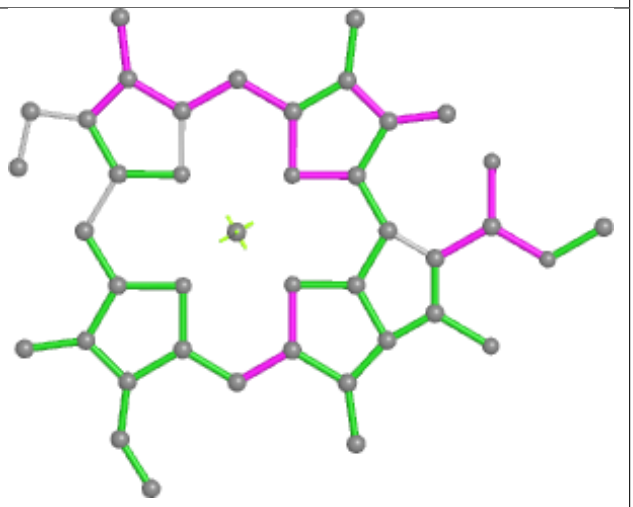


Rings

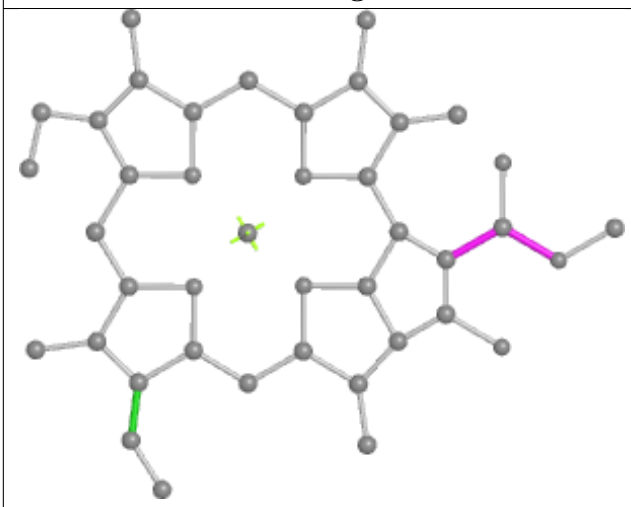
Ligand CLA B 840



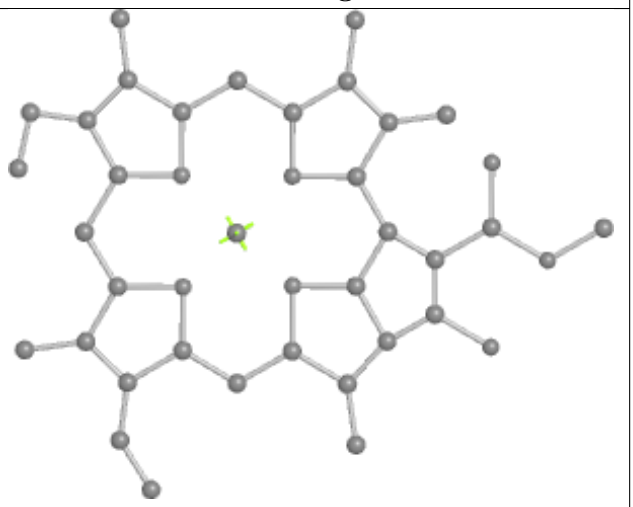
Bond lengths



Bond angles

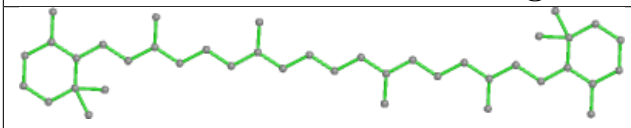


Torsions

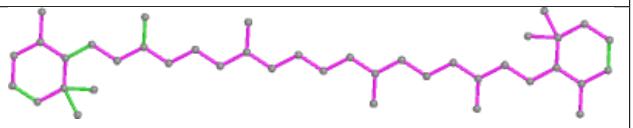


Rings

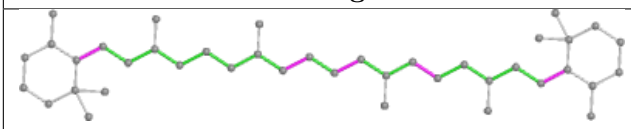
Ligand BCR 6 503



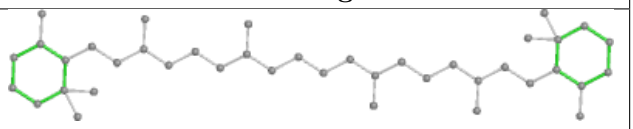
Bond lengths



Bond angles

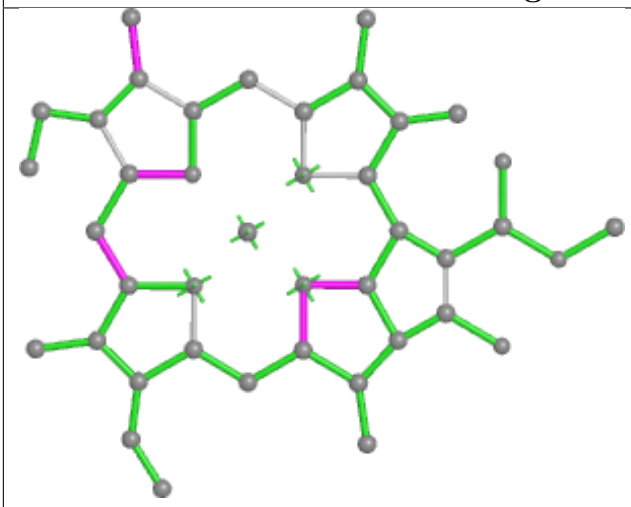


Torsions

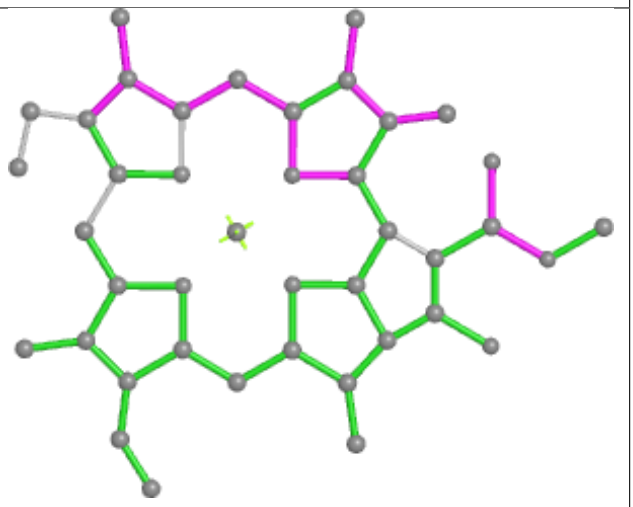


Rings

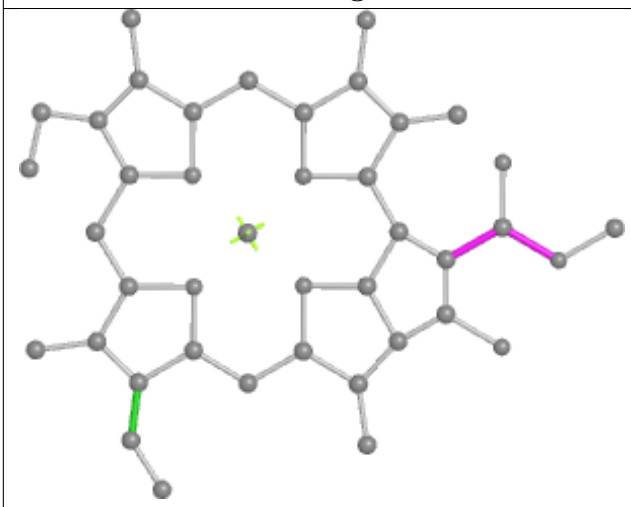
Ligand CLA B 839



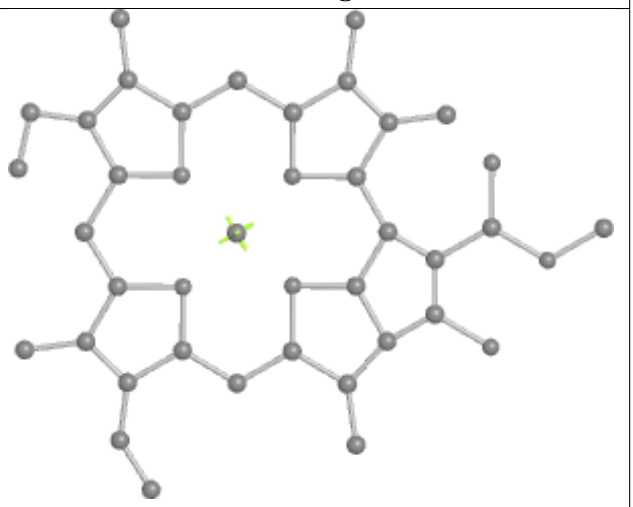
Bond lengths



Bond angles

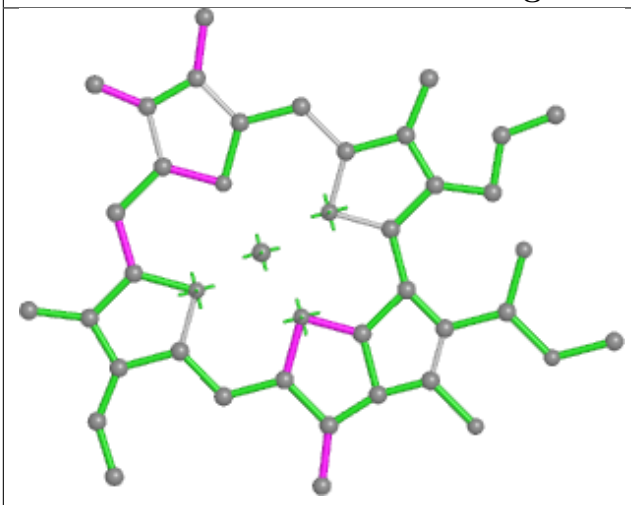


Torsions

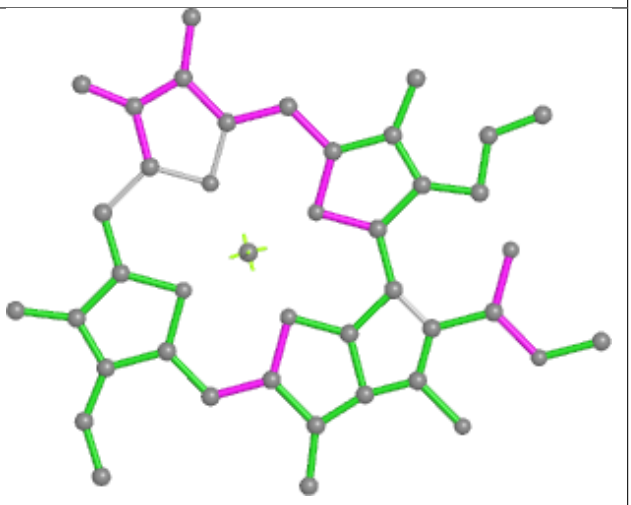


Rings

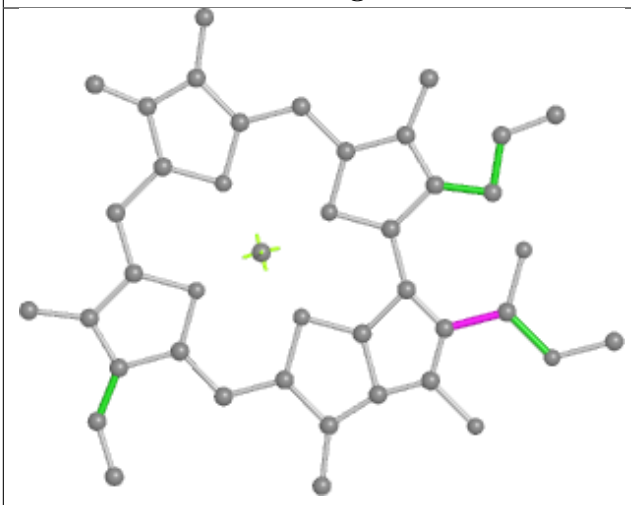
Ligand CLA A 823



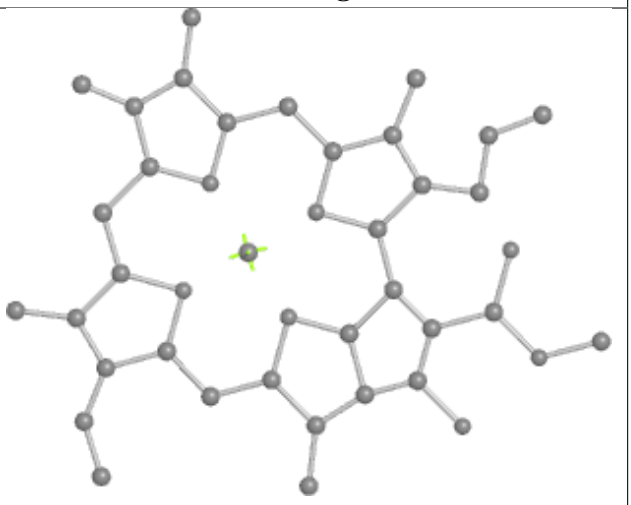
Bond lengths



Bond angles

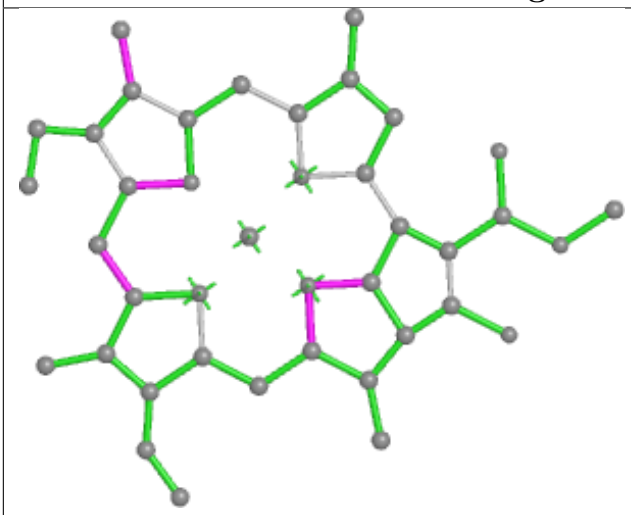


Torsions

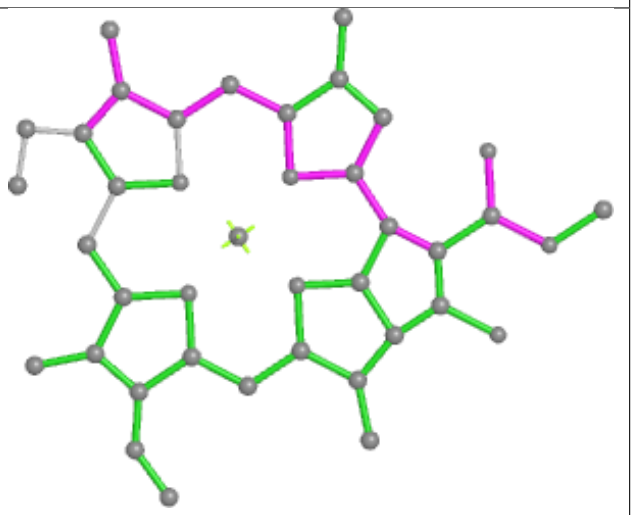


Rings

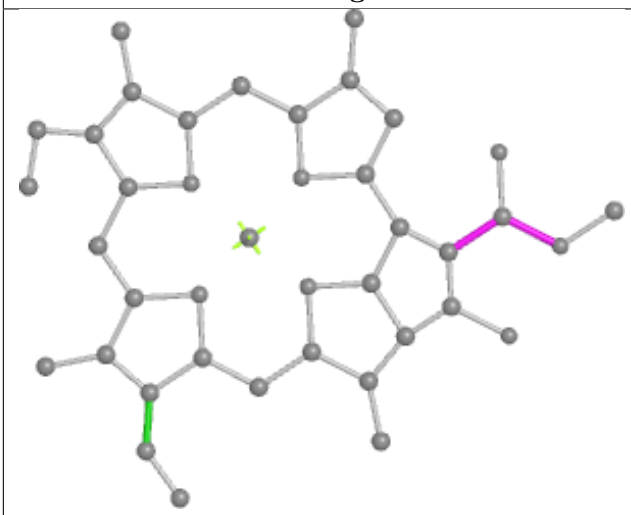
Ligand CLA 3 307



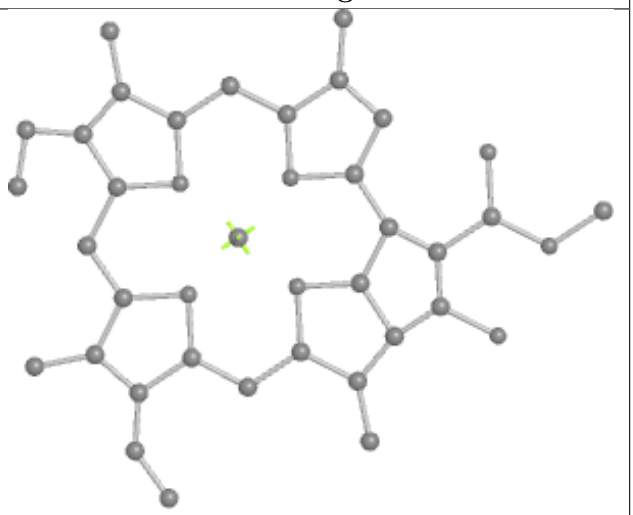
Bond lengths



Bond angles

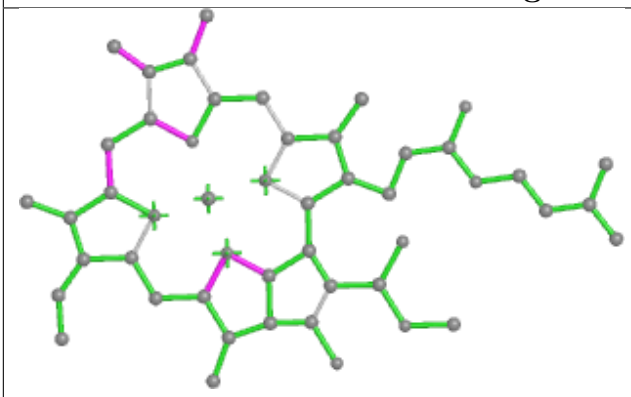


Torsions

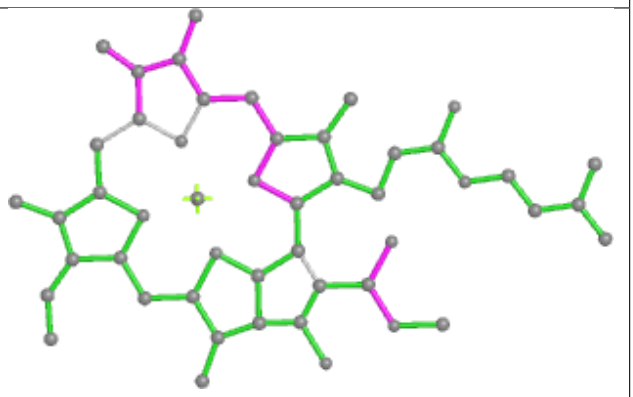


Rings

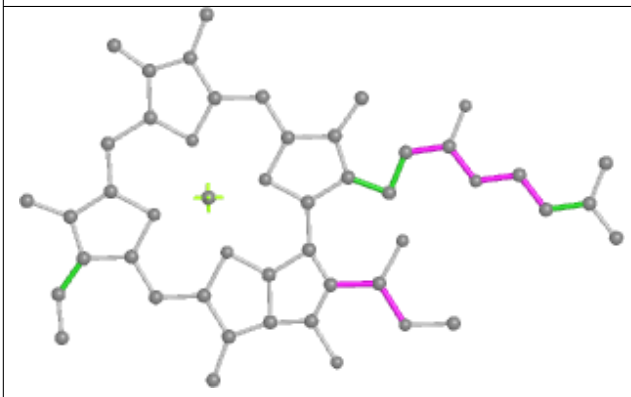
Ligand CLA A 843



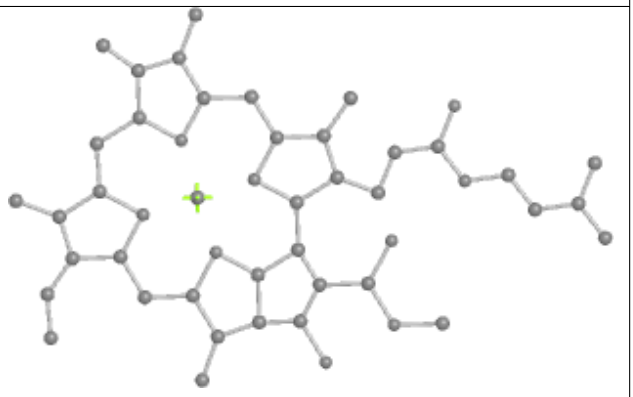
Bond lengths



Bond angles

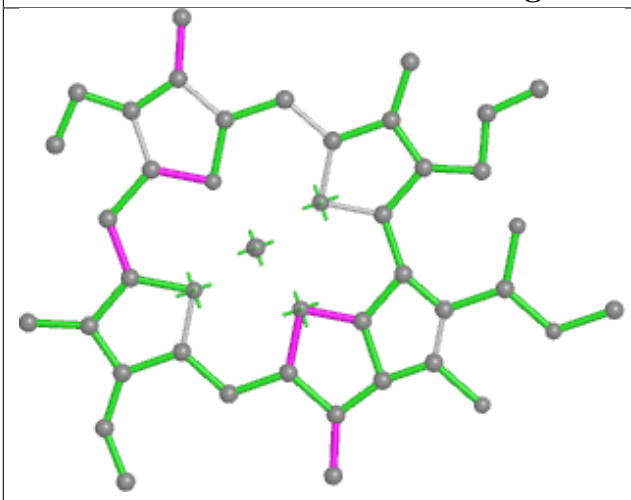


Torsions

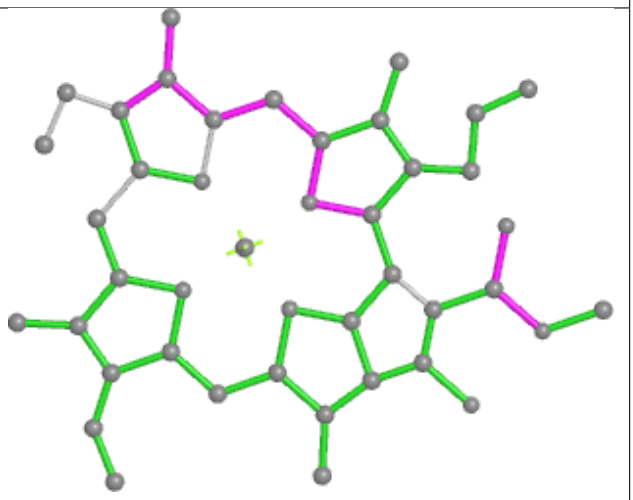


Rings

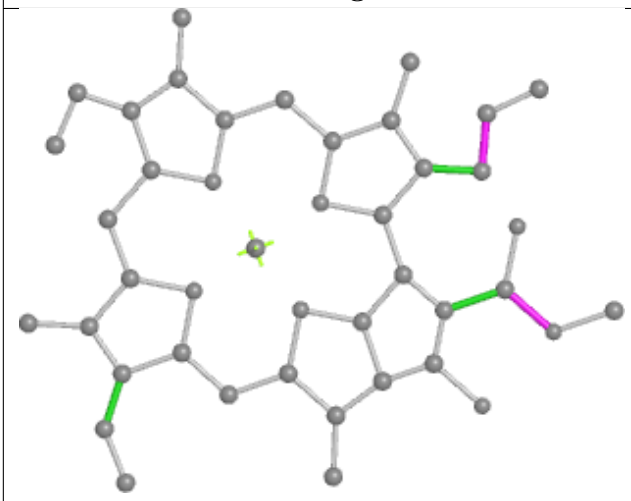
Ligand CLA B 833



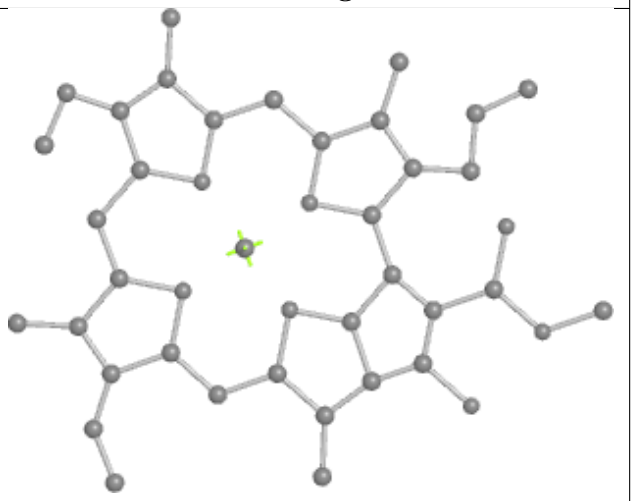
Bond lengths



Bond angles

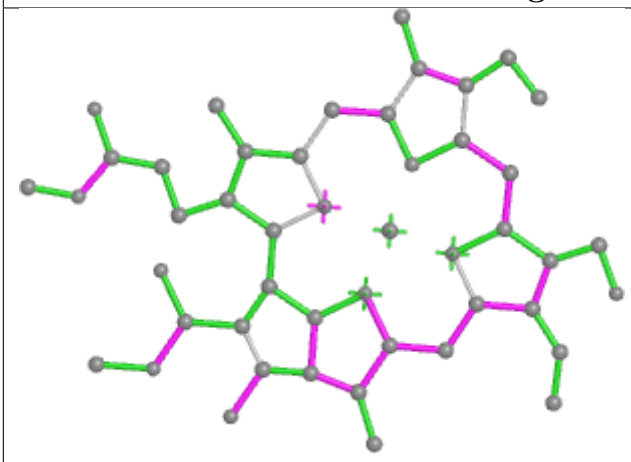


Torsions

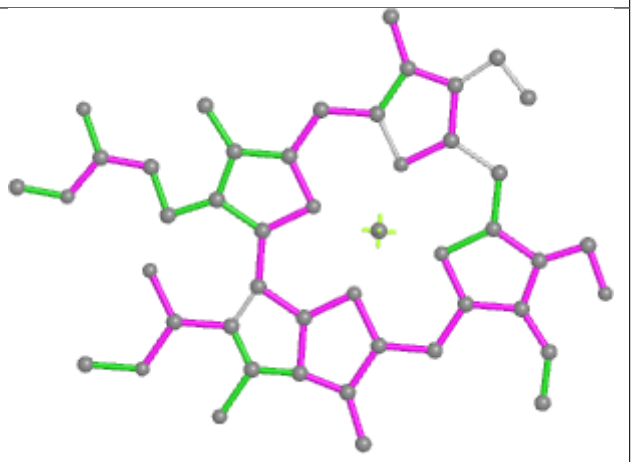


Rings

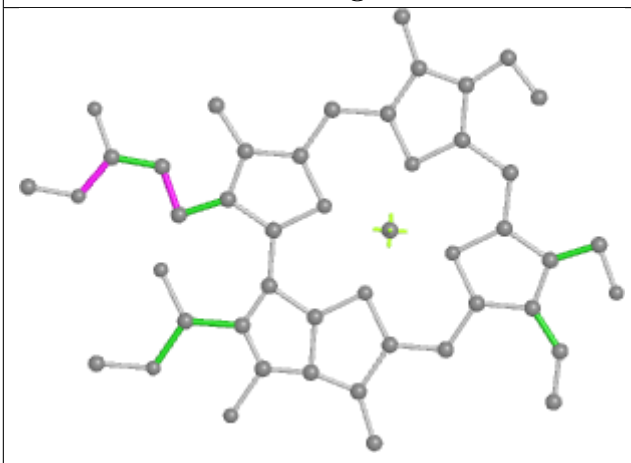
Ligand CHL 1 512



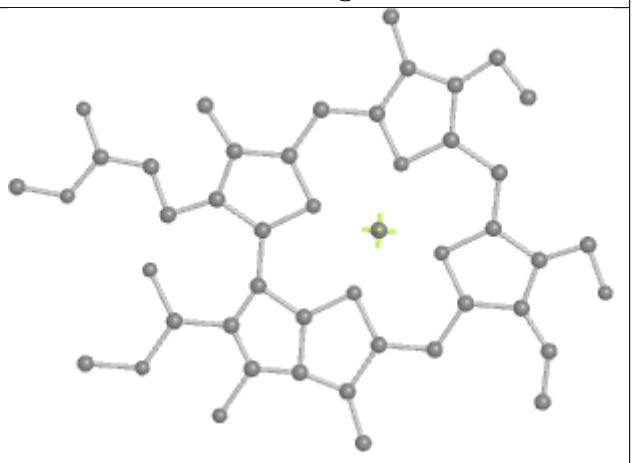
Bond lengths



Bond angles

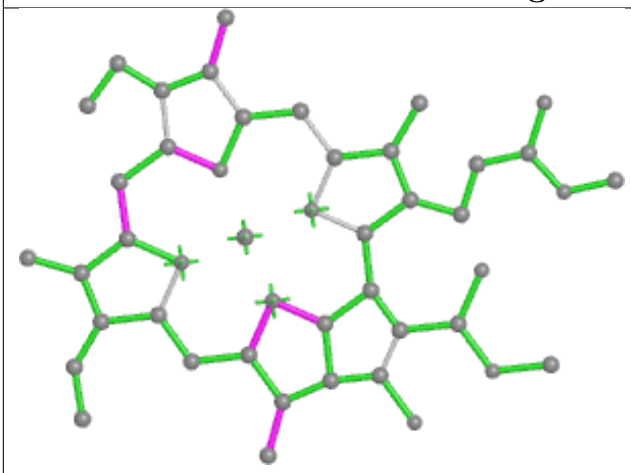


Torsions

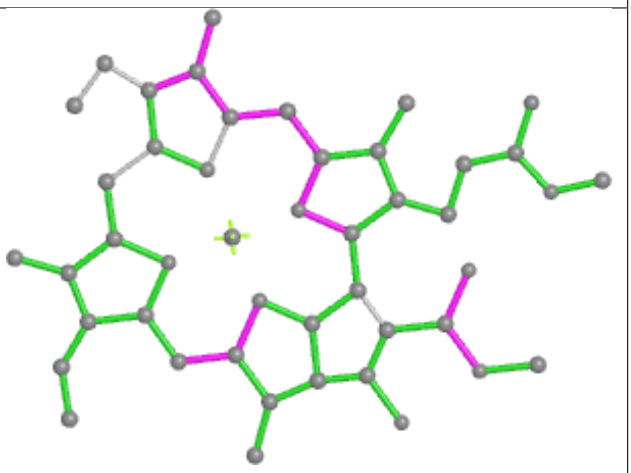


Rings

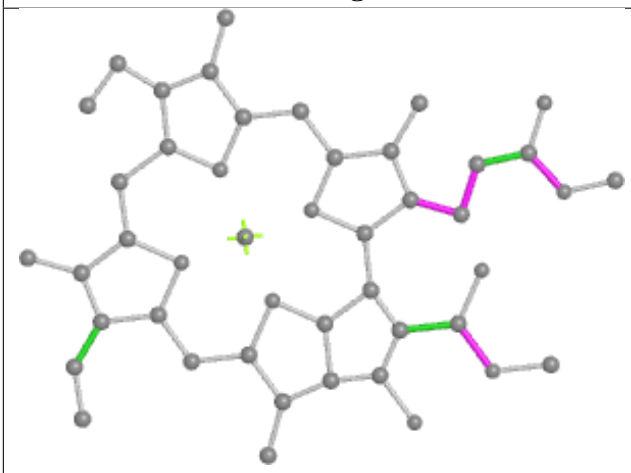
Ligand CLA 3 316



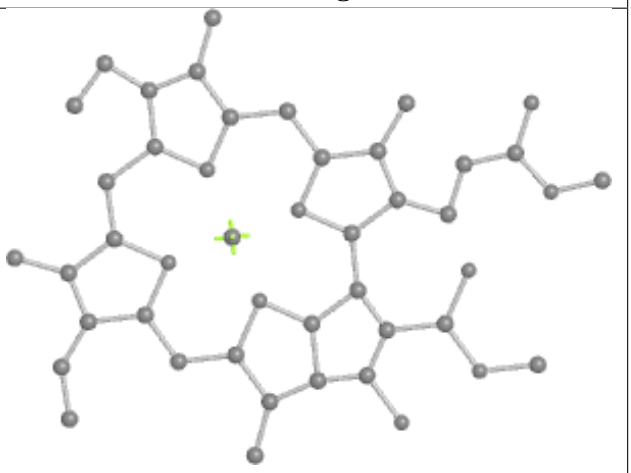
Bond lengths



Bond angles

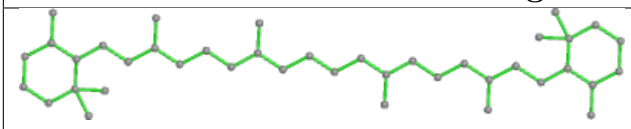


Torsions

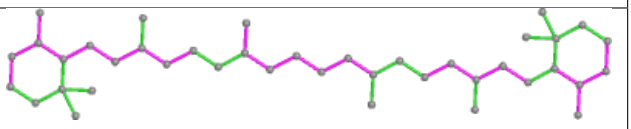


Rings

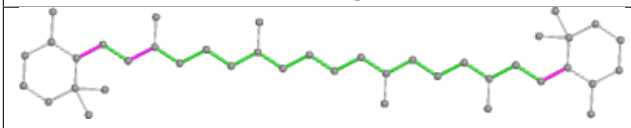
Ligand BCR 4 301



Bond lengths



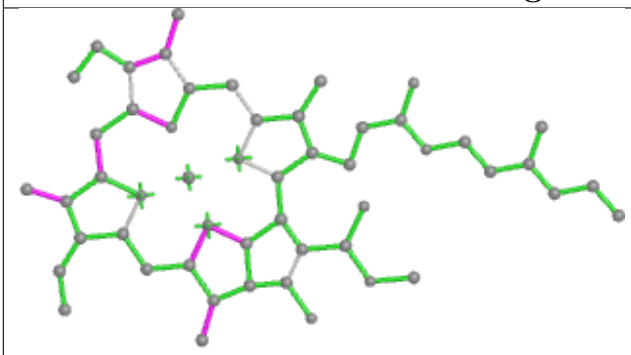
Bond angles



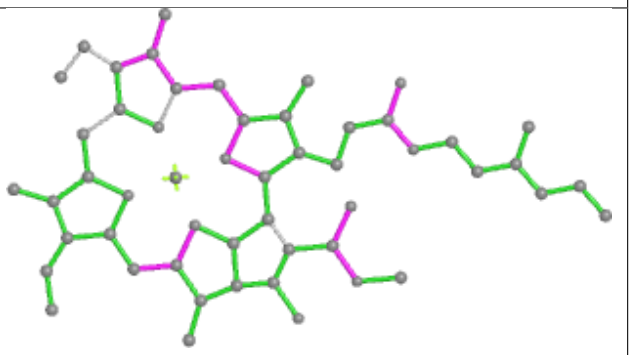
Torsions

Rings

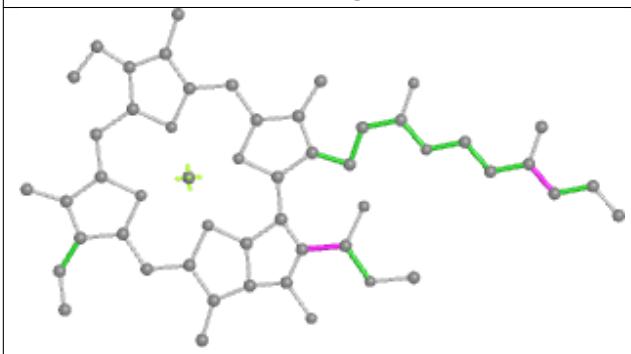
Ligand CLA B 809



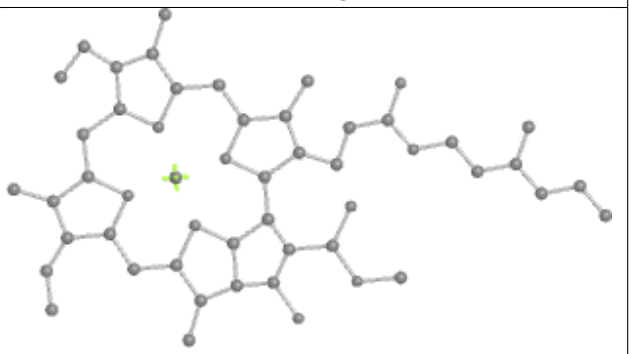
Bond lengths



Bond angles

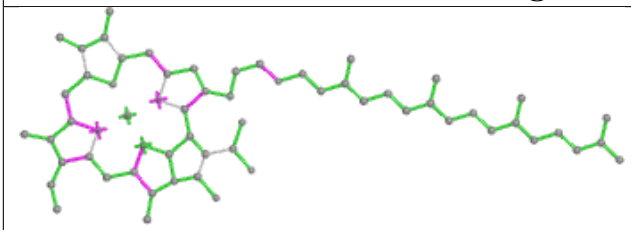


Torsions

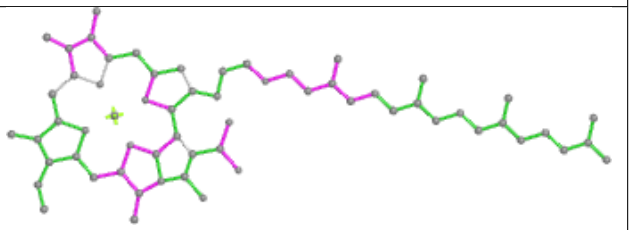


Rings

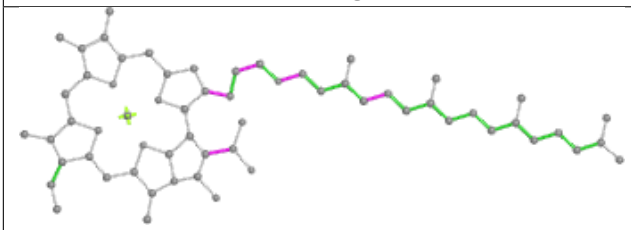
Ligand CL0 A 801



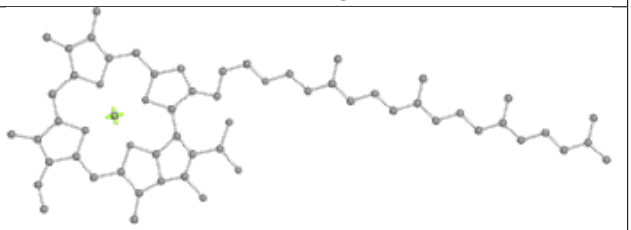
Bond lengths



Bond angles

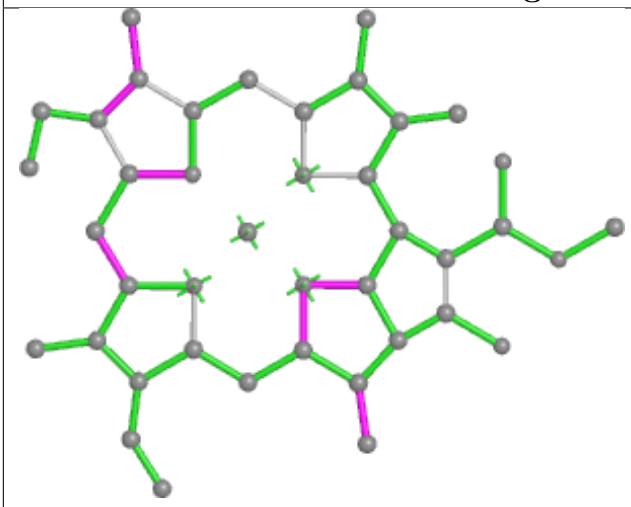


Torsions

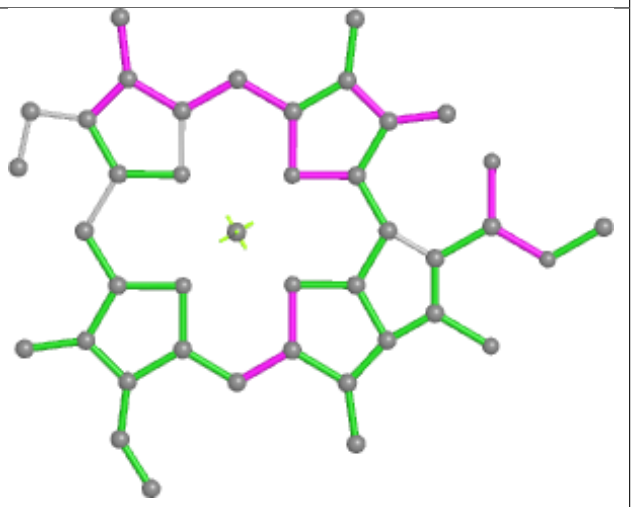


Rings

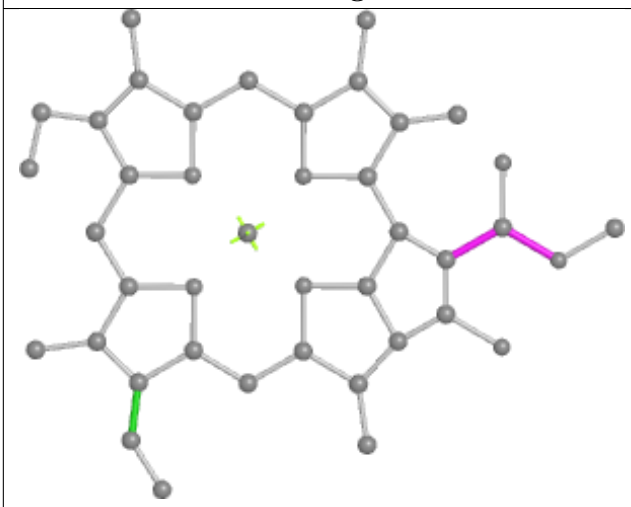
Ligand CLA A 808



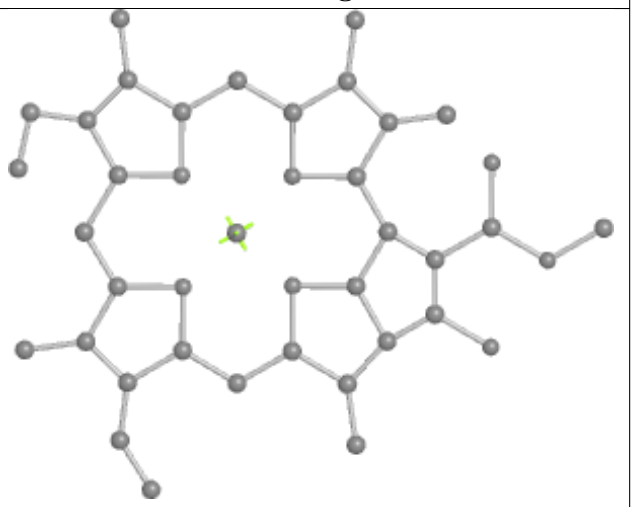
Bond lengths



Bond angles

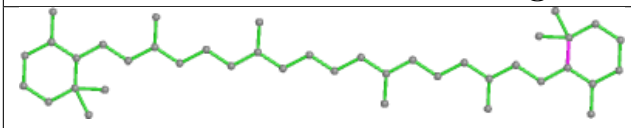


Torsions

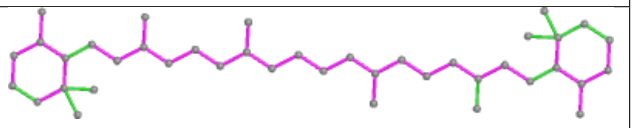


Rings

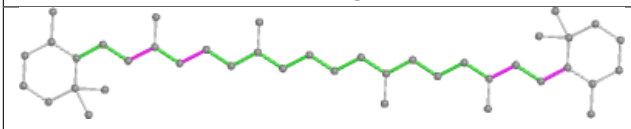
Ligand BCR I 101



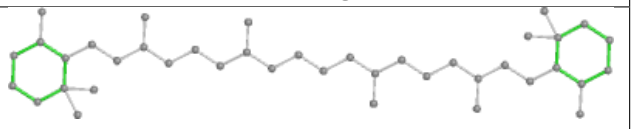
Bond lengths



Bond angles

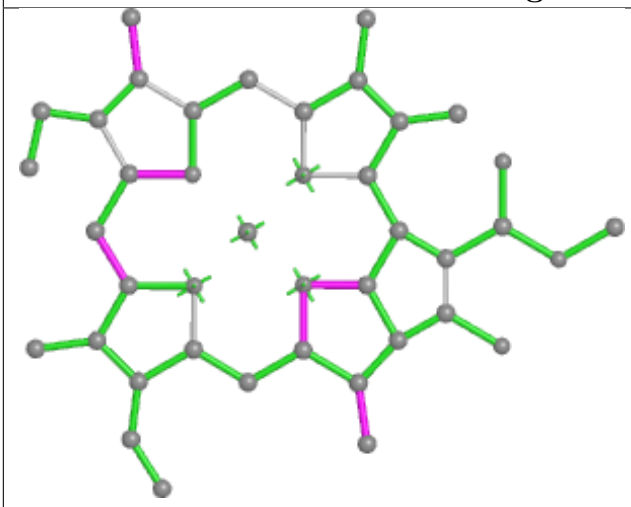


Torsions

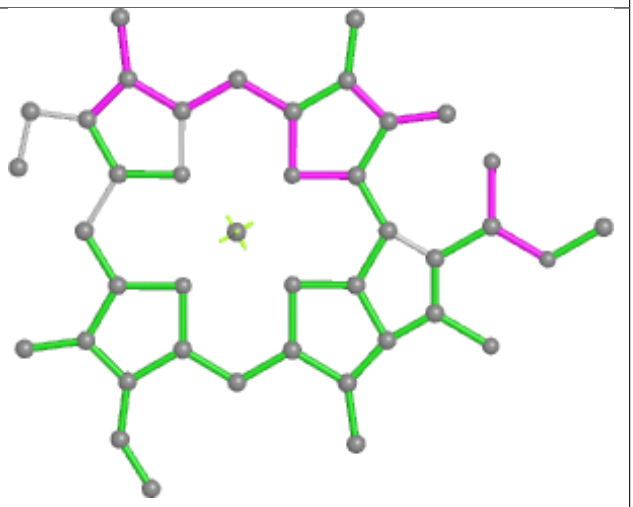


Rings

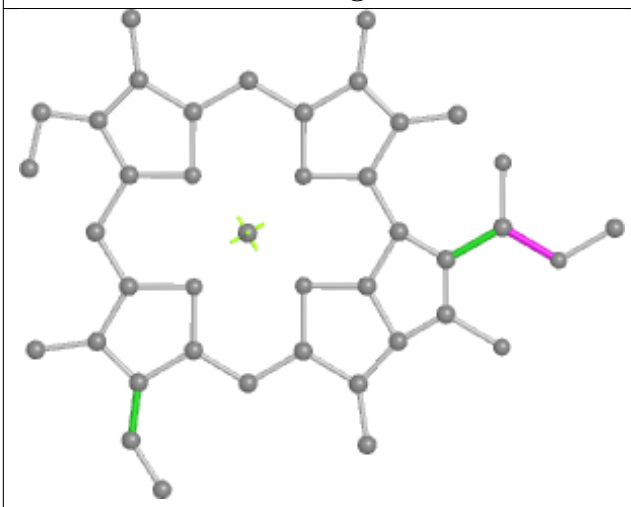
Ligand CLA F 802



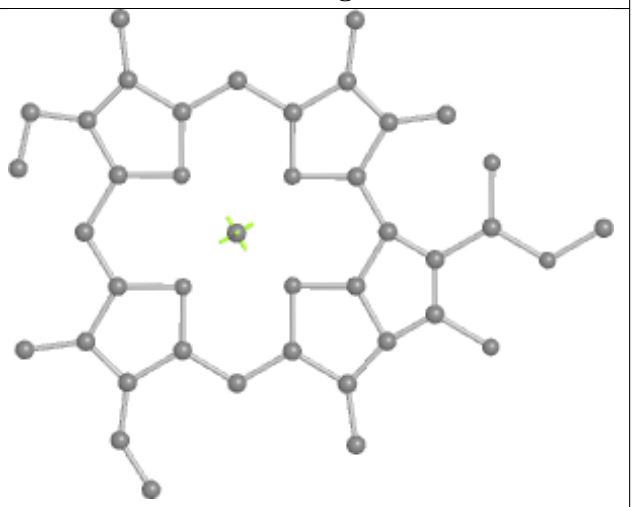
Bond lengths



Bond angles

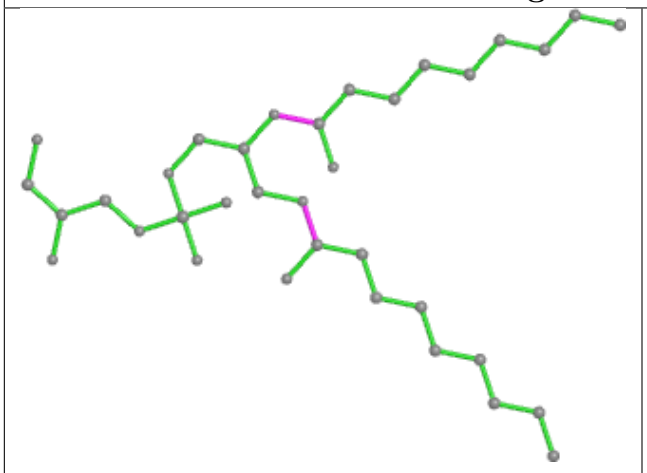


Torsions

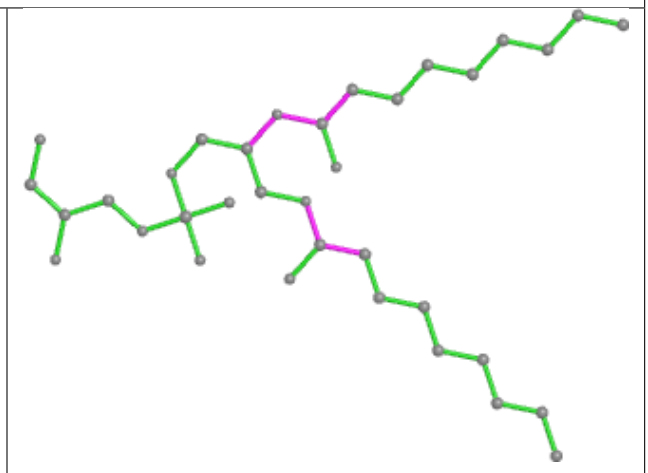


Rings

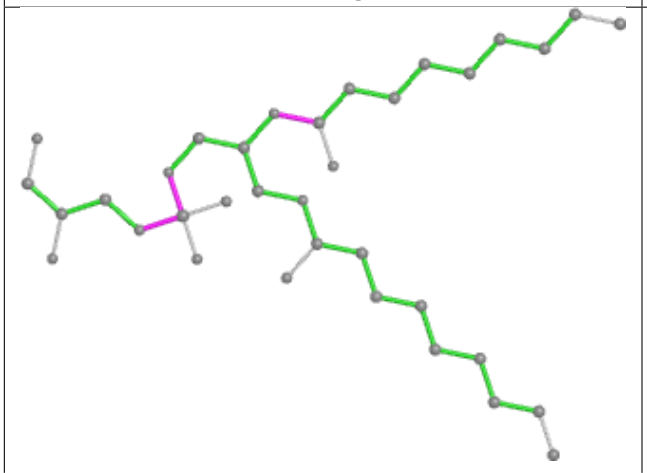
Ligand LHG 6 516



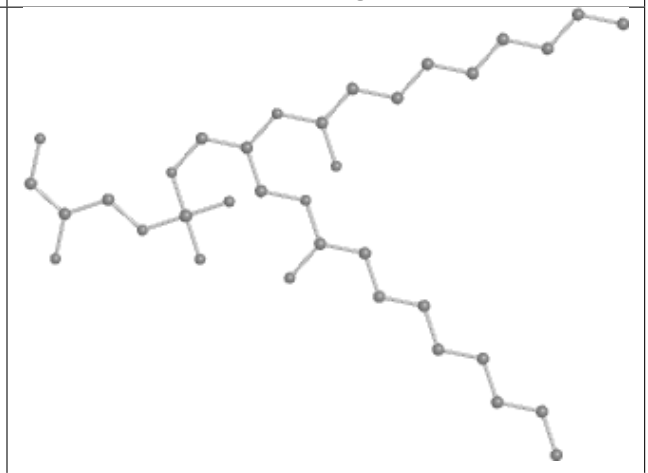
Bond lengths



Bond angles

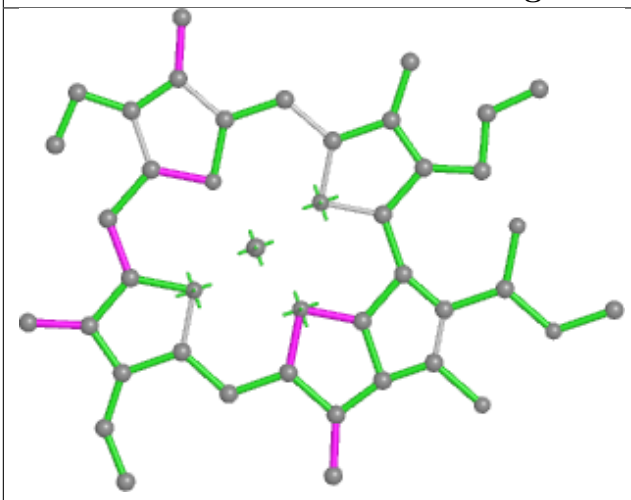


Torsions

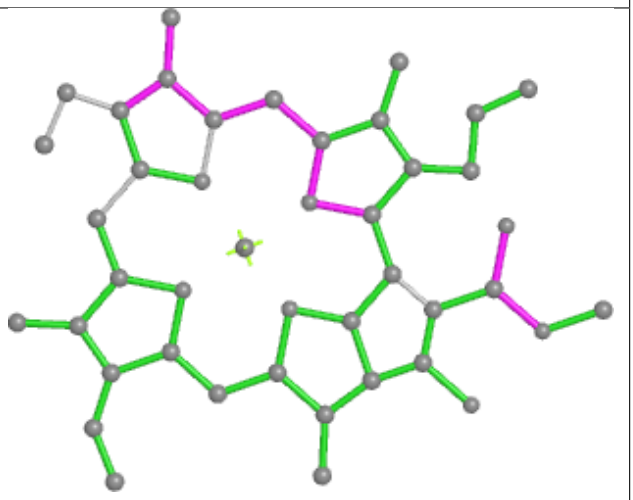


Rings

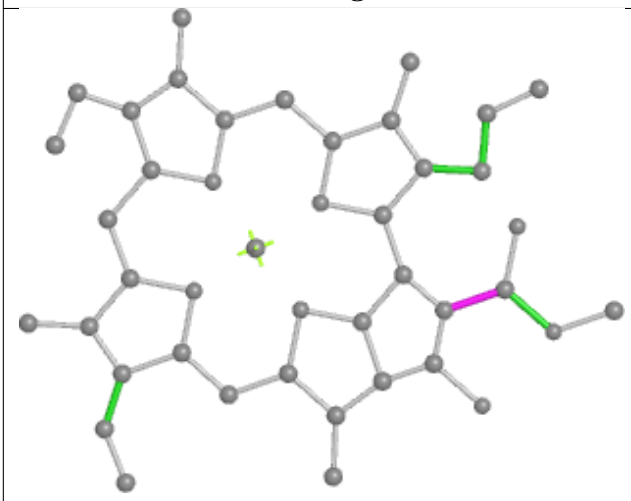
Ligand CLA B 814



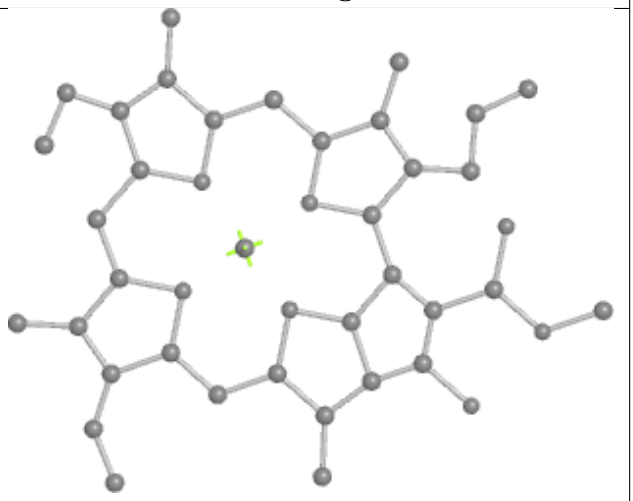
Bond lengths



Bond angles

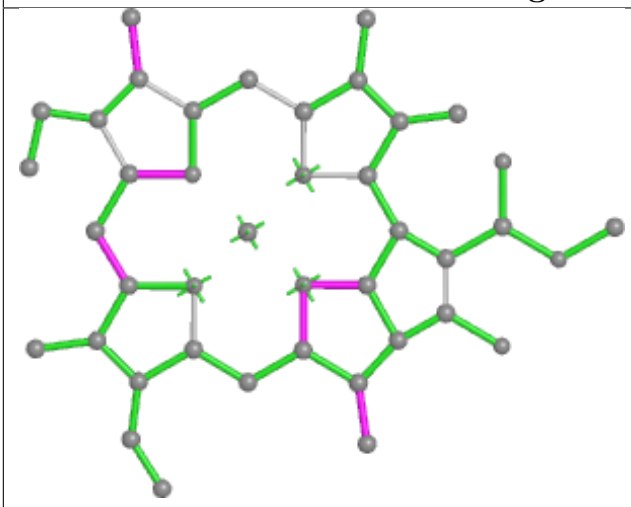


Torsions

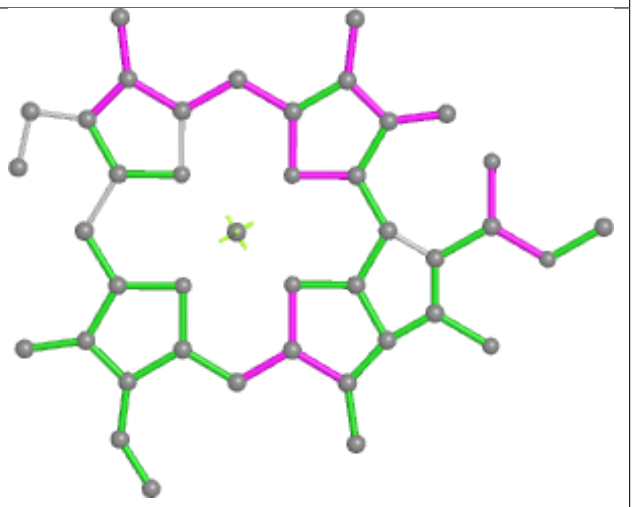


Rings

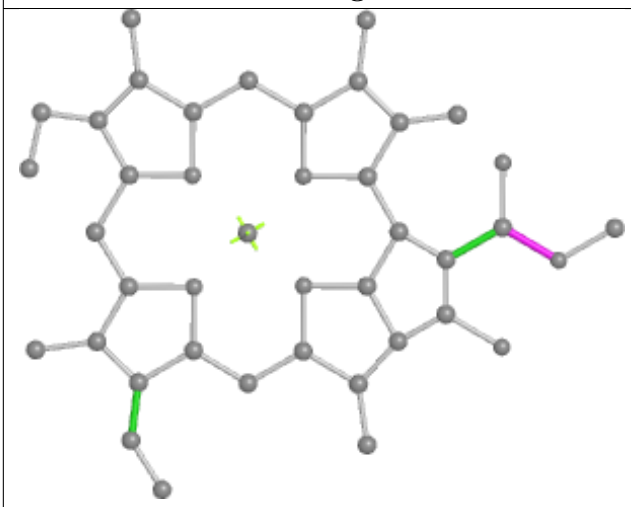
Ligand CLA 4 315



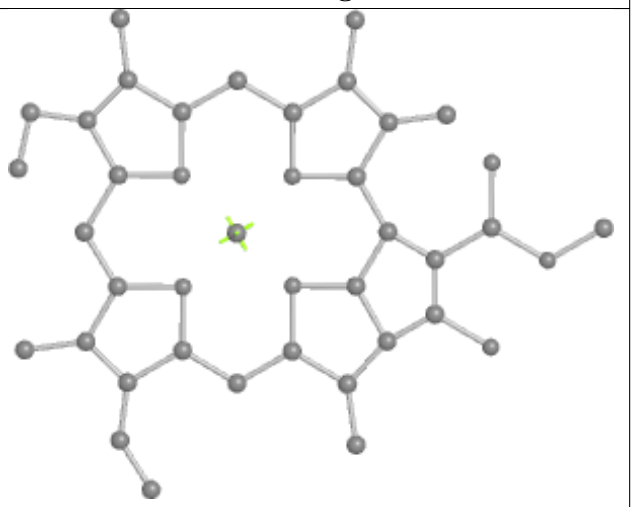
Bond lengths



Bond angles

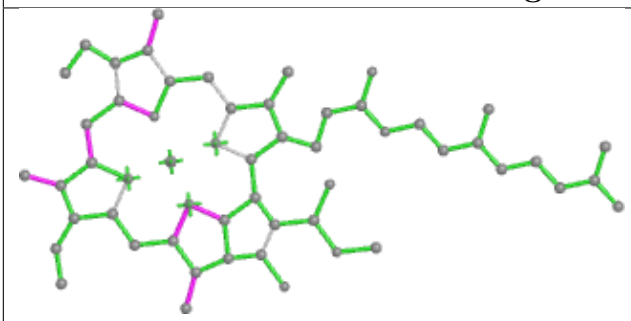


Torsions

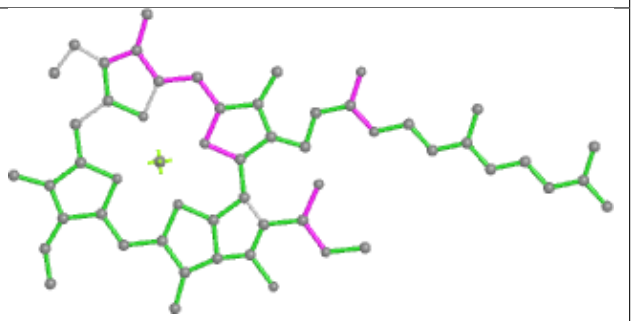


Rings

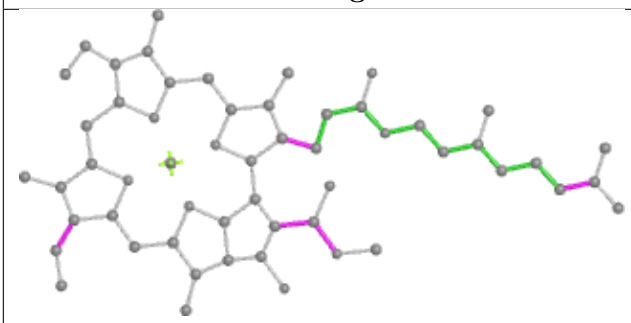
Ligand CLA B 821



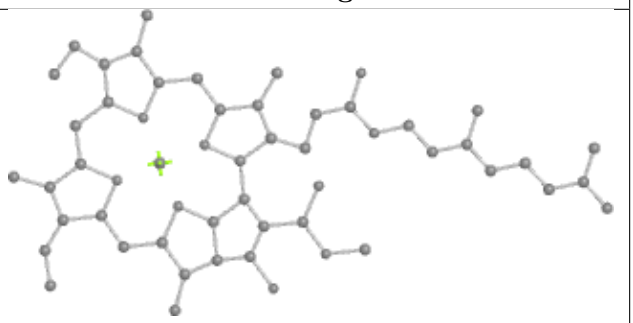
Bond lengths



Bond angles

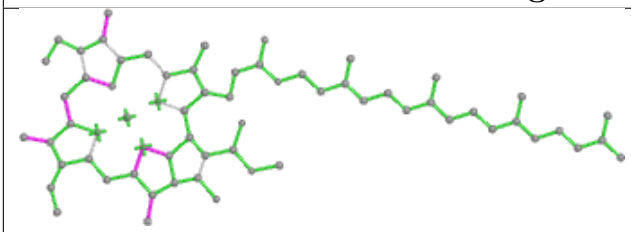


Torsions

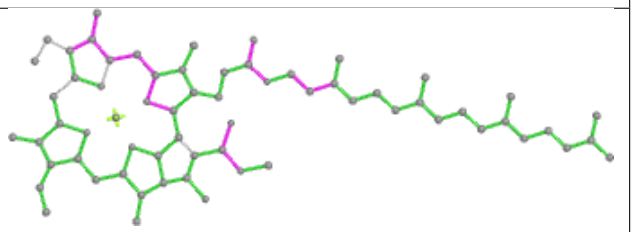


Rings

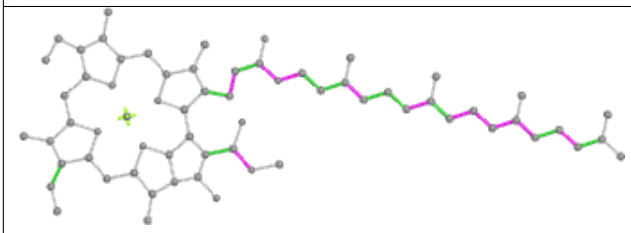
Ligand CLA 4 306



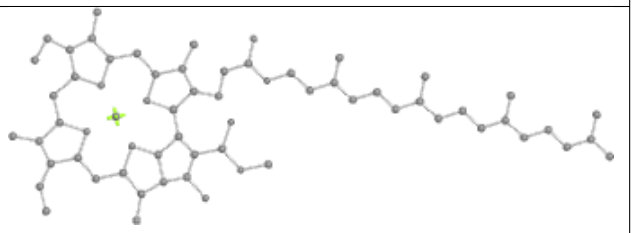
Bond lengths



Bond angles

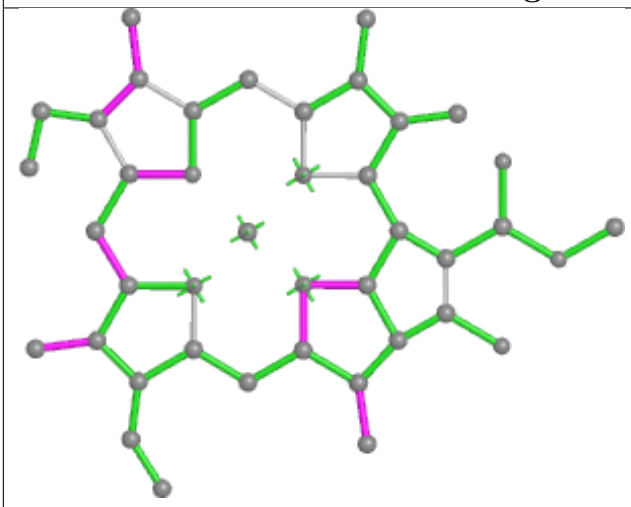


Torsions

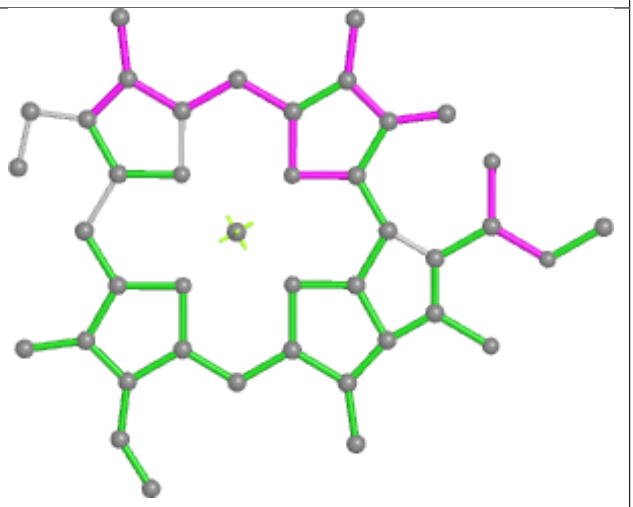


Rings

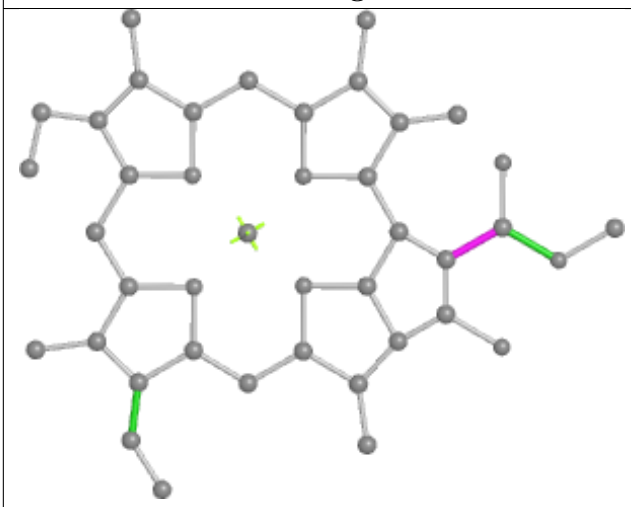
Ligand CLA A 811



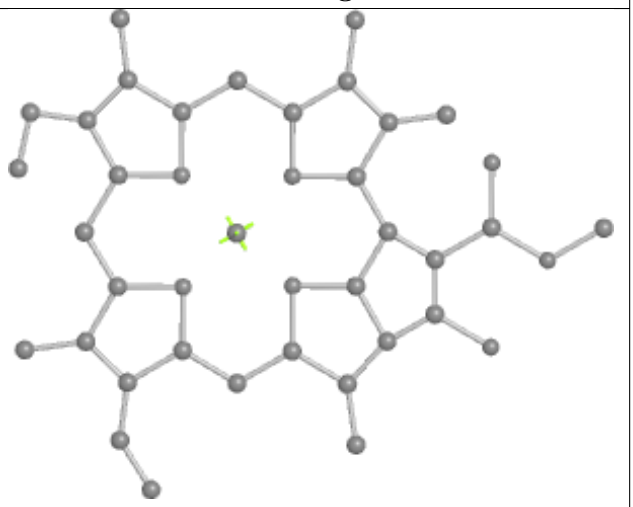
Bond lengths



Bond angles

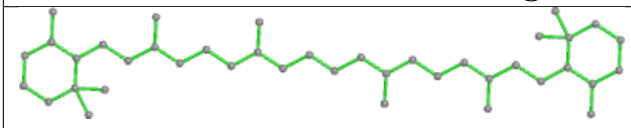


Torsions

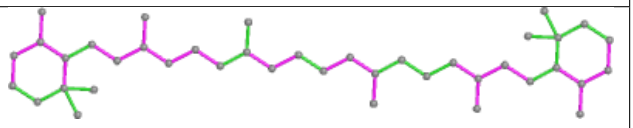


Rings

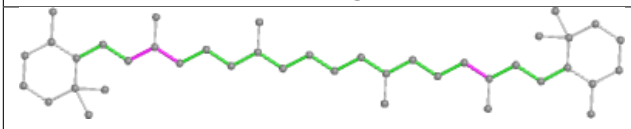
Ligand BCR B 847



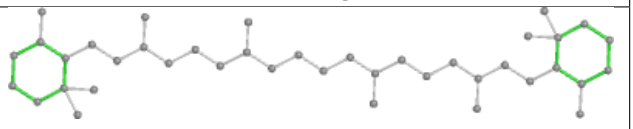
Bond lengths



Bond angles

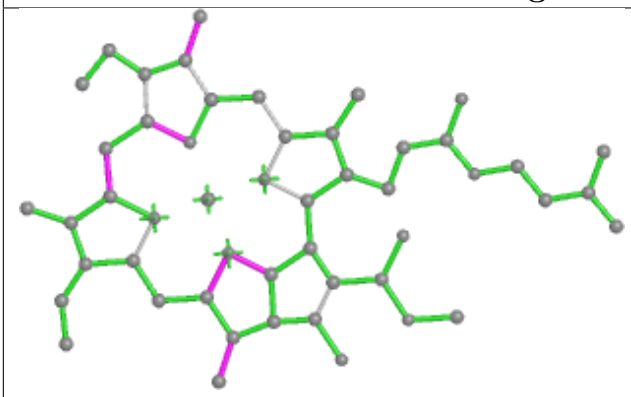


Torsions

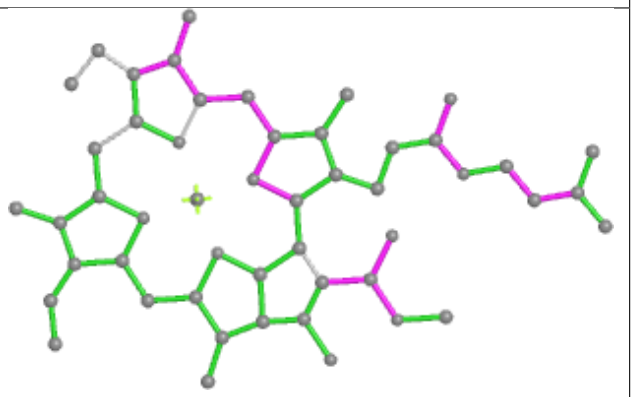


Rings

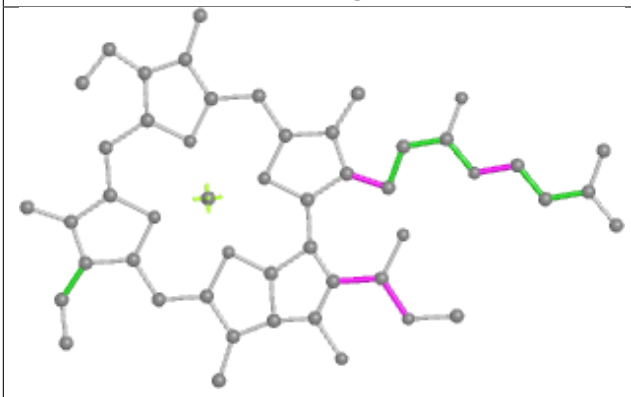
Ligand CLA 4 317



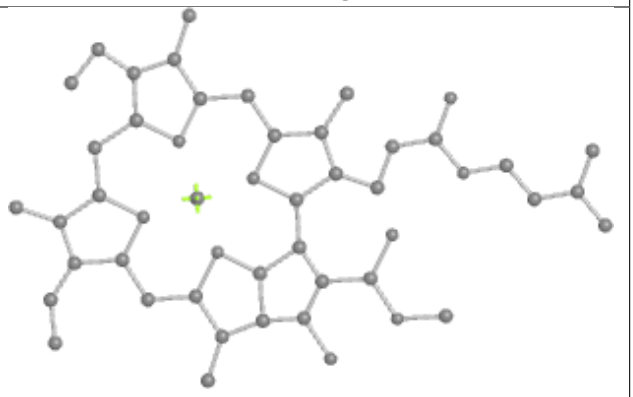
Bond lengths



Bond angles

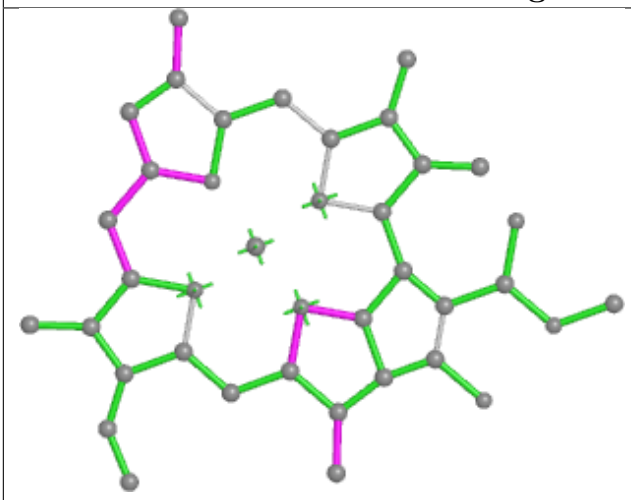


Torsions

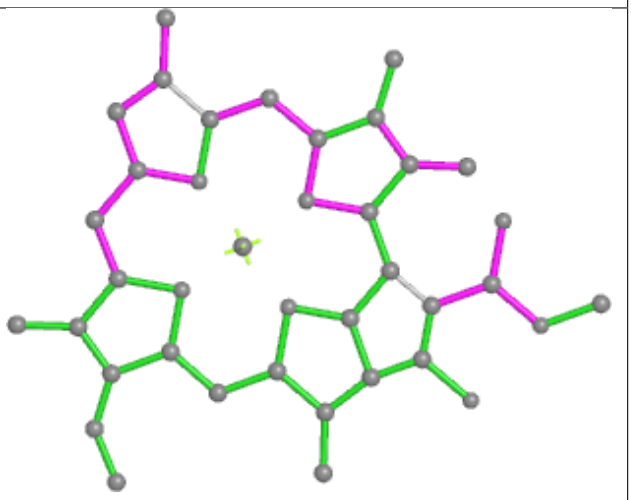


Rings

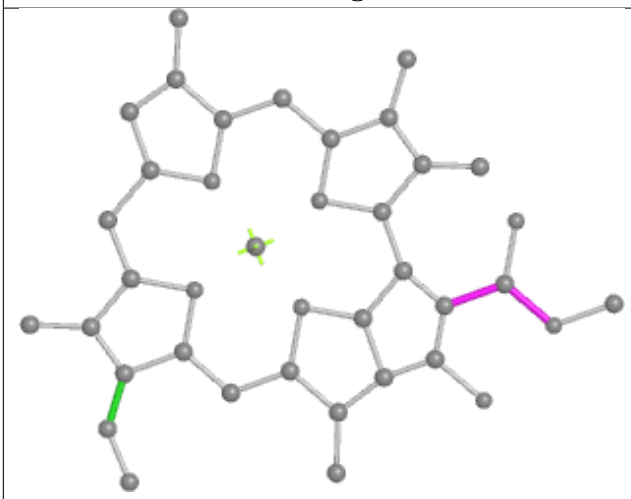
Ligand CLA 6 504



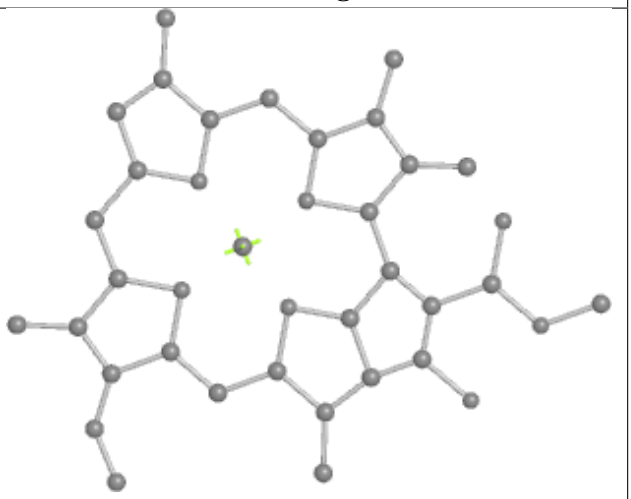
Bond lengths



Bond angles

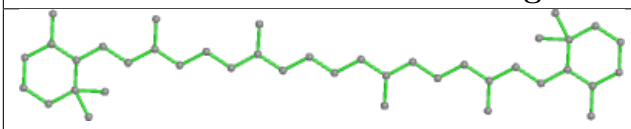


Torsions

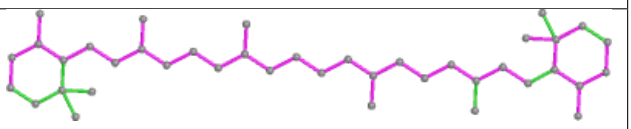


Rings

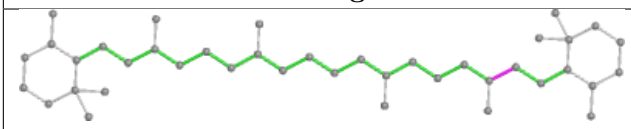
Ligand BCR F 801



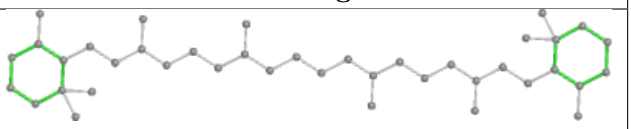
Bond lengths



Bond angles

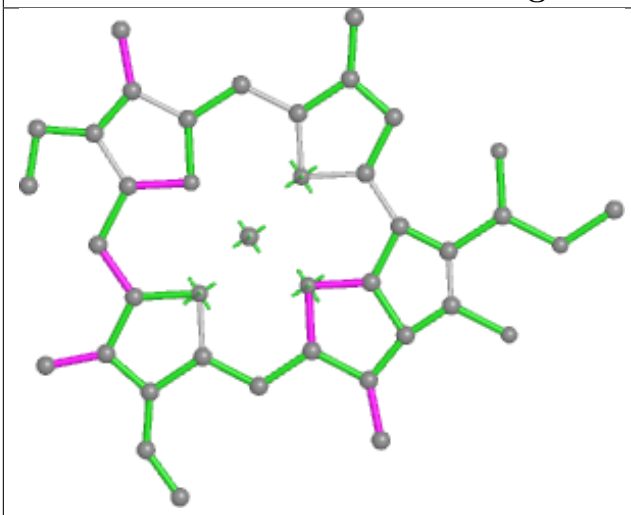


Torsions

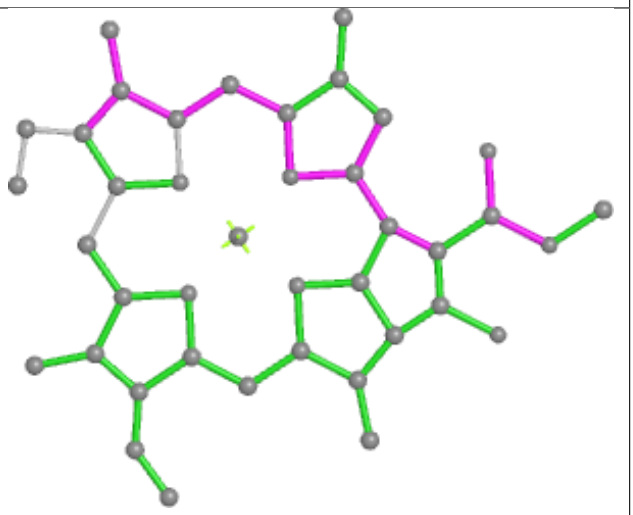


Rings

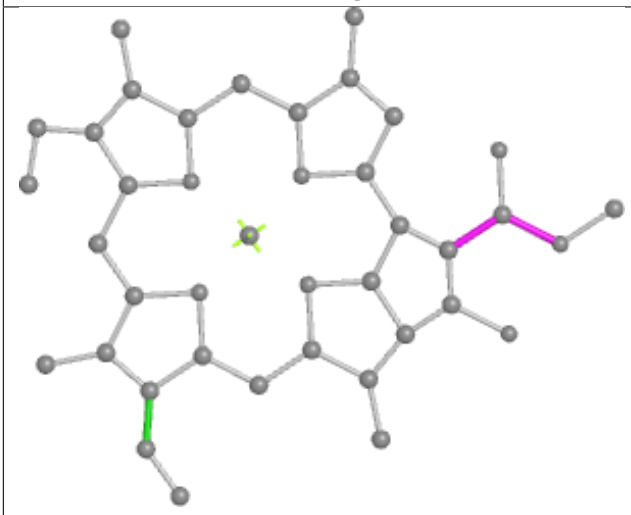
Ligand CLA 1 515



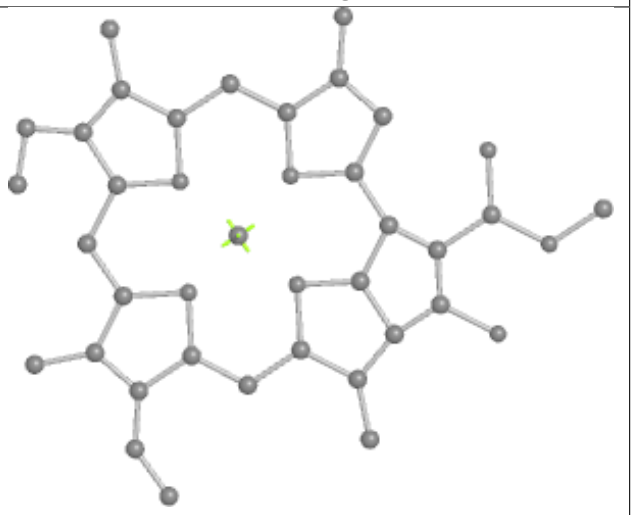
Bond lengths



Bond angles

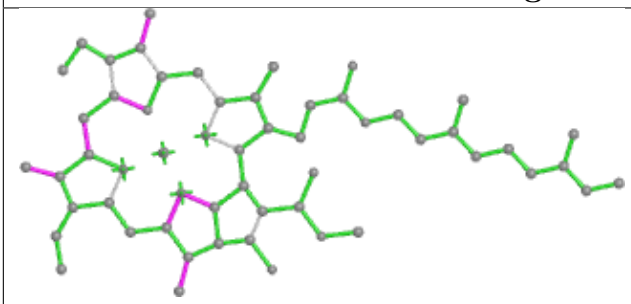


Torsions

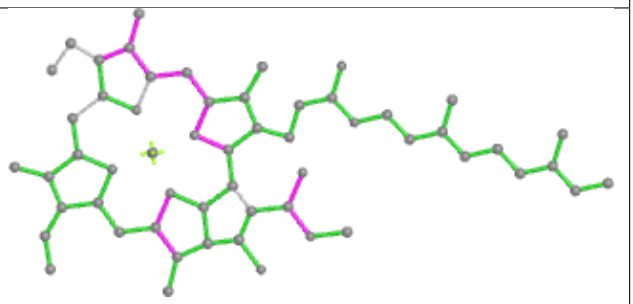


Rings

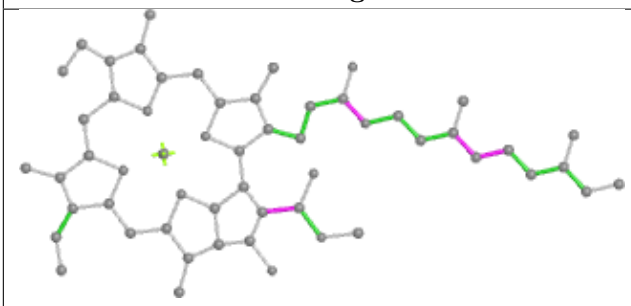
Ligand CLA B 831



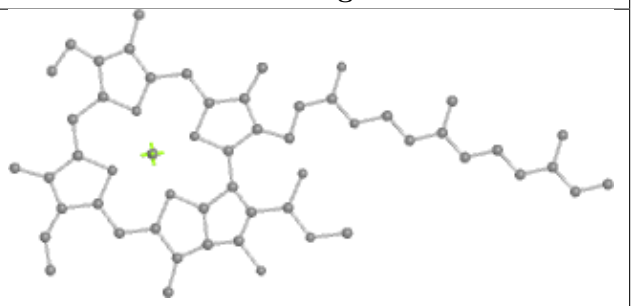
Bond lengths



Bond angles

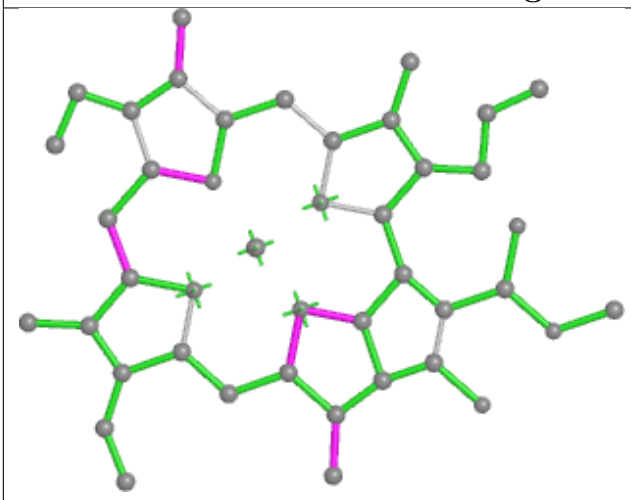


Torsions

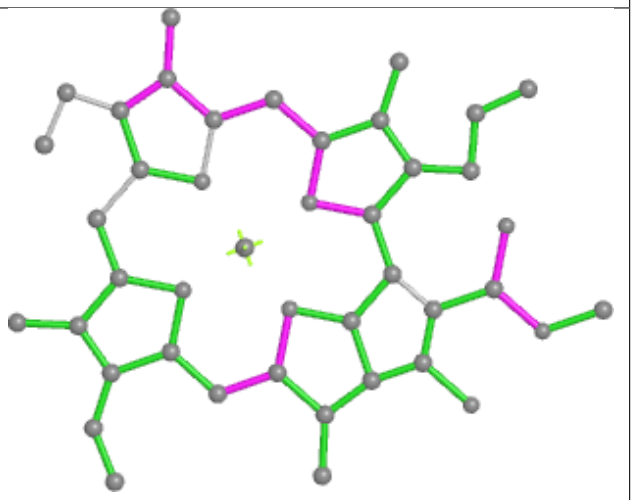


Rings

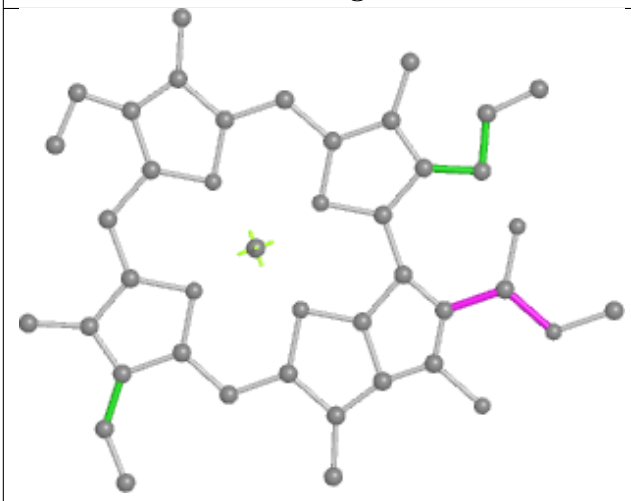
Ligand CLA B 834



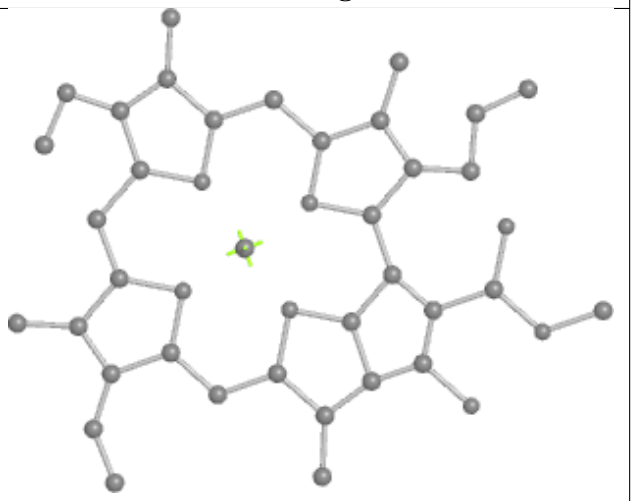
Bond lengths



Bond angles

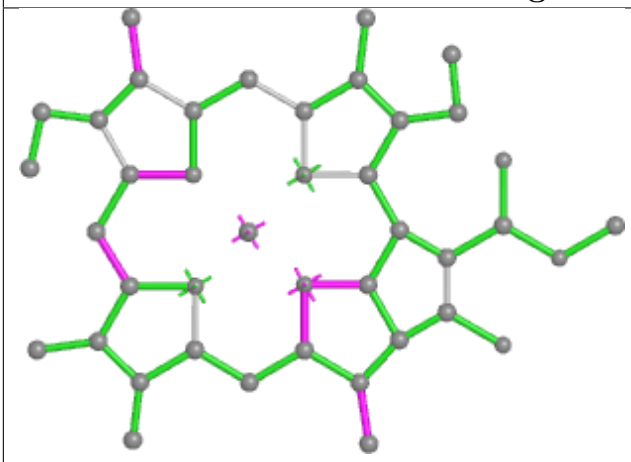


Torsions

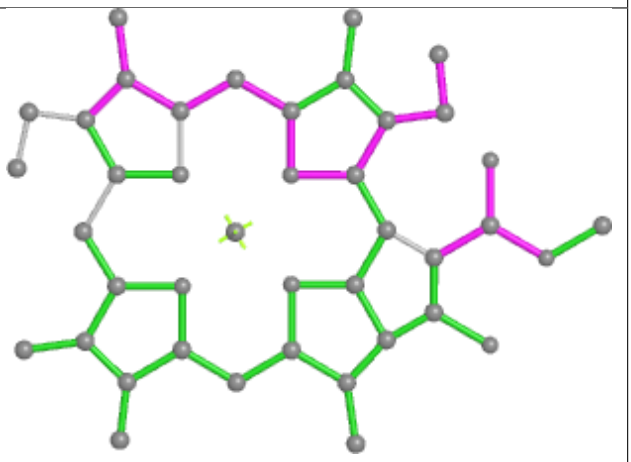


Rings

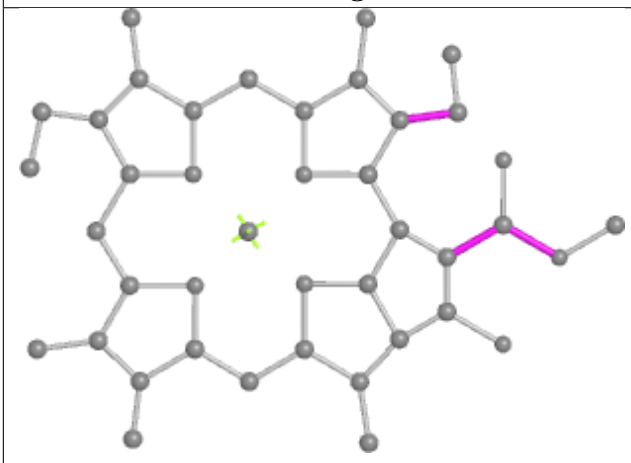
Ligand CLA 1 504



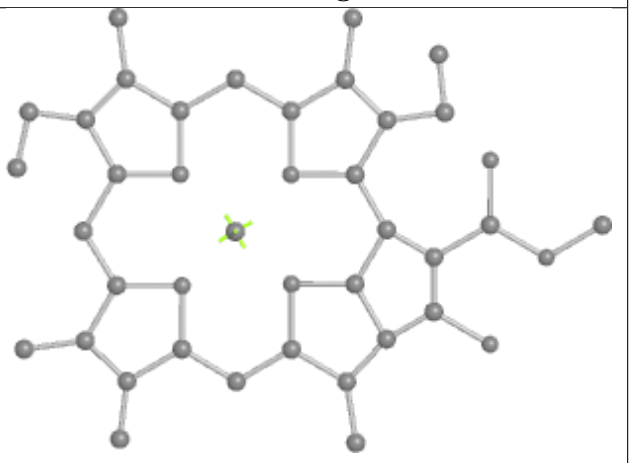
Bond lengths



Bond angles

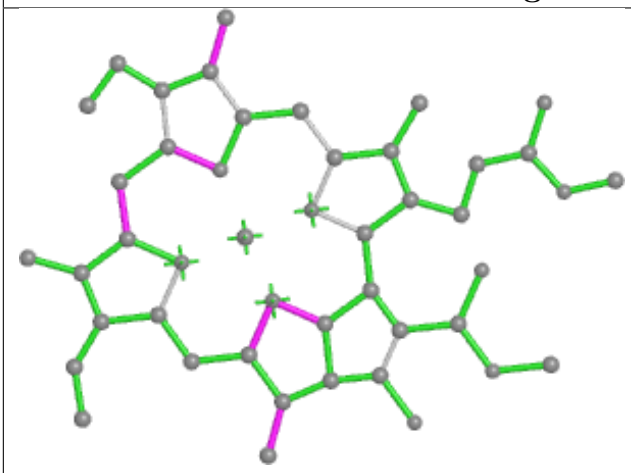


Torsions

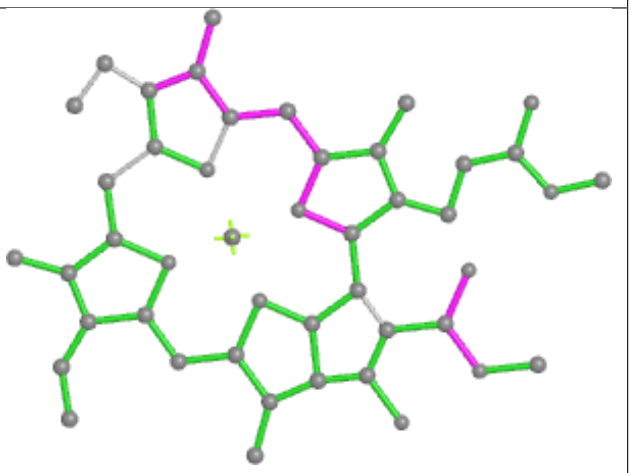


Rings

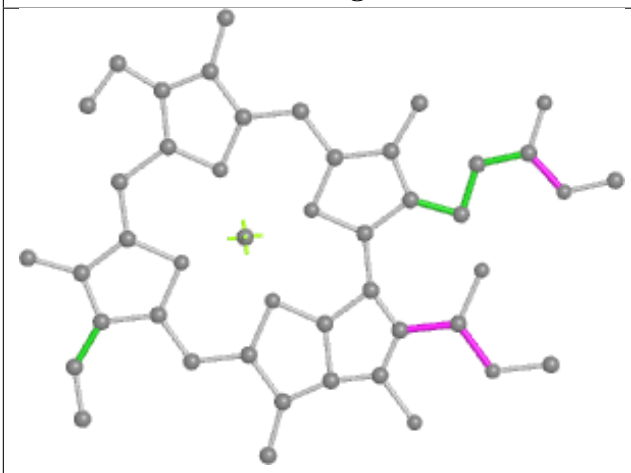
Ligand CLA A 805



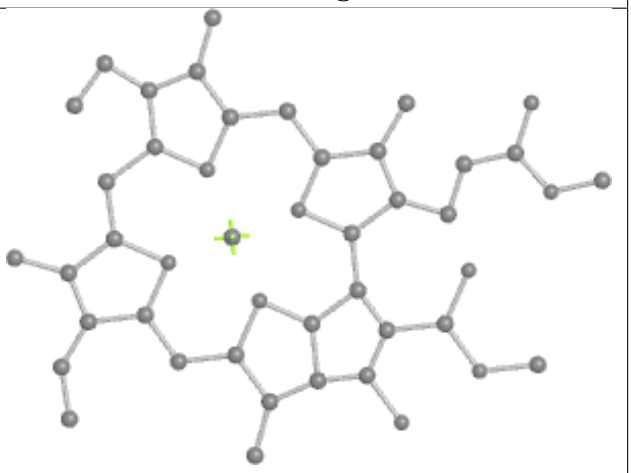
Bond lengths



Bond angles

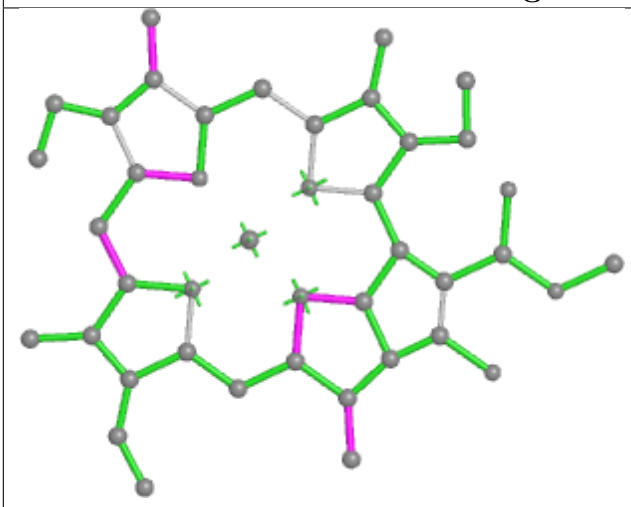


Torsions

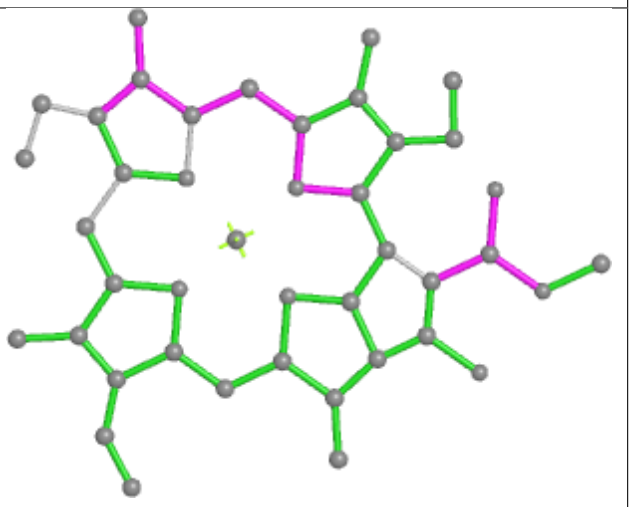


Rings

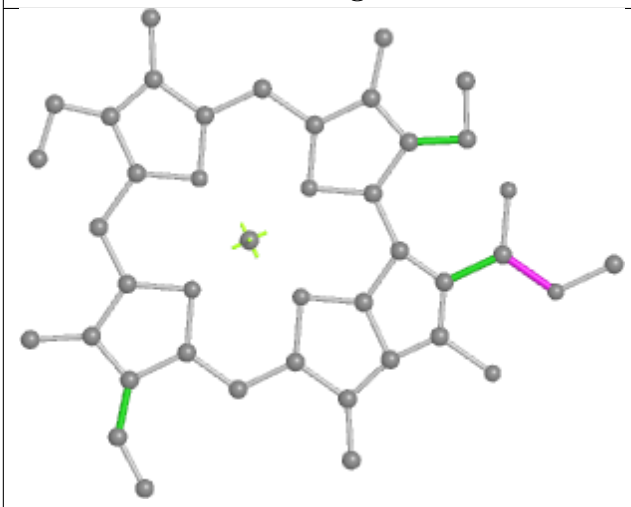
Ligand CLA A 807



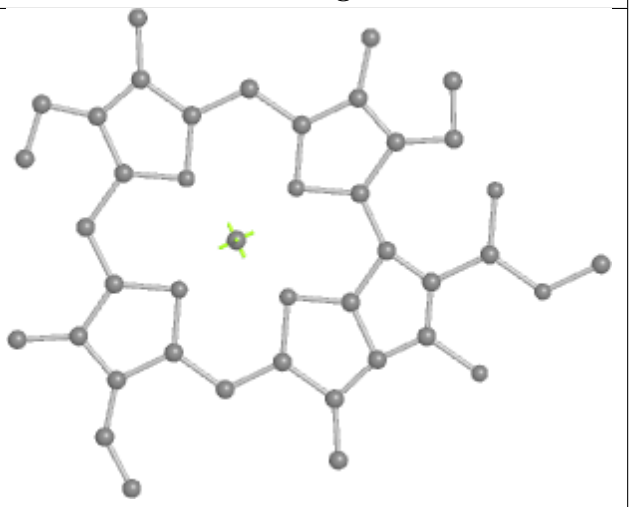
Bond lengths



Bond angles

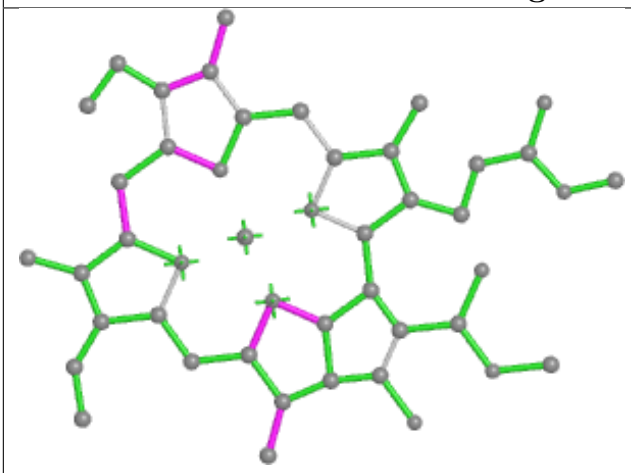


Torsions

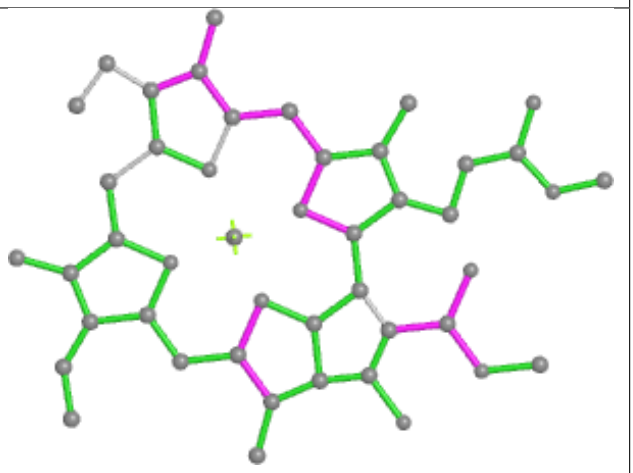


Rings

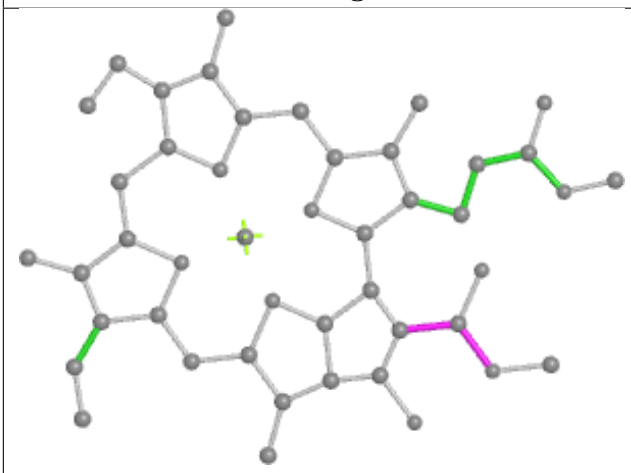
Ligand CLA 4 311



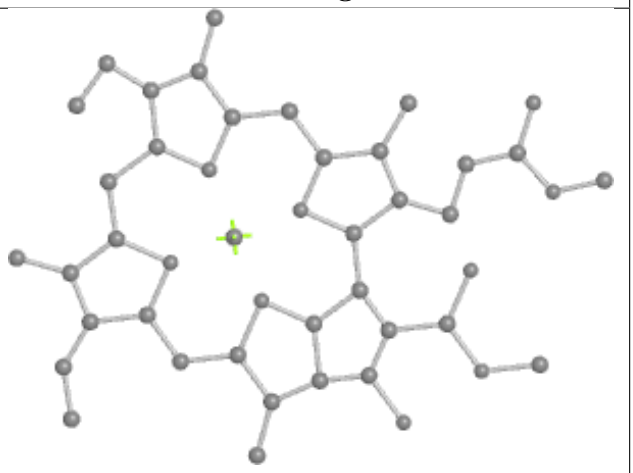
Bond lengths



Bond angles

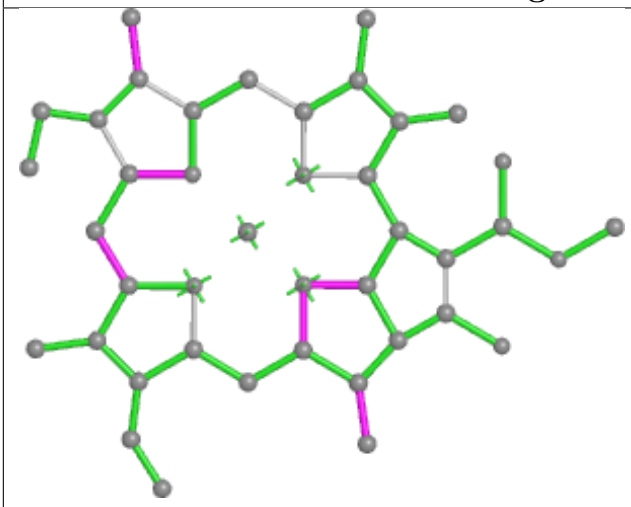


Torsions

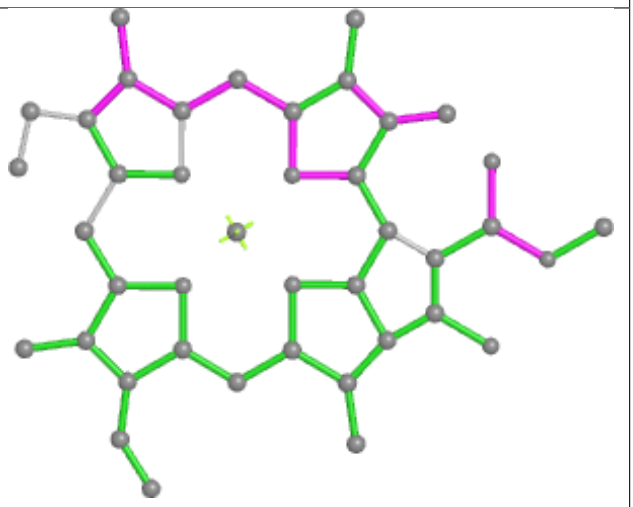


Rings

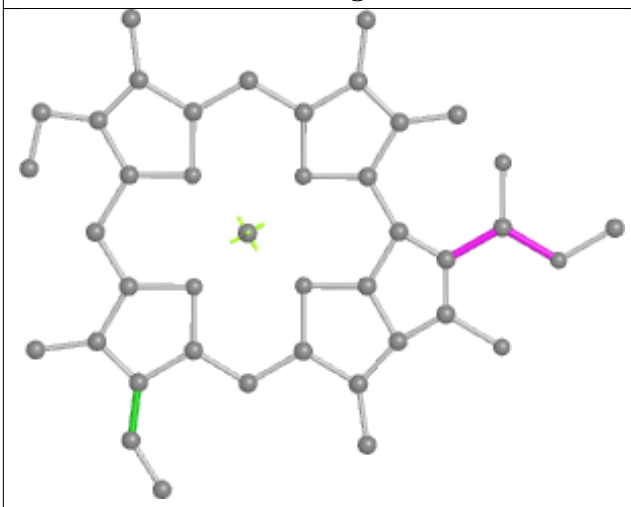
Ligand CLA 4 312



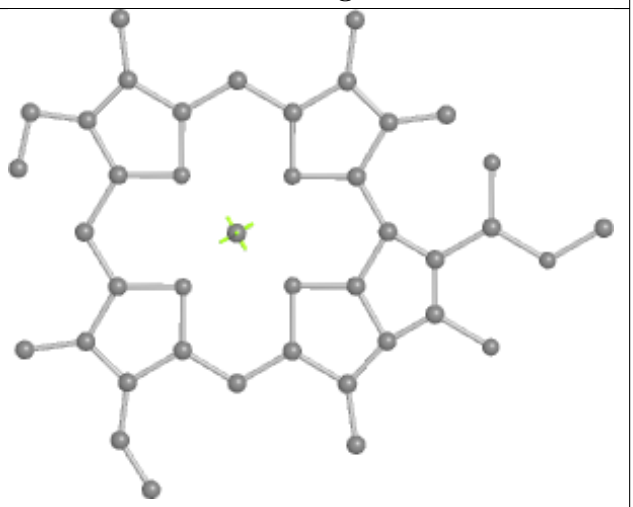
Bond lengths



Bond angles

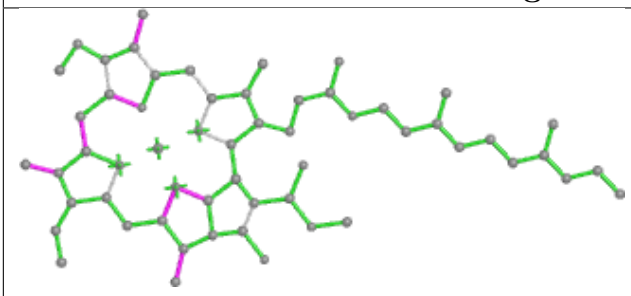


Torsions

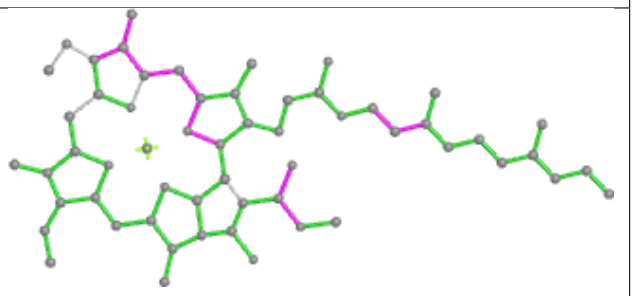


Rings

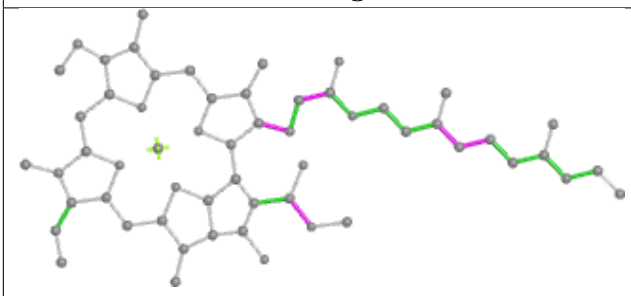
Ligand CLA A 852



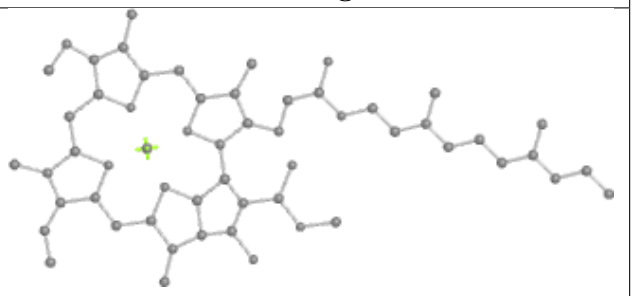
Bond lengths



Bond angles

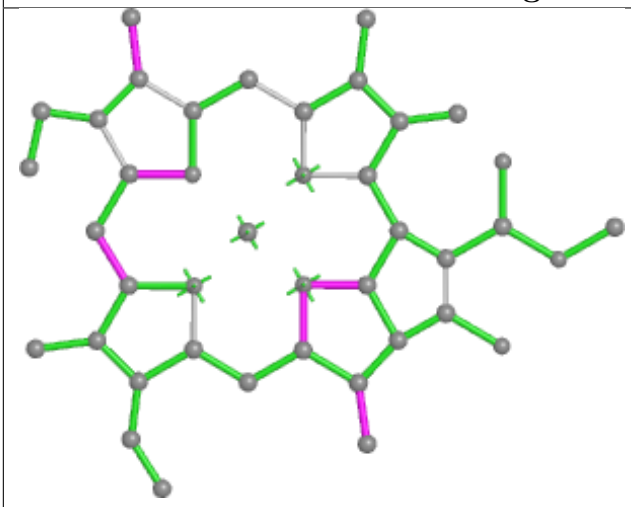


Torsions

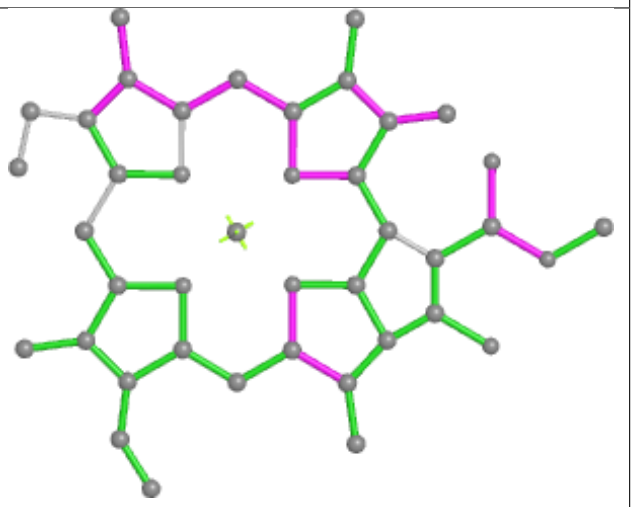


Rings

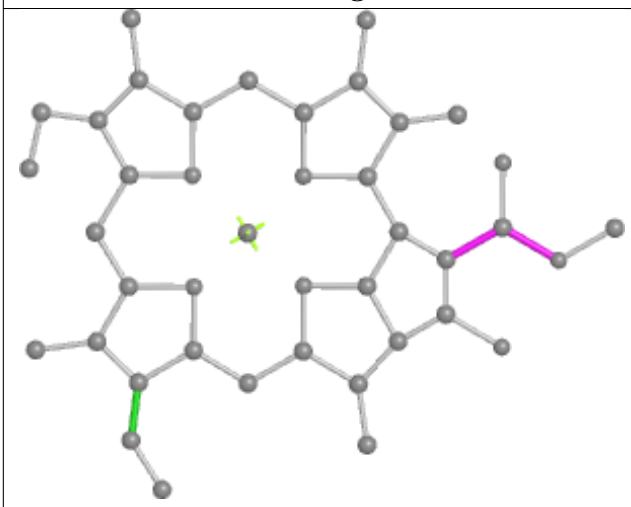
Ligand CLA K 203



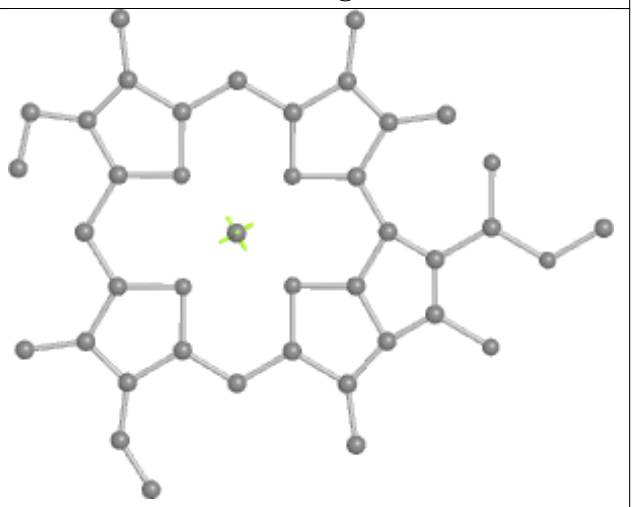
Bond lengths



Bond angles

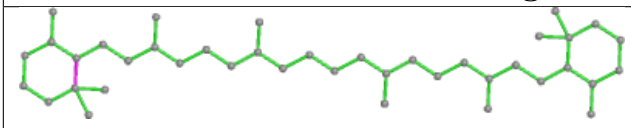


Torsions

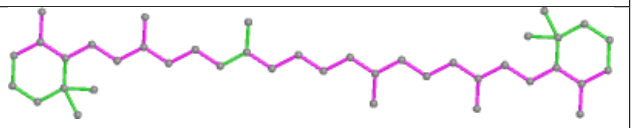


Rings

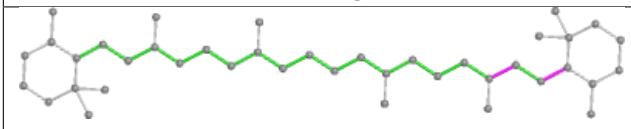
Ligand BCR A 846



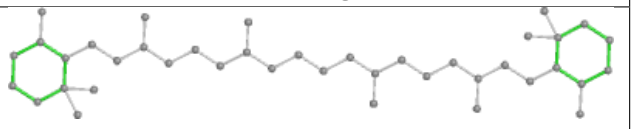
Bond lengths



Bond angles

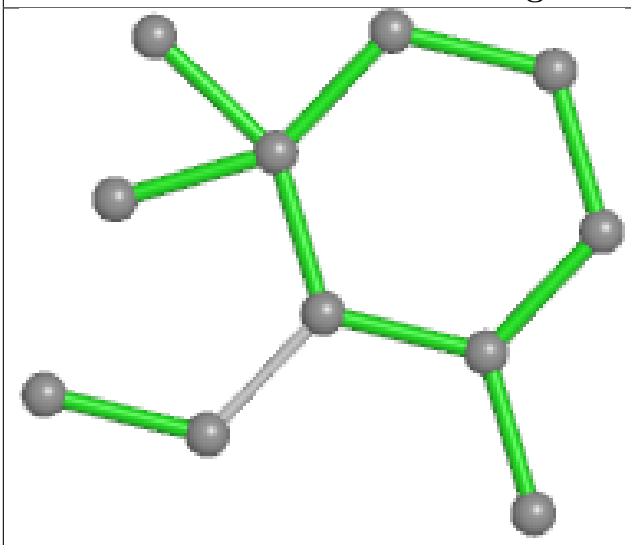


Torsions

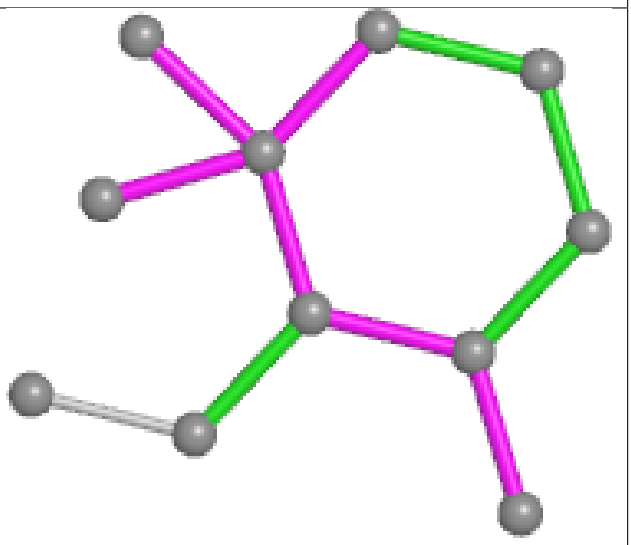


Rings

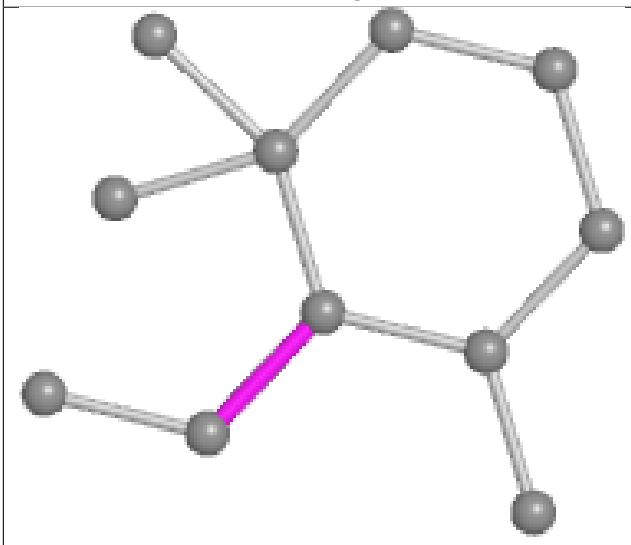
Ligand BCR 1 503



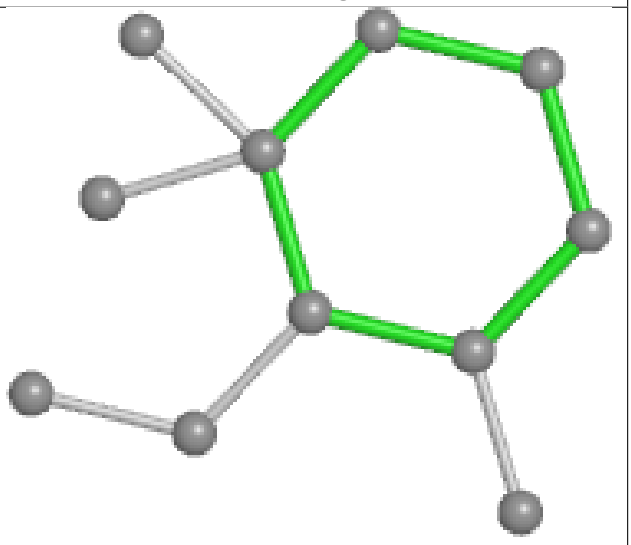
Bond lengths



Bond angles

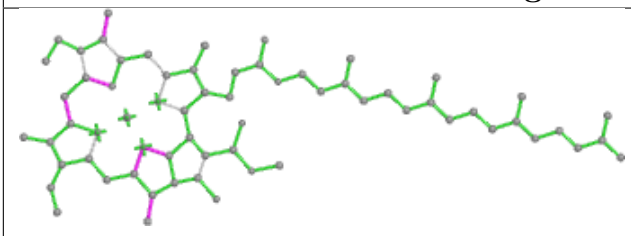


Torsions

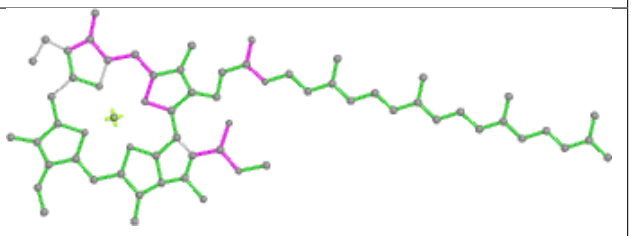


Rings

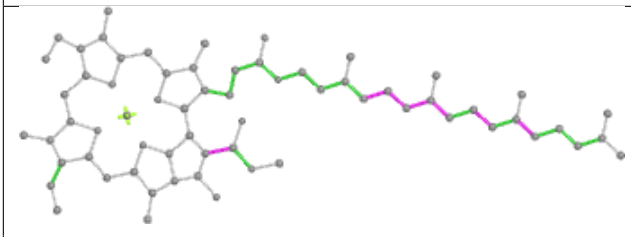
Ligand CLA B 826



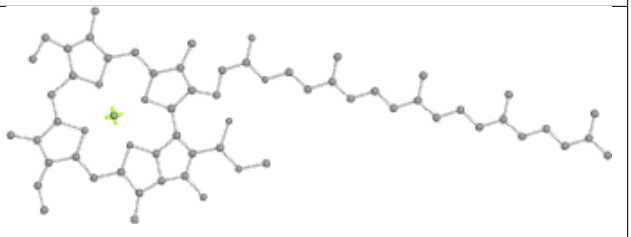
Bond lengths



Bond angles

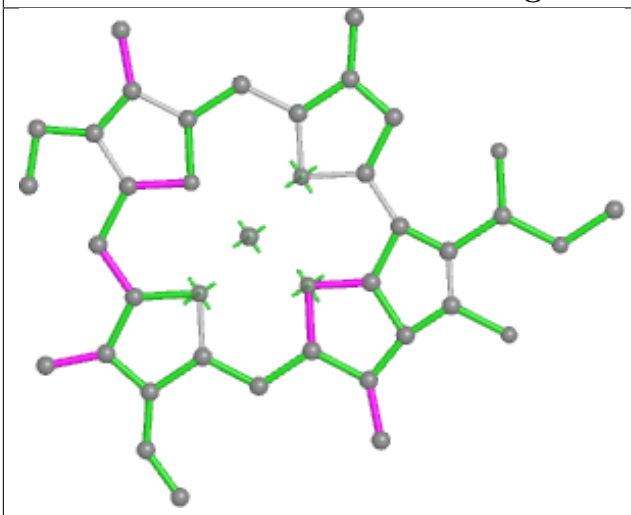


Torsions

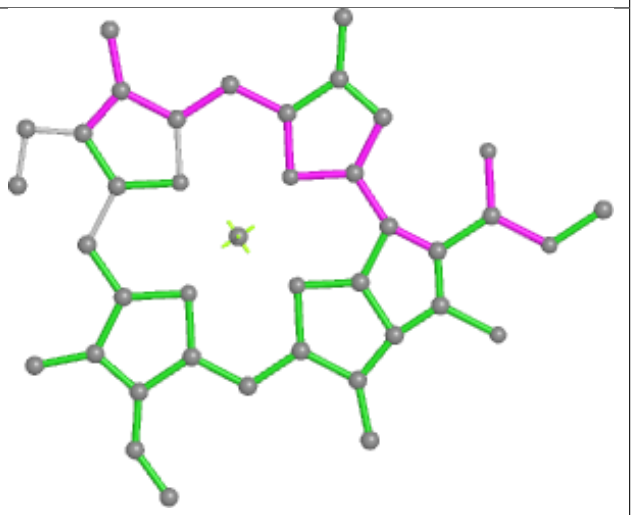


Rings

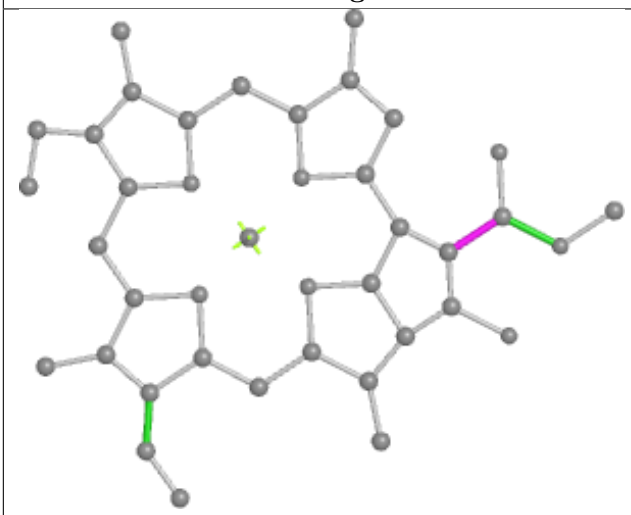
Ligand CLA B 832



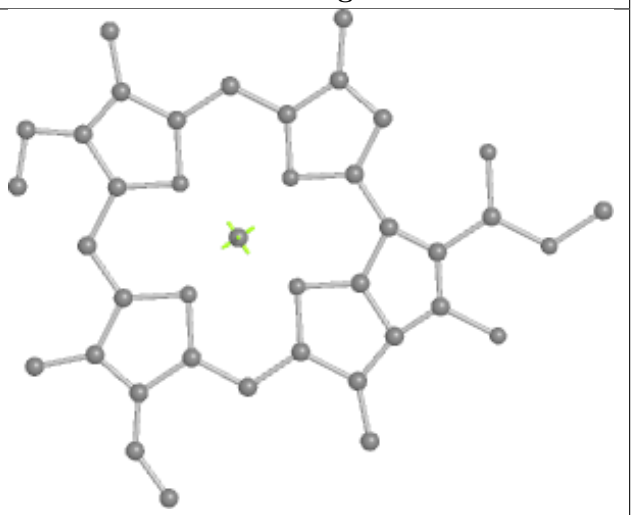
Bond lengths



Bond angles

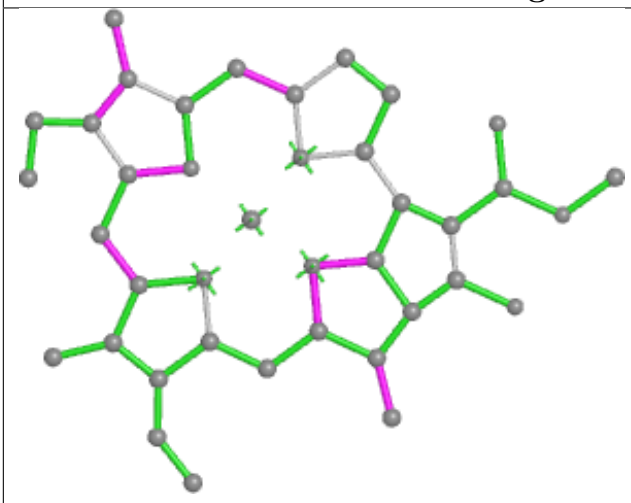


Torsions

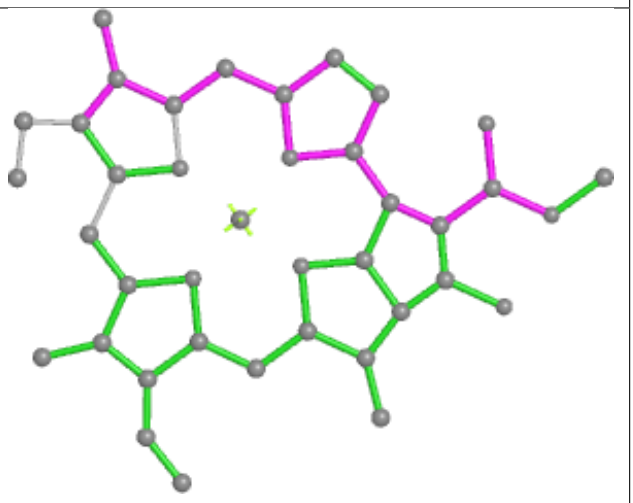


Rings

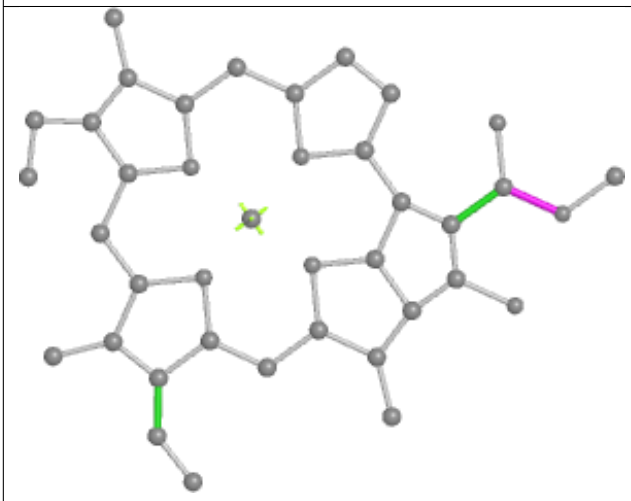
Ligand CLA 1 511



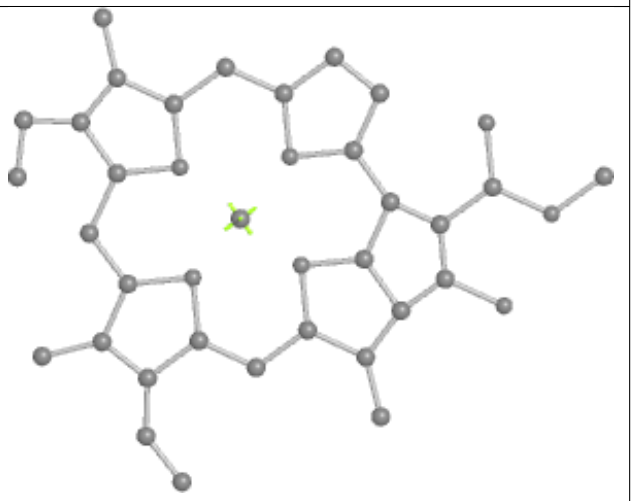
Bond lengths



Bond angles

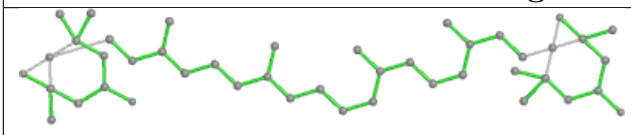


Torsions

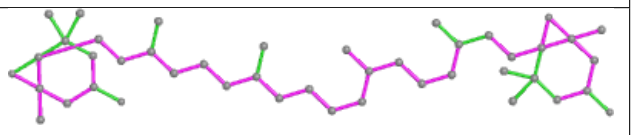


Rings

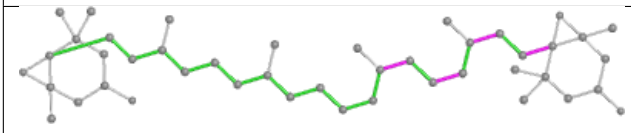
Ligand XAT 6 502



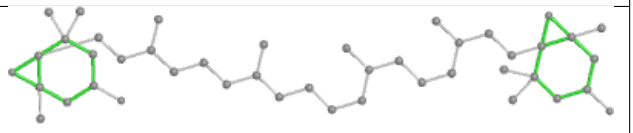
Bond lengths



Bond angles

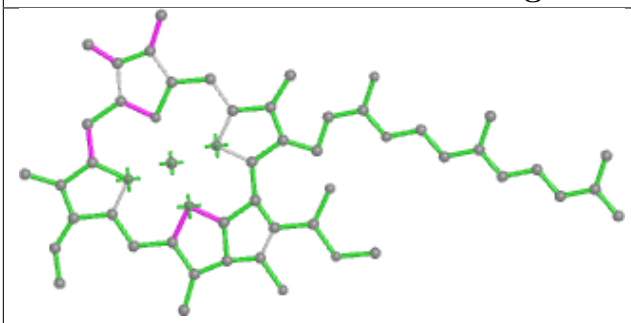


Torsions

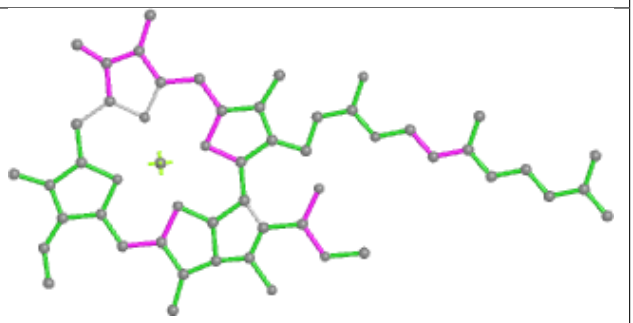


Rings

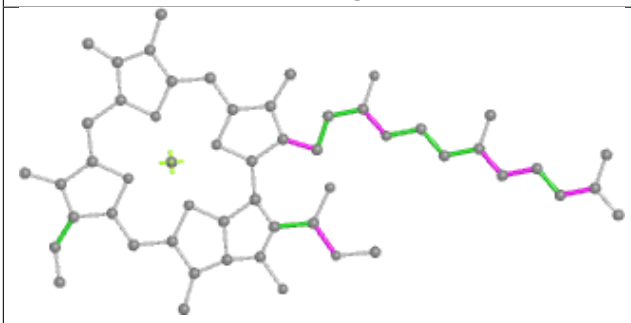
Ligand CLA B 813



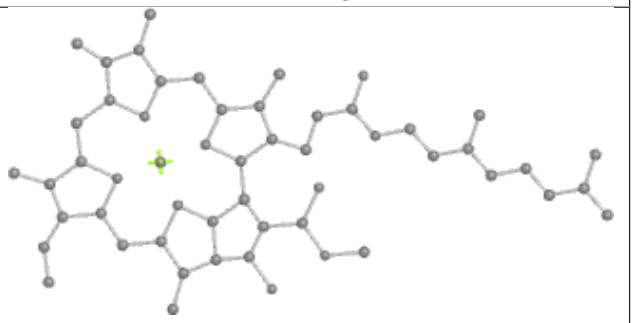
Bond lengths



Bond angles

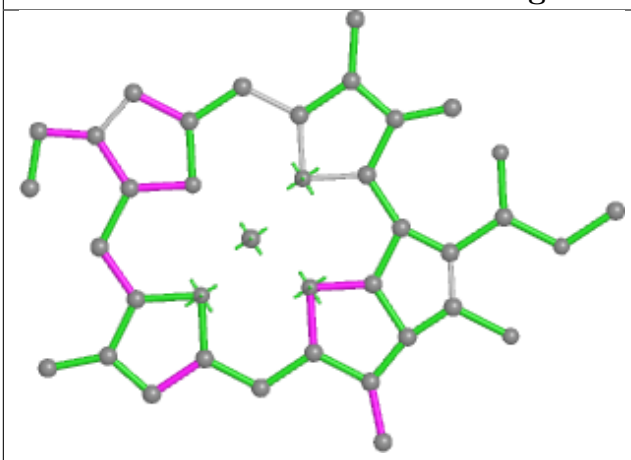


Torsions

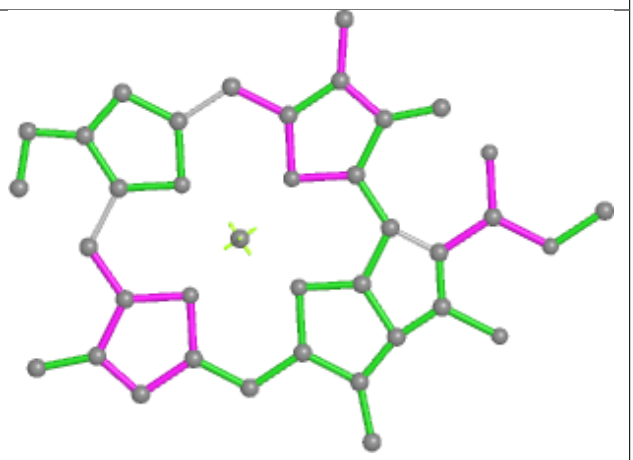


Rings

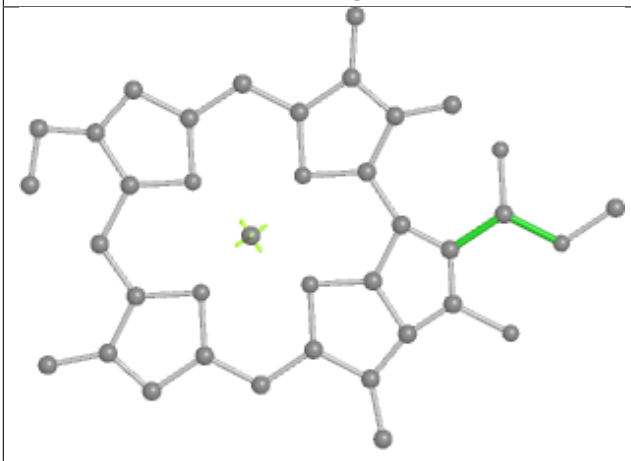
Ligand CLA 3 304



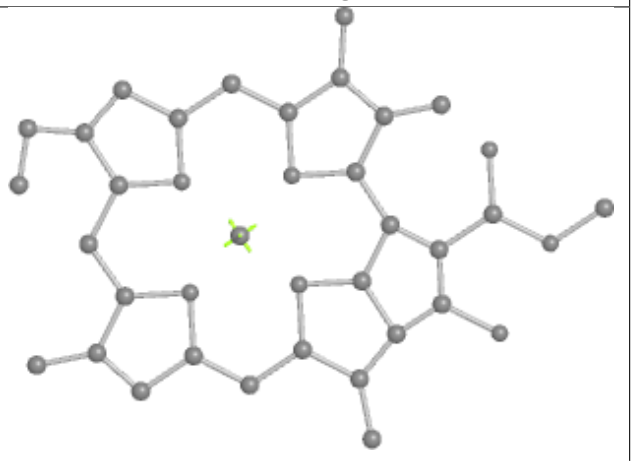
Bond lengths



Bond angles

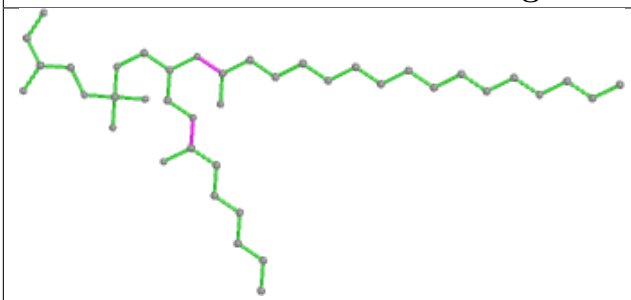


Torsions

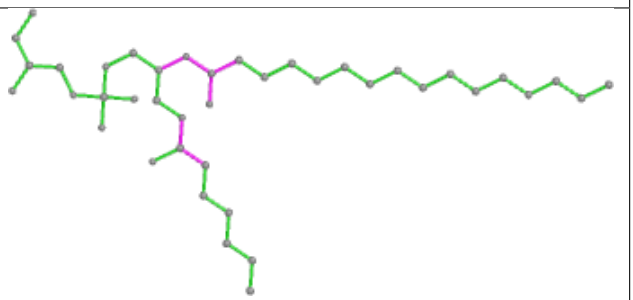


Rings

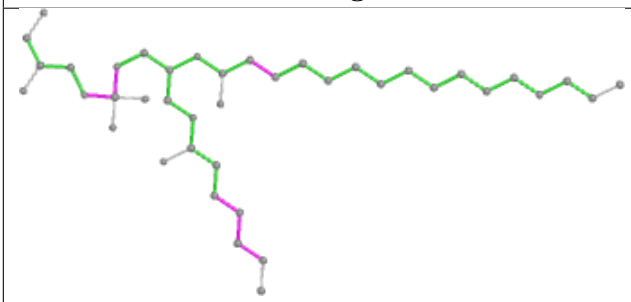
Ligand LHG A 844



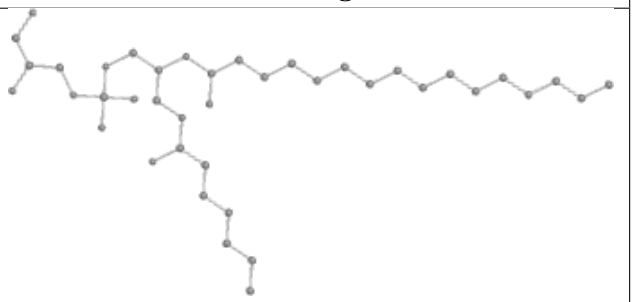
Bond lengths



Bond angles

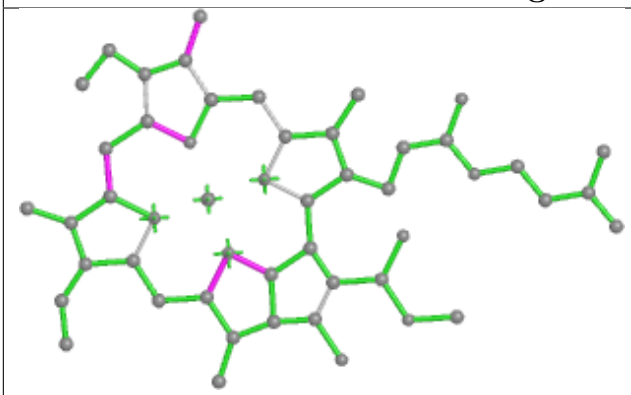


Torsions

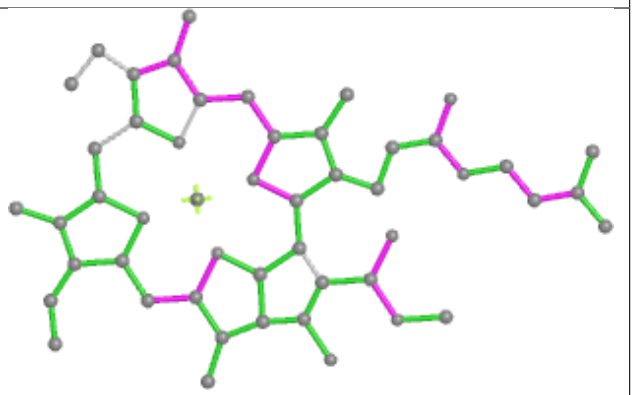


Rings

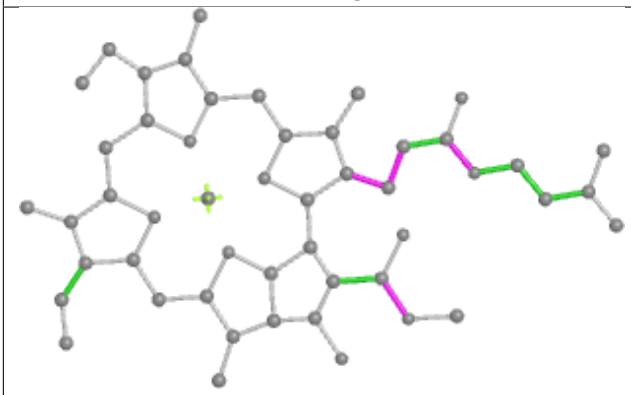
Ligand CLA 6 509



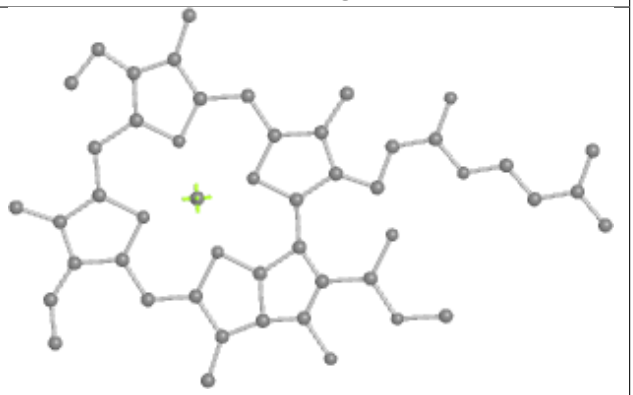
Bond lengths



Bond angles

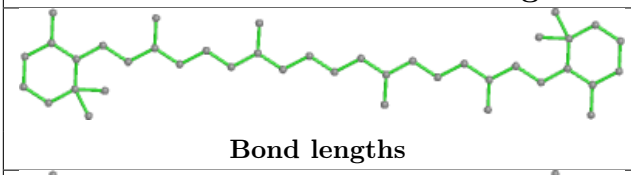


Torsions

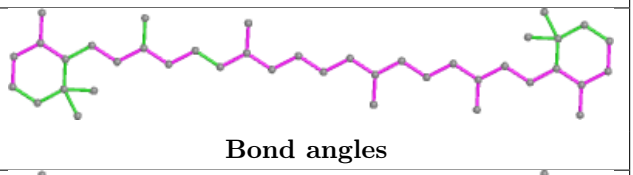


Rings

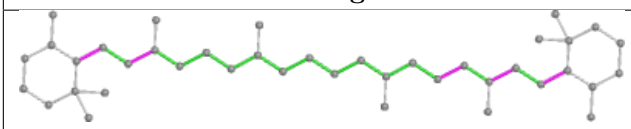
Ligand BCR K 204



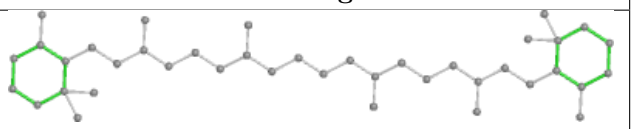
Bond lengths



Bond angles

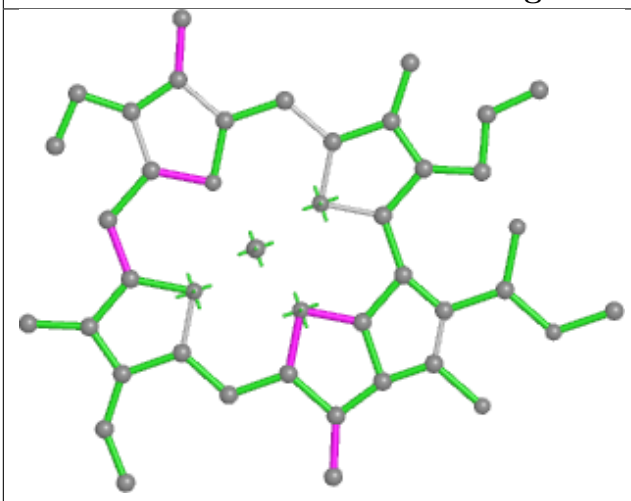


Torsions

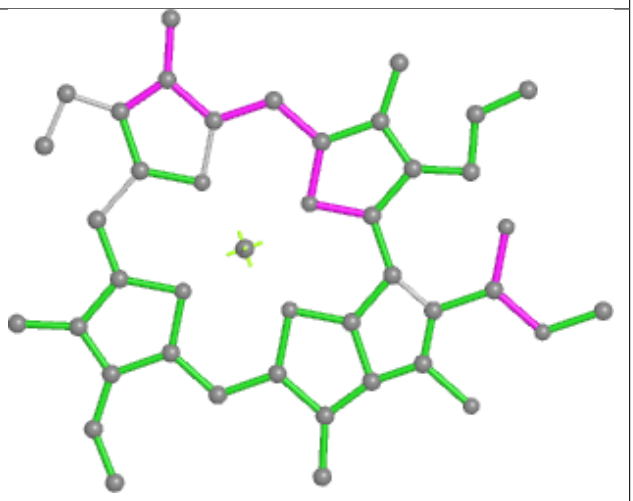


Rings

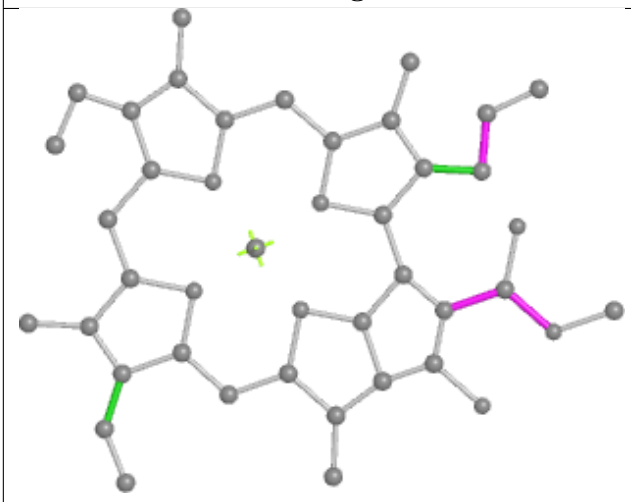
Ligand CLA B 815



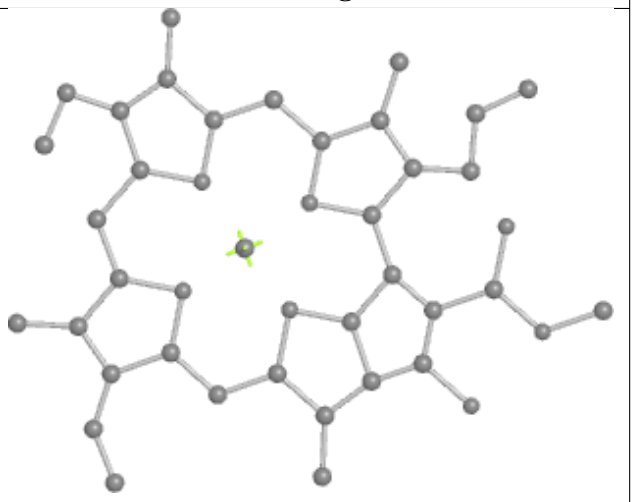
Bond lengths



Bond angles

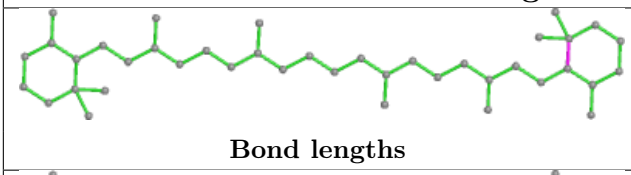


Torsions

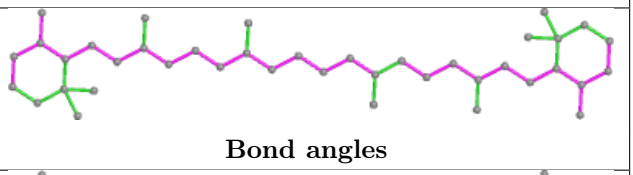


Rings

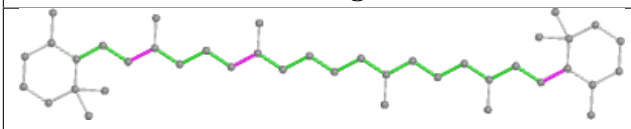
Ligand BCR A 848



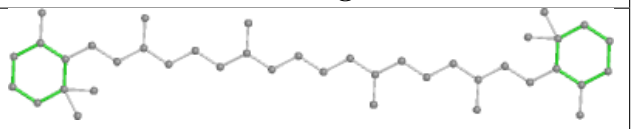
Bond lengths



Bond angles

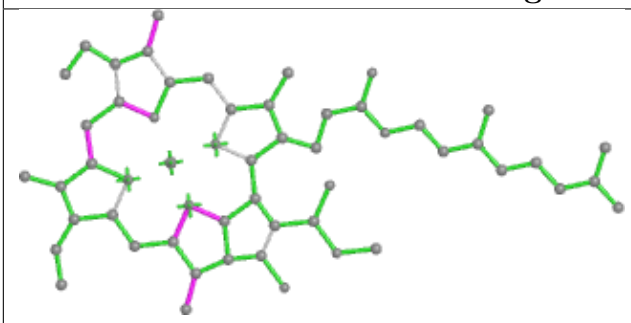


Torsions

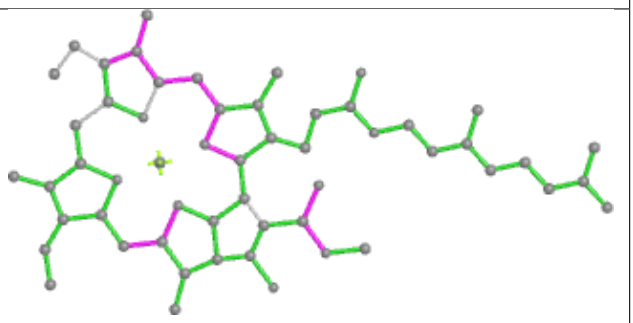


Rings

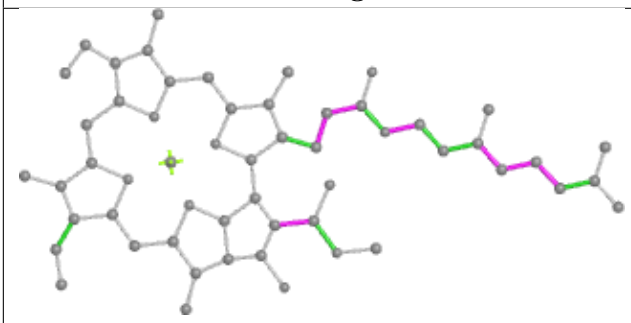
Ligand CLA B 818



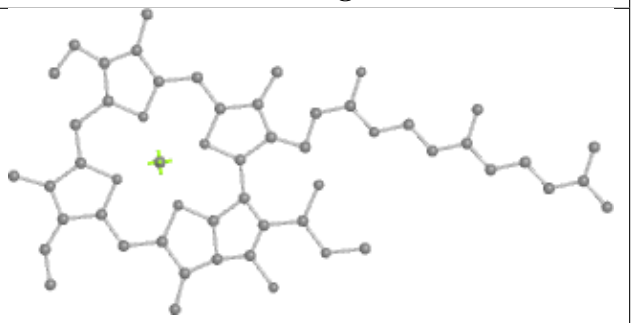
Bond lengths



Bond angles

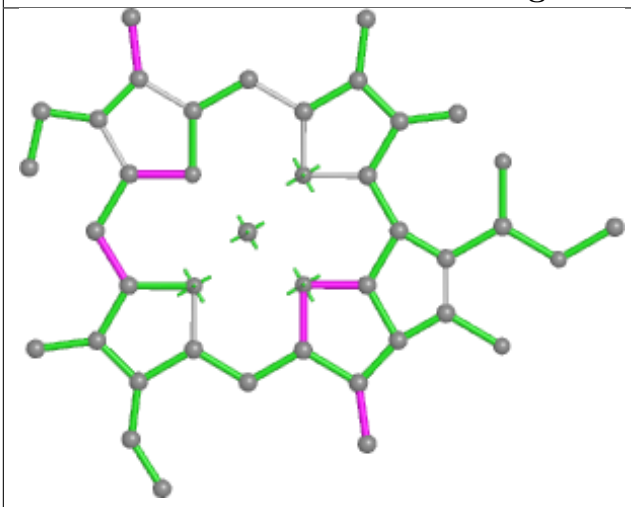


Torsions

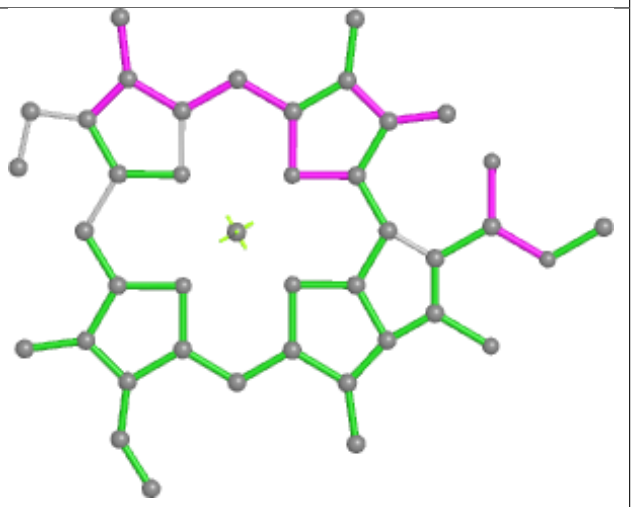


Rings

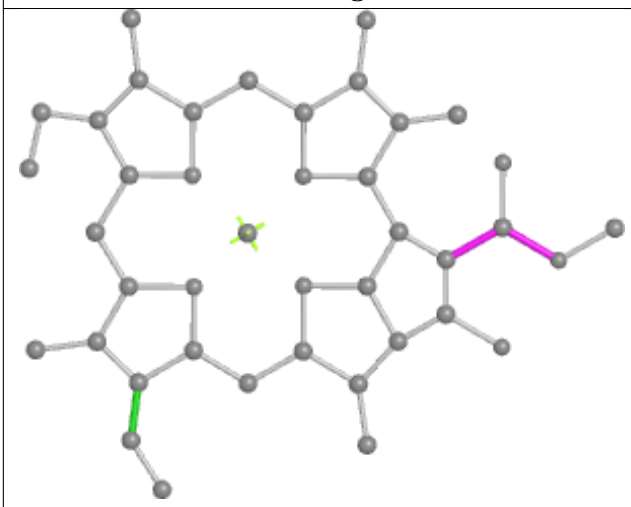
Ligand CLA 3 310



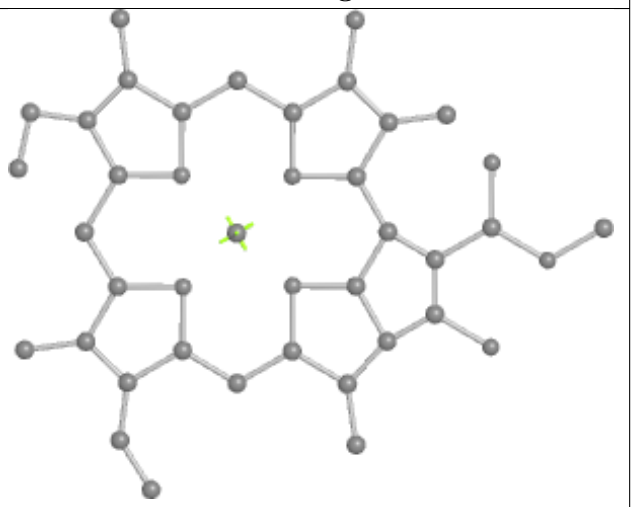
Bond lengths



Bond angles

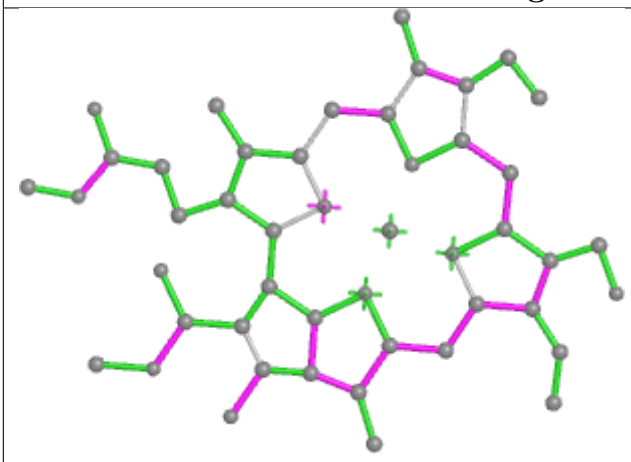


Torsions

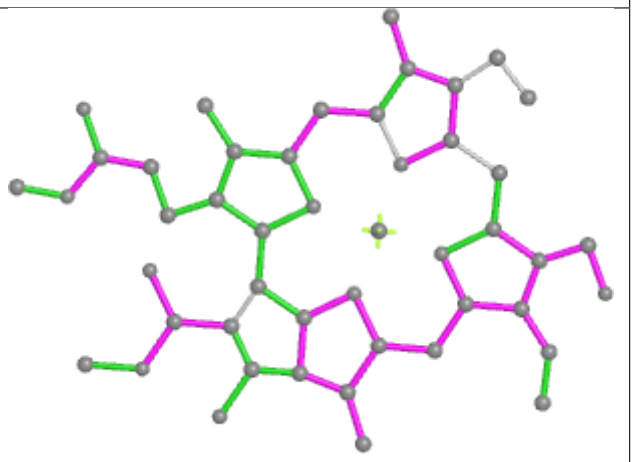


Rings

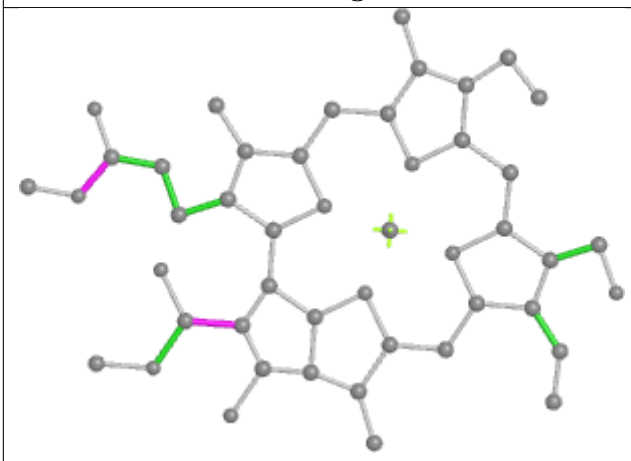
Ligand CHL 6 517



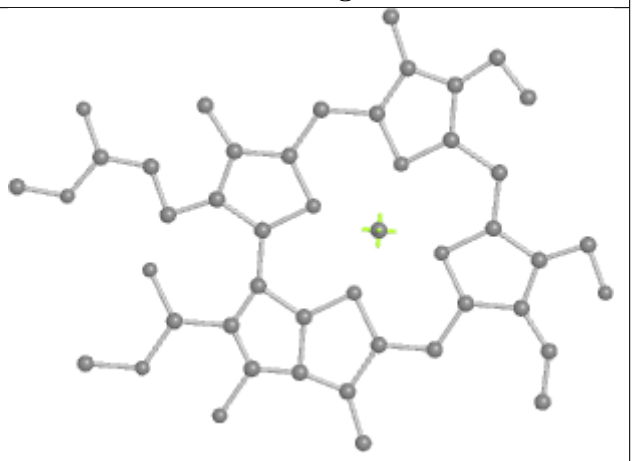
Bond lengths



Bond angles

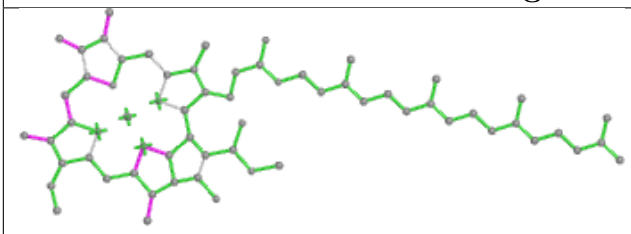


Torsions

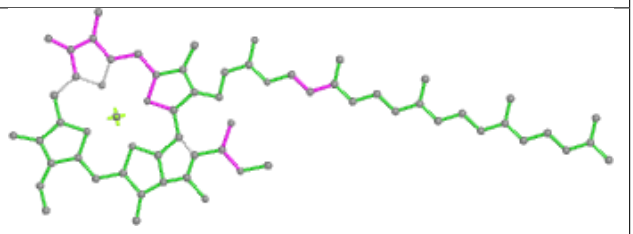


Rings

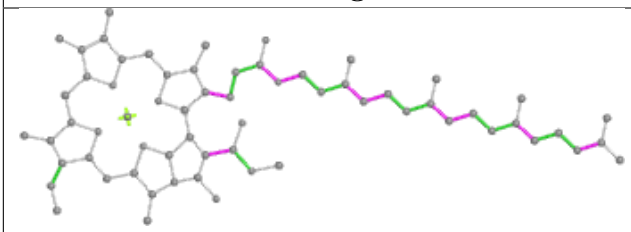
Ligand CLA A 826



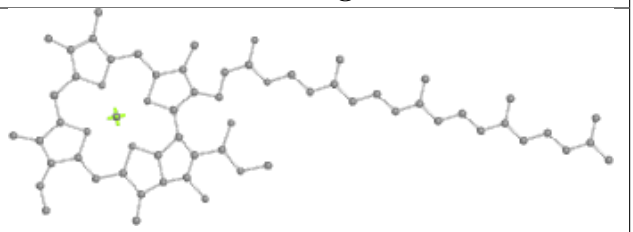
Bond lengths



Bond angles

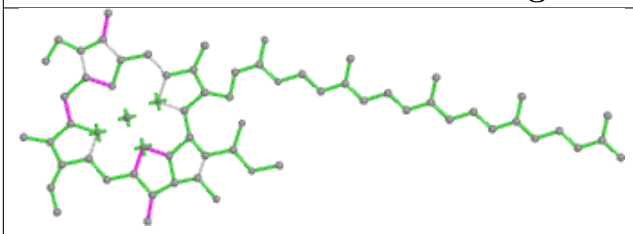


Torsions

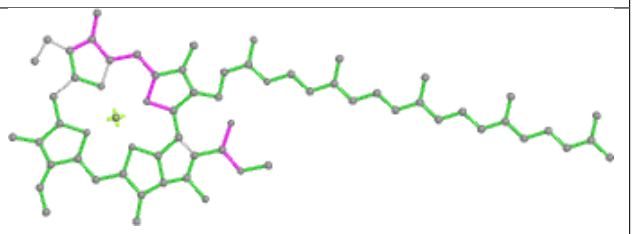


Rings

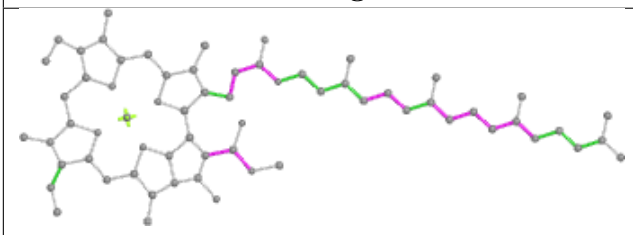
Ligand CLA 6 506



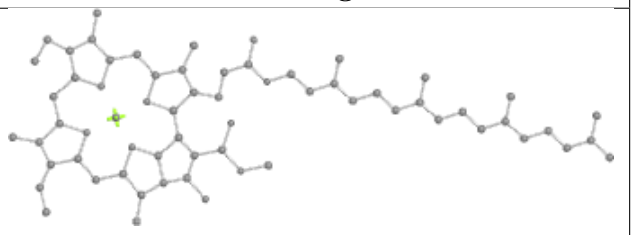
Bond lengths



Bond angles

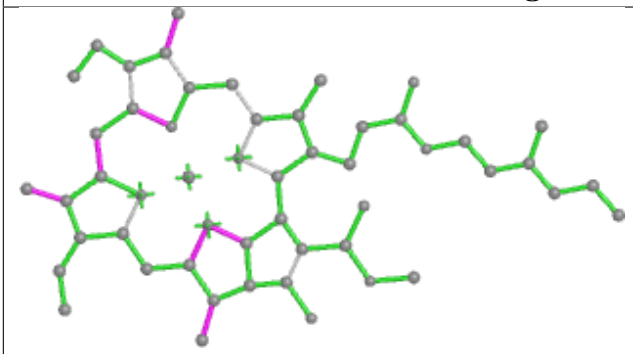


Torsions

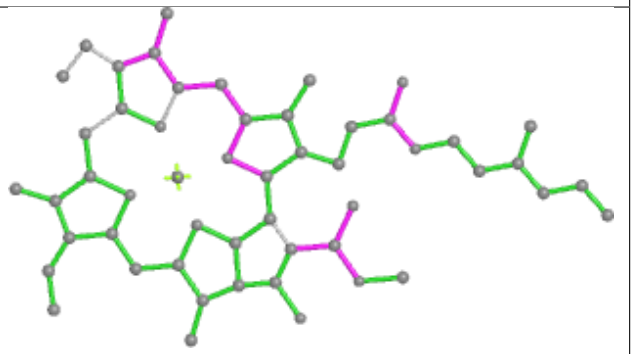


Rings

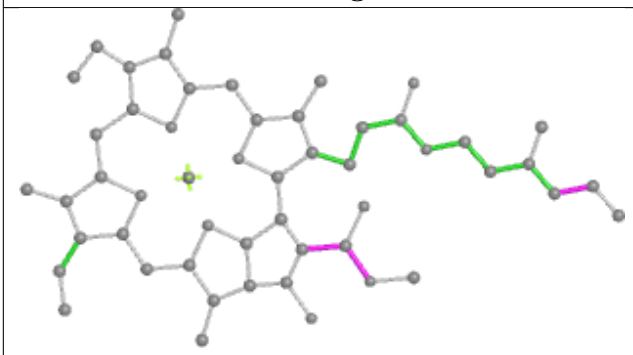
Ligand CLA A 838



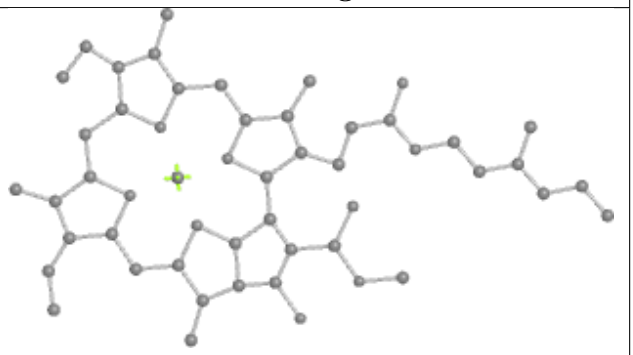
Bond lengths



Bond angles

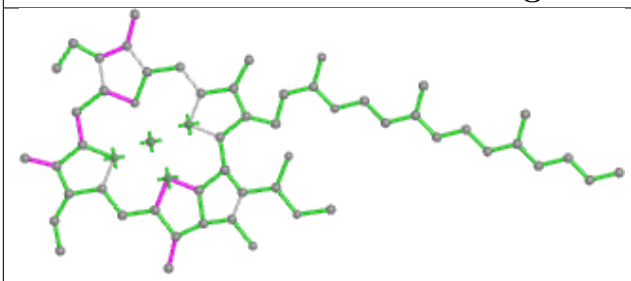


Torsions

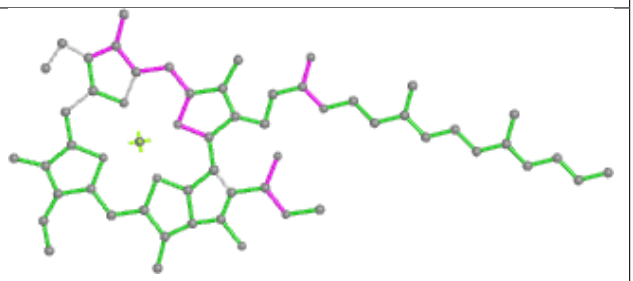


Rings

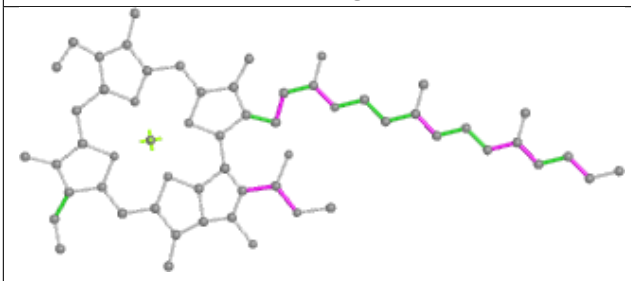
Ligand CLA A 829



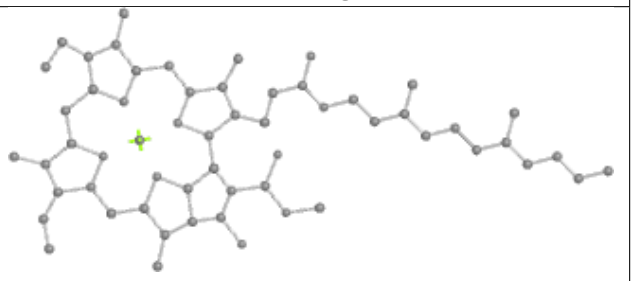
Bond lengths



Bond angles

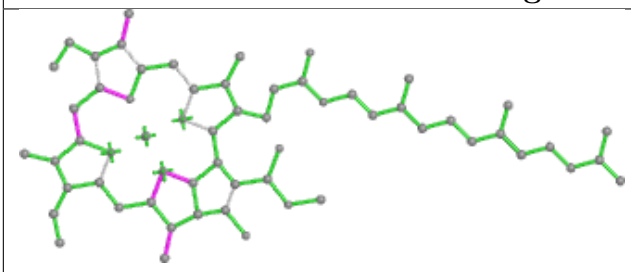


Torsions

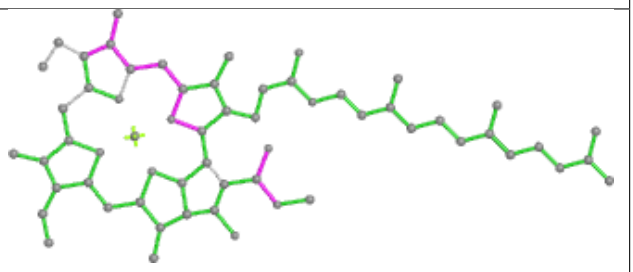


Rings

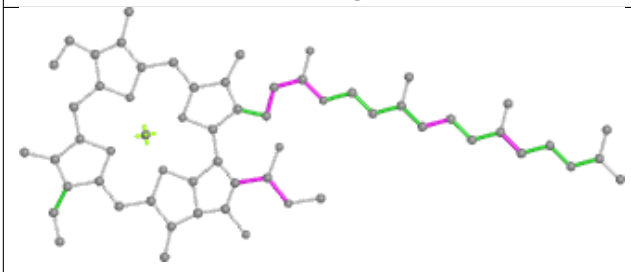
Ligand CLA A 816



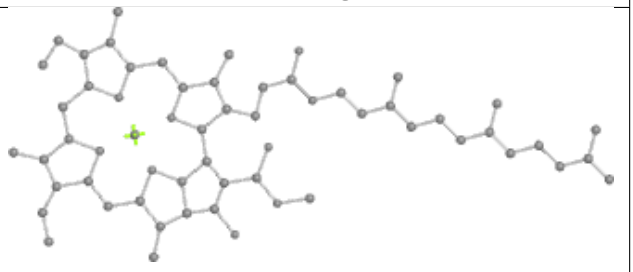
Bond lengths



Bond angles

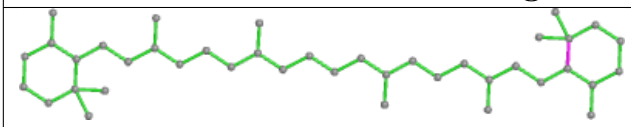


Torsions

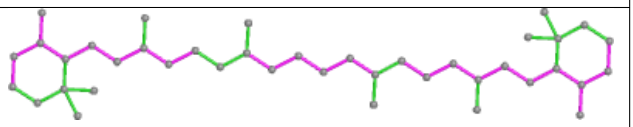


Rings

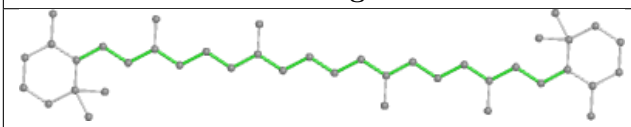
Ligand BCR B 848



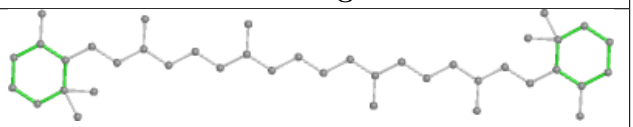
Bond lengths



Bond angles

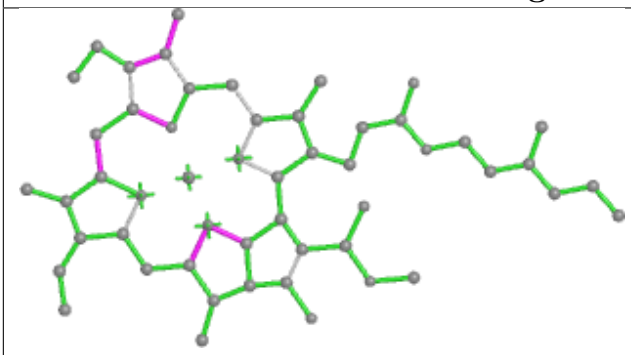


Torsions

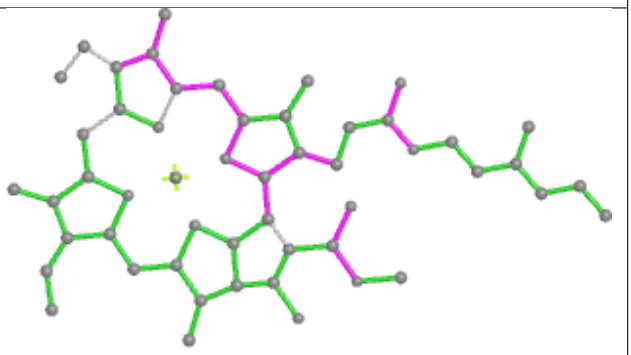


Rings

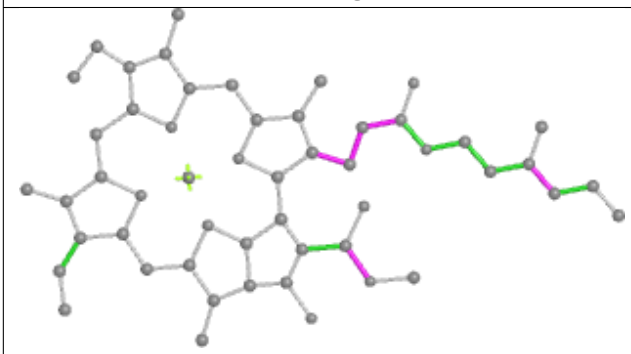
Ligand CLA 3 305



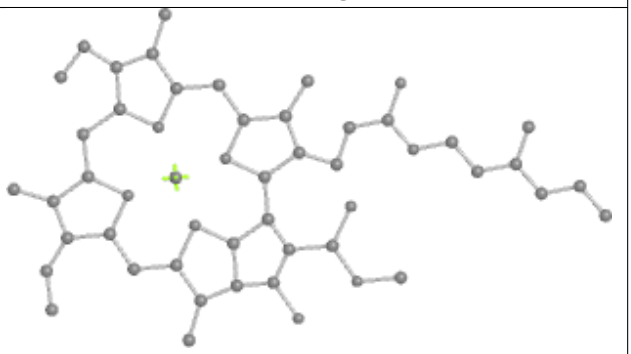
Bond lengths



Bond angles

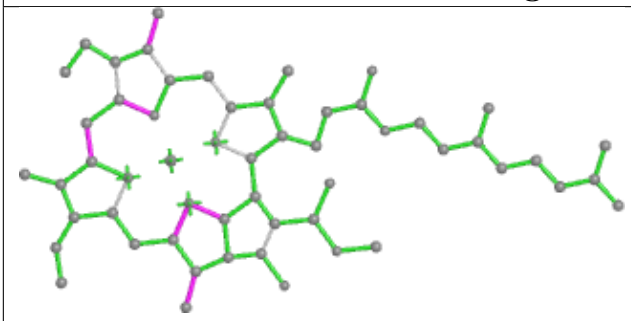


Torsions

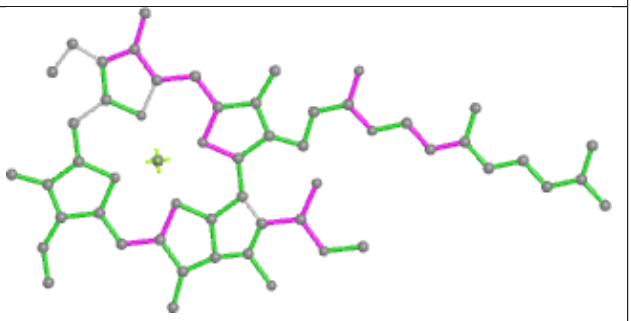


Rings

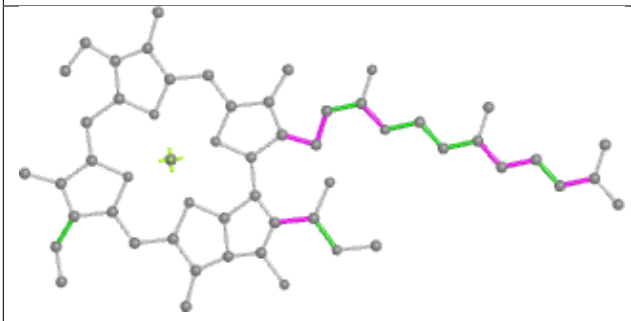
Ligand CLA A 837



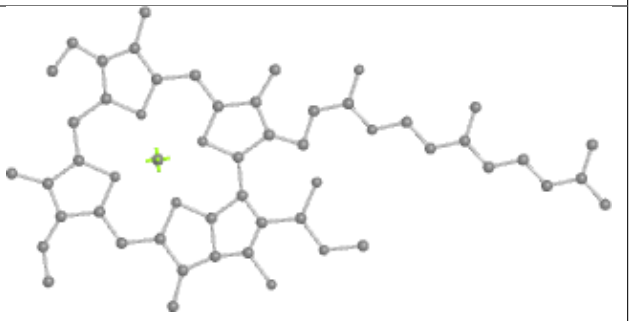
Bond lengths



Bond angles

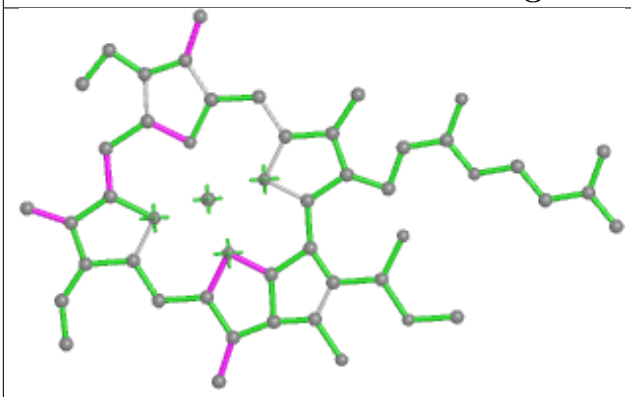


Torsions

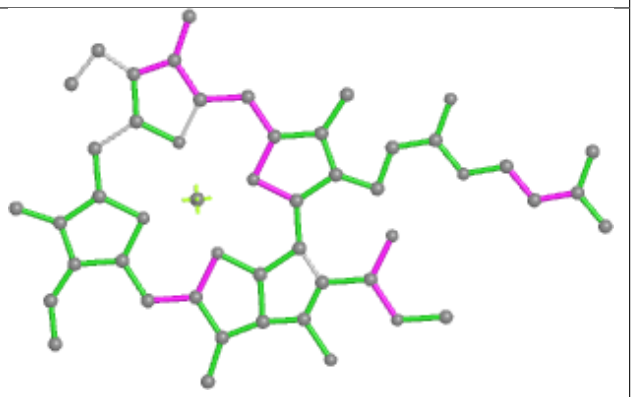


Rings

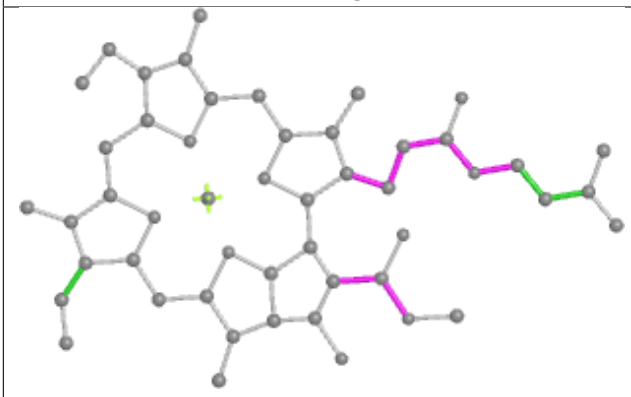
Ligand CLA B 820



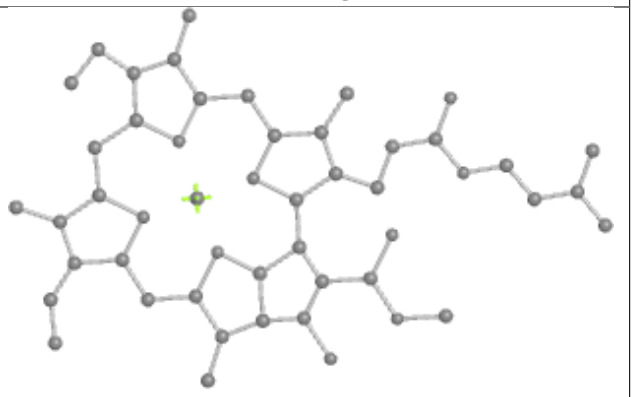
Bond lengths



Bond angles

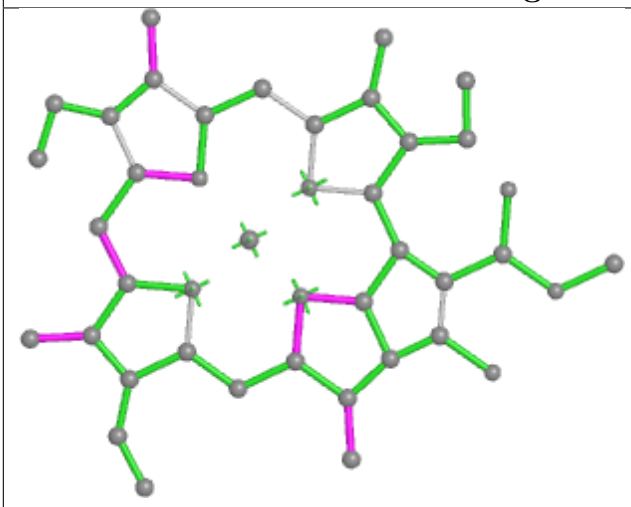


Torsions

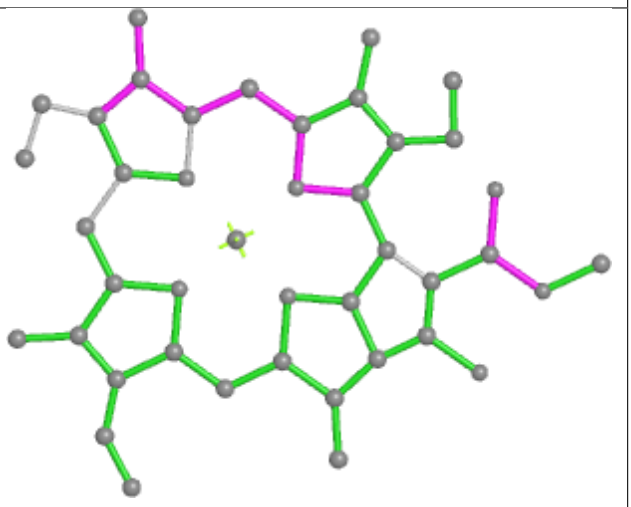


Rings

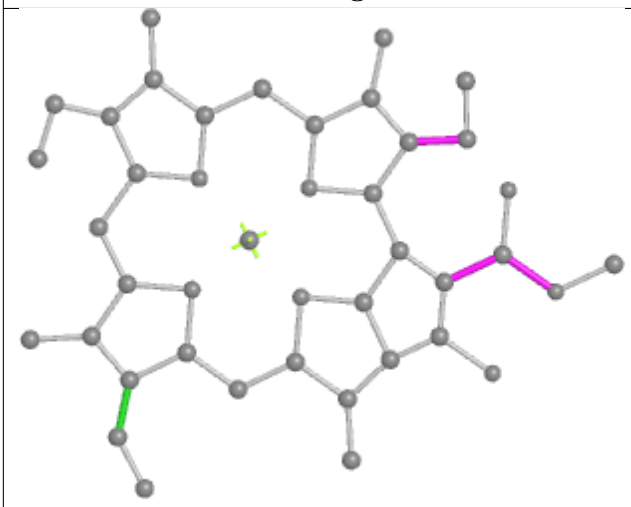
Ligand CLA A 821



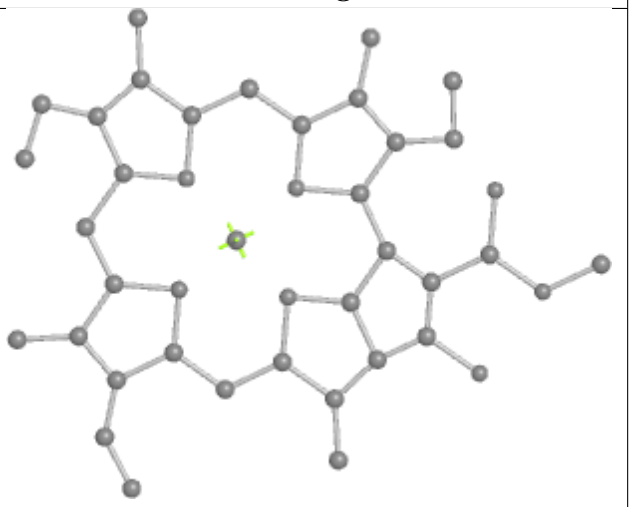
Bond lengths



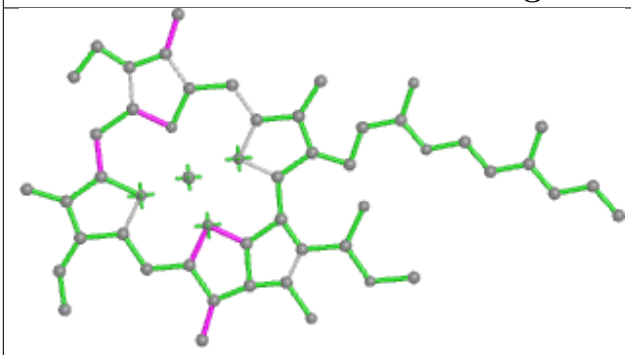
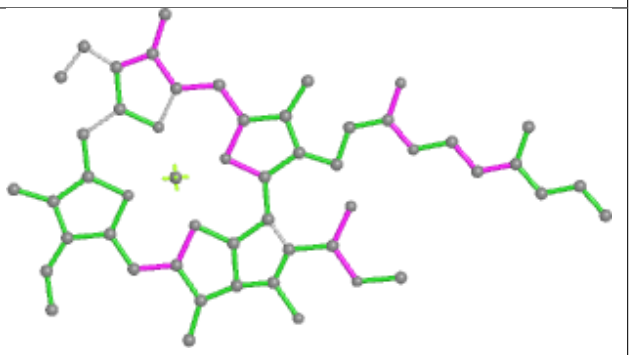
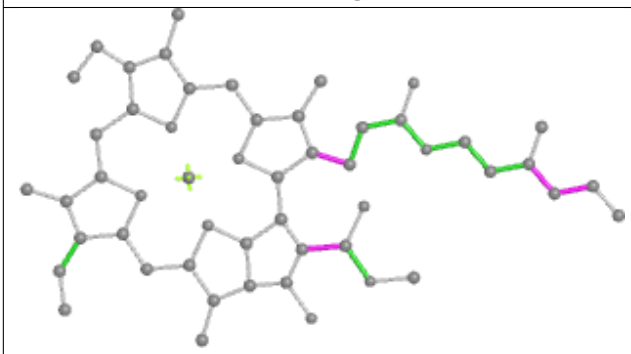
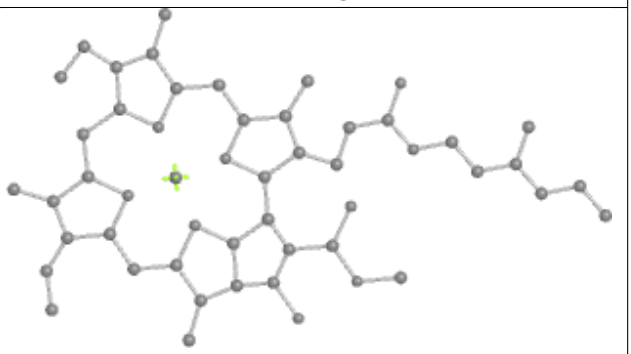
Bond angles

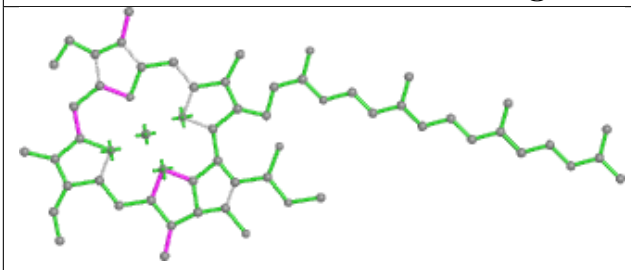
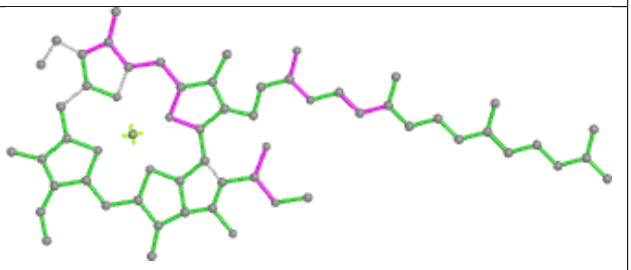
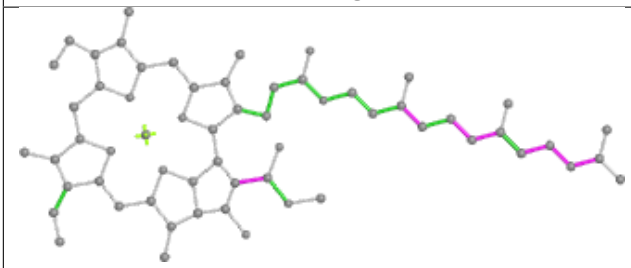
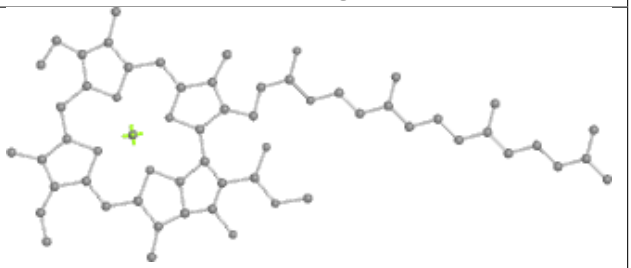


Torsions

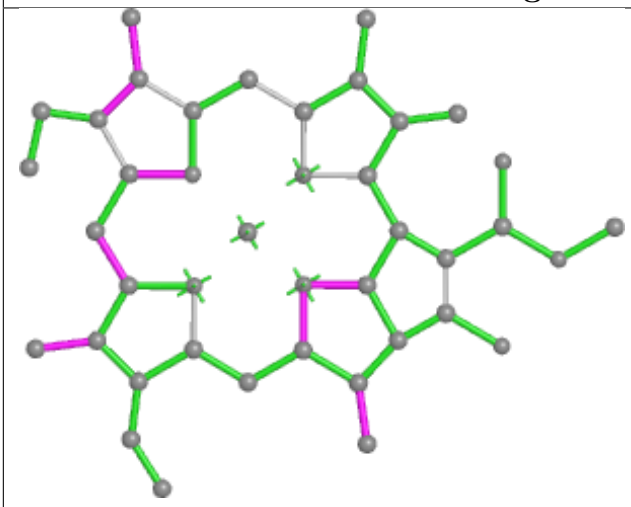


Rings

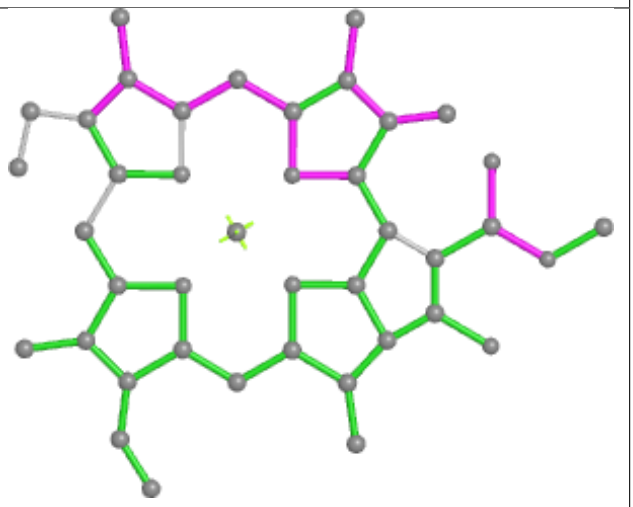
Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

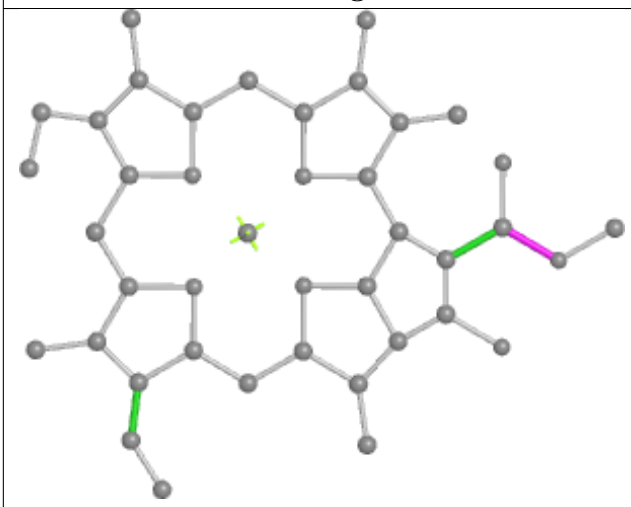
Ligand CLA A 841



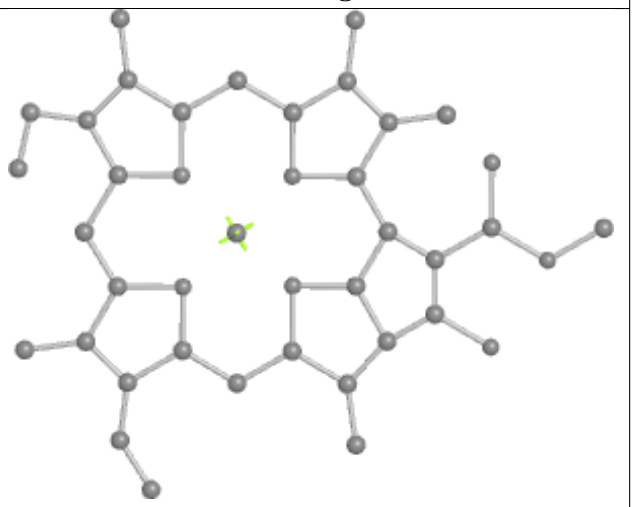
Bond lengths



Bond angles

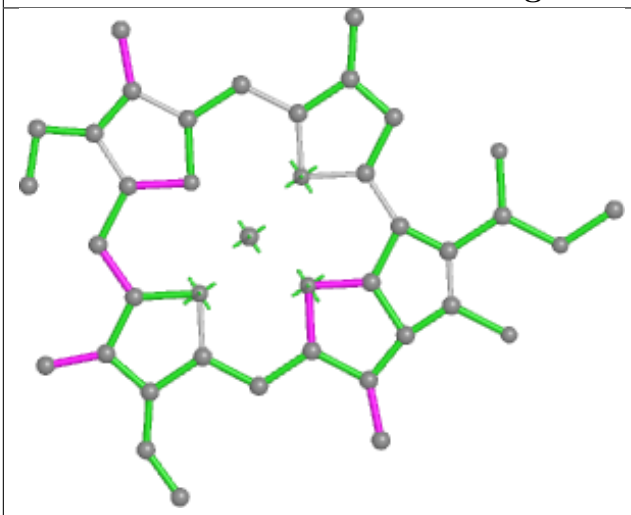


Torsions

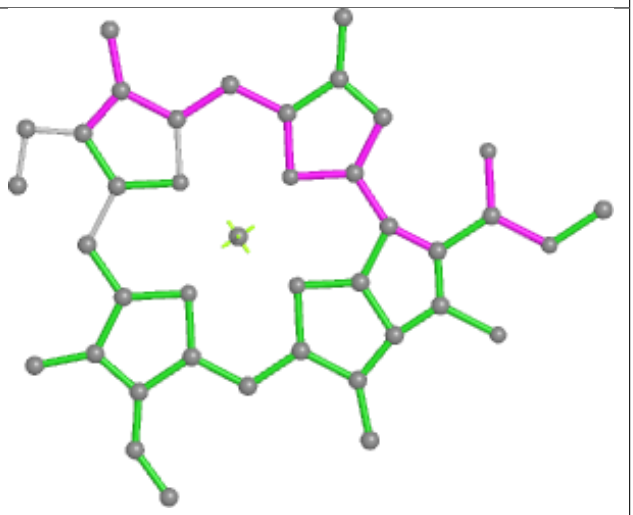


Rings

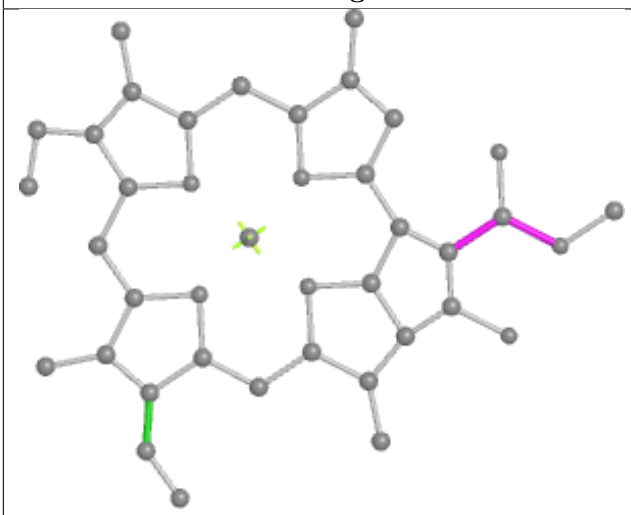
Ligand CLA B 812



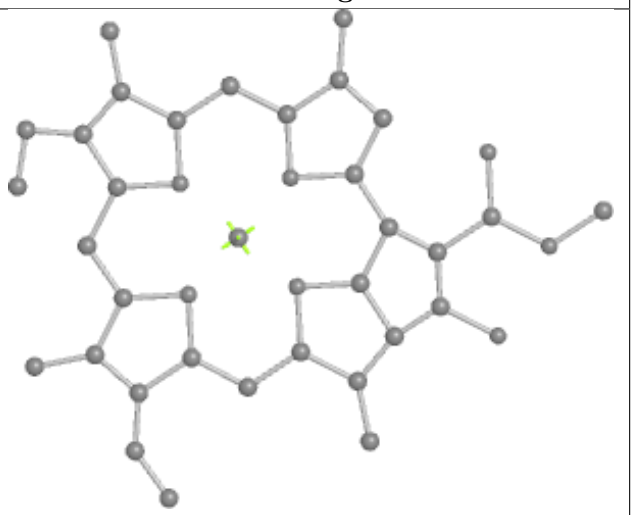
Bond lengths



Bond angles

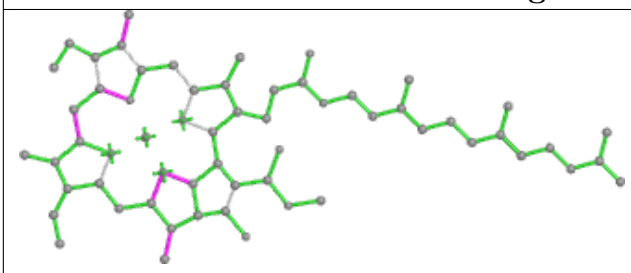


Torsions

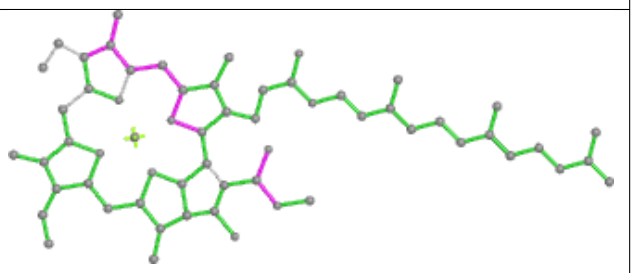


Rings

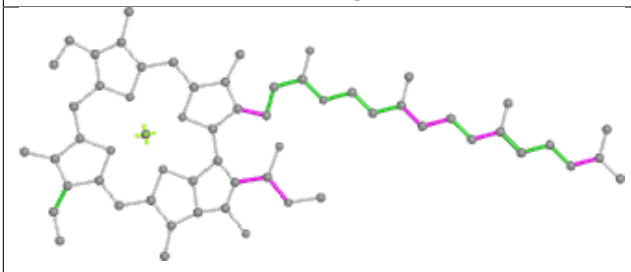
Ligand CLA 6 510



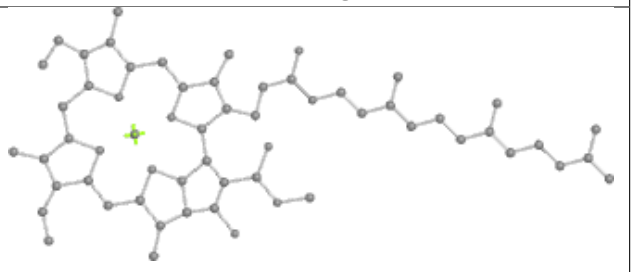
Bond lengths



Bond angles

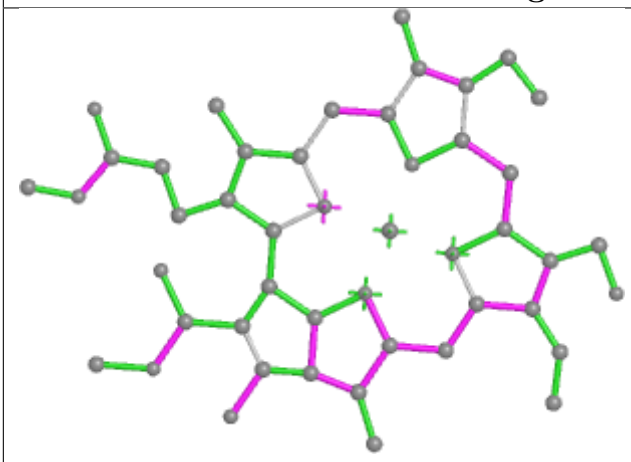


Torsions

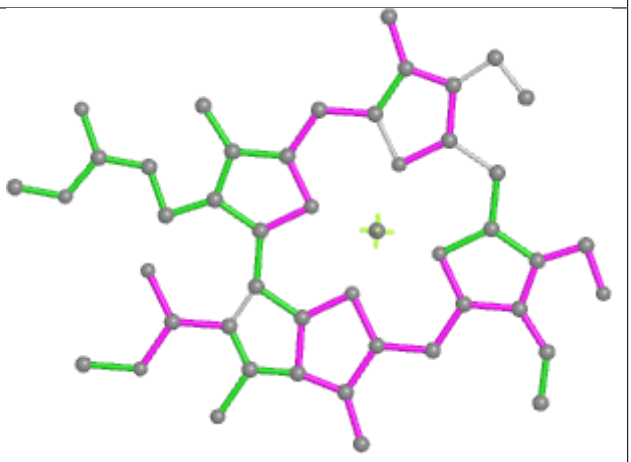


Rings

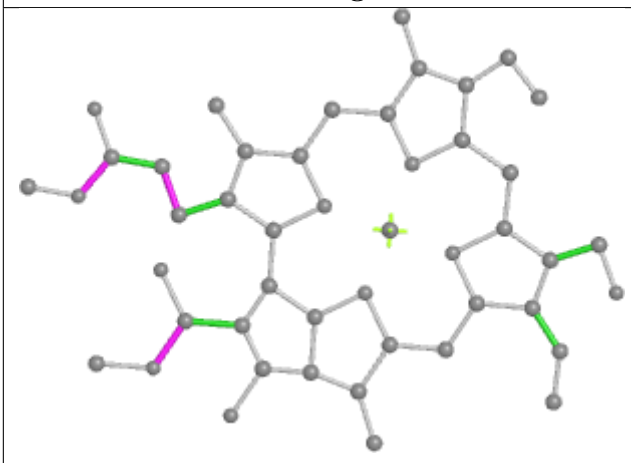
Ligand CHL 6 512



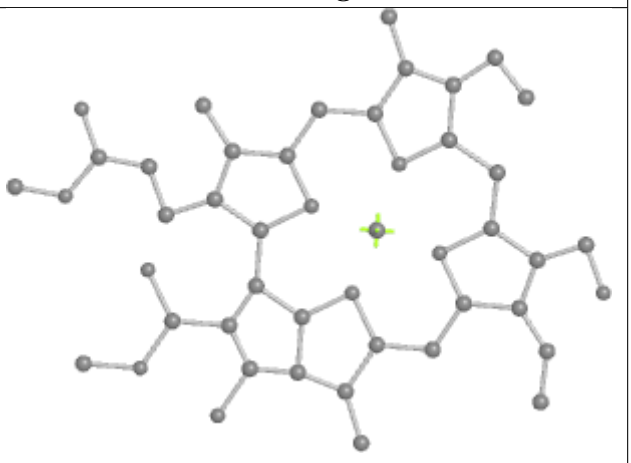
Bond lengths



Bond angles

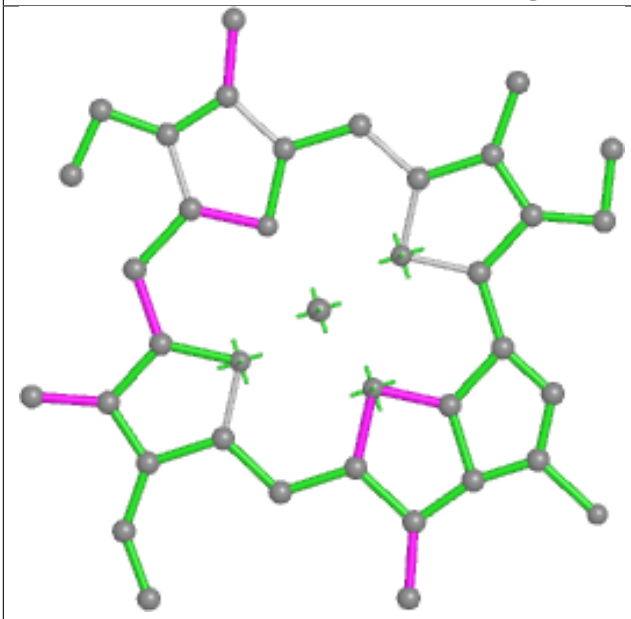


Torsions

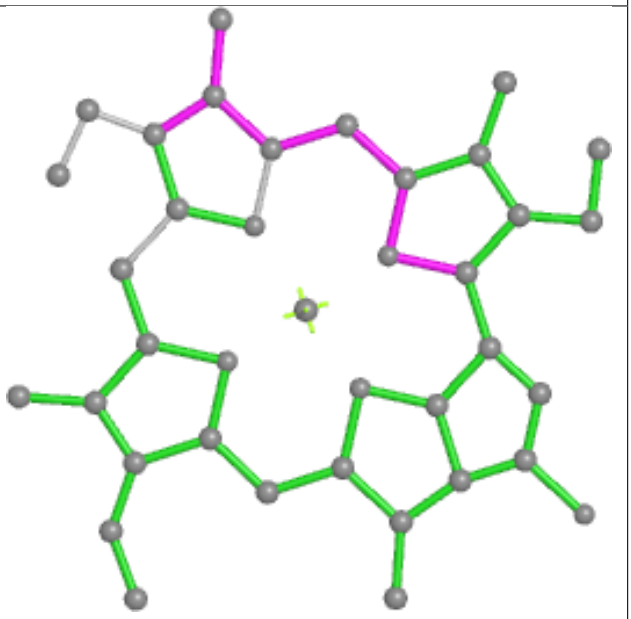


Rings

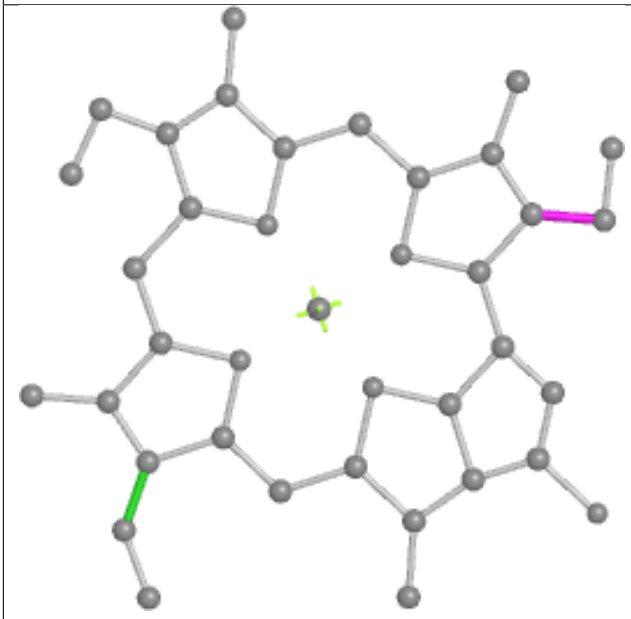
Ligand CLA B 816



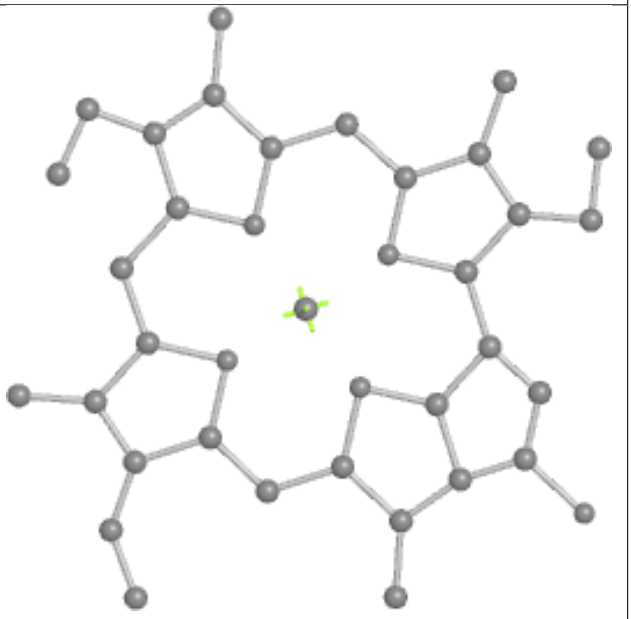
Bond lengths



Bond angles

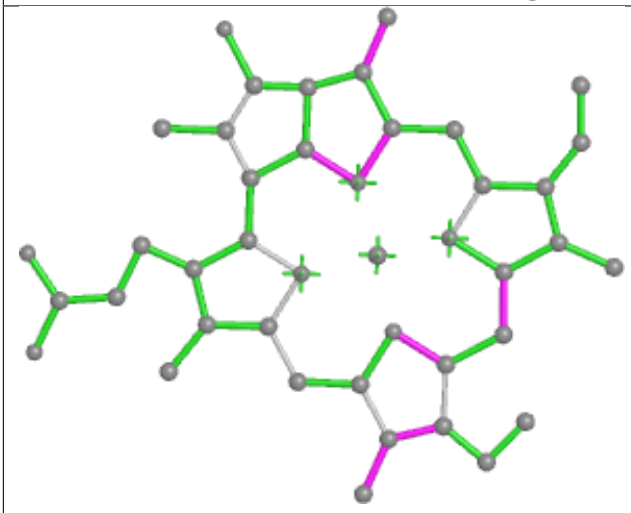


Torsions

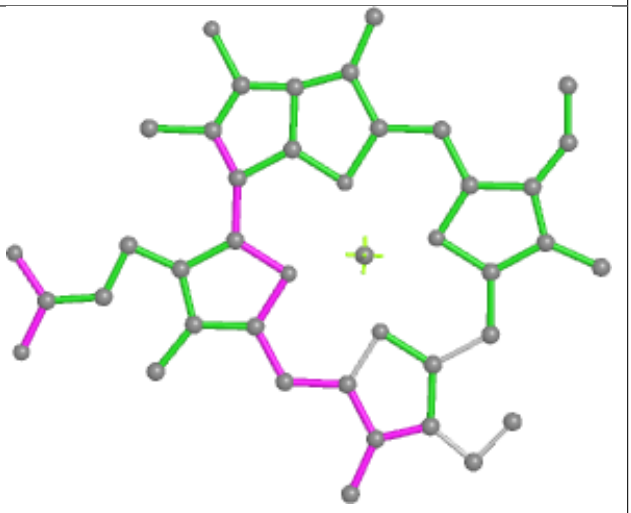


Rings

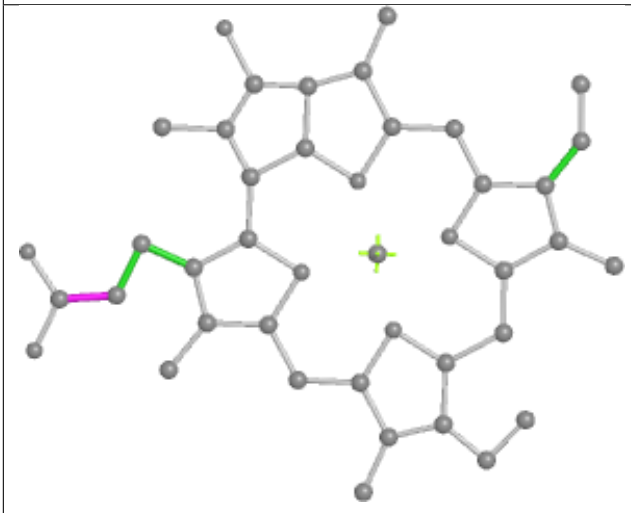
Ligand CLA A 835



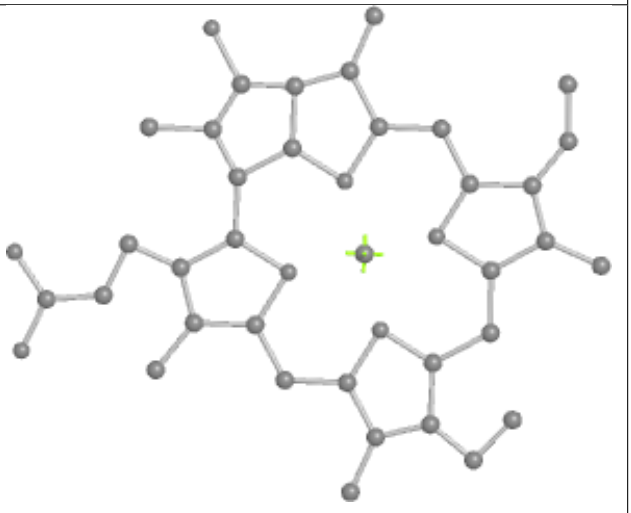
Bond lengths



Bond angles

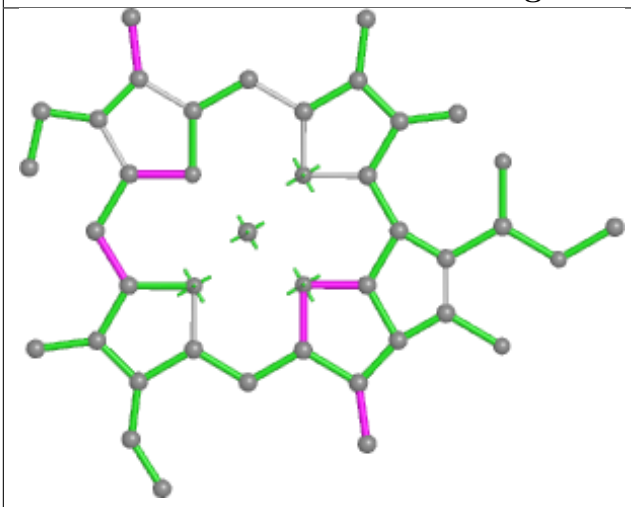


Torsions

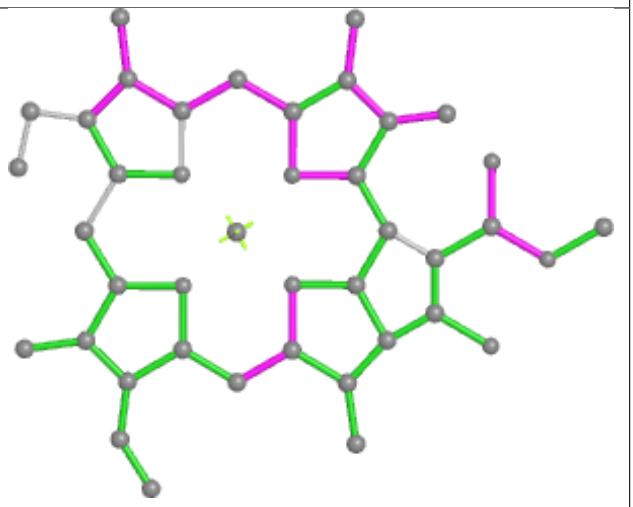


Rings

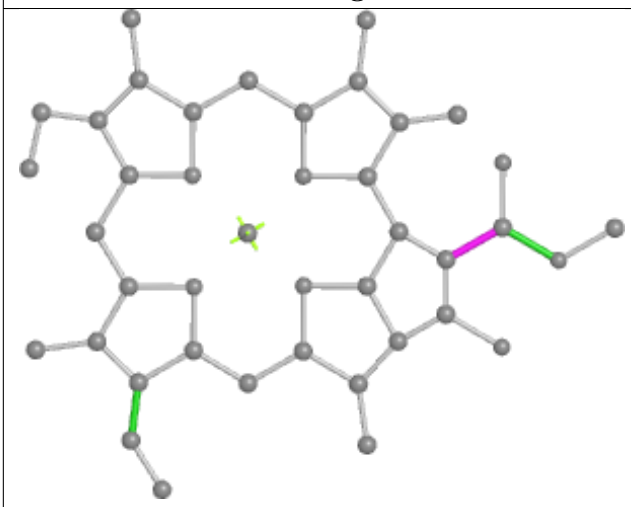
Ligand CLA B 807



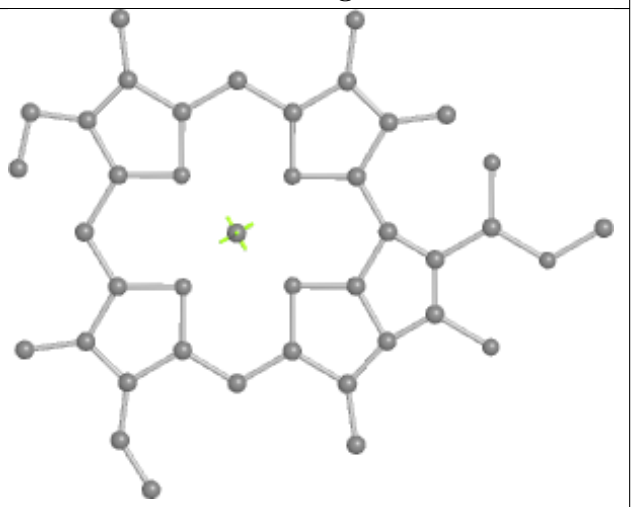
Bond lengths



Bond angles

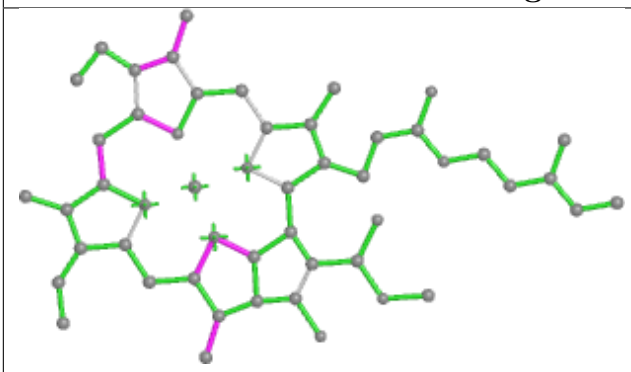


Torsions

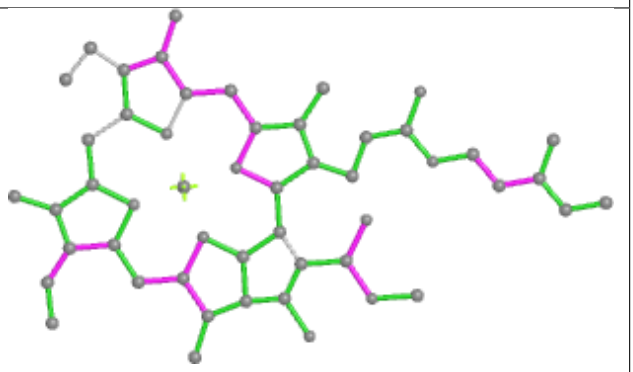


Rings

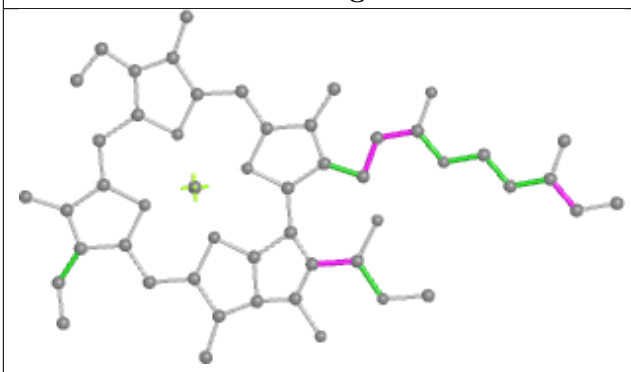
Ligand CLA B 811



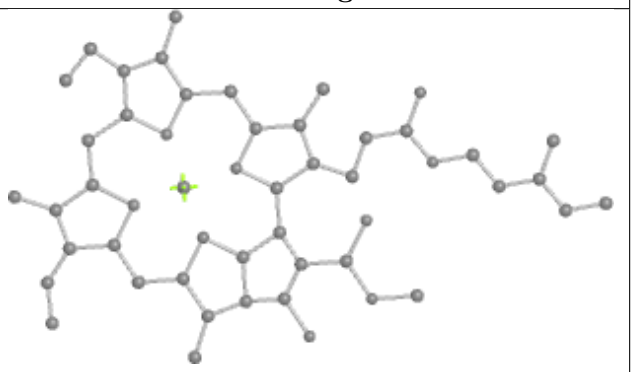
Bond lengths



Bond angles

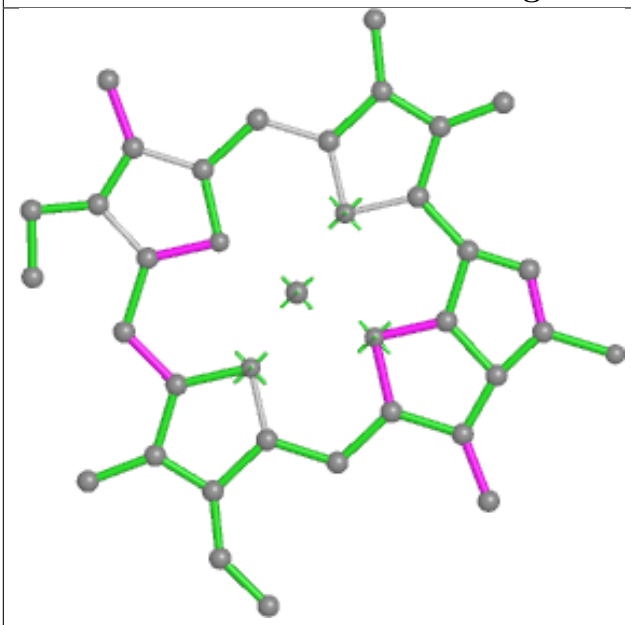


Torsions

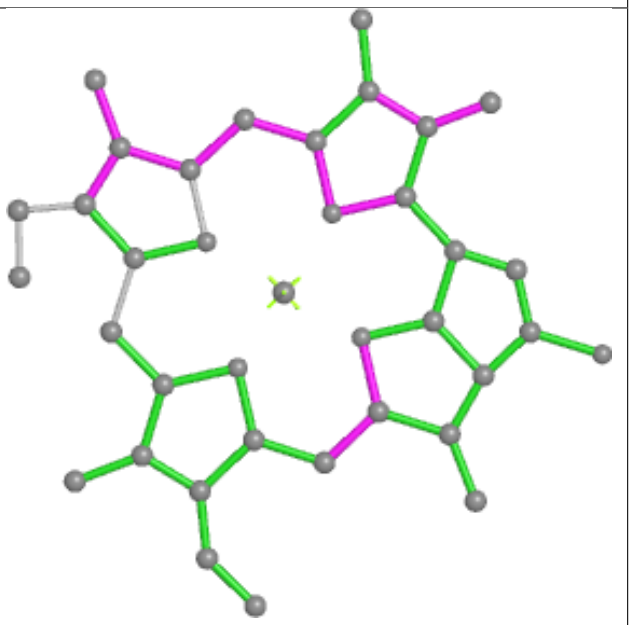


Rings

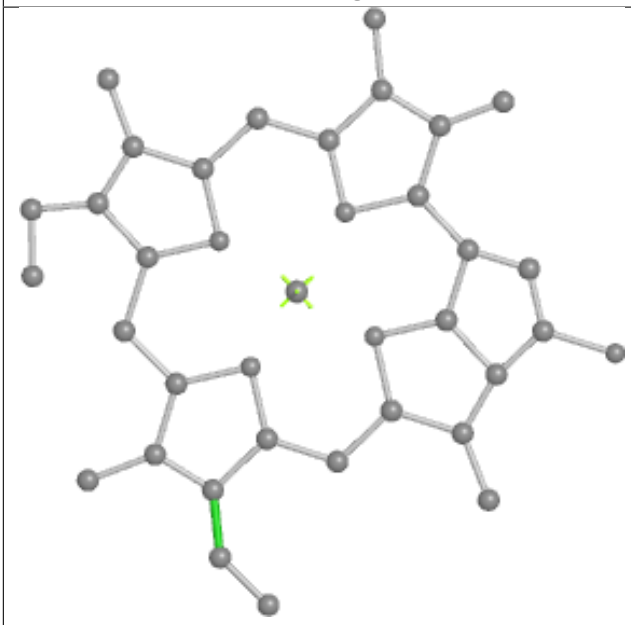
Ligand CLA K 201



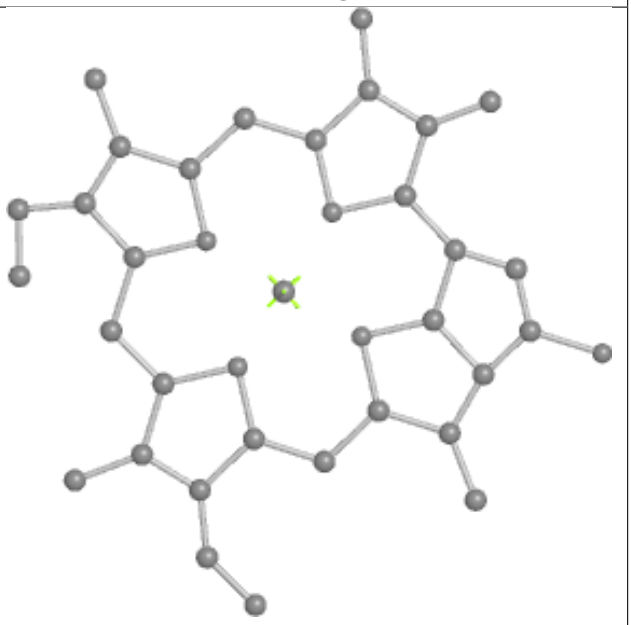
Bond lengths



Bond angles

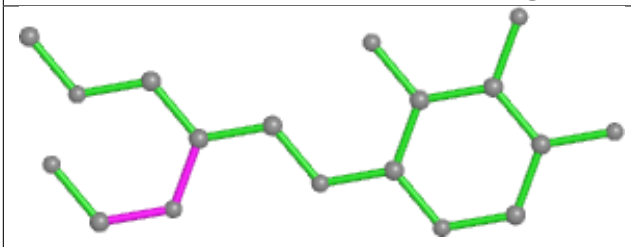


Torsions

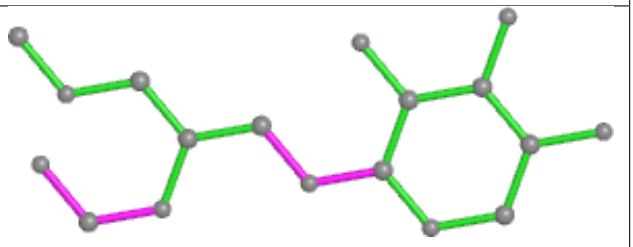


Rings

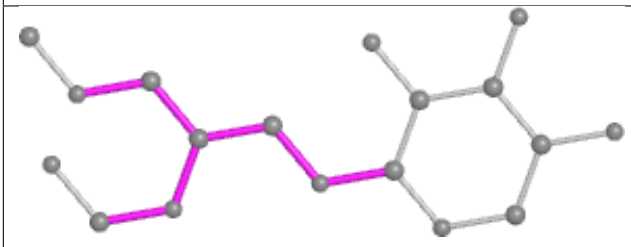
Ligand LMG 4 318



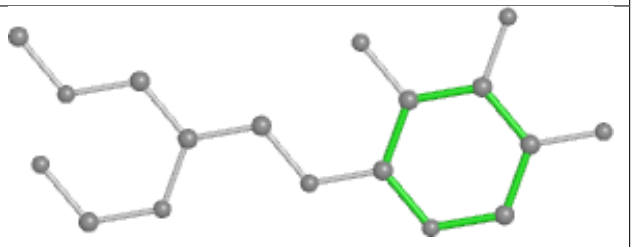
Bond lengths



Bond angles

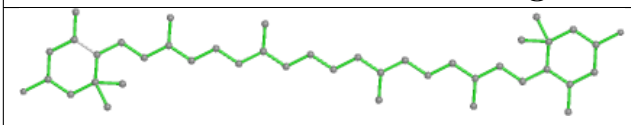


Torsions

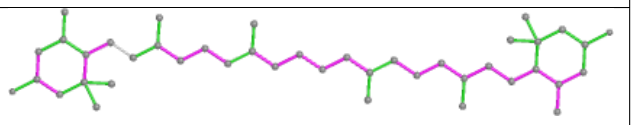


Rings

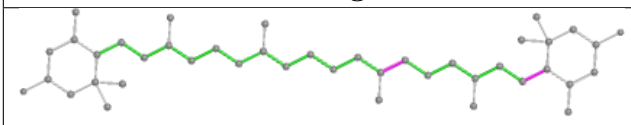
Ligand LUT 6 501



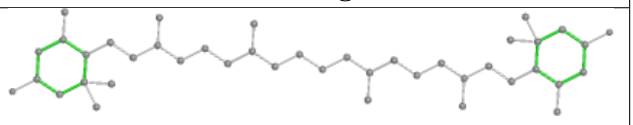
Bond lengths



Bond angles

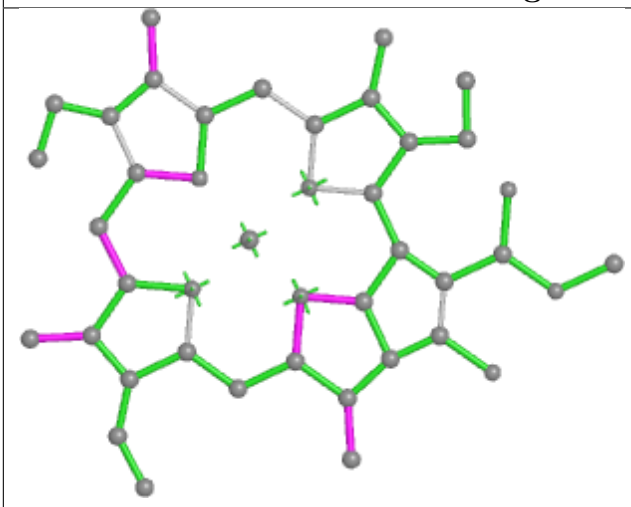


Torsions

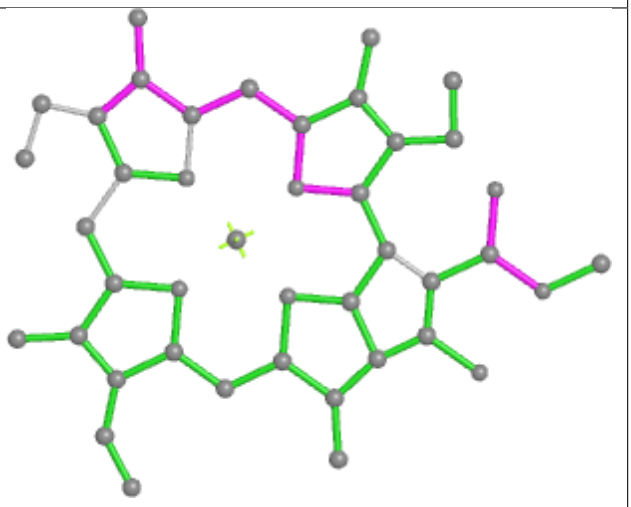


Rings

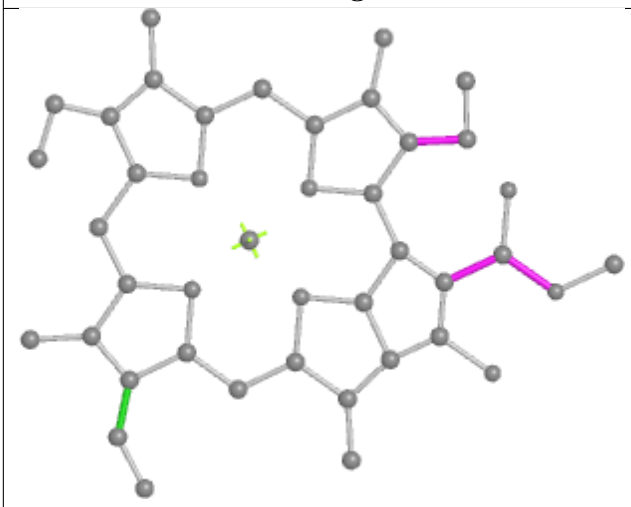
Ligand CLA A 814



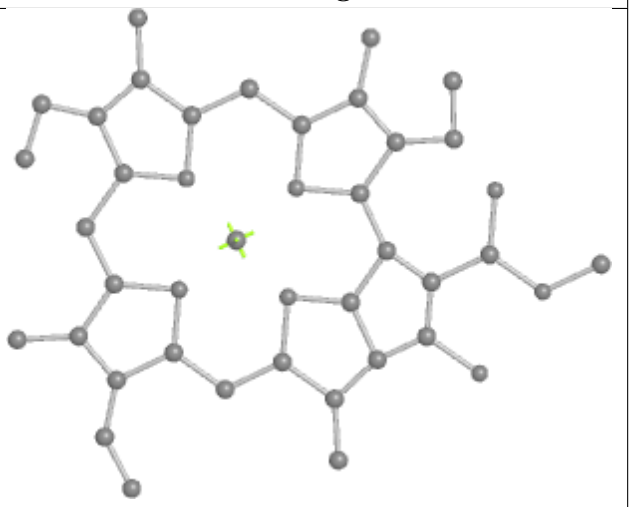
Bond lengths



Bond angles

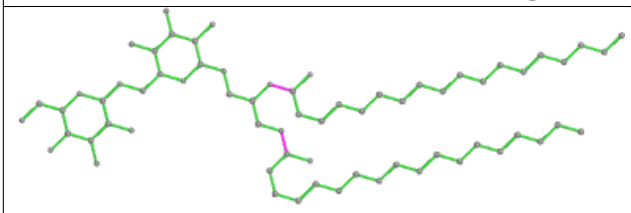


Torsions

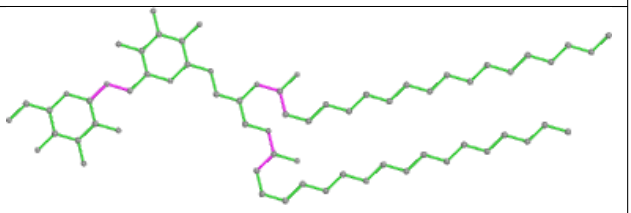


Rings

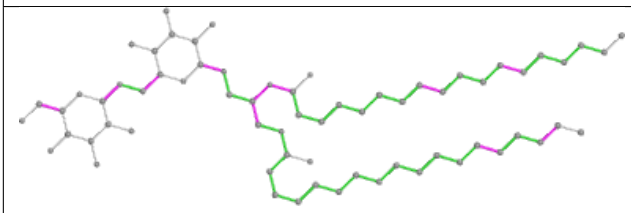
Ligand DGD J 104



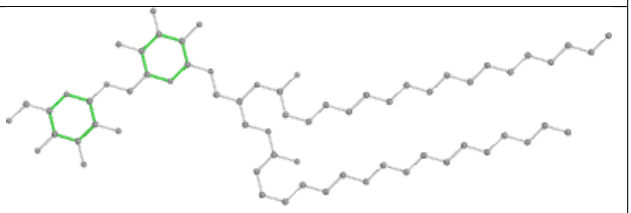
Bond lengths



Bond angles

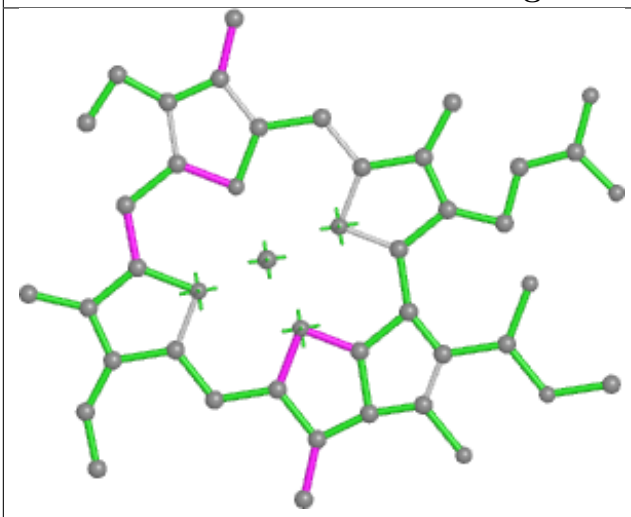


Torsions

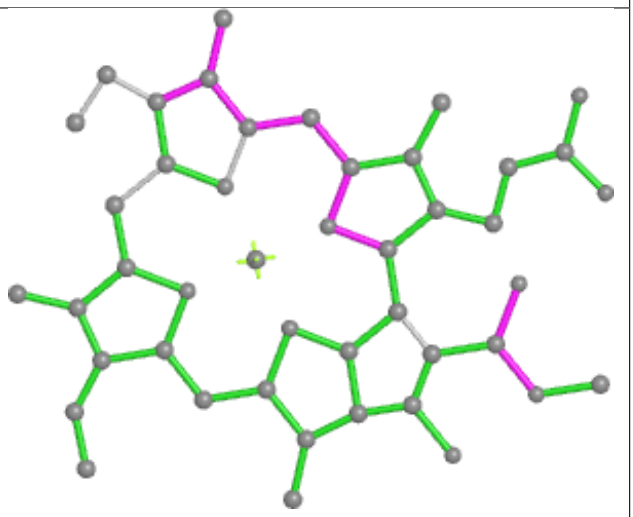


Rings

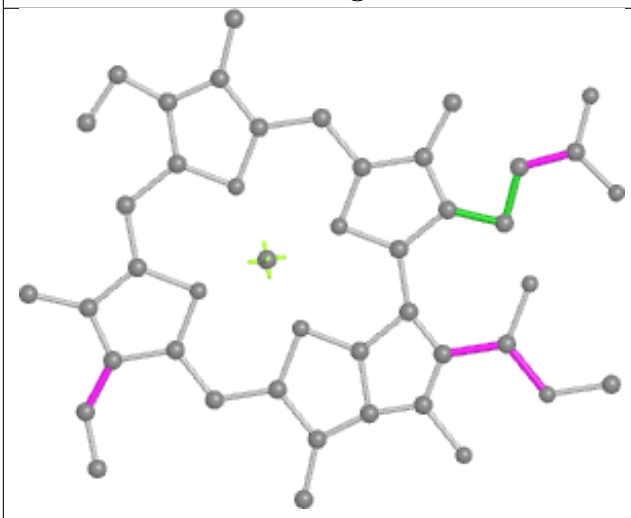
Ligand CLA A 815



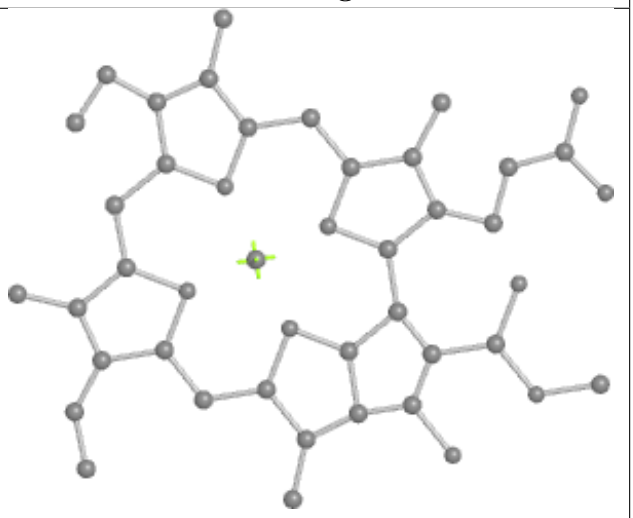
Bond lengths



Bond angles

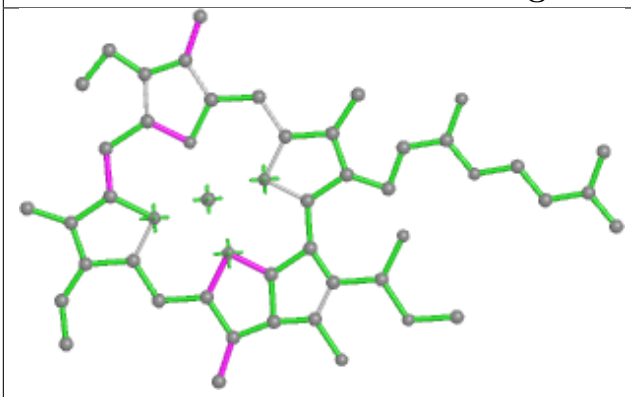


Torsions

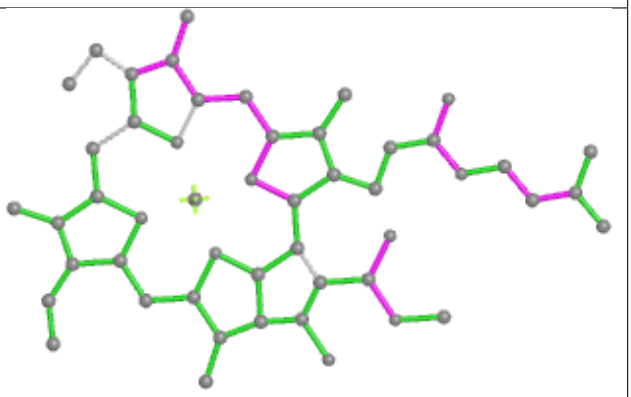


Rings

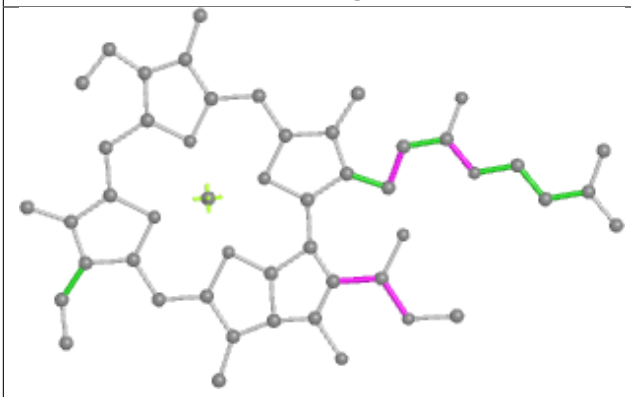
Ligand CLA 4 305



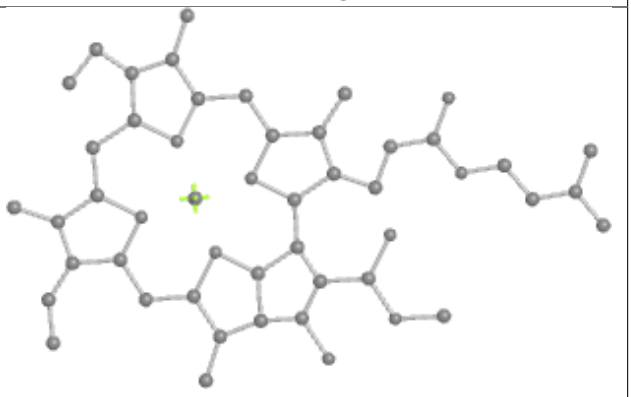
Bond lengths



Bond angles

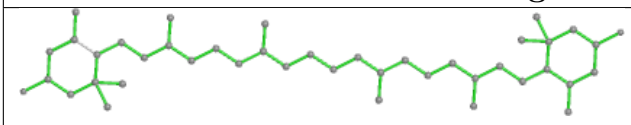


Torsions

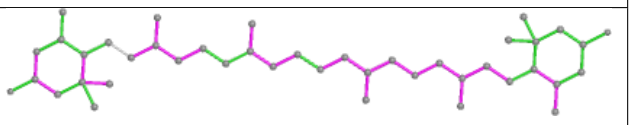


Rings

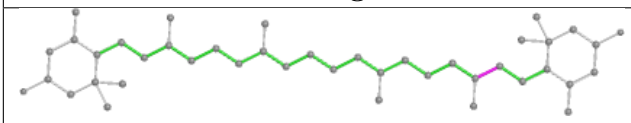
Ligand LUT 1 501



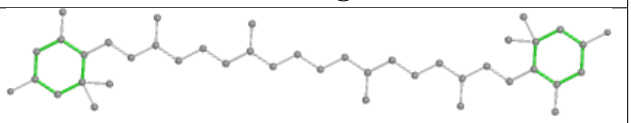
Bond lengths



Bond angles

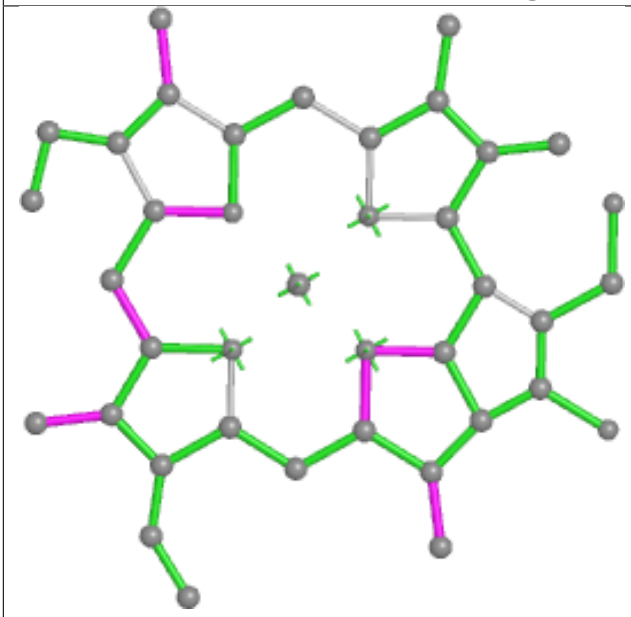


Torsions

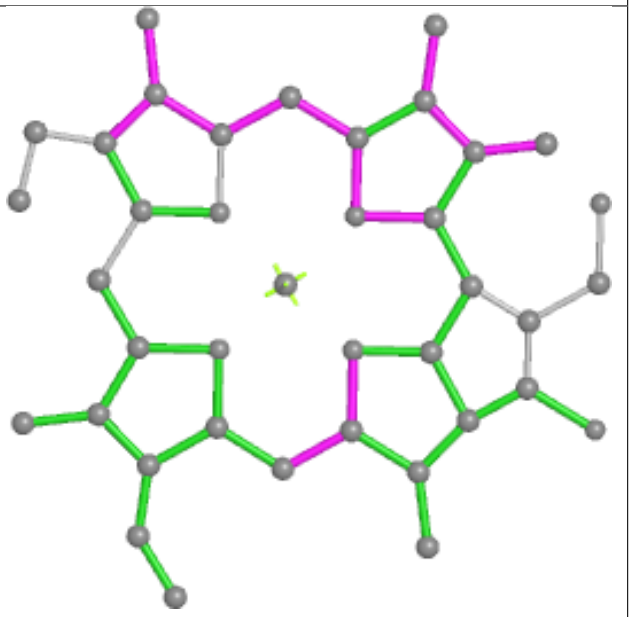


Rings

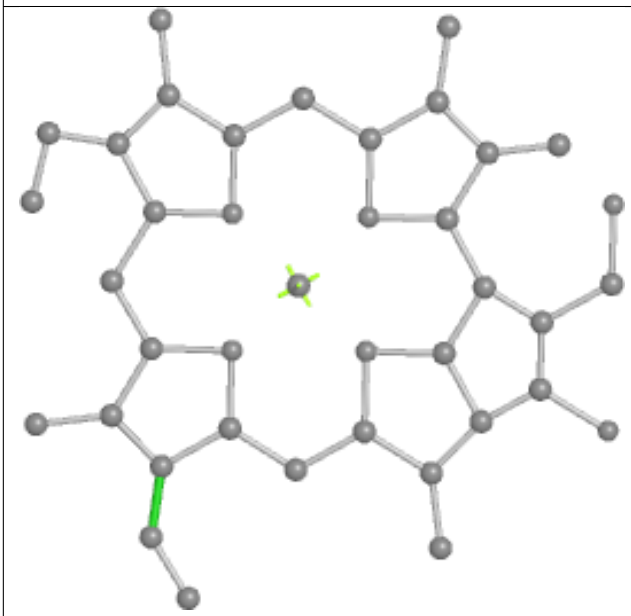
Ligand CLA A 817



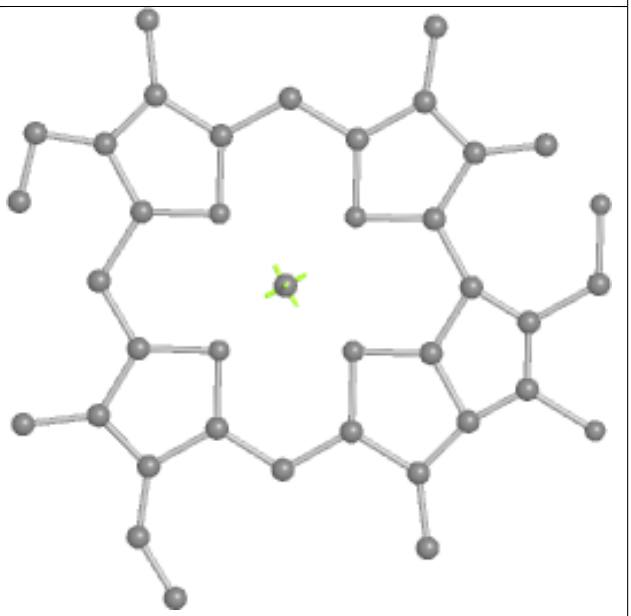
Bond lengths



Bond angles

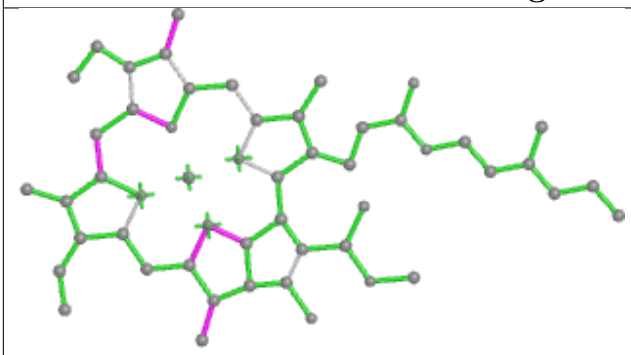


Torsions

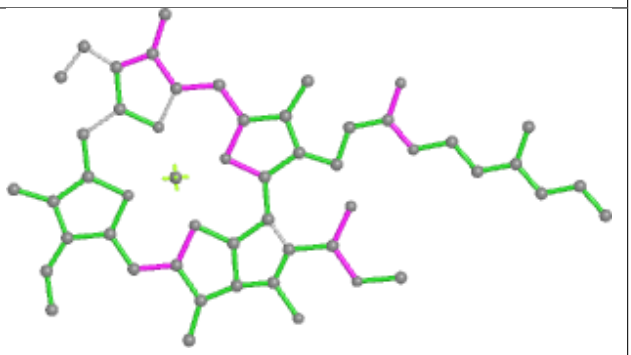


Rings

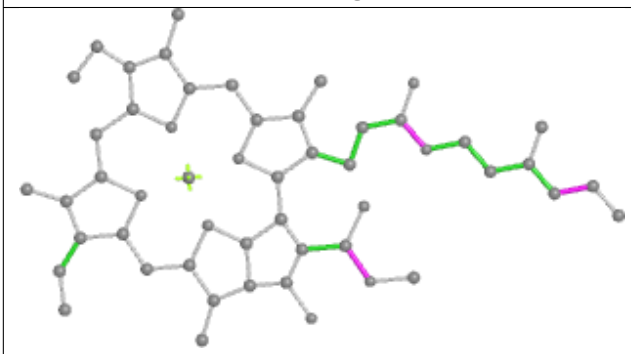
Ligand CLA 1 513



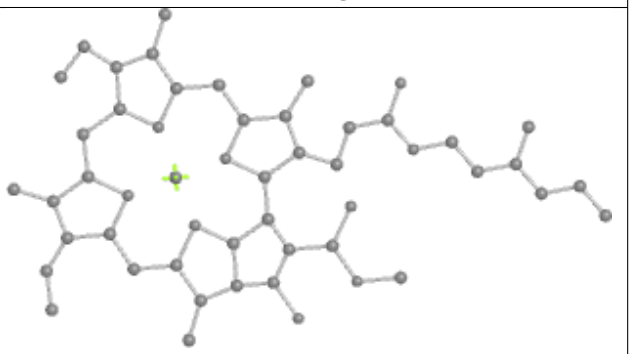
Bond lengths



Bond angles

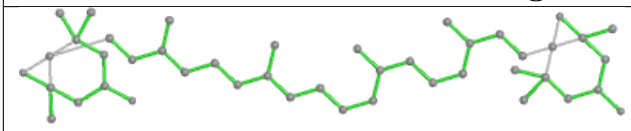


Torsions

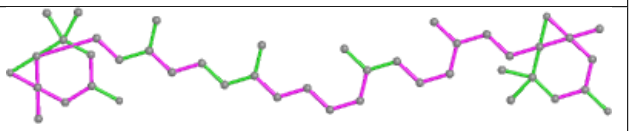


Rings

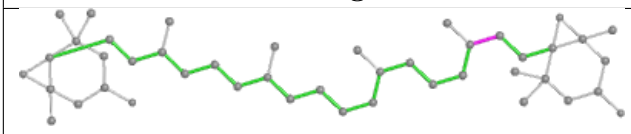
Ligand XAT 4 303



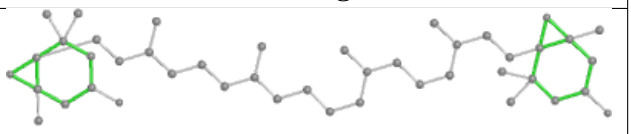
Bond lengths



Bond angles

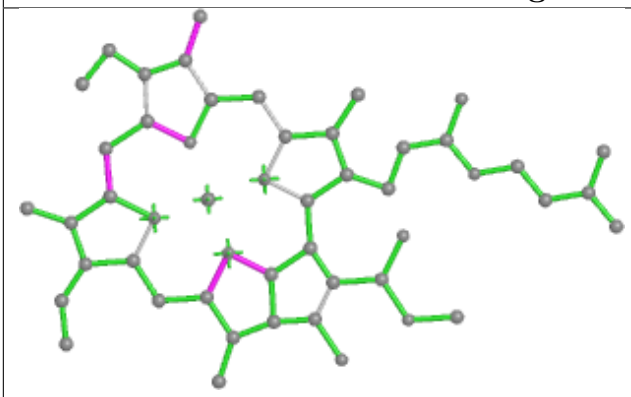


Torsions

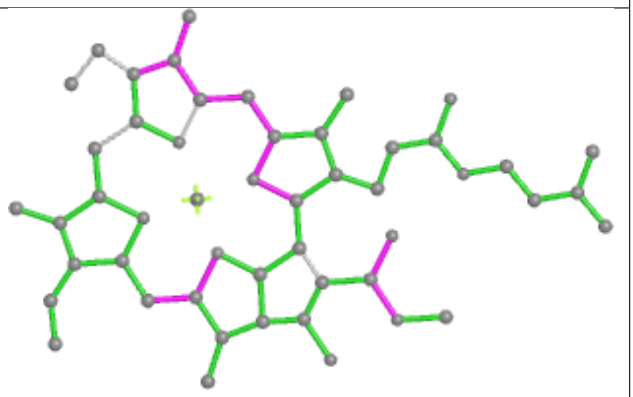


Rings

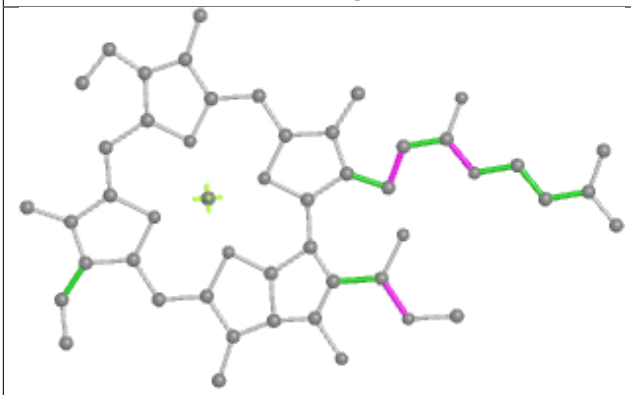
Ligand CLA 3 309



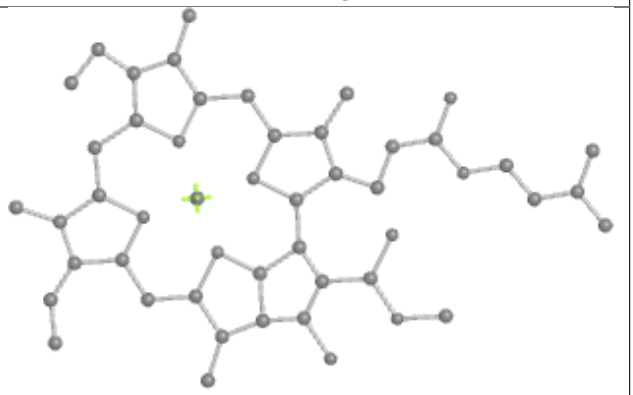
Bond lengths



Bond angles

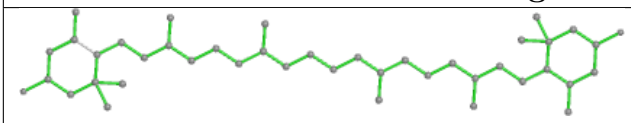


Torsions

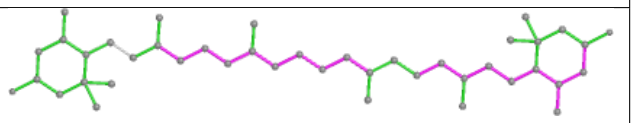


Rings

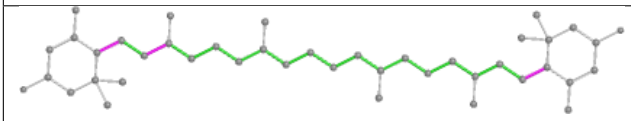
Ligand LUT 3 301



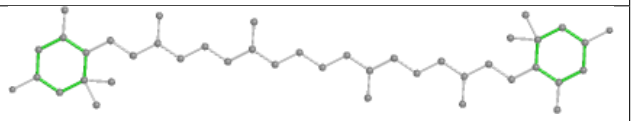
Bond lengths



Bond angles

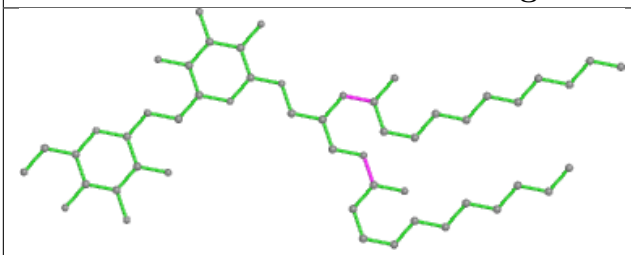


Torsions

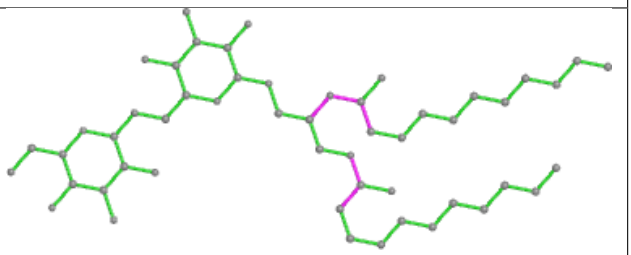


Rings

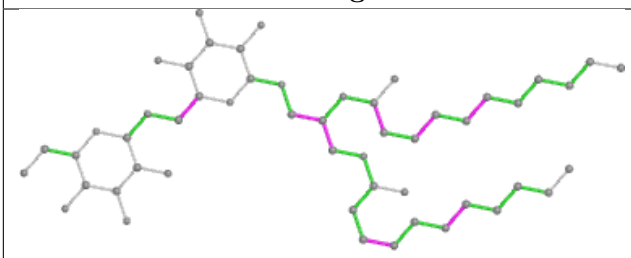
Ligand DGD B 851



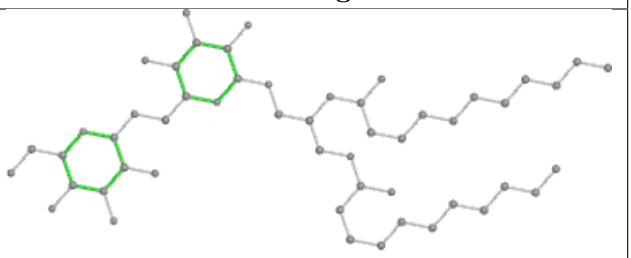
Bond lengths



Bond angles

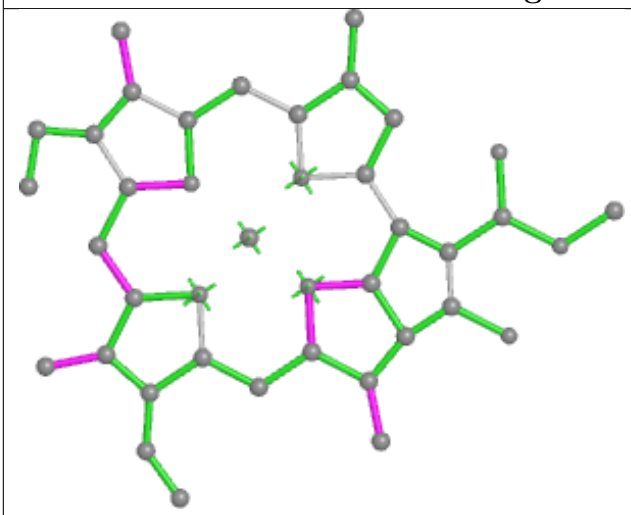


Torsions

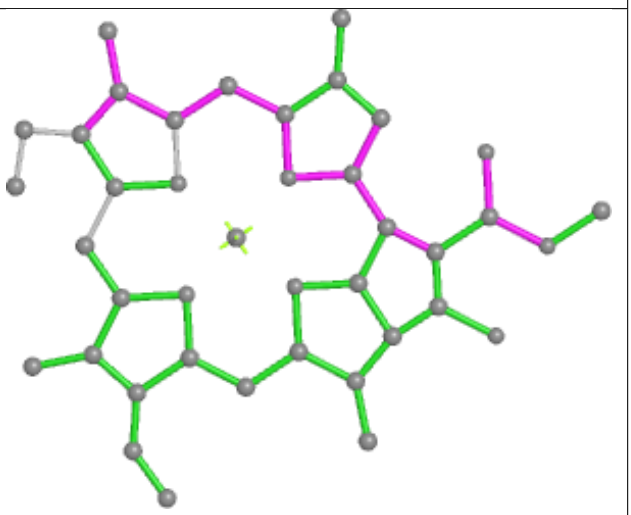


Rings

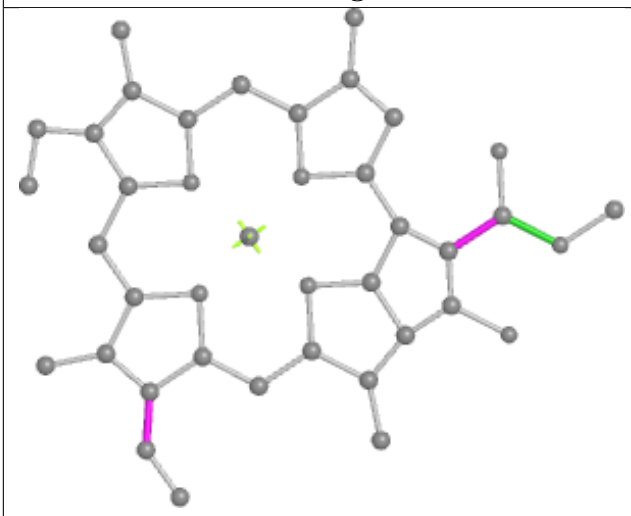
Ligand CLA B 838



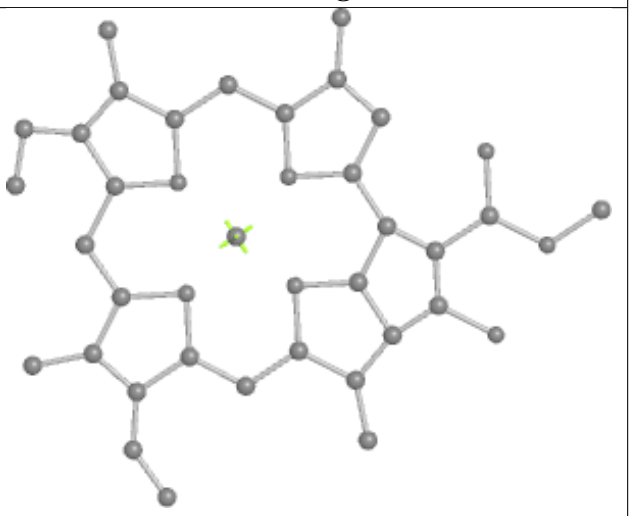
Bond lengths



Bond angles

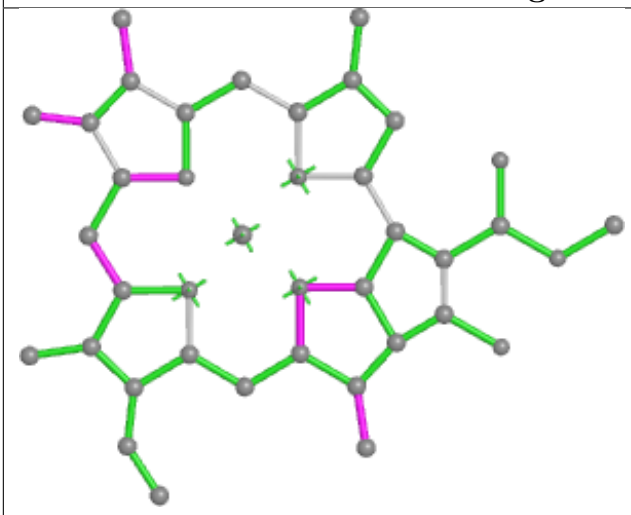


Torsions

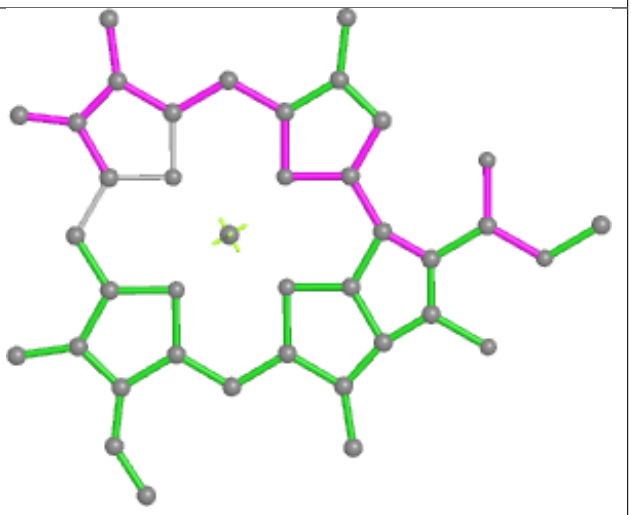


Rings

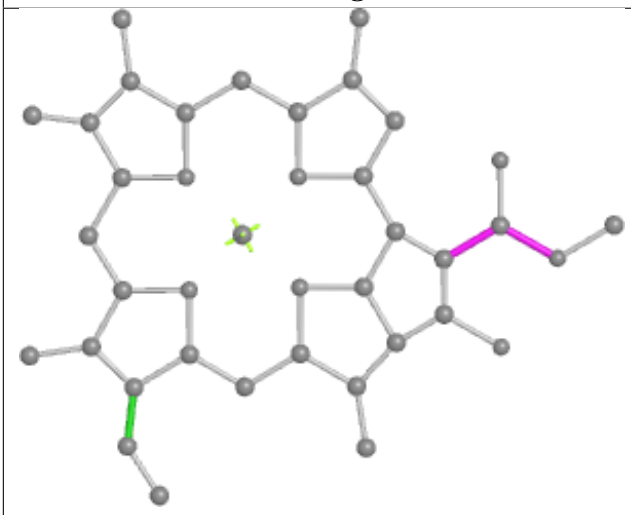
Ligand CLA 4 304



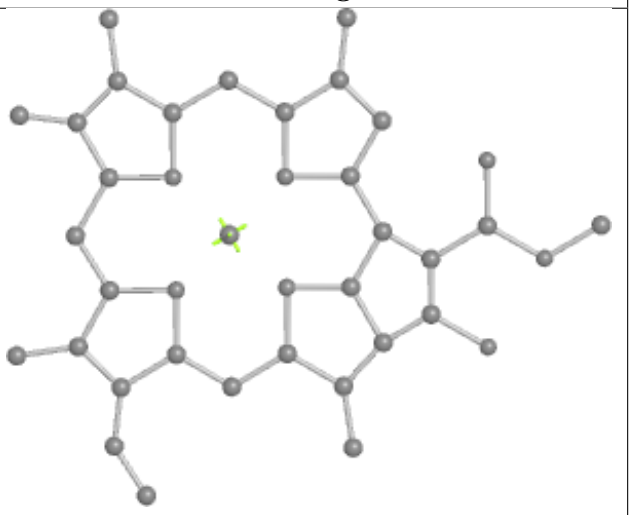
Bond lengths



Bond angles

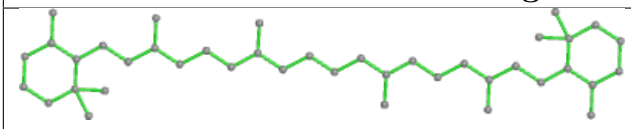


Torsions

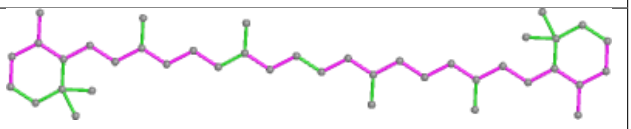


Rings

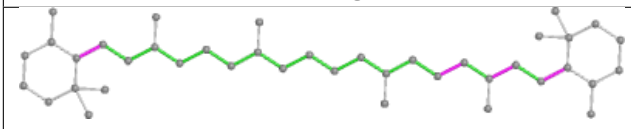
Ligand BCR A 849



Bond lengths



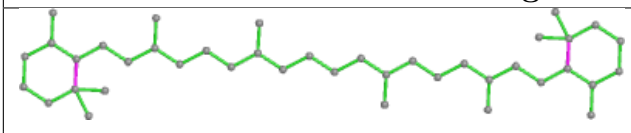
Bond angles



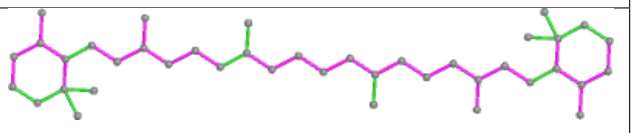
Torsions

Rings

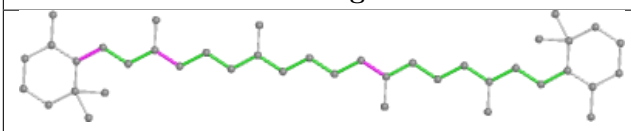
Ligand BCR A 850



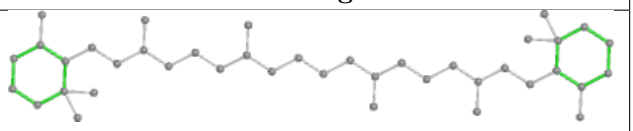
Bond lengths



Bond angles

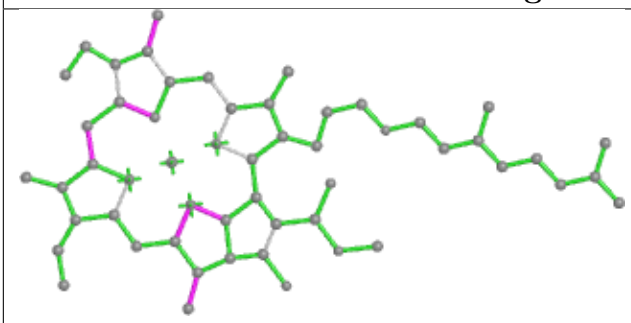


Torsions

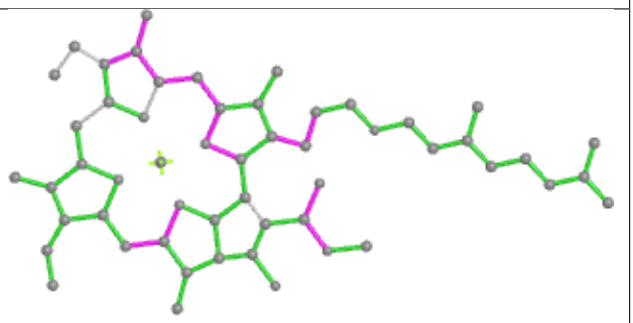


Rings

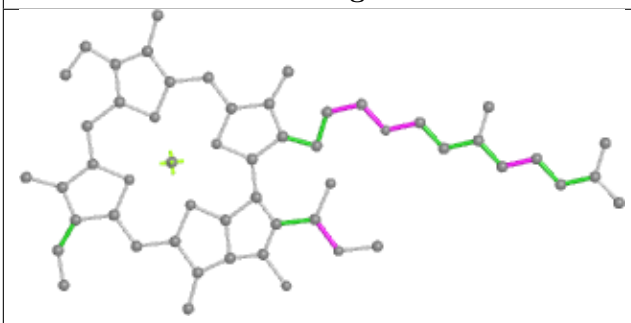
Ligand CLA B 808



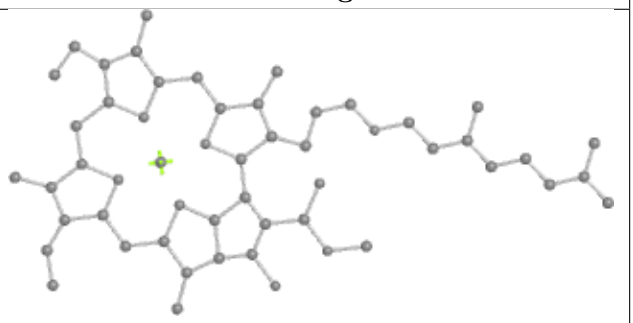
Bond lengths



Bond angles

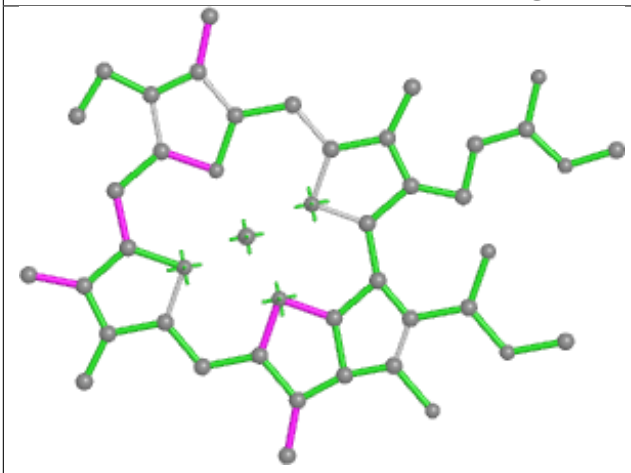


Torsions

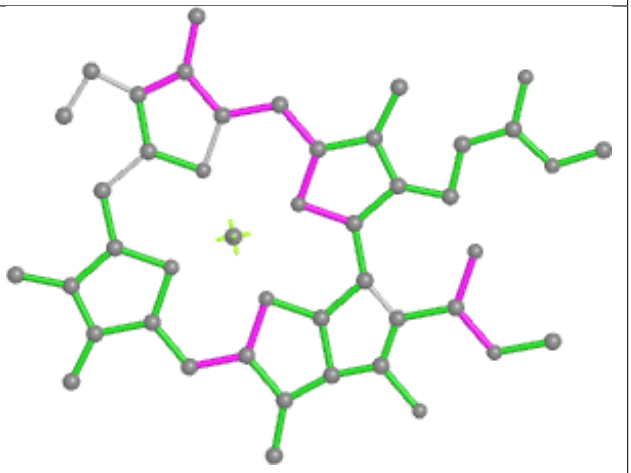


Rings

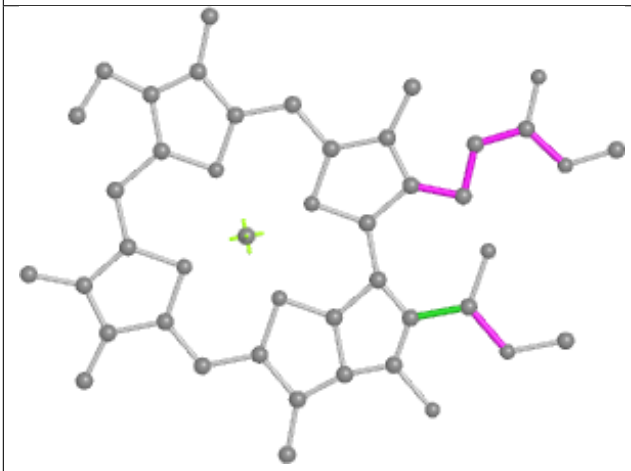
Ligand CLA 3 315



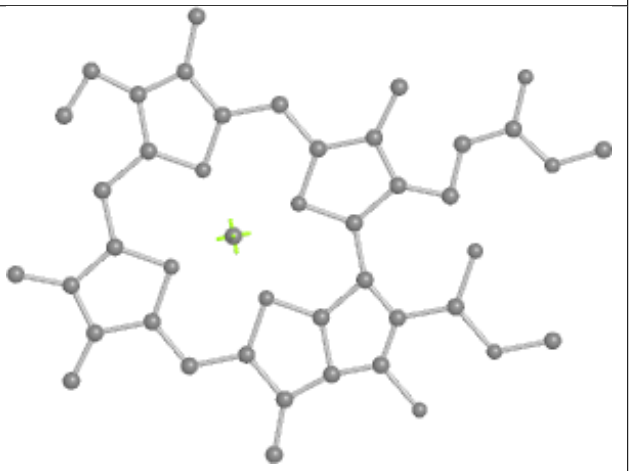
Bond lengths



Bond angles

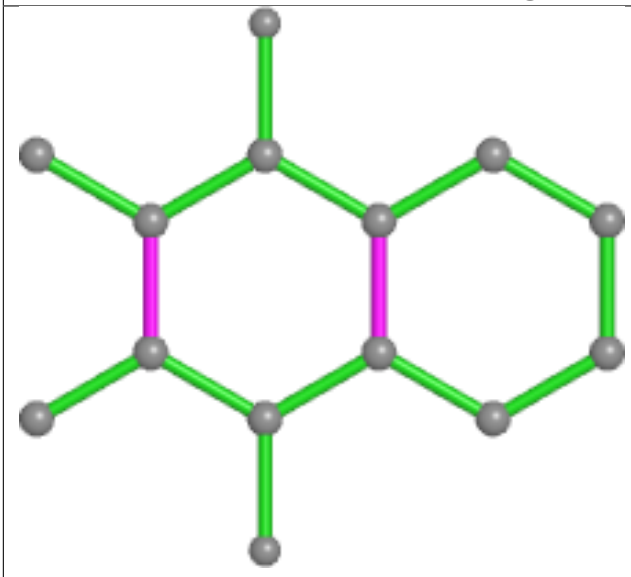


Torsions

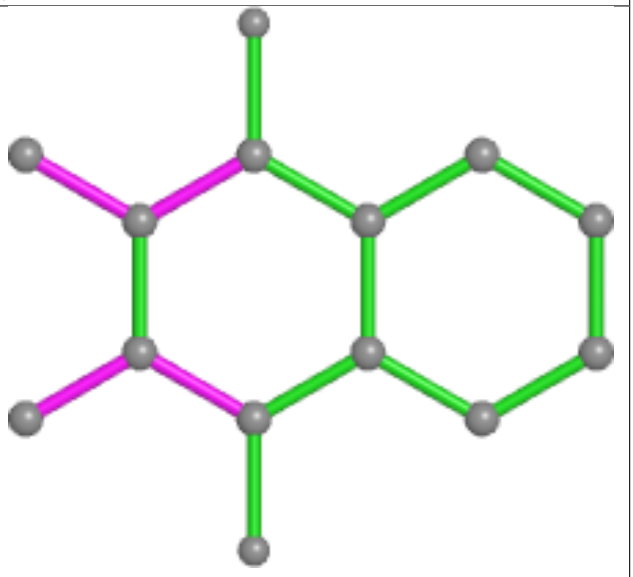


Rings

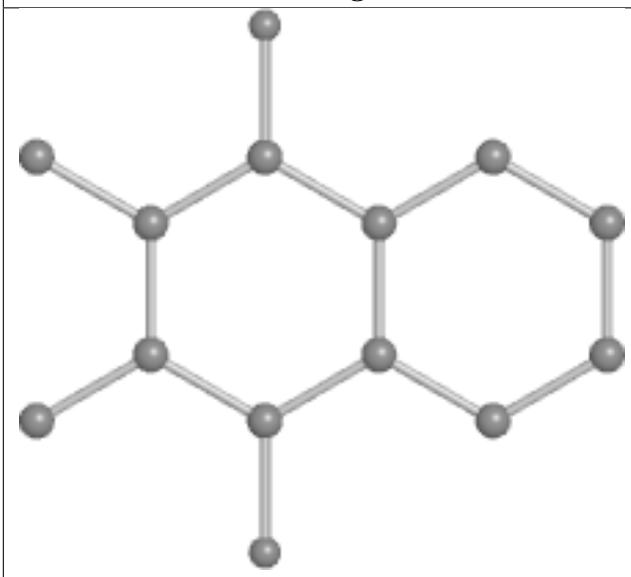
Ligand PQN A 842



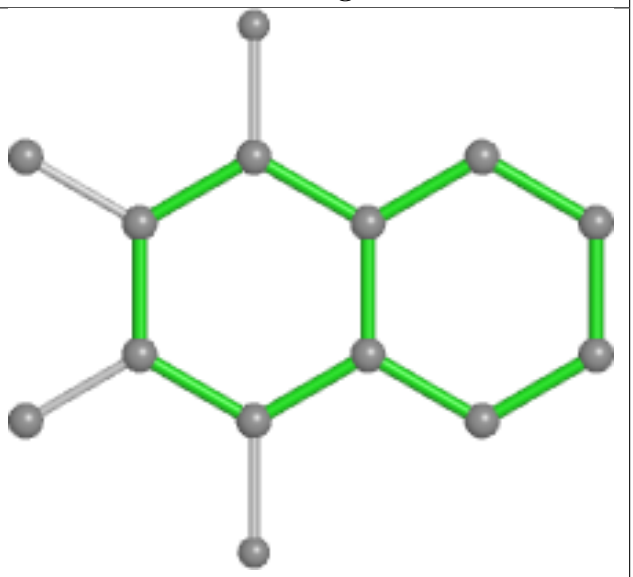
Bond lengths



Bond angles

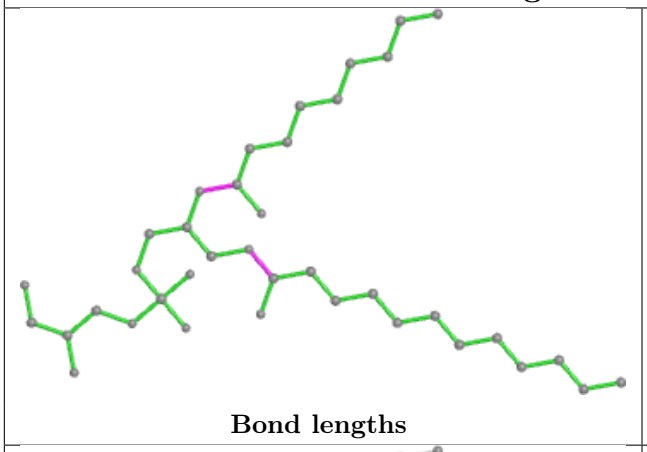


Torsions

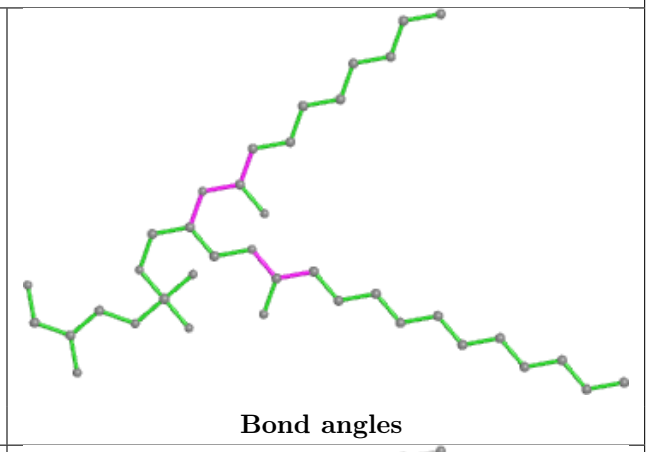


Rings

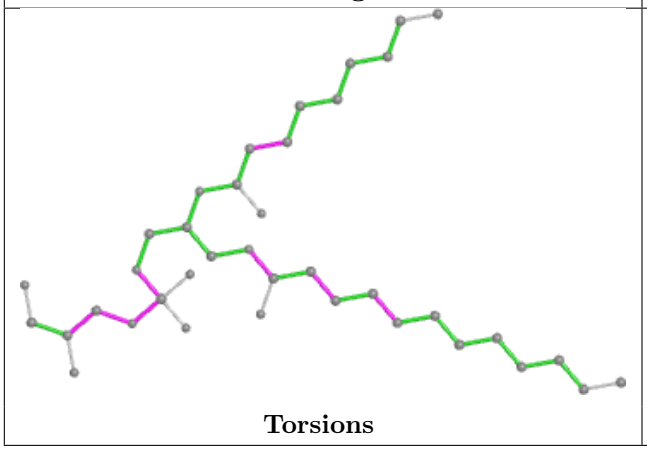
Ligand LHG B 852



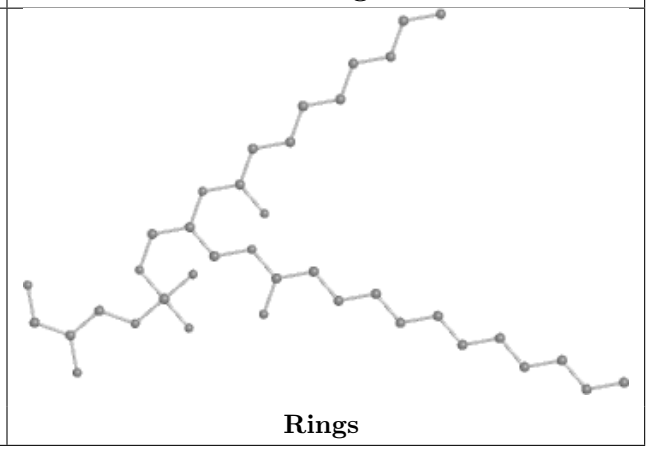
Bond lengths



Bond angles

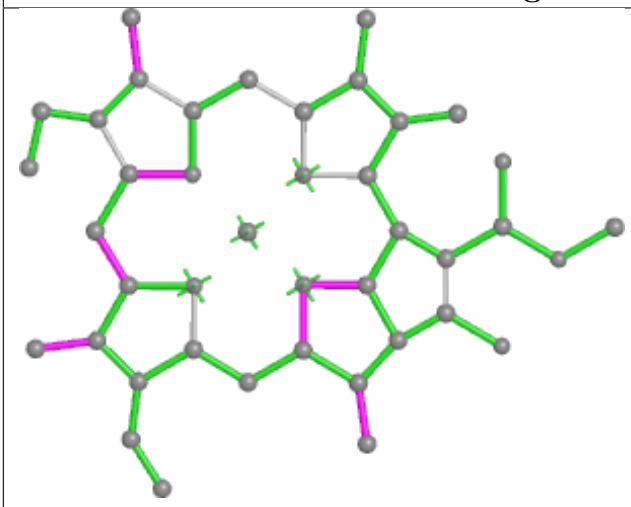


Torsions

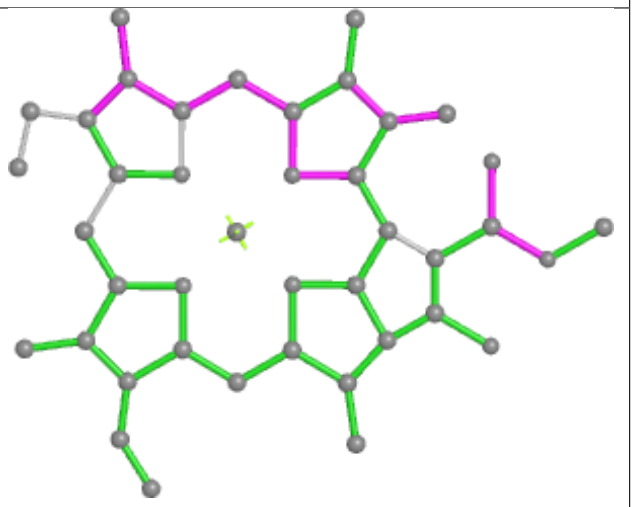


Rings

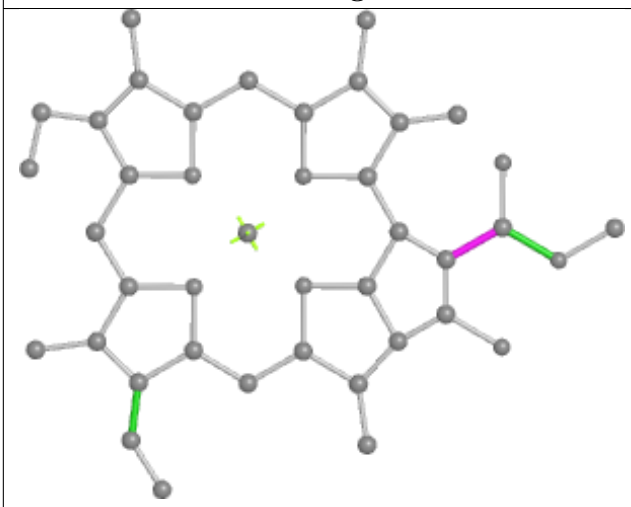
Ligand CLA A 822



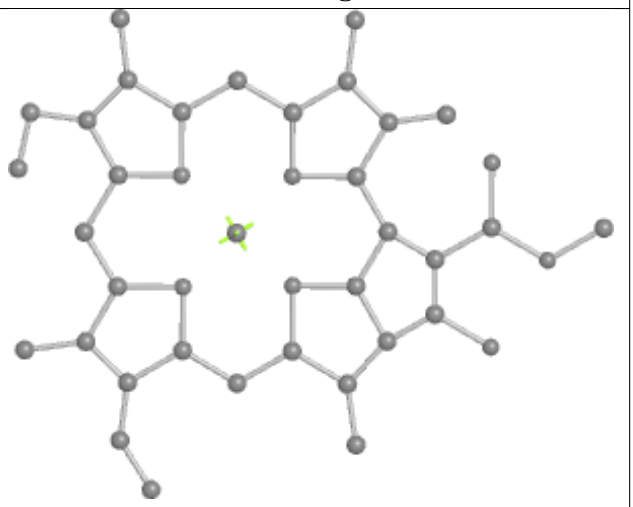
Bond lengths



Bond angles

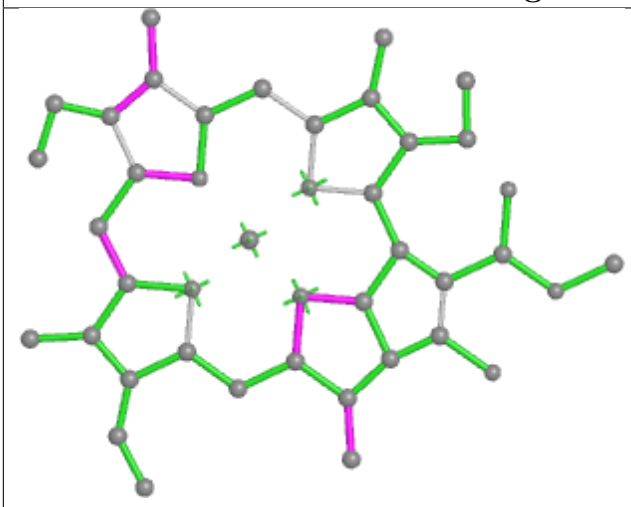


Torsions

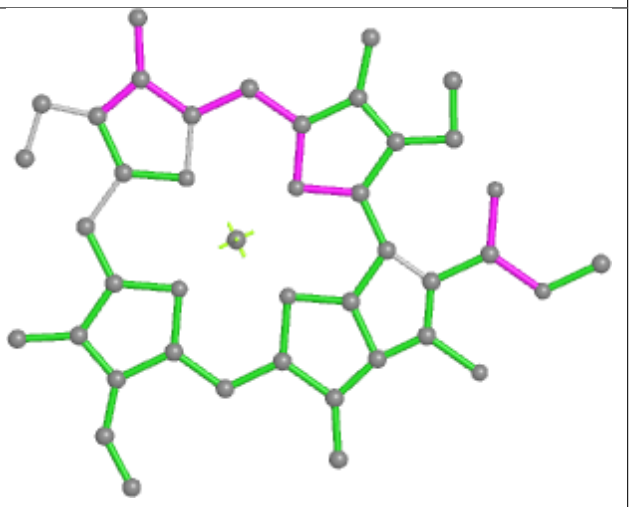


Rings

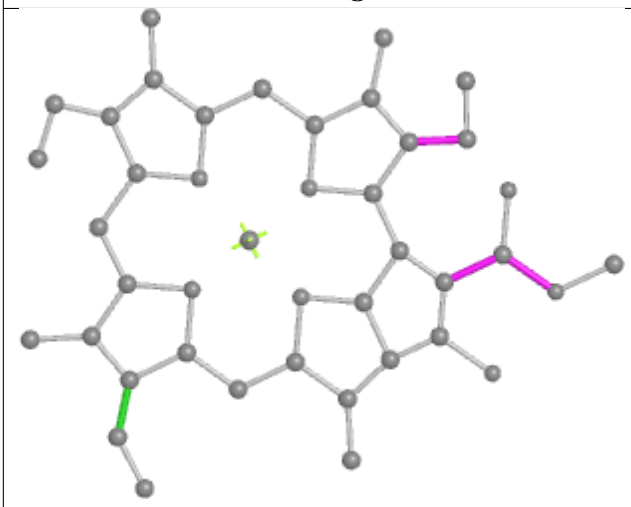
Ligand CLA B 824



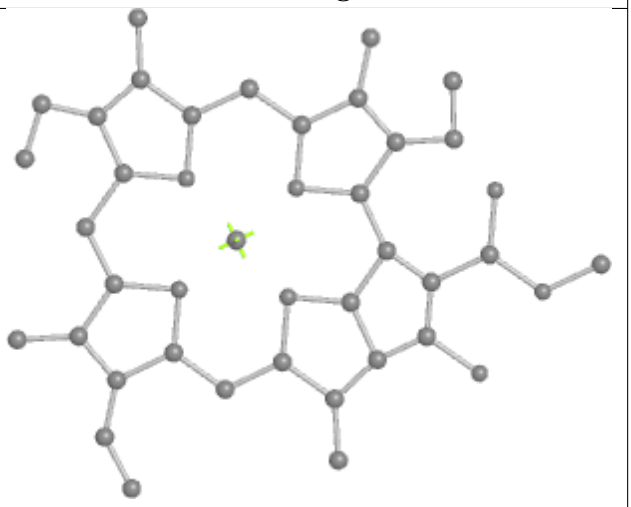
Bond lengths



Bond angles

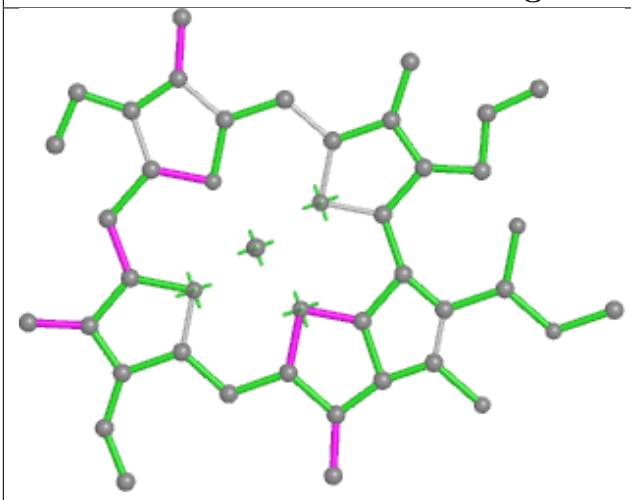


Torsions

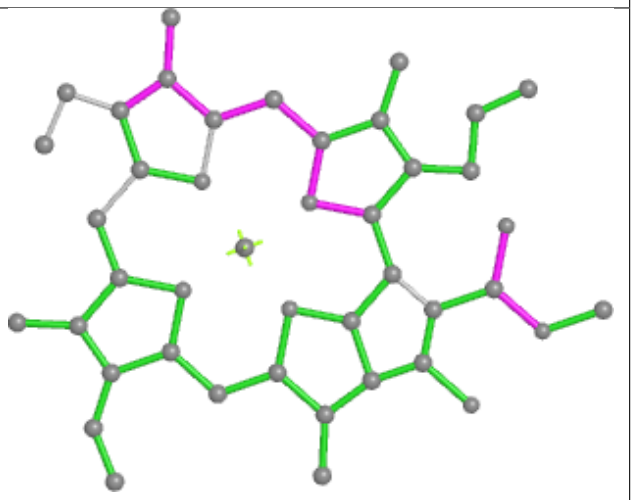


Rings

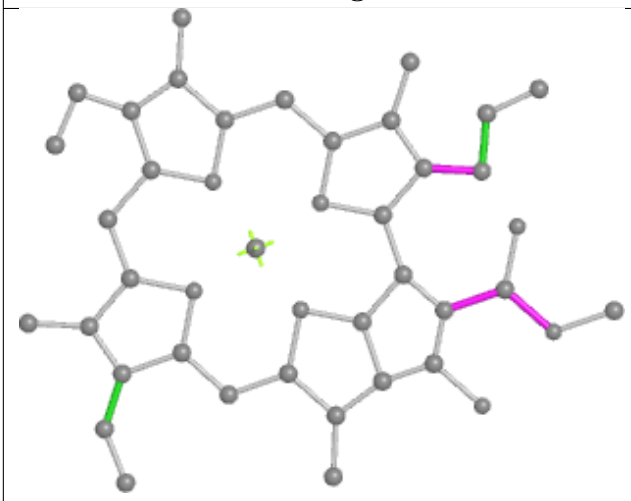
Ligand CLA B 817



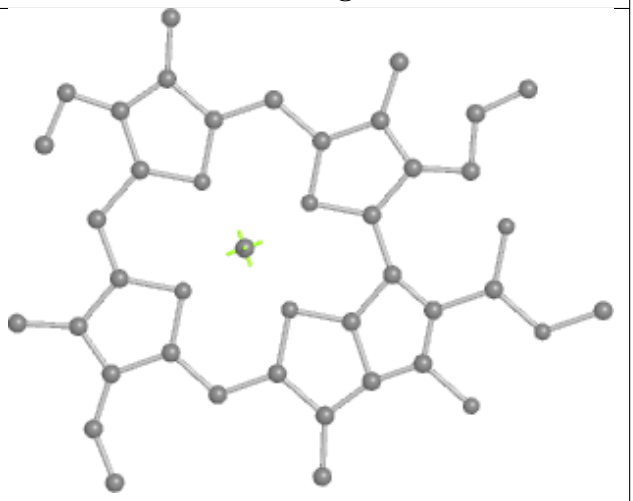
Bond lengths



Bond angles

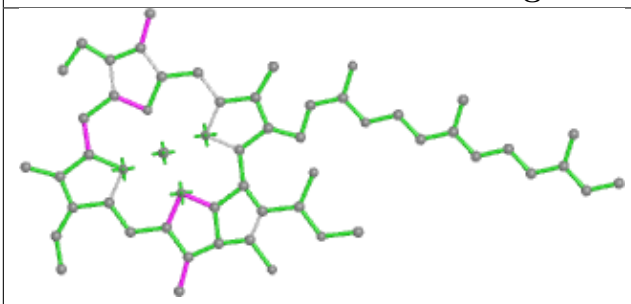


Torsions

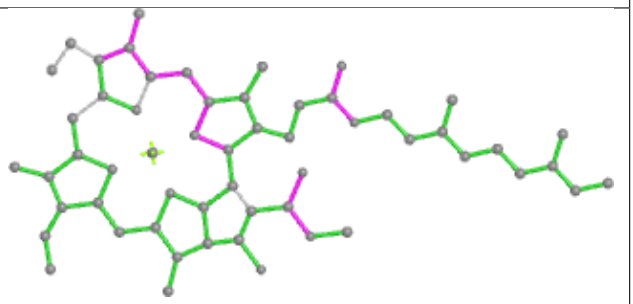


Rings

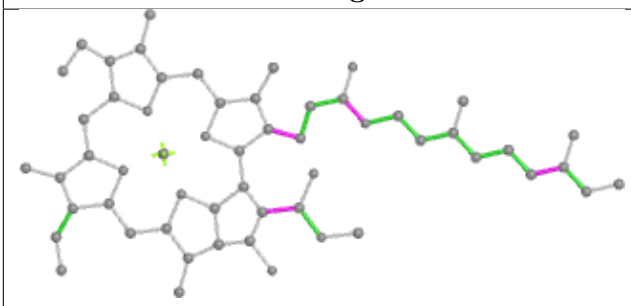
Ligand CLA A 831



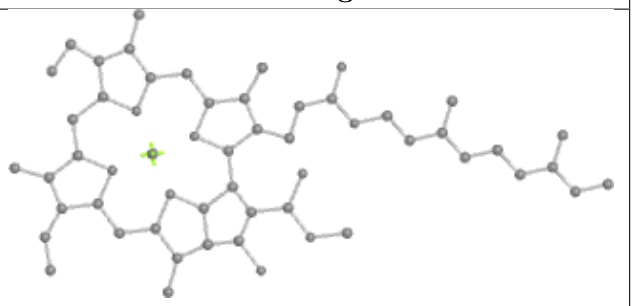
Bond lengths



Bond angles

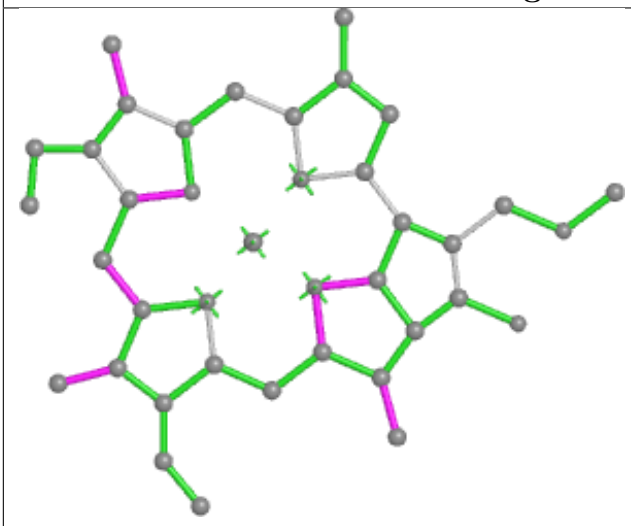


Torsions

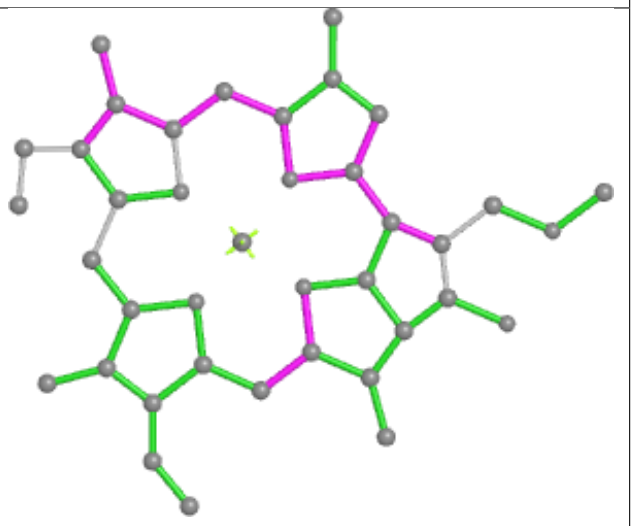


Rings

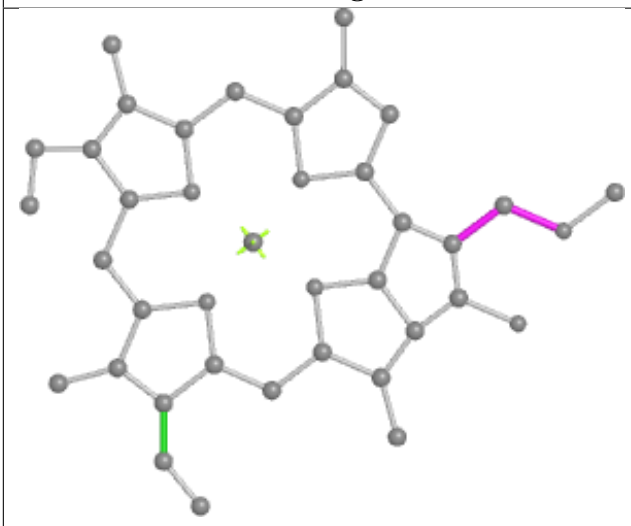
Ligand CLA A 812



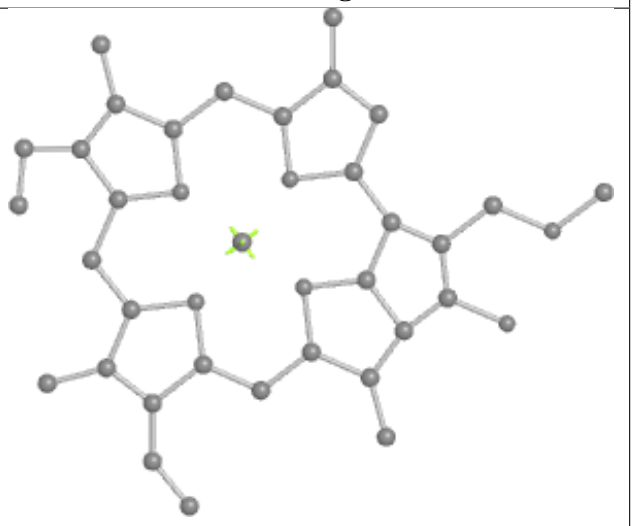
Bond lengths



Bond angles

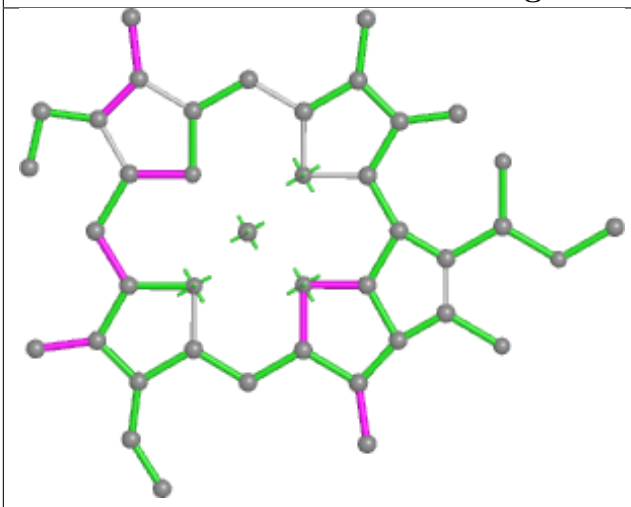


Torsions

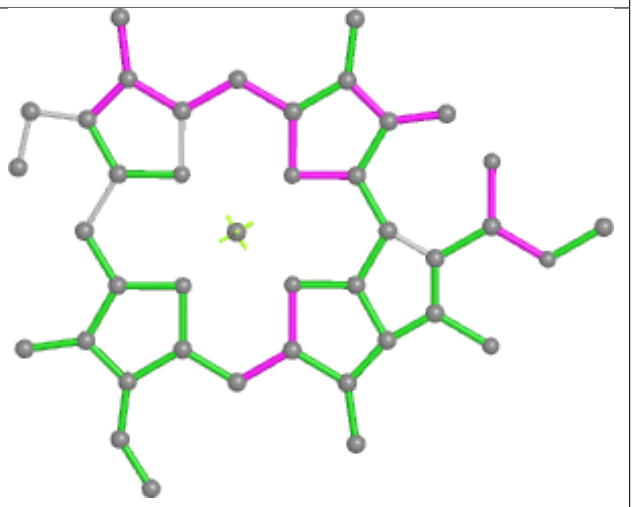


Rings

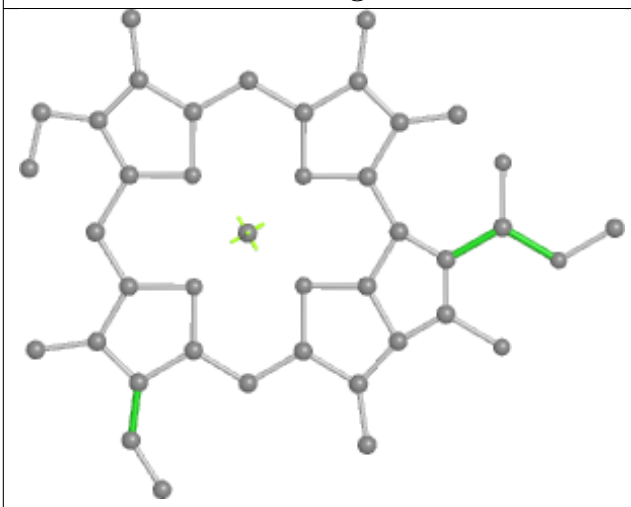
Ligand CLA B 842



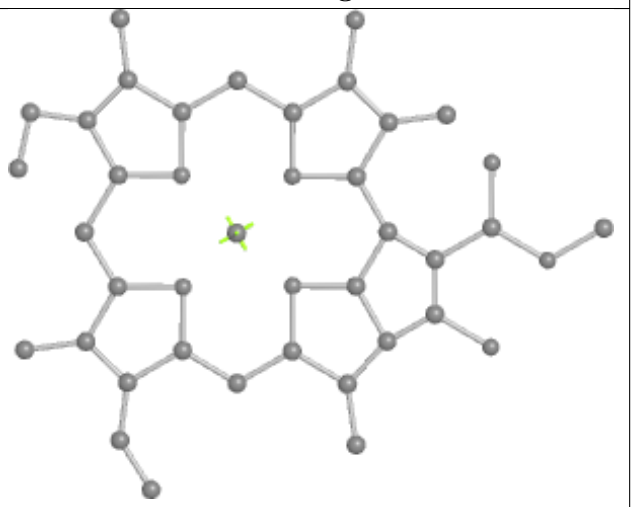
Bond lengths



Bond angles

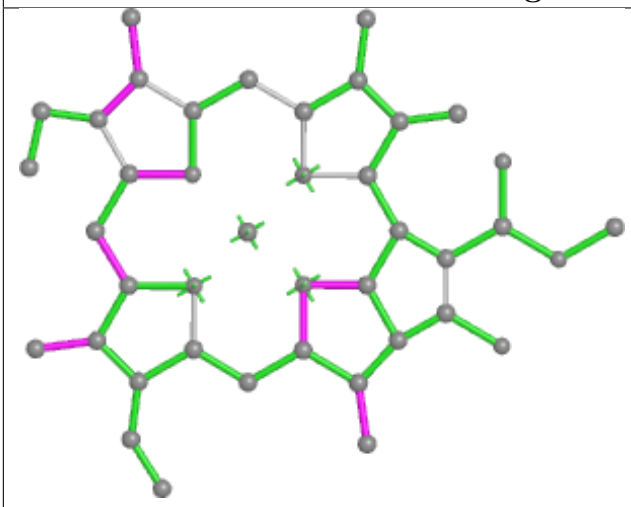


Torsions

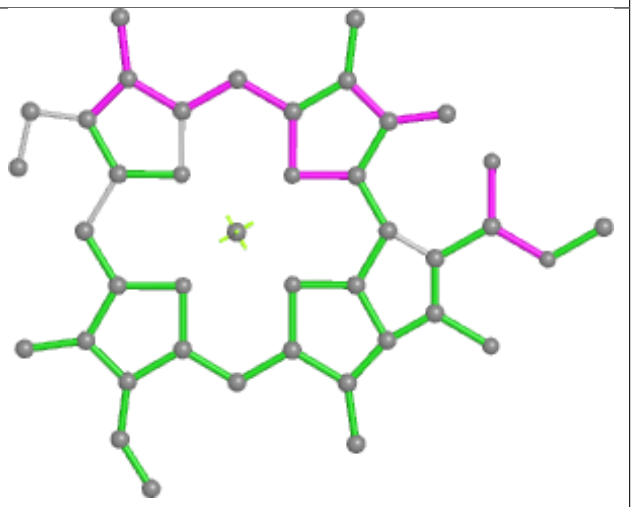


Rings

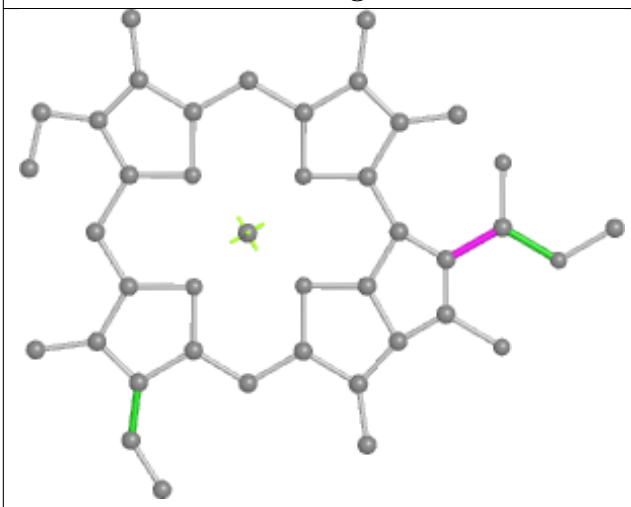
Ligand CLA B 823



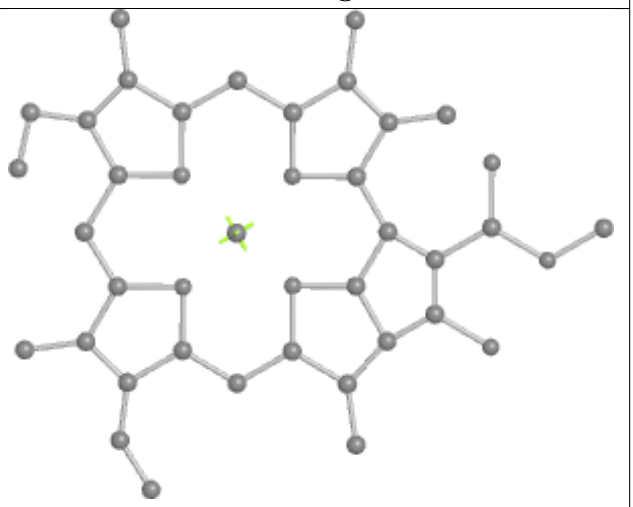
Bond lengths



Bond angles

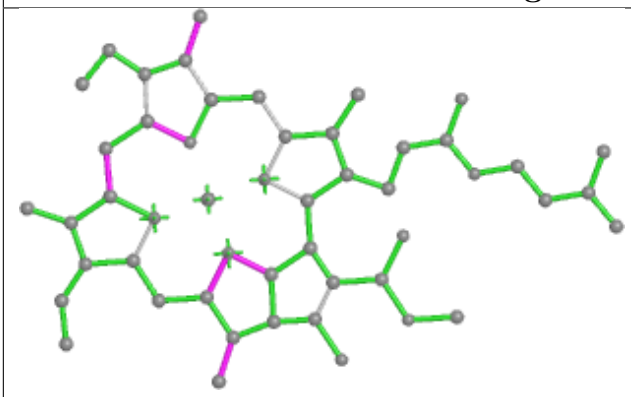


Torsions

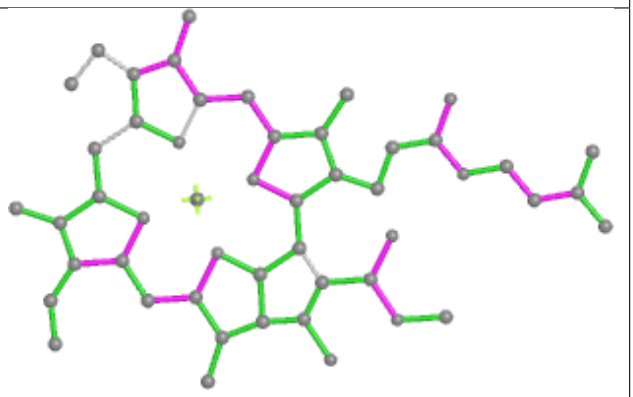


Rings

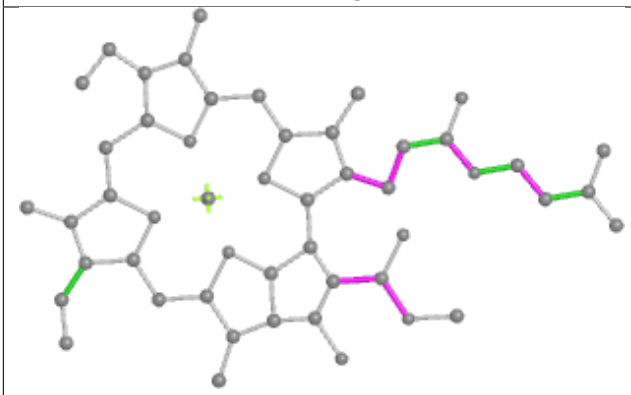
Ligand CLA B 829



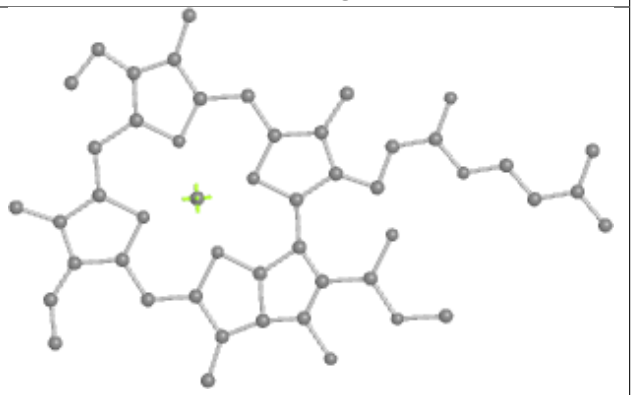
Bond lengths



Bond angles

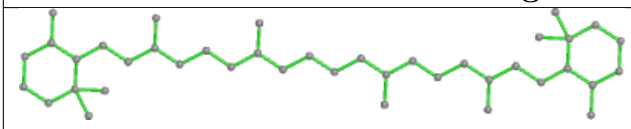


Torsions

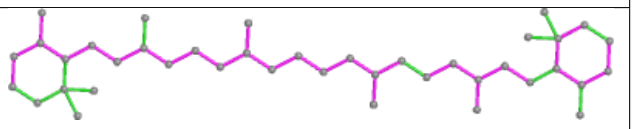


Rings

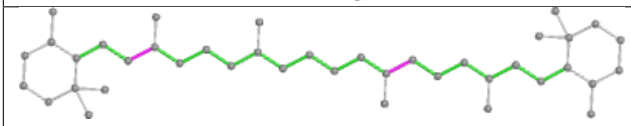
Ligand BCR A 854



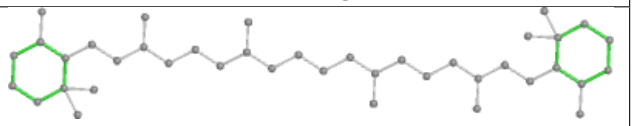
Bond lengths



Bond angles

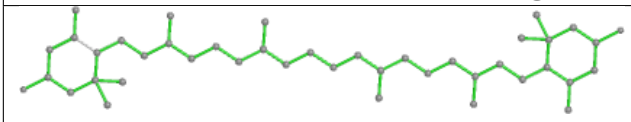


Torsions

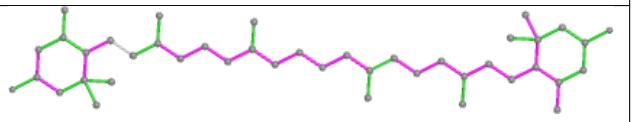


Rings

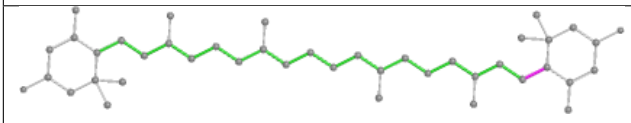
Ligand LUT 4 302



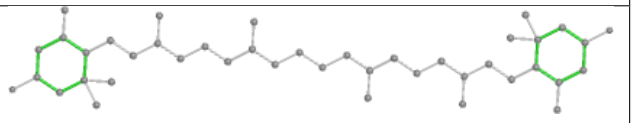
Bond lengths



Bond angles

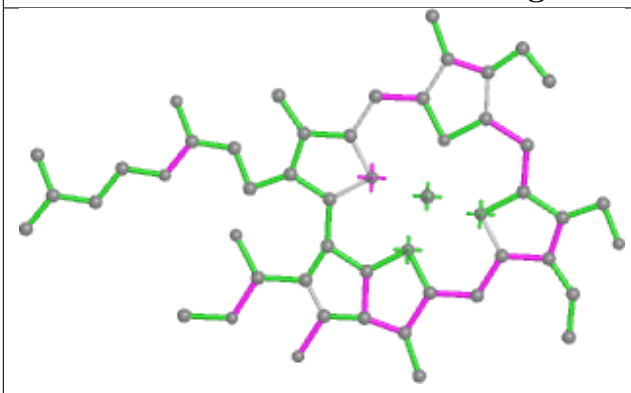


Torsions

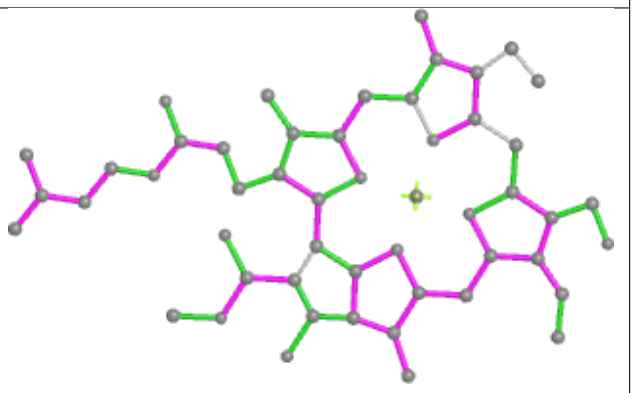


Rings

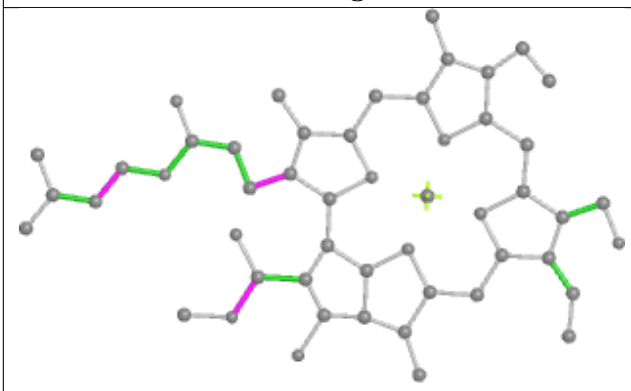
Ligand CHL 4 314



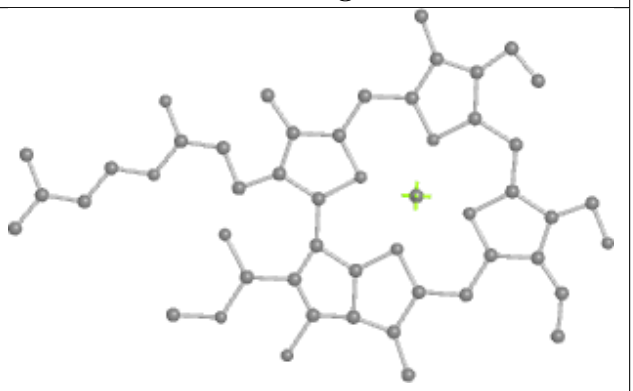
Bond lengths



Bond angles

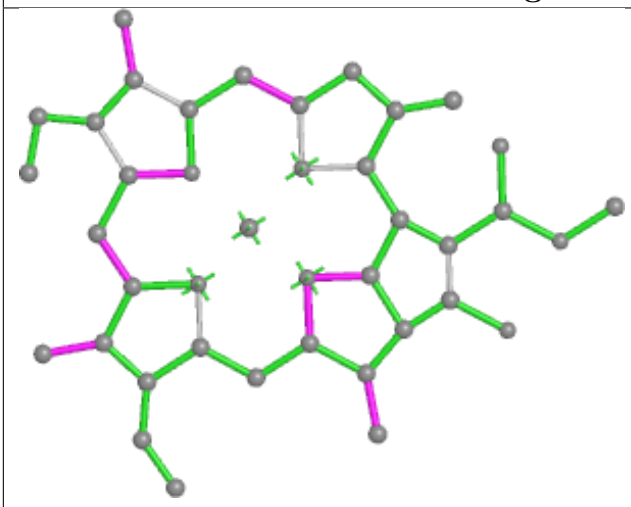


Torsions

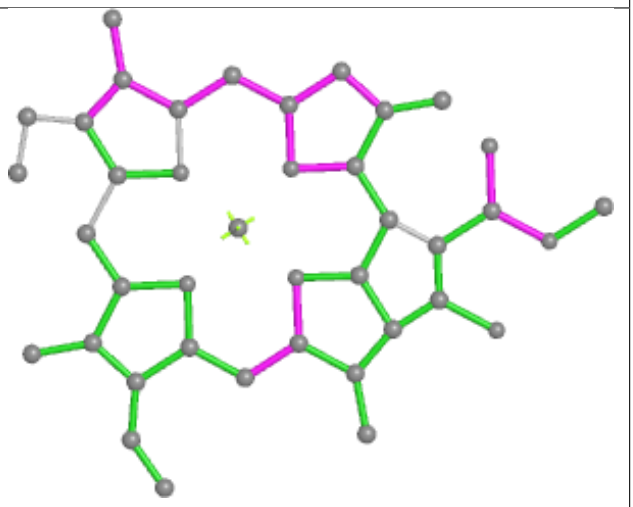


Rings

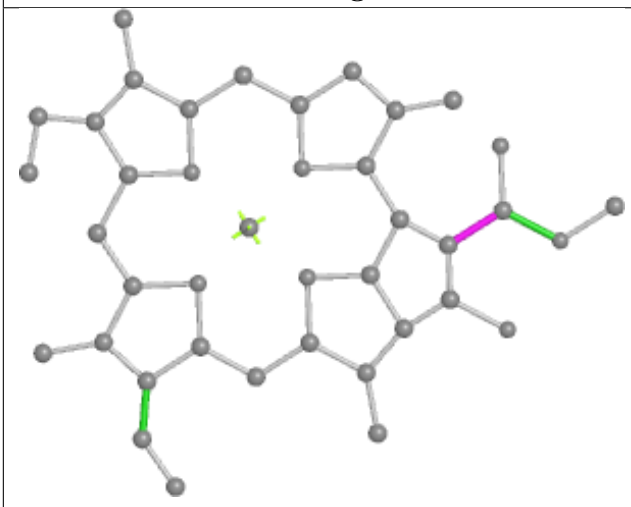
Ligand CLA B 827



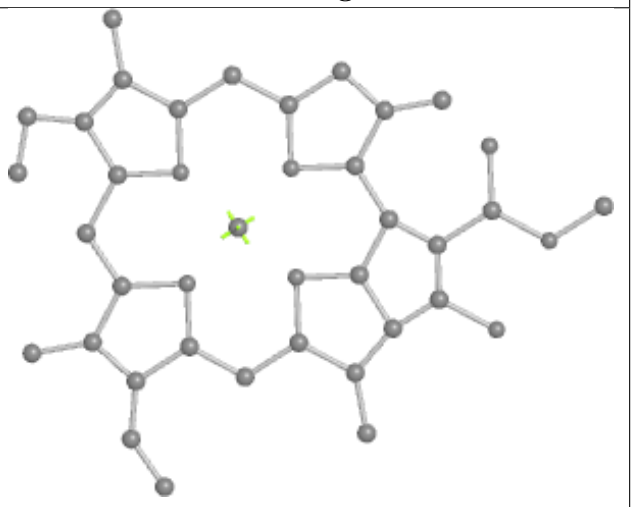
Bond lengths



Bond angles

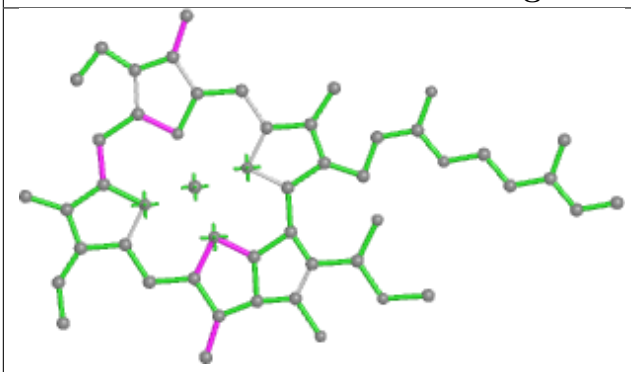


Torsions

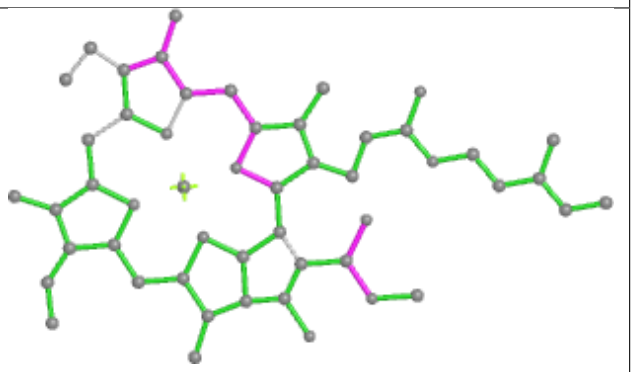


Rings

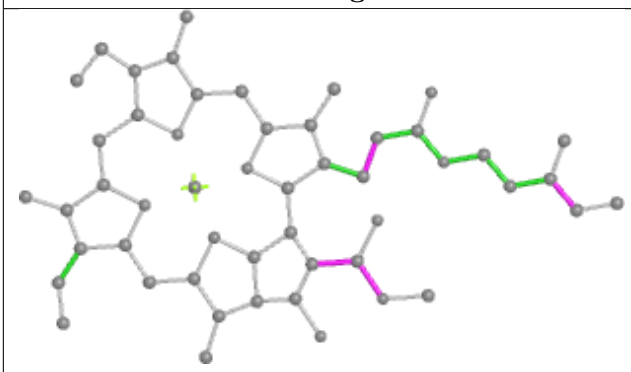
Ligand CLA A 836



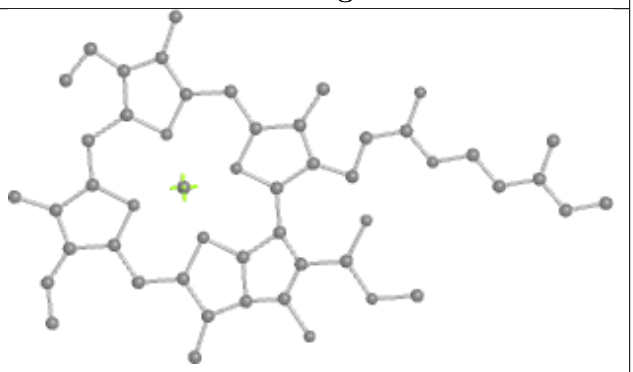
Bond lengths



Bond angles

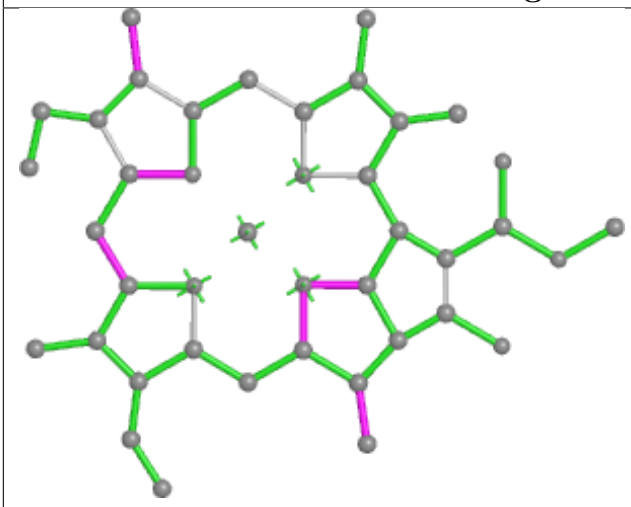


Torsions

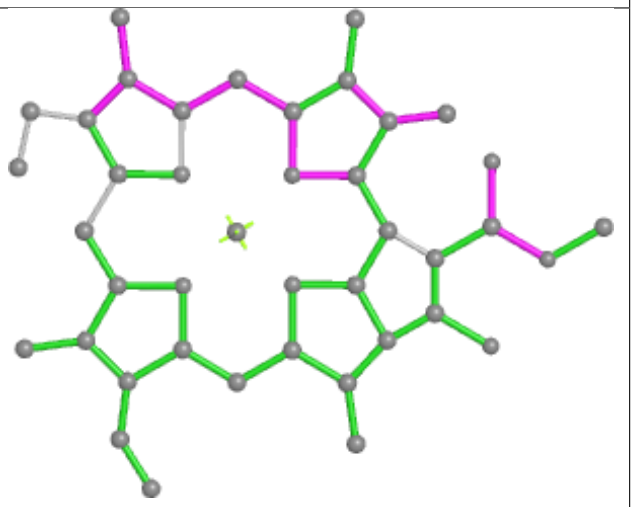


Rings

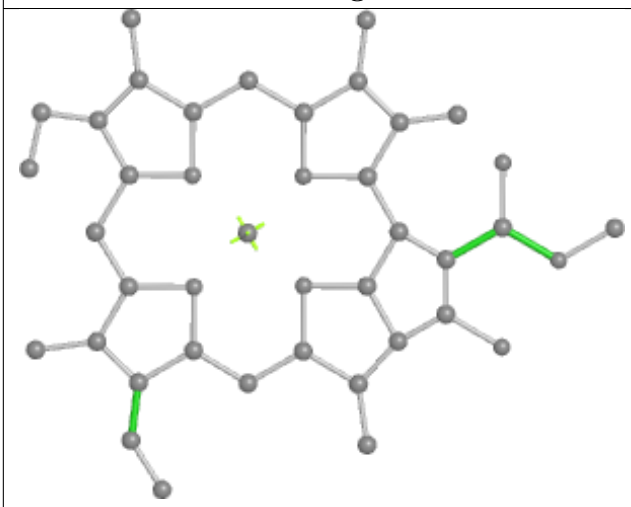
Ligand CLA B 822



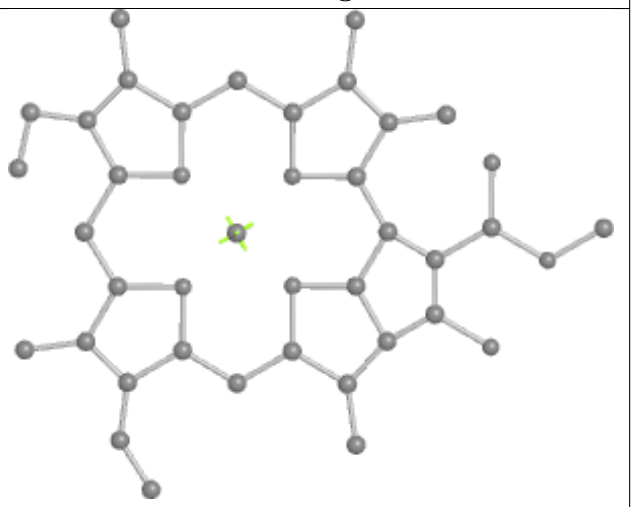
Bond lengths



Bond angles

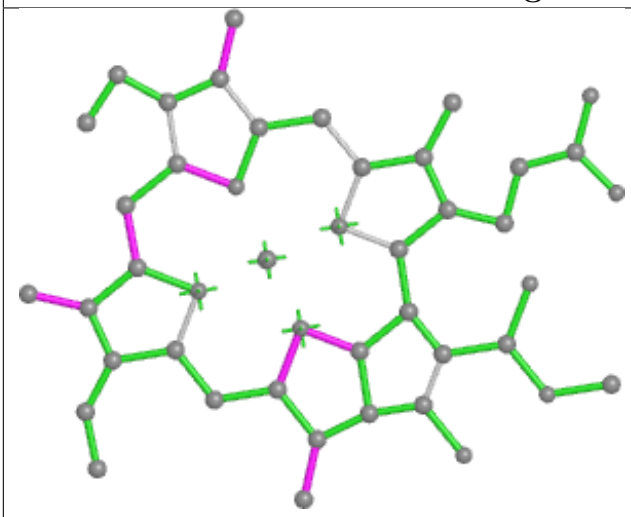


Torsions

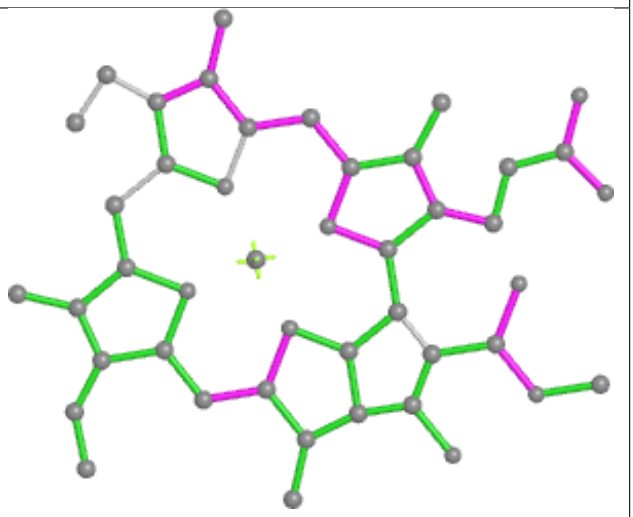


Rings

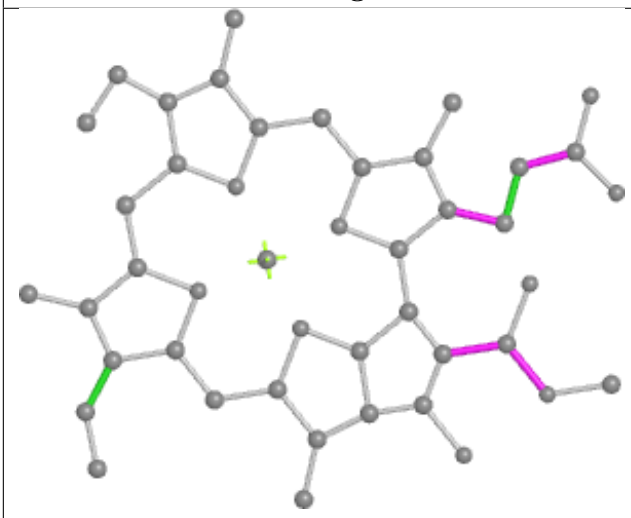
Ligand CLA B 835



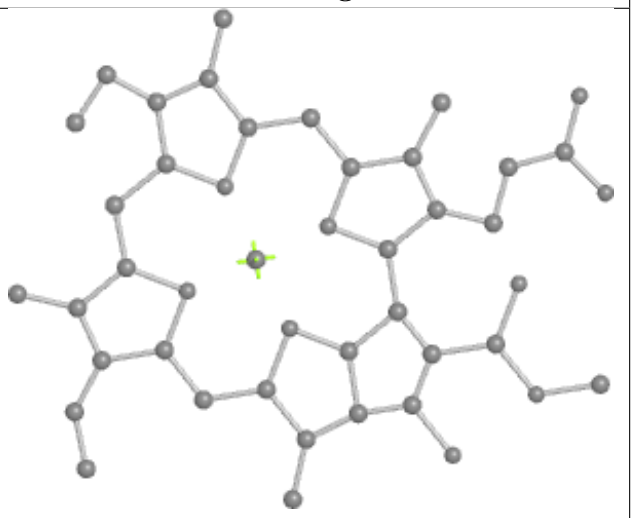
Bond lengths



Bond angles

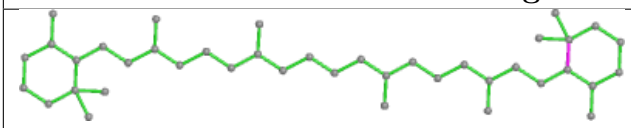


Torsions

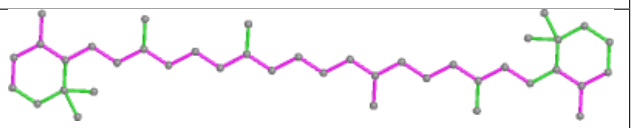


Rings

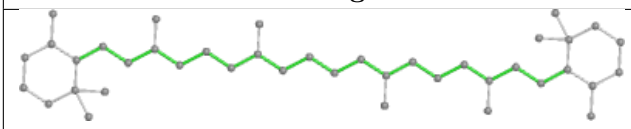
Ligand BCR B 849



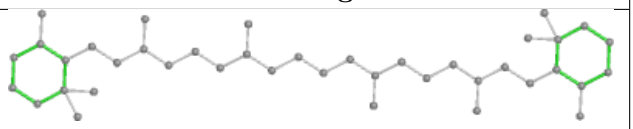
Bond lengths



Bond angles

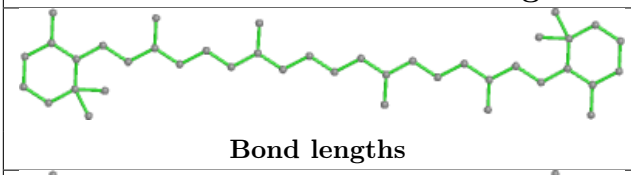


Torsions

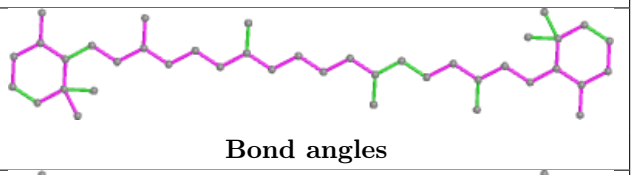


Rings

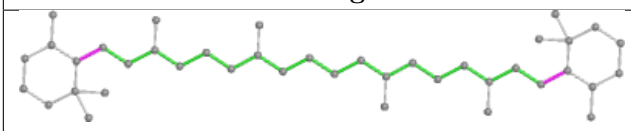
Ligand BCR A 851



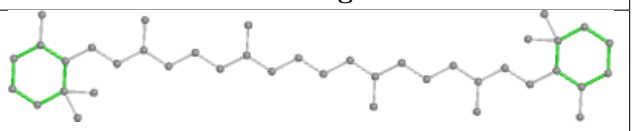
Bond lengths



Bond angles

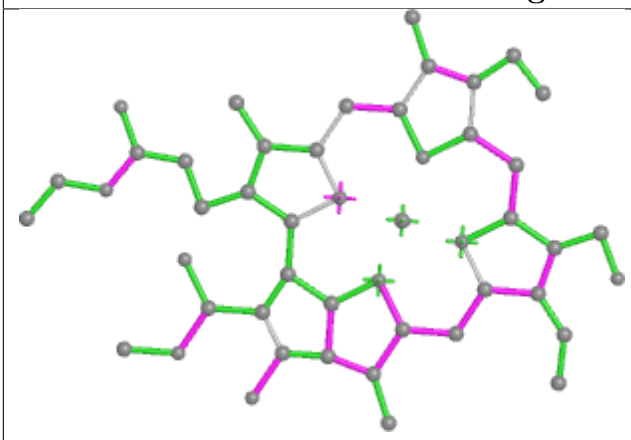


Torsions

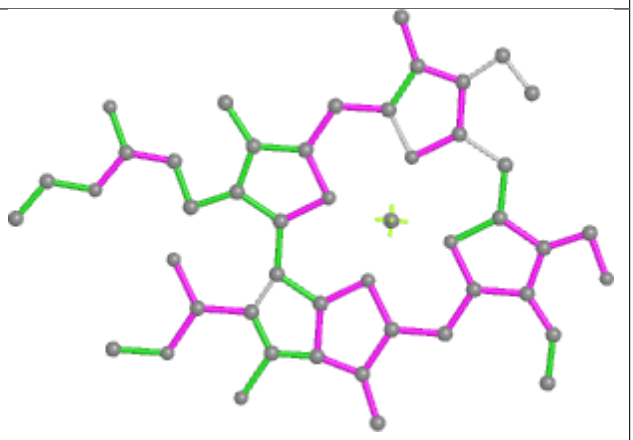


Rings

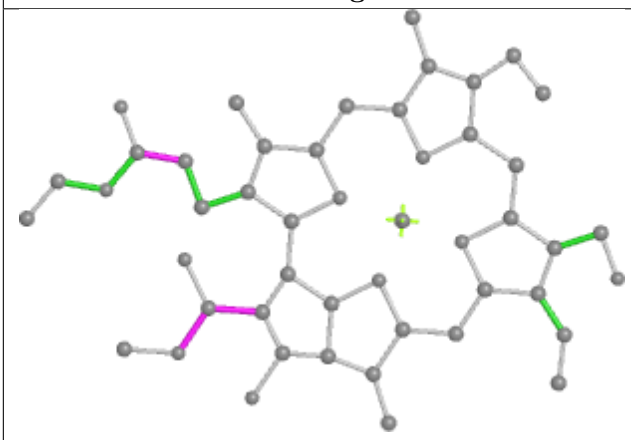
Ligand CHL 6 513



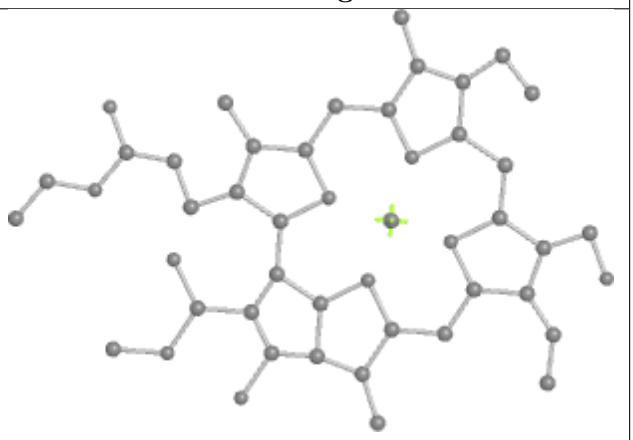
Bond lengths



Bond angles

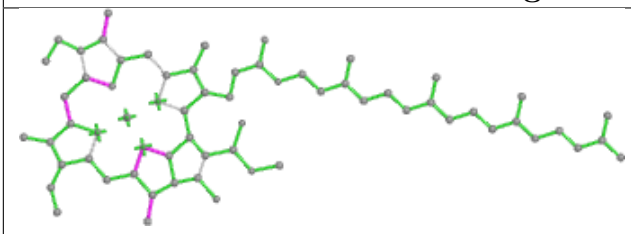


Torsions

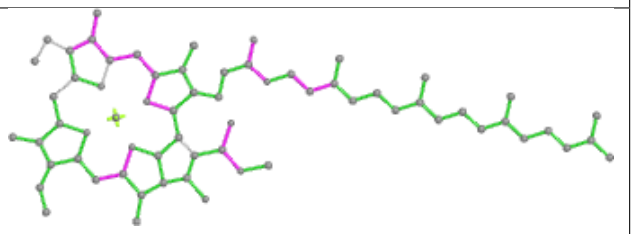


Rings

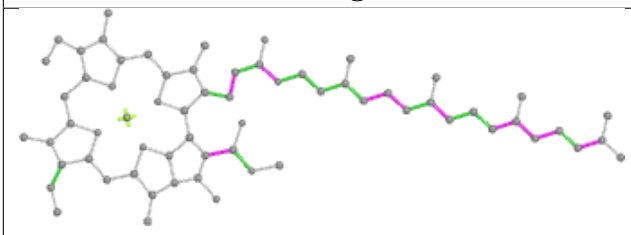
Ligand CLA A 839



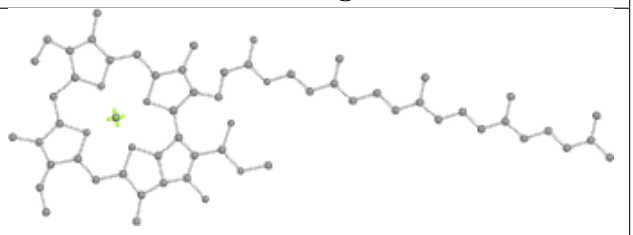
Bond lengths



Bond angles

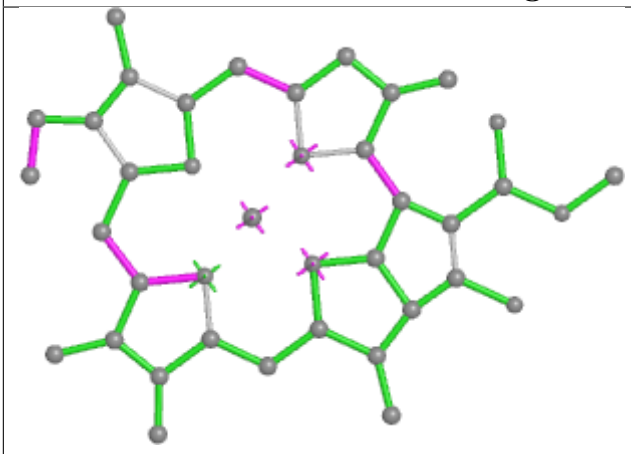


Torsions

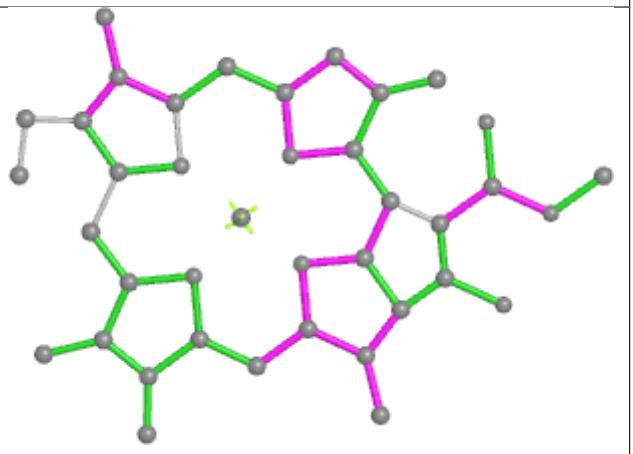


Rings

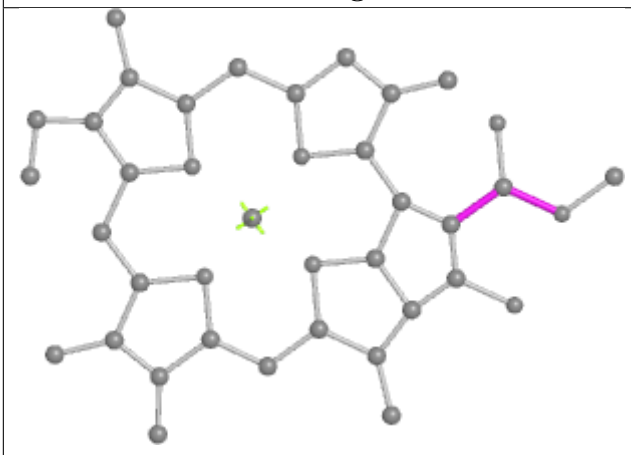
Ligand CLA A 818



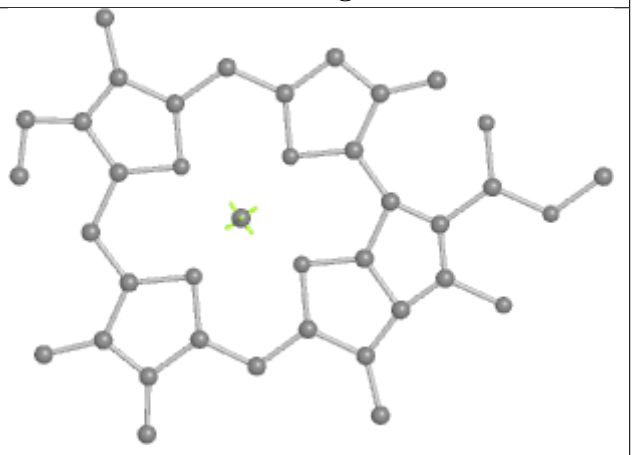
Bond lengths



Bond angles

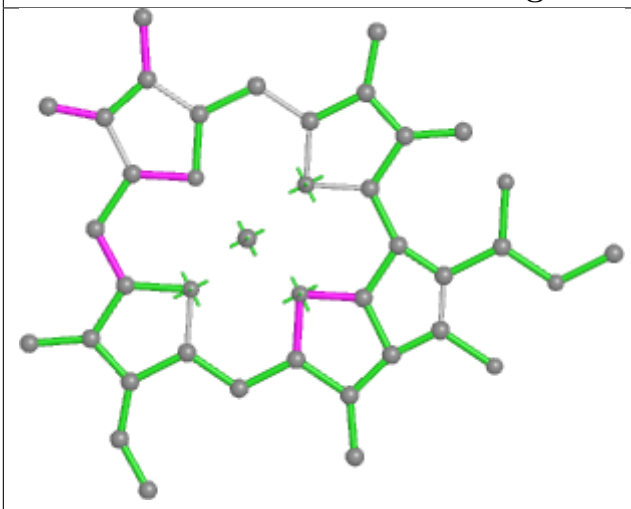


Torsions

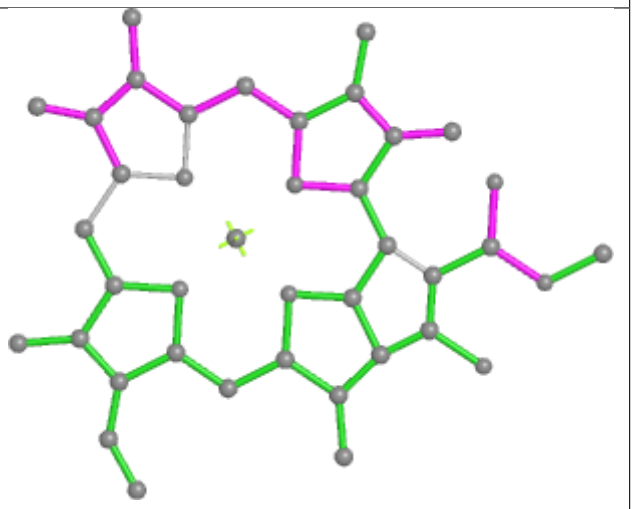


Rings

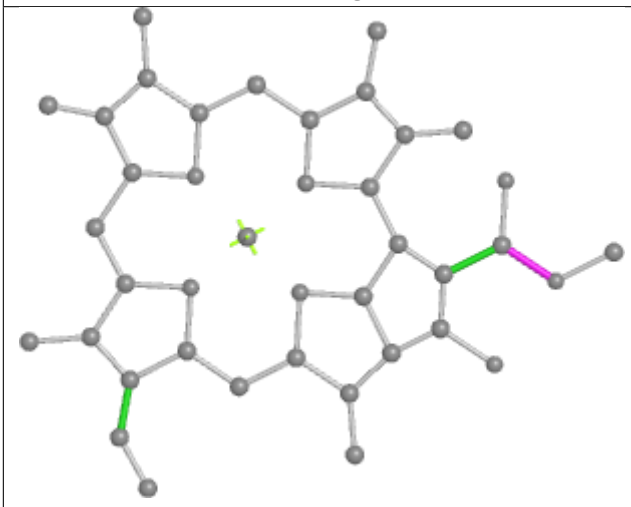
Ligand CLA L 302



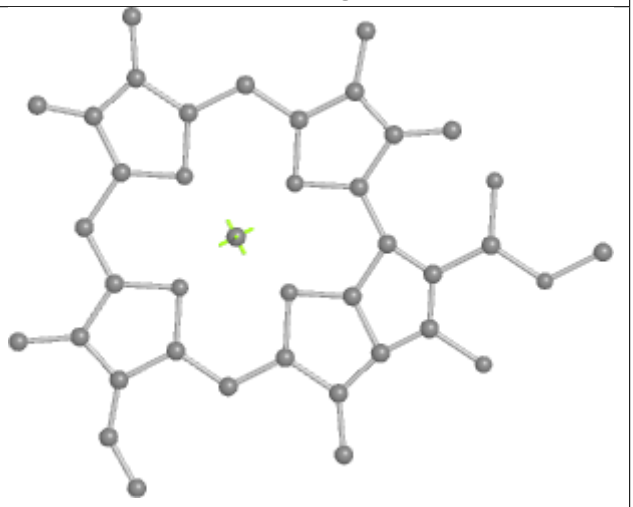
Bond lengths



Bond angles

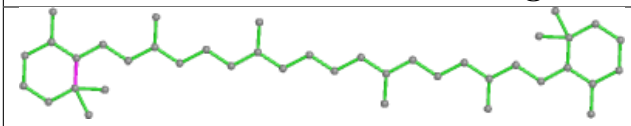


Torsions

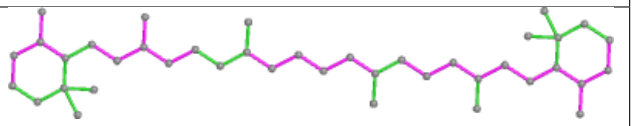


Rings

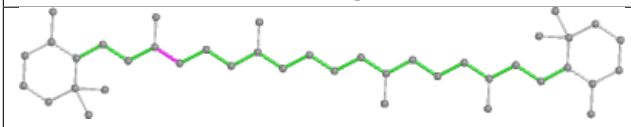
Ligand BCR L 301



Bond lengths



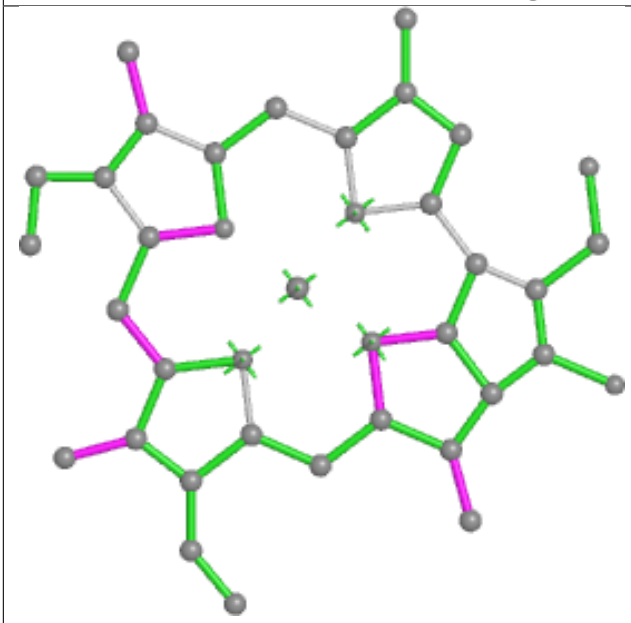
Bond angles



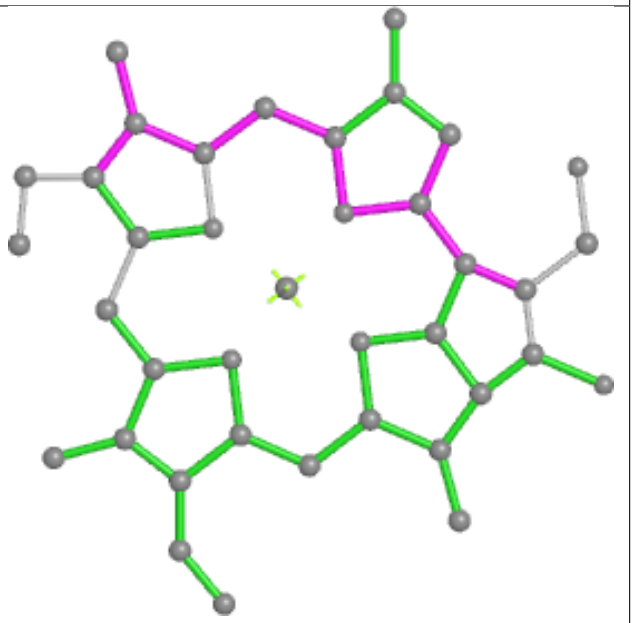
Torsions

Rings

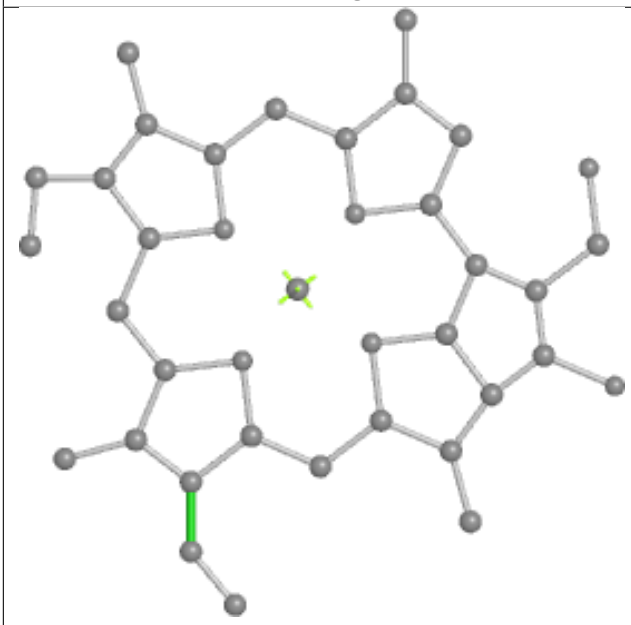
Ligand CLA B 805



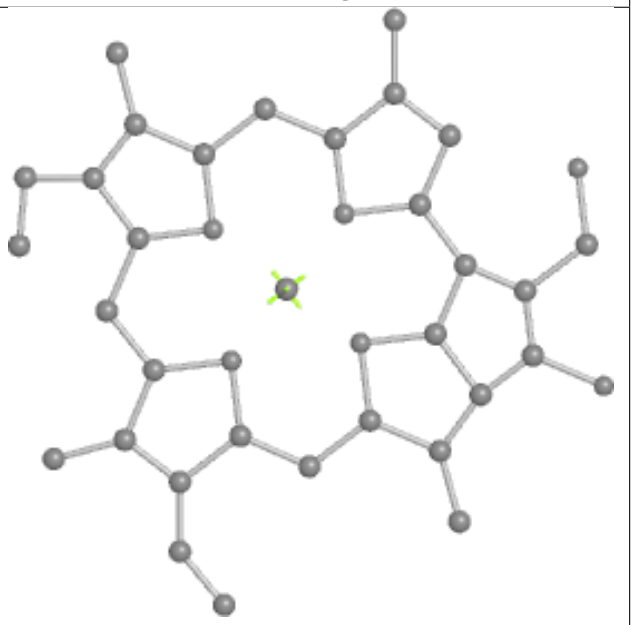
Bond lengths



Bond angles

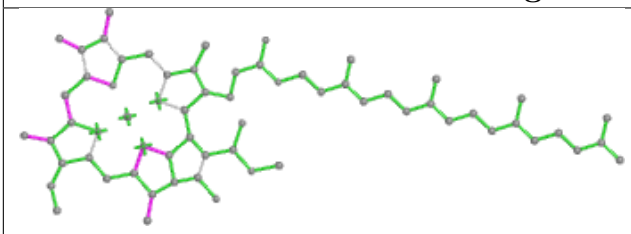


Torsions

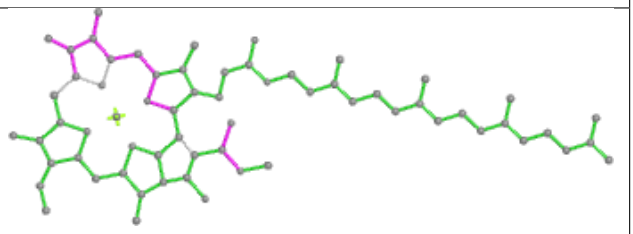


Rings

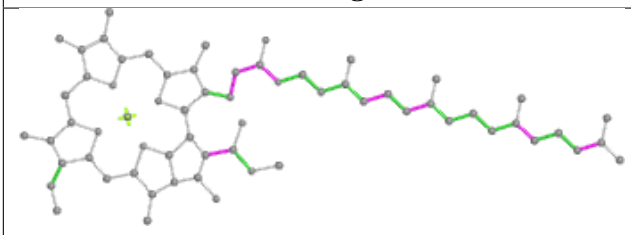
Ligand CLA B 801



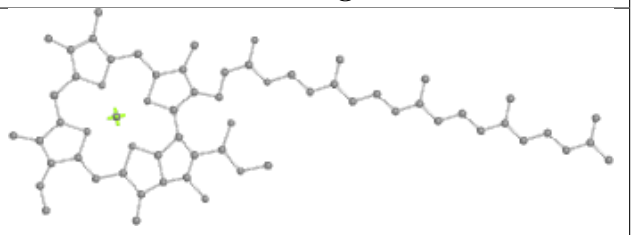
Bond lengths



Bond angles

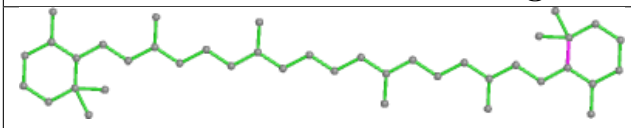


Torsions

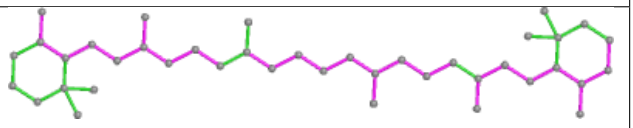


Rings

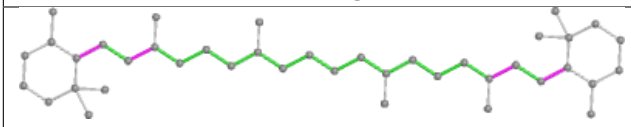
Ligand BCR 3 303



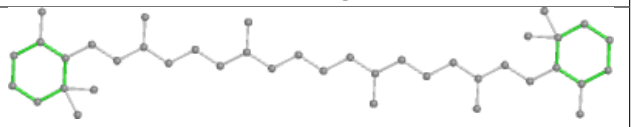
Bond lengths



Bond angles

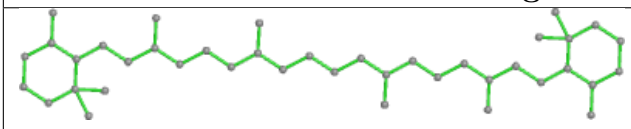


Torsions

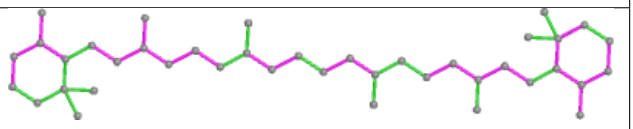


Rings

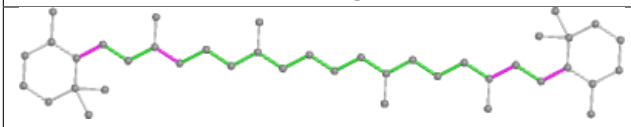
Ligand BCR B 846



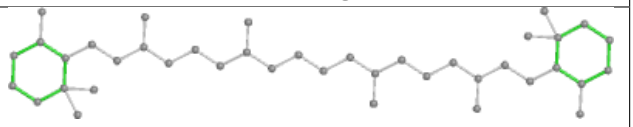
Bond lengths



Bond angles

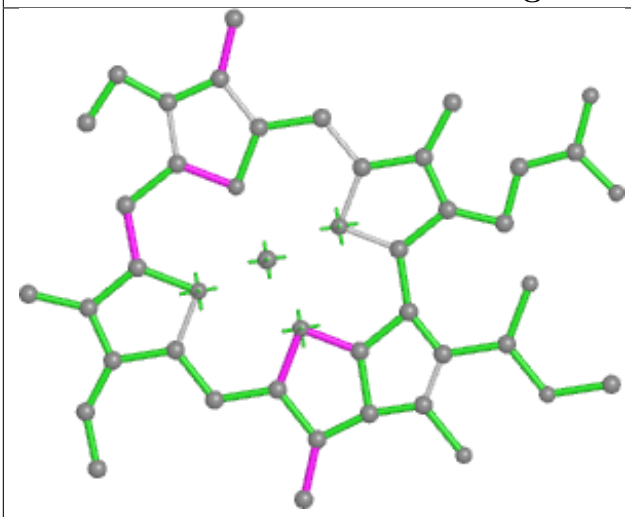


Torsions

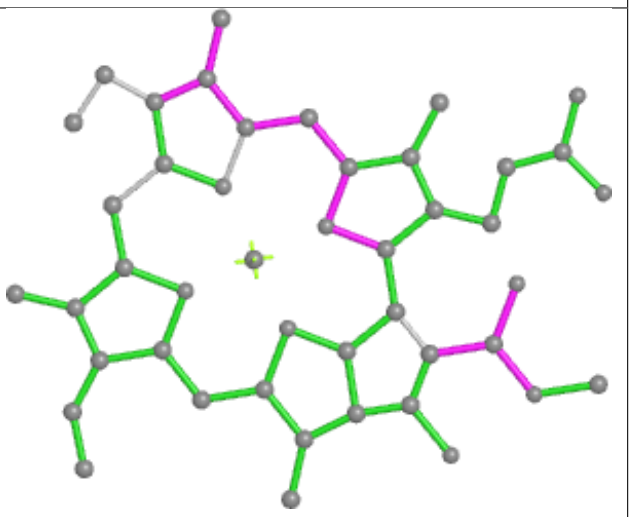


Rings

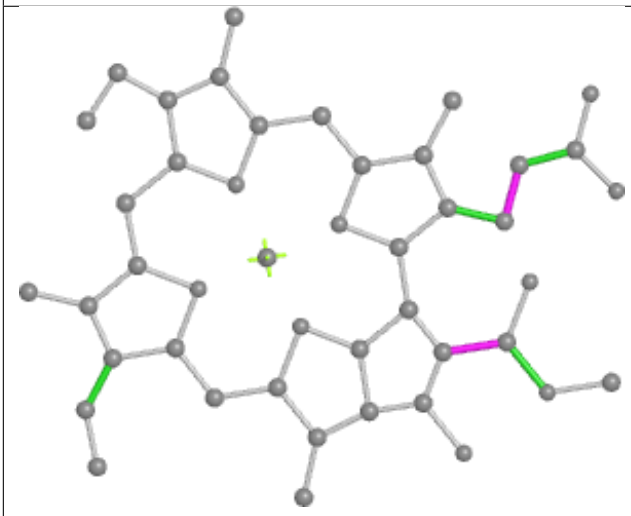
Ligand CLA A 819



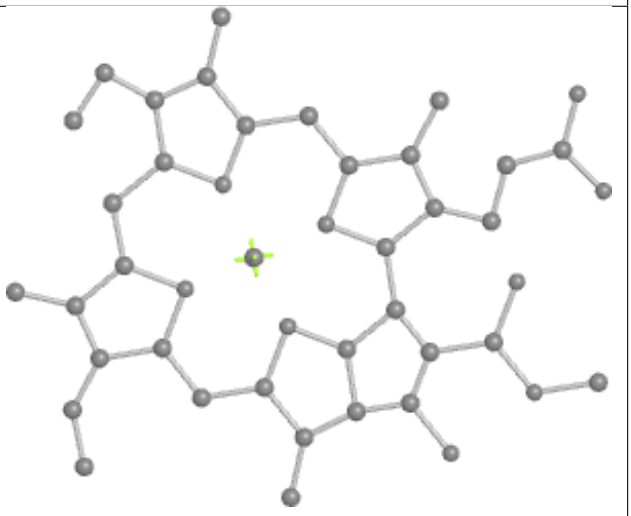
Bond lengths



Bond angles

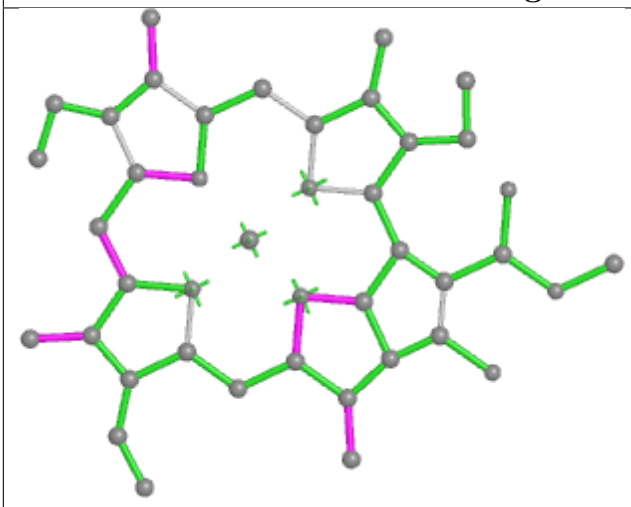


Torsions

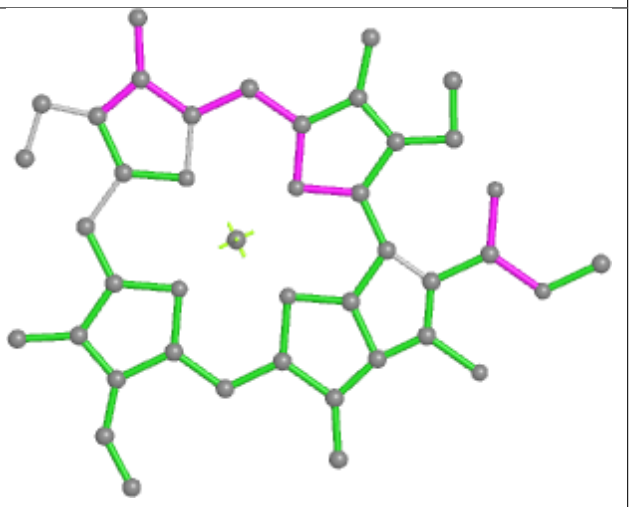


Rings

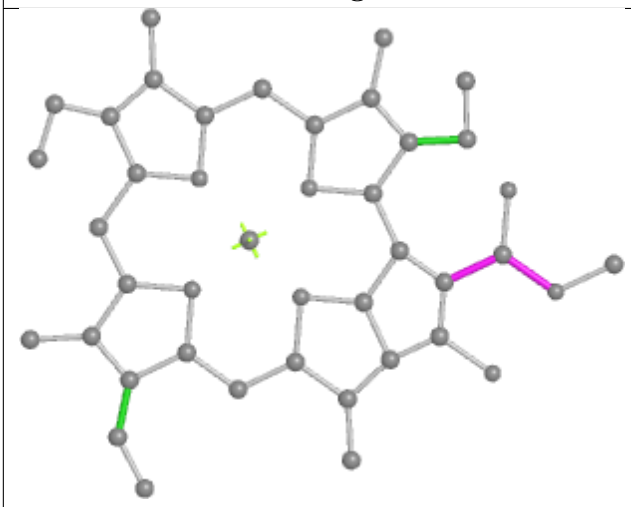
Ligand CLA B 825



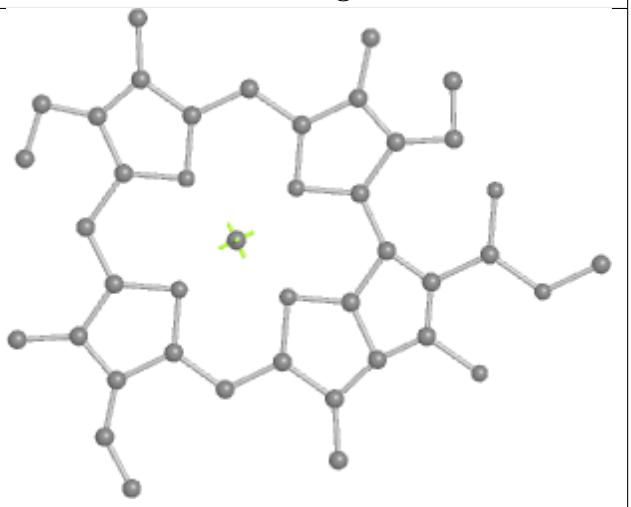
Bond lengths



Bond angles

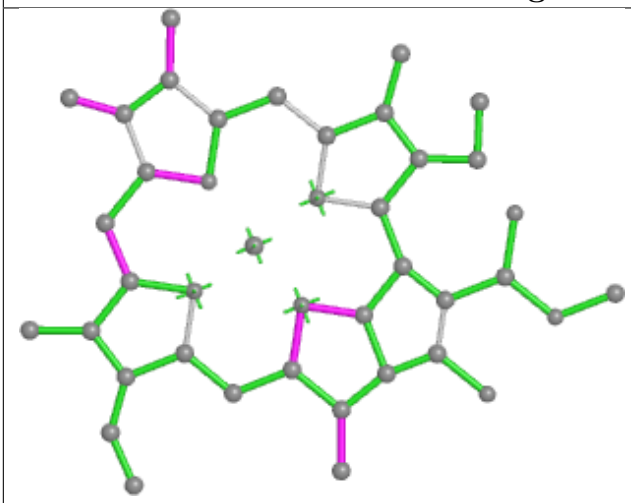


Torsions

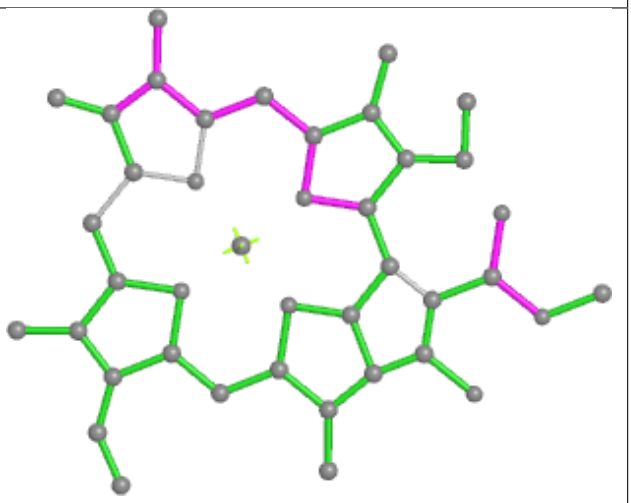


Rings

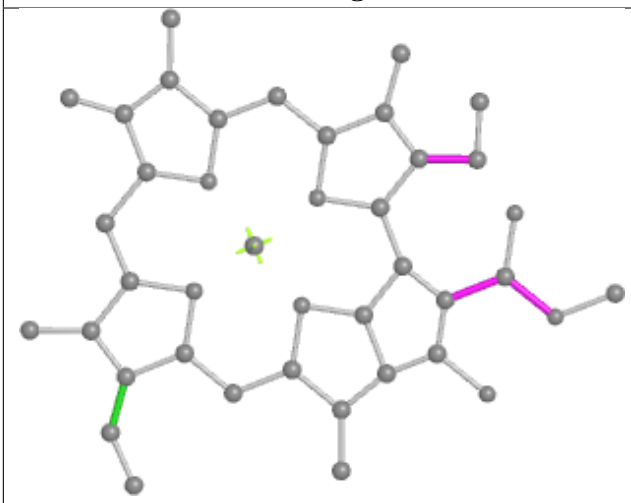
Ligand CLA J 101



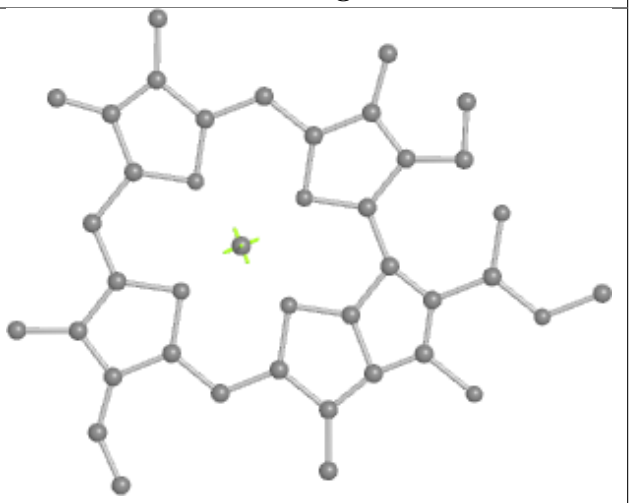
Bond lengths



Bond angles

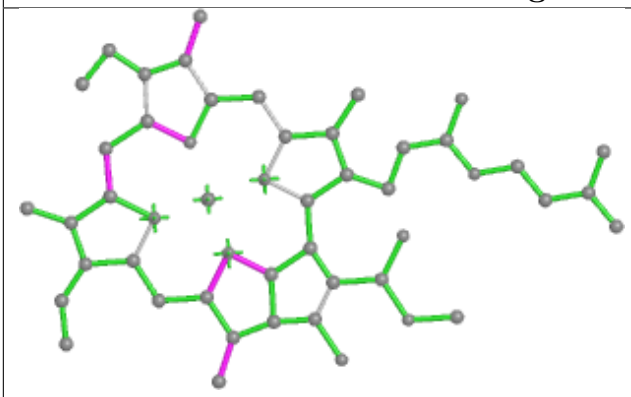


Torsions

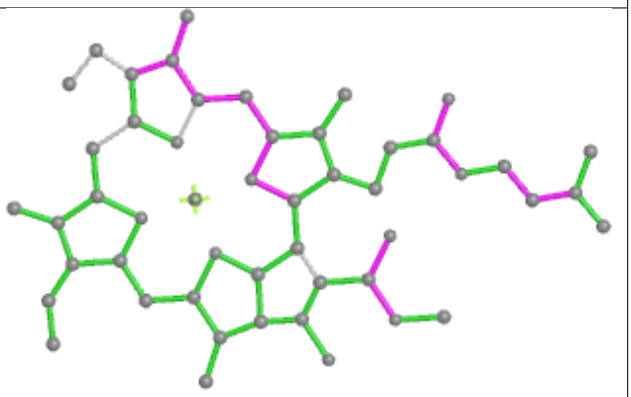


Rings

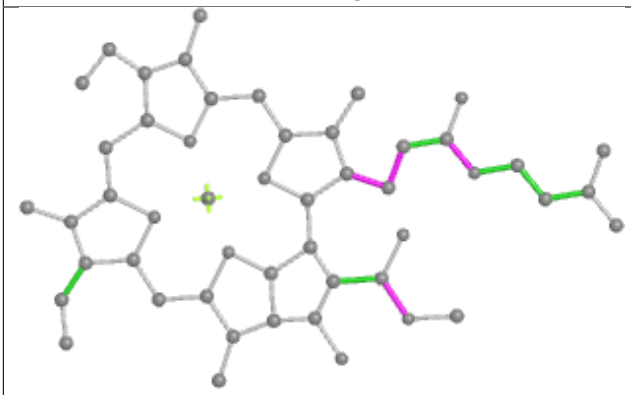
Ligand CLA 4 309



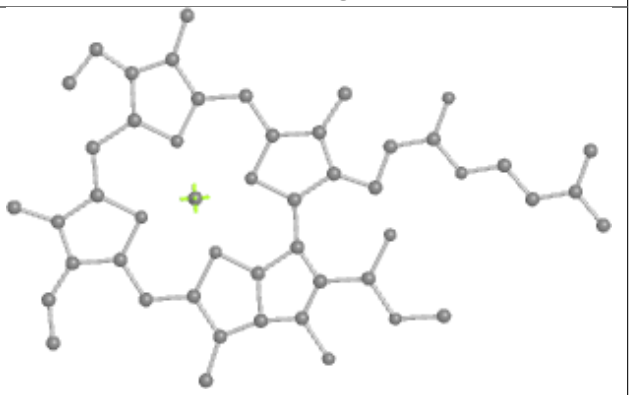
Bond lengths



Bond angles

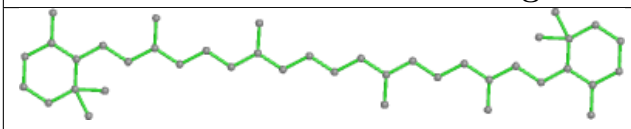


Torsions

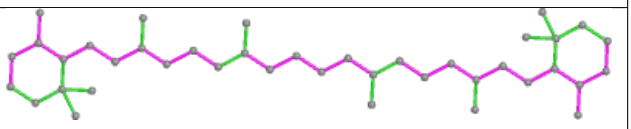


Rings

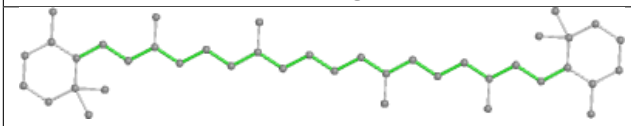
Ligand BCR A 847



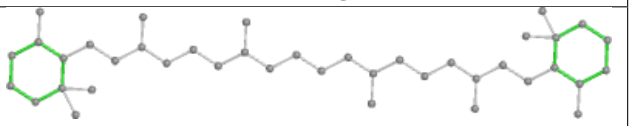
Bond lengths



Bond angles

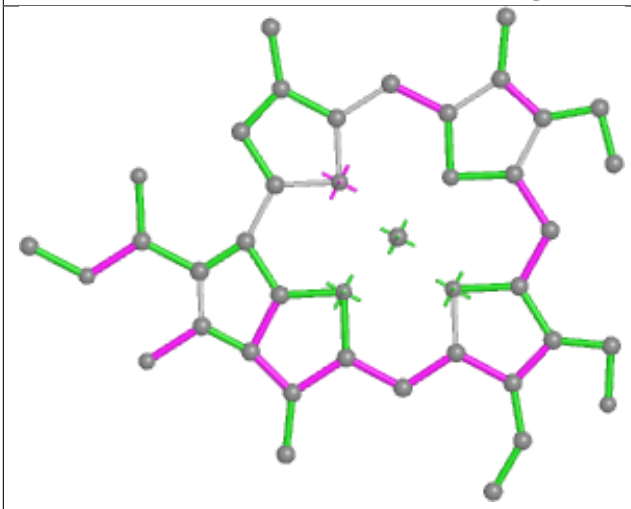


Torsions

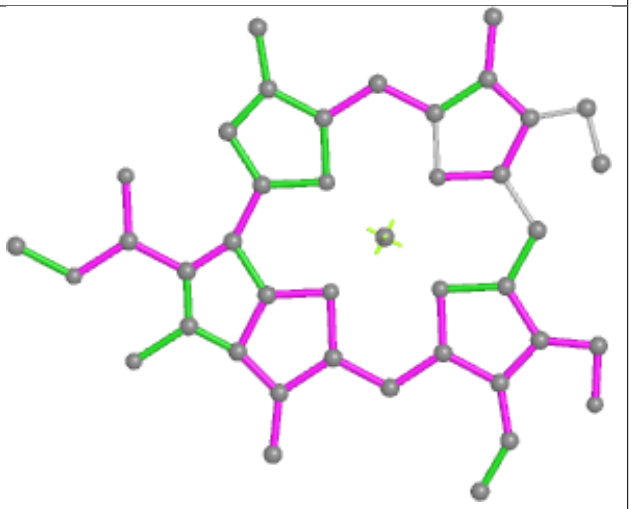


Rings

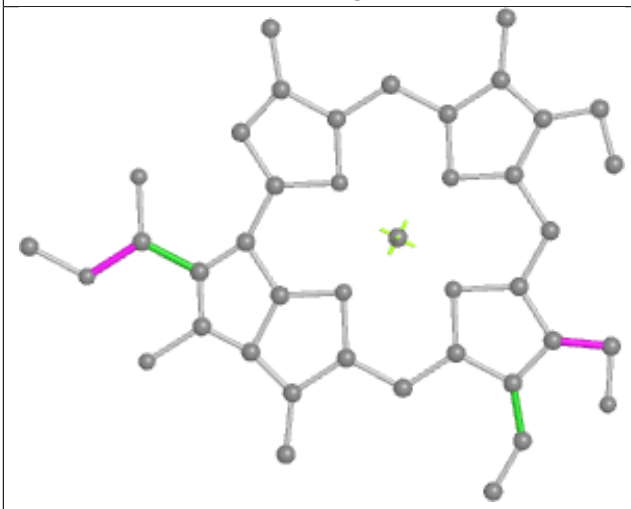
Ligand CHL 6 515



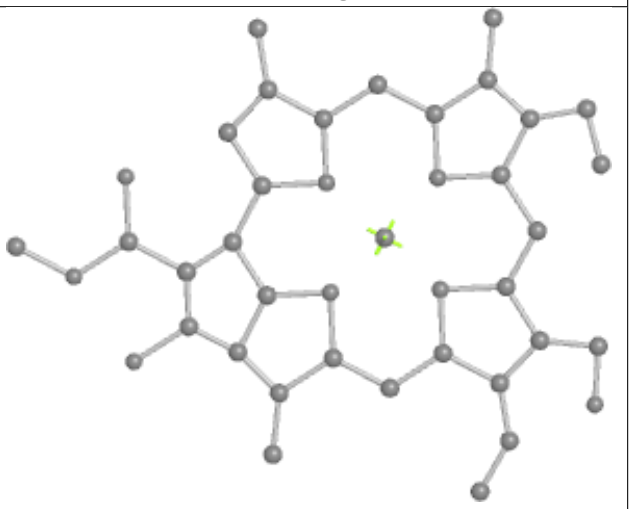
Bond lengths



Bond angles

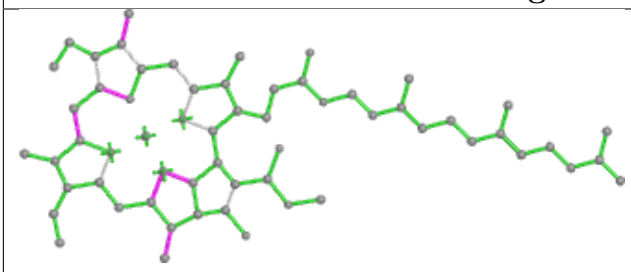


Torsions

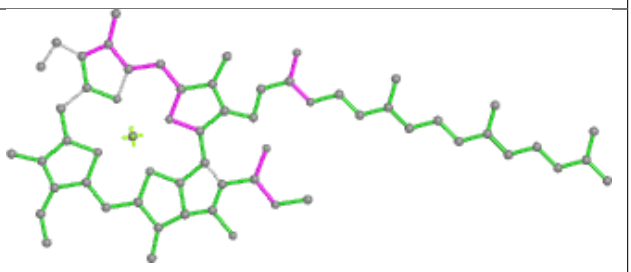


Rings

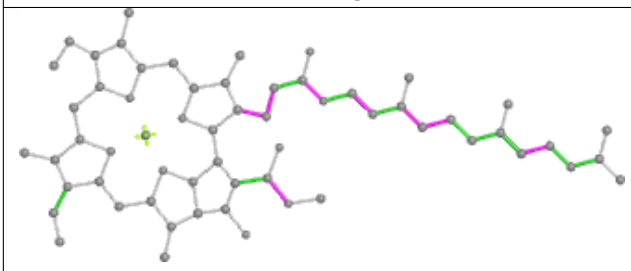
Ligand CLA 3 312



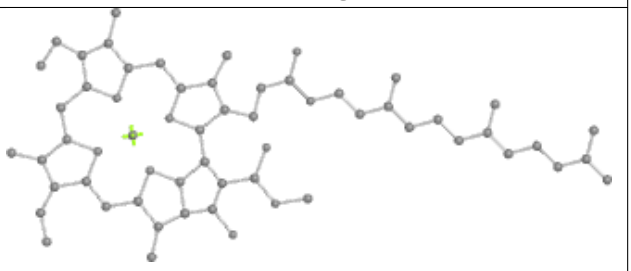
Bond lengths



Bond angles

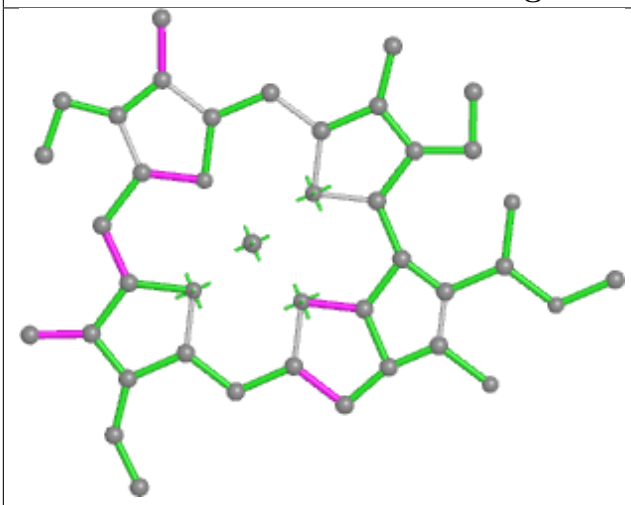


Torsions

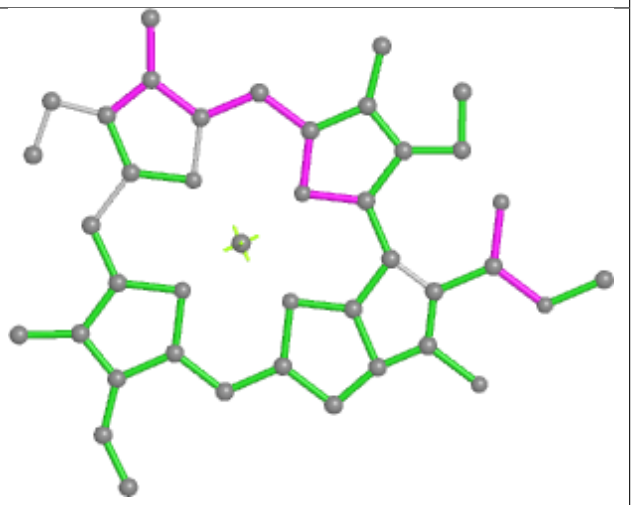


Rings

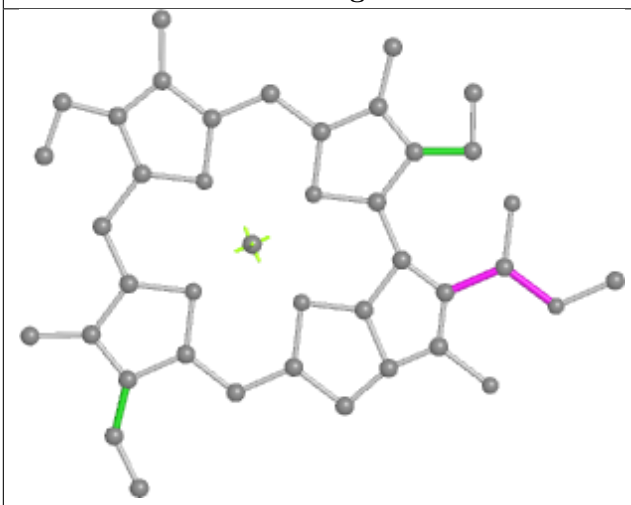
Ligand CLA B 803



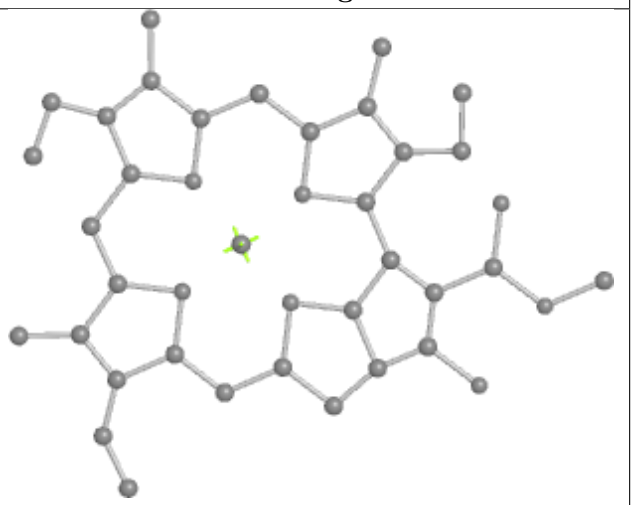
Bond lengths



Bond angles

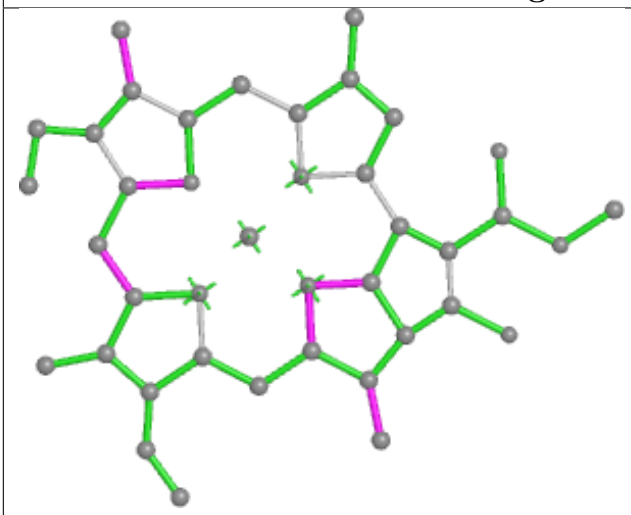


Torsions

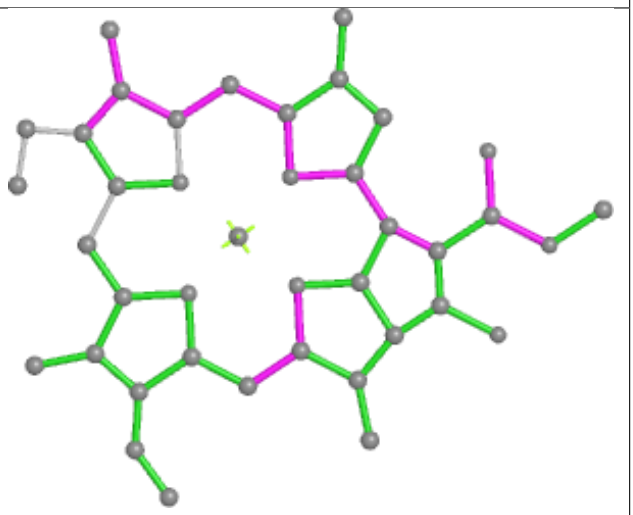


Rings

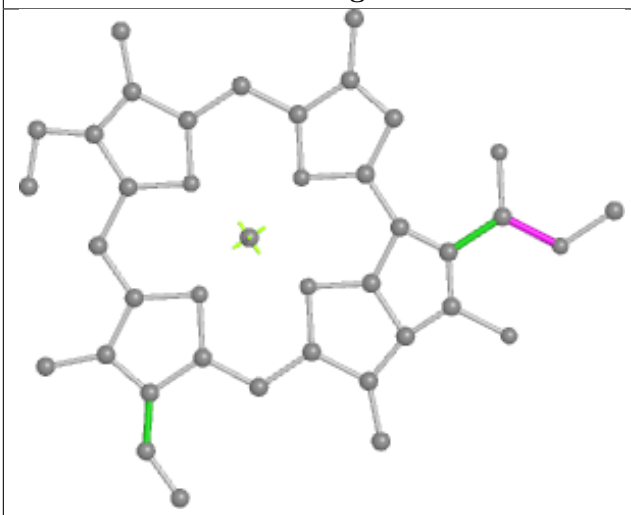
Ligand CLA 3 314



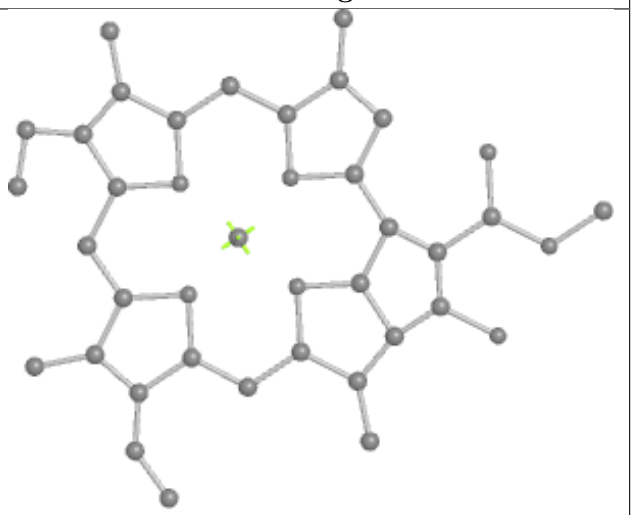
Bond lengths



Bond angles

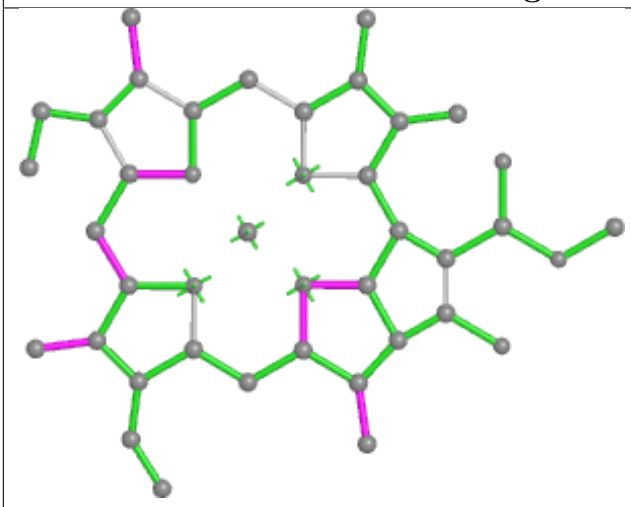


Torsions

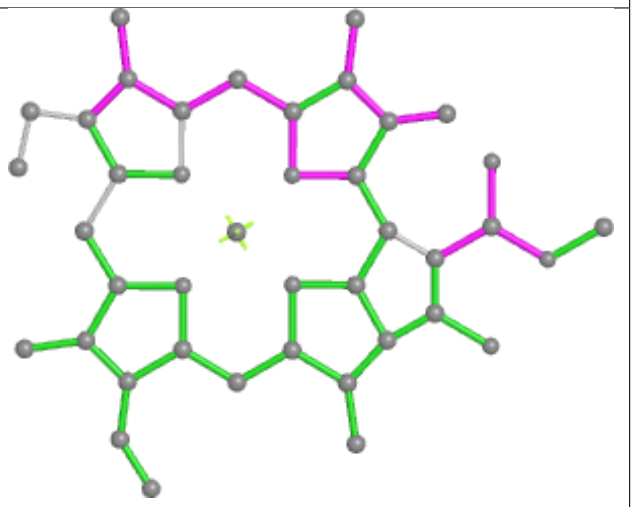


Rings

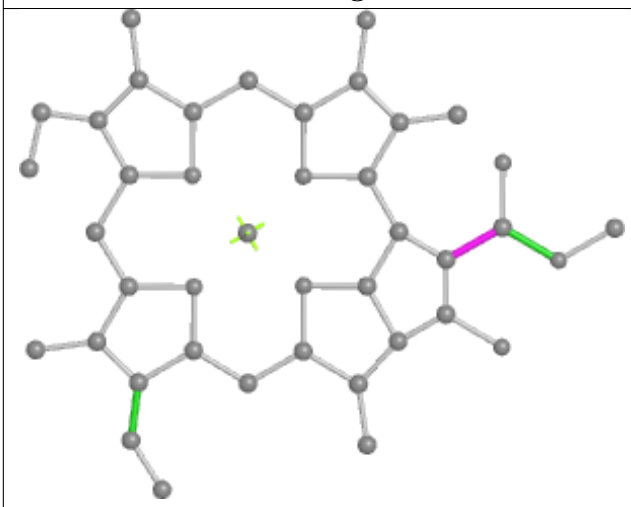
Ligand CLA A 806



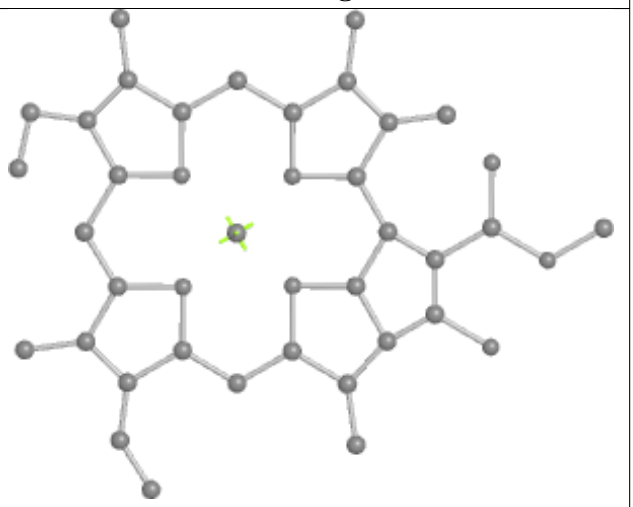
Bond lengths



Bond angles

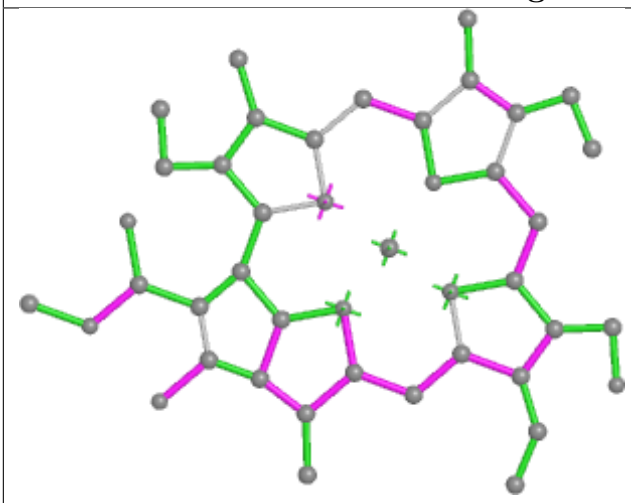


Torsions

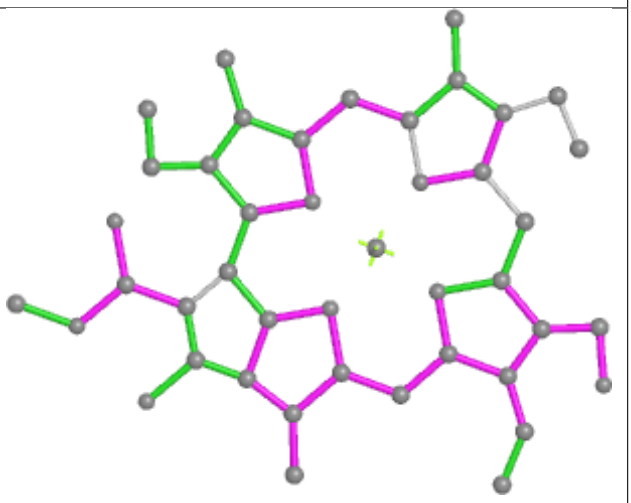


Rings

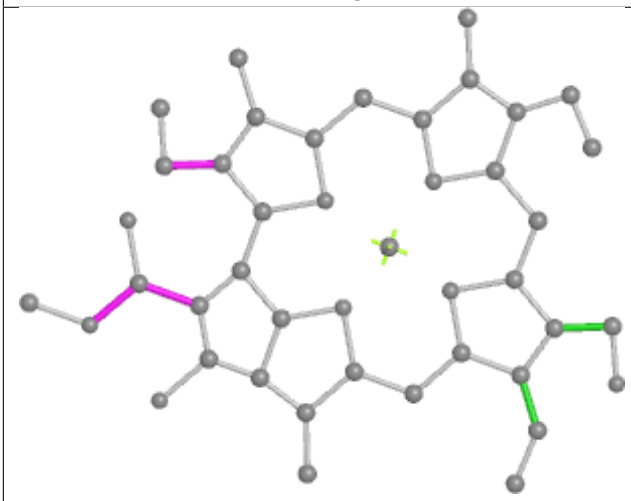
Ligand CHL 1 517



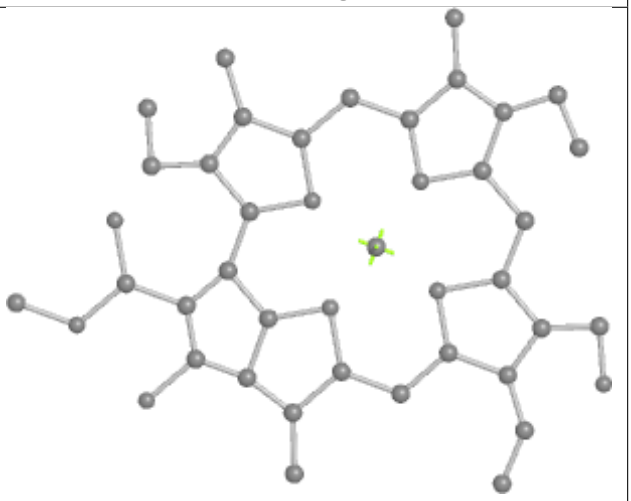
Bond lengths



Bond angles

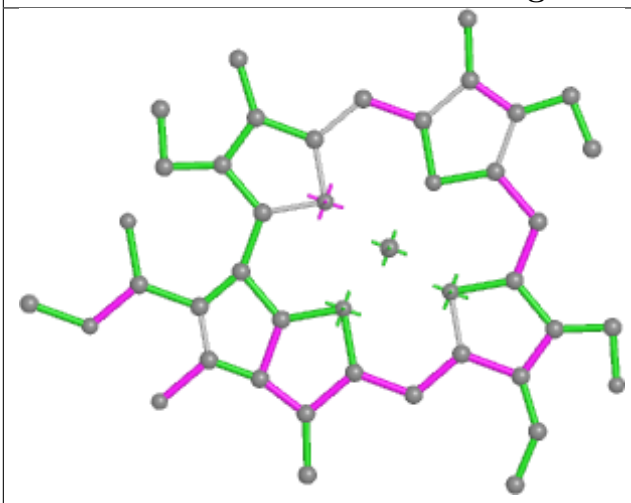


Torsions

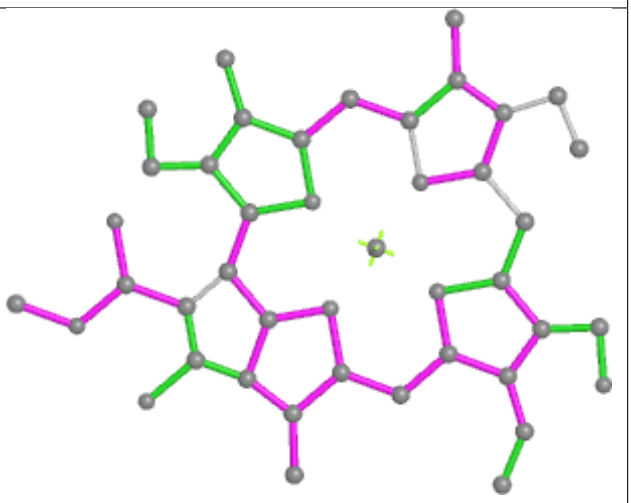


Rings

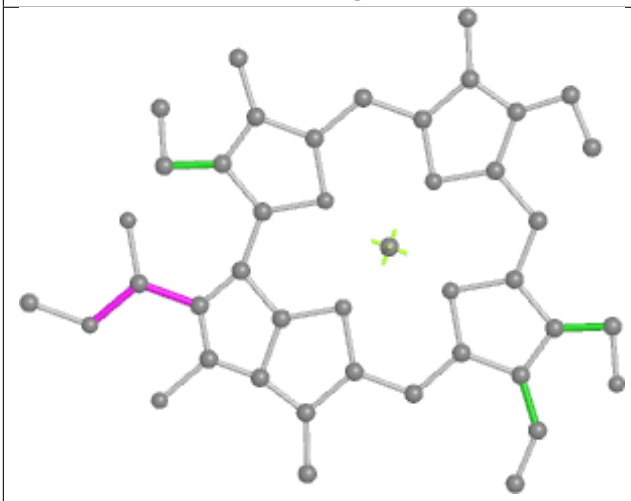
Ligand CHL 4 316



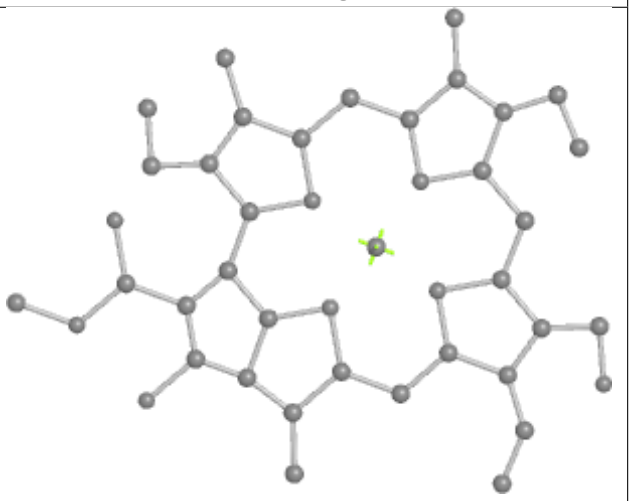
Bond lengths



Bond angles

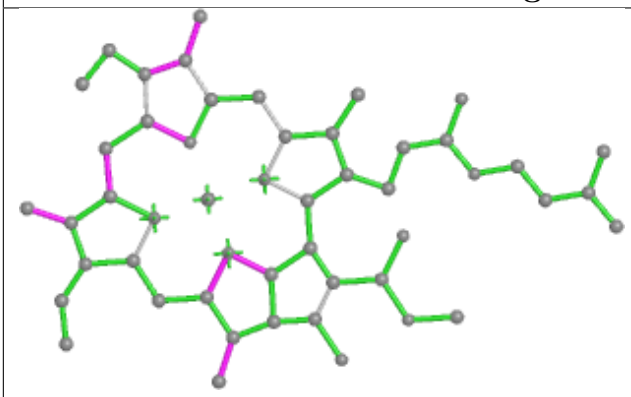


Torsions

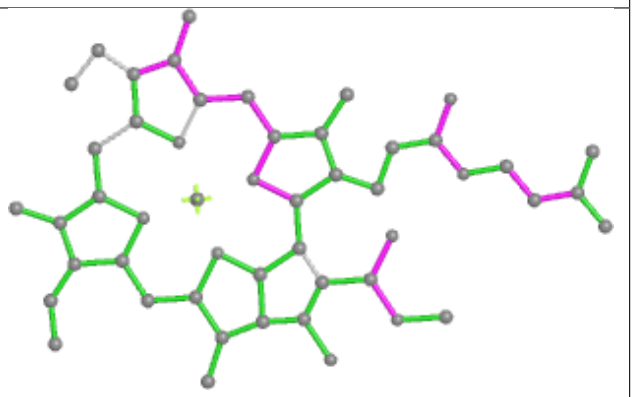


Rings

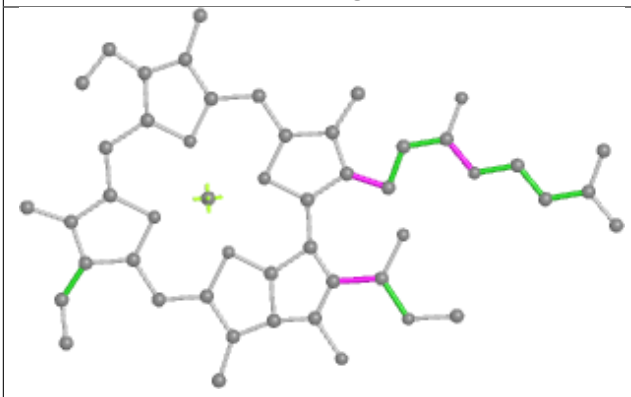
Ligand CLA A 830



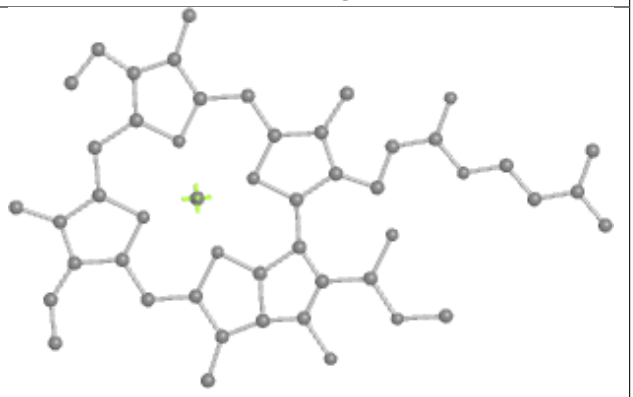
Bond lengths



Bond angles

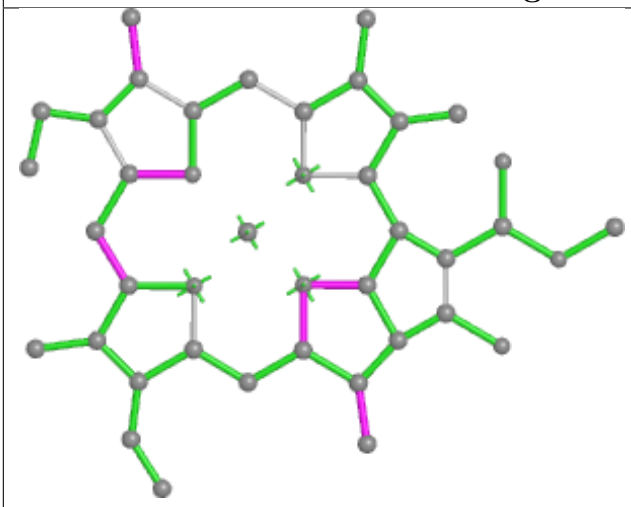


Torsions

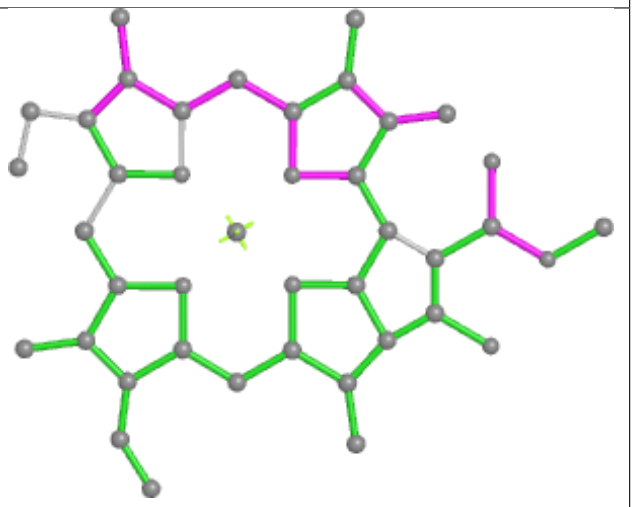


Rings

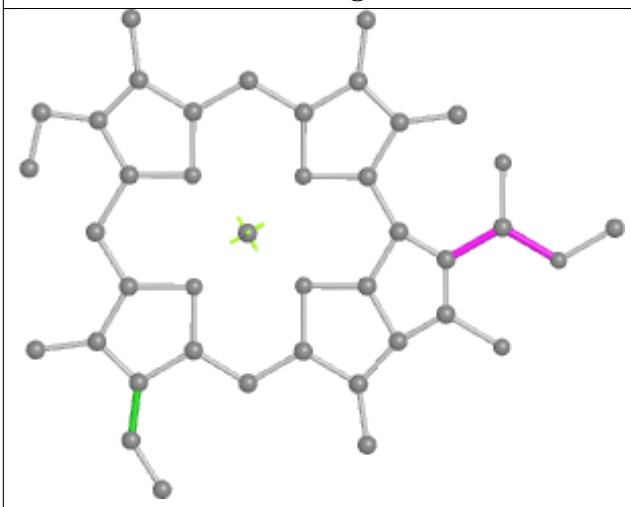
Ligand CLA A 820



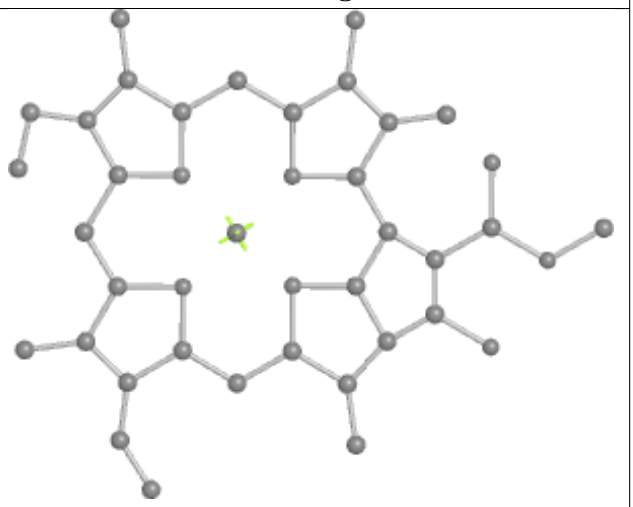
Bond lengths



Bond angles

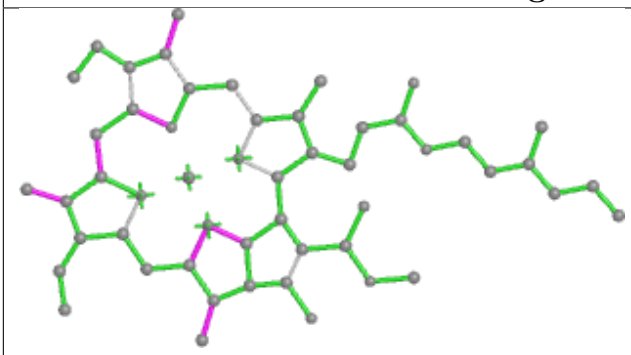


Torsions

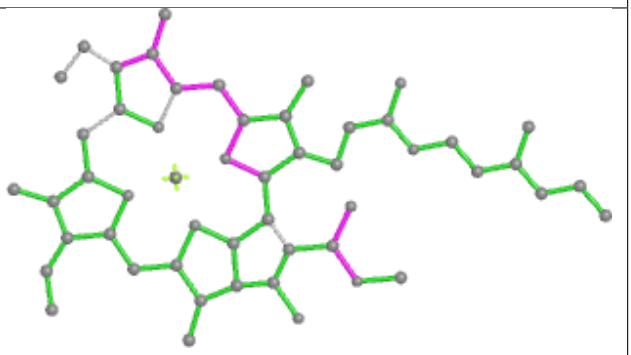


Rings

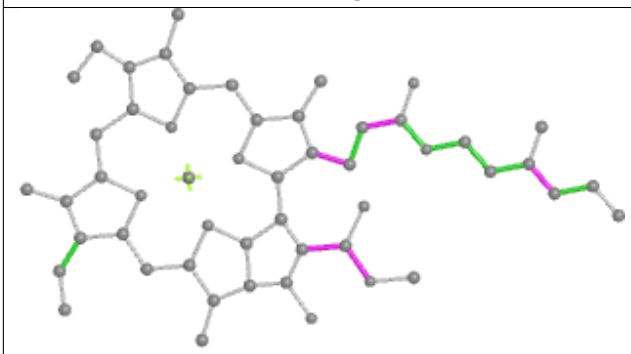
Ligand CLA 6 505



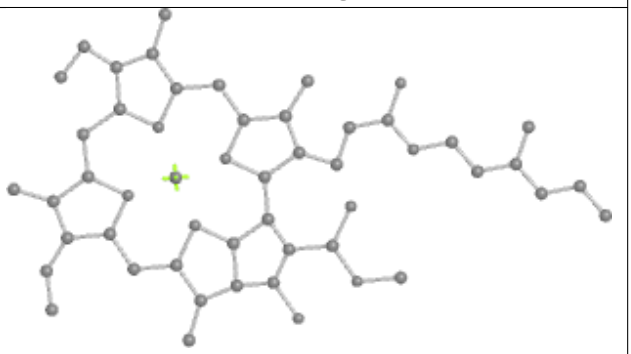
Bond lengths



Bond angles

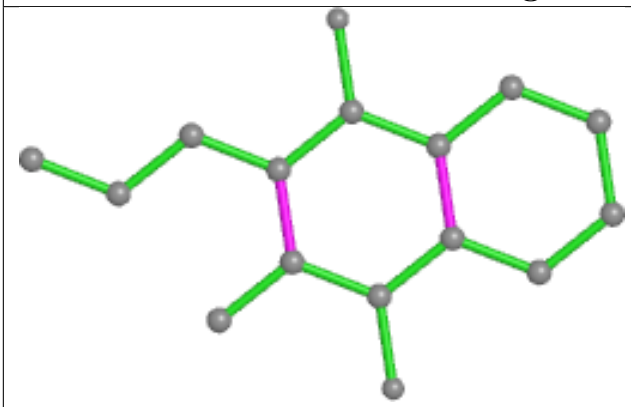


Torsions

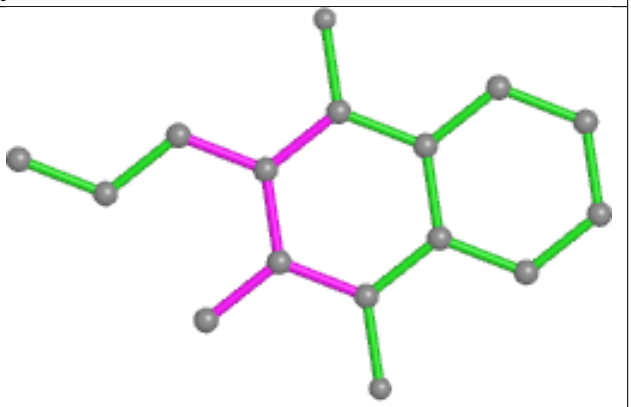


Rings

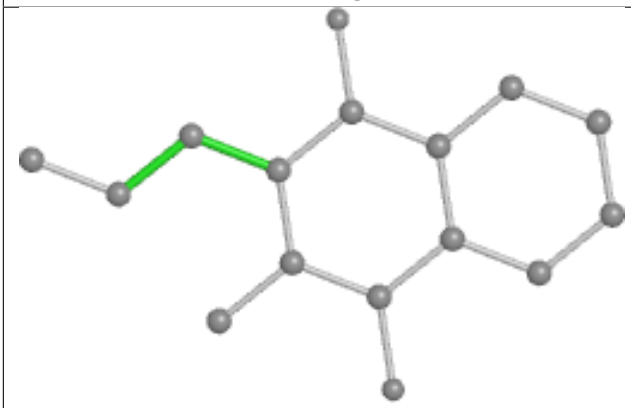
Ligand PQN B 844



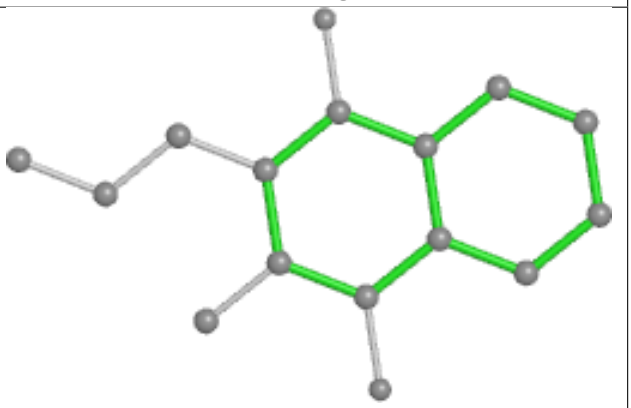
Bond lengths



Bond angles

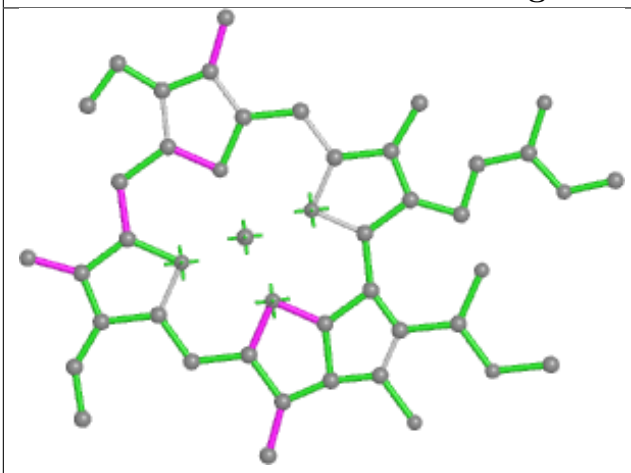


Torsions

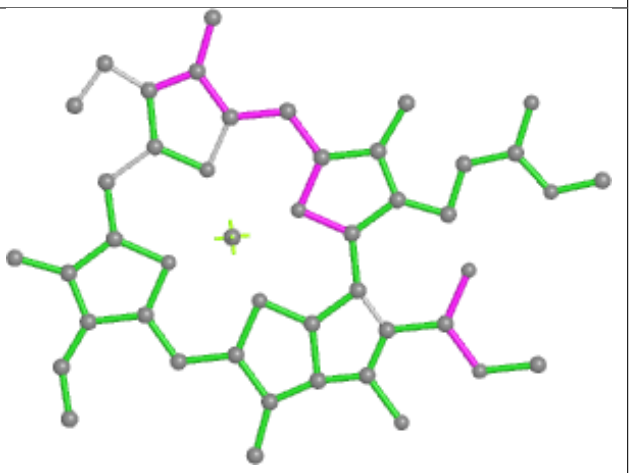


Rings

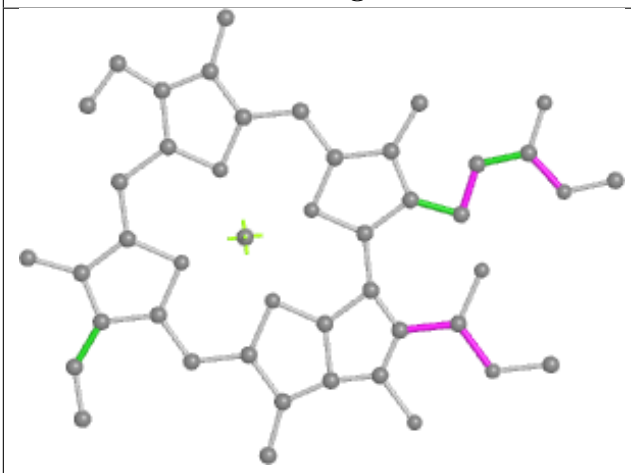
Ligand CLA 1 510



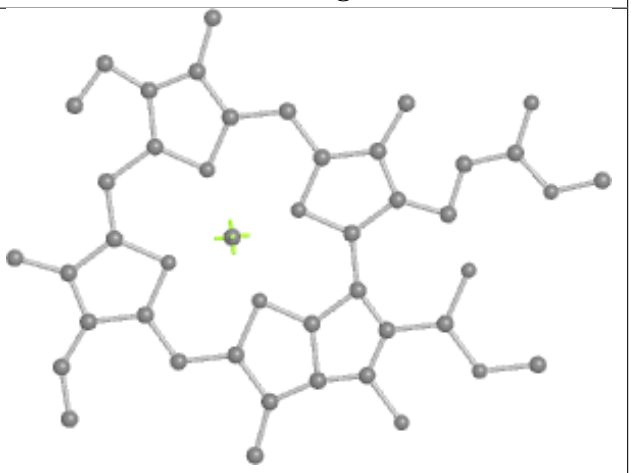
Bond lengths



Bond angles

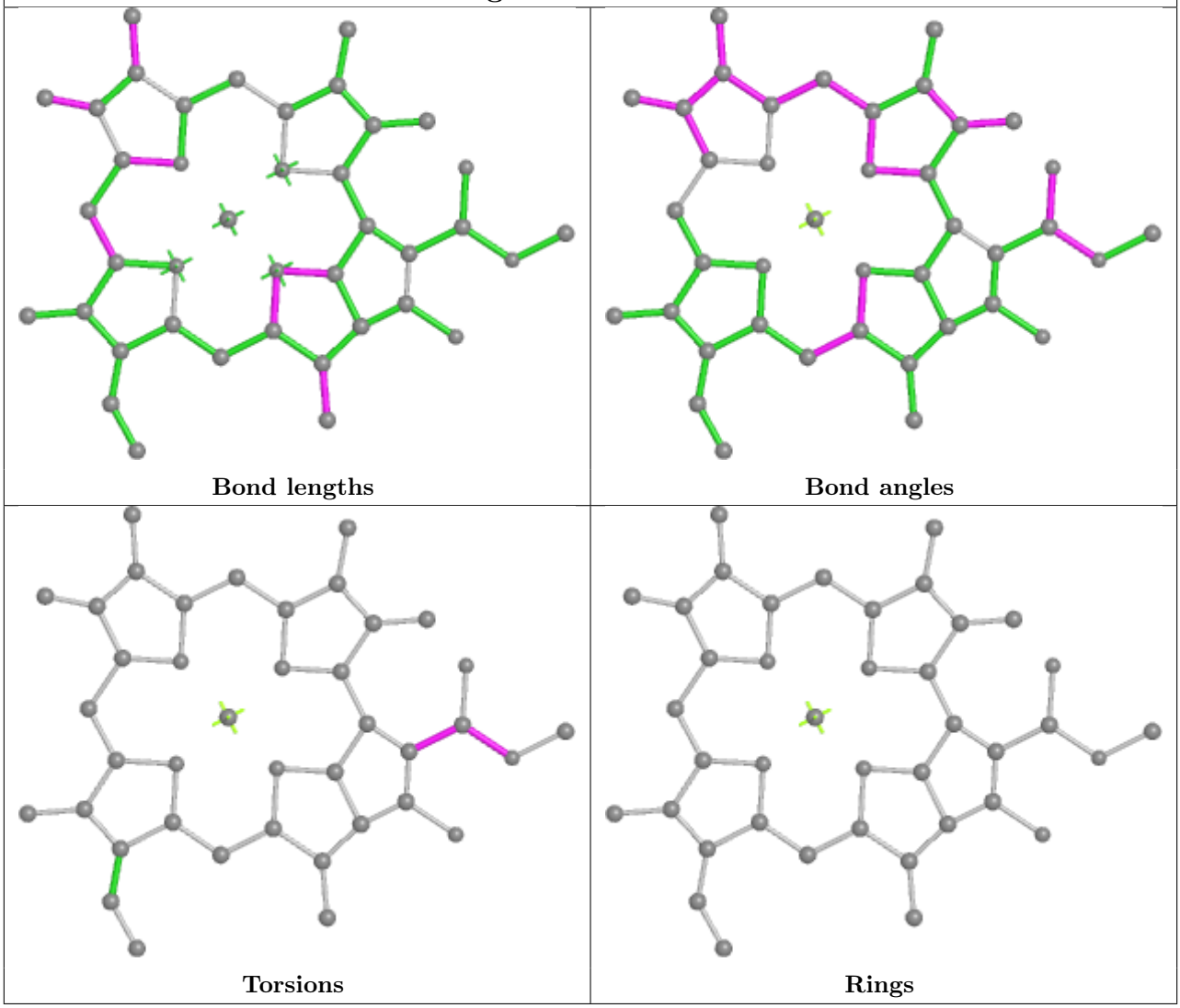


Torsions



Rings

Ligand CLA 1 507



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.

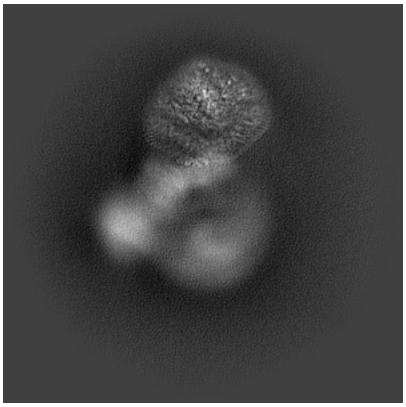
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31350. These allow visual inspection of the internal detail of the map and identification of artifacts.

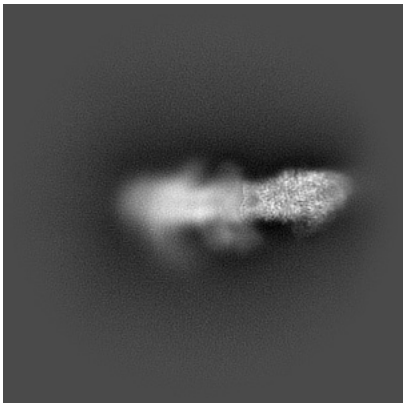
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

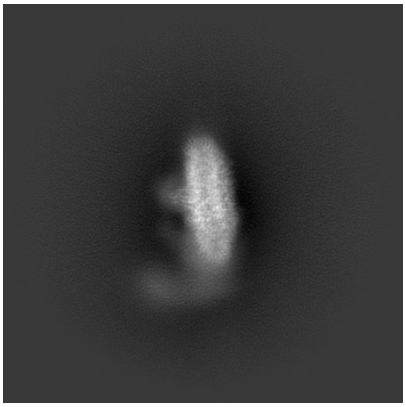
6.1.1 Primary map



X



Y

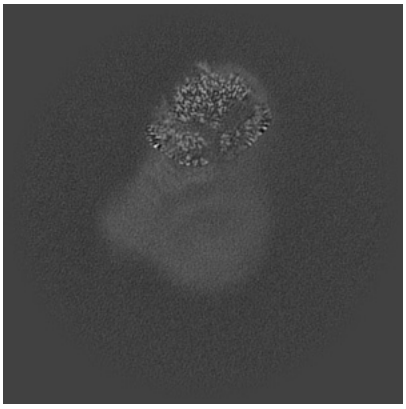


Z

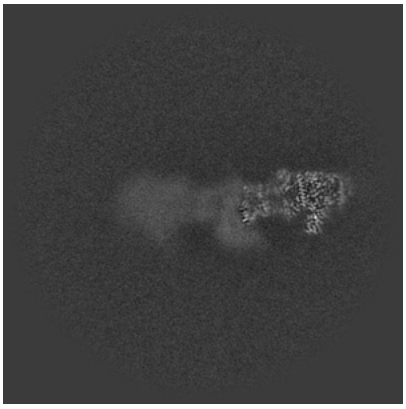
The images above show the map projected in three orthogonal directions.

6.2 Central slices

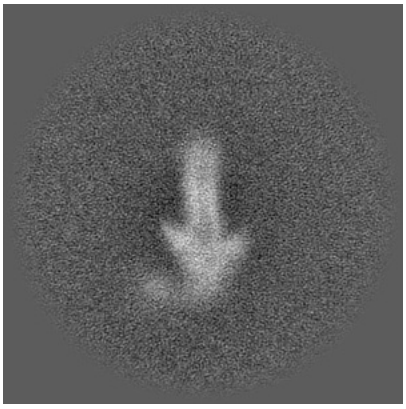
6.2.1 Primary map



X Index: 220



Y Index: 220

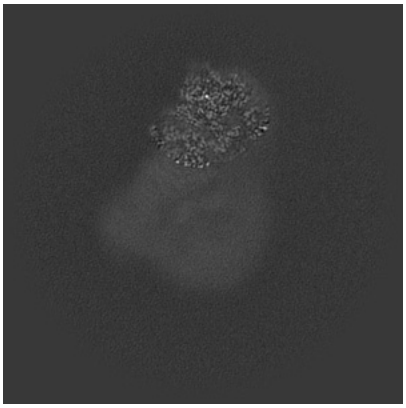


Z Index: 220

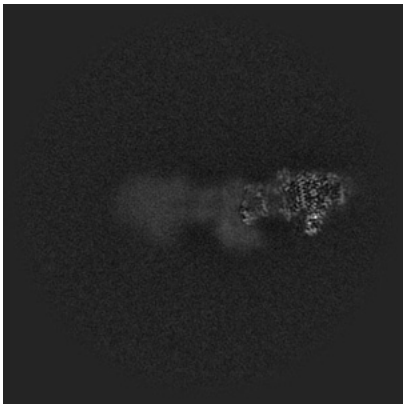
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

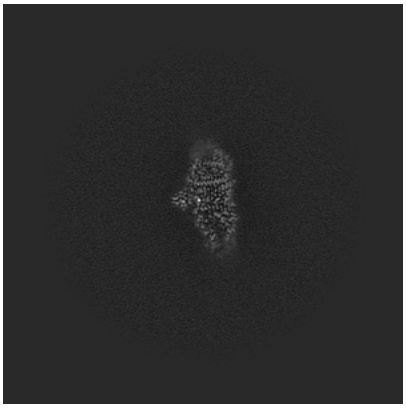
6.3.1 Primary map



X Index: 215



Y Index: 221

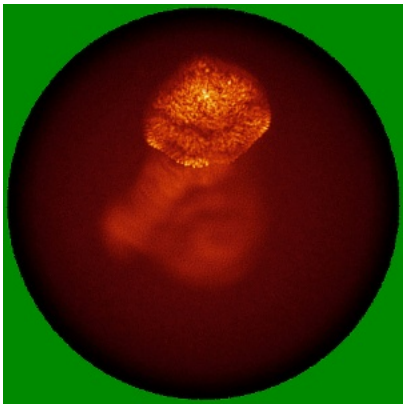


Z Index: 338

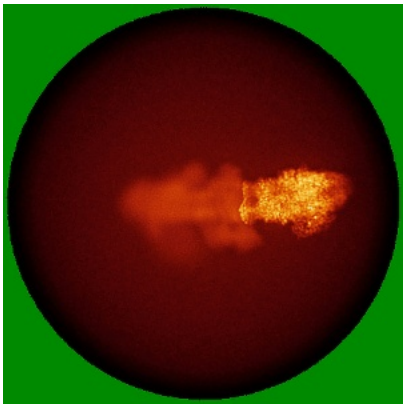
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

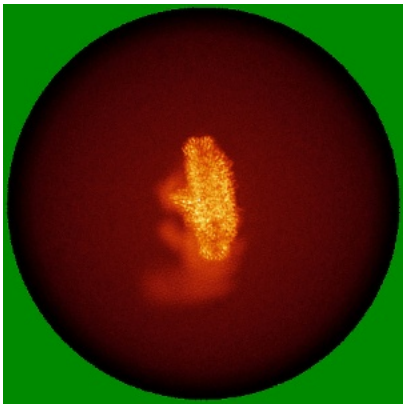
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

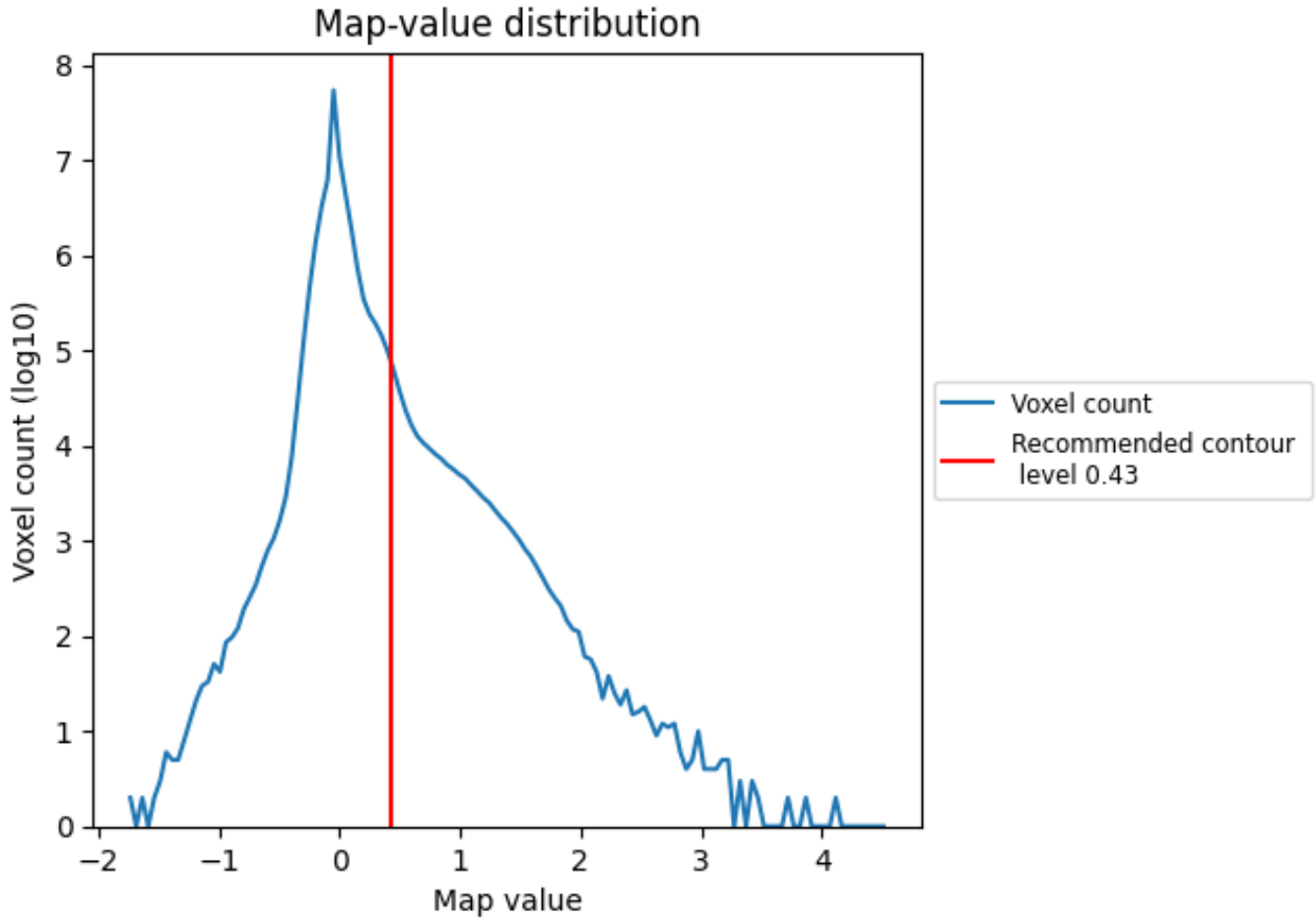
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

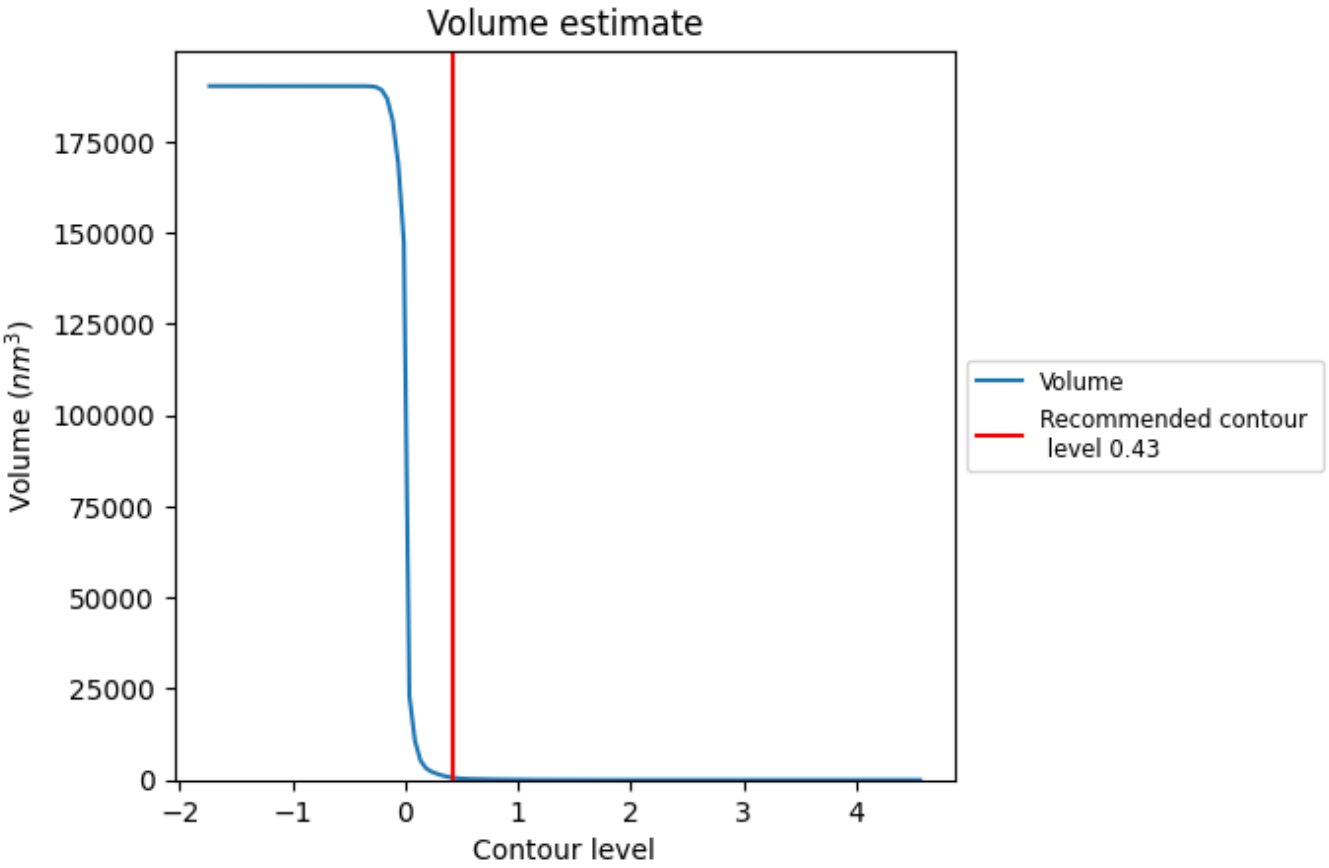
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

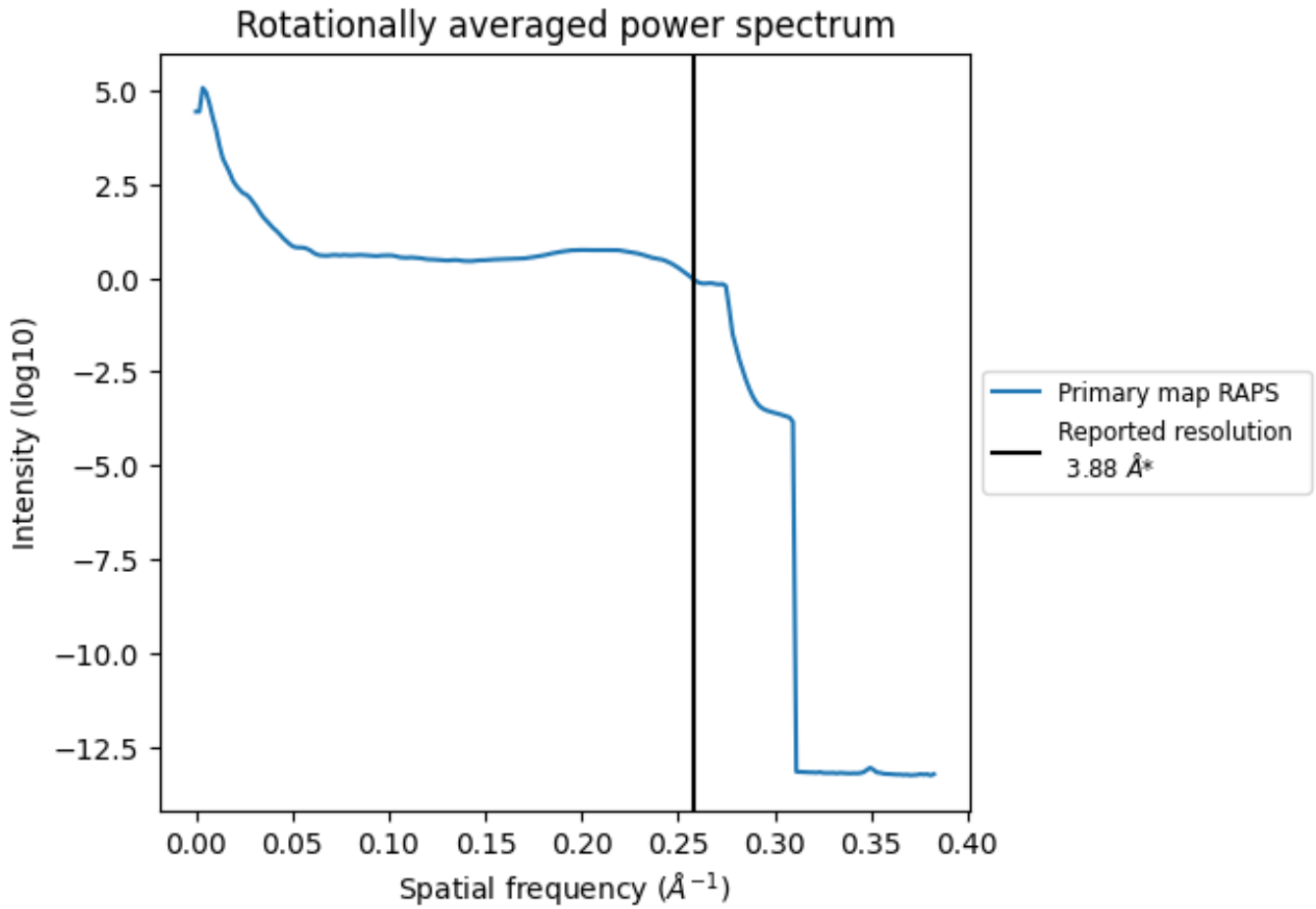
7.2 Volume estimate



The volume at the recommended contour level is 598 nm^3; this corresponds to an approximate mass of 540 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

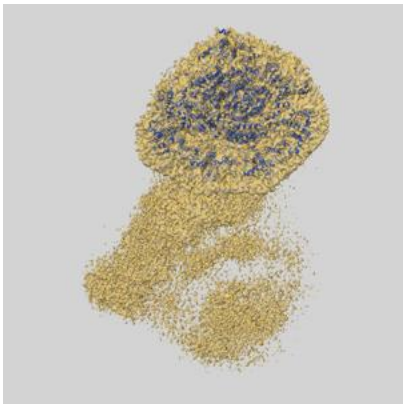
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

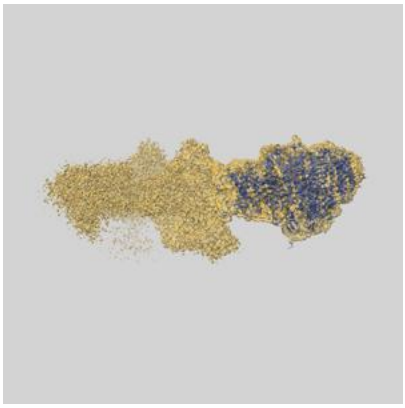
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31350 and PDB model 7EWK. Per-residue inclusion information can be found in section 3 on page 25.

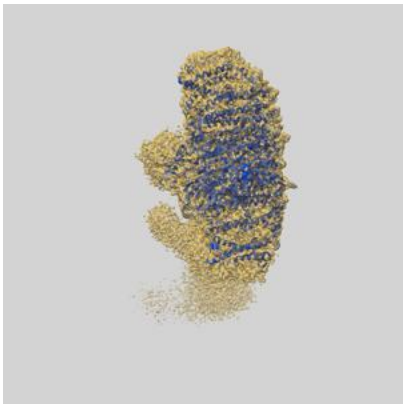
9.1 Map-model overlay



X



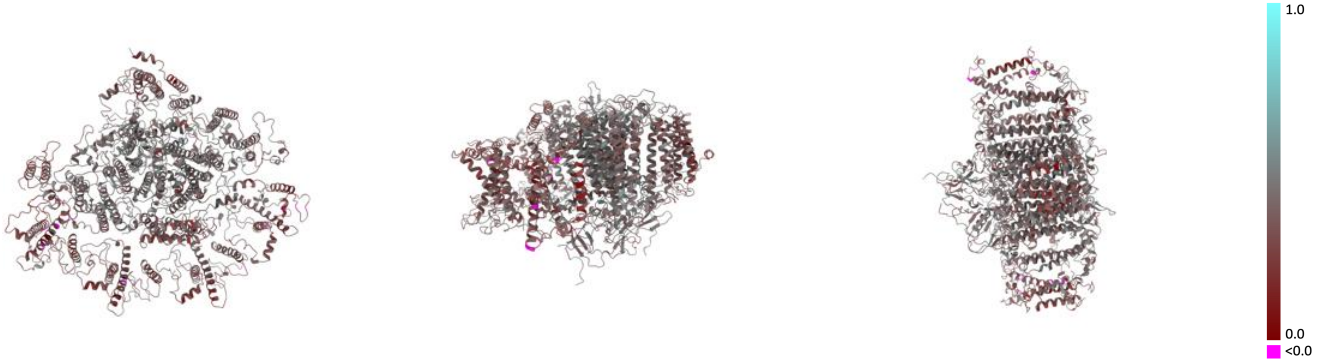
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

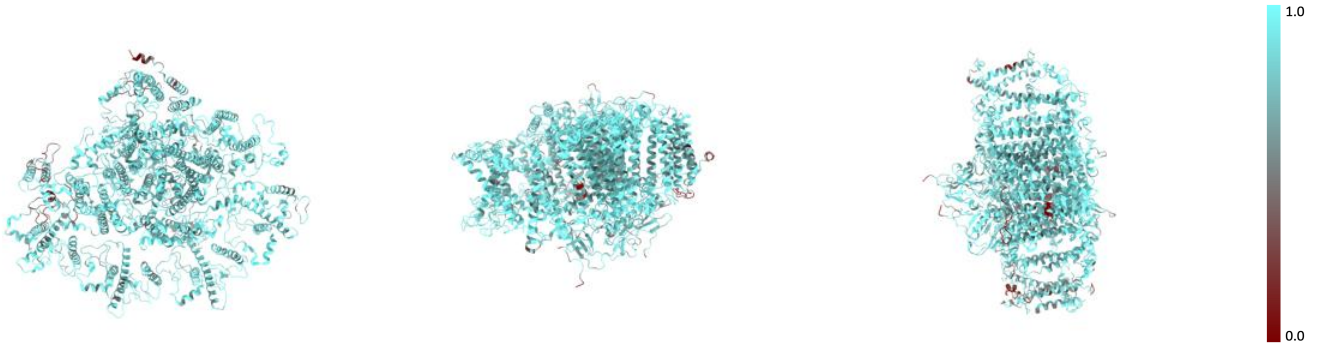
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

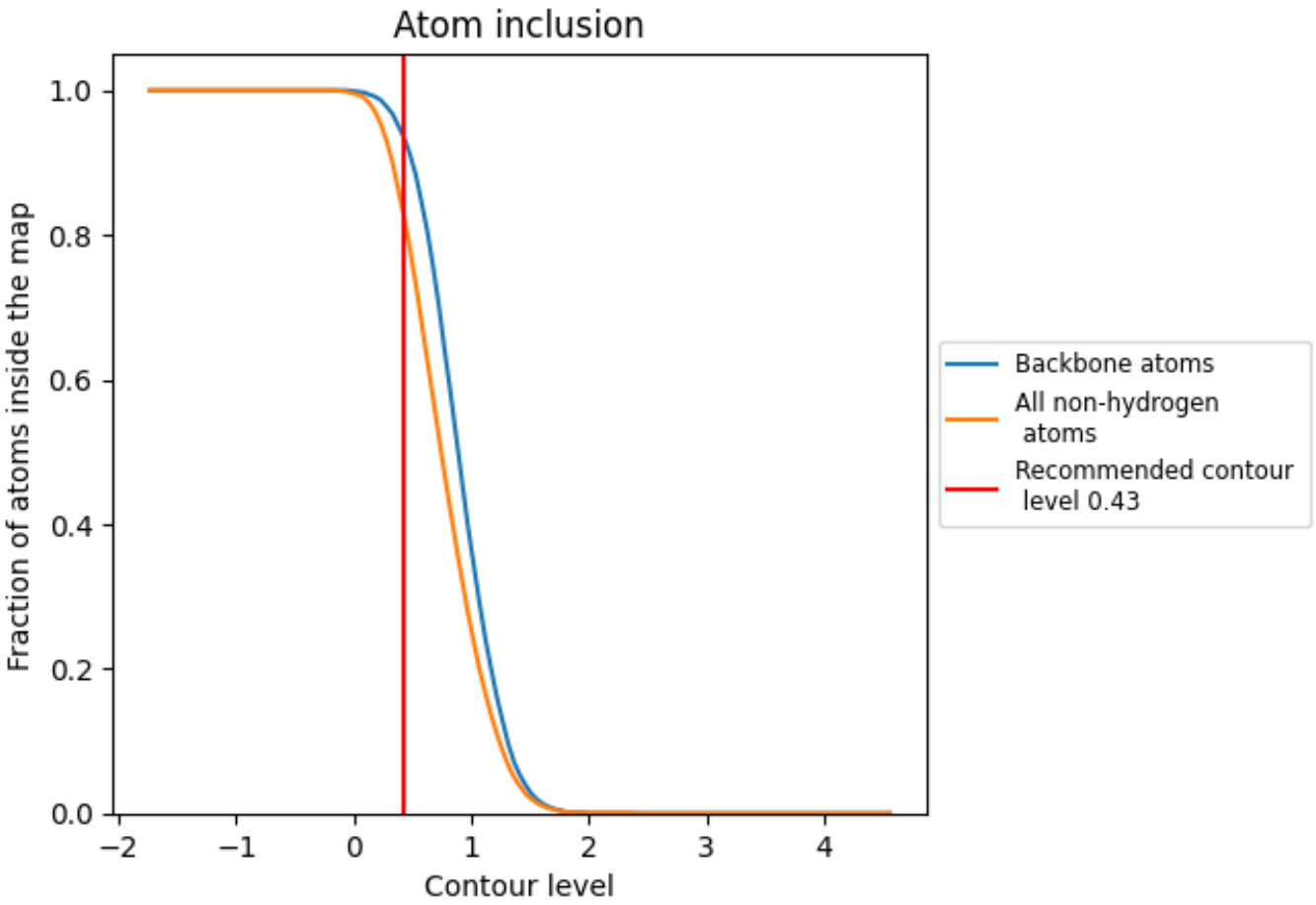
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3960
1	0.8130	0.3100
3	0.7240	0.2960
4	0.8440	0.3590
6	0.8200	0.3440
A	0.8500	0.4450
B	0.8690	0.4350
C	0.9140	0.4250
D	0.8180	0.4190
E	0.7990	0.4320
F	0.8380	0.3750
H	0.6350	0.3430
I	0.7740	0.4220
J	0.7400	0.3940
K	0.6770	0.3280
L	0.7240	0.3620