Full wwPDB EM Validation Report

Oct 1, 2026 – 10:55 AM JST

PDB ID	:	6K33 / pdb_00006k33
EMDB ID	:	EMD-9908
Title	:	Structure of PSI-isiA supercomplex from Thermosynechococcus vulcanus
Authors	:	Akita, F.; Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.
Deposited on	:	2019-05-16
Resolution	:	2.74 Å(reported)
Based on initial model	:	1JB0

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:

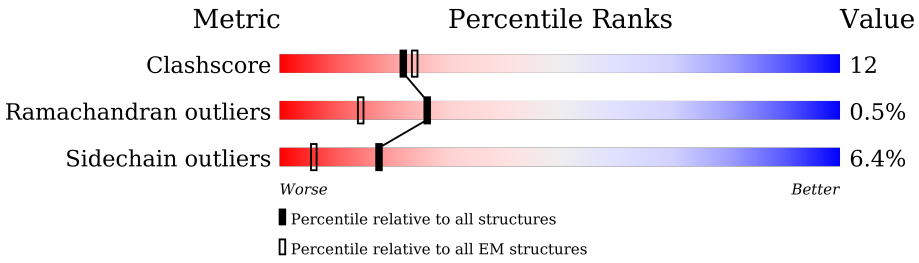
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

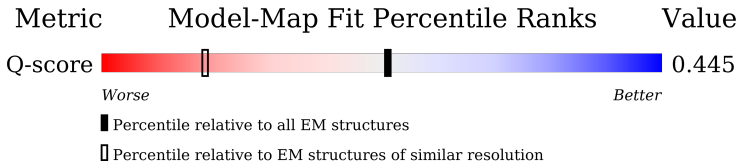
1 Overall quality at a glance

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

The reported resolution of this entry is 2.74 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.





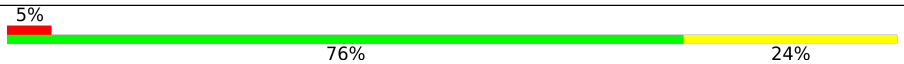
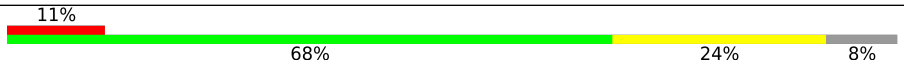
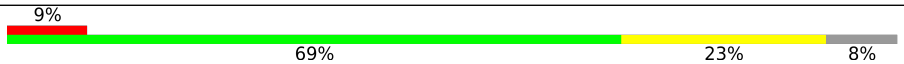
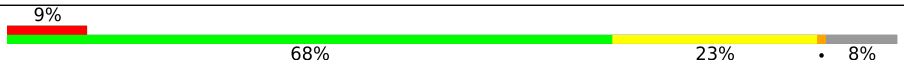
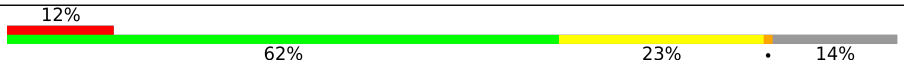
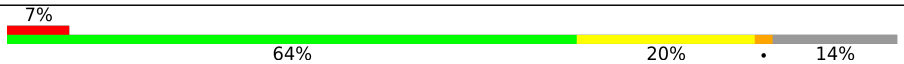
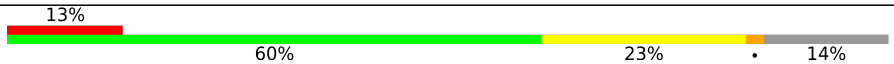
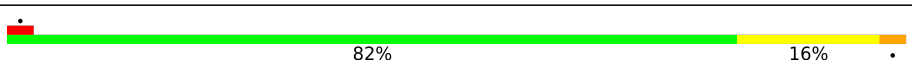
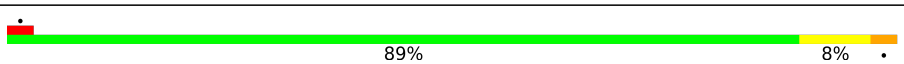
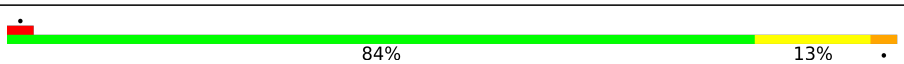
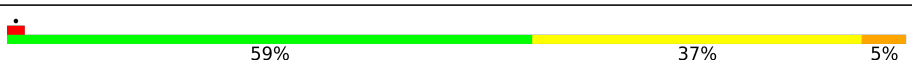
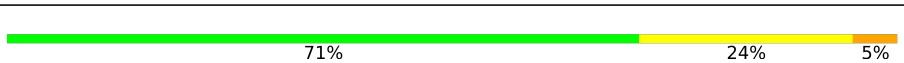
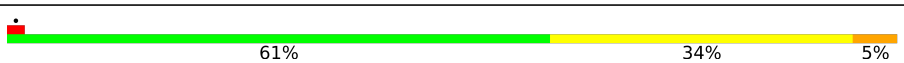
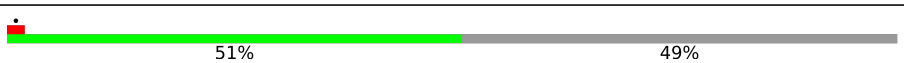
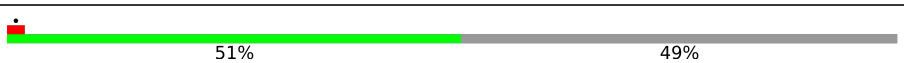
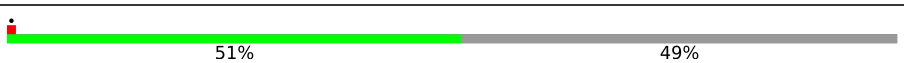
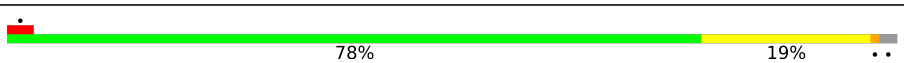
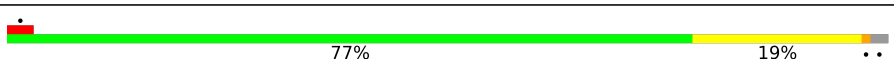
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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	aA	755	75% 21%
1	bA	755	75% 21%
1	cA	755	74% 22%
2	aB	740	77% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	bB	740	
2	cB	740	
3	aC	80	
3	bC	80	
3	cC	80	
4	aD	138	
4	bD	138	
4	cD	138	
5	aE	75	
5	bE	75	
5	cE	75	
6	aF	164	
6	bF	164	
6	cF	164	
7	aI	38	
7	bI	38	
7	cI	38	
8	aJ	41	
8	bJ	41	
8	cJ	41	
9	aK	85	
9	bK	85	
9	cK	85	
10	aL	154	
10	bL	154	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	cL	154	78% 19%
11	aM	31	65% 29% 6%
11	bM	31	65% 29% 6%
11	cM	31	68% 29%
12	aX	35	77% 17%
12	bX	35	77% 6% 17%
12	cX	35	71% 11% 17%
13	a1	358	48% 66% 23% 8%
13	a2	358	52% 63% 26% 9%
13	a3	358	37% 67% 23% 7%
13	a4	358	41% 67% 24% 6%
13	a5	358	48% 67% 23% 7%
13	a6	358	54% 66% 22% 8%
13	b1	358	49% 68% 22% 8%
13	b2	358	53% 65% 23% 9%
13	b3	358	38% 67% 23% 7%
13	b4	358	39% 68% 22% 6%
13	b5	358	48% 69% 21% 7%
13	b6	358	53% 66% 22% 8%
13	c1	358	50% 68% 22% 8%
13	c2	358	52% 64% 24% 9%
13	c3	358	39% 68% 22% 7%
13	c4	358	40% 69% 22% 6%
13	c5	358	48% 66% 23% 7%
13	c6	358	54% 66% 22% 8%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 137634 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	aA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	bA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	cA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	bB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	cB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	cD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	69	Total	C	N	O	0	0
			539	342	93	104		
5	bE	69	Total	C	N	O	0	0
			539	342	93	104		
5	cE	69	Total	C	N	O	0	0
			539	342	93	104		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	bF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	cF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	bI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	cI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		
8	bJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	aK	43	Total	C	N	O	0	0
			208	122	43	43		
9	bK	43	Total	C	N	O	0	0
			208	122	43	43		
9	cK	43	Total	C	N	O	0	0
			208	122	43	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	bL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	cL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

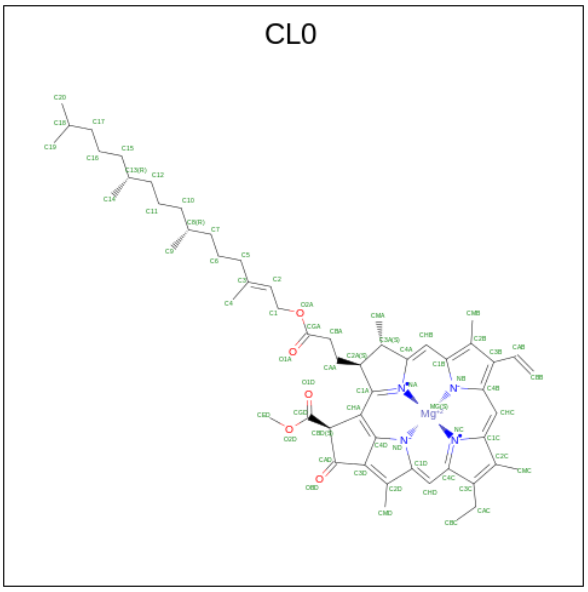
- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			233	164	34	35		
12	bX	29	Total	C	N	O	0	0
			233	164	34	35		
12	cX	29	Total	C	N	O	0	0
			233	164	34	35		

- Molecule 13 is a protein called Iron stress in-duced protein A.

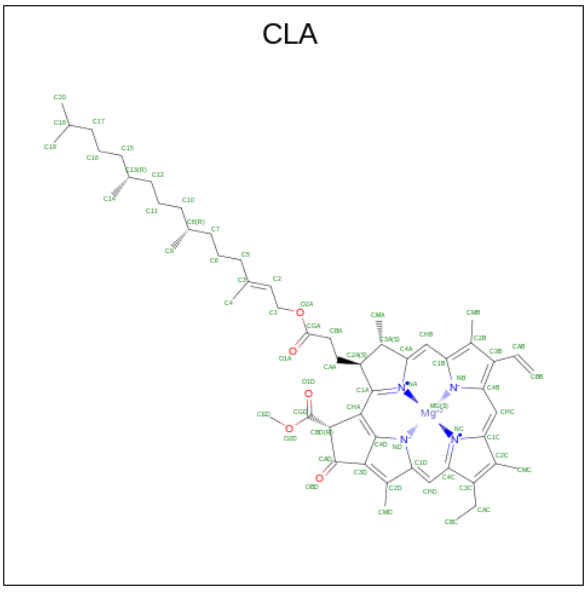
Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	a2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	a3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	a5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	b3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	b5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	c3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	c5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		

- Molecule 14 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	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
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	aK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	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
15	a1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a2	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
15	a2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	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
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	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
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	a6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bA	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
15	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bA	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
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	bA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	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
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	bK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	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
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	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
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	cA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	cK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	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
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

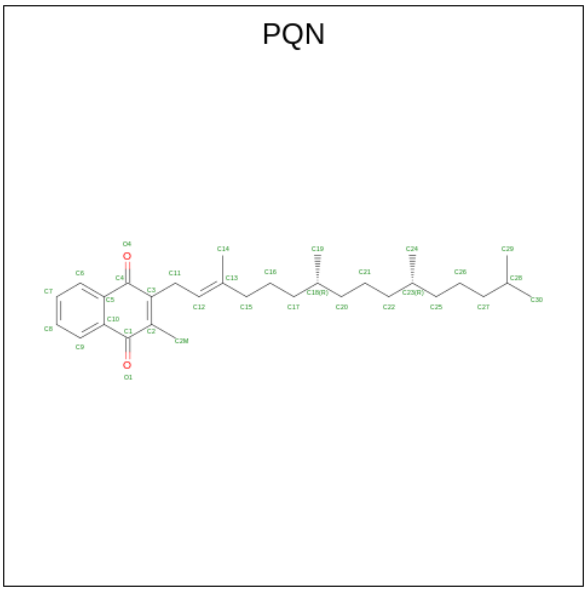
Mol	Chain	Residues	Atoms					AltConf
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	c4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	c5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	c5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

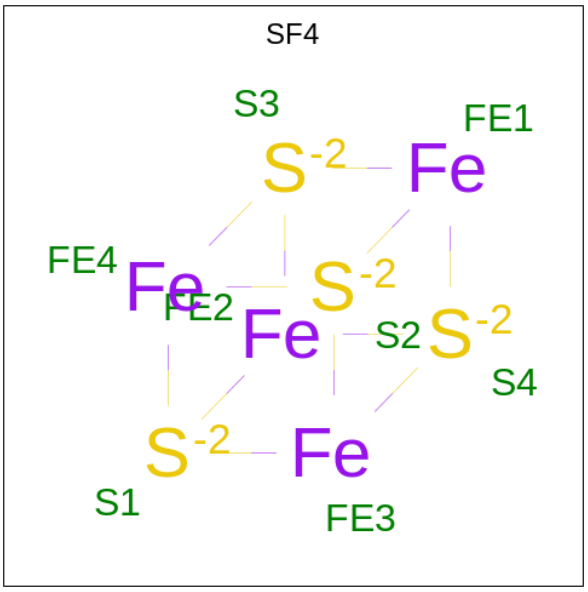
Mol	Chain	Residues	Atoms					AltConf
15	c5	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c5	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c6	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



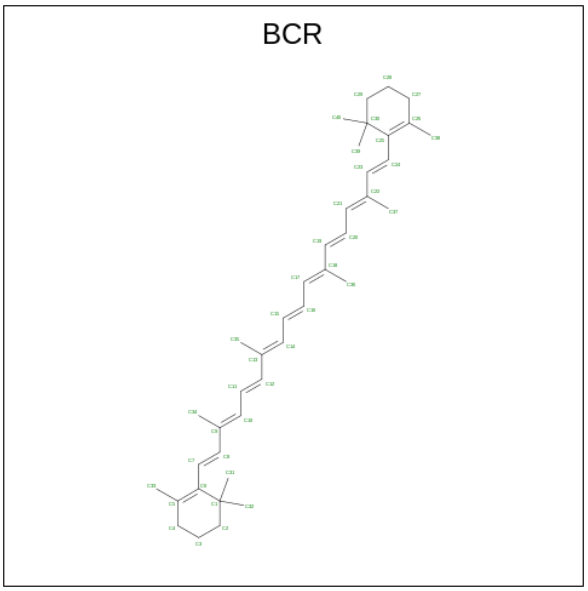
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total Fe S 8 4 4	0
17	aC	1	Total Fe S 8 4 4	0
17	aC	1	Total Fe S 8 4 4	0
17	bA	1	Total Fe S 8 4 4	0
17	bC	1	Total Fe S 8 4 4	0
17	bC	1	Total Fe S 8 4 4	0
17	cA	1	Total Fe S 8 4 4	0
17	cC	1	Total Fe S 8 4 4	0
17	cC	1	Total Fe S 8 4 4	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aA	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 25 25	0
18	aB	1	Total C 40 40	0
18	aB	1	Total C 40 40	0
18	aF	1	Total C 40 40	0
18	aF	1	Total C 40 40	0
18	aF	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aK	1	Total C 40 40	0
18	aL	1	Total C 40 40	0
18	aM	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	bB	1	Total C 25 25	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bF	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bM	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
18	b2	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

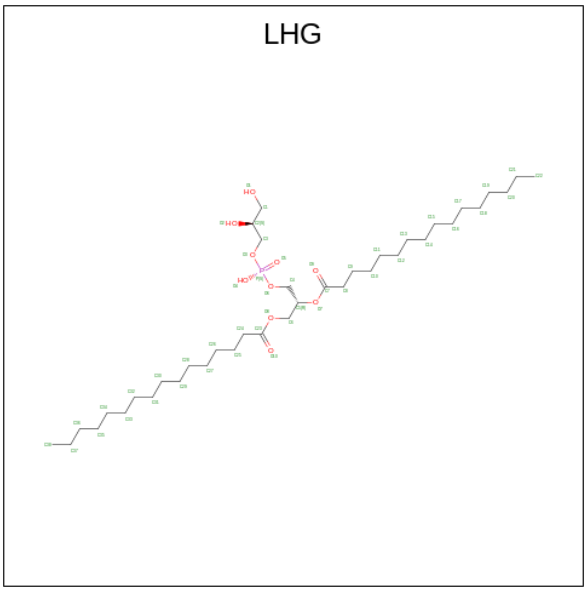
Mol	Chain	Residues	Atoms	AltConf
18	cA	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 25 25	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cK	1	Total C 40 40	0
18	cL	1	Total C 40 40	0
18	cM	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

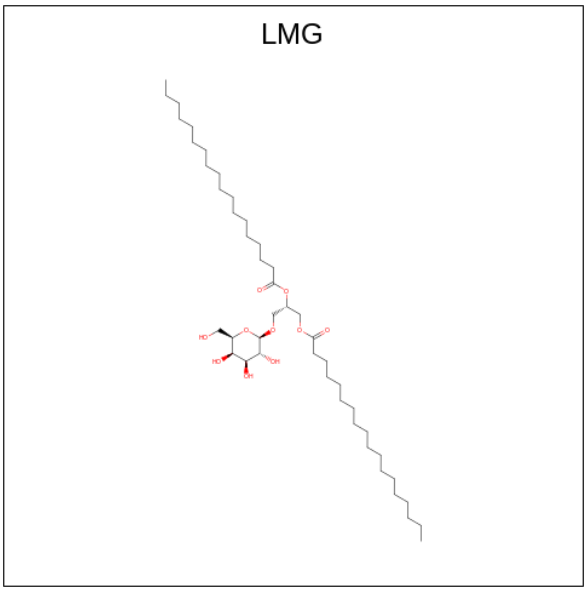
Mol	Chain	Residues	Atoms	AltConf
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms				AltConf
19	aA	1	Total	C	O	P	0
			49	38	10	1	
19	aA	1	Total	C	O	P	0
			27	16	10	1	
19	aX	1	Total	C	O	P	0
			23	12	10	1	
19	bA	1	Total	C	O	P	0
			49	38	10	1	
19	bA	1	Total	C	O	P	0
			27	16	10	1	
19	bX	1	Total	C	O	P	0
			23	12	10	1	
19	cA	1	Total	C	O	P	0
			49	38	10	1	
19	cA	1	Total	C	O	P	0
			27	16	10	1	
19	cX	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
20	aB	1	Total C O 55 45 10	0
20	bB	1	Total C O 55 45 10	0
20	cB	1	Total C O 55 45 10	0

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
21	aL	1	Total Ca 1 1	0
21	bL	1	Total Ca 1 1	0
21	cL	1	Total Ca 1 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	aA	3	Total O 3 3	0
22	aB	3	Total O 3 3	0
22	aL	1	Total O 1 1	0

Continued on next page...

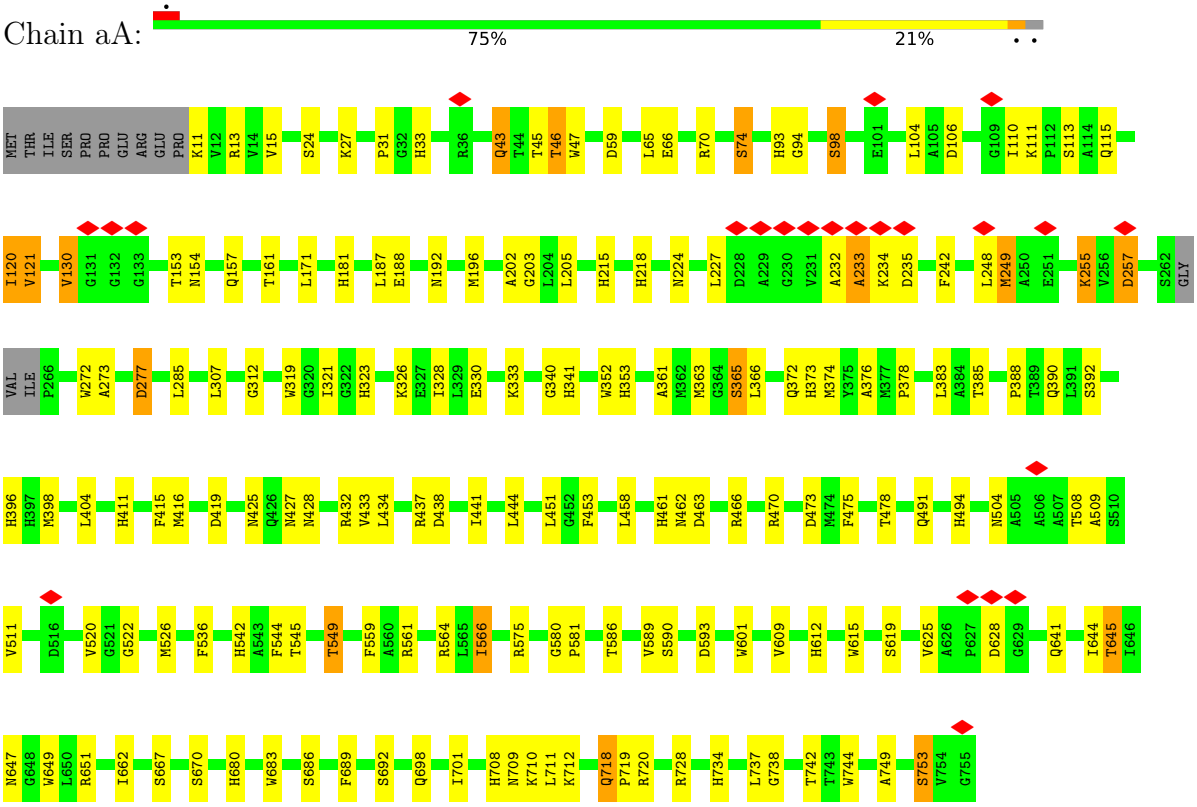
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
22	bA	3	Total O 3 3	0
22	bB	3	Total O 3 3	0
22	bL	1	Total O 1 1	0
22	cA	2	Total O 2 2	0
22	cB	3	Total O 3 3	0
22	cF	1	Total O 1 1	0
22	cL	1	Total O 1 1	0

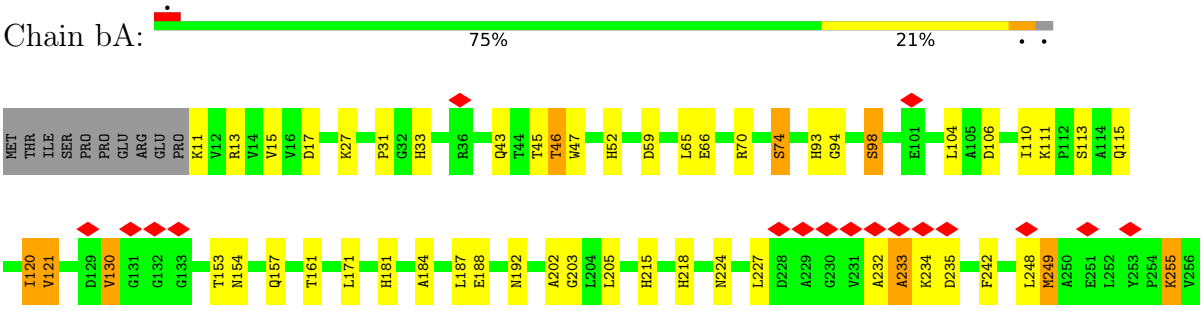
3 Residue-property plots (i)

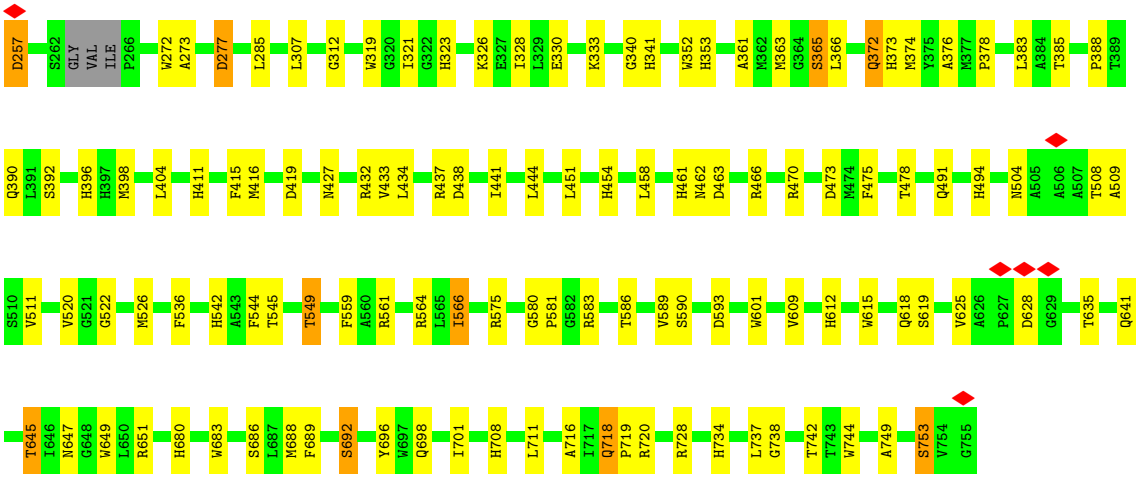
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

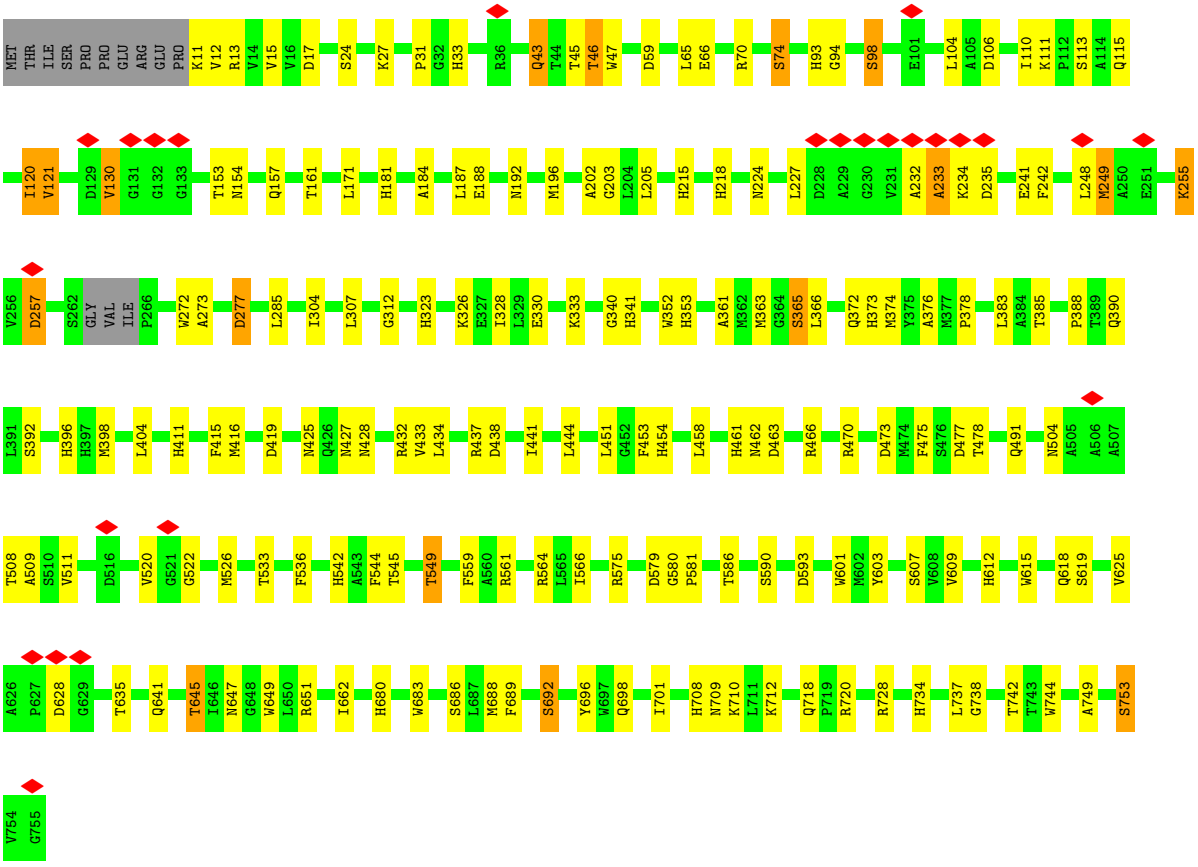




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:

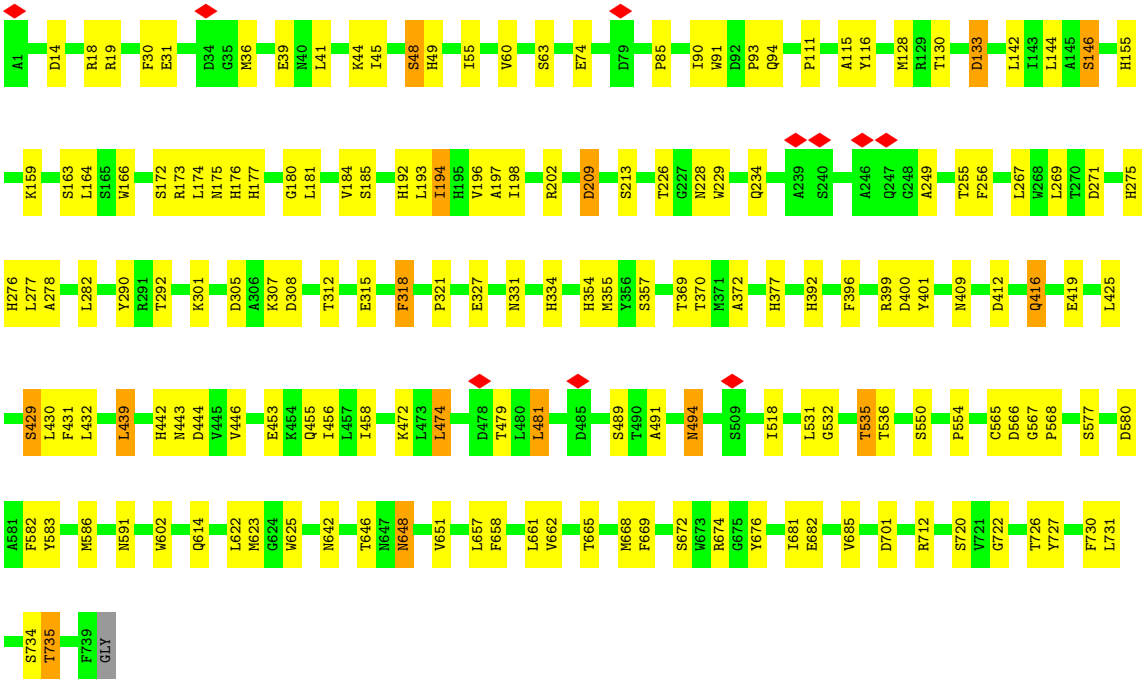




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB:

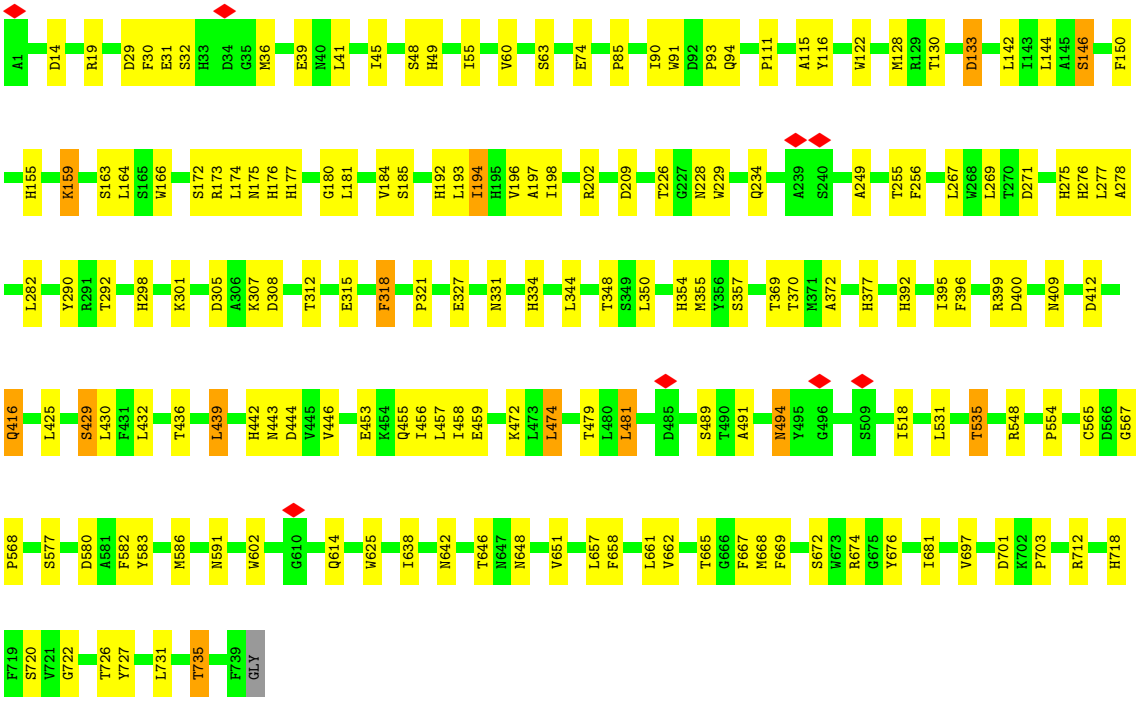




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:

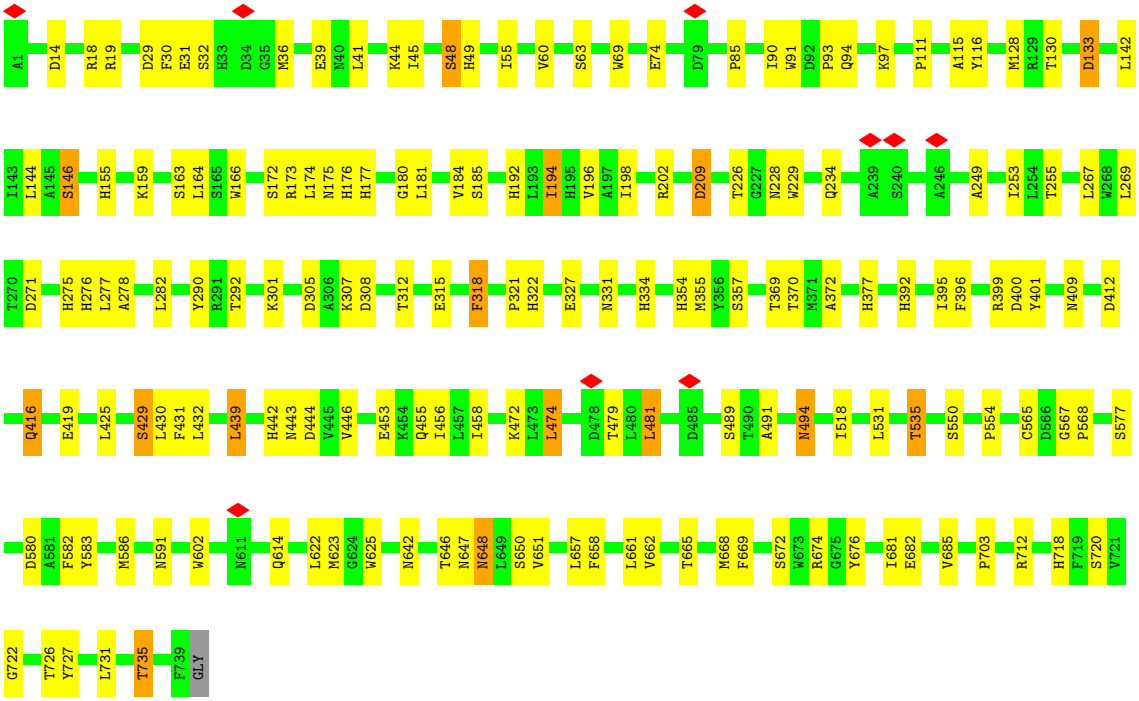




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB:

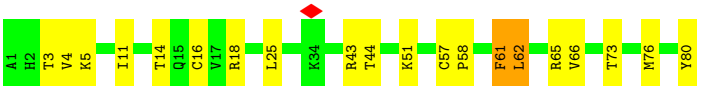




• Molecule 3: Photosystem I iron-sulfur center

Chain aC:

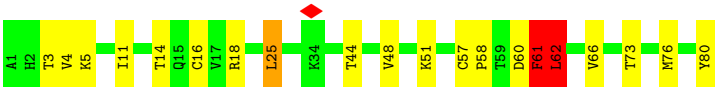




• Molecule 3: Photosystem I iron-sulfur center

Chain bC:

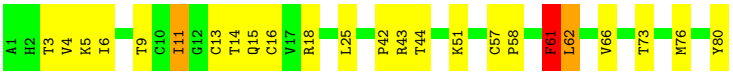




• Molecule 3: Photosystem I iron-sulfur center

Chain cC:

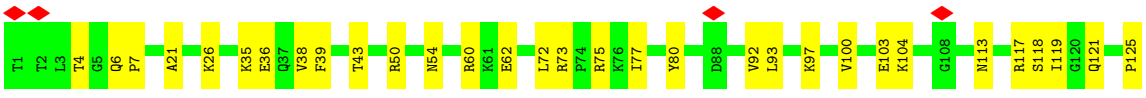


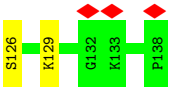


• Molecule 4: Photosystem I reaction center subunit II

Chain aD:

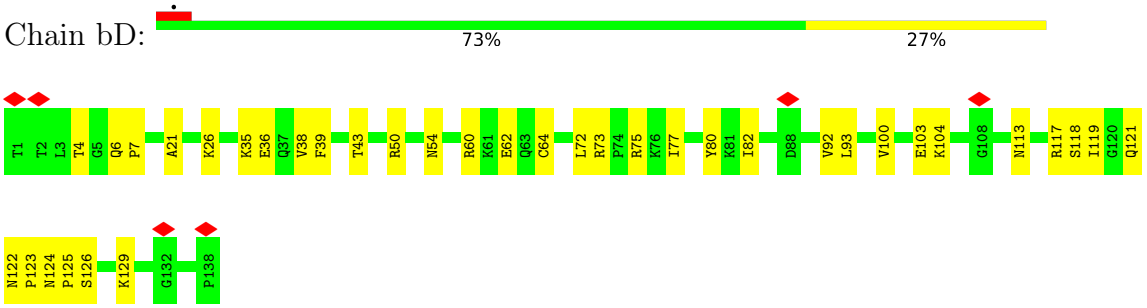






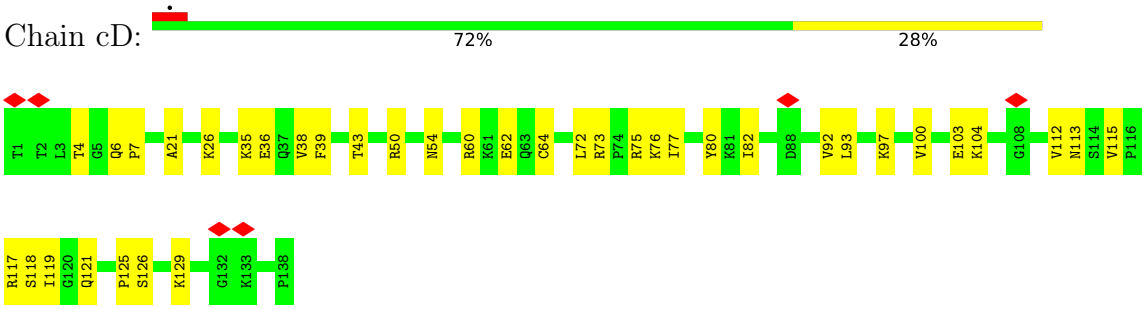
• Molecule 4: Photosystem I reaction center subunit II

Chain bD:



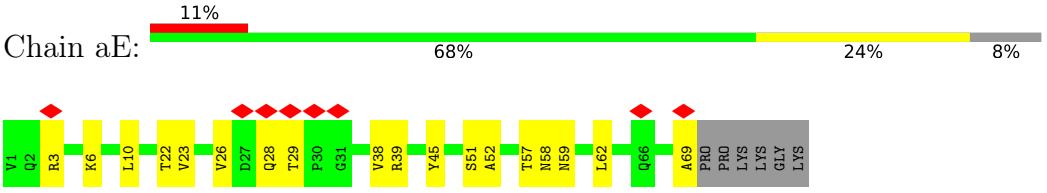
• Molecule 4: Photosystem I reaction center subunit II

Chain cD:



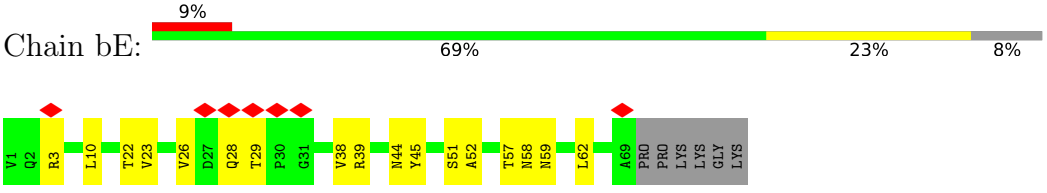
• Molecule 5: Photosystem I reaction center subunit IV

Chain aE:



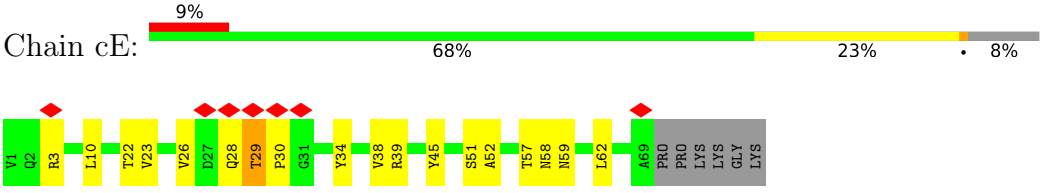
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



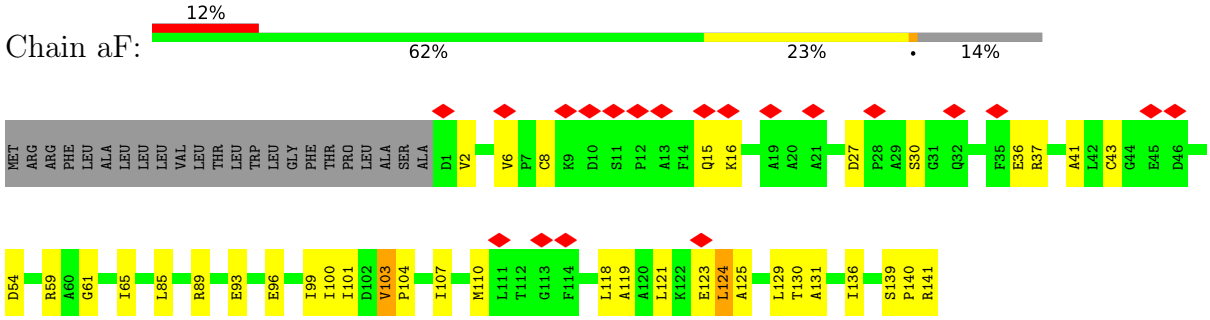
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



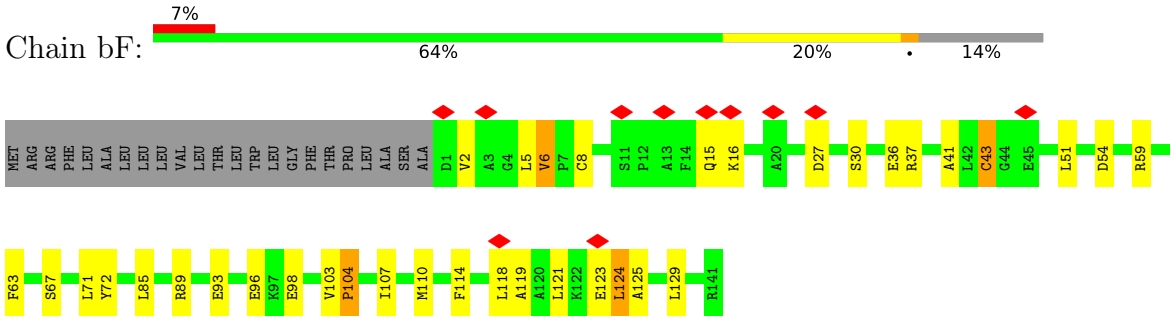
• Molecule 6: Photosystem I reaction center subunit III

Chain aF:



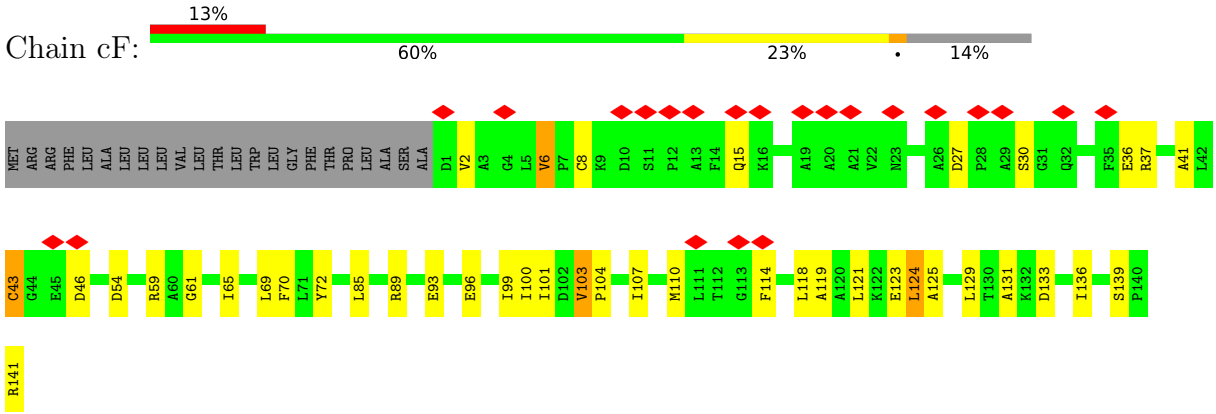
• Molecule 6: Photosystem I reaction center subunit III

Chain bF:



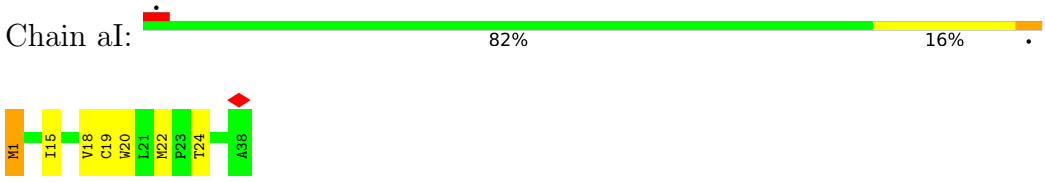
• Molecule 6: Photosystem I reaction center subunit III

Chain cF:



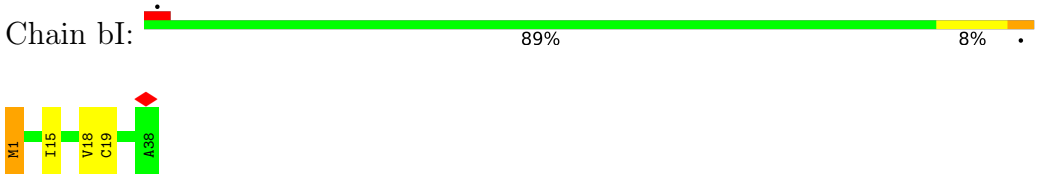
• Molecule 7: Photosystem I reaction center subunit VIII

Chain aI:



• Molecule 7: Photosystem I reaction center subunit VIII

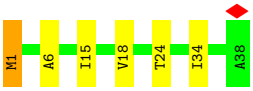
Chain bI:



• Molecule 7: Photosystem I reaction center subunit VIII

Chain cI:

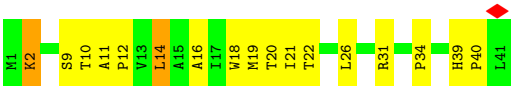




• Molecule 8: Photosystem I reaction center subunit IX

Chain aJ:

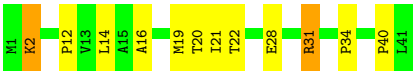




• Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:

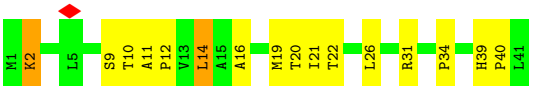




• Molecule 8: Photosystem I reaction center subunit IX

Chain cJ:

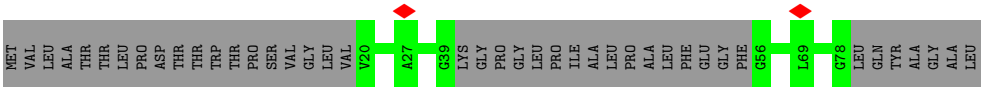




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain aK:

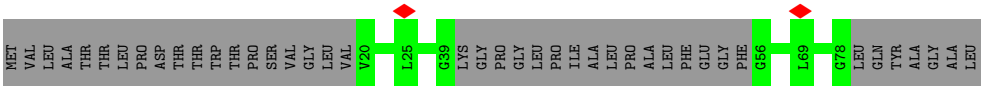




• Molecule 9: Photosystem I reaction center subunit PsaK

Chain bK:

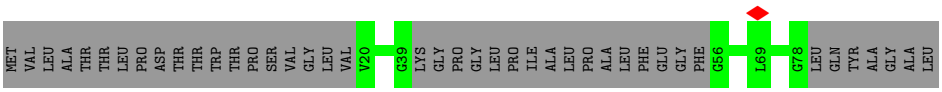




• Molecule 9: Photosystem I reaction center subunit PsaK

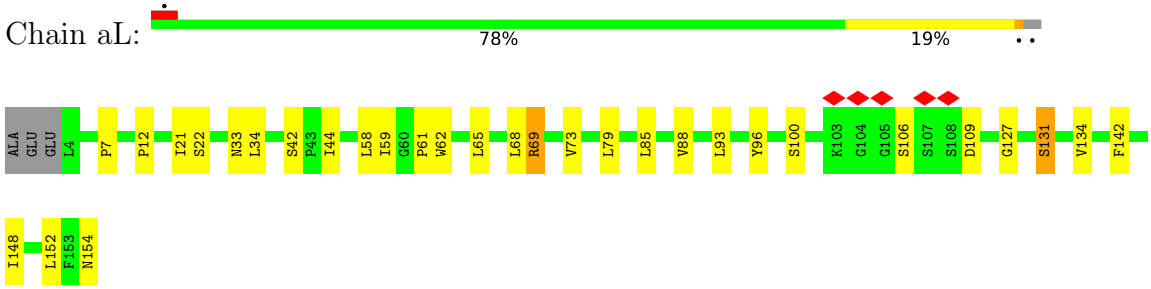
Chain cK:





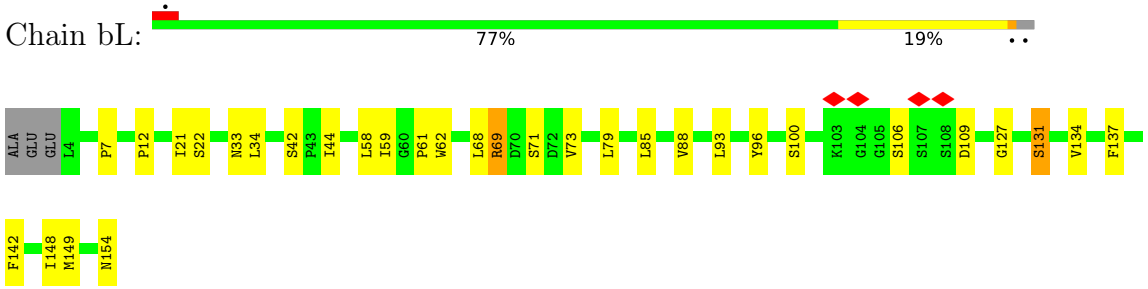
• Molecule 10: Photosystem I reaction center subunit XI

Chain aL:



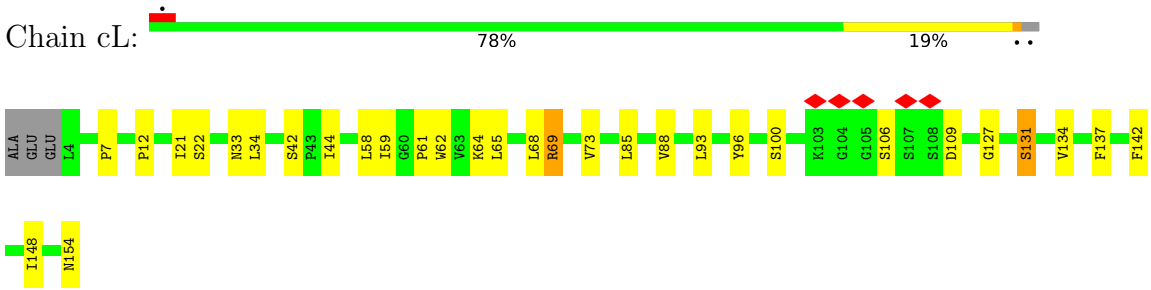
• Molecule 10: Photosystem I reaction center subunit XI

Chain bL:



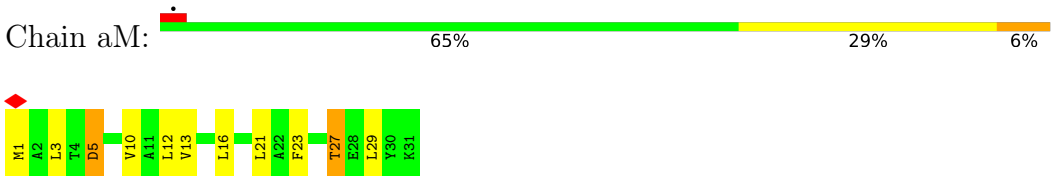
• Molecule 10: Photosystem I reaction center subunit XI

Chain cL:



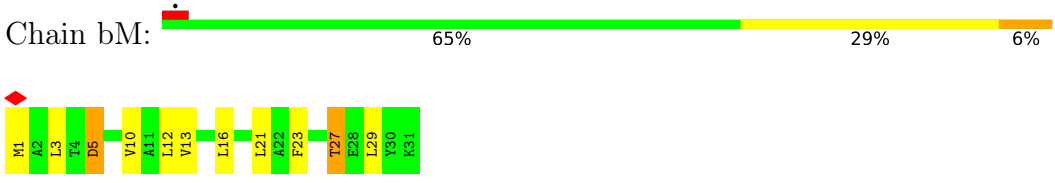
• Molecule 11: Photosystem I reaction center subunit XII

Chain aM:



• Molecule 11: Photosystem I reaction center subunit XII

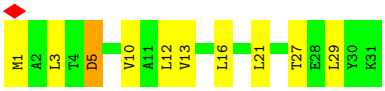
Chain bM:



• Molecule 11: Photosystem I reaction center subunit XII

Chain cM:

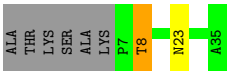




• Molecule 12: Photosystem I reaction center subunit psaX

Chain aX:

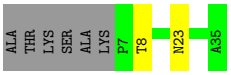




• Molecule 12: Photosystem I reaction center subunit psaX

Chain bX:

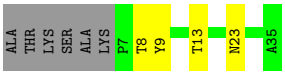




• Molecule 12: Photosystem I reaction center subunit psaX

Chain cX:

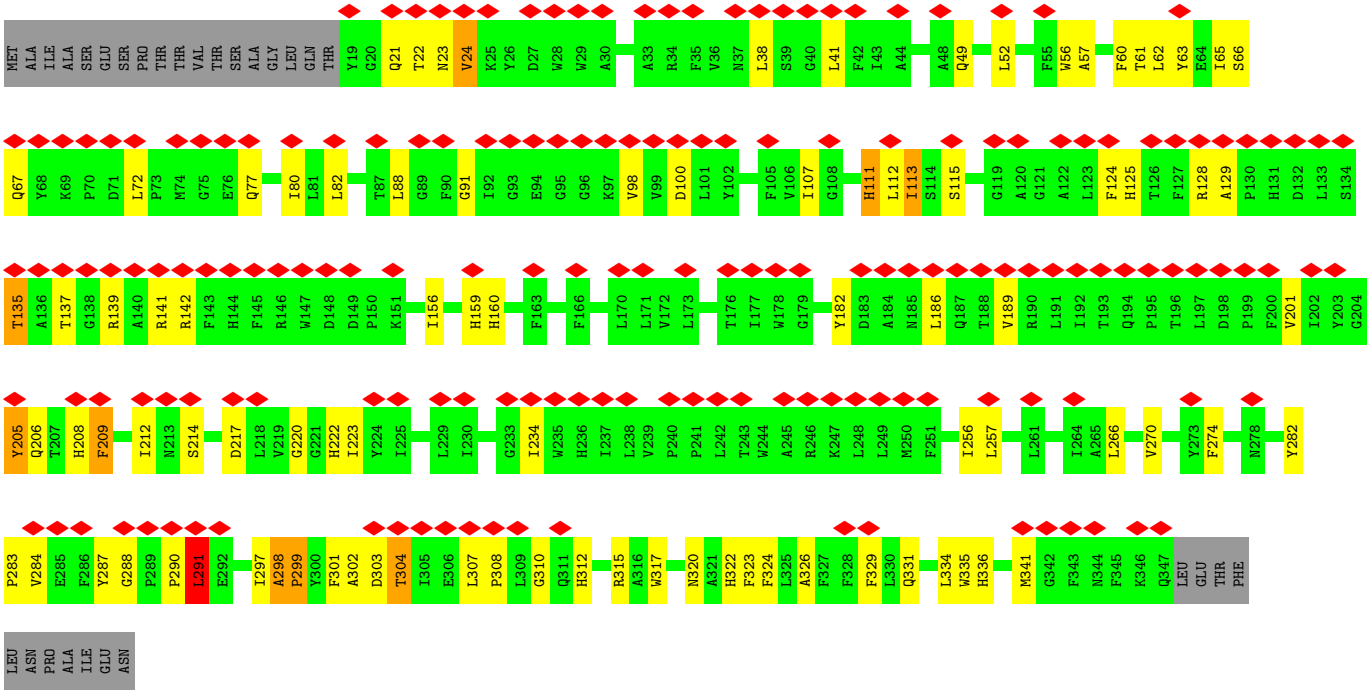




• Molecule 13: Iron stress in-duced protein A

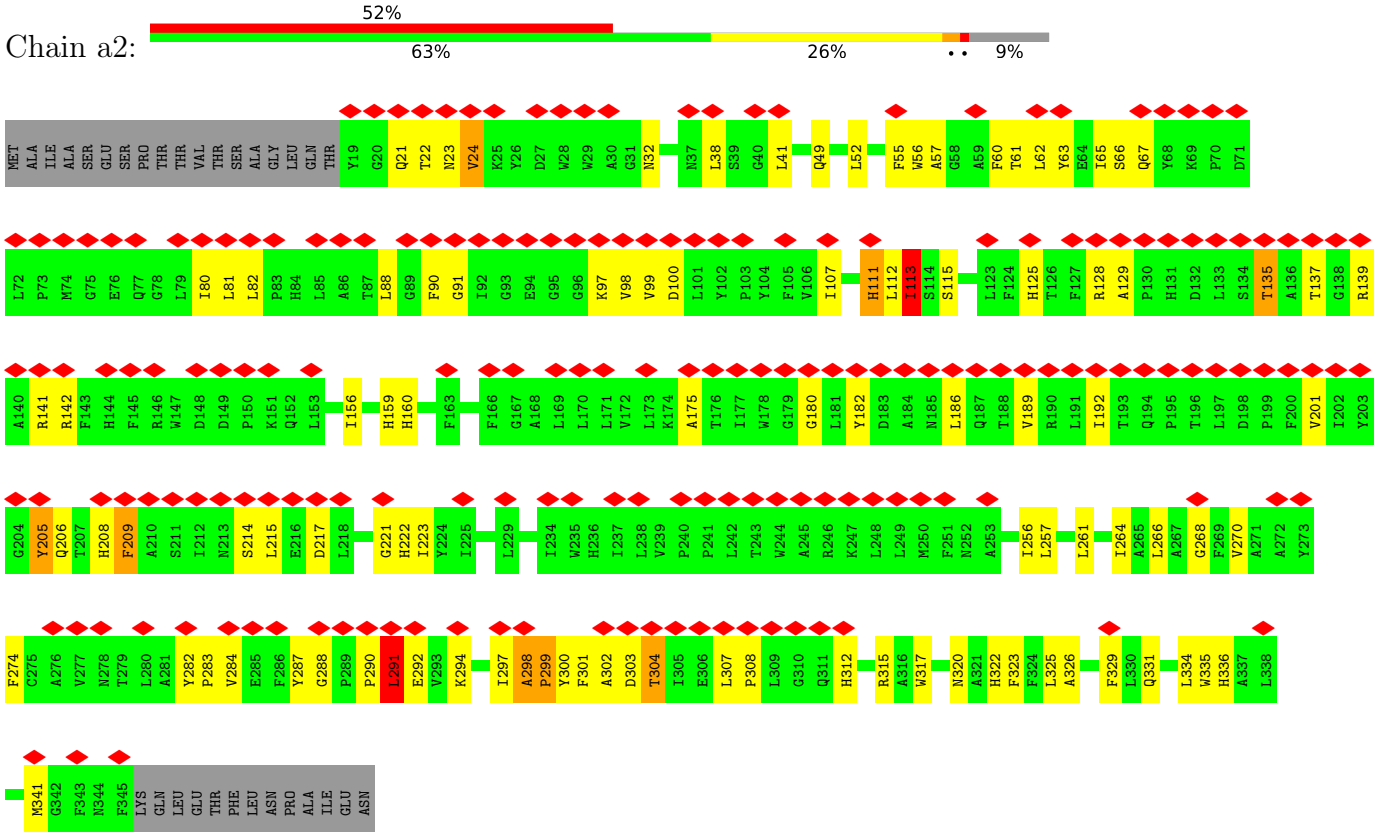
Chain a1:





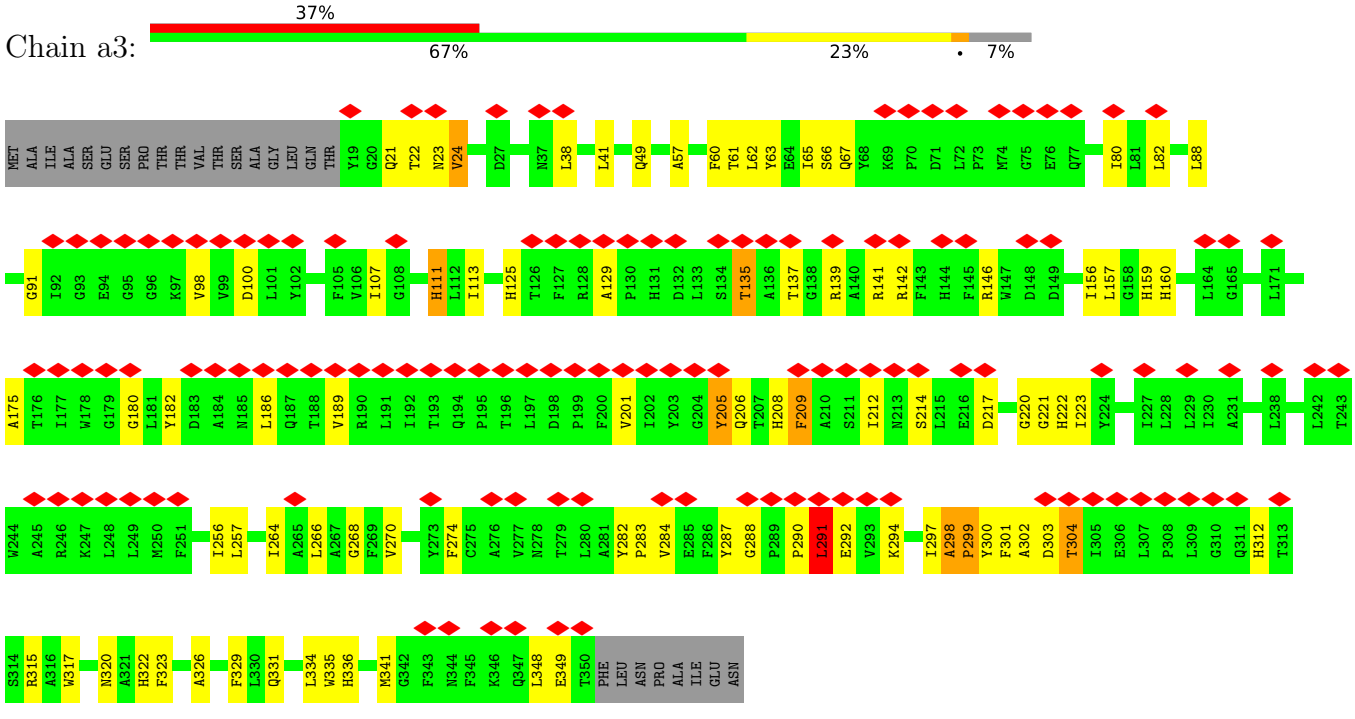
• Molecule 13: Iron stress in-duced protein A

Chain a2:



• Molecule 13: Iron stress in-duced protein A

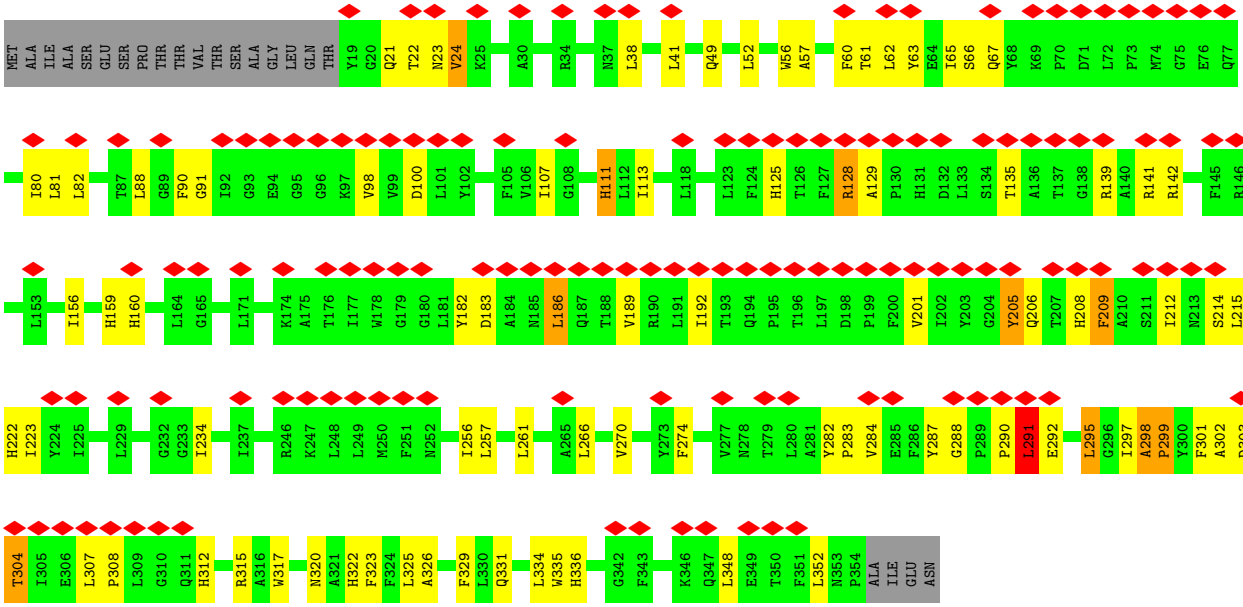
Chain a3:



• Molecule 13: Iron stress in-duced protein A

Chain a4:

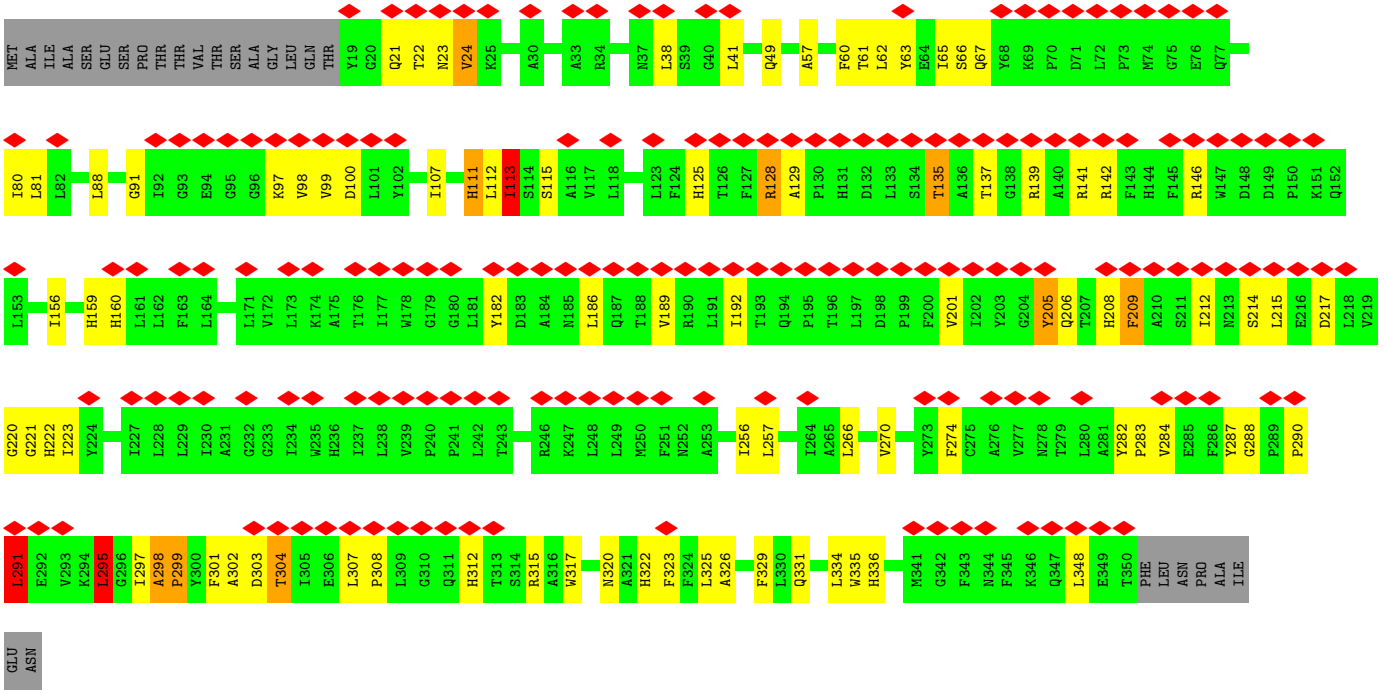




• Molecule 13: Iron stress in-duced protein A

Chain a5:

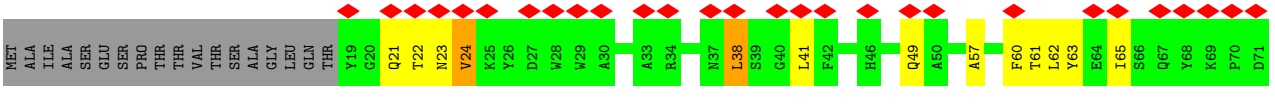


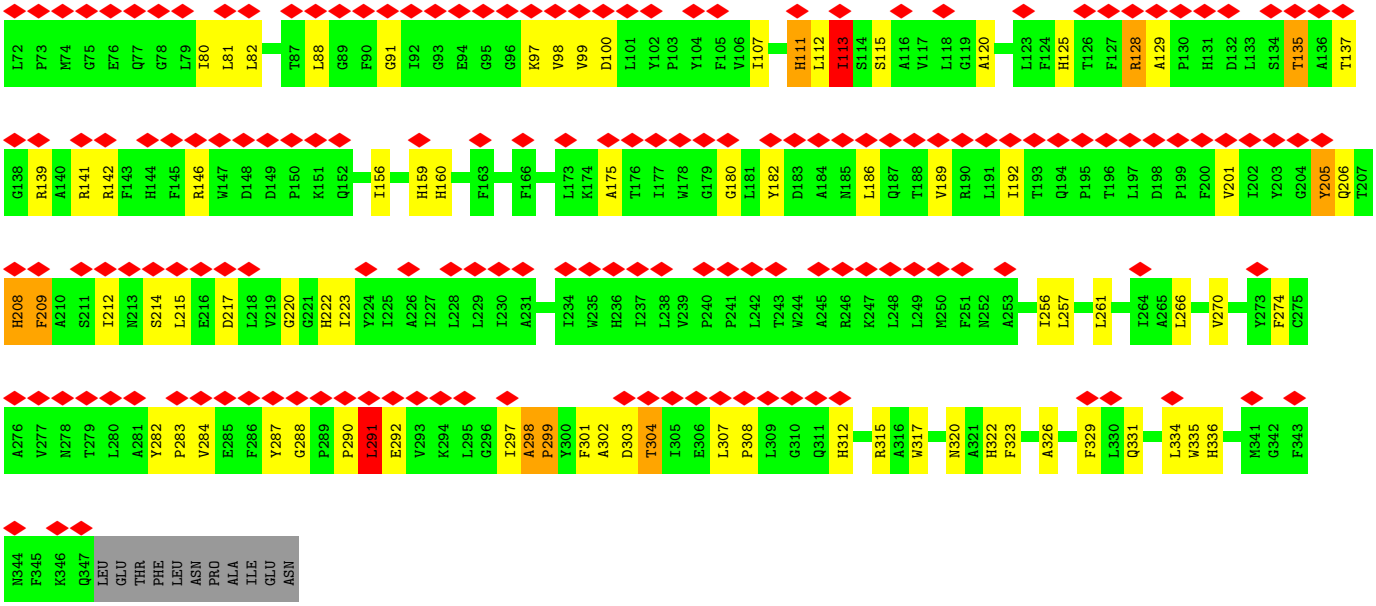


• Molecule 13: Iron stress in-duced protein A

Chain a6:



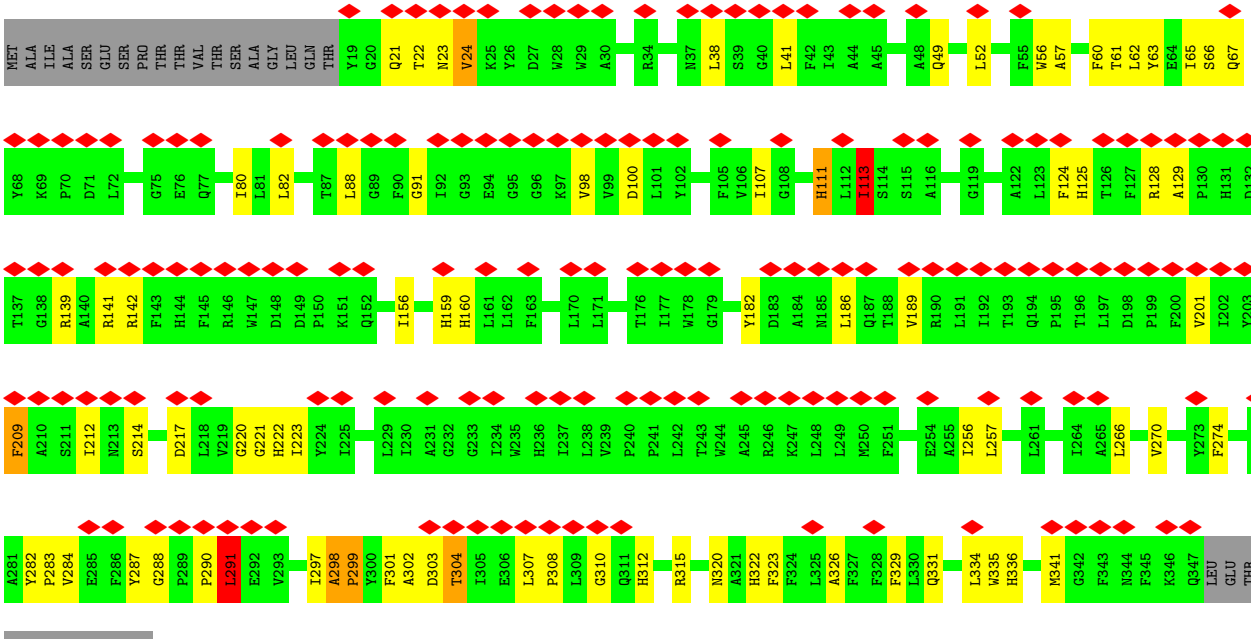




• Molecule 13: Iron stress in-duced protein A

Chain b1:

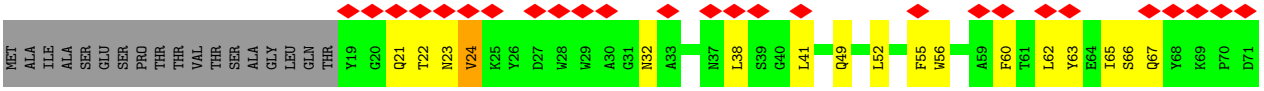


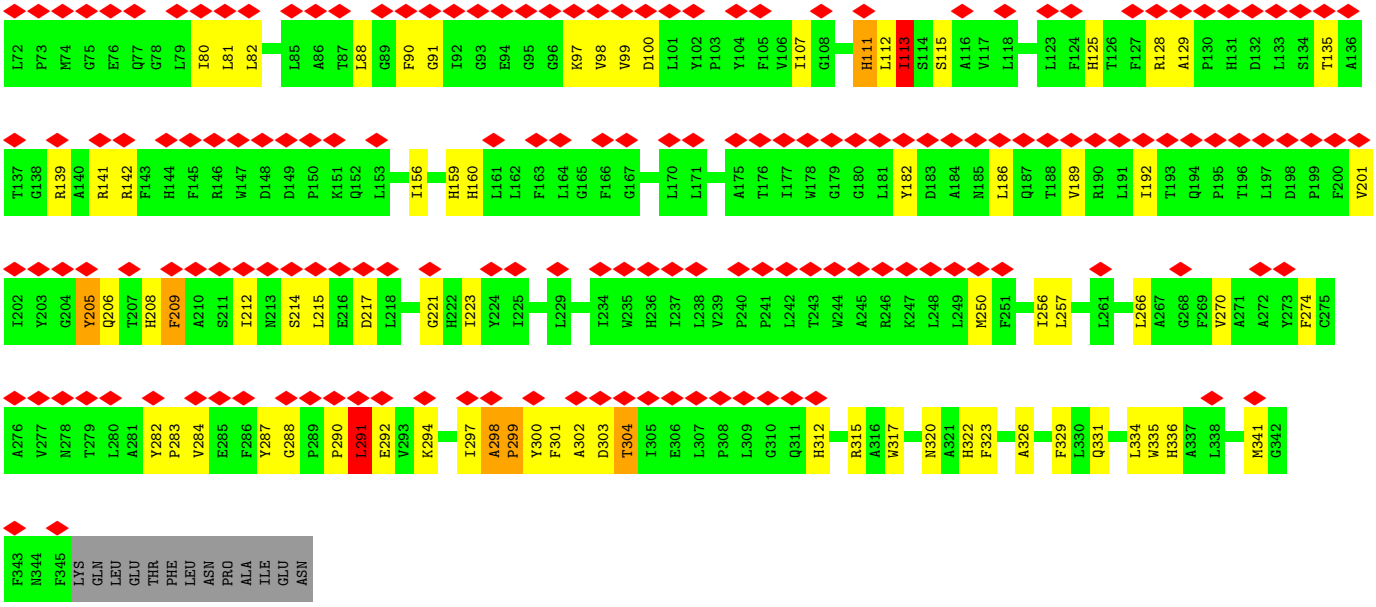


• Molecule 13: Iron stress in-duced protein A

Chain b2:



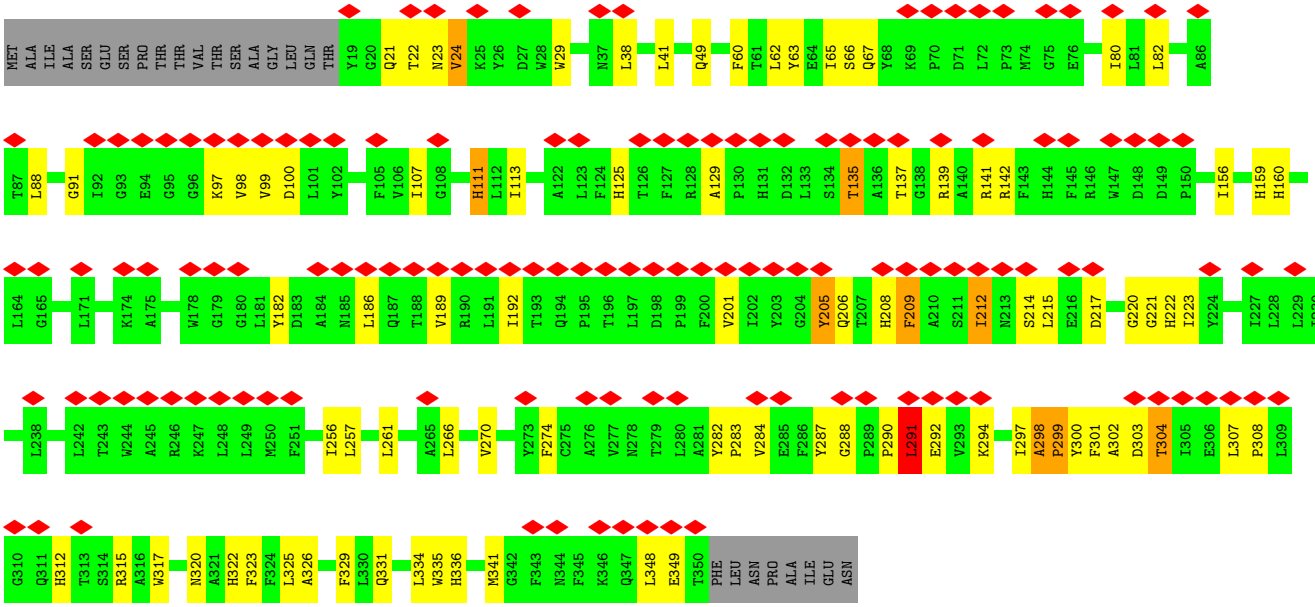




• Molecule 13: Iron stress in-duced protein A

Chain b3:

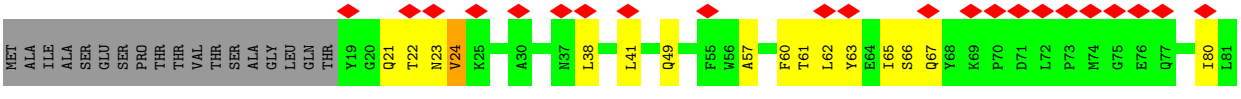


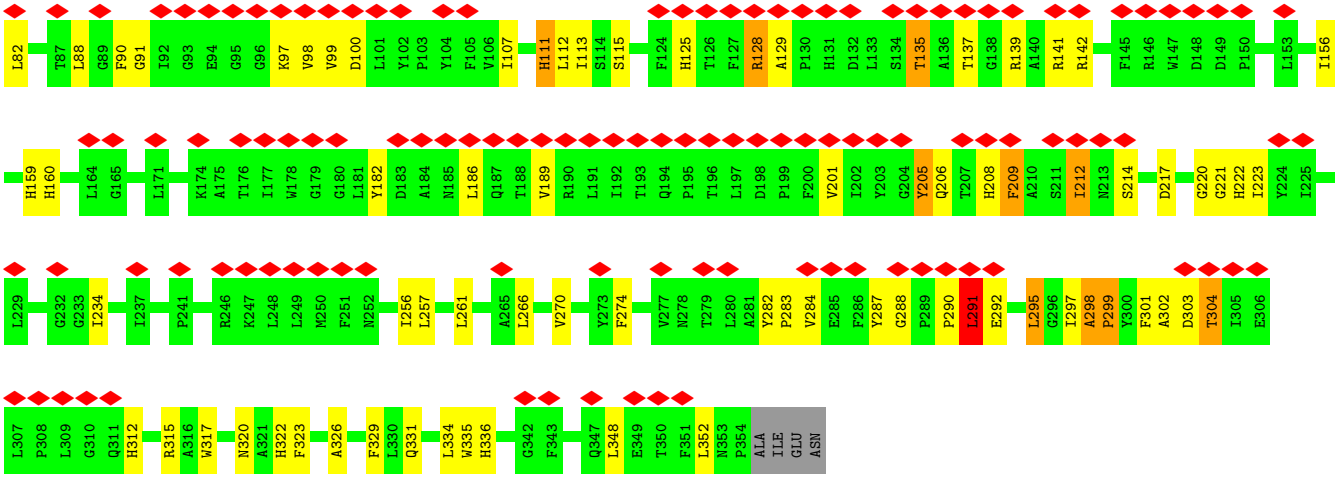


• Molecule 13: Iron stress in-duced protein A

Chain b4:



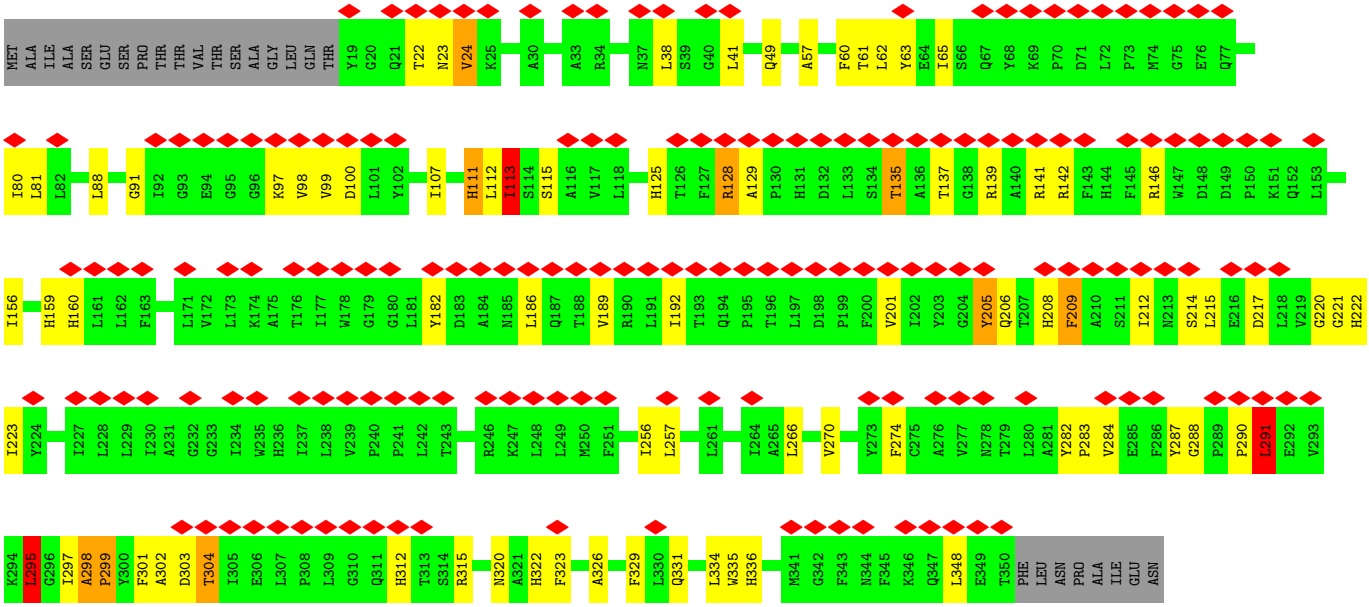




• Molecule 13: Iron stress in-duced protein A

Chain b5:

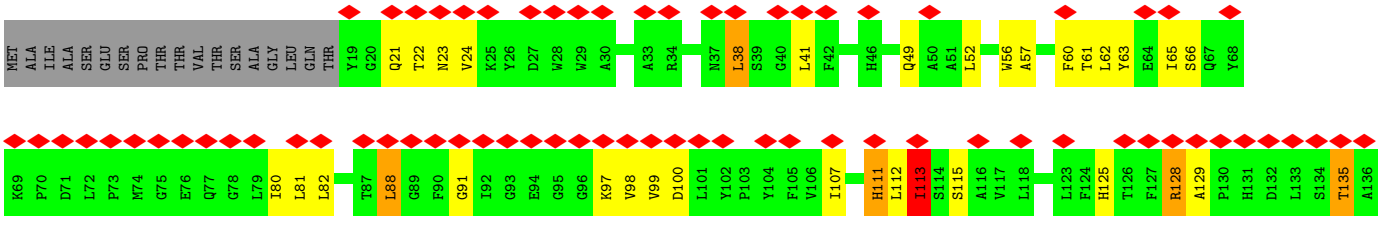


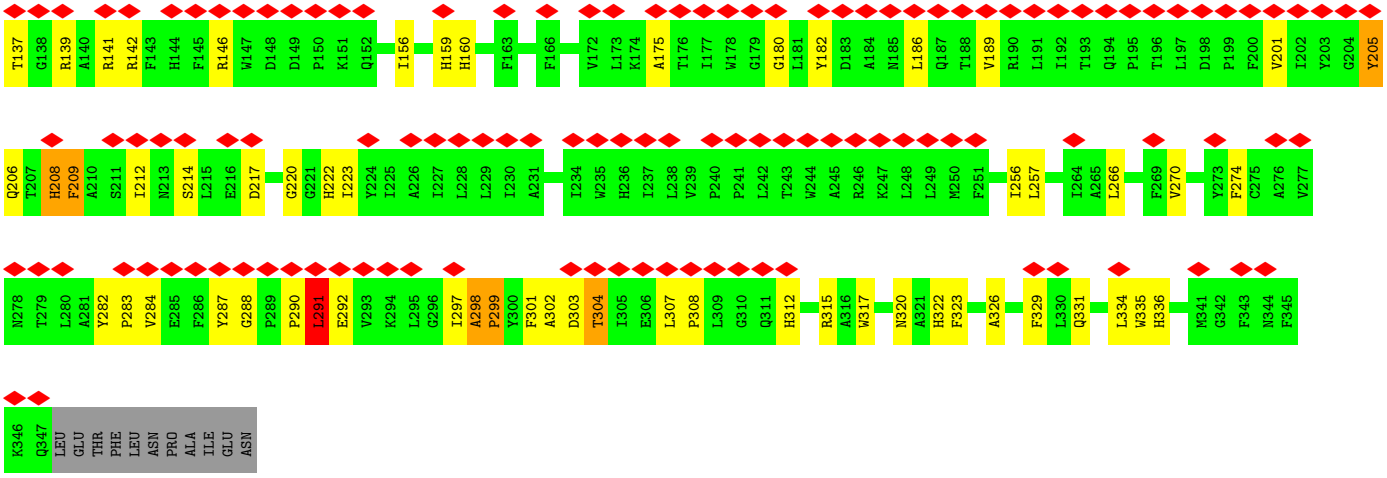


• Molecule 13: Iron stress in-duced protein A

Chain b6:



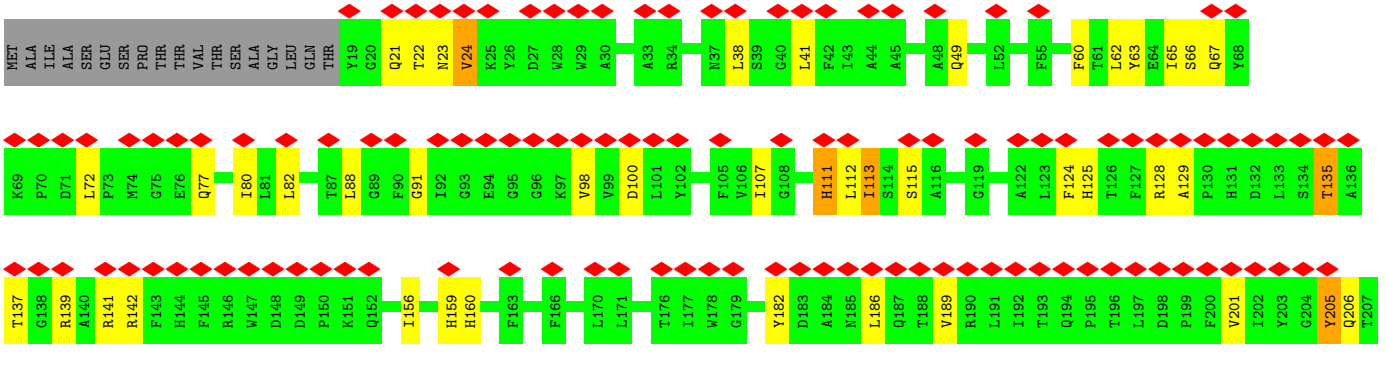




• Molecule 13: Iron stress in-duced protein A

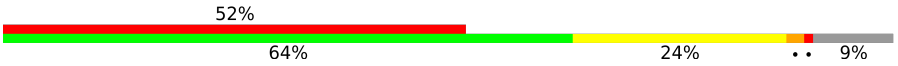
Chain c1:

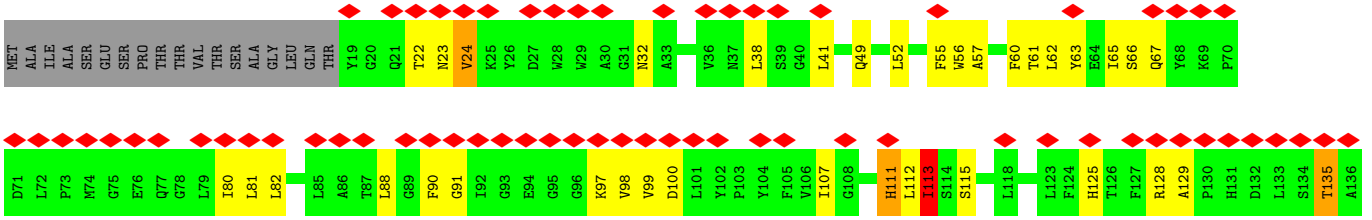


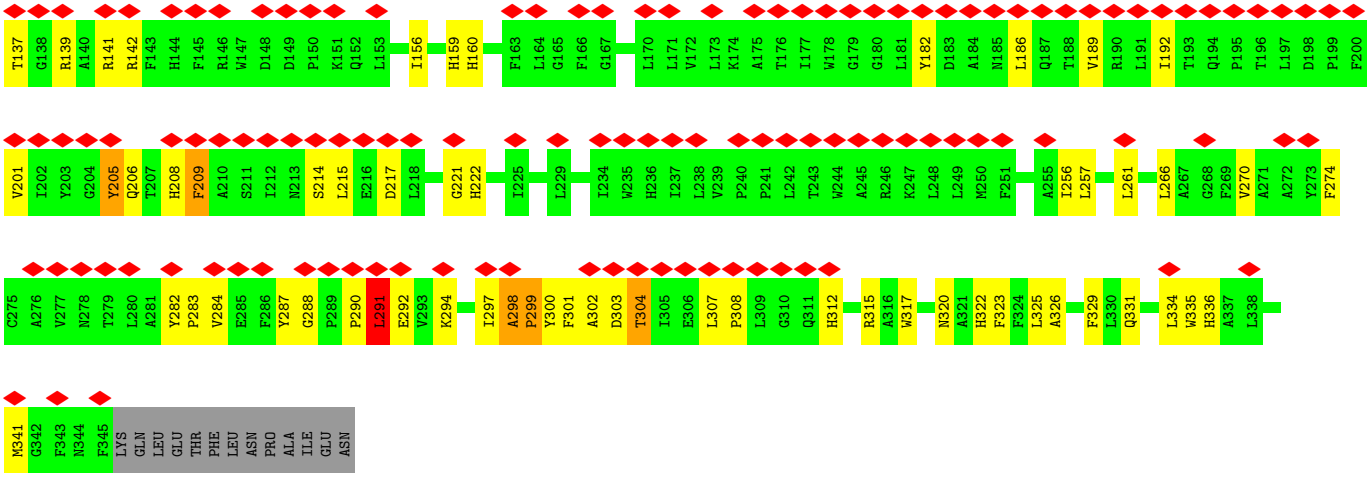


• Molecule 13: Iron stress in-duced protein A

Chain c2:



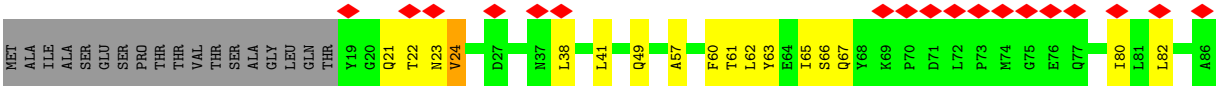


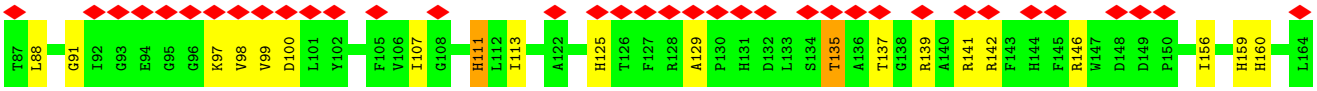


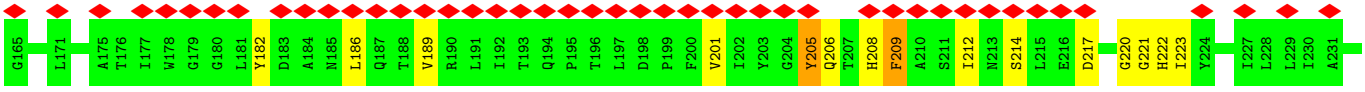
• Molecule 13: Iron stress in-duced protein A

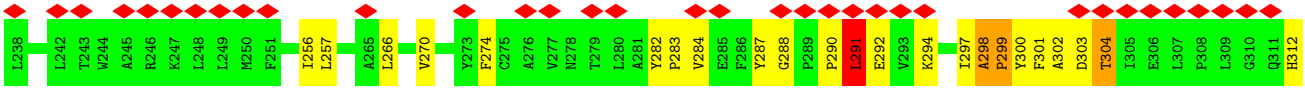
Chain c3:

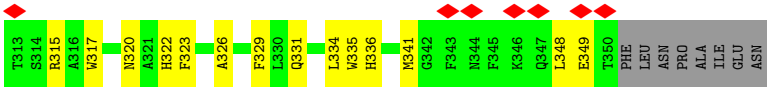








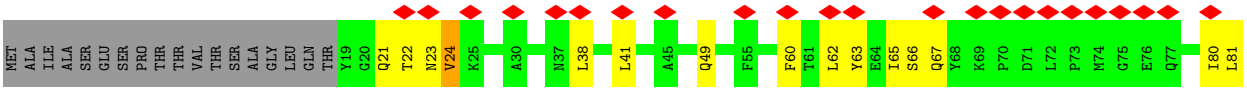


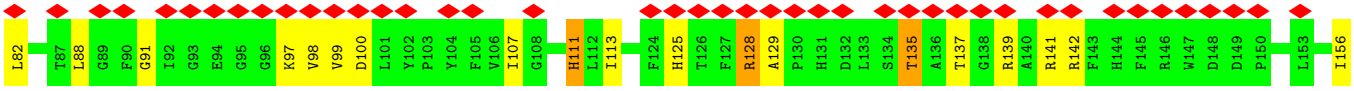


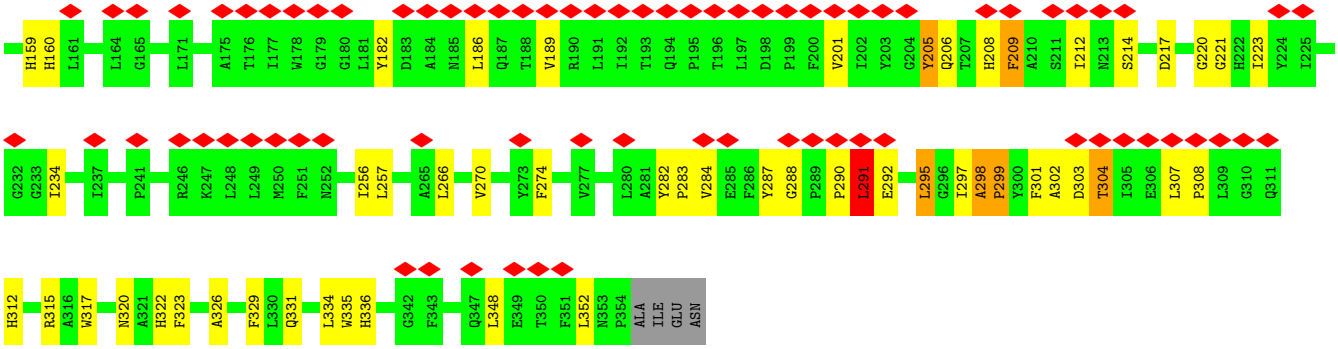
• Molecule 13: Iron stress in-duced protein A

Chain c4:





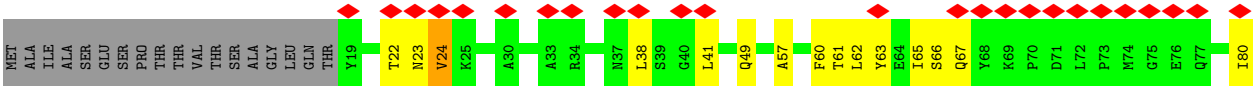


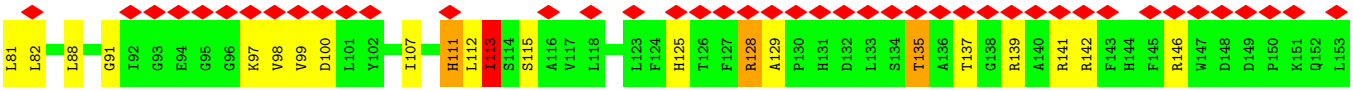


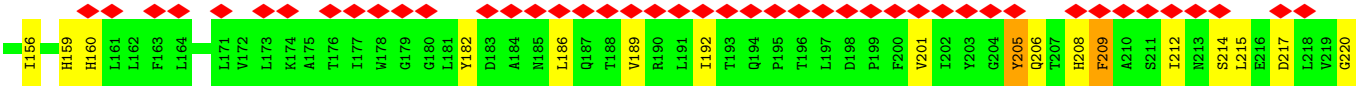
• Molecule 13: Iron stress in-duced protein A

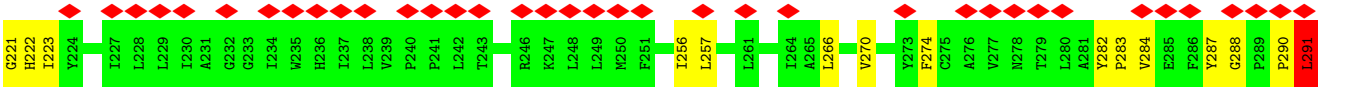
Chain c5:

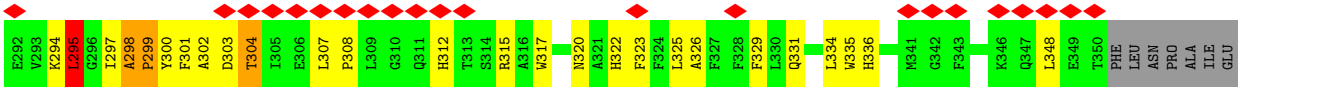










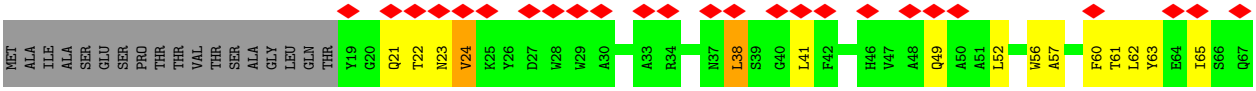


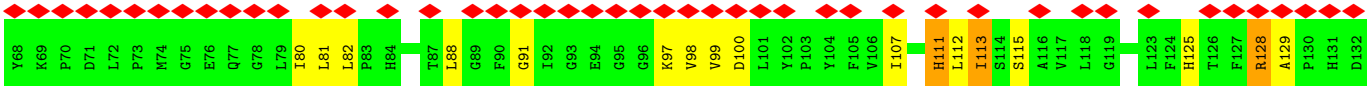


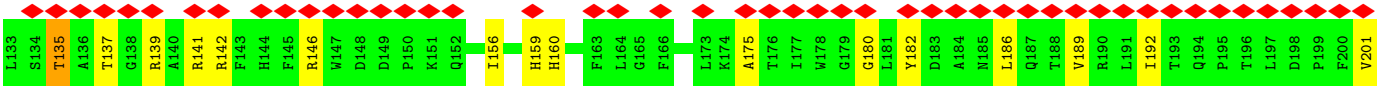
• Molecule 13: Iron stress in-duced protein A

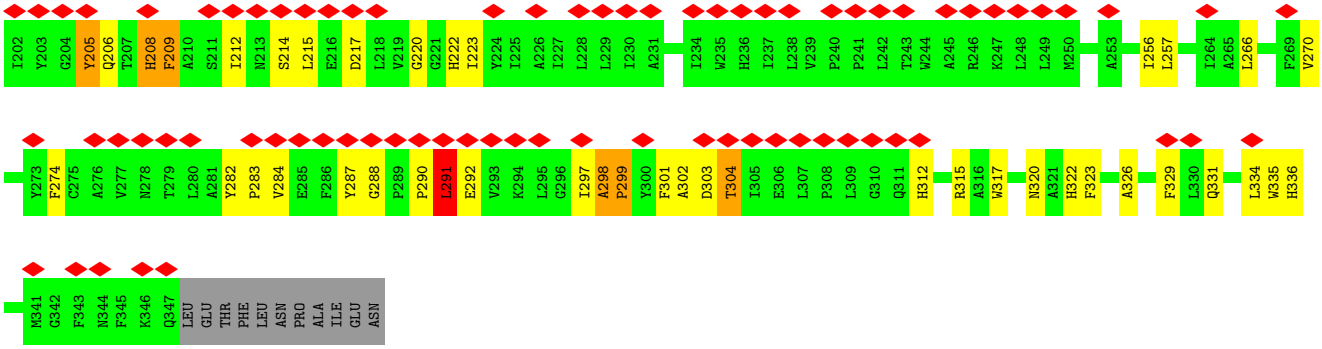
Chain c6:










I202 Y203 G204 Y205 Q206 T207 H208 F209 A210 S211 I212 N213 S214 L215 E216 D217 L218 V219 G220 G221 H222 I223 Y224 I225 A226 I227 L228 L229 I230 A231 I234 W235 H236 I237 L238 V239 P240 P241 L242 T243 W244 A245 R246 K247 L248 L249 M250 A253 I256 L257 I264 A265 L266 F269 V270
Y273 F274 C275 A276 V277 N278 T279 L280 A281 Y282 P283 V284 E285 F286 Y287 G288 P289 P290 L291 E292 V293 K294 L295 G296 I297 A298 P299 Y300 F301 A302 D303 T304 I305 E306 L307 P308 L309 G310 Q311 H312 R315 A316 W317 N320 A321 H322 F323 A326 F329 L330 Q331 L334 W335 H336
M341 G342 F343 N344 F345 K346 Q347 LEU GLU THR PHE LEU ASN PRO ALA ILE GLU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	303983	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.291	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	534.24, 534.24, 534.24	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	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: CL0, LMG, CLA, CA, PQN, SF4, BCR, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	aA	0.53	0/6000	0.54	0/8180
1	bA	0.53	0/6000	0.54	0/8180
1	cA	0.53	0/6000	0.54	0/8180
2	aB	0.52	0/6096	0.57	0/8332
2	bB	0.52	0/6096	0.56	0/8332
2	cB	0.52	0/6096	0.57	0/8332
3	aC	0.52	0/608	0.70	2/824 (0.2%)
3	bC	0.52	0/608	0.70	2/824 (0.2%)
3	cC	0.52	0/608	0.70	2/824 (0.2%)
4	aD	0.42	0/1101	0.51	0/1492
4	bD	0.42	0/1101	0.51	0/1492
4	cD	0.42	0/1101	0.51	0/1492
5	aE	0.35	0/551	0.44	0/750
5	bE	0.35	0/551	0.44	0/750
5	cE	0.35	0/551	0.44	0/750
6	aF	0.41	0/1087	0.56	0/1476
6	bF	0.40	0/1087	0.55	0/1476
6	cF	0.41	0/1087	0.55	0/1476
7	aI	0.55	0/312	0.70	0/425
7	bI	0.55	0/312	0.70	0/425
7	cI	0.55	0/312	0.70	0/425
8	aJ	0.47	0/350	0.64	0/477
8	bJ	0.47	0/350	0.64	0/477
8	cJ	0.47	0/350	0.64	0/477
9	aK	0.23	0/206	0.34	0/281
9	bK	0.23	0/206	0.34	0/281
9	cK	0.23	0/206	0.34	0/281
10	aL	0.52	0/1148	0.54	0/1558
10	bL	0.52	0/1148	0.55	0/1558
10	cL	0.52	0/1148	0.54	0/1558
11	aM	0.44	0/244	0.60	0/332
11	bM	0.44	0/244	0.60	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	cM	0.44	0/244	0.60	0/332
12	aX	0.37	0/242	0.42	0/332
12	bX	0.37	0/242	0.42	0/332
12	cX	0.37	0/242	0.42	0/332
13	a1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	a2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	a3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	a4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	a5	0.41	1/2695 (0.0%)	0.75	15/3680 (0.4%)
13	a6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	b1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	b2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	b3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	b4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	b5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	b6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	c1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	c2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	c3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	c4	0.42	1/2731 (0.0%)	0.72	14/3730 (0.4%)
13	c5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	c6	0.40	1/2671 (0.0%)	0.72	14/3647 (0.4%)
All	All	0.46	18/102183 (0.0%)	0.64	256/139401 (0.2%)

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
2	aB	0	1
2	bB	0	1
2	cB	0	1
6	aF	0	1
6	bF	0	1
6	cF	0	1
11	aM	0	1
11	bM	0	1
11	cM	0	1
13	a1	0	3
13	a2	0	3
13	a3	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	a4	0	3
13	a5	0	3
13	a6	0	3
13	b1	0	3
13	b2	0	3
13	b3	0	3
13	b4	0	3
13	b5	0	3
13	b6	0	3
13	c1	0	3
13	c2	0	3
13	c3	0	3
13	c4	0	3
13	c5	0	3
13	c6	0	3
All	All	0	63

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	b1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	c4	297	ILE	CB-CG2	-6.66	1.30	1.52
13	a4	297	ILE	CB-CG2	-6.64	1.30	1.52
13	b4	297	ILE	CB-CG2	-6.64	1.30	1.52
13	c1	297	ILE	CB-CG2	-6.59	1.30	1.52
13	b5	297	ILE	CB-CG2	-6.56	1.30	1.52
13	a5	297	ILE	CB-CG2	-6.54	1.30	1.52
13	c5	297	ILE	CB-CG2	-6.53	1.30	1.52
13	c3	297	ILE	CB-CG2	-6.49	1.31	1.52
13	a3	297	ILE	CB-CG2	-6.45	1.31	1.52
13	b3	297	ILE	CB-CG2	-6.45	1.31	1.52
13	c6	297	ILE	CB-CG2	-6.41	1.31	1.52
13	a6	297	ILE	CB-CG2	-6.36	1.31	1.52
13	b6	297	ILE	CB-CG2	-6.32	1.31	1.52
13	b2	297	ILE	CB-CG2	-6.16	1.32	1.52
13	c2	297	ILE	CB-CG2	-6.15	1.32	1.52
13	a2	297	ILE	CB-CG2	-6.07	1.32	1.52

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a1	113	ILE	N-CA-CB	-7.92	103.50	112.21
13	c1	113	ILE	N-CA-CB	-7.87	103.55	112.21
13	b6	113	ILE	N-CA-CB	-7.86	103.56	112.21
13	b5	113	ILE	N-CA-CB	-7.62	103.26	112.33
13	a6	113	ILE	N-CA-CB	-7.61	103.84	112.21
13	c5	113	ILE	N-CA-CB	-7.61	103.28	112.33
13	a5	113	ILE	N-CA-CB	-7.58	103.32	112.33
13	b3	209	PHE	CA-C-N	7.39	135.65	121.54
13	b3	209	PHE	C-N-CA	7.39	135.65	121.54
13	c3	209	PHE	CA-C-N	7.35	135.58	121.54
13	c3	209	PHE	C-N-CA	7.35	135.58	121.54
13	a3	209	PHE	CA-C-N	7.33	135.53	121.54
13	a3	209	PHE	C-N-CA	7.33	135.53	121.54
13	a4	209	PHE	CA-C-N	7.25	135.40	121.54
13	a4	209	PHE	C-N-CA	7.25	135.40	121.54
13	c4	209	PHE	CA-C-N	7.25	135.38	121.54
13	c4	209	PHE	C-N-CA	7.25	135.38	121.54
13	b4	209	PHE	CA-C-N	7.23	135.35	121.54
13	b4	209	PHE	C-N-CA	7.23	135.35	121.54
13	b6	209	PHE	CA-C-N	7.20	135.29	121.54
13	b6	209	PHE	C-N-CA	7.20	135.29	121.54
13	c6	209	PHE	CA-C-N	7.17	135.23	121.54
13	c6	209	PHE	C-N-CA	7.17	135.23	121.54
13	a6	209	PHE	CA-C-N	7.16	135.22	121.54
13	a6	209	PHE	C-N-CA	7.16	135.22	121.54
13	c1	209	PHE	CA-C-N	7.13	135.16	121.54
13	c1	209	PHE	C-N-CA	7.13	135.16	121.54
13	a1	209	PHE	CA-C-N	7.09	135.09	121.54
13	a1	209	PHE	C-N-CA	7.09	135.09	121.54
13	b1	209	PHE	CA-C-N	7.09	135.08	121.54
13	b1	209	PHE	C-N-CA	7.09	135.08	121.54
13	c5	209	PHE	CA-C-N	7.08	135.06	121.54
13	c5	209	PHE	C-N-CA	7.08	135.06	121.54
13	a5	209	PHE	CA-C-N	7.07	135.05	121.54
13	a5	209	PHE	C-N-CA	7.07	135.05	121.54
13	b5	209	PHE	CA-C-N	7.07	135.04	121.54
13	b5	209	PHE	C-N-CA	7.07	135.04	121.54
13	b4	299	PRO	N-CD-CG	-6.91	92.83	103.20
13	a4	299	PRO	N-CD-CG	-6.89	92.86	103.20
13	c4	299	PRO	N-CD-CG	-6.87	92.89	103.20
13	b3	135	THR	CA-C-N	6.87	134.06	121.70
13	b3	135	THR	C-N-CA	6.87	134.06	121.70
13	c4	135	THR	CA-C-N	6.87	134.06	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c4	135	THR	C-N-CA	6.87	134.06	121.70
13	c3	135	THR	CA-C-N	6.86	134.05	121.70
13	c3	135	THR	C-N-CA	6.86	134.05	121.70
13	a3	135	THR	CA-C-N	6.86	134.05	121.70
13	a3	135	THR	C-N-CA	6.86	134.05	121.70
13	c2	209	PHE	CA-C-N	6.86	134.63	121.54
13	c2	209	PHE	C-N-CA	6.86	134.63	121.54
13	b4	135	THR	CA-C-N	6.85	134.03	121.70
13	b4	135	THR	C-N-CA	6.85	134.03	121.70
13	a4	135	THR	CA-C-N	6.85	134.02	121.70
13	a4	135	THR	C-N-CA	6.85	134.02	121.70
13	b1	113	ILE	N-CA-CB	-6.83	103.44	112.26
13	a2	209	PHE	CA-C-N	6.83	134.58	121.54
13	a2	209	PHE	C-N-CA	6.83	134.58	121.54
13	b1	135	THR	CA-C-N	6.81	133.97	121.70
13	b1	135	THR	C-N-CA	6.81	133.97	121.70
13	a6	135	THR	CA-C-N	6.81	133.96	121.70
13	a6	135	THR	C-N-CA	6.81	133.96	121.70
13	a1	135	THR	CA-C-N	6.81	133.95	121.70
13	a1	135	THR	C-N-CA	6.81	133.95	121.70
13	c1	135	THR	CA-C-N	6.81	133.95	121.70
13	c1	135	THR	C-N-CA	6.81	133.95	121.70
13	c6	135	THR	CA-C-N	6.81	133.95	121.70
13	c6	135	THR	C-N-CA	6.81	133.95	121.70
13	c5	135	THR	CA-C-N	6.81	133.95	121.70
13	c5	135	THR	C-N-CA	6.81	133.95	121.70
13	a5	135	THR	CA-C-N	6.80	133.95	121.70
13	a5	135	THR	C-N-CA	6.80	133.95	121.70
13	b2	209	PHE	CA-C-N	6.80	134.52	121.54
13	b2	209	PHE	C-N-CA	6.80	134.52	121.54
13	b6	135	THR	CA-C-N	6.79	133.93	121.70
13	b6	135	THR	C-N-CA	6.79	133.93	121.70
13	b5	299	PRO	N-CD-CG	-6.78	93.03	103.20
13	c5	299	PRO	N-CD-CG	-6.78	93.03	103.20
13	b5	135	THR	CA-C-N	6.78	133.90	121.70
13	b5	135	THR	C-N-CA	6.78	133.90	121.70
13	a5	299	PRO	N-CD-CG	-6.76	93.05	103.20
13	c3	299	PRO	N-CD-CG	-6.69	93.17	103.20
13	a2	135	THR	CA-C-N	6.68	133.72	121.70
13	a2	135	THR	C-N-CA	6.68	133.72	121.70
13	b2	135	THR	CA-C-N	6.68	133.72	121.70
13	b2	135	THR	C-N-CA	6.68	133.72	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a3	299	PRO	N-CD-CG	-6.65	93.23	103.20
13	c2	135	THR	CA-C-N	6.65	133.67	121.70
13	c2	135	THR	C-N-CA	6.65	133.67	121.70
13	b3	299	PRO	N-CD-CG	-6.63	93.25	103.20
13	a2	299	PRO	N-CD-CG	-6.62	93.27	103.20
13	b2	299	PRO	N-CD-CG	-6.59	93.31	103.20
13	a6	128	ARG	NE-CZ-NH1	-6.59	114.91	121.50
13	a2	113	ILE	N-CA-CB	-6.59	103.80	112.36
13	b6	299	PRO	N-CD-CG	-6.58	93.33	103.20
13	b2	113	ILE	N-CA-CB	-6.58	103.80	112.36
13	c2	299	PRO	N-CD-CG	-6.56	93.36	103.20
13	a6	299	PRO	N-CD-CG	-6.56	93.36	103.20
13	c6	299	PRO	N-CD-CG	-6.55	93.37	103.20
13	a2	113	ILE	CB-CA-C	6.54	118.12	110.93
13	b2	113	ILE	CB-CA-C	6.54	118.12	110.93
13	c2	113	ILE	N-CA-CB	-6.52	103.89	112.36
13	c2	113	ILE	CB-CA-C	6.50	118.08	110.93
13	b1	299	PRO	N-CD-CG	-6.44	93.54	103.20
13	b6	128	ARG	NE-CZ-NH2	6.39	124.95	119.20
13	c1	299	PRO	N-CD-CG	-6.35	93.68	103.20
13	a1	299	PRO	N-CD-CG	-6.25	93.83	103.20
13	b6	128	ARG	NE-CZ-NH1	-6.22	115.28	121.50
13	c6	128	ARG	NE-CZ-NH2	6.11	124.70	119.20
13	c5	295	LEU	CA-CB-CG	6.10	137.64	116.30
13	b5	295	LEU	CA-CB-CG	6.07	137.54	116.30
13	a5	295	LEU	CA-CB-CG	6.01	137.32	116.30
13	b4	295	LEU	CA-CB-CG	5.94	137.08	116.30
13	c4	295	LEU	CA-CB-CG	5.91	136.97	116.30
13	a4	295	LEU	CA-CB-CG	5.90	136.94	116.30
13	c5	291	LEU	CA-C-N	5.75	132.51	121.54
13	c5	291	LEU	C-N-CA	5.75	132.51	121.54
3	cC	61	PHE	CA-C-N	5.75	132.51	121.54
3	cC	61	PHE	C-N-CA	5.75	132.51	121.54
3	bC	61	PHE	CA-C-N	5.74	132.51	121.54
3	bC	61	PHE	C-N-CA	5.74	132.51	121.54
3	aC	61	PHE	CA-C-N	5.73	132.48	121.54
3	aC	61	PHE	C-N-CA	5.73	132.48	121.54
13	b5	291	LEU	CA-C-N	5.73	132.48	121.54
13	b5	291	LEU	C-N-CA	5.73	132.48	121.54
13	a5	291	LEU	CA-C-N	5.72	132.47	121.54
13	a5	291	LEU	C-N-CA	5.72	132.47	121.54
13	b4	128	ARG	NE-CZ-NH2	5.64	124.28	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a4	128	ARG	NE-CZ-NH2	5.62	124.26	119.20
13	a2	291	LEU	CA-C-N	5.58	132.20	121.54
13	a2	291	LEU	C-N-CA	5.58	132.20	121.54
13	a4	24	VAL	CA-C-N	5.57	131.73	121.70
13	a4	24	VAL	C-N-CA	5.57	131.73	121.70
13	c4	24	VAL	CA-C-N	5.56	131.71	121.70
13	c4	24	VAL	C-N-CA	5.56	131.71	121.70
13	b4	24	VAL	CA-C-N	5.55	131.69	121.70
13	b4	24	VAL	C-N-CA	5.55	131.69	121.70
13	c4	128	ARG	NE-CZ-NH2	5.54	124.18	119.20
13	c2	291	LEU	CA-C-N	5.53	132.10	121.54
13	c2	291	LEU	C-N-CA	5.53	132.10	121.54
13	a3	24	VAL	CA-C-N	5.50	131.59	121.70
13	a3	24	VAL	C-N-CA	5.50	131.59	121.70
13	b4	291	LEU	CA-C-N	5.50	132.04	121.54
13	b4	291	LEU	C-N-CA	5.50	132.04	121.54
13	c4	291	LEU	CA-C-N	5.49	132.03	121.54
13	c4	291	LEU	C-N-CA	5.49	132.03	121.54
13	c6	113	ILE	N-CA-CB	-5.49	103.73	112.07
13	a4	291	LEU	CA-C-N	5.49	132.02	121.54
13	a4	291	LEU	C-N-CA	5.49	132.02	121.54
13	c3	24	VAL	CA-C-N	5.48	131.56	121.70
13	c3	24	VAL	C-N-CA	5.48	131.56	121.70
13	a1	24	VAL	CA-C-N	5.47	131.55	121.70
13	a1	24	VAL	C-N-CA	5.47	131.55	121.70
13	b1	24	VAL	CA-C-N	5.47	131.55	121.70
13	b1	24	VAL	C-N-CA	5.47	131.55	121.70
13	b5	24	VAL	CA-C-N	5.47	131.55	121.70
13	b5	24	VAL	C-N-CA	5.47	131.55	121.70
13	b6	24	VAL	CA-C-N	5.47	131.55	121.70
13	b6	24	VAL	C-N-CA	5.47	131.55	121.70
13	a6	24	VAL	CA-C-N	5.47	131.55	121.70
13	a6	24	VAL	C-N-CA	5.47	131.55	121.70
13	b3	24	VAL	CA-C-N	5.47	131.55	121.70
13	b3	24	VAL	C-N-CA	5.47	131.55	121.70
13	a3	291	LEU	CA-C-N	5.47	131.99	121.54
13	a3	291	LEU	C-N-CA	5.47	131.99	121.54
13	b2	291	LEU	CA-C-N	5.47	131.99	121.54
13	b2	291	LEU	C-N-CA	5.47	131.99	121.54
13	c5	24	VAL	CA-C-N	5.47	131.54	121.70
13	c5	24	VAL	C-N-CA	5.47	131.54	121.70
13	c6	24	VAL	CA-C-N	5.47	131.54	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c6	24	VAL	C-N-CA	5.47	131.54	121.70
13	a1	291	LEU	CA-C-N	5.46	131.98	121.54
13	a1	291	LEU	C-N-CA	5.46	131.98	121.54
13	c1	24	VAL	CA-C-N	5.45	131.52	121.70
13	c1	24	VAL	C-N-CA	5.45	131.52	121.70
13	a5	24	VAL	CA-C-N	5.44	131.50	121.70
13	a5	24	VAL	C-N-CA	5.44	131.50	121.70
13	c3	291	LEU	CA-C-N	5.42	131.90	121.54
13	c3	291	LEU	C-N-CA	5.42	131.90	121.54
13	b3	291	LEU	CA-CB-CG	5.42	135.25	116.30
13	c1	291	LEU	CA-C-N	5.40	131.86	121.54
13	c1	291	LEU	C-N-CA	5.40	131.86	121.54
13	b6	298	ALA	CA-C-N	-5.40	114.23	119.90
13	b6	298	ALA	C-N-CA	-5.40	114.23	119.90
13	c3	291	LEU	CA-CB-CG	5.40	135.20	116.30
13	a6	291	LEU	CA-C-N	5.40	131.85	121.54
13	a6	291	LEU	C-N-CA	5.40	131.85	121.54
13	b6	291	LEU	CA-C-N	5.39	131.84	121.54
13	b6	291	LEU	C-N-CA	5.39	131.84	121.54
13	c5	298	ALA	CA-C-N	-5.39	114.24	119.90
13	c5	298	ALA	C-N-CA	-5.39	114.24	119.90
13	c6	298	ALA	CA-C-N	-5.38	114.25	119.90
13	c6	298	ALA	C-N-CA	-5.38	114.25	119.90
13	c1	298	ALA	CA-C-N	-5.38	114.25	119.90
13	c1	298	ALA	C-N-CA	-5.38	114.25	119.90
13	b5	298	ALA	CA-C-N	-5.38	114.25	119.90
13	b5	298	ALA	C-N-CA	-5.38	114.25	119.90
13	c6	291	LEU	CA-C-N	5.38	131.81	121.54
13	c6	291	LEU	C-N-CA	5.38	131.81	121.54
13	a3	291	LEU	CA-CB-CG	5.38	135.11	116.30
13	b1	291	LEU	CA-C-N	5.37	131.80	121.54
13	b1	291	LEU	C-N-CA	5.37	131.80	121.54
13	c2	291	LEU	CA-CB-CG	5.37	135.10	116.30
13	a6	298	ALA	CA-C-N	-5.37	114.26	119.90
13	a6	298	ALA	C-N-CA	-5.37	114.26	119.90
13	b2	291	LEU	CA-CB-CG	5.37	135.09	116.30
13	a5	298	ALA	CA-C-N	-5.37	114.27	119.90
13	a5	298	ALA	C-N-CA	-5.37	114.27	119.90
13	b3	291	LEU	CA-C-N	5.36	131.77	121.54
13	b3	291	LEU	C-N-CA	5.36	131.77	121.54
13	a2	291	LEU	CA-CB-CG	5.34	135.00	116.30
13	b1	298	ALA	CA-C-N	-5.33	114.30	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b1	298	ALA	C-N-CA	-5.33	114.30	119.90
13	b4	291	LEU	CA-CB-CG	5.33	134.94	116.30
13	c6	291	LEU	CA-CB-CG	5.32	134.92	116.30
13	c4	291	LEU	CA-CB-CG	5.32	134.92	116.30
13	b6	291	LEU	CA-CB-CG	5.32	134.91	116.30
13	a6	128	ARG	NE-CZ-NH2	5.31	123.98	119.20
13	b1	291	LEU	CA-CB-CG	5.31	134.89	116.30
13	b2	24	VAL	CA-C-N	5.31	131.26	121.70
13	b2	24	VAL	C-N-CA	5.31	131.26	121.70
13	a1	298	ALA	CA-C-N	-5.31	114.33	119.90
13	a1	298	ALA	C-N-CA	-5.31	114.33	119.90
13	a5	128	ARG	NE-CZ-NH2	5.30	123.97	119.20
13	a4	291	LEU	CA-CB-CG	5.30	134.84	116.30
13	a6	291	LEU	CA-CB-CG	5.30	134.84	116.30
13	c5	128	ARG	NE-CZ-NH2	5.29	123.96	119.20
13	b5	128	ARG	NE-CZ-NH2	5.28	123.95	119.20
13	c3	298	ALA	CA-C-N	-5.26	114.38	119.90
13	c3	298	ALA	C-N-CA	-5.26	114.38	119.90
13	c1	291	LEU	CA-CB-CG	5.25	134.66	116.30
13	b3	298	ALA	CA-C-N	-5.24	114.40	119.90
13	b3	298	ALA	C-N-CA	-5.24	114.40	119.90
13	a2	24	VAL	CA-C-N	5.23	131.12	121.70
13	a2	24	VAL	C-N-CA	5.23	131.12	121.70
13	c5	291	LEU	CA-CB-CG	5.23	134.61	116.30
13	c2	24	VAL	CA-C-N	5.22	131.10	121.70
13	c2	24	VAL	C-N-CA	5.22	131.10	121.70
13	b5	291	LEU	CA-CB-CG	5.22	134.56	116.30
13	a1	291	LEU	CA-CB-CG	5.21	134.55	116.30
13	b4	298	ALA	CA-C-N	-5.21	114.43	119.90
13	b4	298	ALA	C-N-CA	-5.21	114.43	119.90
13	a3	298	ALA	CA-C-N	-5.21	114.43	119.90
13	a3	298	ALA	C-N-CA	-5.21	114.43	119.90
13	a4	298	ALA	CA-C-N	-5.19	114.45	119.90
13	a4	298	ALA	C-N-CA	-5.19	114.45	119.90
13	a2	298	ALA	CA-C-N	-5.17	114.47	119.90
13	a2	298	ALA	C-N-CA	-5.17	114.47	119.90
13	a5	291	LEU	CA-CB-CG	5.17	134.39	116.30
13	c4	298	ALA	CA-C-N	-5.16	114.48	119.90
13	c4	298	ALA	C-N-CA	-5.16	114.48	119.90
13	b2	298	ALA	CA-C-N	-5.13	114.51	119.90
13	b2	298	ALA	C-N-CA	-5.13	114.51	119.90
13	b5	113	ILE	CB-CA-C	5.10	116.13	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c5	113	ILE	CB-CA-C	5.10	116.13	110.62
13	c2	298	ALA	CA-C-N	-5.09	114.56	119.90
13	c2	298	ALA	C-N-CA	-5.09	114.56	119.90

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a1	282	TYR	Peptide
13	a1	290	PRO	Peptide
13	a1	302	ALA	Peptide
13	a2	282	TYR	Peptide
13	a2	290	PRO	Peptide
13	a2	302	ALA	Peptide
13	a3	282	TYR	Peptide
13	a3	290	PRO	Peptide
13	a3	302	ALA	Peptide
13	a4	282	TYR	Peptide
13	a4	290	PRO	Peptide
13	a4	302	ALA	Peptide
13	a5	282	TYR	Peptide
13	a5	290	PRO	Peptide
13	a5	302	ALA	Peptide
13	a6	282	TYR	Peptide
13	a6	290	PRO	Peptide
13	a6	302	ALA	Peptide
2	aB	234	GLN	Peptide
6	aF	125	ALA	Peptide
11	aM	29	LEU	Peptide
13	b1	282	TYR	Peptide
13	b1	290	PRO	Peptide
13	b1	302	ALA	Peptide
13	b2	282	TYR	Peptide
13	b2	290	PRO	Peptide
13	b2	302	ALA	Peptide
13	b3	282	TYR	Peptide
13	b3	290	PRO	Peptide
13	b3	302	ALA	Peptide
13	b4	282	TYR	Peptide
13	b4	290	PRO	Peptide
13	b4	302	ALA	Peptide
13	b5	282	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	b5	290	PRO	Peptide
13	b5	302	ALA	Peptide
13	b6	282	TYR	Peptide
13	b6	290	PRO	Peptide
13	b6	302	ALA	Peptide
2	bB	234	GLN	Peptide
6	bF	125	ALA	Peptide
11	bM	29	LEU	Peptide
13	c1	282	TYR	Peptide
13	c1	290	PRO	Peptide
13	c1	302	ALA	Peptide
13	c2	282	TYR	Peptide
13	c2	290	PRO	Peptide
13	c2	302	ALA	Peptide
13	c3	282	TYR	Peptide
13	c3	290	PRO	Peptide
13	c3	302	ALA	Peptide
13	c4	282	TYR	Peptide
13	c4	290	PRO	Peptide
13	c4	302	ALA	Peptide
13	c5	282	TYR	Peptide
13	c5	290	PRO	Peptide
13	c5	302	ALA	Peptide
13	c6	282	TYR	Peptide
13	c6	290	PRO	Peptide
13	c6	302	ALA	Peptide
2	cB	234	GLN	Peptide
6	cF	125	ALA	Peptide
11	cM	29	LEU	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	aA	5801	0	5660	126	0
1	bA	5801	0	5660	126	0
1	cA	5801	0	5660	128	0
2	aB	5879	0	5627	119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	bB	5879	0	5627	120	0
2	cB	5879	0	5627	121	0
3	aC	598	0	580	11	0
3	bC	598	0	580	12	0
3	cC	598	0	580	17	0
4	aD	1075	0	1077	20	0
4	bD	1075	0	1077	22	0
4	cD	1075	0	1077	24	0
5	aE	539	0	528	8	0
5	bE	539	0	528	8	0
5	cE	539	0	528	9	0
6	aF	1065	0	1077	29	0
6	bF	1065	0	1077	21	0
6	cF	1065	0	1077	30	0
7	aI	301	0	306	7	0
7	bI	301	0	306	3	0
7	cI	301	0	306	6	0
8	aJ	338	0	347	20	0
8	bJ	338	0	347	9	0
8	cJ	338	0	347	17	0
9	aK	208	0	106	0	0
9	bK	208	0	106	0	0
9	cK	208	0	106	0	0
10	aL	1119	0	1125	21	0
10	bL	1119	0	1125	23	0
10	cL	1119	0	1125	23	0
11	aM	241	0	264	6	0
11	bM	241	0	264	5	0
11	cM	241	0	264	5	0
12	aX	233	0	231	2	0
12	bX	233	0	231	2	0
12	cX	233	0	231	2	0
13	a1	2583	0	2568	69	0
13	a2	2565	0	2545	77	0
13	a3	2607	0	2590	64	0
13	a4	2641	0	2624	67	0
13	a5	2607	0	2591	67	0
13	a6	2583	0	2567	73	0
13	b1	2583	0	2568	69	0
13	b2	2565	0	2545	73	0
13	b3	2607	0	2590	65	0
13	b4	2641	0	2624	67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	b5	2607	0	2591	62	0
13	b6	2583	0	2567	73	0
13	c1	2583	0	2568	69	0
13	c2	2565	0	2545	73	0
13	c3	2607	0	2590	62	0
13	c4	2641	0	2624	63	0
13	c5	2607	0	2591	68	0
13	c6	2583	0	2567	69	0
14	aA	65	0	72	4	0
14	bA	65	0	72	4	0
14	cA	65	0	72	3	0
15	a1	830	0	720	40	0
15	a2	960	0	862	64	0
15	a3	895	0	790	49	0
15	a4	895	0	792	53	0
15	a5	895	0	792	52	0
15	a6	895	0	790	53	0
15	aA	2557	0	2532	109	0
15	aB	2414	0	2369	111	0
15	aJ	127	0	91	5	0
15	aK	45	0	33	0	0
15	aL	195	0	216	11	0
15	aX	45	0	33	2	0
15	b1	830	0	720	41	0
15	b2	960	0	862	67	0
15	b3	895	0	790	47	0
15	b4	895	0	792	54	0
15	b5	895	0	792	56	0
15	b6	895	0	790	53	0
15	bA	2557	0	2532	113	0
15	bB	2414	0	2369	113	0
15	bF	45	0	33	2	0
15	bJ	82	0	58	1	0
15	bK	45	0	33	0	0
15	bL	195	0	216	11	0
15	bX	45	0	33	3	0
15	c1	830	0	720	40	0
15	c2	960	0	862	65	0
15	c3	895	0	790	48	0
15	c4	895	0	792	47	0
15	c5	895	0	792	52	0
15	c6	895	0	790	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	cA	2506	0	2491	112	0
15	cB	2414	0	2369	109	0
15	cF	96	0	74	6	0
15	cJ	82	0	58	1	0
15	cK	45	0	33	0	0
15	cL	195	0	216	13	0
15	cX	45	0	33	2	0
16	aA	33	0	46	3	0
16	aB	33	0	46	3	0
16	bA	33	0	46	3	0
16	bB	33	0	46	4	0
16	cA	33	0	46	4	0
16	cB	33	0	46	3	0
17	aA	8	0	0	0	0
17	aC	16	0	0	0	0
17	bA	8	0	0	0	0
17	bC	16	0	0	0	0
17	cA	8	0	0	0	0
17	cC	16	0	0	0	0
18	a1	200	0	280	15	0
18	a2	160	0	224	14	0
18	a3	160	0	224	9	0
18	a4	160	0	224	13	0
18	a5	120	0	168	10	0
18	a6	200	0	280	14	0
18	aA	200	0	278	13	0
18	aB	225	0	313	16	0
18	aF	120	0	168	15	0
18	aI	120	0	168	10	0
18	aJ	80	0	112	8	0
18	aK	40	0	56	1	0
18	aL	40	0	56	1	0
18	aM	40	0	56	3	0
18	b1	160	0	224	13	0
18	b2	160	0	224	14	0
18	b3	160	0	224	11	0
18	b4	160	0	224	12	0
18	b5	120	0	168	9	0
18	b6	200	0	280	11	0
18	bA	240	0	334	15	0
18	bB	265	0	369	25	0
18	bF	40	0	56	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	bI	80	0	112	4	0
18	bJ	120	0	168	14	0
18	bL	120	0	168	6	0
18	bM	40	0	56	4	0
18	c1	160	0	224	12	0
18	c2	160	0	224	11	0
18	c3	160	0	224	9	0
18	c4	160	0	224	13	0
18	c5	120	0	168	9	0
18	c6	160	0	224	10	0
18	cA	200	0	278	13	0
18	cB	225	0	313	16	0
18	cF	120	0	168	17	0
18	cI	80	0	112	4	0
18	cJ	80	0	112	9	0
18	cK	40	0	56	1	0
18	cL	40	0	56	3	0
18	cM	40	0	56	4	0
19	aA	76	0	98	3	0
19	aX	23	0	16	1	0
19	bA	76	0	98	3	0
19	bX	23	0	16	0	0
19	cA	76	0	98	3	0
19	cX	23	0	16	0	0
20	aB	55	0	86	1	0
20	bB	55	0	86	1	0
20	cB	55	0	86	1	0
21	aL	1	0	0	0	0
21	bL	1	0	0	0	0
21	cL	1	0	0	0	0
22	aA	3	0	0	0	0
22	aB	3	0	0	0	0
22	aL	1	0	0	0	0
22	bA	3	0	0	0	0
22	bB	3	0	0	0	0
22	bL	1	0	0	0	0
22	cA	2	0	0	0	0
22	cB	3	0	0	0	0
22	cF	1	0	0	0	0
22	cL	1	0	0	0	0
All	All	137634	0	136044	3155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (3155) 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)
13:a1:331:GLN:HE22	15:a1:414:CLA:C1B	1.70	1.04
13:c1:331:GLN:HE22	15:c1:415:CLA:C1B	1.70	1.04
13:b1:331:GLN:HE22	15:b1:415:CLA:C1B	1.71	1.03
13:b3:331:GLN:HE22	15:b3:415:CLA:C1B	1.73	1.01
13:c5:331:GLN:HE22	15:c5:415:CLA:C1B	1.74	1.00
13:b6:331:GLN:HE22	15:b6:416:CLA:C1B	1.73	1.00
13:c6:331:GLN:HE22	15:c6:417:CLA:C1B	1.73	1.00
13:a5:331:GLN:HE22	15:a5:415:CLA:C1B	1.73	1.00
13:a6:331:GLN:HE22	15:a6:416:CLA:C1B	1.73	1.00
13:b5:331:GLN:HE22	15:b5:415:CLA:C1B	1.74	1.00
13:c3:331:GLN:HE22	15:c3:415:CLA:C1B	1.73	0.99
13:a3:331:GLN:HE22	15:a3:415:CLA:C1B	1.74	0.99
13:c2:331:GLN:HE22	15:c2:416:CLA:C1B	1.75	0.99
13:b2:331:GLN:HE22	15:b2:416:CLA:C1B	1.74	0.99
13:b4:331:GLN:HE22	15:b4:415:CLA:C1B	1.74	0.98
13:c4:331:GLN:HE22	15:c4:415:CLA:C1B	1.75	0.98
13:a2:331:GLN:HE22	15:a2:416:CLA:C1B	1.75	0.98
13:a4:331:GLN:HE22	15:a4:415:CLA:C1B	1.74	0.98
13:b6:331:GLN:HE22	15:b6:416:CLA:C4B	1.95	0.80
18:a2:420:BCR:H343	15:a3:416:CLA:HBB1	1.64	0.80
13:a6:331:GLN:HE22	15:a6:416:CLA:C4B	1.95	0.79
18:b2:420:BCR:H343	15:b3:416:CLA:HBB1	1.64	0.79
13:a6:128:ARG:NH1	15:a6:422:CLA:H2A	1.97	0.78
13:b2:331:GLN:HE22	15:b2:416:CLA:C4B	1.97	0.78
13:c6:331:GLN:HE22	15:c6:417:CLA:C4B	1.95	0.78
13:c2:331:GLN:HE22	15:c2:416:CLA:C4B	1.97	0.78
18:c2:420:BCR:H343	15:c3:416:CLA:HBB1	1.65	0.76
13:c6:128:ARG:NH1	15:c6:401:CLA:H2A	2.00	0.76
13:a2:331:GLN:HE22	15:a2:416:CLA:C4B	1.97	0.76
13:a1:331:GLN:HE22	15:a1:414:CLA:C4B	2.00	0.74
15:b4:402:CLA:HMA1	18:b4:420:BCR:H401	1.71	0.73
15:aB:821:CLA:HBB1	18:aB:844:BCR:H14C	1.71	0.73
15:bB:821:CLA:HBB1	18:bB:844:BCR:H14C	1.71	0.73
15:c2:402:CLA:HMA1	18:c2:421:BCR:H401	1.71	0.73
15:bB:832:CLA:HBC3	18:bF:202:BCR:H362	1.70	0.72
15:cB:821:CLA:HBB1	18:cB:844:BCR:H14C	1.71	0.72
15:c3:402:CLA:HMA1	18:c3:420:BCR:H401	1.71	0.72
15:c4:402:CLA:HMA1	18:c4:420:BCR:H401	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c6:404:CLA:HMA1	18:c6:421:BCR:H401	1.71	0.72
13:a3:331:GLN:HE22	15:a3:415:CLA:C4B	2.02	0.72
13:b5:331:GLN:HE22	15:b5:415:CLA:C4B	2.02	0.72
15:b5:402:CLA:HMA1	18:b5:419:BCR:H401	1.71	0.72
15:c1:402:CLA:HMA1	18:c1:420:BCR:H401	1.71	0.72
13:b6:128:ARG:NH1	15:b6:422:CLA:H2A	2.03	0.72
1:aA:285:LEU:HD21	1:aA:378:PRO:HD2	1.72	0.72
15:b3:402:CLA:HMA1	18:b3:420:BCR:H401	1.71	0.72
15:a2:402:CLA:HMA1	18:a2:421:BCR:H401	1.71	0.72
15:b1:402:CLA:HMA1	18:b1:420:BCR:H401	1.71	0.72
2:bB:318:PHE:HB2	15:bB:824:CLA:HMA1	1.72	0.72
15:a4:402:CLA:HMA1	18:a4:420:BCR:H401	1.70	0.71
1:bA:285:LEU:HD21	1:bA:378:PRO:HD2	1.72	0.71
15:a5:402:CLA:HMA1	18:a5:419:BCR:H401	1.70	0.71
13:a5:331:GLN:HE22	15:a5:415:CLA:C4B	2.03	0.71
1:cA:285:LEU:HD21	1:cA:378:PRO:HD2	1.72	0.71
15:c5:402:CLA:HMA1	18:c5:419:BCR:H401	1.70	0.71
15:a1:401:CLA:HMA1	18:a1:419:BCR:H401	1.71	0.71
13:c1:331:GLN:NE2	15:c1:415:CLA:C1B	2.47	0.71
15:b6:403:CLA:HMA1	18:b6:420:BCR:H401	1.71	0.71
15:cB:831:CLA:HBC1	18:cB:847:BCR:H23C	1.73	0.71
13:c5:331:GLN:HE22	15:c5:415:CLA:C4B	2.03	0.71
8:aJ:19:MET:HE1	15:aJ:201:CLA:HBC2	1.70	0.71
15:bB:831:CLA:HBC1	18:bB:847:BCR:H23C	1.73	0.71
15:a6:403:CLA:HMA1	18:a6:420:BCR:H401	1.71	0.71
2:cB:318:PHE:HB2	15:cB:824:CLA:HMA1	1.72	0.70
13:a6:287:TYR:HB3	13:a6:315:ARG:HB2	1.74	0.70
15:b2:402:CLA:HMA1	18:b2:421:BCR:H401	1.71	0.70
15:a3:402:CLA:HMA1	18:a3:420:BCR:H401	1.72	0.70
13:b1:331:GLN:HE22	15:b1:415:CLA:C4B	2.04	0.70
13:c1:331:GLN:HE22	15:c1:415:CLA:C4B	2.04	0.70
13:b3:331:GLN:HE22	15:b3:415:CLA:C4B	2.04	0.70
2:aB:318:PHE:HB2	15:aB:824:CLA:HMA1	1.72	0.70
13:b1:331:GLN:NE2	15:b1:415:CLA:C1B	2.47	0.69
13:b6:287:TYR:HB3	13:b6:315:ARG:HB2	1.74	0.69
13:c6:287:TYR:HB3	13:c6:315:ARG:HB2	1.74	0.69
13:b2:287:TYR:HB3	13:b2:315:ARG:HB2	1.75	0.69
6:aF:37:ARG:NH2	8:aJ:34:PRO:O	2.26	0.69
1:bA:647:ASN:HD22	2:bB:657:LEU:HD11	1.58	0.69
13:b4:287:TYR:HB3	13:b4:315:ARG:HB2	1.75	0.69
13:c3:287:TYR:HB3	13:c3:315:ARG:HB2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a2:287:TYR:HB3	13:a2:315:ARG:HB2	1.75	0.69
13:b3:287:TYR:HB3	13:b3:315:ARG:HB2	1.75	0.69
1:aA:709:ASN:HB3	6:aF:136:ILE:HG23	1.75	0.69
15:aB:831:CLA:HBC1	18:aB:847:BCR:H23C	1.73	0.68
6:aF:101:ILE:N	8:aJ:9:SER:O	2.26	0.68
1:bA:396:HIS:HE1	15:bA:829:CLA:ND	1.91	0.68
13:b6:331:GLN:NE2	15:b6:416:CLA:C1B	2.49	0.68
13:a4:287:TYR:HB3	13:a4:315:ARG:HB2	1.76	0.68
13:c2:287:TYR:HB3	13:c2:315:ARG:HB2	1.75	0.68
13:a3:287:TYR:HB3	13:a3:315:ARG:HB2	1.75	0.68
2:bB:94:GLN:OE1	15:bB:811:CLA:NB	2.27	0.68
13:b1:287:TYR:HB3	13:b1:315:ARG:HB2	1.76	0.68
15:bB:814:CLA:H42	18:bB:845:BCR:H19C	1.76	0.68
13:a6:301:PHE:H	13:a6:320:ASN:HD21	1.42	0.68
13:b5:287:TYR:HB3	13:b5:315:ARG:HB2	1.75	0.68
15:cB:814:CLA:H42	18:cB:845:BCR:H19C	1.75	0.68
13:a5:287:TYR:HB3	13:a5:315:ARG:HB2	1.75	0.68
13:c4:287:TYR:HB3	13:c4:315:ARG:HB2	1.75	0.67
15:cF:203:CLA:HBC2	8:cJ:19:MET:HE1	1.75	0.67
13:c1:287:TYR:HB3	13:c1:315:ARG:HB2	1.76	0.67
1:aA:215:HIS:HE1	15:aA:815:CLA:NA	1.92	0.67
13:c5:287:TYR:HB3	13:c5:315:ARG:HB2	1.75	0.67
2:aB:94:GLN:OE1	15:aB:811:CLA:NB	2.27	0.67
2:cB:94:GLN:OE1	15:cB:811:CLA:NB	2.27	0.67
18:cF:202:BCR:H332	18:cJ:103:BCR:HC22	1.77	0.67
13:c3:331:GLN:HE22	15:c3:415:CLA:C4B	2.06	0.67
18:aF:201:BCR:H332	18:aJ:204:BCR:HC22	1.77	0.67
13:c3:301:PHE:H	13:c3:320:ASN:HD21	1.42	0.67
13:b5:295:LEU:HB2	13:b5:299:PRO:HA	1.77	0.67
13:c4:301:PHE:H	13:c4:320:ASN:HD21	1.42	0.67
13:a4:301:PHE:H	13:a4:320:ASN:HD21	1.42	0.67
1:aA:396:HIS:HE1	15:aA:829:CLA:ND	1.91	0.66
6:cF:99:ILE:O	8:cJ:11:ALA:N	2.28	0.66
13:c6:301:PHE:H	13:c6:320:ASN:HD21	1.42	0.66
1:cA:215:HIS:HE1	15:cA:815:CLA:NA	1.92	0.66
2:cB:377:HIS:HE1	15:cB:828:CLA:ND	1.93	0.66
13:c5:295:LEU:HB2	13:c5:299:PRO:HA	1.77	0.66
1:bA:333:LYS:H	15:bA:845:CLA:HBC3	1.60	0.66
13:a1:287:TYR:HB3	13:a1:315:ARG:HB2	1.76	0.66
13:a6:331:GLN:NE2	15:a6:416:CLA:C1B	2.49	0.66
13:c2:336:HIS:HE1	15:c2:409:CLA:NA	1.93	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aB:814:CLA:H42	18:aB:845:BCR:H19C	1.75	0.66
13:a5:295:LEU:HB2	13:a5:299:PRO:HA	1.78	0.66
1:bA:215:HIS:HE1	15:bA:815:CLA:NA	1.92	0.66
13:b3:301:PHE:H	13:b3:320:ASN:HD21	1.42	0.66
15:cA:810:CLA:H122	18:cJ:103:BCR:H272	1.78	0.66
2:aB:377:HIS:HE1	15:aB:828:CLA:ND	1.93	0.66
13:a4:331:GLN:HE22	15:a4:415:CLA:C4B	2.09	0.66
13:b6:331:GLN:NE2	15:b6:416:CLA:C4B	2.54	0.66
1:cA:333:LYS:H	15:cA:844:CLA:HBC3	1.60	0.66
13:a3:301:PHE:H	13:a3:320:ASN:HD21	1.42	0.66
2:aB:55:ILE:HD11	18:aM:101:BCR:HC7	1.77	0.65
13:a3:139:ARG:HB3	13:a3:142:ARG:HG2	1.79	0.65
13:b6:301:PHE:H	13:b6:320:ASN:HD21	1.42	0.65
13:b3:336:HIS:HE1	15:b3:408:CLA:NA	1.94	0.65
13:b4:301:PHE:H	13:b4:320:ASN:HD21	1.42	0.65
13:c5:331:GLN:NE2	15:c5:415:CLA:C4B	2.52	0.65
15:aB:807:CLA:H162	15:aB:829:CLA:HBB2	1.78	0.65
15:bB:807:CLA:H162	15:bB:829:CLA:HBB2	1.78	0.65
13:c3:336:HIS:HE1	15:c3:408:CLA:NA	1.95	0.65
3:aC:5:LYS:HD3	4:aD:113:ASN:HB3	1.79	0.65
13:a1:331:GLN:NE2	15:a1:414:CLA:C1B	2.48	0.65
13:b5:331:GLN:NE2	15:b5:415:CLA:C1B	2.49	0.65
1:cA:111:LYS:HB2	1:cA:130:VAL:HG12	1.78	0.65
13:c4:336:HIS:HE1	15:c4:408:CLA:NA	1.95	0.65
15:aA:841:CLA:H2A	15:aA:841:CLA:HED3	1.78	0.65
18:b4:419:BCR:H343	15:b5:416:CLA:HBB1	1.78	0.65
13:b4:331:GLN:HE22	15:b4:415:CLA:C4B	2.09	0.65
15:aA:810:CLA:H122	18:aJ:204:BCR:H272	1.78	0.65
13:a4:139:ARG:HB3	13:a4:142:ARG:HG2	1.79	0.65
13:b1:301:PHE:H	13:b1:320:ASN:HD21	1.44	0.65
1:cA:396:HIS:HE1	15:cA:829:CLA:ND	1.91	0.65
15:bA:825:CLA:HAC1	18:bA:851:BCR:HC8	1.79	0.65
13:b2:336:HIS:HE1	15:b2:409:CLA:NA	1.94	0.65
18:a4:419:BCR:H343	15:a5:416:CLA:HBB1	1.78	0.65
1:bA:458:LEU:O	1:bA:462:ASN:ND2	2.27	0.65
13:b1:139:ARG:HB3	13:b1:142:ARG:HG2	1.78	0.65
1:cA:458:LEU:O	1:cA:462:ASN:ND2	2.27	0.65
18:c4:419:BCR:H343	15:c5:416:CLA:HBB1	1.78	0.65
6:cF:101:ILE:N	8:cJ:9:SER:O	2.29	0.65
2:aB:133:ASP:N	2:aB:133:ASP:OD1	2.29	0.64
2:cB:55:ILE:HD11	18:cM:101:BCR:HC7	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:133:ASP:OD1	2:cB:133:ASP:N	2.29	0.64
13:c3:139:ARG:HB3	13:c3:142:ARG:HG2	1.79	0.64
15:aB:811:CLA:HED1	18:aI:102:BCR:HC7	1.78	0.64
1:bA:111:LYS:HB2	1:bA:130:VAL:HG12	1.78	0.64
2:cB:192:HIS:HE1	15:cB:815:CLA:NA	1.95	0.64
13:b2:301:PHE:H	13:b2:320:ASN:HD21	1.45	0.64
3:cC:18:ARG:HG2	4:cD:103:GLU:HG2	1.79	0.64
13:c4:331:GLN:HE22	15:c4:415:CLA:C4B	2.09	0.64
13:a5:139:ARG:HB3	13:a5:142:ARG:HG2	1.80	0.64
11:cM:5:ASP:OD1	11:cM:5:ASP:N	2.30	0.64
13:c5:301:PHE:H	13:c5:320:ASN:HD21	1.44	0.64
13:a1:301:PHE:H	13:a1:320:ASN:HD21	1.44	0.64
15:bA:841:CLA:H2A	15:bA:841:CLA:HED3	1.78	0.64
11:bM:5:ASP:OD1	11:bM:5:ASP:N	2.30	0.64
13:b3:139:ARG:HB3	13:b3:142:ARG:HG2	1.79	0.64
13:b3:331:GLN:NE2	15:b3:415:CLA:C1B	2.50	0.64
1:aA:111:LYS:HB2	1:aA:130:VAL:HG12	1.78	0.64
1:aA:333:LYS:H	15:aA:845:CLA:HBC3	1.60	0.64
13:a1:139:ARG:HB3	13:a1:142:ARG:HG2	1.78	0.64
13:c1:139:ARG:HB3	13:c1:142:ARG:HG2	1.79	0.64
13:a2:301:PHE:H	13:a2:320:ASN:HD21	1.44	0.64
15:cB:807:CLA:H162	15:cB:829:CLA:HBB2	1.78	0.64
15:cB:809:CLA:H102	15:cB:809:CLA:H2	1.80	0.64
6:cF:100:ILE:HG12	8:cJ:10:THR:HG22	1.78	0.64
13:c6:331:GLN:NE2	15:c6:417:CLA:C1B	2.49	0.64
13:b4:139:ARG:HB3	13:b4:142:ARG:HG2	1.79	0.64
1:cA:709:ASN:HB3	6:cF:136:ILE:HG23	1.80	0.64
13:c2:139:ARG:HB3	13:c2:142:ARG:HG2	1.80	0.64
13:c2:301:PHE:H	13:c2:320:ASN:HD21	1.44	0.64
13:a2:336:HIS:HE1	15:a2:409:CLA:NA	1.95	0.63
15:bA:810:CLA:H122	18:bJ:103:BCR:H272	1.78	0.63
13:c4:331:GLN:NE2	15:c4:415:CLA:C1B	2.50	0.63
2:bB:377:HIS:HE1	15:bB:828:CLA:ND	1.93	0.63
15:cA:841:CLA:HED3	15:cA:841:CLA:H2A	1.78	0.63
2:bB:133:ASP:N	2:bB:133:ASP:OD1	2.29	0.63
13:c4:139:ARG:HB3	13:c4:142:ARG:HG2	1.79	0.63
2:aB:192:HIS:HE1	15:aB:815:CLA:NA	1.95	0.63
13:a2:139:ARG:HB3	13:a2:142:ARG:HG2	1.80	0.63
13:b2:139:ARG:HB3	13:b2:142:ARG:HG2	1.81	0.63
13:b2:331:GLN:NE2	15:b2:416:CLA:C1B	2.50	0.63
13:b2:331:GLN:NE2	15:b2:416:CLA:C4B	2.54	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aB:809:CLA:H2	15:aB:809:CLA:H102	1.80	0.63
13:a5:301:PHE:H	13:a5:320:ASN:HD21	1.44	0.63
13:b4:336:HIS:HE1	15:b4:408:CLA:NA	1.96	0.63
15:aA:835:CLA:H152	18:aI:102:BCR:H372	1.80	0.63
13:c3:266:LEU:HD12	15:c3:402:CLA:H143	1.81	0.63
15:cA:825:CLA:HAC1	18:cA:849:BCR:HC8	1.79	0.63
13:a2:331:GLN:NE2	15:a2:416:CLA:C1B	2.51	0.63
13:a3:336:HIS:HE1	15:a3:408:CLA:NA	1.95	0.63
13:a6:139:ARG:HB3	13:a6:142:ARG:HG2	1.80	0.62
15:bB:809:CLA:H2	15:bB:809:CLA:H102	1.80	0.62
13:c5:139:ARG:HB3	13:c5:142:ARG:HG2	1.80	0.62
1:aA:710:LYS:O	6:aF:131:ALA:N	2.31	0.62
15:bB:826:CLA:HMA1	18:bB:848:BCR:H14C	1.81	0.62
13:c1:301:PHE:H	13:c1:320:ASN:HD21	1.44	0.62
13:c6:139:ARG:HB3	13:c6:142:ARG:HG2	1.80	0.62
15:aA:825:CLA:HAC1	18:aA:850:BCR:HC8	1.79	0.62
13:a3:266:LEU:HD12	15:a3:402:CLA:H143	1.81	0.62
13:b4:266:LEU:HD12	15:b4:402:CLA:H143	1.81	0.62
13:b5:139:ARG:HB3	13:b5:142:ARG:HG2	1.80	0.62
13:b6:139:ARG:HB3	13:b6:142:ARG:HG2	1.80	0.62
15:cB:826:CLA:HMA1	18:cB:848:BCR:H14C	1.81	0.62
4:bD:60:ARG:NH2	4:bD:62:GLU:OE1	2.33	0.62
13:b4:331:GLN:NE2	15:b4:415:CLA:C1B	2.49	0.62
13:c4:266:LEU:HD12	15:c4:402:CLA:H143	1.81	0.62
13:a4:266:LEU:HD12	15:a4:402:CLA:H143	1.81	0.62
13:a4:331:GLN:NE2	15:a4:415:CLA:C1B	2.50	0.62
13:a5:331:GLN:NE2	15:a5:415:CLA:C4B	2.52	0.62
13:b5:336:HIS:HE1	15:b5:408:CLA:NA	1.97	0.62
2:bB:192:HIS:HE1	15:bB:815:CLA:NA	1.95	0.62
13:b6:336:HIS:HE1	15:b6:409:CLA:NA	1.97	0.62
4:cD:60:ARG:NH2	4:cD:62:GLU:OE1	2.33	0.62
13:a3:331:GLN:NE2	15:a3:415:CLA:C1B	2.50	0.62
13:a4:336:HIS:HE1	15:a4:408:CLA:NA	1.96	0.62
15:aB:826:CLA:HMA1	18:aB:848:BCR:H14C	1.81	0.62
6:aF:99:ILE:O	8:aJ:11:ALA:N	2.33	0.62
13:a1:266:LEU:HD12	15:a1:401:CLA:H143	1.82	0.62
13:b5:301:PHE:H	13:b5:320:ASN:HD21	1.45	0.62
13:a5:331:GLN:NE2	15:a5:415:CLA:C1B	2.49	0.62
13:a6:336:HIS:HE1	15:a6:409:CLA:NA	1.97	0.62
1:bA:154:ASN:OD1	1:bA:157:GLN:NE2	2.32	0.62
13:b1:266:LEU:HD12	15:b1:402:CLA:H143	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:aD:50:ARG:H	4:aD:54:ASN:HD21	1.48	0.61
11:aM:5:ASP:N	11:aM:5:ASP:OD1	2.30	0.61
1:bA:33:HIS:NE2	15:bA:812:CLA:O1A	2.33	0.61
4:bD:50:ARG:H	4:bD:54:ASN:HD21	1.48	0.61
1:aA:458:LEU:O	1:aA:462:ASN:ND2	2.27	0.61
13:a5:336:HIS:HE1	15:a5:408:CLA:NA	1.98	0.61
13:c1:336:HIS:HE1	15:c1:408:CLA:NA	1.98	0.61
13:c3:331:GLN:NE2	15:c3:415:CLA:C4B	2.55	0.61
2:cB:202:ARG:HG2	2:cB:249:ALA:HB1	1.82	0.61
4:aD:60:ARG:NH2	4:aD:62:GLU:OE1	2.33	0.61
1:aA:33:HIS:NE2	15:aA:812:CLA:O1A	2.33	0.61
13:c5:336:HIS:HE1	15:c5:408:CLA:NA	1.96	0.61
13:c6:336:HIS:HE1	15:c6:410:CLA:NA	1.97	0.61
1:aA:437:ARG:NH2	4:aD:43:THR:O	2.34	0.61
2:aB:91:TRP:HB3	7:aI:15:ILE:HG13	1.82	0.61
2:aB:550:SER:HA	6:aF:139:SER:HB3	1.82	0.61
13:a2:266:LEU:HD12	15:a2:402:CLA:H143	1.83	0.61
15:a6:403:CLA:H72	15:a6:403:CLA:HBB1	1.83	0.61
1:bA:470:ARG:HG2	10:cL:154:ASN:HB3	1.82	0.61
15:b1:402:CLA:H72	15:b1:402:CLA:HBB1	1.83	0.61
1:cA:154:ASN:OD1	1:cA:157:GLN:NE2	2.32	0.61
1:cA:437:ARG:NH2	4:cD:43:THR:O	2.34	0.61
1:aA:257:ASP:OD1	1:aA:257:ASP:N	2.34	0.61
1:bA:437:ARG:NH2	4:bD:43:THR:O	2.34	0.61
13:c1:266:LEU:HD12	15:c1:402:CLA:H143	1.83	0.61
15:aA:833:CLA:H42	10:aL:21:ILE:HG23	1.81	0.61
2:aB:412:ASP:O	2:aB:416:GLN:NE2	2.34	0.61
10:aL:154:ASN:HB3	1:cA:470:ARG:HG2	1.83	0.61
1:bA:257:ASP:N	1:bA:257:ASP:OD1	2.34	0.61
13:b3:266:LEU:HD12	15:b3:402:CLA:H143	1.82	0.61
1:aA:647:ASN:OD1	1:aA:651:ARG:NH1	2.34	0.61
13:a5:266:LEU:HD12	15:a5:402:CLA:H143	1.83	0.61
13:b5:266:LEU:HD12	15:b5:402:CLA:H143	1.83	0.61
1:cA:33:HIS:NE2	15:cA:812:CLA:O1A	2.33	0.61
15:cB:801:CLA:H192	10:cL:58:LEU:HD21	1.81	0.61
13:c2:266:LEU:HD12	15:c2:402:CLA:H143	1.83	0.61
13:c5:331:GLN:NE2	15:c5:415:CLA:C1B	2.49	0.61
10:bL:142:PHE:HD1	15:bL:204:CLA:H43	1.66	0.61
2:aB:554:PRO:HB3	6:aF:140:PRO:HG3	1.83	0.60
13:a3:331:GLN:NE2	15:a3:415:CLA:C4B	2.55	0.60
15:a1:415:CLA:HBB1	18:a1:420:BCR:H343	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b6:266:LEU:HD12	15:b6:403:CLA:H143	1.83	0.60
2:cB:412:ASP:O	2:cB:416:GLN:NE2	2.34	0.60
15:cF:203:CLA:HMB2	8:cJ:26:LEU:HD21	1.82	0.60
6:aF:100:ILE:HG12	8:aJ:10:THR:HG22	1.82	0.60
3:bC:5:LYS:HD3	4:bD:113:ASN:HB3	1.82	0.60
2:aB:202:ARG:HG2	2:aB:249:ALA:HB1	1.82	0.60
13:a1:331:GLN:NE2	15:a1:414:CLA:C4B	2.56	0.60
1:aA:154:ASN:OD1	1:aA:157:GLN:NE2	2.32	0.60
15:aA:833:CLA:H193	15:aA:839:CLA:H121	1.83	0.60
1:bA:647:ASN:OD1	1:bA:651:ARG:NH1	2.34	0.60
6:cF:37:ARG:NH2	8:cJ:34:PRO:O	2.35	0.60
10:cL:142:PHE:HD1	15:cL:204:CLA:H43	1.66	0.60
15:c1:402:CLA:H72	15:c1:402:CLA:HBB1	1.83	0.60
1:aA:202:ALA:HB2	1:aA:312:GLY:HA3	1.84	0.60
15:aB:810:CLA:HHB	15:aB:811:CLA:HBB1	1.84	0.60
13:a6:266:LEU:HD12	15:a6:403:CLA:H143	1.84	0.60
1:cA:710:LYS:O	6:cF:131:ALA:N	2.35	0.60
1:aA:581:PRO:HD3	2:aB:567:GLY:HA2	1.83	0.60
2:aB:400:ASP:OD1	4:aD:129:LYS:NZ	2.35	0.60
13:a1:336:HIS:HE1	15:a1:407:CLA:NA	1.99	0.60
4:cD:50:ARG:H	4:cD:54:ASN:HD21	1.48	0.60
15:c6:404:CLA:H72	15:c6:404:CLA:HBB1	1.83	0.60
13:a4:331:GLN:NE2	15:a4:415:CLA:C4B	2.56	0.60
2:bB:412:ASP:O	2:bB:416:GLN:NE2	2.34	0.60
1:bA:202:ALA:HB2	1:bA:312:GLY:HA3	1.84	0.60
13:b1:336:HIS:HE1	15:b1:408:CLA:NA	1.98	0.60
1:cA:202:ALA:HB2	1:cA:312:GLY:HA3	1.84	0.60
13:c6:266:LEU:HD12	15:c6:404:CLA:H143	1.84	0.60
15:b6:403:CLA:H72	15:b6:403:CLA:HBB1	1.83	0.60
1:cA:647:ASN:OD1	1:cA:651:ARG:NH1	2.34	0.60
15:cB:810:CLA:HHB	15:cB:811:CLA:HBB1	1.84	0.59
13:c5:266:LEU:HD12	15:c5:402:CLA:H143	1.83	0.59
13:a4:113:ILE:HG12	15:a4:421:CLA:H172	1.84	0.59
15:a4:402:CLA:H72	15:a4:402:CLA:HBB1	1.85	0.59
2:bB:202:ARG:HG2	2:bB:249:ALA:HB1	1.82	0.59
3:aC:18:ARG:HG2	4:aD:103:GLU:HG2	1.83	0.59
10:aL:142:PHE:HD1	15:aL:203:CLA:H43	1.66	0.59
1:cA:581:PRO:HD3	2:cB:567:GLY:HA2	1.83	0.59
13:b2:128:ARG:NH2	15:b2:422:CLA:O1D	2.29	0.59
15:c3:402:CLA:H72	15:c3:402:CLA:HBB1	1.85	0.59
1:aA:188:GLU:O	1:aA:192:ASN:ND2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aB:833:CLA:H192	18:aF:202:BCR:H17C	1.85	0.59
5:aE:39:ARG:HG3	5:aE:57:THR:HG22	1.85	0.59
15:b4:402:CLA:H72	15:b4:402:CLA:HBB1	1.85	0.59
1:aA:65:LEU:HD11	15:aA:826:CLA:H201	1.84	0.59
13:b4:113:ILE:HG12	15:b4:421:CLA:H172	1.84	0.59
10:aL:152:LEU:O	2:cB:97:LYS:NZ	2.35	0.59
15:a2:402:CLA:H72	15:a2:402:CLA:HBB1	1.85	0.59
1:bA:188:GLU:O	1:bA:192:ASN:ND2	2.36	0.59
13:b2:266:LEU:HD12	15:b2:402:CLA:H143	1.84	0.59
13:c6:331:GLN:NE2	15:c6:417:CLA:C4B	2.54	0.59
1:aA:411:HIS:HE1	15:aA:831:CLA:NA	2.01	0.59
1:cA:188:GLU:O	1:cA:192:ASN:ND2	2.36	0.59
15:cA:833:CLA:H193	15:cA:839:CLA:H121	1.84	0.59
15:cB:833:CLA:H61	18:cF:204:BCR:HC32	1.84	0.59
5:aE:23:VAL:HG12	5:aE:38:VAL:HG22	1.85	0.59
15:bA:834:CLA:H102	15:bB:839:CLA:H52	1.84	0.59
15:bB:810:CLA:HHB	15:bB:811:CLA:HBB1	1.84	0.59
1:bA:411:HIS:HE1	15:bA:831:CLA:NA	2.01	0.58
15:a1:401:CLA:H72	15:a1:401:CLA:HBB1	1.84	0.58
13:a6:128:ARG:HH11	15:a6:422:CLA:H2A	1.68	0.58
5:cE:39:ARG:HG3	5:cE:57:THR:HG22	1.85	0.58
13:b6:331:GLN:HE22	15:b6:416:CLA:NB	1.40	0.58
2:cB:668:MET:O	2:cB:672:SER:OG	2.21	0.58
13:c1:220:GLY:HA2	13:c1:223:ILE:HD12	1.85	0.58
13:c6:331:GLN:HE22	15:c6:417:CLA:NB	1.40	0.58
2:bB:668:MET:O	2:bB:672:SER:OG	2.21	0.58
1:cA:65:LEU:HD11	15:cA:826:CLA:H201	1.84	0.58
13:c5:111:HIS:HE1	15:c5:404:CLA:C4A	2.03	0.58
1:aA:277:ASP:OD1	1:aA:277:ASP:N	2.36	0.58
1:bA:227:LEU:HD21	1:bA:233:ALA:HB2	1.86	0.58
15:bA:833:CLA:H193	15:bA:839:CLA:H121	1.84	0.58
15:b2:402:CLA:H72	15:b2:402:CLA:HBB1	1.85	0.58
13:b3:220:GLY:HA2	13:b3:223:ILE:HD12	1.86	0.58
1:cA:411:HIS:HE1	15:cA:831:CLA:NA	2.01	0.58
13:c4:331:GLN:NE2	15:c4:415:CLA:C4B	2.55	0.58
13:a4:220:GLY:HA2	13:a4:223:ILE:HD12	1.84	0.58
5:bE:39:ARG:HG3	5:bE:57:THR:HG22	1.85	0.58
6:bF:37:ARG:NH2	8:bJ:34:PRO:O	2.37	0.58
15:c4:402:CLA:H72	15:c4:402:CLA:HBB1	1.84	0.58
1:aA:13:ARG:NH2	1:aA:188:GLU:OE2	2.37	0.58
1:aA:255:LYS:NZ	1:aA:273:ALA:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:cE:23:VAL:HG12	5:cE:38:VAL:HG22	1.85	0.58
13:b5:331:GLN:NE2	15:b5:415:CLA:C4B	2.52	0.58
1:cA:257:ASP:N	1:cA:257:ASP:OD1	2.34	0.58
6:cF:103:VAL:HG22	8:cJ:14:LEU:HD11	1.84	0.58
13:c2:331:GLN:NE2	15:c2:416:CLA:C4B	2.55	0.58
13:a6:331:GLN:HE22	15:a6:416:CLA:NB	1.40	0.58
1:bA:65:LEU:HD11	15:bA:826:CLA:H201	1.85	0.58
15:bA:843:CLA:H193	8:bJ:19:MET:HG3	1.86	0.58
2:cB:144:LEU:HD11	15:cB:815:CLA:H152	1.86	0.58
13:c4:113:ILE:HG12	15:c4:421:CLA:H172	1.84	0.58
15:aB:833:CLA:H61	18:aF:202:BCR:HC32	1.86	0.57
6:aF:41:ALA:HA	6:aF:59:ARG:HH22	1.69	0.57
2:bB:439:LEU:O	2:bB:443:ASN:ND2	2.37	0.57
13:b2:270:VAL:HG21	15:b2:402:CLA:H92	1.86	0.57
15:b3:402:CLA:H72	15:b3:402:CLA:HBB1	1.85	0.57
1:cA:13:ARG:NH2	1:cA:188:GLU:OE2	2.37	0.57
2:aB:144:LEU:HD11	15:aB:815:CLA:H152	1.86	0.57
2:aB:439:LEU:O	2:aB:443:ASN:ND2	2.37	0.57
2:bB:181:LEU:O	2:bB:185:SER:OG	2.21	0.57
13:b3:111:HIS:HE1	15:b3:404:CLA:C4A	2.02	0.57
13:c3:111:HIS:HE1	15:c3:404:CLA:C4A	2.02	0.57
15:aA:806:CLA:H12	15:aA:807:CLA:HBB1	1.86	0.57
13:a1:341:MET:HG3	13:c6:128:ARG:HG3	1.85	0.57
1:bA:13:ARG:NH2	1:bA:188:GLU:OE2	2.37	0.57
1:bA:388:PRO:O	1:bA:392:SER:OG	2.22	0.57
2:bB:144:LEU:HD11	15:bB:815:CLA:H152	1.86	0.57
13:b1:331:GLN:NE2	15:b1:415:CLA:C4B	2.56	0.57
13:c2:331:GLN:NE2	15:c2:416:CLA:C1B	2.50	0.57
1:bA:683:TRP:O	1:bA:686:SER:OG	2.22	0.57
5:bE:23:VAL:HG12	5:bE:38:VAL:HG22	1.85	0.57
13:b4:220:GLY:HA2	13:b4:223:ILE:HD12	1.85	0.57
13:c3:331:GLN:NE2	15:c3:415:CLA:C1B	2.49	0.57
1:aA:580:GLY:HA2	2:aB:568:PRO:HD3	1.87	0.57
13:a2:128:ARG:NH2	15:a2:422:CLA:O1D	2.29	0.57
13:a6:220:GLY:HA2	13:a6:223:ILE:HD12	1.86	0.57
15:bA:806:CLA:H12	15:bA:807:CLA:HBB1	1.87	0.57
18:cA:851:BCR:H391	18:cJ:103:BCR:H313	1.86	0.57
2:cB:439:LEU:O	2:cB:443:ASN:ND2	2.37	0.57
18:bA:853:BCR:H391	18:bJ:103:BCR:H313	1.87	0.57
15:bB:809:CLA:H141	15:bB:809:CLA:HBA2	1.87	0.57
13:c2:270:VAL:HG21	15:c2:402:CLA:H92	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c2:331:GLN:HE22	15:c2:416:CLA:NB	1.41	0.57
15:a3:402:CLA:H72	15:a3:402:CLA:HBB1	1.85	0.57
1:cA:227:LEU:HD21	1:cA:233:ALA:HB2	1.85	0.57
13:c6:220:GLY:HA2	13:c6:223:ILE:HD12	1.86	0.57
18:aA:848:BCR:H16C	18:aA:849:BCR:H10C	1.87	0.57
2:aB:668:MET:O	2:aB:672:SER:OG	2.21	0.57
15:aB:811:CLA:HAB	7:aI:19:CYS:HB3	1.86	0.57
1:bA:734:HIS:HE1	15:bA:843:CLA:ND	2.02	0.57
13:b2:331:GLN:HE22	15:b2:416:CLA:NB	1.39	0.57
15:cB:833:CLA:H192	18:cF:204:BCR:H17C	1.86	0.57
13:a2:331:GLN:HE22	15:a2:416:CLA:NB	1.42	0.57
15:b5:402:CLA:H72	15:b5:402:CLA:HBB1	1.87	0.57
15:cA:806:CLA:H12	15:cA:807:CLA:HBB1	1.86	0.57
15:cB:809:CLA:HBA2	15:cB:809:CLA:H141	1.87	0.57
13:a1:159:HIS:CE1	15:a1:413:CLA:ND	2.73	0.56
13:a6:331:GLN:NE2	15:a6:416:CLA:C4B	2.54	0.56
15:bB:801:CLA:H192	10:bL:58:LEU:HD21	1.86	0.56
13:b2:111:HIS:HE1	15:b2:404:CLA:C4A	2.04	0.56
1:cA:734:HIS:HE1	15:cA:842:CLA:ND	2.02	0.56
15:c2:402:CLA:H72	15:c2:402:CLA:HBB1	1.86	0.56
13:c5:335:TRP:HA	15:c5:415:CLA:HMD2	1.87	0.56
1:cA:255:LYS:NZ	1:cA:273:ALA:O	2.37	0.56
2:cB:472:LYS:HE2	2:cB:474:LEU:HD21	1.88	0.56
1:aA:227:LEU:HD21	1:aA:233:ALA:HB2	1.86	0.56
1:bA:255:LYS:NZ	1:bA:273:ALA:O	2.37	0.56
2:bB:472:LYS:HE2	2:bB:474:LEU:HD21	1.88	0.56
8:bJ:40:PRO:HD2	18:bJ:105:BCR:H382	1.87	0.56
13:b3:270:VAL:HG21	15:b3:402:CLA:H92	1.87	0.56
13:b6:326:ALA:HA	13:b6:329:PHE:HB2	1.88	0.56
1:cA:683:TRP:O	1:cA:686:SER:OG	2.22	0.56
18:cA:847:BCR:H16C	18:cA:848:BCR:H10C	1.87	0.56
15:aA:843:CLA:H193	8:aJ:19:MET:HG3	1.86	0.56
13:b5:335:TRP:HA	15:b5:415:CLA:HMD2	1.87	0.56
13:c4:335:TRP:HA	15:c4:415:CLA:HMD2	1.88	0.56
2:aB:472:LYS:HE2	2:aB:474:LEU:HD21	1.88	0.56
15:bB:808:CLA:HHB	15:bB:809:CLA:HHB	1.88	0.56
13:b1:159:HIS:CE1	15:b1:414:CLA:ND	2.73	0.56
15:cA:842:CLA:H193	8:cJ:19:MET:HG3	1.86	0.56
15:cB:839:CLA:H151	10:cL:88:VAL:HG11	1.86	0.56
6:cF:41:ALA:HA	6:cF:59:ARG:HH22	1.69	0.56
13:c4:270:VAL:HG21	15:c4:402:CLA:H92	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aA:835:CLA:H72	18:aI:102:BCR:H17C	1.87	0.56
13:a5:113:ILE:HG13	15:a5:420:CLA:H202	1.88	0.56
13:b4:270:VAL:HG21	15:b4:402:CLA:H92	1.88	0.56
13:a5:111:HIS:HE1	15:a5:404:CLA:C4A	2.03	0.56
15:a5:402:CLA:H72	15:a5:402:CLA:HBB1	1.88	0.56
1:bA:341:HIS:CD2	15:bA:825:CLA:ND	2.74	0.56
18:bA:849:BCR:H16C	18:bA:850:BCR:H10C	1.87	0.56
2:bB:176:HIS:CE1	15:bB:813:CLA:NA	2.74	0.56
6:bF:41:ALA:HA	6:bF:59:ARG:HH22	1.69	0.56
1:cA:580:GLY:HA2	2:cB:568:PRO:HD3	1.87	0.56
15:cA:813:CLA:HBB2	15:cA:821:CLA:H102	1.87	0.56
13:c3:270:VAL:HG21	15:c3:402:CLA:H92	1.87	0.56
13:c5:270:VAL:HG21	15:c5:402:CLA:H92	1.88	0.56
18:aA:852:BCR:H391	18:aJ:204:BCR:H313	1.86	0.56
15:aB:801:CLA:H192	10:aL:58:LEU:HD21	1.86	0.56
15:aB:809:CLA:HBA2	15:aB:809:CLA:H141	1.87	0.56
15:cB:808:CLA:HHB	15:cB:809:CLA:HHB	1.88	0.56
1:aA:683:TRP:O	1:aA:686:SER:OG	2.22	0.56
1:aA:734:HIS:HE1	15:aA:843:CLA:ND	2.02	0.56
13:a6:159:HIS:CE1	15:a6:415:CLA:ND	2.74	0.56
15:bB:814:CLA:H112	18:bB:845:BCR:H381	1.88	0.56
15:cA:833:CLA:H42	10:cL:21:ILE:HG23	1.87	0.56
13:a3:335:TRP:HA	15:a3:415:CLA:HMD2	1.88	0.56
15:bA:833:CLA:H42	10:bL:21:ILE:HG23	1.87	0.56
13:b2:66:SER:OG	13:b2:67:GLN:N	2.38	0.56
13:b3:335:TRP:HA	15:b3:415:CLA:HMD2	1.87	0.56
18:cF:205:BCR:H382	8:cJ:40:PRO:HD2	1.87	0.56
13:c2:66:SER:OG	13:c2:67:GLN:N	2.39	0.56
2:aB:30:PHE:HB3	2:aB:36:MET:HE2	1.88	0.55
2:aB:181:LEU:O	2:aB:185:SER:OG	2.21	0.55
6:aF:85:LEU:HG	6:aF:89:ARG:HH21	1.71	0.55
13:a5:270:VAL:HG21	15:a5:402:CLA:H92	1.87	0.55
2:cB:400:ASP:OD1	4:cD:129:LYS:NZ	2.35	0.55
13:c3:331:GLN:HA	13:c3:334:LEU:HB2	1.88	0.55
13:c3:335:TRP:HA	15:c3:415:CLA:HMD2	1.87	0.55
13:c5:113:ILE:HG13	15:c5:420:CLA:H202	1.88	0.55
13:c6:335:TRP:HA	15:c6:417:CLA:HMD2	1.88	0.55
1:aA:698:GLN:NE2	5:aE:45:TYR:OH	2.40	0.55
2:aB:176:HIS:CE1	15:aB:813:CLA:NA	2.74	0.55
13:a1:220:GLY:HA2	13:a1:223:ILE:HD12	1.86	0.55
13:a1:270:VAL:HG21	15:a1:401:CLA:H92	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a5:331:GLN:HA	13:a5:334:LEU:HB2	1.88	0.55
13:b3:201:VAL:O	13:b3:205:TYR:N	2.33	0.55
2:cB:30:PHE:HB3	2:cB:36:MET:HE2	1.88	0.55
13:c1:159:HIS:CE1	15:c1:414:CLA:ND	2.74	0.55
13:c2:111:HIS:HE1	15:c2:404:CLA:C4A	2.03	0.55
13:c2:128:ARG:HG3	13:c3:341:MET:HG3	1.88	0.55
13:c2:139:ARG:HG3	13:c2:141:ARG:H	1.72	0.55
13:c3:257:LEU:HD22	15:c3:409:CLA:HBC3	1.89	0.55
1:aA:341:HIS:CD2	15:aA:825:CLA:ND	2.74	0.55
15:a4:403:CLA:HBB2	15:a4:410:CLA:H162	1.88	0.55
2:bB:400:ASP:OD1	4:bD:129:LYS:NZ	2.39	0.55
13:b6:139:ARG:HG3	13:b6:141:ARG:H	1.72	0.55
2:cB:176:HIS:CE1	15:cB:813:CLA:NA	2.74	0.55
13:c1:331:GLN:HE22	15:c1:415:CLA:NB	1.43	0.55
13:c4:139:ARG:HG3	13:c4:141:ARG:H	1.72	0.55
13:c5:139:ARG:HG3	13:c5:141:ARG:H	1.72	0.55
13:c6:326:ALA:HA	13:c6:329:PHE:HB2	1.87	0.55
1:aA:202:ALA:HB1	15:aA:821:CLA:HBC3	1.89	0.55
15:aA:813:CLA:HBB2	15:aA:821:CLA:H102	1.87	0.55
18:aF:203:BCR:H382	8:aJ:40:PRO:HD2	1.87	0.55
13:a3:214:SER:OG	13:a3:217:ASP:OD2	2.23	0.55
13:a3:220:GLY:HA2	13:a3:223:ILE:HD12	1.88	0.55
13:a4:111:HIS:HE1	15:a4:404:CLA:C4A	2.05	0.55
1:bA:202:ALA:HB1	15:bA:821:CLA:HBC3	1.89	0.55
13:b5:139:ARG:HG3	13:b5:141:ARG:H	1.72	0.55
10:cL:33:ASN:HB3	15:cL:202:CLA:HAC1	1.89	0.55
13:c1:335:TRP:HA	15:c1:415:CLA:HMD2	1.88	0.55
13:c6:139:ARG:HG3	13:c6:141:ARG:H	1.71	0.55
13:c6:159:HIS:CE1	15:c6:416:CLA:ND	2.74	0.55
10:aL:33:ASN:HB3	15:aL:201:CLA:HAC1	1.89	0.55
13:a2:331:GLN:NE2	15:a2:416:CLA:C4B	2.56	0.55
2:bB:30:PHE:HB3	2:bB:36:MET:HE2	1.89	0.55
15:b4:403:CLA:HBB2	15:b4:410:CLA:H162	1.87	0.55
15:b5:420:CLA:H18	18:b6:402:BCR:H333	1.89	0.55
1:cA:698:GLN:NE2	5:cE:45:TYR:OH	2.39	0.55
2:cB:669:PHE:HA	16:cB:843:PQN:H9	1.89	0.55
15:c5:402:CLA:H72	15:c5:402:CLA:HBB1	1.87	0.55
13:c6:22:THR:OG1	13:c6:23:ASN:N	2.39	0.55
2:aB:531:LEU:O	2:aB:535:THR:OG1	2.21	0.55
2:aB:676:TYR:OH	15:aB:804:CLA:OBD	2.21	0.55
13:a1:335:TRP:HA	15:a1:414:CLA:HMD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a2:270:VAL:HG21	15:a2:402:CLA:H92	1.87	0.55
6:cF:85:LEU:HG	6:cF:89:ARG:HH21	1.71	0.55
15:c4:403:CLA:HBB2	15:c4:410:CLA:H162	1.88	0.55
15:bA:813:CLA:HBB2	15:bA:821:CLA:H102	1.87	0.55
13:b2:128:ARG:HG3	13:b3:341:MET:HG3	1.88	0.55
13:b2:335:TRP:HA	15:b2:416:CLA:HMD2	1.88	0.55
13:b4:335:TRP:HA	15:b4:415:CLA:HMD2	1.87	0.55
13:c2:335:TRP:HA	15:c2:416:CLA:HMD2	1.88	0.55
13:c3:22:THR:OG1	13:c3:23:ASN:N	2.39	0.55
2:aB:307:LYS:NZ	2:aB:315:GLU:O	2.40	0.55
2:aB:682:GLU:HG2	3:aC:80:TYR:HE1	1.72	0.55
1:bA:536:PHE:HA	15:bA:839:CLA:HED1	1.89	0.55
2:bB:531:LEU:O	2:bB:535:THR:OG1	2.21	0.55
15:bB:804:CLA:H111	18:bB:850:BCR:H362	1.89	0.55
6:bF:107:ILE:HA	6:bF:110:MET:HB2	1.89	0.55
13:b1:331:GLN:HE22	15:b1:415:CLA:NB	1.44	0.55
13:b5:270:VAL:HG21	15:b5:402:CLA:H92	1.88	0.55
13:b6:335:TRP:HA	15:b6:416:CLA:HMD2	1.88	0.55
6:cF:61:GLY:HA3	8:cJ:39:HIS:O	2.07	0.55
13:c3:220:GLY:HA2	13:c3:223:ILE:HD12	1.88	0.55
2:aB:669:PHE:HA	16:aB:843:PQN:H9	1.89	0.55
15:aB:814:CLA:H112	18:aB:845:BCR:H381	1.88	0.55
2:bB:307:LYS:NZ	2:bB:315:GLU:O	2.40	0.55
2:bB:676:TYR:OH	15:bB:804:CLA:OBD	2.21	0.55
13:b1:113:ILE:HG12	15:b2:406:CLA:H202	1.88	0.55
13:b4:139:ARG:HG3	13:b4:141:ARG:H	1.72	0.55
13:b5:113:ILE:HG13	15:b5:420:CLA:H202	1.88	0.55
6:cF:107:ILE:HA	6:cF:110:MET:HB2	1.89	0.55
13:c4:214:SER:OG	13:c4:217:ASP:OD2	2.23	0.55
13:c5:159:HIS:CE1	15:c5:414:CLA:ND	2.75	0.55
2:aB:642:ASN:OD1	2:aB:642:ASN:N	2.40	0.55
13:a2:128:ARG:HG3	13:a3:341:MET:HG3	1.88	0.55
13:a6:326:ALA:HA	13:a6:329:PHE:HB2	1.88	0.55
13:a6:335:TRP:HA	15:a6:416:CLA:HMD2	1.88	0.55
10:bL:33:ASN:HB3	15:bL:202:CLA:HAC1	1.89	0.55
13:b2:55:PHE:HZ	15:b3:417:CLA:HMB2	1.72	0.55
13:b6:220:GLY:HA2	13:b6:223:ILE:HD12	1.88	0.55
1:cA:341:HIS:CD2	15:cA:825:CLA:ND	2.74	0.55
16:cA:845:PQN:H111	18:cF:202:BCR:H393	1.89	0.55
2:cB:676:TYR:OH	15:cB:804:CLA:OBD	2.21	0.55
15:aB:839:CLA:H192	7:aI:24:THR:HB	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a2:335:TRP:HA	15:a2:416:CLA:HMD2	1.88	0.54
13:a4:335:TRP:HA	15:a4:415:CLA:HMD2	1.88	0.54
13:a5:335:TRP:HA	15:a5:415:CLA:HMD2	1.87	0.54
15:bA:835:CLA:H152	18:bI:102:BCR:H372	1.89	0.54
6:bF:85:LEU:HG	6:bF:89:ARG:HH21	1.71	0.54
13:b4:326:ALA:HA	13:b4:329:PHE:HB2	1.90	0.54
1:cA:689:PHE:HA	16:cA:845:PQN:H9	1.89	0.54
2:cB:181:LEU:O	2:cB:185:SER:OG	2.21	0.54
15:c5:420:CLA:H18	18:c6:403:BCR:H333	1.89	0.54
13:a3:331:GLN:HA	13:a3:334:LEU:HB2	1.88	0.54
13:a4:270:VAL:HG21	15:a4:402:CLA:H92	1.87	0.54
1:bA:106:ASP:HB3	1:bA:110:ILE:HG12	1.90	0.54
5:bE:58:ASN:ND2	5:bE:59:ASN:O	2.40	0.54
10:bL:7:PRO:HB3	10:bL:12:PRO:HA	1.89	0.54
13:b3:139:ARG:HG3	13:b3:141:ARG:H	1.72	0.54
1:cA:749:ALA:O	1:cA:753:SER:OG	2.26	0.54
13:c2:257:LEU:HD22	15:c2:410:CLA:HBC3	1.90	0.54
15:aA:841:CLA:H203	15:aA:842:CLA:H51	1.89	0.54
15:aB:808:CLA:HHB	15:aB:809:CLA:HHB	1.88	0.54
13:a1:139:ARG:HG3	13:a1:141:ARG:H	1.73	0.54
4:bD:73:ARG:NH2	4:bD:80:TYR:OH	2.40	0.54
13:b4:331:GLN:NE2	15:b4:415:CLA:C4B	2.56	0.54
1:cA:202:ALA:HB1	15:cA:821:CLA:HBC3	1.89	0.54
15:cB:814:CLA:H112	18:cB:845:BCR:H381	1.88	0.54
13:c4:220:GLY:HA2	13:c4:223:ILE:HD12	1.89	0.54
13:a2:139:ARG:HG3	13:a2:141:ARG:H	1.72	0.54
15:a5:420:CLA:H18	18:a6:402:BCR:H333	1.89	0.54
13:a6:214:SER:OG	13:a6:217:ASP:OD2	2.22	0.54
1:bA:698:GLN:NE2	5:bE:45:TYR:OH	2.40	0.54
15:bA:841:CLA:H203	15:bA:842:CLA:H51	1.89	0.54
2:bB:443:ASN:HB3	2:bB:455:GLN:HE21	1.73	0.54
2:bB:669:PHE:HA	16:bB:843:PQN:H9	1.89	0.54
13:b1:335:TRP:HA	15:b1:415:CLA:HMD2	1.88	0.54
1:cA:106:ASP:HB3	1:cA:110:ILE:HG12	1.89	0.54
1:cA:323:HIS:HB3	1:cA:328:ILE:HD11	1.89	0.54
15:cA:841:CLA:H203	15:cF:201:CLA:H51	1.89	0.54
13:c5:220:GLY:HA2	13:c5:223:ILE:HD12	1.90	0.54
13:a3:270:VAL:HG21	15:a3:402:CLA:H92	1.87	0.54
13:a4:139:ARG:HG3	13:a4:141:ARG:H	1.72	0.54
15:bB:832:CLA:HAB	15:bB:833:CLA:H202	1.90	0.54
13:b1:113:ILE:HG13	15:b2:406:CLA:H152	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b3:331:GLN:NE2	15:b3:415:CLA:C4B	2.55	0.54
13:b5:113:ILE:HG21	15:b5:420:CLA:H172	1.90	0.54
13:b6:159:HIS:CE1	15:b6:415:CLA:ND	2.74	0.54
13:c1:270:VAL:HG21	15:c1:402:CLA:H92	1.88	0.54
13:c6:270:VAL:HG21	15:c6:404:CLA:H92	1.90	0.54
1:aA:461:HIS:HE1	15:aA:835:CLA:NA	2.05	0.54
1:aA:536:PHE:HA	15:aA:839:CLA:HED1	1.89	0.54
13:a4:331:GLN:HA	13:a4:334:LEU:HB2	1.89	0.54
13:a5:159:HIS:CE1	15:a5:414:CLA:ND	2.75	0.54
13:b5:159:HIS:CE1	15:b5:414:CLA:ND	2.75	0.54
13:c4:326:ALA:HA	13:c4:329:PHE:HB2	1.89	0.54
1:aA:106:ASP:HB3	1:aA:110:ILE:HG12	1.90	0.54
13:a3:159:HIS:CE1	15:a3:414:CLA:ND	2.76	0.54
13:a3:257:LEU:HD22	15:a3:409:CLA:HBC3	1.89	0.54
13:b2:139:ARG:HG3	13:b2:141:ARG:H	1.72	0.54
13:b5:111:HIS:HE1	15:b5:404:CLA:C4A	2.03	0.54
13:b5:331:GLN:HA	13:b5:334:LEU:HB2	1.89	0.54
1:cA:536:PHE:HA	15:cA:839:CLA:HED1	1.89	0.54
2:cB:443:ASN:HB3	2:cB:455:GLN:HE21	1.73	0.54
15:cB:832:CLA:HAB	15:cB:833:CLA:H202	1.90	0.54
13:c2:326:ALA:HA	13:c2:329:PHE:HB2	1.90	0.54
13:c5:326:ALA:HA	13:c5:329:PHE:HB2	1.90	0.54
1:aA:545:THR:O	1:aA:549:THR:OG1	2.25	0.54
13:b1:331:GLN:HA	13:b1:334:LEU:HB2	1.90	0.54
15:b4:410:CLA:H2	15:b4:410:CLA:HED2	1.90	0.54
5:cE:58:ASN:ND2	5:cE:59:ASN:O	2.40	0.54
13:c5:331:GLN:HA	13:c5:334:LEU:HB2	1.89	0.54
16:aA:846:PQN:H111	18:aF:201:BCR:H393	1.89	0.54
10:aL:127:GLY:O	10:aL:131:SER:OG	2.24	0.54
13:a1:331:GLN:HA	13:a1:334:LEU:HB2	1.89	0.54
13:a6:128:ARG:HH12	15:a6:422:CLA:HED3	1.73	0.54
1:bA:323:HIS:HB3	1:bA:328:ILE:HD11	1.89	0.54
13:b1:270:VAL:HG21	15:b1:402:CLA:H92	1.89	0.54
13:b3:331:GLN:HA	13:b3:334:LEU:HB2	1.89	0.54
1:cA:45:THR:HG21	15:cF:201:CLA:HBB1	1.90	0.54
2:cB:307:LYS:NZ	2:cB:315:GLU:O	2.40	0.54
13:c1:326:ALA:HA	13:c1:329:PHE:HB2	1.90	0.54
13:c3:214:SER:OG	13:c3:217:ASP:OD2	2.23	0.54
13:a2:257:LEU:HD22	15:a2:410:CLA:HBC3	1.90	0.54
2:bB:55:ILE:HD11	18:bM:101:BCR:HC7	1.89	0.54
13:b3:274:PHE:CE1	15:b3:402:CLA:H3A	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b4:159:HIS:CE1	15:b4:414:CLA:ND	2.76	0.54
10:cL:7:PRO:HB3	10:cL:12:PRO:HA	1.89	0.54
13:c6:111:HIS:HE1	15:c6:406:CLA:C4A	2.04	0.54
13:c6:214:SER:OG	13:c6:217:ASP:OD2	2.22	0.54
1:aA:749:ALA:O	1:aA:753:SER:OG	2.26	0.53
15:aB:804:CLA:H111	18:aB:849:BCR:H362	1.89	0.53
13:a4:159:HIS:CE1	15:a4:414:CLA:ND	2.76	0.53
13:a6:139:ARG:HG3	13:a6:141:ARG:H	1.72	0.53
1:bA:451:LEU:HB3	1:bA:544:PHE:HB2	1.90	0.53
2:bB:301:LYS:NZ	2:bB:305:ASP:OD2	2.41	0.53
15:bB:811:CLA:HED1	18:bI:102:BCR:HC7	1.89	0.53
15:b5:415:CLA:O2A	15:b5:415:CLA:H3A	2.08	0.53
15:c1:410:CLA:H2	15:c1:410:CLA:HED2	1.90	0.53
13:c3:139:ARG:HG3	13:c3:141:ARG:H	1.72	0.53
13:c5:113:ILE:HG21	15:c5:420:CLA:H172	1.90	0.53
1:aA:689:PHE:HA	16:aA:846:PQN:H9	1.89	0.53
15:aB:801:CLA:H72	15:aB:801:CLA:HBB1	1.90	0.53
5:aE:58:ASN:ND2	5:aE:59:ASN:O	2.40	0.53
15:bB:801:CLA:H72	15:bB:801:CLA:HBB1	1.90	0.53
13:b3:22:THR:OG1	13:b3:23:ASN:N	2.40	0.53
4:cD:73:ARG:NH2	4:cD:80:TYR:OH	2.41	0.53
6:cF:100:ILE:HA	8:cJ:10:THR:HA	1.90	0.53
1:aA:366:LEU:HD11	15:aA:820:CLA:H71	1.90	0.53
6:aF:107:ILE:HA	6:aF:110:MET:HB2	1.89	0.53
10:aL:7:PRO:HB3	10:aL:12:PRO:HA	1.89	0.53
13:a2:55:PHE:HZ	15:a3:417:CLA:HMB2	1.73	0.53
13:a6:274:PHE:CE1	15:a6:403:CLA:H3A	2.44	0.53
1:bA:45:THR:HG21	15:bA:842:CLA:HBB1	1.90	0.53
1:bA:749:ALA:O	1:bA:753:SER:OG	2.26	0.53
3:cC:5:LYS:HD3	4:cD:113:ASN:HB3	1.89	0.53
13:c1:274:PHE:CE1	15:c1:402:CLA:H3A	2.43	0.53
13:c2:214:SER:OG	13:c2:217:ASP:OD2	2.23	0.53
13:c2:274:PHE:CE1	15:c2:402:CLA:H3A	2.44	0.53
1:aA:323:HIS:HB3	1:aA:328:ILE:HD11	1.89	0.53
2:aB:494:ASN:HB3	15:aB:842:CLA:HED3	1.91	0.53
13:a3:139:ARG:HG3	13:a3:141:ARG:H	1.73	0.53
15:a5:415:CLA:H3A	15:a5:415:CLA:O2A	2.08	0.53
1:bA:366:LEU:HD11	15:bA:820:CLA:H71	1.90	0.53
1:bA:689:PHE:HA	16:bA:846:PQN:H9	1.89	0.53
2:bB:494:ASN:HB3	15:bB:842:CLA:HED3	1.91	0.53
13:b1:274:PHE:CE1	15:b1:402:CLA:H3A	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b1:403:CLA:HBB2	15:b1:410:CLA:H162	1.91	0.53
13:b3:257:LEU:HD22	15:b3:409:CLA:HBC3	1.89	0.53
13:b4:111:HIS:HE1	15:b4:404:CLA:C4A	2.04	0.53
13:b4:214:SER:OG	13:b4:217:ASP:OD2	2.22	0.53
13:b6:22:THR:OG1	13:b6:23:ASN:N	2.39	0.53
13:c3:159:HIS:CE1	15:c3:414:CLA:ND	2.77	0.53
13:a1:274:PHE:CE1	15:a1:401:CLA:H3A	2.43	0.53
18:a2:401:BCR:H333	15:a2:406:CLA:H18	1.91	0.53
2:bB:226:THR:OG1	2:bB:228:ASN:OD1	2.26	0.53
13:b2:274:PHE:CE1	15:b2:402:CLA:H3A	2.44	0.53
18:b2:401:BCR:H333	15:b2:406:CLA:H18	1.90	0.53
1:cA:388:PRO:O	1:cA:392:SER:OG	2.22	0.53
15:cB:801:CLA:H72	15:cB:801:CLA:HBB1	1.90	0.53
13:c1:139:ARG:HG3	13:c1:141:ARG:H	1.73	0.53
13:a3:274:PHE:CE1	15:a3:402:CLA:H3A	2.43	0.53
15:a3:415:CLA:H3A	15:a3:415:CLA:O2A	2.09	0.53
1:bA:461:HIS:HE1	15:bA:835:CLA:NA	2.05	0.53
1:bA:545:THR:O	1:bA:549:THR:OG1	2.25	0.53
13:b2:326:ALA:HA	13:b2:329:PHE:HB2	1.90	0.53
13:b6:274:PHE:CE1	15:b6:403:CLA:H3A	2.44	0.53
1:cA:470:ARG:NH2	15:cA:835:CLA:O1D	2.41	0.53
2:cB:226:THR:OG1	2:cB:228:ASN:OD1	2.26	0.53
15:cB:804:CLA:H111	18:cB:849:BCR:H362	1.89	0.53
13:c1:331:GLN:HA	13:c1:334:LEU:HB2	1.89	0.53
18:c2:401:BCR:H333	15:c2:406:CLA:H18	1.91	0.53
15:c4:410:CLA:H2	15:c4:410:CLA:HED2	1.90	0.53
15:c5:415:CLA:H3A	15:c5:415:CLA:O2A	2.09	0.53
2:aB:443:ASN:HB3	2:aB:455:GLN:HE21	1.73	0.53
15:aB:832:CLA:HAB	15:aB:833:CLA:H202	1.90	0.53
15:aB:837:CLA:H8	18:aF:202:BCR:H372	1.91	0.53
4:aD:73:ARG:NH2	4:aD:80:TYR:OH	2.40	0.53
13:a2:111:HIS:HE1	15:a2:404:CLA:C4A	2.05	0.53
13:a4:326:ALA:HA	13:a4:329:PHE:HB2	1.90	0.53
15:a4:410:CLA:H2	15:a4:410:CLA:HED2	1.90	0.53
2:bB:703:PRO:O	3:bC:80:TYR:OH	2.18	0.53
3:bC:18:ARG:HG2	4:bD:103:GLU:HG2	1.91	0.53
13:b1:113:ILE:HG21	15:b2:406:CLA:H172	1.91	0.53
13:b2:331:GLN:HA	13:b2:334:LEU:HB2	1.91	0.53
13:b3:113:ILE:HG12	15:b3:421:CLA:H172	1.91	0.53
13:b5:274:PHE:CE1	15:b5:402:CLA:H3A	2.44	0.53
2:cB:642:ASN:N	2:cB:642:ASN:OD1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c4:299:PRO:HG2	13:c4:323:PHE:CE2	2.44	0.53
2:aB:301:LYS:NZ	2:aB:305:ASP:OD2	2.41	0.53
13:b5:326:ALA:HA	13:b5:329:PHE:HB2	1.91	0.53
15:cA:839:CLA:H122	15:cL:203:CLA:H203	1.91	0.53
13:c3:113:ILE:HG12	15:c3:421:CLA:H172	1.91	0.53
1:aA:470:ARG:NH2	15:aA:835:CLA:O1D	2.41	0.53
15:a1:409:CLA:HED2	15:a1:409:CLA:H2	1.90	0.53
13:a2:274:PHE:CE1	15:a2:402:CLA:H3A	2.43	0.53
13:a2:298:ALA:HA	15:a2:418:CLA:C4B	2.39	0.53
15:a4:415:CLA:H3A	15:a4:415:CLA:CGA	2.39	0.53
13:a6:331:GLN:HA	13:a6:334:LEU:HB2	1.91	0.53
8:bJ:16:ALA:O	8:bJ:20:THR:OG1	2.24	0.53
1:cA:451:LEU:HB3	1:cA:544:PHE:HB2	1.90	0.53
2:cB:682:GLU:HG2	3:cC:80:TYR:HE1	1.74	0.53
13:c1:113:ILE:HG21	15:c2:406:CLA:H172	1.90	0.53
13:c2:22:THR:OG1	13:c2:23:ASN:N	2.41	0.53
13:a2:66:SER:OG	13:a2:67:GLN:N	2.39	0.53
13:a5:113:ILE:HG21	15:a5:420:CLA:H172	1.90	0.53
13:a5:299:PRO:HG2	13:a5:323:PHE:CE2	2.44	0.53
13:b2:298:ALA:HA	15:b2:418:CLA:C4B	2.39	0.53
13:b3:159:HIS:CE1	15:b3:414:CLA:ND	2.77	0.53
15:cA:807:CLA:H201	19:cA:852:LHG:H221	1.91	0.53
2:cB:494:ASN:HB3	15:cB:842:CLA:HED3	1.91	0.53
6:cF:65:ILE:HG21	8:cJ:39:HIS:CD2	2.44	0.53
13:c4:331:GLN:HA	13:c4:334:LEU:HB2	1.90	0.53
13:c5:299:PRO:HG2	13:c5:323:PHE:CE2	2.44	0.53
1:aA:257:ASP:HB3	13:a1:310:GLY:HA3	1.92	0.52
1:aA:361:ALA:O	1:aA:365:SER:OG	2.27	0.52
15:a2:422:CLA:H72	18:a3:420:BCR:H343	1.91	0.52
13:b6:298:ALA:HA	15:b6:418:CLA:C4B	2.40	0.52
1:cA:366:LEU:HD11	15:cA:820:CLA:H71	1.90	0.52
15:cA:805:CLA:H71	15:cA:810:CLA:H171	1.91	0.52
2:cB:301:LYS:NZ	2:cB:305:ASP:OD2	2.41	0.52
1:aA:416:MET:O	1:aA:561:ARG:NH1	2.38	0.52
15:a4:415:CLA:H3A	15:a4:415:CLA:O2A	2.09	0.52
13:a5:128:ARG:NH1	15:a5:420:CLA:HAA1	2.25	0.52
13:a5:139:ARG:HG3	13:a5:141:ARG:H	1.72	0.52
1:bA:470:ARG:NH2	15:bA:835:CLA:O1D	2.41	0.52
15:bA:839:CLA:H201	15:bL:203:CLA:H102	1.90	0.52
13:b1:139:ARG:HG3	13:b1:141:ARG:H	1.73	0.52
13:b4:299:PRO:HG2	13:b4:323:PHE:CE2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b4:415:CLA:H3A	15:b4:415:CLA:O2A	2.09	0.52
13:b5:128:ARG:NH1	15:b5:420:CLA:HAA1	2.25	0.52
1:cA:564:ARG:O	4:cD:60:ARG:NH1	2.40	0.52
15:cA:803:CLA:H171	15:cA:842:CLA:H51	1.91	0.52
13:c3:299:PRO:HG2	13:c3:323:PHE:CE2	2.44	0.52
1:bA:277:ASP:N	1:bA:277:ASP:OD1	2.36	0.52
15:bA:803:CLA:H171	15:bA:843:CLA:H51	1.91	0.52
15:bB:839:CLA:H151	10:bL:88:VAL:HG11	1.91	0.52
13:b1:326:ALA:HA	13:b1:329:PHE:HB2	1.91	0.52
15:b2:422:CLA:H72	18:b3:420:BCR:H343	1.91	0.52
13:b4:331:GLN:HA	13:b4:334:LEU:HB2	1.89	0.52
13:b5:299:PRO:HG2	13:b5:323:PHE:CE2	2.44	0.52
1:cA:257:ASP:HB3	13:c1:310:GLY:HA3	1.90	0.52
1:cA:545:THR:O	1:cA:549:THR:OG1	2.25	0.52
13:c2:55:PHE:HZ	15:c3:417:CLA:HMB2	1.73	0.52
3:aC:4:VAL:HG22	3:aC:66:VAL:HG22	1.91	0.52
13:a2:331:GLN:HA	13:a2:334:LEU:HB2	1.91	0.52
15:a2:416:CLA:H3A	15:a2:416:CLA:O2A	2.10	0.52
13:a3:113:ILE:HG12	15:a3:421:CLA:H172	1.91	0.52
13:a4:299:PRO:HG2	13:a4:323:PHE:CE2	2.44	0.52
13:b2:257:LEU:HD22	15:b2:410:CLA:HBC3	1.90	0.52
13:b6:270:VAL:HG21	15:b6:403:CLA:H92	1.90	0.52
13:c3:326:ALA:HA	13:c3:329:PHE:HB2	1.91	0.52
13:c4:66:SER:OG	13:c4:67:GLN:N	2.43	0.52
15:c4:415:CLA:CGA	15:c4:415:CLA:H3A	2.40	0.52
13:c5:274:PHE:CE1	15:c5:402:CLA:H3A	2.44	0.52
13:c6:274:PHE:CE1	15:c6:404:CLA:H3A	2.44	0.52
1:aA:45:THR:HG21	15:aA:842:CLA:HBB1	1.90	0.52
1:aA:590:SER:OG	1:aA:593:ASP:OD2	2.28	0.52
6:aF:8:CYS:O	6:aF:15:GLN:NE2	2.43	0.52
13:a3:331:GLN:HE22	15:a3:415:CLA:NB	1.45	0.52
15:a3:403:CLA:HBB2	15:a3:410:CLA:H162	1.91	0.52
15:a6:416:CLA:H3A	15:a6:416:CLA:O2A	2.10	0.52
2:bB:60:VAL:HG21	15:bB:829:CLA:H42	1.92	0.52
2:bB:459:GLU:HG3	6:bF:5:LEU:HD11	1.91	0.52
15:b1:410:CLA:HED2	15:b1:410:CLA:H2	1.90	0.52
13:c1:331:GLN:NE2	15:c1:415:CLA:C4B	2.55	0.52
1:aA:326:LYS:NZ	1:aA:330:GLU:OE2	2.42	0.52
1:aA:451:LEU:HB3	1:aA:544:PHE:HB2	1.90	0.52
1:aA:564:ARG:O	4:aD:60:ARG:NH1	2.40	0.52
2:aB:60:VAL:HG21	15:aB:829:CLA:H42	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a4:257:LEU:HD22	15:a4:409:CLA:HBC3	1.92	0.52
15:bA:805:CLA:H71	15:bA:810:CLA:H171	1.91	0.52
2:bB:642:ASN:N	2:bB:642:ASN:OD1	2.40	0.52
15:b4:415:CLA:H3A	15:b4:415:CLA:CGA	2.40	0.52
13:b5:257:LEU:HD22	15:b5:409:CLA:HBC3	1.92	0.52
1:cA:361:ALA:O	1:cA:365:SER:OG	2.27	0.52
13:c3:274:PHE:CE1	15:c3:402:CLA:H3A	2.44	0.52
2:aB:419:GLU:OE1	6:aF:141:ARG:NH2	2.34	0.52
15:aB:813:CLA:HBB1	15:aB:813:CLA:HHC	1.92	0.52
13:a5:257:LEU:HD22	15:a5:409:CLA:HBC3	1.92	0.52
13:a6:270:VAL:HG21	15:a6:403:CLA:H92	1.90	0.52
13:a6:298:ALA:HA	15:a6:418:CLA:C4B	2.40	0.52
1:bA:361:ALA:O	1:bA:365:SER:OG	2.27	0.52
1:bA:590:SER:OG	1:bA:593:ASP:OD2	2.28	0.52
15:b3:415:CLA:H3A	15:b3:415:CLA:O2A	2.09	0.52
6:cF:8:CYS:O	6:cF:15:GLN:NE2	2.43	0.52
1:aA:738:GLY:O	1:aA:742:THR:OG1	2.24	0.52
2:aB:685:VAL:HG11	3:aC:80:TYR:CG	2.45	0.52
13:a1:113:ILE:HG21	15:a2:406:CLA:H172	1.90	0.52
13:a5:274:PHE:CE1	15:a5:402:CLA:H3A	2.44	0.52
15:bB:837:CLA:H152	18:bF:202:BCR:H402	1.92	0.52
13:b2:201:VAL:O	13:b2:205:TYR:N	2.33	0.52
13:b3:299:PRO:HG2	13:b3:323:PHE:CE2	2.45	0.52
13:b4:257:LEU:HD22	15:b4:409:CLA:HBC3	1.92	0.52
15:b6:416:CLA:H3A	15:b6:416:CLA:O2A	2.10	0.52
15:cA:828:CLA:HBB1	15:cA:836:CLA:HMA2	1.92	0.52
2:cB:60:VAL:HG21	15:cB:829:CLA:H42	1.92	0.52
15:c2:416:CLA:H3A	15:c2:416:CLA:O2A	2.10	0.52
13:c6:298:ALA:HA	15:c6:419:CLA:C4B	2.40	0.52
18:c6:402:BCR:H343	15:c6:418:CLA:HBB1	1.92	0.52
2:aB:275:HIS:HE1	15:aB:818:CLA:ND	2.05	0.52
6:aF:119:ALA:HB2	13:a4:352:LEU:HD22	1.91	0.52
18:aI:103:BCR:H383	10:aL:93:LEU:HD21	1.92	0.52
15:a1:414:CLA:H3A	15:a1:414:CLA:O2A	2.10	0.52
13:a4:57:ALA:O	13:a4:61:THR:OG1	2.26	0.52
13:a5:326:ALA:HA	13:a5:329:PHE:HB2	1.91	0.52
1:bA:257:ASP:HB3	13:b1:310:GLY:HA3	1.92	0.52
15:bB:813:CLA:HHC	15:bB:813:CLA:HBB1	1.92	0.52
15:b1:415:CLA:H3A	15:b1:415:CLA:O2A	2.10	0.52
13:b4:66:SER:OG	13:b4:67:GLN:N	2.43	0.52
18:b6:401:BCR:H343	15:b6:417:CLA:HBB1	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c2:422:CLA:H72	18:c3:420:BCR:H343	1.92	0.52
15:c3:415:CLA:H3A	15:c3:415:CLA:O2A	2.09	0.52
13:c4:159:HIS:CE1	15:c4:414:CLA:ND	2.77	0.52
15:c4:415:CLA:H3A	15:c4:415:CLA:O2A	2.09	0.52
2:aB:722:GLY:O	2:aB:726:THR:OG1	2.21	0.52
13:a1:111:HIS:HE1	15:a1:403:CLA:C4A	2.05	0.52
13:b2:22:THR:OG1	13:b2:23:ASN:N	2.41	0.52
15:b3:403:CLA:HBB2	15:b3:410:CLA:H162	1.91	0.52
1:cA:218:HIS:HE1	15:cA:816:CLA:ND	2.08	0.52
2:cB:31:GLU:OE1	2:cB:334:HIS:NE2	2.43	0.52
11:cM:12:LEU:HB3	18:cM:101:BCR:H21C	1.92	0.52
13:c5:257:LEU:HD22	15:c5:409:CLA:HBC3	1.92	0.52
13:c6:331:GLN:HA	13:c6:334:LEU:HB2	1.92	0.52
1:aA:232:ALA:O	1:aA:235:ASP:N	2.42	0.51
1:aA:737:LEU:HD11	18:aA:852:BCR:HC8	1.92	0.51
15:aA:828:CLA:HBB1	15:aA:836:CLA:HMA2	1.92	0.51
2:aB:209:ASP:OD1	2:aB:209:ASP:N	2.34	0.51
15:aB:811:CLA:H8	15:bL:204:CLA:H112	1.93	0.51
13:a2:159:HIS:CE1	15:a2:415:CLA:ND	2.77	0.51
13:a4:22:THR:OG1	13:a4:23:ASN:N	2.39	0.51
1:bA:326:LYS:NZ	1:bA:330:GLU:OE2	2.42	0.51
1:bA:737:LEU:HD11	18:bA:853:BCR:HC8	1.92	0.51
10:bL:93:LEU:HD21	18:bL:205:BCR:H383	1.92	0.51
13:b6:331:GLN:HA	13:b6:334:LEU:HB2	1.92	0.51
15:cA:803:CLA:H12	2:cB:430:LEU:HD12	1.91	0.51
2:cB:722:GLY:O	2:cB:726:THR:OG1	2.21	0.51
3:cC:4:VAL:HG22	3:cC:66:VAL:HG22	1.91	0.51
13:c2:298:ALA:HA	15:c2:418:CLA:C4B	2.39	0.51
13:c3:298:ALA:HA	15:c3:417:CLA:C4B	2.40	0.51
13:c5:298:ALA:HA	15:c5:417:CLA:C4B	2.41	0.51
15:aA:803:CLA:H12	2:aB:430:LEU:HD12	1.91	0.51
13:a1:299:PRO:HG2	13:a1:323:PHE:CE2	2.45	0.51
13:a1:326:ALA:HA	13:a1:329:PHE:HB2	1.91	0.51
13:a3:299:PRO:HG2	13:a3:323:PHE:CE2	2.44	0.51
15:a3:415:CLA:H3A	15:a3:415:CLA:CGA	2.40	0.51
13:a5:298:ALA:HA	15:a5:417:CLA:C4B	2.41	0.51
18:a6:401:BCR:H343	15:a6:417:CLA:HBB1	1.92	0.51
3:bC:4:VAL:HG22	3:bC:66:VAL:HG22	1.91	0.51
13:b3:298:ALA:HA	15:b3:417:CLA:C4B	2.40	0.51
15:b5:403:CLA:HBB2	15:b5:410:CLA:H162	1.93	0.51
15:b5:415:CLA:H3A	15:b5:415:CLA:CGA	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:cF:123:GLU:O	6:cF:129:LEU:N	2.44	0.51
13:c2:60:PHE:HA	13:c2:63:TYR:HB3	1.92	0.51
13:c4:257:LEU:HD22	15:c4:409:CLA:HBC3	1.92	0.51
13:c5:128:ARG:NH1	15:c5:420:CLA:HAA1	2.25	0.51
13:a6:60:PHE:HA	13:a6:63:TYR:HB3	1.92	0.51
1:bA:564:ARG:O	4:bD:60:ARG:NH1	2.40	0.51
15:bB:801:CLA:H61	15:bB:839:CLA:H43	1.93	0.51
15:b2:406:CLA:H72	18:b2:421:BCR:H343	1.93	0.51
15:b2:416:CLA:H3A	15:b2:416:CLA:O2A	2.11	0.51
13:b6:299:PRO:HG2	13:b6:323:PHE:CE2	2.46	0.51
15:cB:813:CLA:HHC	15:cB:813:CLA:HBB1	1.92	0.51
4:cD:21:ALA:HB1	4:cD:26:LYS:HG3	1.93	0.51
13:c2:331:GLN:HA	13:c2:334:LEU:HB2	1.91	0.51
15:aA:807:CLA:H201	19:aA:853:LHG:H221	1.91	0.51
2:aB:90:ILE:HB	2:aB:111:PRO:HB2	1.92	0.51
13:a1:298:ALA:HA	15:a1:416:CLA:C4B	2.41	0.51
13:a2:270:VAL:O	13:a2:274:PHE:N	2.42	0.51
13:a2:326:ALA:HA	13:a2:329:PHE:HB2	1.90	0.51
15:bA:807:CLA:H201	19:bA:854:LHG:H221	1.91	0.51
15:bA:828:CLA:HBB1	15:bA:836:CLA:HMA2	1.92	0.51
13:b5:220:GLY:HA2	13:b5:223:ILE:HD12	1.91	0.51
13:b6:60:PHE:HA	13:b6:63:TYR:HB3	1.92	0.51
8:cJ:2:LYS:HG2	13:c3:349:GLU:OE1	2.10	0.51
15:c2:406:CLA:H72	18:c2:421:BCR:H343	1.93	0.51
15:c3:403:CLA:HBB2	15:c3:410:CLA:H162	1.91	0.51
2:aB:31:GLU:OE1	2:aB:334:HIS:NE2	2.43	0.51
8:aJ:16:ALA:O	8:aJ:20:THR:OG1	2.24	0.51
13:a5:220:GLY:HA2	13:a5:223:ILE:HD12	1.91	0.51
1:bA:373:HIS:CD2	15:bA:828:CLA:NC	2.79	0.51
8:bJ:2:LYS:HG2	13:b3:349:GLU:OE1	2.11	0.51
13:b1:182:TYR:HA	13:b1:189:VAL:HA	1.93	0.51
1:cA:738:GLY:O	1:cA:742:THR:OG1	2.24	0.51
13:c4:63:TYR:O	13:c4:66:SER:OG	2.27	0.51
13:c4:274:PHE:CE1	15:c4:402:CLA:H3A	2.46	0.51
13:c6:60:PHE:HA	13:c6:63:TYR:HB3	1.92	0.51
15:aA:803:CLA:H171	15:aA:843:CLA:H51	1.91	0.51
6:aF:123:GLU:O	6:aF:129:LEU:N	2.44	0.51
15:a5:415:CLA:H3A	15:a5:415:CLA:CGA	2.40	0.51
13:b1:220:GLY:HA2	13:b1:223:ILE:HD12	1.92	0.51
13:b4:298:ALA:HA	15:b4:417:CLA:C4B	2.41	0.51
13:b6:57:ALA:O	13:b6:61:THR:OG1	2.27	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c1:415:CLA:O2A	15:c1:415:CLA:H3A	2.10	0.51
13:c5:214:SER:OG	13:c5:217:ASP:OD2	2.24	0.51
15:c5:415:CLA:H3A	15:c5:415:CLA:CGA	2.40	0.51
15:c6:417:CLA:H3A	15:c6:417:CLA:O2A	2.10	0.51
1:aA:433:VAL:HG21	15:aA:822:CLA:H192	1.93	0.51
14:bA:801:CL0:H13	15:bB:802:CLA:HAA1	1.93	0.51
13:b5:298:ALA:HA	15:b5:417:CLA:C4B	2.41	0.51
15:b6:416:CLA:H3A	15:b6:416:CLA:CGA	2.41	0.51
10:cL:93:LEU:HD21	18:cL:205:BCR:H383	1.92	0.51
13:c2:159:HIS:CE1	15:c2:415:CLA:ND	2.78	0.51
13:c2:182:TYR:HA	13:c2:189:VAL:HA	1.93	0.51
13:c3:160:HIS:CE1	15:c3:412:CLA:NC	2.77	0.51
15:c3:415:CLA:H3A	15:c3:415:CLA:CGA	2.41	0.51
15:aA:805:CLA:H71	15:aA:810:CLA:H171	1.91	0.51
3:aC:14:THR:OG1	3:aC:18:ARG:NH1	2.44	0.51
11:aM:12:LEU:HB3	18:aM:101:BCR:H21C	1.92	0.51
12:aX:23:ASN:OD1	15:aX:102:CLA:NA	2.44	0.51
13:a2:182:TYR:HA	13:a2:189:VAL:HA	1.93	0.51
13:a3:298:ALA:HA	15:a3:417:CLA:C4B	2.40	0.51
13:a4:182:TYR:HA	13:a4:189:VAL:HA	1.93	0.51
13:a5:274:PHE:CD1	15:a5:402:CLA:H12	2.46	0.51
13:a6:182:TYR:HA	13:a6:189:VAL:HA	1.93	0.51
15:bA:825:CLA:HED3	15:bA:825:CLA:H2A	1.93	0.51
2:bB:392:HIS:HE1	15:bB:830:CLA:NA	2.09	0.51
6:bF:8:CYS:O	6:bF:15:GLN:NE2	2.43	0.51
13:b1:298:ALA:HA	15:b1:417:CLA:C4B	2.41	0.51
13:b1:299:PRO:HG2	13:b1:323:PHE:CE2	2.46	0.51
13:b3:326:ALA:HA	13:b3:329:PHE:HB2	1.91	0.51
1:cA:373:HIS:CD2	15:cA:828:CLA:NC	2.79	0.51
1:cA:461:HIS:HE1	15:cA:835:CLA:NA	2.05	0.51
15:cB:820:CLA:HMB3	15:cB:825:CLA:H52	1.93	0.51
13:c1:201:VAL:O	13:c1:205:TYR:N	2.33	0.51
13:c5:274:PHE:CD1	15:c5:402:CLA:H12	2.46	0.51
8:aJ:26:LEU:HD21	15:aJ:201:CLA:HMB2	1.92	0.51
13:a1:201:VAL:O	13:a1:205:TYR:N	2.33	0.51
15:a1:402:CLA:HBB2	15:a1:409:CLA:H162	1.92	0.51
13:a2:201:VAL:O	13:a2:205:TYR:N	2.33	0.51
15:a2:406:CLA:H72	18:a2:421:BCR:H343	1.93	0.51
13:a4:66:SER:OG	13:a4:67:GLN:N	2.43	0.51
2:bB:36:MET:HE3	2:bB:41:LEU:HA	1.93	0.51
18:bB:849:BCR:HC22	18:bJ:105:BCR:H363	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:bC:14:THR:OG1	3:bC:18:ARG:NH1	2.44	0.51
13:b1:57:ALA:O	13:b1:61:THR:OG1	2.26	0.51
13:b2:159:HIS:CE1	15:b2:415:CLA:ND	2.78	0.51
13:b4:22:THR:OG1	13:b4:23:ASN:N	2.39	0.51
13:b4:274:PHE:CE1	15:b4:402:CLA:H3A	2.46	0.51
15:b5:410:CLA:H2	15:b5:410:CLA:HED2	1.93	0.51
1:cA:473:ASP:OD1	10:cL:69:ARG:NH2	2.44	0.51
2:cB:181:LEU:HD11	15:cB:814:CLA:H12	1.93	0.51
13:c1:182:TYR:HA	13:c1:189:VAL:HA	1.93	0.51
13:c4:182:TYR:HA	13:c4:189:VAL:HA	1.93	0.51
13:c6:182:TYR:HA	13:c6:189:VAL:HA	1.93	0.51
13:c6:299:PRO:HG2	13:c6:323:PHE:CE2	2.46	0.51
13:a1:124:PHE:CG	15:a2:406:CLA:HBA1	2.46	0.51
13:a2:214:SER:OG	13:a2:217:ASP:OD2	2.23	0.51
13:a6:299:PRO:HG2	13:a6:323:PHE:CE2	2.46	0.51
1:bA:218:HIS:HE1	15:bA:816:CLA:ND	2.08	0.51
1:bA:438:ASP:OD2	1:bA:564:ARG:NH1	2.44	0.51
15:bA:831:CLA:H102	15:bA:843:CLA:HAA2	1.93	0.51
2:bB:181:LEU:HD11	15:bB:814:CLA:H12	1.93	0.51
10:bL:127:GLY:O	10:bL:131:SER:OG	2.24	0.51
1:cA:433:VAL:HG21	15:cA:822:CLA:H192	1.93	0.51
15:c1:403:CLA:HBB2	15:c1:410:CLA:H162	1.92	0.51
2:aB:226:THR:OG1	2:aB:228:ASN:OD1	2.26	0.50
13:a3:326:ALA:HA	13:a3:329:PHE:HB2	1.92	0.50
13:a4:214:SER:OG	13:a4:217:ASP:OD2	2.22	0.50
13:a5:331:GLN:HE22	15:a5:415:CLA:NB	1.47	0.50
5:bE:3:ARG:HH12	5:bE:26:VAL:HG12	1.76	0.50
11:bM:12:LEU:HB3	18:bM:101:BCR:H21C	1.92	0.50
13:b2:60:PHE:HA	13:b2:63:TYR:HB3	1.93	0.50
13:b4:63:TYR:O	13:b4:66:SER:OG	2.27	0.50
13:b4:182:TYR:HA	13:b4:189:VAL:HA	1.93	0.50
13:b5:274:PHE:CD1	15:b5:402:CLA:H12	2.46	0.50
1:cA:737:LEU:HD11	18:cA:851:BCR:HC8	1.92	0.50
2:cB:19:ARG:NH2	7:cI:34:ILE:O	2.43	0.50
8:cJ:16:ALA:O	8:cJ:20:THR:OG1	2.24	0.50
13:c2:222:HIS:CE1	15:c2:402:CLA:NA	2.79	0.50
15:c2:416:CLA:H3A	15:c2:416:CLA:CGA	2.41	0.50
1:aA:438:ASP:OD2	1:aA:564:ARG:NH1	2.44	0.50
2:aB:392:HIS:HE1	15:aB:830:CLA:NA	2.09	0.50
8:aJ:2:LYS:HG2	13:a3:349:GLU:OE1	2.11	0.50
13:a1:182:TYR:HA	13:a1:189:VAL:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a2:222:HIS:CE1	15:a2:402:CLA:NA	2.79	0.50
4:bD:21:ALA:HB1	4:bD:26:LYS:HG3	1.93	0.50
12:bX:23:ASN:OD1	15:bX:102:CLA:NA	2.44	0.50
2:cB:392:HIS:HE1	15:cB:830:CLA:NA	2.09	0.50
1:aA:218:HIS:HE1	15:aA:816:CLA:ND	2.08	0.50
13:a4:274:PHE:CE1	15:a4:402:CLA:H3A	2.45	0.50
13:b1:257:LEU:HD22	15:b1:409:CLA:HBC3	1.93	0.50
13:b2:182:TYR:HA	13:b2:189:VAL:HA	1.93	0.50
13:b4:222:HIS:CE1	15:b4:402:CLA:NA	2.79	0.50
13:b5:57:ALA:O	13:b5:61:THR:OG1	2.28	0.50
13:b6:182:TYR:HA	13:b6:189:VAL:HA	1.94	0.50
2:cB:602:TRP:HE1	2:cB:614:GLN:HE21	1.59	0.50
15:cB:837:CLA:HBC2	18:cF:205:BCR:HC7	1.93	0.50
13:c1:299:PRO:HG2	13:c1:323:PHE:CE2	2.46	0.50
15:c6:417:CLA:H3A	15:c6:417:CLA:CGA	2.41	0.50
15:aA:831:CLA:H102	15:aA:843:CLA:HAA2	1.93	0.50
2:aB:731:LEU:O	2:aB:735:THR:OG1	2.27	0.50
13:a2:299:PRO:HG2	13:a2:323:PHE:CE2	2.47	0.50
13:a6:57:ALA:O	13:a6:61:THR:OG1	2.28	0.50
13:a6:111:HIS:HE1	15:a6:405:CLA:C4A	2.04	0.50
2:bB:31:GLU:OE1	2:bB:334:HIS:NE2	2.43	0.50
13:b1:274:PHE:CD1	15:b1:402:CLA:H12	2.47	0.50
13:b4:274:PHE:CD1	15:b4:402:CLA:H12	2.47	0.50
13:b5:182:TYR:HA	13:b5:189:VAL:HA	1.94	0.50
13:b6:111:HIS:HE1	15:b6:405:CLA:C4A	2.04	0.50
15:cA:825:CLA:H2A	15:cA:825:CLA:HED3	1.93	0.50
2:cB:580:ASP:OD1	2:cB:712:ARG:NH1	2.45	0.50
11:cM:10:VAL:HA	11:cM:13:VAL:HG22	1.94	0.50
13:c1:124:PHE:CG	15:c2:406:CLA:HBA1	2.46	0.50
13:c2:160:HIS:CE1	15:c2:413:CLA:NC	2.78	0.50
13:c6:323:PHE:CE1	18:c6:403:BCR:H311	2.46	0.50
1:bA:93:HIS:HE1	15:bA:808:CLA:NA	2.07	0.50
1:bA:232:ALA:O	1:bA:235:ASP:N	2.42	0.50
4:bD:118:SER:OG	4:bD:119:ILE:N	2.44	0.50
13:b1:62:LEU:HD23	13:b1:65:ILE:HD12	1.93	0.50
15:b3:415:CLA:H3A	15:b3:415:CLA:CGA	2.41	0.50
13:b6:323:PHE:CE1	18:b6:402:BCR:H311	2.46	0.50
1:cA:508:THR:OG1	1:cA:509:ALA:N	2.45	0.50
13:c2:62:LEU:HD23	13:c2:65:ILE:HD12	1.94	0.50
13:c2:128:ARG:NH2	15:c2:422:CLA:O1D	2.29	0.50
13:c4:298:ALA:HA	15:c4:417:CLA:C4B	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c6:274:PHE:CD1	15:c6:404:CLA:H12	2.47	0.50
1:aA:373:HIS:CD2	15:aA:828:CLA:NC	2.79	0.50
15:a2:416:CLA:H3A	15:a2:416:CLA:CGA	2.41	0.50
13:a5:182:TYR:HA	13:a5:189:VAL:HA	1.94	0.50
1:bA:508:THR:OG1	1:bA:509:ALA:N	2.45	0.50
4:bD:35:LYS:NZ	4:bD:36:GLU:O	2.45	0.50
6:bF:123:GLU:O	6:bF:129:LEU:N	2.44	0.50
13:b1:128:ARG:HG3	13:b2:341:MET:HG3	1.94	0.50
13:b3:214:SER:OG	13:b3:217:ASP:OD2	2.23	0.50
13:b6:274:PHE:CD1	15:b6:403:CLA:H12	2.47	0.50
2:cB:36:MET:HE3	2:cB:41:LEU:HA	1.93	0.50
3:cC:14:THR:OG1	3:cC:18:ARG:NH1	2.44	0.50
13:c2:299:PRO:HG2	13:c2:323:PHE:CE2	2.46	0.50
13:c4:274:PHE:CD1	15:c4:402:CLA:H12	2.47	0.50
15:aB:820:CLA:HMB3	15:aB:825:CLA:H52	1.93	0.50
15:aB:826:CLA:HBA1	15:aB:827:CLA:HED3	1.94	0.50
15:a5:403:CLA:HBB2	15:a5:410:CLA:H162	1.93	0.50
13:a6:201:VAL:O	13:a6:205:TYR:N	2.33	0.50
14:bA:801:CL0:H61	15:bA:802:CLA:HMA1	1.94	0.50
2:bB:142:LEU:O	2:bB:146:SER:OG	2.30	0.50
13:b4:57:ALA:O	13:b4:61:THR:OG1	2.26	0.50
13:b4:160:HIS:CE1	15:b4:412:CLA:NC	2.77	0.50
1:cA:333:LYS:HB3	1:cA:340:GLY:HA3	1.94	0.50
2:cB:275:HIS:HE1	15:cB:818:CLA:ND	2.06	0.50
12:cX:23:ASN:OD1	15:cX:102:CLA:NA	2.44	0.50
13:c1:111:HIS:HE1	15:c1:404:CLA:C4A	2.04	0.50
13:c1:298:ALA:HA	15:c1:417:CLA:C4B	2.41	0.50
15:c1:415:CLA:H3A	15:c1:415:CLA:CGA	2.42	0.50
13:c3:182:TYR:HA	13:c3:189:VAL:HA	1.94	0.50
1:aA:522:GLY:O	1:aA:625:VAL:N	2.38	0.50
2:aB:142:LEU:O	2:aB:146:SER:OG	2.30	0.50
2:aB:181:LEU:HD11	15:aB:814:CLA:H12	1.93	0.50
4:aD:35:LYS:NZ	4:aD:36:GLU:O	2.45	0.50
12:aX:8:THR:O	19:aX:101:LHG:O2	2.23	0.50
13:a1:22:THR:OG1	13:a1:23:ASN:N	2.40	0.50
13:a1:222:HIS:CE1	15:a1:401:CLA:NA	2.80	0.50
13:a2:274:PHE:CD1	15:a2:402:CLA:H12	2.47	0.50
13:a3:201:VAL:O	13:a3:205:TYR:N	2.33	0.50
15:bB:826:CLA:HBA1	15:bB:827:CLA:HED3	1.94	0.50
15:b2:416:CLA:H3A	15:b2:416:CLA:CGA	2.42	0.50
13:b6:201:VAL:O	13:b6:205:TYR:N	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b6:402:BCR:H343	15:b6:418:CLA:HBB2	1.94	0.50
1:cA:326:LYS:NZ	1:cA:330:GLU:OE2	2.42	0.50
2:cB:90:ILE:HB	2:cB:111:PRO:HB2	1.92	0.50
13:c2:63:TYR:O	13:c2:66:SER:OG	2.27	0.50
2:aB:580:ASP:OD1	2:aB:712:ARG:NH1	2.45	0.50
4:aD:21:ALA:HB1	4:aD:26:LYS:HG3	1.93	0.50
5:aE:3:ARG:HH12	5:aE:26:VAL:HG12	1.76	0.50
8:aJ:18:TRP:HE1	15:aJ:201:CLA:C1D	2.25	0.50
13:a4:222:HIS:CE1	15:a4:402:CLA:NA	2.80	0.50
13:a4:298:ALA:HA	15:a4:417:CLA:C4B	2.41	0.50
15:a6:416:CLA:H3A	15:a6:416:CLA:CGA	2.41	0.50
2:bB:94:GLN:OE1	15:bB:811:CLA:C1B	2.60	0.50
13:b1:201:VAL:O	13:b1:205:TYR:N	2.33	0.50
13:b3:160:HIS:CE1	15:b3:412:CLA:NC	2.76	0.50
13:b4:295:LEU:HB2	13:b4:299:PRO:HA	1.93	0.50
1:cA:438:ASP:OD2	1:cA:564:ARG:NH1	2.44	0.50
13:c4:201:VAL:O	13:c4:205:TYR:N	2.33	0.50
13:c5:182:TYR:HA	13:c5:189:VAL:HA	1.94	0.50
13:c5:206:GLN:HB2	15:c5:416:CLA:HMD2	1.94	0.50
13:c5:331:GLN:HE22	15:c5:415:CLA:NB	1.48	0.50
14:aA:801:CL0:H61	15:aA:802:CLA:HMA1	1.94	0.49
2:aB:425:LEU:O	2:aB:429:SER:OG	2.30	0.49
13:a1:214:SER:OG	13:a1:217:ASP:OD2	2.25	0.49
13:a1:257:LEU:HD22	15:a1:408:CLA:HBC3	1.94	0.49
13:a6:323:PHE:CE1	18:a6:402:BCR:H311	2.46	0.49
2:bB:372:ALA:HB1	2:bB:731:LEU:HD11	1.95	0.49
10:bL:68:LEU:HD23	10:bL:73:VAL:HG23	1.94	0.49
13:b1:124:PHE:CG	15:b2:406:CLA:HBA1	2.46	0.49
1:cA:696:TYR:OH	15:cA:803:CLA:OBD	2.28	0.49
4:cD:35:LYS:NZ	4:cD:36:GLU:O	2.45	0.49
5:cE:3:ARG:HH12	5:cE:26:VAL:HG12	1.76	0.49
13:c4:295:LEU:HB2	13:c4:299:PRO:HA	1.93	0.49
13:c5:112:LEU:O	13:c5:115:SER:OG	2.27	0.49
15:aB:815:CLA:H62	18:aB:846:BCR:H362	1.94	0.49
15:a1:414:CLA:H3A	15:a1:414:CLA:CGA	2.42	0.49
13:a2:57:ALA:O	13:a2:61:THR:OG1	2.28	0.49
13:a3:274:PHE:CD1	15:a3:402:CLA:H12	2.47	0.49
15:a4:421:CLA:HBC1	13:a5:266:LEU:HD11	1.94	0.49
15:a5:410:CLA:H2	15:a5:410:CLA:HED2	1.93	0.49
2:bB:580:ASP:OD1	2:bB:712:ARG:NH1	2.45	0.49
15:b3:421:CLA:HBC1	13:b4:266:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b5:206:GLN:HB2	15:b5:416:CLA:HMD2	1.94	0.49
13:b5:331:GLN:HE22	15:b5:415:CLA:NB	1.47	0.49
2:cB:419:GLU:OE1	6:cF:141:ARG:NH2	2.35	0.49
13:c1:60:PHE:HA	13:c1:63:TYR:HB3	1.94	0.49
13:c1:128:ARG:HG3	13:c2:341:MET:HG3	1.95	0.49
1:aA:662:ILE:HA	2:aB:623:MET:HE3	1.95	0.49
13:a1:274:PHE:CD1	15:a1:401:CLA:H12	2.47	0.49
13:a2:60:PHE:HA	13:a2:63:TYR:HB3	1.93	0.49
13:a4:274:PHE:CD1	15:a4:402:CLA:H12	2.47	0.49
13:a5:49:GLN:HE21	15:a5:409:CLA:HMB3	1.77	0.49
13:a5:206:GLN:HB2	15:a5:416:CLA:HMD2	1.94	0.49
1:bA:696:TYR:OH	15:bA:803:CLA:OBD	2.28	0.49
13:b6:62:LEU:HD23	13:b6:65:ILE:HD12	1.94	0.49
15:cA:831:CLA:H102	15:cA:842:CLA:HAA2	1.93	0.49
2:cB:94:GLN:OE1	15:cB:811:CLA:C1B	2.60	0.49
15:cB:833:CLA:H61	18:cF:204:BCR:H312	1.94	0.49
15:cB:839:CLA:H192	7:cI:24:THR:HB	1.95	0.49
15:c5:403:CLA:HBB2	15:c5:410:CLA:H162	1.94	0.49
15:aA:825:CLA:H2A	15:aA:825:CLA:HED3	1.93	0.49
2:bB:90:ILE:HB	2:bB:111:PRO:HB2	1.92	0.49
15:bB:820:CLA:HMB3	15:bB:825:CLA:H52	1.93	0.49
13:b2:274:PHE:CD1	15:b2:402:CLA:H12	2.47	0.49
13:b6:206:GLN:HB2	15:b6:417:CLA:HMD2	1.95	0.49
4:cD:118:SER:OG	4:cD:119:ILE:N	2.44	0.49
13:c1:257:LEU:HD22	15:c1:409:CLA:HBC3	1.94	0.49
13:c1:274:PHE:CD1	15:c1:402:CLA:H12	2.47	0.49
1:aA:388:PRO:O	1:aA:392:SER:OG	2.22	0.49
2:aB:36:MET:HE3	2:aB:41:LEU:HA	1.93	0.49
2:aB:372:ALA:HB1	2:aB:731:LEU:HD11	1.95	0.49
15:aB:837:CLA:HBC2	18:aF:203:BCR:HC7	1.93	0.49
15:a3:421:CLA:HBC1	13:a4:266:LEU:HD11	1.94	0.49
18:a6:402:BCR:H343	15:a6:418:CLA:HBB2	1.94	0.49
1:bA:433:VAL:HG21	15:bA:822:CLA:H192	1.93	0.49
11:bM:10:VAL:HA	11:bM:13:VAL:HG22	1.94	0.49
13:b2:299:PRO:HG2	13:b2:323:PHE:CE2	2.47	0.49
15:b6:422:CLA:H72	18:c1:420:BCR:H343	1.95	0.49
1:cA:277:ASP:OD1	1:cA:277:ASP:N	2.36	0.49
1:cA:662:ILE:HA	2:cB:623:MET:HE3	1.95	0.49
15:cA:825:CLA:HAB	15:cA:832:CLA:HBC2	1.95	0.49
2:cB:166:TRP:CZ2	15:cB:812:CLA:HHB	2.47	0.49
2:cB:372:ALA:HB1	2:cB:731:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c1:160:HIS:CE1	15:c1:412:CLA:NC	2.78	0.49
13:c3:60:PHE:HA	13:c3:63:TYR:HB3	1.94	0.49
15:aB:839:CLA:H151	10:aL:88:VAL:HG11	1.95	0.49
11:aM:10:VAL:HA	11:aM:13:VAL:HG22	1.94	0.49
13:a6:274:PHE:CD1	15:a6:403:CLA:H12	2.47	0.49
15:a6:404:CLA:HBB2	15:a6:411:CLA:H162	1.95	0.49
2:bB:166:TRP:CZ2	15:bB:812:CLA:HHB	2.47	0.49
13:b1:214:SER:OG	13:b1:217:ASP:OD2	2.24	0.49
13:b1:222:HIS:CE1	15:b1:402:CLA:NA	2.80	0.49
13:b2:214:SER:OG	13:b2:217:ASP:OD2	2.23	0.49
13:b2:266:LEU:HD11	15:b2:406:CLA:HBC1	1.95	0.49
13:b3:222:HIS:CE1	15:b3:402:CLA:NA	2.80	0.49
13:b5:214:SER:OG	13:b5:217:ASP:OD2	2.24	0.49
13:c3:274:PHE:CD1	15:c3:402:CLA:H12	2.48	0.49
1:aA:93:HIS:HE1	15:aA:808:CLA:NA	2.07	0.49
1:aA:508:THR:OG1	1:aA:509:ALA:N	2.45	0.49
13:a1:128:ARG:HG3	13:a2:341:MET:HG3	1.94	0.49
13:a2:62:LEU:HD23	13:a2:65:ILE:HD12	1.94	0.49
15:a2:422:CLA:HBC1	13:a3:266:LEU:HD11	1.94	0.49
13:a3:182:TYR:HA	13:a3:189:VAL:HA	1.94	0.49
13:a5:274:PHE:HD1	15:a5:402:CLA:H12	1.78	0.49
15:a5:420:CLA:HBC1	13:a6:266:LEU:HD11	1.95	0.49
1:bA:153:THR:H	1:bA:157:GLN:HE22	1.60	0.49
15:bA:806:CLA:H151	18:bA:849:BCR:H323	1.95	0.49
13:b3:60:PHE:HA	13:b3:63:TYR:HB3	1.94	0.49
2:cB:425:LEU:O	2:cB:429:SER:OG	2.31	0.49
4:cD:38:VAL:O	4:cD:75:ARG:NH2	2.46	0.49
13:c1:112:LEU:O	13:c1:115:SER:OG	2.25	0.49
15:c4:421:CLA:HBC1	13:c5:266:LEU:HD11	1.94	0.49
13:c5:156:ILE:O	13:c5:160:HIS:ND1	2.46	0.49
13:c5:222:HIS:CE1	15:c5:402:CLA:NA	2.81	0.49
15:c5:410:CLA:HED2	15:c5:410:CLA:H2	1.93	0.49
13:c6:112:LEU:O	13:c6:115:SER:OG	2.25	0.49
15:c6:405:CLA:HBB2	15:c6:412:CLA:H162	1.94	0.49
1:aA:711:LEU:HA	6:aF:130:THR:HA	1.94	0.49
13:a6:113:ILE:HD12	15:a6:422:CLA:H152	1.95	0.49
13:a6:206:GLN:HB2	15:a6:417:CLA:HMD2	1.95	0.49
2:bB:275:HIS:HE1	15:bB:818:CLA:ND	2.06	0.49
2:bB:591:ASN:HB2	15:bB:803:CLA:HBC2	1.95	0.49
3:bC:60:ASP:OD1	5:bE:44:ASN:ND2	2.35	0.49
13:b5:62:LEU:HD23	13:b5:65:ILE:HD12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:45:THR:HG22	1:cA:720:ARG:H	1.77	0.49
2:cB:198:ILE:HG12	2:cB:269:LEU:HB3	1.94	0.49
2:cB:531:LEU:O	2:cB:535:THR:OG1	2.21	0.49
13:c2:57:ALA:O	13:c2:61:THR:OG1	2.28	0.49
13:c6:206:GLN:HB2	15:c6:418:CLA:HMD2	1.95	0.49
1:aA:462:ASN:HD21	1:aA:475:PHE:HB2	1.78	0.49
6:aF:100:ILE:HA	8:aJ:10:THR:HA	1.95	0.49
10:aL:68:LEU:HD23	10:aL:73:VAL:HG23	1.94	0.49
13:a1:270:VAL:O	13:a1:274:PHE:N	2.43	0.49
13:a2:266:LEU:HD11	15:a2:406:CLA:HBC1	1.94	0.49
1:bA:542:HIS:HE1	1:bA:612:HIS:ND1	2.11	0.49
2:bB:198:ILE:HG12	2:bB:269:LEU:HB3	1.94	0.49
1:cA:590:SER:OG	1:cA:593:ASP:OD2	2.28	0.49
15:cA:804:CLA:HHC	15:cA:804:CLA:HBB1	1.95	0.49
2:cB:142:LEU:O	2:cB:146:SER:OG	2.30	0.49
15:cB:826:CLA:HBA1	15:cB:827:CLA:HED3	1.94	0.49
13:c2:266:LEU:HD11	15:c2:406:CLA:HBC1	1.94	0.49
13:c2:274:PHE:CD1	15:c2:402:CLA:H12	2.47	0.49
13:c5:62:LEU:HD23	13:c5:65:ILE:HD12	1.95	0.49
13:c6:128:ARG:HH12	15:c6:401:CLA:HED3	1.78	0.49
2:aB:94:GLN:OE1	15:aB:811:CLA:C1B	2.60	0.49
2:aB:166:TRP:CZ2	15:aB:812:CLA:HHB	2.47	0.49
2:aB:194:ILE:HD13	15:aB:816:CLA:HAC1	1.95	0.49
2:aB:198:ILE:HG12	2:aB:269:LEU:HB3	1.94	0.49
13:a1:60:PHE:HA	13:a1:63:TYR:HB3	1.94	0.49
13:a3:22:THR:OG1	13:a3:23:ASN:N	2.39	0.49
13:a5:60:PHE:HA	13:a5:63:TYR:HB3	1.95	0.49
2:bB:399:ARG:HA	4:bD:125:PRO:HB2	1.95	0.49
2:bB:602:TRP:HE1	2:bB:614:GLN:HE21	1.59	0.49
13:b2:270:VAL:O	13:b2:274:PHE:N	2.42	0.49
13:b5:160:HIS:CE1	15:b5:412:CLA:NC	2.78	0.49
13:b6:112:LEU:O	13:b6:115:SER:OG	2.26	0.49
15:b6:404:CLA:HBB2	15:b6:411:CLA:H162	1.95	0.49
15:cA:813:CLA:HHC	15:cA:813:CLA:HBB1	1.95	0.49
10:cL:68:LEU:HD23	10:cL:73:VAL:HG23	1.94	0.49
13:c1:62:LEU:HD23	13:c1:65:ILE:HD12	1.95	0.49
13:c1:206:GLN:HB2	15:c1:416:CLA:HMD2	1.95	0.49
13:a4:270:VAL:O	13:a4:274:PHE:N	2.42	0.48
1:bA:581:PRO:HD3	2:bB:567:GLY:HA2	1.95	0.48
1:bA:615:TRP:O	1:bA:619:SER:OG	2.25	0.48
2:bB:91:TRP:HB3	7:bI:15:ILE:HG13	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:bE:23:VAL:HA	5:bE:38:VAL:HA	1.95	0.48
13:b3:182:TYR:HA	13:b3:189:VAL:HA	1.93	0.48
13:b5:49:GLN:HE21	15:b5:409:CLA:HMB3	1.77	0.48
13:b5:112:LEU:O	13:b5:115:SER:OG	2.26	0.48
13:b5:201:VAL:O	13:b5:205:TYR:N	2.35	0.48
1:cA:153:THR:H	1:cA:157:GLN:HE22	1.60	0.48
1:cA:232:ALA:O	1:cA:235:ASP:N	2.42	0.48
14:cA:801:CL0:H61	15:cA:802:CLA:HMA1	1.94	0.48
15:cA:827:CLA:HAA1	15:cA:840:CLA:HED2	1.95	0.48
13:c5:60:PHE:HA	13:c5:63:TYR:HB3	1.95	0.48
13:c6:62:LEU:HD23	13:c6:65:ILE:HD12	1.94	0.48
1:aA:45:THR:HG22	1:aA:720:ARG:H	1.77	0.48
1:aA:333:LYS:HB3	1:aA:340:GLY:HA3	1.94	0.48
15:aA:829:CLA:H3A	15:aA:829:CLA:HBA2	1.61	0.48
4:aD:38:VAL:O	4:aD:75:ARG:NH2	2.46	0.48
6:aF:54:ASP:OD1	6:aF:54:ASP:N	2.46	0.48
15:b3:421:CLA:H72	18:b4:420:BCR:H343	1.95	0.48
15:b4:421:CLA:HBC1	13:b5:266:LEU:HD11	1.94	0.48
13:b5:60:PHE:HA	13:b5:63:TYR:HB3	1.95	0.48
15:cA:805:CLA:H62	15:cA:810:CLA:H203	1.96	0.48
15:cA:819:CLA:H3A	15:cA:819:CLA:HBA2	1.61	0.48
4:cD:117:ARG:NE	4:cD:121:GLN:O	2.36	0.48
13:c1:22:THR:OG1	13:c1:23:ASN:N	2.41	0.48
13:c6:222:HIS:CE1	15:c6:404:CLA:NA	2.81	0.48
1:aA:153:THR:H	1:aA:157:GLN:HE22	1.60	0.48
15:aA:826:CLA:HMA2	15:aA:828:CLA:H92	1.96	0.48
2:aB:591:ASN:HB2	15:aB:803:CLA:HBC2	1.95	0.48
4:aD:118:SER:OG	4:aD:119:ILE:N	2.44	0.48
13:a2:206:GLN:HB2	15:a2:417:CLA:HMD2	1.96	0.48
13:a3:60:PHE:HA	13:a3:63:TYR:HB3	1.94	0.48
13:a3:160:HIS:CE1	15:a3:412:CLA:NC	2.76	0.48
15:a3:421:CLA:H72	18:a4:420:BCR:H343	1.96	0.48
2:bB:425:LEU:O	2:bB:429:SER:OG	2.31	0.48
15:bB:833:CLA:H191	15:bB:837:CLA:H112	1.95	0.48
15:bB:833:CLA:H152	6:bF:71:LEU:HD21	1.95	0.48
13:b3:274:PHE:CD1	15:b3:402:CLA:H12	2.48	0.48
13:b5:274:PHE:HD1	15:b5:402:CLA:H12	1.78	0.48
1:cA:477:ASP:OD1	1:cA:533:THR:OG1	2.27	0.48
13:c1:222:HIS:CE1	15:c1:402:CLA:NA	2.81	0.48
15:c2:411:CLA:H2	15:c2:411:CLA:HED2	1.95	0.48
15:c2:413:CLA:H3A	15:c2:413:CLA:HBA1	1.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c3:91:GLY:HA2	13:c3:100:ASP:HB3	1.95	0.48
15:c4:402:CLA:HBC1	15:c4:403:CLA:H93	1.96	0.48
15:aA:805:CLA:H62	15:aA:810:CLA:H203	1.96	0.48
15:aA:825:CLA:HAB	15:aA:832:CLA:HBC2	1.95	0.48
13:a3:222:HIS:CE1	15:a3:402:CLA:NA	2.81	0.48
13:a3:274:PHE:HD1	15:a3:402:CLA:H12	1.79	0.48
2:bB:194:ILE:HD13	15:bB:816:CLA:HAC1	1.95	0.48
13:b1:156:ILE:O	13:b1:160:HIS:ND1	2.47	0.48
15:b2:422:CLA:HBC1	13:b3:266:LEU:HD11	1.94	0.48
15:b5:420:CLA:H72	18:b6:420:BCR:H343	1.95	0.48
13:b6:128:ARG:HH12	15:b6:422:CLA:HED3	1.77	0.48
15:cA:810:CLA:HAA2	18:cJ:104:BCR:H12C	1.95	0.48
15:cB:815:CLA:H62	18:cB:846:BCR:H362	1.94	0.48
13:c3:222:HIS:CE1	15:c3:402:CLA:NA	2.81	0.48
1:aA:504:ASN:HB2	15:aA:837:CLA:HED2	1.96	0.48
1:aA:615:TRP:O	1:aA:619:SER:OG	2.25	0.48
15:aA:842:CLA:HBB2	16:aA:846:PQN:H151	1.96	0.48
2:aB:577:SER:OG	2:aB:580:ASP:OD2	2.31	0.48
13:a3:125:HIS:HA	13:a3:129:ALA:HB3	1.96	0.48
13:a3:312:HIS:CD2	18:a3:418:BCR:H271	2.49	0.48
15:a4:402:CLA:HBC1	15:a4:403:CLA:H93	1.95	0.48
13:a5:222:HIS:CE1	15:a5:402:CLA:NA	2.82	0.48
13:a6:222:HIS:CE1	15:a6:403:CLA:NA	2.81	0.48
1:bA:333:LYS:HB3	1:bA:340:GLY:HA3	1.94	0.48
15:bA:813:CLA:HBB1	15:bA:813:CLA:HHC	1.95	0.48
15:bA:827:CLA:HAA1	15:bA:840:CLA:HED2	1.95	0.48
13:b1:60:PHE:HA	13:b1:63:TYR:HB3	1.94	0.48
13:b6:222:HIS:CE1	15:b6:403:CLA:NA	2.81	0.48
5:cE:23:VAL:HA	5:cE:38:VAL:HA	1.95	0.48
13:c2:206:GLN:HB2	15:c2:417:CLA:HMD2	1.96	0.48
15:c2:422:CLA:HBC1	13:c3:266:LEU:HD11	1.94	0.48
13:c3:125:HIS:HA	13:c3:129:ALA:HB3	1.96	0.48
18:c6:403:BCR:H343	15:c6:419:CLA:HBB2	1.94	0.48
1:aA:376:ALA:HA	1:aA:526:MET:HE3	1.96	0.48
13:a1:206:GLN:HB2	15:a1:415:CLA:HMD2	1.96	0.48
15:a2:403:CLA:HBB2	15:a2:411:CLA:H162	1.95	0.48
1:bA:376:ALA:HA	1:bA:526:MET:HE3	1.96	0.48
1:bA:462:ASN:HD21	1:bA:475:PHE:HB2	1.78	0.48
2:bB:491:ALA:O	2:bB:494:ASN:ND2	2.47	0.48
13:b1:206:GLN:HB2	15:b1:416:CLA:HMD2	1.95	0.48
13:b2:62:LEU:HD23	13:b2:65:ILE:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b6:160:HIS:CE1	15:b6:413:CLA:NC	2.78	0.48
2:cB:399:ARG:HA	4:cD:125:PRO:HB2	1.95	0.48
13:c4:22:THR:OG1	13:c4:23:ASN:N	2.40	0.48
1:aA:542:HIS:HE1	1:aA:612:HIS:ND1	2.11	0.48
15:aA:827:CLA:HAA1	15:aA:840:CLA:HED2	1.96	0.48
15:aB:833:CLA:H191	15:aB:837:CLA:H112	1.95	0.48
15:a3:410:CLA:H2	15:a3:410:CLA:HED2	1.95	0.48
1:bA:45:THR:HG22	1:bA:720:ARG:H	1.77	0.48
1:bA:522:GLY:O	1:bA:625:VAL:N	2.38	0.48
15:bA:825:CLA:HAB	15:bA:832:CLA:HBC2	1.95	0.48
15:bA:826:CLA:HMA2	15:bA:828:CLA:H92	1.96	0.48
13:b5:222:HIS:CE1	15:b5:402:CLA:NA	2.81	0.48
13:c3:274:PHE:HD1	15:c3:402:CLA:H12	1.79	0.48
15:c3:421:CLA:HBC1	13:c4:266:LEU:HD11	1.94	0.48
2:aB:175:ASN:HD22	2:aB:292:THR:HG23	1.79	0.48
1:bA:398:MET:HE2	1:bA:609:VAL:HG11	1.96	0.48
15:bA:810:CLA:HAA2	18:bJ:104:BCR:H12C	1.96	0.48
15:bA:842:CLA:HBB2	16:bA:846:PQN:H151	1.96	0.48
2:bB:701:ASP:OD1	2:bB:701:ASP:N	2.43	0.48
6:bF:54:ASP:N	6:bF:54:ASP:OD1	2.46	0.48
13:b5:156:ILE:O	13:b5:160:HIS:ND1	2.46	0.48
15:b6:417:CLA:HBA2	15:b6:417:CLA:H3A	1.41	0.48
18:c1:419:BCR:H343	15:c2:417:CLA:HBB1	1.95	0.48
15:c2:403:CLA:HBB2	15:c2:411:CLA:H162	1.95	0.48
15:c5:420:CLA:H72	18:c6:421:BCR:H343	1.95	0.48
18:aA:850:BCR:H333	18:aA:851:BCR:H333	1.96	0.48
2:aB:491:ALA:O	2:aB:494:ASN:ND2	2.47	0.48
2:aB:602:TRP:HE1	2:aB:614:GLN:HE21	1.59	0.48
10:aL:61:PRO:HB3	15:aL:203:CLA:HBB1	1.96	0.48
13:a4:201:VAL:O	13:a4:205:TYR:N	2.33	0.48
13:a5:57:ALA:O	13:a5:61:THR:OG1	2.28	0.48
13:a6:62:LEU:HD23	13:a6:65:ILE:HD12	1.94	0.48
15:bA:835:CLA:H72	18:bI:102:BCR:H17C	1.95	0.48
15:bB:815:CLA:H62	18:bB:846:BCR:H362	1.94	0.48
13:b3:125:HIS:HA	13:b3:129:ALA:HB3	1.96	0.48
13:b4:60:PHE:HA	13:b4:63:TYR:HB3	1.96	0.48
13:b6:128:ARG:HG3	13:c1:341:MET:HG3	1.95	0.48
1:cA:398:MET:HE2	1:cA:609:VAL:HG11	1.96	0.48
15:cA:826:CLA:HMA2	15:cA:828:CLA:H92	1.96	0.48
15:cA:834:CLA:H92	15:cB:804:CLA:H141	1.96	0.48
16:cA:845:PQN:H151	15:cF:201:CLA:HBB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:69:TRP:NE1	7:cI:6:ALA:O	2.43	0.48
13:c1:156:ILE:O	13:c1:160:HIS:ND1	2.47	0.48
15:aA:810:CLA:HAA2	18:aJ:205:BCR:H12C	1.96	0.48
15:aA:813:CLA:HHC	15:aA:813:CLA:HBB1	1.94	0.48
13:a2:274:PHE:HD1	15:a2:402:CLA:H12	1.79	0.48
13:a2:323:PHE:CE1	18:a2:401:BCR:H311	2.49	0.48
13:a4:206:GLN:HB2	15:a4:416:CLA:HMD2	1.96	0.48
15:a5:420:CLA:H72	18:a6:420:BCR:H343	1.95	0.48
10:bL:61:PRO:HB3	15:bL:204:CLA:HBB1	1.96	0.48
15:b1:415:CLA:H3A	15:b1:415:CLA:CGA	2.43	0.48
18:b1:419:BCR:H343	15:b2:417:CLA:HBB1	1.94	0.48
13:b2:206:GLN:HB2	15:b2:417:CLA:HMD2	1.95	0.48
13:b4:201:VAL:O	13:b4:205:TYR:N	2.33	0.48
15:b4:402:CLA:HBC1	15:b4:403:CLA:H93	1.96	0.48
1:cA:46:THR:HB	5:cE:52:ALA:HA	1.96	0.48
2:cB:674:ARG:O	2:cB:676:TYR:N	2.47	0.48
13:c4:206:GLN:HB2	15:c4:416:CLA:HMD2	1.96	0.48
1:aA:94:GLY:HA2	1:aA:98:SER:HB3	1.96	0.47
13:a1:156:ILE:O	13:a1:160:HIS:ND1	2.47	0.47
13:a1:322:HIS:CE1	15:a1:402:CLA:NA	2.83	0.47
13:a2:322:HIS:CE1	15:a2:403:CLA:NA	2.82	0.47
1:bA:416:MET:O	1:bA:561:ARG:NH1	2.38	0.47
1:bA:504:ASN:HB2	15:bA:837:CLA:HED2	1.96	0.47
15:bA:819:CLA:HBA2	15:bA:819:CLA:H3A	1.61	0.47
15:bB:819:CLA:HBA2	15:bB:819:CLA:H3A	1.62	0.47
4:bD:38:VAL:O	4:bD:75:ARG:NH2	2.46	0.47
4:bD:117:ARG:NE	4:bD:121:GLN:O	2.37	0.47
15:b5:412:CLA:H3A	15:b5:412:CLA:HBA1	1.54	0.47
13:b6:214:SER:OG	13:b6:217:ASP:OD2	2.22	0.47
18:b6:421:BCR:H333	15:b6:422:CLA:H18	1.95	0.47
1:cA:31:PRO:HB2	1:cA:47:TRP:HH2	1.79	0.47
1:cA:416:MET:O	1:cA:561:ARG:NH1	2.38	0.47
15:cA:806:CLA:H151	18:cA:847:BCR:H323	1.95	0.47
2:cB:491:ALA:O	2:cB:494:ASN:ND2	2.47	0.47
2:cB:554:PRO:HD2	3:cC:61:PHE:CE1	2.49	0.47
13:c4:60:PHE:HA	13:c4:63:TYR:HB3	1.96	0.47
13:c5:49:GLN:HE21	15:c5:409:CLA:HMB3	1.78	0.47
2:aB:85:PRO:HB2	2:aB:115:ALA:HB3	1.96	0.47
13:a1:62:LEU:HD23	13:a1:65:ILE:HD12	1.95	0.47
13:a4:295:LEU:HB2	13:a4:299:PRO:HA	1.95	0.47
1:bA:738:GLY:O	1:bA:742:THR:OG1	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:bA:804:CLA:HHC	15:bA:804:CLA:HBB1	1.95	0.47
6:bF:72:TYR:OH	6:bF:114:PHE:O	2.28	0.47
13:b3:312:HIS:CD2	18:b3:418:BCR:H271	2.49	0.47
13:b4:206:GLN:HB2	15:b4:416:CLA:HMD2	1.96	0.47
15:b5:420:CLA:HBC1	13:b6:266:LEU:HD11	1.95	0.47
13:b6:113:ILE:HD12	15:b6:422:CLA:H152	1.95	0.47
13:b6:128:ARG:HH11	15:b6:422:CLA:H2A	1.79	0.47
13:b6:156:ILE:O	13:b6:160:HIS:ND1	2.48	0.47
15:cA:820:CLA:HBA2	15:cA:820:CLA:H3A	1.61	0.47
2:cB:577:SER:OG	2:cB:580:ASP:OD2	2.31	0.47
2:cB:591:ASN:HB2	15:cB:803:CLA:HBC2	1.95	0.47
15:cB:833:CLA:H191	15:cB:837:CLA:H112	1.95	0.47
13:c2:49:GLN:HE22	15:c2:411:CLA:C4D	2.27	0.47
15:c3:421:CLA:H72	18:c4:420:BCR:H343	1.96	0.47
13:c4:331:GLN:HE22	15:c4:415:CLA:NB	1.51	0.47
13:c5:160:HIS:CE1	15:c5:412:CLA:NC	2.78	0.47
15:aA:806:CLA:H151	18:aA:848:BCR:H323	1.95	0.47
15:aB:808:CLA:HBC1	11:aM:12:LEU:HA	1.97	0.47
13:a1:112:LEU:O	13:a1:115:SER:OG	2.25	0.47
13:a5:23:ASN:HA	13:a5:24:VAL:HA	1.70	0.47
13:a5:112:LEU:O	13:a5:115:SER:OG	2.26	0.47
13:a5:156:ILE:O	13:a5:160:HIS:ND1	2.47	0.47
15:bA:809:CLA:HBA2	15:bA:809:CLA:H3A	1.55	0.47
13:b2:49:GLN:HE22	15:b2:411:CLA:C4D	2.27	0.47
15:b3:410:CLA:H2	15:b3:410:CLA:HED2	1.96	0.47
13:b5:312:HIS:CD2	18:b5:418:BCR:H271	2.50	0.47
15:cB:808:CLA:HBC1	11:cM:12:LEU:HA	1.96	0.47
13:c2:270:VAL:O	13:c2:274:PHE:N	2.42	0.47
13:c5:57:ALA:O	13:c5:61:THR:OG1	2.28	0.47
13:c5:274:PHE:HD1	15:c5:402:CLA:H12	1.78	0.47
15:c5:420:CLA:HBC1	13:c6:266:LEU:HD11	1.95	0.47
1:aA:398:MET:HE2	1:aA:609:VAL:HG11	1.96	0.47
15:aA:834:CLA:H92	15:aB:804:CLA:H141	1.96	0.47
13:a1:113:ILE:HD13	18:a2:401:BCR:C11	2.45	0.47
15:a6:411:CLA:H2	15:a6:411:CLA:HED2	1.96	0.47
18:bA:851:BCR:H333	18:bA:852:BCR:H333	1.96	0.47
13:b1:312:HIS:CD2	18:b1:418:BCR:H271	2.50	0.47
13:b2:323:PHE:CE1	18:b2:401:BCR:H311	2.49	0.47
15:b2:403:CLA:HBB2	15:b2:411:CLA:H162	1.96	0.47
13:b3:274:PHE:HD1	15:b3:402:CLA:H12	1.79	0.47
13:b4:312:HIS:CD2	18:b4:418:BCR:H271	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c5:23:ASN:HA	13:c5:24:VAL:HA	1.70	0.47
1:aA:113:SER:HB2	1:aA:130:VAL:HG11	1.97	0.47
15:aA:841:CLA:H72	15:aB:833:CLA:H42	1.96	0.47
15:aB:841:CLA:C4C	15:aB:842:CLA:HBB1	2.45	0.47
15:a2:403:CLA:H152	15:a2:404:CLA:HHB	1.97	0.47
13:a4:160:HIS:CE1	15:a4:412:CLA:NC	2.77	0.47
15:bA:805:CLA:H62	15:bA:810:CLA:H203	1.96	0.47
15:bB:841:CLA:C4C	15:bB:842:CLA:HBB1	2.45	0.47
13:b6:113:ILE:HG21	15:b6:422:CLA:H172	1.96	0.47
1:cA:462:ASN:HD21	1:cA:475:PHE:HB2	1.78	0.47
1:cA:542:HIS:HE1	1:cA:612:HIS:ND1	2.11	0.47
13:c2:91:GLY:HA2	13:c2:100:ASP:HB3	1.96	0.47
13:c2:201:VAL:O	13:c2:205:TYR:N	2.34	0.47
13:c6:21:GLN:HA	13:c6:22:THR:HA	1.70	0.47
13:c6:257:LEU:HD22	15:c6:411:CLA:HBC3	1.97	0.47
15:aA:804:CLA:H12	15:aA:843:CLA:H93	1.97	0.47
15:aA:822:CLA:H2	15:aA:822:CLA:H61	1.71	0.47
10:aL:96:TYR:O	10:aL:100:SER:OG	2.23	0.47
13:a2:41:LEU:HD11	15:a2:412:CLA:HBA2	1.97	0.47
13:a2:160:HIS:CE1	15:a2:413:CLA:NC	2.77	0.47
15:bA:831:CLA:H18	15:bA:843:CLA:HBA2	1.96	0.47
15:bB:827:CLA:H72	15:bB:827:CLA:H111	1.67	0.47
13:b3:91:GLY:HA2	13:b3:100:ASP:HB3	1.96	0.47
13:b6:312:HIS:CD2	18:b6:419:BCR:H271	2.50	0.47
2:cB:194:ILE:HD13	15:cB:816:CLA:HAC1	1.95	0.47
13:c3:312:HIS:CD2	18:c3:418:BCR:H271	2.49	0.47
13:c4:49:GLN:HE21	15:c4:409:CLA:HMB3	1.80	0.47
15:c4:421:CLA:H72	18:c5:419:BCR:H343	1.96	0.47
13:c6:156:ILE:O	13:c6:160:HIS:ND1	2.48	0.47
1:aA:46:THR:HB	5:aE:52:ALA:HA	1.96	0.47
15:aA:804:CLA:HHC	15:aA:804:CLA:HBB1	1.95	0.47
2:aB:674:ARG:O	2:aB:676:TYR:N	2.47	0.47
13:a1:160:HIS:CE1	15:a1:411:CLA:NC	2.77	0.47
15:a1:411:CLA:H3A	15:a1:411:CLA:HBA1	1.52	0.47
13:a3:91:GLY:HA2	13:a3:100:ASP:HB3	1.95	0.47
13:a4:312:HIS:CD2	18:a4:418:BCR:H271	2.49	0.47
13:a6:49:GLN:HE21	15:a6:410:CLA:HMB3	1.80	0.47
1:bA:46:THR:HB	5:bE:52:ALA:HA	1.96	0.47
15:bA:804:CLA:H12	15:bA:843:CLA:H93	1.97	0.47
2:bB:277:LEU:HG	15:bB:817:CLA:HAB	1.97	0.47
6:bF:104:PRO:HA	13:b3:29:TRP:HZ2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b1:125:HIS:HA	13:b1:129:ALA:HB3	1.97	0.47
18:b1:419:BCR:H343	15:b2:417:CLA:CBB	2.44	0.47
13:b2:21:GLN:HA	13:b2:22:THR:HA	1.71	0.47
13:b2:322:HIS:CE1	15:b2:403:CLA:NA	2.82	0.47
15:b2:417:CLA:H3A	15:b2:417:CLA:HBA2	1.40	0.47
13:b3:62:LEU:HD23	13:b3:65:ILE:HD12	1.96	0.47
13:b6:113:ILE:HG13	15:b6:422:CLA:H202	1.97	0.47
15:b6:403:CLA:HBC1	15:b6:404:CLA:H93	1.97	0.47
1:cA:93:HIS:HE1	15:cA:808:CLA:NA	2.07	0.47
1:cA:113:SER:HB2	1:cA:130:VAL:HG11	1.97	0.47
1:cA:376:ALA:HA	1:cA:526:MET:HE3	1.96	0.47
1:cA:504:ASN:HB2	15:cA:837:CLA:HED2	1.96	0.47
15:cB:806:CLA:HBA1	15:cB:806:CLA:H3A	1.46	0.47
6:cF:54:ASP:OD1	6:cF:54:ASP:N	2.46	0.47
13:c1:113:ILE:HD13	18:c2:401:BCR:C11	2.45	0.47
13:c1:125:HIS:HA	13:c1:129:ALA:HB3	1.97	0.47
13:c1:312:HIS:CD2	18:c1:418:BCR:H271	2.49	0.47
13:c2:41:LEU:HD11	15:c2:412:CLA:HBA2	1.96	0.47
13:c2:274:PHE:HD1	15:c2:402:CLA:H12	1.80	0.47
13:c2:322:HIS:CE1	15:c2:403:CLA:NA	2.83	0.47
13:c4:23:ASN:HA	13:c4:24:VAL:HA	1.72	0.47
13:c4:62:LEU:HD23	13:c4:65:ILE:HD12	1.97	0.47
13:c4:312:HIS:CD2	18:c4:418:BCR:H271	2.50	0.47
13:c6:38:LEU:H	13:c6:38:LEU:HG	1.56	0.47
13:c6:57:ALA:O	13:c6:61:THR:OG1	2.28	0.47
15:c6:412:CLA:H2	15:c6:412:CLA:HED2	1.97	0.47
15:aA:821:CLA:H3A	15:aA:821:CLA:HBA2	1.51	0.47
2:aB:213:SER:O	2:aB:213:SER:OG	2.29	0.47
2:aB:277:LEU:HG	15:aB:817:CLA:HAB	1.97	0.47
2:aB:399:ARG:HA	4:aD:125:PRO:HB2	1.95	0.47
5:aE:23:VAL:HA	5:aE:38:VAL:HA	1.95	0.47
13:a1:49:GLN:HE21	15:a1:408:CLA:HMB3	1.79	0.47
13:a4:91:GLY:HA2	13:a4:100:ASP:HB3	1.97	0.47
13:a5:62:LEU:HD23	13:a5:65:ILE:HD12	1.95	0.47
13:a6:156:ILE:O	13:a6:160:HIS:ND1	2.48	0.47
1:bA:31:PRO:HB2	1:bA:47:TRP:HH2	1.79	0.47
2:bB:175:ASN:HD22	2:bB:292:THR:HG23	1.79	0.47
18:bL:206:BCR:H16C	15:cL:202:CLA:HBA2	1.97	0.47
15:b4:421:CLA:H72	18:b5:419:BCR:H343	1.97	0.47
15:cA:843:CLA:HBA2	15:cA:843:CLA:H3A	1.46	0.47
15:cB:841:CLA:C4C	15:cB:842:CLA:HBB1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:cL:61:PRO:HB3	15:cL:204:CLA:HBB1	1.96	0.47
18:c1:420:BCR:H15C	18:c1:420:BCR:H351	1.81	0.47
13:c3:206:GLN:HB2	15:c3:416:CLA:HMD2	1.97	0.47
18:aF:203:BCR:H15C	18:aF:203:BCR:H351	1.80	0.47
13:a1:21:GLN:HA	13:a1:22:THR:HA	1.71	0.47
13:a1:57:ALA:O	13:a1:61:THR:OG1	2.26	0.47
13:a3:41:LEU:HD11	15:a3:411:CLA:HBA2	1.97	0.47
15:a4:416:CLA:HBA2	15:a4:416:CLA:H3A	1.40	0.47
13:a5:312:HIS:CD2	18:a5:418:BCR:H271	2.50	0.47
15:a6:417:CLA:HBA2	15:a6:417:CLA:H3A	1.41	0.47
1:bA:113:SER:HB2	1:bA:130:VAL:HG11	1.97	0.47
15:bB:828:CLA:H152	15:bB:830:CLA:H162	1.97	0.47
15:bB:833:CLA:H152	15:bB:833:CLA:H112	1.75	0.47
13:b3:49:GLN:HE21	15:b3:409:CLA:HMB3	1.80	0.47
15:b3:412:CLA:HBA1	15:b3:412:CLA:H3A	1.54	0.47
1:cA:94:GLY:HA2	1:cA:98:SER:HB3	1.96	0.47
2:cB:267:LEU:HD22	15:cB:818:CLA:HBA1	1.97	0.47
15:cB:814:CLA:H193	15:cB:814:CLA:H161	1.81	0.47
10:cL:96:TYR:O	10:cL:100:SER:OG	2.23	0.47
13:c3:62:LEU:HD23	13:c3:65:ILE:HD12	1.96	0.47
8:aJ:2:LYS:HA	8:aJ:2:LYS:HD2	1.68	0.47
13:a2:156:ILE:O	13:a2:160:HIS:ND1	2.48	0.47
13:a6:257:LEU:HD22	15:a6:410:CLA:HBC3	1.97	0.47
2:bB:175:ASN:ND2	2:bB:290:TYR:O	2.39	0.47
15:b1:412:CLA:HBA1	15:b1:412:CLA:H3A	1.52	0.47
13:b2:160:HIS:CE1	15:b2:413:CLA:NC	2.77	0.47
13:b3:21:GLN:HA	13:b3:22:THR:HA	1.71	0.47
13:b6:125:HIS:HA	13:b6:129:ALA:HB3	1.97	0.47
13:b6:257:LEU:HD22	15:b6:410:CLA:HBC3	1.97	0.47
1:cA:385:THR:HG21	1:cA:520:VAL:HB	1.97	0.47
2:cB:731:LEU:O	2:cB:735:THR:OG1	2.27	0.47
15:cB:833:CLA:H142	18:cF:204:BCR:H10C	1.97	0.47
15:c1:416:CLA:H3A	15:c1:416:CLA:HBA2	1.41	0.47
13:c2:323:PHE:CE1	18:c2:401:BCR:H311	2.49	0.47
13:c6:49:GLN:HE21	15:c6:411:CLA:HMB3	1.80	0.47
2:aB:267:LEU:HD22	15:aB:818:CLA:HBA1	1.97	0.46
15:aB:811:CLA:CED	18:aI:102:BCR:HC7	2.46	0.46
6:aF:103:VAL:HG22	8:aJ:14:LEU:HD11	1.97	0.46
10:aL:131:SER:HA	10:aL:134:VAL:HG12	1.97	0.46
13:a1:125:HIS:HA	13:a1:129:ALA:HB3	1.97	0.46
15:a1:415:CLA:HBA2	15:a1:415:CLA:H3A	1.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a3:111:HIS:HE1	15:a3:404:CLA:C4A	2.02	0.46
13:a5:270:VAL:O	13:a5:274:PHE:N	2.42	0.46
13:a6:38:LEU:H	13:a6:38:LEU:HG	1.53	0.46
15:bA:803:CLA:O1A	15:bB:803:CLA:HBB2	2.15	0.46
15:bA:844:CLA:H3A	15:bA:844:CLA:HBA2	1.46	0.46
18:bA:848:BCR:H351	18:bA:848:BCR:H15C	1.79	0.46
10:bL:106:SER:OG	10:bL:109:ASP:O	2.33	0.46
15:b6:413:CLA:H3A	15:b6:413:CLA:HBA1	1.52	0.46
1:cA:66:GLU:HB2	1:cA:187:LEU:HB2	1.97	0.46
15:cA:841:CLA:H72	15:cB:833:CLA:H42	1.96	0.46
18:cA:849:BCR:H333	18:cA:850:BCR:H333	1.96	0.46
2:cB:173:ARG:HB2	15:cB:814:CLA:HBC2	1.97	0.46
15:cB:828:CLA:H152	15:cB:830:CLA:H162	1.97	0.46
10:cL:131:SER:HA	10:cL:134:VAL:HG12	1.97	0.46
13:c5:270:VAL:O	13:c5:274:PHE:N	2.43	0.46
15:aB:833:CLA:H152	15:aB:833:CLA:H112	1.75	0.46
4:aD:7:PRO:O	4:aD:50:ARG:NH1	2.45	0.46
13:a1:312:HIS:CD2	18:a1:417:BCR:H271	2.50	0.46
15:a4:421:CLA:H72	18:a5:419:BCR:H343	1.97	0.46
13:a6:91:GLY:HA2	13:a6:100:ASP:HB3	1.98	0.46
13:a6:128:ARG:HG3	13:b1:341:MET:HG3	1.97	0.46
8:bJ:2:LYS:HA	8:bJ:2:LYS:HD2	1.68	0.46
15:b2:403:CLA:H152	15:b2:404:CLA:HHB	1.97	0.46
15:cA:831:CLA:H202	19:cA:852:LHG:H192	1.97	0.46
15:cA:839:CLA:H201	15:cL:203:CLA:H102	1.97	0.46
16:cB:843:PQN:H242	18:cB:849:BCR:H17C	1.97	0.46
13:c3:49:GLN:HE22	15:c3:410:CLA:C4D	2.28	0.46
13:c4:21:GLN:HA	13:c4:22:THR:HA	1.70	0.46
13:c4:91:GLY:HA2	13:c4:100:ASP:HB3	1.97	0.46
15:c5:402:CLA:HBC1	15:c5:403:CLA:H93	1.97	0.46
13:a1:266:LEU:HD11	15:c6:401:CLA:HBC1	1.96	0.46
13:a2:91:GLY:HA2	13:a2:100:ASP:HB3	1.96	0.46
15:a2:411:CLA:HED2	15:a2:411:CLA:H2	1.96	0.46
15:a6:422:CLA:HBC1	13:b1:266:LEU:HD11	1.97	0.46
2:bB:173:ARG:HB2	15:bB:814:CLA:HBC2	1.97	0.46
18:bB:850:BCR:H20C	18:bB:850:BCR:H361	1.79	0.46
13:b1:124:PHE:CD2	15:b2:406:CLA:HBA1	2.50	0.46
2:cB:130:THR:OG1	2:cB:133:ASP:OD1	2.27	0.46
2:cB:209:ASP:OD1	2:cB:209:ASP:N	2.34	0.46
4:cD:7:PRO:O	4:cD:50:ARG:NH1	2.45	0.46
15:cL:202:CLA:HBA2	15:cL:202:CLA:H3A	1.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c3:63:TYR:O	13:c3:66:SER:OG	2.29	0.46
15:c3:410:CLA:H2	15:c3:410:CLA:HED2	1.96	0.46
13:c6:322:HIS:CE1	15:c6:405:CLA:NA	2.84	0.46
13:a1:124:PHE:CD2	15:a2:406:CLA:HBA1	2.50	0.46
15:a1:408:CLA:HBD	15:a1:408:CLA:H121	1.98	0.46
13:a3:62:LEU:HD23	13:a3:65:ILE:HD12	1.97	0.46
13:a4:60:PHE:HA	13:a4:63:TYR:HB3	1.96	0.46
13:a5:91:GLY:HA2	13:a5:100:ASP:HB3	1.97	0.46
15:a5:416:CLA:H3A	15:a5:416:CLA:HBA2	1.41	0.46
15:a6:413:CLA:H3A	15:a6:413:CLA:HBA1	1.52	0.46
2:bB:14:ASP:HB3	2:bB:19:ARG:HB3	1.97	0.46
13:b1:128:ARG:HH12	15:b2:406:CLA:CGD	2.29	0.46
13:b4:91:GLY:HA2	13:b4:100:ASP:HB3	1.97	0.46
1:cA:603:TYR:O	1:cA:607:SER:OG	2.24	0.46
2:cB:85:PRO:HB2	2:cB:115:ALA:HB3	1.96	0.46
2:cB:175:ASN:HD22	2:cB:292:THR:HG23	1.79	0.46
4:cD:39:PHE:HB3	4:cD:75:ARG:HH12	1.81	0.46
13:c3:41:LEU:HD11	15:c3:411:CLA:HBA2	1.97	0.46
13:c4:41:LEU:HD11	15:c4:411:CLA:HBA2	1.98	0.46
13:c5:312:HIS:CD2	18:c5:418:BCR:H271	2.49	0.46
2:aB:172:SER:OG	15:aB:813:CLA:O1D	2.31	0.46
16:aB:843:PQN:H242	18:aB:849:BCR:H17C	1.97	0.46
6:aF:65:ILE:HG21	8:aJ:39:HIS:CD2	2.51	0.46
13:a2:55:PHE:CZ	15:a3:417:CLA:HMB2	2.51	0.46
13:a5:214:SER:OG	13:a5:217:ASP:OD2	2.24	0.46
13:a6:312:HIS:CD2	18:a6:419:BCR:H271	2.50	0.46
1:bA:120:ILE:HD13	1:bA:121:VAL:HG22	1.98	0.46
2:bB:85:PRO:HB2	2:bB:115:ALA:HB3	1.96	0.46
2:bB:577:SER:OG	2:bB:580:ASP:OD2	2.31	0.46
3:bC:62:LEU:H	3:bC:62:LEU:HG	1.47	0.46
13:b1:322:HIS:CE1	15:b1:403:CLA:NA	2.82	0.46
13:b4:49:GLN:HE21	15:b4:409:CLA:HMB3	1.80	0.46
1:cA:522:GLY:O	1:cA:625:VAL:N	2.38	0.46
2:cB:91:TRP:HB3	7:cI:15:ILE:HG13	1.96	0.46
13:c1:124:PHE:CD2	15:c2:406:CLA:HBA1	2.50	0.46
13:c3:23:ASN:HA	13:c3:24:VAL:HA	1.71	0.46
15:aA:831:CLA:H18	15:aA:843:CLA:HBA2	1.96	0.46
15:aA:831:CLA:H202	19:aA:853:LHG:H192	1.97	0.46
13:a3:206:GLN:HB2	15:a3:416:CLA:HMD2	1.97	0.46
1:bA:94:GLY:HA2	1:bA:98:SER:HB3	1.96	0.46
2:bB:548:ARG:NH2	4:bD:124:ASN:OD1	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:bC:16:CYS:HB2	3:bC:25:LEU:HD13	1.97	0.46
4:bD:39:PHE:HA	4:bD:75:ARG:HH22	1.81	0.46
15:b4:416:CLA:HHC	15:b4:416:CLA:HMC1	1.67	0.46
15:b6:418:CLA:H41	15:b6:418:CLA:H62	1.75	0.46
15:cA:804:CLA:H12	15:cA:842:CLA:H93	1.97	0.46
15:cA:831:CLA:H18	15:cA:842:CLA:HBA2	1.96	0.46
6:cF:72:TYR:OH	6:cF:114:PHE:O	2.28	0.46
1:aA:31:PRO:HG2	6:aF:99:ILE:HD12	1.98	0.46
15:aA:807:CLA:H193	15:aA:807:CLA:H161	1.79	0.46
15:aB:821:CLA:HBA2	15:aB:821:CLA:H3A	1.61	0.46
15:aB:837:CLA:C16	18:aF:202:BCR:H23C	2.46	0.46
13:a1:291:LEU:HA	13:a1:304:THR:HG23	1.97	0.46
18:a1:418:BCR:H343	15:a2:417:CLA:CBB	2.45	0.46
13:a2:22:THR:OG1	13:a2:23:ASN:N	2.41	0.46
13:a2:312:HIS:CD2	18:a2:419:BCR:H271	2.51	0.46
13:a3:49:GLN:HE21	15:a3:409:CLA:HMB3	1.80	0.46
13:a4:41:LEU:HD11	15:a4:411:CLA:HBA2	1.98	0.46
13:a6:274:PHE:HD1	15:a6:403:CLA:H12	1.81	0.46
2:bB:321:PRO:HB2	2:bB:409:ASN:HA	1.98	0.46
13:b1:41:LEU:HD11	15:b1:411:CLA:HBA2	1.98	0.46
13:b2:274:PHE:HD1	15:b2:402:CLA:H12	1.79	0.46
15:b3:417:CLA:H62	15:b3:417:CLA:H41	1.77	0.46
13:b4:125:HIS:HA	13:b4:129:ALA:HB3	1.98	0.46
13:b6:63:TYR:O	13:b6:66:SER:OG	2.31	0.46
1:cA:425:ASN:OD1	1:cA:428:ASN:ND2	2.40	0.46
15:cA:812:CLA:H111	15:cA:812:CLA:H151	1.79	0.46
2:cB:277:LEU:HG	15:cB:817:CLA:HAB	1.97	0.46
3:cC:51:LYS:NZ	3:cC:66:VAL:O	2.49	0.46
10:cL:127:GLY:O	10:cL:131:SER:OG	2.24	0.46
13:c1:49:GLN:HE21	15:c1:409:CLA:HMB3	1.80	0.46
13:c1:291:LEU:HA	13:c1:304:THR:HG23	1.97	0.46
13:c3:66:SER:OG	13:c3:67:GLN:N	2.49	0.46
18:c4:420:BCR:H15C	18:c4:420:BCR:H351	1.79	0.46
13:c5:22:THR:OG1	13:c5:23:ASN:N	2.42	0.46
13:c6:91:GLY:HA2	13:c6:100:ASP:HB3	1.98	0.46
15:c6:404:CLA:HBC1	15:c6:405:CLA:H93	1.97	0.46
6:aF:61:GLY:HA3	8:aJ:39:HIS:O	2.16	0.46
13:a1:341:MET:HE2	13:c6:128:ARG:HE	1.81	0.46
18:a1:419:BCR:H343	15:c6:401:CLA:H72	1.97	0.46
13:a4:23:ASN:HA	13:a4:24:VAL:HA	1.71	0.46
1:bA:583:ARG:HG3	3:bC:48:VAL:HB	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:bA:810:CLA:H202	15:bA:810:CLA:H161	1.82	0.46
15:bA:831:CLA:H202	19:bA:854:LHG:H192	1.97	0.46
2:bB:267:LEU:HD22	15:bB:818:CLA:HBA1	1.97	0.46
15:bF:201:CLA:HBA1	15:bF:201:CLA:H3A	1.72	0.46
10:bL:131:SER:HA	10:bL:134:VAL:HG12	1.97	0.46
13:b1:21:GLN:HA	13:b1:22:THR:HA	1.71	0.46
13:b2:156:ILE:O	13:b2:160:HIS:ND1	2.49	0.46
13:b2:312:HIS:CD2	18:b2:419:BCR:H271	2.51	0.46
13:b3:41:LEU:HD11	15:b3:411:CLA:HBA2	1.97	0.46
13:b3:206:GLN:HB2	15:b3:416:CLA:HMD2	1.97	0.46
13:b5:125:HIS:HA	13:b5:129:ALA:HB3	1.98	0.46
15:b5:402:CLA:HBC1	15:b5:403:CLA:H93	1.98	0.46
15:c1:409:CLA:HBD	15:c1:409:CLA:H121	1.98	0.46
13:c4:49:GLN:HE22	15:c4:410:CLA:C4D	2.28	0.46
13:c4:270:VAL:O	13:c4:274:PHE:N	2.43	0.46
13:c6:125:HIS:HA	13:c6:129:ALA:HB3	1.98	0.46
2:aB:173:ARG:HB2	15:aB:814:CLA:HBC2	1.97	0.46
2:aB:276:HIS:CE1	15:aB:819:CLA:NA	2.84	0.46
15:aB:827:CLA:H111	15:aB:827:CLA:H72	1.67	0.46
3:aC:16:CYS:HB2	3:aC:25:LEU:HD13	1.97	0.46
3:aC:43:ARG:HD3	4:aD:97:LYS:HD3	1.97	0.46
3:aC:51:LYS:NZ	3:aC:66:VAL:O	2.49	0.46
10:aL:106:SER:OG	10:aL:109:ASP:O	2.33	0.46
13:a1:274:PHE:HD1	15:a1:401:CLA:H12	1.81	0.46
1:bA:586:THR:O	1:bA:586:THR:OG1	2.31	0.46
1:bA:711:LEU:HD21	15:bB:832:CLA:H3A	1.98	0.46
16:bA:846:PQN:H111	18:bB:849:BCR:H393	1.96	0.46
2:bB:442:HIS:HE1	15:bB:834:CLA:NA	2.13	0.46
16:bB:843:PQN:H242	18:bB:850:BCR:H17C	1.97	0.46
18:b4:401:BCR:H343	15:b4:417:CLA:HBB2	1.98	0.46
2:cB:276:HIS:CE1	15:cB:819:CLA:NA	2.84	0.46
10:cL:106:SER:OG	10:cL:109:ASP:O	2.33	0.46
13:c3:21:GLN:HA	13:c3:22:THR:HA	1.71	0.46
15:c3:412:CLA:HBA1	15:c3:412:CLA:H3A	1.55	0.46
13:c4:125:HIS:HA	13:c4:129:ALA:HB3	1.98	0.46
1:aA:545:THR:HG22	1:aA:601:TRP:HZ3	1.81	0.46
15:aB:801:CLA:H62	15:aB:801:CLA:H41	1.57	0.46
15:aB:814:CLA:H193	15:aB:814:CLA:H161	1.81	0.46
10:aL:79:LEU:HD23	10:bL:137:PHE:CZ	2.51	0.46
13:a1:41:LEU:HD11	15:a1:410:CLA:HBA2	1.98	0.46
13:a1:128:ARG:HH12	15:a2:406:CLA:CGD	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a5:125:HIS:HA	13:a5:129:ALA:HB3	1.98	0.46
15:a5:412:CLA:H3A	15:a5:412:CLA:HBA1	1.53	0.46
15:a5:416:CLA:HHC	15:a5:416:CLA:HMC1	1.69	0.46
18:a6:401:BCR:H20C	18:a6:401:BCR:H361	1.82	0.46
15:bA:807:CLA:H193	15:bA:807:CLA:H161	1.79	0.46
2:bB:228:ASN:OD1	2:bB:228:ASN:N	2.47	0.46
15:bB:831:CLA:HBA2	15:bB:831:CLA:H3A	1.51	0.46
15:bB:836:CLA:H93	12:bX:23:ASN:ND2	2.31	0.46
7:bI:1:MET:HE3	7:bI:1:MET:HB3	1.81	0.46
13:b1:274:PHE:HD1	15:b1:402:CLA:H12	1.80	0.46
13:b2:91:GLY:HA2	13:b2:100:ASP:HB3	1.97	0.46
15:b2:406:CLA:H162	15:b2:417:CLA:HBB2	1.98	0.46
13:b5:323:PHE:CE1	18:b5:401:BCR:H311	2.51	0.46
2:cB:14:ASP:HB3	2:cB:19:ARG:HB3	1.97	0.46
6:cF:70:PHE:HD1	18:cF:202:BCR:H321	1.81	0.46
13:c1:41:LEU:HD11	15:c1:411:CLA:HBA2	1.98	0.46
13:c1:322:HIS:CE1	15:c1:403:CLA:NA	2.83	0.46
18:c1:401:BCR:C9	15:c1:416:CLA:HBB1	2.45	0.46
18:c1:419:BCR:H343	15:c2:417:CLA:CBB	2.45	0.46
13:c6:312:HIS:CD2	18:c6:420:BCR:H271	2.50	0.46
1:aA:31:PRO:HB2	1:aA:47:TRP:HH2	1.79	0.45
1:aA:385:THR:HG21	1:aA:520:VAL:HB	1.97	0.45
15:aA:826:CLA:H143	15:aA:826:CLA:H111	1.77	0.45
15:aA:843:CLA:HBA2	15:aA:843:CLA:H3A	1.77	0.45
2:aB:661:LEU:O	2:aB:665:THR:OG1	2.28	0.45
15:aB:828:CLA:H152	15:aB:830:CLA:H162	1.97	0.45
15:aB:837:CLA:H152	18:aF:202:BCR:H402	1.98	0.45
15:aB:838:CLA:HBC2	15:aX:102:CLA:HBC3	1.98	0.45
4:aD:39:PHE:HB3	4:aD:75:ARG:HH12	1.81	0.45
13:a2:21:GLN:HA	13:a2:22:THR:HA	1.71	0.45
13:a2:49:GLN:HE22	15:a2:411:CLA:C4D	2.28	0.45
13:a6:125:HIS:HA	13:a6:129:ALA:HB3	1.99	0.45
1:bA:385:THR:HG21	1:bA:520:VAL:HB	1.97	0.45
4:bD:39:PHE:HB3	4:bD:75:ARG:HH12	1.81	0.45
10:bL:34:LEU:HD21	15:bL:202:CLA:HBB1	1.98	0.45
13:b1:49:GLN:HE21	15:b1:409:CLA:HMB3	1.79	0.45
13:b2:125:HIS:HA	13:b2:129:ALA:HB3	1.98	0.45
15:b2:406:CLA:H3A	15:b2:406:CLA:HBA2	1.37	0.45
13:b6:49:GLN:HE21	15:b6:410:CLA:HMB3	1.80	0.45
15:b6:411:CLA:H2	15:b6:411:CLA:HED2	1.96	0.45
15:b6:422:CLA:HBC1	13:c1:266:LEU:HD11	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:155:HIS:HE1	15:cB:812:CLA:NA	2.11	0.45
13:c3:201:VAL:O	13:c3:205:TYR:N	2.33	0.45
13:c4:274:PHE:HD1	15:c4:402:CLA:H12	1.81	0.45
13:c6:160:HIS:CE1	15:c6:414:CLA:NC	2.78	0.45
1:aA:66:GLU:HB2	1:aA:187:LEU:HB2	1.97	0.45
2:aB:255:THR:OG1	2:aB:271:ASP:OD1	2.34	0.45
2:aB:369:THR:HG23	2:aB:735:THR:HB	1.98	0.45
4:aD:100:VAL:HG13	4:aD:104:LYS:HE2	1.98	0.45
18:a1:418:BCR:H343	15:a2:417:CLA:HBB1	1.98	0.45
13:a5:21:GLN:HA	13:a5:22:THR:HA	1.72	0.45
1:bA:66:GLU:HB2	1:bA:187:LEU:HB2	1.97	0.45
1:bA:157:GLN:O	1:bA:161:THR:OG1	2.31	0.45
15:bA:803:CLA:H12	2:bB:430:LEU:HD12	1.98	0.45
15:bA:807:CLA:H112	15:bA:807:CLA:H71	1.73	0.45
15:bA:820:CLA:HBA2	15:bA:820:CLA:H3A	1.61	0.45
3:bC:51:LYS:NZ	3:bC:66:VAL:O	2.49	0.45
13:b2:55:PHE:CZ	15:b3:417:CLA:HMB2	2.51	0.45
13:b6:307:LEU:HA	13:b6:308:PRO:HA	1.78	0.45
18:b6:420:BCR:H20C	18:b6:420:BCR:H361	1.83	0.45
2:cB:175:ASN:ND2	2:cB:290:TYR:O	2.40	0.45
2:cB:550:SER:HA	6:cF:139:SER:HB3	1.98	0.45
15:cB:838:CLA:HBC2	15:cX:102:CLA:HBC3	1.97	0.45
1:aA:272:TRP:HZ3	15:aA:818:CLA:H51	1.81	0.45
1:aA:712:LYS:HG3	6:aF:131:ALA:HB2	1.99	0.45
15:a1:401:CLA:HBC1	15:a1:402:CLA:H93	1.98	0.45
13:a2:125:HIS:HA	13:a2:129:ALA:HB3	1.98	0.45
13:a4:125:HIS:HA	13:a4:129:ALA:HB3	1.98	0.45
13:a5:323:PHE:CE1	18:a5:401:BCR:H311	2.51	0.45
15:a6:403:CLA:HBC1	15:a6:404:CLA:H93	1.97	0.45
15:b1:416:CLA:H3A	15:b1:416:CLA:HBA2	1.41	0.45
13:b4:62:LEU:HD23	13:b4:65:ILE:HD12	1.97	0.45
18:cA:848:BCR:H15C	18:cA:848:BCR:H351	1.86	0.45
13:c1:91:GLY:HA2	13:c1:100:ASP:HB3	1.98	0.45
13:c2:55:PHE:CZ	15:c3:417:CLA:HMB2	2.51	0.45
15:c2:403:CLA:H152	15:c2:404:CLA:HHB	1.97	0.45
13:c5:201:VAL:O	13:c5:205:TYR:N	2.35	0.45
4:aD:39:PHE:HA	4:aD:75:ARG:HH22	1.81	0.45
18:a1:418:BCR:H20C	18:a1:418:BCR:H361	1.85	0.45
1:bA:545:THR:HG22	1:bA:601:TRP:HZ3	1.81	0.45
13:b1:160:HIS:CE1	15:b1:412:CLA:NC	2.78	0.45
13:b2:221:GLY:HA3	18:b2:421:BCR:H393	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b2:422:CLA:H92	15:b2:422:CLA:H62	1.83	0.45
13:b3:49:GLN:HE22	15:b3:410:CLA:C4D	2.29	0.45
13:b6:322:HIS:CE1	15:b6:404:CLA:NA	2.84	0.45
1:cA:272:TRP:HZ3	15:cA:818:CLA:H51	1.81	0.45
1:cA:615:TRP:O	1:cA:619:SER:OG	2.25	0.45
15:cA:842:CLA:H142	15:cA:842:CLA:H111	1.82	0.45
4:cD:39:PHE:HA	4:cD:75:ARG:HH22	1.81	0.45
8:cJ:2:LYS:HD2	8:cJ:2:LYS:HA	1.68	0.45
13:c1:128:ARG:HH12	15:c2:406:CLA:CGD	2.29	0.45
13:c2:125:HIS:HA	13:c2:129:ALA:HB3	1.98	0.45
15:c3:402:CLA:HBC1	15:c3:403:CLA:H93	1.99	0.45
13:c5:91:GLY:HA2	13:c5:100:ASP:HB3	1.97	0.45
13:c5:125:HIS:HA	13:c5:129:ALA:HB3	1.98	0.45
15:aA:834:CLA:H102	15:aB:839:CLA:H52	1.98	0.45
2:aB:14:ASP:HB3	2:aB:19:ARG:HB3	1.97	0.45
15:aB:829:CLA:H43	18:aB:845:BCR:H393	1.99	0.45
13:a1:91:GLY:HA2	13:a1:100:ASP:HB3	1.98	0.45
15:a2:406:CLA:H162	15:a2:417:CLA:HBB2	1.98	0.45
13:a3:57:ALA:O	13:a3:61:THR:OG1	2.26	0.45
13:a3:291:LEU:HA	13:a3:304:THR:HG23	1.99	0.45
15:a3:403:CLA:H152	15:a3:404:CLA:HHB	1.99	0.45
15:a3:416:CLA:H3A	15:a3:416:CLA:HBA2	1.40	0.45
13:a4:274:PHE:HD1	15:a4:402:CLA:H12	1.81	0.45
13:a6:113:ILE:HG21	15:a6:422:CLA:H172	1.98	0.45
1:bA:466:ARG:NH1	1:bA:645:THR:OG1	2.50	0.45
1:bA:593:ASP:OD1	1:bA:728:ARG:NH1	2.50	0.45
10:bL:96:TYR:O	10:bL:100:SER:OG	2.23	0.45
13:b4:128:ARG:NH1	15:b4:421:CLA:O1A	2.50	0.45
13:b5:291:LEU:HA	13:b5:304:THR:HG23	1.98	0.45
1:cA:157:GLN:O	1:cA:161:THR:OG1	2.31	0.45
15:cA:834:CLA:H102	15:cB:839:CLA:H52	1.98	0.45
13:c2:156:ILE:O	13:c2:160:HIS:ND1	2.50	0.45
15:c2:402:CLA:HBC1	15:c2:403:CLA:H93	1.99	0.45
13:c4:128:ARG:NH1	15:c4:421:CLA:O1A	2.49	0.45
13:c5:322:HIS:CE1	15:c5:403:CLA:NA	2.85	0.45
1:aA:120:ILE:HD13	1:aA:121:VAL:HG22	1.98	0.45
1:aA:593:ASP:OD1	1:aA:728:ARG:NH1	2.50	0.45
2:aB:321:PRO:HB2	2:aB:409:ASN:HA	1.98	0.45
15:a2:418:CLA:H41	15:a2:418:CLA:H62	1.79	0.45
13:a3:49:GLN:HE22	15:a3:410:CLA:C4D	2.30	0.45
13:a3:66:SER:OG	13:a3:67:GLN:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a3:412:CLA:H3A	15:a3:412:CLA:HBA1	1.55	0.45
13:a4:62:LEU:HD23	13:a4:65:ILE:HD12	1.97	0.45
13:a5:41:LEU:HD11	15:a5:411:CLA:HBA2	1.99	0.45
2:bB:155:HIS:HE1	15:bB:812:CLA:NA	2.11	0.45
2:bB:481:LEU:HA	2:bB:489:SER:HB2	1.99	0.45
13:b1:291:LEU:HA	13:b1:304:THR:HG23	1.98	0.45
15:b1:409:CLA:HBD	15:b1:409:CLA:H121	1.97	0.45
13:b4:112:LEU:O	13:b4:115:SER:OG	2.25	0.45
13:b4:274:PHE:HD1	15:b4:402:CLA:H12	1.81	0.45
1:cA:120:ILE:HD13	1:cA:121:VAL:HG22	1.98	0.45
1:cA:545:THR:HG22	1:cA:601:TRP:HZ3	1.81	0.45
2:cB:49:HIS:NE2	15:cB:806:CLA:C4D	2.75	0.45
2:cB:369:THR:HG23	2:cB:735:THR:HB	1.98	0.45
3:cC:43:ARG:HD3	4:cD:97:LYS:HD3	1.99	0.45
13:c5:307:LEU:HA	13:c5:308:PRO:HA	1.78	0.45
15:aA:839:CLA:H122	15:aL:202:CLA:H203	1.98	0.45
2:aB:566:ASP:OD1	3:aC:65:ARG:NH1	2.41	0.45
2:aB:586:MET:HE3	2:aB:586:MET:HB3	1.80	0.45
18:aI:103:BCR:H15C	18:aI:103:BCR:H351	1.83	0.45
13:a4:49:GLN:HE21	15:a4:409:CLA:HMB3	1.80	0.45
18:a4:401:BCR:H343	15:a4:417:CLA:HBB2	1.99	0.45
13:a6:22:THR:OG1	13:a6:23:ASN:N	2.39	0.45
1:bA:688:MET:O	1:bA:692:SER:OG	2.22	0.45
4:bD:7:PRO:O	4:bD:50:ARG:NH1	2.45	0.45
13:b1:49:GLN:HE22	15:b1:410:CLA:C4D	2.29	0.45
13:b2:41:LEU:HD11	15:b2:412:CLA:HBA2	1.98	0.45
13:b2:112:LEU:O	13:b2:115:SER:OG	2.29	0.45
15:b2:411:CLA:H2	15:b2:411:CLA:HED2	1.97	0.45
15:b3:410:CLA:H162	15:b3:410:CLA:H141	1.86	0.45
13:b4:49:GLN:HE22	15:b4:410:CLA:C4D	2.29	0.45
18:b4:420:BCR:H15C	18:b4:420:BCR:H351	1.79	0.45
13:b5:41:LEU:HD11	15:b5:411:CLA:HBA2	1.99	0.45
13:b5:91:GLY:HA2	13:b5:100:ASP:HB3	1.97	0.45
2:cB:111:PRO:HD2	7:cI:1:MET:HA	1.99	0.45
15:cB:819:CLA:H41	15:cB:819:CLA:H62	1.67	0.45
13:c2:312:HIS:CD2	18:c2:419:BCR:H271	2.51	0.45
15:c3:421:CLA:H203	15:c3:421:CLA:H161	1.81	0.45
15:aA:839:CLA:H142	15:aA:839:CLA:H111	1.83	0.45
2:aB:481:LEU:HA	2:aB:489:SER:HB2	1.99	0.45
10:aL:34:LEU:HD21	15:aL:201:CLA:HBB1	1.98	0.45
15:aL:201:CLA:HBA2	15:aL:201:CLA:H3A	1.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a3:156:ILE:O	13:a3:160:HIS:ND1	2.50	0.45
13:a4:49:GLN:HE22	15:a4:410:CLA:C4D	2.30	0.45
1:bA:181:HIS:CE1	15:bA:812:CLA:NA	2.85	0.45
1:bA:272:TRP:HZ3	15:bA:818:CLA:H51	1.81	0.45
2:bB:49:HIS:NE2	15:bB:806:CLA:C4D	2.75	0.45
13:b1:111:HIS:HE1	15:b1:404:CLA:C4A	2.03	0.45
13:b2:192:ILE:HD11	13:b2:215:LEU:HD13	1.99	0.45
15:b4:417:CLA:H41	15:b4:417:CLA:H62	1.76	0.45
15:cB:817:CLA:HBA2	15:cB:817:CLA:H3A	1.67	0.45
13:c5:291:LEU:HA	13:c5:304:THR:HG23	1.98	0.45
15:aB:833:CLA:H61	18:aF:202:BCR:H312	1.99	0.45
13:a4:291:LEU:HA	13:a4:304:THR:HG23	1.99	0.45
13:a5:192:ILE:HD11	13:a5:215:LEU:HD13	1.99	0.45
15:a5:402:CLA:HBC1	15:a5:403:CLA:H93	1.98	0.45
13:a6:112:LEU:O	13:a6:115:SER:OG	2.27	0.45
2:bB:255:THR:OG1	2:bB:271:ASP:OD1	2.34	0.45
15:bB:810:CLA:H141	15:bB:810:CLA:H162	1.76	0.45
13:b6:91:GLY:HA2	13:b6:100:ASP:HB3	1.98	0.45
13:b6:274:PHE:HD1	15:b6:403:CLA:H12	1.81	0.45
15:cA:830:CLA:H192	15:cA:830:CLA:H162	1.80	0.45
2:cB:321:PRO:HB2	2:cB:409:ASN:HA	1.98	0.45
2:cB:703:PRO:O	3:cC:80:TYR:OH	2.24	0.45
3:cC:13:CYS:O	3:cC:15:GLN:NE2	2.45	0.45
3:cC:16:CYS:HB2	3:cC:25:LEU:HD13	1.97	0.45
13:c1:49:GLN:HE22	15:c1:410:CLA:C4D	2.29	0.45
15:c4:410:CLA:H162	15:c4:410:CLA:H141	1.86	0.45
13:c5:323:PHE:CE1	18:c5:401:BCR:H311	2.51	0.45
13:c6:49:GLN:HE22	15:c6:412:CLA:C4D	2.30	0.45
2:aB:49:HIS:NE2	15:aB:806:CLA:C4D	2.75	0.45
2:aB:155:HIS:HE1	15:aB:812:CLA:NA	2.11	0.45
13:a6:49:GLN:HE22	15:a6:411:CLA:C4D	2.30	0.45
13:a6:307:LEU:HA	13:a6:308:PRO:HA	1.78	0.45
1:bA:491:GLN:HE22	15:bA:838:CLA:HMD3	1.82	0.45
2:bB:150:PHE:HZ	15:cA:844:CLA:H11	1.82	0.45
2:bB:369:THR:HG23	2:bB:735:THR:HB	1.98	0.45
13:b1:80:ILE:HG23	15:b1:405:CLA:HMA1	1.99	0.45
13:b5:22:THR:OG1	13:b5:23:ASN:N	2.42	0.45
1:cA:43:GLN:H	1:cA:43:GLN:HG2	1.49	0.45
2:cB:93:PRO:HG2	15:cB:811:CLA:HHB	1.99	0.45
6:cF:27:ASP:HB3	6:cF:30:SER:HB3	1.99	0.45
15:cF:203:CLA:H3A	15:cF:203:CLA:HBA1	1.72	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c2:406:CLA:H162	15:c2:417:CLA:HBB2	1.99	0.45
13:c3:49:GLN:HE21	15:c3:409:CLA:HMB3	1.80	0.45
13:c3:291:LEU:HA	13:c3:304:THR:HG23	1.99	0.45
13:c5:49:GLN:HE22	15:c5:410:CLA:C4D	2.29	0.45
13:c5:192:ILE:HD11	13:c5:215:LEU:HD13	1.99	0.45
15:aB:819:CLA:HBA2	15:aB:819:CLA:H3A	1.62	0.44
15:aL:203:CLA:H93	15:aL:203:CLA:H111	1.82	0.44
13:a4:128:ARG:NH1	15:a4:421:CLA:O1A	2.49	0.44
15:a4:403:CLA:H152	15:a4:404:CLA:HHB	2.00	0.44
13:a5:49:GLN:HE22	15:a5:410:CLA:C4D	2.30	0.44
13:a5:291:LEU:HA	13:a5:304:THR:HG23	1.98	0.44
1:bA:716:ALA:N	6:bF:98:GLU:OE2	2.47	0.44
15:bA:803:CLA:H121	15:bA:843:CLA:H101	1.99	0.44
15:bA:829:CLA:H93	18:bJ:103:BCR:H361	1.99	0.44
2:bB:722:GLY:O	2:bB:726:THR:OG1	2.21	0.44
13:b1:22:THR:OG1	13:b1:23:ASN:N	2.41	0.44
13:b1:270:VAL:O	13:b1:274:PHE:N	2.44	0.44
13:b2:113:ILE:HD13	13:b2:113:ILE:HA	1.76	0.44
13:b3:80:ILE:HG23	15:b3:405:CLA:HMA1	1.99	0.44
13:b3:156:ILE:O	13:b3:160:HIS:ND1	2.50	0.44
13:b5:322:HIS:CE1	15:b5:403:CLA:NA	2.85	0.44
1:cA:466:ARG:NH2	1:cA:641:GLN:O	2.49	0.44
2:cB:442:HIS:HE1	15:cB:834:CLA:NA	2.13	0.44
13:c1:270:VAL:O	13:c1:274:PHE:N	2.44	0.44
15:c1:403:CLA:H152	15:c1:404:CLA:HHB	2.00	0.44
1:aA:203:GLY:HA3	15:aA:814:CLA:HBB1	1.99	0.44
15:aA:843:CLA:H142	15:aA:843:CLA:H111	1.82	0.44
15:a3:402:CLA:HBC1	15:a3:403:CLA:H93	1.99	0.44
13:a4:307:LEU:HA	13:a4:308:PRO:HA	1.79	0.44
13:a5:160:HIS:CE1	15:a5:412:CLA:NC	2.78	0.44
13:a6:322:HIS:CE1	15:a6:404:CLA:NA	2.84	0.44
1:bA:473:ASP:OD1	10:bL:69:ARG:NH2	2.50	0.44
2:bB:278:ALA:HB1	15:bB:817:CLA:HBC2	2.00	0.44
13:b2:113:ILE:HD12	15:b2:422:CLA:H152	1.99	0.44
15:b3:402:CLA:HBC1	15:b3:403:CLA:H93	1.99	0.44
18:b3:419:BCR:H20C	18:b3:419:BCR:H361	1.83	0.44
13:b4:21:GLN:HA	13:b4:22:THR:HA	1.71	0.44
18:b6:401:BCR:C34	15:b6:417:CLA:HBB1	2.47	0.44
1:cA:203:GLY:HA3	15:cA:814:CLA:HBB1	1.99	0.44
15:cA:829:CLA:HBA2	15:cA:829:CLA:H3A	1.61	0.44
2:cB:685:VAL:HG11	3:cC:80:TYR:CG	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:cD:100:VAL:HG13	4:cD:104:LYS:HE2	1.98	0.44
10:cL:34:LEU:HD22	15:cL:203:CLA:HBD	1.99	0.44
15:cL:204:CLA:H93	15:cL:204:CLA:H111	1.82	0.44
13:c2:112:LEU:O	13:c2:115:SER:OG	2.28	0.44
13:c2:221:GLY:HA3	18:c2:421:BCR:H393	2.00	0.44
15:c2:422:CLA:HBA2	15:c2:422:CLA:H3A	1.80	0.44
15:c6:418:CLA:H3A	15:c6:418:CLA:HBA2	1.41	0.44
2:aB:41:LEU:O	2:aB:45:ILE:HG12	2.18	0.44
15:aB:808:CLA:H2	15:aB:808:CLA:H62	1.82	0.44
13:a1:23:ASN:HA	13:a1:24:VAL:HA	1.71	0.44
18:a2:401:BCR:H343	15:a2:418:CLA:HBB2	2.00	0.44
1:bA:203:GLY:HA3	15:bA:814:CLA:HBB1	1.99	0.44
2:bB:41:LEU:O	2:bB:45:ILE:HG12	2.18	0.44
2:bB:172:SER:OG	15:bB:813:CLA:O1D	2.31	0.44
2:bB:276:HIS:CE1	15:bB:819:CLA:NA	2.84	0.44
2:bB:439:LEU:HD11	18:bJ:105:BCR:H342	1.99	0.44
2:bB:674:ARG:O	2:bB:676:TYR:N	2.47	0.44
15:bB:806:CLA:HBA1	15:bB:806:CLA:H3A	1.46	0.44
13:b4:323:PHE:CE1	18:b4:401:BCR:H311	2.52	0.44
1:cA:396:HIS:HE1	15:cA:829:CLA:C1D	2.30	0.44
1:cA:575:ARG:HD2	19:cA:852:LHG:HC61	2.00	0.44
1:cA:593:ASP:OD1	1:cA:728:ARG:NH1	2.50	0.44
6:cF:119:ALA:HB2	13:c4:352:LEU:HD22	1.99	0.44
18:cI:102:BCR:H20C	18:cI:102:BCR:H361	1.82	0.44
13:c1:274:PHE:HD1	15:c1:402:CLA:H12	1.81	0.44
15:c1:402:CLA:HBC1	15:c1:403:CLA:H93	2.00	0.44
13:c3:156:ILE:O	13:c3:160:HIS:ND1	2.51	0.44
13:c4:323:PHE:CE1	18:c4:401:BCR:H311	2.52	0.44
1:aA:575:ARG:HD2	19:aA:853:LHG:HC61	2.00	0.44
1:aA:647:ASN:HD22	2:aB:657:LEU:HD11	1.83	0.44
15:aA:810:CLA:H2	18:aJ:205:BCR:H16C	1.99	0.44
6:aF:101:ILE:O	8:aJ:9:SER:HB3	2.16	0.44
13:a3:322:HIS:CE1	15:a3:403:CLA:NA	2.85	0.44
13:a6:21:GLN:HA	13:a6:22:THR:HA	1.71	0.44
13:a6:23:ASN:HA	13:a6:24:VAL:HA	1.71	0.44
13:a6:41:LEU:HD11	15:a6:412:CLA:HBA2	2.00	0.44
15:a6:422:CLA:H72	18:b1:420:BCR:H343	1.99	0.44
1:bA:651:ARG:HB2	2:bB:638:ILE:HG22	2.00	0.44
2:bB:93:PRO:HG2	15:bB:811:CLA:HHB	1.99	0.44
15:bB:819:CLA:H62	15:bB:819:CLA:H41	1.67	0.44
18:bB:846:BCR:H20C	18:bB:846:BCR:H361	1.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b4:41:LEU:HD11	15:b4:411:CLA:HBA2	1.98	0.44
13:b6:41:LEU:HD11	15:b6:412:CLA:HBA2	2.00	0.44
13:b6:49:GLN:HE22	15:b6:411:CLA:C4D	2.30	0.44
1:cA:181:HIS:CE1	15:cA:812:CLA:NA	2.85	0.44
1:cA:579:ASP:H	1:cA:586:THR:HG1	1.64	0.44
2:cB:255:THR:OG1	2:cB:271:ASP:OD1	2.34	0.44
13:c2:298:ALA:HA	15:c2:418:CLA:NB	2.33	0.44
13:c4:291:LEU:HA	13:c4:304:THR:HG23	2.00	0.44
15:c4:417:CLA:H62	15:c4:417:CLA:H41	1.77	0.44
18:c6:402:BCR:C34	15:c6:418:CLA:HBB1	2.47	0.44
1:aA:425:ASN:OD1	1:aA:428:ASN:ND2	2.40	0.44
1:aA:466:ARG:NH1	1:aA:645:THR:OG1	2.50	0.44
15:aA:804:CLA:H171	15:aA:804:CLA:H13	1.84	0.44
15:aA:822:CLA:H193	15:aA:825:CLA:HAC2	2.00	0.44
2:aB:355:MET:HE2	2:aB:355:MET:HB3	1.83	0.44
15:a2:413:CLA:H3A	15:a2:413:CLA:HBA1	1.55	0.44
13:a3:221:GLY:HA3	18:a3:420:BCR:H393	2.00	0.44
13:a6:270:VAL:O	13:a6:274:PHE:N	2.45	0.44
15:bB:832:CLA:H11	18:bF:202:BCR:H353	2.00	0.44
3:bC:57:CYS:HA	3:bC:58:PRO:HD3	1.88	0.44
4:bD:72:LEU:HB3	4:bD:77:ILE:HB	2.00	0.44
13:b1:91:GLY:HA2	13:b1:100:ASP:HB3	1.99	0.44
2:cB:355:MET:HE2	2:cB:355:MET:HB3	1.82	0.44
2:cB:625:TRP:CD2	15:cB:802:CLA:H112	2.52	0.44
13:c1:113:ILE:HG12	15:c2:406:CLA:H202	2.00	0.44
15:c2:406:CLA:HBA2	15:c2:406:CLA:H3A	1.37	0.44
18:c4:401:BCR:H343	15:c4:417:CLA:HBB2	1.99	0.44
1:aA:461:HIS:HE1	15:aA:835:CLA:C1A	2.31	0.44
14:aA:801:CL0:H53	14:aA:801:CL0:H60	1.74	0.44
15:aA:809:CLA:H3A	15:aA:809:CLA:HBA2	1.55	0.44
15:aB:839:CLA:HBB2	16:aB:843:PQN:H141	2.00	0.44
15:a1:402:CLA:H152	15:a1:403:CLA:HHB	1.99	0.44
18:a6:401:BCR:C34	15:a6:417:CLA:HBB1	2.47	0.44
15:bA:804:CLA:H143	15:bA:804:CLA:H112	1.79	0.44
15:bA:812:CLA:H111	15:bA:812:CLA:H151	1.79	0.44
2:bB:130:THR:OG1	2:bB:133:ASP:OD1	2.27	0.44
6:bF:27:ASP:HB3	6:bF:30:SER:HB3	1.99	0.44
15:b1:403:CLA:H152	15:b1:404:CLA:HHB	2.00	0.44
18:b2:401:BCR:H343	15:b2:418:CLA:HBB2	2.00	0.44
18:b2:420:BCR:H11C	18:b2:420:BCR:H341	1.84	0.44
13:b3:270:VAL:O	13:b3:274:PHE:N	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b3:291:LEU:HA	13:b3:304:THR:HG23	1.99	0.44
13:b3:322:HIS:CE1	15:b3:403:CLA:NA	2.85	0.44
13:b4:156:ILE:O	13:b4:160:HIS:ND1	2.51	0.44
13:b4:270:VAL:O	13:b4:274:PHE:N	2.42	0.44
1:cA:466:ARG:NH1	1:cA:645:THR:OG1	2.50	0.44
15:cA:803:CLA:H121	15:cA:842:CLA:H101	1.99	0.44
2:cB:18:ARG:HE	2:cB:18:ARG:HB3	1.61	0.44
2:cB:481:LEU:HA	2:cB:489:SER:HB2	1.99	0.44
13:c2:192:ILE:HD11	13:c2:215:LEU:HD13	1.98	0.44
13:c4:221:GLY:HA3	18:c4:420:BCR:H393	2.00	0.44
13:c4:322:HIS:CE1	15:c4:403:CLA:NA	2.86	0.44
13:c5:41:LEU:HD11	15:c5:411:CLA:HBA2	1.99	0.44
1:aA:319:TRP:O	1:aA:321:ILE:N	2.48	0.44
1:aA:396:HIS:HE1	15:aA:829:CLA:C1D	2.30	0.44
15:aA:803:CLA:H121	15:aA:843:CLA:H101	1.99	0.44
2:aB:93:PRO:HG2	15:aB:811:CLA:HHB	1.99	0.44
2:aB:409:ASN:OD1	2:aB:409:ASN:N	2.48	0.44
4:aD:72:LEU:HB3	4:aD:77:ILE:HB	2.00	0.44
6:aF:27:ASP:HB3	6:aF:30:SER:HB3	1.99	0.44
15:a2:402:CLA:HBC1	15:a2:403:CLA:H93	1.99	0.44
15:a4:421:CLA:H92	15:a4:421:CLA:H62	1.87	0.44
15:bA:806:CLA:H71	18:bA:850:BCR:H23C	2.00	0.44
2:bB:344:LEU:O	2:bB:348:THR:OG1	2.31	0.44
15:cA:804:CLA:H143	15:cA:804:CLA:H112	1.79	0.44
15:cA:821:CLA:HBA2	15:cA:821:CLA:H3A	1.51	0.44
15:cA:834:CLA:HBB2	10:cL:65:LEU:HD13	1.99	0.44
18:cA:850:BCR:H20C	18:cA:850:BCR:H361	1.81	0.44
15:cB:839:CLA:HBB2	16:cB:843:PQN:H141	1.99	0.44
18:cL:205:BCR:H20C	18:cL:205:BCR:H361	1.81	0.44
13:c6:41:LEU:HD11	15:c6:413:CLA:HBA2	1.99	0.44
1:aA:181:HIS:CE1	15:aA:812:CLA:NA	2.85	0.44
1:aA:374:MET:HE2	1:aA:374:MET:HB3	1.78	0.44
6:aF:16:LYS:HA	6:aF:16:LYS:HD3	1.84	0.44
15:aL:203:CLA:H3A	15:aL:203:CLA:HBA1	1.76	0.44
13:a1:49:GLN:HE22	15:a1:409:CLA:C4D	2.30	0.44
18:a2:401:BCR:H15C	18:a2:401:BCR:H351	1.82	0.44
13:a4:323:PHE:CE1	18:a4:401:BCR:H311	2.52	0.44
18:a6:420:BCR:H15C	18:a6:420:BCR:H351	1.80	0.44
1:bA:404:LEU:HD21	15:bA:807:CLA:H142	2.00	0.44
1:bA:580:GLY:HA2	2:bB:568:PRO:HD3	2.00	0.44
15:bA:839:CLA:H122	15:bL:203:CLA:H203	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bB:396:PHE:HA	2:bB:400:ASP:HB2	2.00	0.44
2:bB:625:TRP:CD2	15:bB:802:CLA:H112	2.52	0.44
15:b2:406:CLA:H62	15:b2:406:CLA:H92	1.83	0.44
15:b2:413:CLA:H3A	15:b2:413:CLA:HBA1	1.56	0.44
13:b5:192:ILE:HD11	13:b5:215:LEU:HD13	1.99	0.44
13:b6:270:VAL:O	13:b6:274:PHE:N	2.45	0.44
1:cA:242:PHE:HB3	1:cA:249:MET:HG3	2.00	0.44
15:cA:807:CLA:H112	15:cA:807:CLA:H71	1.73	0.44
15:cB:807:CLA:H151	15:cB:807:CLA:H111	1.78	0.44
15:cB:829:CLA:H43	18:cB:845:BCR:H393	1.99	0.44
13:c1:23:ASN:HA	13:c1:24:VAL:HA	1.71	0.44
13:c2:113:ILE:HD12	15:c2:422:CLA:H152	2.00	0.44
15:c4:403:CLA:H152	15:c4:404:CLA:HHB	2.00	0.44
1:aA:441:ILE:HG13	1:aA:559:PHE:HE2	1.83	0.44
15:aA:819:CLA:HBA2	15:aA:819:CLA:H3A	1.61	0.44
15:aA:827:CLA:HMA1	18:aA:851:BCR:H15C	2.00	0.44
18:aA:850:BCR:H15C	18:aA:850:BCR:H351	1.83	0.44
2:aB:532:GLY:O	2:aB:536:THR:OG1	2.27	0.44
15:aB:806:CLA:H3A	15:aB:806:CLA:HBA1	1.46	0.44
7:aI:22:MET:HE3	7:aI:22:MET:HB3	1.92	0.44
13:a2:307:LEU:HA	13:a2:308:PRO:HA	1.78	0.44
15:a2:417:CLA:HMC1	15:a2:417:CLA:HHC	1.69	0.44
13:a5:322:HIS:CE1	15:a5:403:CLA:NA	2.85	0.44
18:a5:401:BCR:H20C	18:a5:401:BCR:H361	1.87	0.44
13:a6:97:LYS:HB3	13:a6:99:VAL:HG13	2.00	0.44
13:a6:120:ALA:HB2	15:a6:422:CLA:H92	1.99	0.44
1:bA:575:ARG:HD2	19:bA:854:LHG:HC61	2.00	0.44
15:bA:822:CLA:H193	15:bA:825:CLA:HAC2	2.00	0.44
15:bB:837:CLA:H3A	15:bB:838:CLA:OBD	2.18	0.44
18:bB:850:BCR:H15C	18:bB:850:BCR:H351	1.88	0.44
13:b2:63:TYR:O	13:b2:66:SER:OG	2.27	0.44
13:b4:291:LEU:HA	13:b4:304:THR:HG23	2.00	0.44
15:b4:416:CLA:HBA2	15:b4:416:CLA:H3A	1.41	0.44
15:cA:822:CLA:H193	15:cA:825:CLA:HAC2	2.00	0.44
2:cB:41:LEU:O	2:cB:45:ILE:HG12	2.18	0.44
2:cB:661:LEU:O	2:cB:665:THR:OG1	2.28	0.44
4:cD:72:LEU:HB3	4:cD:77:ILE:HB	2.00	0.44
13:c2:307:LEU:HA	13:c2:308:PRO:HA	1.78	0.44
13:c6:128:ARG:HH11	15:c6:401:CLA:H2A	1.76	0.44
1:aA:427:ASN:OD1	1:aA:432:ARG:NH1	2.51	0.43
15:aA:839:CLA:H201	15:aL:202:CLA:H102	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:18:ARG:HE	2:aB:18:ARG:HB3	1.61	0.43
2:aB:278:ALA:HB1	15:aB:817:CLA:HBC2	2.00	0.43
18:aB:849:BCR:H20C	18:aB:849:BCR:H361	1.79	0.43
13:a2:113:ILE:HG13	15:a2:422:CLA:H202	2.00	0.43
13:a2:221:GLY:HA3	18:a2:421:BCR:H393	2.00	0.43
1:bA:427:ASN:OD1	1:bA:432:ARG:NH1	2.51	0.43
2:bB:192:HIS:HE1	15:bB:815:CLA:C1A	2.31	0.43
15:bB:837:CLA:CGA	15:bX:102:CLA:HMD3	2.48	0.43
4:bD:100:VAL:HG13	4:bD:104:LYS:HE2	1.98	0.43
6:bF:93:GLU:HG2	6:bF:96:GLU:HB2	2.00	0.43
8:bJ:21:ILE:HA	15:bJ:101:CLA:HBB2	2.00	0.43
10:bL:34:LEU:HD22	15:bL:203:CLA:HBD	1.99	0.43
13:b2:113:ILE:HG13	15:b2:422:CLA:H202	2.00	0.43
13:b3:66:SER:OG	13:b3:67:GLN:N	2.49	0.43
1:cA:461:HIS:HE1	15:cA:835:CLA:C1A	2.31	0.43
15:cA:831:CLA:H13	15:cA:831:CLA:H171	1.85	0.43
2:cB:396:PHE:HA	2:cB:400:ASP:HB2	2.00	0.43
15:cB:808:CLA:H18	15:cB:828:CLA:H201	2.00	0.43
15:cB:828:CLA:HBC3	20:cB:850:LMG:H442	2.00	0.43
15:cB:829:CLA:H3A	15:cB:829:CLA:HBA2	1.73	0.43
15:c3:416:CLA:H3A	15:c3:416:CLA:HBA2	1.41	0.43
18:c4:401:BCR:H15C	18:c4:401:BCR:H351	1.90	0.43
15:c4:409:CLA:HBD	15:c4:409:CLA:H121	2.00	0.43
1:aA:242:PHE:HB3	1:aA:249:MET:HG3	2.00	0.43
15:aA:841:CLA:HAA2	15:aB:832:CLA:HMB1	2.00	0.43
13:a1:80:ILE:HG23	15:a1:404:CLA:HMA1	2.00	0.43
13:a2:192:ILE:HD11	13:a2:215:LEU:HD13	1.99	0.43
15:a6:422:CLA:H171	15:b1:416:CLA:HBB2	2.01	0.43
1:bA:242:PHE:HB3	1:bA:249:MET:HG3	2.00	0.43
1:bA:396:HIS:HE1	15:bA:829:CLA:C1D	2.30	0.43
2:bB:731:LEU:O	2:bB:735:THR:OG1	2.27	0.43
15:bB:829:CLA:H43	18:bB:845:BCR:H393	1.99	0.43
15:b5:420:CLA:H143	15:b5:420:CLA:H111	1.87	0.43
15:cA:810:CLA:H2	18:cJ:104:BCR:H16C	1.99	0.43
15:cB:808:CLA:H2	15:cB:808:CLA:H62	1.82	0.43
15:cB:810:CLA:H91	15:cB:810:CLA:H111	1.85	0.43
10:cL:34:LEU:HD21	15:cL:202:CLA:HBB1	1.98	0.43
13:c2:66:SER:HB2	13:c3:294:LYS:HA	2.01	0.43
13:c2:97:LYS:HB3	13:c2:99:VAL:HG13	2.00	0.43
13:c3:135:THR:HB	13:c3:137:THR:HG23	2.00	0.43
13:c3:322:HIS:CE1	15:c3:403:CLA:NA	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c3:403:CLA:H152	15:c3:404:CLA:HHB	1.99	0.43
13:c6:201:VAL:O	13:c6:205:TYR:N	2.33	0.43
1:aA:491:GLN:HE22	15:aA:838:CLA:HMD3	1.82	0.43
1:aA:649:TRP:CE2	14:aA:801:CL0:H56	2.53	0.43
2:aB:442:HIS:HE1	15:aB:834:CLA:NA	2.13	0.43
8:aJ:21:ILE:HA	15:aJ:202:CLA:HBB2	2.00	0.43
13:a4:21:GLN:HA	13:a4:22:THR:HA	1.70	0.43
18:a4:420:BCR:H20C	18:a4:420:BCR:H361	1.82	0.43
13:a6:80:ILE:HG13	13:a6:81:LEU:HG	2.01	0.43
13:a6:298:ALA:HA	15:a6:418:CLA:NB	2.33	0.43
18:a6:402:BCR:H20C	18:a6:402:BCR:H361	1.90	0.43
15:bA:803:CLA:H91	15:bA:803:CLA:H111	1.83	0.43
15:bA:833:CLA:H41	15:bA:833:CLA:H61	1.83	0.43
15:bB:801:CLA:H41	15:bB:801:CLA:H62	1.57	0.43
18:b4:420:BCR:H20C	18:b4:420:BCR:H361	1.82	0.43
15:b5:416:CLA:H3A	15:b5:416:CLA:HBA2	1.41	0.43
15:cA:802:CLA:H111	15:cA:802:CLA:H142	1.76	0.43
15:cA:806:CLA:H71	18:cA:848:BCR:H23C	2.00	0.43
15:cB:803:CLA:H62	15:cB:803:CLA:H41	1.85	0.43
15:cB:837:CLA:H3A	15:cB:838:CLA:OBD	2.18	0.43
13:c3:80:ILE:HG23	15:c3:405:CLA:HMA1	1.99	0.43
13:c3:221:GLY:HA3	18:c3:420:BCR:H393	2.00	0.43
15:c6:414:CLA:H3A	15:c6:414:CLA:HBA1	1.52	0.43
2:aB:432:LEU:HD11	15:aB:837:CLA:HMB2	2.01	0.43
2:aB:730:PHE:O	2:aB:734:SER:OG	2.31	0.43
15:aB:807:CLA:H111	15:aB:807:CLA:H151	1.79	0.43
15:aB:810:CLA:H141	15:aB:810:CLA:H162	1.76	0.43
18:aF:201:BCR:HC22	18:aF:203:BCR:H363	2.00	0.43
13:a2:113:ILE:HD12	15:a2:422:CLA:H152	2.00	0.43
13:a3:63:TYR:O	13:a3:66:SER:OG	2.29	0.43
15:bA:810:CLA:H2	18:bJ:104:BCR:H16C	1.99	0.43
15:bA:843:CLA:HBA2	15:bA:843:CLA:H3A	1.77	0.43
2:bB:661:LEU:O	2:bB:665:THR:OG1	2.28	0.43
15:b5:412:CLA:HHC	15:b5:412:CLA:HBB1	2.00	0.43
13:b6:97:LYS:HB3	13:b6:99:VAL:HG13	2.00	0.43
15:b6:404:CLA:H152	15:b6:405:CLA:HHB	2.00	0.43
1:cA:710:LYS:NZ	6:cF:133:ASP:OD1	2.29	0.43
15:cA:834:CLA:HAB	15:cA:834:CLA:HHC	1.81	0.43
2:cB:192:HIS:HE1	15:cB:815:CLA:C1A	2.31	0.43
13:c4:156:ILE:O	13:c4:160:HIS:ND1	2.51	0.43
15:aA:829:CLA:H93	18:aJ:204:BCR:H361	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:130:THR:OG1	2:aB:133:ASP:OD1	2.27	0.43
15:aB:829:CLA:H142	15:aB:829:CLA:H111	1.84	0.43
18:aI:102:BCR:H402	15:aL:202:CLA:H52	1.99	0.43
10:aL:34:LEU:HD22	15:aL:202:CLA:HBD	1.99	0.43
13:a1:209:PHE:HE1	13:a1:274:PHE:CE1	2.36	0.43
13:a2:209:PHE:HE1	13:a2:274:PHE:CE1	2.36	0.43
13:a4:221:GLY:HA3	18:a4:420:BCR:H393	2.01	0.43
18:a4:419:BCR:H20C	18:a4:419:BCR:H361	1.86	0.43
15:a6:404:CLA:H152	15:a6:405:CLA:HHB	2.00	0.43
1:bA:649:TRP:CE2	14:bA:801:CL0:H56	2.53	0.43
15:bA:804:CLA:H13	15:bA:804:CLA:H171	1.84	0.43
2:bB:432:LEU:HD11	15:bB:837:CLA:HMB2	2.01	0.43
15:bB:810:CLA:H151	15:bB:810:CLA:H18	1.76	0.43
15:bB:821:CLA:H3A	15:bB:821:CLA:HBA2	1.61	0.43
13:b1:128:ARG:NH1	15:b2:406:CLA:O1D	2.52	0.43
13:b2:52:LEU:O	13:b2:56:TRP:N	2.44	0.43
13:b2:209:PHE:HE1	13:b2:274:PHE:CE1	2.37	0.43
13:b6:80:ILE:HG13	13:b6:81:LEU:HG	2.01	0.43
2:cB:229:TRP:HB2	15:cB:817:CLA:H12	2.01	0.43
8:cJ:12:PRO:HB2	18:cJ:104:BCR:H391	2.00	0.43
13:c1:209:PHE:HE1	13:c1:274:PHE:CE1	2.36	0.43
15:c2:413:CLA:HHC	15:c2:413:CLA:HBB1	2.00	0.43
18:c3:419:BCR:H15C	18:c3:419:BCR:H351	1.84	0.43
15:c4:421:CLA:H203	15:c4:421:CLA:H161	1.88	0.43
15:c5:403:CLA:H152	15:c5:404:CLA:HHB	2.01	0.43
15:c6:418:CLA:HHC	15:c6:418:CLA:HMC1	1.73	0.43
1:aA:744:TRP:CD2	18:aA:852:BCR:HC22	2.54	0.43
2:aB:192:HIS:HE1	15:aB:815:CLA:C1A	2.31	0.43
15:aB:829:CLA:H3A	15:aB:829:CLA:HBA2	1.73	0.43
18:aB:847:BCR:H15C	18:aB:847:BCR:H351	1.92	0.43
6:aF:93:GLU:HG2	6:aF:96:GLU:HB2	2.00	0.43
8:aJ:12:PRO:HB2	18:aJ:205:BCR:H391	2.00	0.43
15:a5:412:CLA:HHC	15:a5:412:CLA:HBB1	2.01	0.43
18:b1:420:BCR:H20C	18:b1:420:BCR:H361	1.84	0.43
13:b5:49:GLN:HE22	15:b5:410:CLA:C4D	2.30	0.43
15:b5:417:CLA:H41	15:b5:417:CLA:H62	1.77	0.43
15:cB:810:CLA:H162	15:cB:810:CLA:H141	1.76	0.43
15:cB:833:CLA:HMC3	18:cF:205:BCR:H12C	2.01	0.43
13:c1:80:ILE:HG23	15:c1:405:CLA:HMA1	2.00	0.43
18:c2:401:BCR:H343	15:c2:418:CLA:HBB2	2.00	0.43
18:c4:420:BCR:H20C	18:c4:420:BCR:H361	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aA:806:CLA:H71	18:aA:849:BCR:H23C	2.00	0.43
2:aB:396:PHE:HA	2:aB:400:ASP:HB2	2.00	0.43
2:aB:625:TRP:CD2	15:aB:802:CLA:H112	2.52	0.43
18:aL:205:BCR:H20C	18:aL:205:BCR:H361	1.81	0.43
13:a2:66:SER:HB2	13:a3:294:LYS:HA	2.00	0.43
13:a2:80:ILE:HG13	13:a2:81:LEU:HG	2.01	0.43
13:a2:298:ALA:HA	15:a2:418:CLA:NB	2.33	0.43
18:a3:419:BCR:H20C	18:a3:419:BCR:H361	1.83	0.43
2:bB:457:LEU:O	6:bF:51:LEU:N	2.35	0.43
2:bB:481:LEU:HD13	15:bB:835:CLA:HED3	2.01	0.43
15:bB:808:CLA:H18	15:bB:828:CLA:H201	2.00	0.43
15:bB:819:CLA:H111	15:bB:819:CLA:H71	1.77	0.43
15:bB:839:CLA:HBB2	16:bB:843:PQN:H141	1.99	0.43
13:b1:23:ASN:HA	13:b1:24:VAL:HA	1.71	0.43
13:b2:66:SER:HB2	13:b3:294:LYS:HA	2.00	0.43
13:b5:80:ILE:HG13	13:b5:81:LEU:HG	2.01	0.43
13:b6:38:LEU:H	13:b6:38:LEU:HG	1.54	0.43
13:b6:298:ALA:HA	15:b6:418:CLA:NB	2.33	0.43
1:cA:227:LEU:HD23	1:cA:227:LEU:HA	1.90	0.43
1:cA:649:TRP:CE2	14:cA:801:CL0:H56	2.53	0.43
2:cB:278:ALA:HB1	15:cB:817:CLA:HBC2	2.00	0.43
2:cB:648:ASN:OD1	2:cB:648:ASN:N	2.41	0.43
3:cC:6:ILE:O	4:cD:115:VAL:N	2.51	0.43
13:c5:325:LEU:O	13:c5:329:PHE:N	2.44	0.43
18:c5:401:BCR:H15C	18:c5:401:BCR:H351	1.87	0.43
15:c5:417:CLA:H41	15:c5:417:CLA:H62	1.77	0.43
13:c6:274:PHE:HD1	15:c6:404:CLA:H12	1.81	0.43
15:c6:419:CLA:H41	15:c6:419:CLA:H62	1.75	0.43
15:aA:806:CLA:H202	15:aA:806:CLA:H162	1.88	0.43
2:aB:39:GLU:HG2	2:aB:164:LEU:HB2	2.01	0.43
2:aB:229:TRP:HB2	15:aB:817:CLA:H12	2.01	0.43
18:aI:103:BCR:H11C	18:aI:103:BCR:H341	1.87	0.43
18:aM:101:BCR:H371	18:aM:101:BCR:H24C	1.78	0.43
15:a1:415:CLA:HBB1	18:a1:420:BCR:C34	2.46	0.43
15:a2:417:CLA:HBA2	15:a2:417:CLA:H3A	1.40	0.43
13:a3:23:ASN:HA	13:a3:24:VAL:HA	1.71	0.43
13:a4:322:HIS:CE1	15:a4:403:CLA:NA	2.85	0.43
15:a4:417:CLA:H62	15:a4:417:CLA:H41	1.77	0.43
15:bA:827:CLA:HMA1	18:bA:852:BCR:H15C	2.00	0.43
2:bB:177:HIS:HA	2:bB:181:LEU:HB3	2.01	0.43
2:bB:602:TRP:HE1	2:bB:614:GLN:NE2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:bF:6:VAL:O	6:bF:43:CYS:N	2.39	0.43
15:b1:402:CLA:HBC1	15:b1:403:CLA:H93	2.00	0.43
15:b3:416:CLA:HBA2	15:b3:416:CLA:H3A	1.41	0.43
13:b4:23:ASN:HA	13:b4:24:VAL:HA	1.72	0.43
15:b4:403:CLA:H152	15:b4:404:CLA:HHB	2.00	0.43
13:b5:135:THR:HB	13:b5:137:THR:HG23	2.01	0.43
14:cA:801:CL0:H8	14:cA:801:CL0:CGD	2.49	0.43
3:cC:11:ILE:H	3:cC:11:ILE:HG12	1.55	0.43
8:cJ:21:ILE:HA	15:cJ:101:CLA:HBB2	2.00	0.43
18:c1:401:BCR:C34	15:c1:416:CLA:HBB1	2.48	0.43
13:c5:80:ILE:HG23	15:c5:405:CLA:HMA1	2.01	0.43
15:c6:411:CLA:HBD	15:c6:411:CLA:H121	2.01	0.43
1:aA:27:LYS:HB2	15:aA:812:CLA:HAA2	2.01	0.43
15:aA:807:CLA:H71	15:aA:807:CLA:H112	1.73	0.43
15:aA:821:CLA:H51	15:aA:821:CLA:H8	1.90	0.43
2:aB:456:ILE:HG22	2:aB:458:ILE:HD11	2.00	0.43
15:aB:828:CLA:HBC3	20:aB:850:LMG:H442	2.00	0.43
15:aB:837:CLA:H3A	15:aB:838:CLA:OBD	2.18	0.43
18:aF:202:BCR:H361	18:aF:202:BCR:H20C	1.75	0.43
13:a1:324:PHE:HE2	18:a1:417:BCR:H403	1.84	0.43
18:a2:420:BCR:H20C	18:a2:420:BCR:H361	1.84	0.43
13:a3:80:ILE:HG23	15:a3:405:CLA:HMA1	2.00	0.43
13:a4:156:ILE:O	13:a4:160:HIS:ND1	2.52	0.43
13:a4:261:LEU:HD23	13:a4:261:LEU:HA	1.88	0.43
13:a5:80:ILE:HG13	13:a5:81:LEU:HG	2.01	0.43
15:a6:422:CLA:H92	15:a6:422:CLA:H62	1.89	0.43
1:bA:52:HIS:HE1	15:bA:804:CLA:ND	2.15	0.43
1:bA:461:HIS:HE1	15:bA:835:CLA:C1A	2.31	0.43
1:bA:744:TRP:CD2	18:bA:853:BCR:HC22	2.54	0.43
15:bA:818:CLA:H62	15:bA:818:CLA:H41	1.83	0.43
2:bB:229:TRP:HB2	15:bB:817:CLA:H12	2.01	0.43
13:b4:221:GLY:HA3	18:b4:420:BCR:H393	2.01	0.43
13:b5:270:VAL:O	13:b5:274:PHE:N	2.42	0.43
15:b6:410:CLA:HBD	15:b6:410:CLA:H121	2.01	0.43
15:cA:821:CLA:H51	15:cA:821:CLA:H8	1.90	0.43
15:cA:829:CLA:H93	18:cJ:103:BCR:H361	1.99	0.43
15:cB:819:CLA:H93	15:cB:819:CLA:H61	1.92	0.43
18:cF:202:BCR:HC22	18:cF:205:BCR:H363	2.00	0.43
13:c6:23:ASN:HA	13:c6:24:VAL:HA	1.71	0.43
13:c6:80:ILE:HG23	15:c6:407:CLA:HMA1	2.01	0.43
13:c6:97:LYS:HB3	13:c6:99:VAL:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:352:TRP:HB3	15:aA:806:CLA:HAC1	2.01	0.43
4:aD:117:ARG:NE	4:aD:121:GLN:O	2.36	0.43
13:a2:52:LEU:O	13:a2:56:TRP:N	2.43	0.43
15:a5:403:CLA:H152	15:a5:404:CLA:HHB	2.01	0.43
1:bA:744:TRP:CG	18:bA:853:BCR:HC22	2.54	0.43
14:bA:801:CL0:CGD	14:bA:801:CL0:H8	2.49	0.43
15:bA:829:CLA:HBA2	15:bA:829:CLA:H3A	1.60	0.43
18:bA:850:BCR:H15C	18:bA:850:BCR:H351	1.85	0.43
2:bB:697:VAL:HG11	15:bB:801:CLA:HAB	2.01	0.43
15:bB:818:CLA:H3A	15:bB:818:CLA:HBA2	1.41	0.43
10:bL:79:LEU:HD23	10:cL:137:PHE:CZ	2.54	0.43
18:bM:101:BCR:H20C	18:bM:101:BCR:H361	1.84	0.43
13:b2:90:PHE:HZ	15:b2:403:CLA:H192	1.84	0.43
15:b2:418:CLA:H41	15:b2:418:CLA:H62	1.79	0.43
13:b3:221:GLY:HA3	18:b3:420:BCR:H393	1.99	0.43
13:b5:221:GLY:HA3	18:b5:419:BCR:H393	2.01	0.43
13:b5:298:ALA:HA	15:b5:417:CLA:NB	2.34	0.43
1:cA:444:LEU:HD22	15:cA:840:CLA:HBB1	2.00	0.43
1:cA:647:ASN:HD22	2:cB:657:LEU:HD11	1.83	0.43
15:cA:827:CLA:HMA1	18:cA:850:BCR:H15C	2.00	0.43
13:c2:209:PHE:HE1	13:c2:274:PHE:CE1	2.37	0.43
15:c3:416:CLA:HHC	15:c3:416:CLA:HMC1	1.69	0.43
15:c4:412:CLA:H3A	15:c4:412:CLA:HBA1	1.55	0.43
1:aA:404:LEU:HD21	15:aA:807:CLA:H142	2.00	0.42
7:aI:1:MET:HE3	7:aI:1:MET:HB3	1.81	0.42
18:a1:421:BCR:C11	13:c6:113:ILE:HD13	2.49	0.42
15:a3:417:CLA:H62	15:a3:417:CLA:H41	1.76	0.42
15:a4:409:CLA:HBD	15:a4:409:CLA:H121	2.00	0.42
13:a5:80:ILE:HG23	15:a5:405:CLA:HMA1	2.01	0.42
1:bA:696:TYR:CE2	15:bA:803:CLA:HMD1	2.54	0.42
15:bA:827:CLA:H111	15:bA:827:CLA:H152	1.84	0.42
18:bL:205:BCR:H15C	18:bL:205:BCR:H351	1.83	0.42
15:b2:422:CLA:H18	18:b3:401:BCR:H333	2.00	0.42
13:b3:209:PHE:HE1	13:b3:274:PHE:CE1	2.37	0.42
15:b3:403:CLA:H152	15:b3:404:CLA:HHB	1.99	0.42
18:b3:419:BCR:H11C	18:b3:419:BCR:H341	1.91	0.42
13:b4:322:HIS:CE1	15:b4:403:CLA:NA	2.86	0.42
1:cA:353:HIS:CD2	1:cA:411:HIS:HD1	2.37	0.42
1:cA:427:ASN:OD1	1:cA:432:ARG:NH1	2.51	0.42
15:cA:841:CLA:HAA2	15:cB:832:CLA:HMB1	2.00	0.42
2:cB:39:GLU:HG2	2:cB:164:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:456:ILE:HG22	2:cB:458:ILE:HD11	2.00	0.42
15:cB:831:CLA:HBA2	15:cB:831:CLA:H3A	1.51	0.42
3:cC:57:CYS:HA	3:cC:58:PRO:HD3	1.88	0.42
13:c2:23:ASN:HA	13:c2:24:VAL:HA	1.71	0.42
13:c2:113:ILE:HG13	15:c2:422:CLA:H202	2.01	0.42
15:c5:412:CLA:HBB1	15:c5:412:CLA:HHC	2.01	0.42
13:c6:298:ALA:HA	15:c6:419:CLA:NB	2.33	0.42
1:aA:494:HIS:HE1	15:aA:836:CLA:NB	2.16	0.42
1:aA:644:ILE:H	1:aA:644:ILE:HG12	1.56	0.42
2:aB:481:LEU:HD13	15:aB:835:CLA:HED3	2.01	0.42
2:aB:701:ASP:OD1	2:aB:701:ASP:N	2.43	0.42
15:a2:406:CLA:H92	15:a2:406:CLA:H62	1.83	0.42
15:a3:416:CLA:HHC	15:a3:416:CLA:HMC1	1.69	0.42
13:a6:160:HIS:CE1	15:a6:413:CLA:NC	2.78	0.42
13:a6:192:ILE:HD11	13:a6:215:LEU:HD13	2.01	0.42
1:bA:59:ASP:OD1	1:bA:59:ASP:N	2.53	0.42
15:bA:821:CLA:HBA2	15:bA:821:CLA:H3A	1.51	0.42
15:bA:839:CLA:H142	15:bA:839:CLA:H111	1.83	0.42
15:bB:817:CLA:HBA2	15:bB:817:CLA:H3A	1.67	0.42
13:b1:66:SER:OG	13:b1:67:GLN:N	2.52	0.42
15:b2:417:CLA:HMC1	15:b2:417:CLA:HHC	1.70	0.42
13:b4:209:PHE:HE1	13:b4:274:PHE:CE1	2.37	0.42
1:cA:404:LEU:HD21	15:cA:807:CLA:H142	2.00	0.42
15:cA:842:CLA:H93	15:cA:842:CLA:H112	1.88	0.42
2:cB:481:LEU:HD13	15:cB:835:CLA:HED3	2.01	0.42
15:cB:821:CLA:H3A	15:cB:821:CLA:HBA2	1.61	0.42
6:cF:93:GLU:HG2	6:cF:96:GLU:HB2	2.00	0.42
13:c2:80:ILE:HG13	13:c2:81:LEU:HG	2.01	0.42
15:c2:417:CLA:HMC1	15:c2:417:CLA:HHC	1.69	0.42
13:c4:209:PHE:HE1	13:c4:274:PHE:CE1	2.37	0.42
15:c5:410:CLA:H162	15:c5:410:CLA:H141	1.88	0.42
15:c5:420:CLA:H92	15:c5:420:CLA:H62	1.88	0.42
15:c6:405:CLA:H152	15:c6:406:CLA:HHB	2.00	0.42
1:aA:157:GLN:O	1:aA:161:THR:OG1	2.31	0.42
14:aA:801:CL0:H8	14:aA:801:CL0:CGD	2.49	0.42
15:aA:822:CLA:H92	15:aA:822:CLA:H62	1.81	0.42
15:a2:406:CLA:H41	15:a2:406:CLA:H61	1.81	0.42
15:a4:417:CLA:H51	15:a4:417:CLA:H12	1.84	0.42
1:bA:441:ILE:HG13	1:bA:559:PHE:HE2	1.83	0.42
2:bB:456:ILE:HG22	2:bB:458:ILE:HD11	2.00	0.42
2:bB:554:PRO:HD2	3:bC:61:PHE:CE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:bJ:104:BCR:H20C	18:bJ:104:BCR:H361	1.78	0.42
13:b1:52:LEU:O	13:b1:56:TRP:N	2.43	0.42
13:b2:298:ALA:HA	15:b2:418:CLA:NB	2.33	0.42
15:b2:402:CLA:HBC1	15:b2:403:CLA:H93	2.01	0.42
13:b4:298:ALA:HA	15:b4:417:CLA:NB	2.35	0.42
2:cB:146:SER:HB3	11:cM:21:LEU:HD12	2.01	0.42
2:cB:396:PHE:O	2:cB:401:TYR:N	2.53	0.42
2:cB:432:LEU:HD11	15:cB:837:CLA:HMB2	2.01	0.42
15:cB:808:CLA:H91	15:cB:808:CLA:H111	1.86	0.42
6:cF:124:LEU:HA	6:cF:129:LEU:HB2	2.02	0.42
18:cJ:103:BCR:H24C	18:cJ:103:BCR:H371	1.83	0.42
13:c1:113:ILE:HG13	15:c2:406:CLA:H152	2.00	0.42
13:c2:52:LEU:O	13:c2:56:TRP:N	2.43	0.42
18:c2:420:BCR:H15C	18:c2:420:BCR:H351	1.85	0.42
15:c2:422:CLA:H18	18:c3:401:BCR:H333	2.00	0.42
15:c4:421:CLA:H171	15:c5:416:CLA:HBB2	2.01	0.42
1:aA:353:HIS:CD2	1:aA:411:HIS:HD1	2.37	0.42
1:aA:667:SER:O	1:aA:670:SER:OG	2.29	0.42
2:aB:177:HIS:HA	2:aB:181:LEU:HB3	2.01	0.42
2:aB:727:TYR:HB2	15:aB:802:CLA:HED3	2.01	0.42
6:aF:124:LEU:HA	6:aF:129:LEU:HB2	2.01	0.42
13:a1:66:SER:OG	13:a1:67:GLN:N	2.51	0.42
13:a3:209:PHE:HE1	13:a3:274:PHE:CE1	2.37	0.42
15:a4:410:CLA:H162	15:a4:410:CLA:H141	1.84	0.42
1:bA:352:TRP:HB3	15:bA:806:CLA:HAC1	2.01	0.42
15:bA:843:CLA:H142	15:bA:843:CLA:H111	1.82	0.42
18:bA:848:BCR:H11C	18:bA:848:BCR:H341	1.95	0.42
15:bB:803:CLA:H62	15:bB:803:CLA:H41	1.85	0.42
16:bB:843:PQN:H222	16:bB:843:PQN:H261	1.92	0.42
8:bJ:12:PRO:HB2	18:bJ:104:BCR:H391	2.00	0.42
15:b5:403:CLA:H152	15:b5:404:CLA:HHB	2.01	0.42
15:b6:418:CLA:H51	15:b6:418:CLA:H12	1.85	0.42
1:cA:374:MET:HE2	1:cA:374:MET:HB3	1.78	0.42
1:cA:744:TRP:CD2	18:cA:851:BCR:HC22	2.54	0.42
15:cB:833:CLA:H152	15:cB:833:CLA:H112	1.75	0.42
15:cB:837:CLA:C16	18:cF:204:BCR:H23C	2.50	0.42
10:cL:34:LEU:HD23	10:cL:34:LEU:HA	1.88	0.42
13:c1:128:ARG:NH1	15:c2:406:CLA:O1D	2.52	0.42
13:c5:298:ALA:HA	15:c5:417:CLA:NB	2.34	0.42
18:c5:419:BCR:H351	18:c5:419:BCR:H15C	1.81	0.42
13:c6:80:ILE:HG13	13:c6:81:LEU:HG	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:586:THR:O	1:aA:586:THR:OG1	2.31	0.42
2:aB:44:LYS:O	2:aB:48:SER:OG	2.32	0.42
2:aB:146:SER:HB3	11:aM:21:LEU:HD12	2.01	0.42
18:aF:203:BCR:H20C	18:aF:203:BCR:H361	1.86	0.42
18:aK:101:BCR:H20C	18:aK:101:BCR:H361	1.88	0.42
15:a1:412:CLA:HBB1	18:a1:418:BCR:H402	2.02	0.42
13:a3:21:GLN:HA	13:a3:22:THR:HA	1.71	0.42
13:a3:135:THR:HB	13:a3:137:THR:HG23	2.00	0.42
13:a3:288:GLY:C	13:a3:315:ARG:HH12	2.27	0.42
13:a4:209:PHE:HE1	13:a4:274:PHE:CE1	2.37	0.42
1:bA:27:LYS:HB2	15:bA:812:CLA:HAA2	2.01	0.42
15:bA:822:CLA:H62	15:bA:822:CLA:H92	1.81	0.42
15:bB:828:CLA:HBC3	20:bB:851:LMG:H442	2.00	0.42
6:bF:121:LEU:HA	6:bF:124:LEU:HB3	2.01	0.42
18:b1:419:BCR:H15C	18:b1:419:BCR:H351	1.90	0.42
13:b2:80:ILE:HG23	15:b2:405:CLA:HMA1	2.01	0.42
15:b6:413:CLA:HBB1	15:b6:413:CLA:HHC	2.02	0.42
15:cA:822:CLA:H92	15:cA:822:CLA:H62	1.81	0.42
15:cA:839:CLA:H41	15:cA:839:CLA:H62	1.82	0.42
2:cB:647:ASN:O	2:cB:650:SER:OG	2.27	0.42
15:cB:807:CLA:H111	15:cB:807:CLA:H72	1.76	0.42
13:c3:288:GLY:C	13:c3:315:ARG:HH12	2.28	0.42
13:c5:135:THR:HB	13:c5:137:THR:HG23	2.02	0.42
13:c5:221:GLY:HA3	18:c5:419:BCR:H393	2.01	0.42
15:aA:803:CLA:H91	15:aA:803:CLA:H111	1.83	0.42
18:aA:848:BCR:H15C	18:aA:848:BCR:H351	1.85	0.42
2:aB:175:ASN:ND2	2:aB:290:TYR:O	2.39	0.42
15:aB:817:CLA:HBA2	15:aB:817:CLA:H3A	1.67	0.42
13:a4:325:LEU:O	13:a4:329:PHE:N	2.45	0.42
18:bB:849:BCR:H11C	18:bB:849:BCR:H341	1.93	0.42
18:bJ:105:BCR:H24C	18:bJ:105:BCR:H371	1.93	0.42
15:b3:421:CLA:H203	15:b3:421:CLA:H161	1.81	0.42
15:b4:409:CLA:HBD	15:b4:409:CLA:H121	2.00	0.42
1:cA:27:LYS:HB2	15:cA:812:CLA:HAA2	2.01	0.42
15:cA:804:CLA:H43	15:cA:842:CLA:H121	2.02	0.42
2:cB:44:LYS:O	2:cB:48:SER:OG	2.32	0.42
13:c1:66:SER:OG	13:c1:67:GLN:N	2.51	0.42
13:c1:135:THR:HB	13:c1:137:THR:HG23	2.02	0.42
13:c4:298:ALA:HA	15:c4:417:CLA:NB	2.35	0.42
13:c6:113:ILE:HG12	15:c6:401:CLA:H202	2.01	0.42
1:aA:59:ASP:OD1	1:aA:59:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aA:809:CLA:HMB3	18:aJ:204:BCR:H20C	2.01	0.42
15:aA:820:CLA:H171	15:aA:836:CLA:H41	2.01	0.42
15:aB:808:CLA:H91	15:aB:808:CLA:H111	1.86	0.42
15:aB:808:CLA:H18	15:aB:828:CLA:H201	2.00	0.42
13:a1:307:LEU:HA	13:a1:308:PRO:HA	1.79	0.42
18:a1:419:BCR:H20C	18:a1:419:BCR:H361	1.85	0.42
13:a2:80:ILE:HG23	15:a2:405:CLA:HMA1	2.01	0.42
13:a2:97:LYS:HB3	13:a2:99:VAL:HG13	2.01	0.42
15:a2:413:CLA:HHC	15:a2:413:CLA:HBB1	2.02	0.42
15:a6:410:CLA:H121	15:a6:410:CLA:HBD	2.01	0.42
1:bA:444:LEU:HD22	15:bA:840:CLA:HBB1	2.01	0.42
1:bA:601:TRP:HE1	15:bB:804:CLA:C1D	2.32	0.42
18:bA:849:BCR:H351	18:bA:849:BCR:H15C	1.85	0.42
2:bB:180:GLY:HA3	15:bB:814:CLA:HBB1	2.02	0.42
2:bB:586:MET:HE3	2:bB:586:MET:HB3	1.80	0.42
15:bB:811:CLA:HAB	7:bI:19:CYS:HB3	2.02	0.42
18:bM:101:BCR:H24C	18:bM:101:BCR:H371	1.78	0.42
18:b2:420:BCR:H20C	18:b2:420:BCR:H361	1.84	0.42
13:b3:97:LYS:HB3	13:b3:99:VAL:HG13	2.01	0.42
13:b6:135:THR:HB	13:b6:137:THR:HG23	2.01	0.42
1:cA:441:ILE:HG13	1:cA:559:PHE:HE2	1.83	0.42
15:cA:818:CLA:H62	15:cA:818:CLA:H41	1.83	0.42
2:cB:172:SER:OG	15:cB:813:CLA:O1D	2.32	0.42
2:cB:177:HIS:HA	2:cB:181:LEU:HB3	2.01	0.42
18:cB:844:BCR:H11C	18:cB:844:BCR:H341	1.87	0.42
6:cF:121:LEU:HA	6:cF:124:LEU:HB3	2.01	0.42
15:c2:404:CLA:H61	15:c2:404:CLA:H2	1.83	0.42
15:c2:417:CLA:HBA2	15:c2:417:CLA:H3A	1.40	0.42
13:c3:209:PHE:HE1	13:c3:274:PHE:CE1	2.37	0.42
15:c5:404:CLA:H61	15:c5:404:CLA:H2	1.82	0.42
1:aA:444:LEU:HD22	15:aA:840:CLA:HBB1	2.01	0.42
15:aB:828:CLA:H92	15:aB:828:CLA:H62	1.76	0.42
18:a1:421:BCR:H333	15:c6:401:CLA:H18	2.02	0.42
15:a4:421:CLA:H171	15:a5:416:CLA:HBB2	2.02	0.42
13:a5:63:TYR:O	13:a5:66:SER:OG	2.31	0.42
13:a5:201:VAL:O	13:a5:205:TYR:N	2.35	0.42
15:a5:420:CLA:HBA2	15:a5:420:CLA:H3A	1.80	0.42
1:bA:319:TRP:O	1:bA:321:ILE:N	2.48	0.42
15:bA:809:CLA:HMB3	18:bJ:103:BCR:H20C	2.01	0.42
15:bA:829:CLA:H61	15:bA:829:CLA:H41	1.88	0.42
2:bB:354:HIS:CD2	15:bB:827:CLA:NC	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bB:727:TYR:HB2	15:bB:802:CLA:HED3	2.01	0.42
15:bB:807:CLA:H111	15:bB:807:CLA:H151	1.78	0.42
15:b4:421:CLA:H92	15:b4:421:CLA:H62	1.87	0.42
13:b5:97:LYS:HB3	13:b5:99:VAL:HG13	2.02	0.42
15:b5:420:CLA:HBA2	15:b5:420:CLA:H3A	1.80	0.42
1:cA:304:ILE:HD13	1:cA:304:ILE:HA	1.81	0.42
1:cA:744:TRP:CG	18:cA:851:BCR:HC22	2.54	0.42
2:cB:74:GLU:HG2	2:cB:130:THR:HA	2.01	0.42
2:cB:116:TYR:HA	2:cB:370:THR:HG22	2.02	0.42
15:cB:830:CLA:H161	15:cB:830:CLA:H141	1.82	0.42
18:cK:101:BCR:H15C	18:cK:101:BCR:H351	1.79	0.42
15:cL:204:CLA:H3A	15:cL:204:CLA:HBA1	1.76	0.42
13:c2:291:LEU:HA	13:c2:304:THR:HG23	2.02	0.42
15:c6:406:CLA:H2	15:c6:406:CLA:H61	1.83	0.42
1:aA:215:HIS:HE1	15:aA:815:CLA:C1A	2.33	0.42
15:aA:843:CLA:H93	15:aA:843:CLA:H112	1.88	0.42
2:aB:163:SER:OG	2:aB:164:LEU:N	2.53	0.42
2:aB:431:PHE:CZ	18:aF:203:BCR:HC41	2.55	0.42
3:aC:57:CYS:HA	3:aC:58:PRO:HD3	1.88	0.42
10:aL:62:TRP:HH2	10:aL:85:LEU:HD22	1.85	0.42
13:a2:49:GLN:HE21	15:a2:410:CLA:HMB3	1.84	0.42
13:a2:291:LEU:HA	13:a2:304:THR:HG23	2.02	0.42
18:a3:419:BCR:H343	15:a4:416:CLA:HBB1	2.02	0.42
13:a4:312:HIS:HB2	13:a4:317:TRP:NE1	2.35	0.42
15:a4:404:CLA:H2	15:a4:404:CLA:H61	1.82	0.42
13:a5:307:LEU:HA	13:a5:308:PRO:HA	1.78	0.42
18:a5:419:BCR:H15C	18:a5:419:BCR:H351	1.81	0.42
13:a6:288:GLY:C	13:a6:315:ARG:HH12	2.28	0.42
1:bA:353:HIS:CD2	1:bA:411:HIS:HD1	2.37	0.42
1:bA:466:ARG:NH2	1:bA:641:GLN:O	2.49	0.42
2:bB:163:SER:OG	2:bB:164:LEU:N	2.53	0.42
13:b1:209:PHE:HE1	13:b1:274:PHE:CE1	2.37	0.42
13:b2:97:LYS:HB3	13:b2:99:VAL:HG13	2.01	0.42
13:b3:135:THR:HB	13:b3:137:THR:HG23	2.01	0.42
13:b6:128:ARG:HE	13:c1:341:MET:HE2	1.85	0.42
13:b6:312:HIS:HB2	13:b6:317:TRP:NE1	2.35	0.42
18:cI:102:BCR:H24C	18:cI:102:BCR:H371	1.79	0.42
15:cL:202:CLA:H2	15:cL:202:CLA:H61	1.78	0.42
13:c2:80:ILE:HG23	15:c2:405:CLA:HMA1	2.01	0.42
13:c3:298:ALA:HA	15:c3:417:CLA:NB	2.35	0.42
13:c6:205:TYR:HA	13:c6:208:HIS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:180:GLY:HA3	15:aB:814:CLA:HBB1	2.02	0.42
6:aF:121:LEU:HA	6:aF:124:LEU:HB3	2.01	0.42
7:aI:20:TRP:CZ3	10:bL:149:MET:HE1	2.55	0.42
13:a1:52:LEU:O	13:a1:56:TRP:N	2.43	0.42
13:a1:128:ARG:NH1	15:a2:406:CLA:O1D	2.51	0.42
13:a3:264:ILE:O	13:a3:268:GLY:N	2.39	0.42
13:a5:221:GLY:HA3	18:a5:419:BCR:H393	2.02	0.42
1:bA:17:ASP:N	1:bA:184:ALA:O	2.50	0.42
1:bA:93:HIS:HE1	15:bA:808:CLA:C1A	2.33	0.42
15:bA:835:CLA:H92	15:bA:835:CLA:H61	1.87	0.42
18:bA:852:BCR:H20C	18:bA:852:BCR:H361	1.81	0.42
2:bB:116:TYR:HA	2:bB:370:THR:HG22	2.01	0.42
18:bB:847:BCR:H15C	18:bB:847:BCR:H351	1.92	0.42
18:bB:849:BCR:H20C	18:bB:849:BCR:H361	1.90	0.42
6:bF:124:LEU:HA	6:bF:129:LEU:HB2	2.01	0.42
13:b2:80:ILE:HG13	13:b2:81:LEU:HG	2.01	0.42
13:b3:212:ILE:H	13:b3:212:ILE:HG12	1.66	0.42
13:b3:288:GLY:C	13:b3:315:ARG:HH12	2.27	0.42
13:b5:80:ILE:HG23	15:b5:405:CLA:HMA1	2.01	0.42
15:b5:416:CLA:HMC1	15:b5:416:CLA:HHC	1.68	0.42
1:cA:352:TRP:HB3	15:cA:806:CLA:HAC1	2.01	0.42
1:cA:491:GLN:HE22	15:cA:838:CLA:HMD3	1.82	0.42
15:cA:804:CLA:H102	15:cA:804:CLA:H62	1.84	0.42
15:cB:827:CLA:H41	15:cB:827:CLA:H62	1.85	0.42
10:cL:58:LEU:HD23	10:cL:58:LEU:HA	1.90	0.42
13:c2:288:GLY:C	13:c2:315:ARG:HH12	2.28	0.42
13:c4:97:LYS:HB3	13:c4:99:VAL:HG13	2.02	0.42
18:c4:419:BCR:H11C	18:c4:419:BCR:H341	1.87	0.42
13:c5:80:ILE:HG13	13:c5:81:LEU:HG	2.02	0.42
1:aA:744:TRP:CG	18:aA:852:BCR:HC22	2.54	0.41
15:aB:819:CLA:H111	15:aB:819:CLA:H71	1.77	0.41
15:aB:837:CLA:H202	15:aB:837:CLA:H162	1.93	0.41
13:a2:264:ILE:O	13:a2:268:GLY:N	2.39	0.41
13:a2:288:GLY:C	13:a2:315:ARG:HH12	2.28	0.41
18:a2:421:BCR:H15C	18:a2:421:BCR:H351	1.81	0.41
15:a2:422:CLA:H18	18:a3:401:BCR:H333	2.01	0.41
13:a5:288:GLY:C	13:a5:315:ARG:HH12	2.28	0.41
18:a5:419:BCR:H361	18:a5:419:BCR:H20C	1.84	0.41
15:a6:418:CLA:H62	15:a6:418:CLA:H41	1.75	0.41
1:bA:718:GLN:HA	1:bA:719:PRO:HD3	1.92	0.41
15:bA:826:CLA:H111	15:bA:826:CLA:H143	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:bB:844:BCR:H11C	18:bB:844:BCR:H341	1.87	0.41
13:b1:307:LEU:HA	13:b1:308:PRO:HA	1.78	0.41
15:b1:404:CLA:H61	15:b1:404:CLA:H2	1.83	0.41
15:b3:416:CLA:HHC	15:b3:416:CLA:HMC1	1.69	0.41
13:b4:261:LEU:HD23	13:b4:261:LEU:HA	1.88	0.41
15:b4:421:CLA:H171	15:b5:416:CLA:HBB2	2.02	0.41
13:b6:209:PHE:HE1	13:b6:274:PHE:CE1	2.38	0.41
1:cA:59:ASP:OD1	1:cA:59:ASP:N	2.53	0.41
15:cA:804:CLA:HED2	15:cA:804:CLA:H2	2.01	0.41
15:cA:809:CLA:H143	15:cA:809:CLA:H161	1.90	0.41
2:cB:727:TYR:HB2	15:cB:802:CLA:HED3	2.01	0.41
3:cC:42:PRO:HB3	4:cD:112:VAL:HG21	2.02	0.41
13:c2:135:THR:HB	13:c2:137:THR:HG23	2.02	0.41
13:c4:80:ILE:HG23	15:c4:405:CLA:HMA1	2.02	0.41
13:c6:192:ILE:HD11	13:c6:215:LEU:HD13	2.01	0.41
2:aB:622:LEU:HD23	2:aB:622:LEU:HA	1.88	0.41
15:aB:833:CLA:H2	15:aB:833:CLA:H62	1.61	0.41
15:a2:410:CLA:HBD	15:a2:410:CLA:H121	2.02	0.41
18:a3:401:BCR:H15C	18:a3:401:BCR:H351	1.90	0.41
15:a4:416:CLA:HHC	15:a4:416:CLA:HMC1	1.67	0.41
18:a4:420:BCR:H15C	18:a4:420:BCR:H351	1.80	0.41
13:a5:298:ALA:HA	15:a5:417:CLA:NB	2.34	0.41
15:a5:409:CLA:HBD	15:a5:409:CLA:H121	2.02	0.41
13:a6:113:ILE:HD13	13:a6:113:ILE:HA	1.83	0.41
13:a6:209:PHE:HE1	13:a6:274:PHE:CE1	2.38	0.41
15:bA:804:CLA:H2	15:bA:804:CLA:HED2	2.01	0.41
2:bB:298:HIS:HE1	15:bB:822:CLA:NB	2.19	0.41
15:bB:837:CLA:H202	15:bB:837:CLA:H162	1.93	0.41
18:bJ:104:BCR:H15C	18:bJ:104:BCR:H351	1.86	0.41
13:b2:23:ASN:HA	13:b2:24:VAL:HA	1.71	0.41
15:b2:410:CLA:H121	15:b2:410:CLA:HBD	2.01	0.41
15:b4:404:CLA:H2	15:b4:404:CLA:H61	1.82	0.41
13:b5:113:ILE:HD12	15:b5:420:CLA:H152	2.02	0.41
15:b5:404:CLA:H61	15:b5:404:CLA:H2	1.82	0.41
15:b5:420:CLA:H61	15:b5:420:CLA:H41	1.80	0.41
13:b6:205:TYR:HA	13:b6:208:HIS:HB2	2.01	0.41
15:b6:410:CLA:H162	15:b6:410:CLA:H141	1.87	0.41
1:cA:215:HIS:HE1	15:cA:815:CLA:C1A	2.33	0.41
15:cB:801:CLA:H13	15:cB:801:CLA:H171	1.87	0.41
6:cF:46:ASP:OD1	6:cF:46:ASP:N	2.50	0.41
18:cI:101:BCR:H15C	18:cI:101:BCR:H351	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c2:410:CLA:HBD	15:c2:410:CLA:H121	2.02	0.41
13:c3:97:LYS:HB3	13:c3:99:VAL:HG13	2.02	0.41
15:c3:417:CLA:H41	15:c3:417:CLA:H62	1.76	0.41
13:c4:160:HIS:CE1	15:c4:412:CLA:NC	2.78	0.41
13:c4:312:HIS:HB2	13:c4:317:TRP:NE1	2.35	0.41
15:c4:417:CLA:H2A	15:c4:417:CLA:O2D	2.20	0.41
15:c5:416:CLA:HBA2	15:c5:416:CLA:H3A	1.41	0.41
2:aB:177:HIS:CD2	15:aB:814:CLA:NB	2.89	0.41
15:aB:818:CLA:HBA2	15:aB:818:CLA:H3A	1.41	0.41
13:a3:312:HIS:HB2	13:a3:317:TRP:NE1	2.36	0.41
13:a4:80:ILE:HG13	13:a4:81:LEU:HG	2.02	0.41
13:a5:113:ILE:HD12	15:a5:420:CLA:H152	2.02	0.41
13:a6:175:ALA:HA	13:a6:180:GLY:HA2	2.02	0.41
1:bA:224:ASN:HA	1:bA:227:LEU:HB2	2.03	0.41
1:bA:494:HIS:HE1	15:bA:836:CLA:NB	2.16	0.41
15:bA:831:CLA:H13	15:bA:831:CLA:H171	1.85	0.41
2:bB:39:GLU:HG2	2:bB:164:LEU:HB2	2.01	0.41
10:bL:62:TRP:HH2	10:bL:85:LEU:HD22	1.85	0.41
13:b4:288:GLY:C	13:b4:315:ARG:HH12	2.28	0.41
13:b6:175:ALA:HA	13:b6:180:GLY:HA2	2.03	0.41
15:cA:844:CLA:HAC1	15:cA:844:CLA:HHD	1.79	0.41
4:cD:64:CYS:HB3	4:cD:82:ILE:HD13	2.02	0.41
13:c2:90:PHE:HZ	15:c2:403:CLA:H192	1.85	0.41
15:c3:421:CLA:H92	15:c3:421:CLA:H62	1.87	0.41
13:c4:111:HIS:HE1	15:c4:404:CLA:C4A	2.04	0.41
1:aA:196:MET:HB2	15:aA:814:CLA:HBC2	2.03	0.41
15:aA:834:CLA:H112	15:aA:834:CLA:H152	1.82	0.41
18:a1:417:BCR:H24C	18:a1:417:BCR:H371	1.88	0.41
13:a2:90:PHE:HZ	15:a2:403:CLA:H192	1.85	0.41
13:a2:294:LYS:HG3	13:a2:300:TYR:CZ	2.56	0.41
13:a4:298:ALA:HA	15:a4:417:CLA:NB	2.35	0.41
13:a6:205:TYR:HA	13:a6:208:HIS:HB2	2.01	0.41
1:bA:31:PRO:HB3	15:bA:804:CLA:HAC1	2.02	0.41
2:bB:350:LEU:HD12	2:bB:350:LEU:HA	1.88	0.41
2:bB:392:HIS:HA	2:bB:395:ILE:HD12	2.02	0.41
15:bB:807:CLA:H111	15:bB:807:CLA:H72	1.76	0.41
15:bB:840:CLA:HBA2	18:bB:850:BCR:H352	2.02	0.41
13:b1:113:ILE:HD13	18:b2:401:BCR:C11	2.49	0.41
13:b2:32:ASN:HD21	15:b2:412:CLA:C1C	2.33	0.41
18:b2:419:BCR:H15C	18:b2:419:BCR:H351	1.92	0.41
18:b2:421:BCR:H20C	18:b2:421:BCR:H361	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b3:261:LEU:HD23	13:b3:261:LEU:HA	1.89	0.41
13:b3:312:HIS:HB2	13:b3:317:TRP:NE1	2.35	0.41
15:b3:409:CLA:HBD	15:b3:409:CLA:H121	2.02	0.41
13:b4:97:LYS:HB3	13:b4:99:VAL:HG13	2.02	0.41
18:b5:401:BCR:H15C	18:b5:401:BCR:H351	1.87	0.41
13:b6:291:LEU:HA	13:b6:304:THR:HG23	2.02	0.41
1:cA:353:HIS:HD2	1:cA:411:HIS:HD1	1.68	0.41
2:cB:177:HIS:CD2	15:cB:814:CLA:NB	2.89	0.41
2:cB:658:PHE:O	2:cB:662:VAL:HG23	2.21	0.41
18:cB:846:BCR:H15C	18:cB:846:BCR:H351	1.86	0.41
12:cX:9:TYR:O	12:cX:13:THR:OG1	2.28	0.41
13:c1:21:GLN:HA	13:c1:22:THR:HA	1.71	0.41
15:c3:404:CLA:H2	15:c3:404:CLA:H61	1.82	0.41
13:c5:113:ILE:HD12	15:c5:420:CLA:H152	2.02	0.41
15:c5:412:CLA:HBA1	15:c5:412:CLA:H3A	1.54	0.41
13:c6:312:HIS:HB2	13:c6:317:TRP:NE1	2.35	0.41
18:c6:420:BCR:H20C	18:c6:420:BCR:H361	1.85	0.41
1:aA:93:HIS:HE1	15:aA:808:CLA:C1A	2.33	0.41
1:aA:224:ASN:HA	1:aA:227:LEU:HB2	2.03	0.41
15:aA:804:CLA:H2	15:aA:804:CLA:HED2	2.01	0.41
15:aA:844:CLA:H3A	15:aA:844:CLA:HBA2	1.46	0.41
2:aB:116:TYR:HA	2:aB:370:THR:HG22	2.01	0.41
2:aB:602:TRP:HE1	2:aB:614:GLN:NE2	2.17	0.41
15:aB:840:CLA:HBA2	15:aB:840:CLA:H3A	1.81	0.41
18:aI:102:BCR:H24C	18:aI:102:BCR:H371	1.79	0.41
13:a1:135:THR:HB	13:a1:137:THR:HG23	2.02	0.41
15:a1:415:CLA:HHC	15:a1:415:CLA:HMC1	1.72	0.41
13:a2:32:ASN:HD21	15:a2:412:CLA:C1C	2.32	0.41
18:a4:401:BCR:H402	15:a4:415:CLA:HED3	2.02	0.41
18:a6:402:BCR:H15C	18:a6:402:BCR:H351	1.86	0.41
15:bA:820:CLA:H171	15:bA:836:CLA:H41	2.01	0.41
2:bB:667:PHE:HB3	15:bB:804:CLA:HMC2	2.02	0.41
15:bB:828:CLA:H62	15:bB:828:CLA:H92	1.76	0.41
15:b1:417:CLA:H51	15:b1:417:CLA:H12	1.87	0.41
18:b1:418:BCR:H24C	18:b1:418:BCR:H371	1.89	0.41
13:b2:49:GLN:HE21	15:b2:410:CLA:HMB3	1.85	0.41
15:b2:406:CLA:H143	15:b2:406:CLA:H111	1.93	0.41
15:b3:421:CLA:H62	15:b3:421:CLA:H92	1.86	0.41
15:b4:416:CLA:HHB	15:b4:416:CLA:HMB3	1.86	0.41
18:b4:419:BCR:H15C	18:b4:419:BCR:H351	1.85	0.41
15:b4:421:CLA:H203	15:b4:421:CLA:H161	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b5:209:PHE:HE1	13:b5:274:PHE:CE1	2.38	0.41
1:cA:17:ASP:N	1:cA:184:ALA:O	2.50	0.41
1:cA:224:ASN:HA	1:cA:227:LEU:HB2	2.03	0.41
2:cB:431:PHE:CZ	18:cF:205:BCR:HC41	2.55	0.41
2:cB:602:TRP:HE1	2:cB:614:GLN:NE2	2.17	0.41
2:cB:622:LEU:HD21	15:cB:802:CLA:H151	2.03	0.41
18:cB:849:BCR:H15C	18:cB:849:BCR:H351	1.88	0.41
13:c1:298:ALA:HA	15:c1:417:CLA:NB	2.35	0.41
13:c2:325:LEU:O	13:c2:329:PHE:N	2.45	0.41
15:c2:406:CLA:H92	15:c2:406:CLA:H62	1.83	0.41
15:c2:418:CLA:H62	15:c2:418:CLA:H41	1.78	0.41
13:c4:80:ILE:HG13	13:c4:81:LEU:HG	2.03	0.41
13:c5:288:GLY:C	13:c5:315:ARG:HH12	2.28	0.41
13:c6:135:THR:HB	13:c6:137:THR:HG23	2.02	0.41
2:aB:74:GLU:HG2	2:aB:130:THR:HA	2.01	0.41
15:aB:811:CLA:C2B	7:aI:20:TRP:HE1	2.34	0.41
18:aB:849:BCR:H15C	18:aB:849:BCR:H351	1.88	0.41
13:a2:175:ALA:HA	13:a2:180:GLY:HA2	2.03	0.41
15:a2:422:CLA:H143	15:a2:422:CLA:H111	1.87	0.41
15:a2:422:CLA:H92	15:a2:422:CLA:H62	1.84	0.41
15:a3:410:CLA:H162	15:a3:410:CLA:H141	1.87	0.41
15:a3:421:CLA:H203	15:a3:421:CLA:H161	1.81	0.41
15:a4:412:CLA:HBA1	15:a4:412:CLA:H3A	1.54	0.41
15:a5:417:CLA:H62	15:a5:417:CLA:H41	1.77	0.41
2:bB:432:LEU:O	2:bB:436:THR:OG1	2.26	0.41
13:b2:291:LEU:HA	13:b2:304:THR:HG23	2.03	0.41
13:b2:312:HIS:HB2	13:b2:317:TRP:NE1	2.36	0.41
15:b2:406:CLA:H41	15:b2:406:CLA:H61	1.80	0.41
13:b3:307:LEU:HA	13:b3:308:PRO:HA	1.78	0.41
18:b4:401:BCR:H402	15:b4:415:CLA:HED3	2.03	0.41
15:b4:421:CLA:H41	15:b4:421:CLA:H61	1.87	0.41
15:b5:409:CLA:HBD	15:b5:409:CLA:H121	2.02	0.41
13:b6:288:GLY:C	13:b6:315:ARG:HH12	2.28	0.41
1:cA:708:HIS:HE1	15:cA:841:CLA:C4D	2.34	0.41
15:cA:820:CLA:H171	15:cA:836:CLA:H41	2.02	0.41
2:cB:128:MET:HE3	15:cB:815:CLA:H2A	2.03	0.41
2:cB:586:MET:HE3	2:cB:586:MET:HB3	1.80	0.41
18:cB:849:BCR:H361	18:cB:849:BCR:H20C	1.79	0.41
18:cF:205:BCR:H15C	18:cF:205:BCR:H351	1.80	0.41
10:cL:64:LYS:HA	10:cL:64:LYS:HD3	1.84	0.41
13:c2:32:ASN:HD21	15:c2:412:CLA:C1C	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c3:421:CLA:H143	15:c3:421:CLA:H111	1.82	0.41
18:c4:401:BCR:H402	15:c4:415:CLA:HED3	2.02	0.41
13:c5:209:PHE:HE1	13:c5:274:PHE:CE1	2.38	0.41
13:c6:52:LEU:O	13:c6:56:TRP:N	2.44	0.41
1:aA:70:ARG:O	1:aA:74:SER:OG	2.39	0.41
1:aA:466:ARG:NH2	1:aA:641:GLN:O	2.49	0.41
15:aA:830:CLA:H192	15:aA:830:CLA:H162	1.80	0.41
2:aB:658:PHE:O	2:aB:662:VAL:HG23	2.21	0.41
15:aJ:201:CLA:H3A	15:aJ:201:CLA:HBA1	1.72	0.41
18:a4:401:BCR:H15C	18:a4:401:BCR:H351	1.90	0.41
15:a4:416:CLA:HMB3	15:a4:416:CLA:HHB	1.86	0.41
13:a5:97:LYS:HB3	13:a5:99:VAL:HG13	2.02	0.41
18:a5:401:BCR:H15C	18:a5:401:BCR:H351	1.87	0.41
13:a6:80:ILE:HG23	15:a6:406:CLA:HMA1	2.02	0.41
13:a6:128:ARG:HE	13:b1:341:MET:HE2	1.85	0.41
1:bA:374:MET:HB3	1:bA:374:MET:HE2	1.78	0.41
1:bA:415:PHE:CD1	1:bA:419:ASP:HB2	2.55	0.41
1:bA:441:ILE:HD13	1:bA:441:ILE:HA	1.86	0.41
1:bA:618:GLN:HB3	1:bA:635:THR:HG23	2.03	0.41
15:bA:805:CLA:HBD	15:bA:812:CLA:H2	2.03	0.41
15:bA:834:CLA:H71	15:bA:834:CLA:H111	1.79	0.41
15:bB:801:CLA:H91	15:bB:801:CLA:H111	1.82	0.41
4:bD:64:CYS:HB3	4:bD:82:ILE:HD13	2.02	0.41
15:b2:422:CLA:H91	15:b2:422:CLA:H112	1.91	0.41
13:b3:23:ASN:HA	13:b3:24:VAL:HA	1.71	0.41
13:b3:298:ALA:HA	15:b3:417:CLA:NB	2.35	0.41
13:b6:80:ILE:HG23	15:b6:406:CLA:HMA1	2.02	0.41
1:cA:415:PHE:CD1	1:cA:419:ASP:HB2	2.55	0.41
1:cA:618:GLN:HB3	1:cA:635:THR:HG23	2.03	0.41
18:cA:847:BCR:H20C	18:cA:847:BCR:H361	1.87	0.41
2:cB:163:SER:OG	2:cB:164:LEU:N	2.53	0.41
15:cB:835:CLA:HAB	18:cB:848:BCR:H333	2.03	0.41
4:cD:76:LYS:HE2	4:cD:76:LYS:HB2	1.90	0.41
6:cF:69:LEU:HD23	18:cF:205:BCR:H361	2.03	0.41
13:c2:261:LEU:HD23	13:c2:261:LEU:HA	1.88	0.41
13:c3:294:LYS:HG3	13:c3:300:TYR:CE2	2.56	0.41
18:c3:420:BCR:H24C	18:c3:420:BCR:H371	1.93	0.41
18:c3:420:BCR:H361	18:c3:420:BCR:H20C	1.84	0.41
13:c4:128:ARG:HH12	15:c4:421:CLA:HBD	1.85	0.41
13:c4:307:LEU:HA	13:c4:308:PRO:HA	1.79	0.41
13:c5:97:LYS:HB3	13:c5:99:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c5:416:CLA:HHC	15:c5:416:CLA:HMC1	1.69	0.41
13:c6:175:ALA:HA	13:c6:180:GLY:HA2	2.03	0.41
13:c6:209:PHE:HE1	13:c6:274:PHE:CE1	2.38	0.41
1:aA:453:PHE:CE2	15:aB:804:CLA:H12	2.56	0.41
1:aA:718:GLN:HA	1:aA:719:PRO:HD3	1.92	0.41
8:aJ:26:LEU:HD23	8:aJ:26:LEU:HA	1.87	0.41
15:a1:409:CLA:H162	15:a1:409:CLA:H141	1.88	0.41
15:a3:421:CLA:H92	15:a3:421:CLA:H62	1.86	0.41
15:a4:417:CLA:O2D	15:a4:417:CLA:H2A	2.21	0.41
15:a5:420:CLA:H61	15:a5:420:CLA:H41	1.80	0.41
13:a6:291:LEU:HA	13:a6:304:THR:HG23	2.02	0.41
15:bB:807:CLA:H162	15:bB:807:CLA:H143	1.95	0.41
15:bB:829:CLA:HBA2	15:bB:829:CLA:H3A	1.73	0.41
8:bJ:28:GLU:OE1	8:bJ:31:ARG:NH2	2.40	0.41
18:bL:206:BCR:H20C	18:bL:206:BCR:H361	1.81	0.41
13:b1:298:ALA:HA	15:b1:417:CLA:NB	2.35	0.41
18:b1:418:BCR:H11C	18:b1:418:BCR:H341	1.94	0.41
18:b2:419:BCR:H11C	18:b2:419:BCR:H341	1.92	0.41
15:b3:404:CLA:H2	15:b3:404:CLA:H61	1.83	0.41
13:b4:312:HIS:HB2	13:b4:317:TRP:NE1	2.35	0.41
18:b5:401:BCR:H343	15:b5:417:CLA:HBB2	2.03	0.41
18:b5:419:BCR:H351	18:b5:419:BCR:H15C	1.81	0.41
1:cA:70:ARG:O	1:cA:74:SER:OG	2.39	0.41
2:cB:180:GLY:HA3	15:cB:814:CLA:HBB1	2.02	0.41
15:cB:818:CLA:HBA2	15:cB:818:CLA:H3A	1.41	0.41
15:c1:413:CLA:HBB1	18:c1:419:BCR:H402	2.03	0.41
18:c1:419:BCR:H20C	18:c1:419:BCR:H361	1.84	0.41
18:c3:420:BCR:H15C	18:c3:420:BCR:H351	1.80	0.41
15:c5:409:CLA:HBD	15:c5:409:CLA:H121	2.03	0.41
15:c6:414:CLA:HHC	15:c6:414:CLA:HBB1	2.03	0.41
1:aA:31:PRO:HB3	15:aA:804:CLA:HAC1	2.02	0.41
1:aA:415:PHE:CD1	1:aA:419:ASP:HB2	2.55	0.41
15:aA:803:CLA:C2	15:aA:803:CLA:H3A	2.51	0.41
15:aA:805:CLA:HBD	15:aA:812:CLA:H2	2.03	0.41
2:aB:354:HIS:CD2	15:aB:827:CLA:NC	2.88	0.41
15:aB:835:CLA:HAB	18:aB:848:BCR:H333	2.03	0.41
11:aM:23:PHE:O	11:aM:27:THR:OG1	2.35	0.41
13:a2:261:LEU:HD23	13:a2:261:LEU:HA	1.88	0.41
13:a3:175:ALA:HA	13:a3:180:GLY:HA2	2.03	0.41
13:a3:294:LYS:HG3	13:a3:300:TYR:CE2	2.56	0.41
15:a3:404:CLA:H61	15:a3:404:CLA:H2	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a4:192:ILE:HD11	13:a4:215:LEU:HD13	2.03	0.41
13:a5:135:THR:HB	13:a5:137:THR:HG23	2.02	0.41
13:a5:209:PHE:HE1	13:a5:274:PHE:CE1	2.38	0.41
18:a5:401:BCR:H343	15:a5:417:CLA:HBB2	2.03	0.41
13:a6:312:HIS:HB2	13:a6:317:TRP:NE1	2.35	0.41
15:a6:413:CLA:HHC	15:a6:413:CLA:HBB1	2.03	0.41
1:bA:566:ILE:HD11	1:bA:589:VAL:HG11	2.03	0.41
2:bB:128:MET:HE3	15:bB:815:CLA:H2A	2.03	0.41
2:bB:355:MET:HE2	2:bB:355:MET:HB3	1.82	0.41
2:bB:658:PHE:O	2:bB:662:VAL:HG23	2.21	0.41
15:bB:830:CLA:H141	15:bB:830:CLA:H161	1.82	0.41
15:bB:835:CLA:HAB	18:bB:848:BCR:H333	2.03	0.41
15:bB:837:CLA:H8	18:bF:202:BCR:H372	2.02	0.41
11:bM:23:PHE:O	11:bM:27:THR:OG1	2.35	0.41
13:b1:288:GLY:C	13:b1:315:ARG:HH12	2.28	0.41
13:b3:325:LEU:O	13:b3:329:PHE:N	2.45	0.41
18:b3:419:BCR:H343	15:b4:416:CLA:HBB1	2.03	0.41
18:b3:420:BCR:H15C	18:b3:420:BCR:H351	1.80	0.41
13:b4:80:ILE:HG23	15:b4:405:CLA:HMA1	2.02	0.41
13:b4:135:THR:HB	13:b4:137:THR:HG23	2.03	0.41
13:b4:299:PRO:HG2	13:b4:323:PHE:HE2	1.86	0.41
13:b5:288:GLY:C	13:b5:315:ARG:HH12	2.28	0.41
15:b5:410:CLA:H162	15:b5:410:CLA:H141	1.87	0.41
13:b6:128:ARG:HH11	13:c1:341:MET:HE2	1.85	0.41
1:cA:93:HIS:HE1	15:cA:808:CLA:C1A	2.33	0.41
1:cA:196:MET:HB2	15:cA:814:CLA:HBC2	2.03	0.41
1:cA:453:PHE:CE2	15:cB:804:CLA:H12	2.56	0.41
1:cA:688:MET:O	1:cA:692:SER:OG	2.22	0.41
2:cB:29:ASP:OD2	2:cB:32:SER:OG	2.33	0.41
2:cB:194:ILE:HG12	2:cB:253:ILE:HB	2.03	0.41
2:cB:322:HIS:CD2	15:cB:824:CLA:ND	2.89	0.41
2:cB:354:HIS:CD2	15:cB:827:CLA:NC	2.88	0.41
15:cB:801:CLA:H111	15:cB:801:CLA:H91	1.82	0.41
15:cB:801:CLA:H62	15:cB:801:CLA:H41	1.57	0.41
15:cB:840:CLA:HBA2	18:cB:849:BCR:H352	2.02	0.41
6:cF:6:VAL:O	6:cF:43:CYS:N	2.39	0.41
18:cM:101:BCR:H15C	18:cM:101:BCR:H351	1.97	0.41
13:c1:324:PHE:HE2	18:c1:418:BCR:H403	1.85	0.41
13:c2:312:HIS:HB2	13:c2:317:TRP:NE1	2.36	0.41
15:c2:411:CLA:H162	15:c2:411:CLA:H141	1.89	0.41
13:c3:312:HIS:HB2	13:c3:317:TRP:NE1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c4:135:THR:HB	13:c4:137:THR:HG23	2.03	0.41
13:c4:288:GLY:C	13:c4:315:ARG:HH12	2.28	0.41
18:c5:401:BCR:H343	15:c5:417:CLA:HBB2	2.03	0.41
15:c6:401:CLA:H91	15:c6:401:CLA:H112	1.96	0.41
1:aA:416:MET:HE1	1:aA:434:LEU:HD11	2.03	0.41
1:aA:473:ASP:OD1	10:aL:69:ARG:NH2	2.54	0.41
15:aA:802:CLA:H142	15:aA:802:CLA:H111	1.76	0.41
15:aA:804:CLA:H43	15:aA:843:CLA:H121	2.02	0.41
15:aA:834:CLA:HBB2	10:aL:65:LEU:HD13	2.03	0.41
2:aB:193:LEU:HA	2:aB:197:ALA:HB3	2.03	0.41
2:aB:256:PHE:HZ	15:aB:818:CLA:H72	1.86	0.41
18:a2:420:BCR:H11C	18:a2:420:BCR:H341	1.84	0.41
13:a3:298:ALA:HA	15:a3:417:CLA:NB	2.35	0.41
1:bA:454:HIS:CE1	15:bA:834:CLA:NA	2.89	0.41
1:bA:708:HIS:HE1	15:bA:841:CLA:C4D	2.34	0.41
2:bB:74:GLU:HG2	2:bB:130:THR:HA	2.01	0.41
2:bB:193:LEU:HA	2:bB:197:ALA:HB3	2.03	0.41
2:bB:327:GLU:O	2:bB:331:ASN:ND2	2.54	0.41
6:bF:63:PHE:O	6:bF:67:SER:OG	2.27	0.41
15:bL:203:CLA:H91	15:bL:203:CLA:H112	1.88	0.41
18:b1:401:BCR:H20C	18:b1:401:BCR:H361	1.87	0.41
13:b2:294:LYS:HG3	13:b2:300:TYR:CZ	2.55	0.41
13:b3:294:LYS:HG3	13:b3:300:TYR:CE2	2.56	0.41
13:b4:90:PHE:HZ	15:b4:403:CLA:H192	1.86	0.41
15:b4:410:CLA:H162	15:b4:410:CLA:H141	1.85	0.41
15:b4:417:CLA:O2D	15:b4:417:CLA:H2A	2.21	0.41
13:b5:23:ASN:HA	13:b5:24:VAL:HA	1.71	0.41
15:cA:804:CLA:H13	15:cA:804:CLA:H171	1.84	0.41
15:cA:809:CLA:HMB3	18:cJ:103:BCR:H20C	2.01	0.41
15:cA:841:CLA:H62	15:cA:841:CLA:H41	1.89	0.41
16:cA:845:PQN:H293	16:cA:845:PQN:H261	1.94	0.41
3:cC:9:THR:HG22	5:cE:34:TYR:CZ	2.56	0.41
18:c2:401:BCR:H20C	18:c2:401:BCR:H361	1.91	0.41
13:c3:57:ALA:O	13:c3:61:THR:OG1	2.26	0.41
15:c3:417:CLA:H51	15:c3:417:CLA:H12	1.87	0.41
18:c4:419:BCR:H15C	18:c4:419:BCR:H351	1.85	0.41
13:c5:294:LYS:HG3	13:c5:300:TYR:CE2	2.56	0.41
18:c5:419:BCR:H20C	18:c5:419:BCR:H361	1.84	0.41
13:c6:288:GLY:C	13:c6:315:ARG:HH12	2.28	0.41
1:aA:43:GLN:H	1:aA:43:GLN:HG2	1.49	0.40
1:aA:470:ARG:HG2	10:bL:154:ASN:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:144:LEU:HD12	2:aB:144:LEU:HA	1.89	0.40
2:aB:648:ASN:OD1	2:aB:648:ASN:N	2.41	0.40
15:aB:826:CLA:C2B	15:aB:838:CLA:H3A	2.52	0.40
15:aB:830:CLA:H141	15:aB:830:CLA:H161	1.81	0.40
15:aB:831:CLA:HBC2	18:aB:847:BCR:H292	2.03	0.40
18:aI:103:BCR:H20C	18:aI:103:BCR:H361	1.81	0.40
13:a1:72:LEU:HB2	13:a1:77:GLN:NE2	2.36	0.40
13:a1:312:HIS:HB2	13:a1:317:TRP:NE1	2.36	0.40
13:a4:80:ILE:HG23	15:a4:405:CLA:HMA1	2.02	0.40
13:a4:288:GLY:C	13:a4:315:ARG:HH12	2.28	0.40
13:a5:325:LEU:O	13:a5:329:PHE:N	2.45	0.40
13:a6:128:ARG:HH12	15:a6:422:CLA:CED	2.34	0.40
13:a6:261:LEU:HA	13:a6:261:LEU:HD23	1.87	0.40
18:a6:421:BCR:H15C	18:a6:421:BCR:H351	1.88	0.40
15:bA:804:CLA:H43	15:bA:843:CLA:H121	2.02	0.40
2:bB:177:HIS:CD2	15:bB:814:CLA:NB	2.89	0.40
15:bB:814:CLA:H122	15:bB:814:CLA:H8	1.83	0.40
18:bB:844:BCR:H15C	18:bB:844:BCR:H351	1.91	0.40
18:bB:847:BCR:H24C	18:bB:847:BCR:H371	1.89	0.40
6:bF:16:LYS:HA	6:bF:16:LYS:HD3	1.84	0.40
6:bF:119:ALA:HB2	13:b4:352:LEU:HD22	2.03	0.40
15:bL:204:CLA:HBA1	15:bL:204:CLA:H3A	1.76	0.40
18:bL:205:BCR:H20C	18:bL:205:BCR:H361	1.81	0.40
18:b4:419:BCR:H20C	18:b4:419:BCR:H361	1.86	0.40
15:b5:417:CLA:H12	15:b5:417:CLA:H51	1.86	0.40
15:b6:405:CLA:H61	15:b6:405:CLA:H2	1.83	0.40
1:cA:454:HIS:CE1	15:cA:834:CLA:NA	2.89	0.40
15:cA:803:CLA:C2	15:cA:803:CLA:H3A	2.51	0.40
2:cB:327:GLU:O	2:cB:331:ASN:ND2	2.54	0.40
2:cB:718:HIS:HE1	15:cB:840:CLA:ND	2.19	0.40
18:cF:202:BCR:H11C	18:cF:202:BCR:H341	1.93	0.40
10:cL:62:TRP:HH2	10:cL:85:LEU:HD22	1.85	0.40
15:cL:204:CLA:H52	15:cL:204:CLA:H8	1.81	0.40
13:c1:72:LEU:HB2	13:c1:77:GLN:NE2	2.37	0.40
13:c1:288:GLY:C	13:c1:315:ARG:HH12	2.29	0.40
13:c5:66:SER:OG	13:c5:67:GLN:N	2.54	0.40
13:c6:291:LEU:HA	13:c6:304:THR:HG23	2.03	0.40
1:aA:24:SER:O	15:aA:812:CLA:HHB	2.21	0.40
1:aA:708:HIS:HE1	15:aA:841:CLA:C4D	2.34	0.40
15:aA:834:CLA:HAB	15:aA:834:CLA:HHC	1.81	0.40
18:aA:848:BCR:H20C	18:aA:848:BCR:H361	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aB:801:CLA:H111	15:aB:801:CLA:H91	1.82	0.40
15:aB:811:CLA:O2A	15:aB:811:CLA:H2A	2.20	0.40
18:aB:848:BCR:H20C	18:aB:848:BCR:H361	1.93	0.40
18:a2:401:BCR:H20C	18:a2:401:BCR:H361	1.91	0.40
15:a3:421:CLA:H143	15:a3:421:CLA:H111	1.82	0.40
13:a4:128:ARG:HH12	15:a4:421:CLA:HBD	1.85	0.40
18:a4:419:BCR:H11C	18:a4:419:BCR:H341	1.88	0.40
13:a6:135:THR:HB	13:a6:137:THR:HG23	2.02	0.40
1:bA:372:GLN:NE2	15:bA:827:CLA:OBD	2.52	0.40
15:bA:803:CLA:H3A	15:bA:803:CLA:C2	2.51	0.40
2:bB:29:ASP:OD2	2:bB:32:SER:OG	2.33	0.40
2:bB:146:SER:HB3	11:bM:21:LEU:HD12	2.02	0.40
15:bB:811:CLA:O2A	15:bB:811:CLA:H2A	2.21	0.40
18:bB:849:BCR:C10	15:bF:201:CLA:HAB	2.52	0.40
18:bB:849:BCR:H332	18:bJ:103:BCR:HC22	2.03	0.40
18:bL:201:BCR:H361	18:bL:201:BCR:H20C	1.81	0.40
13:b1:221:GLY:HA3	18:b1:420:BCR:H393	2.03	0.40
13:b1:307:LEU:HD22	13:b1:308:PRO:HA	2.03	0.40
15:b1:417:CLA:H41	15:b1:417:CLA:H62	1.75	0.40
13:b2:288:GLY:C	13:b2:315:ARG:HH12	2.28	0.40
1:cA:416:MET:HE1	1:cA:434:LEU:HD11	2.03	0.40
15:cA:826:CLA:H111	15:cA:826:CLA:H143	1.77	0.40
15:cB:826:CLA:C2B	15:cB:838:CLA:H3A	2.52	0.40
5:cE:29:THR:HA	5:cE:30:PRO:HD3	1.90	0.40
18:cF:205:BCR:H361	18:cF:205:BCR:H20C	1.86	0.40
18:cI:102:BCR:H15C	18:cI:102:BCR:H351	1.86	0.40
18:cL:205:BCR:H15C	18:cL:205:BCR:H351	1.83	0.40
15:aB:828:CLA:HBA2	15:aB:828:CLA:H3A	1.80	0.40
18:a1:417:BCR:H11C	18:a1:417:BCR:H341	1.93	0.40
13:a2:135:THR:HB	13:a2:137:THR:HG23	2.03	0.40
13:a3:299:PRO:HG2	13:a3:323:PHE:HE2	1.86	0.40
18:a3:420:BCR:H15C	18:a3:420:BCR:H351	1.80	0.40
13:a4:90:PHE:HZ	15:a4:403:CLA:H192	1.87	0.40
15:a6:417:CLA:HMC1	15:a6:417:CLA:HHC	1.73	0.40
2:bB:159:LYS:HE2	2:bB:159:LYS:HB2	1.84	0.40
2:bB:256:PHE:HZ	15:bB:818:CLA:H72	1.86	0.40
15:bB:814:CLA:HHD	15:bB:814:CLA:HAC2	1.95	0.40
4:bD:122:ASN:HA	4:bD:123:PRO:HD3	1.96	0.40
15:bL:204:CLA:H111	15:bL:204:CLA:H93	1.82	0.40
13:b1:128:ARG:NH2	13:b2:250:MET:SD	2.95	0.40
18:b1:401:BCR:C9	15:b1:416:CLA:HBB1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b3:192:ILE:HD11	13:b3:215:LEU:HD13	2.03	0.40
18:b3:418:BCR:H15C	18:b3:418:BCR:H351	1.95	0.40
15:b4:421:CLA:HBA2	15:b4:421:CLA:H3A	1.99	0.40
13:b6:21:GLN:HA	13:b6:22:THR:HA	1.71	0.40
13:b6:88:LEU:HD22	13:b6:88:LEU:HA	1.95	0.40
13:b6:113:ILE:HD13	13:b6:113:ILE:HA	1.91	0.40
1:cA:712:LYS:HG3	6:cF:131:ALA:HB2	2.04	0.40
15:cA:833:CLA:H61	15:cA:833:CLA:H41	1.83	0.40
15:cB:810:CLA:H151	15:cB:810:CLA:H18	1.77	0.40
18:cM:101:BCR:H20C	18:cM:101:BCR:H361	1.84	0.40
15:c1:410:CLA:H162	15:c1:410:CLA:H141	1.87	0.40
15:c1:412:CLA:H3A	15:c1:412:CLA:HBA1	1.52	0.40
13:c3:299:PRO:HG2	13:c3:323:PHE:HE2	1.86	0.40
1:aA:227:LEU:HD23	1:aA:227:LEU:HA	1.90	0.40
1:aA:353:HIS:HD2	1:aA:411:HIS:HD1	1.68	0.40
1:aA:566:ILE:HD11	1:aA:589:VAL:HG11	2.03	0.40
15:aA:810:CLA:H72	15:aA:810:CLA:H111	1.88	0.40
2:aB:128:MET:HE3	15:aB:815:CLA:H2A	2.03	0.40
2:aB:396:PHE:O	2:aB:401:TYR:N	2.53	0.40
18:aB:844:BCR:H15C	18:aB:844:BCR:H351	1.91	0.40
5:aE:6:LYS:HB2	5:aE:69:ALA:HB2	2.04	0.40
13:a1:288:GLY:C	13:a1:315:ARG:HH12	2.29	0.40
13:a1:298:ALA:HA	15:a1:416:CLA:NB	2.36	0.40
13:a1:307:LEU:HD22	13:a1:308:PRO:HA	2.03	0.40
13:a2:312:HIS:HB2	13:a2:317:TRP:NE1	2.36	0.40
13:a2:325:LEU:O	13:a2:329:PHE:N	2.45	0.40
15:a5:420:CLA:H143	15:a5:420:CLA:H111	1.87	0.40
18:a6:419:BCR:H11C	18:a6:419:BCR:H341	1.96	0.40
1:bA:416:MET:HE1	1:bA:434:LEU:HD11	2.03	0.40
15:bA:829:CLA:H172	15:bB:803:CLA:H202	2.03	0.40
15:bA:834:CLA:HAB	15:bA:834:CLA:HHC	1.81	0.40
2:bB:122:TRP:HH2	15:bB:829:CLA:H2	1.87	0.40
10:bL:68:LEU:O	10:bL:71:SER:OG	2.39	0.40
18:b1:420:BCR:H15C	18:b1:420:BCR:H351	1.81	0.40
13:b2:334:LEU:HD11	15:b2:406:CLA:HAB	2.04	0.40
15:b2:422:CLA:HBA2	15:b2:422:CLA:H3A	1.80	0.40
13:b4:212:ILE:H	13:b4:212:ILE:HG12	1.66	0.40
13:b6:52:LEU:O	13:b6:56:TRP:N	2.44	0.40
1:cA:31:PRO:HB3	15:cA:804:CLA:HAC1	2.02	0.40
1:cA:241:GLU:OE1	1:cA:241:GLU:N	2.55	0.40
15:cA:810:CLA:H72	15:cA:810:CLA:H111	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:392:HIS:HA	2:cB:395:ILE:HD12	2.02	0.40
7:cI:1:MET:HE3	7:cI:1:MET:HB3	1.81	0.40
13:c1:221:GLY:HA3	18:c1:420:BCR:H393	2.04	0.40
13:c2:294:LYS:HG3	13:c2:300:TYR:CZ	2.56	0.40
13:c3:270:VAL:O	13:c3:274:PHE:N	2.45	0.40
13:c5:299:PRO:HG2	13:c5:323:PHE:HE2	1.86	0.40
13:c5:312:HIS:HB2	13:c5:317:TRP:NE1	2.37	0.40
18:c6:402:BCR:H11C	18:c6:402:BCR:H341	1.95	0.40
2:aB:327:GLU:O	2:aB:331:ASN:ND2	2.54	0.40
13:a2:23:ASN:HA	13:a2:24:VAL:HA	1.71	0.40
13:a2:41:LEU:HD21	15:a2:412:CLA:HBA2	2.04	0.40
13:a2:112:LEU:O	13:a2:115:SER:OG	2.28	0.40
13:a3:157:LEU:HB2	15:a3:407:CLA:HMD2	2.04	0.40
13:a4:52:LEU:O	13:a4:56:TRP:N	2.44	0.40
13:a4:183:ASP:OD2	13:a4:186:LEU:N	2.51	0.40
13:a5:66:SER:OG	13:a5:67:GLN:N	2.54	0.40
13:a5:312:HIS:HB2	13:a5:317:TRP:NE1	2.36	0.40
1:bA:70:ARG:O	1:bA:74:SER:OG	2.39	0.40
1:bA:353:HIS:HD2	1:bA:411:HIS:HD1	1.68	0.40
1:bA:416:MET:HE3	1:bA:416:MET:HB3	1.93	0.40
15:bA:834:CLA:H112	15:bA:834:CLA:H152	1.82	0.40
2:bB:718:HIS:HE1	15:bB:840:CLA:ND	2.19	0.40
15:bB:831:CLA:HBC2	18:bB:847:BCR:H292	2.03	0.40
18:bF:202:BCR:H373	15:bX:102:CLA:C4B	2.51	0.40
18:bI:102:BCR:H24C	18:bI:102:BCR:H371	1.79	0.40
10:bL:34:LEU:HD23	10:bL:34:LEU:HA	1.88	0.40
13:b2:212:ILE:H	13:b2:212:ILE:HG12	1.68	0.40
18:b3:420:BCR:H24C	18:b3:420:BCR:H371	1.93	0.40
13:b4:128:ARG:HH12	15:b4:421:CLA:HBD	1.85	0.40
15:b5:417:CLA:H2A	15:b5:417:CLA:O2D	2.22	0.40
18:b5:419:BCR:H20C	18:b5:419:BCR:H361	1.84	0.40
18:b6:401:BCR:H11C	18:b6:401:BCR:H341	1.95	0.40
1:cA:24:SER:O	15:cA:812:CLA:HHB	2.21	0.40
15:cA:807:CLA:H193	15:cA:807:CLA:H161	1.79	0.40
15:cA:839:CLA:H142	15:cA:839:CLA:H111	1.82	0.40
15:cA:842:CLA:HBA2	15:cA:842:CLA:H3A	1.77	0.40
15:cB:831:CLA:HBC2	18:cB:847:BCR:H292	2.03	0.40
15:cB:839:CLA:H72	15:cB:839:CLA:H111	1.92	0.40
13:c1:294:LYS:HG3	13:c1:300:TYR:CZ	2.57	0.40
15:c3:409:CLA:HBD	15:c3:409:CLA:H121	2.02	0.40
15:c4:416:CLA:HHC	15:c4:416:CLA:HMC1	1.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c6:270:VAL:O	13:c6:274:PHE:N	2.45	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	aA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48 69
1	bA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48 69
1	cA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48 69
2	aB	737/740 (100%)	699 (95%)	38 (5%)	0	100 100
2	bB	737/740 (100%)	699 (95%)	38 (5%)	0	100 100
2	cB	737/740 (100%)	699 (95%)	38 (5%)	0	100 100
3	aC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4 6
3	bC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4 6
3	cC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4 6
4	aD	136/138 (99%)	126 (93%)	10 (7%)	0	100 100
4	bD	136/138 (99%)	126 (93%)	10 (7%)	0	100 100
4	cD	136/138 (99%)	126 (93%)	10 (7%)	0	100 100
5	aE	67/75 (89%)	64 (96%)	3 (4%)	0	100 100
5	bE	67/75 (89%)	64 (96%)	3 (4%)	0	100 100
5	cE	67/75 (89%)	64 (96%)	3 (4%)	0	100 100
6	aF	139/164 (85%)	133 (96%)	6 (4%)	0	100 100
6	bF	139/164 (85%)	133 (96%)	6 (4%)	0	100 100
6	cF	139/164 (85%)	133 (96%)	6 (4%)	0	100 100
7	aI	36/38 (95%)	36 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	bI	36/38 (95%)	36 (100%)	0	0	100	100
7	cI	36/38 (95%)	36 (100%)	0	0	100	100
8	aJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	aK	39/85 (46%)	39 (100%)	0	0	100	100
9	bK	39/85 (46%)	39 (100%)	0	0	100	100
9	cK	39/85 (46%)	39 (100%)	0	0	100	100
10	aL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	bL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	cL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
11	aM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	bM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	cM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	aX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	bX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	cX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
13	a1	327/358 (91%)	301 (92%)	24 (7%)	2 (1%)	21	36
13	a2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	a3	330/358 (92%)	303 (92%)	24 (7%)	3 (1%)	14	26
13	a4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	a5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	a6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	b1	327/358 (91%)	299 (91%)	26 (8%)	2 (1%)	21	36
13	b2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	b3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	b4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	b5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	b6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	c1	327/358 (91%)	300 (92%)	25 (8%)	2 (1%)	21	36
13	c2	325/358 (91%)	298 (92%)	24 (7%)	3 (1%)	14	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	c3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	c4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	c5	330/358 (92%)	302 (92%)	26 (8%)	2 (1%)	21	36
13	c6	327/358 (91%)	298 (91%)	26 (8%)	3 (1%)	14	26
All	All	12561/13452 (93%)	11740 (94%)	764 (6%)	57 (0%)	26	40

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	aA	233	ALA
13	a1	283	PRO
13	a2	283	PRO
13	a3	283	PRO
13	a4	283	PRO
13	a5	283	PRO
13	a6	283	PRO
1	bA	233	ALA
13	b1	283	PRO
13	b2	283	PRO
13	b3	283	PRO
13	b4	283	PRO
13	b5	283	PRO
13	b6	283	PRO
1	cA	233	ALA
13	c1	283	PRO
13	c2	283	PRO
13	c3	283	PRO
13	c4	283	PRO
13	c5	283	PRO
13	c6	283	PRO
3	aC	61	PHE
3	bC	61	PHE
3	cC	61	PHE
3	aC	62	LEU
13	a2	292	GLU
13	a2	303	ASP
13	a3	303	ASP
13	a4	303	ASP
13	a5	303	ASP
13	a6	292	GLU
13	a6	303	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	bC	62	LEU
13	b2	292	GLU
13	b2	303	ASP
13	b3	303	ASP
13	b4	303	ASP
13	b5	303	ASP
13	b6	292	GLU
13	b6	303	ASP
3	cC	62	LEU
13	c2	292	GLU
13	c2	303	ASP
13	c4	303	ASP
13	c5	303	ASP
13	c6	292	GLU
13	c6	303	ASP
13	a1	303	ASP
13	a3	292	GLU
13	b1	303	ASP
13	c1	303	ASP
13	c3	303	ASP
13	a4	292	GLU
13	b3	292	GLU
13	b4	292	GLU
13	c3	292	GLU
13	c4	292	GLU

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	aA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	bA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	cA	592/604 (98%)	554 (94%)	38 (6%)	16	29
2	aB	595/597 (100%)	559 (94%)	36 (6%)	17	30
2	bB	595/597 (100%)	559 (94%)	36 (6%)	17	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	cB	595/597 (100%)	559 (94%)	36 (6%)	17 30
3	aC	67/67 (100%)	61 (91%)	6 (9%)	9 17
3	bC	67/67 (100%)	60 (90%)	7 (10%)	7 13
3	cC	67/67 (100%)	61 (91%)	6 (9%)	9 17
4	aD	115/115 (100%)	110 (96%)	5 (4%)	26 46
4	bD	115/115 (100%)	110 (96%)	5 (4%)	26 46
4	cD	115/115 (100%)	110 (96%)	5 (4%)	26 46
5	aE	59/64 (92%)	53 (90%)	6 (10%)	7 13
5	bE	59/64 (92%)	53 (90%)	6 (10%)	7 13
5	cE	59/64 (92%)	53 (90%)	6 (10%)	7 13
6	aF	109/128 (85%)	101 (93%)	8 (7%)	13 24
6	bF	109/128 (85%)	101 (93%)	8 (7%)	13 24
6	cF	109/128 (85%)	101 (93%)	8 (7%)	13 24
7	aI	32/32 (100%)	30 (94%)	2 (6%)	16 29
7	bI	32/32 (100%)	30 (94%)	2 (6%)	16 29
7	cI	32/32 (100%)	30 (94%)	2 (6%)	16 29
8	aJ	36/36 (100%)	32 (89%)	4 (11%)	6 11
8	bJ	36/36 (100%)	32 (89%)	4 (11%)	6 11
8	cJ	36/36 (100%)	32 (89%)	4 (11%)	6 11
10	aL	117/119 (98%)	110 (94%)	7 (6%)	17 31
10	bL	117/119 (98%)	110 (94%)	7 (6%)	17 31
10	cL	117/119 (98%)	110 (94%)	7 (6%)	17 31
11	aM	26/26 (100%)	21 (81%)	5 (19%)	1 2
11	bM	26/26 (100%)	21 (81%)	5 (19%)	1 2
11	cM	26/26 (100%)	21 (81%)	5 (19%)	1 2
12	aX	20/24 (83%)	19 (95%)	1 (5%)	22 40
12	bX	20/24 (83%)	19 (95%)	1 (5%)	22 40
12	cX	20/24 (83%)	19 (95%)	1 (5%)	22 40
13	a1	255/279 (91%)	240 (94%)	15 (6%)	18 32
13	a2	253/279 (91%)	238 (94%)	15 (6%)	18 32
13	a3	258/279 (92%)	242 (94%)	16 (6%)	16 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	a4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	a5	258/279 (92%)	241 (93%)	17 (7%)	15	28
13	a6	255/279 (91%)	239 (94%)	16 (6%)	16	29
13	b1	255/279 (91%)	240 (94%)	15 (6%)	18	32
13	b2	253/279 (91%)	238 (94%)	15 (6%)	18	32
13	b3	258/279 (92%)	243 (94%)	15 (6%)	18	33
13	b4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	b5	258/279 (92%)	241 (93%)	17 (7%)	15	28
13	b6	255/279 (91%)	239 (94%)	16 (6%)	16	29
13	c1	255/279 (91%)	240 (94%)	15 (6%)	18	32
13	c2	253/279 (91%)	239 (94%)	14 (6%)	19	35
13	c3	258/279 (92%)	242 (94%)	16 (6%)	16	30
13	c4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	c5	258/279 (92%)	240 (93%)	18 (7%)	14	26
13	c6	255/279 (91%)	240 (94%)	15 (6%)	18	32
All	All	9927/10458 (95%)	9291 (94%)	636 (6%)	18	29

All (636) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	11	LYS
1	aA	15	VAL
1	aA	43	GLN
1	aA	46	THR
1	aA	74	SER
1	aA	98	SER
1	aA	104	LEU
1	aA	115	GLN
1	aA	120	ILE
1	aA	121	VAL
1	aA	130	VAL
1	aA	171	LEU
1	aA	205	LEU
1	aA	234	LYS
1	aA	248	LEU
1	aA	249	MET
1	aA	255	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	aA	257	ASP
1	aA	277	ASP
1	aA	307	LEU
1	aA	363	MET
1	aA	365	SER
1	aA	372	GLN
1	aA	383	LEU
1	aA	390	GLN
1	aA	463	ASP
1	aA	478	THR
1	aA	511	VAL
1	aA	549	THR
1	aA	566	ILE
1	aA	628	ASP
1	aA	645	THR
1	aA	680	HIS
1	aA	692	SER
1	aA	701	ILE
1	aA	718	GLN
1	aA	753	SER
2	aB	48	SER
2	aB	63	SER
2	aB	133	ASP
2	aB	146	SER
2	aB	159	LYS
2	aB	174	LEU
2	aB	184	VAL
2	aB	194	ILE
2	aB	196	VAL
2	aB	209	ASP
2	aB	282	LEU
2	aB	308	ASP
2	aB	312	THR
2	aB	318	PHE
2	aB	357	SER
2	aB	416	GLN
2	aB	429	SER
2	aB	439	LEU
2	aB	444	ASP
2	aB	446	VAL
2	aB	453	GLU
2	aB	474	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	aB	479	THR
2	aB	481	LEU
2	aB	494	ASN
2	aB	518	ILE
2	aB	535	THR
2	aB	565	CYS
2	aB	582	PHE
2	aB	583	TYR
2	aB	646	THR
2	aB	648	ASN
2	aB	651	VAL
2	aB	681	ILE
2	aB	720	SER
2	aB	735	THR
3	aC	3	THR
3	aC	11	ILE
3	aC	44	THR
3	aC	62	LEU
3	aC	73	THR
3	aC	76	MET
4	aD	4	THR
4	aD	6	GLN
4	aD	92	VAL
4	aD	93	LEU
4	aD	126	SER
5	aE	10	LEU
5	aE	22	THR
5	aE	28	GLN
5	aE	29	THR
5	aE	51	SER
5	aE	62	LEU
6	aF	2	VAL
6	aF	6	VAL
6	aF	36	GLU
6	aF	43	CYS
6	aF	103	VAL
6	aF	104	PRO
6	aF	118	LEU
6	aF	124	LEU
7	aI	1	MET
7	aI	18	VAL
8	aJ	2	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	aJ	14	LEU
8	aJ	22	THR
8	aJ	31	ARG
10	aL	22	SER
10	aL	42	SER
10	aL	44	ILE
10	aL	59	ILE
10	aL	69	ARG
10	aL	131	SER
10	aL	148	ILE
11	aM	1	MET
11	aM	3	LEU
11	aM	5	ASP
11	aM	16	LEU
11	aM	27	THR
12	aX	8	THR
13	a1	38	LEU
13	a1	82	LEU
13	a1	88	LEU
13	a1	98	VAL
13	a1	107	ILE
13	a1	111	HIS
13	a1	186	LEU
13	a1	205	TYR
13	a1	208	HIS
13	a1	212	ILE
13	a1	234	ILE
13	a1	256	ILE
13	a1	284	VAL
13	a1	291	LEU
13	a1	304	THR
13	a2	38	LEU
13	a2	82	LEU
13	a2	88	LEU
13	a2	98	VAL
13	a2	107	ILE
13	a2	111	HIS
13	a2	113	ILE
13	a2	186	LEU
13	a2	205	TYR
13	a2	208	HIS
13	a2	223	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a2	256	ILE
13	a2	284	VAL
13	a2	291	LEU
13	a2	304	THR
13	a3	38	LEU
13	a3	82	LEU
13	a3	88	LEU
13	a3	98	VAL
13	a3	107	ILE
13	a3	111	HIS
13	a3	146	ARG
13	a3	186	LEU
13	a3	205	TYR
13	a3	208	HIS
13	a3	212	ILE
13	a3	256	ILE
13	a3	284	VAL
13	a3	291	LEU
13	a3	304	THR
13	a3	348	LEU
13	a4	38	LEU
13	a4	82	LEU
13	a4	88	LEU
13	a4	98	VAL
13	a4	107	ILE
13	a4	111	HIS
13	a4	186	LEU
13	a4	205	TYR
13	a4	208	HIS
13	a4	212	ILE
13	a4	234	ILE
13	a4	256	ILE
13	a4	284	VAL
13	a4	291	LEU
13	a4	304	THR
13	a4	348	LEU
13	a5	38	LEU
13	a5	88	LEU
13	a5	98	VAL
13	a5	107	ILE
13	a5	111	HIS
13	a5	113	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a5	146	ARG
13	a5	186	LEU
13	a5	205	TYR
13	a5	208	HIS
13	a5	212	ILE
13	a5	256	ILE
13	a5	284	VAL
13	a5	291	LEU
13	a5	295	LEU
13	a5	304	THR
13	a5	348	LEU
13	a6	38	LEU
13	a6	82	LEU
13	a6	88	LEU
13	a6	98	VAL
13	a6	107	ILE
13	a6	111	HIS
13	a6	113	ILE
13	a6	146	ARG
13	a6	186	LEU
13	a6	205	TYR
13	a6	208	HIS
13	a6	212	ILE
13	a6	256	ILE
13	a6	284	VAL
13	a6	291	LEU
13	a6	304	THR
1	bA	11	LYS
1	bA	15	VAL
1	bA	43	GLN
1	bA	46	THR
1	bA	74	SER
1	bA	98	SER
1	bA	104	LEU
1	bA	115	GLN
1	bA	120	ILE
1	bA	121	VAL
1	bA	130	VAL
1	bA	171	LEU
1	bA	205	LEU
1	bA	234	LYS
1	bA	248	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	bA	249	MET
1	bA	255	LYS
1	bA	257	ASP
1	bA	277	ASP
1	bA	307	LEU
1	bA	363	MET
1	bA	365	SER
1	bA	372	GLN
1	bA	383	LEU
1	bA	390	GLN
1	bA	463	ASP
1	bA	478	THR
1	bA	511	VAL
1	bA	549	THR
1	bA	566	ILE
1	bA	628	ASP
1	bA	645	THR
1	bA	680	HIS
1	bA	692	SER
1	bA	701	ILE
1	bA	718	GLN
1	bA	753	SER
2	bB	48	SER
2	bB	63	SER
2	bB	133	ASP
2	bB	146	SER
2	bB	159	LYS
2	bB	174	LEU
2	bB	184	VAL
2	bB	194	ILE
2	bB	196	VAL
2	bB	209	ASP
2	bB	282	LEU
2	bB	308	ASP
2	bB	312	THR
2	bB	318	PHE
2	bB	357	SER
2	bB	416	GLN
2	bB	429	SER
2	bB	439	LEU
2	bB	444	ASP
2	bB	446	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	bB	453	GLU
2	bB	474	LEU
2	bB	479	THR
2	bB	481	LEU
2	bB	494	ASN
2	bB	518	ILE
2	bB	535	THR
2	bB	565	CYS
2	bB	582	PHE
2	bB	583	TYR
2	bB	646	THR
2	bB	648	ASN
2	bB	651	VAL
2	bB	681	ILE
2	bB	720	SER
2	bB	735	THR
3	bC	3	THR
3	bC	11	ILE
3	bC	25	LEU
3	bC	44	THR
3	bC	62	LEU
3	bC	73	THR
3	bC	76	MET
4	bD	4	THR
4	bD	6	GLN
4	bD	92	VAL
4	bD	93	LEU
4	bD	126	SER
5	bE	10	LEU
5	bE	22	THR
5	bE	28	GLN
5	bE	29	THR
5	bE	51	SER
5	bE	62	LEU
6	bF	2	VAL
6	bF	6	VAL
6	bF	36	GLU
6	bF	43	CYS
6	bF	103	VAL
6	bF	104	PRO
6	bF	118	LEU
6	bF	124	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	bI	1	MET
7	bI	18	VAL
8	bJ	2	LYS
8	bJ	14	LEU
8	bJ	22	THR
8	bJ	31	ARG
10	bL	22	SER
10	bL	42	SER
10	bL	44	ILE
10	bL	59	ILE
10	bL	69	ARG
10	bL	131	SER
10	bL	148	ILE
11	bM	1	MET
11	bM	3	LEU
11	bM	5	ASP
11	bM	16	LEU
11	bM	27	THR
12	bX	8	THR
13	b1	38	LEU
13	b1	82	LEU
13	b1	88	LEU
13	b1	98	VAL
13	b1	107	ILE
13	b1	111	HIS
13	b1	113	ILE
13	b1	186	LEU
13	b1	205	TYR
13	b1	208	HIS
13	b1	212	ILE
13	b1	256	ILE
13	b1	284	VAL
13	b1	291	LEU
13	b1	304	THR
13	b2	38	LEU
13	b2	82	LEU
13	b2	88	LEU
13	b2	98	VAL
13	b2	107	ILE
13	b2	111	HIS
13	b2	113	ILE
13	b2	186	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	b2	205	TYR
13	b2	208	HIS
13	b2	223	ILE
13	b2	256	ILE
13	b2	284	VAL
13	b2	291	LEU
13	b2	304	THR
13	b3	38	LEU
13	b3	82	LEU
13	b3	88	LEU
13	b3	98	VAL
13	b3	107	ILE
13	b3	111	HIS
13	b3	186	LEU
13	b3	205	TYR
13	b3	208	HIS
13	b3	212	ILE
13	b3	256	ILE
13	b3	284	VAL
13	b3	291	LEU
13	b3	304	THR
13	b3	348	LEU
13	b4	38	LEU
13	b4	82	LEU
13	b4	88	LEU
13	b4	98	VAL
13	b4	107	ILE
13	b4	111	HIS
13	b4	186	LEU
13	b4	205	TYR
13	b4	208	HIS
13	b4	212	ILE
13	b4	234	ILE
13	b4	256	ILE
13	b4	284	VAL
13	b4	291	LEU
13	b4	304	THR
13	b4	348	LEU
13	b5	38	LEU
13	b5	88	LEU
13	b5	98	VAL
13	b5	107	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	b5	111	HIS
13	b5	113	ILE
13	b5	146	ARG
13	b5	186	LEU
13	b5	205	TYR
13	b5	208	HIS
13	b5	212	ILE
13	b5	256	ILE
13	b5	284	VAL
13	b5	291	LEU
13	b5	295	LEU
13	b5	304	THR
13	b5	348	LEU
13	b6	38	LEU
13	b6	82	LEU
13	b6	88	LEU
13	b6	98	VAL
13	b6	107	ILE
13	b6	111	HIS
13	b6	113	ILE
13	b6	146	ARG
13	b6	186	LEU
13	b6	205	TYR
13	b6	208	HIS
13	b6	212	ILE
13	b6	256	ILE
13	b6	284	VAL
13	b6	291	LEU
13	b6	304	THR
1	cA	11	LYS
1	cA	12	VAL
1	cA	15	VAL
1	cA	43	GLN
1	cA	46	THR
1	cA	74	SER
1	cA	98	SER
1	cA	104	LEU
1	cA	115	GLN
1	cA	120	ILE
1	cA	121	VAL
1	cA	130	VAL
1	cA	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	cA	205	LEU
1	cA	234	LYS
1	cA	248	LEU
1	cA	249	MET
1	cA	255	LYS
1	cA	257	ASP
1	cA	277	ASP
1	cA	307	LEU
1	cA	363	MET
1	cA	365	SER
1	cA	372	GLN
1	cA	383	LEU
1	cA	390	GLN
1	cA	463	ASP
1	cA	478	THR
1	cA	511	VAL
1	cA	549	THR
1	cA	566	ILE
1	cA	628	ASP
1	cA	645	THR
1	cA	680	HIS
1	cA	692	SER
1	cA	701	ILE
1	cA	718	GLN
1	cA	753	SER
2	cB	48	SER
2	cB	63	SER
2	cB	133	ASP
2	cB	146	SER
2	cB	159	LYS
2	cB	174	LEU
2	cB	184	VAL
2	cB	194	ILE
2	cB	196	VAL
2	cB	209	ASP
2	cB	282	LEU
2	cB	308	ASP
2	cB	312	THR
2	cB	318	PHE
2	cB	357	SER
2	cB	416	GLN
2	cB	429	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	cB	439	LEU
2	cB	444	ASP
2	cB	446	VAL
2	cB	453	GLU
2	cB	474	LEU
2	cB	479	THR
2	cB	481	LEU
2	cB	494	ASN
2	cB	518	ILE
2	cB	535	THR
2	cB	565	CYS
2	cB	582	PHE
2	cB	583	TYR
2	cB	646	THR
2	cB	648	ASN
2	cB	651	VAL
2	cB	681	ILE
2	cB	720	SER
2	cB	735	THR
3	cC	3	THR
3	cC	11	ILE
3	cC	44	THR
3	cC	62	LEU
3	cC	73	THR
3	cC	76	MET
4	cD	4	THR
4	cD	6	GLN
4	cD	92	VAL
4	cD	93	LEU
4	cD	126	SER
5	cE	10	LEU
5	cE	22	THR
5	cE	28	GLN
5	cE	29	THR
5	cE	51	SER
5	cE	62	LEU
6	cF	2	VAL
6	cF	6	VAL
6	cF	36	GLU
6	cF	43	CYS
6	cF	103	VAL
6	cF	104	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	cF	118	LEU
6	cF	124	LEU
7	cI	1	MET
7	cI	18	VAL
8	cJ	2	LYS
8	cJ	14	LEU
8	cJ	22	THR
8	cJ	31	ARG
10	cL	22	SER
10	cL	42	SER
10	cL	44	ILE
10	cL	59	ILE
10	cL	69	ARG
10	cL	131	SER
10	cL	148	ILE
11	cM	1	MET
11	cM	3	LEU
11	cM	5	ASP
11	cM	16	LEU
11	cM	27	THR
12	cX	8	THR
13	c1	38	LEU
13	c1	82	LEU
13	c1	88	LEU
13	c1	98	VAL
13	c1	107	ILE
13	c1	111	HIS
13	c1	186	LEU
13	c1	205	TYR
13	c1	208	HIS
13	c1	212	ILE
13	c1	234	ILE
13	c1	256	ILE
13	c1	284	VAL
13	c1	291	LEU
13	c1	304	THR
13	c2	38	LEU
13	c2	82	LEU
13	c2	88	LEU
13	c2	98	VAL
13	c2	107	ILE
13	c2	111	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c2	113	ILE
13	c2	186	LEU
13	c2	205	TYR
13	c2	208	HIS
13	c2	256	ILE
13	c2	284	VAL
13	c2	291	LEU
13	c2	304	THR
13	c3	38	LEU
13	c3	82	LEU
13	c3	88	LEU
13	c3	98	VAL
13	c3	107	ILE
13	c3	111	HIS
13	c3	146	ARG
13	c3	186	LEU
13	c3	205	TYR
13	c3	208	HIS
13	c3	212	ILE
13	c3	256	ILE
13	c3	284	VAL
13	c3	291	LEU
13	c3	304	THR
13	c3	348	LEU
13	c4	38	LEU
13	c4	82	LEU
13	c4	88	LEU
13	c4	98	VAL
13	c4	107	ILE
13	c4	111	HIS
13	c4	186	LEU
13	c4	205	TYR
13	c4	208	HIS
13	c4	212	ILE
13	c4	234	ILE
13	c4	256	ILE
13	c4	284	VAL
13	c4	291	LEU
13	c4	304	THR
13	c4	348	LEU
13	c5	38	LEU
13	c5	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	c5	88	LEU
13	c5	98	VAL
13	c5	107	ILE
13	c5	111	HIS
13	c5	113	ILE
13	c5	146	ARG
13	c5	186	LEU
13	c5	205	TYR
13	c5	208	HIS
13	c5	212	ILE
13	c5	256	ILE
13	c5	284	VAL
13	c5	291	LEU
13	c5	295	LEU
13	c5	304	THR
13	c5	348	LEU
13	c6	38	LEU
13	c6	82	LEU
13	c6	88	LEU
13	c6	98	VAL
13	c6	107	ILE
13	c6	111	HIS
13	c6	146	ARG
13	c6	186	LEU
13	c6	205	TYR
13	c6	208	HIS
13	c6	212	ILE
13	c6	256	ILE
13	c6	284	VAL
13	c6	291	LEU
13	c6	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	192	ASN
1	aA	216	GLN
1	aA	286	ASN
1	aA	353	HIS
1	aA	359	ASN
1	aA	372	GLN
1	aA	483	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	aA	542	HIS
2	aB	33	HIS
2	aB	234	GLN
2	aB	235	ASN
2	aB	247	GLN
2	aB	261	HIS
2	aB	330	ASN
2	aB	406	ASN
2	aB	455	GLN
2	aB	494	ASN
2	aB	611	ASN
2	aB	614	GLN
2	aB	616	ASN
2	aB	639	ASN
2	aB	678	GLN
2	aB	688	HIS
2	aB	710	GLN
4	aD	54	ASN
4	aD	70	GLN
4	aD	71	GLN
5	aE	18	ASN
6	aF	23	ASN
6	aF	50	HIS
10	aL	16	HIS
13	a1	187	GLN
13	a1	320	ASN
13	a2	131	HIS
13	a2	320	ASN
13	a3	320	ASN
13	a4	131	HIS
13	a4	320	ASN
13	a5	320	ASN
13	a6	320	ASN
1	bA	192	ASN
1	bA	216	GLN
1	bA	286	ASN
1	bA	353	HIS
1	bA	359	ASN
1	bA	372	GLN
1	bA	483	GLN
1	bA	542	HIS
2	bB	33	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	bB	234	GLN
2	bB	235	ASN
2	bB	261	HIS
2	bB	330	ASN
2	bB	406	ASN
2	bB	455	GLN
2	bB	494	ASN
2	bB	611	ASN
2	bB	614	GLN
2	bB	616	ASN
2	bB	639	ASN
2	bB	678	GLN
2	bB	688	HIS
4	bD	54	ASN
4	bD	70	GLN
4	bD	71	GLN
5	bE	18	ASN
6	bF	95	ASN
10	bL	16	HIS
13	b1	320	ASN
13	b2	320	ASN
13	b3	320	ASN
13	b4	320	ASN
13	b5	320	ASN
13	b6	320	ASN
1	cA	192	ASN
1	cA	216	GLN
1	cA	286	ASN
1	cA	353	HIS
1	cA	359	ASN
1	cA	372	GLN
1	cA	483	GLN
1	cA	542	HIS
2	cB	33	HIS
2	cB	234	GLN
2	cB	235	ASN
2	cB	247	GLN
2	cB	261	HIS
2	cB	330	ASN
2	cB	406	ASN
2	cB	455	GLN
2	cB	494	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	cB	611	ASN
2	cB	614	GLN
2	cB	616	ASN
2	cB	639	ASN
2	cB	678	GLN
2	cB	688	HIS
2	cB	710	GLN
4	cD	54	ASN
4	cD	70	GLN
4	cD	71	GLN
5	cE	18	ASN
10	cL	16	HIS
13	c1	320	ASN
13	c2	320	ASN
13	c3	320	ASN
13	c4	131	HIS
13	c4	320	ASN
13	c5	320	ASN
13	c6	320	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 759 ligands modelled in this entry, 3 are monoatomic - leaving 756 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLA	cA	818	1	58,62,73	1.33	10 (17%)	69,99,113	1.60	9 (13%)
15	CLA	a4	407	-	49,53,73	1.47	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	c4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	b1	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.66	9 (15%)
16	PQN	aA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	c3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	a3	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	CLA	c2	405	-	49,53,73	1.58	9 (18%)	59,89,113	1.94	19 (32%)
15	CLA	c2	414	13	49,53,73	1.52	10 (20%)	59,89,113	1.52	6 (10%)
15	CLA	bA	838	1	55,59,73	1.46	10 (18%)	66,96,113	1.69	12 (18%)
15	CLA	aA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	a6	415	13	45,49,73	1.52	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	bA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
16	PQN	cB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
18	BCR	b3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	a3	413	13	49,53,73	1.51	11 (22%)	59,89,113	1.50	6 (10%)
15	CLA	aA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
15	CLA	bB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	b2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	cA	831	1	69,73,73	1.37	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	cB	835	2	49,53,73	1.42	9 (18%)	59,89,113	1.72	6 (10%)
19	LHG	bX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a6	411	13	68,72,73	1.32	11 (16%)	81,111,113	1.57	15 (18%)
15	CLA	cB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	a2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.47	7 (11%)
15	CLA	a6	414	13	49,53,73	1.50	12 (24%)	59,89,113	1.68	10 (16%)
15	CLA	cA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	bA	842	22	55,59,73	1.41	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	bA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	b5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	16 (22%)
15	CLA	a1	413	13	45,49,73	1.49	9 (20%)	54,84,113	1.58	7 (12%)
15	CLA	c2	415	13	45,49,73	1.51	7 (15%)	54,84,113	1.60	5 (9%)
17	SF4	aC	101	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c2	413	13	49,53,73	1.58	10 (20%)	59,89,113	1.63	15 (25%)
15	CLA	aA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	bB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)
15	CLA	c5	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
15	CLA	c5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	a6	412	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	11 (18%)
15	CLA	b6	414	13	49,53,73	1.53	10 (20%)	59,89,113	1.69	10 (16%)
15	CLA	aB	836	2	64,68,73	1.37	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	bA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
15	CLA	cA	810	1	69,73,73	1.25	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	c2	411	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	a4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.68	16 (19%)
18	BCR	a3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
15	CLA	b2	402	13	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
15	CLA	aB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	b5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.37	6 (7%)
18	BCR	b1	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	8 (14%)
15	CLA	aA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.58	11 (13%)
15	CLA	aB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	cB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	aA	818	1	58,62,73	1.34	10 (17%)	69,99,113	1.62	8 (11%)
15	CLA	b5	403	13	69,73,73	1.22	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	b2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.61	5 (9%)
18	BCR	c1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.65	12 (21%)
15	CLA	b5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	a3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	18 (25%)
15	CLA	bB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.50	8 (11%)
15	CLA	bB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	aA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.68	12 (18%)
15	CLA	aJ	203	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
18	BCR	b4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	b2	417	-	54,58,73	1.57	11 (20%)	65,95,113	2.32	18 (27%)
15	CLA	bB	817	2	59,63,73	1.36	8 (13%)	71,101,113	1.63	14 (19%)
15	CLA	a2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	b2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	cA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.48	10 (12%)
15	CLA	aB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)
15	CLA	aL	202	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
15	CLA	a4	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.95	16 (22%)
15	CLA	cL	202	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
18	BCR	b3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
19	LHG	aA	854	15	26,26,48	0.97	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	bA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	a5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	cF	201	22	55,59,73	1.42	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	aA	842	22	55,59,73	1.41	9 (16%)	66,96,113	1.33	8 (12%)
15	CLA	aB	816	2	49,53,73	1.40	10 (20%)	59,89,113	1.73	7 (11%)
15	CLA	a5	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.94	15 (21%)
15	CLA	c1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	17 (23%)
18	BCR	aB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
15	CLA	aB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.77	15 (18%)
18	BCR	aB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	bB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
15	CLA	bA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	b3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
18	BCR	c2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.84	11 (19%)
15	CLA	a3	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	11 (18%)
15	CLA	b3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.52	5 (8%)
15	CLA	c6	401	13	69,73,73	1.42	14 (20%)	83,113,113	1.98	20 (24%)
18	BCR	c1	401	-	41,41,41	1.16	3 (7%)	56,56,56	1.54	9 (16%)
15	CLA	a4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	cA	820	1	69,73,73	1.30	10 (14%)	83,113,113	1.51	11 (13%)
15	CLA	cB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	c2	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.93	15 (21%)
15	CLA	cA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.36	9 (10%)
15	CLA	b2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
15	CLA	c1	405	-	49,53,73	1.55	9 (18%)	59,89,113	1.91	19 (32%)
15	CLA	c1	409	13	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.83	11 (18%)
18	BCR	a6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	b2	401	-	41,41,41	1.24	4 (9%)	56,56,56	1.82	12 (21%)
18	BCR	b3	418	-	41,41,41	1.43	5 (12%)	56,56,56	1.55	10 (17%)
18	BCR	b4	420	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	aA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
18	BCR	a6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	a3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.64	10 (16%)
15	CLA	a2	414	13	49,53,73	1.51	9 (18%)	59,89,113	1.52	5 (8%)
15	CLA	bA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
19	LHG	aA	853	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	b3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	bB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	bB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	10 (12%)
15	CLA	a6	406	-	49,53,73	1.57	8 (16%)	59,89,113	1.92	19 (32%)
15	CLA	b3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.63	6 (11%)
18	BCR	a1	419	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
19	LHG	cA	852	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
18	BCR	a3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.67	9 (16%)
15	CLA	cA	832	1	54,58,73	1.36	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	c6	416	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	bA	821	1	65,69,73	1.30	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	aB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)
15	CLA	c2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	c2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	c6	408	13	49,53,73	1.45	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	b6	406	-	49,53,73	1.58	8 (16%)	59,89,113	1.92	19 (32%)
15	CLA	b4	415	13	49,53,73	1.48	9 (18%)	59,89,113	1.86	13 (22%)
19	LHG	bA	855	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	bB	836	2	64,68,73	1.38	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	bB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.52	9 (14%)
15	CLA	bB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.51	14 (16%)
15	CLA	a2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.60	5 (9%)
15	CLA	c2	408	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	10 (16%)
15	CLA	a4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	cA	851	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	cB	827	2	69,73,73	1.29	10 (14%)	83,113,113	1.55	14 (16%)
15	CLA	bA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	aL	203	22	69,73,73	1.31	9 (13%)	83,113,113	1.32	9 (10%)
15	CLA	aA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
15	CLA	a2	417	-	54,58,73	1.57	11 (20%)	65,95,113	2.36	20 (30%)
18	BCR	a1	418	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	bB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
17	SF4	aC	102	3	0,12,12	-	-	-		
15	CLA	b5	413	13	49,53,73	1.50	10 (20%)	59,89,113	1.49	5 (8%)
17	SF4	cA	846	1,2	0,12,12	-	-	-		
18	BCR	c2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	bJ	101	8	49,53,73	1.46	12 (24%)	59,89,113	1.66	7 (11%)
15	CLA	c4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	cA	840	1	51,55,73	1.53	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	b6	407	13	49,53,73	1.46	9 (18%)	59,89,113	1.49	7 (11%)
18	BCR	a4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	cA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
18	BCR	b5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	10 (17%)
18	BCR	c4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.49	10 (17%)
15	CLA	c5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	aA	812	1	69,73,73	1.26	11 (15%)	83,113,113	1.35	9 (10%)
15	CLA	c5	413	13	49,53,73	1.50	11 (22%)	59,89,113	1.51	5 (8%)
14	CL0	aA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	aB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	11 (13%)
15	CLA	aA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	18 (26%)
18	BCR	b3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	10 (17%)
15	CLA	bL	204	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
15	CLA	cA	807	1	69,73,73	1.36	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	bB	840	2	69,73,73	1.31	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	bB	811	2	69,73,73	1.29	10 (14%)	83,113,113	1.70	12 (14%)
15	CLA	cL	204	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
18	BCR	bA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	cA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	c5	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.65	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.27	17 (26%)
17	SF4	bA	847	1,2	0,12,12	-	-	-		
18	BCR	a6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	c6	413	13	49,53,73	1.49	10 (20%)	59,89,113	1.64	11 (18%)
15	CLA	aA	809	1	69,73,73	1.24	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	b4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	c2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
18	BCR	bA	852	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	cB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
15	CLA	cA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.56	11 (13%)
15	CLA	c6	411	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	9 (10%)
15	CLA	aA	816	1	49,53,73	1.46	11 (22%)	59,89,113	1.65	6 (10%)
15	CLA	c2	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.39	9 (10%)
15	CLA	c5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	7 (12%)
15	CLA	aB	818	2	63,67,73	1.30	10 (15%)	75,105,113	1.48	13 (17%)
18	BCR	a2	401	-	41,41,41	1.26	4 (9%)	56,56,56	1.83	12 (21%)
15	CLA	a1	410	13	49,53,73	1.49	11 (22%)	59,89,113	1.65	8 (13%)
18	BCR	b6	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	8 (14%)
15	CLA	c3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.92	18 (25%)
15	CLA	b1	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	b4	403	13	69,73,73	1.22	8 (11%)	83,113,113	1.40	8 (9%)
15	CLA	bA	844	-	46,49,73	1.47	9 (19%)	55,83,113	1.59	5 (9%)
15	CLA	bB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.49	9 (12%)
19	LHG	bA	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	bJ	102	8	42,45,73	1.51	11 (26%)	50,78,113	1.64	5 (10%)
15	CLA	b6	422	13	69,73,73	1.45	13 (18%)	83,113,113	2.00	20 (24%)
15	CLA	c6	418	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
18	BCR	b6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
15	CLA	a3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
15	CLA	cA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.69	12 (18%)
15	CLA	a3	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	10 (16%)
18	BCR	c6	421	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	c3	402	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
15	CLA	bB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.64	8 (13%)
18	BCR	cM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	bB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	b6	412	13	49,53,73	1.48	10 (20%)	59,89,113	1.64	11 (18%)
15	CLA	bA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.69	8 (12%)
18	BCR	c6	402	-	41,41,41	1.18	4 (9%)	56,56,56	1.53	11 (19%)
15	CLA	c4	414	13	45,49,73	1.53	9 (20%)	54,84,113	1.59	5 (9%)
15	CLA	aB	819	2	64,68,73	1.30	11 (17%)	77,107,113	1.60	10 (12%)
18	BCR	a1	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.59	9 (16%)
15	CLA	cB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	aB	839	22	69,73,73	1.24	11 (15%)	83,113,113	1.42	9 (10%)
18	BCR	bJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	c6	405	13	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
18	BCR	aJ	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	bA	834	1	69,73,73	1.34	12 (17%)	83,113,113	1.56	11 (13%)
15	CLA	a6	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.91	14 (19%)
15	CLA	bB	842	-	49,53,73	1.47	7 (14%)	59,89,113	1.40	3 (5%)
15	CLA	cB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)
15	CLA	c6	414	13	49,53,73	1.56	10 (20%)	59,89,113	1.60	14 (23%)
15	CLA	bB	826	22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
15	CLA	aA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
15	CLA	bA	818	1	58,62,73	1.34	11 (18%)	69,99,113	1.61	9 (13%)
15	CLA	c5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.85	17 (20%)
15	CLA	cA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
15	CLA	c1	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	5 (8%)
15	CLA	aA	821	1	65,69,73	1.32	12 (18%)	78,108,113	1.41	7 (8%)
18	BCR	cF	202	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	9 (16%)
15	CLA	cB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.56	5 (8%)
18	BCR	b6	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	c5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.53	12 (21%)
15	CLA	cA	835	1	69,73,73	1.27	9 (13%)	83,113,113	1.55	10 (12%)
18	BCR	bJ	105	-	41,41,41	1.20	5 (12%)	56,56,56	1.35	9 (16%)
15	CLA	a5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)
15	CLA	cA	803	-	69,73,73	1.28	12 (17%)	83,113,113	1.74	15 (18%)
18	BCR	cI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.28	5 (8%)
15	CLA	aB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.52	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
18	BCR	c1	418	-	41,41,41	1.37	5 (12%)	56,56,56	1.54	11 (19%)
14	CL0	cA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	bB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	b4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	b5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.50	8 (13%)
15	CLA	b4	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.60	14 (17%)
18	BCR	b6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	b3	403	13	69,73,73	1.21	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	a3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.62	6 (11%)
15	CLA	bB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
18	BCR	c1	420	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	aB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
18	BCR	bB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	9 (16%)
15	CLA	c3	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.37	7 (8%)
18	BCR	a3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	9 (16%)
15	CLA	a4	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.40	9 (10%)
15	CLA	bB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	12 (20%)
15	CLA	aB	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.56	14 (16%)
15	CLA	a5	415	13	49,53,73	1.49	10 (20%)	59,89,113	1.85	12 (20%)
15	CLA	aB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	a5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
15	CLA	b5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)
18	BCR	aF	203	-	41,41,41	1.20	4 (9%)	56,56,56	1.35	9 (16%)
15	CLA	b5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	6 (11%)
15	CLA	cA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	b4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.69	16 (19%)
15	CLA	cB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.63	8 (13%)
15	CLA	c5	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	a5	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.65	10 (16%)
15	CLA	c3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.50	6 (10%)
18	BCR	cB	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
15	CLA	bB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	12 (14%)
15	CLA	bA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	10 (12%)
18	BCR	aL	205	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c1	415	13	49,53,73	1.47	9 (18%)	59,89,113	1.83	11 (18%)
15	CLA	c3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
18	BCR	c4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
19	LHG	cX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
18	BCR	cB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	9 (16%)
18	BCR	c3	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.54	10 (17%)
15	CLA	a2	411	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
14	CL0	bA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	a1	409	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
15	CLA	bA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	17 (25%)
15	CLA	b6	410	13	69,73,73	1.25	9 (13%)	83,113,113	1.33	9 (10%)
15	CLA	cB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	a5	414	13	45,49,73	1.49	9 (20%)	54,84,113	1.62	7 (12%)
15	CLA	c3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.62	14 (17%)
15	CLA	aA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	bB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.55	9 (10%)
15	CLA	aB	802	2	69,73,73	1.37	10 (14%)	83,113,113	1.51	9 (10%)
15	CLA	a1	414	13	49,53,73	1.48	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	aJ	202	8	49,53,73	1.45	12 (24%)	59,89,113	1.65	7 (11%)
15	CLA	a2	405	-	49,53,73	1.58	8 (16%)	59,89,113	1.95	19 (32%)
15	CLA	b2	411	13	68,72,73	1.30	11 (16%)	81,111,113	1.58	15 (18%)
18	BCR	bB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	bA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	9 (13%)
18	BCR	c4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	b1	414	13	45,49,73	1.51	9 (20%)	54,84,113	1.57	8 (14%)
15	CLA	c5	412	13	49,53,73	1.55	9 (18%)	59,89,113	1.62	14 (23%)
15	CLA	bB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	bA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
18	BCR	a2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	bA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	cA	823	1	53,57,73	1.39	9 (16%)	62,93,113	1.47	6 (9%)
15	CLA	b3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.61	12 (20%)
15	CLA	a2	416	13	49,53,73	1.48	9 (18%)	59,89,113	1.81	11 (18%)
18	BCR	bB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	a6	417	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
18	BCR	cA	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
20	LMG	bB	851	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
18	BCR	bA	853	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	6 (10%)
15	CLA	bA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	a4	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	b6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.55	9 (15%)
15	CLA	c2	412	13	49,53,73	1.51	11 (22%)	59,89,113	1.66	10 (16%)
15	CLA	cA	842	1	69,73,73	1.32	10 (14%)	83,113,113	1.51	8 (9%)
15	CLA	cA	805	1	63,67,73	1.34	11 (17%)	75,105,113	1.53	11 (14%)
15	CLA	c5	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.37	9 (10%)
15	CLA	aA	807	1	69,73,73	1.35	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	c5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	10 (16%)
20	LMG	cB	850	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	b1	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.43	4 (6%)
15	CLA	bB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.74	7 (11%)
15	CLA	b6	417	-	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
18	BCR	cF	204	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	b1	405	-	49,53,73	1.55	8 (16%)	59,89,113	1.91	20 (33%)
15	CLA	c1	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	c5	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.63	15 (18%)
15	CLA	c2	417	-	54,58,73	1.58	11 (20%)	65,95,113	2.35	19 (29%)
15	CLA	c6	404	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
15	CLA	aA	823	1	53,57,73	1.40	9 (16%)	62,93,113	1.46	6 (9%)
15	CLA	cB	836	2	64,68,73	1.38	10 (15%)	77,107,113	1.49	10 (12%)
15	CLA	c6	410	13	49,53,73	1.46	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	a6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.82	11 (18%)
18	BCR	b4	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.56	9 (16%)
19	LHG	cA	853	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	a4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.58	8 (13%)
15	CLA	a3	416	-	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	c6	419	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	14 (19%)
18	BCR	cF	205	-	41,41,41	1.21	5 (12%)	56,56,56	1.34	8 (14%)
18	BCR	a2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.44	8 (14%)
15	CLA	a1	401	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c1	403	13	69,73,73	1.24	9 (13%)	83,113,113	1.43	10 (12%)
18	BCR	a5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	11 (19%)
15	CLA	bA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)
15	CLA	c3	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.63	6 (11%)
15	CLA	aA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	10 (12%)
15	CLA	a4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	aB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	c4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
15	CLA	cA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.50	11 (13%)
15	CLA	a1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	bL	203	10	69,73,73	1.26	10 (14%)	83,113,113	1.60	11 (13%)
15	CLA	c5	407	-	49,53,73	1.46	8 (16%)	59,89,113	1.54	9 (15%)
15	CLA	c3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.61	15 (18%)
18	BCR	cL	205	-	41,41,41	1.30	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	b3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	cA	821	1	65,69,73	1.31	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	b6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
15	CLA	cA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
18	BCR	aB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	b1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
15	CLA	bA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
15	CLA	b5	408	13	49,53,73	1.45	11 (22%)	59,89,113	1.62	9 (15%)
18	BCR	aB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	aB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	a5	403	13	69,73,73	1.23	10 (14%)	83,113,113	1.42	10 (12%)
15	CLA	b6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.38	9 (10%)
15	CLA	aA	814	1	64,68,73	1.36	11 (17%)	77,107,113	1.38	7 (9%)
15	CLA	b2	406	13	69,73,73	1.41	12 (17%)	83,113,113	1.89	21 (25%)
15	CLA	b6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	bB	821	2	51,55,73	1.45	11 (21%)	61,91,113	1.46	4 (6%)
18	BCR	c6	420	-	41,41,41	1.36	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	c3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)
18	BCR	a1	417	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	8 (14%)
15	CLA	bA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	cB	803	-	69,73,73	1.31	8 (11%)	83,113,113	1.51	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aB	821	2	51,55,73	1.46	11 (21%)	61,91,113	1.48	4 (6%)
15	CLA	b4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.49	5 (8%)
15	CLA	c6	409	-	49,53,73	1.46	9 (18%)	59,89,113	1.52	8 (13%)
16	PQN	bB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
18	BCR	bI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	cJ	101	8	49,53,73	1.46	11 (22%)	59,89,113	1.64	7 (11%)
15	CLA	aA	805	1	63,67,73	1.33	10 (15%)	75,105,113	1.54	11 (14%)
15	CLA	aA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
18	BCR	bI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	a5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.51	8 (13%)
15	CLA	b2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
15	CLA	c3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	bB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	c4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.59	8 (13%)
18	BCR	aA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
18	BCR	a6	402	-	41,41,41	1.24	4 (9%)	56,56,56	1.71	10 (17%)
18	BCR	b1	401	-	41,41,41	1.16	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	bA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	11 (13%)
15	CLA	c2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.58	9 (15%)
17	SF4	aA	847	1,2	0,12,12	-	-	-		
15	CLA	aB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	bA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	b6	413	13	49,53,73	1.55	10 (20%)	59,89,113	1.59	14 (23%)
15	CLA	a6	413	13	49,53,73	1.56	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	c4	405	-	49,53,73	1.55	11 (22%)	59,89,113	1.96	21 (35%)
18	BCR	aA	852	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
15	CLA	cA	844	19	56,60,73	1.41	12 (21%)	67,97,113	2.01	17 (25%)
15	CLA	c1	410	13	68,72,73	1.29	11 (16%)	81,111,113	1.60	15 (18%)
15	CLA	cK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
18	BCR	bA	849	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	b2	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.39	9 (10%)
18	BCR	a4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	bA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	aA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	cA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	bB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.49	9 (10%)
15	CLA	b1	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.79	11 (18%)
15	CLA	a5	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.55	10 (16%)
15	CLA	b6	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	cB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	aA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
15	CLA	bB	823	-	59,63,73	1.30	10 (16%)	71,101,113	1.51	7 (9%)
15	CLA	b3	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.63	10 (16%)
15	CLA	b2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	a2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
18	BCR	aA	848	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	a6	422	13	69,73,73	1.50	15 (21%)	83,113,113	2.17	21 (25%)
15	CLA	b5	407	-	49,53,73	1.45	8 (16%)	59,89,113	1.55	10 (16%)
15	CLA	a2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	8 (9%)
15	CLA	cF	203	-	49,53,73	1.51	10 (20%)	59,89,113	1.67	11 (18%)
18	BCR	bB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	c1	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.59	8 (13%)
15	CLA	a4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.35	8 (9%)
15	CLA	c4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.33	10 (12%)
18	BCR	bF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	b2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
15	CLA	b4	406	13	49,53,73	1.44	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	cA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	cB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.53	9 (10%)
15	CLA	cB	834	2	62,66,73	1.31	11 (17%)	74,104,113	1.48	9 (12%)
18	BCR	cK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
18	BCR	bJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	aA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)
15	CLA	cA	814	1	64,68,73	1.35	10 (15%)	77,107,113	1.38	7 (9%)
15	CLA	bA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
15	CLA	b2	405	-	49,53,73	1.59	8 (16%)	59,89,113	1.94	19 (32%)
15	CLA	bA	823	1	53,57,73	1.41	10 (18%)	62,93,113	1.46	6 (9%)
15	CLA	aA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	a4	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	b2	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.55	9 (16%)
15	CLA	b5	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.66	10 (16%)
15	CLA	a6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.62	8 (13%)
15	CLA	bA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.65	6 (10%)
15	CLA	a1	415	-	54,58,73	1.54	11 (20%)	65,95,113	2.28	18 (27%)
18	BCR	bL	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	b4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	a6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
18	BCR	b5	419	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	aB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	aX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	12 (20%)
15	CLA	a5	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
18	BCR	c2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.52	9 (16%)
18	BCR	c3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	cA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.49	12 (14%)
15	CLA	bB	827	2	69,73,73	1.29	11 (15%)	83,113,113	1.55	14 (16%)
15	CLA	a1	411	13	49,53,73	1.56	11 (22%)	59,89,113	1.70	14 (23%)
15	CLA	cA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.48	10 (15%)
15	CLA	cB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
18	BCR	a3	418	-	41,41,41	1.44	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	c5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.94	15 (21%)
15	CLA	aA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
15	CLA	a2	413	13	49,53,73	1.57	11 (22%)	59,89,113	1.65	15 (25%)
15	CLA	a1	406	-	49,53,73	1.46	9 (18%)	59,89,113	1.57	9 (15%)
18	BCR	aI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	b4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	7 (8%)
15	CLA	b3	402	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
15	CLA	c3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.60	10 (16%)
15	CLA	a2	409	13	49,53,73	1.44	9 (18%)	59,89,113	1.57	8 (13%)
18	BCR	aA	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	a4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.37	8 (9%)
15	CLA	bA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.37	7 (8%)
15	CLA	cA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	cX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	11 (18%)
15	CLA	a2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	aB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	b5	405	-	49,53,73	1.54	10 (20%)	59,89,113	1.97	22 (37%)
15	CLA	b2	414	13	49,53,73	1.52	9 (18%)	59,89,113	1.53	6 (10%)
15	CLA	b1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	c5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.36	6 (7%)
15	CLA	c5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
18	BCR	a1	420	-	41,41,41	1.14	3 (7%)	56,56,56	1.51	10 (17%)
20	LMG	aB	850	-	55,55,55	1.07	4 (7%)	63,63,63	1.62	8 (12%)
15	CLA	bA	836	1	58,62,73	1.34	10 (17%)	69,99,113	1.40	6 (8%)
15	CLA	aA	844	-	46,49,73	1.46	8 (17%)	55,83,113	1.60	4 (7%)
15	CLA	b6	415	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	a2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	bA	803	-	69,73,73	1.28	13 (18%)	83,113,113	1.74	15 (18%)
15	CLA	aB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.59	7 (11%)
15	CLA	a4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	b4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	cA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	aB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.53	8 (12%)
15	CLA	b6	411	13	68,72,73	1.31	12 (17%)	81,111,113	1.57	15 (18%)
18	BCR	a2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	b3	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.62	14 (23%)
15	CLA	c1	411	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	aA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	10 (14%)
15	CLA	aB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.52	15 (18%)
15	CLA	aA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	c5	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
15	CLA	a6	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.34	9 (10%)
15	CLA	b3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.55	10 (16%)
15	CLA	c6	415	13	49,53,73	1.52	7 (14%)	59,89,113	1.64	8 (13%)
18	BCR	bB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
15	CLA	a3	421	13	69,73,73	1.40	11 (15%)	83,113,113	1.62	15 (18%)
15	CLA	cB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.54	8 (9%)
15	CLA	cB	811	2	69,73,73	1.28	8 (11%)	83,113,113	1.70	12 (14%)
15	CLA	cA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.48	9 (12%)
15	CLA	aA	843	1	69,73,73	1.31	10 (14%)	83,113,113	1.52	8 (9%)
15	CLA	a1	403	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	c4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.60	14 (23%)
15	CLA	aA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.48	7 (11%)
15	CLA	cB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	b1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	b1	403	13	69,73,73	1.24	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	aB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	cB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.60	7 (11%)
18	BCR	b1	420	-	41,41,41	1.20	4 (9%)	56,56,56	1.45	11 (19%)
18	BCR	cA	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	cB	832	2	53,57,73	1.44	8 (15%)	62,93,113	1.53	8 (12%)
15	CLA	bB	802	2	69,73,73	1.38	10 (14%)	83,113,113	1.50	9 (10%)
15	CLA	b3	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	cA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	11 (14%)
18	BCR	bL	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	a6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.54	9 (15%)
15	CLA	a4	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.86	13 (22%)
15	CLA	bA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	c6	412	13	68,72,73	1.31	11 (16%)	81,111,113	1.57	15 (18%)
15	CLA	a5	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.62	15 (18%)
15	CLA	b1	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	8 (9%)
15	CLA	b3	417	13	59,63,73	1.57	8 (13%)	71,101,113	1.93	18 (25%)
18	BCR	bA	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	9 (16%)
18	BCR	cJ	104	-	41,41,41	1.31	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	cA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.55	9 (13%)
15	CLA	a3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.83	12 (20%)
15	CLA	cA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
15	CLA	aK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
15	CLA	aB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	a4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
18	BCR	c4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	b3	405	-	49,53,73	1.55	11 (22%)	59,89,113	1.93	18 (30%)
15	CLA	bA	805	1	63,67,73	1.33	11 (17%)	75,105,113	1.54	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	cB	812	2	49,53,73	1.46	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	cA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)
15	CLA	cB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	17 (20%)
15	CLA	a3	405	-	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
15	CLA	cB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	c6	407	-	49,53,73	1.57	9 (18%)	59,89,113	1.93	19 (32%)
15	CLA	cB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	cA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.66	6 (10%)
15	CLA	a1	407	13	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
18	BCR	aJ	204	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	a3	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.60	14 (17%)
15	CLA	aA	815	1	49,53,73	1.48	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	cB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	bA	802	22	69,73,73	1.41	12 (17%)	83,113,113	1.44	10 (12%)
15	CLA	aB	807	2	69,73,73	1.39	11 (15%)	83,113,113	1.49	10 (12%)
15	CLA	b1	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.56	8 (13%)
15	CLA	cB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	aA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
15	CLA	cB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.78	15 (18%)
18	BCR	bA	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
15	CLA	c6	417	13	49,53,73	1.51	8 (16%)	59,89,113	1.82	11 (18%)
15	CLA	cB	841	-	49,53,73	1.52	11 (22%)	59,89,113	1.55	9 (15%)
15	CLA	c4	415	13	49,53,73	1.47	8 (16%)	59,89,113	1.85	12 (20%)
15	CLA	b5	410	13	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	aB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	bB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.79	15 (18%)
15	CLA	b5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.27	16 (24%)
15	CLA	cB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.68	12 (14%)
15	CLA	c3	405	-	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
15	CLA	c4	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.49	6 (10%)
18	BCR	b6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	a1	404	-	49,53,73	1.54	9 (18%)	59,89,113	1.91	19 (32%)
18	BCR	aI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
18	BCR	bL	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
18	BCR	cB	848	-	41,41,41	1.33	4 (9%)	56,56,56	1.50	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	b2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)
15	CLA	c4	411	13	49,53,73	1.49	11 (22%)	59,89,113	1.66	9 (15%)
18	BCR	b1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
18	BCR	c3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	8 (14%)
15	CLA	bL	202	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	bB	806	2	69,73,73	1.26	12 (17%)	83,113,113	1.53	9 (10%)
15	CLA	b5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
18	BCR	aK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
15	CLA	cB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.50	10 (12%)
18	BCR	b5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
18	BCR	aI	103	-	41,41,41	1.31	4 (9%)	56,56,56	1.44	9 (16%)
15	CLA	b4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
15	CLA	cJ	102	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
15	CLA	b4	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	8 (13%)
15	CLA	c1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.45	8 (13%)
15	CLA	a5	416	-	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
15	CLA	aA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	a3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	bB	822	2	49,53,73	1.44	8 (16%)	59,89,113	1.62	8 (13%)
15	CLA	cB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	9 (10%)
15	CLA	cB	802	2	69,73,73	1.38	11 (15%)	83,113,113	1.51	10 (12%)
15	CLA	c3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.54	10 (16%)
15	CLA	a5	413	13	49,53,73	1.50	9 (18%)	59,89,113	1.50	5 (8%)
15	CLA	cA	843	-	46,49,73	1.47	8 (17%)	55,83,113	1.59	5 (9%)
15	CLA	aB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	cA	827	22	69,73,73	1.31	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	bA	807	1	69,73,73	1.35	12 (17%)	83,113,113	1.49	14 (16%)
15	CLA	aB	826	22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
15	CLA	c4	421	13	69,73,73	1.38	14 (20%)	83,113,113	1.69	16 (19%)
18	BCR	bB	849	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	10 (17%)
15	CLA	a4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	bB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	bB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.61	7 (11%)
18	BCR	a5	418	-	41,41,41	1.39	6 (14%)	56,56,56	1.53	10 (17%)
18	BCR	a5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	c1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	CLA	c1	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	c1	416	-	54,58,73	1.52	11 (20%)	65,95,113	2.27	17 (26%)
15	CLA	cB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	c2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
16	PQN	bA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
18	BCR	cA	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	9 (16%)
18	BCR	cB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	bB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	cB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.43	7 (8%)
15	CLA	b2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.59	10 (16%)
15	CLA	a6	407	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	b4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.66	9 (15%)
18	BCR	c3	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
15	CLA	cB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
18	BCR	c5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	b2	413	13	49,53,73	1.57	10 (20%)	59,89,113	1.66	15 (25%)
15	CLA	aA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.62	13 (15%)
15	CLA	a5	404	13	69,73,73	1.25	9 (13%)	83,113,113	1.38	8 (9%)
16	PQN	aB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
15	CLA	cB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
15	CLA	c1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
18	BCR	cA	850	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	cB	826	22	50,54,73	1.43	10 (20%)	60,90,113	1.75	11 (18%)
15	CLA	c2	403	13	69,73,73	1.23	9 (13%)	83,113,113	1.42	9 (10%)
15	CLA	b3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.60	15 (18%)
15	CLA	aA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	a1	405	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	cB	821	2	51,55,73	1.47	11 (21%)	61,91,113	1.46	4 (6%)
17	SF4	bC	101	3	0,12,12	-	-	-		
15	CLA	aJ	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
19	LHG	aX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	a6	404	13	69,73,73	1.22	9 (13%)	83,113,113	1.42	10 (12%)
17	SF4	bC	102	3	0,12,12	-	-	-		
18	BCR	aF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	aB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
15	CLA	aA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	c6	406	13	69,73,73	1.27	10 (14%)	83,113,113	1.39	9 (10%)
15	CLA	bA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
18	BCR	a4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.49	11 (19%)
18	BCR	aB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	9 (16%)
15	CLA	aB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	11 (13%)
18	BCR	c5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.41	11 (19%)
15	CLA	bA	843	1	69,73,73	1.32	10 (14%)	83,113,113	1.50	8 (9%)
15	CLA	aB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.62	8 (13%)
15	CLA	a3	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.37	8 (9%)
15	CLA	aA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.45	6 (9%)
15	CLA	a3	403	13	69,73,73	1.21	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	c1	412	13	49,53,73	1.56	11 (22%)	59,89,113	1.67	13 (22%)
15	CLA	bA	811	1	49,53,73	1.45	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	c2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	bB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)
18	BCR	b2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	aB	811	2	69,73,73	1.29	9 (13%)	83,113,113	1.69	12 (14%)
15	CLA	a3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	bB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	bB	804	-	69,73,73	1.36	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	b6	404	13	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
15	CLA	b4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
18	BCR	b2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	c2	422	13	69,73,73	1.36	11 (15%)	83,113,113	1.80	19 (22%)
18	BCR	a6	421	-	41,41,41	1.11	4 (9%)	56,56,56	1.55	9 (16%)
18	BCR	bB	850	-	41,41,41	1.41	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	c4	402	13	69,73,73	1.22	8 (11%)	83,113,113	1.38	8 (9%)
18	BCR	bM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	aB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
18	BCR	cI	102	-	41,41,41	1.37	3 (7%)	56,56,56	1.41	9 (16%)
15	CLA	c3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.63	10 (16%)
15	CLA	a2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
15	CLA	c4	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.40	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a5	409	13	69,73,73	1.28	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	b1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	16 (22%)
15	CLA	bA	814	1	64,68,73	1.36	10 (15%)	77,107,113	1.37	7 (9%)
18	BCR	aB	845	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	6 (10%)
18	BCR	aA	851	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	a4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.48	5 (8%)
18	BCR	aF	201	-	41,41,41	1.31	4 (9%)	56,56,56	1.37	9 (16%)
15	CLA	bA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
17	SF4	cC	101	3	0,12,12	-	-	-		
15	CLA	a2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
18	BCR	b4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.50	9 (16%)
18	BCR	cB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	bA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	7 (11%)
17	SF4	cC	102	3	0,12,12	-	-	-		
15	CLA	aB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	b4	405	-	49,53,73	1.55	10 (20%)	59,89,113	1.97	18 (30%)
15	CLA	bA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	bK	101	-	49,53,73	1.48	11 (22%)	59,89,113	1.52	10 (16%)
15	CLA	b5	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
15	CLA	c4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	8 (9%)
15	CLA	aL	201	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	a6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.37	8 (9%)
15	CLA	bA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
15	CLA	aB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	a2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	aB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	a5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
15	CLA	c4	410	13	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	a1	416	13	59,63,73	1.54	9 (15%)	71,101,113	1.93	17 (23%)
15	CLA	b2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	cB	820	22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	cL	203	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
18	BCR	cJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
18	BCR	cB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	aB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CLA	a1	412	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	4 (6%)
15	CLA	b1	416	-	54,58,73	1.52	9 (16%)	65,95,113	2.25	17 (26%)
18	BCR	a4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	7 (12%)
15	CLA	cA	813	1	58,62,73	1.42	10 (17%)	69,99,113	1.42	10 (14%)
15	CLA	a1	408	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	9 (10%)
15	CLA	aA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	4 (6%)
15	CLA	c3	403	13	69,73,73	1.22	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	b1	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.66	14 (23%)
15	CLA	aB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
16	PQN	cA	845	-	34,34,34	1.40	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	b4	416	-	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	a2	404	13	69,73,73	1.27	10 (14%)	83,113,113	1.40	9 (10%)
15	CLA	b1	408	13	49,53,73	1.44	9 (18%)	59,89,113	1.60	9 (15%)
18	BCR	c2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
18	BCR	c6	403	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
18	BCR	aM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	bB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	bF	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
15	CLA	aA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	bX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.68	11 (18%)
15	CLA	aA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	cA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
15	CLA	aA	803	-	69,73,73	1.27	12 (17%)	83,113,113	1.74	15 (18%)

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
15	CLA	cA	818	1	-	6/26/102/115	-
15	CLA	a4	407	-	-	8/15/91/115	-
15	CLA	c4	407	-	-	8/15/91/115	-
15	CLA	b1	411	13	-	5/15/91/115	-
16	PQN	aA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	c3	406	13	-	4/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a3	402	13	-	17/39/115/115	-
15	CLA	c2	405	-	-	3/15/91/115	-
15	CLA	c2	414	13	-	4/15/91/115	-
15	CLA	bA	838	1	-	8/23/99/115	-
15	CLA	aA	835	1	-	14/39/115/115	-
15	CLA	a6	415	13	-	4/10/86/115	-
15	CLA	bA	808	1	-	4/23/99/115	-
16	PQN	cB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	b3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	a3	413	13	-	3/15/91/115	-
15	CLA	aA	837	1	-	7/15/91/115	-
15	CLA	bB	825	2	-	10/26/102/115	-
15	CLA	b2	403	13	-	14/39/115/115	-
15	CLA	cA	831	1	-	8/39/115/115	-
15	CLA	cB	835	2	-	9/15/91/115	-
19	LHG	bX	101	-	-	11/26/26/53	-
15	CLA	a6	411	13	-	13/38/114/115	-
15	CLA	cB	833	2	-	18/39/115/115	-
15	CLA	a2	407	13	-	4/15/91/115	-
15	CLA	a6	414	13	-	4/15/91/115	-
15	CLA	cA	815	1	-	4/15/91/115	-
15	CLA	bA	842	22	-	10/23/99/115	-
15	CLA	bA	815	1	-	4/15/91/115	-
15	CLA	b5	417	13	-	10/27/103/115	-
15	CLA	a1	413	13	-	4/10/86/115	-
15	CLA	c2	415	13	-	4/10/86/115	-
17	SF4	aC	101	3	-	-	0/6/5/5
15	CLA	c2	413	13	-	9/15/91/115	-
15	CLA	aA	840	1	-	4/18/94/115	-
15	CLA	bB	828	2	-	21/39/115/115	-
15	CLA	c5	405	-	-	4/15/91/115	-
15	CLA	c5	409	13	-	6/39/115/115	-
15	CLA	a6	412	13	-	4/15/91/115	-
15	CLA	b6	414	13	-	4/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	836	2	-	11/33/109/115	-
15	CLA	bA	824	1	-	14/23/99/115	-
15	CLA	cA	810	1	-	18/39/115/115	-
15	CLA	c2	411	13	-	12/38/114/115	-
15	CLA	a4	421	13	-	13/39/115/115	-
18	BCR	a3	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	836	1	-	8/26/102/115	-
15	CLA	b2	402	13	-	17/39/115/115	-
15	CLA	aB	841	-	-	4/15/91/115	-
15	CLA	b5	402	13	-	17/39/115/115	-
18	BCR	b1	418	-	-	9/29/63/63	0/2/2/2
15	CLA	aA	834	1	-	12/39/115/115	-
15	CLA	aB	805	2	-	5/26/102/115	-
15	CLA	cB	810	2	-	16/39/115/115	-
15	CLA	aA	818	1	-	6/26/102/115	-
15	CLA	b5	403	13	-	14/39/115/115	-
15	CLA	b2	415	13	-	4/10/86/115	-
18	BCR	c1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	415	13	-	7/15/91/115	-
15	CLA	a3	417	13	-	12/27/103/115	-
15	CLA	bB	805	2	-	5/26/102/115	-
15	CLA	bB	841	-	-	4/15/91/115	-
15	CLA	aA	838	1	-	8/23/99/115	-
15	CLA	aJ	203	8	-	2/4/76/115	-
18	BCR	b4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	417	-	-	9/21/97/115	-
15	CLA	bB	817	2	-	12/27/103/115	-
15	CLA	a2	418	13	-	11/27/103/115	-
15	CLA	c3	416	-	-	11/21/97/115	-
15	CLA	b2	410	13	-	7/39/115/115	-
15	CLA	cA	826	-	-	10/39/115/115	-
15	CLA	aB	814	2	-	25/39/115/115	-
15	CLA	aL	202	10	-	10/39/115/115	-
15	CLA	a4	417	13	-	9/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cL	202	10	-	15/39/115/115	-
18	BCR	b3	419	-	-	11/29/63/63	0/2/2/2
19	LHG	aA	854	15	-	15/31/31/53	-
15	CLA	bA	825	1	-	17/32/108/115	-
15	CLA	a5	408	13	-	5/15/91/115	-
15	CLA	cF	201	22	-	10/23/99/115	-
15	CLA	aA	842	22	-	10/23/99/115	-
15	CLA	aB	816	2	-	6/15/91/115	-
15	CLA	a5	417	13	-	9/27/103/115	-
15	CLA	c1	417	13	-	9/27/103/115	-
18	BCR	aB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	830	2	-	6/39/115/115	-
18	BCR	aB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	bB	819	2	-	12/33/109/115	-
15	CLA	bA	841	1	-	17/39/115/115	-
15	CLA	b3	416	-	-	11/21/97/115	-
18	BCR	c2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a3	408	13	-	5/15/91/115	-
15	CLA	b3	413	13	-	3/15/91/115	-
15	CLA	c6	401	13	-	16/39/115/115	-
18	BCR	c1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	416	-	-	11/21/97/115	-
15	CLA	cA	820	1	-	18/39/115/115	-
15	CLA	cB	818	2	-	10/32/108/115	-
15	CLA	c2	418	13	-	11/27/103/115	-
15	CLA	cA	812	1	-	13/39/115/115	-
15	CLA	b2	408	-	-	7/15/91/115	-
15	CLA	c1	405	-	-	3/15/91/115	-
15	CLA	c1	409	13	-	6/39/115/115	-
15	CLA	b6	416	13	-	7/15/91/115	-
18	BCR	a6	420	-	-	12/29/63/63	0/2/2/2
18	BCR	b2	401	-	-	12/29/63/63	0/2/2/2
18	BCR	b3	418	-	-	10/29/63/63	0/2/2/2
18	BCR	b4	420	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	806	1	-	23/39/115/115	-
18	BCR	a6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	a3	411	13	-	5/15/91/115	-
15	CLA	a2	414	13	-	3/15/91/115	-
15	CLA	bA	826	-	-	10/39/115/115	-
19	LHG	aA	853	-	-	19/53/53/53	-
15	CLA	b3	406	13	-	4/15/91/115	-
15	CLA	bB	820	22	-	10/39/115/115	-
15	CLA	bB	837	2	-	15/39/115/115	-
15	CLA	a6	406	-	-	3/15/91/115	-
15	CLA	b3	414	13	-	4/10/86/115	-
18	BCR	a1	419	-	-	12/29/63/63	0/2/2/2
19	LHG	cA	852	-	-	19/53/53/53	-
18	BCR	a3	401	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	832	1	-	8/21/97/115	-
15	CLA	c6	416	13	-	4/10/86/115	-
15	CLA	bA	821	1	-	15/35/111/115	-
15	CLA	aB	828	2	-	21/39/115/115	-
15	CLA	c2	402	13	-	17/39/115/115	-
15	CLA	c2	416	13	-	7/15/91/115	-
15	CLA	c6	408	13	-	4/15/91/115	-
15	CLA	b6	406	-	-	3/15/91/115	-
15	CLA	b4	415	13	-	7/15/91/115	-
19	LHG	bA	855	15	-	15/31/31/53	-
15	CLA	bB	836	2	-	11/33/109/115	-
15	CLA	bB	832	2	-	8/20/96/115	-
15	CLA	bB	803	-	-	11/39/115/115	-
15	CLA	a2	415	13	-	4/10/86/115	-
15	CLA	c2	408	-	-	8/15/91/115	-
15	CLA	a4	412	13	-	9/15/91/115	-
18	BCR	cA	851	-	-	22/29/63/63	0/2/2/2
15	CLA	cB	827	2	-	15/39/115/115	-
15	CLA	bA	833	1	-	11/39/115/115	-
15	CLA	aL	203	22	-	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	829	1	-	22/39/115/115	-
15	CLA	a2	417	-	-	9/21/97/115	-
18	BCR	a1	418	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	839	22	-	10/39/115/115	-
17	SF4	aC	102	3	-	-	0/6/5/5
15	CLA	b5	413	13	-	3/15/91/115	-
18	BCR	c2	420	-	-	11/29/63/63	0/2/2/2
17	SF4	cA	846	1,2	-	-	0/6/5/5
15	CLA	bJ	101	8	-	8/15/91/115	-
15	CLA	c4	406	13	-	4/15/91/115	-
15	CLA	cA	840	1	-	5/18/94/115	-
15	CLA	b6	407	13	-	4/15/91/115	-
18	BCR	a4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	822	-	-	18/39/115/115	-
18	BCR	b5	418	-	-	11/29/63/63	0/2/2/2
18	BCR	c4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	c5	415	13	-	7/15/91/115	-
15	CLA	aA	812	1	-	13/39/115/115	-
15	CLA	c5	413	13	-	3/15/91/115	-
14	CL0	aA	801	1	-	6/39/115/115	-
15	CLA	aB	801	-	-	12/39/115/115	-
15	CLA	aA	845	19	-	13/24/100/115	-
18	BCR	b3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bL	204	22	-	15/39/115/115	-
15	CLA	cA	807	1	-	11/39/115/115	-
15	CLA	bB	840	2	-	16/39/115/115	-
15	CLA	bB	811	2	-	13/39/115/115	-
15	CLA	cL	204	22	-	15/39/115/115	-
18	BCR	bA	850	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	809	1	-	21/39/115/115	-
15	CLA	c5	411	13	-	3/15/91/115	-
15	CLA	c4	416	-	-	11/21/97/115	-
17	SF4	bA	847	1,2	-	-	0/6/5/5
18	BCR	a6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c6	413	13	-	4/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	809	1	-	21/39/115/115	-
15	CLA	b4	412	13	-	9/15/91/115	-
15	CLA	c2	407	13	-	4/15/91/115	-
18	BCR	bA	852	-	-	8/29/63/63	0/2/2/2
15	CLA	cB	809	2	-	13/39/115/115	-
15	CLA	cA	834	1	-	12/39/115/115	-
15	CLA	c6	411	13	-	6/39/115/115	-
15	CLA	aA	816	1	-	3/15/91/115	-
15	CLA	c2	404	13	-	11/39/115/115	-
15	CLA	c5	414	13	-	4/10/86/115	-
15	CLA	aB	818	2	-	10/32/108/115	-
18	BCR	a2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a1	410	13	-	4/15/91/115	-
18	BCR	b6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	c3	417	13	-	11/27/103/115	-
15	CLA	b1	410	13	-	14/38/114/115	-
15	CLA	b4	403	13	-	14/39/115/115	-
15	CLA	bA	844	-	-	7/9/81/115	-
15	CLA	bB	834	2	-	15/31/107/115	-
19	LHG	bA	854	-	-	19/53/53/53	-
15	CLA	bJ	102	8	-	2/4/76/115	-
15	CLA	b6	422	13	-	17/39/115/115	-
15	CLA	c6	418	-	-	11/21/97/115	-
18	BCR	b6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	a3	412	13	-	9/15/91/115	-
15	CLA	cA	838	1	-	8/23/99/115	-
15	CLA	a3	407	-	-	7/15/91/115	-
18	BCR	c6	421	-	-	12/29/63/63	0/2/2/2
15	CLA	c3	402	13	-	17/39/115/115	-
15	CLA	bB	838	2	-	2/18/94/115	-
18	BCR	cM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	409	13	-	6/39/115/115	-
15	CLA	bB	808	2	-	14/39/115/115	-
15	CLA	b6	412	13	-	4/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	832	1	-	8/21/97/115	-
18	BCR	c6	402	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	414	13	-	4/10/86/115	-
15	CLA	aB	819	2	-	12/33/109/115	-
18	BCR	a1	421	-	-	14/29/63/63	0/2/2/2
15	CLA	cB	801	-	-	12/39/115/115	-
15	CLA	aB	839	22	-	10/39/115/115	-
18	BCR	bJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	c6	405	13	-	14/39/115/115	-
18	BCR	aJ	205	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	834	1	-	12/39/115/115	-
15	CLA	a6	418	13	-	11/27/103/115	-
15	CLA	bB	842	-	-	2/15/91/115	-
15	CLA	cB	817	2	-	12/27/103/115	-
15	CLA	c6	414	13	-	9/15/91/115	-
15	CLA	bB	826	22	-	8/17/93/115	-
15	CLA	aA	826	-	-	10/39/115/115	-
15	CLA	bA	818	1	-	6/26/102/115	-
15	CLA	c5	420	13	-	12/39/115/115	-
15	CLA	cA	836	1	-	8/26/102/115	-
15	CLA	c1	413	13	-	4/15/91/115	-
15	CLA	aA	821	1	-	15/35/111/115	-
18	BCR	cF	202	-	-	14/29/63/63	0/2/2/2
15	CLA	cB	831	2	-	8/15/91/115	-
18	BCR	b6	420	-	-	12/29/63/63	0/2/2/2
18	BCR	c5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	835	1	-	14/39/115/115	-
18	BCR	bJ	105	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	420	13	-	12/39/115/115	-
15	CLA	cA	803	-	-	16/39/115/115	-
18	BCR	cI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	806	2	-	21/39/115/115	-
15	CLA	cA	806	1	-	23/39/115/115	-
18	BCR	c1	418	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL0	cA	801	1	-	6/39/115/115	-
15	CLA	bB	829	2	-	16/39/115/115	-
15	CLA	b4	409	13	-	6/39/115/115	-
15	CLA	b5	406	13	-	4/15/91/115	-
15	CLA	b4	410	13	-	13/38/114/115	-
18	BCR	b6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b3	403	13	-	13/39/115/115	-
15	CLA	a3	414	13	-	4/10/86/115	-
15	CLA	bB	812	2	-	3/15/91/115	-
18	BCR	c1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	804	-	-	12/39/115/115	-
18	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	c3	404	13	-	12/39/115/115	-
18	BCR	a3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	403	13	-	14/39/115/115	-
15	CLA	bB	824	2	-	5/15/91/115	-
15	CLA	aB	827	2	-	15/39/115/115	-
15	CLA	a5	415	13	-	7/15/91/115	-
15	CLA	aB	815	2	-	17/39/115/115	-
15	CLA	a5	402	13	-	17/39/115/115	-
15	CLA	b5	420	13	-	12/39/115/115	-
18	BCR	aF	203	-	-	11/29/63/63	0/2/2/2
15	CLA	b5	414	13	-	4/10/86/115	-
15	CLA	cA	811	1	-	10/15/91/115	-
15	CLA	b4	421	13	-	13/39/115/115	-
15	CLA	cB	822	2	-	2/15/91/115	-
15	CLA	c5	403	13	-	14/39/115/115	-
15	CLA	a5	411	13	-	3/15/91/115	-
15	CLA	c3	413	13	-	4/15/91/115	-
18	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	bB	810	2	-	16/39/115/115	-
15	CLA	bA	806	1	-	23/39/115/115	-
18	BCR	aL	205	-	-	14/29/63/63	0/2/2/2
15	CLA	c1	415	13	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c3	412	13	-	9/15/91/115	-
18	BCR	c4	419	-	-	11/29/63/63	0/2/2/2
19	LHG	cX	101	-	-	11/26/26/53	-
18	BCR	cB	849	-	-	11/29/63/63	0/2/2/2
18	BCR	c3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	a2	411	13	-	13/38/114/115	-
14	CL0	bA	801	1	-	6/39/115/115	-
15	CLA	a1	409	13	-	14/38/114/115	-
15	CLA	bA	845	19	-	13/24/100/115	-
15	CLA	b6	410	13	-	6/39/115/115	-
15	CLA	cB	823	-	-	5/27/103/115	-
15	CLA	a5	414	13	-	4/10/86/115	-
15	CLA	c3	410	13	-	12/38/114/115	-
15	CLA	aA	839	1	-	16/39/115/115	-
15	CLA	bB	809	2	-	13/39/115/115	-
15	CLA	aB	802	2	-	13/39/115/115	-
15	CLA	a1	414	13	-	7/15/91/115	-
15	CLA	aJ	202	8	-	8/15/91/115	-
15	CLA	a2	405	-	-	4/15/91/115	-
15	CLA	b2	411	13	-	13/38/114/115	-
18	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	813	1	-	8/26/102/115	-
18	BCR	c4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	b1	414	13	-	4/10/86/115	-
15	CLA	c5	412	13	-	9/15/91/115	-
15	CLA	bB	833	2	-	18/39/115/115	-
15	CLA	bA	810	1	-	18/39/115/115	-
18	BCR	a2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	827	22	-	10/39/115/115	-
15	CLA	cA	823	1	-	6/20/96/115	-
15	CLA	b3	408	13	-	5/15/91/115	-
15	CLA	a2	416	13	-	7/15/91/115	-
18	BCR	bB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	a6	417	-	-	11/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b3	410	13	-	12/38/114/115	-
18	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
20	LMG	bB	851	-	-	26/50/70/70	0/1/1/1
18	BCR	bA	853	-	-	22/29/63/63	0/2/2/2
15	CLA	bA	809	1	-	21/39/115/115	-
15	CLA	a4	410	13	-	13/38/114/115	-
15	CLA	b6	408	-	-	7/15/91/115	-
15	CLA	c2	412	13	-	3/15/91/115	-
15	CLA	cA	842	1	-	14/39/115/115	-
15	CLA	cA	805	1	-	11/32/108/115	-
15	CLA	c5	404	13	-	11/39/115/115	-
15	CLA	aA	807	1	-	11/39/115/115	-
15	CLA	c5	408	13	-	5/15/91/115	-
20	LMG	cB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	b1	413	13	-	4/15/91/115	-
15	CLA	bB	816	2	-	6/15/91/115	-
15	CLA	b6	417	-	-	11/21/97/115	-
18	BCR	cF	204	-	-	12/29/63/63	0/2/2/2
15	CLA	b1	405	-	-	3/15/91/115	-
15	CLA	c1	414	13	-	4/10/86/115	-
15	CLA	c5	410	13	-	13/38/114/115	-
15	CLA	c2	417	-	-	9/21/97/115	-
15	CLA	c6	404	13	-	17/39/115/115	-
15	CLA	aA	823	1	-	6/20/96/115	-
15	CLA	cB	836	2	-	11/33/109/115	-
15	CLA	c6	410	13	-	5/15/91/115	-
15	CLA	a6	416	13	-	7/15/91/115	-
18	BCR	b4	418	-	-	9/29/63/63	0/2/2/2
19	LHG	cA	853	15	-	15/31/31/53	-
15	CLA	a4	408	13	-	5/15/91/115	-
15	CLA	a3	416	-	-	11/21/97/115	-
15	CLA	c6	419	13	-	11/27/103/115	-
18	BCR	cF	205	-	-	11/29/63/63	0/2/2/2
18	BCR	a2	420	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a1	401	13	-	17/39/115/115	-
15	CLA	c1	403	13	-	14/39/115/115	-
18	BCR	a5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	817	-	-	6/20/96/115	-
15	CLA	c3	414	13	-	4/10/86/115	-
15	CLA	aA	820	1	-	18/39/115/115	-
15	CLA	a4	411	13	-	5/15/91/115	-
15	CLA	aB	833	2	-	18/39/115/115	-
15	CLA	c4	417	13	-	9/27/103/115	-
15	CLA	cA	830	1	-	13/39/115/115	-
15	CLA	a1	402	13	-	14/39/115/115	-
15	CLA	bL	203	10	-	10/39/115/115	-
15	CLA	c5	407	-	-	8/15/91/115	-
15	CLA	c3	421	13	-	12/39/115/115	-
18	BCR	cL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	b3	409	13	-	5/39/115/115	-
15	CLA	cA	821	1	-	15/35/111/115	-
15	CLA	b6	403	13	-	17/39/115/115	-
15	CLA	cA	837	1	-	7/15/91/115	-
18	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	b1	402	13	-	17/39/115/115	-
15	CLA	bA	829	1	-	22/39/115/115	-
15	CLA	b5	408	13	-	5/15/91/115	-
18	BCR	aB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	831	2	-	8/15/91/115	-
15	CLA	a5	403	13	-	14/39/115/115	-
15	CLA	b6	405	13	-	11/39/115/115	-
15	CLA	aA	814	1	-	16/33/109/115	-
15	CLA	b2	406	13	-	10/39/115/115	-
15	CLA	b6	409	13	-	5/15/91/115	-
15	CLA	bB	821	2	-	13/18/94/115	-
18	BCR	c6	420	-	-	10/29/63/63	0/2/2/2
15	CLA	c3	415	13	-	7/15/91/115	-
18	BCR	a1	417	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	835	1	-	14/39/115/115	-
15	CLA	cB	803	-	-	11/39/115/115	-
15	CLA	aB	821	2	-	13/18/94/115	-
15	CLA	b4	413	13	-	4/15/91/115	-
15	CLA	c6	409	-	-	7/15/91/115	-
16	PQN	bB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	cJ	101	8	-	8/15/91/115	-
15	CLA	aA	805	1	-	11/32/108/115	-
15	CLA	aA	830	1	-	13/39/115/115	-
18	BCR	bI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	406	13	-	4/15/91/115	-
15	CLA	b2	412	13	-	3/15/91/115	-
15	CLA	c3	409	13	-	6/39/115/115	-
15	CLA	bB	835	2	-	9/15/91/115	-
15	CLA	c4	408	13	-	5/15/91/115	-
18	BCR	aA	850	-	-	13/29/63/63	0/2/2/2
18	BCR	a6	402	-	-	14/29/63/63	0/2/2/2
18	BCR	b1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	820	1	-	18/39/115/115	-
15	CLA	c2	409	13	-	5/15/91/115	-
17	SF4	aA	847	1,2	-	-	0/6/5/5
15	CLA	aB	825	2	-	10/26/102/115	-
15	CLA	bA	822	-	-	18/39/115/115	-
15	CLA	b6	413	13	-	9/15/91/115	-
15	CLA	a6	413	13	-	9/15/91/115	-
15	CLA	c4	405	-	-	4/15/91/115	-
18	BCR	aA	852	-	-	22/29/63/63	0/2/2/2
15	CLA	cA	844	19	-	13/24/100/115	-
15	CLA	c1	410	13	-	15/38/114/115	-
15	CLA	cK	102	-	-	10/15/91/115	-
18	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	404	13	-	11/39/115/115	-
18	BCR	a4	418	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	831	1	-	8/39/115/115	-
15	CLA	aA	828	1	-	14/39/115/115	-
15	CLA	cA	839	1	-	16/39/115/115	-
15	CLA	cB	824	2	-	5/15/91/115	-
15	CLA	bB	807	2	-	15/39/115/115	-
15	CLA	b1	415	13	-	7/15/91/115	-
15	CLA	a5	407	-	-	8/15/91/115	-
15	CLA	b6	418	13	-	11/27/103/115	-
15	CLA	cB	825	2	-	10/26/102/115	-
15	CLA	aA	841	1	-	17/39/115/115	-
15	CLA	bB	823	-	-	5/27/103/115	-
15	CLA	b3	411	13	-	5/15/91/115	-
15	CLA	b2	422	13	-	12/39/115/115	-
15	CLA	a2	412	13	-	3/15/91/115	-
18	BCR	aA	848	-	-	11/29/63/63	0/2/2/2
15	CLA	a6	422	13	-	19/39/115/115	-
15	CLA	b5	407	-	-	8/15/91/115	-
15	CLA	a2	403	13	-	14/39/115/115	-
15	CLA	cF	203	-	-	10/15/91/115	-
18	BCR	bB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	c1	408	13	-	5/15/91/115	-
15	CLA	a4	404	13	-	12/39/115/115	-
15	CLA	c4	409	13	-	6/39/115/115	-
18	BCR	bF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	407	13	-	4/15/91/115	-
15	CLA	b4	406	13	-	4/15/91/115	-
15	CLA	cA	833	1	-	11/39/115/115	-
15	CLA	cB	806	2	-	21/39/115/115	-
15	CLA	cB	834	2	-	15/31/107/115	-
18	BCR	cK	101	-	-	10/29/63/63	0/2/2/2
18	BCR	bJ	103	-	-	14/29/63/63	0/2/2/2
15	CLA	aA	802	22	-	16/39/115/115	-
15	CLA	cA	814	1	-	16/33/109/115	-
15	CLA	bA	812	1	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b2	405	-	-	4/15/91/115	-
15	CLA	bA	823	1	-	6/20/96/115	-
15	CLA	aA	822	-	-	18/39/115/115	-
15	CLA	a4	405	-	-	4/15/91/115	-
18	BCR	b2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b5	411	13	-	3/15/91/115	-
15	CLA	a6	409	13	-	5/15/91/115	-
15	CLA	bA	816	1	-	3/15/91/115	-
15	CLA	a1	415	-	-	11/21/97/115	-
18	BCR	bL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	b4	402	13	-	17/39/115/115	-
15	CLA	a6	403	13	-	17/39/115/115	-
18	BCR	b5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	823	-	-	5/27/103/115	-
15	CLA	aX	102	12	-	8/15/91/115	-
15	CLA	a5	405	-	-	4/15/91/115	-
18	BCR	c2	419	-	-	10/29/63/63	0/2/2/2
18	BCR	c3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	829	1	-	22/39/115/115	-
15	CLA	bB	827	2	-	15/39/115/115	-
15	CLA	a1	411	13	-	9/15/91/115	-
15	CLA	cA	808	1	-	4/23/99/115	-
15	CLA	cB	837	2	-	15/39/115/115	-
18	BCR	a3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c5	417	13	-	10/27/103/115	-
15	CLA	aA	819	1	-	10/26/102/115	-
15	CLA	a2	413	13	-	9/15/91/115	-
15	CLA	a1	406	-	-	8/15/91/115	-
18	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	b4	404	13	-	12/39/115/115	-
15	CLA	b3	402	13	-	17/39/115/115	-
15	CLA	c3	408	13	-	5/15/91/115	-
15	CLA	a2	409	13	-	5/15/91/115	-
18	BCR	aA	849	-	-	13/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a4	402	13	-	17/39/115/115	-
15	CLA	bA	828	1	-	14/39/115/115	-
15	CLA	cA	804	1	-	10/39/115/115	-
15	CLA	cX	102	12	-	8/15/91/115	-
15	CLA	a2	410	13	-	6/39/115/115	-
15	CLA	b3	415	13	-	7/15/91/115	-
15	CLA	aB	824	2	-	5/15/91/115	-
15	CLA	b5	405	-	-	4/15/91/115	-
15	CLA	b2	414	13	-	3/15/91/115	-
15	CLA	b1	406	13	-	4/15/91/115	-
15	CLA	c5	402	13	-	17/39/115/115	-
15	CLA	c5	416	-	-	11/21/97/115	-
18	BCR	a1	420	-	-	12/29/63/63	0/2/2/2
20	LMG	aB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	bA	836	1	-	8/26/102/115	-
15	CLA	aA	844	-	-	7/9/81/115	-
15	CLA	b6	415	13	-	4/10/86/115	-
15	CLA	a2	422	13	-	13/39/115/115	-
15	CLA	bA	803	-	-	16/39/115/115	-
15	CLA	aB	813	2	-	4/15/91/115	-
15	CLA	a4	409	13	-	5/39/115/115	-
15	CLA	b4	407	-	-	8/15/91/115	-
15	CLA	cA	828	1	-	14/39/115/115	-
15	CLA	aB	832	2	-	8/20/96/115	-
15	CLA	b6	411	13	-	14/38/114/115	-
18	BCR	a2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	412	13	-	9/15/91/115	-
15	CLA	c1	411	13	-	5/15/91/115	-
15	CLA	aA	813	1	-	8/26/102/115	-
15	CLA	aB	803	-	-	11/39/115/115	-
15	CLA	aA	804	1	-	10/39/115/115	-
15	CLA	c5	406	13	-	4/15/91/115	-
15	CLA	a6	410	13	-	6/39/115/115	-
15	CLA	b3	407	-	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c6	415	13	-	4/15/91/115	-
18	BCR	bB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	a3	421	13	-	12/39/115/115	-
15	CLA	cB	828	2	-	21/39/115/115	-
15	CLA	cB	811	2	-	13/39/115/115	-
15	CLA	cA	802	22	-	16/39/115/115	-
15	CLA	aB	834	2	-	15/31/107/115	-
15	CLA	aA	843	1	-	14/39/115/115	-
15	CLA	a1	403	13	-	13/39/115/115	-
15	CLA	c4	412	13	-	9/15/91/115	-
15	CLA	aA	811	1	-	10/15/91/115	-
15	CLA	cB	815	2	-	17/39/115/115	-
15	CLA	b1	404	13	-	14/39/115/115	-
15	CLA	b1	403	13	-	14/39/115/115	-
15	CLA	aB	810	2	-	16/39/115/115	-
15	CLA	cB	813	2	-	4/15/91/115	-
18	BCR	b1	420	-	-	12/29/63/63	0/2/2/2
18	BCR	cA	847	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	832	2	-	8/20/96/115	-
15	CLA	bB	802	2	-	13/39/115/115	-
15	CLA	b3	404	13	-	12/39/115/115	-
15	CLA	cA	825	1	-	17/32/108/115	-
18	BCR	bL	206	-	-	14/29/63/63	0/2/2/2
15	CLA	a6	408	-	-	7/15/91/115	-
15	CLA	a4	415	13	-	7/15/91/115	-
15	CLA	bA	840	1	-	5/18/94/115	-
15	CLA	c6	412	13	-	12/38/114/115	-
15	CLA	a5	410	13	-	14/38/114/115	-
15	CLA	b1	409	13	-	6/39/115/115	-
15	CLA	b3	417	13	-	11/27/103/115	-
18	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
18	BCR	cJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	cA	819	1	-	10/26/102/115	-
15	CLA	a3	415	13	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cA	841	1	-	17/39/115/115	-
15	CLA	aK	102	-	-	10/15/91/115	-
15	CLA	aB	840	2	-	16/39/115/115	-
15	CLA	a4	414	13	-	4/10/86/115	-
18	BCR	c4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	405	-	-	3/15/91/115	-
15	CLA	bA	805	1	-	11/32/108/115	-
15	CLA	cB	812	2	-	3/15/91/115	-
15	CLA	cA	817	-	-	6/20/96/115	-
15	CLA	cB	814	2	-	25/39/115/115	-
15	CLA	a3	405	-	-	3/15/91/115	-
15	CLA	cB	839	22	-	10/39/115/115	-
15	CLA	c6	407	-	-	3/15/91/115	-
15	CLA	cB	805	2	-	5/26/102/115	-
15	CLA	cA	816	1	-	3/15/91/115	-
15	CLA	a1	407	13	-	5/15/91/115	-
18	BCR	aJ	204	-	-	14/29/63/63	0/2/2/2
15	CLA	a3	410	13	-	12/38/114/115	-
15	CLA	aA	815	1	-	4/15/91/115	-
15	CLA	cB	804	-	-	12/39/115/115	-
15	CLA	bA	802	22	-	16/39/115/115	-
15	CLA	aB	807	2	-	15/39/115/115	-
15	CLA	b1	407	-	-	7/15/91/115	-
15	CLA	cB	816	2	-	6/15/91/115	-
15	CLA	aA	808	1	-	4/23/99/115	-
15	CLA	cB	830	2	-	6/39/115/115	-
18	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
15	CLA	c6	417	13	-	7/15/91/115	-
15	CLA	cB	841	-	-	4/15/91/115	-
15	CLA	c4	415	13	-	7/15/91/115	-
15	CLA	b5	410	13	-	14/38/114/115	-
15	CLA	aB	829	2	-	16/39/115/115	-
15	CLA	bB	830	2	-	6/39/115/115	-
15	CLA	b5	416	-	-	11/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	840	2	-	16/39/115/115	-
15	CLA	c3	405	-	-	3/15/91/115	-
15	CLA	c4	413	13	-	4/15/91/115	-
18	BCR	b6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	a1	404	-	-	3/15/91/115	-
18	BCR	aI	102	-	-	11/29/63/63	0/2/2/2
18	BCR	bL	201	-	-	14/29/63/63	0/2/2/2
18	BCR	cB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	b2	416	13	-	7/15/91/115	-
15	CLA	c4	411	13	-	4/15/91/115	-
18	BCR	b1	419	-	-	11/29/63/63	0/2/2/2
18	BCR	c3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bL	202	10	-	15/39/115/115	-
15	CLA	bB	806	2	-	21/39/115/115	-
15	CLA	b5	412	13	-	9/15/91/115	-
18	BCR	aK	101	-	-	10/29/63/63	0/2/2/2
15	CLA	cB	807	2	-	15/39/115/115	-
18	BCR	b5	401	-	-	14/29/63/63	0/2/2/2
18	BCR	aI	103	-	-	9/29/63/63	0/2/2/2
15	CLA	b4	414	13	-	4/10/86/115	-
15	CLA	cJ	102	8	-	2/4/76/115	-
15	CLA	b4	408	13	-	5/15/91/115	-
15	CLA	c1	406	13	-	4/15/91/115	-
15	CLA	a5	416	-	-	11/21/97/115	-
15	CLA	aA	833	1	-	11/39/115/115	-
15	CLA	a3	406	13	-	4/15/91/115	-
15	CLA	bB	822	2	-	2/15/91/115	-
15	CLA	cB	829	2	-	16/39/115/115	-
15	CLA	cB	802	2	-	13/39/115/115	-
15	CLA	c3	407	-	-	7/15/91/115	-
15	CLA	a5	413	13	-	3/15/91/115	-
15	CLA	cA	843	-	-	7/9/81/115	-
15	CLA	aB	820	22	-	10/39/115/115	-
15	CLA	cA	827	22	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bA	807	1	-	11/39/115/115	-
15	CLA	aB	826	22	-	8/17/93/115	-
15	CLA	c4	421	13	-	12/39/115/115	-
18	BCR	bB	849	-	-	14/29/63/63	0/2/2/2
15	CLA	a4	406	13	-	4/15/91/115	-
15	CLA	bB	801	-	-	12/39/115/115	-
15	CLA	bB	813	2	-	4/15/91/115	-
18	BCR	a5	418	-	-	11/29/63/63	0/2/2/2
18	BCR	a5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	c1	402	13	-	17/39/115/115	-
15	CLA	c1	407	-	-	8/15/91/115	-
15	CLA	c1	416	-	-	11/21/97/115	-
15	CLA	cB	838	2	-	2/18/94/115	-
15	CLA	c2	406	13	-	11/39/115/115	-
16	PQN	bA	846	-	-	5/23/43/43	0/2/2/2
18	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
18	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	bB	815	2	-	17/39/115/115	-
15	CLA	cB	808	2	-	14/39/115/115	-
15	CLA	b2	409	13	-	5/15/91/115	-
15	CLA	a6	407	13	-	4/15/91/115	-
15	CLA	b4	411	13	-	5/15/91/115	-
18	BCR	c3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cB	819	2	-	12/33/109/115	-
18	BCR	c5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	413	13	-	9/15/91/115	-
15	CLA	aA	831	1	-	8/39/115/115	-
15	CLA	a5	404	13	-	11/39/115/115	-
16	PQN	aB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	cB	842	-	-	2/15/91/115	-
15	CLA	c1	404	13	-	13/39/115/115	-
18	BCR	cA	850	-	-	8/29/63/63	0/2/2/2
15	CLA	cB	826	22	-	8/17/93/115	-
15	CLA	c2	403	13	-	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b3	421	13	-	12/39/115/115	-
15	CLA	aA	810	1	-	18/39/115/115	-
15	CLA	a1	405	13	-	4/15/91/115	-
15	CLA	cB	821	2	-	13/18/94/115	-
17	SF4	bC	101	3	-	-	0/6/5/5
15	CLA	aJ	201	-	-	10/15/91/115	-
19	LHG	aX	101	-	-	11/26/26/53	-
15	CLA	a6	404	13	-	14/39/115/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
18	BCR	aF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	812	2	-	3/15/91/115	-
15	CLA	aA	825	1	-	17/32/108/115	-
15	CLA	c6	406	13	-	11/39/115/115	-
15	CLA	bA	819	1	-	10/26/102/115	-
18	BCR	a4	401	-	-	13/29/63/63	0/2/2/2
18	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	837	2	-	15/39/115/115	-
18	BCR	c5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	843	1	-	14/39/115/115	-
15	CLA	aB	822	2	-	2/15/91/115	-
15	CLA	a3	404	13	-	12/39/115/115	-
15	CLA	aA	824	1	-	14/23/99/115	-
15	CLA	a3	403	13	-	13/39/115/115	-
15	CLA	c1	412	13	-	9/15/91/115	-
15	CLA	bA	811	1	-	10/15/91/115	-
15	CLA	c2	410	13	-	6/39/115/115	-
15	CLA	bB	814	2	-	25/39/115/115	-
18	BCR	b2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	811	2	-	13/39/115/115	-
15	CLA	a3	409	13	-	5/39/115/115	-
15	CLA	bB	818	2	-	10/32/108/115	-
15	CLA	bB	804	-	-	12/39/115/115	-
15	CLA	b6	404	13	-	14/39/115/115	-
15	CLA	b4	417	13	-	9/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	422	13	-	13/39/115/115	-
18	BCR	a6	421	-	-	13/29/63/63	0/2/2/2
18	BCR	bB	850	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	402	13	-	17/39/115/115	-
18	BCR	bM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	809	2	-	13/39/115/115	-
18	BCR	cI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	c3	411	13	-	5/15/91/115	-
15	CLA	a2	406	13	-	11/39/115/115	-
15	CLA	c4	403	13	-	14/39/115/115	-
15	CLA	a5	409	13	-	6/39/115/115	-
15	CLA	b1	417	13	-	12/27/103/115	-
15	CLA	bA	814	1	-	16/33/109/115	-
18	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
18	BCR	aA	851	-	-	8/29/63/63	0/2/2/2
15	CLA	a4	413	13	-	4/15/91/115	-
18	BCR	aF	201	-	-	14/29/63/63	0/2/2/2
15	CLA	bA	839	1	-	16/39/115/115	-
18	BCR	b4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	a2	408	-	-	8/15/91/115	-
18	BCR	cB	847	-	-	9/18/35/63	0/1/1/2
17	SF4	cC	101	3	-	-	0/6/5/5
15	CLA	bA	837	1	-	7/15/91/115	-
17	SF4	cC	102	3	-	-	0/6/5/5
15	CLA	aB	835	2	-	9/15/91/115	-
15	CLA	b4	405	-	-	4/15/91/115	-
15	CLA	bA	804	1	-	10/39/115/115	-
15	CLA	bK	101	-	-	10/15/91/115	-
15	CLA	b5	404	13	-	11/39/115/115	-
15	CLA	c4	404	13	-	11/39/115/115	-
15	CLA	aL	201	10	-	15/39/115/115	-
15	CLA	a6	405	13	-	11/39/115/115	-
15	CLA	bA	830	1	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	838	2	-	2/18/94/115	-
15	CLA	a2	402	13	-	17/39/115/115	-
15	CLA	aB	808	2	-	14/39/115/115	-
15	CLA	a5	412	13	-	9/15/91/115	-
15	CLA	c4	410	13	-	13/38/114/115	-
15	CLA	a1	416	13	-	10/27/103/115	-
15	CLA	b2	418	13	-	11/27/103/115	-
15	CLA	cB	820	22	-	10/39/115/115	-
15	CLA	cL	203	10	-	10/39/115/115	-
18	BCR	cJ	103	-	-	14/29/63/63	0/2/2/2
18	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	817	2	-	12/27/103/115	-
15	CLA	a1	412	13	-	4/15/91/115	-
15	CLA	b1	416	-	-	11/21/97/115	-
18	BCR	a4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	813	1	-	8/26/102/115	-
15	CLA	a1	408	13	-	6/39/115/115	-
15	CLA	aA	817	-	-	6/20/96/115	-
15	CLA	c3	403	13	-	13/39/115/115	-
15	CLA	b1	412	13	-	9/15/91/115	-
15	CLA	aB	842	-	-	2/15/91/115	-
16	PQN	cA	845	-	-	5/23/43/43	0/2/2/2
15	CLA	b4	416	-	-	11/21/97/115	-
15	CLA	a2	404	13	-	12/39/115/115	-
15	CLA	b1	408	13	-	5/15/91/115	-
18	BCR	c2	421	-	-	12/29/63/63	0/2/2/2
18	BCR	c6	403	-	-	13/29/63/63	0/2/2/2
18	BCR	aM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	831	2	-	8/15/91/115	-
15	CLA	bF	201	-	-	10/15/91/115	-
15	CLA	aA	827	22	-	10/39/115/115	-
15	CLA	bX	102	12	-	8/15/91/115	-
15	CLA	aA	832	1	-	8/21/97/115	-
15	CLA	cA	824	1	-	14/23/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	803	-	-	16/39/115/115	-

All (6339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	aA	846	PQN	C3-C2	6.92	1.47	1.35
16	bA	846	PQN	C3-C2	6.88	1.47	1.35
16	cA	845	PQN	C3-C2	6.86	1.47	1.35
16	cB	843	PQN	C3-C2	6.78	1.47	1.35
16	aB	843	PQN	C3-C2	6.78	1.47	1.35
16	bB	843	PQN	C3-C2	6.77	1.47	1.35
15	b6	418	CLA	C3B-C4B	5.52	1.55	1.42
15	a6	418	CLA	C3B-C4B	5.49	1.55	1.42
15	a2	418	CLA	C3B-C4B	5.49	1.55	1.42
15	c6	419	CLA	C3B-C4B	5.48	1.55	1.42
15	b2	418	CLA	C3B-C4B	5.47	1.55	1.42
15	c2	418	CLA	C3B-C4B	5.42	1.55	1.42
15	b5	417	CLA	C3B-C4B	5.33	1.55	1.42
15	b4	417	CLA	C3B-C4B	5.33	1.55	1.42
15	c5	417	CLA	C3B-C4B	5.32	1.55	1.42
15	b3	417	CLA	C3B-C4B	5.32	1.55	1.42
15	a5	417	CLA	C3B-C4B	5.31	1.55	1.42
15	a3	417	CLA	C3B-C4B	5.30	1.55	1.42
15	a4	417	CLA	C3B-C4B	5.30	1.55	1.42
15	c4	417	CLA	C3B-C4B	5.27	1.55	1.42
15	c3	417	CLA	C3B-C4B	5.26	1.55	1.42
15	b1	417	CLA	C3B-C4B	5.18	1.54	1.42
15	c1	417	CLA	C3B-C4B	5.14	1.54	1.42
15	a1	416	CLA	C3B-C4B	5.07	1.54	1.42
15	b2	418	CLA	C1D-ND	4.97	1.43	1.37
14	aA	801	CL0	C1B-NB	-4.95	1.31	1.37
15	c6	419	CLA	C1D-ND	4.93	1.43	1.37
14	bA	801	CL0	C1B-NB	-4.92	1.31	1.37
15	b6	418	CLA	C1D-ND	4.91	1.43	1.37
14	cA	801	CL0	C1B-NB	-4.89	1.31	1.37
15	a6	418	CLA	C1D-ND	4.86	1.43	1.37
15	a2	418	CLA	C1D-ND	4.83	1.43	1.37
15	c1	417	CLA	C1D-ND	4.74	1.43	1.37
15	c2	418	CLA	C1D-ND	4.72	1.43	1.37
15	a1	416	CLA	C1D-ND	4.71	1.43	1.37
15	b1	417	CLA	C1D-ND	4.69	1.43	1.37
14	aA	801	CL0	O2D-CGD	4.68	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	801	CL0	O2D-CGD	4.68	1.44	1.33
14	bA	801	CL0	O2D-CGD	4.67	1.44	1.33
15	a3	417	CLA	C1D-ND	4.63	1.43	1.37
15	aA	806	CLA	C4D-ND	-4.63	1.31	1.37
15	cA	806	CLA	C4D-ND	-4.61	1.31	1.37
15	bA	806	CLA	C4D-ND	-4.61	1.31	1.37
14	bA	801	CL0	C3C-C2C	4.61	1.46	1.36
15	b3	417	CLA	C1D-ND	4.60	1.43	1.37
14	cA	801	CL0	C3C-C2C	4.59	1.46	1.36
14	aA	801	CL0	C3C-C2C	4.59	1.46	1.36
15	b4	417	CLA	C4B-NB	4.55	1.43	1.37
15	c4	417	CLA	C4B-NB	4.54	1.43	1.37
15	c3	417	CLA	C1D-ND	4.54	1.43	1.37
14	aA	801	CL0	C4B-NB	-4.52	1.32	1.37
14	bA	801	CL0	C4B-NB	-4.51	1.32	1.37
15	c2	405	CLA	C1D-ND	4.49	1.43	1.37
15	bB	802	CLA	C4D-ND	-4.49	1.31	1.37
15	b3	417	CLA	C4B-NB	4.48	1.43	1.37
15	c3	417	CLA	C4B-NB	4.48	1.43	1.37
15	a4	417	CLA	C4B-NB	4.48	1.43	1.37
15	c5	417	CLA	C1D-ND	4.47	1.43	1.37
15	b2	405	CLA	C1D-ND	4.46	1.43	1.37
15	a2	405	CLA	C1D-ND	4.46	1.43	1.37
15	a2	418	CLA	C4B-NB	4.46	1.43	1.37
15	b5	417	CLA	C1D-ND	4.45	1.43	1.37
14	cA	801	CL0	C4B-NB	-4.45	1.32	1.37
15	a5	417	CLA	C1D-ND	4.45	1.43	1.37
15	b2	418	CLA	C4B-NB	4.45	1.43	1.37
15	cB	802	CLA	C4D-ND	-4.44	1.31	1.37
15	c2	418	CLA	C4B-NB	4.43	1.43	1.37
15	aB	802	CLA	C4D-ND	-4.43	1.31	1.37
15	b6	418	CLA	C4B-NB	4.42	1.43	1.37
15	b6	406	CLA	C1D-ND	4.42	1.43	1.37
15	cA	840	CLA	C4D-ND	-4.40	1.31	1.37
15	c6	419	CLA	C4B-NB	4.39	1.43	1.37
15	a6	418	CLA	C4B-NB	4.39	1.43	1.37
15	a6	406	CLA	C1D-ND	4.39	1.43	1.37
15	bA	840	CLA	C4D-ND	-4.37	1.31	1.37
15	aA	840	CLA	C4D-ND	-4.37	1.31	1.37
15	c4	417	CLA	C1D-ND	4.36	1.43	1.37
15	c6	407	CLA	C1D-ND	4.36	1.43	1.37
15	bA	834	CLA	C4D-ND	-4.34	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	417	CLA	C4B-NB	4.34	1.43	1.37
15	aL	203	CLA	C4D-ND	-4.34	1.31	1.37
15	cA	802	CLA	C4D-ND	-4.34	1.31	1.37
15	cB	806	CLA	C4D-ND	-4.34	1.31	1.37
15	aA	834	CLA	C4D-ND	-4.34	1.31	1.37
15	a5	417	CLA	C4B-NB	4.34	1.43	1.37
15	bB	804	CLA	C4D-ND	-4.33	1.31	1.37
15	aL	202	CLA	C4D-ND	-4.33	1.31	1.37
15	aB	807	CLA	C4D-ND	-4.32	1.31	1.37
15	bL	204	CLA	C4D-ND	-4.32	1.31	1.37
15	a4	417	CLA	C1D-ND	4.31	1.43	1.37
15	cB	828	CLA	C4D-ND	-4.31	1.31	1.37
15	aB	804	CLA	C4D-ND	-4.31	1.31	1.37
15	b5	417	CLA	C4B-NB	4.31	1.43	1.37
15	bL	203	CLA	C4D-ND	-4.30	1.31	1.37
15	b4	417	CLA	C1D-ND	4.30	1.43	1.37
15	bB	806	CLA	C4D-ND	-4.30	1.31	1.37
15	aA	843	CLA	C4D-ND	-4.30	1.31	1.37
15	cB	807	CLA	C4D-ND	-4.30	1.31	1.37
15	cA	831	CLA	CMB-C2B	-4.29	1.41	1.50
15	bA	831	CLA	CMB-C2B	-4.29	1.41	1.50
15	aA	831	CLA	CMB-C2B	-4.29	1.41	1.50
15	c5	417	CLA	C4B-NB	4.29	1.43	1.37
15	cA	834	CLA	C4D-ND	-4.29	1.31	1.37
15	cL	203	CLA	C4D-ND	-4.29	1.31	1.37
15	cL	204	CLA	C4D-ND	-4.29	1.31	1.37
15	bA	843	CLA	C4D-ND	-4.29	1.31	1.37
15	cB	804	CLA	C4D-ND	-4.29	1.31	1.37
15	aB	828	CLA	C4D-ND	-4.29	1.31	1.37
15	aB	806	CLA	C4D-ND	-4.28	1.31	1.37
15	b1	417	CLA	C4B-NB	4.28	1.43	1.37
15	aA	802	CLA	C4D-ND	-4.28	1.31	1.37
15	bB	828	CLA	C4D-ND	-4.28	1.31	1.37
15	bB	807	CLA	C4D-ND	-4.26	1.31	1.37
15	cA	839	CLA	C4D-ND	-4.25	1.31	1.37
15	bA	802	CLA	C4D-ND	-4.24	1.31	1.37
15	cA	842	CLA	C4D-ND	-4.24	1.31	1.37
15	c2	417	CLA	C4D-ND	-4.23	1.31	1.37
15	aA	839	CLA	C4D-ND	-4.23	1.31	1.37
15	c1	417	CLA	C4B-NB	4.23	1.43	1.37
15	b2	417	CLA	C4D-ND	-4.23	1.31	1.37
15	bA	839	CLA	C4D-ND	-4.23	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	405	CLA	C1D-ND	4.21	1.43	1.37
15	bA	833	CLA	C4D-ND	-4.21	1.31	1.37
15	cA	807	CLA	C4D-ND	-4.20	1.31	1.37
15	bB	803	CLA	C4D-ND	-4.20	1.31	1.37
15	a2	417	CLA	C4D-ND	-4.19	1.31	1.37
15	aA	814	CLA	C4D-ND	-4.19	1.31	1.37
15	aA	833	CLA	C4D-ND	-4.18	1.32	1.37
15	cB	836	CLA	C4D-ND	-4.18	1.32	1.37
15	cB	837	CLA	C4D-ND	-4.17	1.32	1.37
15	aA	845	CLA	C4D-ND	-4.17	1.32	1.37
15	aA	813	CLA	C4D-ND	-4.17	1.32	1.37
15	aB	837	CLA	C4D-ND	-4.16	1.32	1.37
15	bL	202	CLA	C4D-ND	-4.16	1.32	1.37
15	c3	405	CLA	C1D-ND	4.16	1.42	1.37
15	bB	837	CLA	C4D-ND	-4.16	1.32	1.37
15	bA	807	CLA	C4D-ND	-4.16	1.32	1.37
15	aB	803	CLA	C4D-ND	-4.16	1.32	1.37
15	bB	819	CLA	C4D-ND	-4.16	1.32	1.37
15	aB	838	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	833	CLA	C4D-ND	-4.15	1.32	1.37
15	aL	201	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	827	CLA	C4D-ND	-4.15	1.32	1.37
15	cB	803	CLA	C4D-ND	-4.15	1.32	1.37
15	a4	405	CLA	C1D-ND	4.15	1.42	1.37
15	bA	845	CLA	C4D-ND	-4.15	1.32	1.37
15	cA	844	CLA	C4D-ND	-4.15	1.32	1.37
15	b3	405	CLA	C1D-ND	4.15	1.42	1.37
15	bB	836	CLA	C4D-ND	-4.14	1.32	1.37
15	cB	838	CLA	C4D-ND	-4.14	1.32	1.37
15	aA	807	CLA	C4D-ND	-4.14	1.32	1.37
15	bA	838	CLA	C4D-ND	-4.14	1.32	1.37
15	b4	405	CLA	C1D-ND	4.14	1.42	1.37
15	cA	814	CLA	C4D-ND	-4.13	1.32	1.37
15	aB	830	CLA	CMB-C2B	-4.13	1.42	1.50
15	cB	819	CLA	C4D-ND	-4.13	1.32	1.37
15	bA	814	CLA	C4D-ND	-4.13	1.32	1.37
15	b1	405	CLA	C1D-ND	4.13	1.42	1.37
15	bA	827	CLA	C4D-ND	-4.13	1.32	1.37
15	aB	836	CLA	C4D-ND	-4.12	1.32	1.37
15	bA	813	CLA	C4D-ND	-4.12	1.32	1.37
15	b5	405	CLA	C1D-ND	4.12	1.42	1.37
15	c1	405	CLA	C1D-ND	4.12	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	838	CLA	C4D-ND	-4.11	1.32	1.37
15	c4	405	CLA	C1D-ND	4.11	1.42	1.37
15	a5	405	CLA	C1D-ND	4.11	1.42	1.37
15	cA	813	CLA	C4D-ND	-4.11	1.32	1.37
15	cL	202	CLA	C4D-ND	-4.11	1.32	1.37
15	cB	830	CLA	CMB-C2B	-4.11	1.42	1.50
18	bB	850	BCR	C30-C25	-4.10	1.48	1.53
15	aB	819	CLA	C4D-ND	-4.10	1.32	1.37
15	cA	838	CLA	C4D-ND	-4.10	1.32	1.37
15	b4	416	CLA	C4D-ND	-4.10	1.32	1.37
15	c3	416	CLA	C4D-ND	-4.09	1.32	1.37
18	cB	849	BCR	C30-C25	-4.09	1.48	1.53
19	aA	853	LHG	O7-C5	-4.09	1.36	1.46
15	a1	416	CLA	C4B-NB	4.08	1.42	1.37
15	a3	416	CLA	C4D-ND	-4.08	1.32	1.37
15	bB	830	CLA	CMB-C2B	-4.08	1.42	1.50
15	aA	827	CLA	C4D-ND	-4.08	1.32	1.37
15	aA	838	CLA	C4D-ND	-4.07	1.32	1.37
15	a1	404	CLA	C1D-ND	4.07	1.42	1.37
15	c5	405	CLA	C1D-ND	4.07	1.42	1.37
19	cA	852	LHG	O7-C5	-4.06	1.36	1.46
15	b3	416	CLA	C4D-ND	-4.06	1.32	1.37
19	bA	854	LHG	O7-C5	-4.06	1.36	1.46
15	aB	813	CLA	C4D-ND	-4.06	1.32	1.37
15	a4	416	CLA	C4D-ND	-4.05	1.32	1.37
15	cB	832	CLA	C4D-ND	-4.05	1.32	1.37
15	c4	416	CLA	C4D-ND	-4.05	1.32	1.37
15	aB	832	CLA	C4D-ND	-4.05	1.32	1.37
15	cB	813	CLA	C4D-ND	-4.05	1.32	1.37
15	bB	832	CLA	C4D-ND	-4.04	1.32	1.37
18	aB	849	BCR	C30-C25	-4.04	1.48	1.53
15	aB	827	CLA	C4D-ND	-4.04	1.32	1.37
16	bA	846	PQN	C10-C5	4.04	1.47	1.40
15	cB	833	CLA	C4D-ND	-4.03	1.32	1.37
15	bB	833	CLA	C4D-ND	-4.03	1.32	1.37
15	bB	840	CLA	C4D-ND	-4.03	1.32	1.37
15	cB	827	CLA	C4D-ND	-4.01	1.32	1.37
15	bB	827	CLA	C4D-ND	-4.01	1.32	1.37
15	aB	810	CLA	C4D-ND	-4.00	1.32	1.37
15	bB	810	CLA	C4D-ND	-4.00	1.32	1.37
15	bB	813	CLA	C4D-ND	-4.00	1.32	1.37
15	cB	840	CLA	C4D-ND	-3.99	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	416	CLA	C4D-ND	-3.98	1.32	1.37
18	b4	418	BCR	C30-C25	-3.98	1.48	1.53
15	cA	829	CLA	C4D-ND	-3.98	1.32	1.37
18	cB	848	BCR	C30-C25	-3.98	1.48	1.53
15	a5	416	CLA	C4D-ND	-3.98	1.32	1.37
18	a4	418	BCR	C30-C25	-3.98	1.48	1.53
16	aA	846	PQN	C10-C5	3.97	1.47	1.40
16	cA	845	PQN	C10-C5	3.96	1.47	1.40
15	aA	828	CLA	C4D-ND	-3.96	1.32	1.37
15	aB	833	CLA	C4D-ND	-3.95	1.32	1.37
15	aB	840	CLA	C4D-ND	-3.95	1.32	1.37
15	bA	831	CLA	C4D-ND	-3.95	1.32	1.37
15	bA	828	CLA	C4D-ND	-3.94	1.32	1.37
15	cB	810	CLA	C4D-ND	-3.94	1.32	1.37
15	aB	811	CLA	C4D-ND	-3.94	1.32	1.37
15	aA	819	CLA	C4D-ND	-3.93	1.32	1.37
15	cA	819	CLA	C4D-ND	-3.93	1.32	1.37
15	bA	829	CLA	C4D-ND	-3.92	1.32	1.37
15	cA	828	CLA	C4D-ND	-3.92	1.32	1.37
18	aB	848	BCR	C30-C25	-3.91	1.48	1.53
18	c4	418	BCR	C30-C25	-3.91	1.48	1.53
18	c2	419	BCR	C30-C25	-3.91	1.48	1.53
15	c5	416	CLA	C4D-ND	-3.91	1.32	1.37
15	bB	811	CLA	C4D-ND	-3.91	1.32	1.37
15	a6	416	CLA	C1D-ND	3.91	1.42	1.37
15	cA	831	CLA	C4D-ND	-3.90	1.32	1.37
15	c6	418	CLA	C4D-ND	-3.90	1.32	1.37
15	aA	829	CLA	C4D-ND	-3.90	1.32	1.37
15	bA	803	CLA	C4D-ND	-3.90	1.32	1.37
15	cA	803	CLA	C4D-ND	-3.90	1.32	1.37
18	bB	848	BCR	C30-C25	-3.90	1.48	1.53
15	c1	412	CLA	C1D-ND	3.90	1.42	1.37
15	aA	830	CLA	C4D-ND	-3.90	1.32	1.37
15	cB	811	CLA	C4D-ND	-3.90	1.32	1.37
15	b6	422	CLA	C4B-NB	3.89	1.42	1.37
15	b6	416	CLA	C1D-ND	3.89	1.42	1.37
15	a6	417	CLA	C4D-ND	-3.89	1.32	1.37
15	b6	414	CLA	C1D-ND	3.89	1.42	1.37
18	b1	418	BCR	C30-C25	-3.89	1.48	1.53
15	bA	830	CLA	C4D-ND	-3.88	1.32	1.37
18	a3	418	BCR	C30-C25	-3.88	1.48	1.53
15	bA	819	CLA	C4D-ND	-3.88	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	416	CLA	C4D-ND	-3.88	1.32	1.37
15	aA	826	CLA	C4D-ND	-3.88	1.32	1.37
15	a1	415	CLA	C4D-ND	-3.88	1.32	1.37
15	b6	417	CLA	C4D-ND	-3.88	1.32	1.37
15	cB	839	CLA	C4D-ND	-3.88	1.32	1.37
15	a1	411	CLA	C1D-ND	3.88	1.42	1.37
15	c6	417	CLA	C1D-ND	3.87	1.42	1.37
15	bA	823	CLA	C4D-ND	-3.87	1.32	1.37
15	bB	818	CLA	C4D-ND	-3.87	1.32	1.37
15	cA	830	CLA	C4D-ND	-3.87	1.32	1.37
15	bB	839	CLA	C4D-ND	-3.87	1.32	1.37
15	aA	831	CLA	C4D-ND	-3.87	1.32	1.37
18	c3	418	BCR	C30-C25	-3.87	1.48	1.53
18	c1	418	BCR	C30-C25	-3.87	1.48	1.53
14	cA	801	CL0	O2A-CGA	3.87	1.44	1.33
15	aA	803	CLA	C4D-ND	-3.87	1.32	1.37
15	aB	821	CLA	C4D-ND	-3.86	1.32	1.37
18	a2	419	BCR	C30-C25	-3.86	1.48	1.53
15	cB	814	CLA	C4D-ND	-3.86	1.32	1.37
15	b1	412	CLA	C1D-ND	3.86	1.42	1.37
14	aA	801	CL0	O2A-CGA	3.86	1.44	1.33
15	cB	821	CLA	C4D-ND	-3.86	1.32	1.37
15	bA	826	CLA	C4D-ND	-3.86	1.32	1.37
15	b1	416	CLA	C4D-ND	-3.85	1.32	1.37
14	bA	801	CL0	O2A-CGA	3.85	1.44	1.33
18	a1	417	BCR	C30-C25	-3.85	1.48	1.53
15	aA	823	CLA	C4D-ND	-3.85	1.32	1.37
15	cK	102	CLA	C4D-ND	-3.84	1.32	1.37
15	c6	415	CLA	C1D-ND	3.84	1.42	1.37
15	aB	814	CLA	C4D-ND	-3.84	1.32	1.37
15	cA	812	CLA	C4D-ND	-3.84	1.32	1.37
15	aB	839	CLA	C4D-ND	-3.83	1.32	1.37
15	cA	823	CLA	C4D-ND	-3.83	1.32	1.37
15	a6	413	CLA	C1D-ND	3.83	1.42	1.37
15	b5	420	CLA	C4B-NB	3.83	1.42	1.37
18	b3	418	BCR	C30-C25	-3.83	1.48	1.53
15	cB	818	CLA	C4D-ND	-3.82	1.32	1.37
18	b2	419	BCR	C30-C25	-3.82	1.48	1.53
15	cA	826	CLA	C4D-ND	-3.82	1.32	1.37
15	bB	814	CLA	C4D-ND	-3.82	1.32	1.37
18	a6	419	BCR	C30-C25	-3.82	1.48	1.53
15	a4	421	CLA	C4B-NB	3.81	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	413	CLA	C1D-ND	3.81	1.42	1.37
15	aA	812	CLA	C4D-ND	-3.81	1.32	1.37
15	aB	818	CLA	C4D-ND	-3.81	1.32	1.37
15	c6	419	CLA	CHC-C1C	3.80	1.46	1.38
15	cA	820	CLA	C4D-ND	-3.80	1.32	1.37
15	bK	101	CLA	C4D-ND	-3.80	1.32	1.37
15	aK	102	CLA	C4D-ND	-3.80	1.32	1.37
16	aB	843	PQN	C10-C5	3.80	1.47	1.40
15	bB	821	CLA	C4D-ND	-3.80	1.32	1.37
15	b6	413	CLA	C1D-ND	3.80	1.42	1.37
15	a5	420	CLA	C4B-NB	3.79	1.42	1.37
18	b6	419	BCR	C30-C25	-3.79	1.48	1.53
15	cB	825	CLA	C4D-ND	-3.78	1.32	1.37
15	bB	825	CLA	C4D-ND	-3.78	1.32	1.37
15	bA	812	CLA	C4D-ND	-3.78	1.32	1.37
15	bA	820	CLA	C4D-ND	-3.78	1.32	1.37
15	b4	421	CLA	C4B-NB	3.78	1.42	1.37
16	bB	843	PQN	C10-C5	3.78	1.46	1.40
15	c5	420	CLA	C4B-NB	3.77	1.42	1.37
15	c2	406	CLA	C4B-NB	3.77	1.42	1.37
15	aA	820	CLA	C4D-ND	-3.76	1.32	1.37
15	c1	407	CLA	C1D-ND	3.76	1.42	1.37
15	cA	822	CLA	C4D-ND	-3.76	1.32	1.37
15	a6	422	CLA	C4B-NB	3.75	1.42	1.37
18	cI	102	BCR	C30-C25	-3.75	1.48	1.53
15	a5	417	CLA	CHC-C1C	3.75	1.46	1.38
15	c4	412	CLA	C1D-ND	3.75	1.42	1.37
18	a5	418	BCR	C30-C25	-3.75	1.48	1.53
16	cB	843	PQN	C10-C5	3.74	1.46	1.40
15	bX	102	CLA	C4D-ND	-3.74	1.32	1.37
15	b2	406	CLA	C4B-NB	3.74	1.42	1.37
15	a6	418	CLA	CHC-C1C	3.74	1.46	1.38
15	b6	418	CLA	CHC-C1C	3.74	1.46	1.38
18	c6	420	BCR	C30-C25	-3.74	1.48	1.53
15	a2	406	CLA	C4B-NB	3.74	1.42	1.37
15	b3	415	CLA	C1D-ND	3.74	1.42	1.37
18	c5	418	BCR	C30-C25	-3.73	1.48	1.53
15	aX	102	CLA	C4D-ND	-3.73	1.32	1.37
15	c6	414	CLA	C1D-ND	3.73	1.42	1.37
15	aA	822	CLA	C4D-ND	-3.73	1.32	1.37
18	b5	418	BCR	C30-C25	-3.73	1.48	1.53
18	bI	102	BCR	C30-C25	-3.73	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	417	CLA	CHC-C1C	3.72	1.46	1.38
15	bA	822	CLA	C4D-ND	-3.72	1.32	1.37
15	bB	830	CLA	C4D-ND	-3.72	1.32	1.37
15	b2	413	CLA	C1D-ND	3.72	1.42	1.37
15	cX	102	CLA	C4D-ND	-3.72	1.32	1.37
15	a6	415	CLA	C4B-NB	3.71	1.42	1.37
14	aA	801	CL0	CHC-C1C	3.71	1.46	1.38
18	aI	102	BCR	C30-C25	-3.71	1.48	1.53
18	bA	852	BCR	C30-C25	-3.71	1.48	1.53
15	c4	417	CLA	CHC-C1C	3.70	1.46	1.38
14	bA	801	CL0	CHC-C1C	3.70	1.46	1.38
15	a2	413	CLA	C1D-ND	3.70	1.42	1.37
15	b4	417	CLA	CHC-C1C	3.70	1.46	1.38
15	b5	417	CLA	CHC-C1C	3.69	1.46	1.38
15	cB	829	CLA	C4D-ND	-3.69	1.32	1.37
15	c5	417	CLA	CHC-C1C	3.69	1.46	1.38
15	cB	830	CLA	C4D-ND	-3.69	1.32	1.37
15	a5	415	CLA	C1D-ND	3.69	1.42	1.37
15	c5	415	CLA	C1D-ND	3.69	1.42	1.37
15	c6	416	CLA	C4B-NB	3.69	1.42	1.37
15	c2	416	CLA	C1D-ND	3.69	1.42	1.37
15	bB	842	CLA	C1D-ND	3.69	1.42	1.37
15	aB	825	CLA	C4D-ND	-3.68	1.32	1.37
15	b6	405	CLA	C1D-ND	3.68	1.42	1.37
15	a6	405	CLA	C1D-ND	3.68	1.42	1.37
14	cA	801	CL0	CHC-C1C	3.68	1.46	1.38
15	aA	833	CLA	C1B-NB	-3.68	1.33	1.37
15	cA	802	CLA	CMB-C2B	-3.67	1.43	1.50
15	c4	421	CLA	C4B-NB	3.67	1.42	1.37
15	a2	422	CLA	C4D-ND	-3.67	1.32	1.37
18	cJ	103	BCR	C1-C6	-3.67	1.48	1.53
15	b4	412	CLA	C1D-ND	3.67	1.42	1.37
15	a2	416	CLA	C1D-ND	3.67	1.42	1.37
15	a1	406	CLA	C1D-ND	3.67	1.42	1.37
15	b1	407	CLA	C1D-ND	3.67	1.42	1.37
15	bB	829	CLA	C4D-ND	-3.67	1.32	1.37
18	cA	850	BCR	C30-C25	-3.67	1.48	1.53
15	a3	417	CLA	CHC-C1C	3.67	1.46	1.38
15	b2	416	CLA	C1D-ND	3.67	1.42	1.37
15	b6	415	CLA	C4B-NB	3.67	1.42	1.37
15	a3	414	CLA	C4B-NB	3.66	1.42	1.37
15	c3	417	CLA	CHC-C1C	3.66	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	802	CLA	CMB-C2B	-3.66	1.43	1.50
15	a4	415	CLA	C4D-ND	-3.66	1.32	1.37
15	bA	833	CLA	C1B-NB	-3.66	1.33	1.37
15	bA	804	CLA	C4D-ND	-3.66	1.32	1.37
15	aB	829	CLA	C4D-ND	-3.66	1.32	1.37
15	a3	415	CLA	C1D-ND	3.66	1.42	1.37
18	bJ	103	BCR	C1-C6	-3.66	1.48	1.53
18	aA	851	BCR	C30-C25	-3.65	1.48	1.53
15	cA	833	CLA	C1B-NB	-3.65	1.33	1.37
15	bA	808	CLA	C4D-ND	-3.65	1.32	1.37
15	cA	805	CLA	C4D-ND	-3.65	1.32	1.37
15	bA	802	CLA	CMB-C2B	-3.65	1.43	1.50
15	aA	805	CLA	C4D-ND	-3.65	1.32	1.37
15	a5	407	CLA	C1D-ND	3.65	1.42	1.37
15	c6	416	CLA	C1D-ND	3.65	1.42	1.37
15	bA	809	CLA	C4D-ND	-3.65	1.32	1.37
15	b1	414	CLA	C4B-NB	3.64	1.42	1.37
15	cB	842	CLA	C1D-ND	3.64	1.42	1.37
15	c1	414	CLA	C4B-NB	3.64	1.42	1.37
15	b2	422	CLA	C4D-ND	-3.64	1.32	1.37
15	bA	821	CLA	C4D-ND	-3.64	1.32	1.37
15	b3	417	CLA	CHC-C1C	3.64	1.45	1.38
15	bB	824	CLA	C1D-ND	3.64	1.42	1.37
15	aA	804	CLA	C4D-ND	-3.64	1.32	1.37
15	cB	801	CLA	C4D-ND	-3.64	1.32	1.37
15	bA	805	CLA	C4D-ND	-3.64	1.32	1.37
15	cA	808	CLA	C4D-ND	-3.64	1.32	1.37
15	b6	415	CLA	C1D-ND	3.64	1.42	1.37
15	bA	831	CLA	MG-NB	-3.64	1.98	2.05
15	c1	417	CLA	CHC-C1C	3.64	1.45	1.38
15	aB	842	CLA	C1D-ND	3.64	1.42	1.37
15	a3	421	CLA	C4B-NB	3.64	1.42	1.37
15	b5	415	CLA	C1D-ND	3.64	1.42	1.37
15	c6	409	CLA	C1D-ND	3.63	1.42	1.37
15	aB	830	CLA	C4D-ND	-3.63	1.32	1.37
15	aB	830	CLA	C1B-NB	-3.63	1.33	1.37
15	cA	809	CLA	C4D-ND	-3.63	1.32	1.37
18	bL	205	BCR	C30-C25	-3.63	1.48	1.53
15	b5	414	CLA	C1D-ND	3.63	1.42	1.37
15	b5	414	CLA	C4B-NB	3.63	1.42	1.37
15	bB	801	CLA	C4D-ND	-3.63	1.32	1.37
14	cA	801	CL0	CHD-C1D	3.63	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	830	CLA	C1B-NB	-3.63	1.33	1.37
14	bA	801	CL0	CHD-C1D	3.62	1.45	1.38
15	b1	417	CLA	CHC-C1C	3.62	1.45	1.38
15	aA	821	CLA	C4D-ND	-3.62	1.32	1.37
18	aJ	204	BCR	C1-C6	-3.62	1.48	1.53
15	a2	418	CLA	CHC-C1C	3.62	1.45	1.38
15	aB	801	CLA	C4D-ND	-3.62	1.32	1.37
15	aA	831	CLA	MG-NB	-3.62	1.98	2.05
15	b3	421	CLA	C4B-NB	3.62	1.42	1.37
15	aA	836	CLA	C4D-ND	-3.62	1.32	1.37
15	c5	407	CLA	C1D-ND	3.61	1.42	1.37
15	c6	401	CLA	C4B-NB	3.61	1.42	1.37
15	cA	821	CLA	C4D-ND	-3.61	1.32	1.37
15	aA	808	CLA	C4D-ND	-3.61	1.32	1.37
15	cA	836	CLA	C4D-ND	-3.61	1.32	1.37
15	c2	408	CLA	C1D-ND	3.61	1.42	1.37
15	b1	404	CLA	C1D-ND	3.61	1.42	1.37
15	c5	412	CLA	C1D-ND	3.61	1.42	1.37
15	a6	415	CLA	C1D-ND	3.61	1.42	1.37
15	c4	415	CLA	C1D-ND	3.61	1.42	1.37
15	bB	820	CLA	C4D-ND	-3.61	1.32	1.37
18	bJ	104	BCR	C1-C6	-3.61	1.48	1.53
15	bA	825	CLA	C4D-ND	-3.61	1.32	1.37
14	aA	801	CL0	CHD-C1D	3.61	1.45	1.38
15	a1	413	CLA	C4B-NB	3.60	1.42	1.37
15	a4	412	CLA	C1D-ND	3.60	1.42	1.37
15	c2	422	CLA	C4D-ND	-3.60	1.32	1.37
15	a5	414	CLA	C4B-NB	3.60	1.42	1.37
15	b1	414	CLA	C1D-ND	3.60	1.42	1.37
15	cA	831	CLA	MG-NB	-3.60	1.98	2.05
15	cA	804	CLA	C4D-ND	-3.60	1.32	1.37
15	c5	414	CLA	C1D-ND	3.60	1.42	1.37
15	a6	408	CLA	C1D-ND	3.60	1.42	1.37
15	bB	818	CLA	C1D-ND	3.60	1.42	1.37
15	b5	407	CLA	C1D-ND	3.60	1.42	1.37
15	aB	804	CLA	CMC-C2C	-3.60	1.43	1.50
15	c3	415	CLA	C1D-ND	3.60	1.42	1.37
15	aA	825	CLA	C4D-ND	-3.60	1.32	1.37
15	aB	831	CLA	C4D-ND	-3.60	1.32	1.37
15	b6	408	CLA	C1D-ND	3.60	1.42	1.37
15	b3	407	CLA	C4D-ND	-3.59	1.32	1.37
15	aA	809	CLA	C4D-ND	-3.59	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	cJ	104	BCR	C1-C6	-3.59	1.48	1.53
15	bB	803	CLA	MG-NB	-3.59	1.98	2.05
15	a3	409	CLA	C4D-ND	-3.59	1.32	1.37
15	bB	817	CLA	C4D-ND	-3.59	1.32	1.37
15	b4	415	CLA	C1D-ND	3.59	1.42	1.37
15	aB	805	CLA	C4D-ND	-3.59	1.32	1.37
15	cB	824	CLA	C1D-ND	3.59	1.42	1.37
15	aA	818	CLA	C4D-ND	-3.59	1.32	1.37
15	bB	804	CLA	CMC-C2C	-3.59	1.43	1.50
15	aB	820	CLA	C4D-ND	-3.59	1.32	1.37
15	c3	421	CLA	C4B-NB	3.58	1.42	1.37
15	c2	418	CLA	CHC-C1C	3.58	1.45	1.38
15	b4	415	CLA	C4D-ND	-3.58	1.32	1.37
15	a3	411	CLA	C4D-ND	-3.58	1.32	1.37
15	b2	418	CLA	CHC-C1C	3.58	1.45	1.38
15	a3	407	CLA	C4D-ND	-3.58	1.32	1.37
15	cB	804	CLA	CMC-C2C	-3.58	1.43	1.50
15	aB	824	CLA	C1D-ND	3.58	1.42	1.37
15	cA	811	CLA	C4D-ND	-3.58	1.32	1.37
15	bA	802	CLA	MG-NB	-3.58	1.98	2.05
15	cA	825	CLA	C4D-ND	-3.58	1.32	1.37
18	aJ	205	BCR	C1-C6	-3.58	1.48	1.53
15	bB	805	CLA	C4D-ND	-3.57	1.32	1.37
15	cA	841	CLA	C4B-NB	3.57	1.42	1.37
15	cB	817	CLA	C4D-ND	-3.57	1.32	1.37
15	cB	831	CLA	C4D-ND	-3.57	1.32	1.37
15	cB	803	CLA	MG-NB	-3.57	1.98	2.05
15	aB	818	CLA	C1D-ND	3.57	1.42	1.37
18	aK	101	BCR	C1-C6	-3.57	1.48	1.53
15	a6	422	CLA	C2A-C1A	3.57	1.60	1.52
15	aA	841	CLA	C4B-NB	3.57	1.42	1.37
15	aJ	201	CLA	C4D-ND	-3.57	1.32	1.37
15	cB	830	CLA	C1B-NB	-3.57	1.33	1.37
15	b5	412	CLA	C1D-ND	3.56	1.42	1.37
15	c1	414	CLA	C1D-ND	3.56	1.42	1.37
15	b2	408	CLA	C1D-ND	3.56	1.42	1.37
18	cK	101	BCR	C1-C6	-3.56	1.48	1.53
18	bA	848	BCR	C1-C6	-3.56	1.48	1.53
15	c2	415	CLA	C4B-NB	3.56	1.42	1.37
15	aA	811	CLA	C4D-ND	-3.56	1.32	1.37
15	aB	808	CLA	C4D-ND	-3.56	1.32	1.37
15	aB	809	CLA	C4D-ND	-3.56	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	407	CLA	C4D-ND	-3.56	1.32	1.37
15	a2	408	CLA	C1D-ND	3.56	1.42	1.37
15	bA	841	CLA	C4B-NB	3.56	1.42	1.37
15	c6	406	CLA	C1D-ND	3.56	1.42	1.37
15	cB	812	CLA	C4D-ND	-3.56	1.32	1.37
15	a1	416	CLA	CHC-C1C	3.55	1.45	1.38
20	cB	850	LMG	O1-C7	-3.55	1.37	1.43
15	b3	414	CLA	C4B-NB	3.55	1.42	1.37
18	aI	103	BCR	C30-C25	-3.55	1.48	1.53
18	bJ	104	BCR	C30-C25	-3.55	1.48	1.53
18	cL	205	BCR	C30-C25	-3.55	1.48	1.53
15	c1	404	CLA	C1D-ND	3.55	1.42	1.37
15	bA	841	CLA	C4D-ND	-3.55	1.32	1.37
15	c5	414	CLA	C4B-NB	3.55	1.42	1.37
15	a1	413	CLA	C1D-ND	3.54	1.42	1.37
15	c4	414	CLA	C4B-NB	3.54	1.42	1.37
20	aB	850	LMG	O1-C7	-3.54	1.37	1.43
15	cB	805	CLA	C4D-ND	-3.54	1.32	1.37
15	bA	811	CLA	C4D-ND	-3.54	1.32	1.37
15	cB	824	CLA	C4D-ND	-3.54	1.32	1.37
18	aJ	205	BCR	C30-C25	-3.54	1.48	1.53
15	cB	820	CLA	C4D-ND	-3.54	1.32	1.37
15	cF	203	CLA	C4D-ND	-3.54	1.32	1.37
15	b2	415	CLA	C4B-NB	3.54	1.42	1.37
15	c3	415	CLA	C4D-ND	-3.53	1.32	1.37
15	aB	803	CLA	MG-NB	-3.53	1.98	2.05
15	bA	836	CLA	C4D-ND	-3.53	1.32	1.37
15	aA	824	CLA	C4D-ND	-3.53	1.32	1.37
15	aB	817	CLA	C4D-ND	-3.53	1.32	1.37
15	bB	812	CLA	C4D-ND	-3.53	1.32	1.37
15	c4	414	CLA	C1D-ND	3.53	1.42	1.37
15	b5	411	CLA	C4D-ND	-3.53	1.32	1.37
15	bB	831	CLA	C4D-ND	-3.53	1.32	1.37
15	c3	411	CLA	C4D-ND	-3.53	1.32	1.37
15	c2	415	CLA	C1D-ND	3.52	1.42	1.37
15	b2	402	CLA	C1D-ND	3.52	1.42	1.37
15	c1	402	CLA	C1D-ND	3.52	1.42	1.37
15	a1	403	CLA	C1D-ND	3.52	1.42	1.37
15	a4	414	CLA	C4B-NB	3.52	1.42	1.37
15	a4	415	CLA	C1D-ND	3.52	1.42	1.37
15	aB	822	CLA	C4D-ND	-3.52	1.32	1.37
15	aB	824	CLA	C4D-ND	-3.52	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	405	CLA	C1D-ND	3.52	1.42	1.37
15	a5	414	CLA	C1D-ND	3.52	1.42	1.37
15	cA	802	CLA	MG-NB	-3.52	1.98	2.05
15	a3	412	CLA	C1D-ND	3.52	1.42	1.37
15	cB	809	CLA	C4D-ND	-3.52	1.32	1.37
20	bB	851	LMG	O1-C7	-3.52	1.37	1.43
15	a3	415	CLA	C4D-ND	-3.52	1.32	1.37
15	b4	404	CLA	C4D-ND	-3.52	1.32	1.37
15	a2	415	CLA	C4B-NB	3.52	1.42	1.37
15	c4	415	CLA	C4D-ND	-3.51	1.32	1.37
15	b6	403	CLA	C1D-ND	3.51	1.42	1.37
15	bB	822	CLA	C4D-ND	-3.51	1.32	1.37
15	c3	414	CLA	C4B-NB	3.51	1.42	1.37
15	b3	411	CLA	C4D-ND	-3.51	1.32	1.37
15	a5	411	CLA	C4D-ND	-3.51	1.32	1.37
15	a2	404	CLA	C1D-ND	3.51	1.42	1.37
15	b4	414	CLA	C4B-NB	3.51	1.42	1.37
18	cJ	104	BCR	C30-C25	-3.51	1.48	1.53
15	bB	809	CLA	C4D-ND	-3.51	1.32	1.37
15	cB	818	CLA	C1D-ND	3.51	1.42	1.37
15	b3	409	CLA	C4D-ND	-3.51	1.32	1.37
15	c4	413	CLA	C1D-ND	3.51	1.42	1.37
15	bF	201	CLA	C4D-ND	-3.51	1.32	1.37
15	aB	822	CLA	C1D-ND	3.51	1.42	1.37
15	b2	407	CLA	C1D-ND	3.50	1.42	1.37
15	cA	827	CLA	CMD-C2D	-3.50	1.43	1.50
15	aA	802	CLA	MG-NB	-3.50	1.98	2.05
15	cB	822	CLA	C4D-ND	-3.50	1.32	1.37
15	a2	415	CLA	C1D-ND	3.50	1.42	1.37
15	cB	822	CLA	C1D-ND	3.50	1.42	1.37
15	bB	808	CLA	C4D-ND	-3.50	1.32	1.37
15	aB	812	CLA	C4D-ND	-3.50	1.32	1.37
15	cB	808	CLA	C4D-ND	-3.50	1.32	1.37
15	cA	841	CLA	C4D-ND	-3.49	1.32	1.37
15	bA	818	CLA	C4D-ND	-3.49	1.32	1.37
15	b5	402	CLA	C1D-ND	3.49	1.42	1.37
15	c5	411	CLA	C4D-ND	-3.49	1.32	1.37
15	b4	414	CLA	C1D-ND	3.49	1.42	1.37
15	cA	824	CLA	C4D-ND	-3.49	1.32	1.37
15	bA	824	CLA	C4D-ND	-3.49	1.32	1.37
15	b6	407	CLA	C1D-ND	3.49	1.42	1.37
18	a3	418	BCR	C1-C6	-3.49	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	818	CLA	C4D-ND	-3.49	1.32	1.37
15	c3	409	CLA	C4D-ND	-3.49	1.32	1.37
15	bB	816	CLA	C1D-ND	3.48	1.42	1.37
15	aA	827	CLA	CMD-C2D	-3.48	1.43	1.50
15	a5	402	CLA	C1D-ND	3.48	1.42	1.37
15	c1	415	CLA	C1D-ND	3.48	1.42	1.37
15	aA	816	CLA	C4D-ND	-3.48	1.32	1.37
15	c4	404	CLA	C4D-ND	-3.48	1.32	1.37
15	bB	822	CLA	C1D-ND	3.48	1.42	1.37
15	bA	810	CLA	C4D-ND	-3.48	1.32	1.37
15	cB	830	CLA	MG-NB	-3.48	1.98	2.05
15	b1	415	CLA	C1D-ND	3.48	1.42	1.37
15	a6	403	CLA	C1D-ND	3.48	1.42	1.37
15	c2	422	CLA	C4B-NB	3.47	1.42	1.37
18	c3	418	BCR	C1-C6	-3.47	1.49	1.53
15	bA	827	CLA	CMD-C2D	-3.47	1.43	1.50
15	bB	810	CLA	CMB-C2B	-3.47	1.43	1.50
15	a3	412	CLA	C4D-ND	-3.47	1.32	1.37
15	b2	404	CLA	C1D-ND	3.47	1.42	1.37
15	c1	406	CLA	C1D-ND	3.47	1.42	1.37
15	aB	816	CLA	C1D-ND	3.47	1.42	1.37
15	b1	402	CLA	C1D-ND	3.47	1.42	1.37
15	b2	415	CLA	C1D-ND	3.47	1.42	1.37
15	a5	406	CLA	C1D-ND	3.47	1.42	1.37
15	a5	412	CLA	C1D-ND	3.47	1.42	1.37
15	c4	404	CLA	C1D-ND	3.47	1.42	1.37
15	c2	407	CLA	C1D-ND	3.47	1.42	1.37
15	b3	412	CLA	C4D-ND	-3.47	1.32	1.37
15	cA	810	CLA	C4D-ND	-3.47	1.32	1.37
15	aB	841	CLA	C4D-ND	-3.47	1.32	1.37
15	c5	402	CLA	C1D-ND	3.47	1.42	1.37
15	aB	826	CLA	C4D-ND	-3.46	1.32	1.37
15	aA	838	CLA	MG-NB	-3.46	1.98	2.05
15	a6	422	CLA	C1D-ND	3.46	1.42	1.37
15	c2	404	CLA	C1D-ND	3.46	1.42	1.37
15	aA	817	CLA	C1D-ND	3.46	1.42	1.37
15	aB	810	CLA	CMB-C2B	-3.46	1.43	1.50
15	a4	414	CLA	C1D-ND	3.46	1.42	1.37
15	c2	402	CLA	C1D-ND	3.46	1.42	1.37
15	cB	810	CLA	CMB-C2B	-3.46	1.43	1.50
15	aA	831	CLA	C1B-NB	-3.46	1.33	1.37
15	bA	816	CLA	C4D-ND	-3.46	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a5	415	CLA	C4D-ND	-3.45	1.32	1.37
15	bB	830	CLA	MG-NB	-3.45	1.98	2.05
15	bA	832	CLA	C4D-ND	-3.45	1.32	1.37
15	bB	824	CLA	C4D-ND	-3.45	1.32	1.37
15	cB	836	CLA	MG-NB	-3.45	1.98	2.05
15	cB	816	CLA	C1D-ND	3.45	1.42	1.37
15	b3	415	CLA	C4D-ND	-3.45	1.33	1.37
15	cA	816	CLA	C4D-ND	-3.45	1.33	1.37
15	a1	401	CLA	C1D-ND	3.45	1.42	1.37
15	b5	415	CLA	C4D-ND	-3.45	1.33	1.37
15	a4	404	CLA	C4D-ND	-3.45	1.33	1.37
15	cJ	101	CLA	C1D-ND	3.45	1.42	1.37
15	a4	409	CLA	C4D-ND	-3.45	1.33	1.37
15	b5	406	CLA	C1D-ND	3.45	1.42	1.37
15	b3	421	CLA	C4D-ND	-3.45	1.33	1.37
15	bJ	101	CLA	C1D-ND	3.44	1.42	1.37
15	aA	832	CLA	C4D-ND	-3.44	1.33	1.37
15	a4	407	CLA	C4D-ND	-3.44	1.33	1.37
15	c6	404	CLA	C1D-ND	3.44	1.42	1.37
15	cA	840	CLA	MG-NB	-3.44	1.99	2.05
15	b3	413	CLA	C1D-ND	3.44	1.42	1.37
18	b3	418	BCR	C1-C6	-3.44	1.49	1.53
15	b2	413	CLA	C4D-ND	-3.44	1.33	1.37
15	c6	408	CLA	C1D-ND	3.44	1.42	1.37
15	b6	422	CLA	C1D-ND	3.44	1.42	1.37
15	c4	407	CLA	C4D-ND	-3.44	1.33	1.37
15	aA	839	CLA	C1B-NB	-3.44	1.33	1.37
15	bB	826	CLA	C4D-ND	-3.44	1.33	1.37
15	cA	815	CLA	C4D-ND	-3.44	1.33	1.37
15	aB	830	CLA	MG-NB	-3.44	1.99	2.05
15	bA	838	CLA	MG-NB	-3.44	1.99	2.05
15	b2	408	CLA	C4D-ND	-3.44	1.33	1.37
15	b3	412	CLA	C1D-ND	3.43	1.42	1.37
15	cA	816	CLA	C1D-ND	3.43	1.42	1.37
15	bB	841	CLA	C4D-ND	-3.43	1.33	1.37
15	b3	404	CLA	C1D-ND	3.43	1.42	1.37
15	cA	838	CLA	MG-NB	-3.43	1.99	2.05
15	aJ	202	CLA	C1D-ND	3.43	1.42	1.37
15	c3	412	CLA	C1D-ND	3.43	1.42	1.37
15	c4	411	CLA	C1D-ND	3.43	1.42	1.37
15	a2	422	CLA	C4B-NB	3.43	1.42	1.37
15	cA	839	CLA	C1B-NB	-3.43	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	414	CLA	C1D-ND	3.43	1.42	1.37
15	c6	412	CLA	C1D-ND	3.43	1.42	1.37
15	c3	412	CLA	C4D-ND	-3.43	1.33	1.37
15	bA	840	CLA	MG-NB	-3.42	1.99	2.05
15	aA	841	CLA	C4D-ND	-3.42	1.33	1.37
15	cA	832	CLA	C4D-ND	-3.42	1.33	1.37
18	aF	201	BCR	C30-C25	-3.42	1.49	1.53
15	b1	406	CLA	C1D-ND	3.42	1.42	1.37
15	c2	413	CLA	C4D-ND	-3.42	1.33	1.37
15	c5	415	CLA	C4D-ND	-3.42	1.33	1.37
15	a6	407	CLA	C1D-ND	3.42	1.42	1.37
15	a2	402	CLA	C1D-ND	3.42	1.42	1.37
15	cA	817	CLA	C1D-ND	3.42	1.42	1.37
15	bA	815	CLA	C4D-ND	-3.42	1.33	1.37
15	aA	815	CLA	C4D-ND	-3.42	1.33	1.37
15	a6	413	CLA	C4D-ND	-3.42	1.33	1.37
15	b4	411	CLA	C1D-ND	3.42	1.42	1.37
15	a2	407	CLA	C1D-ND	3.42	1.42	1.37
15	c3	414	CLA	C1D-ND	3.41	1.42	1.37
15	b4	407	CLA	C4D-ND	-3.41	1.33	1.37
15	cB	841	CLA	C4D-ND	-3.41	1.33	1.37
15	b1	411	CLA	C1D-ND	3.41	1.42	1.37
15	bB	836	CLA	MG-NB	-3.41	1.99	2.05
15	bB	842	CLA	C4B-NB	3.41	1.42	1.37
15	b4	410	CLA	C1D-ND	3.41	1.42	1.37
15	b3	407	CLA	C1D-ND	3.41	1.42	1.37
15	b6	411	CLA	C1D-ND	3.41	1.42	1.37
15	b1	410	CLA	C1D-ND	3.41	1.42	1.37
15	b3	414	CLA	C1D-ND	3.41	1.42	1.37
15	b4	409	CLA	C4D-ND	-3.41	1.33	1.37
15	c4	411	CLA	C4D-ND	-3.41	1.33	1.37
15	c2	410	CLA	C4D-ND	-3.41	1.33	1.37
15	a6	411	CLA	C1D-ND	3.41	1.42	1.37
15	bA	831	CLA	C1B-NB	-3.41	1.33	1.37
15	b4	413	CLA	C1D-ND	3.41	1.42	1.37
15	b3	409	CLA	C1D-ND	3.40	1.42	1.37
15	bA	839	CLA	C1B-NB	-3.40	1.33	1.37
15	aB	836	CLA	MG-NB	-3.40	1.99	2.05
18	cF	202	BCR	C30-C25	-3.40	1.49	1.53
15	c4	409	CLA	C1D-ND	3.40	1.42	1.37
15	b4	411	CLA	C4D-ND	-3.40	1.33	1.37
15	c3	409	CLA	C1D-ND	3.40	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	407	CLA	C1D-ND	3.40	1.42	1.37
15	cB	826	CLA	C4D-ND	-3.40	1.33	1.37
15	a4	409	CLA	C1D-ND	3.40	1.42	1.37
15	a2	410	CLA	C4D-ND	-3.40	1.33	1.37
15	a4	410	CLA	C1D-ND	3.39	1.42	1.37
15	bA	816	CLA	C1D-ND	3.39	1.42	1.37
15	a4	411	CLA	C4D-ND	-3.39	1.33	1.37
15	c4	409	CLA	C4D-ND	-3.39	1.33	1.37
15	aA	810	CLA	C4D-ND	-3.39	1.33	1.37
15	b6	413	CLA	C4D-ND	-3.39	1.33	1.37
18	aB	844	BCR	C1-C6	-3.39	1.49	1.53
15	cA	831	CLA	C1B-NB	-3.39	1.33	1.37
15	b2	404	CLA	C4D-ND	-3.39	1.33	1.37
15	b6	410	CLA	C4D-ND	-3.39	1.33	1.37
15	a3	409	CLA	C1D-ND	3.39	1.42	1.37
15	bA	837	CLA	C1D-ND	3.39	1.42	1.37
15	aA	840	CLA	MG-NB	-3.39	1.99	2.05
15	c6	414	CLA	C4D-ND	-3.39	1.33	1.37
15	a5	410	CLA	C1D-ND	3.39	1.41	1.37
15	c4	410	CLA	C1D-ND	3.39	1.41	1.37
15	a2	413	CLA	C4D-ND	-3.39	1.33	1.37
15	b2	422	CLA	C4B-NB	3.39	1.41	1.37
15	a3	421	CLA	C4D-ND	-3.39	1.33	1.37
15	c2	416	CLA	C4D-ND	-3.38	1.33	1.37
15	b2	412	CLA	C1D-ND	3.38	1.41	1.37
15	c5	406	CLA	C1D-ND	3.38	1.41	1.37
15	a1	410	CLA	C1D-ND	3.38	1.41	1.37
18	cB	844	BCR	C1-C6	-3.38	1.49	1.53
15	b4	404	CLA	C1D-ND	3.38	1.41	1.37
15	aB	842	CLA	C4B-NB	3.38	1.41	1.37
15	b4	408	CLA	C4D-ND	-3.38	1.33	1.37
15	a4	404	CLA	C1D-ND	3.38	1.41	1.37
15	a4	413	CLA	C1D-ND	3.38	1.41	1.37
15	cA	835	CLA	C4D-ND	-3.37	1.33	1.37
15	c3	421	CLA	C4D-ND	-3.37	1.33	1.37
15	aA	816	CLA	C1D-ND	3.37	1.41	1.37
15	a2	408	CLA	C4D-ND	-3.37	1.33	1.37
15	aA	835	CLA	C4D-ND	-3.37	1.33	1.37
15	a5	409	CLA	C4D-ND	-3.37	1.33	1.37
15	b6	412	CLA	C4D-ND	-3.37	1.33	1.37
15	bA	815	CLA	C1D-ND	3.37	1.41	1.37
15	bA	817	CLA	C1D-ND	3.37	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	406	CLA	C4B-NB	3.37	1.41	1.37
15	b5	404	CLA	C1D-ND	3.37	1.41	1.37
15	a5	403	CLA	C4D-ND	-3.37	1.33	1.37
15	b2	416	CLA	C4D-ND	-3.37	1.33	1.37
15	c5	403	CLA	C4D-ND	-3.37	1.33	1.37
15	a6	405	CLA	C4B-NB	3.37	1.41	1.37
15	cA	837	CLA	C1D-ND	3.37	1.41	1.37
15	c2	408	CLA	C4D-ND	-3.37	1.33	1.37
15	b5	409	CLA	C4D-ND	-3.36	1.33	1.37
15	b1	409	CLA	C1D-ND	3.36	1.41	1.37
15	aA	837	CLA	C1D-ND	3.36	1.41	1.37
15	bA	835	CLA	C4D-ND	-3.36	1.33	1.37
15	b5	410	CLA	C1D-ND	3.36	1.41	1.37
15	c6	413	CLA	C4D-ND	-3.36	1.33	1.37
15	a4	411	CLA	C1D-ND	3.36	1.41	1.37
18	bB	849	BCR	C30-C25	-3.36	1.49	1.53
15	c1	411	CLA	C1D-ND	3.36	1.41	1.37
18	bB	844	BCR	C1-C6	-3.36	1.49	1.53
15	a3	413	CLA	C1D-ND	3.36	1.41	1.37
15	a4	407	CLA	C1D-ND	3.36	1.41	1.37
18	cA	849	BCR	C1-C6	-3.35	1.49	1.53
15	cA	815	CLA	C1D-ND	3.35	1.41	1.37
15	a3	404	CLA	C4D-ND	-3.35	1.33	1.37
15	aA	844	CLA	C4D-ND	-3.35	1.33	1.37
15	a4	408	CLA	C4D-ND	-3.35	1.33	1.37
15	c6	411	CLA	C4D-ND	-3.35	1.33	1.37
15	a5	416	CLA	MG-NB	-3.35	1.99	2.05
15	a3	414	CLA	C1D-ND	3.35	1.41	1.37
15	c2	411	CLA	C1D-ND	3.35	1.41	1.37
15	c3	404	CLA	C4D-ND	-3.35	1.33	1.37
18	b4	418	BCR	C1-C6	-3.35	1.49	1.53
15	aB	835	CLA	C4D-ND	-3.34	1.33	1.37
15	aB	829	CLA	CMD-C2D	-3.34	1.43	1.50
15	a3	407	CLA	C1D-ND	3.34	1.41	1.37
15	c5	409	CLA	C4D-ND	-3.34	1.33	1.37
15	b4	412	CLA	C4D-ND	-3.34	1.33	1.37
15	cB	842	CLA	C4B-NB	3.34	1.41	1.37
15	c2	412	CLA	C1D-ND	3.34	1.41	1.37
15	a4	412	CLA	C4D-ND	-3.34	1.33	1.37
15	cA	843	CLA	C4D-ND	-3.34	1.33	1.37
15	c1	403	CLA	C4D-ND	-3.34	1.33	1.37
15	b4	409	CLA	C1D-ND	3.34	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	405	CLA	C4B-NB	3.34	1.41	1.37
15	c6	401	CLA	C1D-ND	3.34	1.41	1.37
15	c4	407	CLA	C1D-ND	3.34	1.41	1.37
15	b6	410	CLA	C1D-ND	3.34	1.41	1.37
15	a6	410	CLA	C4D-ND	-3.34	1.33	1.37
15	aA	815	CLA	C1D-ND	3.33	1.41	1.37
15	cB	835	CLA	C4D-ND	-3.33	1.33	1.37
15	b2	410	CLA	C1D-ND	3.33	1.41	1.37
15	c6	413	CLA	C1D-ND	3.33	1.41	1.37
15	bA	844	CLA	C4D-ND	-3.33	1.33	1.37
15	a2	404	CLA	C4D-ND	-3.33	1.33	1.37
15	a2	416	CLA	C4D-ND	-3.33	1.33	1.37
15	a1	409	CLA	C1D-ND	3.33	1.41	1.37
15	b5	403	CLA	C4D-ND	-3.33	1.33	1.37
15	b3	402	CLA	C1D-ND	3.33	1.41	1.37
15	a2	414	CLA	C4D-ND	-3.33	1.33	1.37
15	bB	835	CLA	C4D-ND	-3.33	1.33	1.37
15	c3	413	CLA	C1D-ND	3.33	1.41	1.37
15	b5	404	CLA	C4D-ND	-3.32	1.33	1.37
15	c4	406	CLA	C1D-ND	3.32	1.41	1.37
15	a1	415	CLA	MG-NB	-3.32	1.99	2.05
15	a4	416	CLA	MG-NB	-3.32	1.99	2.05
15	b3	408	CLA	C4D-ND	-3.32	1.33	1.37
15	cA	817	CLA	C4D-ND	-3.32	1.33	1.37
15	c3	408	CLA	C4D-ND	-3.32	1.33	1.37
15	c5	416	CLA	MG-NB	-3.32	1.99	2.05
15	a1	410	CLA	C4D-ND	-3.32	1.33	1.37
15	c1	410	CLA	C1D-ND	3.32	1.41	1.37
15	c2	410	CLA	C1D-ND	3.32	1.41	1.37
15	c6	417	CLA	C4B-NB	3.32	1.41	1.37
15	c4	412	CLA	C4D-ND	-3.32	1.33	1.37
15	b5	416	CLA	MG-NB	-3.32	1.99	2.05
15	a3	411	CLA	C1D-ND	3.32	1.41	1.37
15	c3	403	CLA	C4D-ND	-3.32	1.33	1.37
15	bB	829	CLA	CMD-C2D	-3.32	1.43	1.50
15	a2	417	CLA	C1B-NB	-3.32	1.33	1.37
15	c3	404	CLA	C1D-ND	3.32	1.41	1.37
15	b1	411	CLA	C4D-ND	-3.32	1.33	1.37
15	aJ	201	CLA	MG-NB	-3.31	1.99	2.05
15	a2	414	CLA	C1D-ND	3.31	1.41	1.37
15	a6	412	CLA	C4D-ND	-3.31	1.33	1.37
15	c4	416	CLA	MG-NB	-3.31	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b1	419	BCR	C1-C6	-3.31	1.49	1.53
15	a2	410	CLA	C1D-ND	3.31	1.41	1.37
18	bB	850	BCR	C1-C6	-3.31	1.49	1.53
15	c5	410	CLA	C1D-ND	3.31	1.41	1.37
18	aF	201	BCR	C1-C6	-3.31	1.49	1.53
15	a3	403	CLA	C4D-ND	-3.31	1.33	1.37
15	bF	201	CLA	MG-NB	-3.31	1.99	2.05
15	b3	404	CLA	C4D-ND	-3.31	1.33	1.37
15	c2	406	CLA	C4D-ND	-3.31	1.33	1.37
15	a2	411	CLA	C1D-ND	3.31	1.41	1.37
15	b4	416	CLA	MG-NB	-3.31	1.99	2.05
15	c4	416	CLA	C1B-NB	-3.31	1.33	1.37
15	a4	406	CLA	C1D-ND	3.31	1.41	1.37
18	aA	850	BCR	C1-C6	-3.31	1.49	1.53
15	aA	837	CLA	C4D-ND	-3.31	1.33	1.37
15	b6	405	CLA	C4D-ND	-3.31	1.33	1.37
15	c5	404	CLA	C4D-ND	-3.30	1.33	1.37
15	a1	408	CLA	C4D-ND	-3.30	1.33	1.37
15	a2	412	CLA	C1D-ND	3.30	1.41	1.37
15	c5	412	CLA	C4D-ND	-3.30	1.33	1.37
15	b3	405	CLA	C4D-ND	-3.30	1.33	1.37
15	c2	414	CLA	C4D-ND	-3.30	1.33	1.37
15	c2	417	CLA	C1B-NB	-3.30	1.33	1.37
15	bA	817	CLA	C4D-ND	-3.30	1.33	1.37
15	b6	404	CLA	C4D-ND	-3.30	1.33	1.37
15	b2	414	CLA	C1D-ND	3.30	1.41	1.37
15	b3	406	CLA	C1D-ND	3.30	1.41	1.37
15	c5	404	CLA	C1D-ND	3.30	1.41	1.37
15	cB	817	CLA	CMC-C2C	-3.29	1.43	1.50
15	a6	412	CLA	C1D-ND	3.29	1.41	1.37
15	a1	402	CLA	C4D-ND	-3.29	1.33	1.37
15	b5	412	CLA	C4D-ND	-3.29	1.33	1.37
18	bA	851	BCR	C1-C6	-3.29	1.49	1.53
15	aA	825	CLA	C1D-ND	3.29	1.41	1.37
15	b1	403	CLA	C1D-ND	3.29	1.41	1.37
15	b6	412	CLA	C1D-ND	3.29	1.41	1.37
15	cB	829	CLA	CMD-C2D	-3.29	1.43	1.50
15	bA	837	CLA	C4D-ND	-3.29	1.33	1.37
15	c3	407	CLA	C1D-ND	3.29	1.41	1.37
15	c6	406	CLA	C4D-ND	-3.29	1.33	1.37
18	c6	421	BCR	C1-C6	-3.29	1.49	1.53
15	a4	416	CLA	C1B-NB	-3.29	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	402	CLA	C1D-ND	3.29	1.41	1.37
15	a6	416	CLA	C4B-NB	3.29	1.41	1.37
15	aB	834	CLA	C1D-ND	3.29	1.41	1.37
15	b4	406	CLA	C1D-ND	3.29	1.41	1.37
18	a1	418	BCR	C1-C6	-3.29	1.49	1.53
15	a2	406	CLA	C4D-ND	-3.29	1.33	1.37
15	b2	406	CLA	C4D-ND	-3.29	1.33	1.37
15	b1	413	CLA	C4B-NB	3.29	1.41	1.37
15	aA	804	CLA	CMD-C2D	-3.29	1.43	1.50
14	aA	801	CL0	CHD-C4C	3.29	1.46	1.39
15	c3	406	CLA	C4D-ND	-3.29	1.33	1.37
18	c4	418	BCR	C1-C6	-3.29	1.49	1.53
15	bA	842	CLA	C4D-ND	-3.29	1.33	1.37
18	aB	849	BCR	C1-C6	-3.29	1.49	1.53
15	c5	408	CLA	C4D-ND	-3.29	1.33	1.37
15	a6	405	CLA	C4D-ND	-3.28	1.33	1.37
18	cB	846	BCR	C30-C25	-3.28	1.49	1.53
15	b5	416	CLA	C1B-NB	-3.28	1.33	1.37
15	b2	410	CLA	C4D-ND	-3.28	1.33	1.37
15	cA	837	CLA	C4D-ND	-3.28	1.33	1.37
15	aA	842	CLA	CMD-C2D	-3.28	1.43	1.50
15	a3	405	CLA	C4D-ND	-3.28	1.33	1.37
15	c1	411	CLA	C4D-ND	-3.28	1.33	1.37
15	c6	411	CLA	C1D-ND	3.28	1.41	1.37
15	a5	412	CLA	C4D-ND	-3.28	1.33	1.37
15	b2	404	CLA	C4B-NB	3.28	1.41	1.37
15	cA	825	CLA	C1D-ND	3.28	1.41	1.37
15	b1	409	CLA	C4D-ND	-3.28	1.33	1.37
15	bB	841	CLA	C1D-ND	3.28	1.41	1.37
15	b2	411	CLA	C1D-ND	3.28	1.41	1.37
15	b2	417	CLA	C1B-NB	-3.28	1.33	1.37
15	a3	408	CLA	C4D-ND	-3.28	1.33	1.37
15	cF	203	CLA	MG-NB	-3.28	1.99	2.05
15	a3	413	CLA	C4D-ND	-3.27	1.33	1.37
14	cA	801	CL0	CHD-C4C	3.27	1.46	1.39
15	bA	842	CLA	CMD-C2D	-3.27	1.43	1.50
15	c2	414	CLA	C1D-ND	3.27	1.41	1.37
15	a5	404	CLA	C4D-ND	-3.27	1.33	1.37
15	a6	409	CLA	C1D-ND	3.27	1.41	1.37
15	a3	404	CLA	C1D-ND	3.27	1.41	1.37
15	a6	410	CLA	C1D-ND	3.27	1.41	1.37
15	bB	834	CLA	C1D-ND	3.27	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	817	CLA	CMC-C2C	-3.27	1.43	1.50
15	c2	404	CLA	C4D-ND	-3.27	1.33	1.37
15	bA	838	CLA	C1B-NB	-3.27	1.33	1.37
15	bA	804	CLA	CMD-C2D	-3.27	1.43	1.50
15	bA	813	CLA	C3B-C4B	3.27	1.50	1.42
15	a5	408	CLA	C4D-ND	-3.27	1.33	1.37
15	c3	413	CLA	C4D-ND	-3.27	1.33	1.37
18	cB	849	BCR	C1-C6	-3.27	1.49	1.53
14	bA	801	CL0	CHD-C4C	3.27	1.46	1.39
15	cF	201	CLA	C4D-ND	-3.27	1.33	1.37
15	a5	413	CLA	C1D-ND	3.27	1.41	1.37
15	b5	408	CLA	C4D-ND	-3.27	1.33	1.37
15	c6	410	CLA	C1D-ND	3.26	1.41	1.37
15	c1	409	CLA	C4D-ND	-3.26	1.33	1.37
15	aA	813	CLA	C3B-C4B	3.26	1.50	1.42
15	cF	201	CLA	CMD-C2D	-3.26	1.43	1.50
15	a3	402	CLA	C1D-ND	3.26	1.41	1.37
15	aA	835	CLA	C1D-ND	3.26	1.41	1.37
15	b6	416	CLA	C4B-NB	3.26	1.41	1.37
15	bA	825	CLA	C1D-ND	3.26	1.41	1.37
15	cA	804	CLA	CMD-C2D	-3.26	1.43	1.50
15	b4	402	CLA	C1D-ND	3.26	1.41	1.37
15	c4	414	CLA	C4D-ND	-3.26	1.33	1.37
15	c4	408	CLA	C4D-ND	-3.26	1.33	1.37
15	cA	838	CLA	C1B-NB	-3.26	1.33	1.37
18	a4	418	BCR	C1-C6	-3.26	1.49	1.53
15	aB	817	CLA	CMC-C2C	-3.26	1.43	1.50
15	c4	405	CLA	C4D-ND	-3.26	1.33	1.37
15	bA	835	CLA	C1D-ND	3.26	1.41	1.37
15	b2	409	CLA	C1D-ND	3.26	1.41	1.37
18	cF	202	BCR	C1-C6	-3.26	1.49	1.53
15	c1	406	CLA	C4B-NB	3.26	1.41	1.37
15	aA	842	CLA	C4D-ND	-3.26	1.33	1.37
15	c1	412	CLA	C4D-ND	-3.26	1.33	1.37
15	cA	813	CLA	C3B-C4B	3.25	1.50	1.42
15	b3	403	CLA	C4D-ND	-3.25	1.33	1.37
15	a3	406	CLA	C1D-ND	3.25	1.41	1.37
15	c3	405	CLA	C4D-ND	-3.25	1.33	1.37
15	cB	833	CLA	C4B-NB	3.25	1.41	1.37
15	c1	409	CLA	C4B-NB	3.25	1.41	1.37
15	c3	406	CLA	C1D-ND	3.25	1.41	1.37
15	b3	413	CLA	C4D-ND	-3.25	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	406	CLA	C4B-NB	3.25	1.41	1.37
15	c1	413	CLA	C4B-NB	3.25	1.41	1.37
15	aB	810	CLA	MG-NB	-3.25	1.99	2.05
15	bB	841	CLA	C4B-NB	3.25	1.41	1.37
15	a4	405	CLA	C4D-ND	-3.25	1.33	1.37
15	b1	403	CLA	C4D-ND	-3.25	1.33	1.37
15	b5	402	CLA	C4B-NB	3.25	1.41	1.37
15	c5	413	CLA	C1D-ND	3.25	1.41	1.37
15	c6	405	CLA	C4D-ND	-3.25	1.33	1.37
15	b3	406	CLA	C4D-ND	-3.25	1.33	1.37
15	b4	416	CLA	C1B-NB	-3.25	1.33	1.37
15	b2	414	CLA	C4D-ND	-3.24	1.33	1.37
15	c6	408	CLA	C4D-ND	-3.24	1.33	1.37
15	a5	416	CLA	C1B-NB	-3.24	1.33	1.37
15	cB	841	CLA	C1D-ND	3.24	1.41	1.37
18	a3	418	BCR	C38-C26	-3.24	1.45	1.50
15	cJ	102	CLA	C1D-ND	3.24	1.41	1.37
15	a4	403	CLA	C4D-ND	-3.24	1.33	1.37
15	a1	408	CLA	C1D-ND	3.24	1.41	1.37
15	aA	819	CLA	C1D-ND	3.24	1.41	1.37
15	b4	414	CLA	C4D-ND	-3.24	1.33	1.37
15	a4	402	CLA	C1D-ND	3.24	1.41	1.37
15	a2	406	CLA	C1D-ND	3.24	1.41	1.37
15	cA	835	CLA	C1D-ND	3.24	1.41	1.37
15	c3	411	CLA	C1D-ND	3.24	1.41	1.37
15	a1	407	CLA	C1D-ND	3.24	1.41	1.37
15	a1	408	CLA	C4B-NB	3.24	1.41	1.37
15	a1	402	CLA	C1D-ND	3.23	1.41	1.37
15	a2	404	CLA	C4B-NB	3.23	1.41	1.37
15	aB	834	CLA	C4D-ND	-3.23	1.33	1.37
15	bK	101	CLA	C1D-ND	3.23	1.41	1.37
15	c4	406	CLA	C4B-NB	3.23	1.41	1.37
15	a5	404	CLA	C1D-ND	3.23	1.41	1.37
15	aJ	203	CLA	C1D-ND	3.23	1.41	1.37
15	a1	411	CLA	C4D-ND	-3.23	1.33	1.37
15	a1	412	CLA	C4B-NB	3.23	1.41	1.37
15	b6	409	CLA	C1D-ND	3.23	1.41	1.37
15	aB	828	CLA	MG-NB	-3.23	1.99	2.05
15	a5	402	CLA	C4B-NB	3.23	1.41	1.37
15	aB	833	CLA	C4B-NB	3.23	1.41	1.37
15	a1	414	CLA	C4D-ND	-3.23	1.33	1.37
15	a2	417	CLA	MG-NB	-3.23	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	406	CLA	C4B-NB	3.23	1.41	1.37
18	c1	419	BCR	C1-C6	-3.23	1.49	1.53
15	bB	811	CLA	MG-NB	-3.23	1.99	2.05
18	c4	418	BCR	C38-C26	-3.23	1.45	1.50
15	a6	407	CLA	C4D-ND	-3.23	1.33	1.37
18	bB	846	BCR	C30-C25	-3.23	1.49	1.53
18	bM	101	BCR	C1-C6	-3.23	1.49	1.53
15	aB	841	CLA	C1D-ND	3.23	1.41	1.37
15	a4	406	CLA	C4B-NB	3.23	1.41	1.37
18	bB	849	BCR	C1-C6	-3.22	1.49	1.53
15	a5	406	CLA	C4D-ND	-3.22	1.33	1.37
15	c1	403	CLA	C1D-ND	3.22	1.41	1.37
15	c1	409	CLA	C1D-ND	3.22	1.41	1.37
15	c1	415	CLA	C4D-ND	-3.22	1.33	1.37
18	b6	420	BCR	C1-C6	-3.22	1.49	1.53
15	bJ	102	CLA	C1D-ND	3.22	1.41	1.37
15	b5	409	CLA	C1D-ND	3.22	1.41	1.37
15	cB	811	CLA	MG-NB	-3.22	1.99	2.05
15	bB	834	CLA	C4D-ND	-3.22	1.33	1.37
15	cB	834	CLA	C1D-ND	3.22	1.41	1.37
15	cB	841	CLA	C4B-NB	3.22	1.41	1.37
15	c4	402	CLA	C1D-ND	3.22	1.41	1.37
18	aM	101	BCR	C1-C6	-3.22	1.49	1.53
15	aA	817	CLA	C4D-ND	-3.22	1.33	1.37
15	c5	409	CLA	C1D-ND	3.22	1.41	1.37
15	b4	405	CLA	C4D-ND	-3.21	1.33	1.37
18	a4	418	BCR	C38-C26	-3.21	1.45	1.50
15	b5	413	CLA	C1D-ND	3.21	1.41	1.37
15	cB	828	CLA	MG-NB	-3.21	1.99	2.05
15	b3	406	CLA	C4B-NB	3.21	1.41	1.37
14	bA	801	CL0	CHB-C1B	3.21	1.46	1.39
15	a2	409	CLA	C1D-ND	3.21	1.41	1.37
18	aB	846	BCR	C30-C25	-3.21	1.49	1.53
18	b4	418	BCR	C38-C26	-3.21	1.45	1.50
15	bA	834	CLA	C1B-NB	-3.21	1.33	1.37
15	a1	412	CLA	C4D-ND	-3.21	1.33	1.37
15	a4	414	CLA	C4D-ND	-3.21	1.33	1.37
18	a6	420	BCR	C1-C6	-3.21	1.49	1.53
15	a3	406	CLA	C4D-ND	-3.21	1.33	1.37
15	c3	402	CLA	C4D-ND	-3.21	1.33	1.37
15	bB	832	CLA	MG-NB	-3.21	1.99	2.05
15	c1	416	CLA	MG-NB	-3.21	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	aB	846	BCR	C1-C6	-3.21	1.49	1.53
14	aA	801	CL0	CHB-C1B	3.20	1.46	1.39
15	b6	407	CLA	C4D-ND	-3.20	1.33	1.37
15	c1	407	CLA	C4D-ND	-3.20	1.33	1.37
15	c3	410	CLA	C1D-ND	3.20	1.41	1.37
15	c1	404	CLA	C4D-ND	-3.20	1.33	1.37
18	cM	101	BCR	C1-C6	-3.20	1.49	1.53
15	aB	811	CLA	MG-NB	-3.20	1.99	2.05
15	bB	811	CLA	C1D-ND	3.20	1.41	1.37
15	c1	408	CLA	C1D-ND	3.20	1.41	1.37
15	a5	408	CLA	C1D-ND	3.20	1.41	1.37
15	a5	411	CLA	C1D-ND	3.20	1.41	1.37
15	c4	403	CLA	C4D-ND	-3.20	1.33	1.37
15	b2	406	CLA	C1D-ND	3.20	1.41	1.37
15	a1	403	CLA	C4B-NB	3.20	1.41	1.37
15	bB	817	CLA	C1B-NB	-3.20	1.33	1.37
15	a6	404	CLA	C4D-ND	-3.20	1.33	1.37
15	bB	813	CLA	C3B-C4B	3.20	1.50	1.42
15	a5	409	CLA	C1D-ND	3.20	1.41	1.37
15	c5	402	CLA	C4B-NB	3.20	1.41	1.37
15	aA	838	CLA	C1B-NB	-3.20	1.33	1.37
15	cK	102	CLA	C1D-ND	3.20	1.41	1.37
15	bB	810	CLA	MG-NB	-3.20	1.99	2.05
15	c5	416	CLA	C1B-NB	-3.20	1.33	1.37
15	cA	834	CLA	C1B-NB	-3.19	1.33	1.37
15	c2	412	CLA	C4D-ND	-3.19	1.33	1.37
15	c2	409	CLA	C1D-ND	3.19	1.41	1.37
15	b1	415	CLA	C4D-ND	-3.19	1.33	1.37
15	c2	403	CLA	C4D-ND	-3.19	1.33	1.37
15	c2	406	CLA	C1D-ND	3.19	1.41	1.37
15	b4	413	CLA	C4D-ND	-3.19	1.33	1.37
18	b3	418	BCR	C38-C26	-3.19	1.45	1.50
15	c5	406	CLA	C4B-NB	3.19	1.41	1.37
15	cA	804	CLA	C3B-C4B	3.19	1.50	1.42
15	b1	412	CLA	C4D-ND	-3.19	1.33	1.37
14	cA	801	CL0	CHB-C1B	3.19	1.46	1.39
15	c1	404	CLA	C4B-NB	3.19	1.41	1.37
15	aA	834	CLA	C1B-NB	-3.19	1.33	1.37
15	aB	811	CLA	C1D-ND	3.19	1.41	1.37
15	a3	406	CLA	C4B-NB	3.19	1.41	1.37
15	c5	409	CLA	C4B-NB	3.19	1.41	1.37
18	bB	846	BCR	C1-C6	-3.19	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	413	CLA	C4D-ND	-3.19	1.33	1.37
15	b1	406	CLA	C4B-NB	3.19	1.41	1.37
15	b3	404	CLA	C4B-NB	3.19	1.41	1.37
15	c2	417	CLA	MG-NB	-3.19	1.99	2.05
18	cA	850	BCR	C1-C6	-3.19	1.49	1.53
15	b5	411	CLA	C1D-ND	3.19	1.41	1.37
15	cB	810	CLA	MG-NB	-3.19	1.99	2.05
15	bB	840	CLA	CMB-C2B	-3.18	1.44	1.50
15	bA	829	CLA	C1D-ND	3.18	1.41	1.37
15	bB	833	CLA	C4B-NB	3.18	1.41	1.37
15	b1	408	CLA	C1D-ND	3.18	1.41	1.37
15	c5	408	CLA	C1D-ND	3.18	1.41	1.37
15	aB	813	CLA	C3B-C4B	3.18	1.50	1.42
15	bA	844	CLA	C1D-ND	3.18	1.41	1.37
20	bB	851	LMG	O8-C9	-3.18	1.37	1.45
18	aA	851	BCR	C1-C6	-3.18	1.49	1.53
15	bA	839	CLA	MG-NB	-3.18	1.99	2.05
15	c2	403	CLA	C1D-ND	3.18	1.41	1.37
15	a4	406	CLA	C4D-ND	-3.18	1.33	1.37
15	cB	834	CLA	C4D-ND	-3.18	1.33	1.37
15	aB	832	CLA	MG-NB	-3.18	1.99	2.05
15	a5	406	CLA	C4B-NB	3.18	1.41	1.37
15	cB	832	CLA	MG-NB	-3.18	1.99	2.05
15	a2	412	CLA	C4D-ND	-3.18	1.33	1.37
15	b1	405	CLA	C4D-ND	-3.18	1.33	1.37
15	b2	409	CLA	C4D-ND	-3.18	1.33	1.37
15	cA	843	CLA	C1D-ND	3.18	1.41	1.37
18	aA	852	BCR	C30-C25	-3.18	1.49	1.53
18	cF	204	BCR	C1-C6	-3.18	1.49	1.53
15	bB	842	CLA	C4D-ND	-3.18	1.33	1.37
15	aK	102	CLA	C1D-ND	3.18	1.41	1.37
15	a2	409	CLA	C4D-ND	-3.18	1.33	1.37
15	b3	411	CLA	C1D-ND	3.18	1.41	1.37
15	c5	411	CLA	C1D-ND	3.18	1.41	1.37
15	b4	403	CLA	C4D-ND	-3.18	1.33	1.37
15	b6	417	CLA	MG-NB	-3.18	1.99	2.05
15	a3	404	CLA	C4B-NB	3.18	1.41	1.37
15	b1	409	CLA	C4B-NB	3.17	1.41	1.37
15	b4	406	CLA	C4D-ND	-3.17	1.33	1.37
15	a3	416	CLA	MG-NB	-3.17	1.99	2.05
18	bA	853	BCR	C30-C25	-3.17	1.49	1.53
18	b3	420	BCR	C1-C6	-3.17	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	405	CLA	C4B-NB	3.17	1.41	1.37
15	a5	407	CLA	C4D-ND	-3.17	1.33	1.37
15	a5	413	CLA	C4D-ND	-3.17	1.33	1.37
15	b2	417	CLA	MG-NB	-3.17	1.99	2.05
15	cB	816	CLA	C4D-ND	-3.17	1.33	1.37
15	c5	413	CLA	C4D-ND	-3.17	1.33	1.37
18	b1	420	BCR	C1-C6	-3.17	1.49	1.53
15	bA	819	CLA	C1D-ND	3.17	1.41	1.37
15	bA	804	CLA	C3B-C4B	3.17	1.50	1.42
15	b1	413	CLA	C4D-ND	-3.17	1.33	1.37
15	c6	418	CLA	MG-NB	-3.17	1.99	2.05
20	cB	850	LMG	O8-C9	-3.17	1.37	1.45
15	bB	816	CLA	C4D-ND	-3.17	1.33	1.37
15	cB	813	CLA	C3B-C4B	3.17	1.50	1.42
15	bB	828	CLA	MG-NB	-3.17	1.99	2.05
18	bA	852	BCR	C1-C6	-3.17	1.49	1.53
15	cB	840	CLA	CMB-C2B	-3.17	1.44	1.50
15	a6	422	CLA	C4D-ND	-3.17	1.33	1.37
15	b5	408	CLA	C1D-ND	3.17	1.41	1.37
15	c3	404	CLA	C4B-NB	3.17	1.41	1.37
18	b6	419	BCR	C1-C6	-3.17	1.49	1.53
20	aB	850	LMG	O8-C9	-3.17	1.37	1.45
15	c4	413	CLA	C4D-ND	-3.16	1.33	1.37
15	a1	406	CLA	C4D-ND	-3.16	1.33	1.37
15	b1	416	CLA	MG-NB	-3.16	1.99	2.05
15	b5	406	CLA	C4D-ND	-3.16	1.33	1.37
15	aA	844	CLA	C1D-ND	3.16	1.41	1.37
18	c3	418	BCR	C38-C26	-3.16	1.45	1.50
18	cA	847	BCR	C1-C6	-3.16	1.49	1.53
15	cB	842	CLA	C4D-ND	-3.16	1.33	1.37
15	c2	415	CLA	C4D-ND	-3.16	1.33	1.37
15	aA	804	CLA	C3B-C4B	3.16	1.50	1.42
15	aB	840	CLA	CMB-C2B	-3.16	1.44	1.50
15	aB	841	CLA	C4B-NB	3.16	1.41	1.37
18	cB	846	BCR	C1-C6	-3.16	1.49	1.53
15	a6	417	CLA	MG-NB	-3.16	1.99	2.05
15	cA	808	CLA	C1D-ND	3.16	1.41	1.37
15	aB	815	CLA	C1D-ND	3.16	1.41	1.37
15	c2	404	CLA	C4B-NB	3.16	1.41	1.37
15	c3	416	CLA	MG-NB	-3.16	1.99	2.05
15	b3	402	CLA	C4D-ND	-3.16	1.33	1.37
15	c5	405	CLA	C4D-ND	-3.16	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	803	CLA	C1B-NB	-3.16	1.33	1.37
15	b3	416	CLA	MG-NB	-3.16	1.99	2.05
15	b1	404	CLA	C4B-NB	3.16	1.41	1.37
15	b1	416	CLA	C1B-NB	-3.16	1.33	1.37
15	cA	819	CLA	C1D-ND	3.16	1.41	1.37
18	c5	418	BCR	C38-C26	-3.15	1.45	1.50
18	aA	848	BCR	C1-C6	-3.15	1.49	1.53
15	cB	801	CLA	C1D-ND	3.15	1.41	1.37
18	b5	418	BCR	C38-C26	-3.15	1.45	1.50
18	bA	849	BCR	C1-C6	-3.15	1.49	1.53
15	a2	417	CLA	MG-ND	-3.15	1.99	2.05
15	b2	403	CLA	C4D-ND	-3.15	1.33	1.37
15	b5	405	CLA	C4D-ND	-3.15	1.33	1.37
15	bB	815	CLA	C1D-ND	3.15	1.41	1.37
15	cA	839	CLA	MG-NB	-3.15	1.99	2.05
15	b1	407	CLA	C4D-ND	-3.15	1.33	1.37
15	c1	413	CLA	C4D-ND	-3.15	1.33	1.37
18	c1	420	BCR	C1-C6	-3.14	1.49	1.53
15	bX	102	CLA	C4B-NB	3.14	1.41	1.37
15	c2	412	CLA	C4B-NB	3.14	1.41	1.37
15	a3	402	CLA	C4D-ND	-3.14	1.33	1.37
15	c2	409	CLA	C4D-ND	-3.14	1.33	1.37
18	aI	103	BCR	C1-C6	-3.14	1.49	1.53
15	b5	409	CLA	C4B-NB	3.14	1.41	1.37
15	cA	829	CLA	C1D-ND	3.14	1.41	1.37
15	a3	410	CLA	C1D-ND	3.14	1.41	1.37
15	a6	411	CLA	C4D-ND	-3.14	1.33	1.37
15	aA	839	CLA	MG-NB	-3.14	1.99	2.05
15	bA	837	CLA	C4B-NB	3.14	1.41	1.37
14	aA	801	CL0	C1D-ND	3.14	1.41	1.37
15	a1	403	CLA	C4D-ND	-3.14	1.33	1.37
15	a2	403	CLA	C4D-ND	-3.14	1.33	1.37
15	b2	412	CLA	C4D-ND	-3.14	1.33	1.37
15	b5	407	CLA	C4D-ND	-3.14	1.33	1.37
15	cB	811	CLA	C1D-ND	3.14	1.41	1.37
15	c3	406	CLA	C4B-NB	3.14	1.41	1.37
15	c6	414	CLA	C3B-C4B	3.14	1.50	1.42
15	aB	808	CLA	C4B-NB	3.14	1.41	1.37
15	c6	410	CLA	C4D-ND	-3.14	1.33	1.37
15	aA	808	CLA	C1D-ND	3.14	1.41	1.37
15	bB	803	CLA	C1B-NB	-3.14	1.33	1.37
15	c2	417	CLA	MG-ND	-3.14	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	408	CLA	C4D-ND	-3.13	1.33	1.37
15	c4	406	CLA	C4D-ND	-3.13	1.33	1.37
15	aB	801	CLA	C1D-ND	3.13	1.41	1.37
15	cA	837	CLA	C4B-NB	3.13	1.41	1.37
15	bB	808	CLA	C4B-NB	3.13	1.41	1.37
15	b6	408	CLA	C4D-ND	-3.13	1.33	1.37
15	bA	842	CLA	C1D-ND	3.13	1.41	1.37
15	aB	833	CLA	C3B-C4B	3.13	1.50	1.42
15	b6	411	CLA	C4D-ND	-3.13	1.33	1.37
15	b5	402	CLA	C4D-ND	-3.13	1.33	1.37
15	a5	409	CLA	C4B-NB	3.13	1.41	1.37
15	b2	412	CLA	C4B-NB	3.13	1.41	1.37
18	a6	419	BCR	C1-C6	-3.13	1.49	1.53
18	bF	202	BCR	C1-C6	-3.13	1.49	1.53
15	aB	823	CLA	C4D-ND	-3.13	1.33	1.37
15	bA	833	CLA	MG-NB	-3.13	1.99	2.05
18	a5	418	BCR	C38-C26	-3.13	1.45	1.50
15	cB	808	CLA	C4B-NB	3.13	1.41	1.37
15	b5	413	CLA	C4D-ND	-3.13	1.33	1.37
18	a1	419	BCR	C1-C6	-3.13	1.49	1.53
15	c6	411	CLA	C4B-NB	3.13	1.41	1.37
15	cF	201	CLA	C1D-ND	3.12	1.41	1.37
15	a5	405	CLA	C4D-ND	-3.12	1.33	1.37
15	b6	406	CLA	C4D-ND	-3.12	1.33	1.37
15	c5	406	CLA	C4D-ND	-3.12	1.33	1.37
15	b6	416	CLA	C4D-ND	-3.12	1.33	1.37
15	aA	842	CLA	C1D-ND	3.12	1.41	1.37
15	a4	413	CLA	C4B-NB	3.12	1.41	1.37
15	aB	842	CLA	C4D-ND	-3.12	1.33	1.37
14	bA	801	CL0	C1D-ND	3.12	1.41	1.37
14	cA	801	CL0	C1D-ND	3.12	1.41	1.37
15	bA	808	CLA	C1D-ND	3.12	1.41	1.37
15	b4	411	CLA	C4B-NB	3.12	1.41	1.37
15	bB	823	CLA	C4D-ND	-3.12	1.33	1.37
15	b5	420	CLA	C1D-ND	3.12	1.41	1.37
15	cB	823	CLA	C4D-ND	-3.12	1.33	1.37
15	c5	404	CLA	C4B-NB	3.12	1.41	1.37
15	a6	416	CLA	C4D-ND	-3.12	1.33	1.37
18	c2	419	BCR	C38-C26	-3.12	1.45	1.50
15	cA	837	CLA	C3B-C4B	3.12	1.50	1.42
15	b6	404	CLA	C1D-ND	3.12	1.41	1.37
15	c6	417	CLA	C4D-ND	-3.11	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	837	CLA	C4B-NB	3.11	1.41	1.37
18	aF	202	BCR	C1-C6	-3.11	1.49	1.53
14	cA	801	CL0	C3D-C4D	-3.11	1.37	1.44
15	c5	402	CLA	C4D-ND	-3.11	1.33	1.37
15	b6	413	CLA	C3B-C4B	3.11	1.50	1.42
15	bB	801	CLA	C1D-ND	3.11	1.41	1.37
15	cA	834	CLA	MG-NB	-3.11	1.99	2.05
18	a2	419	BCR	C38-C26	-3.11	1.45	1.50
15	aA	814	CLA	C1D-ND	3.11	1.41	1.37
15	bB	833	CLA	C3B-C4B	3.11	1.50	1.42
15	aB	814	CLA	C3B-C4B	3.11	1.50	1.42
15	bA	837	CLA	C3B-C4B	3.11	1.50	1.42
15	a2	403	CLA	C1D-ND	3.11	1.41	1.37
15	c5	407	CLA	C4D-ND	-3.11	1.33	1.37
15	bA	807	CLA	C1B-NB	-3.11	1.34	1.37
15	aB	816	CLA	C4D-ND	-3.11	1.33	1.37
18	aI	101	BCR	C1-C6	-3.11	1.49	1.53
15	aB	802	CLA	MG-NB	-3.11	1.99	2.05
15	c3	414	CLA	C4D-ND	-3.11	1.33	1.37
18	a5	418	BCR	C1-C6	-3.11	1.49	1.53
15	c6	418	CLA	C1B-NB	-3.10	1.34	1.37
15	aA	837	CLA	C3B-C4B	3.10	1.50	1.42
15	a5	404	CLA	C4B-NB	3.10	1.41	1.37
15	bA	814	CLA	C1D-ND	3.10	1.41	1.37
15	c6	405	CLA	C1D-ND	3.10	1.41	1.37
18	cI	101	BCR	C1-C6	-3.10	1.49	1.53
15	cB	833	CLA	C3B-C4B	3.10	1.50	1.42
15	a1	401	CLA	C4D-ND	-3.10	1.33	1.37
15	bA	841	CLA	C1D-ND	3.10	1.41	1.37
15	a2	411	CLA	C4D-ND	-3.10	1.33	1.37
15	b6	414	CLA	C4B-NB	3.10	1.41	1.37
15	bA	828	CLA	CMC-C2C	-3.10	1.44	1.50
18	a3	420	BCR	C1-C6	-3.10	1.49	1.53
15	cA	833	CLA	MG-NB	-3.10	1.99	2.05
15	cB	802	CLA	MG-NB	-3.10	1.99	2.05
15	b3	410	CLA	C4D-ND	-3.10	1.33	1.37
15	aA	833	CLA	MG-NB	-3.10	1.99	2.05
15	bA	834	CLA	MG-NB	-3.10	1.99	2.05
15	a4	403	CLA	C1D-ND	3.10	1.41	1.37
15	b1	404	CLA	C4D-ND	-3.10	1.33	1.37
15	b2	403	CLA	C1D-ND	3.10	1.41	1.37
15	cA	828	CLA	CMC-C2C	-3.10	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	813	CLA	C4B-NB	3.10	1.41	1.37
15	b3	410	CLA	C1D-ND	3.10	1.41	1.37
15	c6	415	CLA	C4B-NB	3.10	1.41	1.37
15	b1	406	CLA	C4D-ND	-3.10	1.33	1.37
18	c6	420	BCR	C1-C6	-3.10	1.49	1.53
18	a2	419	BCR	C1-C6	-3.09	1.49	1.53
18	c2	419	BCR	C1-C6	-3.09	1.49	1.53
15	cA	827	CLA	MG-NB	-3.09	1.99	2.05
15	aA	807	CLA	C1B-NB	-3.09	1.34	1.37
15	aA	807	CLA	MG-NB	-3.09	1.99	2.05
15	cA	807	CLA	C1B-NB	-3.09	1.34	1.37
15	a3	414	CLA	C4D-ND	-3.09	1.33	1.37
15	a2	412	CLA	C4B-NB	3.09	1.41	1.37
15	cB	814	CLA	C3B-C4B	3.09	1.50	1.42
18	c5	418	BCR	C1-C6	-3.09	1.49	1.53
15	a5	420	CLA	C1D-ND	3.09	1.41	1.37
15	cB	803	CLA	C1B-NB	-3.09	1.34	1.37
15	a6	413	CLA	C3B-C4B	3.09	1.50	1.42
15	aX	102	CLA	C4B-NB	3.09	1.41	1.37
15	b2	415	CLA	C4D-ND	-3.09	1.33	1.37
15	a3	416	CLA	CMD-C2D	-3.09	1.44	1.50
18	bI	101	BCR	C1-C6	-3.09	1.49	1.53
15	a2	407	CLA	C4D-ND	-3.09	1.33	1.37
15	bA	843	CLA	C4B-NB	3.09	1.41	1.37
18	c3	420	BCR	C1-C6	-3.08	1.49	1.53
15	aA	824	CLA	C1D-ND	3.08	1.41	1.37
15	b6	414	CLA	C4D-ND	-3.08	1.33	1.37
20	aB	850	LMG	O7-C8	-3.08	1.38	1.46
15	bB	814	CLA	C3B-C4B	3.08	1.50	1.42
18	b2	419	BCR	C38-C26	-3.08	1.45	1.50
18	a1	417	BCR	C1-C6	-3.08	1.49	1.53
15	a4	416	CLA	MG-ND	-3.08	1.99	2.05
15	cB	823	CLA	C1D-ND	3.08	1.41	1.37
15	b4	402	CLA	C4D-ND	-3.08	1.33	1.37
15	c6	407	CLA	C4D-ND	-3.08	1.33	1.37
15	c4	416	CLA	MG-ND	-3.08	1.99	2.05
15	b2	407	CLA	C4D-ND	-3.08	1.33	1.37
15	bB	802	CLA	MG-NB	-3.08	1.99	2.05
15	a5	412	CLA	C3B-C4B	3.08	1.50	1.42
18	bA	850	BCR	C30-C25	-3.08	1.49	1.53
18	cA	851	BCR	C30-C25	-3.08	1.49	1.53
15	cB	815	CLA	C1D-ND	3.08	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c4	413	CLA	C4B-NB	3.08	1.41	1.37
15	aA	827	CLA	MG-NB	-3.08	1.99	2.05
15	cA	841	CLA	C1D-ND	3.08	1.41	1.37
15	c1	405	CLA	C4D-ND	-3.07	1.33	1.37
18	bL	205	BCR	C1-C6	-3.07	1.49	1.53
14	bA	801	CL0	C3D-C4D	-3.07	1.37	1.44
15	bB	831	CLA	C1D-ND	3.07	1.41	1.37
15	b4	416	CLA	MG-ND	-3.07	1.99	2.05
15	a1	404	CLA	C4D-ND	-3.07	1.33	1.37
18	b5	419	BCR	C1-C6	-3.07	1.49	1.53
18	c6	420	BCR	C38-C26	-3.07	1.45	1.50
15	c4	404	CLA	C4B-NB	3.07	1.41	1.37
15	c5	412	CLA	C3B-C4B	3.07	1.49	1.42
15	a6	409	CLA	C4D-ND	-3.07	1.33	1.37
15	b3	414	CLA	C4D-ND	-3.07	1.33	1.37
20	cB	850	LMG	O7-C8	-3.07	1.38	1.46
15	c2	407	CLA	C4B-NB	3.07	1.41	1.37
15	a2	415	CLA	C4D-ND	-3.07	1.33	1.37
18	c5	419	BCR	C1-C6	-3.07	1.49	1.53
15	b6	417	CLA	C1B-NB	-3.07	1.34	1.37
15	cX	102	CLA	C4B-NB	3.07	1.41	1.37
15	c6	409	CLA	C4D-ND	-3.07	1.33	1.37
15	c6	412	CLA	C4D-ND	-3.07	1.33	1.37
15	aB	817	CLA	C1B-NB	-3.07	1.34	1.37
15	aB	831	CLA	C1D-ND	3.07	1.41	1.37
15	b2	407	CLA	C4B-NB	3.07	1.41	1.37
15	a6	406	CLA	C4D-ND	-3.07	1.33	1.37
15	b5	404	CLA	C4B-NB	3.07	1.41	1.37
15	bB	819	CLA	MG-NB	-3.07	1.99	2.05
15	c1	402	CLA	C4D-ND	-3.07	1.33	1.37
15	c4	402	CLA	C4D-ND	-3.07	1.33	1.37
18	a6	419	BCR	C38-C26	-3.07	1.45	1.50
15	aA	829	CLA	C1D-ND	3.06	1.41	1.37
15	a2	407	CLA	C4B-NB	3.06	1.41	1.37
15	bA	807	CLA	MG-NB	-3.06	1.99	2.05
18	aA	849	BCR	C30-C25	-3.06	1.49	1.53
15	a1	410	CLA	C4B-NB	3.06	1.41	1.37
15	b2	402	CLA	C4B-NB	3.06	1.41	1.37
15	b6	410	CLA	C4B-NB	3.06	1.41	1.37
15	c2	411	CLA	C4D-ND	-3.06	1.33	1.37
15	b3	416	CLA	CMD-C2D	-3.06	1.44	1.50
15	cJ	101	CLA	C4D-ND	-3.06	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	407	CLA	C4D-ND	-3.06	1.33	1.37
15	a6	414	CLA	C1D-ND	3.06	1.41	1.37
15	cA	824	CLA	C1D-ND	3.06	1.41	1.37
15	b6	409	CLA	C4D-ND	-3.06	1.33	1.37
14	aA	801	CL0	C3D-C4D	-3.06	1.37	1.44
15	cA	807	CLA	MG-NB	-3.06	1.99	2.05
15	aA	828	CLA	CMC-C2C	-3.06	1.44	1.50
15	cB	817	CLA	C1B-NB	-3.06	1.34	1.37
15	c1	416	CLA	C1B-NB	-3.06	1.34	1.37
15	cA	840	CLA	C1B-NB	-3.06	1.34	1.37
15	aJ	202	CLA	C4D-ND	-3.06	1.33	1.37
15	c5	416	CLA	MG-ND	-3.06	1.99	2.05
15	b4	413	CLA	C4B-NB	3.06	1.41	1.37
15	aA	834	CLA	MG-NB	-3.06	1.99	2.05
15	cB	825	CLA	C1D-ND	3.06	1.41	1.37
15	c6	415	CLA	C4D-ND	-3.06	1.33	1.37
18	b3	401	BCR	C1-C6	-3.06	1.49	1.53
18	cL	205	BCR	C1-C6	-3.06	1.49	1.53
15	c3	416	CLA	CMD-C2D	-3.06	1.44	1.50
18	cF	205	BCR	C30-C25	-3.05	1.49	1.53
15	c1	411	CLA	C4B-NB	3.05	1.41	1.37
18	a1	418	BCR	C34-C9	-3.05	1.44	1.50
20	bB	851	LMG	O7-C8	-3.05	1.39	1.46
15	b5	412	CLA	C3B-C4B	3.05	1.49	1.42
15	bA	827	CLA	MG-NB	-3.05	1.99	2.05
15	bA	824	CLA	C1D-ND	3.05	1.41	1.37
15	b2	417	CLA	MG-ND	-3.05	1.99	2.05
15	b4	421	CLA	C1D-ND	3.05	1.41	1.37
15	bB	802	CLA	CMC-C2C	-3.05	1.44	1.50
15	bJ	101	CLA	C4D-ND	-3.05	1.33	1.37
15	bB	813	CLA	C4B-NB	3.05	1.41	1.37
15	bB	801	CLA	CMB-C2B	-3.05	1.44	1.50
15	bB	825	CLA	C1B-NB	-3.05	1.34	1.37
15	cB	813	CLA	C4B-NB	3.05	1.41	1.37
15	a1	405	CLA	C4D-ND	-3.04	1.33	1.37
15	bB	830	CLA	CMD-C2D	-3.04	1.44	1.50
18	b6	419	BCR	C38-C26	-3.04	1.45	1.50
15	cB	825	CLA	C1B-NB	-3.04	1.34	1.37
15	a3	416	CLA	C1B-NB	-3.04	1.34	1.37
18	a5	419	BCR	C1-C6	-3.04	1.49	1.53
18	cA	848	BCR	C30-C25	-3.04	1.49	1.53
15	aB	830	CLA	CMD-C2D	-3.04	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	402	CLA	C4B-NB	3.04	1.41	1.37
15	cB	830	CLA	CMD-C2D	-3.04	1.44	1.50
15	c1	406	CLA	C4D-ND	-3.04	1.33	1.37
15	c4	403	CLA	C1D-ND	3.04	1.41	1.37
18	aF	203	BCR	C30-C25	-3.04	1.49	1.53
15	a6	417	CLA	C1B-NB	-3.04	1.34	1.37
15	aB	802	CLA	CMC-C2C	-3.04	1.44	1.50
15	a6	404	CLA	C1D-ND	3.03	1.41	1.37
15	cB	819	CLA	MG-NB	-3.03	1.99	2.05
15	a3	410	CLA	C4D-ND	-3.03	1.33	1.37
15	aB	825	CLA	C1B-NB	-3.03	1.34	1.37
15	cB	831	CLA	C1D-ND	3.03	1.41	1.37
18	bJ	103	BCR	C30-C25	-3.03	1.49	1.53
18	aJ	204	BCR	C30-C25	-3.03	1.49	1.53
15	a1	415	CLA	MG-ND	-3.03	1.99	2.05
15	b1	416	CLA	CMD-C2D	-3.03	1.44	1.50
15	aB	819	CLA	MG-NB	-3.03	1.99	2.05
15	a4	421	CLA	C1D-ND	3.03	1.41	1.37
15	b3	412	CLA	C3B-C4B	3.03	1.49	1.42
18	cB	848	BCR	C1-C6	-3.03	1.49	1.53
15	aB	807	CLA	MG-NB	-3.03	1.99	2.05
15	b2	411	CLA	C4D-ND	-3.03	1.33	1.37
15	aB	825	CLA	C1D-ND	3.03	1.41	1.37
15	cB	815	CLA	C4B-NB	3.03	1.41	1.37
15	a6	410	CLA	C4B-NB	3.03	1.41	1.37
15	b2	405	CLA	C4B-NB	3.03	1.41	1.37
15	bA	838	CLA	CMD-C2D	-3.03	1.44	1.50
15	a4	411	CLA	C4B-NB	3.03	1.41	1.37
15	aB	801	CLA	CMB-C2B	-3.03	1.44	1.50
15	c2	417	CLA	CMD-C2D	-3.03	1.44	1.50
15	aA	838	CLA	CMD-C2D	-3.03	1.44	1.50
15	bB	825	CLA	C1D-ND	3.03	1.41	1.37
15	cA	814	CLA	C1D-ND	3.03	1.41	1.37
15	b4	403	CLA	C1D-ND	3.02	1.41	1.37
15	cA	842	CLA	C4B-NB	3.02	1.41	1.37
14	cA	801	CL0	C3D-C2D	3.02	1.47	1.39
18	bB	848	BCR	C1-C6	-3.02	1.49	1.53
15	aB	823	CLA	C1D-ND	3.02	1.41	1.37
15	a4	404	CLA	C4B-NB	3.02	1.41	1.37
15	c1	408	CLA	C4D-ND	-3.02	1.33	1.37
15	a5	416	CLA	MG-ND	-3.02	1.99	2.05
18	b5	418	BCR	C1-C6	-3.02	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	417	CLA	CMD-C2D	-3.02	1.44	1.50
18	b1	419	BCR	C34-C9	-3.02	1.44	1.50
18	b2	419	BCR	C1-C6	-3.02	1.49	1.53
18	b1	418	BCR	C1-C6	-3.02	1.49	1.53
18	cJ	103	BCR	C30-C25	-3.02	1.49	1.53
15	a1	415	CLA	CMD-C2D	-3.02	1.44	1.50
15	aA	843	CLA	C4B-NB	3.02	1.41	1.37
15	bB	807	CLA	MG-NB	-3.02	1.99	2.05
15	b1	416	CLA	MG-ND	-3.02	1.99	2.05
15	a4	402	CLA	C4D-ND	-3.02	1.33	1.37
15	c3	416	CLA	C1B-NB	-3.02	1.34	1.37
15	cB	802	CLA	CMC-C2C	-3.02	1.44	1.50
15	a2	414	CLA	C4B-NB	3.01	1.41	1.37
15	bA	840	CLA	C1B-NB	-3.01	1.34	1.37
15	c5	420	CLA	C1D-ND	3.01	1.41	1.37
15	cB	801	CLA	CMB-C2B	-3.01	1.44	1.50
15	a5	420	CLA	C4D-ND	-3.01	1.33	1.37
15	c3	421	CLA	C1D-ND	3.01	1.41	1.37
15	a6	417	CLA	MG-ND	-3.01	1.99	2.05
15	c5	420	CLA	C4D-ND	-3.01	1.33	1.37
18	a3	401	BCR	C33-C5	-3.01	1.46	1.50
15	a5	402	CLA	C4D-ND	-3.01	1.33	1.37
15	b6	407	CLA	C4B-NB	3.01	1.41	1.37
15	c1	416	CLA	MG-ND	-3.01	1.99	2.05
15	c3	410	CLA	C4D-ND	-3.01	1.33	1.37
15	b3	416	CLA	C1B-NB	-3.01	1.34	1.37
15	c1	416	CLA	CMD-C2D	-3.01	1.44	1.50
14	aA	801	CL0	C3D-C2D	3.01	1.47	1.39
15	bL	204	CLA	MG-NB	-3.01	1.99	2.05
18	c2	401	BCR	C1-C6	-3.01	1.49	1.53
15	c2	402	CLA	C4D-ND	-3.01	1.33	1.37
15	a5	413	CLA	C4B-NB	3.01	1.41	1.37
18	b1	418	BCR	C38-C26	-3.01	1.46	1.50
18	c3	401	BCR	C33-C5	-3.01	1.46	1.50
18	a1	417	BCR	C38-C26	-3.01	1.46	1.50
18	c1	418	BCR	C1-C6	-3.01	1.49	1.53
15	b5	416	CLA	MG-ND	-3.01	1.99	2.05
15	a1	415	CLA	C1B-NB	-3.01	1.34	1.37
15	a6	414	CLA	C4D-ND	-3.01	1.33	1.37
18	bJ	105	BCR	C30-C25	-3.00	1.49	1.53
15	b2	414	CLA	C4B-NB	3.00	1.41	1.37
18	c3	401	BCR	C1-C6	-3.00	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	407	CLA	C4B-NB	3.00	1.41	1.37
15	b1	402	CLA	C4D-ND	-3.00	1.33	1.37
15	aA	840	CLA	C1B-NB	-3.00	1.34	1.37
15	aB	815	CLA	C4B-NB	3.00	1.41	1.37
15	a2	408	CLA	C4B-NB	3.00	1.41	1.37
15	cA	822	CLA	CMB-C2B	-3.00	1.44	1.50
15	bA	822	CLA	CMB-C2B	-3.00	1.44	1.50
18	a3	401	BCR	C1-C6	-3.00	1.49	1.53
18	b2	420	BCR	C1-C6	-3.00	1.49	1.53
15	a6	417	CLA	CMD-C2D	-3.00	1.44	1.50
15	aL	203	CLA	MG-NB	-3.00	1.99	2.05
15	aA	841	CLA	C1D-ND	3.00	1.41	1.37
15	a6	415	CLA	C4D-ND	-3.00	1.33	1.37
15	b4	404	CLA	C4B-NB	3.00	1.41	1.37
15	cA	809	CLA	C1D-ND	2.99	1.41	1.37
15	aB	829	CLA	MG-NB	-2.99	1.99	2.05
15	c6	405	CLA	C3B-C4B	2.99	1.49	1.42
15	c2	403	CLA	C3B-C4B	2.99	1.49	1.42
15	bB	815	CLA	C4D-ND	-2.99	1.33	1.37
15	aB	837	CLA	MG-NB	-2.99	1.99	2.05
18	c1	419	BCR	C34-C9	-2.99	1.44	1.50
15	b2	403	CLA	C3B-C4B	2.99	1.49	1.42
15	bA	836	CLA	CMB-C2B	-2.99	1.44	1.50
15	a2	405	CLA	C4B-NB	2.99	1.41	1.37
15	c5	413	CLA	C4B-NB	2.99	1.41	1.37
18	b3	401	BCR	C33-C5	-2.99	1.46	1.50
15	bB	829	CLA	MG-NB	-2.99	1.99	2.05
18	a2	401	BCR	C1-C6	-2.99	1.49	1.53
18	c4	420	BCR	C1-C6	-2.99	1.49	1.53
15	a6	403	CLA	C4D-ND	-2.98	1.33	1.37
15	c3	412	CLA	C3B-C4B	2.98	1.49	1.42
15	cL	204	CLA	MG-NB	-2.98	1.99	2.05
15	cA	838	CLA	CMD-C2D	-2.98	1.44	1.50
15	c6	418	CLA	MG-ND	-2.98	1.99	2.05
15	a4	410	CLA	C4D-ND	-2.98	1.33	1.37
15	b4	410	CLA	C4D-ND	-2.98	1.33	1.37
18	aB	848	BCR	C1-C6	-2.98	1.49	1.53
15	bB	823	CLA	C1D-ND	2.98	1.41	1.37
15	aA	822	CLA	CMB-C2B	-2.98	1.44	1.50
18	c1	418	BCR	C38-C26	-2.98	1.46	1.50
15	cB	807	CLA	MG-NB	-2.97	1.99	2.05
15	a1	407	CLA	C4D-ND	-2.97	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	801	CL0	C3D-C2D	2.97	1.47	1.39
15	b2	402	CLA	C4D-ND	-2.97	1.33	1.37
15	c6	401	CLA	C4D-ND	-2.97	1.33	1.37
15	a5	403	CLA	C3B-C4B	2.97	1.49	1.42
15	cA	827	CLA	C1B-NB	-2.97	1.34	1.37
15	a3	421	CLA	MG-ND	-2.97	1.99	2.05
15	b1	408	CLA	C4D-ND	-2.97	1.33	1.37
18	a4	420	BCR	C1-C6	-2.97	1.49	1.53
15	a6	404	CLA	C3B-C4B	2.97	1.49	1.42
15	c2	405	CLA	C4B-NB	2.97	1.41	1.37
15	a2	417	CLA	CMD-C2D	-2.97	1.44	1.50
15	a6	414	CLA	C4B-NB	2.97	1.41	1.37
15	c2	408	CLA	C4B-NB	2.97	1.41	1.37
15	cB	837	CLA	MG-NB	-2.97	1.99	2.05
14	bA	801	CL0	CHC-C4B	2.97	1.46	1.39
15	c6	401	CLA	C2A-C1A	2.97	1.58	1.52
18	b4	420	BCR	C1-C6	-2.96	1.49	1.53
15	b6	404	CLA	C3B-C4B	2.96	1.49	1.42
18	aB	847	BCR	C30-C25	-2.96	1.49	1.53
15	aA	821	CLA	C1D-ND	2.96	1.41	1.37
15	b3	421	CLA	C1D-ND	2.96	1.41	1.37
15	a2	402	CLA	C4D-ND	-2.96	1.33	1.37
15	c5	403	CLA	C1D-ND	2.96	1.41	1.37
15	c6	418	CLA	CMD-C2D	-2.96	1.44	1.50
15	aB	815	CLA	C4D-ND	-2.96	1.33	1.37
15	c4	421	CLA	C1D-ND	2.96	1.41	1.37
15	c6	408	CLA	C4B-NB	2.96	1.41	1.37
15	cA	836	CLA	CMB-C2B	-2.96	1.44	1.50
15	cB	804	CLA	MG-NB	-2.96	1.99	2.05
15	b2	413	CLA	C4B-NB	2.96	1.41	1.37
15	c4	402	CLA	C4B-NB	2.96	1.41	1.37
15	c3	408	CLA	C1D-ND	2.96	1.41	1.37
18	c2	421	BCR	C1-C6	-2.96	1.49	1.53
15	a2	403	CLA	C3B-C4B	2.96	1.49	1.42
15	c6	416	CLA	C4D-ND	-2.96	1.33	1.37
18	a2	420	BCR	C1-C6	-2.96	1.49	1.53
15	cA	834	CLA	MG-ND	-2.96	1.99	2.05
15	aL	203	CLA	C1D-ND	2.96	1.41	1.37
15	c2	414	CLA	C4B-NB	2.96	1.41	1.37
15	c5	407	CLA	C4B-NB	2.96	1.41	1.37
18	c6	403	BCR	C33-C5	-2.96	1.46	1.50
15	bA	834	CLA	MG-ND	-2.96	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	809	CLA	MG-NB	-2.96	1.99	2.05
18	aI	101	BCR	C30-C25	-2.96	1.49	1.53
15	b6	413	CLA	C4B-NB	2.96	1.41	1.37
15	aB	807	CLA	CMD-C2D	-2.96	1.44	1.50
18	aL	205	BCR	C1-C6	-2.96	1.49	1.53
18	a6	402	BCR	C33-C5	-2.96	1.46	1.50
15	cB	839	CLA	C1D-ND	2.96	1.41	1.37
15	c6	404	CLA	C4D-ND	-2.96	1.33	1.37
15	a4	409	CLA	C4B-NB	2.96	1.41	1.37
15	c4	411	CLA	C4B-NB	2.96	1.41	1.37
15	b4	414	CLA	C3B-C4B	2.95	1.49	1.42
15	cB	810	CLA	C1B-NB	-2.95	1.34	1.37
15	b6	403	CLA	C4D-ND	-2.95	1.33	1.37
15	bB	815	CLA	C4B-NB	2.95	1.41	1.37
15	c3	409	CLA	C4B-NB	2.95	1.41	1.37
15	aA	836	CLA	CMB-C2B	-2.95	1.44	1.50
15	c3	416	CLA	MG-ND	-2.95	1.99	2.05
15	bA	809	CLA	C1D-ND	2.95	1.41	1.37
15	c5	415	CLA	C4B-NB	2.95	1.41	1.37
18	b2	401	BCR	C1-C6	-2.95	1.49	1.53
15	aA	822	CLA	MG-NB	-2.95	1.99	2.05
15	c4	410	CLA	C4D-ND	-2.95	1.33	1.37
15	b6	417	CLA	MG-ND	-2.95	1.99	2.05
15	cB	803	CLA	MG-ND	-2.95	1.99	2.05
15	aB	804	CLA	MG-NB	-2.95	1.99	2.05
15	c4	409	CLA	C4B-NB	2.95	1.41	1.37
18	bI	101	BCR	C30-C25	-2.95	1.49	1.53
15	a3	421	CLA	C1D-ND	2.95	1.41	1.37
15	cB	829	CLA	MG-NB	-2.95	1.99	2.05
15	c2	410	CLA	C4B-NB	2.95	1.41	1.37
15	a4	412	CLA	C3B-C4B	2.95	1.49	1.42
15	aA	826	CLA	MG-NB	-2.94	1.99	2.05
15	bB	804	CLA	MG-NB	-2.94	1.99	2.05
18	a2	421	BCR	C1-C6	-2.94	1.49	1.53
15	aA	802	CLA	MG-ND	-2.94	2.00	2.05
15	cA	826	CLA	MG-NB	-2.94	2.00	2.05
18	c2	420	BCR	C1-C6	-2.94	1.49	1.53
15	b4	408	CLA	C1D-ND	2.94	1.41	1.37
15	b2	417	CLA	CMD-C2D	-2.94	1.44	1.50
15	aA	809	CLA	C1D-ND	2.94	1.41	1.37
15	cB	815	CLA	C4D-ND	-2.94	1.33	1.37
15	bB	814	CLA	MG-NB	-2.94	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	411	CLA	C4B-NB	2.94	1.41	1.37
15	bA	819	CLA	C3B-C4B	2.94	1.49	1.42
15	aB	803	CLA	MG-ND	-2.94	2.00	2.05
15	bA	802	CLA	C1B-NB	-2.94	1.34	1.37
15	b5	413	CLA	C4B-NB	2.94	1.41	1.37
14	cA	801	CL0	CHC-C4B	2.94	1.46	1.39
15	cB	813	CLA	C1B-NB	-2.94	1.34	1.37
15	b5	420	CLA	C4D-ND	-2.94	1.33	1.37
15	aA	802	CLA	C1B-NB	-2.94	1.34	1.37
15	bB	803	CLA	MG-ND	-2.94	2.00	2.05
15	aB	838	CLA	MG-NB	-2.94	2.00	2.05
18	a1	419	BCR	C30-C25	-2.94	1.49	1.53
15	aB	813	CLA	C1B-NB	-2.94	1.34	1.37
15	b4	412	CLA	C3B-C4B	2.94	1.49	1.42
15	a3	412	CLA	C3B-C4B	2.93	1.49	1.42
15	b1	414	CLA	C3B-C4B	2.93	1.49	1.42
15	bB	805	CLA	C1D-ND	2.93	1.41	1.37
15	cB	807	CLA	CMD-C2D	-2.93	1.44	1.50
15	b3	416	CLA	MG-ND	-2.93	2.00	2.05
14	aA	801	CL0	CHC-C4B	2.93	1.46	1.39
15	bB	827	CLA	MG-NB	-2.93	2.00	2.05
15	cA	802	CLA	MG-ND	-2.93	2.00	2.05
15	cA	822	CLA	MG-NB	-2.93	2.00	2.05
15	c2	413	CLA	C4B-NB	2.93	1.41	1.37
15	bA	828	CLA	C3B-C4B	2.93	1.49	1.42
15	c5	411	CLA	C4B-NB	2.93	1.41	1.37
15	c6	409	CLA	C4B-NB	2.93	1.41	1.37
15	bB	838	CLA	MG-NB	-2.93	2.00	2.05
15	aB	809	CLA	MG-NB	-2.93	2.00	2.05
15	b5	411	CLA	C4B-NB	2.93	1.41	1.37
15	c2	402	CLA	C4B-NB	2.93	1.41	1.37
15	c5	403	CLA	C3B-C4B	2.93	1.49	1.42
15	c2	405	CLA	C4D-ND	-2.93	1.33	1.37
15	bB	839	CLA	C1D-ND	2.93	1.41	1.37
15	bB	807	CLA	CMD-C2D	-2.93	1.44	1.50
15	c5	415	CLA	CMD-C2D	-2.93	1.44	1.50
15	bB	820	CLA	MG-NB	-2.93	2.00	2.05
15	cA	841	CLA	C3B-C4B	2.93	1.49	1.42
15	aB	814	CLA	MG-NB	-2.93	2.00	2.05
15	b5	403	CLA	C3B-C4B	2.92	1.49	1.42
15	bB	837	CLA	MG-NB	-2.92	2.00	2.05
15	a5	403	CLA	C1D-ND	2.92	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	416	CLA	C3B-C4B	2.92	1.49	1.42
15	a6	403	CLA	C4B-NB	2.92	1.41	1.37
18	c1	420	BCR	C30-C25	-2.92	1.49	1.53
15	bA	817	CLA	C4B-NB	2.92	1.41	1.37
15	bA	802	CLA	MG-ND	-2.92	2.00	2.05
15	cA	819	CLA	C3B-C4B	2.92	1.49	1.42
15	aA	834	CLA	MG-ND	-2.92	2.00	2.05
15	cB	814	CLA	MG-NB	-2.92	2.00	2.05
15	cF	203	CLA	CMB-C2B	-2.92	1.44	1.50
15	a3	413	CLA	C4B-NB	2.92	1.41	1.37
15	bA	841	CLA	C3B-C4B	2.92	1.49	1.42
15	bA	822	CLA	MG-NB	-2.92	2.00	2.05
15	cA	802	CLA	C1B-NB	-2.92	1.34	1.37
15	aA	841	CLA	C3B-C4B	2.92	1.49	1.42
15	c2	413	CLA	C3B-C4B	2.92	1.49	1.42
15	bA	827	CLA	C1B-NB	-2.92	1.34	1.37
15	aA	819	CLA	C3B-C4B	2.92	1.49	1.42
15	c6	414	CLA	C4B-NB	2.92	1.41	1.37
15	c4	412	CLA	C3B-C4B	2.92	1.49	1.42
15	a3	409	CLA	C4B-NB	2.92	1.41	1.37
15	c3	403	CLA	C1D-ND	2.92	1.41	1.37
15	aB	810	CLA	C1B-NB	-2.92	1.34	1.37
15	aJ	201	CLA	CMB-C2B	-2.92	1.44	1.50
15	a2	405	CLA	C4D-ND	-2.91	1.33	1.37
15	b5	414	CLA	C4D-ND	-2.91	1.33	1.37
15	b6	415	CLA	C4D-ND	-2.91	1.33	1.37
15	b6	415	CLA	C3B-C4B	2.91	1.49	1.42
18	bB	847	BCR	C30-C25	-2.91	1.49	1.53
15	aB	820	CLA	MG-NB	-2.91	2.00	2.05
15	b3	421	CLA	MG-ND	-2.91	2.00	2.05
18	cB	847	BCR	C30-C25	-2.91	1.49	1.53
15	c5	414	CLA	C4D-ND	-2.91	1.33	1.37
18	bL	201	BCR	C1-C6	-2.91	1.49	1.53
15	b1	403	CLA	C3B-C4B	2.91	1.49	1.42
15	b3	412	CLA	C4B-NB	2.91	1.41	1.37
15	c3	413	CLA	C4B-NB	2.91	1.41	1.37
18	cI	101	BCR	C30-C25	-2.91	1.49	1.53
18	b4	418	BCR	C40-C30	-2.91	1.48	1.53
15	aA	830	CLA	MG-NB	-2.91	2.00	2.05
18	a4	418	BCR	C40-C30	-2.91	1.48	1.53
15	cA	812	CLA	C1D-ND	2.91	1.41	1.37
15	c5	403	CLA	C4B-NB	2.91	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	826	CLA	MG-NB	-2.91	2.00	2.05
15	a6	408	CLA	C4B-NB	2.91	1.41	1.37
15	a1	402	CLA	C3B-C4B	2.91	1.49	1.42
15	c4	415	CLA	CMD-C2D	-2.91	1.44	1.50
18	b2	421	BCR	C1-C6	-2.91	1.49	1.53
15	cB	820	CLA	MG-NB	-2.91	2.00	2.05
15	a2	422	CLA	C1D-ND	2.91	1.41	1.37
18	a2	421	BCR	C30-C25	-2.91	1.49	1.53
15	cA	828	CLA	C3B-C4B	2.91	1.49	1.42
15	aB	836	CLA	C1B-NB	-2.91	1.34	1.37
15	bF	201	CLA	CMB-C2B	-2.91	1.44	1.50
15	b6	422	CLA	C4D-ND	-2.91	1.33	1.37
15	bB	828	CLA	CMD-C2D	-2.90	1.44	1.50
15	aA	843	CLA	C3B-C4B	2.90	1.49	1.42
15	cA	836	CLA	C1D-ND	2.90	1.41	1.37
15	a3	416	CLA	MG-ND	-2.90	2.00	2.05
15	bA	807	CLA	MG-ND	-2.90	2.00	2.05
15	b2	405	CLA	C4D-ND	-2.90	1.33	1.37
15	c3	421	CLA	MG-ND	-2.90	2.00	2.05
15	b5	410	CLA	C4D-ND	-2.90	1.33	1.37
15	aA	828	CLA	C3B-C4B	2.90	1.49	1.42
15	aB	833	CLA	C1B-NB	-2.90	1.34	1.37
15	bA	812	CLA	C1D-ND	2.90	1.41	1.37
15	bL	204	CLA	C1D-ND	2.90	1.41	1.37
15	aA	827	CLA	C1B-NB	-2.90	1.34	1.37
15	aJ	203	CLA	C4B-NB	2.90	1.41	1.37
15	bB	833	CLA	C1B-NB	-2.90	1.34	1.37
15	b2	410	CLA	C4B-NB	2.90	1.41	1.37
15	bB	815	CLA	C3B-C4B	2.90	1.49	1.42
15	c4	414	CLA	C3B-C4B	2.90	1.49	1.42
15	b2	403	CLA	C4B-NB	2.90	1.41	1.37
18	b6	402	BCR	C33-C5	-2.90	1.46	1.50
15	bB	813	CLA	C1B-NB	-2.90	1.34	1.37
15	bB	821	CLA	C4B-NB	2.90	1.41	1.37
15	cB	809	CLA	MG-NB	-2.90	2.00	2.05
15	cB	805	CLA	C1D-ND	2.90	1.41	1.37
15	cB	827	CLA	MG-NB	-2.90	2.00	2.05
15	a4	414	CLA	C3B-C4B	2.90	1.49	1.42
15	b1	413	CLA	C1D-ND	2.90	1.41	1.37
15	c4	408	CLA	C1D-ND	2.90	1.41	1.37
15	bA	830	CLA	MG-NB	-2.90	2.00	2.05
15	cB	838	CLA	MG-NB	-2.90	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	840	CLA	MG-NB	-2.90	2.00	2.05
15	b4	416	CLA	CMD-C2D	-2.90	1.44	1.50
15	bB	810	CLA	C1B-NB	-2.89	1.34	1.37
15	aB	839	CLA	C1D-ND	2.89	1.41	1.37
15	cA	821	CLA	C1D-ND	2.89	1.41	1.37
15	bB	836	CLA	C1B-NB	-2.89	1.34	1.37
15	c1	403	CLA	C3B-C4B	2.89	1.49	1.42
18	bL	206	BCR	C1-C6	-2.89	1.49	1.53
15	aA	815	CLA	MG-NB	-2.89	2.00	2.05
15	c5	414	CLA	C3B-C4B	2.89	1.49	1.42
15	aB	804	CLA	C1B-NB	-2.89	1.34	1.37
15	bB	824	CLA	C4B-NB	2.89	1.41	1.37
15	cB	821	CLA	C4B-NB	2.89	1.41	1.37
18	c2	421	BCR	C30-C25	-2.89	1.49	1.53
15	a2	413	CLA	C3B-C4B	2.89	1.49	1.42
15	bA	843	CLA	C3B-C4B	2.89	1.49	1.42
15	cJ	102	CLA	C4B-NB	2.89	1.41	1.37
15	a5	416	CLA	CMD-C2D	-2.89	1.44	1.50
15	a5	415	CLA	CMD-C2D	-2.89	1.44	1.50
15	cB	828	CLA	CMD-C2D	-2.89	1.44	1.50
18	c6	402	BCR	C1-C6	-2.89	1.49	1.53
15	aB	812	CLA	C1D-ND	2.89	1.41	1.37
15	a1	401	CLA	C4B-NB	2.89	1.41	1.37
15	cB	801	CLA	C4B-NB	2.89	1.41	1.37
15	b5	416	CLA	CMD-C2D	-2.89	1.44	1.50
15	bL	202	CLA	MG-NB	-2.89	2.00	2.05
18	b1	420	BCR	C30-C25	-2.89	1.49	1.53
15	b6	406	CLA	C4B-NB	2.89	1.41	1.37
15	bA	815	CLA	MG-NB	-2.89	2.00	2.05
15	a1	413	CLA	C3B-C4B	2.89	1.49	1.42
15	aL	201	CLA	MG-NB	-2.89	2.00	2.05
15	cA	830	CLA	MG-NB	-2.88	2.00	2.05
15	b3	408	CLA	C1D-ND	2.88	1.41	1.37
15	cL	204	CLA	C1D-ND	2.88	1.41	1.37
15	b2	412	CLA	C3B-C4B	2.88	1.49	1.42
15	a6	413	CLA	C4B-NB	2.88	1.41	1.37
15	aA	807	CLA	CMD-C2D	-2.88	1.44	1.50
15	aA	828	CLA	C4B-NB	2.88	1.41	1.37
15	b4	409	CLA	C4B-NB	2.88	1.41	1.37
18	b3	420	BCR	C30-C25	-2.88	1.49	1.53
15	aB	815	CLA	C3B-C4B	2.88	1.49	1.42
15	cA	817	CLA	C4B-NB	2.88	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	422	CLA	C1D-ND	2.88	1.41	1.37
15	a5	407	CLA	C4B-NB	2.88	1.41	1.37
15	bA	821	CLA	C1D-ND	2.88	1.41	1.37
15	a2	410	CLA	C4B-NB	2.88	1.41	1.37
15	a3	408	CLA	C1D-ND	2.88	1.41	1.37
15	a4	415	CLA	CMD-C2D	-2.88	1.44	1.50
15	aA	811	CLA	C4B-NB	2.88	1.41	1.37
15	b2	422	CLA	MG-ND	-2.88	2.00	2.05
15	a6	415	CLA	C3B-C4B	2.88	1.49	1.42
15	a6	406	CLA	C4B-NB	2.88	1.41	1.37
15	cA	807	CLA	MG-ND	-2.88	2.00	2.05
18	c5	419	BCR	C30-C25	-2.88	1.49	1.53
15	c5	416	CLA	CMD-C2D	-2.88	1.44	1.50
15	a4	408	CLA	C1D-ND	2.88	1.41	1.37
15	b3	409	CLA	C4B-NB	2.88	1.41	1.37
15	c6	407	CLA	C4B-NB	2.88	1.41	1.37
15	b2	408	CLA	C4B-NB	2.87	1.41	1.37
15	a1	409	CLA	C4D-ND	-2.87	1.33	1.37
15	b5	415	CLA	CMD-C2D	-2.87	1.44	1.50
15	a2	412	CLA	C3B-C4B	2.87	1.49	1.42
15	a4	421	CLA	C4D-ND	-2.87	1.33	1.37
15	cA	805	CLA	MG-NB	-2.87	2.00	2.05
15	b4	415	CLA	CMD-C2D	-2.87	1.44	1.50
15	aA	817	CLA	C4B-NB	2.87	1.41	1.37
15	a4	402	CLA	C4B-NB	2.87	1.41	1.37
15	c2	412	CLA	C3B-C4B	2.87	1.49	1.42
15	aB	827	CLA	MG-NB	-2.87	2.00	2.05
15	cA	804	CLA	C4B-NB	2.87	1.41	1.37
15	bA	805	CLA	MG-NB	-2.87	2.00	2.05
15	b3	413	CLA	C4B-NB	2.87	1.41	1.37
15	b5	415	CLA	C4B-NB	2.87	1.41	1.37
15	a5	410	CLA	C4D-ND	-2.87	1.33	1.37
18	a5	419	BCR	C30-C25	-2.87	1.49	1.53
15	c3	412	CLA	MG-NB	-2.87	2.00	2.05
15	aA	807	CLA	MG-ND	-2.87	2.00	2.05
15	aB	806	CLA	MG-ND	-2.87	2.00	2.05
15	cA	842	CLA	C3B-C4B	2.87	1.49	1.42
15	cB	833	CLA	C1B-NB	-2.86	1.34	1.37
15	a5	414	CLA	C4D-ND	-2.86	1.33	1.37
15	b5	414	CLA	C3B-C4B	2.86	1.49	1.42
15	cA	815	CLA	MG-NB	-2.86	2.00	2.05
15	b2	422	CLA	C1D-ND	2.86	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	408	CLA	C4B-NB	2.86	1.41	1.37
15	c1	413	CLA	C1D-ND	2.86	1.41	1.37
15	cB	825	CLA	MG-NB	-2.86	2.00	2.05
15	a5	414	CLA	C3B-C4B	2.86	1.49	1.42
15	b6	422	CLA	C2A-C1A	2.86	1.58	1.52
15	cL	202	CLA	MG-NB	-2.86	2.00	2.05
15	cA	806	CLA	CMC-C2C	-2.86	1.44	1.50
15	b4	402	CLA	C4B-NB	2.86	1.41	1.37
18	a6	401	BCR	C1-C6	-2.86	1.49	1.53
15	bA	811	CLA	C4B-NB	2.86	1.41	1.37
15	bJ	102	CLA	C4B-NB	2.86	1.41	1.37
15	c1	402	CLA	C4B-NB	2.86	1.41	1.37
15	cJ	102	CLA	C4D-ND	-2.86	1.33	1.37
15	b3	403	CLA	C3B-C4B	2.86	1.49	1.42
15	aA	805	CLA	MG-NB	-2.86	2.00	2.05
15	bB	804	CLA	C1B-NB	-2.86	1.34	1.37
15	aB	840	CLA	MG-NB	-2.86	2.00	2.05
15	cB	807	CLA	C1B-NB	-2.86	1.34	1.37
15	b2	413	CLA	C3B-C4B	2.86	1.49	1.42
15	a3	408	CLA	CMD-C2D	-2.86	1.44	1.50
18	aB	845	BCR	C1-C6	-2.86	1.49	1.53
15	aB	807	CLA	C1B-NB	-2.86	1.34	1.37
15	b3	402	CLA	C4B-NB	2.86	1.41	1.37
15	b5	403	CLA	C1D-ND	2.86	1.41	1.37
15	cA	811	CLA	C4B-NB	2.86	1.41	1.37
15	bB	825	CLA	MG-NB	-2.86	2.00	2.05
15	bA	830	CLA	C1B-NB	-2.85	1.34	1.37
15	aJ	203	CLA	C4D-ND	-2.85	1.33	1.37
18	c4	418	BCR	C40-C30	-2.85	1.48	1.53
15	b1	403	CLA	C4B-NB	2.85	1.41	1.37
15	cB	841	CLA	C3B-C4B	2.85	1.49	1.42
15	a2	413	CLA	C4B-NB	2.85	1.41	1.37
15	b5	403	CLA	C4B-NB	2.85	1.41	1.37
15	c5	410	CLA	C4D-ND	-2.85	1.33	1.37
15	bA	820	CLA	MG-ND	-2.85	2.00	2.05
15	c1	410	CLA	C4D-ND	-2.85	1.33	1.37
15	bB	812	CLA	C1D-ND	2.85	1.41	1.37
15	b5	407	CLA	C4B-NB	2.85	1.41	1.37
15	a5	403	CLA	C4B-NB	2.85	1.41	1.37
15	a5	411	CLA	C4B-NB	2.85	1.41	1.37
15	aB	821	CLA	C4B-NB	2.85	1.41	1.37
15	bB	840	CLA	MG-NB	-2.85	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	812	CLA	C1D-ND	2.85	1.41	1.37
15	a4	412	CLA	MG-NB	-2.85	2.00	2.05
15	cA	810	CLA	C1D-ND	2.85	1.41	1.37
15	c3	403	CLA	C3B-C4B	2.85	1.49	1.42
18	cB	845	BCR	C1-C6	-2.85	1.49	1.53
18	c4	420	BCR	C30-C25	-2.85	1.49	1.53
15	aB	825	CLA	MG-NB	-2.85	2.00	2.05
15	aB	841	CLA	C3B-C4B	2.84	1.49	1.42
15	c5	412	CLA	C4B-NB	2.84	1.41	1.37
15	aB	817	CLA	MG-NB	-2.84	2.00	2.05
18	bA	853	BCR	C1-C6	-2.84	1.49	1.53
15	cA	803	CLA	MG-NB	-2.84	2.00	2.05
15	cB	836	CLA	C1B-NB	-2.84	1.34	1.37
15	aA	832	CLA	MG-NB	-2.84	2.00	2.05
15	c4	416	CLA	CMD-C2D	-2.84	1.44	1.50
18	bB	845	BCR	C1-C6	-2.84	1.49	1.53
15	bB	817	CLA	MG-NB	-2.84	2.00	2.05
18	aA	852	BCR	C1-C6	-2.84	1.49	1.53
18	a3	420	BCR	C30-C25	-2.84	1.49	1.53
15	aB	805	CLA	C1D-ND	2.84	1.41	1.37
15	bB	832	CLA	C1B-NB	-2.84	1.34	1.37
15	c6	410	CLA	C3B-C4B	2.84	1.49	1.42
15	b6	403	CLA	C4B-NB	2.84	1.41	1.37
15	c6	404	CLA	C4B-NB	2.84	1.41	1.37
15	bK	101	CLA	MG-NB	-2.84	2.00	2.05
15	b3	411	CLA	C4B-NB	2.84	1.41	1.37
18	b6	401	BCR	C1-C6	-2.84	1.49	1.53
15	b4	412	CLA	MG-NB	-2.84	2.00	2.05
15	cB	815	CLA	C3B-C4B	2.84	1.49	1.42
15	b1	410	CLA	C4D-ND	-2.84	1.33	1.37
15	cA	805	CLA	C1B-NB	-2.84	1.34	1.37
15	b3	412	CLA	MG-NB	-2.83	2.00	2.05
15	aA	806	CLA	CMC-C2C	-2.83	1.44	1.50
15	cB	828	CLA	C1B-NB	-2.83	1.34	1.37
15	b2	415	CLA	C3B-C4B	2.83	1.49	1.42
15	b1	402	CLA	C4B-NB	2.83	1.41	1.37
15	c3	402	CLA	C4B-NB	2.83	1.41	1.37
15	c3	403	CLA	C4B-NB	2.83	1.41	1.37
15	b1	414	CLA	C4D-ND	-2.83	1.33	1.37
15	aB	828	CLA	CMD-C2D	-2.83	1.44	1.50
15	cB	804	CLA	CMD-C2D	-2.83	1.44	1.50
15	aB	801	CLA	C4B-NB	2.83	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	832	CLA	C1B-NB	-2.83	1.34	1.37
15	bA	807	CLA	CMD-C2D	-2.83	1.44	1.50
18	c2	419	BCR	C40-C30	-2.83	1.48	1.53
18	b2	421	BCR	C30-C25	-2.83	1.49	1.53
15	bB	801	CLA	C4B-NB	2.83	1.41	1.37
15	bA	803	CLA	CMC-C2C	-2.83	1.44	1.50
18	c3	420	BCR	C30-C25	-2.83	1.49	1.53
15	cA	807	CLA	CMD-C2D	-2.83	1.44	1.50
15	aB	804	CLA	CMD-C2D	-2.83	1.44	1.50
15	bB	806	CLA	MG-ND	-2.83	2.00	2.05
15	c4	412	CLA	MG-NB	-2.83	2.00	2.05
15	a1	414	CLA	C4B-NB	2.83	1.41	1.37
18	aF	202	BCR	C30-C25	-2.83	1.49	1.53
18	c6	402	BCR	C34-C9	-2.83	1.45	1.50
15	bA	806	CLA	CMC-C2C	-2.83	1.44	1.50
15	a3	403	CLA	C1D-ND	2.83	1.41	1.37
15	c3	412	CLA	C4B-NB	2.83	1.41	1.37
15	bB	841	CLA	C3B-C4B	2.83	1.49	1.42
15	c1	403	CLA	C4B-NB	2.83	1.41	1.37
15	aA	811	CLA	C1D-ND	2.82	1.41	1.37
15	c2	403	CLA	C4B-NB	2.82	1.41	1.37
15	cB	817	CLA	MG-NB	-2.82	2.00	2.05
15	c4	403	CLA	C3B-C4B	2.82	1.49	1.42
15	a4	416	CLA	CMD-C2D	-2.82	1.44	1.50
15	a2	415	CLA	C3B-C4B	2.82	1.49	1.42
15	c1	414	CLA	C3B-C4B	2.82	1.49	1.42
15	cA	830	CLA	C1B-NB	-2.82	1.34	1.37
15	a2	422	CLA	MG-ND	-2.82	2.00	2.05
15	cA	820	CLA	C1B-NB	-2.82	1.34	1.37
15	bA	836	CLA	C1D-ND	2.82	1.41	1.37
15	a3	402	CLA	C4B-NB	2.82	1.41	1.37
15	bF	201	CLA	C1B-NB	-2.82	1.34	1.37
15	cF	203	CLA	C1B-NB	-2.82	1.34	1.37
18	aA	849	BCR	C1-C6	-2.82	1.49	1.53
18	bF	202	BCR	C30-C25	-2.82	1.49	1.53
15	c2	415	CLA	C3B-C4B	2.82	1.49	1.42
15	cB	827	CLA	CMC-C2C	-2.82	1.44	1.50
15	cB	812	CLA	C1D-ND	2.82	1.41	1.37
15	bA	803	CLA	MG-NB	-2.82	2.00	2.05
15	bB	804	CLA	CMD-C2D	-2.82	1.44	1.50
15	aB	824	CLA	C4B-NB	2.82	1.41	1.37
15	a3	403	CLA	C4B-NB	2.82	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a4	420	BCR	C30-C25	-2.82	1.49	1.53
15	b4	403	CLA	C3B-C4B	2.82	1.49	1.42
15	b6	412	CLA	C4B-NB	2.82	1.41	1.37
18	b6	401	BCR	C34-C9	-2.82	1.45	1.50
15	cB	832	CLA	C1D-ND	2.81	1.41	1.37
15	c1	415	CLA	C4B-NB	2.81	1.41	1.37
15	aA	831	CLA	MG-ND	-2.81	2.00	2.05
15	a4	412	CLA	CMB-C2B	-2.81	1.44	1.50
15	b1	412	CLA	C3B-C4B	2.81	1.49	1.42
15	a2	403	CLA	C4B-NB	2.81	1.41	1.37
18	cA	851	BCR	C1-C6	-2.81	1.49	1.53
15	cA	820	CLA	MG-NB	-2.81	2.00	2.05
15	aB	832	CLA	C1B-NB	-2.81	1.34	1.37
15	a6	409	CLA	C4B-NB	2.81	1.41	1.37
15	b4	403	CLA	C4B-NB	2.81	1.41	1.37
15	b6	409	CLA	C4B-NB	2.81	1.41	1.37
15	a3	403	CLA	C3B-C4B	2.81	1.49	1.42
15	aA	804	CLA	C4B-NB	2.81	1.41	1.37
15	a5	415	CLA	C4B-NB	2.81	1.41	1.37
15	cA	803	CLA	CMC-C2C	-2.81	1.44	1.50
15	a3	412	CLA	MG-NB	-2.81	2.00	2.05
15	aA	805	CLA	C1B-NB	-2.81	1.34	1.37
15	a3	411	CLA	C4B-NB	2.81	1.41	1.37
18	bB	844	BCR	C30-C25	-2.81	1.49	1.53
15	aA	820	CLA	MG-ND	-2.81	2.00	2.05
15	b1	415	CLA	C4B-NB	2.81	1.41	1.37
15	b3	403	CLA	C1D-ND	2.81	1.41	1.37
15	bB	827	CLA	CMC-C2C	-2.81	1.44	1.50
15	c3	408	CLA	CMD-C2D	-2.81	1.44	1.50
15	cB	802	CLA	C1D-ND	2.81	1.41	1.37
15	b4	421	CLA	C4D-ND	-2.81	1.33	1.37
15	b5	411	CLA	C3B-C4B	2.81	1.49	1.42
15	a4	403	CLA	C3B-C4B	2.81	1.49	1.42
18	c1	401	BCR	C34-C9	-2.81	1.45	1.50
15	c4	412	CLA	CMB-C2B	-2.81	1.44	1.50
15	cB	809	CLA	C1B-NB	-2.81	1.34	1.37
18	b5	419	BCR	C30-C25	-2.81	1.49	1.53
15	bA	843	CLA	MG-NB	-2.81	2.00	2.05
15	cA	828	CLA	MG-NB	-2.81	2.00	2.05
15	bA	805	CLA	C1B-NB	-2.81	1.34	1.37
15	bA	832	CLA	MG-NB	-2.81	2.00	2.05
15	aK	102	CLA	MG-NB	-2.80	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	410	CLA	C4B-NB	2.80	1.41	1.37
15	bA	828	CLA	C4B-NB	2.80	1.41	1.37
15	a1	407	CLA	C3B-C4B	2.80	1.49	1.42
15	bJ	102	CLA	C4D-ND	-2.80	1.33	1.37
15	aB	828	CLA	C1B-NB	-2.80	1.34	1.37
15	c4	421	CLA	C4D-ND	-2.80	1.33	1.37
15	cB	817	CLA	MG-ND	-2.80	2.00	2.05
15	cK	102	CLA	MG-NB	-2.80	2.00	2.05
15	b2	416	CLA	C4B-NB	2.80	1.41	1.37
15	c6	417	CLA	CMD-C2D	-2.80	1.44	1.50
15	a5	411	CLA	C3B-C4B	2.80	1.49	1.42
18	a2	419	BCR	C40-C30	-2.80	1.48	1.53
18	bA	850	BCR	C1-C6	-2.80	1.49	1.53
15	bA	820	CLA	C1B-NB	-2.80	1.34	1.37
15	bA	810	CLA	C1D-ND	2.80	1.41	1.37
15	cB	806	CLA	C1B-NB	-2.80	1.34	1.37
15	aA	836	CLA	C1D-ND	2.80	1.41	1.37
15	bB	809	CLA	C1B-NB	-2.80	1.34	1.37
15	c1	415	CLA	CMD-C2D	-2.80	1.44	1.50
18	b4	419	BCR	C1-C6	-2.80	1.49	1.53
15	aA	826	CLA	C1B-NB	-2.80	1.34	1.37
15	aA	842	CLA	C4B-NB	2.80	1.41	1.37
15	bA	804	CLA	C4B-NB	2.80	1.41	1.37
15	bA	828	CLA	MG-NB	-2.80	2.00	2.05
15	aB	827	CLA	CMC-C2C	-2.80	1.44	1.50
18	cF	204	BCR	C30-C25	-2.79	1.49	1.53
15	b3	408	CLA	CMD-C2D	-2.79	1.44	1.50
15	b5	402	CLA	C1B-C2B	2.79	1.49	1.43
15	bB	807	CLA	C1B-NB	-2.79	1.34	1.37
15	c2	416	CLA	C4B-NB	2.79	1.41	1.37
18	cA	848	BCR	C1-C6	-2.79	1.49	1.53
15	aA	828	CLA	MG-NB	-2.79	2.00	2.05
15	cA	831	CLA	MG-ND	-2.79	2.00	2.05
15	a3	414	CLA	C3B-C4B	2.79	1.49	1.42
15	b4	412	CLA	CMB-C2B	-2.79	1.44	1.50
15	bB	805	CLA	C1B-NB	-2.79	1.34	1.37
15	a6	416	CLA	CMD-C2D	-2.79	1.44	1.50
18	a4	419	BCR	C1-C6	-2.79	1.49	1.53
15	a1	412	CLA	C1D-ND	2.79	1.41	1.37
15	aA	803	CLA	CMC-C2C	-2.79	1.44	1.50
18	a6	401	BCR	C34-C9	-2.79	1.45	1.50
15	cB	822	CLA	C4B-NB	2.79	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	801	CL0	C1C-NC	-2.79	1.33	1.37
15	a5	402	CLA	C1B-C2B	2.79	1.49	1.43
15	c4	411	CLA	C3B-C4B	2.79	1.49	1.42
15	cA	813	CLA	C1B-NB	-2.79	1.34	1.37
15	aB	814	CLA	C1D-ND	2.79	1.41	1.37
15	c5	402	CLA	C1B-C2B	2.79	1.49	1.43
15	cA	832	CLA	MG-NB	-2.79	2.00	2.05
15	cA	811	CLA	C1D-ND	2.78	1.41	1.37
15	cB	804	CLA	C1B-NB	-2.78	1.34	1.37
15	b5	404	CLA	C3B-C4B	2.78	1.49	1.42
15	bA	840	CLA	MG-ND	-2.78	2.00	2.05
15	aB	817	CLA	MG-ND	-2.78	2.00	2.05
15	cB	806	CLA	MG-ND	-2.78	2.00	2.05
15	aA	820	CLA	C1B-NB	-2.78	1.34	1.37
15	a2	416	CLA	C4B-NB	2.78	1.41	1.37
15	bA	842	CLA	C4B-NB	2.78	1.41	1.37
15	bJ	101	CLA	C4B-NB	2.78	1.41	1.37
15	cB	831	CLA	MG-NB	-2.78	2.00	2.05
15	b3	414	CLA	C3B-C4B	2.78	1.49	1.42
15	a6	404	CLA	C4B-NB	2.78	1.41	1.37
15	aA	840	CLA	MG-ND	-2.78	2.00	2.05
15	cA	840	CLA	MG-ND	-2.78	2.00	2.05
15	a1	402	CLA	C4B-NB	2.78	1.41	1.37
15	b1	405	CLA	C4B-NB	2.78	1.41	1.37
15	b6	409	CLA	C3B-C4B	2.78	1.49	1.42
15	aA	835	CLA	C4B-NB	2.78	1.41	1.37
15	a1	414	CLA	CMD-C2D	-2.78	1.44	1.50
15	aJ	201	CLA	C1B-NB	-2.78	1.34	1.37
15	b1	408	CLA	C4B-NB	2.78	1.41	1.37
15	b1	404	CLA	C3B-C4B	2.78	1.49	1.42
14	bA	801	CL0	C1C-NC	-2.78	1.33	1.37
15	aB	802	CLA	CMD-C2D	-2.78	1.44	1.50
15	cA	820	CLA	MG-ND	-2.78	2.00	2.05
15	c2	409	CLA	C3B-C4B	2.78	1.49	1.42
15	c5	404	CLA	C3B-C4B	2.78	1.49	1.42
15	aB	832	CLA	C1D-ND	2.78	1.41	1.37
18	bI	102	BCR	C1-C6	-2.78	1.49	1.53
18	c2	401	BCR	C33-C5	-2.78	1.46	1.50
18	aI	102	BCR	C1-C6	-2.78	1.50	1.53
15	b4	412	CLA	C4B-NB	2.78	1.41	1.37
15	aA	830	CLA	C1B-NB	-2.77	1.34	1.37
15	cA	813	CLA	C4B-NB	2.77	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	410	CLA	C4B-NB	2.77	1.41	1.37
15	aA	803	CLA	MG-NB	-2.77	2.00	2.05
15	a1	411	CLA	MG-NB	-2.77	2.00	2.05
15	c2	422	CLA	MG-ND	-2.77	2.00	2.05
15	c1	408	CLA	C3B-C4B	2.77	1.49	1.42
15	c3	415	CLA	CMD-C2D	-2.77	1.44	1.50
15	aA	821	CLA	C4B-NB	2.77	1.41	1.37
15	c3	411	CLA	C4B-NB	2.77	1.41	1.37
15	cB	805	CLA	C1B-NB	-2.77	1.34	1.37
15	c1	405	CLA	C4B-NB	2.77	1.41	1.37
15	a4	412	CLA	C4B-NB	2.77	1.41	1.37
15	aA	808	CLA	C4B-NB	2.77	1.41	1.37
15	cA	820	CLA	C1D-ND	2.77	1.41	1.37
15	aB	805	CLA	C1B-NB	-2.77	1.34	1.37
15	b1	415	CLA	CMD-C2D	-2.77	1.44	1.50
15	aB	809	CLA	C1B-NB	-2.77	1.34	1.37
15	bA	835	CLA	C4B-NB	2.77	1.41	1.37
15	cA	818	CLA	C4B-NB	2.77	1.41	1.37
15	b6	416	CLA	CMD-C2D	-2.77	1.44	1.50
15	a1	403	CLA	C3B-C4B	2.77	1.49	1.42
18	cI	102	BCR	C1-C6	-2.77	1.50	1.53
15	a5	408	CLA	CMD-C2D	-2.76	1.44	1.50
15	cA	819	CLA	CMC-C2C	-2.76	1.44	1.50
15	a5	412	CLA	C4B-NB	2.76	1.41	1.37
15	aA	820	CLA	C1D-ND	2.76	1.41	1.37
15	bA	820	CLA	MG-NB	-2.76	2.00	2.05
15	aA	832	CLA	CMD-C2D	-2.76	1.44	1.50
15	aB	812	CLA	C4B-NB	2.76	1.41	1.37
15	aA	820	CLA	MG-NB	-2.76	2.00	2.05
15	a5	404	CLA	C3B-C4B	2.76	1.49	1.42
15	bB	828	CLA	C1B-NB	-2.76	1.34	1.37
15	cF	201	CLA	C4B-NB	2.76	1.41	1.37
15	a2	413	CLA	MG-NB	-2.76	2.00	2.05
15	c6	413	CLA	C3B-C4B	2.76	1.49	1.42
15	bA	831	CLA	MG-ND	-2.76	2.00	2.05
15	c3	414	CLA	C3B-C4B	2.76	1.49	1.42
15	c1	414	CLA	C4D-ND	-2.76	1.33	1.37
18	a4	401	BCR	C1-C6	-2.76	1.50	1.53
15	a6	411	CLA	C4B-NB	2.76	1.41	1.37
15	bA	818	CLA	C4B-NB	2.76	1.41	1.37
15	bB	812	CLA	C4B-NB	2.76	1.41	1.37
15	b2	413	CLA	CMB-C2B	-2.76	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	802	CLA	CMD-C2D	-2.76	1.45	1.50
15	a1	406	CLA	C4B-NB	2.76	1.41	1.37
15	b5	412	CLA	C4B-NB	2.76	1.41	1.37
15	c4	403	CLA	C4B-NB	2.76	1.41	1.37
15	bA	820	CLA	C1D-ND	2.76	1.41	1.37
15	bA	823	CLA	C1D-ND	2.76	1.41	1.37
15	bB	832	CLA	C1D-ND	2.76	1.41	1.37
15	b4	408	CLA	C3B-C4B	2.76	1.49	1.42
15	c1	404	CLA	C3B-C4B	2.76	1.49	1.42
18	a6	420	BCR	C30-C25	-2.76	1.50	1.53
15	a6	412	CLA	C3B-C4B	2.76	1.49	1.42
15	aA	810	CLA	C1D-ND	2.76	1.41	1.37
15	aA	813	CLA	C4B-NB	2.76	1.41	1.37
15	bA	826	CLA	C1B-NB	-2.76	1.34	1.37
15	bB	802	CLA	C1D-ND	2.76	1.41	1.37
15	bB	814	CLA	C1D-ND	2.75	1.41	1.37
15	bA	827	CLA	MG-ND	-2.75	2.00	2.05
15	a3	412	CLA	C4B-NB	2.75	1.41	1.37
15	cX	102	CLA	MG-NB	-2.75	2.00	2.05
18	b4	401	BCR	C1-C6	-2.75	1.50	1.53
15	cA	842	CLA	CMC-C2C	-2.75	1.45	1.50
15	c1	412	CLA	C3B-C4B	2.75	1.49	1.42
15	cB	809	CLA	CMB-C2B	-2.75	1.45	1.50
15	a4	411	CLA	C3B-C4B	2.75	1.49	1.42
15	aA	827	CLA	MG-ND	-2.75	2.00	2.05
15	bB	831	CLA	MG-NB	-2.75	2.00	2.05
15	cB	834	CLA	C4B-NB	2.75	1.41	1.37
15	bB	802	CLA	CMD-C2D	-2.75	1.45	1.50
15	b5	408	CLA	CMD-C2D	-2.75	1.45	1.50
15	bB	817	CLA	MG-ND	-2.75	2.00	2.05
15	a6	409	CLA	C3B-C4B	2.75	1.49	1.42
15	a1	404	CLA	C4B-NB	2.75	1.41	1.37
15	c4	408	CLA	C3B-C4B	2.75	1.49	1.42
15	b4	410	CLA	C4B-NB	2.75	1.41	1.37
15	b4	416	CLA	CHC-C4B	-2.75	1.33	1.39
15	cA	824	CLA	C3B-C4B	2.75	1.49	1.42
15	b4	411	CLA	C3B-C4B	2.75	1.49	1.42
15	bB	834	CLA	C4B-NB	2.75	1.41	1.37
18	a2	401	BCR	C33-C5	-2.75	1.46	1.50
15	c2	413	CLA	MG-NB	-2.75	2.00	2.05
18	aB	844	BCR	C30-C25	-2.75	1.50	1.53
15	c5	405	CLA	C4B-NB	2.75	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	405	CLA	C4B-NB	2.75	1.41	1.37
15	b4	421	CLA	O1D-CGD	2.75	1.28	1.21
15	bA	832	CLA	CMD-C2D	-2.74	1.45	1.50
15	bA	808	CLA	C4B-NB	2.74	1.41	1.37
15	bB	806	CLA	C1B-NB	-2.74	1.34	1.37
15	bB	834	CLA	CMC-C2C	-2.74	1.45	1.50
18	c4	401	BCR	C30-C25	-2.74	1.50	1.53
15	aB	830	CLA	MG-ND	-2.74	2.00	2.05
15	aA	840	CLA	CMB-C2B	-2.74	1.45	1.50
15	c2	413	CLA	CMB-C2B	-2.74	1.45	1.50
15	aA	804	CLA	MG-NB	-2.74	2.00	2.05
15	cA	842	CLA	MG-NB	-2.74	2.00	2.05
15	bB	822	CLA	C4B-NB	2.74	1.41	1.37
15	cA	808	CLA	C4B-NB	2.74	1.41	1.37
15	cA	828	CLA	C4B-NB	2.74	1.41	1.37
15	a3	412	CLA	CMB-C2B	-2.74	1.45	1.50
15	aA	825	CLA	C4B-NB	2.74	1.41	1.37
15	aB	806	CLA	C1B-NB	-2.74	1.34	1.37
15	b2	413	CLA	MG-NB	-2.74	2.00	2.05
15	bA	819	CLA	CMC-C2C	-2.74	1.45	1.50
15	cB	824	CLA	C4B-NB	2.74	1.41	1.37
15	a2	409	CLA	C3B-C4B	2.74	1.49	1.42
15	a5	405	CLA	C4B-NB	2.74	1.41	1.37
15	aB	836	CLA	CMB-C2B	-2.74	1.45	1.50
15	c6	413	CLA	C4B-NB	2.74	1.41	1.37
15	bX	102	CLA	MG-NB	-2.74	2.00	2.05
15	c5	411	CLA	C3B-C4B	2.74	1.49	1.42
14	aA	801	CL0	OBD-CAD	2.74	1.27	1.22
15	aB	831	CLA	MG-NB	-2.74	2.00	2.05
15	b5	405	CLA	C4B-NB	2.74	1.41	1.37
15	cA	835	CLA	C4B-NB	2.74	1.41	1.37
15	cB	821	CLA	C1B-NB	-2.74	1.34	1.37
15	aA	843	CLA	MG-NB	-2.74	2.00	2.05
15	c3	416	CLA	CHC-C4B	-2.74	1.33	1.39
15	aB	809	CLA	CMD-C2D	-2.74	1.45	1.50
15	cA	820	CLA	CMB-C2B	-2.74	1.45	1.50
15	b1	408	CLA	C3B-C4B	2.74	1.49	1.42
15	cA	829	CLA	MG-NB	-2.74	2.00	2.05
15	aA	818	CLA	C4B-NB	2.73	1.41	1.37
15	a4	403	CLA	C4B-NB	2.73	1.41	1.37
15	cA	804	CLA	MG-NB	-2.73	2.00	2.05
15	c4	412	CLA	C4B-NB	2.73	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	843	CLA	CMC-C2C	-2.73	1.45	1.50
15	cA	810	CLA	CMD-C2D	-2.73	1.45	1.50
15	c1	413	CLA	CMB-C2B	-2.73	1.45	1.50
15	aA	843	CLA	CMC-C2C	-2.73	1.45	1.50
15	c4	421	CLA	O1D-CGD	2.73	1.28	1.21
15	a6	412	CLA	C4B-NB	2.73	1.41	1.37
15	a1	411	CLA	C3B-C4B	2.73	1.49	1.42
15	bA	813	CLA	C4B-NB	2.73	1.41	1.37
15	cA	825	CLA	C4B-NB	2.73	1.41	1.37
15	aA	819	CLA	CMC-C2C	-2.73	1.45	1.50
15	b6	412	CLA	C3B-C4B	2.73	1.49	1.42
15	bB	809	CLA	CMB-C2B	-2.73	1.45	1.50
15	a6	414	CLA	CMB-C2B	-2.73	1.45	1.50
15	aA	829	CLA	MG-NB	-2.73	2.00	2.05
18	a1	417	BCR	C40-C30	-2.73	1.48	1.53
15	c5	408	CLA	CMD-C2D	-2.73	1.45	1.50
15	aA	838	CLA	MG-ND	-2.73	2.00	2.05
15	b4	404	CLA	C3B-C4B	2.73	1.49	1.42
15	b6	404	CLA	C4B-NB	2.73	1.41	1.37
15	a1	413	CLA	C4D-ND	-2.73	1.33	1.37
15	c4	416	CLA	CHC-C4B	-2.73	1.33	1.39
14	aA	801	CL0	C1C-NC	-2.73	1.33	1.37
15	a2	417	CLA	C1C-NC	-2.73	1.33	1.37
15	bA	811	CLA	C1D-ND	2.73	1.41	1.37
15	aA	824	CLA	C3B-C4B	2.73	1.49	1.42
15	aA	818	CLA	C1D-ND	2.73	1.41	1.37
15	aB	802	CLA	C1D-ND	2.73	1.41	1.37
15	cA	806	CLA	MG-NB	-2.73	2.00	2.05
15	bA	810	CLA	CMD-C2D	-2.73	1.45	1.50
18	c4	401	BCR	C1-C6	-2.73	1.50	1.53
15	cB	836	CLA	CMB-C2B	-2.72	1.45	1.50
15	cL	202	CLA	CMB-C2B	-2.72	1.45	1.50
15	bA	829	CLA	MG-NB	-2.72	2.00	2.05
18	a6	401	BCR	C30-C25	-2.72	1.50	1.53
18	c4	419	BCR	C1-C6	-2.72	1.50	1.53
15	a4	421	CLA	O1D-CGD	2.72	1.28	1.21
15	cB	812	CLA	C4B-NB	2.72	1.41	1.37
15	aA	810	CLA	CMD-C2D	-2.72	1.45	1.50
15	bB	836	CLA	CMB-C2B	-2.72	1.45	1.50
18	b4	420	BCR	C30-C25	-2.72	1.50	1.53
15	a4	408	CLA	C3B-C4B	2.72	1.49	1.42
15	bA	824	CLA	C3B-C4B	2.72	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	422	CLA	MG-NB	-2.72	2.00	2.05
15	aB	809	CLA	CMB-C2B	-2.72	1.45	1.50
15	a4	416	CLA	CHC-C4B	-2.72	1.33	1.39
15	b2	409	CLA	C3B-C4B	2.72	1.49	1.42
18	cB	844	BCR	C30-C25	-2.72	1.50	1.53
15	aX	102	CLA	MG-ND	-2.72	2.00	2.05
15	cA	827	CLA	MG-ND	-2.72	2.00	2.05
15	aB	834	CLA	C4B-NB	2.72	1.41	1.37
15	bB	821	CLA	C1B-NB	-2.72	1.34	1.37
18	b2	401	BCR	C33-C5	-2.72	1.46	1.50
15	aA	806	CLA	MG-NB	-2.72	2.00	2.05
15	aX	102	CLA	MG-NB	-2.72	2.00	2.05
15	a2	413	CLA	CMB-C2B	-2.72	1.45	1.50
15	b6	409	CLA	CMD-C2D	-2.72	1.45	1.50
15	cB	801	CLA	MG-NB	-2.72	2.00	2.05
15	bA	803	CLA	CMD-C2D	-2.72	1.45	1.50
15	cA	803	CLA	CMD-C2D	-2.72	1.45	1.50
15	a3	415	CLA	CMD-C2D	-2.72	1.45	1.50
15	bA	840	CLA	CMB-C2B	-2.71	1.45	1.50
15	cB	834	CLA	CMC-C2C	-2.71	1.45	1.50
15	bA	813	CLA	C1B-NB	-2.71	1.34	1.37
15	cB	835	CLA	C1D-ND	2.71	1.41	1.37
15	c3	408	CLA	C3B-C4B	2.71	1.49	1.42
15	cB	809	CLA	CMD-C2D	-2.71	1.45	1.50
15	aJ	202	CLA	C4B-NB	2.71	1.41	1.37
15	c3	412	CLA	CMB-C2B	-2.71	1.45	1.50
15	cB	814	CLA	C1D-ND	2.71	1.41	1.37
15	c5	408	CLA	C3B-C4B	2.71	1.49	1.42
15	bA	806	CLA	MG-NB	-2.71	2.00	2.05
15	bB	801	CLA	MG-NB	-2.71	2.00	2.05
18	b2	419	BCR	C40-C30	-2.71	1.48	1.53
15	cB	825	CLA	CMD-C2D	-2.71	1.45	1.50
15	b2	411	CLA	C3B-C4B	2.71	1.49	1.42
15	b3	415	CLA	CMD-C2D	-2.71	1.45	1.50
15	aA	815	CLA	C4B-NB	2.71	1.41	1.37
15	c4	410	CLA	C4B-NB	2.71	1.41	1.37
15	aB	810	CLA	CMD-C2D	-2.71	1.45	1.50
15	a2	405	CLA	C1D-C2D	2.71	1.50	1.45
15	aA	839	CLA	CMB-C2B	-2.71	1.45	1.50
15	bA	812	CLA	CMC-C2C	-2.71	1.45	1.50
15	cA	832	CLA	CMD-C2D	-2.71	1.45	1.50
15	a5	409	CLA	C3B-C4B	2.71	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	823	CLA	C1D-ND	2.71	1.41	1.37
15	bB	835	CLA	C1D-ND	2.71	1.41	1.37
15	bB	809	CLA	CMD-C2D	-2.71	1.45	1.50
18	b1	418	BCR	C40-C30	-2.71	1.48	1.53
15	b5	409	CLA	C3B-C4B	2.71	1.49	1.42
15	b3	403	CLA	C4B-NB	2.71	1.41	1.37
15	bB	818	CLA	MG-NB	-2.71	2.00	2.05
15	c2	414	CLA	CMB-C2B	-2.71	1.45	1.50
15	aA	821	CLA	MG-NB	-2.71	2.00	2.05
15	b1	412	CLA	MG-NB	-2.71	2.00	2.05
15	a4	404	CLA	C3B-C4B	2.71	1.49	1.42
15	cJ	101	CLA	C4B-NB	2.71	1.41	1.37
15	c2	417	CLA	C1C-NC	-2.71	1.33	1.37
15	b2	414	CLA	CMB-C2B	-2.71	1.45	1.50
15	cB	837	CLA	C1B-NB	-2.70	1.34	1.37
15	c1	410	CLA	C4B-NB	2.70	1.41	1.37
15	bA	838	CLA	MG-ND	-2.70	2.00	2.05
15	bB	812	CLA	C3B-C4B	2.70	1.49	1.42
15	c6	407	CLA	C3B-C4B	2.70	1.49	1.42
18	c3	418	BCR	C33-C5	-2.70	1.46	1.50
15	aB	821	CLA	C1B-NB	-2.70	1.34	1.37
15	aA	820	CLA	CMB-C2B	-2.70	1.45	1.50
15	bA	825	CLA	C4B-NB	2.70	1.41	1.37
15	cA	823	CLA	C1D-ND	2.70	1.41	1.37
15	cA	816	CLA	C3B-C4B	2.70	1.49	1.42
15	bB	807	CLA	CAA-C2A	-2.70	1.49	1.54
15	bA	820	CLA	CMB-C2B	-2.70	1.45	1.50
15	cB	841	CLA	CMB-C2B	-2.70	1.45	1.50
15	c2	414	CLA	MG-NB	-2.70	2.00	2.05
15	b1	416	CLA	CHC-C4B	-2.70	1.33	1.39
15	cA	838	CLA	MG-ND	-2.70	2.00	2.05
15	b3	408	CLA	C3B-C4B	2.70	1.49	1.42
15	cA	826	CLA	C1B-NB	-2.70	1.34	1.37
15	b2	405	CLA	C1D-C2D	2.70	1.50	1.45
15	bX	102	CLA	MG-ND	-2.70	2.00	2.05
15	a5	408	CLA	C3B-C4B	2.70	1.49	1.42
15	bB	825	CLA	CMD-C2D	-2.70	1.45	1.50
15	cB	810	CLA	CMD-C2D	-2.70	1.45	1.50
15	aA	803	CLA	CMD-C2D	-2.70	1.45	1.50
15	bB	837	CLA	C1D-ND	2.70	1.41	1.37
15	a6	422	CLA	MG-ND	-2.70	2.00	2.05
15	aB	825	CLA	MG-ND	-2.70	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	801	CL0	OBD-CAD	2.70	1.27	1.22
15	a6	409	CLA	CMD-C2D	-2.70	1.45	1.50
15	cA	840	CLA	CMB-C2B	-2.70	1.45	1.50
15	aA	816	CLA	C3B-C4B	2.70	1.49	1.42
15	aB	821	CLA	C1D-ND	2.70	1.41	1.37
15	a6	406	CLA	C3B-C4B	2.70	1.49	1.42
15	cB	807	CLA	CAA-C2A	-2.70	1.49	1.54
15	cA	842	CLA	CMD-C2D	-2.70	1.45	1.50
15	aB	838	CLA	C1B-NB	-2.70	1.34	1.37
15	a3	416	CLA	CHC-C4B	-2.70	1.33	1.39
15	bA	843	CLA	CMD-C2D	-2.70	1.45	1.50
15	aB	835	CLA	C1D-ND	2.70	1.41	1.37
15	a2	411	CLA	C3B-C4B	2.70	1.49	1.42
15	bA	840	CLA	C1D-ND	2.69	1.41	1.37
15	cA	840	CLA	C1D-ND	2.69	1.41	1.37
15	bB	841	CLA	CMB-C2B	-2.69	1.45	1.50
15	c2	410	CLA	C3B-C4B	2.69	1.49	1.42
15	b3	407	CLA	MG-NB	-2.69	2.00	2.05
15	aB	834	CLA	CMC-C2C	-2.69	1.45	1.50
15	aB	841	CLA	CMB-C2B	-2.69	1.45	1.50
15	bA	829	CLA	CMD-C2D	-2.69	1.45	1.50
15	cA	839	CLA	CMB-C2B	-2.69	1.45	1.50
15	a3	408	CLA	C3B-C4B	2.69	1.49	1.42
15	bB	830	CLA	MG-ND	-2.69	2.00	2.05
15	c1	412	CLA	MG-NB	-2.69	2.00	2.05
15	cB	820	CLA	C1D-ND	2.69	1.41	1.37
15	aB	840	CLA	CMD-C2D	-2.69	1.45	1.50
15	cB	830	CLA	MG-ND	-2.69	2.00	2.05
15	cX	102	CLA	MG-ND	-2.69	2.00	2.05
15	cA	805	CLA	CMB-C2B	-2.69	1.45	1.50
15	c5	409	CLA	C3B-C4B	2.69	1.49	1.42
15	b3	416	CLA	CHC-C4B	-2.69	1.33	1.39
18	b4	401	BCR	C30-C25	-2.69	1.50	1.53
15	b2	410	CLA	C3B-C4B	2.69	1.49	1.42
15	b4	421	CLA	MG-ND	-2.69	2.00	2.05
15	c2	411	CLA	C3B-C4B	2.69	1.49	1.42
15	b3	412	CLA	CMB-C2B	-2.69	1.45	1.50
15	aA	813	CLA	C1B-NB	-2.69	1.34	1.37
15	aB	822	CLA	C4B-NB	2.69	1.41	1.37
15	cA	830	CLA	MG-ND	-2.69	2.00	2.05
15	b3	404	CLA	C3B-C4B	2.69	1.49	1.42
15	aA	829	CLA	CMD-C2D	-2.69	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	818	CLA	MG-NB	-2.69	2.00	2.05
15	bA	804	CLA	MG-NB	-2.69	2.00	2.05
15	c1	407	CLA	C4B-NB	2.69	1.41	1.37
15	bA	830	CLA	MG-ND	-2.69	2.00	2.05
15	bA	815	CLA	C4B-NB	2.69	1.41	1.37
18	c3	419	BCR	C1-C6	-2.69	1.50	1.53
15	aA	839	CLA	C1D-ND	2.69	1.41	1.37
15	bB	827	CLA	C1D-ND	2.69	1.41	1.37
15	cB	838	CLA	C1B-NB	-2.69	1.34	1.37
15	c2	411	CLA	C4B-NB	2.69	1.41	1.37
18	b3	419	BCR	C1-C6	-2.69	1.50	1.53
18	c6	421	BCR	C30-C25	-2.69	1.50	1.53
15	cB	837	CLA	C1D-ND	2.69	1.41	1.37
15	aB	807	CLA	CAA-C2A	-2.69	1.49	1.54
15	bA	816	CLA	C3B-C4B	2.69	1.49	1.42
15	cB	826	CLA	C3B-C4B	2.69	1.49	1.42
15	cB	818	CLA	MG-NB	-2.69	2.00	2.05
15	bA	839	CLA	CMB-C2B	-2.69	1.45	1.50
15	aB	842	CLA	C3B-C4B	2.69	1.49	1.42
15	c1	413	CLA	MG-NB	-2.69	2.00	2.05
15	bB	828	CLA	MG-ND	-2.69	2.00	2.05
15	b1	413	CLA	MG-NB	-2.69	2.00	2.05
15	cA	813	CLA	MG-ND	-2.69	2.00	2.05
15	a2	409	CLA	CMD-C2D	-2.69	1.45	1.50
15	a1	409	CLA	C4B-NB	2.69	1.41	1.37
15	cA	821	CLA	C4B-NB	2.69	1.41	1.37
15	bB	826	CLA	C3B-C4B	2.68	1.49	1.42
15	aA	805	CLA	CMB-C2B	-2.68	1.45	1.50
15	cA	812	CLA	CMC-C2C	-2.68	1.45	1.50
15	b1	412	CLA	C4B-NB	2.68	1.41	1.37
15	aA	814	CLA	CMD-C2D	-2.68	1.45	1.50
15	bL	204	CLA	C1B-NB	-2.68	1.34	1.37
15	c6	414	CLA	CMB-C2B	-2.68	1.45	1.50
15	b5	416	CLA	CHC-C4B	-2.68	1.33	1.39
15	c6	414	CLA	MG-NB	-2.68	2.00	2.05
15	bF	201	CLA	C1D-ND	2.68	1.41	1.37
15	aB	825	CLA	CMD-C2D	-2.68	1.45	1.50
18	b6	420	BCR	C30-C25	-2.68	1.50	1.53
18	c1	401	BCR	C1-C6	-2.68	1.50	1.53
14	bA	801	CL0	OBD-CAD	2.68	1.27	1.22
18	a5	418	BCR	C40-C30	-2.68	1.48	1.53
15	b1	409	CLA	C3B-C4B	2.68	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a5	416	CLA	CHC-C4B	-2.68	1.33	1.39
15	bA	835	CLA	CMD-C2D	-2.68	1.45	1.50
15	bB	807	CLA	MG-ND	-2.68	2.00	2.05
15	c3	407	CLA	MG-NB	-2.68	2.00	2.05
15	aA	845	CLA	C1D-ND	2.68	1.41	1.37
15	aB	801	CLA	MG-NB	-2.68	2.00	2.05
15	c5	416	CLA	CHC-C4B	-2.68	1.33	1.39
15	c2	416	CLA	CMD-C2D	-2.68	1.45	1.50
15	bB	836	CLA	C1D-ND	2.68	1.41	1.37
15	a1	415	CLA	CHC-C4B	-2.68	1.33	1.39
18	b3	418	BCR	C33-C5	-2.68	1.46	1.50
15	a6	411	CLA	C3B-C4B	2.68	1.49	1.42
15	b6	405	CLA	C3B-C4B	2.68	1.49	1.42
15	aA	830	CLA	MG-ND	-2.67	2.00	2.05
15	bA	813	CLA	MG-ND	-2.67	2.00	2.05
15	b6	411	CLA	C4B-NB	2.67	1.41	1.37
15	cA	829	CLA	CMD-C2D	-2.67	1.45	1.50
15	c6	410	CLA	CMD-C2D	-2.67	1.45	1.50
18	a1	420	BCR	C30-C25	-2.67	1.50	1.53
15	aB	826	CLA	C3B-C4B	2.67	1.49	1.42
15	cB	812	CLA	C3B-C4B	2.67	1.49	1.42
15	aB	813	CLA	C1D-ND	2.67	1.41	1.37
15	b4	405	CLA	C4B-NB	2.67	1.41	1.37
15	cB	836	CLA	C1D-ND	2.67	1.41	1.37
15	b5	411	CLA	MG-NB	-2.67	2.00	2.05
15	bA	805	CLA	CMB-C2B	-2.67	1.45	1.50
15	cA	814	CLA	MG-NB	-2.67	2.00	2.05
15	cA	844	CLA	C4B-NB	2.67	1.41	1.37
15	cB	821	CLA	C1D-ND	2.67	1.41	1.37
15	c4	415	CLA	C4B-NB	2.67	1.41	1.37
15	bB	836	CLA	MG-ND	-2.67	2.00	2.05
15	cA	813	CLA	C1D-ND	2.67	1.41	1.37
18	a1	420	BCR	C1-C6	-2.67	1.50	1.53
15	cB	840	CLA	CMD-C2D	-2.67	1.45	1.50
15	c3	421	CLA	C1B-C2B	2.67	1.49	1.43
15	c6	412	CLA	C3B-C4B	2.67	1.49	1.42
15	a4	421	CLA	MG-ND	-2.67	2.00	2.05
15	c1	412	CLA	CMB-C2B	-2.67	1.45	1.50
15	c4	408	CLA	C4B-NB	2.67	1.41	1.37
15	cJ	101	CLA	C3B-C4B	2.67	1.49	1.42
15	b1	407	CLA	C4B-NB	2.67	1.41	1.37
18	c5	418	BCR	C40-C30	-2.67	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c5	412	CLA	CMB-C2B	-2.67	1.45	1.50
15	c2	405	CLA	C1D-C2D	2.67	1.50	1.45
15	a3	407	CLA	MG-NB	-2.67	2.00	2.05
15	cA	808	CLA	MG-NB	-2.67	2.00	2.05
15	bA	816	CLA	C4B-NB	2.67	1.41	1.37
18	b6	401	BCR	C30-C25	-2.67	1.50	1.53
15	a1	407	CLA	CMD-C2D	-2.67	1.45	1.50
18	a4	401	BCR	C30-C25	-2.67	1.50	1.53
15	bF	201	CLA	MG-ND	-2.67	2.00	2.05
15	b5	408	CLA	C3B-C4B	2.67	1.49	1.42
15	b6	411	CLA	C3B-C4B	2.67	1.49	1.42
15	aL	201	CLA	CMB-C2B	-2.67	1.45	1.50
15	aB	836	CLA	MG-ND	-2.67	2.00	2.05
15	a4	410	CLA	C4B-NB	2.67	1.41	1.37
15	bB	820	CLA	C1D-ND	2.67	1.41	1.37
15	aB	812	CLA	C1B-NB	-2.66	1.34	1.37
15	bA	813	CLA	C1D-ND	2.66	1.41	1.37
18	c1	418	BCR	C40-C30	-2.66	1.48	1.53
15	a2	407	CLA	C3B-C4B	2.66	1.49	1.42
15	cA	817	CLA	C3B-C4B	2.66	1.49	1.42
15	bL	202	CLA	C1D-ND	2.66	1.41	1.37
15	aA	835	CLA	CMD-C2D	-2.66	1.45	1.50
15	bB	837	CLA	C1B-NB	-2.66	1.34	1.37
15	cA	826	CLA	C1D-ND	2.66	1.41	1.37
15	c4	404	CLA	C3B-C4B	2.66	1.49	1.42
15	cA	821	CLA	C1B-NB	-2.66	1.34	1.37
15	c2	415	CLA	C1B-C2B	2.66	1.49	1.43
15	c5	410	CLA	C3B-C4B	2.66	1.49	1.42
15	aA	812	CLA	CMC-C2C	-2.66	1.45	1.50
15	bB	840	CLA	CMD-C2D	-2.66	1.45	1.50
15	b4	407	CLA	MG-NB	-2.66	2.00	2.05
15	c6	412	CLA	C4B-NB	2.66	1.41	1.37
15	a1	411	CLA	CMB-C2B	-2.66	1.45	1.50
15	c4	421	CLA	MG-ND	-2.66	2.00	2.05
18	c1	401	BCR	C30-C25	-2.66	1.50	1.53
15	a1	408	CLA	C3B-C4B	2.66	1.49	1.42
15	cA	815	CLA	C4B-NB	2.66	1.41	1.37
15	cB	807	CLA	MG-ND	-2.66	2.00	2.05
15	bA	821	CLA	MG-NB	-2.66	2.00	2.05
15	bB	810	CLA	CMD-C2D	-2.66	1.45	1.50
15	a1	407	CLA	C4B-NB	2.66	1.41	1.37
15	bA	821	CLA	C4B-NB	2.66	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	814	CLA	C3B-C4B	2.66	1.49	1.42
15	aA	840	CLA	C1D-ND	2.66	1.41	1.37
15	cA	839	CLA	C1D-ND	2.66	1.41	1.37
15	cL	204	CLA	C1B-NB	-2.66	1.34	1.37
15	bA	814	CLA	CMD-C2D	-2.66	1.45	1.50
15	cA	836	CLA	CMD-C2D	-2.66	1.45	1.50
15	aJ	201	CLA	C1D-ND	2.66	1.41	1.37
15	b4	417	CLA	C1B-NB	-2.66	1.34	1.37
15	c2	407	CLA	C3B-C4B	2.66	1.49	1.42
15	bB	810	CLA	MG-ND	-2.65	2.00	2.05
15	aJ	202	CLA	C3B-C4B	2.65	1.49	1.42
15	cA	835	CLA	CMD-C2D	-2.65	1.45	1.50
15	a5	412	CLA	MG-NB	-2.65	2.00	2.05
15	c3	411	CLA	C1B-NB	-2.65	1.34	1.37
15	bJ	101	CLA	C3B-C4B	2.65	1.49	1.42
15	a6	405	CLA	C3B-C4B	2.65	1.49	1.42
15	aA	843	CLA	CMD-C2D	-2.65	1.45	1.50
15	a1	412	CLA	CMB-C2B	-2.65	1.45	1.50
15	bB	814	CLA	CMC-C2C	-2.65	1.45	1.50
15	c2	409	CLA	CMD-C2D	-2.65	1.45	1.50
15	aB	812	CLA	C3B-C4B	2.65	1.49	1.42
15	a5	410	CLA	C3B-C4B	2.65	1.49	1.42
15	bA	816	CLA	MG-NB	-2.65	2.00	2.05
15	a4	415	CLA	C4B-NB	2.65	1.41	1.37
15	b4	410	CLA	C3B-C4B	2.65	1.49	1.42
15	aB	820	CLA	C1D-ND	2.65	1.41	1.37
15	a1	411	CLA	C4B-NB	2.65	1.41	1.37
15	a1	412	CLA	MG-NB	-2.65	2.00	2.05
15	c3	402	CLA	C1B-C2B	2.65	1.49	1.43
15	cB	842	CLA	C3B-C4B	2.65	1.49	1.42
15	bA	845	CLA	C4B-NB	2.65	1.41	1.37
15	cB	813	CLA	C1D-ND	2.65	1.41	1.37
15	c5	408	CLA	C4B-NB	2.65	1.41	1.37
15	b3	413	CLA	MG-NB	-2.65	2.00	2.05
15	c1	416	CLA	CHC-C4B	-2.65	1.33	1.39
15	a3	402	CLA	C1B-C2B	2.65	1.49	1.43
15	c4	407	CLA	MG-NB	-2.65	2.00	2.05
15	cA	844	CLA	C1D-ND	2.65	1.41	1.37
15	a2	410	CLA	C3B-C4B	2.65	1.49	1.42
15	a5	408	CLA	C4B-NB	2.65	1.41	1.37
15	b6	414	CLA	CMB-C2B	-2.65	1.45	1.50
15	bB	825	CLA	MG-ND	-2.65	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	836	CLA	MG-ND	-2.65	2.00	2.05
15	aX	102	CLA	C3B-C4B	2.65	1.49	1.42
15	a3	404	CLA	C3B-C4B	2.65	1.49	1.42
15	b6	406	CLA	C3B-C4B	2.65	1.49	1.42
15	b2	416	CLA	CMD-C2D	-2.65	1.45	1.50
15	c5	412	CLA	MG-NB	-2.65	2.00	2.05
15	bA	842	CLA	C3B-C4B	2.65	1.49	1.42
15	cB	810	CLA	MG-ND	-2.65	2.00	2.05
15	c5	410	CLA	MG-NB	-2.65	2.00	2.05
15	b2	402	CLA	C1B-C2B	2.65	1.49	1.43
15	bA	814	CLA	MG-NB	-2.65	2.00	2.05
15	cB	825	CLA	MG-ND	-2.65	2.00	2.05
15	cA	822	CLA	C1B-NB	-2.65	1.34	1.37
18	c6	402	BCR	C30-C25	-2.65	1.50	1.53
18	b3	418	BCR	C40-C30	-2.64	1.48	1.53
15	a2	414	CLA	CMB-C2B	-2.64	1.45	1.50
15	bA	830	CLA	CMD-C2D	-2.64	1.45	1.50
15	a5	411	CLA	MG-NB	-2.64	2.00	2.05
18	a3	419	BCR	C1-C6	-2.64	1.50	1.53
18	b1	401	BCR	C30-C25	-2.64	1.50	1.53
15	bA	809	CLA	C3B-C4B	2.64	1.49	1.42
15	aA	839	CLA	CMD-C2D	-2.64	1.45	1.50
15	b5	413	CLA	CMB-C2B	-2.64	1.45	1.50
15	c3	413	CLA	CMB-C2B	-2.64	1.45	1.50
15	b5	408	CLA	C4B-NB	2.64	1.41	1.37
15	aA	842	CLA	C3B-C4B	2.64	1.49	1.42
15	b2	407	CLA	C3B-C4B	2.64	1.49	1.42
15	a4	407	CLA	MG-NB	-2.64	2.00	2.05
15	b1	402	CLA	C1B-C2B	2.64	1.49	1.43
15	a2	422	CLA	MG-NB	-2.64	2.00	2.05
15	cA	821	CLA	MG-NB	-2.64	2.00	2.05
15	bL	202	CLA	CMB-C2B	-2.64	1.45	1.50
15	bB	813	CLA	C1D-ND	2.64	1.41	1.37
15	cB	827	CLA	C1B-NB	-2.64	1.34	1.37
15	aA	808	CLA	MG-NB	-2.64	2.00	2.05
15	a2	417	CLA	CHC-C4B	-2.64	1.33	1.39
15	aA	845	CLA	C4B-NB	2.64	1.41	1.37
15	bA	818	CLA	C1D-ND	2.64	1.41	1.37
15	b5	410	CLA	C3B-C4B	2.64	1.48	1.42
15	aB	828	CLA	MG-ND	-2.64	2.00	2.05
15	b3	413	CLA	CMB-C2B	-2.64	1.45	1.50
15	cA	814	CLA	CMD-C2D	-2.64	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	408	CLA	C3B-C4B	2.64	1.48	1.42
15	bA	845	CLA	C1D-ND	2.64	1.41	1.37
15	bB	821	CLA	C1D-ND	2.64	1.41	1.37
15	b2	409	CLA	CMD-C2D	-2.64	1.45	1.50
15	c1	412	CLA	C4B-NB	2.64	1.41	1.37
15	b1	413	CLA	CMB-C2B	-2.64	1.45	1.50
18	a4	418	BCR	C33-C5	-2.64	1.46	1.50
15	cB	814	CLA	CMC-C2C	-2.64	1.45	1.50
15	b1	413	CLA	C3B-C4B	2.64	1.48	1.42
15	aA	813	CLA	MG-ND	-2.64	2.00	2.05
15	cB	833	CLA	MG-NB	-2.64	2.00	2.05
15	b3	402	CLA	C1B-C2B	2.64	1.49	1.43
15	cA	813	CLA	MG-NB	-2.64	2.00	2.05
15	b2	417	CLA	CHC-C4B	-2.64	1.33	1.39
15	b4	408	CLA	C4B-NB	2.64	1.41	1.37
15	a5	410	CLA	MG-NB	-2.64	2.00	2.05
18	a3	418	BCR	C33-C5	-2.64	1.46	1.50
15	a5	413	CLA	CMB-C2B	-2.64	1.45	1.50
15	c1	409	CLA	C3B-C4B	2.64	1.48	1.42
15	bA	808	CLA	MG-NB	-2.64	2.00	2.05
15	c4	410	CLA	C3B-C4B	2.63	1.48	1.42
15	b3	415	CLA	MG-NB	-2.63	2.00	2.05
15	aL	203	CLA	C1B-NB	-2.63	1.34	1.37
15	aA	814	CLA	MG-NB	-2.63	2.00	2.05
15	b5	412	CLA	MG-NB	-2.63	2.00	2.05
15	aB	810	CLA	CMC-C2C	-2.63	1.45	1.50
15	bA	817	CLA	C3B-C4B	2.63	1.48	1.42
15	aB	836	CLA	C1D-ND	2.63	1.41	1.37
15	aA	814	CLA	C3B-C4B	2.63	1.48	1.42
15	bA	813	CLA	MG-NB	-2.63	2.00	2.05
15	cX	102	CLA	C3B-C4B	2.63	1.48	1.42
15	cB	827	CLA	C1D-ND	2.63	1.41	1.37
18	c6	420	BCR	C40-C30	-2.63	1.48	1.53
15	aA	836	CLA	CMD-C2D	-2.63	1.45	1.50
15	c3	404	CLA	C3B-C4B	2.63	1.48	1.42
15	bA	839	CLA	CMD-C2D	-2.63	1.45	1.50
15	c2	422	CLA	MG-NB	-2.63	2.00	2.05
15	bA	806	CLA	CMD-C2D	-2.63	1.45	1.50
15	b3	411	CLA	CMB-C2B	-2.63	1.45	1.50
15	a2	411	CLA	MG-NB	-2.63	2.00	2.05
15	c6	406	CLA	C3B-C4B	2.63	1.48	1.42
15	aA	820	CLA	CMC-C2C	-2.63	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	836	CLA	CMD-C2D	-2.63	1.45	1.50
15	bB	842	CLA	C3B-C4B	2.63	1.48	1.42
15	b3	415	CLA	C4B-NB	2.63	1.41	1.37
15	b1	411	CLA	MG-NB	-2.63	2.00	2.05
15	aB	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	cA	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	aB	810	CLA	MG-ND	-2.63	2.00	2.05
15	aB	827	CLA	C1D-ND	2.63	1.41	1.37
15	c2	417	CLA	CHC-C4B	-2.63	1.33	1.39
15	aA	821	CLA	C1B-NB	-2.63	1.34	1.37
15	bB	812	CLA	C1B-NB	-2.63	1.34	1.37
15	aA	823	CLA	MG-NB	-2.63	2.00	2.05
15	bA	814	CLA	CMC-C2C	-2.63	1.45	1.50
15	a2	414	CLA	MG-NB	-2.63	2.00	2.05
15	c3	411	CLA	C3B-C4B	2.63	1.48	1.42
15	aB	807	CLA	CMC-C2C	-2.63	1.45	1.50
15	bB	815	CLA	CMD-C2D	-2.63	1.45	1.50
15	a1	416	CLA	C1B-NB	-2.63	1.34	1.37
15	a3	421	CLA	C1B-C2B	2.63	1.49	1.43
15	aA	816	CLA	C4B-NB	2.63	1.41	1.37
15	cB	804	CLA	MG-ND	-2.63	2.00	2.05
15	c1	413	CLA	C3B-C4B	2.63	1.48	1.42
15	aA	813	CLA	MG-NB	-2.63	2.00	2.05
15	b5	409	CLA	MG-NB	-2.63	2.00	2.05
15	bA	815	CLA	C3B-C4B	2.62	1.48	1.42
15	aB	804	CLA	MG-ND	-2.62	2.00	2.05
15	aA	809	CLA	C3B-C4B	2.62	1.48	1.42
15	bA	821	CLA	C1B-NB	-2.62	1.34	1.37
15	cL	202	CLA	C1D-ND	2.62	1.41	1.37
15	a2	415	CLA	C1B-C2B	2.62	1.49	1.43
15	cA	843	CLA	C4B-NB	2.62	1.41	1.37
15	c3	415	CLA	C4B-NB	2.62	1.41	1.37
15	bX	102	CLA	C3B-C4B	2.62	1.48	1.42
15	a6	413	CLA	CMB-C2B	-2.62	1.45	1.50
15	cA	806	CLA	CMD-C2D	-2.62	1.45	1.50
15	cF	201	CLA	C3B-C4B	2.62	1.48	1.42
15	bB	838	CLA	C1B-NB	-2.62	1.34	1.37
15	aB	839	CLA	CMD-C2D	-2.62	1.45	1.50
15	cA	835	CLA	CMB-C2B	-2.62	1.45	1.50
15	aB	807	CLA	MG-ND	-2.62	2.00	2.05
15	a3	413	CLA	MG-NB	-2.62	2.00	2.05
15	c3	413	CLA	MG-NB	-2.62	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	827	CLA	C1B-NB	-2.62	1.34	1.37
15	a3	407	CLA	C4B-NB	2.62	1.41	1.37
15	cA	816	CLA	C4B-NB	2.62	1.41	1.37
15	cA	809	CLA	C3B-C4B	2.62	1.48	1.42
15	aJ	201	CLA	MG-ND	-2.62	2.00	2.05
15	cA	820	CLA	CMC-C2C	-2.62	1.45	1.50
15	c1	408	CLA	CMD-C2D	-2.62	1.45	1.50
15	c4	408	CLA	CMD-C2D	-2.62	1.45	1.50
18	c5	401	BCR	C30-C25	-2.62	1.50	1.53
15	aL	201	CLA	C1D-ND	2.62	1.41	1.37
15	a3	411	CLA	C1B-NB	-2.62	1.34	1.37
15	c1	408	CLA	C4B-NB	2.62	1.41	1.37
15	b6	403	CLA	C1B-C2B	2.62	1.49	1.43
15	c4	413	CLA	CMB-C2B	-2.62	1.45	1.50
15	a2	402	CLA	C1B-C2B	2.62	1.49	1.43
15	bA	835	CLA	CMB-C2B	-2.62	1.45	1.50
15	aA	806	CLA	CMD-C2D	-2.62	1.45	1.50
15	bB	807	CLA	CMC-C2C	-2.62	1.45	1.50
15	b5	410	CLA	MG-NB	-2.62	2.00	2.05
15	c3	411	CLA	CMB-C2B	-2.62	1.45	1.50
15	bA	839	CLA	C1D-ND	2.62	1.41	1.37
15	b1	417	CLA	C1B-NB	-2.62	1.34	1.37
15	b5	412	CLA	CMB-C2B	-2.61	1.45	1.50
15	b5	413	CLA	MG-NB	-2.61	2.00	2.05
15	aB	833	CLA	MG-NB	-2.61	2.00	2.05
15	a4	410	CLA	C3B-C4B	2.61	1.48	1.42
15	a5	406	CLA	C3B-C4B	2.61	1.48	1.42
15	b1	410	CLA	C3B-C4B	2.61	1.48	1.42
15	b6	413	CLA	CMB-C2B	-2.61	1.45	1.50
15	c4	402	CLA	C1B-C2B	2.61	1.49	1.43
15	cA	814	CLA	C3B-C4B	2.61	1.48	1.42
18	b4	418	BCR	C33-C5	-2.61	1.46	1.50
15	cF	203	CLA	MG-ND	-2.61	2.00	2.05
15	aA	829	CLA	C3B-C4B	2.61	1.48	1.42
15	aB	831	CLA	C1B-C2B	2.61	1.49	1.43
15	bA	820	CLA	CMC-C2C	-2.61	1.45	1.50
15	cB	815	CLA	CMD-C2D	-2.61	1.45	1.50
18	b6	419	BCR	C40-C30	-2.61	1.48	1.53
15	bA	829	CLA	C3B-C4B	2.61	1.48	1.42
18	b1	401	BCR	C34-C9	-2.61	1.45	1.50
15	a4	413	CLA	CMB-C2B	-2.61	1.45	1.50
15	a6	414	CLA	MG-NB	-2.61	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	407	CLA	C1B-C2B	2.61	1.49	1.43
15	b3	421	CLA	C1B-C2B	2.61	1.49	1.43
15	cB	828	CLA	MG-ND	-2.61	2.00	2.05
15	c5	411	CLA	MG-NB	-2.61	2.00	2.05
15	cF	203	CLA	C1D-ND	2.61	1.41	1.37
15	aA	817	CLA	C3B-C4B	2.61	1.48	1.42
15	aB	820	CLA	CMB-C2B	-2.61	1.45	1.50
15	c6	404	CLA	C1B-C2B	2.61	1.49	1.43
18	aF	203	BCR	C1-C6	-2.61	1.50	1.53
18	a5	401	BCR	C30-C25	-2.61	1.50	1.53
15	cA	816	CLA	MG-NB	-2.61	2.00	2.05
15	a1	405	CLA	C3B-C4B	2.61	1.48	1.42
15	a3	413	CLA	CMB-C2B	-2.61	1.45	1.50
15	cA	833	CLA	MG-ND	-2.61	2.00	2.05
15	aA	815	CLA	C3B-C4B	2.61	1.48	1.42
18	c3	418	BCR	C40-C30	-2.61	1.48	1.53
15	aA	814	CLA	CMC-C2C	-2.60	1.45	1.50
15	b3	411	CLA	C3B-C4B	2.60	1.48	1.42
15	cA	815	CLA	C3B-C4B	2.60	1.48	1.42
15	bB	838	CLA	C1D-ND	2.60	1.41	1.37
15	c4	405	CLA	C4B-NB	2.60	1.41	1.37
15	c5	413	CLA	CMB-C2B	-2.60	1.45	1.50
15	aA	803	CLA	C1B-NB	-2.60	1.34	1.37
15	cA	804	CLA	CMC-C2C	-2.60	1.45	1.50
15	a6	403	CLA	C1B-C2B	2.60	1.49	1.43
15	a1	412	CLA	C3B-C4B	2.60	1.48	1.42
15	b2	415	CLA	C1B-C2B	2.60	1.49	1.43
15	bB	810	CLA	CMC-C2C	-2.60	1.45	1.50
15	bB	827	CLA	C1B-NB	-2.60	1.34	1.37
15	c1	406	CLA	C3B-C4B	2.60	1.48	1.42
15	c5	406	CLA	C3B-C4B	2.60	1.48	1.42
15	cA	839	CLA	CMD-C2D	-2.60	1.45	1.50
15	b3	414	CLA	C1B-C2B	2.60	1.49	1.43
15	c6	415	CLA	C1B-C2B	2.60	1.49	1.43
15	b6	422	CLA	MG-ND	-2.60	2.00	2.05
15	cA	818	CLA	C1D-ND	2.60	1.41	1.37
15	a4	408	CLA	CMD-C2D	-2.60	1.45	1.50
15	b4	407	CLA	C4B-NB	2.60	1.41	1.37
15	b2	411	CLA	MG-NB	-2.60	2.00	2.05
15	c6	401	CLA	MG-ND	-2.60	2.00	2.05
15	a2	416	CLA	CMD-C2D	-2.60	1.45	1.50
15	a3	411	CLA	CMB-C2B	-2.60	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	416	CLA	MG-NB	-2.60	2.00	2.05
15	b1	412	CLA	CMB-C2B	-2.60	1.45	1.50
18	cF	205	BCR	C1-C6	-2.60	1.50	1.53
15	a5	413	CLA	MG-NB	-2.60	2.00	2.05
15	bA	804	CLA	CMC-C2C	-2.60	1.45	1.50
15	cB	832	CLA	MG-ND	-2.60	2.00	2.05
15	cA	830	CLA	CMD-C2D	-2.60	1.45	1.50
15	c1	417	CLA	C1B-NB	-2.60	1.34	1.37
18	c3	401	BCR	C30-C25	-2.60	1.50	1.53
15	b2	405	CLA	C3B-C4B	2.60	1.48	1.42
15	c5	403	CLA	CMD-C2D	-2.60	1.45	1.50
18	a3	418	BCR	C40-C30	-2.60	1.48	1.53
15	aA	813	CLA	C1D-ND	2.60	1.41	1.37
15	cB	821	CLA	MG-ND	-2.60	2.00	2.05
15	b6	407	CLA	C3B-C4B	2.60	1.48	1.42
15	cB	812	CLA	C1B-NB	-2.60	1.34	1.37
18	a3	401	BCR	C30-C25	-2.60	1.50	1.53
18	a6	402	BCR	C1-C6	-2.60	1.50	1.53
18	b5	418	BCR	C40-C30	-2.60	1.48	1.53
15	aA	834	CLA	CMD-C2D	-2.59	1.45	1.50
15	a6	410	CLA	C3B-C4B	2.59	1.48	1.42
15	aA	816	CLA	MG-NB	-2.59	2.00	2.05
15	c5	413	CLA	MG-NB	-2.59	2.00	2.05
15	c5	410	CLA	C4B-NB	2.59	1.41	1.37
15	b1	403	CLA	MG-NB	-2.59	2.00	2.05
15	a5	412	CLA	CMB-C2B	-2.59	1.45	1.50
15	b4	413	CLA	CMB-C2B	-2.59	1.45	1.50
18	b2	401	BCR	C30-C25	-2.59	1.50	1.53
15	aA	835	CLA	CMB-C2B	-2.59	1.45	1.50
15	c2	402	CLA	C1B-C2B	2.59	1.49	1.43
15	aB	837	CLA	C1D-ND	2.59	1.41	1.37
15	a4	407	CLA	C4B-NB	2.59	1.41	1.37
15	cB	839	CLA	CMD-C2D	-2.59	1.45	1.50
18	b5	401	BCR	C1-C6	-2.59	1.50	1.53
15	b5	406	CLA	C3B-C4B	2.59	1.48	1.42
15	a3	417	CLA	C1B-NB	-2.59	1.34	1.37
15	bA	826	CLA	C1D-ND	2.59	1.41	1.37
15	b3	417	CLA	C1B-NB	-2.59	1.34	1.37
15	c2	407	CLA	C1B-C2B	2.59	1.49	1.43
15	b6	417	CLA	CHC-C4B	-2.59	1.33	1.39
15	b4	405	CLA	C1B-C2B	2.59	1.49	1.43
15	a1	410	CLA	MG-NB	-2.59	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	413	CLA	MG-NB	-2.59	2.00	2.05
15	aA	802	CLA	CMD-C2D	-2.59	1.45	1.50
18	b6	419	BCR	C33-C5	-2.59	1.46	1.50
15	c1	410	CLA	C3B-C4B	2.59	1.48	1.42
18	a4	419	BCR	C30-C25	-2.59	1.50	1.53
15	aA	826	CLA	C1D-ND	2.59	1.41	1.37
15	c3	407	CLA	C4B-NB	2.59	1.41	1.37
15	cA	811	CLA	MG-NB	-2.59	2.00	2.05
15	cA	829	CLA	C3B-C4B	2.59	1.48	1.42
15	bA	806	CLA	C1B-NB	-2.59	1.34	1.37
15	b4	415	CLA	C4B-NB	2.59	1.41	1.37
15	c6	417	CLA	C3B-C4B	2.59	1.48	1.42
15	b3	410	CLA	MG-NB	-2.59	2.00	2.05
15	aB	820	CLA	C4B-NB	2.59	1.41	1.37
15	aB	838	CLA	C1D-ND	2.59	1.41	1.37
15	bA	838	CLA	C1D-ND	2.59	1.41	1.37
15	c2	409	CLA	C4B-NB	2.59	1.41	1.37
15	bB	823	CLA	C3B-C4B	2.59	1.48	1.42
15	b4	408	CLA	CMD-C2D	-2.59	1.45	1.50
15	cB	820	CLA	CMB-C2B	-2.59	1.45	1.50
15	b4	402	CLA	C1B-C2B	2.59	1.49	1.43
18	a2	401	BCR	C30-C25	-2.59	1.50	1.53
15	b3	408	CLA	C4B-NB	2.59	1.41	1.37
15	cB	831	CLA	C1B-C2B	2.59	1.49	1.43
15	bA	802	CLA	CMC-C2C	-2.59	1.45	1.50
15	a1	409	CLA	C3B-C4B	2.59	1.48	1.42
18	b1	401	BCR	C1-C6	-2.59	1.50	1.53
15	b1	411	CLA	C3B-C4B	2.59	1.48	1.42
15	bA	844	CLA	C4B-NB	2.58	1.41	1.37
15	a6	407	CLA	C3B-C4B	2.58	1.48	1.42
15	bA	819	CLA	MG-NB	-2.58	2.00	2.05
18	aA	848	BCR	C30-C25	-2.58	1.50	1.53
15	aA	804	CLA	CMC-C2C	-2.58	1.45	1.50
15	b3	409	CLA	C3B-C4B	2.58	1.48	1.42
15	aA	830	CLA	CMD-C2D	-2.58	1.45	1.50
15	b5	403	CLA	CMD-C2D	-2.58	1.45	1.50
15	b5	406	CLA	C1B-C2B	2.58	1.49	1.43
15	aB	837	CLA	C1B-NB	-2.58	1.34	1.37
15	cA	819	CLA	MG-NB	-2.58	2.00	2.05
15	bA	818	CLA	CMD-C2D	-2.58	1.45	1.50
15	b1	408	CLA	CMD-C2D	-2.58	1.45	1.50
15	cB	807	CLA	CMC-C2C	-2.58	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	406	CLA	C3B-C4B	2.58	1.48	1.42
15	cB	810	CLA	CMC-C2C	-2.58	1.45	1.50
15	c4	409	CLA	C3B-C4B	2.58	1.48	1.42
15	bB	804	CLA	MG-ND	-2.58	2.00	2.05
15	bB	831	CLA	C1B-C2B	2.58	1.49	1.43
15	aA	824	CLA	C4B-NB	2.58	1.41	1.37
15	aA	802	CLA	CMC-C2C	-2.58	1.45	1.50
15	bA	833	CLA	MG-ND	-2.58	2.00	2.05
15	cA	844	CLA	MG-NB	-2.58	2.00	2.05
15	aA	803	CLA	CMB-C2B	-2.58	1.45	1.50
15	c6	415	CLA	CMB-C2B	-2.58	1.45	1.50
15	a3	408	CLA	C4B-NB	2.58	1.41	1.37
15	bA	822	CLA	C1B-NB	-2.58	1.34	1.37
15	aB	815	CLA	CMD-C2D	-2.58	1.45	1.50
15	bB	820	CLA	CMB-C2B	-2.58	1.45	1.50
15	cA	840	CLA	CMD-C2D	-2.58	1.45	1.50
15	aA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	cA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	aB	819	CLA	C1D-ND	2.58	1.41	1.37
15	a3	415	CLA	C4B-NB	2.58	1.41	1.37
15	a6	416	CLA	C3B-C4B	2.58	1.48	1.42
15	bA	831	CLA	CMC-C2C	-2.58	1.45	1.50
15	cA	842	CLA	CMB-C2B	-2.58	1.45	1.50
15	b2	414	CLA	MG-NB	-2.58	2.00	2.05
15	bA	823	CLA	MG-NB	-2.58	2.00	2.05
15	cL	204	CLA	MG-ND	-2.58	2.00	2.05
15	aB	811	CLA	CMB-C2B	-2.58	1.45	1.50
15	a4	408	CLA	C4B-NB	2.57	1.40	1.37
15	a3	411	CLA	C3B-C4B	2.57	1.48	1.42
15	c5	406	CLA	C1B-C2B	2.57	1.49	1.43
18	a6	419	BCR	C40-C30	-2.57	1.48	1.53
15	c1	403	CLA	MG-NB	-2.57	2.00	2.05
15	aB	823	CLA	C3B-C4B	2.57	1.48	1.42
15	a2	411	CLA	C4B-NB	2.57	1.40	1.37
15	a3	415	CLA	MG-NB	-2.57	2.00	2.05
15	cB	820	CLA	C4B-NB	2.57	1.40	1.37
15	b6	410	CLA	C3B-C4B	2.57	1.48	1.42
15	aA	819	CLA	MG-NB	-2.57	2.00	2.05
15	aB	821	CLA	MG-ND	-2.57	2.00	2.05
15	cA	834	CLA	CMD-C2D	-2.57	1.45	1.50
15	b4	413	CLA	MG-NB	-2.57	2.00	2.05
15	bA	803	CLA	CMB-C2B	-2.57	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c2	412	CLA	MG-NB	-2.57	2.00	2.05
15	bB	821	CLA	MG-ND	-2.57	2.00	2.05
15	bB	833	CLA	MG-NB	-2.57	2.00	2.05
15	a2	405	CLA	C3B-C4B	2.57	1.48	1.42
15	b2	417	CLA	C3B-C4B	2.57	1.48	1.42
15	a4	410	CLA	MG-NB	-2.57	2.00	2.05
15	aA	810	CLA	CMB-C2B	-2.57	1.45	1.50
15	b6	414	CLA	C1B-C2B	2.57	1.49	1.43
15	bA	824	CLA	C4B-NB	2.57	1.40	1.37
15	bA	834	CLA	CMD-C2D	-2.57	1.45	1.50
18	b4	419	BCR	C30-C25	-2.57	1.50	1.53
15	a3	411	CLA	MG-NB	-2.57	2.00	2.05
15	a4	413	CLA	MG-NB	-2.57	2.00	2.05
15	cA	823	CLA	MG-NB	-2.57	2.00	2.05
15	a2	409	CLA	C4B-NB	2.57	1.40	1.37
15	bB	819	CLA	C1D-ND	2.57	1.40	1.37
15	cA	812	CLA	MG-NB	-2.57	2.00	2.05
15	a2	416	CLA	MG-NB	-2.57	2.00	2.05
15	bA	845	CLA	MG-NB	-2.57	2.00	2.05
18	c6	403	BCR	C1-C6	-2.57	1.50	1.53
15	b3	411	CLA	MG-NB	-2.57	2.00	2.05
15	c2	411	CLA	MG-NB	-2.57	2.00	2.05
18	b6	402	BCR	C1-C6	-2.57	1.50	1.53
15	aA	806	CLA	C1B-NB	-2.57	1.34	1.37
15	b5	410	CLA	C4B-NB	2.57	1.40	1.37
15	b2	417	CLA	C1C-NC	-2.57	1.34	1.37
15	c2	414	CLA	C1B-C2B	2.57	1.49	1.43
15	cB	802	CLA	MG-ND	-2.57	2.00	2.05
15	bA	802	CLA	CMD-C2D	-2.57	1.45	1.50
15	a4	405	CLA	C4B-NB	2.57	1.40	1.37
15	aA	832	CLA	CMB-C2B	-2.57	1.45	1.50
15	a2	407	CLA	C1B-C2B	2.57	1.49	1.43
15	c1	402	CLA	C1B-C2B	2.57	1.49	1.43
15	c2	405	CLA	C3B-C4B	2.57	1.48	1.42
18	b3	401	BCR	C30-C25	-2.57	1.50	1.53
15	aB	832	CLA	MG-ND	-2.57	2.00	2.05
15	b2	404	CLA	C3B-C4B	2.56	1.48	1.42
15	a1	401	CLA	C1B-C2B	2.56	1.49	1.43
15	a5	409	CLA	MG-NB	-2.56	2.00	2.05
15	bA	822	CLA	MG-ND	-2.56	2.00	2.05
15	c6	411	CLA	C3B-C4B	2.56	1.48	1.42
15	bA	844	CLA	C3B-C4B	2.56	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c4	414	CLA	C1B-C2B	2.56	1.49	1.43
15	c3	415	CLA	MG-NB	-2.56	2.00	2.05
15	b3	405	CLA	MG-NB	-2.56	2.00	2.05
15	cA	803	CLA	CMB-C2B	-2.56	1.45	1.50
15	b4	421	CLA	C2A-C1A	2.56	1.58	1.52
15	aA	833	CLA	MG-ND	-2.56	2.00	2.05
15	cA	806	CLA	MG-ND	-2.56	2.00	2.05
18	a5	401	BCR	C1-C6	-2.56	1.50	1.53
15	bB	836	CLA	C3B-C4B	2.56	1.48	1.42
15	a5	403	CLA	CMD-C2D	-2.56	1.45	1.50
15	cA	832	CLA	CMB-C2B	-2.56	1.45	1.50
15	a2	404	CLA	MG-NB	-2.56	2.00	2.05
15	aB	802	CLA	MG-ND	-2.56	2.00	2.05
15	bB	832	CLA	MG-ND	-2.56	2.00	2.05
15	bL	204	CLA	MG-ND	-2.56	2.00	2.05
15	a4	402	CLA	C1B-C2B	2.56	1.49	1.43
15	aB	836	CLA	C3B-C4B	2.56	1.48	1.42
15	a3	410	CLA	MG-NB	-2.56	2.00	2.05
15	bB	839	CLA	CMD-C2D	-2.56	1.45	1.50
15	c4	407	CLA	C4B-NB	2.56	1.40	1.37
15	a1	412	CLA	C1B-C2B	2.56	1.49	1.43
15	aL	203	CLA	MG-ND	-2.56	2.00	2.05
15	a6	413	CLA	MG-NB	-2.56	2.00	2.05
15	b2	404	CLA	MG-NB	-2.56	2.00	2.05
15	b3	411	CLA	C1B-NB	-2.56	1.34	1.37
15	bA	818	CLA	CMC-C2C	-2.56	1.45	1.50
15	cA	802	CLA	CMD-C2D	-2.56	1.45	1.50
15	bA	811	CLA	MG-NB	-2.56	2.00	2.05
15	c6	404	CLA	C3B-C4B	2.56	1.48	1.42
15	aA	844	CLA	C4B-NB	2.56	1.40	1.37
15	b2	409	CLA	C4B-NB	2.56	1.40	1.37
15	b4	409	CLA	C3B-C4B	2.56	1.48	1.42
15	aA	811	CLA	MG-NB	-2.56	2.00	2.05
18	c4	418	BCR	C33-C5	-2.56	1.46	1.50
15	a4	414	CLA	C1B-C2B	2.56	1.49	1.43
15	aA	812	CLA	C4B-NB	2.56	1.40	1.37
15	a1	403	CLA	C1B-C2B	2.56	1.49	1.43
15	a3	414	CLA	C1B-C2B	2.56	1.49	1.43
15	bJ	102	CLA	C3B-C4B	2.56	1.48	1.42
15	aA	840	CLA	CMD-C2D	-2.55	1.45	1.50
15	bX	102	CLA	CMD-C2D	-2.55	1.45	1.50
15	cA	824	CLA	C4B-NB	2.55	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	819	CLA	C1D-ND	2.55	1.40	1.37
15	c1	411	CLA	C3B-C4B	2.55	1.48	1.42
15	a6	417	CLA	CHC-C4B	-2.55	1.33	1.39
15	cA	805	CLA	C1D-ND	2.55	1.40	1.37
15	c4	421	CLA	C2A-C1A	2.55	1.58	1.52
15	c3	411	CLA	MG-NB	-2.55	2.00	2.05
15	a3	421	CLA	CMD-C2D	-2.55	1.45	1.50
15	c3	414	CLA	C1B-C2B	2.55	1.49	1.43
18	c4	419	BCR	C30-C25	-2.55	1.50	1.53
15	a2	404	CLA	C3B-C4B	2.55	1.48	1.42
15	cA	824	CLA	MG-NB	-2.55	2.00	2.05
15	aB	829	CLA	C1B-NB	-2.55	1.34	1.37
15	bB	820	CLA	C4B-NB	2.55	1.40	1.37
15	aA	843	CLA	CMB-C2B	-2.55	1.45	1.50
15	bA	823	CLA	C1B-C2B	2.55	1.49	1.43
15	cA	804	CLA	C1B-NB	-2.55	1.34	1.37
15	b1	404	CLA	C1B-C2B	2.55	1.49	1.43
15	bA	805	CLA	C1D-ND	2.55	1.40	1.37
18	a3	419	BCR	C30-C25	-2.55	1.50	1.53
18	c2	401	BCR	C30-C25	-2.55	1.50	1.53
15	bA	832	CLA	CMB-C2B	-2.55	1.45	1.50
15	aA	823	CLA	C4B-NB	2.55	1.40	1.37
15	bB	835	CLA	C4B-NB	2.55	1.40	1.37
15	a4	409	CLA	C3B-C4B	2.55	1.48	1.42
15	cB	811	CLA	CMB-C2B	-2.55	1.45	1.50
15	cB	813	CLA	CMB-C2B	-2.55	1.45	1.50
15	a2	414	CLA	C1B-C2B	2.55	1.49	1.43
15	cA	831	CLA	CMD-C2D	-2.55	1.45	1.50
18	c6	420	BCR	C33-C5	-2.55	1.46	1.50
15	cA	818	CLA	MG-NB	-2.55	2.00	2.05
18	bJ	105	BCR	C1-C6	-2.55	1.50	1.53
15	cB	835	CLA	C4B-NB	2.55	1.40	1.37
15	a6	415	CLA	C1B-C2B	2.55	1.49	1.43
15	b4	414	CLA	C1B-C2B	2.55	1.49	1.43
15	aA	824	CLA	MG-NB	-2.55	2.00	2.05
15	c4	405	CLA	C1B-C2B	2.55	1.49	1.43
15	cB	823	CLA	C3B-C4B	2.55	1.48	1.42
15	cA	807	CLA	CMC-C2C	-2.55	1.45	1.50
18	c5	401	BCR	C1-C6	-2.55	1.50	1.53
15	c4	413	CLA	MG-NB	-2.55	2.00	2.05
15	bA	823	CLA	C4B-NB	2.55	1.40	1.37
15	cA	818	CLA	CMD-C2D	-2.55	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	845	CLA	MG-NB	-2.55	2.00	2.05
15	bA	812	CLA	MG-NB	-2.54	2.00	2.05
15	bB	802	CLA	MG-ND	-2.54	2.00	2.05
15	c2	416	CLA	MG-NB	-2.54	2.00	2.05
18	b5	418	BCR	C33-C5	-2.54	1.46	1.50
15	aA	844	CLA	C1B-C2B	2.54	1.49	1.43
15	cA	819	CLA	C4B-NB	2.54	1.40	1.37
15	bA	806	CLA	MG-ND	-2.54	2.00	2.05
15	bA	824	CLA	MG-NB	-2.54	2.00	2.05
15	c1	411	CLA	MG-NB	-2.54	2.00	2.05
15	bA	819	CLA	C4B-NB	2.54	1.40	1.37
15	cB	838	CLA	C1D-ND	2.54	1.40	1.37
15	aA	812	CLA	MG-NB	-2.54	2.00	2.05
15	cA	822	CLA	MG-ND	-2.54	2.00	2.05
15	cB	825	CLA	CMC-C2C	-2.54	1.45	1.50
15	a2	412	CLA	MG-NB	-2.54	2.00	2.05
15	a3	409	CLA	C3B-C4B	2.54	1.48	1.42
15	b6	416	CLA	C3B-C4B	2.54	1.48	1.42
15	aA	822	CLA	MG-ND	-2.54	2.00	2.05
15	aA	835	CLA	MG-NB	-2.54	2.00	2.05
15	c3	409	CLA	C3B-C4B	2.54	1.48	1.42
15	aA	818	CLA	CMD-C2D	-2.54	1.45	1.50
15	aL	201	CLA	CMD-C2D	-2.54	1.45	1.50
15	cA	843	CLA	C3B-C4B	2.54	1.48	1.42
18	a6	419	BCR	C33-C5	-2.54	1.46	1.50
15	a6	414	CLA	C1B-C2B	2.54	1.49	1.43
15	cA	825	CLA	C3B-C4B	2.54	1.48	1.42
15	b2	414	CLA	C1B-C2B	2.54	1.49	1.43
18	cA	847	BCR	C30-C25	-2.54	1.50	1.53
15	cB	818	CLA	CMC-C2C	-2.54	1.45	1.50
15	aJ	203	CLA	C3B-C4B	2.54	1.48	1.42
15	a3	421	CLA	MG-NB	-2.54	2.00	2.05
15	cA	818	CLA	CMC-C2C	-2.54	1.45	1.50
15	aA	822	CLA	C1B-NB	-2.54	1.34	1.37
15	c3	408	CLA	C4B-NB	2.54	1.40	1.37
15	c2	404	CLA	MG-NB	-2.54	2.00	2.05
15	b1	415	CLA	C3B-C4B	2.54	1.48	1.42
15	a1	405	CLA	C1B-C2B	2.54	1.49	1.43
15	a5	412	CLA	C1B-NB	-2.54	1.34	1.37
15	aA	819	CLA	C4B-NB	2.54	1.40	1.37
15	cA	810	CLA	CMB-C2B	-2.54	1.45	1.50
15	a1	404	CLA	C3B-C4B	2.54	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	410	CLA	MG-NB	-2.54	2.00	2.05
15	aL	203	CLA	CMB-C2B	-2.54	1.45	1.50
15	bB	809	CLA	CMC-C2C	-2.54	1.45	1.50
15	bB	811	CLA	CMB-C2B	-2.54	1.45	1.50
15	a3	406	CLA	C3B-C4B	2.54	1.48	1.42
15	bA	803	CLA	C1B-NB	-2.54	1.34	1.37
15	bA	804	CLA	C1B-NB	-2.54	1.34	1.37
15	a3	408	CLA	MG-NB	-2.54	2.00	2.05
15	a6	403	CLA	C3B-C4B	2.54	1.48	1.42
15	b3	406	CLA	C1B-C2B	2.54	1.49	1.43
15	c3	405	CLA	C1B-C2B	2.54	1.49	1.43
15	bB	826	CLA	C1D-ND	2.54	1.40	1.37
15	b4	410	CLA	MG-NB	-2.54	2.00	2.05
15	b1	407	CLA	C3B-C4B	2.53	1.48	1.42
15	a5	410	CLA	C4B-NB	2.53	1.40	1.37
15	aA	831	CLA	CMD-C2D	-2.53	1.45	1.50
15	aB	820	CLA	CMD-C2D	-2.53	1.45	1.50
15	a1	402	CLA	MG-NB	-2.53	2.00	2.05
15	cA	810	CLA	MG-NB	-2.53	2.00	2.05
18	a1	420	BCR	C34-C9	-2.53	1.45	1.50
15	b3	405	CLA	C4B-NB	2.53	1.40	1.37
15	cA	838	CLA	C1D-ND	2.53	1.40	1.37
15	bA	840	CLA	CMD-C2D	-2.53	1.45	1.50
15	c5	411	CLA	C1B-NB	-2.53	1.34	1.37
15	b2	412	CLA	MG-NB	-2.53	2.00	2.05
15	c3	408	CLA	MG-NB	-2.53	2.00	2.05
15	c2	413	CLA	MG-ND	-2.53	2.00	2.05
15	cA	820	CLA	C4B-NB	2.53	1.40	1.37
15	aA	806	CLA	MG-ND	-2.53	2.00	2.05
15	a5	411	CLA	CMB-C2B	-2.53	1.45	1.50
15	bA	831	CLA	CMD-C2D	-2.53	1.45	1.50
15	aB	818	CLA	CMC-C2C	-2.53	1.45	1.50
15	bB	840	CLA	C4B-NB	2.53	1.40	1.37
15	b6	415	CLA	C1B-C2B	2.53	1.49	1.43
18	b3	419	BCR	C30-C25	-2.53	1.50	1.53
15	a4	421	CLA	MG-NB	-2.53	2.00	2.05
15	b3	421	CLA	MG-NB	-2.53	2.00	2.05
15	c4	411	CLA	MG-NB	-2.53	2.00	2.05
15	aA	838	CLA	C1D-ND	2.53	1.40	1.37
15	c3	417	CLA	C1B-NB	-2.53	1.34	1.37
15	a1	402	CLA	CMD-C2D	-2.53	1.45	1.50
18	b6	402	BCR	C30-C25	-2.53	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	828	CLA	C1B-NB	-2.53	1.34	1.37
15	bB	813	CLA	CMB-C2B	-2.53	1.45	1.50
15	a5	406	CLA	C1B-C2B	2.53	1.49	1.43
15	a4	417	CLA	C1B-NB	-2.53	1.34	1.37
15	aA	825	CLA	C3B-C4B	2.53	1.48	1.42
15	aA	810	CLA	MG-NB	-2.53	2.00	2.05
15	cA	812	CLA	C4B-NB	2.53	1.40	1.37
15	cA	812	CLA	C3B-C4B	2.53	1.48	1.42
15	a6	422	CLA	CMB-C2B	-2.53	1.45	1.50
15	bA	807	CLA	CMC-C2C	-2.53	1.45	1.50
15	aB	826	CLA	C1D-ND	2.53	1.40	1.37
15	cL	204	CLA	CMB-C2B	-2.53	1.45	1.50
15	c5	409	CLA	MG-NB	-2.53	2.00	2.05
15	c6	416	CLA	C1B-C2B	2.53	1.49	1.43
15	a4	412	CLA	C1B-NB	-2.53	1.34	1.37
15	b5	411	CLA	C1B-NB	-2.53	1.34	1.37
15	c1	411	CLA	C1B-NB	-2.53	1.34	1.37
18	a1	418	BCR	C30-C25	-2.53	1.50	1.53
15	cA	802	CLA	CMC-C2C	-2.53	1.45	1.50
15	bA	843	CLA	CMB-C2B	-2.53	1.45	1.50
15	aA	818	CLA	CMC-C2C	-2.52	1.45	1.50
15	c3	406	CLA	C3B-C4B	2.52	1.48	1.42
15	aB	819	CLA	MG-ND	-2.52	2.00	2.05
15	c3	410	CLA	MG-NB	-2.52	2.00	2.05
15	cA	823	CLA	C4B-NB	2.52	1.40	1.37
15	a3	406	CLA	C1B-C2B	2.52	1.49	1.43
15	a4	405	CLA	C1B-C2B	2.52	1.49	1.43
15	aB	821	CLA	MG-NB	-2.52	2.00	2.05
18	aK	101	BCR	C30-C25	-2.52	1.50	1.53
15	a1	410	CLA	C3B-C4B	2.52	1.48	1.42
15	aA	823	CLA	C1B-C2B	2.52	1.49	1.43
15	b6	412	CLA	MG-NB	-2.52	2.00	2.05
15	cA	809	CLA	MG-NB	-2.52	2.00	2.05
15	aA	812	CLA	C3B-C4B	2.52	1.48	1.42
15	aA	844	CLA	C3B-C4B	2.52	1.48	1.42
15	bA	825	CLA	C3B-C4B	2.52	1.48	1.42
15	a5	413	CLA	C1B-C2B	2.52	1.49	1.43
15	a1	406	CLA	C3B-C4B	2.52	1.48	1.42
15	cA	818	CLA	C3B-C4B	2.52	1.48	1.42
15	bA	810	CLA	CMB-C2B	-2.52	1.45	1.50
15	bB	808	CLA	MG-NB	-2.52	2.00	2.05
15	cJ	102	CLA	C3B-C4B	2.52	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b5	401	BCR	C30-C25	-2.52	1.50	1.53
15	c6	413	CLA	MG-NB	-2.52	2.00	2.05
15	b6	408	CLA	C3B-C4B	2.52	1.48	1.42
15	bB	828	CLA	CMB-C2B	-2.52	1.45	1.50
15	bB	808	CLA	C1B-C2B	2.52	1.49	1.43
18	c3	419	BCR	C30-C25	-2.52	1.50	1.53
15	a4	421	CLA	C2A-C1A	2.52	1.57	1.52
15	c3	406	CLA	C1B-C2B	2.52	1.49	1.43
15	c5	413	CLA	C1B-C2B	2.52	1.49	1.43
15	a1	415	CLA	CMB-C2B	-2.52	1.45	1.50
15	aA	809	CLA	MG-NB	-2.52	2.00	2.05
15	b1	403	CLA	CMD-C2D	-2.52	1.45	1.50
15	cL	204	CLA	CMD-C2D	-2.52	1.45	1.50
15	c6	418	CLA	CHC-C4B	-2.52	1.33	1.39
15	c1	406	CLA	C1B-C2B	2.52	1.49	1.43
15	b3	403	CLA	MG-NB	-2.52	2.00	2.05
15	cB	836	CLA	C3B-C4B	2.52	1.48	1.42
15	bB	822	CLA	C1B-C2B	2.52	1.49	1.43
15	a2	406	CLA	MG-ND	-2.52	2.00	2.05
15	b2	403	CLA	MG-NB	-2.52	2.00	2.05
15	bL	204	CLA	CMB-C2B	-2.52	1.45	1.50
15	b6	422	CLA	C1B-C2B	2.52	1.49	1.43
15	cA	826	CLA	MG-ND	-2.52	2.00	2.05
15	aB	813	CLA	CMB-C2B	-2.52	1.45	1.50
15	bA	809	CLA	MG-NB	-2.52	2.00	2.05
15	cA	835	CLA	MG-NB	-2.52	2.00	2.05
15	aL	203	CLA	CMD-C2D	-2.52	1.45	1.50
15	c2	413	CLA	C1B-NB	-2.52	1.34	1.37
15	c3	421	CLA	C2A-C1A	2.51	1.57	1.52
15	b5	411	CLA	CMB-C2B	-2.51	1.45	1.50
15	a6	408	CLA	C3B-C4B	2.51	1.48	1.42
15	aX	102	CLA	CMD-C2D	-2.51	1.45	1.50
15	cB	827	CLA	MG-ND	-2.51	2.00	2.05
15	c5	412	CLA	MG-ND	-2.51	2.00	2.05
15	cB	833	CLA	CMB-C2B	-2.51	1.45	1.50
15	aB	806	CLA	C1D-ND	2.51	1.40	1.37
15	aB	808	CLA	C1B-C2B	2.51	1.49	1.43
15	a1	408	CLA	C1B-C2B	2.51	1.49	1.43
15	cJ	102	CLA	C1B-C2B	2.51	1.49	1.43
15	c3	421	CLA	CMD-C2D	-2.51	1.45	1.50
15	c4	412	CLA	MG-ND	-2.51	2.00	2.05
15	b2	406	CLA	CAA-CBA	-2.51	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	836	CLA	CMD-C2D	-2.51	1.45	1.50
15	a3	405	CLA	MG-NB	-2.51	2.00	2.05
15	aB	835	CLA	C4B-NB	2.51	1.40	1.37
15	aB	835	CLA	C3B-C4B	2.51	1.48	1.42
15	bA	818	CLA	C3B-C4B	2.51	1.48	1.42
15	cB	839	CLA	C3B-C4B	2.51	1.48	1.42
15	bB	825	CLA	CMC-C2C	-2.51	1.45	1.50
15	aA	836	CLA	MG-NB	-2.51	2.00	2.05
15	bA	836	CLA	MG-NB	-2.51	2.00	2.05
15	cB	819	CLA	MG-ND	-2.51	2.00	2.05
15	cL	202	CLA	CMD-C2D	-2.51	1.45	1.50
15	bB	819	CLA	C1B-NB	-2.51	1.34	1.37
15	a3	421	CLA	C2A-C1A	2.51	1.57	1.52
15	a2	406	CLA	CAA-CBA	-2.51	1.45	1.52
15	b1	413	CLA	C1B-C2B	2.51	1.49	1.43
15	a1	409	CLA	MG-NB	-2.51	2.00	2.05
18	a6	402	BCR	C30-C25	-2.51	1.50	1.53
15	aB	809	CLA	C1D-ND	2.51	1.40	1.37
15	c2	422	CLA	CMD-C2D	-2.51	1.45	1.50
15	cB	820	CLA	CMD-C2D	-2.51	1.45	1.50
15	c2	406	CLA	CMD-C2D	-2.51	1.45	1.50
15	a6	422	CLA	CAA-C2A	2.51	1.58	1.54
15	a1	414	CLA	C3B-C4B	2.51	1.48	1.42
15	aA	804	CLA	C1B-NB	-2.51	1.34	1.37
15	cB	826	CLA	C1D-ND	2.51	1.40	1.37
15	a4	411	CLA	MG-NB	-2.51	2.00	2.05
15	c4	410	CLA	MG-NB	-2.51	2.00	2.05
15	aJ	203	CLA	C1B-C2B	2.51	1.49	1.43
15	bB	821	CLA	MG-NB	-2.51	2.00	2.05
15	cA	823	CLA	C1B-C2B	2.51	1.49	1.43
15	cB	808	CLA	C1B-C2B	2.51	1.49	1.43
15	c2	408	CLA	C1B-C2B	2.51	1.49	1.43
15	aA	807	CLA	CMC-C2C	-2.51	1.45	1.50
18	a5	418	BCR	C33-C5	-2.51	1.46	1.50
15	a6	406	CLA	C1D-C2D	2.51	1.50	1.45
15	aB	827	CLA	MG-ND	-2.51	2.00	2.05
15	cB	836	CLA	CMD-C2D	-2.51	1.45	1.50
15	aB	834	CLA	C3B-C4B	2.51	1.48	1.42
15	bA	818	CLA	MG-NB	-2.51	2.00	2.05
15	b6	406	CLA	C1D-C2D	2.51	1.50	1.45
15	cA	843	CLA	C1B-C2B	2.51	1.49	1.43
15	a3	405	CLA	C4B-NB	2.51	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	820	CLA	CMD-C2D	-2.51	1.45	1.50
15	bA	810	CLA	MG-NB	-2.51	2.00	2.05
15	c4	403	CLA	CMD-C2D	-2.51	1.45	1.50
15	bB	829	CLA	C1B-NB	-2.51	1.34	1.37
15	cB	829	CLA	C1B-NB	-2.51	1.34	1.37
15	aB	825	CLA	CMC-C2C	-2.51	1.45	1.50
15	b3	410	CLA	C3B-C4B	2.50	1.48	1.42
15	bB	827	CLA	MG-ND	-2.50	2.00	2.05
15	aA	818	CLA	C3B-C4B	2.50	1.48	1.42
15	b3	421	CLA	CMD-C2D	-2.50	1.45	1.50
15	b1	411	CLA	C1B-NB	-2.50	1.34	1.37
15	c1	405	CLA	C3B-C4B	2.50	1.48	1.42
15	c2	417	CLA	C3B-C4B	2.50	1.48	1.42
15	b4	412	CLA	C1B-NB	-2.50	1.34	1.37
15	bA	817	CLA	CMB-C2B	-2.50	1.45	1.50
15	aB	839	CLA	C3B-C4B	2.50	1.48	1.42
15	b6	403	CLA	C3B-C4B	2.50	1.48	1.42
15	cB	824	CLA	MG-NB	-2.50	2.00	2.05
15	bB	833	CLA	CMB-C2B	-2.50	1.45	1.50
15	bL	202	CLA	CMD-C2D	-2.50	1.45	1.50
15	cB	835	CLA	CMC-C2C	-2.50	1.45	1.50
15	a4	408	CLA	MG-NB	-2.50	2.00	2.05
15	aB	803	CLA	CMC-C2C	-2.50	1.45	1.50
15	bB	838	CLA	CMB-C2B	-2.50	1.45	1.50
15	a2	417	CLA	C3B-C4B	2.50	1.48	1.42
15	c1	407	CLA	C3B-C4B	2.50	1.48	1.42
15	a1	410	CLA	C1B-NB	-2.50	1.34	1.37
15	c4	417	CLA	C1B-NB	-2.50	1.34	1.37
15	b2	413	CLA	MG-ND	-2.50	2.00	2.05
15	c4	412	CLA	C1B-NB	-2.50	1.34	1.37
15	cB	828	CLA	CMB-C2B	-2.50	1.45	1.50
15	bA	844	CLA	C1B-C2B	2.50	1.49	1.43
15	a2	422	CLA	CMD-C2D	-2.50	1.45	1.50
15	cB	838	CLA	CMB-C2B	-2.50	1.45	1.50
15	c1	403	CLA	CMD-C2D	-2.50	1.45	1.50
15	aA	805	CLA	C1D-ND	2.50	1.40	1.37
15	bA	835	CLA	C1B-NB	-2.50	1.34	1.37
15	cB	822	CLA	C1B-C2B	2.50	1.49	1.43
15	a5	411	CLA	C1B-NB	-2.50	1.34	1.37
15	c5	412	CLA	C1B-NB	-2.50	1.34	1.37
15	bB	819	CLA	CMD-C2D	-2.50	1.45	1.50
15	b2	406	CLA	CMD-C2D	-2.50	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	819	CLA	CMD-C2D	-2.50	1.45	1.50
15	cA	821	CLA	C1B-C2B	2.50	1.49	1.43
15	c3	410	CLA	C3B-C4B	2.50	1.48	1.42
15	a4	403	CLA	CMD-C2D	-2.50	1.45	1.50
15	bL	204	CLA	CMD-C2D	-2.50	1.45	1.50
15	c3	410	CLA	C4B-NB	2.50	1.40	1.37
15	cB	809	CLA	CMC-C2C	-2.50	1.45	1.50
15	b1	405	CLA	C3B-C4B	2.50	1.48	1.42
15	b5	412	CLA	C1B-NB	-2.50	1.34	1.37
15	aB	822	CLA	C1B-C2B	2.50	1.49	1.43
15	cX	102	CLA	CMD-C2D	-2.50	1.45	1.50
15	bA	812	CLA	C3B-C4B	2.50	1.48	1.42
15	b3	406	CLA	C3B-C4B	2.50	1.48	1.42
18	a2	420	BCR	C30-C25	-2.49	1.50	1.53
15	cL	203	CLA	CMC-C2C	-2.49	1.45	1.50
15	b3	410	CLA	C4B-NB	2.49	1.40	1.37
15	b1	409	CLA	C1B-C2B	2.49	1.49	1.43
15	c6	411	CLA	C1B-C2B	2.49	1.49	1.43
15	c3	421	CLA	MG-NB	-2.49	2.00	2.05
15	cB	834	CLA	C3B-C4B	2.49	1.48	1.42
15	c1	416	CLA	CMB-C2B	-2.49	1.45	1.50
15	cA	806	CLA	C1B-NB	-2.49	1.34	1.37
15	a3	403	CLA	MG-NB	-2.49	2.00	2.05
15	a4	404	CLA	MG-NB	-2.49	2.00	2.05
15	aB	809	CLA	CMC-C2C	-2.49	1.45	1.50
15	bA	820	CLA	C3B-C4B	2.49	1.48	1.42
15	c6	409	CLA	C3B-C4B	2.49	1.48	1.42
15	c6	406	CLA	C1B-C2B	2.49	1.49	1.43
15	c5	411	CLA	CMB-C2B	-2.49	1.45	1.50
15	bJ	102	CLA	C1B-C2B	2.49	1.49	1.43
15	bA	835	CLA	CMC-C2C	-2.49	1.45	1.50
15	b6	410	CLA	MG-NB	-2.49	2.00	2.05
15	cA	836	CLA	MG-NB	-2.49	2.00	2.05
15	bA	812	CLA	C4B-NB	2.49	1.40	1.37
15	c3	405	CLA	C4B-NB	2.49	1.40	1.37
15	b1	416	CLA	CMB-C2B	-2.49	1.45	1.50
15	c2	404	CLA	C3B-C4B	2.49	1.48	1.42
15	c1	404	CLA	C1B-C2B	2.49	1.49	1.43
15	b2	422	CLA	CMD-C2D	-2.49	1.45	1.50
15	b4	416	CLA	CMB-C2B	-2.49	1.45	1.50
15	a6	410	CLA	C1B-C2B	2.49	1.49	1.43
15	b5	413	CLA	C1B-C2B	2.49	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	835	CLA	CMC-C2C	-2.49	1.45	1.50
18	b6	421	BCR	C1-C6	-2.49	1.50	1.53
15	aA	826	CLA	C3B-C4B	2.49	1.48	1.42
15	b1	412	CLA	C1B-NB	-2.49	1.34	1.37
15	cB	840	CLA	C4B-NB	2.49	1.40	1.37
15	bB	842	CLA	C1B-C2B	2.49	1.49	1.43
15	b6	422	CLA	CMD-C2D	-2.49	1.45	1.50
15	b5	403	CLA	MG-NB	-2.49	2.00	2.05
15	a3	410	CLA	C4B-NB	2.49	1.40	1.37
15	c2	406	CLA	CAA-CBA	-2.49	1.45	1.52
15	bB	818	CLA	CMC-C2C	-2.49	1.45	1.50
15	c4	416	CLA	CMB-C2B	-2.49	1.45	1.50
15	aA	820	CLA	C3B-C4B	2.49	1.48	1.42
15	a4	403	CLA	MG-NB	-2.49	2.00	2.05
15	aL	202	CLA	CMC-C2C	-2.49	1.45	1.50
15	bB	803	CLA	CMC-C2C	-2.49	1.45	1.50
15	a6	405	CLA	C1B-C2B	2.49	1.49	1.43
15	a3	404	CLA	C1B-C2B	2.49	1.49	1.43
15	b1	406	CLA	C1B-C2B	2.49	1.49	1.43
15	aB	824	CLA	MG-NB	-2.48	2.00	2.05
15	a6	412	CLA	MG-NB	-2.48	2.00	2.05
15	b6	411	CLA	MG-NB	-2.48	2.00	2.05
15	cB	803	CLA	CMC-C2C	-2.48	1.45	1.50
15	cB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	b3	407	CLA	C4B-NB	2.48	1.40	1.37
15	cA	803	CLA	C1B-NB	-2.48	1.34	1.37
15	cB	814	CLA	C1B-NB	-2.48	1.34	1.37
15	a5	405	CLA	C1D-C2D	2.48	1.50	1.45
15	aB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	a4	412	CLA	MG-ND	-2.48	2.00	2.05
15	c6	412	CLA	MG-NB	-2.48	2.00	2.05
15	a2	413	CLA	MG-ND	-2.48	2.00	2.05
15	a6	411	CLA	MG-NB	-2.48	2.00	2.05
15	aA	814	CLA	MG-ND	-2.48	2.00	2.05
15	a2	406	CLA	CMD-C2D	-2.48	1.45	1.50
15	a5	420	CLA	C3B-C4B	2.48	1.48	1.42
15	aA	803	CLA	MG-ND	-2.48	2.00	2.05
15	bA	835	CLA	MG-NB	-2.48	2.00	2.05
15	b3	408	CLA	MG-NB	-2.48	2.00	2.05
15	a3	416	CLA	CMB-C2B	-2.48	1.45	1.50
15	bB	811	CLA	CMC-C2C	-2.48	1.45	1.50
15	c1	413	CLA	C1B-C2B	2.48	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	405	CLA	MG-NB	-2.48	2.00	2.05
15	c4	413	CLA	C1B-C2B	2.48	1.49	1.43
15	bB	822	CLA	C3B-C4B	2.48	1.48	1.42
15	b4	412	CLA	MG-ND	-2.48	2.00	2.05
15	c6	411	CLA	MG-NB	-2.48	2.00	2.05
15	a2	416	CLA	CMB-C2B	-2.48	1.45	1.50
15	aA	818	CLA	MG-NB	-2.48	2.00	2.05
15	a5	403	CLA	MG-NB	-2.48	2.00	2.05
15	bA	814	CLA	MG-ND	-2.48	2.00	2.05
15	aA	821	CLA	C1B-C2B	2.48	1.49	1.43
15	bB	839	CLA	C3B-C4B	2.48	1.48	1.42
15	c4	421	CLA	MG-NB	-2.48	2.00	2.05
15	c2	405	CLA	C1B-C2B	2.48	1.49	1.43
15	b4	408	CLA	MG-NB	-2.48	2.00	2.05
15	a3	405	CLA	C1B-C2B	2.48	1.49	1.43
15	aA	835	CLA	CMC-C2C	-2.48	1.45	1.50
15	a5	412	CLA	MG-ND	-2.48	2.00	2.05
15	c2	416	CLA	CMB-C2B	-2.48	1.45	1.50
15	cB	821	CLA	MG-NB	-2.48	2.00	2.05
15	c4	408	CLA	MG-NB	-2.48	2.00	2.05
15	bB	809	CLA	C1D-ND	2.48	1.40	1.37
15	aB	826	CLA	CMD-C2D	-2.48	1.45	1.50
15	c3	416	CLA	CMB-C2B	-2.48	1.45	1.50
15	b3	416	CLA	C4C-C3C	2.48	1.49	1.45
15	aB	833	CLA	CMB-C2B	-2.48	1.45	1.50
18	c6	403	BCR	C30-C25	-2.48	1.50	1.53
15	b4	406	CLA	C1B-C2B	2.48	1.49	1.43
15	aA	833	CLA	CMD-C2D	-2.47	1.45	1.50
15	aB	828	CLA	CMB-C2B	-2.47	1.45	1.50
15	c5	417	CLA	C1B-C2B	2.47	1.49	1.43
15	a4	416	CLA	CMB-C2B	-2.47	1.45	1.50
15	a4	405	CLA	C1D-C2D	2.47	1.50	1.45
15	aB	808	CLA	MG-NB	-2.47	2.00	2.05
15	cB	808	CLA	MG-NB	-2.47	2.00	2.05
15	b2	406	CLA	MG-ND	-2.47	2.00	2.05
15	c5	402	CLA	C3B-C4B	2.47	1.48	1.42
18	c2	420	BCR	C30-C25	-2.47	1.50	1.53
15	cL	203	CLA	CMD-C2D	-2.47	1.45	1.50
15	c3	405	CLA	C1D-C2D	2.47	1.50	1.45
15	b6	408	CLA	C1B-C2B	2.47	1.49	1.43
18	bA	849	BCR	C30-C25	-2.47	1.50	1.53
15	b3	405	CLA	C1B-C2B	2.47	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aJ	202	CLA	MG-NB	-2.47	2.00	2.05
15	b4	403	CLA	MG-NB	-2.47	2.00	2.05
15	a3	410	CLA	C3B-C4B	2.47	1.48	1.42
15	b2	408	CLA	MG-NB	-2.47	2.00	2.05
15	b4	411	CLA	MG-NB	-2.47	2.00	2.05
15	cA	821	CLA	MG-ND	-2.47	2.00	2.05
15	aB	840	CLA	C4B-NB	2.47	1.40	1.37
15	bB	836	CLA	CMD-C2D	-2.47	1.45	1.50
15	cA	835	CLA	CMC-C2C	-2.47	1.45	1.50
15	aA	826	CLA	MG-ND	-2.47	2.00	2.05
15	cA	826	CLA	C3B-C4B	2.47	1.48	1.42
15	bA	826	CLA	MG-ND	-2.47	2.00	2.05
15	b4	421	CLA	MG-NB	-2.47	2.00	2.05
15	cB	819	CLA	C1B-NB	-2.47	1.34	1.37
15	aB	838	CLA	CMB-C2B	-2.47	1.45	1.50
15	c5	403	CLA	MG-NB	-2.47	2.00	2.05
15	b2	402	CLA	C3B-C4B	2.47	1.48	1.42
18	bB	845	BCR	C30-C25	-2.47	1.50	1.53
15	a4	403	CLA	C1B-C2B	2.47	1.49	1.43
15	bA	821	CLA	C1B-C2B	2.47	1.49	1.43
15	a3	412	CLA	C1B-NB	-2.47	1.34	1.37
15	cA	842	CLA	C1B-NB	-2.47	1.34	1.37
15	bA	845	CLA	C3B-C4B	2.47	1.48	1.42
15	b4	404	CLA	C1B-C2B	2.47	1.49	1.43
15	aB	817	CLA	C3B-C4B	2.47	1.48	1.42
15	a2	403	CLA	MG-NB	-2.47	2.00	2.05
15	b5	416	CLA	C3C-C2C	2.47	1.42	1.36
15	bB	806	CLA	C1D-ND	2.47	1.40	1.37
15	aA	805	CLA	CMC-C2C	-2.47	1.45	1.50
15	aB	811	CLA	C1B-C2B	2.47	1.49	1.43
15	bL	203	CLA	CMD-C2D	-2.47	1.45	1.50
15	bA	828	CLA	C1B-NB	-2.47	1.34	1.37
15	c1	409	CLA	C1B-C2B	2.47	1.49	1.43
15	bB	835	CLA	CMB-C2B	-2.47	1.45	1.50
15	b6	405	CLA	C1B-C2B	2.46	1.49	1.43
15	a4	412	CLA	CMC-C2C	-2.46	1.45	1.50
15	b2	405	CLA	C1B-C2B	2.46	1.49	1.43
15	c4	405	CLA	C1D-C2D	2.46	1.50	1.45
15	c1	404	CLA	MG-NB	-2.46	2.00	2.05
15	bB	835	CLA	CMC-C2C	-2.46	1.45	1.50
15	aB	816	CLA	C3B-C4B	2.46	1.48	1.42
15	cB	809	CLA	C1D-ND	2.46	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a1	414	CLA	CMB-C2B	-2.46	1.45	1.50
15	cA	817	CLA	CMB-C2B	-2.46	1.45	1.50
15	bB	823	CLA	C1B-C2B	2.46	1.49	1.43
15	b2	416	CLA	CMB-C2B	-2.46	1.45	1.50
15	a6	408	CLA	C1B-C2B	2.46	1.49	1.43
15	b4	403	CLA	CMD-C2D	-2.46	1.45	1.50
15	b4	411	CLA	CMB-C2B	-2.46	1.45	1.50
15	bB	824	CLA	MG-NB	-2.46	2.00	2.05
15	c5	407	CLA	MG-NB	-2.46	2.00	2.05
15	aB	835	CLA	CMB-C2B	-2.46	1.45	1.50
15	a3	416	CLA	C4C-C3C	2.46	1.49	1.45
15	aB	805	CLA	MG-NB	-2.46	2.00	2.05
15	c2	403	CLA	MG-NB	-2.46	2.00	2.05
18	c1	419	BCR	C30-C25	-2.46	1.50	1.53
15	c6	401	CLA	CMD-C2D	-2.46	1.45	1.50
15	aB	842	CLA	C1B-C2B	2.46	1.49	1.43
15	a5	417	CLA	C1B-C2B	2.46	1.49	1.43
15	c4	412	CLA	CMC-C2C	-2.46	1.45	1.50
15	bB	835	CLA	C3B-C4B	2.46	1.48	1.42
15	aB	805	CLA	C4B-NB	2.46	1.40	1.37
15	b2	411	CLA	C4B-NB	2.46	1.40	1.37
15	a5	407	CLA	C3B-C4B	2.46	1.48	1.42
15	b1	414	CLA	C1B-C2B	2.46	1.49	1.43
15	bJ	101	CLA	MG-NB	-2.46	2.00	2.05
15	cB	817	CLA	C3B-C4B	2.46	1.48	1.42
15	a6	417	CLA	CMB-C2B	-2.46	1.45	1.50
15	cB	842	CLA	C1B-C2B	2.46	1.49	1.43
15	cA	833	CLA	CMD-C2D	-2.46	1.45	1.50
15	b1	410	CLA	MG-NB	-2.46	2.00	2.05
15	b5	412	CLA	MG-ND	-2.46	2.00	2.05
15	aA	817	CLA	CMB-C2B	-2.46	1.45	1.50
15	bB	819	CLA	MG-ND	-2.46	2.00	2.05
15	a2	404	CLA	C1B-C2B	2.46	1.49	1.43
15	a4	413	CLA	C1B-C2B	2.46	1.49	1.43
15	bL	203	CLA	C1B-NB	-2.46	1.34	1.37
15	bB	837	CLA	CMC-C2C	-2.46	1.45	1.50
15	cB	820	CLA	C3B-C4B	2.46	1.48	1.42
15	c4	406	CLA	C1B-C2B	2.46	1.49	1.43
15	aA	821	CLA	MG-ND	-2.46	2.00	2.05
15	bL	203	CLA	CMC-C2C	-2.46	1.45	1.50
15	a2	406	CLA	C3B-C4B	2.46	1.48	1.42
15	a2	408	CLA	MG-NB	-2.46	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	aB	845	BCR	C30-C25	-2.46	1.50	1.53
15	b4	412	CLA	CMC-C2C	-2.46	1.45	1.50
18	c5	418	BCR	C33-C5	-2.46	1.46	1.50
18	b1	419	BCR	C30-C25	-2.46	1.50	1.53
15	cB	826	CLA	CMD-C2D	-2.46	1.45	1.50
15	cB	837	CLA	CMC-C2C	-2.46	1.45	1.50
15	c4	417	CLA	C1B-C2B	2.46	1.49	1.43
15	a6	410	CLA	MG-NB	-2.46	2.00	2.05
15	a5	416	CLA	C3C-C2C	2.46	1.41	1.36
18	aB	849	BCR	C38-C26	-2.46	1.46	1.50
15	aA	845	CLA	C3B-C4B	2.46	1.48	1.42
15	a5	402	CLA	C3B-C4B	2.46	1.48	1.42
15	b5	402	CLA	C3B-C4B	2.46	1.48	1.42
15	b5	420	CLA	C3B-C4B	2.46	1.48	1.42
18	cB	845	BCR	C30-C25	-2.45	1.50	1.53
15	cL	202	CLA	C1B-NB	-2.45	1.34	1.37
15	b4	415	CLA	MG-NB	-2.45	2.00	2.05
15	cB	802	CLA	CMB-C2B	-2.45	1.45	1.50
15	aA	811	CLA	C3B-C4B	2.45	1.48	1.42
15	bL	203	CLA	MG-NB	-2.45	2.00	2.05
15	b3	421	CLA	C2A-C1A	2.45	1.57	1.52
15	aB	819	CLA	CMD-C2D	-2.45	1.45	1.50
15	cB	838	CLA	CMD-C2D	-2.45	1.45	1.50
15	a2	413	CLA	C1B-NB	-2.45	1.34	1.37
15	cA	836	CLA	C4B-NB	2.45	1.40	1.37
15	bB	834	CLA	C3B-C4B	2.45	1.48	1.42
15	b5	413	CLA	C3B-C4B	2.45	1.48	1.42
15	cA	820	CLA	C3B-C4B	2.45	1.48	1.42
15	aL	202	CLA	CMD-C2D	-2.45	1.45	1.50
15	cA	825	CLA	MG-NB	-2.45	2.00	2.05
15	c3	403	CLA	MG-NB	-2.45	2.00	2.05
15	aB	808	CLA	C1D-ND	2.45	1.40	1.37
15	bL	202	CLA	C1B-NB	-2.45	1.34	1.37
15	c2	412	CLA	CMB-C2B	-2.45	1.45	1.50
15	bB	820	CLA	C3B-C4B	2.45	1.48	1.42
15	bA	828	CLA	CMB-C2B	-2.45	1.45	1.50
15	bB	827	CLA	CMB-C2B	-2.45	1.45	1.50
15	b3	412	CLA	MG-ND	-2.45	2.00	2.05
15	aA	836	CLA	C4B-NB	2.45	1.40	1.37
15	bB	838	CLA	CMD-C2D	-2.45	1.45	1.50
15	c1	415	CLA	CMB-C2B	-2.45	1.45	1.50
15	a1	406	CLA	C1B-C2B	2.45	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	838	CLA	CMD-C2D	-2.45	1.45	1.50
15	c4	403	CLA	MG-NB	-2.45	2.00	2.05
15	cB	828	CLA	CMC-C2C	-2.45	1.45	1.50
15	aB	820	CLA	C3B-C4B	2.45	1.48	1.42
15	aA	835	CLA	C1B-NB	-2.45	1.34	1.37
15	b1	416	CLA	C3C-C2C	2.45	1.41	1.36
15	aX	102	CLA	CMB-C2B	-2.45	1.45	1.50
15	b1	415	CLA	CMB-C2B	-2.45	1.45	1.50
15	bA	836	CLA	C4B-NB	2.45	1.40	1.37
15	bA	828	CLA	C1D-ND	2.45	1.40	1.37
15	c5	420	CLA	C3B-C4B	2.45	1.48	1.42
15	c5	408	CLA	MG-NB	-2.45	2.00	2.05
15	bB	828	CLA	CMC-C2C	-2.45	1.45	1.50
15	a1	401	CLA	C3B-C4B	2.45	1.48	1.42
15	a3	405	CLA	C3B-C4B	2.45	1.48	1.42
15	b1	402	CLA	C3B-C4B	2.45	1.48	1.42
15	cB	811	CLA	CMD-C2D	-2.45	1.45	1.50
15	aA	810	CLA	C4B-NB	2.45	1.40	1.37
15	c6	401	CLA	C3B-C4B	2.45	1.48	1.42
15	aB	809	CLA	MG-ND	-2.45	2.00	2.05
15	cB	835	CLA	C3B-C4B	2.45	1.48	1.42
15	cB	835	CLA	CMB-C2B	-2.45	1.45	1.50
15	aB	824	CLA	C3B-C4B	2.45	1.48	1.42
15	b5	415	CLA	MG-NB	-2.45	2.00	2.05
15	c3	412	CLA	MG-ND	-2.45	2.00	2.05
15	a4	406	CLA	C1B-C2B	2.45	1.49	1.43
15	aB	822	CLA	C3B-C4B	2.45	1.48	1.42
15	c3	407	CLA	C3B-C4B	2.45	1.48	1.42
15	cJ	101	CLA	C1B-NB	-2.45	1.34	1.37
15	c5	404	CLA	C1B-C2B	2.45	1.49	1.43
15	cA	844	CLA	C3B-C4B	2.45	1.48	1.42
15	aB	815	CLA	MG-NB	-2.45	2.00	2.05
15	bA	821	CLA	MG-ND	-2.45	2.00	2.05
15	bA	825	CLA	MG-NB	-2.45	2.00	2.05
15	c6	409	CLA	C1B-C2B	2.45	1.49	1.43
15	cA	828	CLA	CMB-C2B	-2.44	1.45	1.50
15	c2	406	CLA	MG-ND	-2.44	2.00	2.05
15	aB	815	CLA	CMC-C2C	-2.44	1.45	1.50
15	aB	837	CLA	CMC-C2C	-2.44	1.45	1.50
15	aL	202	CLA	C1B-NB	-2.44	1.34	1.37
15	c6	407	CLA	C1D-C2D	2.44	1.50	1.45
15	bA	833	CLA	CMD-C2D	-2.44	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	417	CLA	C1B-NB	-2.44	1.34	1.37
15	cA	828	CLA	C1D-ND	2.44	1.40	1.37
15	bB	816	CLA	C3B-C4B	2.44	1.48	1.42
15	cJ	101	CLA	MG-NB	-2.44	2.00	2.05
15	bA	826	CLA	C3B-C4B	2.44	1.48	1.42
15	aB	823	CLA	C1B-C2B	2.44	1.49	1.43
15	a2	408	CLA	C1B-C2B	2.44	1.49	1.43
15	cA	830	CLA	CMC-C2C	-2.44	1.45	1.50
15	b4	406	CLA	C3B-C4B	2.44	1.48	1.42
15	cA	828	CLA	C1B-NB	-2.44	1.34	1.37
15	a6	413	CLA	MG-ND	-2.44	2.00	2.05
15	b3	415	CLA	CMB-C2B	-2.44	1.45	1.50
15	b2	408	CLA	C1B-C2B	2.44	1.49	1.43
15	bB	814	CLA	C1B-NB	-2.44	1.34	1.37
15	b3	412	CLA	C1B-NB	-2.44	1.34	1.37
15	aL	202	CLA	MG-NB	-2.44	2.00	2.05
15	c3	405	CLA	C3B-C4B	2.44	1.48	1.42
15	aB	811	CLA	CMD-C2D	-2.44	1.45	1.50
15	aB	828	CLA	CMC-C2C	-2.44	1.45	1.50
15	c6	418	CLA	CMB-C2B	-2.44	1.45	1.50
15	aA	825	CLA	MG-NB	-2.44	2.00	2.05
15	a4	406	CLA	C3B-C4B	2.44	1.48	1.42
15	a5	415	CLA	C3B-C4B	2.44	1.48	1.42
15	bA	838	CLA	CMB-C2B	-2.44	1.45	1.50
15	bB	815	CLA	CMC-C2C	-2.44	1.45	1.50
15	b4	404	CLA	MG-NB	-2.44	2.01	2.05
15	b2	416	CLA	C3B-C4B	2.44	1.48	1.42
15	cL	203	CLA	C3B-C4B	2.44	1.48	1.42
15	aA	812	CLA	CMD-C2D	-2.44	1.45	1.50
15	bA	806	CLA	CMB-C2B	-2.44	1.45	1.50
15	b3	416	CLA	CMB-C2B	-2.44	1.45	1.50
15	aB	826	CLA	C1B-NB	-2.44	1.34	1.37
15	bA	820	CLA	C4B-NB	2.44	1.40	1.37
15	cB	806	CLA	C1D-ND	2.44	1.40	1.37
15	c6	413	CLA	C1B-NB	-2.44	1.34	1.37
15	c3	416	CLA	C4C-C3C	2.44	1.49	1.45
15	bA	803	CLA	MG-ND	-2.44	2.01	2.05
15	c1	415	CLA	C3B-C4B	2.44	1.48	1.42
15	a4	404	CLA	C1B-C2B	2.44	1.49	1.43
15	a4	421	CLA	CMD-C2D	-2.44	1.45	1.50
15	bB	811	CLA	CMD-C2D	-2.44	1.45	1.50
15	cA	806	CLA	CMB-C2B	-2.44	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	809	CLA	MG-ND	-2.44	2.01	2.05
15	cB	822	CLA	C3B-C4B	2.44	1.48	1.42
15	aA	819	CLA	CMD-C2D	-2.44	1.45	1.50
15	aB	814	CLA	MG-ND	-2.44	2.01	2.05
15	a4	402	CLA	C3B-C4B	2.44	1.48	1.42
15	cB	821	CLA	C3B-C4B	2.44	1.48	1.42
15	a1	403	CLA	MG-NB	-2.44	2.01	2.05
15	cA	835	CLA	C1B-NB	-2.44	1.34	1.37
15	b3	404	CLA	C1B-C2B	2.44	1.49	1.43
15	bB	811	CLA	C1B-C2B	2.44	1.49	1.43
15	aA	813	CLA	CMD-C2D	-2.44	1.45	1.50
15	b6	417	CLA	CMB-C2B	-2.44	1.45	1.50
15	a2	403	CLA	C1B-C2B	2.44	1.49	1.43
15	a1	415	CLA	C3C-C2C	2.44	1.41	1.36
15	aL	201	CLA	C1B-NB	-2.44	1.34	1.37
15	aB	802	CLA	CMB-C2B	-2.44	1.45	1.50
15	cA	805	CLA	CMC-C2C	-2.44	1.45	1.50
15	b5	404	CLA	C1B-C2B	2.44	1.49	1.43
15	c4	415	CLA	MG-NB	-2.43	2.01	2.05
15	aA	806	CLA	CMB-C2B	-2.43	1.45	1.50
15	a3	410	CLA	CMB-C2B	-2.43	1.45	1.50
15	a6	413	CLA	CMC-C2C	-2.43	1.45	1.50
15	bB	824	CLA	C3B-C4B	2.43	1.48	1.42
15	aB	819	CLA	C1B-NB	-2.43	1.34	1.37
15	aB	820	CLA	C1B-NB	-2.43	1.34	1.37
15	bA	804	CLA	MG-ND	-2.43	2.01	2.05
15	a6	406	CLA	C1B-C2B	2.43	1.49	1.43
15	a3	412	CLA	MG-ND	-2.43	2.01	2.05
15	c1	405	CLA	C1B-C2B	2.43	1.49	1.43
15	cA	825	CLA	CMD-C2D	-2.43	1.45	1.50
18	bB	850	BCR	C38-C26	-2.43	1.46	1.50
15	b5	417	CLA	C1B-C2B	2.43	1.49	1.43
15	c4	404	CLA	C1B-C2B	2.43	1.49	1.43
15	c5	416	CLA	C3C-C2C	2.43	1.41	1.36
15	b2	417	CLA	CMB-C2B	-2.43	1.45	1.50
15	c2	422	CLA	C1B-C2B	2.43	1.49	1.43
15	bA	812	CLA	CMD-C2D	-2.43	1.45	1.50
15	a5	417	CLA	C1B-NB	-2.43	1.34	1.37
15	aA	813	CLA	CMB-C2B	-2.43	1.45	1.50
15	bA	805	CLA	CMC-C2C	-2.43	1.45	1.50
15	bB	826	CLA	CMD-C2D	-2.43	1.45	1.50
15	bX	102	CLA	CMB-C2B	-2.43	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	414	CLA	MG-ND	-2.43	2.01	2.05
15	cA	810	CLA	C4B-NB	2.43	1.40	1.37
15	c6	408	CLA	C1B-C2B	2.43	1.49	1.43
15	c4	405	CLA	MG-NB	-2.43	2.01	2.05
18	a1	421	BCR	C1-C6	-2.43	1.50	1.53
15	b1	405	CLA	C1D-C2D	2.43	1.50	1.45
15	aA	828	CLA	CMB-C2B	-2.43	1.45	1.50
15	aA	820	CLA	C4B-NB	2.43	1.40	1.37
15	c2	408	CLA	C3B-C4B	2.43	1.48	1.42
15	cB	823	CLA	C1B-C2B	2.43	1.49	1.43
15	a2	412	CLA	CMB-C2B	-2.43	1.45	1.50
15	bB	809	CLA	MG-ND	-2.43	2.01	2.05
15	c5	415	CLA	MG-NB	-2.43	2.01	2.05
15	a1	404	CLA	C1D-C2D	2.43	1.50	1.45
15	a3	407	CLA	C3B-C4B	2.43	1.48	1.42
15	cA	811	CLA	C3B-C4B	2.43	1.48	1.42
15	cL	203	CLA	MG-NB	-2.43	2.01	2.05
15	a3	413	CLA	C1B-C2B	2.43	1.49	1.43
15	aA	828	CLA	C1D-ND	2.43	1.40	1.37
15	a6	422	CLA	CMD-C2D	-2.43	1.45	1.50
15	bB	817	CLA	C3B-C4B	2.43	1.48	1.42
15	c2	406	CLA	C3B-C4B	2.43	1.48	1.42
15	c5	405	CLA	C1D-C2D	2.43	1.50	1.45
15	cB	816	CLA	C3B-C4B	2.43	1.48	1.42
18	cB	849	BCR	C38-C26	-2.43	1.46	1.50
15	a5	405	CLA	C3B-C4B	2.43	1.48	1.42
15	bA	808	CLA	C3B-C4B	2.43	1.48	1.42
15	a4	417	CLA	C1B-C2B	2.43	1.49	1.43
15	b2	418	CLA	C1B-C2B	2.43	1.49	1.43
15	b6	404	CLA	MG-NB	-2.43	2.01	2.05
18	b2	420	BCR	C30-C25	-2.43	1.50	1.53
15	a2	402	CLA	C3B-C4B	2.43	1.48	1.42
15	aB	814	CLA	C1B-NB	-2.43	1.34	1.37
15	a5	404	CLA	MG-NB	-2.43	2.01	2.05
15	b5	406	CLA	MG-NB	-2.43	2.01	2.05
15	c4	421	CLA	CMD-C2D	-2.43	1.45	1.50
15	c5	405	CLA	C3B-C4B	2.43	1.48	1.42
15	b4	413	CLA	C1B-C2B	2.43	1.49	1.43
15	bB	831	CLA	CMD-C2D	-2.43	1.45	1.50
15	cB	827	CLA	CMD-C2D	-2.43	1.45	1.50
15	c4	406	CLA	C3B-C4B	2.43	1.48	1.42
15	c4	404	CLA	MG-NB	-2.43	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	802	CLA	CMB-C2B	-2.43	1.45	1.50
15	cA	834	CLA	CMB-C2B	-2.43	1.45	1.50
15	a5	404	CLA	C1B-C2B	2.43	1.49	1.43
15	b4	417	CLA	C1B-C2B	2.43	1.49	1.43
15	b6	412	CLA	C1B-NB	-2.43	1.34	1.37
15	c1	402	CLA	C3B-C4B	2.43	1.48	1.42
15	a3	416	CLA	C3C-C2C	2.43	1.41	1.36
15	b3	413	CLA	C1B-C2B	2.43	1.49	1.43
15	cA	809	CLA	CMB-C2B	-2.43	1.45	1.50
15	a2	408	CLA	C3B-C4B	2.43	1.48	1.42
15	cB	827	CLA	CMB-C2B	-2.42	1.45	1.50
18	b6	421	BCR	C33-C5	-2.42	1.47	1.50
15	b4	403	CLA	C1B-C2B	2.42	1.49	1.43
15	cA	842	CLA	MG-ND	-2.42	2.01	2.05
15	bB	840	CLA	C1B-NB	-2.42	1.34	1.37
15	b5	408	CLA	MG-NB	-2.42	2.01	2.05
15	b2	408	CLA	C3B-C4B	2.42	1.48	1.42
15	aB	831	CLA	CMD-C2D	-2.42	1.45	1.50
15	bA	809	CLA	CMD-C2D	-2.42	1.45	1.50
15	cA	812	CLA	CMD-C2D	-2.42	1.45	1.50
15	c1	412	CLA	MG-ND	-2.42	2.01	2.05
15	c1	414	CLA	C1B-C2B	2.42	1.49	1.43
15	c1	416	CLA	C3C-C2C	2.42	1.41	1.36
15	aA	820	CLA	CMD-C2D	-2.42	1.45	1.50
15	aA	838	CLA	CMB-C2B	-2.42	1.45	1.50
15	cB	832	CLA	CMD-C2D	-2.42	1.45	1.50
18	a5	401	BCR	C33-C5	-2.42	1.47	1.50
15	b5	407	CLA	C3B-C4B	2.42	1.48	1.42
15	cA	803	CLA	MG-ND	-2.42	2.01	2.05
15	aA	843	CLA	C1B-NB	-2.42	1.34	1.37
15	c2	418	CLA	C1B-NB	-2.42	1.34	1.37
15	cA	819	CLA	CMD-C2D	-2.42	1.45	1.50
15	bA	816	CLA	CMC-C2C	-2.42	1.45	1.50
15	cA	820	CLA	CMD-C2D	-2.42	1.45	1.50
15	c6	417	CLA	CMB-C2B	-2.42	1.45	1.50
15	a6	407	CLA	C1B-C2B	2.42	1.49	1.43
15	bA	843	CLA	MG-ND	-2.42	2.01	2.05
15	b3	402	CLA	C3B-C4B	2.42	1.48	1.42
15	b3	407	CLA	C3B-C4B	2.42	1.48	1.42
15	c5	407	CLA	C3B-C4B	2.42	1.48	1.42
15	cA	813	CLA	CMD-C2D	-2.42	1.45	1.50
15	cB	823	CLA	CMD-C2D	-2.42	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	833	CLA	MG-ND	-2.42	2.01	2.05
15	b1	407	CLA	MG-NB	-2.42	2.01	2.05
15	bL	203	CLA	C3B-C4B	2.42	1.48	1.42
15	aB	834	CLA	CMB-C2B	-2.42	1.45	1.50
15	bA	834	CLA	CMB-C2B	-2.42	1.45	1.50
15	c2	408	CLA	MG-NB	-2.42	2.01	2.05
15	a1	413	CLA	C1B-C2B	2.42	1.49	1.43
15	a2	405	CLA	C1B-C2B	2.42	1.49	1.43
15	bA	830	CLA	CMC-C2C	-2.42	1.45	1.50
15	cA	804	CLA	CMB-C2B	-2.42	1.45	1.50
15	c2	402	CLA	C3B-C4B	2.42	1.48	1.42
15	aB	801	CLA	C1B-NB	-2.42	1.34	1.37
15	c5	404	CLA	MG-NB	-2.42	2.01	2.05
15	b5	415	CLA	C3B-C4B	2.42	1.48	1.42
15	aA	804	CLA	MG-ND	-2.42	2.01	2.05
15	c3	410	CLA	CMB-C2B	-2.42	1.45	1.50
15	c4	411	CLA	CMB-C2B	-2.42	1.45	1.50
15	aA	843	CLA	MG-ND	-2.42	2.01	2.05
15	cA	838	CLA	CMB-C2B	-2.42	1.45	1.50
15	bA	819	CLA	CMD-C2D	-2.42	1.45	1.50
15	cB	839	CLA	CMC-C2C	-2.42	1.45	1.50
15	c2	417	CLA	CMB-C2B	-2.42	1.45	1.50
15	cA	814	CLA	MG-ND	-2.42	2.01	2.05
15	cB	823	CLA	MG-NB	-2.42	2.01	2.05
15	a6	412	CLA	C1B-NB	-2.42	1.34	1.37
15	b3	410	CLA	C1B-NB	-2.42	1.34	1.37
15	cB	805	CLA	C4B-NB	2.42	1.40	1.37
15	b4	405	CLA	C1D-C2D	2.42	1.50	1.45
15	a2	410	CLA	MG-NB	-2.42	2.01	2.05
15	b4	405	CLA	MG-NB	-2.42	2.01	2.05
15	aB	817	CLA	C1D-ND	2.42	1.40	1.37
15	cA	830	CLA	C1D-ND	2.42	1.40	1.37
15	bA	811	CLA	C3B-C4B	2.42	1.48	1.42
18	cK	101	BCR	C30-C25	-2.42	1.50	1.53
15	a6	416	CLA	CMB-C2B	-2.42	1.45	1.50
15	b2	410	CLA	MG-NB	-2.42	2.01	2.05
15	b5	404	CLA	MG-NB	-2.42	2.01	2.05
15	c1	405	CLA	C1D-C2D	2.42	1.50	1.45
15	bA	810	CLA	C4B-NB	2.42	1.40	1.37
15	c3	412	CLA	C1B-NB	-2.42	1.34	1.37
15	c2	417	CLA	C4C-C3C	2.42	1.49	1.45
15	c5	413	CLA	C3B-C4B	2.42	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	410	CLA	CMB-C2B	-2.42	1.45	1.50
15	cB	805	CLA	MG-NB	-2.42	2.01	2.05
18	c5	401	BCR	C33-C5	-2.42	1.47	1.50
15	cB	824	CLA	C3B-C4B	2.42	1.48	1.42
15	aB	814	CLA	CMD-C2D	-2.42	1.45	1.50
15	bB	815	CLA	MG-NB	-2.42	2.01	2.05
15	cA	843	CLA	MG-NB	-2.42	2.01	2.05
15	aB	827	CLA	CMD-C2D	-2.42	1.45	1.50
15	a2	417	CLA	CMB-C2B	-2.42	1.45	1.50
15	c4	403	CLA	C1B-C2B	2.42	1.48	1.43
15	b2	412	CLA	CMB-C2B	-2.41	1.45	1.50
15	b6	416	CLA	CMB-C2B	-2.41	1.45	1.50
15	c5	417	CLA	C1B-NB	-2.41	1.34	1.37
15	c2	404	CLA	C1B-C2B	2.41	1.48	1.43
15	cA	808	CLA	C3B-C4B	2.41	1.48	1.42
15	c2	416	CLA	C3B-C4B	2.41	1.48	1.42
15	aA	825	CLA	CMD-C2D	-2.41	1.45	1.50
15	aA	833	CLA	CMB-C2B	-2.41	1.45	1.50
15	b6	413	CLA	CMC-C2C	-2.41	1.45	1.50
15	cB	831	CLA	CMD-C2D	-2.41	1.45	1.50
15	b5	405	CLA	C1D-C2D	2.41	1.50	1.45
15	a4	411	CLA	CMB-C2B	-2.41	1.45	1.50
15	b3	412	CLA	CMC-C2C	-2.41	1.45	1.50
15	c4	417	CLA	C4D-ND	-2.41	1.34	1.37
18	bB	848	BCR	C33-C5	-2.41	1.47	1.50
18	b1	418	BCR	C33-C5	-2.41	1.47	1.50
15	bA	830	CLA	C1D-ND	2.41	1.40	1.37
15	c6	419	CLA	C1B-NB	-2.41	1.34	1.37
15	b3	415	CLA	MG-ND	-2.41	2.01	2.05
15	aA	810	CLA	MG-ND	-2.41	2.01	2.05
15	bB	814	CLA	MG-ND	-2.41	2.01	2.05
15	bB	823	CLA	C4B-NB	2.41	1.40	1.37
15	cB	805	CLA	CMC-C2C	-2.41	1.45	1.50
15	b5	405	CLA	C3B-C4B	2.41	1.48	1.42
15	c4	402	CLA	C3B-C4B	2.41	1.48	1.42
15	a3	402	CLA	C3B-C4B	2.41	1.48	1.42
15	c3	415	CLA	CMB-C2B	-2.41	1.45	1.50
15	bB	801	CLA	C1B-NB	-2.41	1.34	1.37
15	c5	415	CLA	C3B-C4B	2.41	1.48	1.42
15	aA	845	CLA	CMD-C2D	-2.41	1.45	1.50
15	bA	808	CLA	CMB-C2B	-2.41	1.45	1.50
15	bB	827	CLA	CMD-C2D	-2.41	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	830	CLA	CMC-C2C	-2.41	1.45	1.50
15	c6	414	CLA	CMC-C2C	-2.41	1.45	1.50
15	a4	405	CLA	MG-NB	-2.41	2.01	2.05
15	cL	203	CLA	MG-ND	-2.41	2.01	2.05
15	cX	102	CLA	C1B-NB	-2.41	1.34	1.37
15	cB	821	CLA	CMD-C2D	-2.41	1.45	1.50
15	b6	407	CLA	C1B-C2B	2.41	1.48	1.43
15	aA	808	CLA	C3B-C4B	2.41	1.48	1.42
15	b4	416	CLA	C3C-C2C	2.41	1.41	1.36
15	b2	404	CLA	C1B-C2B	2.41	1.48	1.43
15	b6	406	CLA	C1B-C2B	2.41	1.48	1.43
15	c3	404	CLA	C1B-C2B	2.41	1.48	1.43
15	c3	413	CLA	C1B-C2B	2.41	1.48	1.43
15	b6	418	CLA	C1B-C2B	2.41	1.48	1.43
15	cA	844	CLA	CMD-C2D	-2.41	1.45	1.50
15	b4	402	CLA	C3B-C4B	2.41	1.48	1.42
15	a5	408	CLA	MG-NB	-2.41	2.01	2.05
15	c3	402	CLA	C3B-C4B	2.41	1.48	1.42
15	cB	802	CLA	C1B-C2B	2.41	1.48	1.43
15	a3	405	CLA	C1D-C2D	2.41	1.50	1.45
15	a4	405	CLA	C3B-C4B	2.41	1.48	1.42
15	aA	830	CLA	C1D-ND	2.41	1.40	1.37
15	a3	407	CLA	C1B-C2B	2.41	1.48	1.43
15	c3	402	CLA	MG-NB	-2.41	2.01	2.05
15	c1	407	CLA	C1B-C2B	2.41	1.48	1.43
15	c4	421	CLA	C1B-C2B	2.41	1.48	1.43
15	a6	422	CLA	MG-NB	-2.41	2.01	2.05
15	aB	832	CLA	CMD-C2D	-2.41	1.45	1.50
15	bA	813	CLA	CMB-C2B	-2.41	1.45	1.50
15	cA	804	CLA	MG-ND	-2.41	2.01	2.05
15	c5	406	CLA	MG-NB	-2.41	2.01	2.05
15	bB	805	CLA	CMC-C2C	-2.41	1.45	1.50
15	b5	409	CLA	C1B-C2B	2.41	1.48	1.43
15	b5	407	CLA	MG-NB	-2.40	2.01	2.05
15	aB	827	CLA	CMB-C2B	-2.40	1.45	1.50
15	aB	805	CLA	CMC-C2C	-2.40	1.45	1.50
15	aB	821	CLA	C3B-C4B	2.40	1.48	1.42
15	cB	816	CLA	C1B-C2B	2.40	1.48	1.43
15	a1	406	CLA	MG-NB	-2.40	2.01	2.05
15	cA	809	CLA	CMD-C2D	-2.40	1.45	1.50
15	a5	409	CLA	C1B-C2B	2.40	1.48	1.43
15	a6	418	CLA	C1B-C2B	2.40	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	839	CLA	CMC-C2C	-2.40	1.45	1.50
15	aB	834	CLA	CMD-C2D	-2.40	1.45	1.50
15	a1	411	CLA	MG-ND	-2.40	2.01	2.05
15	a5	420	CLA	MG-ND	-2.40	2.01	2.05
15	a4	411	CLA	C1B-NB	-2.40	1.34	1.37
15	c1	412	CLA	C1B-NB	-2.40	1.34	1.37
15	aB	823	CLA	CMD-C2D	-2.40	1.45	1.50
15	bA	813	CLA	CMD-C2D	-2.40	1.45	1.50
15	a6	404	CLA	MG-NB	-2.40	2.01	2.05
15	cJ	102	CLA	MG-NB	-2.40	2.01	2.05
15	c1	407	CLA	MG-NB	-2.40	2.01	2.05
15	bA	820	CLA	CMD-C2D	-2.40	1.45	1.50
15	b1	412	CLA	CMC-C2C	-2.40	1.45	1.50
15	cA	816	CLA	CMC-C2C	-2.40	1.45	1.50
15	aL	202	CLA	C3B-C4B	2.40	1.48	1.42
15	bX	102	CLA	C1B-NB	-2.40	1.34	1.37
15	b2	417	CLA	C4C-C3C	2.40	1.49	1.45
15	a3	406	CLA	MG-NB	-2.40	2.01	2.05
15	b3	402	CLA	MG-NB	-2.40	2.01	2.05
18	b5	401	BCR	C33-C5	-2.40	1.47	1.50
15	c4	416	CLA	C3C-C2C	2.40	1.41	1.36
15	cA	810	CLA	C3B-C4B	2.40	1.48	1.42
15	aB	802	CLA	C1B-C2B	2.40	1.48	1.43
15	b6	410	CLA	C1B-C2B	2.40	1.48	1.43
15	b4	405	CLA	C3B-C4B	2.40	1.48	1.42
15	cB	833	CLA	CMD-C2D	-2.40	1.45	1.50
15	c5	412	CLA	CMC-C2C	-2.40	1.45	1.50
15	b2	406	CLA	C1B-C2B	2.40	1.48	1.43
15	a4	409	CLA	MG-NB	-2.40	2.01	2.05
15	a4	415	CLA	MG-NB	-2.40	2.01	2.05
15	a5	406	CLA	MG-NB	-2.40	2.01	2.05
15	a3	415	CLA	CMB-C2B	-2.40	1.45	1.50
15	b2	406	CLA	C3B-C4B	2.40	1.48	1.42
15	bB	821	CLA	CMD-C2D	-2.40	1.45	1.50
15	bB	834	CLA	CMD-C2D	-2.40	1.45	1.50
15	cX	102	CLA	CMB-C2B	-2.40	1.45	1.50
15	a5	407	CLA	MG-NB	-2.40	2.01	2.05
15	b6	413	CLA	MG-ND	-2.40	2.01	2.05
15	c6	415	CLA	C3B-C4B	2.40	1.48	1.42
15	aB	833	CLA	MG-ND	-2.40	2.01	2.05
15	a4	413	CLA	C3B-C4B	2.40	1.48	1.42
15	a4	416	CLA	C3C-C2C	2.40	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	810	CLA	MG-ND	-2.40	2.01	2.05
15	c4	409	CLA	MG-NB	-2.40	2.01	2.05
15	aA	816	CLA	CMC-C2C	-2.40	1.45	1.50
15	c6	407	CLA	C1B-C2B	2.40	1.48	1.43
15	cA	813	CLA	CMB-C2B	-2.40	1.45	1.50
18	c1	418	BCR	C33-C5	-2.40	1.47	1.50
15	a3	404	CLA	MG-NB	-2.40	2.01	2.05
15	c6	405	CLA	MG-NB	-2.40	2.01	2.05
15	cB	814	CLA	MG-ND	-2.40	2.01	2.05
15	c5	409	CLA	C1B-C2B	2.40	1.48	1.43
15	aB	832	CLA	CMB-C2B	-2.40	1.45	1.50
15	bB	833	CLA	CMD-C2D	-2.40	1.45	1.50
18	a1	418	BCR	C33-C5	-2.40	1.47	1.50
15	a2	416	CLA	C3B-C4B	2.40	1.48	1.42
15	c4	405	CLA	C3B-C4B	2.40	1.48	1.42
15	cL	203	CLA	C1B-NB	-2.40	1.34	1.37
15	bB	805	CLA	MG-NB	-2.40	2.01	2.05
15	bJ	102	CLA	MG-NB	-2.40	2.01	2.05
15	cF	203	CLA	C3B-C4B	2.39	1.48	1.42
15	aB	839	CLA	CMC-C2C	-2.39	1.45	1.50
15	bB	832	CLA	CMD-C2D	-2.39	1.45	1.50
15	a2	409	CLA	MG-NB	-2.39	2.01	2.05
15	a3	415	CLA	MG-ND	-2.39	2.01	2.05
15	aB	808	CLA	C3B-C4B	2.39	1.48	1.42
15	c6	405	CLA	CMD-C2D	-2.39	1.45	1.50
15	bB	816	CLA	C1B-C2B	2.39	1.48	1.43
15	a3	410	CLA	C1B-NB	-2.39	1.34	1.37
15	a4	417	CLA	C4D-ND	-2.39	1.34	1.37
15	bA	833	CLA	CMB-C2B	-2.39	1.45	1.50
15	a1	404	CLA	C1B-C2B	2.39	1.48	1.43
15	a2	418	CLA	C1B-C2B	2.39	1.48	1.43
15	cB	801	CLA	C1B-NB	-2.39	1.34	1.37
18	bA	848	BCR	C30-C25	-2.39	1.50	1.53
15	c3	416	CLA	C3C-C2C	2.39	1.41	1.36
15	bF	201	CLA	C3B-C4B	2.39	1.48	1.42
15	a5	412	CLA	CMC-C2C	-2.39	1.45	1.50
15	b6	414	CLA	MG-NB	-2.39	2.01	2.05
15	c5	414	CLA	C1B-C2B	2.39	1.48	1.43
15	cB	814	CLA	CMD-C2D	-2.39	1.45	1.50
18	a1	417	BCR	C33-C5	-2.39	1.47	1.50
15	b4	421	CLA	C1B-C2B	2.39	1.48	1.43
15	bA	825	CLA	CMD-C2D	-2.39	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	845	CLA	CMD-C2D	-2.39	1.45	1.50
15	aJ	202	CLA	C1B-NB	-2.39	1.34	1.37
15	b3	421	CLA	C3B-C4B	2.39	1.48	1.42
15	bB	826	CLA	MG-NB	-2.39	2.01	2.05
15	aB	803	CLA	CMD-C2D	-2.39	1.45	1.50
15	bB	803	CLA	CMB-C2B	-2.39	1.45	1.50
15	b5	412	CLA	CMC-C2C	-2.39	1.45	1.50
15	cB	825	CLA	CAC-C3C	-2.39	1.45	1.51
15	bB	817	CLA	C1D-ND	2.39	1.40	1.37
15	cB	823	CLA	C4B-NB	2.39	1.40	1.37
15	a5	414	CLA	C1B-C2B	2.39	1.48	1.43
15	b1	405	CLA	C1B-C2B	2.39	1.48	1.43
15	cB	811	CLA	C1B-C2B	2.39	1.48	1.43
15	bL	203	CLA	MG-ND	-2.39	2.01	2.05
15	cL	202	CLA	MG-ND	-2.39	2.01	2.05
15	aB	833	CLA	CMD-C2D	-2.39	1.45	1.50
15	cB	815	CLA	CMC-C2C	-2.39	1.45	1.50
15	bB	821	CLA	C3B-C4B	2.39	1.48	1.42
15	b2	422	CLA	C1B-C2B	2.39	1.48	1.43
15	c6	419	CLA	C1B-C2B	2.39	1.48	1.43
15	aJ	201	CLA	C3B-C4B	2.39	1.48	1.42
15	aA	810	CLA	C3B-C4B	2.39	1.48	1.42
15	a6	417	CLA	C3C-C2C	2.39	1.41	1.36
15	bB	825	CLA	CAC-C3C	-2.39	1.45	1.51
15	aB	840	CLA	C1B-NB	-2.39	1.34	1.37
15	aA	809	CLA	CMD-C2D	-2.39	1.45	1.50
15	cB	826	CLA	MG-NB	-2.39	2.01	2.05
15	cB	829	CLA	MG-ND	-2.39	2.01	2.05
15	b2	414	CLA	C3B-C4B	2.39	1.48	1.42
15	bB	803	CLA	CMD-C2D	-2.39	1.45	1.50
15	aB	825	CLA	CAC-C3C	-2.39	1.45	1.51
15	a5	407	CLA	C1B-C2B	2.39	1.48	1.43
15	bA	844	CLA	MG-NB	-2.39	2.01	2.05
18	b1	419	BCR	C33-C5	-2.39	1.47	1.50
15	cF	201	CLA	C1B-C2B	2.39	1.48	1.43
15	a5	413	CLA	C3B-C4B	2.39	1.48	1.42
15	aA	804	CLA	CMB-C2B	-2.39	1.45	1.50
15	bB	834	CLA	CMB-C2B	-2.39	1.45	1.50
15	cB	819	CLA	CAC-C3C	-2.39	1.45	1.51
15	c2	406	CLA	C1B-C2B	2.39	1.48	1.43
15	aA	834	CLA	CMB-C2B	-2.39	1.45	1.50
15	aL	202	CLA	MG-ND	-2.39	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	418	CLA	C1B-NB	-2.39	1.34	1.37
15	cB	815	CLA	MG-NB	-2.39	2.01	2.05
15	bB	825	CLA	C3B-C4B	2.39	1.48	1.42
15	aX	102	CLA	C1B-NB	-2.38	1.34	1.37
15	aB	821	CLA	CMD-C2D	-2.38	1.45	1.50
15	aA	844	CLA	MG-NB	-2.38	2.01	2.05
15	aB	819	CLA	CAC-C3C	-2.38	1.45	1.51
15	b5	407	CLA	C1B-C2B	2.38	1.48	1.43
15	bB	808	CLA	C3B-C4B	2.38	1.48	1.42
15	bA	804	CLA	C1D-ND	2.38	1.40	1.37
15	aB	829	CLA	MG-ND	-2.38	2.01	2.05
15	b6	414	CLA	C3B-C4B	2.38	1.48	1.42
15	c3	421	CLA	C3B-C4B	2.38	1.48	1.42
15	cA	808	CLA	CMB-C2B	-2.38	1.45	1.50
15	aB	825	CLA	C3B-C4B	2.38	1.48	1.42
15	b4	421	CLA	C3B-C4B	2.38	1.48	1.42
15	bA	817	CLA	MG-NB	-2.38	2.01	2.05
15	b1	404	CLA	MG-NB	-2.38	2.01	2.05
15	b3	406	CLA	MG-NB	-2.38	2.01	2.05
15	b4	409	CLA	MG-NB	-2.38	2.01	2.05
15	b5	420	CLA	MG-ND	-2.38	2.01	2.05
15	c6	415	CLA	MG-NB	-2.38	2.01	2.05
15	b2	413	CLA	C1B-NB	-2.38	1.34	1.37
15	cA	809	CLA	CHC-C1C	2.38	1.43	1.38
15	b5	414	CLA	C1B-C2B	2.38	1.48	1.43
15	bA	809	CLA	CMB-C2B	-2.38	1.45	1.50
15	bA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	cB	806	CLA	CMD-C2D	-2.38	1.45	1.50
15	b3	405	CLA	C1D-C2D	2.38	1.50	1.45
15	a2	406	CLA	C1B-C2B	2.38	1.48	1.43
15	aA	818	CLA	C1B-NB	-2.38	1.34	1.37
15	a1	411	CLA	C1B-NB	-2.38	1.34	1.37
15	cA	818	CLA	C1B-NB	-2.38	1.34	1.37
15	a4	402	CLA	MG-NB	-2.38	2.01	2.05
15	bB	832	CLA	CMB-C2B	-2.38	1.45	1.50
15	bJ	101	CLA	C1B-NB	-2.38	1.34	1.37
15	a1	414	CLA	MG-NB	-2.38	2.01	2.05
15	c1	408	CLA	MG-NB	-2.38	2.01	2.05
15	c4	413	CLA	C3B-C4B	2.38	1.48	1.42
15	cB	834	CLA	CMB-C2B	-2.38	1.45	1.50
15	aB	816	CLA	MG-NB	-2.38	2.01	2.05
15	cB	825	CLA	C3B-C4B	2.38	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	b4	410	CLA	CMB-C2B	-2.38	1.45	1.50
15	b4	421	CLA	CMD-C2D	-2.38	1.45	1.50
15	bB	823	CLA	MG-NB	-2.38	2.01	2.05
15	a2	418	CLA	C1B-NB	-2.38	1.34	1.37
15	c5	407	CLA	C1B-C2B	2.38	1.48	1.43
15	bA	810	CLA	MG-ND	-2.38	2.01	2.05
15	c2	403	CLA	C1B-C2B	2.38	1.48	1.43
15	b3	405	CLA	C3B-C4B	2.38	1.48	1.42
15	aB	840	CLA	MG-ND	-2.38	2.01	2.05
15	c3	415	CLA	MG-ND	-2.38	2.01	2.05
15	c3	410	CLA	C1B-NB	-2.38	1.34	1.37
15	cA	805	CLA	CMD-C2D	-2.38	1.45	1.50
15	c5	420	CLA	MG-ND	-2.38	2.01	2.05
15	c2	418	CLA	C1B-C2B	2.38	1.48	1.43
15	bA	811	CLA	CMD-C2D	-2.38	1.45	1.50
15	cA	826	CLA	CMD-C2D	-2.38	1.45	1.50
15	b6	407	CLA	MG-NB	-2.38	2.01	2.05
15	cA	833	CLA	CMB-C2B	-2.38	1.45	1.50
15	cA	839	CLA	CMC-C2C	-2.38	1.45	1.50
15	bB	823	CLA	CMD-C2D	-2.38	1.45	1.50
15	cA	811	CLA	CMD-C2D	-2.38	1.45	1.50
15	c6	413	CLA	CMB-C2B	-2.38	1.45	1.50
15	cB	803	CLA	CMD-C2D	-2.38	1.45	1.50
15	bB	816	CLA	MG-NB	-2.38	2.01	2.05
15	c3	403	CLA	CMD-C2D	-2.38	1.45	1.50
15	bB	802	CLA	C1B-C2B	2.38	1.48	1.43
15	c3	404	CLA	MG-NB	-2.37	2.01	2.05
15	bB	805	CLA	C4B-NB	2.37	1.40	1.37
15	b6	422	CLA	C3B-C4B	2.37	1.48	1.42
15	a3	412	CLA	CMC-C2C	-2.37	1.45	1.50
15	bB	832	CLA	CMC-C2C	-2.37	1.45	1.50
15	c2	408	CLA	CMD-C2D	-2.37	1.45	1.50
15	cA	805	CLA	MG-ND	-2.37	2.01	2.05
15	bB	808	CLA	C1D-ND	2.37	1.40	1.37
15	c6	406	CLA	MG-NB	-2.37	2.01	2.05
15	cB	808	CLA	C1D-ND	2.37	1.40	1.37
15	cB	820	CLA	C1B-NB	-2.37	1.34	1.37
15	bA	830	CLA	CMB-C2B	-2.37	1.45	1.50
15	cA	830	CLA	CMB-C2B	-2.37	1.45	1.50
15	aK	102	CLA	C3B-C4B	2.37	1.48	1.42
15	bB	837	CLA	C3B-C4B	2.37	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	804	CLA	CMB-C2B	-2.37	1.45	1.50
15	b1	407	CLA	C1B-C2B	2.37	1.48	1.43
15	c3	406	CLA	MG-NB	-2.37	2.01	2.05
15	a1	415	CLA	C1C-NC	-2.37	1.34	1.37
15	aA	809	CLA	CMB-C2B	-2.37	1.45	1.50
15	bA	810	CLA	C3B-C4B	2.37	1.48	1.42
15	bA	811	CLA	CMB-C2B	-2.37	1.45	1.50
15	b5	420	CLA	C1B-C2B	2.37	1.48	1.43
15	b1	406	CLA	MG-NB	-2.37	2.01	2.05
15	c3	407	CLA	C1B-C2B	2.37	1.48	1.43
15	c6	401	CLA	C1B-C2B	2.37	1.48	1.43
15	aA	808	CLA	CMB-C2B	-2.37	1.45	1.50
15	cB	832	CLA	CMB-C2B	-2.37	1.45	1.50
15	aJ	203	CLA	MG-NB	-2.37	2.01	2.05
15	a5	415	CLA	MG-NB	-2.37	2.01	2.05
15	aB	826	CLA	MG-NB	-2.37	2.01	2.05
15	a6	405	CLA	MG-NB	-2.37	2.01	2.05
15	b2	409	CLA	MG-NB	-2.37	2.01	2.05
15	cF	203	CLA	CMD-C2D	-2.37	1.45	1.50
15	cB	808	CLA	C3B-C4B	2.37	1.48	1.42
15	bA	832	CLA	C1B-NB	-2.37	1.34	1.37
15	aA	842	CLA	MG-ND	-2.37	2.01	2.05
15	aB	816	CLA	C1B-C2B	2.37	1.48	1.43
15	aB	801	CLA	CMD-C2D	-2.37	1.45	1.50
15	a1	411	CLA	CMC-C2C	-2.37	1.45	1.50
15	bB	829	CLA	MG-ND	-2.37	2.01	2.05
15	aB	823	CLA	MG-NB	-2.37	2.01	2.05
15	aA	830	CLA	CMB-C2B	-2.37	1.45	1.50
15	aA	842	CLA	C1B-C2B	2.37	1.48	1.43
15	a5	415	CLA	CMB-C2B	-2.37	1.45	1.50
15	cA	811	CLA	CMB-C2B	-2.37	1.45	1.50
15	cB	840	CLA	C1B-NB	-2.37	1.34	1.37
15	c2	410	CLA	C1B-C2B	2.37	1.48	1.43
15	b6	412	CLA	CMB-C2B	-2.37	1.45	1.50
15	bA	841	CLA	MG-NB	-2.37	2.01	2.05
15	bA	842	CLA	MG-ND	-2.37	2.01	2.05
15	cB	816	CLA	MG-NB	-2.37	2.01	2.05
15	a5	405	CLA	C1B-C2B	2.37	1.48	1.43
15	c1	416	CLA	C4C-C3C	2.36	1.49	1.45
18	aF	201	BCR	C32-C1	-2.36	1.49	1.53
15	aA	811	CLA	CMB-C2B	-2.36	1.45	1.50
15	bK	101	CLA	MG-ND	-2.36	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	416	CLA	C3C-C2C	2.36	1.41	1.36
15	cB	832	CLA	CMC-C2C	-2.36	1.45	1.50
15	aA	841	CLA	MG-NB	-2.36	2.01	2.05
18	c1	419	BCR	C33-C5	-2.36	1.47	1.50
15	a2	411	CLA	CMB-C2B	-2.36	1.45	1.50
15	a4	415	CLA	CMB-C2B	-2.36	1.45	1.50
15	bB	810	CLA	CHC-C4B	-2.36	1.34	1.39
15	bB	814	CLA	CMD-C2D	-2.36	1.45	1.50
15	a5	402	CLA	MG-NB	-2.36	2.01	2.05
15	cA	841	CLA	MG-NB	-2.36	2.01	2.05
15	cF	201	CLA	MG-ND	-2.36	2.01	2.05
15	bA	809	CLA	CHC-C1C	2.36	1.43	1.38
15	bB	810	CLA	CAA-C2A	-2.36	1.49	1.54
15	cB	826	CLA	C1B-NB	-2.36	1.34	1.37
15	a3	403	CLA	CMD-C2D	-2.36	1.45	1.50
15	cB	834	CLA	CMD-C2D	-2.36	1.45	1.50
15	cA	817	CLA	MG-NB	-2.36	2.01	2.05
15	cK	102	CLA	C3B-C4B	2.36	1.48	1.42
15	c3	412	CLA	CMC-C2C	-2.36	1.45	1.50
15	a1	405	CLA	MG-NB	-2.36	2.01	2.05
15	b2	403	CLA	C1B-C2B	2.36	1.48	1.43
15	bB	840	CLA	MG-ND	-2.36	2.01	2.05
15	bL	202	CLA	MG-ND	-2.36	2.01	2.05
18	a3	401	BCR	C4-C5	-2.36	1.46	1.51
15	cA	811	CLA	C1B-C2B	2.36	1.48	1.43
15	a2	403	CLA	CMD-C2D	-2.36	1.45	1.50
15	cB	803	CLA	CMB-C2B	-2.36	1.45	1.50
15	bA	843	CLA	C1B-NB	-2.36	1.34	1.37
15	a1	409	CLA	C3C-C2C	2.36	1.41	1.36
15	cB	833	CLA	MG-ND	-2.36	2.01	2.05
15	c2	414	CLA	C3B-C4B	2.36	1.48	1.42
15	cB	801	CLA	CMD-C2D	-2.36	1.45	1.50
15	bB	819	CLA	CAC-C3C	-2.36	1.45	1.51
15	a2	410	CLA	C1B-C2B	2.36	1.48	1.43
15	a1	409	CLA	CMB-C2B	-2.36	1.45	1.50
15	b2	406	CLA	MG-NB	-2.36	2.01	2.05
15	a6	422	CLA	C1B-C2B	2.36	1.48	1.43
15	aB	837	CLA	C3B-C4B	2.36	1.48	1.42
15	cB	837	CLA	C3B-C4B	2.36	1.48	1.42
15	a3	402	CLA	MG-NB	-2.36	2.01	2.05
15	b6	408	CLA	MG-NB	-2.36	2.01	2.05
15	aB	829	CLA	C1D-ND	2.36	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	829	CLA	C1D-ND	2.36	1.40	1.37
18	a2	419	BCR	C33-C5	-2.36	1.47	1.50
15	c5	405	CLA	C1B-C2B	2.36	1.48	1.43
15	b5	402	CLA	MG-NB	-2.36	2.01	2.05
15	b4	411	CLA	C1B-NB	-2.36	1.34	1.37
15	aA	822	CLA	CMD-C2D	-2.36	1.45	1.50
15	aB	806	CLA	CMD-C2D	-2.36	1.45	1.50
15	bB	842	CLA	CMB-C2B	-2.36	1.45	1.50
15	b4	413	CLA	C3B-C4B	2.36	1.48	1.42
15	b1	412	CLA	MG-ND	-2.35	2.01	2.05
15	c1	406	CLA	MG-NB	-2.35	2.01	2.05
15	b6	404	CLA	CMD-C2D	-2.35	1.45	1.50
15	aB	805	CLA	CMB-C2B	-2.35	1.45	1.50
15	bB	801	CLA	CMD-C2D	-2.35	1.45	1.50
15	cB	810	CLA	CHC-C4B	-2.35	1.34	1.39
15	c4	410	CLA	CMB-C2B	-2.35	1.45	1.50
15	aA	817	CLA	MG-NB	-2.35	2.01	2.05
15	bA	805	CLA	MG-ND	-2.35	2.01	2.05
15	bA	839	CLA	CMC-C2C	-2.35	1.45	1.50
15	a6	411	CLA	C3C-C2C	2.35	1.41	1.36
15	c1	405	CLA	MG-NB	-2.35	2.01	2.05
15	a2	422	CLA	C1B-C2B	2.35	1.48	1.43
15	aA	811	CLA	CMD-C2D	-2.35	1.45	1.50
15	a2	417	CLA	C4C-C3C	2.35	1.49	1.45
15	bA	832	CLA	C1B-C2B	2.35	1.48	1.43
15	cB	818	CLA	C3B-C4B	2.35	1.48	1.42
15	a2	408	CLA	CMD-C2D	-2.35	1.45	1.50
15	b1	408	CLA	MG-NB	-2.35	2.01	2.05
18	aB	848	BCR	C33-C5	-2.35	1.47	1.50
15	bB	806	CLA	CMD-C2D	-2.35	1.45	1.50
15	bB	840	CLA	CMC-C2C	-2.35	1.45	1.50
15	a1	408	CLA	MG-NB	-2.35	2.01	2.05
15	c4	407	CLA	C1B-C2B	2.35	1.48	1.43
15	aA	837	CLA	CMD-C2D	-2.35	1.45	1.50
15	aB	803	CLA	CMB-C2B	-2.35	1.45	1.50
15	aA	819	CLA	CMB-C2B	-2.35	1.45	1.50
15	bK	101	CLA	C3B-C4B	2.35	1.48	1.42
15	b4	402	CLA	MG-NB	-2.35	2.01	2.05
15	aA	805	CLA	CMD-C2D	-2.35	1.45	1.50
15	a4	410	CLA	CMB-C2B	-2.35	1.45	1.50
15	aB	810	CLA	CHC-C4B	-2.35	1.34	1.39
15	a3	407	CLA	MG-ND	-2.35	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	824	CLA	CMD-C2D	-2.35	1.45	1.50
15	bB	804	CLA	C3B-C4B	2.35	1.48	1.42
15	c2	409	CLA	MG-NB	-2.35	2.01	2.05
15	c5	415	CLA	CMB-C2B	-2.35	1.45	1.50
15	b5	405	CLA	C1B-C2B	2.35	1.48	1.43
15	a6	408	CLA	MG-NB	-2.35	2.01	2.05
15	bB	822	CLA	MG-NB	-2.35	2.01	2.05
15	c3	407	CLA	MG-ND	-2.35	2.01	2.05
15	bA	824	CLA	CMD-C2D	-2.35	1.45	1.50
15	bB	820	CLA	C1B-NB	-2.35	1.34	1.37
15	b6	418	CLA	C1B-NB	-2.35	1.34	1.37
18	a6	421	BCR	C33-C5	-2.35	1.47	1.50
15	aJ	202	CLA	CMB-C2B	-2.35	1.45	1.50
15	bA	805	CLA	CMD-C2D	-2.35	1.45	1.50
15	aB	832	CLA	CMC-C2C	-2.35	1.45	1.50
15	bJ	101	CLA	CMB-C2B	-2.34	1.45	1.50
15	cB	840	CLA	MG-ND	-2.34	2.01	2.05
15	aB	822	CLA	MG-NB	-2.34	2.01	2.05
15	a4	421	CLA	C1B-C2B	2.34	1.48	1.43
15	bB	802	CLA	C1B-NB	-2.34	1.34	1.37
15	cB	817	CLA	C1D-ND	2.34	1.40	1.37
15	bB	839	CLA	CMC-C2C	-2.34	1.45	1.50
18	bB	849	BCR	C32-C1	-2.34	1.49	1.53
15	c2	410	CLA	MG-NB	-2.34	2.01	2.05
15	c4	402	CLA	MG-NB	-2.34	2.01	2.05
15	aB	823	CLA	C4B-NB	2.34	1.40	1.37
15	b3	407	CLA	C1B-C2B	2.34	1.48	1.43
15	bB	841	CLA	MG-NB	-2.34	2.01	2.05
15	aB	810	CLA	CAA-C2A	-2.34	1.49	1.54
15	bB	812	CLA	MG-NB	-2.34	2.01	2.05
15	a1	415	CLA	C4C-C3C	2.34	1.49	1.45
15	c2	422	CLA	C3B-C4B	2.34	1.48	1.42
15	bA	818	CLA	C1B-NB	-2.34	1.34	1.37
15	b3	404	CLA	MG-NB	-2.34	2.01	2.05
15	a3	417	CLA	C1B-C2B	2.34	1.48	1.43
15	b2	410	CLA	C1B-C2B	2.34	1.48	1.43
15	b1	410	CLA	CMB-C2B	-2.34	1.45	1.50
15	cA	804	CLA	C1D-ND	2.34	1.40	1.37
15	a2	402	CLA	MG-NB	-2.34	2.01	2.05
15	a4	406	CLA	MG-NB	-2.34	2.01	2.05
15	b2	403	CLA	CMD-C2D	-2.34	1.45	1.50
15	b4	407	CLA	C3B-C4B	2.34	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a5	420	CLA	C1B-C2B	2.34	1.48	1.43
15	b1	405	CLA	MG-NB	-2.34	2.01	2.05
15	aA	822	CLA	CMC-C2C	-2.34	1.45	1.50
15	b1	409	CLA	MG-NB	-2.34	2.01	2.05
15	cB	835	CLA	MG-NB	-2.34	2.01	2.05
15	b4	417	CLA	C4D-ND	-2.34	1.34	1.37
15	aK	102	CLA	C1B-C2B	2.34	1.48	1.43
15	c3	417	CLA	C1B-C2B	2.34	1.48	1.43
15	cB	810	CLA	CAA-C2A	-2.34	1.49	1.54
15	c4	411	CLA	C1B-NB	-2.34	1.34	1.37
15	bB	805	CLA	CMD-C2D	-2.34	1.45	1.50
15	a1	401	CLA	MG-NB	-2.33	2.01	2.05
15	cB	822	CLA	MG-NB	-2.33	2.01	2.05
15	bA	813	CLA	CMC-C2C	-2.33	1.45	1.50
15	c5	420	CLA	C1B-C2B	2.33	1.48	1.43
15	bA	822	CLA	CMD-C2D	-2.33	1.45	1.50
15	aA	813	CLA	CMC-C2C	-2.33	1.45	1.50
15	aA	811	CLA	C1B-C2B	2.33	1.48	1.43
15	aA	832	CLA	C1B-C2B	2.33	1.48	1.43
15	aB	801	CLA	MG-ND	-2.33	2.01	2.05
15	aA	809	CLA	CHC-C1C	2.33	1.43	1.38
15	cB	804	CLA	C3B-C4B	2.33	1.48	1.42
15	bA	811	CLA	C1B-C2B	2.33	1.48	1.43
15	aA	805	CLA	MG-ND	-2.33	2.01	2.05
15	b3	407	CLA	MG-ND	-2.33	2.01	2.05
15	b2	402	CLA	CMD-C2D	-2.33	1.45	1.50
15	c4	409	CLA	C1B-C2B	2.33	1.48	1.43
15	bB	808	CLA	CMD-C2D	-2.33	1.45	1.50
15	a3	413	CLA	C3B-C4B	2.33	1.48	1.42
15	b5	416	CLA	C4C-C3C	2.33	1.49	1.45
15	a6	411	CLA	C1B-NB	-2.33	1.34	1.37
15	bB	835	CLA	MG-NB	-2.33	2.01	2.05
15	c2	402	CLA	MG-NB	-2.33	2.01	2.05
15	cA	824	CLA	CMD-C2D	-2.33	1.45	1.50
15	b5	415	CLA	CMB-C2B	-2.33	1.45	1.50
15	cA	839	CLA	MG-ND	-2.33	2.01	2.05
18	c2	419	BCR	C33-C5	-2.33	1.47	1.50
15	bF	201	CLA	CMD-C2D	-2.33	1.45	1.50
15	c2	414	CLA	MG-ND	-2.33	2.01	2.05
15	a2	409	CLA	C1B-C2B	2.33	1.48	1.43
18	b3	401	BCR	C4-C5	-2.33	1.46	1.51
15	aL	201	CLA	MG-ND	-2.33	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	826	CLA	C1B-NB	-2.33	1.34	1.37
15	bB	840	CLA	CHC-C4B	-2.33	1.34	1.39
15	b3	402	CLA	CMD-C2D	-2.33	1.45	1.50
15	cB	808	CLA	CMD-C2D	-2.33	1.45	1.50
15	aA	805	CLA	C3B-C4B	2.33	1.48	1.42
15	cA	837	CLA	CMD-C2D	-2.33	1.45	1.50
15	aB	840	CLA	CHC-C4B	-2.33	1.34	1.39
15	aB	813	CLA	MG-NB	-2.33	2.01	2.05
15	c5	402	CLA	MG-NB	-2.33	2.01	2.05
15	cK	102	CLA	MG-ND	-2.33	2.01	2.05
15	c6	405	CLA	C1B-C2B	2.33	1.48	1.43
15	a5	416	CLA	C4C-C3C	2.33	1.49	1.45
15	aA	833	CLA	CMC-C2C	-2.33	1.45	1.50
15	cB	831	CLA	CMB-C2B	-2.33	1.45	1.50
15	aB	804	CLA	C3B-C4B	2.33	1.48	1.42
15	aB	805	CLA	CMD-C2D	-2.33	1.45	1.50
15	aJ	201	CLA	CMD-C2D	-2.33	1.45	1.50
15	a6	412	CLA	CMB-C2B	-2.33	1.45	1.50
15	b4	415	CLA	CMB-C2B	-2.33	1.45	1.50
15	a2	414	CLA	MG-ND	-2.32	2.01	2.05
15	a6	404	CLA	CMD-C2D	-2.32	1.45	1.50
15	b4	407	CLA	MG-ND	-2.32	2.01	2.05
15	cB	841	CLA	MG-NB	-2.32	2.01	2.05
15	bA	842	CLA	C1B-C2B	2.32	1.48	1.43
15	c6	418	CLA	C3C-C2C	2.32	1.41	1.36
15	b6	405	CLA	MG-NB	-2.32	2.01	2.05
15	aA	822	CLA	C1D-ND	2.32	1.40	1.37
15	aB	842	CLA	CMB-C2B	-2.32	1.45	1.50
15	cB	805	CLA	CMB-C2B	-2.32	1.45	1.50
15	cB	805	CLA	CMD-C2D	-2.32	1.45	1.50
15	cK	102	CLA	C1B-C2B	2.32	1.48	1.43
15	a1	407	CLA	MG-NB	-2.32	2.01	2.05
15	c3	413	CLA	C1B-NB	-2.32	1.34	1.37
15	a6	422	CLA	O2D-CGD	2.32	1.38	1.33
15	c1	409	CLA	MG-NB	-2.32	2.01	2.05
15	c1	415	CLA	MG-NB	-2.32	2.01	2.05
18	b2	420	BCR	C34-C9	-2.32	1.46	1.50
15	c6	408	CLA	MG-NB	-2.32	2.01	2.05
15	c5	403	CLA	C1B-C2B	2.32	1.48	1.43
15	cA	819	CLA	CMB-C2B	-2.32	1.45	1.50
15	cJ	102	CLA	CMB-C2B	-2.32	1.45	1.50
15	c2	403	CLA	CMD-C2D	-2.32	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a6	421	BCR	C1-C6	-2.32	1.50	1.53
15	cB	840	CLA	CHC-C4B	-2.32	1.34	1.39
15	bB	818	CLA	C3B-C4B	2.32	1.48	1.42
15	aK	102	CLA	MG-ND	-2.32	2.01	2.05
15	aB	830	CLA	CHC-C4B	-2.32	1.34	1.39
15	b1	411	CLA	CMB-C2B	-2.32	1.45	1.50
15	a4	407	CLA	C3B-C4B	2.32	1.48	1.42
15	bB	813	CLA	MG-NB	-2.32	2.01	2.05
15	cB	801	CLA	MG-ND	-2.32	2.01	2.05
15	b2	411	CLA	CMB-C2B	-2.32	1.45	1.50
15	c1	410	CLA	C3C-C2C	2.32	1.41	1.36
15	aJ	203	CLA	CMB-C2B	-2.32	1.45	1.50
15	c1	410	CLA	CMB-C2B	-2.32	1.45	1.50
15	bA	805	CLA	C3B-C4B	2.32	1.48	1.42
15	b6	417	CLA	C3C-C2C	2.32	1.41	1.36
15	b2	414	CLA	MG-ND	-2.32	2.01	2.05
15	cA	823	CLA	C3B-C4B	2.32	1.48	1.42
15	b2	408	CLA	CMD-C2D	-2.32	1.45	1.50
15	cA	822	CLA	CMD-C2D	-2.32	1.45	1.50
15	c5	416	CLA	C4C-C3C	2.32	1.49	1.45
15	b6	411	CLA	C3C-C2C	2.32	1.41	1.36
18	c3	401	BCR	C4-C5	-2.32	1.46	1.51
15	b4	407	CLA	C1B-C2B	2.32	1.48	1.43
15	a6	407	CLA	MG-NB	-2.32	2.01	2.05
15	cK	102	CLA	CMD-C2D	-2.32	1.45	1.50
15	aA	839	CLA	MG-ND	-2.32	2.01	2.05
15	b3	403	CLA	CMD-C2D	-2.32	1.45	1.50
15	a3	409	CLA	MG-NB	-2.32	2.01	2.05
15	bA	837	CLA	CMD-C2D	-2.32	1.45	1.50
15	c3	402	CLA	CMD-C2D	-2.32	1.45	1.50
15	aA	832	CLA	C1D-ND	2.32	1.40	1.37
15	bK	101	CLA	C4B-NB	2.32	1.40	1.37
15	b2	418	CLA	C1B-NB	-2.32	1.34	1.37
15	cB	829	CLA	C1D-ND	2.32	1.40	1.37
15	b1	410	CLA	C3C-C2C	2.32	1.41	1.36
15	aB	807	CLA	C1D-ND	2.31	1.40	1.37
15	b6	409	CLA	MG-NB	-2.31	2.01	2.05
15	aB	806	CLA	CMC-C2C	-2.31	1.45	1.50
15	bB	805	CLA	CMB-C2B	-2.31	1.45	1.50
15	bK	101	CLA	CMD-C2D	-2.31	1.45	1.50
15	aA	804	CLA	C1D-ND	2.31	1.40	1.37
15	cB	816	CLA	C4B-NB	2.31	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a2	414	CLA	C3B-C4B	2.31	1.48	1.42
15	aA	845	CLA	CMB-C2B	-2.31	1.45	1.50
15	c5	416	CLA	CMB-C2B	-2.31	1.45	1.50
15	c6	410	CLA	MG-NB	-2.31	2.01	2.05
15	c1	412	CLA	CMC-C2C	-2.31	1.45	1.50
15	bA	834	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	813	CLA	CMC-C2C	-2.31	1.45	1.50
15	b2	416	CLA	MG-ND	-2.31	2.01	2.05
15	b3	413	CLA	C1B-NB	-2.31	1.34	1.37
15	b4	406	CLA	MG-NB	-2.31	2.01	2.05
15	b3	417	CLA	C1B-C2B	2.31	1.48	1.43
15	aA	834	CLA	CMC-C2C	-2.31	1.45	1.50
15	cA	833	CLA	CMC-C2C	-2.31	1.45	1.50
15	aA	832	CLA	C1B-NB	-2.31	1.34	1.37
18	cF	202	BCR	C32-C1	-2.31	1.49	1.53
15	bA	845	CLA	CMB-C2B	-2.31	1.45	1.50
15	bB	801	CLA	CMC-C2C	-2.31	1.45	1.50
15	cB	808	CLA	CMC-C2C	-2.31	1.45	1.50
15	c6	412	CLA	C3C-C2C	2.31	1.41	1.36
15	cA	832	CLA	C1B-C2B	2.31	1.48	1.43
15	b3	408	CLA	CMC-C2C	-2.31	1.45	1.50
15	c2	411	CLA	C3C-C2C	2.31	1.41	1.36
15	aB	835	CLA	MG-NB	-2.31	2.01	2.05
15	cA	805	CLA	C3B-C4B	2.31	1.48	1.42
15	bA	809	CLA	C4B-NB	2.31	1.40	1.37
15	cB	807	CLA	C1D-ND	2.31	1.40	1.37
15	cA	838	CLA	CHC-C4B	-2.31	1.34	1.39
15	b2	405	CLA	MG-NB	-2.31	2.01	2.05
15	bA	819	CLA	CMB-C2B	-2.31	1.45	1.50
15	b4	421	CLA	CMB-C2B	-2.31	1.45	1.50
15	c3	413	CLA	C3B-C4B	2.31	1.48	1.42
15	a1	404	CLA	MG-NB	-2.31	2.01	2.05
15	c6	409	CLA	MG-NB	-2.31	2.01	2.05
15	a4	407	CLA	C1B-C2B	2.31	1.48	1.43
15	b3	409	CLA	C1B-C2B	2.31	1.48	1.43
15	c2	412	CLA	C1B-NB	-2.31	1.34	1.37
15	aB	809	CLA	C3B-C4B	2.31	1.48	1.42
15	bA	808	CLA	CMD-C2D	-2.31	1.45	1.50
15	bA	826	CLA	CMB-C2B	-2.31	1.45	1.50
15	bA	833	CLA	CMC-C2C	-2.31	1.45	1.50
15	bA	839	CLA	MG-ND	-2.31	2.01	2.05
15	c4	407	CLA	C3B-C4B	2.31	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	404	CLA	C1B-C2B	2.31	1.48	1.43
15	aA	838	CLA	CHC-C4B	-2.31	1.34	1.39
15	bB	841	CLA	CMD-C2D	-2.31	1.45	1.50
15	a4	407	CLA	MG-ND	-2.31	2.01	2.05
15	cB	821	CLA	C1B-C2B	2.31	1.48	1.43
18	cB	848	BCR	C33-C5	-2.31	1.47	1.50
15	cB	831	CLA	C4B-NB	2.31	1.40	1.37
15	aB	840	CLA	CMC-C2C	-2.30	1.45	1.50
15	cA	808	CLA	CMD-C2D	-2.30	1.45	1.50
15	c4	416	CLA	C4C-C3C	2.30	1.49	1.45
15	cB	837	CLA	CMD-C2D	-2.30	1.45	1.50
15	bA	832	CLA	C1D-ND	2.30	1.40	1.37
15	bB	830	CLA	CHC-C4B	-2.30	1.34	1.39
15	c2	411	CLA	C1B-C2B	2.30	1.48	1.43
15	a6	409	CLA	MG-NB	-2.30	2.01	2.05
15	aB	831	CLA	C4B-NB	2.30	1.40	1.37
15	bK	101	CLA	C1B-NB	-2.30	1.35	1.37
15	c4	415	CLA	CMB-C2B	-2.30	1.45	1.50
15	aB	837	CLA	CMD-C2D	-2.30	1.45	1.50
15	aJ	201	CLA	C4B-NB	2.30	1.40	1.37
15	bA	822	CLA	CMC-C2C	-2.30	1.45	1.50
15	b3	407	CLA	CMD-C2D	-2.30	1.45	1.50
15	a1	414	CLA	MG-ND	-2.30	2.01	2.05
15	a2	416	CLA	MG-ND	-2.30	2.01	2.05
15	cA	822	CLA	CMC-C2C	-2.30	1.45	1.50
15	c2	402	CLA	CMD-C2D	-2.30	1.45	1.50
15	c6	404	CLA	CMD-C2D	-2.30	1.45	1.50
15	a4	410	CLA	C3C-C2C	2.30	1.41	1.36
15	c4	410	CLA	C3C-C2C	2.30	1.41	1.36
15	cB	806	CLA	CMC-C2C	-2.30	1.45	1.50
15	aB	812	CLA	MG-NB	-2.30	2.01	2.05
15	aB	808	CLA	CMD-C2D	-2.30	1.45	1.50
15	aA	828	CLA	CMD-C2D	-2.30	1.45	1.50
15	bB	831	CLA	CMB-C2B	-2.30	1.45	1.50
15	a6	422	CLA	C3B-C4B	2.30	1.48	1.42
15	bB	808	CLA	CMC-C2C	-2.30	1.45	1.50
15	a4	421	CLA	C3B-C4B	2.30	1.48	1.42
15	b2	411	CLA	C3C-C2C	2.30	1.41	1.36
15	a3	403	CLA	MG-ND	-2.30	2.01	2.05
15	bB	837	CLA	MG-ND	-2.30	2.01	2.05
15	bB	807	CLA	C1D-ND	2.30	1.40	1.37
15	a2	406	CLA	MG-NB	-2.30	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a6	404	CLA	C1B-C2B	2.30	1.48	1.43
15	c1	415	CLA	MG-ND	-2.30	2.01	2.05
15	aB	808	CLA	CMC-C2C	-2.30	1.45	1.50
15	bA	823	CLA	C3B-C4B	2.30	1.48	1.42
15	b1	415	CLA	MG-NB	-2.30	2.01	2.05
15	aB	814	CLA	CHC-C1C	2.30	1.43	1.38
15	aA	808	CLA	C1B-C2B	2.30	1.48	1.43
15	c2	409	CLA	C1B-C2B	2.30	1.48	1.43
15	cB	814	CLA	CHC-C1C	2.30	1.43	1.38
15	cA	822	CLA	C1D-ND	2.30	1.40	1.37
15	cB	830	CLA	CHC-C4B	-2.29	1.34	1.39
15	cB	810	CLA	C1D-ND	2.29	1.40	1.37
15	b1	416	CLA	C4C-C3C	2.29	1.49	1.45
15	cB	809	CLA	C3B-C4B	2.29	1.48	1.42
15	c3	409	CLA	MG-NB	-2.29	2.01	2.05
15	bA	838	CLA	CHC-C4B	-2.29	1.34	1.39
15	aK	102	CLA	CMD-C2D	-2.29	1.45	1.50
15	cJ	101	CLA	CMB-C2B	-2.29	1.45	1.50
15	aB	818	CLA	C3B-C4B	2.29	1.48	1.42
15	a2	422	CLA	C3B-C4B	2.29	1.48	1.42
15	bB	801	CLA	MG-ND	-2.29	2.01	2.05
15	c1	411	CLA	CMB-C2B	-2.29	1.45	1.50
15	aX	102	CLA	C1D-ND	2.29	1.40	1.37
15	c6	401	CLA	MG-NB	-2.29	2.01	2.05
15	bK	101	CLA	C1B-C2B	2.29	1.48	1.43
15	cB	842	CLA	CMB-C2B	-2.29	1.45	1.50
15	c2	411	CLA	CMB-C2B	-2.29	1.45	1.50
15	cA	807	CLA	CAA-C2A	-2.29	1.49	1.54
15	cA	832	CLA	C1B-NB	-2.29	1.35	1.37
15	a1	410	CLA	CMB-C2B	-2.29	1.45	1.50
15	c6	412	CLA	CMB-C2B	-2.29	1.45	1.50
15	c5	405	CLA	MG-NB	-2.29	2.01	2.05
15	c6	417	CLA	MG-NB	-2.29	2.01	2.05
15	c3	407	CLA	CMD-C2D	-2.29	1.45	1.50
15	c2	416	CLA	MG-ND	-2.29	2.01	2.05
15	bB	821	CLA	C1B-C2B	2.29	1.48	1.43
15	aA	823	CLA	C3B-C4B	2.29	1.48	1.42
15	bB	839	CLA	MG-NB	-2.29	2.01	2.05
15	c1	417	CLA	C1B-C2B	2.29	1.48	1.43
15	aB	810	CLA	C1D-ND	2.29	1.40	1.37
15	bB	810	CLA	C1D-ND	2.29	1.40	1.37
15	cA	805	CLA	C4B-NB	2.29	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	403	CLA	MG-ND	-2.29	2.01	2.05
15	c2	406	CLA	MG-NB	-2.29	2.01	2.05
18	a2	420	BCR	C34-C9	-2.29	1.46	1.50
15	bB	806	CLA	CMC-C2C	-2.29	1.45	1.50
15	cB	821	CLA	CMB-C2B	-2.29	1.45	1.50
15	aA	809	CLA	C4B-NB	2.29	1.40	1.37
15	aA	832	CLA	C4B-NB	2.29	1.40	1.37
15	aB	840	CLA	C1D-ND	2.29	1.40	1.37
15	a5	408	CLA	CMB-C2B	-2.29	1.45	1.50
15	a5	403	CLA	C1B-C2B	2.29	1.48	1.43
18	b2	419	BCR	C33-C5	-2.29	1.47	1.50
15	a6	417	CLA	C4C-C3C	2.29	1.49	1.45
15	cB	836	CLA	CMC-C2C	-2.29	1.46	1.50
15	cK	102	CLA	C1B-NB	-2.29	1.35	1.37
15	b3	413	CLA	C3B-C4B	2.29	1.48	1.42
15	b5	405	CLA	MG-NB	-2.29	2.01	2.05
15	aA	826	CLA	CMB-C2B	-2.29	1.46	1.50
15	aB	807	CLA	CMB-C2B	-2.29	1.46	1.50
15	cA	808	CLA	C1B-C2B	2.29	1.48	1.43
15	c5	420	CLA	MG-NB	-2.29	2.01	2.05
15	cB	840	CLA	CMC-C2C	-2.29	1.46	1.50
15	b3	416	CLA	C3B-C4B	2.29	1.48	1.42
15	bA	822	CLA	C1D-ND	2.29	1.40	1.37
15	bA	828	CLA	CMD-C2D	-2.29	1.46	1.50
15	cB	801	CLA	CMC-C2C	-2.29	1.46	1.50
15	b6	422	CLA	MG-NB	-2.29	2.01	2.05
15	a6	414	CLA	C3B-C4B	2.29	1.48	1.42
15	b2	422	CLA	C3B-C4B	2.28	1.48	1.42
15	bA	840	CLA	CHC-C4B	-2.28	1.34	1.39
15	cA	828	CLA	CMD-C2D	-2.28	1.46	1.50
15	c4	407	CLA	MG-ND	-2.28	2.01	2.05
15	c6	418	CLA	C4C-C3C	2.28	1.49	1.45
15	b6	411	CLA	C1B-NB	-2.28	1.35	1.37
15	c4	421	CLA	C3B-C4B	2.28	1.48	1.42
15	aA	824	CLA	CMB-C2B	-2.28	1.46	1.50
15	aK	102	CLA	C1B-NB	-2.28	1.35	1.37
15	aL	201	CLA	C4B-NB	2.28	1.40	1.37
15	a4	409	CLA	C1B-C2B	2.28	1.48	1.43
15	b1	415	CLA	MG-ND	-2.28	2.01	2.05
15	cA	836	CLA	MG-ND	-2.28	2.01	2.05
15	cA	826	CLA	CMB-C2B	-2.28	1.46	1.50
15	c4	415	CLA	MG-ND	-2.28	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	402	CLA	MG-NB	-2.28	2.01	2.05
15	aB	837	CLA	CMB-C2B	-2.28	1.46	1.50
15	a2	422	CLA	CMB-C2B	-2.28	1.46	1.50
15	bB	836	CLA	CMC-C2C	-2.28	1.46	1.50
15	b2	411	CLA	MG-ND	-2.28	2.01	2.05
15	c6	412	CLA	C1B-NB	-2.28	1.35	1.37
15	bA	808	CLA	C1B-C2B	2.28	1.48	1.43
15	a5	405	CLA	MG-NB	-2.28	2.01	2.05
15	aK	102	CLA	C4B-NB	2.28	1.40	1.37
15	a6	407	CLA	CMB-C2B	-2.28	1.46	1.50
15	a6	411	CLA	CMB-C2B	-2.28	1.46	1.50
15	c5	410	CLA	CMB-C2B	-2.28	1.46	1.50
15	aB	831	CLA	CMB-C2B	-2.28	1.46	1.50
15	aB	841	CLA	CMD-C2D	-2.28	1.46	1.50
15	cA	840	CLA	CHC-C4B	-2.28	1.34	1.39
15	bF	201	CLA	C4B-NB	2.28	1.40	1.37
15	cA	832	CLA	C1D-ND	2.28	1.40	1.37
15	b3	409	CLA	MG-NB	-2.28	2.01	2.05
15	cB	837	CLA	CMB-C2B	-2.28	1.46	1.50
15	bB	809	CLA	C3B-C4B	2.28	1.48	1.42
15	c4	406	CLA	MG-NB	-2.28	2.01	2.05
15	cA	841	CLA	C1B-C2B	2.28	1.48	1.43
15	bB	814	CLA	CHC-C1C	2.28	1.43	1.38
15	b6	416	CLA	MG-NB	-2.28	2.01	2.05
15	aB	815	CLA	CMB-C2B	-2.28	1.46	1.50
15	a3	409	CLA	C1B-C2B	2.28	1.48	1.43
15	cA	809	CLA	CMC-C2C	-2.28	1.46	1.50
15	cA	844	CLA	CMB-C2B	-2.28	1.46	1.50
15	cB	812	CLA	MG-NB	-2.28	2.01	2.05
15	bB	831	CLA	C4B-NB	2.28	1.40	1.37
15	bX	102	CLA	C1D-ND	2.28	1.40	1.37
15	cA	822	CLA	C3B-C4B	2.28	1.48	1.42
15	b5	416	CLA	CMB-C2B	-2.28	1.46	1.50
15	aB	841	CLA	MG-NB	-2.28	2.01	2.05
15	b5	403	CLA	C1B-C2B	2.28	1.48	1.43
15	a3	402	CLA	CMD-C2D	-2.28	1.46	1.50
15	c2	405	CLA	MG-NB	-2.28	2.01	2.05
15	aA	845	CLA	C1B-NB	-2.28	1.35	1.37
15	a2	411	CLA	C3C-C2C	2.28	1.41	1.36
15	a5	410	CLA	C3C-C2C	2.28	1.41	1.36
15	aA	825	CLA	MG-ND	-2.28	2.01	2.05
15	a5	415	CLA	MG-ND	-2.28	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	813	CLA	MG-NB	-2.28	2.01	2.05
15	bB	809	CLA	C4B-NB	2.28	1.40	1.37
15	cB	841	CLA	C1B-NB	-2.28	1.35	1.37
15	aB	821	CLA	C1B-C2B	2.28	1.48	1.43
18	bB	849	BCR	C33-C5	-2.27	1.47	1.50
15	b4	410	CLA	C3C-C2C	2.27	1.41	1.36
15	b6	411	CLA	CMB-C2B	-2.27	1.46	1.50
15	cB	840	CLA	C1D-ND	2.27	1.40	1.37
15	b3	406	CLA	CMB-C2B	-2.27	1.46	1.50
15	b2	412	CLA	C1B-NB	-2.27	1.35	1.37
15	aA	825	CLA	CMB-C2B	-2.27	1.46	1.50
15	bL	202	CLA	C4B-NB	2.27	1.40	1.37
18	c6	403	BCR	C4-C5	-2.27	1.46	1.51
15	b4	409	CLA	C1B-C2B	2.27	1.48	1.43
15	cB	841	CLA	CMD-C2D	-2.27	1.46	1.50
15	bA	841	CLA	C1B-C2B	2.27	1.48	1.43
15	cA	825	CLA	MG-ND	-2.27	2.01	2.05
15	cB	813	CLA	MG-ND	-2.27	2.01	2.05
15	b5	415	CLA	MG-ND	-2.27	2.01	2.05
15	bB	815	CLA	CMB-C2B	-2.27	1.46	1.50
15	a4	416	CLA	C4C-C3C	2.27	1.48	1.45
15	b4	409	CLA	CMD-C2D	-2.27	1.46	1.50
15	c3	409	CLA	C1B-C2B	2.27	1.48	1.43
15	a6	403	CLA	CMD-C2D	-2.27	1.46	1.50
15	bJ	102	CLA	CMB-C2B	-2.27	1.46	1.50
15	bA	842	CLA	MG-NB	-2.27	2.01	2.05
15	a3	421	CLA	C3B-C4B	2.27	1.48	1.42
15	aB	801	CLA	CMC-C2C	-2.27	1.46	1.50
15	bA	836	CLA	MG-ND	-2.27	2.01	2.05
15	b4	416	CLA	C4C-C3C	2.27	1.48	1.45
15	b5	410	CLA	CMB-C2B	-2.27	1.46	1.50
15	cA	823	CLA	CMD-C2D	-2.27	1.46	1.50
15	b4	415	CLA	MG-ND	-2.27	2.01	2.05
15	cB	839	CLA	MG-NB	-2.27	2.01	2.05
15	c3	408	CLA	C1B-C2B	2.27	1.48	1.43
15	bA	832	CLA	C4B-NB	2.27	1.40	1.37
18	cF	202	BCR	C33-C5	-2.27	1.47	1.50
15	bA	807	CLA	CAA-C2A	-2.27	1.49	1.54
15	cA	827	CLA	CMB-C2B	-2.27	1.46	1.50
15	b1	413	CLA	C1B-NB	-2.27	1.35	1.37
15	b5	410	CLA	MG-ND	-2.27	2.01	2.05
15	c5	415	CLA	MG-ND	-2.27	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a5	410	CLA	CMB-C2B	-2.27	1.46	1.50
15	a5	416	CLA	CMB-C2B	-2.27	1.46	1.50
15	aA	841	CLA	C1B-C2B	2.27	1.48	1.43
15	a4	415	CLA	MG-ND	-2.27	2.01	2.05
15	aA	810	CLA	C1B-NB	-2.27	1.35	1.37
15	c4	413	CLA	C1B-NB	-2.27	1.35	1.37
15	a3	407	CLA	CMD-C2D	-2.27	1.46	1.50
15	bA	823	CLA	CMD-C2D	-2.27	1.46	1.50
15	a2	422	CLA	CMC-C2C	-2.26	1.46	1.50
18	aM	101	BCR	C30-C25	-2.26	1.50	1.53
15	aB	802	CLA	C1B-NB	-2.26	1.35	1.37
15	b6	417	CLA	C4C-C3C	2.26	1.48	1.45
15	bA	825	CLA	CMB-C2B	-2.26	1.46	1.50
15	bA	841	CLA	CMC-C2C	-2.26	1.46	1.50
15	b5	408	CLA	CMB-C2B	-2.26	1.46	1.50
15	bA	824	CLA	CMB-C2B	-2.26	1.46	1.50
15	a4	413	CLA	C1B-NB	-2.26	1.35	1.37
15	c1	413	CLA	MG-ND	-2.26	2.01	2.05
15	a4	409	CLA	CMD-C2D	-2.26	1.46	1.50
15	bB	821	CLA	CMB-C2B	-2.26	1.46	1.50
15	a5	417	CLA	C4D-ND	-2.26	1.34	1.37
18	c2	420	BCR	C34-C9	-2.26	1.46	1.50
15	aA	842	CLA	MG-NB	-2.26	2.01	2.05
15	b5	420	CLA	MG-NB	-2.26	2.01	2.05
15	bB	840	CLA	C1D-ND	2.26	1.40	1.37
15	aB	834	CLA	C1B-C2B	2.26	1.48	1.43
15	aA	822	CLA	C3B-C4B	2.26	1.48	1.42
15	a2	411	CLA	MG-ND	-2.26	2.01	2.05
18	aI	103	BCR	C33-C5	-2.26	1.47	1.50
15	aL	203	CLA	C3B-C4B	2.26	1.48	1.42
15	aB	839	CLA	MG-NB	-2.26	2.01	2.05
18	b6	402	BCR	C4-C5	-2.26	1.46	1.51
15	a3	408	CLA	CMC-C2C	-2.26	1.46	1.50
15	b6	403	CLA	CMD-C2D	-2.26	1.46	1.50
15	c3	416	CLA	C3B-C4B	2.26	1.48	1.42
15	b6	407	CLA	CMB-C2B	-2.26	1.46	1.50
15	c1	413	CLA	C1B-NB	-2.26	1.35	1.37
15	a1	416	CLA	C1B-C2B	2.26	1.48	1.43
15	aB	837	CLA	MG-ND	-2.26	2.01	2.05
15	aB	833	CLA	CMC-C2C	-2.26	1.46	1.50
15	a4	421	CLA	CMB-C2B	-2.26	1.46	1.50
15	b5	402	CLA	CMD-C2D	-2.26	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	408	CLA	CMC-C2C	-2.26	1.46	1.50
15	b2	417	CLA	C3C-C2C	2.26	1.41	1.36
15	cB	837	CLA	MG-ND	-2.26	2.01	2.05
15	aA	808	CLA	CMD-C2D	-2.26	1.46	1.50
15	cB	807	CLA	CMB-C2B	-2.26	1.46	1.50
15	c4	407	CLA	CMD-C2D	-2.26	1.46	1.50
15	a2	412	CLA	C1B-NB	-2.26	1.35	1.37
15	cA	809	CLA	MG-ND	-2.26	2.01	2.05
15	bA	827	CLA	CMB-C2B	-2.26	1.46	1.50
15	bB	837	CLA	CMD-C2D	-2.26	1.46	1.50
15	cA	834	CLA	CMC-C2C	-2.26	1.46	1.50
18	aA	851	BCR	C38-C26	-2.26	1.47	1.50
15	aB	804	CLA	CMB-C2B	-2.26	1.46	1.50
15	bA	806	CLA	CMA-C3A	-2.26	1.48	1.53
15	a2	407	CLA	MG-NB	-2.26	2.01	2.05
15	aJ	203	CLA	C1B-NB	-2.26	1.35	1.37
15	c5	408	CLA	CMB-C2B	-2.26	1.46	1.50
15	aA	840	CLA	CHC-C4B	-2.26	1.34	1.39
15	a1	407	CLA	C1B-C2B	2.26	1.48	1.43
15	b4	406	CLA	CMB-C2B	-2.26	1.46	1.50
15	a6	416	CLA	MG-NB	-2.25	2.01	2.05
18	a6	402	BCR	C4-C5	-2.25	1.46	1.51
18	bA	852	BCR	C38-C26	-2.25	1.47	1.50
15	aB	826	CLA	CMB-C2B	-2.25	1.46	1.50
15	bA	812	CLA	CMB-C2B	-2.25	1.46	1.50
15	cB	815	CLA	CMB-C2B	-2.25	1.46	1.50
15	cB	830	CLA	CMC-C2C	-2.25	1.46	1.50
15	c5	402	CLA	CMD-C2D	-2.25	1.46	1.50
15	c5	420	CLA	CMD-C2D	-2.25	1.46	1.50
15	a3	410	CLA	MG-ND	-2.25	2.01	2.05
15	bB	839	CLA	C1B-NB	-2.25	1.35	1.37
15	cB	802	CLA	C1B-NB	-2.25	1.35	1.37
15	a2	402	CLA	CMD-C2D	-2.25	1.46	1.50
15	c4	421	CLA	CMB-C2B	-2.25	1.46	1.50
15	b3	403	CLA	MG-ND	-2.25	2.01	2.05
15	bB	829	CLA	CMC-C2C	-2.25	1.46	1.50
15	bB	837	CLA	CMB-C2B	-2.25	1.46	1.50
18	cM	101	BCR	C30-C25	-2.25	1.50	1.53
15	bB	842	CLA	CMD-C2D	-2.25	1.46	1.50
15	cA	841	CLA	CMB-C2B	-2.25	1.46	1.50
15	aA	838	CLA	CMC-C2C	-2.25	1.46	1.50
15	b4	413	CLA	C1B-NB	-2.25	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	834	CLA	C1D-ND	2.25	1.40	1.37
15	cF	203	CLA	C4B-NB	2.25	1.40	1.37
15	bB	833	CLA	CMC-C2C	-2.25	1.46	1.50
15	aA	809	CLA	MG-ND	-2.25	2.01	2.05
15	c6	412	CLA	MG-ND	-2.25	2.01	2.05
15	cA	809	CLA	C4B-NB	2.25	1.40	1.37
15	aA	809	CLA	CMC-C2C	-2.25	1.46	1.50
15	aB	841	CLA	CHC-C1C	2.25	1.43	1.38
15	a6	406	CLA	CMB-C2B	-2.25	1.46	1.50
15	b3	403	CLA	C1B-C2B	2.25	1.48	1.43
15	b4	408	CLA	C1B-C2B	2.25	1.48	1.43
15	aB	841	CLA	C1B-NB	-2.25	1.35	1.37
15	cA	832	CLA	C4B-NB	2.25	1.40	1.37
15	cB	818	CLA	C1B-NB	-2.25	1.35	1.37
15	bB	841	CLA	CHC-C1C	2.25	1.43	1.38
15	aB	821	CLA	CMB-C2B	-2.25	1.46	1.50
15	b1	408	CLA	C1B-C2B	2.25	1.48	1.43
15	a1	408	CLA	CHC-C1C	2.25	1.43	1.38
15	bB	834	CLA	C1B-C2B	2.25	1.48	1.43
15	aA	823	CLA	CMD-C2D	-2.25	1.46	1.50
15	c4	406	CLA	CMB-C2B	-2.25	1.46	1.50
15	c6	407	CLA	CMB-C2B	-2.25	1.46	1.50
15	cB	839	CLA	C4B-NB	2.25	1.40	1.37
15	c5	417	CLA	C4D-ND	-2.25	1.34	1.37
15	cF	201	CLA	MG-NB	-2.25	2.01	2.05
15	aB	839	CLA	C4B-NB	2.25	1.40	1.37
15	bB	841	CLA	C1B-NB	-2.25	1.35	1.37
15	cA	812	CLA	CMB-C2B	-2.25	1.46	1.50
15	cA	821	CLA	CMB-C2B	-2.25	1.46	1.50
15	c4	410	CLA	MG-ND	-2.25	2.01	2.05
15	bB	807	CLA	CMB-C2B	-2.25	1.46	1.50
15	b6	404	CLA	MG-ND	-2.25	2.01	2.05
15	b2	409	CLA	CMC-C2C	-2.25	1.46	1.50
15	c2	413	CLA	CMC-C2C	-2.25	1.46	1.50
15	a6	411	CLA	MG-ND	-2.25	2.01	2.05
15	c3	417	CLA	C4D-ND	-2.25	1.34	1.37
15	cA	841	CLA	CMC-C2C	-2.25	1.46	1.50
15	bA	807	CLA	C3B-C4B	2.25	1.48	1.42
15	a5	420	CLA	CMC-C2C	-2.24	1.46	1.50
15	cA	824	CLA	CMB-C2B	-2.24	1.46	1.50
15	a2	411	CLA	C1B-C2B	2.24	1.48	1.43
15	bJ	101	CLA	C1B-C2B	2.24	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c4	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	a1	412	CLA	MG-ND	-2.24	2.01	2.05
18	a6	421	BCR	C30-C25	-2.24	1.50	1.53
15	aA	807	CLA	C3B-C4B	2.24	1.48	1.42
15	aA	841	CLA	CMB-C2B	-2.24	1.46	1.50
15	a2	409	CLA	CMC-C2C	-2.24	1.46	1.50
15	bA	809	CLA	MG-ND	-2.24	2.01	2.05
15	aB	842	CLA	CMD-C2D	-2.24	1.46	1.50
15	cJ	102	CLA	C1B-NB	-2.24	1.35	1.37
15	aA	812	CLA	CMB-C2B	-2.24	1.46	1.50
15	a5	402	CLA	CMD-C2D	-2.24	1.46	1.50
15	cA	806	CLA	CMA-C3A	-2.24	1.48	1.53
15	b1	413	CLA	MG-ND	-2.24	2.01	2.05
15	cX	102	CLA	C1D-ND	2.24	1.40	1.37
15	aB	836	CLA	CMC-C2C	-2.24	1.46	1.50
15	c5	408	CLA	CMC-C2C	-2.24	1.46	1.50
15	bA	822	CLA	C3B-C4B	2.24	1.48	1.42
18	a1	421	BCR	C33-C5	-2.24	1.47	1.50
15	a3	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	cB	826	CLA	CMB-C2B	-2.24	1.46	1.50
15	c5	410	CLA	C3C-C2C	2.24	1.41	1.36
15	aA	807	CLA	CAA-C2A	-2.24	1.49	1.54
15	bB	806	CLA	CMB-C2B	-2.24	1.46	1.50
15	a6	403	CLA	MG-NB	-2.24	2.01	2.05
15	bA	829	CLA	MG-ND	-2.24	2.01	2.05
15	b2	410	CLA	CHC-C1C	2.24	1.43	1.38
15	cB	841	CLA	CHC-C1C	2.24	1.43	1.38
15	bL	204	CLA	C3B-C4B	2.24	1.48	1.42
15	aB	829	CLA	CMC-C2C	-2.24	1.46	1.50
15	cA	812	CLA	C1B-C2B	2.24	1.48	1.43
15	a3	406	CLA	CMB-C2B	-2.24	1.46	1.50
15	bB	818	CLA	C1B-NB	-2.24	1.35	1.37
15	a6	409	CLA	CMC-C2C	-2.24	1.46	1.50
15	bA	841	CLA	CMB-C2B	-2.24	1.46	1.50
15	cA	817	CLA	CMD-C2D	-2.24	1.46	1.50
15	bA	825	CLA	MG-ND	-2.24	2.01	2.05
15	c6	405	CLA	MG-ND	-2.24	2.01	2.05
15	cB	817	CLA	CMD-C2D	-2.24	1.46	1.50
15	cB	842	CLA	CMD-C2D	-2.24	1.46	1.50
18	b6	421	BCR	C30-C25	-2.24	1.50	1.53
15	c5	410	CLA	C1B-NB	-2.24	1.35	1.37
18	cA	850	BCR	C38-C26	-2.24	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	827	CLA	CMB-C2B	-2.24	1.46	1.50
15	a4	404	CLA	CMB-C2B	-2.24	1.46	1.50
15	bB	835	CLA	CMD-C2D	-2.24	1.46	1.50
15	c4	410	CLA	CMD-C2D	-2.24	1.46	1.50
15	bA	816	CLA	C1B-C2B	2.24	1.48	1.43
15	cB	834	CLA	C1B-C2B	2.24	1.48	1.43
15	a5	410	CLA	MG-ND	-2.24	2.01	2.05
15	aB	816	CLA	C4B-NB	2.24	1.40	1.37
15	bB	834	CLA	MG-ND	-2.24	2.01	2.05
15	b1	403	CLA	C1B-C2B	2.24	1.48	1.43
15	b2	422	CLA	CMC-C2C	-2.24	1.46	1.50
15	b2	409	CLA	C1B-C2B	2.24	1.48	1.43
15	cB	829	CLA	C1B-C2B	2.24	1.48	1.43
15	cL	204	CLA	C3B-C4B	2.24	1.48	1.42
15	a5	409	CLA	CMD-C2D	-2.24	1.46	1.50
15	c2	422	CLA	CMC-C2C	-2.24	1.46	1.50
15	cJ	101	CLA	C1B-C2B	2.23	1.48	1.43
15	c2	407	CLA	MG-NB	-2.23	2.01	2.05
15	aA	805	CLA	C4B-NB	2.23	1.40	1.37
15	bB	839	CLA	C4B-NB	2.23	1.40	1.37
15	bA	809	CLA	CMC-C2C	-2.23	1.46	1.50
15	b6	411	CLA	MG-ND	-2.23	2.01	2.05
15	cA	816	CLA	C1B-NB	-2.23	1.35	1.37
15	bB	817	CLA	CMD-C2D	-2.23	1.46	1.50
15	bJ	102	CLA	C1B-NB	-2.23	1.35	1.37
15	cA	838	CLA	CMC-C2C	-2.23	1.46	1.50
15	aA	836	CLA	MG-ND	-2.23	2.01	2.05
15	cB	804	CLA	CMB-C2B	-2.23	1.46	1.50
15	bB	831	CLA	MG-ND	-2.23	2.01	2.05
15	cA	807	CLA	C3B-C4B	2.23	1.48	1.42
15	aA	816	CLA	C1B-NB	-2.23	1.35	1.37
15	cA	837	CLA	CMB-C2B	-2.23	1.46	1.50
15	bB	830	CLA	CMC-C2C	-2.23	1.46	1.50
15	c3	409	CLA	CMD-C2D	-2.23	1.46	1.50
18	bM	101	BCR	C30-C25	-2.23	1.50	1.53
15	b5	417	CLA	C4D-ND	-2.23	1.34	1.37
15	b1	417	CLA	C1B-C2B	2.23	1.48	1.43
15	aJ	202	CLA	C1B-C2B	2.23	1.48	1.43
15	bA	838	CLA	CMC-C2C	-2.23	1.46	1.50
15	b2	402	CLA	MG-NB	-2.23	2.01	2.05
15	b1	402	CLA	CMD-C2D	-2.23	1.46	1.50
15	c2	422	CLA	CMB-C2B	-2.23	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c6	408	CLA	CMB-C2B	-2.23	1.46	1.50
15	bA	812	CLA	C1B-C2B	2.23	1.48	1.43
15	b4	402	CLA	CMD-C2D	-2.23	1.46	1.50
15	bB	828	CLA	C1D-ND	2.23	1.40	1.37
15	aB	813	CLA	MG-ND	-2.23	2.01	2.05
15	b1	417	CLA	CMD-C2D	-2.23	1.46	1.50
15	b5	408	CLA	CMC-C2C	-2.23	1.46	1.50
15	cB	806	CLA	MG-NB	-2.23	2.01	2.05
15	bB	816	CLA	C4B-NB	2.23	1.40	1.37
15	a2	417	CLA	C3C-C2C	2.23	1.41	1.36
15	bB	826	CLA	CMB-C2B	-2.23	1.46	1.50
15	cB	824	CLA	CMD-C2D	-2.23	1.46	1.50
15	bA	834	CLA	C1D-ND	2.23	1.40	1.37
15	aB	808	CLA	CMB-C2B	-2.23	1.46	1.50
15	bB	819	CLA	CMC-C2C	-2.23	1.46	1.50
15	b2	413	CLA	CMC-C2C	-2.23	1.46	1.50
15	a2	418	CLA	C4D-ND	-2.23	1.34	1.37
15	cB	820	CLA	MG-ND	-2.23	2.01	2.05
15	b5	410	CLA	C3C-C2C	2.23	1.41	1.36
15	bB	804	CLA	CMB-C2B	-2.23	1.46	1.50
15	a5	420	CLA	MG-NB	-2.23	2.01	2.05
15	a5	420	CLA	CMD-C2D	-2.23	1.46	1.50
15	cB	808	CLA	CMB-C2B	-2.23	1.46	1.50
15	cK	102	CLA	C4B-NB	2.23	1.40	1.37
15	aB	821	CLA	CMC-C2C	-2.23	1.46	1.50
15	cB	833	CLA	CMC-C2C	-2.23	1.46	1.50
15	cB	834	CLA	MG-ND	-2.23	2.01	2.05
15	c4	408	CLA	C1B-C2B	2.22	1.48	1.43
15	a3	411	CLA	CMC-C2C	-2.22	1.46	1.50
15	b3	404	CLA	CMB-C2B	-2.22	1.46	1.50
15	bA	810	CLA	C1B-NB	-2.22	1.35	1.37
15	c6	407	CLA	MG-NB	-2.22	2.01	2.05
15	a6	413	CLA	C1B-NB	-2.22	1.35	1.37
15	bA	809	CLA	C1B-NB	-2.22	1.35	1.37
15	b2	414	CLA	C1B-NB	-2.22	1.35	1.37
15	a4	413	CLA	CMD-C2D	-2.22	1.46	1.50
15	b4	407	CLA	CMD-C2D	-2.22	1.46	1.50
15	b2	418	CLA	CMC-C2C	-2.22	1.46	1.50
15	b5	409	CLA	CMD-C2D	-2.22	1.46	1.50
15	cB	806	CLA	CMB-C2B	-2.22	1.46	1.50
15	c2	405	CLA	CMB-C2B	-2.22	1.46	1.50
15	c3	406	CLA	CMB-C2B	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	834	CLA	MG-ND	-2.22	2.01	2.05
15	a6	404	CLA	MG-ND	-2.22	2.01	2.05
15	cB	809	CLA	C4B-NB	2.22	1.40	1.37
15	cB	839	CLA	C1B-NB	-2.22	1.35	1.37
15	cA	816	CLA	C1B-C2B	2.22	1.48	1.43
15	a3	416	CLA	C3B-C4B	2.22	1.48	1.42
15	aA	837	CLA	CMB-C2B	-2.22	1.46	1.50
15	cA	810	CLA	C1B-NB	-2.22	1.35	1.37
15	a3	408	CLA	C1B-C2B	2.22	1.48	1.43
15	bA	831	CLA	CHC-C4B	-2.22	1.34	1.39
15	c6	410	CLA	CMC-C2C	-2.22	1.46	1.50
15	aA	812	CLA	C1B-C2B	2.22	1.48	1.43
15	c2	417	CLA	C3C-C2C	2.22	1.41	1.36
18	aF	201	BCR	C33-C5	-2.22	1.47	1.50
15	a4	408	CLA	C1B-C2B	2.22	1.48	1.43
15	aA	809	CLA	C1B-NB	-2.22	1.35	1.37
15	a5	408	CLA	CMC-C2C	-2.22	1.46	1.50
15	b4	410	CLA	CMD-C2D	-2.22	1.46	1.50
15	bB	806	CLA	MG-NB	-2.22	2.01	2.05
15	cB	835	CLA	CMD-C2D	-2.22	1.46	1.50
15	c2	409	CLA	CMC-C2C	-2.22	1.46	1.50
15	b2	411	CLA	C1B-C2B	2.22	1.48	1.43
15	bA	817	CLA	CMD-C2D	-2.22	1.46	1.50
15	bA	837	CLA	CMB-C2B	-2.22	1.46	1.50
15	a5	409	CLA	CHC-C1C	2.22	1.43	1.38
15	aB	818	CLA	C1B-NB	-2.22	1.35	1.37
15	aB	835	CLA	CMD-C2D	-2.22	1.46	1.50
15	b4	404	CLA	CMB-C2B	-2.22	1.46	1.50
15	cJ	101	CLA	CMD-C2D	-2.22	1.46	1.50
15	cA	825	CLA	CMB-C2B	-2.22	1.46	1.50
15	c5	410	CLA	MG-ND	-2.22	2.01	2.05
15	bB	813	CLA	MG-ND	-2.22	2.01	2.05
15	b1	402	CLA	MG-NB	-2.22	2.01	2.05
15	aA	817	CLA	CMD-C2D	-2.22	1.46	1.50
15	aB	830	CLA	CMC-C2C	-2.22	1.46	1.50
15	a4	410	CLA	C1B-NB	-2.22	1.35	1.37
15	bA	816	CLA	C1B-NB	-2.22	1.35	1.37
15	bA	829	CLA	C1B-NB	-2.22	1.35	1.37
15	b4	408	CLA	CMC-C2C	-2.22	1.46	1.50
15	bF	201	CLA	CMC-C2C	-2.22	1.46	1.50
15	b5	410	CLA	C1B-NB	-2.22	1.35	1.37
15	aA	806	CLA	CMA-C3A	-2.22	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	406	CLA	CMB-C2B	-2.22	1.46	1.50
15	cF	203	CLA	CMC-C2C	-2.22	1.46	1.50
18	cL	205	BCR	C33-C5	-2.22	1.47	1.50
15	a2	405	CLA	MG-NB	-2.21	2.01	2.05
15	aB	817	CLA	CMD-C2D	-2.21	1.46	1.50
15	aB	807	CLA	C1B-C2B	2.21	1.48	1.43
15	a3	404	CLA	CMB-C2B	-2.21	1.46	1.50
15	aB	823	CLA	C1B-NB	-2.21	1.35	1.37
15	a6	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	bJ	102	CLA	CMC-C2C	-2.21	1.46	1.50
15	aA	824	CLA	C1B-C2B	2.21	1.48	1.43
15	aB	829	CLA	C1B-C2B	2.21	1.48	1.43
15	cL	202	CLA	C4B-NB	2.21	1.40	1.37
15	a4	402	CLA	CMD-C2D	-2.21	1.46	1.50
15	aA	816	CLA	C1B-C2B	2.21	1.48	1.43
15	aA	829	CLA	C1B-NB	-2.21	1.35	1.37
15	a2	411	CLA	C1B-NB	-2.21	1.35	1.37
15	cA	802	CLA	C4B-NB	2.21	1.40	1.37
15	a1	409	CLA	MG-ND	-2.21	2.01	2.05
15	a4	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	b4	405	CLA	CMD-C2D	-2.21	1.46	1.50
15	c6	404	CLA	MG-NB	-2.21	2.01	2.05
15	c1	409	CLA	CHC-C1C	2.21	1.43	1.38
15	b3	408	CLA	C1B-C2B	2.21	1.48	1.43
15	c4	407	CLA	C1B-NB	-2.21	1.35	1.37
15	bB	818	CLA	CMB-C2B	-2.21	1.46	1.50
15	a3	415	CLA	C3B-C4B	2.21	1.47	1.42
15	c1	403	CLA	C1B-C2B	2.21	1.48	1.43
15	bA	841	CLA	CMD-C2D	-2.21	1.46	1.50
15	a4	408	CLA	CMC-C2C	-2.21	1.46	1.50
15	c3	404	CLA	CMB-C2B	-2.21	1.46	1.50
15	cB	838	CLA	MG-ND	-2.21	2.01	2.05
15	a4	421	CLA	C1B-NB	-2.21	1.35	1.37
15	bA	845	CLA	C1B-NB	-2.21	1.35	1.37
15	aJ	201	CLA	CMC-C2C	-2.21	1.46	1.50
15	b3	411	CLA	CMD-C2D	-2.21	1.46	1.50
15	c1	409	CLA	CMD-C2D	-2.21	1.46	1.50
15	c4	402	CLA	CMD-C2D	-2.21	1.46	1.50
15	b6	403	CLA	MG-NB	-2.21	2.01	2.05
15	aA	831	CLA	CHC-C4B	-2.21	1.34	1.39
15	bA	802	CLA	C4B-NB	2.21	1.40	1.37
15	a4	410	CLA	MG-ND	-2.21	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b3	411	CLA	CMC-C2C	-2.21	1.46	1.50
15	b5	420	CLA	CMD-C2D	-2.21	1.46	1.50
15	cA	841	CLA	CMD-C2D	-2.21	1.46	1.50
18	cL	205	BCR	C38-C26	-2.21	1.47	1.50
15	bB	829	CLA	C1B-C2B	2.21	1.48	1.43
15	cB	807	CLA	C1B-C2B	2.21	1.48	1.43
15	bB	820	CLA	MG-ND	-2.21	2.01	2.05
15	bB	838	CLA	MG-ND	-2.21	2.01	2.05
15	a3	413	CLA	C1B-NB	-2.21	1.35	1.37
15	bA	805	CLA	C4B-NB	2.21	1.40	1.37
15	cB	818	CLA	CMB-C2B	-2.21	1.46	1.50
15	cB	829	CLA	CMC-C2C	-2.21	1.46	1.50
18	bL	205	BCR	C33-C5	-2.21	1.47	1.50
15	c2	418	CLA	C4D-ND	-2.21	1.34	1.37
15	cA	809	CLA	C1B-NB	-2.21	1.35	1.37
15	aA	829	CLA	MG-ND	-2.21	2.01	2.05
15	c2	403	CLA	MG-ND	-2.21	2.01	2.05
15	aL	203	CLA	CMC-C2C	-2.21	1.46	1.50
15	aA	821	CLA	CAC-C3C	-2.21	1.45	1.51
18	aF	202	BCR	C33-C5	-2.21	1.47	1.50
15	a6	406	CLA	MG-NB	-2.20	2.01	2.05
15	aA	841	CLA	CMC-C2C	-2.20	1.46	1.50
15	b4	413	CLA	CMD-C2D	-2.20	1.46	1.50
15	b1	409	CLA	CMD-C2D	-2.20	1.46	1.50
15	bB	813	CLA	CHC-C1C	2.20	1.43	1.38
15	a4	407	CLA	CMD-C2D	-2.20	1.46	1.50
15	c3	411	CLA	CMC-C2C	-2.20	1.46	1.50
15	c3	403	CLA	C1B-C2B	2.20	1.48	1.43
15	a4	407	CLA	C1B-NB	-2.20	1.35	1.37
15	b6	406	CLA	MG-NB	-2.20	2.01	2.05
15	cA	829	CLA	MG-ND	-2.20	2.01	2.05
15	a1	408	CLA	CMD-C2D	-2.20	1.46	1.50
15	c2	418	CLA	CMC-C2C	-2.20	1.46	1.50
15	c3	411	CLA	CMD-C2D	-2.20	1.46	1.50
15	cB	835	CLA	C1B-C2B	2.20	1.48	1.43
15	b6	405	CLA	CMD-C2D	-2.20	1.46	1.50
15	aB	819	CLA	CMC-C2C	-2.20	1.46	1.50
15	aJ	202	CLA	CMD-C2D	-2.20	1.46	1.50
15	cB	831	CLA	CMC-C2C	-2.20	1.46	1.50
15	aB	813	CLA	CHC-C1C	2.20	1.43	1.38
15	cB	819	CLA	CMC-C2C	-2.20	1.46	1.50
18	cF	204	BCR	C33-C5	-2.20	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aB	809	CLA	C4B-NB	2.20	1.40	1.37
15	c1	403	CLA	MG-ND	-2.20	2.01	2.05
15	c1	410	CLA	MG-ND	-2.20	2.01	2.05
15	a2	413	CLA	CMC-C2C	-2.20	1.46	1.50
15	c2	406	CLA	CMC-C2C	-2.20	1.46	1.50
15	c4	405	CLA	CMD-C2D	-2.20	1.46	1.50
15	bA	834	CLA	CMA-C3A	-2.20	1.48	1.53
15	aB	828	CLA	C1D-ND	2.20	1.40	1.37
15	cA	829	CLA	C1B-NB	-2.20	1.35	1.37
18	a1	421	BCR	C30-C25	-2.20	1.50	1.53
15	aB	813	CLA	CMC-C2C	-2.20	1.46	1.50
15	aB	831	CLA	C3B-C4B	2.20	1.47	1.42
15	a6	410	CLA	CHC-C1C	2.20	1.43	1.38
15	aA	818	CLA	CMB-C2B	-2.20	1.46	1.50
15	c4	404	CLA	CMB-C2B	-2.20	1.46	1.50
15	bA	824	CLA	C1B-C2B	2.20	1.48	1.43
15	cA	836	CLA	CMC-C2C	-2.20	1.46	1.50
15	cB	813	CLA	CMD-C2D	-2.20	1.46	1.50
15	c2	411	CLA	MG-ND	-2.20	2.01	2.05
15	a1	402	CLA	C1B-C2B	2.20	1.48	1.43
15	b5	408	CLA	C1B-C2B	2.20	1.48	1.43
15	b4	407	CLA	C1B-NB	-2.20	1.35	1.37
15	c4	410	CLA	C1B-C2B	2.20	1.48	1.43
15	cA	815	CLA	C1B-C2B	2.20	1.48	1.43
15	aB	838	CLA	MG-ND	-2.20	2.01	2.05
15	a2	422	CLA	C1B-NB	-2.20	1.35	1.37
15	c3	413	CLA	MG-ND	-2.20	2.01	2.05
15	aA	842	CLA	CMB-C2B	-2.19	1.46	1.50
15	cA	824	CLA	CMC-C2C	-2.19	1.46	1.50
15	cA	826	CLA	CMC-C2C	-2.19	1.46	1.50
15	b4	421	CLA	C1B-NB	-2.19	1.35	1.37
15	c1	410	CLA	CMD-C2D	-2.19	1.46	1.50
15	b2	418	CLA	C4D-ND	-2.19	1.34	1.37
15	aB	831	CLA	MG-ND	-2.19	2.01	2.05
15	bB	838	CLA	C3B-C4B	2.19	1.47	1.42
15	aB	818	CLA	CMB-C2B	-2.19	1.46	1.50
15	a3	411	CLA	CMD-C2D	-2.19	1.46	1.50
15	bA	814	CLA	C1B-NB	-2.19	1.35	1.37
15	aB	806	CLA	CMB-C2B	-2.19	1.46	1.50
15	bB	813	CLA	CMC-C2C	-2.19	1.46	1.50
15	c4	413	CLA	CMD-C2D	-2.19	1.46	1.50
15	cA	842	CLA	C1D-ND	2.19	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	410	CLA	MG-ND	-2.19	2.01	2.05
15	a2	410	CLA	CMD-C2D	-2.19	1.46	1.50
15	bA	836	CLA	CMC-C2C	-2.19	1.46	1.50
15	b4	410	CLA	C1B-NB	-2.19	1.35	1.37
15	bJ	101	CLA	CMD-C2D	-2.19	1.46	1.50
15	b6	409	CLA	CMC-C2C	-2.19	1.46	1.50
15	aA	834	CLA	C1D-ND	2.19	1.40	1.37
15	c4	408	CLA	CMC-C2C	-2.19	1.46	1.50
15	c3	411	CLA	MG-ND	-2.19	2.01	2.05
15	c2	410	CLA	CHC-C1C	2.19	1.43	1.38
15	a3	404	CLA	CMD-C2D	-2.19	1.46	1.50
15	bA	827	CLA	CMC-C2C	-2.19	1.46	1.50
15	bB	823	CLA	C1B-NB	-2.19	1.35	1.37
15	cA	844	CLA	C1B-NB	-2.19	1.35	1.37
15	b1	410	CLA	MG-ND	-2.19	2.01	2.05
14	cA	801	CL0	C4D-CHA	2.19	1.46	1.38
15	bB	831	CLA	C3B-C4B	2.19	1.47	1.42
15	aA	836	CLA	CMC-C2C	-2.19	1.46	1.50
15	b6	422	CLA	CMB-C2B	-2.19	1.46	1.50
15	aA	802	CLA	C4B-NB	2.19	1.40	1.37
15	c1	406	CLA	CMC-C2C	-2.19	1.46	1.50
15	bA	821	CLA	CAC-C3C	-2.19	1.45	1.51
15	bA	810	CLA	C1B-C2B	2.19	1.48	1.43
15	bA	829	CLA	CMC-C2C	-2.19	1.46	1.50
15	bB	812	CLA	C1B-C2B	2.19	1.48	1.43
15	bB	808	CLA	CMB-C2B	-2.19	1.46	1.50
15	b1	409	CLA	CHC-C1C	2.19	1.43	1.38
15	c3	410	CLA	C3C-C2C	2.19	1.41	1.36
15	cA	834	CLA	CMA-C3A	-2.19	1.48	1.53
15	c1	410	CLA	C1B-C2B	2.19	1.48	1.43
15	bB	813	CLA	CMD-C2D	-2.19	1.46	1.50
15	bB	831	CLA	CMC-C2C	-2.19	1.46	1.50
15	aB	838	CLA	C3B-C4B	2.19	1.47	1.42
15	b1	410	CLA	C1B-C2B	2.19	1.48	1.43
18	bF	202	BCR	C33-C5	-2.19	1.47	1.50
15	aA	829	CLA	CMC-C2C	-2.19	1.46	1.50
15	b1	406	CLA	CMD-C2D	-2.19	1.46	1.50
15	b5	406	CLA	CMD-C2D	-2.19	1.46	1.50
15	b3	408	CLA	MG-ND	-2.19	2.01	2.05
15	cL	202	CLA	C3B-C4B	2.19	1.47	1.42
15	aB	828	CLA	C1C-NC	-2.19	1.34	1.37
15	aA	821	CLA	CMB-C2B	-2.19	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b5	420	CLA	CMC-C2C	-2.19	1.46	1.50
15	bB	835	CLA	C1B-C2B	2.19	1.48	1.43
15	cA	824	CLA	C1B-C2B	2.19	1.48	1.43
15	cA	831	CLA	CHC-C4B	-2.19	1.34	1.39
15	aA	828	CLA	MG-ND	-2.19	2.01	2.05
15	c6	406	CLA	CMD-C2D	-2.19	1.46	1.50
15	aB	806	CLA	MG-NB	-2.19	2.01	2.05
15	c1	408	CLA	C1B-C2B	2.19	1.48	1.43
15	a4	406	CLA	CMB-C2B	-2.19	1.46	1.50
15	a6	411	CLA	C1B-C2B	2.18	1.48	1.43
15	b2	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	cB	813	CLA	CMC-C2C	-2.18	1.46	1.50
15	a3	403	CLA	C1B-C2B	2.18	1.48	1.43
15	bL	202	CLA	C3B-C4B	2.18	1.47	1.42
15	b1	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	b4	407	CLA	CMB-C2B	-2.18	1.46	1.50
15	aA	827	CLA	CMC-C2C	-2.18	1.46	1.50
15	bB	824	CLA	CMD-C2D	-2.18	1.46	1.50
15	bA	818	CLA	CMB-C2B	-2.18	1.46	1.50
15	cB	838	CLA	C3B-C4B	2.18	1.47	1.42
15	cB	828	CLA	C1C-NC	-2.18	1.34	1.37
15	b1	404	CLA	MG-ND	-2.18	2.01	2.05
15	a4	409	CLA	CHC-C1C	2.18	1.43	1.38
15	aA	810	CLA	C1B-C2B	2.18	1.48	1.43
15	a4	407	CLA	CMB-C2B	-2.18	1.46	1.50
15	a4	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	cF	201	CLA	CMB-C2B	-2.18	1.46	1.50
15	b2	404	CLA	MG-ND	-2.18	2.01	2.05
15	aA	834	CLA	CMA-C3A	-2.18	1.48	1.53
15	c6	413	CLA	C1B-C2B	2.18	1.48	1.43
15	aA	811	CLA	CMC-C2C	-2.18	1.46	1.50
15	a3	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	a5	405	CLA	CMB-C2B	-2.18	1.46	1.50
15	aA	814	CLA	C1B-NB	-2.18	1.35	1.37
15	bB	821	CLA	CMC-C2C	-2.18	1.46	1.50
15	c1	417	CLA	CMD-C2D	-2.18	1.46	1.50
15	bA	811	CLA	CMC-C2C	-2.18	1.46	1.50
15	b3	409	CLA	CMD-C2D	-2.18	1.46	1.50
15	cA	810	CLA	C1B-C2B	2.18	1.48	1.43
15	c3	421	CLA	MG-NA	2.18	2.11	2.06
15	aB	824	CLA	CMD-C2D	-2.18	1.46	1.50
15	cA	814	CLA	C1B-NB	-2.18	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	815	CLA	C1B-C2B	2.18	1.48	1.43
15	b4	415	CLA	C3B-C4B	2.18	1.47	1.42
15	c5	411	CLA	MG-ND	-2.18	2.01	2.05
15	c2	411	CLA	C1B-NB	-2.18	1.35	1.37
15	a4	411	CLA	CMC-C2C	-2.18	1.46	1.50
15	a5	406	CLA	CMB-C2B	-2.18	1.46	1.50
15	bA	821	CLA	CMB-C2B	-2.18	1.46	1.50
15	b5	405	CLA	CMB-C2B	-2.18	1.46	1.50
15	cL	204	CLA	CMC-C2C	-2.18	1.46	1.50
15	bB	804	CLA	C1B-C2B	2.18	1.48	1.43
15	aL	201	CLA	C3B-C4B	2.18	1.47	1.42
15	b3	413	CLA	MG-ND	-2.18	2.01	2.05
15	bL	203	CLA	CMB-C2B	-2.18	1.46	1.50
15	b6	415	CLA	CMD-C2D	-2.18	1.46	1.50
15	b4	409	CLA	CHC-C1C	2.18	1.42	1.38
15	c5	409	CLA	CHC-C1C	2.18	1.42	1.38
15	bA	828	CLA	MG-ND	-2.18	2.01	2.05
15	bA	816	CLA	CMD-C2D	-2.18	1.46	1.50
15	cJ	102	CLA	CMC-C2C	-2.18	1.46	1.50
15	c5	405	CLA	CMB-C2B	-2.18	1.46	1.50
15	c1	417	CLA	C4D-ND	-2.18	1.34	1.37
15	b2	406	CLA	CHC-C1C	2.18	1.42	1.38
15	b3	417	CLA	CMC-C2C	-2.18	1.46	1.50
15	c5	417	CLA	CMC-C2C	-2.18	1.46	1.50
15	bA	826	CLA	CMC-C2C	-2.18	1.46	1.50
15	c5	410	CLA	CMD-C2D	-2.18	1.46	1.50
15	c6	411	CLA	CHC-C1C	2.17	1.42	1.38
15	a5	417	CLA	CMC-C2C	-2.17	1.46	1.50
15	b6	417	CLA	C3B-C4B	2.17	1.47	1.42
15	aB	812	CLA	CMD-C2D	-2.17	1.46	1.50
15	b6	408	CLA	CMD-C2D	-2.17	1.46	1.50
15	c5	420	CLA	CMC-C2C	-2.17	1.46	1.50
15	bL	202	CLA	CMC-C2C	-2.17	1.46	1.50
15	c5	409	CLA	CMD-C2D	-2.17	1.46	1.50
15	bB	826	CLA	MG-ND	-2.17	2.01	2.05
15	bA	815	CLA	C1B-C2B	2.17	1.48	1.43
15	a5	410	CLA	C1B-NB	-2.17	1.35	1.37
15	a2	403	CLA	MG-ND	-2.17	2.01	2.05
15	cA	821	CLA	CAC-C3C	-2.17	1.45	1.51
15	a2	410	CLA	CHC-C1C	2.17	1.42	1.38
15	c1	406	CLA	CMB-C2B	-2.17	1.46	1.50
15	c4	411	CLA	CMC-C2C	-2.17	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b1	404	CLA	CMB-C2B	-2.17	1.46	1.50
15	aA	827	CLA	C3B-C4B	2.17	1.47	1.42
15	cB	824	CLA	C1B-C2B	2.17	1.48	1.43
15	c6	412	CLA	C1B-C2B	2.17	1.48	1.43
18	a4	401	BCR	C33-C5	-2.17	1.47	1.50
15	c5	406	CLA	CMD-C2D	-2.17	1.46	1.50
15	b3	417	CLA	C4D-ND	-2.17	1.34	1.37
15	a4	415	CLA	C3B-C4B	2.17	1.47	1.42
15	a6	408	CLA	CMD-C2D	-2.17	1.46	1.50
15	bA	824	CLA	CMC-C2C	-2.17	1.46	1.50
15	bA	842	CLA	CMB-C2B	-2.17	1.46	1.50
15	a4	410	CLA	C1B-C2B	2.17	1.48	1.43
15	cB	828	CLA	C1D-ND	2.17	1.40	1.37
14	bA	801	CL0	C4D-CHA	2.17	1.46	1.38
15	b2	407	CLA	MG-NB	-2.17	2.01	2.05
15	b3	404	CLA	CMD-C2D	-2.17	1.46	1.50
15	b5	409	CLA	CHC-C1C	2.17	1.42	1.38
15	c2	406	CLA	CHC-C1C	2.17	1.42	1.38
15	aA	824	CLA	CMC-C2C	-2.17	1.46	1.50
15	a1	406	CLA	CMB-C2B	-2.17	1.46	1.50
15	cL	203	CLA	CMB-C2B	-2.17	1.46	1.50
15	cB	802	CLA	CAA-C2A	-2.17	1.50	1.54
15	aB	804	CLA	C1B-C2B	2.17	1.48	1.43
15	b4	410	CLA	C1B-C2B	2.17	1.48	1.43
15	b3	411	CLA	MG-ND	-2.17	2.01	2.05
18	bB	850	BCR	C33-C5	-2.17	1.47	1.50
15	cB	831	CLA	C3B-C4B	2.17	1.47	1.42
15	b5	411	CLA	MG-ND	-2.17	2.01	2.05
15	aA	841	CLA	CMD-C2D	-2.17	1.46	1.50
15	cB	829	CLA	CMB-C2B	-2.17	1.46	1.50
15	b2	403	CLA	MG-ND	-2.17	2.01	2.05
15	b2	405	CLA	CMB-C2B	-2.17	1.46	1.50
15	b4	408	CLA	CMB-C2B	-2.17	1.46	1.50
15	a5	408	CLA	C1B-C2B	2.17	1.48	1.43
18	bL	205	BCR	C38-C26	-2.17	1.47	1.50
15	aB	820	CLA	MG-ND	-2.17	2.01	2.05
15	a2	404	CLA	MG-ND	-2.17	2.01	2.05
15	a3	411	CLA	MG-ND	-2.17	2.01	2.05
15	aB	829	CLA	CMB-C2B	-2.17	1.46	1.50
15	aB	839	CLA	C1B-NB	-2.17	1.35	1.37
15	bA	831	CLA	C1D-ND	2.17	1.40	1.37
15	aB	802	CLA	CAA-C2A	-2.17	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	415	CLA	C3B-C4B	2.17	1.47	1.42
15	c4	415	CLA	C3B-C4B	2.17	1.47	1.42
15	a1	403	CLA	MG-ND	-2.17	2.01	2.05
18	b4	401	BCR	C33-C5	-2.17	1.47	1.50
15	aB	835	CLA	C1B-C2B	2.17	1.48	1.43
15	a1	409	CLA	CMD-C2D	-2.17	1.46	1.50
15	bB	841	CLA	CMC-C2C	-2.17	1.46	1.50
15	bB	807	CLA	C1B-C2B	2.17	1.48	1.43
15	c6	409	CLA	CMD-C2D	-2.17	1.46	1.50
15	c1	417	CLA	CMC-C2C	-2.17	1.46	1.50
18	cB	849	BCR	C33-C5	-2.17	1.47	1.50
15	bA	834	CLA	C1B-C2B	2.17	1.48	1.43
15	bA	839	CLA	C3B-C4B	2.16	1.47	1.42
15	c4	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	a1	412	CLA	C1B-NB	-2.16	1.35	1.37
15	bA	843	CLA	C1D-ND	2.16	1.40	1.37
15	b1	406	CLA	CMC-C2C	-2.16	1.46	1.50
15	a3	408	CLA	MG-ND	-2.16	2.01	2.05
15	a5	411	CLA	MG-ND	-2.16	2.01	2.05
15	a2	406	CLA	CMC-C2C	-2.16	1.46	1.50
15	b3	410	CLA	CMD-C2D	-2.16	1.46	1.50
15	bA	845	CLA	CHC-C1C	2.16	1.42	1.38
15	aB	813	CLA	CMD-C2D	-2.16	1.46	1.50
15	a6	417	CLA	C3B-C4B	2.16	1.47	1.42
15	aB	826	CLA	MG-ND	-2.16	2.01	2.05
15	a3	413	CLA	MG-ND	-2.16	2.01	2.05
15	cA	828	CLA	MG-ND	-2.16	2.01	2.05
15	cB	821	CLA	CMC-C2C	-2.16	1.46	1.50
15	c2	404	CLA	CMD-C2D	-2.16	1.46	1.50
15	b2	422	CLA	CMB-C2B	-2.16	1.46	1.50
15	aA	831	CLA	C4B-NB	2.16	1.40	1.37
15	aA	843	CLA	C1D-ND	2.16	1.40	1.37
15	b2	404	CLA	CMD-C2D	-2.16	1.46	1.50
15	b5	406	CLA	CMB-C2B	-2.16	1.46	1.50
15	c2	404	CLA	MG-ND	-2.16	2.01	2.05
15	cB	839	CLA	CMB-C2B	-2.16	1.46	1.50
15	bB	828	CLA	C1C-NC	-2.16	1.34	1.37
15	aA	815	CLA	CMD-C2D	-2.16	1.46	1.50
15	b3	405	CLA	CMD-C2D	-2.16	1.46	1.50
18	bL	206	BCR	C30-C25	-2.16	1.50	1.53
15	b6	410	CLA	CHC-C1C	2.16	1.42	1.38
15	a6	414	CLA	C1B-NB	-2.16	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aJ	203	CLA	CMC-C2C	-2.16	1.46	1.50
15	aL	202	CLA	CMB-C2B	-2.16	1.46	1.50
15	b3	410	CLA	MG-ND	-2.16	2.01	2.05
15	c6	418	CLA	C3B-C4B	2.16	1.47	1.42
15	aA	808	CLA	CMC-C2C	-2.16	1.46	1.50
15	a4	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	a6	409	CLA	CMB-C2B	-2.16	1.46	1.50
15	aA	831	CLA	C1D-ND	2.16	1.40	1.37
15	cA	834	CLA	C1B-C2B	2.16	1.48	1.43
15	b4	414	CLA	CMD-C2D	-2.16	1.46	1.50
15	cB	841	CLA	CMC-C2C	-2.16	1.46	1.50
15	cA	807	CLA	C4B-NB	2.16	1.40	1.37
15	bL	204	CLA	CMC-C2C	-2.16	1.46	1.50
15	c3	404	CLA	CMD-C2D	-2.16	1.46	1.50
15	c3	410	CLA	C1B-C2B	2.16	1.48	1.43
18	aI	103	BCR	C38-C26	-2.16	1.47	1.50
15	a1	405	CLA	CMD-C2D	-2.16	1.46	1.50
15	b5	417	CLA	CMC-C2C	-2.16	1.46	1.50
15	aB	834	CLA	C1B-NB	-2.16	1.35	1.37
15	aB	827	CLA	C3B-C4B	2.16	1.47	1.42
15	a1	401	CLA	CMB-C2B	-2.16	1.46	1.50
15	cA	811	CLA	CMC-C2C	-2.16	1.46	1.50
15	c4	406	CLA	CMD-C2D	-2.16	1.46	1.50
15	bB	812	CLA	CMD-C2D	-2.15	1.46	1.50
15	c4	421	CLA	C1B-NB	-2.15	1.35	1.37
15	c6	410	CLA	CMB-C2B	-2.15	1.46	1.50
15	cA	828	CLA	CHC-C1C	2.15	1.42	1.38
15	a5	406	CLA	CMD-C2D	-2.15	1.46	1.50
15	cB	812	CLA	CMD-C2D	-2.15	1.46	1.50
15	c4	404	CLA	CMD-C2D	-2.15	1.46	1.50
14	bA	801	CL0	C1B-C2B	2.15	1.48	1.43
15	a6	414	CLA	MG-ND	-2.15	2.01	2.05
15	b1	407	CLA	CMB-C2B	-2.15	1.46	1.50
18	cB	847	BCR	C12-C13	-2.15	1.44	1.50
15	cA	822	CLA	C4B-NB	2.15	1.40	1.37
15	a2	405	CLA	CMB-C2B	-2.15	1.46	1.50
15	c3	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	cA	844	CLA	CHC-C1C	2.15	1.42	1.38
15	cA	836	CLA	C3B-C4B	2.15	1.47	1.42
15	aA	826	CLA	CMC-C2C	-2.15	1.46	1.50
15	a2	418	CLA	CMC-C2C	-2.15	1.46	1.50
15	cA	829	CLA	CMC-C2C	-2.15	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	aA	801	CL0	C4D-CHA	2.15	1.46	1.38
15	b2	406	CLA	CMC-C2C	-2.15	1.46	1.50
15	cB	813	CLA	CHC-C1C	2.15	1.42	1.38
15	c3	405	CLA	CMD-C2D	-2.15	1.46	1.50
15	c4	410	CLA	C1B-NB	-2.15	1.35	1.37
15	a3	417	CLA	C4D-ND	-2.15	1.34	1.37
15	a6	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	cA	808	CLA	CMC-C2C	-2.15	1.46	1.50
15	a1	409	CLA	C1B-C2B	2.15	1.48	1.43
15	cB	831	CLA	MG-ND	-2.15	2.01	2.05
15	c5	406	CLA	CMB-C2B	-2.15	1.46	1.50
15	aA	828	CLA	CHC-C1C	2.15	1.42	1.38
15	cA	831	CLA	C1D-ND	2.15	1.40	1.37
15	b4	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	c1	404	CLA	MG-ND	-2.15	2.01	2.05
15	aA	816	CLA	CMD-C2D	-2.15	1.46	1.50
15	a3	421	CLA	MG-NA	2.15	2.11	2.06
15	cA	816	CLA	MG-ND	-2.15	2.01	2.05
18	cM	101	BCR	C33-C5	-2.15	1.47	1.50
15	a3	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	aA	834	CLA	C1B-C2B	2.15	1.48	1.43
14	cA	801	CL0	C1B-C2B	2.15	1.48	1.43
15	aB	841	CLA	CMC-C2C	-2.15	1.46	1.50
15	c3	408	CLA	MG-ND	-2.15	2.01	2.05
15	c2	422	CLA	C1B-NB	-2.15	1.35	1.37
15	a1	405	CLA	CMC-C2C	-2.15	1.46	1.50
15	bB	818	CLA	CMD-C2D	-2.15	1.46	1.50
15	c4	407	CLA	CMB-C2B	-2.15	1.46	1.50
15	aA	839	CLA	C3B-C4B	2.15	1.47	1.42
15	a2	404	CLA	CMD-C2D	-2.15	1.46	1.50
15	b1	417	CLA	CMC-C2C	-2.15	1.46	1.50
15	b4	405	CLA	CMC-C2C	-2.15	1.46	1.50
15	cA	816	CLA	CMD-C2D	-2.15	1.46	1.50
15	c1	406	CLA	CMD-C2D	-2.15	1.46	1.50
15	a5	410	CLA	CMD-C2D	-2.15	1.46	1.50
15	c1	402	CLA	CMB-C2B	-2.15	1.46	1.50
15	b1	403	CLA	MG-ND	-2.15	2.01	2.05
15	cA	807	CLA	C1D-ND	2.14	1.40	1.37
15	a1	402	CLA	MG-ND	-2.14	2.01	2.05
15	c1	402	CLA	CMD-C2D	-2.14	1.46	1.50
15	c5	404	CLA	MG-ND	-2.14	2.01	2.05
15	bB	834	CLA	C1B-NB	-2.14	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c2	401	BCR	C4-C5	-2.14	1.46	1.51
15	bB	802	CLA	CAA-C2A	-2.14	1.50	1.54
15	aJ	203	CLA	CMD-C2D	-2.14	1.46	1.50
15	cB	818	CLA	CMD-C2D	-2.14	1.46	1.50
18	aB	849	BCR	C33-C5	-2.14	1.47	1.50
15	cB	823	CLA	C1B-NB	-2.14	1.35	1.37
15	aB	831	CLA	CMC-C2C	-2.14	1.46	1.50
15	b6	415	CLA	CMC-C2C	-2.14	1.46	1.50
15	cA	839	CLA	C3B-C4B	2.14	1.47	1.42
18	aB	847	BCR	C12-C13	-2.14	1.44	1.50
15	a4	414	CLA	CMD-C2D	-2.14	1.46	1.50
15	cA	815	CLA	CMD-C2D	-2.14	1.46	1.50
15	c5	420	CLA	CMB-C2B	-2.14	1.46	1.50
15	aA	803	CLA	C4B-NB	2.14	1.40	1.37
15	a2	412	CLA	MG-ND	-2.14	2.01	2.05
15	bB	829	CLA	CMB-C2B	-2.14	1.46	1.50
15	cA	837	CLA	MG-NB	-2.14	2.01	2.05
15	c5	408	CLA	C1B-C2B	2.14	1.48	1.43
15	b4	404	CLA	CMD-C2D	-2.14	1.46	1.50
15	cA	818	CLA	CMB-C2B	-2.14	1.46	1.50
15	cA	827	CLA	CMC-C2C	-2.14	1.46	1.50
15	c6	411	CLA	CMD-C2D	-2.14	1.46	1.50
15	c2	408	CLA	MG-ND	-2.14	2.01	2.05
14	aA	801	CL0	C1B-C2B	2.14	1.48	1.43
15	bB	816	CLA	CMC-C2C	-2.14	1.46	1.50
15	aB	812	CLA	C1B-C2B	2.14	1.48	1.43
15	cB	804	CLA	C1B-C2B	2.14	1.48	1.43
15	b6	413	CLA	C1B-NB	-2.14	1.35	1.37
15	a4	404	CLA	CMD-C2D	-2.14	1.46	1.50
15	b4	403	CLA	MG-ND	-2.14	2.01	2.05
15	cB	826	CLA	MG-ND	-2.14	2.01	2.05
15	b3	421	CLA	MG-NA	2.14	2.11	2.06
15	a3	414	CLA	CMB-C2B	-2.14	1.46	1.50
15	cA	837	CLA	CMC-C2C	-2.14	1.46	1.50
15	cB	812	CLA	C1B-C2B	2.14	1.48	1.43
15	aA	806	CLA	C3B-C4B	2.14	1.47	1.42
15	bB	804	CLA	C4B-NB	2.14	1.40	1.37
15	b2	422	CLA	C1B-NB	-2.14	1.35	1.37
15	b5	404	CLA	MG-ND	-2.14	2.01	2.05
15	a1	416	CLA	CMD-C2D	-2.14	1.46	1.50
15	a6	412	CLA	C1B-C2B	2.14	1.48	1.43
15	c6	409	CLA	MG-ND	-2.14	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a4	406	CLA	CMD-C2D	-2.14	1.46	1.50
15	b4	411	CLA	CMC-C2C	-2.14	1.46	1.50
15	c2	412	CLA	MG-ND	-2.14	2.01	2.05
15	b3	415	CLA	C3B-C4B	2.14	1.47	1.42
15	a6	415	CLA	CMC-C2C	-2.14	1.46	1.50
15	b3	404	CLA	MG-ND	-2.14	2.01	2.05
15	a3	412	CLA	CMD-C2D	-2.14	1.46	1.50
15	a1	410	CLA	CMC-C2C	-2.14	1.46	1.50
15	a4	408	CLA	CMB-C2B	-2.14	1.46	1.50
15	b2	404	CLA	CMB-C2B	-2.14	1.46	1.50
15	c3	410	CLA	MG-ND	-2.14	2.01	2.05
15	cA	806	CLA	C3B-C4B	2.14	1.47	1.42
15	cB	834	CLA	C1B-NB	-2.14	1.35	1.37
15	c1	410	CLA	C1B-NB	-2.14	1.35	1.37
15	a4	403	CLA	MG-ND	-2.13	2.01	2.05
15	c3	414	CLA	CHC-C1C	2.13	1.42	1.38
15	c3	405	CLA	CMC-C2C	-2.13	1.46	1.50
15	bB	833	CLA	C1D-ND	2.13	1.40	1.37
15	a1	405	CLA	CMB-C2B	-2.13	1.46	1.50
15	a5	405	CLA	CMD-C2D	-2.13	1.46	1.50
15	c1	405	CLA	CMB-C2B	-2.13	1.46	1.50
15	c4	411	CLA	CMD-C2D	-2.13	1.46	1.50
15	aB	804	CLA	C4B-NB	2.13	1.40	1.37
15	aB	833	CLA	C1D-ND	2.13	1.40	1.37
15	bA	807	CLA	C4B-NB	2.13	1.40	1.37
15	a5	411	CLA	CMC-C2C	-2.13	1.46	1.50
15	a5	420	CLA	CMB-C2B	-2.13	1.46	1.50
15	cJ	102	CLA	CMD-C2D	-2.13	1.46	1.50
15	c6	408	CLA	CMD-C2D	-2.13	1.46	1.50
18	bB	847	BCR	C12-C13	-2.13	1.44	1.50
15	bA	844	CLA	CMD-C2D	-2.13	1.46	1.50
15	c5	404	CLA	CMD-C2D	-2.13	1.46	1.50
15	bB	827	CLA	C3B-C4B	2.13	1.47	1.42
15	b2	412	CLA	MG-ND	-2.13	2.01	2.05
18	aA	850	BCR	C33-C5	-2.13	1.47	1.50
18	bL	201	BCR	C30-C25	-2.13	1.50	1.53
15	b6	409	CLA	CMB-C2B	-2.13	1.46	1.50
15	c2	414	CLA	C1B-NB	-2.13	1.35	1.37
15	c5	403	CLA	C1B-NB	-2.13	1.35	1.37
15	aA	832	CLA	CMC-C2C	-2.13	1.46	1.50
15	b1	402	CLA	CMB-C2B	-2.13	1.46	1.50
15	b3	412	CLA	CMD-C2D	-2.13	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	406	CLA	CMD-C2D	-2.13	1.46	1.50
15	b4	411	CLA	CMD-C2D	-2.13	1.46	1.50
15	a4	414	CLA	CMB-C2B	-2.13	1.46	1.50
15	bJ	102	CLA	CMD-C2D	-2.13	1.46	1.50
15	b1	402	CLA	CMC-C2C	-2.13	1.46	1.50
15	c5	414	CLA	CMD-C2D	-2.13	1.46	1.50
15	aA	807	CLA	C1D-ND	2.13	1.40	1.37
15	b3	410	CLA	C1B-C2B	2.13	1.48	1.43
15	bB	839	CLA	CMB-C2B	-2.13	1.46	1.50
15	cA	815	CLA	CMB-C2B	-2.13	1.46	1.50
15	aA	815	CLA	CHC-C1C	2.13	1.42	1.38
15	cA	807	CLA	CAC-C3C	-2.13	1.45	1.51
15	aA	807	CLA	C4B-NB	2.13	1.40	1.37
15	c6	413	CLA	MG-ND	-2.13	2.01	2.05
15	aB	827	CLA	C1B-C2B	2.13	1.48	1.43
15	c1	404	CLA	CMB-C2B	-2.13	1.46	1.50
15	c5	411	CLA	CMC-C2C	-2.13	1.46	1.50
19	cA	853	LHG	O8-C6	-2.13	1.40	1.45
15	a1	415	CLA	C3B-C4B	2.13	1.47	1.42
15	aB	838	CLA	C4B-NB	2.13	1.40	1.37
15	a1	411	CLA	CMD-C2D	-2.13	1.46	1.50
15	a4	405	CLA	CMC-C2C	-2.13	1.46	1.50
15	b5	404	CLA	CMB-C2B	-2.13	1.46	1.50
15	b5	414	CLA	CMD-C2D	-2.13	1.46	1.50
18	cB	844	BCR	C33-C5	-2.13	1.47	1.50
15	a3	405	CLA	MG-ND	-2.13	2.01	2.05
15	c4	409	CLA	CHC-C1C	2.13	1.42	1.38
15	a6	403	CLA	CMB-C2B	-2.13	1.46	1.50
15	b1	408	CLA	CMC-C2C	-2.13	1.46	1.50
15	aA	836	CLA	C3B-C4B	2.13	1.47	1.42
15	aB	816	CLA	CMC-C2C	-2.13	1.46	1.50
15	cB	816	CLA	CMB-C2B	-2.13	1.46	1.50
15	cL	202	CLA	CMC-C2C	-2.13	1.46	1.50
15	bA	827	CLA	C3B-C4B	2.13	1.47	1.42
15	cA	827	CLA	C3B-C4B	2.13	1.47	1.42
18	bM	101	BCR	C33-C5	-2.13	1.47	1.50
15	aB	822	CLA	CMD-C2D	-2.13	1.46	1.50
15	aB	838	CLA	CMC-C2C	-2.13	1.46	1.50
15	a1	416	CLA	CMC-C2C	-2.13	1.46	1.50
15	cA	821	CLA	CMD-C2D	-2.13	1.46	1.50
15	a4	411	CLA	CHC-C1C	2.13	1.42	1.38
15	b3	403	CLA	C1B-NB	-2.13	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cJ	101	CLA	MG-ND	-2.13	2.01	2.05
15	b3	414	CLA	CMB-C2B	-2.13	1.46	1.50
15	c4	414	CLA	CMD-C2D	-2.13	1.46	1.50
15	bB	822	CLA	CMD-C2D	-2.13	1.46	1.50
15	c4	408	CLA	CMB-C2B	-2.13	1.46	1.50
18	a6	421	BCR	C4-C5	-2.12	1.46	1.51
15	aB	825	CLA	CMB-C2B	-2.12	1.46	1.50
15	a1	407	CLA	CMB-C2B	-2.12	1.46	1.50
15	bA	808	CLA	CMC-C2C	-2.12	1.46	1.50
15	a6	415	CLA	CMD-C2D	-2.12	1.46	1.50
15	bA	815	CLA	CMD-C2D	-2.12	1.46	1.50
15	bB	814	CLA	CMB-C2B	-2.12	1.46	1.50
15	b5	410	CLA	CMD-C2D	-2.12	1.46	1.50
15	b5	411	CLA	CMC-C2C	-2.12	1.46	1.50
15	cB	827	CLA	C1B-C2B	2.12	1.48	1.43
15	a6	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	c1	414	CLA	CMD-C2D	-2.12	1.46	1.50
15	c3	409	CLA	CMC-C2C	-2.12	1.46	1.50
15	b6	411	CLA	C1B-C2B	2.12	1.48	1.43
15	b3	405	CLA	MG-ND	-2.12	2.01	2.05
15	aB	818	CLA	CMD-C2D	-2.12	1.46	1.50
15	aB	839	CLA	CMB-C2B	-2.12	1.46	1.50
15	bA	815	CLA	CMB-C2B	-2.12	1.46	1.50
15	b1	405	CLA	CMB-C2B	-2.12	1.46	1.50
15	a6	414	CLA	CAC-C3C	-2.12	1.45	1.51
15	bA	806	CLA	C3B-C4B	2.12	1.47	1.42
15	cB	826	CLA	CMC-C2C	-2.12	1.46	1.50
15	c1	404	CLA	CMD-C2D	-2.12	1.46	1.50
15	bJ	101	CLA	MG-ND	-2.12	2.01	2.05
15	c6	414	CLA	C1B-NB	-2.12	1.35	1.37
18	c4	401	BCR	C33-C5	-2.12	1.47	1.50
15	c4	405	CLA	CMC-C2C	-2.12	1.46	1.50
15	bA	816	CLA	MG-ND	-2.12	2.01	2.05
19	cX	101	LHG	P-O6	2.12	1.67	1.59
15	b3	405	CLA	CMC-C2C	-2.12	1.46	1.50
15	b4	402	CLA	CMB-C2B	-2.12	1.46	1.50
15	aA	807	CLA	CAC-C3C	-2.12	1.45	1.51
19	bX	101	LHG	P-O6	2.12	1.67	1.59
15	aA	837	CLA	MG-NB	-2.12	2.01	2.05
15	bB	805	CLA	MG-ND	-2.12	2.01	2.05
15	bA	836	CLA	C3B-C4B	2.12	1.47	1.42
15	b6	403	CLA	CMB-C2B	-2.12	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	816	CLA	CMD-C2D	-2.12	1.46	1.50
15	c1	414	CLA	CMC-C2C	-2.12	1.46	1.50
18	a2	401	BCR	C4-C5	-2.12	1.46	1.51
15	a4	411	CLA	CMD-C2D	-2.12	1.46	1.50
15	c2	410	CLA	CMD-C2D	-2.12	1.46	1.50
15	c5	408	CLA	MG-ND	-2.12	2.01	2.05
15	bB	824	CLA	C1B-C2B	2.12	1.48	1.43
15	cB	827	CLA	C3B-C4B	2.12	1.47	1.42
15	bB	816	CLA	CMB-C2B	-2.12	1.46	1.50
18	aM	101	BCR	C33-C5	-2.12	1.47	1.50
15	aK	102	CLA	CMC-C2C	-2.12	1.46	1.50
15	a3	406	CLA	CMC-C2C	-2.12	1.46	1.50
15	c5	404	CLA	CMB-C2B	-2.12	1.46	1.50
15	b6	412	CLA	MG-ND	-2.12	2.01	2.05
15	c1	407	CLA	CMB-C2B	-2.12	1.46	1.50
15	b4	411	CLA	CHC-C1C	2.12	1.42	1.38
19	aX	101	LHG	P-O6	2.12	1.67	1.59
15	b5	420	CLA	CMB-C2B	-2.12	1.46	1.50
15	bB	838	CLA	CMC-C2C	-2.12	1.46	1.50
15	c1	408	CLA	CMC-C2C	-2.12	1.46	1.50
18	aI	102	BCR	C34-C9	-2.12	1.46	1.50
15	a6	412	CLA	MG-ND	-2.12	2.01	2.05
15	c4	413	CLA	MG-ND	-2.12	2.01	2.05
15	b1	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	a6	408	CLA	MG-ND	-2.12	2.01	2.05
15	cB	805	CLA	MG-ND	-2.12	2.01	2.05
15	a5	414	CLA	CMC-C2C	-2.12	1.46	1.50
15	b5	414	CLA	CMB-C2B	-2.12	1.46	1.50
15	bA	803	CLA	CAC-C3C	-2.12	1.45	1.51
15	bA	825	CLA	C1B-NB	-2.12	1.35	1.37
15	b4	412	CLA	CMD-C2D	-2.12	1.46	1.50
15	b5	407	CLA	CMD-C2D	-2.12	1.46	1.50
15	cB	837	CLA	C4B-NB	2.11	1.40	1.37
15	aA	821	CLA	CMD-C2D	-2.11	1.46	1.50
15	a1	404	CLA	CMB-C2B	-2.11	1.46	1.50
15	b2	408	CLA	MG-ND	-2.11	2.01	2.05
15	aB	824	CLA	C1B-C2B	2.11	1.48	1.43
15	bA	828	CLA	CHC-C1C	2.11	1.42	1.38
15	b3	407	CLA	CMC-C2C	-2.11	1.46	1.50
18	cI	102	BCR	C34-C9	-2.11	1.46	1.50
18	aL	205	BCR	C30-C25	-2.11	1.50	1.53
18	cA	849	BCR	C33-C5	-2.11	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	415	CLA	CHC-C1C	2.11	1.42	1.38
15	cB	823	CLA	CMB-C2B	-2.11	1.46	1.50
15	a5	404	CLA	MG-ND	-2.11	2.01	2.05
15	c6	416	CLA	CMD-C2D	-2.11	1.46	1.50
15	b3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	cB	816	CLA	MG-ND	-2.11	2.01	2.05
15	aA	826	CLA	C1B-C2B	2.11	1.48	1.43
15	b5	413	CLA	MG-ND	-2.11	2.01	2.05
15	bA	818	CLA	C1B-C2B	2.11	1.48	1.43
15	a3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	b3	410	CLA	C3C-C2C	2.11	1.41	1.36
15	bA	807	CLA	CAC-C3C	-2.11	1.45	1.51
15	cB	816	CLA	CMC-C2C	-2.11	1.46	1.50
15	bA	837	CLA	MG-NB	-2.11	2.01	2.05
15	bA	829	CLA	CMB-C2B	-2.11	1.46	1.50
15	b1	414	CLA	CMD-C2D	-2.11	1.46	1.50
15	cA	832	CLA	CMC-C2C	-2.11	1.46	1.50
15	c5	414	CLA	CMB-C2B	-2.11	1.46	1.50
15	b4	414	CLA	CMB-C2B	-2.11	1.46	1.50
15	aA	802	CLA	C5-C3	-2.11	1.46	1.51
15	a2	406	CLA	CHC-C1C	2.11	1.42	1.38
15	a5	403	CLA	MG-ND	-2.11	2.01	2.05
18	aA	851	BCR	C10-C9	-2.11	1.33	1.35
15	b2	411	CLA	CMD-C2D	-2.11	1.46	1.50
15	cB	822	CLA	CMD-C2D	-2.11	1.46	1.50
15	aB	816	CLA	MG-ND	-2.11	2.01	2.05
15	aA	837	CLA	CMC-C2C	-2.11	1.46	1.50
15	b3	405	CLA	CMB-C2B	-2.11	1.46	1.50
15	c1	403	CLA	C1B-NB	-2.11	1.35	1.37
15	b1	408	CLA	CMB-C2B	-2.11	1.46	1.50
15	c6	404	CLA	CMB-C2B	-2.11	1.46	1.50
15	a1	413	CLA	CMC-C2C	-2.11	1.46	1.50
15	aA	803	CLA	CAC-C3C	-2.11	1.45	1.51
15	c3	416	CLA	C1C-NC	-2.11	1.34	1.37
15	aA	844	CLA	CMD-C2D	-2.11	1.46	1.50
15	bB	816	CLA	CMD-C2D	-2.11	1.46	1.50
15	bB	826	CLA	CMC-C2C	-2.11	1.46	1.50
15	c3	412	CLA	CMD-C2D	-2.11	1.46	1.50
15	aA	816	CLA	MG-ND	-2.11	2.01	2.05
18	b6	401	BCR	C4-C5	-2.11	1.46	1.51
15	a6	422	CLA	C1B-NB	-2.11	1.35	1.37
15	b1	406	CLA	CMB-C2B	-2.11	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b2	412	CLA	CMD-C2D	-2.11	1.46	1.50
15	aA	845	CLA	CHC-C1C	2.11	1.42	1.38
15	bB	815	CLA	CHC-C1C	2.11	1.42	1.38
15	b6	410	CLA	CMD-C2D	-2.11	1.46	1.50
15	c5	403	CLA	MG-ND	-2.11	2.01	2.05
15	cA	803	CLA	CAC-C3C	-2.11	1.45	1.51
15	c6	419	CLA	C4D-ND	-2.11	1.34	1.37
15	b2	413	CLA	CMD-C2D	-2.11	1.46	1.50
15	c3	414	CLA	CMC-C2C	-2.11	1.46	1.50
15	bB	827	CLA	C1B-C2B	2.11	1.48	1.43
15	aA	824	CLA	MG-ND	-2.11	2.01	2.05
15	a5	407	CLA	MG-ND	-2.11	2.01	2.05
15	cK	102	CLA	CMC-C2C	-2.11	1.46	1.50
15	c4	414	CLA	CMB-C2B	-2.11	1.46	1.50
19	bA	855	LHG	O8-C6	-2.11	1.40	1.45
15	bA	819	CLA	C1B-C2B	2.10	1.48	1.43
15	bA	807	CLA	C1D-ND	2.10	1.40	1.37
18	bI	102	BCR	C34-C9	-2.10	1.46	1.50
15	a1	416	CLA	C4D-ND	-2.10	1.34	1.37
15	bA	815	CLA	CHC-C1C	2.10	1.42	1.38
15	a4	404	CLA	MG-ND	-2.10	2.01	2.05
15	c4	404	CLA	MG-ND	-2.10	2.01	2.05
15	bA	814	CLA	C1B-C2B	2.10	1.48	1.43
15	b6	412	CLA	C1B-C2B	2.10	1.48	1.43
15	a3	405	CLA	CMD-C2D	-2.10	1.46	1.50
15	a6	422	CLA	CMC-C2C	-2.10	1.46	1.50
15	aA	830	CLA	C3B-C4B	2.10	1.47	1.42
15	b3	414	CLA	CHC-C1C	2.10	1.42	1.38
15	b4	413	CLA	MG-ND	-2.10	2.01	2.05
15	aB	816	CLA	CMD-C2D	-2.10	1.46	1.50
15	b3	406	CLA	CMD-C2D	-2.10	1.46	1.50
15	aA	815	CLA	CMB-C2B	-2.10	1.46	1.50
15	aB	814	CLA	CMB-C2B	-2.10	1.46	1.50
15	a1	401	CLA	CMD-C2D	-2.10	1.46	1.50
18	bA	848	BCR	C33-C5	-2.10	1.47	1.50
15	c6	417	CLA	MG-ND	-2.10	2.01	2.05
15	bA	832	CLA	CMC-C2C	-2.10	1.46	1.50
15	bB	838	CLA	C4B-NB	2.10	1.40	1.37
15	a1	403	CLA	CMB-C2B	-2.10	1.46	1.50
15	a1	413	CLA	CMD-C2D	-2.10	1.46	1.50
15	c5	406	CLA	CMC-C2C	-2.10	1.46	1.50
15	a3	410	CLA	C1B-C2B	2.10	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	803	CLA	C3B-C4B	2.10	1.47	1.42
15	cA	815	CLA	CHC-C1C	2.10	1.42	1.38
15	cX	102	CLA	CMC-C2C	-2.10	1.46	1.50
15	a6	408	CLA	CMB-C2B	-2.10	1.46	1.50
15	bA	821	CLA	CMD-C2D	-2.10	1.46	1.50
15	c4	402	CLA	CMB-C2B	-2.10	1.46	1.50
15	a5	408	CLA	MG-ND	-2.10	2.01	2.05
15	b1	410	CLA	C1B-NB	-2.10	1.35	1.37
15	b6	408	CLA	CMB-C2B	-2.10	1.46	1.50
15	aA	829	CLA	CMB-C2B	-2.10	1.46	1.50
15	aB	823	CLA	CMB-C2B	-2.10	1.46	1.50
15	a3	407	CLA	CMC-C2C	-2.10	1.46	1.50
15	a5	413	CLA	MG-ND	-2.10	2.01	2.05
15	cA	814	CLA	C1B-C2B	2.10	1.48	1.43
15	a5	404	CLA	CMB-C2B	-2.10	1.46	1.50
15	b1	411	CLA	CMC-C2C	-2.10	1.46	1.50
15	b5	414	CLA	CMC-C2C	-2.10	1.46	1.50
15	c1	407	CLA	CMD-C2D	-2.10	1.46	1.50
15	aA	845	CLA	MG-ND	-2.10	2.01	2.05
15	bA	826	CLA	C1B-C2B	2.10	1.48	1.43
15	cA	819	CLA	C1B-NB	-2.10	1.35	1.37
15	a3	410	CLA	C3C-C2C	2.10	1.41	1.36
15	c1	412	CLA	CHC-C4B	-2.10	1.34	1.39
15	cA	843	CLA	CMD-C2D	-2.10	1.46	1.50
15	c2	413	CLA	CMD-C2D	-2.10	1.46	1.50
15	c5	409	CLA	CMB-C2B	-2.10	1.46	1.50
15	aB	833	CLA	CHC-C1C	2.10	1.42	1.38
15	bA	845	CLA	MG-ND	-2.10	2.01	2.05
15	cA	803	CLA	C4B-NB	2.10	1.40	1.37
15	a1	407	CLA	CMC-C2C	-2.10	1.46	1.50
15	bA	824	CLA	MG-ND	-2.10	2.01	2.05
15	a4	402	CLA	CMB-C2B	-2.10	1.46	1.50
15	c3	417	CLA	CMC-C2C	-2.10	1.46	1.50
15	aB	815	CLA	CHC-C1C	2.10	1.42	1.38
15	bB	816	CLA	MG-ND	-2.10	2.01	2.05
15	b4	414	CLA	CMC-C2C	-2.10	1.46	1.50
15	a2	408	CLA	MG-ND	-2.10	2.01	2.05
18	a6	401	BCR	C4-C5	-2.10	1.46	1.51
15	cK	102	CLA	CMB-C2B	-2.10	1.46	1.50
18	aB	845	BCR	C38-C26	-2.10	1.47	1.50
15	c1	411	CLA	CMD-C2D	-2.09	1.46	1.50
15	c3	409	CLA	CMB-C2B	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	421	CLA	CMC-C2C	-2.09	1.46	1.50
15	bA	822	CLA	C4B-NB	2.09	1.40	1.37
15	cA	815	CLA	C1B-NB	-2.09	1.35	1.37
15	aA	818	CLA	C1B-C2B	2.09	1.48	1.43
15	a5	410	CLA	C1B-C2B	2.09	1.48	1.43
15	aB	806	CLA	CHC-C4B	-2.09	1.34	1.39
15	cB	814	CLA	CMB-C2B	-2.09	1.46	1.50
15	c6	416	CLA	CMC-C2C	-2.09	1.46	1.50
18	aB	844	BCR	C33-C5	-2.09	1.47	1.50
15	aB	818	CLA	MG-ND	-2.09	2.01	2.05
15	a3	421	CLA	CMC-C2C	-2.09	1.46	1.50
15	c3	407	CLA	CMC-C2C	-2.09	1.46	1.50
18	b1	401	BCR	C4-C5	-2.09	1.46	1.51
18	cB	848	BCR	C38-C26	-2.09	1.47	1.50
15	b6	416	CLA	MG-ND	-2.09	2.01	2.05
15	cA	803	CLA	C3B-C4B	2.09	1.47	1.42
15	b5	420	CLA	CHC-C1C	2.09	1.42	1.38
18	bB	845	BCR	C38-C26	-2.09	1.47	1.50
15	a5	402	CLA	CMC-C2C	-2.09	1.46	1.50
15	a6	418	CLA	CMC-C2C	-2.09	1.46	1.50
15	b2	415	CLA	CMD-C2D	-2.09	1.46	1.50
15	cB	825	CLA	CMB-C2B	-2.09	1.46	1.50
18	b2	401	BCR	C4-C5	-2.09	1.46	1.51
15	bA	821	CLA	C3B-C4B	2.09	1.47	1.42
15	b5	404	CLA	CMD-C2D	-2.09	1.46	1.50
15	c1	411	CLA	CMC-C2C	-2.09	1.46	1.50
15	c3	414	CLA	CMB-C2B	-2.09	1.46	1.50
15	c6	413	CLA	CMD-C2D	-2.09	1.46	1.50
15	b6	414	CLA	CAC-C3C	-2.09	1.45	1.51
15	bA	830	CLA	C3B-C4B	2.09	1.47	1.42
15	a2	413	CLA	CMD-C2D	-2.09	1.46	1.50
15	bL	203	CLA	C4B-NB	2.09	1.40	1.37
15	a4	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	aL	201	CLA	CMC-C2C	-2.09	1.46	1.50
15	cB	838	CLA	CMC-C2C	-2.09	1.46	1.50
15	c1	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	cL	203	CLA	C4B-NB	2.09	1.40	1.37
15	c3	403	CLA	C1B-NB	-2.09	1.35	1.37
15	bB	803	CLA	C3B-C4B	2.09	1.47	1.42
15	aA	814	CLA	C1B-C2B	2.09	1.48	1.43
15	c2	408	CLA	CMC-C2C	-2.09	1.46	1.50
15	c5	405	CLA	CMD-C2D	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	806	CLA	CHC-C4B	-2.09	1.34	1.39
15	a5	414	CLA	CMD-C2D	-2.09	1.46	1.50
15	c4	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	bA	837	CLA	CMC-C2C	-2.09	1.46	1.50
15	c3	407	CLA	CMB-C2B	-2.09	1.46	1.50
15	c1	416	CLA	C1C-NC	-2.09	1.34	1.37
15	a3	403	CLA	C1B-NB	-2.09	1.35	1.37
15	a4	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	bB	825	CLA	CMB-C2B	-2.09	1.46	1.50
15	cA	818	CLA	C1B-C2B	2.09	1.48	1.43
15	b5	403	CLA	MG-ND	-2.09	2.01	2.05
15	b3	409	CLA	CMB-C2B	-2.09	1.46	1.50
15	bA	802	CLA	C5-C3	-2.09	1.46	1.51
18	c6	402	BCR	C4-C5	-2.09	1.46	1.51
15	a2	415	CLA	CMD-C2D	-2.09	1.46	1.50
15	cA	829	CLA	CMB-C2B	-2.09	1.46	1.50
18	b5	401	BCR	C4-C5	-2.09	1.46	1.51
15	b3	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	bB	805	CLA	C3B-C4B	2.09	1.47	1.42
15	a5	404	CLA	CMD-C2D	-2.09	1.46	1.50
15	a6	413	CLA	CMD-C2D	-2.09	1.46	1.50
19	bA	854	LHG	O6-C4	-2.09	1.36	1.44
15	bA	803	CLA	C1D-ND	2.09	1.40	1.37
15	cB	838	CLA	C4B-NB	2.09	1.40	1.37
15	c5	420	CLA	CHC-C1C	2.09	1.42	1.38
15	c4	414	CLA	CMC-C2C	-2.09	1.46	1.50
15	c5	420	CLA	C2A-C1A	2.09	1.56	1.52
15	c4	403	CLA	MG-ND	-2.09	2.01	2.05
15	bA	810	CLA	CMC-C2C	-2.09	1.46	1.50
15	b6	412	CLA	CMD-C2D	-2.09	1.46	1.50
15	b1	414	CLA	CMB-C2B	-2.09	1.46	1.50
15	a5	414	CLA	CMB-C2B	-2.08	1.46	1.50
15	c4	417	CLA	CMD-C2D	-2.08	1.46	1.50
15	cA	830	CLA	C3B-C4B	2.08	1.47	1.42
15	b6	405	CLA	CMB-C2B	-2.08	1.46	1.50
15	c4	411	CLA	CHC-C1C	2.08	1.42	1.38
15	aB	805	CLA	MG-ND	-2.08	2.01	2.05
15	bA	803	CLA	C4B-NB	2.08	1.40	1.37
15	cA	811	CLA	C1B-NB	-2.08	1.35	1.37
15	aK	102	CLA	CMB-C2B	-2.08	1.46	1.50
15	cB	815	CLA	CHC-C1C	2.08	1.42	1.38
18	cK	101	BCR	C33-C5	-2.08	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	805	CLA	C3B-C4B	2.08	1.47	1.42
15	a6	422	CLA	C4D-CHA	2.08	1.45	1.38
15	a1	410	CLA	CHC-C1C	2.08	1.42	1.38
15	cA	815	CLA	MG-ND	-2.08	2.01	2.05
15	b6	418	CLA	CMC-C2C	-2.08	1.46	1.50
15	c5	407	CLA	CMD-C2D	-2.08	1.46	1.50
15	c6	414	CLA	CMD-C2D	-2.08	1.46	1.50
15	aA	819	CLA	C1B-C2B	2.08	1.48	1.43
15	bB	818	CLA	C1B-C2B	2.08	1.48	1.43
15	aA	819	CLA	MG-ND	-2.08	2.01	2.05
15	a1	409	CLA	C1B-NB	-2.08	1.35	1.37
15	a5	420	CLA	CHC-C1C	2.08	1.42	1.38
15	b5	410	CLA	C1B-C2B	2.08	1.48	1.43
15	bB	811	CLA	CAC-C3C	-2.08	1.45	1.51
15	b4	417	CLA	CMD-C2D	-2.08	1.46	1.50
15	cA	835	CLA	C1B-C2B	2.08	1.48	1.43
16	bB	843	PQN	C9-C10	-2.08	1.36	1.39
15	cA	821	CLA	C3B-C4B	2.08	1.47	1.42
15	aA	811	CLA	MG-ND	-2.08	2.01	2.05
15	cA	844	CLA	MG-ND	-2.08	2.01	2.05
15	bB	815	CLA	C1B-C2B	2.08	1.48	1.43
15	aA	819	CLA	C1B-NB	-2.08	1.35	1.37
15	bA	815	CLA	MG-ND	-2.08	2.01	2.05
15	bA	819	CLA	MG-ND	-2.08	2.01	2.05
15	aB	818	CLA	C1B-C2B	2.08	1.48	1.43
15	bB	801	CLA	C3B-C4B	2.08	1.47	1.42
15	a5	409	CLA	CMC-C2C	-2.08	1.46	1.50
15	cA	810	CLA	CMC-C2C	-2.08	1.46	1.50
15	c3	415	CLA	O2A-CGA	2.08	1.37	1.30
19	cA	852	LHG	O6-C4	-2.08	1.36	1.44
15	cA	824	CLA	C1B-NB	-2.08	1.35	1.37
18	bB	844	BCR	C33-C5	-2.08	1.47	1.50
15	cA	824	CLA	MG-ND	-2.08	2.01	2.05
15	cB	811	CLA	CAC-C3C	-2.08	1.45	1.51
15	a3	408	CLA	CMB-C2B	-2.08	1.46	1.50
15	a4	417	CLA	CMD-C2D	-2.08	1.46	1.50
15	a2	409	CLA	MG-ND	-2.08	2.01	2.05
15	aB	815	CLA	C1B-C2B	2.08	1.48	1.43
15	aB	803	CLA	C3B-C4B	2.08	1.47	1.42
15	aA	840	CLA	CMC-C2C	-2.08	1.46	1.50
15	cB	833	CLA	CHC-C1C	2.08	1.42	1.38
15	aB	826	CLA	CMC-C2C	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	409	CLA	C1B-C2B	2.08	1.48	1.43
15	a2	404	CLA	CMB-C2B	-2.08	1.46	1.50
15	a2	407	CLA	CMD-C2D	-2.08	1.46	1.50
15	a3	407	CLA	CMB-C2B	-2.08	1.46	1.50
15	bB	823	CLA	CMB-C2B	-2.08	1.46	1.50
15	cB	818	CLA	C1B-C2B	2.08	1.48	1.43
15	a3	405	CLA	CMB-C2B	-2.07	1.46	1.50
15	b2	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	b2	411	CLA	C1B-NB	-2.07	1.35	1.37
15	cB	833	CLA	C1D-ND	2.07	1.40	1.37
19	aA	853	LHG	O6-C4	-2.07	1.36	1.44
15	b5	409	CLA	CMB-C2B	-2.07	1.46	1.50
15	b6	407	CLA	CMC-C2C	-2.07	1.46	1.50
19	aA	854	LHG	O8-C6	-2.07	1.40	1.45
15	a5	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	c5	407	CLA	MG-ND	-2.07	2.01	2.05
15	aA	838	CLA	C1C-NC	-2.07	1.34	1.37
15	aA	833	CLA	CAC-C3C	-2.07	1.45	1.51
15	aX	102	CLA	CMC-C2C	-2.07	1.46	1.50
15	c6	419	CLA	CMC-C2C	-2.07	1.46	1.50
15	a5	414	CLA	CHC-C1C	2.07	1.42	1.38
15	a5	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	b6	407	CLA	CMD-C2D	-2.07	1.46	1.50
15	cA	814	CLA	CMB-C2B	-2.07	1.46	1.50
15	b6	418	CLA	C4D-ND	-2.07	1.34	1.37
15	cB	819	CLA	C1B-C2B	2.07	1.48	1.43
15	c2	404	CLA	CMC-C2C	-2.07	1.46	1.50
15	a6	418	CLA	C4D-ND	-2.07	1.34	1.37
15	b1	417	CLA	C4D-ND	-2.07	1.34	1.37
15	bB	833	CLA	CHC-C1C	2.07	1.42	1.38
15	b5	407	CLA	MG-ND	-2.07	2.01	2.05
15	b6	405	CLA	MG-ND	-2.07	2.01	2.05
15	b3	421	CLA	CMC-C2C	-2.07	1.46	1.50
15	c5	414	CLA	CHC-C1C	2.07	1.42	1.38
15	aA	835	CLA	C1B-C2B	2.07	1.48	1.43
15	aB	809	CLA	C1B-C2B	2.07	1.48	1.43
15	b3	407	CLA	CMB-C2B	-2.07	1.46	1.50
18	aB	848	BCR	C38-C26	-2.07	1.47	1.50
15	b5	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	c1	408	CLA	CMB-C2B	-2.07	1.46	1.50
15	bA	811	CLA	C1B-NB	-2.07	1.35	1.37
15	cA	826	CLA	C1B-C2B	2.07	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a3	413	CLA	CMD-C2D	-2.07	1.46	1.50
15	c1	413	CLA	CMD-C2D	-2.07	1.46	1.50
15	c2	404	CLA	CMB-C2B	-2.07	1.46	1.50
18	aA	848	BCR	C38-C26	-2.07	1.47	1.50
15	aB	814	CLA	C4B-NB	2.07	1.40	1.37
15	aB	805	CLA	C3B-C4B	2.07	1.47	1.42
15	a2	412	CLA	CMD-C2D	-2.07	1.46	1.50
15	b6	408	CLA	MG-ND	-2.07	2.01	2.05
15	bA	835	CLA	C1B-C2B	2.07	1.48	1.43
15	bK	101	CLA	CMC-C2C	-2.07	1.46	1.50
15	b3	406	CLA	CMC-C2C	-2.07	1.46	1.50
15	a6	414	CLA	CMD-C2D	-2.07	1.46	1.50
15	bA	825	CLA	CMC-C2C	-2.07	1.46	1.50
15	cA	819	CLA	C1B-C2B	2.07	1.48	1.43
18	aK	101	BCR	C33-C5	-2.07	1.47	1.50
18	cF	205	BCR	C38-C26	-2.07	1.47	1.50
15	aB	816	CLA	CMB-C2B	-2.07	1.46	1.50
15	a5	402	CLA	CMB-C2B	-2.07	1.46	1.50
15	bA	837	CLA	C1B-C2B	2.07	1.48	1.43
15	aA	836	CLA	C1B-C2B	2.07	1.48	1.43
15	bB	809	CLA	C1B-C2B	2.07	1.48	1.43
15	bX	102	CLA	CMC-C2C	-2.07	1.46	1.50
15	c6	406	CLA	CMB-C2B	-2.07	1.46	1.50
15	a3	404	CLA	MG-ND	-2.07	2.01	2.05
15	bB	819	CLA	C1B-C2B	2.07	1.48	1.43
15	aB	819	CLA	C1B-C2B	2.07	1.48	1.43
15	b6	422	CLA	CMC-C2C	-2.07	1.46	1.50
15	a1	411	CLA	CHC-C4B	-2.07	1.34	1.39
15	a4	411	CLA	C1B-C2B	2.07	1.48	1.43
15	c6	410	CLA	C1B-C2B	2.07	1.48	1.43
15	c5	413	CLA	MG-ND	-2.07	2.01	2.05
15	c6	416	CLA	CHC-C1C	2.07	1.42	1.38
15	c5	414	CLA	CMC-C2C	-2.07	1.46	1.50
15	aA	808	CLA	C1B-NB	-2.07	1.35	1.37
15	aA	815	CLA	C1B-NB	-2.07	1.35	1.37
15	cA	802	CLA	C1D-ND	2.07	1.40	1.37
15	cB	830	CLA	C4B-NB	2.07	1.40	1.37
18	aF	203	BCR	C33-C5	-2.07	1.47	1.50
15	aA	845	CLA	CMC-C2C	-2.07	1.46	1.50
15	a6	412	CLA	CMD-C2D	-2.07	1.46	1.50
15	aB	811	CLA	CAC-C3C	-2.07	1.45	1.51
15	aA	814	CLA	CMB-C2B	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c5	401	BCR	C4-C5	-2.06	1.46	1.51
15	b1	403	CLA	C1B-NB	-2.06	1.35	1.37
15	c2	403	CLA	CHC-C1C	2.06	1.42	1.38
15	c6	409	CLA	CMB-C2B	-2.06	1.46	1.50
15	b3	409	CLA	CMC-C2C	-2.06	1.46	1.50
15	b4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	aA	825	CLA	C1B-NB	-2.06	1.35	1.37
15	cA	844	CLA	CMC-C2C	-2.06	1.46	1.50
15	b2	409	CLA	MG-ND	-2.06	2.01	2.05
15	aB	807	CLA	CAC-C3C	-2.06	1.45	1.51
18	cA	850	BCR	C10-C9	-2.06	1.33	1.35
15	cB	840	CLA	C3B-C4B	2.06	1.47	1.42
15	a6	405	CLA	CMB-C2B	-2.06	1.46	1.50
15	c3	402	CLA	CMB-C2B	-2.06	1.46	1.50
15	b6	409	CLA	MG-ND	-2.06	2.01	2.05
15	bB	819	CLA	C3B-C4B	2.06	1.47	1.42
15	aJ	202	CLA	MG-ND	-2.06	2.01	2.05
18	cF	202	BCR	C38-C26	-2.06	1.47	1.50
15	aB	828	CLA	C3B-C4B	2.06	1.47	1.42
15	bJ	101	CLA	CMC-C2C	-2.06	1.46	1.50
15	b1	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c6	412	CLA	CMD-C2D	-2.06	1.46	1.50
15	cB	806	CLA	CHC-C4B	-2.06	1.34	1.39
15	b3	402	CLA	CMB-C2B	-2.06	1.46	1.50
15	c3	406	CLA	CMD-C2D	-2.06	1.46	1.50
15	c5	410	CLA	C1B-C2B	2.06	1.48	1.43
15	cA	834	CLA	CAA-C2A	-2.06	1.50	1.54
18	bA	849	BCR	C38-C26	-2.06	1.47	1.50
15	aJ	202	CLA	CMC-C2C	-2.06	1.46	1.50
15	c6	408	CLA	CMC-C2C	-2.06	1.46	1.50
15	a1	413	CLA	CHC-C1C	2.06	1.42	1.38
15	a6	409	CLA	MG-ND	-2.06	2.01	2.05
15	b4	404	CLA	MG-ND	-2.06	2.01	2.05
15	bA	819	CLA	C1B-NB	-2.06	1.35	1.37
15	cB	804	CLA	C4B-NB	2.06	1.40	1.37
15	c2	416	CLA	O2A-CGA	2.06	1.37	1.30
15	b2	403	CLA	CHC-C1C	2.06	1.42	1.38
15	b5	408	CLA	MG-ND	-2.06	2.01	2.05
15	cB	819	CLA	CMB-C2B	-2.06	1.46	1.50
18	bA	852	BCR	C33-C5	-2.06	1.47	1.50
15	c3	405	CLA	MG-ND	-2.06	2.01	2.05
15	c2	409	CLA	MG-ND	-2.06	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	bA	851	BCR	C33-C5	-2.06	1.47	1.50
15	cA	838	CLA	C1C-NC	-2.06	1.34	1.37
15	c2	412	CLA	CMD-C2D	-2.06	1.46	1.50
15	aB	801	CLA	C3B-C4B	2.06	1.47	1.42
15	aA	815	CLA	MG-ND	-2.06	2.01	2.05
15	c1	407	CLA	MG-ND	-2.06	2.01	2.05
15	b1	412	CLA	CMD-C2D	-2.06	1.46	1.50
15	c2	407	CLA	CMD-C2D	-2.06	1.46	1.50
15	c2	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	a4	406	CLA	CMC-C2C	-2.06	1.46	1.50
15	b5	405	CLA	CMD-C2D	-2.06	1.46	1.50
15	c1	402	CLA	CMC-C2C	-2.06	1.46	1.50
15	bA	808	CLA	C1B-NB	-2.06	1.35	1.37
15	cA	825	CLA	C1B-NB	-2.06	1.35	1.37
18	aA	851	BCR	C33-C5	-2.06	1.47	1.50
15	a3	409	CLA	CMC-C2C	-2.06	1.46	1.50
15	b6	411	CLA	CMD-C2D	-2.06	1.46	1.50
15	c4	421	CLA	CMC-C2C	-2.06	1.46	1.50
15	c5	405	CLA	CMC-C2C	-2.06	1.46	1.50
15	aJ	203	CLA	MG-ND	-2.06	2.01	2.05
15	a1	406	CLA	CMD-C2D	-2.06	1.46	1.50
15	bA	845	CLA	C1B-C2B	2.06	1.48	1.43
15	bA	839	CLA	CHC-C4B	-2.06	1.34	1.39
15	a4	407	CLA	CMC-C2C	-2.06	1.46	1.50
15	b2	408	CLA	CMC-C2C	-2.06	1.46	1.50
15	aB	819	CLA	CMB-C2B	-2.06	1.46	1.50
15	bA	814	CLA	CMB-C2B	-2.06	1.46	1.50
15	a2	412	CLA	O2A-CGA	2.06	1.37	1.30
15	a3	402	CLA	CMB-C2B	-2.06	1.46	1.50
15	b6	413	CLA	CMD-C2D	-2.06	1.46	1.50
15	c3	405	CLA	CMB-C2B	-2.06	1.46	1.50
15	a6	416	CLA	MG-ND	-2.06	2.01	2.05
15	c4	421	CLA	C4D-CHA	2.06	1.45	1.38
15	a6	407	CLA	CMC-C2C	-2.06	1.46	1.50
15	c5	402	CLA	CMB-C2B	-2.06	1.46	1.50
15	b4	404	CLA	CMC-C2C	-2.05	1.46	1.50
15	c2	415	CLA	CMD-C2D	-2.05	1.46	1.50
15	a5	403	CLA	C1B-NB	-2.05	1.35	1.37
15	bK	101	CLA	CMB-C2B	-2.05	1.46	1.50
15	cJ	101	CLA	CMC-C2C	-2.05	1.46	1.50
15	cB	818	CLA	MG-ND	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c1	411	CLA	MG-ND	-2.05	2.01	2.05
15	bB	837	CLA	C4B-NB	2.05	1.40	1.37
15	c1	411	CLA	CHC-C1C	2.05	1.42	1.38
15	bA	812	CLA	MG-ND	-2.05	2.01	2.05
15	bA	840	CLA	CMC-C2C	-2.05	1.46	1.50
15	a4	421	CLA	O2D-CGD	2.05	1.38	1.33
15	bA	844	CLA	CBD-CAD	2.05	1.56	1.51
18	bJ	103	BCR	C33-C5	-2.05	1.47	1.50
15	aA	810	CLA	CMC-C2C	-2.05	1.46	1.50
15	a3	414	CLA	CHC-C1C	2.05	1.42	1.38
15	aA	821	CLA	CHC-C4B	-2.05	1.34	1.39
15	a3	414	CLA	CMC-C2C	-2.05	1.46	1.50
15	b5	402	CLA	CMC-C2C	-2.05	1.46	1.50
15	b6	416	CLA	C1B-C2B	2.05	1.48	1.43
15	cB	803	CLA	C3B-C4B	2.05	1.47	1.42
15	a4	413	CLA	MG-ND	-2.05	2.01	2.05
15	aA	802	CLA	C1D-ND	2.05	1.40	1.37
15	cA	841	CLA	CHC-C1C	2.05	1.42	1.38
15	bA	836	CLA	C1B-C2B	2.05	1.48	1.43
15	cB	801	CLA	C3B-C4B	2.05	1.47	1.42
15	c1	414	CLA	CMB-C2B	-2.05	1.46	1.50
15	c4	407	CLA	CMC-C2C	-2.05	1.46	1.50
15	aB	812	CLA	CHC-C1C	2.05	1.42	1.38
15	aB	840	CLA	C3B-C4B	2.05	1.47	1.42
15	b1	414	CLA	CMC-C2C	-2.05	1.46	1.50
15	b2	412	CLA	O2A-CGA	2.05	1.37	1.30
15	a2	408	CLA	CMC-C2C	-2.05	1.46	1.50
15	b2	416	CLA	O2A-CGA	2.05	1.37	1.30
15	cB	815	CLA	C1B-C2B	2.05	1.48	1.43
15	a3	404	CLA	C1B-NB	-2.05	1.35	1.37
16	aB	843	PQN	C9-C10	-2.05	1.36	1.39
15	a1	410	CLA	MG-ND	-2.05	2.01	2.05
15	aB	837	CLA	C4B-NB	2.05	1.40	1.37
15	a3	407	CLA	C1B-NB	-2.05	1.35	1.37
15	bA	831	CLA	C4B-NB	2.05	1.40	1.37
18	cA	847	BCR	C38-C26	-2.05	1.47	1.50
15	a3	409	CLA	CMB-C2B	-2.05	1.46	1.50
15	cJ	102	CLA	MG-ND	-2.05	2.01	2.05
15	a6	415	CLA	CHC-C1C	2.05	1.42	1.38
15	bB	828	CLA	C3B-C4B	2.05	1.47	1.42
15	b4	421	CLA	CMC-C2C	-2.05	1.46	1.50
15	bB	818	CLA	MG-ND	-2.05	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cA	812	CLA	MG-ND	-2.05	2.01	2.05
15	bA	823	CLA	C1B-NB	-2.05	1.35	1.37
15	b5	403	CLA	C1B-NB	-2.05	1.35	1.37
15	cA	833	CLA	C1D-ND	2.05	1.40	1.37
18	aA	852	BCR	C38-C26	-2.05	1.47	1.50
15	a1	403	CLA	CMD-C2D	-2.05	1.46	1.50
15	b5	402	CLA	CMB-C2B	-2.05	1.46	1.50
15	aA	822	CLA	C4B-NB	2.05	1.40	1.37
15	b5	420	CLA	C2A-C1A	2.05	1.56	1.52
15	a4	404	CLA	CMC-C2C	-2.05	1.46	1.50
15	cA	811	CLA	MG-ND	-2.05	2.01	2.05
15	c4	408	CLA	MG-ND	-2.05	2.01	2.05
15	aB	828	CLA	CHC-C4B	-2.05	1.34	1.39
15	bB	828	CLA	CHC-C4B	-2.05	1.34	1.39
15	cA	839	CLA	CHC-C4B	-2.05	1.34	1.39
15	a2	415	CLA	CMC-C2C	-2.05	1.46	1.50
15	bA	833	CLA	C1D-ND	2.05	1.40	1.37
15	a6	405	CLA	MG-ND	-2.05	2.01	2.05
15	c6	410	CLA	MG-ND	-2.05	2.01	2.05
15	b5	405	CLA	CMC-C2C	-2.05	1.46	1.50
15	cA	815	CLA	CMC-C2C	-2.05	1.46	1.50
15	c6	401	CLA	CMB-C2B	-2.05	1.46	1.50
18	aJ	204	BCR	C33-C5	-2.05	1.47	1.50
15	b1	407	CLA	MG-ND	-2.04	2.01	2.05
15	c6	401	CLA	CHC-C1C	2.04	1.42	1.38
16	cB	843	PQN	C9-C10	-2.04	1.36	1.39
15	bA	803	CLA	C1B-C2B	2.04	1.48	1.43
15	cB	836	CLA	C4B-NB	2.04	1.40	1.37
18	bA	852	BCR	C10-C9	-2.04	1.33	1.35
15	a3	405	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	402	CLA	CMC-C2C	-2.04	1.46	1.50
15	a4	421	CLA	C4D-CHA	2.04	1.45	1.38
15	a2	414	CLA	C1B-NB	-2.04	1.35	1.37
15	a2	403	CLA	CHC-C1C	2.04	1.42	1.38
15	aA	821	CLA	C3B-C4B	2.04	1.47	1.42
15	bB	819	CLA	CMB-C2B	-2.04	1.46	1.50
15	aA	841	CLA	CHC-C1C	2.04	1.42	1.38
15	c4	411	CLA	C1B-C2B	2.04	1.48	1.43
15	a2	411	CLA	CMD-C2D	-2.04	1.46	1.50
15	c4	405	CLA	CMB-C2B	-2.04	1.46	1.50
15	cA	836	CLA	C1B-C2B	2.04	1.48	1.43
15	aB	842	CLA	MG-NB	-2.04	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aA	815	CLA	CMC-C2C	-2.04	1.46	1.50
15	c5	402	CLA	CMC-C2C	-2.04	1.46	1.50
15	cB	828	CLA	CHC-C4B	-2.04	1.34	1.39
15	c2	412	CLA	O2A-CGA	2.04	1.37	1.30
15	a1	402	CLA	C1B-NB	-2.04	1.35	1.37
15	cA	819	CLA	MG-ND	-2.04	2.01	2.05
15	a1	406	CLA	CMC-C2C	-2.04	1.46	1.50
15	a1	410	CLA	CMD-C2D	-2.04	1.46	1.50
15	b4	421	CLA	C4D-CHA	2.04	1.45	1.38
15	a6	414	CLA	CHC-C4B	-2.04	1.34	1.39
15	a1	412	CLA	CMD-C2D	-2.04	1.46	1.50
15	a2	402	CLA	CMB-C2B	-2.04	1.46	1.50
15	a5	420	CLA	C2A-C1A	2.04	1.56	1.52
15	bA	815	CLA	CMC-C2C	-2.04	1.46	1.50
15	aA	834	CLA	CAA-C2A	-2.04	1.50	1.54
15	a2	416	CLA	O2A-CGA	2.04	1.37	1.30
18	bB	849	BCR	C38-C26	-2.04	1.47	1.50
18	bJ	105	BCR	C33-C5	-2.04	1.47	1.50
18	cB	845	BCR	C38-C26	-2.04	1.47	1.50
15	c2	405	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	413	CLA	CMD-C2D	-2.04	1.46	1.50
15	c4	404	CLA	CMC-C2C	-2.04	1.46	1.50
15	b6	414	CLA	C1B-NB	-2.04	1.35	1.37
15	b6	422	CLA	CAA-C2A	2.04	1.57	1.54
15	aA	812	CLA	MG-ND	-2.04	2.01	2.05
15	cA	832	CLA	MG-ND	-2.04	2.01	2.05
15	bB	806	CLA	CMA-C3A	-2.04	1.48	1.53
18	aJ	205	BCR	C33-C5	-2.04	1.47	1.50
15	b3	409	CLA	CHC-C1C	2.04	1.42	1.38
15	cB	812	CLA	CHC-C1C	2.04	1.42	1.38
15	c4	404	CLA	CHC-C1C	2.04	1.42	1.38
15	bA	811	CLA	MG-ND	-2.04	2.01	2.05
15	a1	414	CLA	O2A-CGA	2.04	1.37	1.30
15	aB	812	CLA	CMC-C2C	-2.04	1.46	1.50
15	a1	401	CLA	CMC-C2C	-2.04	1.46	1.50
18	aJ	205	BCR	C38-C26	-2.04	1.47	1.50
15	a6	409	CLA	C1B-C2B	2.04	1.48	1.43
15	aA	835	CLA	CAC-C3C	-2.04	1.45	1.51
15	cB	819	CLA	C3B-C4B	2.04	1.47	1.42
15	b3	408	CLA	CMB-C2B	-2.04	1.46	1.50
15	a6	416	CLA	C1B-C2B	2.04	1.48	1.43
15	b4	421	CLA	O2D-CGD	2.04	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b4	407	CLA	CMC-C2C	-2.04	1.46	1.50
15	cA	840	CLA	CMC-C2C	-2.04	1.46	1.50
15	cB	807	CLA	CAC-C3C	-2.04	1.45	1.51
18	bI	102	BCR	C17-C18	-2.04	1.33	1.35
15	bB	824	CLA	CMC-C2C	-2.04	1.46	1.50
15	c3	414	CLA	CMD-C2D	-2.04	1.46	1.50
15	cB	809	CLA	C1B-C2B	2.04	1.48	1.43
15	bB	811	CLA	C1B-NB	-2.04	1.35	1.37
15	cA	802	CLA	C5-C3	-2.04	1.47	1.51
15	b4	405	CLA	CMB-C2B	-2.04	1.46	1.50
15	aB	834	CLA	MG-NB	-2.04	2.01	2.05
18	b1	420	BCR	C31-C1	-2.04	1.49	1.53
15	cA	837	CLA	C1B-C2B	2.04	1.48	1.43
15	aA	803	CLA	C1D-ND	2.04	1.40	1.37
15	a2	415	CLA	CMB-C2B	-2.04	1.46	1.50
15	a5	412	CLA	CMD-C2D	-2.04	1.46	1.50
15	bA	833	CLA	CAC-C3C	-2.04	1.45	1.51
15	bA	838	CLA	C1C-NC	-2.04	1.34	1.37
15	b4	414	CLA	MG-ND	-2.04	2.01	2.05
15	bB	807	CLA	CAC-C3C	-2.04	1.45	1.51
18	aF	203	BCR	C38-C26	-2.04	1.47	1.50
15	a4	405	CLA	CMB-C2B	-2.04	1.46	1.50
15	c6	401	CLA	CMC-C2C	-2.04	1.46	1.50
15	c1	416	CLA	C3B-C4B	2.04	1.47	1.42
15	c4	414	CLA	MG-ND	-2.03	2.01	2.05
15	a1	413	CLA	CMB-C2B	-2.03	1.46	1.50
15	c1	405	CLA	CMD-C2D	-2.03	1.46	1.50
15	bA	834	CLA	CHC-C4B	-2.03	1.34	1.39
15	aA	837	CLA	C1B-C2B	2.03	1.48	1.43
15	c6	406	CLA	MG-ND	-2.03	2.01	2.05
15	aB	830	CLA	C4B-NB	2.03	1.40	1.37
15	cA	823	CLA	C1B-NB	-2.03	1.35	1.37
18	aB	849	BCR	C36-C18	-2.03	1.46	1.50
15	b3	415	CLA	O2A-CGA	2.03	1.37	1.30
15	aA	803	CLA	C3B-C4B	2.03	1.47	1.42
15	aB	819	CLA	C3B-C4B	2.03	1.47	1.42
15	bA	845	CLA	CMC-C2C	-2.03	1.46	1.50
15	b1	413	CLA	CMD-C2D	-2.03	1.46	1.50
15	aA	814	CLA	C4B-NB	2.03	1.40	1.37
15	bA	802	CLA	C1D-ND	2.03	1.40	1.37
15	a2	404	CLA	CMC-C2C	-2.03	1.46	1.50
15	bX	102	CLA	C1B-C2B	2.03	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	aL	202	CLA	C4B-NB	2.03	1.40	1.37
15	aL	202	CLA	C1D-ND	2.03	1.40	1.37
15	c5	413	CLA	C1B-NB	-2.03	1.35	1.37
15	bB	840	CLA	C3B-C4B	2.03	1.47	1.42
15	a3	409	CLA	CHC-C1C	2.03	1.42	1.38
15	b4	404	CLA	CHC-C1C	2.03	1.42	1.38
15	bA	823	CLA	CMC-C2C	-2.03	1.46	1.50
20	aB	850	LMG	O4-C4	-2.03	1.38	1.43
15	b4	411	CLA	C1B-C2B	2.03	1.48	1.43
18	bJ	104	BCR	C38-C26	-2.03	1.47	1.50
18	cJ	104	BCR	C38-C26	-2.03	1.47	1.50
15	cA	843	CLA	CBD-CAD	2.03	1.56	1.51
15	a5	415	CLA	O2A-CGA	2.03	1.37	1.30
18	cA	851	BCR	C38-C26	-2.03	1.47	1.50
15	aA	825	CLA	CMC-C2C	-2.03	1.46	1.50
15	a5	407	CLA	CMB-C2B	-2.03	1.46	1.50
15	cB	814	CLA	C4B-NB	2.03	1.40	1.37
15	aB	839	CLA	MG-ND	-2.03	2.01	2.05
15	a4	414	CLA	MG-ND	-2.03	2.01	2.05
15	bA	834	CLA	CAA-C2A	-2.03	1.50	1.54
15	a5	409	CLA	CMB-C2B	-2.03	1.46	1.50
15	b2	415	CLA	CMC-C2C	-2.03	1.46	1.50
18	a5	401	BCR	C4-C5	-2.03	1.47	1.51
15	bJ	102	CLA	MG-ND	-2.03	2.01	2.05
15	c3	404	CLA	MG-ND	-2.03	2.01	2.05
15	bA	824	CLA	C1B-NB	-2.03	1.35	1.37
15	b2	408	CLA	C1B-NB	-2.03	1.35	1.37
15	a4	421	CLA	CMC-C2C	-2.03	1.46	1.50
15	b3	413	CLA	CMD-C2D	-2.03	1.46	1.50
15	cB	824	CLA	CMC-C2C	-2.03	1.46	1.50
15	aB	806	CLA	C1B-C2B	2.03	1.48	1.43
18	bJ	105	BCR	C36-C18	-2.03	1.46	1.50
15	bA	823	CLA	MG-ND	-2.03	2.01	2.05
15	cA	834	CLA	CHC-C4B	-2.03	1.34	1.39
15	bA	832	CLA	MG-ND	-2.03	2.01	2.05
18	bB	848	BCR	C38-C26	-2.03	1.47	1.50
15	b5	413	CLA	CMC-C2C	-2.03	1.46	1.50
15	cB	802	CLA	CAC-C3C	-2.03	1.45	1.51
15	b2	402	CLA	CMB-C2B	-2.03	1.46	1.50
18	aB	846	BCR	C38-C26	-2.03	1.47	1.50
14	aA	801	CL0	CMD-C2D	-2.03	1.46	1.50
15	a5	417	CLA	CMD-C2D	-2.03	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c3	408	CLA	CMB-C2B	-2.03	1.46	1.50
15	c6	401	CLA	CAA-C2A	2.03	1.57	1.54
15	b5	409	CLA	CMC-C2C	-2.03	1.46	1.50
15	b5	411	CLA	CMD-C2D	-2.03	1.46	1.50
15	cB	839	CLA	MG-ND	-2.03	2.01	2.05
15	cB	826	CLA	CHC-C1C	2.03	1.42	1.38
15	cA	844	CLA	C1B-C2B	2.03	1.48	1.43
15	a5	411	CLA	CMD-C2D	-2.03	1.46	1.50
15	b6	405	CLA	CMC-C2C	-2.03	1.46	1.50
15	cB	806	CLA	C1B-C2B	2.03	1.48	1.43
18	bB	850	BCR	C36-C18	-2.03	1.46	1.50
18	a5	418	BCR	C27-C26	-2.03	1.47	1.51
15	cA	825	CLA	CMC-C2C	-2.03	1.46	1.50
18	cF	205	BCR	C33-C5	-2.03	1.47	1.50
15	b1	404	CLA	CMD-C2D	-2.03	1.46	1.50
15	a3	415	CLA	O2A-CGA	2.03	1.37	1.30
14	cA	801	CL0	CMD-C2D	-2.03	1.46	1.50
15	c6	406	CLA	CMC-C2C	-2.03	1.46	1.50
15	b5	408	CLA	C1B-NB	-2.03	1.35	1.37
15	c6	401	CLA	C4D-CHA	2.03	1.45	1.38
18	bL	206	BCR	C33-C5	-2.02	1.47	1.50
15	aA	845	CLA	C1B-C2B	2.02	1.48	1.43
15	bB	806	CLA	C1B-C2B	2.02	1.48	1.43
15	cA	831	CLA	C4B-NB	2.02	1.40	1.37
15	a5	413	CLA	CMC-C2C	-2.02	1.46	1.50
15	b2	415	CLA	CMB-C2B	-2.02	1.46	1.50
15	cB	828	CLA	C3B-C4B	2.02	1.47	1.42
18	bJ	105	BCR	C38-C26	-2.02	1.47	1.50
15	b6	422	CLA	CHC-C1C	2.02	1.42	1.38
15	bB	807	CLA	CHC-C4B	-2.02	1.34	1.39
15	cA	821	CLA	CHC-C4B	-2.02	1.34	1.39
15	bA	802	CLA	C3B-C4B	2.02	1.47	1.42
15	c1	407	CLA	CMC-C2C	-2.02	1.46	1.50
15	aA	833	CLA	C1D-ND	2.02	1.40	1.37
15	aX	102	CLA	C1B-C2B	2.02	1.48	1.43
15	bA	842	CLA	CMC-C2C	-2.02	1.46	1.50
15	a6	411	CLA	CMD-C2D	-2.02	1.46	1.50
15	c5	413	CLA	CMD-C2D	-2.02	1.46	1.50
15	bA	815	CLA	C1B-NB	-2.02	1.35	1.37
15	bB	814	CLA	C4B-NB	2.02	1.40	1.37
15	bB	830	CLA	C4B-NB	2.02	1.40	1.37
15	cA	803	CLA	C1D-ND	2.02	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	839	CLA	CHC-C1C	2.02	1.42	1.38
15	cA	833	CLA	CAC-C3C	-2.02	1.45	1.51
15	bA	821	CLA	CHC-C4B	-2.02	1.34	1.39
18	bB	846	BCR	C38-C26	-2.02	1.47	1.50
15	cA	823	CLA	MG-ND	-2.02	2.01	2.05
15	b2	412	CLA	CMC-C2C	-2.02	1.46	1.50
15	c2	414	CLA	CMD-C2D	-2.02	1.46	1.50
15	aA	839	CLA	CHC-C4B	-2.02	1.34	1.39
15	a1	407	CLA	MG-ND	-2.02	2.01	2.05
15	aB	826	CLA	CHC-C1C	2.02	1.42	1.38
15	aA	802	CLA	C3B-C4B	2.02	1.47	1.42
15	bB	806	CLA	C3B-C4B	2.02	1.47	1.42
15	a3	402	CLA	CMC-C2C	-2.02	1.46	1.50
15	aA	834	CLA	CHC-C4B	-2.02	1.34	1.39
15	bA	803	CLA	CHC-C4B	-2.02	1.34	1.39
15	b1	414	CLA	CHC-C1C	2.02	1.42	1.38
18	cJ	103	BCR	C33-C5	-2.02	1.47	1.50
15	a5	403	CLA	CHC-C1C	2.02	1.42	1.38
15	a4	402	CLA	CMC-C2C	-2.02	1.46	1.50
15	b3	414	CLA	CMD-C2D	-2.02	1.46	1.50
15	aA	823	CLA	CMC-C2C	-2.02	1.46	1.50
15	c1	414	CLA	CHC-C1C	2.02	1.42	1.38
15	aB	811	CLA	MG-ND	-2.02	2.01	2.05
15	bL	203	CLA	C1D-ND	2.02	1.40	1.37
18	cA	850	BCR	C33-C5	-2.02	1.47	1.50
18	bL	201	BCR	C33-C5	-2.02	1.47	1.50
15	c3	409	CLA	CHC-C1C	2.02	1.42	1.38
15	b6	411	CLA	CHC-C1C	2.02	1.42	1.38
15	a5	415	CLA	C1B-C2B	2.02	1.48	1.43
15	aB	824	CLA	CMC-C2C	-2.02	1.46	1.50
15	a3	406	CLA	CMD-C2D	-2.02	1.46	1.50
15	bB	822	CLA	CMB-C2B	-2.02	1.46	1.50
15	cB	842	CLA	MG-NB	-2.02	2.01	2.05
18	aL	205	BCR	C33-C5	-2.02	1.47	1.50
15	c2	412	CLA	CMC-C2C	-2.01	1.46	1.50
15	c3	406	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	841	CLA	CHC-C1C	2.01	1.42	1.38
15	aA	824	CLA	C1B-NB	-2.01	1.35	1.37
15	aA	832	CLA	MG-ND	-2.01	2.01	2.05
15	bB	823	CLA	CMC-C2C	-2.01	1.46	1.50
18	c1	420	BCR	C35-C13	-2.01	1.46	1.50
15	b2	412	CLA	CHC-C1C	2.01	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	839	CLA	MG-ND	-2.01	2.01	2.05
15	b5	412	CLA	CMD-C2D	-2.01	1.46	1.50
15	c6	407	CLA	CMD-C2D	-2.01	1.46	1.50
18	cF	205	BCR	C36-C18	-2.01	1.46	1.50
15	c1	415	CLA	O2A-CGA	2.01	1.37	1.30
15	bB	811	CLA	MG-ND	-2.01	2.01	2.05
15	a2	413	CLA	CHC-C4B	-2.01	1.34	1.39
15	bB	834	CLA	MG-NB	-2.01	2.01	2.05
15	aA	823	CLA	C1B-NB	-2.01	1.35	1.37
15	cA	808	CLA	C1B-NB	-2.01	1.35	1.37
15	b2	406	CLA	CMB-C2B	-2.01	1.46	1.50
18	b1	420	BCR	C35-C13	-2.01	1.46	1.50
15	bB	812	CLA	CMC-C2C	-2.01	1.46	1.50
15	c2	415	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	802	CLA	O2D-CED	-2.01	1.40	1.45
15	aA	812	CLA	C1B-NB	-2.01	1.35	1.37
15	bB	827	CLA	C4B-NB	2.01	1.40	1.37
15	c3	402	CLA	C1B-NB	-2.01	1.35	1.37
15	b4	415	CLA	O2A-CGA	2.01	1.37	1.30
15	b5	414	CLA	CHC-C1C	2.01	1.42	1.38
15	c1	408	CLA	MG-ND	-2.01	2.01	2.05
14	bA	801	CL0	CMD-C2D	-2.01	1.46	1.50
15	c5	413	CLA	CMC-C2C	-2.01	1.46	1.50
15	cB	807	CLA	CHC-C4B	-2.01	1.34	1.39
18	aI	102	BCR	C33-C5	-2.01	1.47	1.50
18	bJ	104	BCR	C33-C5	-2.01	1.47	1.50
15	bB	835	CLA	MG-ND	-2.01	2.01	2.05
15	a2	412	CLA	C1B-C2B	2.01	1.48	1.43
15	aB	839	CLA	CHC-C1C	2.01	1.42	1.38
15	cF	201	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	805	CLA	CAA-C2A	-2.01	1.50	1.54
15	aJ	202	CLA	O2A-CGA	2.01	1.37	1.30
15	b5	413	CLA	C1B-NB	-2.01	1.35	1.37
15	cB	839	CLA	CHC-C1C	2.01	1.42	1.38
15	a6	405	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	807	CLA	CMB-C2B	-2.01	1.46	1.50
15	a4	408	CLA	MG-ND	-2.01	2.01	2.05
15	cB	834	CLA	MG-NB	-2.01	2.01	2.05
15	a6	412	CLA	CMC-C2C	-2.01	1.46	1.50
15	cA	802	CLA	C3B-C4B	2.01	1.47	1.42
15	c5	415	CLA	O2A-CGA	2.01	1.37	1.30
18	cB	849	BCR	C36-C18	-2.01	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bJ	101	CLA	O2A-CGA	2.01	1.37	1.30
15	cB	806	CLA	CMA-C3A	-2.01	1.48	1.53
15	aB	826	CLA	C4B-NB	2.01	1.40	1.37
15	a5	405	CLA	CMC-C2C	-2.01	1.46	1.50
15	bA	844	CLA	CMB-C2B	-2.01	1.46	1.50
15	aA	803	CLA	C1B-C2B	2.01	1.48	1.43
15	b3	414	CLA	MG-ND	-2.01	2.01	2.05
15	aA	816	CLA	CMB-C2B	-2.01	1.46	1.50
15	a1	404	CLA	CMC-C2C	-2.01	1.46	1.50
15	aB	806	CLA	CMA-C3A	-2.01	1.48	1.53
15	aA	811	CLA	C1B-NB	-2.01	1.35	1.37
15	b4	402	CLA	CMC-C2C	-2.01	1.46	1.50
15	cA	803	CLA	C1B-C2B	2.01	1.48	1.43
15	c5	404	CLA	CMC-C2C	-2.01	1.46	1.50
15	bB	812	CLA	CHC-C1C	2.01	1.42	1.38
15	a2	408	CLA	C1B-NB	-2.01	1.35	1.37
15	aB	835	CLA	MG-ND	-2.00	2.01	2.05
15	bA	818	CLA	MG-ND	-2.00	2.01	2.05
18	a1	419	BCR	C35-C13	-2.00	1.46	1.50
15	cX	102	CLA	C1B-C2B	2.00	1.48	1.43
15	a2	412	CLA	CMC-C2C	-2.00	1.46	1.50
15	a6	415	CLA	CMB-C2B	-2.00	1.46	1.50
15	b6	410	CLA	MG-ND	-2.00	2.01	2.05
15	a4	404	CLA	CHC-C1C	2.00	1.42	1.38
15	a6	404	CLA	CHC-C1C	2.00	1.42	1.38
15	bB	826	CLA	CHC-C1C	2.00	1.42	1.38
15	bB	826	CLA	C4B-NB	2.00	1.40	1.37
15	c2	402	CLA	CMB-C2B	-2.00	1.46	1.50
15	cA	805	CLA	CAA-C2A	-2.00	1.50	1.54
15	a3	414	CLA	CMD-C2D	-2.00	1.46	1.50
15	bA	835	CLA	CAC-C3C	-2.00	1.46	1.51
15	cL	203	CLA	C1D-ND	2.00	1.40	1.37
18	b4	418	BCR	C27-C26	-2.00	1.47	1.51
15	a3	414	CLA	MG-ND	-2.00	2.01	2.05
15	b4	408	CLA	MG-ND	-2.00	2.01	2.05
15	aA	844	CLA	CBD-CAD	2.00	1.56	1.51
18	c3	418	BCR	C27-C26	-2.00	1.47	1.51
15	c5	409	CLA	CMC-C2C	-2.00	1.46	1.50
15	b5	415	CLA	O2A-CGA	2.00	1.37	1.30
15	c4	405	CLA	MG-ND	-2.00	2.01	2.05
15	a3	404	CLA	CMC-C2C	-2.00	1.46	1.50
15	cB	841	CLA	MG-ND	-2.00	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b6	414	CLA	CHC-C4B	-2.00	1.34	1.39
15	a3	413	CLA	CMC-C2C	-2.00	1.46	1.50

All (7568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	bB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	aB	804	CLA	C4A-NA-C1A	10.44	111.40	106.71
15	aA	803	CLA	C4A-NA-C1A	9.96	111.19	106.71
15	cA	803	CLA	C4A-NA-C1A	9.91	111.16	106.71
15	bA	803	CLA	C4A-NA-C1A	9.83	111.13	106.71
15	cB	840	CLA	C4A-NA-C1A	9.66	111.05	106.71
15	bB	811	CLA	C4A-NA-C1A	9.63	111.04	106.71
15	cB	811	CLA	C4A-NA-C1A	9.60	111.02	106.71
15	aB	840	CLA	C4A-NA-C1A	9.58	111.01	106.71
15	bB	840	CLA	C4A-NA-C1A	9.55	111.00	106.71
15	aB	811	CLA	C4A-NA-C1A	9.50	110.97	106.71
15	bB	809	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	cA	840	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	aA	840	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	cA	806	CLA	C4A-NA-C1A	9.04	110.77	106.71
15	cB	809	CLA	C4A-NA-C1A	9.03	110.76	106.71
15	bA	806	CLA	C4A-NA-C1A	9.02	110.76	106.71
15	bA	840	CLA	C4A-NA-C1A	9.01	110.75	106.71
15	aA	806	CLA	C4A-NA-C1A	9.00	110.75	106.71
15	aB	809	CLA	C4A-NA-C1A	8.97	110.74	106.71
15	c5	420	CLA	C4A-NA-C1A	8.79	110.66	106.71
15	bL	203	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	cL	203	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	b5	420	CLA	C4A-NA-C1A	8.70	110.62	106.71
15	aL	202	CLA	C4A-NA-C1A	8.70	110.62	106.71
14	cA	801	CL0	C1D-ND-C4D	-8.66	100.19	106.33
15	a5	420	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	aA	843	CLA	C4A-NA-C1A	8.62	110.58	106.71
14	bA	801	CL0	C1D-ND-C4D	-8.60	100.22	106.33
15	cA	832	CLA	C4A-NA-C1A	8.56	110.56	106.71
14	aA	801	CL0	C1D-ND-C4D	-8.55	100.26	106.33
15	cA	842	CLA	C4A-NA-C1A	8.55	110.55	106.71
15	bA	832	CLA	C4A-NA-C1A	8.53	110.54	106.71
15	aA	832	CLA	C4A-NA-C1A	8.53	110.54	106.71
15	aA	834	CLA	C4A-NA-C1A	8.51	110.53	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	818	CLA	C4A-NA-C1A	8.47	110.52	106.71
15	bA	843	CLA	C4A-NA-C1A	8.47	110.51	106.71
15	bB	816	CLA	C4A-NA-C1A	8.43	110.50	106.71
15	bA	818	CLA	C4A-NA-C1A	8.40	110.48	106.71
15	c2	406	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	a2	406	CLA	C4A-NA-C1A	8.34	110.46	106.71
15	cB	823	CLA	C4A-NA-C1A	8.34	110.46	106.71
15	bB	823	CLA	C4A-NA-C1A	8.32	110.44	106.71
15	bA	834	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	aB	823	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	cA	834	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	aB	816	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	cA	818	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	cB	822	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	bB	808	CLA	C4A-NA-C1A	8.27	110.42	106.71
15	cA	810	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	aB	808	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	cA	816	CLA	C4A-NA-C1A	8.25	110.42	106.71
15	aA	810	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	aB	822	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	bB	822	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	cB	816	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	cB	828	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	bA	810	CLA	C4A-NA-C1A	8.21	110.40	106.71
15	cB	808	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	b2	406	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	bB	835	CLA	C4A-NA-C1A	8.17	110.38	106.71
15	aA	816	CLA	C4A-NA-C1A	8.17	110.38	106.71
15	bA	816	CLA	C4A-NA-C1A	8.15	110.37	106.71
15	aA	844	CLA	C4A-NA-C1A	8.13	110.36	106.71
15	bB	805	CLA	C4A-NA-C1A	8.12	110.36	106.71
15	b6	422	CLA	C4A-NA-C1A	8.11	110.35	106.71
15	cB	835	CLA	C4A-NA-C1A	8.09	110.34	106.71
15	aB	835	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	aB	838	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	bJ	101	CLA	C4A-NA-C1A	8.07	110.34	106.71
15	aB	821	CLA	C4A-NA-C1A	8.07	110.33	106.71
15	bB	828	CLA	C4A-NA-C1A	8.06	110.33	106.71
15	bA	844	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	aB	805	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	aB	828	CLA	C4A-NA-C1A	8.05	110.32	106.71
15	cB	805	CLA	C4A-NA-C1A	8.04	110.32	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	838	CLA	C4A-NA-C1A	8.04	110.32	106.71
15	cA	843	CLA	C4A-NA-C1A	8.03	110.31	106.71
15	a2	422	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	c6	401	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	a4	415	CLA	C4A-NA-C1A	7.99	110.30	106.71
15	cB	806	CLA	C4A-NA-C1A	7.97	110.29	106.71
15	c2	422	CLA	C4A-NA-C1A	7.96	110.29	106.71
15	bB	806	CLA	C4A-NA-C1A	7.96	110.28	106.71
15	bA	826	CLA	C4A-NA-C1A	7.95	110.28	106.71
15	aJ	202	CLA	C4A-NA-C1A	7.94	110.28	106.71
15	cJ	101	CLA	C4A-NA-C1A	7.94	110.27	106.71
15	b4	415	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	cB	821	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	c4	415	CLA	C4A-NA-C1A	7.93	110.27	106.71
15	bB	819	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	bB	821	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	b2	422	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	aB	802	CLA	C4A-NA-C1A	7.90	110.26	106.71
15	bB	838	CLA	C4A-NA-C1A	7.90	110.26	106.71
15	a6	422	CLA	C4A-NA-C1A	7.89	110.25	106.71
15	a5	415	CLA	C4A-NA-C1A	7.88	110.25	106.71
15	cB	802	CLA	C4A-NA-C1A	7.87	110.25	106.71
15	aB	807	CLA	C4A-NA-C1A	7.87	110.24	106.71
15	b2	415	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	aA	826	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	b5	415	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	cB	819	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	cB	831	CLA	C4A-NA-C1A	7.83	110.23	106.71
15	c5	415	CLA	C4A-NA-C1A	7.82	110.22	106.71
15	aB	819	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	bB	802	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	cB	807	CLA	C4A-NA-C1A	7.81	110.22	106.71
15	aB	827	CLA	C4A-NA-C1A	7.79	110.21	106.71
15	cA	826	CLA	C4A-NA-C1A	7.79	110.21	106.71
15	aB	806	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	a2	415	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	bB	807	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	bB	831	CLA	C4A-NA-C1A	7.78	110.20	106.71
15	aB	831	CLA	C4A-NA-C1A	7.77	110.20	106.71
15	c2	415	CLA	C4A-NA-C1A	7.76	110.20	106.71
15	bB	827	CLA	C4A-NA-C1A	7.74	110.19	106.71
15	b6	416	CLA	C4A-NA-C1A	7.73	110.18	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	810	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	bB	813	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	aB	810	CLA	C4A-NA-C1A	7.71	110.17	106.71
15	c6	417	CLA	C4A-NA-C1A	7.69	110.16	106.71
15	cB	827	CLA	C4A-NA-C1A	7.67	110.16	106.71
15	b6	415	CLA	C4A-NA-C1A	7.67	110.16	106.71
15	cB	813	CLA	C4A-NA-C1A	7.66	110.15	106.71
15	bA	845	CLA	C4A-NA-C1A	7.65	110.14	106.71
15	a6	415	CLA	C4A-NA-C1A	7.64	110.14	106.71
14	aA	801	CL0	C2B-C1B-NB	7.63	115.35	110.23
15	bB	810	CLA	C4A-NA-C1A	7.62	110.13	106.71
15	b5	414	CLA	C4A-NA-C1A	7.62	110.13	106.71
14	bA	801	CL0	C2B-C1B-NB	7.62	115.34	110.23
15	a4	414	CLA	C4A-NA-C1A	7.61	110.13	106.71
15	b4	414	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	b3	403	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	aA	845	CLA	C4A-NA-C1A	7.60	110.12	106.71
15	c1	415	CLA	C4A-NA-C1A	7.60	110.12	106.71
14	cA	801	CL0	C2B-C1B-NB	7.59	115.32	110.23
15	cA	837	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c6	416	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c3	403	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	c5	414	CLA	C4A-NA-C1A	7.58	110.11	106.71
15	aB	813	CLA	C4A-NA-C1A	7.57	110.11	106.71
15	cX	102	CLA	C4A-NA-C1A	7.56	110.10	106.71
15	c4	414	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	cA	844	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	bA	837	CLA	C4A-NA-C1A	7.55	110.10	106.71
15	a3	415	CLA	C4A-NA-C1A	7.54	110.10	106.71
15	bX	102	CLA	C4A-NA-C1A	7.53	110.09	106.71
15	aA	829	CLA	C4A-NA-C1A	7.52	110.09	106.71
15	a1	414	CLA	C4A-NA-C1A	7.52	110.09	106.71
15	c3	414	CLA	C4A-NA-C1A	7.52	110.08	106.71
15	a6	416	CLA	C4A-NA-C1A	7.51	110.08	106.71
15	bA	829	CLA	C4A-NA-C1A	7.50	110.08	106.71
15	aA	837	CLA	C4A-NA-C1A	7.49	110.07	106.71
15	a2	403	CLA	C4A-NA-C1A	7.49	110.07	106.71
15	aX	102	CLA	C4A-NA-C1A	7.46	110.06	106.71
15	b1	403	CLA	C4A-NA-C1A	7.44	110.05	106.71
15	b3	415	CLA	C4A-NA-C1A	7.43	110.05	106.71
15	c5	403	CLA	C4A-NA-C1A	7.43	110.05	106.71
15	a5	403	CLA	C4A-NA-C1A	7.42	110.04	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	414	CLA	C4A-NA-C1A	7.42	110.04	106.71
15	cA	829	CLA	C4A-NA-C1A	7.41	110.04	106.71
15	cJ	102	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	a3	403	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	a5	414	CLA	C4A-NA-C1A	7.40	110.03	106.71
15	b6	404	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	a5	404	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	c4	416	CLA	C4A-NA-C1A	7.39	110.03	106.71
15	c2	403	CLA	C4A-NA-C1A	7.38	110.02	106.71
15	b1	416	CLA	C4A-NA-C1A	7.38	110.02	106.71
15	aJ	203	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	b5	403	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	b2	416	CLA	C4A-NA-C1A	7.37	110.02	106.71
15	a6	404	CLA	C4A-NA-C1A	7.36	110.02	106.71
15	c6	405	CLA	C4A-NA-C1A	7.36	110.01	106.71
15	c3	415	CLA	C4A-NA-C1A	7.35	110.01	106.71
15	c2	416	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	bA	839	CLA	C4A-NA-C1A	7.34	110.01	106.71
15	a1	402	CLA	C4A-NA-C1A	7.34	110.00	106.71
15	c4	403	CLA	C4A-NA-C1A	7.33	110.00	106.71
15	a4	416	CLA	C4A-NA-C1A	7.32	110.00	106.71
15	a1	416	CLA	CMB-C2B-C1B	-7.32	114.22	125.37
15	a3	414	CLA	C4A-NA-C1A	7.32	110.00	106.71
15	a1	403	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	cA	839	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	c1	414	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	b2	403	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	aA	839	CLA	C4A-NA-C1A	7.31	109.99	106.71
15	c1	403	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b1	404	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b4	403	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b4	416	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	b1	415	CLA	C4A-NA-C1A	7.30	109.99	106.71
15	cA	821	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	b1	417	CLA	CMB-C2B-C1B	-7.28	114.28	125.37
15	b6	417	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	cA	824	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	c5	404	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	c6	418	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	a2	417	CLA	C4A-NA-C1A	7.28	109.98	106.71
15	a1	413	CLA	C4A-NA-C1A	7.27	109.98	106.71
15	a6	417	CLA	C4A-NA-C1A	7.27	109.98	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	417	CLA	CMB-C2B-C1B	-7.27	114.30	125.37
15	a2	404	CLA	C4A-NA-C1A	7.27	109.97	106.71
15	c1	416	CLA	C4A-NA-C1A	7.27	109.97	106.71
15	a3	404	CLA	C4A-NA-C1A	7.26	109.97	106.71
15	bA	824	CLA	C4A-NA-C1A	7.26	109.97	106.71
15	a5	417	CLA	CMB-C2B-C1B	-7.26	114.32	125.37
15	c6	406	CLA	C4A-NA-C1A	7.25	109.96	106.71
15	bA	821	CLA	C4A-NA-C1A	7.24	109.96	106.71
15	a4	403	CLA	C4A-NA-C1A	7.24	109.96	106.71
15	b5	417	CLA	CMB-C2B-C1B	-7.24	114.35	125.37
15	b2	417	CLA	C4A-NA-C1A	7.23	109.96	106.71
15	b3	417	CLA	CMB-C2B-C1B	-7.23	114.36	125.37
15	b4	411	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	c5	417	CLA	CMB-C2B-C1B	-7.22	114.37	125.37
15	a1	415	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	a3	416	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	b1	407	CLA	C4A-NA-C1A	7.22	109.95	106.71
15	c3	417	CLA	CMB-C2B-C1B	-7.22	114.38	125.37
15	b2	404	CLA	C4A-NA-C1A	7.21	109.95	106.71
15	a4	417	CLA	CMB-C2B-C1B	-7.21	114.38	125.37
15	b5	404	CLA	C4A-NA-C1A	7.21	109.95	106.71
15	aA	824	CLA	C4A-NA-C1A	7.20	109.94	106.71
15	a3	417	CLA	CMB-C2B-C1B	-7.20	114.41	125.37
15	bJ	102	CLA	C4A-NA-C1A	7.20	109.94	106.71
15	b4	421	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	b5	416	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	aA	821	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	a1	406	CLA	C4A-NA-C1A	7.19	109.94	106.71
15	c4	417	CLA	CMB-C2B-C1B	-7.19	114.43	125.37
15	c4	421	CLA	C4A-NA-C1A	7.18	109.94	106.71
15	c1	407	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	c2	404	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	a1	410	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	b4	417	CLA	CMB-C2B-C1B	-7.17	114.45	125.37
15	bA	835	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	b6	412	CLA	C4A-NA-C1A	7.17	109.93	106.71
15	aA	835	CLA	C4A-NA-C1A	7.16	109.92	106.71
15	c3	416	CLA	C4A-NA-C1A	7.16	109.92	106.71
15	b1	402	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a2	416	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a5	402	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	a5	416	CLA	C4A-NA-C1A	7.15	109.92	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	404	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	c3	404	CLA	C4A-NA-C1A	7.15	109.92	106.71
15	b3	404	CLA	C4A-NA-C1A	7.14	109.92	106.71
15	c2	417	CLA	C4A-NA-C1A	7.13	109.91	106.71
15	b3	416	CLA	C4A-NA-C1A	7.13	109.91	106.71
15	a1	401	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	b6	405	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	a4	421	CLA	C4A-NA-C1A	7.12	109.91	106.71
15	a3	411	CLA	C4A-NA-C1A	7.11	109.90	106.71
15	b1	411	CLA	C4A-NA-C1A	7.11	109.90	106.71
15	aA	823	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	b1	414	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	cB	829	CLA	C4A-NA-C1A	7.10	109.90	106.71
15	c1	411	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	cA	801	CL0	C2D-C1D-ND	7.09	115.33	110.10
15	a6	405	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	c5	416	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	cA	823	CLA	C4A-NA-C1A	7.09	109.89	106.71
15	b5	402	CLA	C4A-NA-C1A	7.08	109.89	106.71
15	b3	411	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	c2	418	CLA	CMB-C2B-C1B	-7.06	114.61	125.37
15	c6	413	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	a4	411	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	cA	836	CLA	C4A-NA-C1A	7.06	109.88	106.71
15	b2	412	CLA	C4A-NA-C1A	7.05	109.88	106.71
14	bA	801	CL0	C2D-C1D-ND	7.05	115.30	110.10
15	a2	412	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	b5	411	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	a2	418	CLA	CMB-C2B-C1B	-7.04	114.64	125.37
15	aA	808	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	cA	838	CLA	C4A-NA-C1A	7.04	109.87	106.71
15	b6	418	CLA	CMB-C2B-C1B	-7.04	114.65	125.37
14	aA	801	CL0	C2D-C1D-ND	7.03	115.29	110.10
15	b2	418	CLA	CMB-C2B-C1B	-7.03	114.67	125.37
15	a6	412	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	bA	808	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	bB	829	CLA	C4A-NA-C1A	7.02	109.86	106.71
15	a6	410	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	a3	402	CLA	C4A-NA-C1A	7.01	109.86	106.71
15	a6	418	CLA	CMB-C2B-C1B	-7.01	114.70	125.37
15	cA	835	CLA	C4A-NA-C1A	7.00	109.86	106.71
15	aA	836	CLA	C4A-NA-C1A	7.00	109.85	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	829	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	bA	838	CLA	C4A-NA-C1A	7.00	109.85	106.71
15	cA	808	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	bA	823	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	c6	419	CLA	CMB-C2B-C1B	-6.99	114.73	125.37
15	bB	839	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	c4	411	CLA	C4A-NA-C1A	6.99	109.85	106.71
15	c6	404	CLA	C4A-NA-C1A	6.98	109.85	106.71
15	c4	402	CLA	C4A-NA-C1A	6.98	109.84	106.71
15	cB	837	CLA	C4A-NA-C1A	6.98	109.84	106.71
15	bB	834	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	aA	838	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	a5	411	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	cB	839	CLA	C4A-NA-C1A	6.97	109.84	106.71
15	bB	837	CLA	C4A-NA-C1A	6.96	109.84	106.71
15	c5	411	CLA	C4A-NA-C1A	6.96	109.84	106.71
15	c1	402	CLA	C4A-NA-C1A	6.96	109.83	106.71
15	cA	822	CLA	C4A-NA-C1A	6.96	109.83	106.71
15	b4	402	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	a6	422	CLA	CAA-CBA-CGA	-6.95	92.94	113.25
15	c4	404	CLA	C4A-NA-C1A	6.95	109.83	106.71
15	aB	839	CLA	C4A-NA-C1A	6.94	109.83	106.71
15	bA	836	CLA	C4A-NA-C1A	6.94	109.82	106.71
15	a6	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	b4	406	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	b6	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	aB	834	CLA	C4A-NA-C1A	6.93	109.82	106.71
15	aB	837	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	c3	411	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	b5	407	CLA	C4A-NA-C1A	6.92	109.82	106.71
15	a4	404	CLA	C4A-NA-C1A	6.92	109.81	106.71
15	c4	406	CLA	C4A-NA-C1A	6.91	109.81	106.71
15	bA	809	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	bB	842	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	aA	827	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	aB	842	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	b4	404	CLA	C4A-NA-C1A	6.90	109.81	106.71
15	a5	407	CLA	C4A-NA-C1A	6.89	109.81	106.71
15	b6	408	CLA	C4A-NA-C1A	6.89	109.80	106.71
15	bA	827	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	cA	809	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	c2	412	CLA	C4A-NA-C1A	6.88	109.80	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	842	CLA	C4A-NA-C1A	6.88	109.80	106.71
15	cB	834	CLA	C4A-NA-C1A	6.87	109.79	106.71
15	aA	822	CLA	C4A-NA-C1A	6.86	109.79	106.71
15	bA	822	CLA	C4A-NA-C1A	6.85	109.79	106.71
15	b6	410	CLA	C4A-NA-C1A	6.85	109.78	106.71
15	c5	402	CLA	C4A-NA-C1A	6.85	109.78	106.71
15	aA	809	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	cA	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	c5	407	CLA	C4A-NA-C1A	6.84	109.78	106.71
15	a5	409	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	a4	406	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	b3	406	CLA	C4A-NA-C1A	6.83	109.78	106.71
15	c6	411	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	a6	408	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	c5	406	CLA	C4A-NA-C1A	6.82	109.77	106.71
15	cA	841	CLA	C4A-NA-C1A	6.81	109.77	106.71
15	b3	409	CLA	C4A-NA-C1A	6.80	109.76	106.71
15	b3	407	CLA	C4A-NA-C1A	6.80	109.76	106.71
15	a5	406	CLA	C4A-NA-C1A	6.79	109.76	106.71
15	b5	406	CLA	C4A-NA-C1A	6.78	109.76	106.71
15	c4	407	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	c3	402	CLA	C4A-NA-C1A	6.78	109.75	106.71
15	a3	407	CLA	C4A-NA-C1A	6.77	109.75	106.71
15	c3	406	CLA	C4A-NA-C1A	6.77	109.75	106.71
15	aA	841	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	a4	402	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	bA	811	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	b5	409	CLA	C4A-NA-C1A	6.76	109.74	106.71
15	c3	407	CLA	C4A-NA-C1A	6.74	109.74	106.71
15	aA	811	CLA	C4A-NA-C1A	6.74	109.73	106.71
15	bA	805	CLA	C4A-NA-C1A	6.73	109.73	106.71
15	b4	407	CLA	C4A-NA-C1A	6.72	109.73	106.71
15	bA	841	CLA	C4A-NA-C1A	6.71	109.72	106.71
15	aA	807	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	aA	805	CLA	C4A-NA-C1A	6.70	109.72	106.71
15	a3	409	CLA	C4A-NA-C1A	6.69	109.71	106.71
15	b3	402	CLA	C4A-NA-C1A	6.69	109.71	106.71
15	c6	409	CLA	C4A-NA-C1A	6.69	109.71	106.71
15	bA	807	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	c3	409	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	a3	406	CLA	C4A-NA-C1A	6.68	109.71	106.71
15	a4	407	CLA	C4A-NA-C1A	6.67	109.71	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	407	CLA	C4A-NA-C1A	6.67	109.70	106.71
15	cA	811	CLA	C4A-NA-C1A	6.67	109.70	106.71
15	b6	407	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	cA	805	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	a2	408	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	c5	409	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	c6	408	CLA	C4A-NA-C1A	6.66	109.70	106.71
15	aB	841	CLA	C4A-NA-C1A	6.65	109.69	106.71
15	bB	841	CLA	C4A-NA-C1A	6.64	109.69	106.71
15	a2	410	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	c2	407	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	b2	410	CLA	C4A-NA-C1A	6.63	109.69	106.71
15	c1	416	CLA	CMC-C2C-C1C	-6.62	114.96	125.04
15	aB	820	CLA	C4A-NA-C1A	6.62	109.68	106.71
15	a2	407	CLA	C4A-NA-C1A	6.61	109.68	106.71
15	b2	408	CLA	C4A-NA-C1A	6.61	109.68	106.71
15	a6	407	CLA	C4A-NA-C1A	6.59	109.67	106.71
15	bA	833	CLA	C4A-NA-C1A	6.59	109.67	106.71
15	c4	416	CLA	CMC-C2C-C1C	-6.59	115.01	125.04
15	cA	807	CLA	C4A-NA-C1A	6.58	109.67	106.71
15	b4	416	CLA	CMC-C2C-C1C	-6.58	115.02	125.04
15	c2	408	CLA	C4A-NA-C1A	6.58	109.66	106.71
15	a4	416	CLA	CMC-C2C-C1C	-6.56	115.05	125.04
15	bA	830	CLA	C4A-NA-C1A	6.56	109.65	106.71
15	a1	408	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	cA	833	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	b2	414	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	b1	416	CLA	CMC-C2C-C1C	-6.55	115.07	125.04
15	cB	820	CLA	C4A-NA-C1A	6.55	109.65	106.71
15	b2	402	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	bB	820	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	aA	830	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	cB	841	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	cB	815	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	c2	402	CLA	C4A-NA-C1A	6.53	109.64	106.71
15	c2	410	CLA	C4A-NA-C1A	6.50	109.63	106.71
15	cA	830	CLA	C4A-NA-C1A	6.49	109.62	106.71
15	aB	815	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	aA	833	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	a2	414	CLA	C4A-NA-C1A	6.48	109.62	106.71
15	aA	828	CLA	C4A-NA-C1A	6.47	109.62	106.71
15	a2	402	CLA	C4A-NA-C1A	6.47	109.62	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	406	CLA	C4A-NA-C1A	6.47	109.61	106.71
15	cA	828	CLA	C4A-NA-C1A	6.47	109.61	106.71
15	b1	409	CLA	C4A-NA-C1A	6.47	109.61	106.71
14	aA	801	CL0	O2D-CGD-CBD	6.46	122.74	111.27
15	b5	416	CLA	CMC-C2C-C1C	-6.45	115.22	125.04
14	bA	801	CL0	O2D-CGD-CBD	6.45	122.73	111.27
14	cA	801	CL0	O2D-CGD-CBD	6.45	122.73	111.27
15	bB	815	CLA	C4A-NA-C1A	6.45	109.61	106.71
15	a4	409	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	cA	814	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	cA	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	c4	409	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	aB	826	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	bA	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
15	a1	415	CLA	CMC-C2C-C1C	-6.44	115.24	125.04
15	bB	826	CLA	C4A-NA-C1A	6.43	109.60	106.71
15	a5	416	CLA	CMC-C2C-C1C	-6.43	115.25	125.04
15	c2	414	CLA	C4A-NA-C1A	6.42	109.59	106.71
15	aA	814	CLA	C4A-NA-C1A	6.41	109.59	106.71
15	c5	416	CLA	CMC-C2C-C1C	-6.41	115.28	125.04
15	bK	101	CLA	C4A-NA-C1A	6.40	109.58	106.71
15	a3	416	CLA	CMC-C2C-C1C	-6.39	115.31	125.04
15	aA	820	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	bA	814	CLA	C4A-NA-C1A	6.39	109.58	106.71
15	b3	416	CLA	CMC-C2C-C1C	-6.37	115.33	125.04
15	b6	417	CLA	CMC-C2C-C1C	-6.36	115.35	125.04
15	c3	416	CLA	CMC-C2C-C1C	-6.36	115.35	125.04
15	a6	417	CLA	CMC-C2C-C1C	-6.36	115.36	125.04
15	cB	826	CLA	C4A-NA-C1A	6.35	109.56	106.71
15	a1	405	CLA	C4A-NA-C1A	6.35	109.56	106.71
15	c6	418	CLA	CMC-C2C-C1C	-6.34	115.38	125.04
15	b4	409	CLA	C4A-NA-C1A	6.34	109.56	106.71
15	c1	409	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	cA	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	bA	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	bA	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
15	cA	819	CLA	C4A-NA-C1A	6.32	109.55	106.71
15	b6	414	CLA	C4A-NA-C1A	6.31	109.54	106.71
15	aA	815	CLA	C4A-NA-C1A	6.30	109.54	106.71
15	c1	406	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	aK	102	CLA	C4A-NA-C1A	6.28	109.53	106.71
15	aJ	201	CLA	C4A-NA-C1A	6.28	109.53	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	413	CLA	C4A-NA-C1A	6.27	109.53	106.71
15	bF	201	CLA	C4A-NA-C1A	6.27	109.52	106.71
15	cK	102	CLA	C4A-NA-C1A	6.26	109.52	106.71
15	c3	421	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	a3	421	CLA	C4A-NA-C1A	6.24	109.51	106.71
15	bB	825	CLA	C4A-NA-C1A	6.23	109.51	106.71
15	cF	203	CLA	C4A-NA-C1A	6.23	109.51	106.71
15	aB	825	CLA	C4A-NA-C1A	6.22	109.50	106.71
15	a3	413	CLA	C4A-NA-C1A	6.19	109.49	106.71
15	bA	819	CLA	C4A-NA-C1A	6.19	109.49	106.71
15	bB	818	CLA	C4A-NA-C1A	6.18	109.48	106.71
15	c5	413	CLA	C4A-NA-C1A	6.18	109.48	106.71
15	aA	845	CLA	CAC-C3C-C4C	-6.17	116.80	124.81
15	cA	844	CLA	CAC-C3C-C4C	-6.17	116.81	124.81
15	bA	845	CLA	CAC-C3C-C4C	-6.16	116.81	124.81
15	cA	812	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	aB	818	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	c3	413	CLA	C4A-NA-C1A	6.15	109.47	106.71
15	b2	417	CLA	CMC-C2C-C1C	-6.14	115.68	125.04
15	bA	817	CLA	C4A-NA-C1A	6.14	109.47	106.71
15	c2	417	CLA	CMC-C2C-C1C	-6.14	115.69	125.04
15	cB	818	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	aA	804	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	aA	819	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	a2	417	CLA	CMC-C2C-C1C	-6.13	115.71	125.04
15	aA	817	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	cA	817	CLA	C4A-NA-C1A	6.13	109.46	106.71
15	cB	825	CLA	C4A-NA-C1A	6.12	109.46	106.71
15	a1	412	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	aA	812	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	b3	421	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	bA	812	CLA	C4A-NA-C1A	6.10	109.45	106.71
15	b4	408	CLA	C4A-NA-C1A	6.09	109.44	106.71
15	a6	414	CLA	C4A-NA-C1A	6.09	109.44	106.71
15	a5	413	CLA	C4A-NA-C1A	6.07	109.44	106.71
15	bA	804	CLA	C4A-NA-C1A	6.06	109.43	106.71
15	cA	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
15	c4	413	CLA	C4A-NA-C1A	6.03	109.42	106.71
15	c6	415	CLA	C4A-NA-C1A	6.03	109.42	106.71
15	a2	417	CLA	CMB-C2B-C1B	-6.03	116.19	125.37
15	a4	413	CLA	C4A-NA-C1A	6.02	109.41	106.71
15	c1	413	CLA	C4A-NA-C1A	6.02	109.41	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	408	CLA	C4A-NA-C1A	6.01	109.41	106.71
15	c2	417	CLA	CMB-C2B-C1B	-5.99	116.24	125.37
15	b5	413	CLA	C4A-NA-C1A	5.98	109.40	106.71
18	c2	401	BCR	C11-C10-C9	-5.98	118.78	127.31
15	aB	836	CLA	C4A-NA-C1A	5.97	109.39	106.71
15	b4	413	CLA	C4A-NA-C1A	5.96	109.39	106.71
14	aA	801	CL0	CHD-C4C-C3C	-5.96	116.08	124.84
14	bA	801	CL0	CHD-C4C-C3C	-5.96	116.08	124.84
18	a2	401	BCR	C11-C10-C9	-5.95	118.81	127.31
15	c6	419	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	a5	408	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	bB	836	CLA	C4A-NA-C1A	5.95	109.38	106.71
15	b1	410	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	cA	801	CL0	CHD-C4C-C3C	-5.94	116.10	124.84
15	c3	410	CLA	C4A-NA-C1A	5.94	109.38	106.71
15	cB	836	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	b3	410	CLA	C4A-NA-C1A	5.93	109.37	106.71
15	b1	413	CLA	C4A-NA-C1A	5.92	109.37	106.71
15	c2	411	CLA	C4A-NA-C1A	5.92	109.37	106.71
15	bB	830	CLA	C4A-NA-C1A	5.91	109.36	106.71
15	c4	416	CLA	CMB-C2B-C1B	-5.90	116.38	125.37
15	a4	408	CLA	C4A-NA-C1A	5.89	109.35	106.71
15	a2	411	CLA	C4A-NA-C1A	5.88	109.35	106.71
15	b4	416	CLA	CMB-C2B-C1B	-5.88	116.42	125.37
15	c2	418	CLA	C4A-NA-C1A	5.87	109.35	106.71
15	c5	408	CLA	C4A-NA-C1A	5.87	109.35	106.71
15	a6	409	CLA	C4A-NA-C1A	5.87	109.34	106.71
15	a1	409	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	b2	418	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	b4	410	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	cB	801	CLA	C4A-NA-C1A	5.86	109.34	106.71
15	aB	801	CLA	C4A-NA-C1A	5.85	109.34	106.71
15	bB	801	CLA	C4A-NA-C1A	5.85	109.34	106.71
18	a1	421	BCR	C11-C10-C9	-5.84	118.98	127.31
15	b2	409	CLA	C4A-NA-C1A	5.84	109.33	106.71
15	a4	416	CLA	CMB-C2B-C1B	-5.84	116.48	125.37
15	b2	417	CLA	CMB-C2B-C1B	-5.82	116.50	125.37
15	aB	833	CLA	C4A-NA-C1A	5.81	109.32	106.71
15	a2	409	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	c2	409	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	c4	408	CLA	C4A-NA-C1A	5.80	109.31	106.71
15	cB	830	CLA	C4A-NA-C1A	5.79	109.31	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	832	CLA	C4A-NA-C1A	5.78	109.31	106.71
15	cB	832	CLA	C4A-NA-C1A	5.77	109.30	106.71
15	a5	416	CLA	CMB-C2B-C1B	-5.77	116.58	125.37
15	a1	416	CLA	C4A-NA-C1A	5.76	109.30	106.71
15	a4	410	CLA	C4A-NA-C1A	5.75	109.29	106.71
15	c5	416	CLA	CMB-C2B-C1B	-5.75	116.62	125.37
18	b2	401	BCR	C11-C10-C9	-5.75	119.11	127.31
15	a3	410	CLA	C4A-NA-C1A	5.74	109.29	106.71
15	b6	418	CLA	C4A-NA-C1A	5.74	109.29	106.71
15	cB	833	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	c1	410	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	b1	408	CLA	C4A-NA-C1A	5.73	109.28	106.71
15	c1	417	CLA	C4A-NA-C1A	5.72	109.28	106.71
15	b5	416	CLA	CMB-C2B-C1B	-5.72	116.66	125.37
15	b6	409	CLA	C4A-NA-C1A	5.71	109.28	106.71
15	aB	830	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	a6	418	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	bB	833	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	b1	417	CLA	C4A-NA-C1A	5.70	109.27	106.71
15	b3	417	CLA	C4A-NA-C1A	5.70	109.27	106.71
14	cA	801	CL0	C2C-C1C-NC	5.70	115.31	109.97
14	bA	801	CL0	C2C-C1C-NC	5.69	115.31	109.97
15	a3	408	CLA	C4A-NA-C1A	5.69	109.27	106.71
15	bA	845	CLA	CAC-C3C-C2C	5.69	137.26	127.53
15	bB	832	CLA	C4A-NA-C1A	5.68	109.26	106.71
15	c4	410	CLA	C4A-NA-C1A	5.68	109.26	106.71
14	aA	801	CL0	C2C-C1C-NC	5.68	115.29	109.97
15	cA	844	CLA	CAC-C3C-C2C	5.67	137.23	127.53
15	aA	845	CLA	CAC-C3C-C2C	5.67	137.23	127.53
15	bB	812	CLA	C4A-NA-C1A	5.67	109.25	106.71
15	b2	411	CLA	C4A-NA-C1A	5.67	109.25	106.71
15	a2	418	CLA	C4A-NA-C1A	5.65	109.25	106.71
15	c6	410	CLA	C4A-NA-C1A	5.64	109.24	106.71
15	cL	202	CLA	C4A-NA-C1A	5.63	109.23	106.71
15	cB	812	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	bL	202	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	c3	408	CLA	C4A-NA-C1A	5.62	109.23	106.71
15	b3	408	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	a5	410	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	c3	417	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	a3	417	CLA	C4A-NA-C1A	5.61	109.23	106.71
15	aL	201	CLA	C4A-NA-C1A	5.61	109.23	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	842	CLA	C4A-NA-C1A	5.56	109.21	106.71
15	aB	812	CLA	C4A-NA-C1A	5.55	109.20	106.71
15	c5	410	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	a1	407	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	aB	803	CLA	C4A-NA-C1A	5.54	109.20	106.71
15	c1	408	CLA	C4A-NA-C1A	5.54	109.19	106.71
15	bA	842	CLA	C4A-NA-C1A	5.53	109.19	106.71
15	b5	410	CLA	C4A-NA-C1A	5.53	109.19	106.71
15	c6	418	CLA	CMB-C2B-C1B	-5.53	116.94	125.37
15	bB	803	CLA	C4A-NA-C1A	5.51	109.19	106.71
15	b6	417	CLA	CMB-C2B-C1B	-5.51	116.98	125.37
18	b3	401	BCR	C3-C4-C5	-5.51	104.25	114.08
15	a6	417	CLA	CMB-C2B-C1B	-5.50	116.98	125.37
15	cB	803	CLA	C4A-NA-C1A	5.49	109.17	106.71
15	a6	422	CLA	C2A-C1A-CHA	5.49	133.46	123.86
18	a3	401	BCR	C3-C4-C5	-5.49	104.28	114.08
15	cF	201	CLA	C4A-NA-C1A	5.48	109.17	106.71
18	c3	401	BCR	C3-C4-C5	-5.45	104.34	114.08
15	c5	417	CLA	C4A-NA-C1A	5.43	109.14	106.71
15	c4	417	CLA	C4A-NA-C1A	5.40	109.13	106.71
15	cL	204	CLA	C4A-NA-C1A	5.40	109.13	106.71
15	aB	830	CLA	CMB-C2B-C1B	-5.39	117.16	125.37
15	bB	830	CLA	CMB-C2B-C1B	-5.39	117.16	125.37
15	cB	830	CLA	CMB-C2B-C1B	-5.38	117.18	125.37
15	bL	204	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	aL	203	CLA	C4A-NA-C1A	5.37	109.12	106.71
15	a1	415	CLA	CMC-C2C-C3C	5.35	140.64	126.12
15	c2	417	CLA	CMC-C2C-C3C	5.33	140.59	126.12
15	bA	831	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	bA	813	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	a5	417	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	a2	417	CLA	CMC-C2C-C3C	5.32	140.56	126.12
15	cA	813	CLA	C4A-NA-C1A	5.32	109.10	106.71
15	aA	813	CLA	C4A-NA-C1A	5.31	109.09	106.71
15	aA	831	CLA	C4A-NA-C1A	5.31	109.09	106.71
15	b2	417	CLA	CMC-C2C-C3C	5.29	140.47	126.12
15	c1	416	CLA	CMC-C2C-C3C	5.28	140.46	126.12
15	bA	825	CLA	C4A-NA-C1A	5.28	109.08	106.71
15	a4	417	CLA	C4A-NA-C1A	5.27	109.07	106.71
15	cA	825	CLA	C4A-NA-C1A	5.26	109.07	106.71
15	a2	417	CLA	C2C-C1C-NC	5.25	114.89	109.97
15	cA	831	CLA	C4A-NA-C1A	5.24	109.06	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	416	CLA	CMB-C2B-C1B	-5.24	117.39	125.37
15	a5	416	CLA	CMC-C2C-C3C	5.23	140.31	126.12
15	b5	416	CLA	CMC-C2C-C3C	5.23	140.30	126.12
15	b4	417	CLA	C4A-NA-C1A	5.22	109.05	106.71
15	b1	416	CLA	CMC-C2C-C3C	5.22	140.28	126.12
15	b6	417	CLA	CMC-C2C-C3C	5.22	140.28	126.12
18	a6	402	BCR	C11-C10-C9	-5.22	119.87	127.31
15	c3	416	CLA	CMC-C2C-C3C	5.21	140.27	126.12
18	a3	401	BCR	C11-C10-C9	-5.21	119.87	127.31
15	c5	416	CLA	CMC-C2C-C3C	5.21	140.26	126.12
15	a3	416	CLA	CMC-C2C-C3C	5.21	140.26	126.12
15	b3	416	CLA	CMC-C2C-C3C	5.21	140.25	126.12
15	b5	417	CLA	C4A-NA-C1A	5.20	109.05	106.71
15	a6	417	CLA	CMC-C2C-C3C	5.20	140.25	126.12
15	aA	825	CLA	C4A-NA-C1A	5.20	109.05	106.71
15	c4	416	CLA	CMC-C2C-C3C	5.20	140.24	126.12
15	cA	831	CLA	CMB-C2B-C1B	-5.20	117.45	125.37
18	c3	401	BCR	C11-C10-C9	-5.20	119.89	127.31
15	c6	418	CLA	CMC-C2C-C3C	5.20	140.22	126.12
15	a4	416	CLA	CMC-C2C-C3C	5.19	140.22	126.12
15	b4	416	CLA	CMC-C2C-C3C	5.19	140.21	126.12
18	b3	401	BCR	C11-C10-C9	-5.18	119.92	127.31
15	c2	417	CLA	C2C-C1C-NC	5.17	114.82	109.97
15	bA	831	CLA	CMB-C2B-C1B	-5.17	117.49	125.37
15	a3	416	CLA	CMB-C2B-C1B	-5.17	117.49	125.37
15	b3	416	CLA	CMB-C2B-C1B	-5.17	117.50	125.37
15	b1	416	CLA	CMB-C2B-C1B	-5.17	117.50	125.37
15	b4	405	CLA	C4A-NA-C1A	5.16	109.03	106.71
15	a4	405	CLA	C4A-NA-C1A	5.16	109.02	106.71
15	c4	405	CLA	C4A-NA-C1A	5.16	109.02	106.71
15	aA	831	CLA	CMB-C2B-C1B	-5.15	117.52	125.37
14	bA	801	CL0	C3B-C2B-C1B	-5.15	100.94	107.16
15	a1	415	CLA	CMB-C2B-C1B	-5.15	117.53	125.37
18	b6	402	BCR	C11-C10-C9	-5.15	119.96	127.31
14	aA	801	CL0	C3B-C2B-C1B	-5.14	100.95	107.16
18	c6	403	BCR	C11-C10-C9	-5.13	119.98	127.31
15	c5	405	CLA	CAC-C3C-C4C	5.13	131.47	124.81
14	cA	801	CL0	C3B-C2B-C1B	-5.12	100.97	107.16
15	b6	422	CLA	CBA-CAA-C2A	5.12	128.99	113.86
15	c3	416	CLA	CMB-C2B-C1B	-5.12	117.56	125.37
15	c6	412	CLA	C4A-NA-C1A	5.12	109.01	106.71
15	a6	411	CLA	C4A-NA-C1A	5.12	109.01	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a6	421	BCR	C11-C10-C9	-5.11	120.01	127.31
15	b6	411	CLA	C4A-NA-C1A	5.11	109.00	106.71
15	b5	405	CLA	CAC-C3C-C4C	5.11	131.44	124.81
15	c6	407	CLA	CAC-C3C-C4C	5.10	131.43	124.81
18	a6	402	BCR	C3-C4-C5	-5.10	104.97	114.08
15	b6	406	CLA	CAC-C3C-C4C	5.10	131.42	124.81
18	c6	403	BCR	C3-C4-C5	-5.10	104.98	114.08
15	a3	405	CLA	C4A-NA-C1A	5.09	109.00	106.71
15	c3	405	CLA	C4A-NA-C1A	5.09	108.99	106.71
15	a6	406	CLA	CAC-C3C-C4C	5.09	131.41	124.81
18	b6	402	BCR	C3-C4-C5	-5.09	105.00	114.08
15	bB	830	CLA	O2D-CGD-CBD	5.06	120.25	111.27
15	cB	830	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	aB	830	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	a5	405	CLA	CAC-C3C-C4C	5.04	131.35	124.81
15	cA	831	CLA	CHB-C1B-NB	5.03	129.58	124.26
15	cA	802	CLA	C4A-NA-C1A	5.02	108.96	106.71
15	b2	405	CLA	CAC-C3C-C4C	5.01	131.31	124.81
15	bA	831	CLA	CHB-C1B-NB	5.00	129.55	124.26
15	aA	831	CLA	CHB-C1B-NB	5.00	129.55	124.26
15	b2	417	CLA	C2C-C1C-NC	4.99	114.65	109.97
15	a5	405	CLA	C4A-NA-C1A	4.99	108.95	106.71
15	a2	405	CLA	CAC-C3C-C4C	4.99	131.28	124.81
15	bA	802	CLA	C4A-NA-C1A	4.96	108.94	106.71
15	c2	405	CLA	CAC-C3C-C4C	4.96	131.24	124.81
18	b6	421	BCR	C11-C10-C9	-4.95	120.25	127.31
18	a2	401	BCR	C3-C4-C5	-4.95	105.24	114.08
15	c3	405	CLA	CAC-C3C-C4C	4.94	131.22	124.81
18	b1	419	BCR	C11-C10-C9	-4.94	120.26	127.31
18	c1	419	BCR	C11-C10-C9	-4.94	120.27	127.31
18	a1	418	BCR	C11-C10-C9	-4.94	120.27	127.31
15	b3	405	CLA	CAC-C3C-C4C	4.93	131.20	124.81
15	a1	404	CLA	C4A-NA-C1A	4.92	108.92	106.71
18	c2	401	BCR	C3-C4-C5	-4.91	105.32	114.08
15	aA	802	CLA	C4A-NA-C1A	4.90	108.91	106.71
15	c6	401	CLA	C2A-C1A-CHA	4.89	132.42	123.86
15	b1	405	CLA	CAC-C3C-C4C	4.89	131.15	124.81
18	b2	401	BCR	C3-C4-C5	-4.89	105.35	114.08
15	a3	405	CLA	CAC-C3C-C4C	4.88	131.15	124.81
15	b3	405	CLA	C4A-NA-C1A	4.85	108.89	106.71
15	cB	814	CLA	CBC-CAC-C3C	4.84	125.78	112.43
15	bB	814	CLA	CBC-CAC-C3C	4.84	125.78	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	405	CLA	C4A-NA-C1A	4.84	108.88	106.71
15	aB	814	CLA	CBC-CAC-C3C	4.84	125.77	112.43
15	a4	417	CLA	O2D-CGD-O1D	-4.83	114.39	123.84
15	b2	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	c5	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	c3	410	CLA	CBC-CAC-C3C	4.79	125.64	112.43
18	b2	419	BCR	C29-C30-C25	4.79	117.86	110.48
15	a2	405	CLA	C4A-NA-C1A	4.79	108.86	106.71
15	b2	406	CLA	C1-C2-C3	-4.79	117.77	126.04
15	b3	410	CLA	CBC-CAC-C3C	4.78	125.61	112.43
15	b6	422	CLA	C2A-C1A-CHA	4.77	132.20	123.86
15	c1	405	CLA	C4A-NA-C1A	4.77	108.85	106.71
15	c2	406	CLA	C1-C2-C3	-4.76	117.80	126.04
15	a3	410	CLA	CBC-CAC-C3C	4.76	125.56	112.43
15	c4	405	CLA	CAC-C3C-C4C	4.76	130.99	124.81
15	a2	406	CLA	C1-C2-C3	-4.76	117.81	126.04
15	c4	417	CLA	O2D-CGD-O1D	-4.76	114.54	123.84
14	aA	801	CL0	CAA-C2A-C3A	-4.76	99.75	112.78
15	c2	405	CLA	C4A-NA-C1A	4.76	108.84	106.71
14	bA	801	CL0	CAA-C2A-C3A	-4.75	99.76	112.78
15	c1	405	CLA	CAC-C3C-C4C	4.75	130.97	124.81
14	cA	801	CL0	CAA-C2A-C3A	-4.75	99.78	112.78
18	a2	419	BCR	C29-C30-C25	4.74	117.78	110.48
15	b4	417	CLA	O2D-CGD-O1D	-4.74	114.56	123.84
15	c6	407	CLA	C4A-NA-C1A	4.74	108.84	106.71
18	a4	418	BCR	C29-C30-C25	4.74	117.78	110.48
18	c2	419	BCR	C29-C30-C25	4.73	117.77	110.48
15	b4	405	CLA	CAC-C3C-C4C	4.73	130.94	124.81
15	cB	804	CLA	CAC-C3C-C4C	4.73	130.94	124.81
15	bB	804	CLA	CAC-C3C-C4C	4.72	130.93	124.81
15	b1	410	CLA	CBC-CAC-C3C	4.72	125.43	112.43
15	c5	420	CLA	C2A-C1A-CHA	4.71	132.09	123.86
18	b3	418	BCR	C29-C30-C25	4.70	117.72	110.48
15	c6	401	CLA	CBA-CAA-C2A	4.70	127.74	113.86
15	aB	804	CLA	CAC-C3C-C4C	4.70	130.91	124.81
15	a4	405	CLA	CAC-C3C-C4C	4.70	130.91	124.81
15	a1	404	CLA	CAC-C3C-C4C	4.70	130.90	124.81
15	a5	420	CLA	C2A-C1A-CHA	4.69	132.07	123.86
15	bA	835	CLA	O2D-CGD-O1D	-4.69	114.67	123.84
15	c1	410	CLA	CBC-CAC-C3C	4.68	125.33	112.43
15	cA	835	CLA	O2D-CGD-O1D	-4.68	114.69	123.84
15	b1	405	CLA	C4A-NA-C1A	4.67	108.81	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c3	418	BCR	C29-C30-C25	4.67	117.67	110.48
15	b5	420	CLA	C2A-C1A-CHA	4.67	132.02	123.86
18	b4	418	BCR	C29-C30-C25	4.67	117.67	110.48
18	a3	418	BCR	C29-C30-C25	4.67	117.67	110.48
15	aA	835	CLA	O2D-CGD-O1D	-4.66	114.72	123.84
20	cB	850	LMG	O1-C1-C2	-4.66	101.03	108.30
15	a1	409	CLA	CBC-CAC-C3C	4.66	125.28	112.43
20	bB	851	LMG	O1-C1-C2	-4.66	101.03	108.30
15	b5	410	CLA	CBC-CAC-C3C	4.66	125.27	112.43
20	aB	850	LMG	O1-C1-C2	-4.66	101.03	108.30
15	a6	422	CLA	CAA-C2A-C1A	4.65	127.22	111.97
18	a6	419	BCR	C29-C30-C25	4.65	117.64	110.48
18	c6	420	BCR	C29-C30-C25	4.65	117.64	110.48
15	b6	406	CLA	C4A-NA-C1A	4.65	108.80	106.71
15	a5	410	CLA	CBC-CAC-C3C	4.65	125.25	112.43
15	a6	422	CLA	CED-O2D-CGD	4.64	126.44	115.94
18	a1	417	BCR	C29-C30-C25	4.64	117.63	110.48
15	a1	416	CLA	CMB-C2B-C3B	4.64	137.83	126.59
18	b6	419	BCR	C29-C30-C25	4.64	117.62	110.48
18	c4	418	BCR	C29-C30-C25	4.63	117.61	110.48
15	a6	406	CLA	C4A-NA-C1A	4.62	108.78	106.71
18	b1	418	BCR	C29-C30-C25	4.62	117.59	110.48
15	c5	410	CLA	CBC-CAC-C3C	4.61	125.15	112.43
15	aA	802	CLA	CMB-C2B-C1B	-4.59	118.37	125.37
15	a6	411	CLA	CBC-CAC-C3C	4.59	125.09	112.43
15	cA	802	CLA	CMB-C2B-C1B	-4.59	118.38	125.37
15	c6	412	CLA	CBC-CAC-C3C	4.57	125.03	112.43
19	aA	854	LHG	O4-P-O5	4.57	134.82	112.24
15	bA	802	CLA	CMB-C2B-C1B	-4.56	118.42	125.37
19	cA	853	LHG	O4-P-O5	4.56	134.80	112.24
15	a4	410	CLA	CBC-CAC-C3C	4.56	125.01	112.43
15	b6	411	CLA	CBC-CAC-C3C	4.56	125.00	112.43
19	bA	855	LHG	O4-P-O5	4.56	134.77	112.24
15	cB	814	CLA	C4A-NA-C1A	4.56	108.75	106.71
15	c2	417	CLA	CBC-CAC-C3C	-4.56	99.87	112.43
15	b2	411	CLA	CBC-CAC-C3C	4.55	124.98	112.43
15	c4	421	CLA	C2A-C1A-CHA	4.55	131.82	123.86
18	b1	420	BCR	C2-C1-C6	4.55	117.49	110.48
15	c1	417	CLA	CMB-C2B-C3B	4.55	137.60	126.59
15	b4	421	CLA	C2A-C1A-CHA	4.55	131.81	123.86
18	c1	418	BCR	C29-C30-C25	4.54	117.48	110.48
15	a2	411	CLA	CBC-CAC-C3C	4.54	124.94	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	410	CLA	CBC-CAC-C3C	4.54	124.94	112.43
18	c5	418	BCR	C29-C30-C25	4.53	117.46	110.48
15	b1	417	CLA	CMB-C2B-C3B	4.53	137.57	126.59
15	a1	411	CLA	C4A-NA-C1A	4.53	108.74	106.71
15	b2	417	CLA	CBC-CAC-C3C	-4.52	99.97	112.43
18	a5	418	BCR	C29-C30-C25	4.52	117.44	110.48
15	a4	421	CLA	C2A-C1A-CHA	4.52	131.76	123.86
18	b5	418	BCR	C29-C30-C25	4.52	117.43	110.48
15	a1	415	CLA	C2C-C1C-NC	4.51	114.20	109.97
15	c2	411	CLA	CBC-CAC-C3C	4.51	124.86	112.43
15	b4	410	CLA	CBC-CAC-C3C	4.51	124.86	112.43
15	bB	814	CLA	C4A-NA-C1A	4.49	108.73	106.71
15	aB	814	CLA	C4A-NA-C1A	4.49	108.72	106.71
15	c1	412	CLA	C4A-NA-C1A	4.49	108.72	106.71
15	b1	412	CLA	C4A-NA-C1A	4.48	108.72	106.71
15	b6	422	CLA	CAA-C2A-C1A	4.48	126.64	111.97
15	a5	417	CLA	CMB-C2B-C3B	4.47	137.43	126.59
15	a2	417	CLA	CBC-CAC-C3C	-4.47	100.11	112.43
18	cF	202	BCR	C2-C1-C6	4.45	117.34	110.48
15	a5	416	CLA	CMB-C2B-C3B	4.45	137.36	126.59
18	c1	420	BCR	C2-C1-C6	4.44	117.32	110.48
15	cB	817	CLA	C4A-NA-C1A	4.44	108.70	106.71
15	c2	418	CLA	CMB-C2B-C3B	4.44	137.35	126.59
15	cB	824	CLA	C4A-NA-C1A	4.44	108.70	106.71
15	a2	418	CLA	CMB-C2B-C3B	4.44	137.35	126.59
18	aF	201	BCR	C2-C1-C6	4.44	117.31	110.48
15	a5	417	CLA	O2D-CGD-O1D	-4.44	115.17	123.84
15	c5	417	CLA	CMB-C2B-C3B	4.43	137.33	126.59
18	bB	849	BCR	C2-C1-C6	4.43	117.31	110.48
15	b2	418	CLA	CMB-C2B-C3B	4.43	137.32	126.59
15	b5	417	CLA	CMB-C2B-C3B	4.43	137.32	126.59
15	c5	416	CLA	CMB-C2B-C3B	4.43	137.31	126.59
15	b5	417	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
15	b5	416	CLA	CMB-C2B-C3B	4.42	137.30	126.59
15	c4	416	CLA	CMB-C2B-C3B	4.42	137.30	126.59
15	c5	417	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
15	bB	817	CLA	C4A-NA-C1A	4.41	108.69	106.71
15	c4	421	CLA	CAA-C2A-C1A	4.41	126.42	111.97
15	aB	824	CLA	C4A-NA-C1A	4.41	108.69	106.71
15	a4	417	CLA	CMB-C2B-C3B	4.41	137.26	126.59
15	a4	416	CLA	CMB-C2B-C3B	4.41	137.26	126.59
15	b4	416	CLA	CMB-C2B-C3B	4.41	137.26	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	417	CLA	CMB-C2B-C3B	4.40	137.25	126.59
15	c6	419	CLA	CMB-C2B-C3B	4.40	137.25	126.59
15	aA	819	CLA	CAC-C3C-C4C	4.40	130.52	124.81
14	aA	801	CL0	C3C-C4C-NC	4.40	115.50	110.57
18	a1	419	BCR	C2-C1-C6	4.39	117.25	110.48
15	b6	418	CLA	CMB-C2B-C3B	4.39	137.23	126.59
15	bB	824	CLA	C4A-NA-C1A	4.39	108.68	106.71
15	cA	819	CLA	CAC-C3C-C4C	4.39	130.51	124.81
15	b4	417	CLA	CMB-C2B-C3B	4.39	137.22	126.59
15	b4	421	CLA	CAA-C2A-C1A	4.39	126.35	111.97
15	c3	417	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
15	a6	422	CLA	CBA-CAA-C2A	4.38	126.80	113.86
15	b1	416	CLA	CBC-CAC-C3C	-4.38	100.35	112.43
15	a3	417	CLA	CMB-C2B-C3B	4.38	137.20	126.59
15	a6	418	CLA	CMB-C2B-C3B	4.38	137.20	126.59
15	a4	405	CLA	C2D-C1D-ND	-4.38	106.88	110.10
15	a3	417	CLA	O2D-CGD-O1D	-4.37	115.29	123.84
15	bA	819	CLA	CAC-C3C-C4C	4.37	130.48	124.81
15	c6	401	CLA	CAA-C2A-C1A	4.37	126.29	111.97
15	c2	422	CLA	C2A-C1A-CHA	4.37	131.49	123.86
14	cA	801	CL0	C3C-C4C-NC	4.37	115.47	110.57
15	b3	417	CLA	CMB-C2B-C3B	4.36	137.16	126.59
15	c3	417	CLA	CMB-C2B-C3B	4.36	137.15	126.59
15	a4	421	CLA	CAA-C2A-C1A	4.36	126.26	111.97
14	bA	801	CL0	C3C-C4C-NC	4.35	115.45	110.57
14	bA	801	CL0	C1D-CHD-C4C	-4.35	116.67	126.06
18	b5	401	BCR	C3-C4-C5	-4.35	106.31	114.08
14	cA	801	CL0	C1D-CHD-C4C	-4.35	116.67	126.06
15	aB	817	CLA	C4A-NA-C1A	4.35	108.66	106.71
15	a2	422	CLA	C2A-C1A-CHA	4.35	131.46	123.86
15	b3	417	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
15	c5	420	CLA	CAA-C2A-C1A	4.34	126.21	111.97
18	c5	401	BCR	C3-C4-C5	-4.34	106.32	114.08
14	aA	801	CL0	C1D-CHD-C4C	-4.34	116.70	126.06
15	bB	828	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
19	bA	854	LHG	O4-P-O5	4.33	133.65	112.24
15	c4	405	CLA	C2D-C1D-ND	-4.33	106.92	110.10
19	cA	852	LHG	O4-P-O5	4.32	133.62	112.24
15	a6	413	CLA	C4A-NA-C1A	4.32	108.65	106.71
15	aB	828	CLA	O2D-CGD-O1D	-4.32	115.38	123.84
15	cB	828	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
18	a5	401	BCR	C3-C4-C5	-4.32	106.36	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	aA	853	LHG	O4-P-O5	4.32	133.58	112.24
15	b5	420	CLA	CAA-C2A-C1A	4.31	126.09	111.97
15	a2	417	CLA	CMB-C2B-C3B	4.31	137.02	126.59
15	c2	417	CLA	CMB-C2B-C3B	4.30	137.01	126.59
15	b2	422	CLA	C2A-C1A-CHA	4.30	131.38	123.86
15	b6	417	CLA	CBC-CAC-C3C	-4.30	100.58	112.43
15	a5	420	CLA	CAA-C2A-C1A	4.29	126.04	111.97
15	aA	840	CLA	O2D-CGD-O1D	-4.28	115.46	123.84
15	b5	411	CLA	CMB-C2B-C1B	-4.28	118.86	125.37
15	bA	840	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
15	a2	417	CLA	CHD-C4C-C3C	4.27	131.12	124.84
15	c1	416	CLA	CBC-CAC-C3C	-4.26	100.68	112.43
15	c3	410	CLA	CMC-C2C-C1C	-4.26	118.55	125.04
15	c2	417	CLA	CHD-C4C-C3C	4.26	131.10	124.84
15	c6	418	CLA	CBC-CAC-C3C	-4.26	100.70	112.43
15	cA	840	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
15	b5	412	CLA	C4A-NA-C1A	4.24	108.61	106.71
15	b4	405	CLA	C2D-C1D-ND	-4.24	106.98	110.10
15	c5	411	CLA	CMB-C2B-C1B	-4.24	118.92	125.37
15	b4	410	CLA	CMC-C2C-C1C	-4.24	118.59	125.04
14	aA	801	CL0	C4A-NA-C1A	-4.23	104.81	106.71
20	bB	851	LMG	O1-C7-C8	-4.23	100.70	110.90
15	a4	417	CLA	O2D-CGD-CBD	4.23	118.78	111.27
14	bA	801	CL0	C4A-NA-C1A	-4.22	104.81	106.71
14	cA	801	CL0	C4A-NA-C1A	-4.22	104.81	106.71
20	cB	850	LMG	O1-C7-C8	-4.22	100.71	110.90
15	b6	413	CLA	C4A-NA-C1A	4.22	108.60	106.71
19	bX	101	LHG	O4-P-O5	4.22	133.11	112.24
20	aB	850	LMG	O1-C7-C8	-4.22	100.71	110.90
15	b3	405	CLA	C2D-C1D-ND	-4.22	107.00	110.10
15	b3	410	CLA	CMC-C2C-C1C	-4.22	118.62	125.04
19	aX	101	LHG	O4-P-O5	4.22	133.08	112.24
15	a6	417	CLA	CBC-CAC-C3C	-4.21	100.82	112.43
19	cX	101	LHG	O4-P-O5	4.21	133.06	112.24
15	a5	411	CLA	CMB-C2B-C1B	-4.21	118.96	125.37
15	a1	416	CLA	O2D-CGD-O1D	-4.21	115.61	123.84
15	bB	830	CLA	C2D-C1D-ND	-4.21	107.00	110.10
15	a1	415	CLA	CBC-CAC-C3C	-4.21	100.83	112.43
15	c2	412	CLA	CMB-C2B-C1B	-4.20	118.97	125.37
15	cB	830	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	c1	417	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
15	a2	412	CLA	CMB-C2B-C1B	-4.20	118.97	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	405	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	c5	405	CLA	C2D-C1D-ND	-4.20	107.01	110.10
15	c4	410	CLA	CMC-C2C-C1C	-4.19	118.65	125.04
18	c4	420	BCR	C2-C1-C6	4.19	116.94	110.48
15	b2	417	CLA	CHD-C4C-C3C	4.19	131.00	124.84
15	c5	410	CLA	CMC-C2C-C1C	-4.19	118.66	125.04
15	a1	411	CLA	CHB-C1B-NB	4.19	128.69	124.26
15	a3	410	CLA	CMC-C2C-C1C	-4.19	118.66	125.04
15	b2	412	CLA	CMB-C2B-C1B	-4.19	118.99	125.37
15	a6	418	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
15	aA	828	CLA	C3B-C4B-NB	-4.18	106.64	110.52
15	c4	411	CLA	CMB-C2B-C1B	-4.18	119.00	125.37
18	c3	420	BCR	C2-C1-C6	4.18	116.92	110.48
15	a3	412	CLA	C4A-NA-C1A	4.18	108.58	106.71
15	b6	418	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
15	c6	419	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
15	a1	409	CLA	CMC-C2C-C1C	-4.18	118.68	125.04
15	b1	417	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
18	a3	420	BCR	C2-C1-C6	4.17	116.91	110.48
15	b4	417	CLA	O2D-CGD-CBD	4.17	118.68	111.27
18	b4	420	BCR	C2-C1-C6	4.17	116.90	110.48
15	b1	411	CLA	CMB-C2B-C1B	-4.17	119.02	125.37
15	b2	406	CLA	C2A-C1A-CHA	4.17	131.15	123.86
18	a4	420	BCR	C2-C1-C6	4.17	116.90	110.48
18	b3	420	BCR	C2-C1-C6	4.17	116.90	110.48
15	c2	418	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
15	aB	830	CLA	C2D-C1D-ND	-4.16	107.04	110.10
15	b5	416	CLA	CBC-CAC-C3C	-4.16	100.96	112.43
15	a2	405	CLA	C2D-C1D-ND	-4.16	107.04	110.10
15	c5	416	CLA	CBC-CAC-C3C	-4.16	100.97	112.43
15	c1	410	CLA	CMC-C2C-C1C	-4.16	118.71	125.04
15	b2	417	CLA	CMB-C2B-C3B	4.15	136.65	126.59
18	b2	421	BCR	C2-C1-C6	4.15	116.87	110.48
15	c3	416	CLA	C2C-C1C-NC	4.15	113.86	109.97
15	bA	828	CLA	C3B-C4B-NB	-4.15	106.67	110.52
18	a2	421	BCR	C2-C1-C6	4.15	116.87	110.48
15	c3	416	CLA	CHD-C4C-C3C	4.15	130.94	124.84
15	a5	416	CLA	CBC-CAC-C3C	-4.14	101.01	112.43
15	b1	410	CLA	CMC-C2C-C1C	-4.14	118.73	125.04
15	b5	405	CLA	C2D-C1D-ND	-4.14	107.05	110.10
15	c4	417	CLA	O2D-CGD-CBD	4.14	118.62	111.27
15	c3	405	CLA	C2D-C1D-ND	-4.14	107.06	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	416	CLA	C2C-C1C-NC	4.14	113.85	109.97
15	a4	410	CLA	CMC-C2C-C1C	-4.13	118.75	125.04
15	a3	416	CLA	C2C-C1C-NC	4.13	113.84	109.97
15	a1	410	CLA	CMB-C2B-C1B	-4.12	119.09	125.37
15	b2	405	CLA	C2D-C1D-ND	-4.12	107.07	110.10
15	b2	406	CLA	CAA-CBA-CGA	-4.12	101.21	113.25
15	a3	405	CLA	C2D-C1D-ND	-4.12	107.07	110.10
15	a5	412	CLA	C4A-NA-C1A	4.11	108.56	106.71
15	b2	411	CLA	CMC-C2C-C1C	-4.11	118.78	125.04
15	a2	411	CLA	CMC-C2C-C1C	-4.11	118.78	125.04
15	c2	405	CLA	C2D-C1D-ND	-4.11	107.08	110.10
15	c2	406	CLA	CAA-CBA-CGA	-4.11	101.24	113.25
15	b1	412	CLA	CHB-C1B-NB	4.11	128.61	124.26
15	c6	418	CLA	CMB-C2B-C3B	4.11	136.53	126.59
15	a6	417	CLA	CMB-C2B-C3B	4.10	136.53	126.59
18	c2	421	BCR	C2-C1-C6	4.10	116.80	110.48
15	c1	411	CLA	CMB-C2B-C1B	-4.10	119.12	125.37
15	a2	418	CLA	O2D-CGD-O1D	-4.10	115.82	123.84
15	a1	415	CLA	CHD-C4C-C3C	4.10	130.86	124.84
15	a3	416	CLA	CHD-C4C-C3C	4.09	130.86	124.84
15	a4	411	CLA	CMB-C2B-C1B	-4.09	119.13	125.37
15	a5	410	CLA	CMC-C2C-C1C	-4.09	118.81	125.04
15	a6	417	CLA	CHD-C4C-C3C	4.09	130.85	124.84
15	b3	416	CLA	CHD-C4C-C3C	4.09	130.85	124.84
15	cA	828	CLA	C3B-C4B-NB	-4.09	106.72	110.52
15	a2	406	CLA	CAA-CBA-CGA	-4.09	101.30	113.25
15	cB	811	CLA	CHC-C4B-NB	4.09	128.58	124.26
15	b5	410	CLA	CMC-C2C-C1C	-4.09	118.82	125.04
14	cA	801	CL0	C3D-C4D-ND	4.08	116.84	110.24
15	aB	811	CLA	CHC-C4B-NB	4.08	128.58	124.26
15	c2	406	CLA	C2A-C1A-CHA	4.08	131.00	123.86
15	a2	406	CLA	C2A-C1A-CHA	4.08	130.99	123.86
18	cB	844	BCR	C24-C23-C22	-4.08	120.07	126.23
15	bB	828	CLA	O2D-CGD-CBD	4.08	118.52	111.27
15	c2	413	CLA	CHB-C1B-NB	4.08	128.57	124.26
15	a6	417	CLA	C2C-C1C-NC	4.08	113.79	109.97
15	b6	417	CLA	CMB-C2B-C3B	4.08	136.46	126.59
15	b4	411	CLA	CMB-C2B-C1B	-4.08	119.16	125.37
15	a2	413	CLA	CHB-C1B-NB	4.08	128.57	124.26
15	c6	418	CLA	CHD-C4C-C3C	4.08	130.83	124.84
15	b6	417	CLA	CHD-C4C-C3C	4.08	130.83	124.84
15	bB	811	CLA	CHC-C4B-NB	4.07	128.57	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	411	CLA	CMC-C2C-C1C	-4.07	118.84	125.04
18	aB	844	BCR	C24-C23-C22	-4.07	120.09	126.23
15	bB	830	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
15	b2	418	CLA	O2D-CGD-O1D	-4.07	115.89	123.84
15	cB	828	CLA	O2D-CGD-CBD	4.07	118.49	111.27
15	c6	414	CLA	C4A-NA-C1A	4.06	108.53	106.71
15	b2	413	CLA	CHB-C1B-NB	4.06	128.56	124.26
15	cA	831	CLA	C2B-C1B-NB	-4.06	107.51	110.23
14	bA	801	CL0	C3D-C4D-ND	4.06	116.80	110.24
15	bB	830	CLA	CHB-C1B-NB	4.06	128.55	124.26
15	bA	820	CLA	CMB-C2B-C1B	-4.06	119.19	125.37
15	cB	830	CLA	CHB-C1B-NB	4.06	128.55	124.26
15	c6	401	CLA	C1-C2-C3	-4.05	119.03	126.04
15	aB	828	CLA	O2D-CGD-CBD	4.05	118.47	111.27
18	b5	419	BCR	C2-C1-C6	4.05	116.72	110.48
15	aB	817	CLA	C3B-C4B-NB	-4.05	106.76	110.52
18	bB	844	BCR	C24-C23-C22	-4.05	120.12	126.23
15	c6	418	CLA	C2C-C1C-NC	4.05	113.76	109.97
18	c5	419	BCR	C2-C1-C6	4.04	116.71	110.48
15	b6	417	CLA	C2C-C1C-NC	4.04	113.76	109.97
15	aA	820	CLA	CMB-C2B-C1B	-4.04	119.21	125.37
15	c3	411	CLA	CMB-C2B-C1B	-4.04	119.21	125.37
18	a6	420	BCR	C2-C1-C6	4.04	116.70	110.48
15	cB	817	CLA	C3B-C4B-NB	-4.04	106.77	110.52
15	aB	830	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
14	aA	801	CL0	C3D-C4D-ND	4.04	116.77	110.24
15	cB	830	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
15	bB	817	CLA	C3B-C4B-NB	-4.03	106.77	110.52
15	cB	816	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
15	aB	830	CLA	CHB-C1B-NB	4.03	128.52	124.26
15	cA	804	CLA	C3B-C4B-NB	-4.03	106.78	110.52
15	c5	416	CLA	CHD-C4C-C3C	4.03	130.76	124.84
15	a5	416	CLA	CHD-C4C-C3C	4.02	130.76	124.84
15	aB	816	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
15	bA	804	CLA	C3B-C4B-NB	-4.02	106.78	110.52
15	a6	422	CLA	C1-C2-C3	-4.02	119.09	126.04
15	b3	416	CLA	CBC-CAC-C3C	-4.02	101.35	112.43
15	b2	413	CLA	C4A-NA-C1A	4.02	108.51	106.71
15	c1	416	CLA	CHD-C4C-C3C	4.01	130.74	124.84
18	c6	421	BCR	C2-C1-C6	4.01	116.66	110.48
18	a5	419	BCR	C2-C1-C6	4.01	116.66	110.48
15	b5	416	CLA	CHD-C4C-C3C	4.01	130.74	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	416	CLA	CBC-CAC-C3C	-4.01	101.38	112.43
15	a5	412	CLA	CHB-C1B-NB	4.01	128.50	124.26
15	a4	416	CLA	CHD-C4C-C3C	4.01	130.73	124.84
15	c4	412	CLA	CHB-C1B-NB	4.01	128.50	124.26
15	c4	416	CLA	CHD-C4C-C3C	4.00	130.72	124.84
15	cA	820	CLA	CMB-C2B-C1B	-4.00	119.28	125.37
15	a4	412	CLA	CHB-C1B-NB	4.00	128.49	124.26
15	c3	412	CLA	C4A-NA-C1A	3.99	108.50	106.71
15	aA	804	CLA	C3B-C4B-NB	-3.99	106.81	110.52
18	b6	420	BCR	C2-C1-C6	3.99	116.62	110.48
15	c1	416	CLA	CMB-C2B-C3B	3.99	136.25	126.59
15	bB	816	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
15	c1	412	CLA	CHB-C1B-NB	3.99	128.48	124.26
15	b4	416	CLA	CBC-CAC-C3C	-3.98	101.45	112.43
15	bB	802	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
15	b4	412	CLA	CHB-C1B-NB	3.98	128.47	124.26
15	cB	802	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
15	aA	805	CLA	CMB-C2B-C1B	-3.98	119.31	125.37
15	aB	802	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
15	a3	411	CLA	CMB-C2B-C1B	-3.97	119.32	125.37
15	c4	416	CLA	CBC-CAC-C3C	-3.97	101.49	112.43
15	b4	416	CLA	CHD-C4C-C3C	3.97	130.67	124.84
15	a5	416	CLA	C2C-C1C-NC	3.97	113.69	109.97
15	c5	416	CLA	C2C-C1C-NC	3.96	113.69	109.97
15	c5	412	CLA	CHB-C1B-NB	3.96	128.45	124.26
18	c6	402	BCR	C34-C9-C8	-3.96	111.84	118.08
15	bA	805	CLA	CMB-C2B-C1B	-3.96	119.34	125.37
15	bA	831	CLA	C2B-C1B-NB	-3.96	107.58	110.23
15	c5	412	CLA	C4A-NA-C1A	3.96	108.48	106.71
15	aA	845	CLA	CBC-CAC-C3C	3.95	123.33	112.43
15	cB	803	CLA	CMB-C2B-C1B	-3.95	119.35	125.37
15	cA	844	CLA	CBC-CAC-C3C	3.95	123.33	112.43
15	cA	805	CLA	CMB-C2B-C1B	-3.95	119.35	125.37
15	b5	412	CLA	CHB-C1B-NB	3.95	128.44	124.26
15	cA	838	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
15	c6	412	CLA	CMC-C2C-C1C	-3.94	119.03	125.04
15	b1	416	CLA	CMB-C2B-C3B	3.94	136.14	126.59
15	a5	420	CLA	C1-C2-C3	-3.94	119.22	126.04
15	b5	420	CLA	C1-C2-C3	-3.94	119.23	126.04
15	b1	416	CLA	CHD-C4C-C3C	3.94	130.63	124.84
15	b3	411	CLA	CMB-C2B-C1B	-3.94	119.37	125.37
15	bA	838	CLA	O2D-CGD-O1D	-3.94	116.14	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	413	CLA	C4A-NA-C1A	3.94	108.48	106.71
15	a4	412	CLA	C4A-NA-C1A	3.94	108.48	106.71
15	a6	412	CLA	CMB-C2B-C1B	-3.94	119.37	125.37
15	a4	416	CLA	CBC-CAC-C3C	-3.93	101.58	112.43
15	c5	420	CLA	O2D-CGD-O1D	-3.93	116.14	123.84
18	a6	401	BCR	C34-C9-C8	-3.93	111.88	118.08
15	bA	845	CLA	CBC-CAC-C3C	3.93	123.27	112.43
15	a1	415	CLA	CMB-C2B-C3B	3.93	136.11	126.59
18	cL	205	BCR	C24-C23-C22	-3.93	120.30	126.23
15	a3	416	CLA	CBC-CAC-C3C	-3.93	101.59	112.43
15	aB	803	CLA	CMB-C2B-C1B	-3.93	119.38	125.37
15	bB	803	CLA	CMB-C2B-C1B	-3.93	119.39	125.37
15	a5	420	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
15	b6	411	CLA	CMC-C2C-C1C	-3.93	119.06	125.04
15	a5	417	CLA	O2D-CGD-CBD	3.93	118.25	111.27
15	b6	422	CLA	C1-C2-C3	-3.93	119.25	126.04
15	aA	838	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
15	b5	416	CLA	C2C-C1C-NC	3.92	113.65	109.97
15	aB	840	CLA	CAC-C3C-C4C	3.92	129.90	124.81
15	c6	413	CLA	CMB-C2B-C1B	-3.92	119.40	125.37
15	c5	420	CLA	C1-C2-C3	-3.92	119.27	126.04
15	c1	416	CLA	C2C-C1C-NC	3.92	113.64	109.97
18	b6	401	BCR	C34-C9-C8	-3.92	111.91	118.08
15	b3	412	CLA	CHB-C1B-NB	3.91	128.40	124.26
15	b6	412	CLA	CMB-C2B-C1B	-3.91	119.42	125.37
15	bB	840	CLA	CAC-C3C-C4C	3.91	129.88	124.81
15	cB	840	CLA	CAC-C3C-C4C	3.91	129.88	124.81
18	aI	103	BCR	C24-C23-C22	-3.91	120.33	126.23
15	c3	412	CLA	CHB-C1B-NB	3.90	128.39	124.26
15	aA	831	CLA	C2B-C1B-NB	-3.90	107.61	110.23
18	c1	401	BCR	C34-C9-C8	-3.90	111.93	118.08
15	a6	411	CLA	CMC-C2C-C1C	-3.90	119.10	125.04
15	aB	836	CLA	C3B-C4B-NB	-3.90	106.90	110.52
15	b5	420	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
18	bL	205	BCR	C24-C23-C22	-3.89	120.35	126.23
15	b4	412	CLA	C4A-NA-C1A	3.89	108.46	106.71
15	a3	416	CLA	CMB-C2B-C3B	3.89	136.01	126.59
15	aJ	203	CLA	CAA-C2A-C3A	-3.89	107.02	116.10
15	a3	412	CLA	CHB-C1B-NB	3.89	128.38	124.26
15	c5	417	CLA	O2D-CGD-CBD	3.89	118.18	111.27
15	bJ	102	CLA	CAA-C2A-C3A	-3.89	107.03	116.10
15	b5	417	CLA	O2D-CGD-CBD	3.89	118.18	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	412	CLA	C4A-NA-C1A	3.89	108.45	106.71
18	b6	421	BCR	C3-C4-C5	-3.87	107.16	114.08
15	b3	416	CLA	CMB-C2B-C3B	3.87	135.97	126.59
14	aA	801	CL0	O2D-CGD-O1D	-3.87	116.28	123.84
15	c3	421	CLA	CAA-CBA-CGA	-3.86	101.96	113.25
15	cJ	102	CLA	CAA-C2A-C3A	-3.86	107.09	116.10
15	c3	416	CLA	CMB-C2B-C3B	3.86	135.94	126.59
18	c4	401	BCR	C3-C4-C5	-3.86	107.19	114.08
15	c6	414	CLA	CHB-C1B-NB	3.86	128.34	124.26
18	aA	851	BCR	C24-C23-C22	-3.86	120.41	126.23
18	a4	401	BCR	C2-C1-C6	3.85	116.41	110.48
18	b4	401	BCR	C3-C4-C5	-3.85	107.20	114.08
18	bA	852	BCR	C24-C23-C22	-3.85	120.41	126.23
14	cA	801	CL0	O2D-CGD-O1D	-3.85	116.31	123.84
15	b6	406	CLA	C2D-C1D-ND	-3.85	107.27	110.10
14	bA	801	CL0	O2D-CGD-O1D	-3.85	116.31	123.84
15	cB	836	CLA	C3B-C4B-NB	-3.85	106.94	110.52
15	bB	804	CLA	CMB-C2B-C1B	-3.85	119.51	125.37
18	c4	401	BCR	C2-C1-C6	3.85	116.40	110.48
15	bA	835	CLA	O2D-CGD-CBD	3.85	118.10	111.27
15	c5	417	CLA	CHC-C4B-NB	-3.84	120.19	124.26
15	bB	836	CLA	C3B-C4B-NB	-3.84	106.95	110.52
15	a6	413	CLA	CHB-C1B-NB	3.84	128.32	124.26
15	cB	804	CLA	CMB-C2B-C1B	-3.84	119.52	125.37
15	b6	422	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
18	cA	850	BCR	C24-C23-C22	-3.84	120.43	126.23
15	b1	416	CLA	C2C-C1C-NC	3.84	113.56	109.97
18	a4	401	BCR	C3-C4-C5	-3.83	107.23	114.08
15	b1	405	CLA	C2D-C1D-ND	-3.83	107.28	110.10
15	c6	410	CLA	CMB-C2B-C1B	-3.83	119.53	125.37
15	a5	417	CLA	CHC-C4B-NB	-3.83	120.20	124.26
18	b4	401	BCR	C2-C1-C6	3.83	116.37	110.48
15	aB	815	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
15	a3	421	CLA	CAA-CBA-CGA	-3.82	102.09	113.25
15	cB	815	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
15	a1	404	CLA	C2D-C1D-ND	-3.81	107.30	110.10
15	c6	419	CLA	CHC-C4B-NB	-3.81	120.22	124.26
15	aB	804	CLA	CMB-C2B-C1B	-3.81	119.57	125.37
15	bB	815	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
15	cA	835	CLA	O2D-CGD-CBD	3.81	118.03	111.27
15	cA	803	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
15	aB	814	CLA	C3B-C4B-NB	-3.80	106.99	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	803	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
15	bA	803	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
15	a6	418	CLA	CHC-C4B-NB	-3.79	120.24	124.26
15	cB	814	CLA	C3B-C4B-NB	-3.79	107.00	110.52
15	b3	421	CLA	CAA-CBA-CGA	-3.79	102.18	113.25
15	c6	401	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
15	aA	835	CLA	O2D-CGD-CBD	3.78	117.99	111.27
15	b6	409	CLA	CMB-C2B-C1B	-3.78	119.61	125.37
15	b5	417	CLA	CHC-C4B-NB	-3.78	120.26	124.26
15	b6	418	CLA	CHC-C4B-NB	-3.78	120.26	124.26
15	a6	409	CLA	CMB-C2B-C1B	-3.78	119.62	125.37
15	bB	814	CLA	C3B-C4B-NB	-3.77	107.01	110.52
15	c2	413	CLA	C4A-NA-C1A	3.77	108.40	106.71
15	a6	406	CLA	C2D-C1D-ND	-3.77	107.33	110.10
15	cB	835	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
15	b6	413	CLA	CHB-C1B-NB	3.75	128.23	124.26
15	c6	407	CLA	C2D-C1D-ND	-3.75	107.34	110.10
15	aL	202	CLA	CHB-C4A-NA	3.75	129.69	124.51
15	c5	405	CLA	CAC-C3C-C2C	-3.74	121.12	127.53
15	c1	415	CLA	CHB-C4A-NA	3.74	129.68	124.51
15	bB	835	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
15	aB	835	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
15	b4	417	CLA	CHC-C4B-NB	-3.73	120.30	124.26
15	bA	806	CLA	CAA-C2A-C3A	-3.73	102.56	112.78
18	b1	401	BCR	C11-C10-C9	-3.73	121.99	127.31
15	cA	806	CLA	CAA-C2A-C3A	-3.73	102.57	112.78
15	b5	405	CLA	CAC-C3C-C2C	-3.73	121.16	127.53
15	b2	418	CLA	CHC-C4B-NB	-3.72	120.31	124.26
15	c1	405	CLA	C2D-C1D-ND	-3.72	107.36	110.10
15	cL	203	CLA	CHB-C4A-NA	3.72	129.65	124.51
15	aA	843	CLA	C1-O2A-CGA	3.72	126.19	116.44
15	aA	806	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
15	a2	418	CLA	CHC-C4B-NB	-3.71	120.33	124.26
15	a4	417	CLA	CHC-C4B-NB	-3.71	120.33	124.26
15	cA	842	CLA	C1-O2A-CGA	3.70	126.15	116.44
15	bL	203	CLA	CHB-C4A-NA	3.69	129.62	124.51
15	c6	401	CLA	CAA-CBA-CGA	-3.69	102.47	113.25
15	a4	415	CLA	CHB-C4A-NA	3.69	129.62	124.51
15	bA	843	CLA	C1-O2A-CGA	3.69	126.12	116.44
14	cA	801	CL0	CMD-C2D-C1D	3.68	131.21	124.71
15	bA	832	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
15	c3	417	CLA	O2D-CGD-CBD	3.68	117.81	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	415	CLA	CHB-C4A-NA	3.68	129.60	124.51
15	a1	414	CLA	CHB-C4A-NA	3.68	129.60	124.51
15	bB	833	CLA	CHB-C1B-NB	3.68	128.15	124.26
15	a5	405	CLA	CAC-C3C-C2C	-3.68	121.24	127.53
18	cB	848	BCR	C15-C16-C17	-3.67	115.95	123.47
15	aB	817	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
15	bA	803	CLA	CMB-C2B-C1B	-3.67	119.78	125.37
15	b2	422	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
15	cA	832	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
18	aB	848	BCR	C15-C16-C17	-3.67	115.96	123.47
15	a2	422	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
15	a3	417	CLA	O2D-CGD-CBD	3.66	117.78	111.27
15	b1	415	CLA	CHB-C4A-NA	3.66	129.58	124.51
15	cA	803	CLA	CMB-C2B-C1B	-3.66	119.79	125.37
15	b6	418	CLA	O2D-CGD-CBD	3.66	117.77	111.27
15	a3	415	CLA	CHB-C4A-NA	3.66	129.57	124.51
15	aA	832	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	cB	817	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	bB	817	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
15	c6	407	CLA	CAC-C3C-C2C	-3.66	121.28	127.53
15	c2	422	CLA	C1-C2-C3	-3.65	119.72	126.04
15	bX	102	CLA	CHB-C4A-NA	3.65	129.56	124.51
15	a6	418	CLA	O2D-CGD-CBD	3.65	117.75	111.27
15	c5	415	CLA	CHB-C4A-NA	3.65	129.56	124.51
15	cB	833	CLA	CHB-C1B-NB	3.65	128.12	124.26
15	aX	102	CLA	CHB-C4A-NA	3.65	129.56	124.51
18	aA	850	BCR	C15-C16-C17	-3.65	116.01	123.47
18	bB	848	BCR	C15-C16-C17	-3.65	116.01	123.47
15	b4	415	CLA	CHB-C4A-NA	3.64	129.55	124.51
15	aB	833	CLA	CHB-C1B-NB	3.64	128.12	124.26
15	c4	417	CLA	CHC-C4B-NB	-3.64	120.40	124.26
15	cX	102	CLA	CHB-C4A-NA	3.64	129.55	124.51
15	a1	416	CLA	O2D-CGD-CBD	3.64	117.74	111.27
15	a4	416	CLA	C2C-C1C-NC	3.64	113.38	109.97
15	c2	418	CLA	CHC-C4B-NB	-3.64	120.40	124.26
14	bA	801	CL0	CMD-C2D-C1D	3.64	131.13	124.71
15	b4	416	CLA	C2C-C1C-NC	3.64	113.38	109.97
14	aA	801	CL0	CMD-C2D-C1D	3.64	131.13	124.71
15	c1	417	CLA	O2D-CGD-CBD	3.64	117.73	111.27
15	b3	421	CLA	C2A-C1A-CHA	3.64	130.22	123.86
18	a6	421	BCR	C3-C4-C5	-3.64	107.58	114.08
15	b5	415	CLA	CHB-C4A-NA	3.63	129.53	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	830	CLA	CMB-C2B-C1B	-3.63	119.84	125.37
15	bB	806	CLA	CHB-C4A-NA	3.63	129.53	124.51
18	bA	851	BCR	C15-C16-C17	-3.63	116.05	123.47
15	b6	406	CLA	CAC-C3C-C2C	-3.62	121.33	127.53
18	bA	848	BCR	C15-C16-C17	-3.62	116.05	123.47
15	aB	809	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
15	cA	830	CLA	CMB-C2B-C1B	-3.62	119.85	125.37
15	cB	806	CLA	CHB-C4A-NA	3.62	129.52	124.51
18	cA	849	BCR	C15-C16-C17	-3.62	116.06	123.47
15	c3	421	CLA	C2A-C1A-CHA	3.62	130.19	123.86
18	c1	418	BCR	C2-C1-C6	3.62	116.05	110.48
15	a3	421	CLA	C2A-C1A-CHA	3.62	130.19	123.86
15	c4	412	CLA	C4A-NA-C1A	3.62	108.33	106.71
15	b6	416	CLA	CHB-C4A-NA	3.62	129.52	124.51
15	bB	803	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
18	cK	101	BCR	C15-C16-C17	-3.62	116.06	123.47
15	aB	803	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
15	c4	415	CLA	CHB-C4A-NA	3.61	129.51	124.51
14	aA	801	CL0	CMA-C3A-C2A	-3.61	99.25	113.83
15	a2	405	CLA	CAC-C3C-C2C	-3.61	121.35	127.53
15	aA	803	CLA	CMB-C2B-C1B	-3.61	119.87	125.37
15	a6	422	CLA	C3A-C2A-C1A	3.61	106.75	101.34
15	aA	806	CLA	CHB-C4A-NA	3.61	129.50	124.51
18	a1	417	BCR	C2-C1-C6	3.61	116.03	110.48
14	bA	801	CL0	CMA-C3A-C2A	-3.61	99.27	113.83
15	c6	419	CLA	O2D-CGD-CBD	3.61	117.68	111.27
15	cA	806	CLA	CHB-C4A-NA	3.61	129.50	124.51
15	cB	803	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
15	b2	405	CLA	CAC-C3C-C2C	-3.61	121.36	127.53
15	bA	830	CLA	CMB-C2B-C1B	-3.61	119.88	125.37
15	aB	806	CLA	CHB-C4A-NA	3.60	129.50	124.51
15	b6	422	CLA	CED-O2D-CGD	3.60	124.08	115.94
15	bB	808	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
18	aK	101	BCR	C15-C16-C17	-3.60	116.10	123.47
15	c4	416	CLA	C2C-C1C-NC	3.60	113.34	109.97
14	cA	801	CL0	CMA-C3A-C2A	-3.60	99.32	113.83
15	b1	417	CLA	O2D-CGD-CBD	3.60	117.66	111.27
15	b3	417	CLA	O2D-CGD-CBD	3.60	117.66	111.27
15	bB	802	CLA	CHC-C4B-NB	3.60	128.06	124.26
15	cJ	101	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
15	cB	809	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
15	bA	838	CLA	CMB-C2B-C1B	-3.59	119.90	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a3	418	BCR	C30-C25-C26	-3.59	117.55	122.61
15	c3	415	CLA	CHB-C4A-NA	3.59	129.48	124.51
15	cA	838	CLA	CMB-C2B-C1B	-3.59	119.90	125.37
15	bB	809	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
15	b2	422	CLA	C1-C2-C3	-3.59	119.84	126.04
18	bB	844	BCR	C28-C27-C26	-3.59	107.67	114.08
15	c6	417	CLA	CHB-C4A-NA	3.59	129.47	124.51
15	cB	808	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
15	cA	842	CLA	C3B-C4B-NB	-3.59	107.19	110.52
15	a2	422	CLA	C1-C2-C3	-3.59	119.84	126.04
15	c3	405	CLA	CAC-C3C-C2C	-3.59	121.39	127.53
14	bA	801	CL0	C1C-C2C-C3C	-3.59	103.19	106.96
15	b3	405	CLA	CAC-C3C-C2C	-3.58	121.40	127.53
15	c2	405	CLA	CAC-C3C-C2C	-3.58	121.40	127.53
15	cA	802	CLA	CHB-C1B-NB	3.58	128.05	124.26
14	cA	801	CL0	C1C-C2C-C3C	-3.58	103.19	106.96
18	b3	418	BCR	C30-C25-C26	-3.58	117.57	122.61
18	bB	848	BCR	C24-C23-C22	-3.58	120.83	126.23
15	a6	416	CLA	CHB-C4A-NA	3.58	129.46	124.51
15	a6	406	CLA	CAC-C3C-C2C	-3.58	121.41	127.53
15	aJ	202	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
18	aB	848	BCR	C24-C23-C22	-3.58	120.83	126.23
18	aB	844	BCR	C28-C27-C26	-3.58	107.69	114.08
15	aA	802	CLA	CHB-C1B-NB	3.58	128.04	124.26
15	cB	836	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
15	c3	417	CLA	CHC-C4B-NB	-3.57	120.47	124.26
18	cB	844	BCR	C28-C27-C26	-3.57	107.70	114.08
15	aB	836	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
15	bB	836	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
15	bJ	101	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
15	aA	838	CLA	CMB-C2B-C1B	-3.57	119.93	125.37
14	aA	801	CL0	C1C-C2C-C3C	-3.57	103.20	106.96
18	aJ	205	BCR	C2-C1-C6	3.57	115.97	110.48
15	bA	802	CLA	CHB-C1B-NB	3.57	128.03	124.26
15	a2	422	CLA	O2D-CGD-CBD	3.57	117.61	111.27
15	cB	802	CLA	CHC-C4B-NB	3.56	128.03	124.26
15	a6	422	CLA	CGD-CBD-CAD	-3.56	99.19	110.73
14	bA	801	CL0	C3B-C4B-NB	3.56	113.82	110.52
15	bA	806	CLA	CHB-C4A-NA	3.56	129.44	124.51
18	b2	419	BCR	C2-C1-C6	3.56	115.97	110.48
18	cJ	104	BCR	C2-C1-C6	3.56	115.96	110.48
18	aA	850	BCR	C15-C14-C13	-3.56	122.23	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bA	851	BCR	C15-C14-C13	-3.56	122.23	127.31
15	aB	808	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	c3	421	CLA	CAA-C2A-C1A	3.56	123.64	111.97
18	a1	421	BCR	C3-C4-C5	-3.56	107.72	114.08
18	cB	848	BCR	C24-C23-C22	-3.56	120.86	126.23
18	b2	401	BCR	C2-C1-C6	3.56	115.96	110.48
15	b3	415	CLA	CHB-C4A-NA	3.56	129.43	124.51
15	aA	843	CLA	C3B-C4B-NB	-3.56	107.21	110.52
15	aB	802	CLA	CHC-C4B-NB	3.56	128.03	124.26
15	c2	422	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	cA	839	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
15	a3	417	CLA	CHC-C4B-NB	-3.56	120.49	124.26
15	bA	843	CLA	C3B-C4B-NB	-3.56	107.22	110.52
18	b1	418	BCR	C2-C1-C6	3.55	115.95	110.48
15	a3	421	CLA	CAA-C2A-C1A	3.55	123.62	111.97
15	a3	405	CLA	CAC-C3C-C2C	-3.55	121.45	127.53
15	c2	416	CLA	CHB-C4A-NA	3.55	129.42	124.51
18	bJ	104	BCR	C2-C1-C6	3.55	115.94	110.48
15	c2	418	CLA	O2D-CGD-CBD	3.55	117.58	111.27
15	b3	421	CLA	CAA-C2A-C1A	3.55	123.60	111.97
15	a2	418	CLA	O2D-CGD-CBD	3.55	117.57	111.27
18	cA	849	BCR	C15-C14-C13	-3.55	122.25	127.31
15	bA	839	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
18	c2	401	BCR	C2-C1-C6	3.54	115.94	110.48
15	cA	840	CLA	CHB-C4A-NA	3.54	129.41	124.51
14	cA	801	CL0	C3B-C4B-NB	3.54	113.80	110.52
18	c2	419	BCR	C2-C1-C6	3.54	115.92	110.48
15	b3	417	CLA	CHC-C4B-NB	-3.53	120.52	124.26
15	aA	805	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
15	cA	805	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
18	a2	401	BCR	C2-C1-C6	3.53	115.91	110.48
15	bA	805	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
14	aA	801	CL0	C3B-C4B-NB	3.53	113.79	110.52
15	bB	825	CLA	O2D-CGD-CBD	3.52	117.53	111.27
18	a3	419	BCR	C2-C1-C6	3.52	115.90	110.48
18	bA	853	BCR	C40-C30-C25	3.52	116.01	110.30
15	b3	421	CLA	C1-C2-C3	-3.52	119.96	126.04
15	c3	421	CLA	C1-C2-C3	-3.52	119.96	126.04
15	aB	825	CLA	O2D-CGD-CBD	3.52	117.52	111.27
18	b3	419	BCR	C2-C1-C6	3.52	115.89	110.48
18	c3	419	BCR	C2-C1-C6	3.52	115.89	110.48
18	aA	852	BCR	C40-C30-C25	3.52	116.00	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	839	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
18	a2	419	BCR	C2-C1-C6	3.51	115.89	110.48
15	cB	825	CLA	O2D-CGD-CBD	3.51	117.50	111.27
15	cB	826	CLA	CHB-C4A-NA	3.51	129.37	124.51
15	bA	840	CLA	CHB-C4A-NA	3.51	129.36	124.51
15	aB	827	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
15	aA	840	CLA	CHB-C4A-NA	3.50	129.36	124.51
15	aA	820	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
15	a2	416	CLA	CHB-C4A-NA	3.50	129.36	124.51
18	c3	418	BCR	C30-C25-C26	-3.50	117.68	122.61
15	aB	810	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
15	aA	812	CLA	CAA-CBA-CGA	3.50	123.48	113.25
15	bA	812	CLA	CAA-CBA-CGA	3.50	123.48	113.25
18	b5	401	BCR	C2-C1-C6	3.50	115.87	110.48
15	b2	416	CLA	CHB-C4A-NA	3.50	129.35	124.51
15	cB	840	CLA	CHB-C4A-NA	3.50	129.35	124.51
15	a5	408	CLA	CMB-C2B-C1B	-3.50	120.04	125.37
15	cB	827	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
18	cA	851	BCR	C40-C30-C25	3.50	115.97	110.30
15	bB	810	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
18	b2	419	BCR	C30-C25-C26	-3.50	117.69	122.61
18	a1	420	BCR	C11-C10-C9	-3.49	122.32	127.31
18	b5	418	BCR	C2-C1-C6	3.49	115.86	110.48
18	b2	420	BCR	C11-C10-C9	-3.49	122.33	127.31
18	c1	419	BCR	C34-C9-C10	-3.49	118.03	122.92
15	bB	827	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
15	cB	810	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
15	bB	826	CLA	CHB-C4A-NA	3.49	129.33	124.51
18	c5	401	BCR	C2-C1-C6	3.49	115.85	110.48
15	cA	812	CLA	CAA-CBA-CGA	3.48	123.43	113.25
18	b6	401	BCR	C2-C1-C6	3.48	115.84	110.48
15	aB	840	CLA	CHB-C4A-NA	3.48	129.33	124.51
15	aB	826	CLA	CHB-C4A-NA	3.48	129.32	124.51
15	cA	820	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
15	c6	401	CLA	C3A-C2A-C1A	3.48	106.55	101.34
18	a5	401	BCR	C2-C1-C6	3.48	115.83	110.48
15	b2	418	CLA	O2D-CGD-CBD	3.47	117.44	111.27
14	cA	801	CL0	CMA-C3A-C4A	-3.47	102.44	111.77
18	a5	418	BCR	C2-C1-C6	3.47	115.83	110.48
15	b5	408	CLA	CMB-C2B-C1B	-3.47	120.08	125.37
18	c6	420	BCR	C30-C25-C26	-3.47	117.72	122.61
14	bA	801	CL0	CMA-C3A-C4A	-3.47	102.44	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c2	420	BCR	C11-C10-C9	-3.47	122.36	127.31
15	a3	421	CLA	C1-C2-C3	-3.47	120.04	126.04
15	bA	820	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
18	c5	418	BCR	C2-C1-C6	3.47	115.82	110.48
15	c4	421	CLA	C1-C2-C3	-3.47	120.04	126.04
15	a6	414	CLA	CAC-C3C-C4C	3.47	129.31	124.81
15	b4	405	CLA	CAC-C3C-C2C	-3.47	121.60	127.53
15	aB	817	CLA	CMB-C2B-C3B	3.47	134.99	126.59
18	b6	419	BCR	C30-C25-C26	-3.47	117.73	122.61
15	bB	817	CLA	CMB-C2B-C3B	3.47	134.99	126.59
15	aB	804	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
18	b1	401	BCR	C2-C1-C6	3.47	115.82	110.48
15	b2	422	CLA	CAA-C2A-C1A	3.47	123.33	111.97
18	a6	419	BCR	C30-C25-C26	-3.46	117.74	122.61
18	a4	419	BCR	C2-C1-C6	3.46	115.81	110.48
15	bF	201	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
15	a3	403	CLA	CMB-C2B-C1B	-3.46	120.10	125.37
15	c2	422	CLA	CAA-C2A-C1A	3.46	123.32	111.97
14	aA	801	CL0	CMA-C3A-C4A	-3.46	102.47	111.77
15	b4	421	CLA	C1-C2-C3	-3.46	120.06	126.04
15	a5	420	CLA	C3A-C2A-C1A	3.46	106.52	101.34
18	a4	418	BCR	C30-C25-C26	-3.46	117.74	122.61
15	a4	405	CLA	CAC-C3C-C2C	-3.46	121.61	127.53
15	cA	804	CLA	CHB-C1B-NB	3.46	127.92	124.26
15	cB	804	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
15	a2	422	CLA	CAA-C2A-C1A	3.46	123.31	111.97
15	bB	840	CLA	CHB-C4A-NA	3.46	129.29	124.51
15	bB	804	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
18	a6	402	BCR	C2-C1-C6	3.46	115.80	110.48
15	c5	420	CLA	C3A-C2A-C1A	3.46	106.52	101.34
18	c6	402	BCR	C2-C1-C6	3.46	115.80	110.48
15	b2	422	CLA	O2D-CGD-CBD	3.45	117.41	111.27
15	cB	838	CLA	CHB-C4A-NA	3.45	129.29	124.51
18	c6	403	BCR	C2-C1-C6	3.45	115.80	110.48
15	c5	408	CLA	CMB-C2B-C1B	-3.45	120.11	125.37
14	bA	801	CL0	C3D-C2D-C1D	-3.45	101.12	105.83
14	cA	801	CL0	C3D-C2D-C1D	-3.45	101.12	105.83
15	aJ	201	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
18	c4	419	BCR	C2-C1-C6	3.45	115.79	110.48
18	b4	418	BCR	C30-C25-C26	-3.45	117.76	122.61
15	bA	822	CLA	CHB-C1B-NB	3.45	127.91	124.26
15	cB	817	CLA	CMB-C2B-C3B	3.44	134.93	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	844	CLA	CHB-C4A-NA	3.44	129.28	124.51
15	b3	403	CLA	CMB-C2B-C1B	-3.44	120.13	125.37
18	a2	420	BCR	C11-C10-C9	-3.44	122.40	127.31
15	bA	804	CLA	CHB-C1B-NB	3.44	127.90	124.26
15	aA	804	CLA	CHB-C1B-NB	3.44	127.90	124.26
15	cF	203	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
18	bA	848	BCR	C15-C14-C13	-3.44	122.41	127.31
18	aK	101	BCR	C15-C14-C13	-3.43	122.41	127.31
18	aL	205	BCR	C2-C1-C6	3.43	115.77	110.48
18	b5	418	BCR	C30-C25-C26	-3.43	117.78	122.61
16	bA	846	PQN	C11-C12-C13	-3.43	121.08	126.79
18	c4	418	BCR	C30-C25-C26	-3.43	117.78	122.61
18	c5	401	BCR	C11-C10-C9	-3.43	122.41	127.31
18	bL	201	BCR	C2-C1-C6	3.43	115.76	110.48
15	c4	405	CLA	CAC-C3C-C2C	-3.43	121.66	127.53
15	c2	422	CLA	O2D-CGD-CBD	3.43	117.36	111.27
18	b4	419	BCR	C2-C1-C6	3.43	115.76	110.48
15	bB	838	CLA	CHB-C4A-NA	3.43	129.25	124.51
18	bJ	103	BCR	C15-C16-C17	-3.43	116.45	123.47
18	b6	402	BCR	C2-C1-C6	3.43	115.76	110.48
15	bA	844	CLA	CHB-C4A-NA	3.43	129.25	124.51
18	cK	101	BCR	C15-C14-C13	-3.43	122.42	127.31
15	c4	408	CLA	CMB-C2B-C1B	-3.43	120.15	125.37
14	aA	801	CL0	C3D-C2D-C1D	-3.42	101.16	105.83
15	aA	822	CLA	CHB-C1B-NB	3.42	127.88	124.26
15	aB	838	CLA	CHB-C4A-NA	3.42	129.25	124.51
18	a6	401	BCR	C2-C1-C6	3.42	115.75	110.48
18	bA	849	BCR	C15-C16-C17	-3.42	116.47	123.47
15	a1	407	CLA	CMB-C2B-C1B	-3.42	120.16	125.37
18	bL	206	BCR	C2-C1-C6	3.42	115.74	110.48
18	aJ	204	BCR	C15-C16-C17	-3.42	116.47	123.47
18	aA	848	BCR	C15-C16-C17	-3.41	116.48	123.47
16	aA	846	PQN	C11-C12-C13	-3.41	121.11	126.79
15	c1	408	CLA	CMB-C2B-C1B	-3.41	120.17	125.37
18	a1	418	BCR	C34-C9-C10	-3.41	118.15	122.92
18	cJ	103	BCR	C15-C16-C17	-3.41	116.49	123.47
18	c4	418	BCR	C2-C1-C6	3.41	115.73	110.48
15	bB	833	CLA	C3B-C4B-NB	-3.41	107.36	110.52
18	cA	847	BCR	C15-C16-C17	-3.40	116.50	123.47
15	cA	843	CLA	CHB-C4A-NA	3.40	129.22	124.51
18	a2	419	BCR	C30-C25-C26	-3.40	117.82	122.61
15	b5	420	CLA	C3A-C2A-C1A	3.40	106.43	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c5	418	BCR	C30-C25-C26	-3.39	117.83	122.61
16	cA	845	PQN	C11-C12-C13	-3.39	121.14	126.79
15	a2	413	CLA	CMC-C2C-C1C	-3.39	119.87	125.04
18	b4	418	BCR	C2-C1-C6	3.39	115.71	110.48
18	a5	401	BCR	C11-C10-C9	-3.39	122.47	127.31
15	aB	833	CLA	C3B-C4B-NB	-3.39	107.37	110.52
15	a4	421	CLA	C1-C2-C3	-3.39	120.18	126.04
15	aA	818	CLA	CHB-C4A-NA	3.39	129.20	124.51
15	b1	408	CLA	CMB-C2B-C1B	-3.39	120.21	125.37
15	b5	412	CLA	CMC-C2C-C1C	-3.39	119.88	125.04
15	cA	842	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
18	b1	419	BCR	C34-C9-C10	-3.39	118.18	122.92
15	aA	843	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
18	a5	418	BCR	C30-C25-C26	-3.38	117.85	122.61
15	bB	836	CLA	CHB-C1B-NB	3.38	127.84	124.26
15	aB	832	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
15	aB	836	CLA	CHB-C1B-NB	3.38	127.84	124.26
15	b1	405	CLA	CAC-C3C-C2C	-3.38	121.75	127.53
15	a4	408	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
15	c3	403	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
14	aA	801	CL0	CHD-C1D-ND	-3.38	121.35	124.45
18	a4	418	BCR	C2-C1-C6	3.38	115.68	110.48
15	b2	413	CLA	CMC-C2C-C1C	-3.37	119.90	125.04
18	bA	851	BCR	C24-C23-C22	-3.37	121.14	126.23
18	b2	401	BCR	C7-C8-C9	-3.37	121.14	126.23
15	a5	412	CLA	CMC-C2C-C1C	-3.37	119.90	125.04
15	b6	422	CLA	C6-C5-C3	-3.37	104.61	113.45
15	bB	814	CLA	C1-C2-C3	-3.37	120.21	126.04
18	cA	849	BCR	C24-C23-C22	-3.37	121.14	126.23
15	c1	405	CLA	CAC-C3C-C2C	-3.37	121.77	127.53
15	aL	201	CLA	C3B-C4B-NB	-3.37	107.39	110.52
15	bA	818	CLA	CHB-C4A-NA	3.37	129.17	124.51
15	aB	814	CLA	CMB-C2B-C1B	-3.37	120.24	125.37
15	bL	202	CLA	C3B-C4B-NB	-3.37	107.39	110.52
14	bA	801	CL0	CHD-C1D-ND	-3.36	121.36	124.45
18	b2	420	BCR	C2-C1-C6	3.36	115.66	110.48
15	c5	412	CLA	CMC-C2C-C1C	-3.36	119.92	125.04
14	cA	801	CL0	CHD-C1D-ND	-3.36	121.37	124.45
15	bB	814	CLA	CMB-C2B-C1B	-3.36	120.26	125.37
15	bA	843	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
15	cA	822	CLA	CHB-C1B-NB	3.36	127.81	124.26
15	cB	832	CLA	O2D-CGD-O1D	-3.35	117.28	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aA	850	BCR	C24-C23-C22	-3.35	121.17	126.23
15	aA	813	CLA	CHB-C1B-NB	3.35	127.80	124.26
15	cA	818	CLA	CHB-C4A-NA	3.35	129.15	124.51
15	b4	408	CLA	CMB-C2B-C1B	-3.35	120.27	125.37
18	bB	847	BCR	C40-C30-C25	3.35	115.73	110.30
15	cB	814	CLA	C1-C2-C3	-3.35	120.25	126.04
18	bF	202	BCR	C16-C15-C14	-3.35	116.62	123.47
18	c2	401	BCR	C7-C8-C9	-3.35	121.18	126.23
15	cA	837	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
18	c2	420	BCR	C2-C1-C6	3.35	115.63	110.48
15	cB	814	CLA	CMB-C2B-C1B	-3.35	120.27	125.37
18	a2	420	BCR	C2-C1-C6	3.34	115.63	110.48
18	b5	401	BCR	C11-C10-C9	-3.34	122.54	127.31
15	cB	833	CLA	C3B-C4B-NB	-3.34	107.42	110.52
15	bB	832	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
18	cF	204	BCR	C16-C15-C14	-3.34	116.63	123.47
18	c3	418	BCR	C2-C1-C6	3.34	115.62	110.48
15	a5	403	CLA	CMB-C2B-C1B	-3.34	120.28	125.37
15	c6	419	CLA	C2B-C1B-NB	3.34	112.47	110.23
15	bA	837	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
15	aB	814	CLA	C1-C2-C3	-3.34	120.28	126.04
15	aA	837	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
14	cA	801	CL0	CBC-CAC-C3C	-3.33	103.24	112.43
15	cF	203	CLA	CMB-C2B-C1B	-3.33	120.29	125.37
14	bA	801	CL0	CBC-CAC-C3C	-3.33	103.25	112.43
15	bB	816	CLA	CHB-C4A-NA	3.33	129.12	124.51
15	aA	813	CLA	C3B-C4B-NB	-3.33	107.42	110.52
15	b2	403	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
15	bA	813	CLA	CHB-C1B-NB	3.33	127.78	124.26
15	a1	414	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
15	aA	827	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
18	aB	847	BCR	C40-C30-C25	3.33	115.69	110.30
15	cA	813	CLA	C3B-C4B-NB	-3.33	107.43	110.52
15	c2	422	CLA	CGD-CBD-CAD	-3.33	99.96	110.73
15	cA	827	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
18	aF	202	BCR	C16-C15-C14	-3.33	116.66	123.47
18	b6	419	BCR	C2-C1-C6	3.32	115.60	110.48
15	cB	836	CLA	CHB-C1B-NB	3.32	127.78	124.26
14	aA	801	CL0	CBC-CAC-C3C	-3.32	103.27	112.43
18	c6	420	BCR	C2-C1-C6	3.32	115.59	110.48
15	b2	406	CLA	C3B-C4B-NB	-3.32	107.43	110.52
15	bA	827	CLA	O2D-CGD-O1D	-3.32	117.35	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c2	419	BCR	C30-C25-C26	-3.32	117.94	122.61
15	aB	816	CLA	CHB-C4A-NA	3.32	129.10	124.51
18	cB	847	BCR	C40-C30-C25	3.31	115.67	110.30
18	bB	848	BCR	C11-C10-C9	-3.31	122.58	127.31
15	a2	406	CLA	C6-C5-C3	-3.31	104.77	113.45
15	a2	422	CLA	CGD-CBD-CAD	-3.31	100.01	110.73
15	a6	422	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	cA	813	CLA	CHB-C1B-NB	3.31	127.76	124.26
15	c2	406	CLA	C6-C5-C3	-3.31	104.78	113.45
15	aA	804	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	c6	401	CLA	C6-C5-C3	-3.31	104.78	113.45
18	c1	401	BCR	C11-C10-C9	-3.31	122.59	127.31
15	a2	406	CLA	C3B-C4B-NB	-3.31	107.45	110.52
18	a6	419	BCR	C2-C1-C6	3.31	115.57	110.48
15	b1	403	CLA	CMB-C2B-C1B	-3.30	120.34	125.37
18	cB	846	BCR	C15-C16-C17	-3.30	116.71	123.47
15	cL	202	CLA	C3B-C4B-NB	-3.30	107.45	110.52
15	bA	813	CLA	C3B-C4B-NB	-3.30	107.45	110.52
15	bA	804	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
15	aJ	201	CLA	CMB-C2B-C1B	-3.30	120.34	125.37
15	c2	406	CLA	C3B-C4B-NB	-3.30	107.45	110.52
15	cB	816	CLA	CHB-C4A-NA	3.30	129.07	124.51
18	a2	401	BCR	C7-C8-C9	-3.30	121.25	126.23
15	a1	404	CLA	CAC-C3C-C2C	-3.30	121.89	127.53
15	cA	804	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
15	b2	406	CLA	C6-C5-C3	-3.30	104.81	113.45
15	b5	403	CLA	CMB-C2B-C1B	-3.30	120.35	125.37
18	a1	420	BCR	C2-C1-C6	3.30	115.56	110.48
19	bA	855	LHG	O8-C23-C24	3.30	120.02	111.38
19	cA	853	LHG	O8-C23-C24	3.30	120.02	111.38
18	bL	205	BCR	C11-C10-C9	-3.29	122.61	127.31
18	bB	846	BCR	C15-C16-C17	-3.29	116.73	123.47
15	bB	830	CLA	C2B-C1B-NB	-3.29	108.02	110.23
15	bJ	101	CLA	CHB-C4A-NA	3.29	129.07	124.51
18	cB	848	BCR	C11-C10-C9	-3.29	122.61	127.31
15	bF	201	CLA	CMB-C2B-C1B	-3.29	120.35	125.37
15	cA	809	CLA	CHB-C4A-NA	3.29	129.06	124.51
15	c5	403	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
15	aB	820	CLA	C3B-C4B-NB	-3.29	107.46	110.52
18	cJ	103	BCR	C15-C14-C13	-3.29	122.62	127.31
15	aB	818	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
15	c5	410	CLA	C2D-C1D-ND	-3.29	107.68	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	809	CLA	CHB-C4A-NA	3.29	129.06	124.51
15	a6	413	CLA	CMC-C2C-C1C	-3.29	120.04	125.04
15	b2	422	CLA	CGD-CBD-CAD	-3.28	100.10	110.73
18	aB	846	BCR	C15-C16-C17	-3.28	116.75	123.47
18	aB	848	BCR	C11-C10-C9	-3.28	122.62	127.31
15	cB	818	CLA	CMB-C2B-C1B	-3.28	120.37	125.37
15	bA	810	CLA	CHB-C4A-NA	3.28	129.05	124.51
15	cA	816	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
15	aA	834	CLA	CHB-C4A-NA	3.28	129.05	124.51
18	a3	418	BCR	C2-C1-C6	3.28	115.53	110.48
15	a1	402	CLA	CMB-C2B-C1B	-3.28	120.38	125.37
19	aA	854	LHG	O8-C23-C24	3.28	119.98	111.38
15	c1	403	CLA	CMB-C2B-C1B	-3.28	120.38	125.37
15	cB	830	CLA	C2B-C1B-NB	-3.28	108.04	110.23
15	cA	810	CLA	CHB-C4A-NA	3.28	129.04	124.51
15	c1	405	CLA	CHD-C1D-ND	-3.27	121.44	124.45
18	cB	848	BCR	C2-C1-C6	3.27	115.52	110.48
15	bB	818	CLA	CMB-C2B-C1B	-3.27	120.38	125.37
15	a3	408	CLA	CMB-C2B-C1B	-3.27	120.39	125.37
15	aA	809	CLA	CHB-C4A-NA	3.27	129.04	124.51
15	aJ	202	CLA	CHB-C4A-NA	3.27	129.03	124.51
18	aF	203	BCR	C2-C1-C6	3.27	115.51	110.48
18	bJ	105	BCR	C2-C1-C6	3.27	115.51	110.48
15	c2	413	CLA	CMC-C2C-C1C	-3.27	120.06	125.04
15	cA	807	CLA	C3B-C4B-NB	-3.27	107.48	110.52
18	c3	420	BCR	C28-C27-C26	-3.27	108.25	114.08
15	b3	408	CLA	CMB-C2B-C1B	-3.27	120.40	125.37
15	bB	825	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
15	aA	810	CLA	CHB-C4A-NA	3.26	129.02	124.51
15	aB	825	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
18	aB	848	BCR	C2-C1-C6	3.26	115.50	110.48
15	aB	810	CLA	CBA-CAA-C2A	-3.26	104.24	113.86
15	cJ	101	CLA	CHB-C4A-NA	3.26	129.02	124.51
15	aA	807	CLA	C3B-C4B-NB	-3.26	107.49	110.52
18	bJ	103	BCR	C15-C14-C13	-3.26	122.66	127.31
15	a2	418	CLA	C2B-C1B-NB	3.26	112.42	110.23
15	cB	810	CLA	CBA-CAA-C2A	-3.26	104.25	113.86
15	aA	816	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
15	aA	845	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
18	aJ	204	BCR	C15-C14-C13	-3.25	122.67	127.31
15	c2	403	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
15	c6	405	CLA	CMB-C2B-C1B	-3.25	120.42	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	833	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
15	aA	809	CLA	C3B-C4B-NB	-3.25	107.50	110.52
15	bA	830	CLA	CHB-C4A-NA	3.25	129.00	124.51
18	b3	418	BCR	C2-C1-C6	3.25	115.48	110.48
15	bB	810	CLA	CBA-CAA-C2A	-3.25	104.28	113.86
15	cB	833	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	cB	825	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	b5	410	CLA	C2D-C1D-ND	-3.25	107.71	110.10
15	b2	406	CLA	C16-C15-C13	-3.25	105.42	115.92
18	b2	401	BCR	C15-C14-C13	-3.25	122.68	127.31
15	cB	820	CLA	C3B-C4B-NB	-3.25	107.50	110.52
18	c2	401	BCR	C15-C14-C13	-3.25	122.68	127.31
15	aB	833	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
15	cB	803	CLA	CMB-C2B-C3B	3.24	134.45	126.59
15	a1	415	CLA	CHB-C4A-NA	3.24	129.00	124.51
15	b1	405	CLA	CHD-C1D-ND	-3.24	121.47	124.45
15	bB	803	CLA	CMB-C2B-C3B	3.24	134.44	126.59
15	bB	836	CLA	O2D-CGD-CBD	3.24	117.03	111.27
15	aB	836	CLA	O2D-CGD-CBD	3.24	117.03	111.27
15	bB	820	CLA	C3B-C4B-NB	-3.24	107.51	110.52
15	cL	204	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
15	cA	830	CLA	CHB-C4A-NA	3.24	128.99	124.51
15	cB	836	CLA	O2D-CGD-CBD	3.24	117.02	111.27
15	aL	203	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
18	cL	205	BCR	C11-C10-C9	-3.24	122.69	127.31
15	aB	830	CLA	C2B-C1B-NB	-3.24	108.06	110.23
15	bA	834	CLA	CHB-C4A-NA	3.23	128.99	124.51
18	cA	848	BCR	C2-C1-C6	3.23	115.46	110.48
15	cB	837	CLA	C3B-C4B-NB	-3.23	107.52	110.52
15	bA	809	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	a1	419	BCR	C28-C27-C26	-3.23	108.31	114.08
15	bA	816	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	c2	404	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	a2	404	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	cB	823	CLA	CHB-C4A-NA	3.23	128.98	124.51
15	c6	414	CLA	CMC-C2C-C1C	-3.23	120.12	125.04
15	cB	838	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
15	c1	415	CLA	CMB-C2B-C1B	-3.23	120.45	125.37
15	aA	830	CLA	CHB-C4A-NA	3.23	128.98	124.51
15	aB	803	CLA	CMB-C2B-C3B	3.23	134.41	126.59
18	a1	421	BCR	C2-C1-C6	3.23	115.45	110.48
15	bL	204	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aI	103	BCR	C11-C10-C9	-3.23	122.70	127.31
15	cB	819	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
15	c1	416	CLA	CHB-C4A-NA	3.23	128.97	124.51
18	a3	420	BCR	C28-C27-C26	-3.22	108.32	114.08
15	cA	834	CLA	CHB-C4A-NA	3.22	128.97	124.51
15	bA	809	CLA	C3B-C4B-NB	-3.22	107.53	110.52
15	c4	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
18	cF	205	BCR	C2-C1-C6	3.22	115.44	110.48
15	cA	844	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
18	b1	418	BCR	C30-C25-C26	-3.22	118.08	122.61
15	a5	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
15	b4	410	CLA	C2D-C1D-ND	-3.22	107.73	110.10
15	bB	823	CLA	CHB-C4A-NA	3.22	128.96	124.51
15	cA	809	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
15	aA	809	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
15	bB	838	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	aA	849	BCR	C2-C1-C6	3.22	115.43	110.48
18	bB	848	BCR	C2-C1-C6	3.22	115.43	110.48
15	c3	408	CLA	CMB-C2B-C1B	-3.22	120.47	125.37
15	b3	408	CLA	C2D-C1D-ND	-3.21	107.73	110.10
16	cB	843	PQN	C11-C12-C13	-3.21	121.44	126.79
15	aA	831	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
15	bL	203	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
15	a2	417	CLA	CHB-C4A-NA	3.21	128.96	124.51
18	c1	401	BCR	C2-C1-C6	3.21	115.43	110.48
15	a6	422	CLA	O2D-CGD-CBD	3.21	116.98	111.27
15	bA	808	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	bA	850	BCR	C2-C1-C6	3.21	115.42	110.48
15	b1	417	CLA	CHC-C4B-NB	-3.21	120.86	124.26
15	c2	416	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
18	b1	401	BCR	C34-C9-C8	-3.21	113.03	118.08
15	aL	202	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
15	bB	825	CLA	CHB-C4A-NA	3.21	128.94	124.51
15	cA	808	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
15	a1	404	CLA	CHD-C1D-ND	-3.20	121.51	124.45
15	c2	418	CLA	C2B-C1B-NB	3.20	112.38	110.23
15	b4	415	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
15	a4	410	CLA	C2D-C1D-ND	-3.20	107.74	110.10
15	aA	804	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
18	bB	847	BCR	C27-C26-C25	3.20	127.38	122.73
15	bB	819	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
14	aA	801	CL0	C4C-C3C-C2C	-3.20	102.23	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	420	BCR	C28-C27-C26	-3.20	108.36	114.08
15	bB	835	CLA	CHB-C4A-NA	3.20	128.94	124.51
15	bA	807	CLA	C3B-C4B-NB	-3.20	107.54	110.52
15	bA	845	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	b5	420	CLA	CHB-C4A-NA	3.20	128.94	124.51
15	cA	804	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
18	b4	420	BCR	C28-C27-C26	-3.20	108.36	114.08
15	aB	823	CLA	CHB-C4A-NA	3.20	128.94	124.51
15	aB	812	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	bA	831	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
15	b1	405	CLA	CMD-C2D-C1D	3.20	130.35	124.71
15	b2	409	CLA	CMB-C2B-C1B	-3.20	120.50	125.37
18	c2	421	BCR	C28-C27-C26	-3.20	108.37	114.08
15	bB	837	CLA	C3B-C4B-NB	-3.20	107.55	110.52
18	c6	402	BCR	C11-C10-C9	-3.20	122.75	127.31
18	a1	417	BCR	C30-C25-C26	-3.20	118.11	122.61
18	a4	420	BCR	C28-C27-C26	-3.20	108.37	114.08
15	a2	416	CLA	CMB-C2B-C1B	-3.19	120.50	125.37
15	bA	804	CLA	CMD-C2D-C1D	-3.19	119.08	124.71
15	b1	415	CLA	CMB-C2B-C1B	-3.19	120.50	125.37
15	cA	840	CLA	CHC-C4B-NB	3.19	127.64	124.26
15	c5	420	CLA	CHB-C4A-NA	3.19	128.93	124.51
15	a4	405	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
16	bB	843	PQN	C11-C12-C13	-3.19	121.48	126.79
18	a2	421	BCR	C28-C27-C26	-3.19	108.38	114.08
18	b3	418	BCR	C3-C4-C5	-3.19	108.38	114.08
15	aB	825	CLA	CHB-C4A-NA	3.19	128.93	124.51
15	a6	404	CLA	CMB-C2B-C1B	-3.19	120.51	125.37
15	b2	418	CLA	C2B-C1B-NB	3.19	112.37	110.23
15	aA	815	CLA	C3B-C4B-NB	-3.19	107.56	110.52
15	cB	835	CLA	CHB-C4A-NA	3.19	128.92	124.51
15	bB	837	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
15	cA	809	CLA	C3B-C4B-NB	-3.19	107.56	110.52
15	cF	203	CLA	C3B-C4B-NB	-3.19	107.56	110.52
18	c4	420	BCR	C28-C27-C26	-3.19	108.39	114.08
15	bA	840	CLA	CHC-C4B-NB	3.19	127.63	124.26
15	bB	812	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
15	b1	416	CLA	CHB-C4A-NA	3.19	128.92	124.51
15	c6	401	CLA	CED-O2D-CGD	3.19	123.14	115.94
15	bA	845	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
15	cA	831	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
14	bA	801	CL0	C4C-C3C-C2C	-3.18	102.26	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	801	CL0	C4C-C3C-C2C	-3.18	102.26	106.90
15	cF	203	CLA	CHB-C1B-NB	3.18	127.63	124.26
15	aA	845	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
15	cA	844	CLA	O2A-CGA-O1A	-3.18	115.56	123.59
15	aB	817	CLA	CMB-C2B-C1B	-3.18	120.52	125.37
18	c1	418	BCR	C30-C25-C26	-3.18	118.13	122.61
15	aB	838	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
15	b6	406	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
15	cB	812	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	aB	819	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	c6	417	CLA	CMB-C2B-C1B	-3.18	120.52	125.37
15	cL	203	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	aJ	201	CLA	CHB-C1B-NB	3.18	127.62	124.26
15	bA	815	CLA	C3B-C4B-NB	-3.18	107.56	110.52
15	aB	835	CLA	CHB-C4A-NA	3.18	128.91	124.51
15	aB	809	CLA	CBA-CAA-C2A	3.18	123.25	113.86
18	a2	401	BCR	C15-C14-C13	-3.18	122.77	127.31
15	cB	825	CLA	CHB-C4A-NA	3.18	128.91	124.51
15	a3	412	CLA	CMC-C2C-C1C	-3.18	120.20	125.04
15	a3	421	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
15	bF	201	CLA	CHB-C1B-NB	3.18	127.62	124.26
15	cB	817	CLA	CMB-C2B-C1B	-3.18	120.53	125.37
15	b6	418	CLA	C2B-C1B-NB	3.18	112.36	110.23
15	aA	808	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
15	aB	837	CLA	C3B-C4B-NB	-3.18	107.57	110.52
15	bB	811	CLA	CHB-C4A-NA	3.18	128.90	124.51
15	b2	417	CLA	CHB-C4A-NA	3.18	128.90	124.51
15	bB	829	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
18	a6	401	BCR	C11-C10-C9	-3.17	122.78	127.31
16	aB	843	PQN	C11-C12-C13	-3.17	121.51	126.79
15	b2	416	CLA	CMB-C2B-C1B	-3.17	120.53	125.37
15	a3	410	CLA	C2D-C1D-ND	-3.17	107.77	110.10
18	aB	847	BCR	C27-C26-C25	3.17	127.34	122.73
15	c1	405	CLA	CMD-C2D-C1D	3.17	130.31	124.71
15	b4	415	CLA	CMB-C2B-C1B	-3.17	120.54	125.37
15	c2	406	CLA	C16-C15-C13	-3.17	105.67	115.92
15	cB	811	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	aB	811	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	cB	837	CLA	CHB-C4A-NA	3.17	128.90	124.51
15	aB	841	CLA	C3B-C4B-NB	-3.17	107.57	110.52
15	cB	809	CLA	CBA-CAA-C2A	3.17	123.22	113.86
15	cB	814	CLA	CHB-C1B-NB	3.17	127.61	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cB	847	BCR	C27-C26-C25	3.17	127.33	122.73
15	b3	412	CLA	CMC-C2C-C1C	-3.17	120.21	125.04
15	aB	837	CLA	CHB-C4A-NA	3.17	128.89	124.51
18	b6	421	BCR	C2-C1-C6	3.17	115.36	110.48
14	cA	801	CL0	CHC-C1C-C2C	-3.17	117.93	126.73
15	b4	405	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
15	b3	421	CLA	CHA-C1A-NA	-3.17	119.15	126.40
15	bB	809	CLA	CBA-CAA-C2A	3.17	123.21	113.86
15	bA	820	CLA	O2D-CGD-CBD	3.16	116.89	111.27
20	aB	850	LMG	O6-C1-O1	-3.16	102.48	109.97
20	bB	851	LMG	O6-C1-O1	-3.16	102.48	109.97
15	bA	832	CLA	O2D-CGD-CBD	3.16	116.89	111.27
15	b6	404	CLA	CMB-C2B-C1B	-3.16	120.55	125.37
15	c4	405	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
14	bA	801	CL0	CHC-C1C-C2C	-3.16	117.94	126.73
15	bB	837	CLA	CHB-C4A-NA	3.16	128.89	124.51
15	bB	817	CLA	CMB-C2B-C1B	-3.16	120.55	125.37
15	a3	403	CLA	C3B-C4B-NB	-3.16	107.58	110.52
15	b6	416	CLA	CMB-C2B-C1B	-3.16	120.55	125.37
15	b3	421	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	cB	837	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	aB	837	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	b3	410	CLA	C2D-C1D-ND	-3.16	107.78	110.10
15	cB	832	CLA	CMB-C2B-C1B	-3.16	120.56	125.37
15	c6	415	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
15	aB	829	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
15	a6	418	CLA	C2B-C1B-NB	3.16	112.35	110.23
15	a1	403	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
14	aA	801	CL0	CHC-C1C-C2C	-3.16	117.96	126.73
15	bB	841	CLA	C3B-C4B-NB	-3.16	107.59	110.52
15	bF	201	CLA	C3B-C4B-NB	-3.16	107.59	110.52
18	b1	420	BCR	C28-C27-C26	-3.16	108.44	114.08
15	a2	422	CLA	C16-C15-C13	-3.16	105.72	115.92
20	cB	850	LMG	O6-C1-O1	-3.16	102.50	109.97
15	a6	406	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
15	a5	420	CLA	CHB-C4A-NA	3.16	128.88	124.51
15	cB	841	CLA	C3B-C4B-NB	-3.16	107.59	110.52
15	c2	422	CLA	C16-C15-C13	-3.15	105.72	115.92
15	b3	404	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
15	a3	421	CLA	CHA-C1A-NA	-3.15	119.17	126.40
15	c6	407	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
15	b6	411	CLA	C2D-C1D-ND	-3.15	107.78	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	820	CLA	O2D-CGD-CBD	3.15	116.87	111.27
18	c1	420	BCR	C28-C27-C26	-3.15	108.45	114.08
15	cA	820	CLA	O2D-CGD-CBD	3.15	116.87	111.27
15	b2	404	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
18	a4	401	BCR	C11-C10-C9	-3.15	122.81	127.31
15	c3	403	CLA	C3B-C4B-NB	-3.15	107.59	110.52
15	a3	408	CLA	C2D-C1D-ND	-3.15	107.78	110.10
15	c1	417	CLA	CHC-C4B-NB	-3.15	120.92	124.26
15	cB	826	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
15	c3	421	CLA	CHA-C1A-NA	-3.15	119.19	126.40
15	b6	407	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
15	b2	422	CLA	C16-C15-C13	-3.15	105.75	115.92
15	aA	814	CLA	C3B-C4B-NB	-3.15	107.60	110.52
18	b4	401	BCR	C11-C10-C9	-3.14	122.82	127.31
15	a2	406	CLA	C16-C15-C13	-3.14	105.76	115.92
15	cB	840	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
15	a1	411	CLA	CMC-C2C-C1C	-3.14	120.25	125.04
15	cA	832	CLA	O2D-CGD-CBD	3.14	116.85	111.27
15	cB	829	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
18	b6	401	BCR	C11-C10-C9	-3.14	122.83	127.31
15	aA	840	CLA	CHC-C4B-NB	3.14	127.58	124.26
15	aB	832	CLA	CMB-C2B-C1B	-3.14	120.59	125.37
15	c5	408	CLA	C2D-C1D-ND	-3.14	107.79	110.10
15	c2	417	CLA	CHB-C4A-NA	3.14	128.85	124.51
15	a6	414	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
15	b6	413	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
15	cA	815	CLA	C3B-C4B-NB	-3.13	107.61	110.52
15	a1	407	CLA	C2D-C1D-ND	-3.13	107.79	110.10
15	cA	803	CLA	CHB-C4A-NA	3.13	128.85	124.51
15	bB	828	CLA	CHB-C4A-NA	3.13	128.84	124.51
15	c4	415	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
15	a2	403	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
15	a6	416	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
15	aA	832	CLA	O2D-CGD-CBD	3.13	116.83	111.27
15	c3	412	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
15	bA	807	CLA	CHB-C4A-NA	3.13	128.84	124.51
15	aJ	201	CLA	C3B-C4B-NB	-3.13	107.61	110.52
18	a3	418	BCR	C3-C4-C5	-3.13	108.49	114.08
15	a6	414	CLA	C2D-C1D-ND	-3.13	107.80	110.10
15	b3	415	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
15	aB	840	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
15	bB	840	CLA	O2D-CGD-O1D	-3.13	117.73	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	410	CLA	C2D-C1D-ND	-3.13	107.80	110.10
15	aB	811	CLA	C2B-C1B-NB	-3.13	108.14	110.23
18	b2	421	BCR	C28-C27-C26	-3.12	108.50	114.08
15	bB	826	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
15	aA	834	CLA	CHC-C4B-NB	3.12	127.56	124.26
15	aB	834	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
15	bA	803	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	cB	829	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	aB	826	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	cA	829	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	aA	803	CLA	CHB-C4A-NA	3.12	128.83	124.51
15	a1	404	CLA	CMD-C2D-C1D	3.12	130.21	124.71
15	c6	407	CLA	CHD-C1D-ND	-3.12	121.59	124.45
15	bA	814	CLA	C3B-C4B-NB	-3.12	107.62	110.52
15	cA	834	CLA	CHC-C4B-NB	3.12	127.56	124.26
15	bB	817	CLA	O2D-CGD-CBD	3.12	116.81	111.27
15	bA	816	CLA	CMB-C2B-C1B	-3.12	120.62	125.37
15	aA	829	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
15	b6	405	CLA	C3B-C4B-NB	-3.12	107.62	110.52
15	b4	417	CLA	C2C-C1C-NC	-3.12	107.05	109.97
15	aB	817	CLA	O2D-CGD-CBD	3.12	116.81	111.27
15	aB	828	CLA	CHB-C4A-NA	3.12	128.82	124.51
15	c4	417	CLA	C2C-C1C-NC	-3.12	107.05	109.97
15	cA	816	CLA	CMB-C2B-C1B	-3.12	120.62	125.37
15	a3	416	CLA	CHB-C4A-NA	3.11	128.82	124.51
15	c1	408	CLA	C2D-C1D-ND	-3.11	107.81	110.10
15	c1	416	CLA	C1-C2-C3	-3.11	121.72	126.75
15	a2	405	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	b4	405	CLA	CMD-C2D-C1D	3.11	130.19	124.71
15	cA	837	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	a3	404	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	b3	416	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	cI	102	BCR	C15-C14-C13	-3.11	122.87	127.31
15	aA	807	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	a6	407	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	a6	417	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	a6	421	BCR	C2-C1-C6	3.11	115.26	110.48
18	c4	401	BCR	C11-C10-C9	-3.11	122.88	127.31
15	cB	828	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	c3	405	CLA	CMD-C2D-C1D	3.11	130.19	124.71
15	cA	807	CLA	CHB-C4A-NA	3.11	128.81	124.51
15	aA	816	CLA	CMB-C2B-C1B	-3.11	120.64	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	832	CLA	CMB-C2B-C1B	-3.10	120.64	125.37
15	bA	834	CLA	CHC-C4B-NB	3.10	127.54	124.26
15	c3	415	CLA	CMB-C2B-C1B	-3.10	120.64	125.37
15	aB	829	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	a4	415	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
15	c6	418	CLA	CHB-C4A-NA	3.10	128.80	124.51
18	cA	851	BCR	C39-C30-C25	-3.10	105.27	110.30
15	cB	805	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
18	c4	419	BCR	C24-C23-C22	-3.10	121.55	126.23
15	a3	405	CLA	CMD-C2D-C1D	3.10	130.18	124.71
15	a6	405	CLA	C3B-C4B-NB	-3.10	107.64	110.52
15	bX	102	CLA	C3B-C4B-NB	-3.10	107.64	110.52
18	bI	102	BCR	C15-C14-C13	-3.10	122.89	127.31
15	aB	814	CLA	CHB-C1B-NB	3.10	127.54	124.26
15	b2	418	CLA	CHB-C4A-NA	3.10	128.80	124.51
15	b6	422	CLA	CGD-CBD-CAD	-3.10	100.70	110.73
15	a3	415	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
15	a4	402	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
15	c2	416	CLA	C2D-C1D-ND	-3.10	107.82	110.10
15	b6	422	CLA	C3A-C2A-C1A	3.10	105.97	101.34
18	aI	102	BCR	C15-C14-C13	-3.09	122.89	127.31
15	c6	408	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
18	c1	419	BCR	C3-C4-C5	-3.09	108.55	114.08
15	a4	417	CLA	C2C-C1C-NC	-3.09	107.07	109.97
15	b2	405	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
15	cA	835	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	bA	829	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
15	aA	837	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	a5	402	CLA	C1-C2-C3	-3.09	120.70	126.04
15	bB	805	CLA	CMB-C2B-C1B	-3.09	120.66	125.37
15	cB	834	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	a1	418	BCR	C3-C4-C5	-3.09	108.56	114.08
15	c3	416	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	cA	814	CLA	C3B-C4B-NB	-3.09	107.65	110.52
15	c6	406	CLA	C3B-C4B-NB	-3.09	107.65	110.52
15	bB	829	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	aA	835	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	b5	408	CLA	C2D-C1D-ND	-3.09	107.83	110.10
15	c5	402	CLA	C1-C2-C3	-3.09	120.70	126.04
15	bB	834	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
15	cB	817	CLA	O2D-CGD-CBD	3.09	116.75	111.27
15	c3	408	CLA	C2D-C1D-ND	-3.09	107.83	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	418	CLA	CHB-C4A-NA	3.09	128.78	124.51
15	bA	842	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
15	a5	415	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
15	aB	827	CLA	CHB-C4A-NA	3.08	128.78	124.51
15	a2	409	CLA	CMB-C2B-C1B	-3.08	120.67	125.37
15	c5	413	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	c4	405	CLA	CMD-C2D-C1D	3.08	130.14	124.71
15	aB	813	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	b1	404	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
15	c2	411	CLA	C2D-C1D-ND	-3.08	107.83	110.10
15	a5	405	CLA	CMD-C2D-C1D	3.08	130.14	124.71
15	c2	405	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
18	bA	853	BCR	C39-C30-C25	-3.08	105.31	110.30
15	c1	404	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
15	c4	402	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
15	b6	417	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	c1	417	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	b5	405	CLA	CMD-C2D-C1D	3.08	130.13	124.71
15	a2	422	CLA	C3B-C4B-NB	-3.08	107.66	110.52
15	aB	818	CLA	CHB-C4A-NA	3.08	128.77	124.51
15	c3	421	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
15	c5	417	CLA	C2C-C1C-NC	-3.08	107.09	109.97
15	a5	413	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	a6	411	CLA	C2D-C1D-ND	-3.07	107.84	110.10
15	c5	415	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	c2	417	CLA	C1C-C2C-C3C	-3.07	103.72	106.96
15	a5	408	CLA	C2D-C1D-ND	-3.07	107.84	110.10
15	b3	421	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	b6	420	BCR	C28-C27-C26	-3.07	108.59	114.08
15	a5	406	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
15	c2	418	CLA	CHB-C4A-NA	3.07	128.76	124.51
15	c2	409	CLA	CMB-C2B-C1B	-3.07	120.69	125.37
15	a1	416	CLA	CHB-C4A-NA	3.07	128.75	124.51
15	c6	412	CLA	C2D-C1D-ND	-3.07	107.84	110.10
15	aX	102	CLA	C3B-C4B-NB	-3.07	107.67	110.52
15	a6	406	CLA	CHD-C1D-ND	-3.07	121.64	124.45
15	a2	417	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
15	bB	813	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
15	bB	814	CLA	CHB-C1B-NB	3.07	127.50	124.26
15	c5	405	CLA	CMD-C2D-C1D	3.07	130.12	124.71
15	aB	805	CLA	CMB-C2B-C1B	-3.06	120.70	125.37
18	aA	852	BCR	C39-C30-C25	-3.06	105.33	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	403	CLA	C3B-C4B-NB	-3.06	107.67	110.52
15	b4	402	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	a3	404	CLA	C1-C2-C3	-3.06	120.74	126.04
15	aA	807	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
15	bB	802	CLA	C3B-C4B-NB	-3.06	107.67	110.52
15	a4	415	CLA	CMB-C2B-C1B	-3.06	120.70	125.37
15	c6	401	CLA	CHB-C4A-NA	3.06	128.75	124.51
15	b5	413	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	bB	827	CLA	CHB-C4A-NA	3.06	128.75	124.51
15	bB	813	CLA	C3B-C4B-NB	-3.06	107.67	110.52
15	cF	201	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
15	a3	421	CLA	C3B-C4B-NB	-3.06	107.68	110.52
18	c5	419	BCR	C28-C27-C26	-3.06	108.61	114.08
15	b6	406	CLA	CHD-C1D-ND	-3.06	121.64	124.45
15	b4	411	CLA	CHB-C4A-NA	3.06	128.74	124.51
15	b2	422	CLA	C3B-C4B-NB	-3.06	107.68	110.52
15	cB	818	CLA	CHB-C4A-NA	3.06	128.74	124.51
15	b6	414	CLA	CHD-C1D-ND	-3.06	121.64	124.45
15	b3	405	CLA	CMD-C2D-C1D	3.06	130.10	124.71
15	b5	417	CLA	C2C-C1C-NC	-3.06	107.11	109.97
18	c3	418	BCR	C3-C4-C5	-3.06	108.62	114.08
15	b1	417	CLA	C2C-C1C-NC	-3.06	107.11	109.97
15	a6	404	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	bA	807	CLA	CAA-C2A-C3A	-3.05	104.41	112.78
15	cA	807	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
15	cX	102	CLA	C3B-C4B-NB	-3.05	107.68	110.52
15	c5	403	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	b5	402	CLA	C1-C2-C3	-3.05	120.76	126.04
15	c3	404	CLA	C1-C2-C3	-3.05	120.76	126.04
15	a6	406	CLA	CMD-C2D-C1D	3.05	130.09	124.71
15	bA	837	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	a4	405	CLA	CMD-C2D-C1D	3.05	130.09	124.71
15	aB	827	CLA	CMB-C2B-C1B	-3.05	120.72	125.37
15	cB	813	CLA	C3B-C4B-NB	-3.05	107.68	110.52
15	cB	813	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
15	bB	818	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	aB	802	CLA	C3B-C4B-NB	-3.05	107.69	110.52
15	b6	404	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
15	cB	827	CLA	CHB-C4A-NA	3.05	128.73	124.51
15	bB	809	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
15	c5	404	CLA	C3B-C4B-NB	-3.05	107.69	110.52
15	bA	835	CLA	C2D-C1D-ND	-3.05	107.86	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	408	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	cA	848	BCR	C15-C16-C17	-3.04	117.24	123.47
15	cB	811	CLA	C2B-C1B-NB	-3.04	108.19	110.23
18	c6	420	BCR	C3-C4-C5	-3.04	108.64	114.08
18	b4	419	BCR	C24-C23-C22	-3.04	121.64	126.23
18	aA	849	BCR	C15-C16-C17	-3.04	117.24	123.47
15	cA	828	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
15	bB	820	CLA	CHB-C1B-NB	3.04	127.48	124.26
15	bA	830	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
15	aB	813	CLA	C3B-C4B-NB	-3.04	107.69	110.52
18	cB	847	BCR	C15-C16-C17	-3.04	117.24	123.47
15	cA	830	CLA	CMB-C2B-C3B	3.04	133.96	126.59
15	cB	802	CLA	C3B-C4B-NB	-3.04	107.69	110.52
15	c1	404	CLA	C3B-C4B-NB	-3.04	107.69	110.52
15	aB	826	CLA	CAA-C2A-C1A	-3.04	102.01	111.97
15	cA	830	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
18	aB	847	BCR	C15-C16-C17	-3.04	117.25	123.47
15	aA	842	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
15	aA	827	CLA	CAA-CBA-CGA	-3.04	104.37	113.25
18	b5	419	BCR	C28-C27-C26	-3.04	108.65	114.08
15	b6	414	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
15	aA	830	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
18	c6	421	BCR	C28-C27-C26	-3.04	108.66	114.08
18	bA	850	BCR	C15-C16-C17	-3.04	117.25	123.47
15	bA	830	CLA	CMB-C2B-C3B	3.04	133.94	126.59
15	aB	820	CLA	CHB-C1B-NB	3.03	127.47	124.26
15	aA	830	CLA	CMB-C2B-C3B	3.03	133.94	126.59
15	b5	403	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	cB	826	CLA	CAA-C2A-C1A	-3.03	102.03	111.97
15	bA	828	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	bA	826	CLA	CHB-C4A-NA	3.03	128.71	124.51
18	a4	419	BCR	C24-C23-C22	-3.03	121.65	126.23
15	aB	809	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
15	cA	827	CLA	CAA-CBA-CGA	-3.03	104.39	113.25
15	c2	412	CLA	CHB-C1B-NB	3.03	127.47	124.26
15	a2	418	CLA	C2C-C1C-NC	-3.03	107.13	109.97
15	b5	406	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
18	b1	419	BCR	C3-C4-C5	-3.03	108.67	114.08
15	cB	820	CLA	CHB-C1B-NB	3.03	127.47	124.26
18	b6	419	BCR	C3-C4-C5	-3.03	108.67	114.08
15	c4	403	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
18	a5	419	BCR	C28-C27-C26	-3.03	108.67	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	406	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
15	bA	827	CLA	CAA-CBA-CGA	-3.03	104.40	113.25
18	a6	420	BCR	C28-C27-C26	-3.03	108.67	114.08
15	b1	403	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
15	aA	820	CLA	CHB-C1B-NB	3.03	127.46	124.26
15	b1	417	CLA	CHB-C4A-NA	3.03	128.70	124.51
15	b5	416	CLA	CHB-C4A-NA	3.03	128.70	124.51
15	a1	409	CLA	C2D-C1D-ND	-3.03	107.87	110.10
15	bB	826	CLA	CAA-C2A-C1A	-3.03	102.06	111.97
15	aB	804	CLA	CMB-C2B-C3B	3.03	133.92	126.59
18	b4	418	BCR	C27-C26-C25	3.03	127.12	122.73
15	c2	405	CLA	CMD-C2D-C1D	3.02	130.04	124.71
15	a5	403	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
15	aB	839	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
15	b2	411	CLA	C2D-C1D-ND	-3.02	107.88	110.10
15	b2	405	CLA	CMD-C2D-C1D	3.02	130.04	124.71
15	cB	825	CLA	CMB-C2B-C1B	-3.02	120.76	125.37
15	bB	811	CLA	C2B-C1B-NB	-3.02	108.20	110.23
15	c5	409	CLA	C3B-C4B-NB	-3.02	107.71	110.52
18	c4	418	BCR	C27-C26-C25	3.02	127.12	122.73
15	bB	839	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
18	bB	844	BCR	C11-C10-C9	-3.02	123.00	127.31
15	c1	417	CLA	C2C-C1C-NC	-3.02	107.14	109.97
15	c3	421	CLA	C3B-C4B-NB	-3.02	107.71	110.52
18	a6	419	BCR	C3-C4-C5	-3.02	108.68	114.08
15	aA	828	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	a1	402	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	c1	403	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	c6	418	CLA	CHB-C1B-NB	3.02	127.45	124.26
15	aA	826	CLA	CHB-C4A-NA	3.02	128.69	124.51
15	b5	415	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
15	c4	415	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
18	bB	847	BCR	C15-C16-C17	-3.02	117.30	123.47
15	cB	839	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
15	bB	825	CLA	CMB-C2B-C1B	-3.02	120.78	125.37
15	a4	409	CLA	C3B-C4B-NB	-3.01	107.72	110.52
15	c1	412	CLA	CMC-C2C-C1C	-3.01	120.45	125.04
15	bB	804	CLA	CMB-C2B-C3B	3.01	133.89	126.59
18	aI	102	BCR	C2-C1-C6	3.01	115.12	110.48
15	cB	809	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
15	c3	408	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
15	bB	819	CLA	CHB-C4A-NA	3.01	128.68	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	804	CLA	CMB-C2B-C3B	3.01	133.88	126.59
15	aB	825	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
15	bA	820	CLA	CHB-C1B-NB	3.01	127.44	124.26
15	b2	404	CLA	C3B-C4B-NB	-3.01	107.72	110.52
15	c4	416	CLA	CHB-C4A-NA	3.01	128.67	124.51
15	b2	403	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
15	c6	407	CLA	CMD-C2D-C1D	3.01	130.01	124.71
15	c5	420	CLA	C3B-C4B-NB	-3.01	107.73	110.52
15	a4	404	CLA	C3B-C4B-NB	-3.00	107.73	110.52
15	b4	403	CLA	CMB-C2B-C1B	-3.00	120.79	125.37
15	a2	407	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	b2	415	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	c6	401	CLA	C3B-C4B-NB	-3.00	107.73	110.52
15	a2	416	CLA	C2D-C1D-ND	-3.00	107.89	110.10
15	cA	820	CLA	CHB-C1B-NB	3.00	127.44	124.26
15	aL	202	CLA	O2D-CGD-CBD	3.00	116.60	111.27
15	a2	405	CLA	CMD-C2D-C1D	3.00	130.00	124.71
15	cA	826	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	bA	810	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	bB	827	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
15	c6	405	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
15	a1	409	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	aB	844	BCR	C15-C16-C17	-3.00	117.33	123.47
15	cJ	102	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	c5	416	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	b5	420	CLA	C3B-C4B-NB	-3.00	107.73	110.52
15	b5	415	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
18	cB	844	BCR	C15-C16-C17	-3.00	117.33	123.47
18	c1	419	BCR	C2-C1-C6	3.00	115.10	110.48
18	cI	102	BCR	C2-C1-C6	3.00	115.10	110.48
18	bI	101	BCR	C2-C1-C6	3.00	115.09	110.48
18	c4	420	BCR	C15-C14-C13	-3.00	123.03	127.31
15	a5	416	CLA	CHB-C4A-NA	3.00	128.66	124.51
15	b2	418	CLA	C2C-C1C-NC	-3.00	107.17	109.97
15	c3	415	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	b1	408	CLA	C2D-C1D-ND	-3.00	107.90	110.10
15	a6	422	CLA	C16-C15-C13	-3.00	106.23	115.92
15	cA	827	CLA	CMB-C2B-C1B	-3.00	120.81	125.37
18	aI	101	BCR	C2-C1-C6	3.00	115.09	110.48
15	b6	406	CLA	CMD-C2D-C1D	2.99	129.99	124.71
18	a1	418	BCR	C2-C1-C6	2.99	115.09	110.48
15	aL	203	CLA	C3B-C4B-NB	-2.99	107.74	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	827	CLA	CMB-C2B-C1B	-2.99	120.81	125.37
15	aB	839	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	a3	409	CLA	C3B-C4B-NB	-2.99	107.74	110.52
15	b3	404	CLA	C3B-C4B-NB	-2.99	107.74	110.52
15	c5	417	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	cB	839	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	b6	414	CLA	C3C-C4C-NC	-2.99	107.22	110.57
15	b5	404	CLA	C3B-C4B-NB	-2.99	107.74	110.52
15	bA	818	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
15	bB	805	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	cX	102	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
18	bB	844	BCR	C15-C16-C17	-2.99	117.35	123.47
15	aB	833	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	cA	829	CLA	CMB-C2B-C1B	-2.99	120.82	125.37
15	a4	411	CLA	CHB-C4A-NA	2.99	128.65	124.51
15	a4	403	CLA	CMB-C2B-C1B	-2.99	120.82	125.37
15	bB	839	CLA	CHB-C4A-NA	2.99	128.64	124.51
15	b3	411	CLA	CHB-C4A-NA	2.99	128.64	124.51
15	a5	420	CLA	C3B-C4B-NB	-2.99	107.74	110.52
15	aA	810	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b3	408	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b5	405	CLA	CHD-C1D-ND	-2.99	121.71	124.45
15	c2	407	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	cA	810	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
15	b3	404	CLA	C1-C2-C3	-2.99	120.88	126.04
15	b4	405	CLA	C3C-C4C-NC	-2.99	107.22	110.57
15	a5	405	CLA	CHD-C1D-ND	-2.99	121.71	124.45
15	b2	412	CLA	CHB-C1B-NB	2.98	127.42	124.26
18	cA	849	BCR	C11-C10-C9	-2.98	123.05	127.31
18	a4	418	BCR	C27-C26-C25	2.98	127.06	122.73
15	bL	203	CLA	O2D-CGD-CBD	2.98	116.57	111.27
15	c5	405	CLA	CHD-C1D-ND	-2.98	121.71	124.45
15	cL	203	CLA	O2D-CGD-CBD	2.98	116.57	111.27
15	cL	204	CLA	C3B-C4B-NB	-2.98	107.75	110.52
15	b4	404	CLA	C1-C2-C3	-2.98	120.88	126.04
15	aA	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
15	bX	102	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
18	cB	844	BCR	C11-C10-C9	-2.98	123.05	127.31
15	cB	817	CLA	CHB-C4A-NA	2.98	128.64	124.51
15	aA	802	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
15	cB	819	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	aB	806	CLA	O2A-C1-C2	-2.98	100.80	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	409	CLA	C3B-C4B-NB	-2.98	107.75	110.52
15	aB	819	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	cI	101	BCR	C2-C1-C6	2.98	115.06	110.48
15	a2	403	CLA	CMB-C2B-C1B	-2.98	120.84	125.37
15	b5	414	CLA	CAA-C2A-C3A	-2.98	109.15	116.10
15	cB	833	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	bA	827	CLA	CMB-C2B-C1B	-2.98	120.84	125.37
15	a1	406	CLA	CHB-C4A-NA	2.98	128.63	124.51
15	b6	418	CLA	C2C-C1C-NC	-2.97	107.19	109.97
15	b4	402	CLA	C1-C2-C3	-2.97	120.90	126.04
15	aX	102	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
18	bI	102	BCR	C2-C1-C6	2.97	115.06	110.48
18	aB	844	BCR	C11-C10-C9	-2.97	123.06	127.31
15	c6	401	CLA	C6-C7-C8	-2.97	106.31	115.92
15	b1	406	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
15	c4	409	CLA	C3B-C4B-NB	-2.97	107.76	110.52
15	b3	415	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
18	b2	419	BCR	C27-C26-C25	2.97	127.05	122.73
15	bB	833	CLA	CHB-C4A-NA	2.97	128.62	124.51
15	c4	410	CLA	CMC-C2C-C3C	2.97	134.18	126.12
15	bB	806	CLA	O2A-C1-C2	-2.97	100.83	108.64
15	b2	416	CLA	C2D-C1D-ND	-2.97	107.92	110.10
18	bJ	103	BCR	C24-C23-C22	-2.97	121.75	126.23
15	b1	407	CLA	CHB-C4A-NA	2.97	128.62	124.51
18	aJ	205	BCR	C15-C16-C17	-2.97	117.39	123.47
15	a1	416	CLA	C2C-C1C-NC	-2.97	107.19	109.97
18	cJ	104	BCR	C15-C16-C17	-2.97	117.40	123.47
15	b6	422	CLA	C6-C7-C8	-2.97	106.33	115.92
15	a1	403	CLA	C3B-C4B-NB	-2.97	107.76	110.52
15	cB	806	CLA	O2A-C1-C2	-2.97	100.84	108.64
15	a4	414	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	bB	817	CLA	CHB-C4A-NA	2.97	128.61	124.51
15	b6	422	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	bA	851	BCR	C11-C10-C9	-2.96	123.08	127.31
15	cA	818	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
15	a2	404	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	c3	409	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	c2	418	CLA	C2C-C1C-NC	-2.96	107.19	109.97
15	b1	410	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	bJ	104	BCR	C15-C16-C17	-2.96	117.40	123.47
15	c2	415	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	b6	420	BCR	C15-C14-C13	-2.96	123.08	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	422	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	c3	404	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
15	b1	412	CLA	CMC-C2C-C1C	-2.96	120.53	125.04
15	bA	829	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
15	cA	802	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
15	b1	416	CLA	C1-C2-C3	-2.96	121.96	126.75
18	c2	420	BCR	C24-C23-C22	-2.96	121.76	126.23
15	a2	403	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	b4	404	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	cB	839	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	a2	415	CLA	CHB-C4A-NA	2.96	128.60	124.51
15	c6	415	CLA	CHD-C1D-ND	-2.96	121.73	124.45
14	bA	801	CL0	CAC-C3C-C4C	2.96	128.65	124.81
15	a6	422	CLA	C6-C5-C3	-2.96	105.69	113.45
15	a5	415	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
15	b4	421	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	cB	805	CLA	CHB-C4A-NA	2.96	128.60	124.51
15	b4	405	CLA	CHD-C1D-ND	-2.96	121.74	124.45
18	aA	850	BCR	C11-C10-C9	-2.96	123.09	127.31
18	b1	419	BCR	C2-C1-C6	2.96	115.03	110.48
15	a4	402	CLA	C1-C2-C3	-2.96	120.93	126.04
15	bB	834	CLA	C2D-C1D-ND	-2.96	107.92	110.10
15	bB	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	a5	409	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	b2	403	CLA	C3B-C4B-NB	-2.96	107.77	110.52
15	b2	417	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
18	cI	102	BCR	C15-C16-C17	-2.96	117.42	123.47
15	c2	411	CLA	CMC-C2C-C3C	2.96	134.14	126.12
15	cA	839	CLA	C3B-C4B-NB	-2.96	107.77	110.52
18	a6	420	BCR	C15-C14-C13	-2.96	123.09	127.31
15	aA	829	CLA	CMB-C2B-C1B	-2.96	120.87	125.37
15	aB	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	c6	402	BCR	C24-C23-C22	-2.95	121.77	126.23
15	c4	421	CLA	CAA-CBA-CGA	-2.95	104.62	113.25
15	a5	404	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	a5	417	CLA	C2C-C1C-NC	-2.95	107.20	109.97
14	aA	801	CL0	CAC-C3C-C4C	2.95	128.64	124.81
15	a1	405	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	cA	833	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	c6	406	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
15	a4	421	CLA	C6-C7-C8	-2.95	106.38	115.92
15	bJ	102	CLA	CHB-C4A-NA	2.95	128.59	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bL	203	CLA	C3B-C4B-NB	-2.95	107.78	110.52
15	aA	827	CLA	CMB-C2B-C1B	-2.95	120.87	125.37
15	aJ	203	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	b4	410	CLA	CMC-C2C-C3C	2.95	134.13	126.12
15	b4	416	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	b2	402	CLA	C1-C2-C3	-2.95	120.94	126.04
15	b1	403	CLA	C3B-C4B-NB	-2.95	107.78	110.52
15	b6	422	CLA	C3B-C4B-NB	-2.95	107.78	110.52
15	cB	829	CLA	C2D-C1D-ND	-2.95	107.93	110.10
15	a6	422	CLA	C6-C7-C8	-2.95	106.38	115.92
15	c4	411	CLA	CHB-C4A-NA	2.95	128.59	124.51
15	b4	412	CLA	CMC-C2C-C1C	-2.95	120.55	125.04
16	bB	843	PQN	C14-C13-C15	2.95	120.23	115.27
15	a4	404	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	bA	833	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
18	bB	848	BCR	C3-C4-C5	-2.95	108.81	114.08
15	c4	421	CLA	C6-C7-C8	-2.95	106.39	115.92
15	aA	833	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	a6	403	CLA	C1-C2-C3	-2.95	120.95	126.04
15	bL	204	CLA	C3B-C4B-NB	-2.95	107.78	110.52
15	b3	409	CLA	C3B-C4B-NB	-2.95	107.78	110.52
15	a3	414	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	bA	802	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
15	c6	404	CLA	C1-C2-C3	-2.95	120.95	126.04
18	aJ	204	BCR	C24-C23-C22	-2.95	121.78	126.23
18	c6	421	BCR	C15-C14-C13	-2.94	123.11	127.31
15	aB	835	CLA	C3B-C4B-NB	-2.94	107.78	110.52
15	a6	404	CLA	C3B-C4B-NB	-2.94	107.78	110.52
15	a5	404	CLA	CHB-C4A-NA	2.94	128.58	124.51
15	a2	412	CLA	CHB-C1B-NB	2.94	127.37	124.26
15	b5	405	CLA	C3C-C4C-NC	-2.94	107.27	110.57
18	a6	401	BCR	C24-C23-C22	-2.94	121.79	126.23
15	b4	421	CLA	C6-C7-C8	-2.94	106.41	115.92
18	cB	848	BCR	C3-C4-C5	-2.94	108.82	114.08
15	bA	839	CLA	C3B-C4B-NB	-2.94	107.78	110.52
15	b2	407	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
15	a5	405	CLA	C3C-C4C-NC	-2.94	107.27	110.57
15	c5	414	CLA	CAA-C2A-C3A	-2.94	109.23	116.10
15	cB	817	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
15	bA	838	CLA	CMB-C2B-C3B	2.94	133.71	126.59
15	a5	404	CLA	C3B-C4B-NB	-2.94	107.79	110.52
15	aA	826	CLA	C2A-C1A-CHA	2.94	129.00	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a6	401	BCR	C15-C16-C17	-2.94	117.45	123.47
15	bB	841	CLA	CHB-C1B-NB	2.94	127.37	124.26
15	c1	410	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	aL	202	CLA	C3B-C4B-NB	-2.94	107.79	110.52
15	aA	804	CLA	O2D-CGD-CBD	2.94	116.49	111.27
15	a1	409	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	a6	422	CLA	CHB-C4A-NA	2.94	128.57	124.51
15	b1	410	CLA	CMC-C2C-C3C	2.94	134.09	126.12
18	aI	102	BCR	C15-C16-C17	-2.94	117.46	123.47
15	bA	822	CLA	CMB-C2B-C1B	-2.94	120.90	125.37
15	cA	826	CLA	C2A-C1A-CHA	2.94	128.99	123.86
15	b5	417	CLA	CHB-C4A-NA	2.94	128.57	124.51
15	b2	411	CLA	CMC-C2C-C3C	2.94	134.09	126.12
15	c3	404	CLA	C3B-C4B-NB	-2.94	107.79	110.52
15	c4	404	CLA	C3B-C4B-NB	-2.94	107.79	110.52
18	b4	420	BCR	C15-C14-C13	-2.94	123.12	127.31
15	c4	402	CLA	C1-C2-C3	-2.93	120.97	126.04
15	a4	416	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a5	417	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a2	411	CLA	CMC-C2C-C3C	2.93	134.08	126.12
15	a6	405	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
16	aB	843	PQN	C14-C13-C15	2.93	120.21	115.27
14	cA	801	CL0	CAC-C3C-C4C	2.93	128.62	124.81
15	cL	203	CLA	C3B-C4B-NB	-2.93	107.79	110.52
15	aB	841	CLA	CHB-C1B-NB	2.93	127.36	124.26
15	a2	412	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	a6	416	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	b1	411	CLA	CMB-C2B-C3B	2.93	133.69	126.59
15	a6	417	CLA	CHB-C1B-NB	2.93	127.36	124.26
15	bA	805	CLA	CHB-C1B-NB	2.93	127.36	124.26
15	b5	411	CLA	CHB-C1B-NB	2.93	127.36	124.26
15	cB	814	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	b2	412	CLA	CHB-C4A-NA	2.93	128.57	124.51
15	aB	839	CLA	C3B-C4B-NB	-2.93	107.80	110.52
15	bA	827	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
15	a1	416	CLA	CHC-C4B-NB	-2.93	121.15	124.26
15	aA	824	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	c1	407	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	c2	412	CLA	CHB-C4A-NA	2.93	128.56	124.51
18	bJ	105	BCR	C15-C14-C13	-2.93	123.13	127.31
15	b4	414	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	a1	412	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	817	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	bA	845	CLA	C3B-C4B-NB	-2.93	107.80	110.52
15	aA	806	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
15	b6	403	CLA	C1-C2-C3	-2.93	120.98	126.04
15	c5	411	CLA	CMB-C2B-C3B	2.93	133.68	126.59
15	a3	417	CLA	C2C-C1C-NC	-2.93	107.23	109.97
15	aA	822	CLA	CMB-C2B-C1B	-2.93	120.91	125.37
15	cA	827	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
15	b5	411	CLA	CMB-C2B-C3B	2.93	133.68	126.59
15	bA	806	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
15	c4	404	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	a4	410	CLA	CMC-C2C-C3C	2.93	134.06	126.12
15	c6	409	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
15	aB	805	CLA	CHB-C4A-NA	2.93	128.56	124.51
15	a6	418	CLA	C2C-C1C-NC	-2.93	107.23	109.97
18	cJ	104	BCR	C11-C10-C9	-2.93	123.14	127.31
15	b4	421	CLA	CAA-CBA-CGA	-2.93	104.70	113.25
18	b1	419	BCR	C15-C16-C17	-2.93	117.48	123.47
15	a4	421	CLA	CAA-CBA-CGA	-2.92	104.71	113.25
15	bB	835	CLA	C3B-C4B-NB	-2.92	107.80	110.52
15	a2	411	CLA	C2D-C1D-ND	-2.92	107.95	110.10
15	c2	422	CLA	CED-O2D-CGD	2.92	122.55	115.94
18	bI	102	BCR	C15-C16-C17	-2.92	117.48	123.47
15	a4	421	CLA	CHA-C1A-NA	-2.92	119.70	126.40
15	c4	404	CLA	C1-C2-C3	-2.92	120.99	126.04
15	a3	411	CLA	CHB-C4A-NA	2.92	128.56	124.51
15	a1	416	CLA	C2B-C1B-NB	2.92	112.19	110.23
15	a3	406	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
15	aA	805	CLA	CHB-C1B-NB	2.92	127.35	124.26
15	bA	813	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
15	bA	826	CLA	C2A-C1A-CHA	2.92	128.97	123.86
15	aA	838	CLA	CMB-C2B-C3B	2.92	133.67	126.59
15	b4	421	CLA	CHA-C1A-NA	-2.92	119.70	126.40
15	c6	417	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
18	a1	420	BCR	C24-C23-C22	-2.92	121.82	126.23
15	c1	410	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	c5	414	CLA	CHB-C4A-NA	2.92	128.55	124.51
18	aF	203	BCR	C15-C14-C13	-2.92	123.14	127.31
15	c2	402	CLA	C1-C2-C3	-2.92	120.99	126.04
18	aJ	205	BCR	C11-C10-C9	-2.92	123.14	127.31
15	aB	818	CLA	CMB-C2B-C3B	2.92	133.66	126.59
15	cA	806	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	410	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	cA	819	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	c4	414	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	cB	818	CLA	CMB-C2B-C3B	2.92	133.66	126.59
18	b4	418	BCR	C40-C30-C29	-2.92	97.23	108.91
15	aA	845	CLA	C3B-C4B-NB	-2.92	107.81	110.52
15	cB	811	CLA	C3B-C4B-NB	-2.92	107.81	110.52
15	b2	416	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
15	cA	826	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
15	c2	404	CLA	C3B-C4B-NB	-2.92	107.81	110.52
15	cB	841	CLA	CHB-C1B-NB	2.92	127.35	124.26
15	b3	416	CLA	C1-C2-C3	-2.92	122.03	126.75
15	b6	416	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
15	c3	404	CLA	CHB-C4A-NA	2.92	128.55	124.51
15	c5	404	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
15	bB	818	CLA	CMB-C2B-C3B	2.92	133.65	126.59
15	a4	421	CLA	C3B-C4B-NB	-2.92	107.81	110.52
15	c2	403	CLA	C3B-C4B-NB	-2.92	107.81	110.52
15	c5	415	CLA	CMB-C2B-C1B	-2.92	120.93	125.37
15	cA	824	CLA	CHB-C4A-NA	2.92	128.54	124.51
15	c6	410	CLA	C2D-C1D-ND	-2.92	107.95	110.10
15	a5	411	CLA	CHB-C1B-NB	2.92	127.34	124.26
15	a6	408	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
15	bB	817	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
15	cA	838	CLA	CMB-C2B-C3B	2.92	133.65	126.59
15	a4	405	CLA	C3C-C4C-NC	-2.91	107.30	110.57
15	a4	406	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	b1	415	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	bA	824	CLA	CHB-C4A-NA	2.91	128.54	124.51
15	cB	815	CLA	C3B-C4B-NB	-2.91	107.81	110.52
15	bB	829	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	b6	409	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	bA	826	CLA	CMB-C2B-C1B	-2.91	120.93	125.37
18	aB	848	BCR	C3-C4-C5	-2.91	108.88	114.08
18	cF	205	BCR	C15-C14-C13	-2.91	123.15	127.31
18	c1	419	BCR	C24-C23-C22	-2.91	121.83	126.23
15	cA	844	CLA	C3B-C4B-NB	-2.91	107.81	110.52
15	c1	413	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	c4	407	CLA	CHB-C4A-NA	2.91	128.54	124.51
18	a2	420	BCR	C24-C23-C22	-2.91	121.84	126.23
16	cB	843	PQN	C14-C13-C15	2.91	120.17	115.27
15	b5	414	CLA	CHB-C4A-NA	2.91	128.54	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	839	CLA	C3B-C4B-NB	-2.91	107.81	110.52
15	b5	409	CLA	C3B-C4B-NB	-2.91	107.81	110.52
15	b4	404	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
15	c3	410	CLA	CMC-C2C-C3C	2.91	134.01	126.12
15	b1	404	CLA	C3B-C4B-NB	-2.91	107.82	110.52
18	a4	420	BCR	C15-C14-C13	-2.91	123.16	127.31
15	a5	414	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	b2	401	BCR	C1-C6-C5	-2.91	118.52	122.61
18	a4	418	BCR	C40-C30-C29	-2.91	97.28	108.91
15	b5	404	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
15	c4	412	CLA	CMC-C2C-C1C	-2.91	120.61	125.04
15	cA	805	CLA	CHB-C1B-NB	2.91	127.33	124.26
15	c4	421	CLA	CHA-C1A-NA	-2.91	119.74	126.40
15	b4	406	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	c2	404	CLA	C1-C2-C3	-2.91	121.02	126.04
15	aA	827	CLA	CAA-C2A-C1A	-2.91	102.45	111.97
18	cJ	103	BCR	C24-C23-C22	-2.91	121.84	126.23
15	c1	410	CLA	C2D-C1D-ND	-2.91	107.96	110.10
15	a3	415	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
15	bA	819	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	cB	826	CLA	CMB-C2B-C1B	-2.90	120.94	125.37
15	c5	411	CLA	CHB-C1B-NB	2.90	127.33	124.26
15	cA	804	CLA	O2D-CGD-CBD	2.90	116.43	111.27
15	b4	417	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	c3	411	CLA	CHB-C4A-NA	2.90	128.53	124.51
15	b3	414	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
15	b6	410	CLA	C3B-C4B-NB	-2.90	107.82	110.52
15	c1	403	CLA	C3B-C4B-NB	-2.90	107.82	110.52
15	a4	404	CLA	C1-C2-C3	-2.90	121.02	126.04
15	b6	408	CLA	CHB-C4A-NA	2.90	128.53	124.51
18	bJ	104	BCR	C11-C10-C9	-2.90	123.17	127.31
15	aA	813	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
15	b2	405	CLA	CHD-C1D-ND	-2.90	121.79	124.45
15	a2	406	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	b1	417	CLA	C2B-C1B-NB	2.90	112.18	110.23
15	a6	409	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	aA	826	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
15	aA	830	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	b4	407	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c4	417	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c6	418	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	a6	414	CLA	CAC-C3C-C2C	-2.90	122.57	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a1	418	BCR	C24-C23-C22	-2.90	121.86	126.23
15	cA	830	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	c3	417	CLA	C2C-C1C-NC	-2.90	107.26	109.97
15	c3	416	CLA	C1-C2-C3	-2.90	122.06	126.75
15	a4	405	CLA	CHD-C1D-ND	-2.90	121.79	124.45
15	bA	804	CLA	O2D-CGD-CBD	2.90	116.42	111.27
15	b1	402	CLA	C1-C2-C3	-2.90	121.03	126.04
15	aB	829	CLA	C2D-C1D-ND	-2.90	107.97	110.10
15	c4	414	CLA	CAA-C2A-C3A	-2.90	109.34	116.10
15	aA	813	CLA	CMB-C2B-C1B	-2.90	120.96	125.37
15	c5	410	CLA	CMB-C2B-C1B	-2.90	120.96	125.37
15	bA	809	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
15	a1	414	CLA	C2D-C1D-ND	-2.90	107.97	110.10
18	c4	418	BCR	C40-C30-C29	-2.90	97.32	108.91
15	c1	408	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	c3	408	CLA	CHB-C4A-NA	2.90	128.52	124.51
15	bB	839	CLA	C3B-C4B-NB	-2.90	107.83	110.52
15	cB	835	CLA	C3B-C4B-NB	-2.90	107.83	110.52
15	bB	801	CLA	CHB-C1B-NB	2.90	127.32	124.26
15	c5	404	CLA	CHB-C4A-NA	2.89	128.51	124.51
15	c2	416	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	cA	813	CLA	CMB-C2B-C1B	-2.89	120.96	125.37
15	a2	405	CLA	C3C-C4C-NC	-2.89	107.33	110.57
15	c2	405	CLA	CHD-C1D-ND	-2.89	121.80	124.45
15	b6	417	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	bB	814	CLA	CMB-C2B-C3B	2.89	133.60	126.59
15	b6	417	CLA	CHB-C1B-NB	2.89	127.32	124.26
15	cB	810	CLA	CHC-C4B-NB	2.89	127.32	124.26
15	a6	410	CLA	C3B-C4B-NB	-2.89	107.83	110.52
15	c6	405	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	c6	402	BCR	C15-C16-C17	-2.89	117.55	123.47
15	cA	813	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	c2	403	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
15	a2	402	CLA	C1-C2-C3	-2.89	121.04	126.04
15	b1	404	CLA	C1-C2-C3	-2.89	121.04	126.04
15	a5	414	CLA	CAA-C2A-C3A	-2.89	109.35	116.10
15	c5	410	CLA	CMC-C2C-C3C	2.89	133.97	126.12
15	aB	817	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
15	bA	822	CLA	CHB-C4A-NA	2.89	128.51	124.51
15	b1	410	CLA	C2D-C1D-ND	-2.89	107.97	110.10
15	b1	413	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	a6	402	BCR	C7-C8-C9	-2.89	121.87	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	815	CLA	C3B-C4B-NB	-2.89	107.83	110.52
18	c2	401	BCR	C1-C6-C5	-2.89	118.54	122.61
18	b1	419	BCR	C24-C23-C22	-2.89	121.87	126.23
18	b2	420	BCR	C24-C23-C22	-2.89	121.87	126.23
15	a2	412	CLA	CMB-C2B-C3B	2.89	133.59	126.59
15	a5	411	CLA	CMB-C2B-C3B	2.89	133.59	126.59
15	bB	826	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
18	b6	401	BCR	C24-C23-C22	-2.89	121.87	126.23
15	aB	801	CLA	CHB-C1B-NB	2.89	127.31	124.26
15	b4	414	CLA	CAA-C2A-C3A	-2.89	109.36	116.10
15	cB	814	CLA	CMB-C2B-C3B	2.89	133.58	126.59
15	c6	419	CLA	C2C-C1C-NC	-2.89	107.27	109.97
15	bA	838	CLA	CHB-C4A-NA	2.89	128.50	124.51
15	cA	822	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	bI	102	BCR	C24-C23-C22	-2.89	121.87	126.23
15	bA	813	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
15	aB	826	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
15	a6	422	CLA	C3B-C4B-NB	-2.88	107.84	110.52
15	a4	413	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	bB	810	CLA	CHC-C4B-NB	2.88	127.31	124.26
15	aB	803	CLA	C3B-C4B-NB	-2.88	107.84	110.52
15	a5	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	b1	401	BCR	C15-C16-C17	-2.88	117.57	123.47
15	cA	822	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
15	c4	411	CLA	CMB-C2B-C3B	2.88	133.57	126.59
15	aL	201	CLA	CHB-C1B-NB	2.88	127.31	124.26
18	a2	401	BCR	C1-C6-C5	-2.88	118.55	122.61
15	c4	405	CLA	C3C-C4C-NC	-2.88	107.34	110.57
15	b2	414	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	a3	416	CLA	C1-C2-C3	-2.88	122.09	126.75
15	b5	404	CLA	CHB-C4A-NA	2.88	128.50	124.51
18	aA	849	BCR	C3-C4-C5	-2.88	108.93	114.08
15	cB	816	CLA	O2D-CGD-CBD	2.88	116.39	111.27
18	b6	401	BCR	C15-C16-C17	-2.88	117.57	123.47
15	a1	406	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
15	b6	422	CLA	CAA-CBA-CGA	-2.88	104.83	113.25
15	c2	412	CLA	CMB-C2B-C3B	2.88	133.56	126.59
15	b3	408	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	cA	838	CLA	CHB-C4A-NA	2.88	128.50	124.51
15	a3	404	CLA	C3B-C4B-NB	-2.88	107.84	110.52
15	aA	816	CLA	CHB-C4A-NA	2.88	128.49	124.51
15	b6	409	CLA	O2D-CGD-O1D	-2.88	118.21	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	403	CLA	CMB-C2B-C3B	2.88	133.56	126.59
15	a2	416	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
15	aB	834	CLA	C2D-C1D-ND	-2.88	107.98	110.10
15	bB	811	CLA	C3B-C4B-NB	-2.88	107.84	110.52
18	cJ	104	BCR	C27-C26-C25	2.88	126.91	122.73
18	aI	102	BCR	C24-C23-C22	-2.88	121.89	126.23
15	aB	814	CLA	CMB-C2B-C3B	2.88	133.56	126.59
18	a1	420	BCR	C15-C16-C17	-2.88	117.58	123.47
15	aA	843	CLA	CHB-C4A-NA	2.88	128.49	124.51
15	cB	803	CLA	C3B-C4B-NB	-2.88	107.85	110.52
15	c6	406	CLA	C1-C2-C3	-2.88	121.07	126.04
15	b2	417	CLA	CHB-C1B-NB	2.88	127.30	124.26
15	bK	101	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	a4	412	CLA	CMC-C2C-C1C	-2.87	120.66	125.04
15	b6	405	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	b4	421	CLA	CHB-C4A-NA	2.87	128.49	124.51
15	cL	202	CLA	CHB-C1B-NB	2.87	127.30	124.26
15	cA	809	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
15	b4	413	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	bB	815	CLA	C3B-C4B-NB	-2.87	107.85	110.52
15	a1	415	CLA	C1-C2-C3	-2.87	122.10	126.75
15	a4	414	CLA	CAA-C2A-C3A	-2.87	109.39	116.10
15	a1	415	CLA	CHB-C1B-NB	2.87	127.30	124.26
15	cB	813	CLA	CHB-C1B-NB	2.87	127.30	124.26
15	b3	406	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
15	aB	816	CLA	O2D-CGD-CBD	2.87	116.37	111.27
15	a2	404	CLA	C1-C2-C3	-2.87	121.08	126.04
15	b2	405	CLA	C3C-C4C-NC	-2.87	107.35	110.57
15	cB	804	CLA	CBC-CAC-C3C	2.87	120.35	112.43
15	aA	804	CLA	CHB-C4A-NA	2.87	128.48	124.51
15	aB	810	CLA	CHC-C4B-NB	2.87	127.30	124.26
15	a1	402	CLA	C3B-C4B-NB	-2.87	107.85	110.52
15	c3	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	b3	417	CLA	C2C-C1C-NC	-2.87	107.28	109.97
15	b2	412	CLA	CMB-C2B-C3B	2.87	133.54	126.59
18	a2	419	BCR	C40-C30-C29	-2.87	97.43	108.91
18	b3	418	BCR	C27-C26-C25	2.87	126.90	122.73
15	b1	412	CLA	CMB-C2B-C1B	-2.87	121.00	125.37
15	c2	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	a3	402	CLA	C1-C2-C3	-2.87	121.08	126.04
15	aB	811	CLA	C3B-C4B-NB	-2.87	107.85	110.52
15	a1	403	CLA	C1-C2-C3	-2.87	121.08	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	403	CLA	CMB-C2B-C3B	2.87	133.54	126.59
15	c5	410	CLA	CHB-C4A-NA	2.87	128.48	124.51
15	bL	202	CLA	CHB-C1B-NB	2.87	127.29	124.26
15	bB	803	CLA	C3B-C4B-NB	-2.87	107.85	110.52
15	bA	820	CLA	CMB-C2B-C3B	2.87	133.53	126.59
15	aA	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	c4	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	b3	410	CLA	CMC-C2C-C3C	2.87	133.90	126.12
16	cB	843	PQN	C16-C17-C18	-2.87	106.65	115.92
15	cA	842	CLA	CHB-C4A-NA	2.87	128.48	124.51
18	b2	401	BCR	C15-C16-C17	-2.87	117.60	123.47
15	bB	804	CLA	CBC-CAC-C3C	2.87	120.33	112.43
15	a2	417	CLA	CHB-C1B-NB	2.87	127.29	124.26
15	bA	830	CLA	C2D-C1D-ND	-2.87	107.99	110.10
16	bB	843	PQN	C16-C17-C18	-2.87	106.66	115.92
15	a1	407	CLA	CHB-C4A-NA	2.87	128.47	124.51
15	c3	414	CLA	CHB-C4A-NA	2.87	128.47	124.51
18	b6	402	BCR	C7-C8-C9	-2.86	121.91	126.23
18	bB	845	BCR	C28-C27-C26	-2.86	108.96	114.08
15	bA	820	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	a6	417	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	cB	801	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	a3	418	BCR	C27-C26-C25	2.86	126.89	122.73
15	aB	804	CLA	CBC-CAC-C3C	2.86	120.33	112.43
18	aJ	205	BCR	C27-C26-C25	2.86	126.89	122.73
15	c2	405	CLA	C3C-C4C-NC	-2.86	107.36	110.57
15	b6	408	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	cB	820	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	bJ	104	BCR	C27-C26-C25	2.86	126.89	122.73
15	c3	403	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	b3	403	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	c6	403	BCR	C7-C8-C9	-2.86	121.91	126.23
15	cA	829	CLA	CMB-C2B-C3B	2.86	133.52	126.59
15	aK	102	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	c1	406	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	b6	419	BCR	C27-C26-C25	2.86	126.89	122.73
15	c2	417	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
15	b3	417	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	aA	809	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
15	c3	414	CLA	CAA-C2A-C3A	-2.86	109.42	116.10
15	a1	410	CLA	CMB-C2B-C3B	2.86	133.52	126.59
16	aB	843	PQN	C16-C17-C18	-2.86	106.67	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b4	420	BCR	C35-C13-C14	-2.86	118.92	122.92
15	a4	417	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	a6	408	CLA	CHB-C4A-NA	2.86	128.47	124.51
15	cK	102	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
15	c4	411	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
15	aB	815	CLA	CHB-C4A-NA	2.86	128.46	124.51
18	cB	845	BCR	C28-C27-C26	-2.86	108.97	114.08
18	a1	418	BCR	C15-C16-C17	-2.86	117.62	123.47
15	b1	408	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	b3	407	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	cA	816	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	b5	410	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	a6	409	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
15	cB	818	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	c2	419	BCR	C40-C30-C29	-2.86	97.48	108.91
15	c3	410	CLA	CAC-C3C-C2C	2.86	132.41	127.53
15	aK	102	CLA	C3B-C4B-NB	-2.86	107.87	110.52
15	cK	102	CLA	C3B-C4B-NB	-2.86	107.87	110.52
15	c6	411	CLA	C3B-C4B-NB	-2.86	107.87	110.52
15	c6	410	CLA	CMB-C2B-C3B	2.86	133.50	126.59
18	a1	421	BCR	C15-C16-C17	-2.86	117.62	123.47
18	a6	421	BCR	C15-C16-C17	-2.86	117.62	123.47
18	bA	850	BCR	C3-C4-C5	-2.86	108.98	114.08
15	cB	822	CLA	CHB-C4A-NA	2.86	128.46	124.51
15	cB	801	CLA	CHB-C1B-NB	2.85	127.28	124.26
15	c1	407	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	c2	406	CLA	C6-C7-C8	-2.85	106.69	115.92
18	c1	401	BCR	C15-C16-C17	-2.85	117.63	123.47
18	b3	419	BCR	C24-C23-C22	-2.85	121.92	126.23
15	a1	410	CLA	CHB-C1B-NB	2.85	127.28	124.26
15	bB	813	CLA	CHB-C1B-NB	2.85	127.28	124.26
18	aB	845	BCR	C28-C27-C26	-2.85	108.98	114.08
15	a2	405	CLA	CHD-C1D-ND	-2.85	121.83	124.45
15	c3	405	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	a3	419	BCR	C24-C23-C22	-2.85	121.92	126.23
18	a6	419	BCR	C27-C26-C25	2.85	126.87	122.73
18	c1	419	BCR	C15-C16-C17	-2.85	117.63	123.47
18	b1	401	BCR	C24-C23-C22	-2.85	121.92	126.23
15	bB	801	CLA	C3B-C4B-NB	-2.85	107.87	110.52
15	c3	417	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	a6	412	CLA	CMB-C2B-C3B	2.85	133.50	126.59
15	cA	820	CLA	CMB-C2B-C3B	2.85	133.50	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	816	CLA	O2D-CGD-CBD	2.85	116.34	111.27
15	bA	829	CLA	CMB-C2B-C3B	2.85	133.50	126.59
15	bA	816	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	cA	804	CLA	CHB-C4A-NA	2.85	128.46	124.51
15	c4	408	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	aA	829	CLA	CMB-C2B-C3B	2.85	133.49	126.59
15	bB	822	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	cA	848	BCR	C3-C4-C5	-2.85	108.99	114.08
15	c1	417	CLA	C2B-C1B-NB	2.85	112.14	110.23
15	c5	405	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	b2	413	CLA	C2D-C1D-ND	-2.85	108.00	110.10
15	aA	822	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c1	402	CLA	C1-C2-C3	-2.85	121.12	126.04
18	c6	420	BCR	C27-C26-C25	2.85	126.87	122.73
18	cB	845	BCR	C30-C25-C26	-2.85	118.60	122.61
18	cF	204	BCR	C30-C25-C26	-2.85	118.60	122.61
15	cA	826	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
15	a1	415	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
15	c5	405	CLA	C3C-C4C-NC	-2.85	107.38	110.57
15	cA	841	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	bL	206	BCR	C3-C4-C5	-2.85	108.99	114.08
15	bA	843	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c4	405	CLA	CHD-C1D-ND	-2.85	121.84	124.45
15	a3	417	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c1	404	CLA	C1-C2-C3	-2.85	121.12	126.04
18	b4	419	BCR	C15-C14-C13	-2.85	123.25	127.31
15	a5	410	CLA	CMC-C2C-C3C	2.85	133.84	126.12
15	b3	404	CLA	CHB-C4A-NA	2.85	128.45	124.51
15	c6	418	CLA	C1-C2-C3	-2.85	122.15	126.75
15	a1	411	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	b1	411	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	c4	419	BCR	C15-C14-C13	-2.85	123.25	127.31
15	aA	820	CLA	CMB-C2B-C3B	2.85	133.48	126.59
15	a2	417	CLA	CHC-C1C-C2C	-2.85	118.83	126.73
15	aB	822	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a2	406	CLA	C6-C7-C8	-2.84	106.73	115.92
18	c3	419	BCR	C24-C23-C22	-2.84	121.94	126.23
15	b2	406	CLA	C6-C7-C8	-2.84	106.73	115.92
15	a4	407	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	b2	419	BCR	C40-C30-C29	-2.84	97.53	108.91
18	a2	419	BCR	C27-C26-C25	2.84	126.86	122.73
15	c2	409	CLA	C2D-C1D-ND	-2.84	108.01	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	409	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	a5	418	BCR	C3-C4-C5	-2.84	109.00	114.08
15	aB	818	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	c2	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	aB	848	BCR	C15-C14-C13	-2.84	123.25	127.31
15	bA	804	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	c4	421	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	c6	419	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a1	401	CLA	C1-C2-C3	-2.84	121.13	126.04
15	b3	402	CLA	C1-C2-C3	-2.84	121.13	126.04
15	a2	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	c3	414	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
15	cB	811	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
15	aA	819	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	a3	410	CLA	CMC-C2C-C3C	2.84	133.83	126.12
15	c6	409	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	b2	422	CLA	CED-O2D-CGD	2.84	122.36	115.94
15	b5	405	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	bB	820	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	c2	414	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	c1	410	CLA	CAC-C3C-C2C	2.84	132.38	127.53
15	cB	834	CLA	C2D-C1D-ND	-2.84	108.01	110.10
15	b6	409	CLA	CMB-C2B-C3B	2.84	133.46	126.59
15	c3	403	CLA	CMB-C2B-C3B	2.84	133.46	126.59
15	b6	404	CLA	C3B-C4B-NB	-2.84	107.88	110.52
15	aA	826	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
15	bA	841	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	a1	411	CLA	C2D-C1D-ND	-2.84	108.01	110.10
15	b2	417	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
15	b1	407	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	b5	410	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
15	aA	838	CLA	CHB-C4A-NA	2.84	128.43	124.51
15	b1	411	CLA	CHB-C1B-NB	2.83	127.26	124.26
15	b5	410	CLA	CMC-C2C-C3C	2.83	133.81	126.12
18	cI	102	BCR	C24-C23-C22	-2.83	121.95	126.23
15	aB	813	CLA	CHB-C1B-NB	2.83	127.26	124.26
15	bA	824	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	aB	801	CLA	C3B-C4B-NB	-2.83	107.89	110.52
15	cB	815	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	c2	409	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	c5	411	CLA	CHB-C4A-NA	2.83	128.43	124.51
15	aA	824	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	405	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	c4	411	CLA	CHB-C1B-NB	2.83	127.25	124.26
15	c4	413	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	c2	417	CLA	CHB-C1B-NB	2.83	127.25	124.26
15	a5	410	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
15	b4	403	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	bA	826	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
15	a1	411	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
15	c6	412	CLA	CMC-C2C-C3C	2.83	133.80	126.12
15	c1	411	CLA	CMB-C2B-C3B	2.83	133.44	126.59
15	bK	101	CLA	C3B-C4B-NB	-2.83	107.89	110.52
15	aB	820	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c6	413	CLA	CMB-C2B-C3B	2.83	133.44	126.59
15	c1	415	CLA	C2D-C1D-ND	-2.83	108.02	110.10
15	b6	405	CLA	C1-C2-C3	-2.83	121.15	126.04
15	bA	825	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c1	411	CLA	CHB-C4A-NA	2.83	128.42	124.51
18	c5	418	BCR	C40-C30-C29	-2.83	97.59	108.91
15	c3	402	CLA	C1-C2-C3	-2.83	121.15	126.04
15	b2	406	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c5	402	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	c5	420	CLA	C16-C15-C13	-2.83	106.78	115.92
18	c2	401	BCR	C35-C13-C14	-2.83	118.96	122.92
15	a5	411	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	a3	408	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	c3	407	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	b2	404	CLA	C1-C2-C3	-2.83	121.15	126.04
15	aB	811	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
15	aA	820	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	b3	414	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	aA	809	CLA	O2D-CGD-CBD	2.83	116.29	111.27
15	bB	815	CLA	CHB-C4A-NA	2.83	128.42	124.51
15	a6	405	CLA	C1-C2-C3	-2.83	121.16	126.04
15	a5	402	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
18	bL	201	BCR	C3-C4-C5	-2.82	109.03	114.08
15	a3	407	CLA	CHB-C4A-NA	2.82	128.42	124.51
15	b2	406	CLA	CHB-C4A-NA	2.82	128.42	124.51
15	b1	416	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
15	c1	416	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
15	b5	403	CLA	C3B-C4B-NB	-2.82	107.89	110.52
15	cA	828	CLA	CHB-C1B-NB	2.82	127.25	124.26
15	cA	824	CLA	O2D-CGD-O1D	-2.82	118.32	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c5	418	BCR	C3-C4-C5	-2.82	109.04	114.08
15	aA	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	aA	839	CLA	CHB-C1B-NB	2.82	127.25	124.26
18	a4	419	BCR	C15-C14-C13	-2.82	123.28	127.31
15	c6	410	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	c2	419	BCR	C27-C26-C25	2.82	126.83	122.73
15	a6	409	CLA	CMB-C2B-C3B	2.82	133.42	126.59
15	a5	420	CLA	C16-C15-C13	-2.82	106.80	115.92
18	c1	401	BCR	C24-C23-C22	-2.82	121.97	126.23
15	bB	834	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	cA	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	c1	412	CLA	C2D-C1D-ND	-2.82	108.03	110.10
18	bB	846	BCR	C15-C14-C13	-2.82	123.29	127.31
15	bB	809	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	a5	403	CLA	C3B-C4B-NB	-2.82	107.90	110.52
15	bB	811	CLA	O2A-CGA-O1A	-2.82	116.48	123.59
15	b2	402	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
15	a4	421	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	b6	409	CLA	CHB-C4A-NA	2.82	128.41	124.51
15	b3	405	CLA	CHD-C1D-ND	-2.82	121.86	124.45
15	cA	821	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	cJ	103	BCR	C35-C13-C14	-2.82	118.98	122.92
18	bF	202	BCR	C30-C25-C26	-2.82	118.65	122.61
15	bB	818	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	c3	401	BCR	C15-C16-C17	-2.81	117.71	123.47
18	bB	848	BCR	C15-C14-C13	-2.81	123.29	127.31
15	b5	404	CLA	C1-C2-C3	-2.81	121.17	126.04
18	aF	202	BCR	C30-C25-C26	-2.81	118.65	122.61
15	c6	406	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	aJ	204	BCR	C35-C13-C14	-2.81	118.98	122.92
15	a6	411	CLA	CMC-C2C-C3C	2.81	133.76	126.12
15	b6	411	CLA	CMC-C2C-C3C	2.81	133.76	126.12
15	bL	203	CLA	CHD-C1D-ND	-2.81	121.87	124.45
15	aA	842	CLA	C3B-C4B-NB	-2.81	107.91	110.52
15	b4	408	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	a1	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	a6	409	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	bL	205	BCR	C15-C14-C13	-2.81	123.30	127.31
18	cB	846	BCR	C15-C14-C13	-2.81	123.30	127.31
15	c2	413	CLA	C2D-C1D-ND	-2.81	108.03	110.10
15	a2	406	CLA	CHB-C4A-NA	2.81	128.40	124.51
15	cA	820	CLA	CHB-C4A-NA	2.81	128.40	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a2	401	BCR	C35-C13-C14	-2.81	118.99	122.92
15	cA	809	CLA	O2D-CGD-CBD	2.81	116.26	111.27
15	a4	408	CLA	C2D-C1D-ND	-2.81	108.03	110.10
15	bA	842	CLA	C3B-C4B-NB	-2.81	107.91	110.52
15	c3	405	CLA	C3C-C4C-NC	-2.81	107.42	110.57
15	a4	403	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	a3	404	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	a5	418	BCR	C40-C30-C29	-2.81	97.67	108.91
18	aL	205	BCR	C3-C4-C5	-2.81	109.06	114.08
18	c3	418	BCR	C40-C30-C29	-2.81	97.67	108.91
15	a2	414	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
15	c3	416	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
15	a2	409	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	bJ	103	BCR	C35-C13-C14	-2.81	118.99	122.92
18	cL	205	BCR	C15-C14-C13	-2.81	123.30	127.31
15	a6	422	CLA	CHA-C1A-NA	-2.81	119.97	126.40
15	a4	411	CLA	CMB-C2B-C3B	2.81	133.39	126.59
15	a6	412	CLA	CHB-C4A-NA	2.81	128.39	124.51
15	a2	409	CLA	C2D-C1D-ND	-2.81	108.04	110.10
18	c2	401	BCR	C15-C16-C17	-2.81	117.73	123.47
15	cB	814	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
18	b2	401	BCR	C35-C13-C14	-2.81	118.99	122.92
15	bB	824	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	a1	417	BCR	C40-C30-C29	-2.81	97.69	108.91
15	a4	403	CLA	C3B-C4B-NB	-2.80	107.91	110.52
15	c1	411	CLA	CHB-C1B-NB	2.80	127.23	124.26
15	a3	405	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
15	a3	405	CLA	C3C-C4C-NC	-2.80	107.43	110.57
15	c4	403	CLA	C3B-C4B-NB	-2.80	107.91	110.52
18	b3	418	BCR	C40-C30-C29	-2.80	97.69	108.91
18	cB	849	BCR	C27-C26-C25	2.80	126.80	122.73
15	cL	203	CLA	CHD-C1D-ND	-2.80	121.88	124.45
15	c4	421	CLA	C3B-C4B-NB	-2.80	107.92	110.52
15	c5	403	CLA	C3B-C4B-NB	-2.80	107.92	110.52
15	b1	404	CLA	CHB-C4A-NA	2.80	128.39	124.51
15	b6	417	CLA	C1-C2-C3	-2.80	122.22	126.75
18	aJ	204	BCR	C7-C8-C9	-2.80	122.00	126.23
15	b6	412	CLA	CMB-C2B-C3B	2.80	133.37	126.59
15	a3	416	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
15	c2	410	CLA	C3B-C4B-NB	-2.80	107.92	110.52
15	cF	201	CLA	C3B-C4B-NB	-2.80	107.92	110.52
15	a1	413	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a3	403	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
15	a6	417	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
15	c6	418	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
15	a3	414	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	cB	809	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	cA	833	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
18	a4	418	BCR	C3-C4-C5	-2.80	109.08	114.08
15	bA	845	CLA	CHB-C4A-NA	2.80	128.38	124.51
15	b5	402	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
15	b3	416	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
15	b6	417	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
15	a6	417	CLA	C1-C2-C3	-2.80	122.23	126.75
18	cA	848	BCR	C40-C30-C25	2.80	114.84	110.30
18	b5	418	BCR	C40-C30-C29	-2.80	97.72	108.91
18	bB	850	BCR	C27-C26-C25	2.80	126.79	122.73
18	b6	419	BCR	C40-C30-C29	-2.80	97.72	108.91
15	c6	416	CLA	CHB-C4A-NA	2.80	128.38	124.51
18	a2	401	BCR	C15-C16-C17	-2.80	117.75	123.47
15	a5	408	CLA	CHB-C4A-NA	2.79	128.38	124.51
15	c6	413	CLA	CHB-C4A-NA	2.79	128.38	124.51
18	cF	204	BCR	C35-C13-C14	-2.79	119.01	122.92
15	b4	411	CLA	CMB-C2B-C3B	2.79	133.36	126.59
15	b1	412	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
15	a4	416	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
15	aA	821	CLA	CHB-C4A-NA	2.79	128.38	124.51
18	a3	418	BCR	C40-C30-C29	-2.79	97.73	108.91
18	a1	420	BCR	C34-C9-C8	-2.79	113.67	118.08
15	c1	414	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	aA	849	BCR	C27-C26-C25	2.79	126.79	122.73
15	b6	405	CLA	CHB-C4A-NA	2.79	128.38	124.51
15	c3	411	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	a3	420	BCR	C15-C14-C13	-2.79	123.32	127.31
15	bA	819	CLA	C3B-C4B-NB	-2.79	107.92	110.52
15	bB	834	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
18	aB	845	BCR	C30-C25-C26	-2.79	118.68	122.61
15	a4	407	CLA	C2A-C1A-CHA	2.79	128.74	123.86
15	bA	809	CLA	O2D-CGD-CBD	2.79	116.23	111.27
15	b5	420	CLA	C16-C15-C13	-2.79	106.89	115.92
18	aB	849	BCR	C27-C26-C25	2.79	126.78	122.73
18	c3	419	BCR	C15-C16-C17	-2.79	117.76	123.47
18	c4	418	BCR	C3-C4-C5	-2.79	109.09	114.08
18	bB	848	BCR	C27-C26-C25	2.79	126.78	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	809	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	c2	406	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	c1	412	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	cJ	103	BCR	C7-C8-C9	-2.79	122.02	126.23
15	bA	818	CLA	CMB-C2B-C1B	-2.79	121.12	125.37
18	bB	845	BCR	C30-C25-C26	-2.79	118.69	122.61
19	bA	854	LHG	O8-C23-C24	2.79	120.66	111.91
15	c3	411	CLA	CMB-C2B-C3B	2.79	133.34	126.59
15	bB	814	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
18	c4	420	BCR	C35-C13-C14	-2.79	119.02	122.92
18	bA	850	BCR	C27-C26-C25	2.79	126.78	122.73
15	b3	414	CLA	CAA-C2A-C3A	-2.79	109.59	116.10
19	cA	852	LHG	O8-C23-C24	2.79	120.65	111.91
15	aA	845	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	b6	418	CLA	CHB-C4A-NA	2.79	128.37	124.51
15	b2	406	CLA	CGD-CBD-CAD	-2.79	101.71	110.73
15	aB	814	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
18	aA	849	BCR	C40-C30-C25	2.79	114.82	110.30
15	aB	834	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
18	a6	419	BCR	C40-C30-C29	-2.79	97.77	108.91
15	c4	403	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
18	a4	420	BCR	C35-C13-C14	-2.78	119.02	122.92
15	c4	416	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
18	bA	850	BCR	C40-C30-C25	2.78	114.81	110.30
15	b4	403	CLA	C3B-C4B-NB	-2.78	107.93	110.52
15	aB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
15	cB	834	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
19	aA	853	LHG	O8-C23-C24	2.78	120.64	111.91
20	cB	850	LMG	C40-C39-C38	-2.78	100.30	114.42
15	b1	402	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
15	aA	828	CLA	CHB-C1B-NB	2.78	127.20	124.26
15	b4	416	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
18	b6	421	BCR	C15-C16-C17	-2.78	117.78	123.47
18	bJ	103	BCR	C7-C8-C9	-2.78	122.03	126.23
15	a3	414	CLA	CAA-C2A-C3A	-2.78	109.61	116.10
15	aA	819	CLA	C3B-C4B-NB	-2.78	107.94	110.52
18	c3	418	BCR	C27-C26-C25	2.78	126.77	122.73
15	bA	821	CLA	CHB-C4A-NA	2.78	128.36	124.51
15	cB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	c6	420	BCR	C40-C30-C29	-2.78	97.79	108.91
15	aA	833	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
15	a2	413	CLA	C2D-C1D-ND	-2.78	108.06	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	839	CLA	CHB-C1B-NB	2.78	127.20	124.26
14	bA	801	CL0	CHB-C4A-NA	2.78	128.35	124.51
15	a1	410	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	cA	823	CLA	C3B-C4B-NB	-2.78	107.94	110.52
15	aA	811	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
15	bA	831	CLA	C2D-C1D-ND	-2.78	108.06	110.10
15	c6	410	CLA	CHB-C4A-NA	2.78	128.35	124.51
18	b4	419	BCR	C11-C10-C9	-2.78	123.35	127.31
15	cA	818	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
15	bA	828	CLA	CHB-C1B-NB	2.78	127.20	124.26
18	cA	848	BCR	C27-C26-C25	2.78	126.76	122.73
15	aB	841	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	bB	808	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	c1	404	CLA	CHB-C4A-NA	2.78	128.35	124.51
15	b1	405	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
15	a3	421	CLA	C6-C7-C8	-2.78	106.95	115.92
18	c4	419	BCR	C15-C16-C17	-2.78	117.79	123.47
15	aA	803	CLA	CAA-CBA-CGA	-2.77	105.14	113.25
15	b5	411	CLA	CHB-C4A-NA	2.77	128.35	124.51
15	b5	408	CLA	CHB-C4A-NA	2.77	128.35	124.51
18	c5	418	BCR	C27-C26-C25	2.77	126.76	122.73
15	c2	406	CLA	CGD-CBD-CAD	-2.77	101.75	110.73
15	a5	404	CLA	C1-C2-C3	-2.77	121.25	126.04
15	a1	408	CLA	C3B-C4B-NB	-2.77	107.94	110.52
15	a2	422	CLA	CED-O2D-CGD	2.77	122.21	115.94
18	aB	846	BCR	C15-C14-C13	-2.77	123.35	127.31
15	b3	421	CLA	C6-C7-C8	-2.77	106.96	115.92
15	cA	819	CLA	C3B-C4B-NB	-2.77	107.94	110.52
15	a2	406	CLA	CGD-CBD-CAD	-2.77	101.75	110.73
15	bA	832	CLA	CHC-C4B-NB	2.77	127.19	124.26
15	b4	411	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	b5	412	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
15	bA	817	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	c6	401	CLA	CGD-CBD-CAD	-2.77	101.76	110.73
14	cA	801	CL0	CHB-C4A-NA	2.77	128.34	124.51
15	a3	409	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	cA	803	CLA	CAA-CBA-CGA	-2.77	105.16	113.25
15	b4	417	CLA	C2B-C1B-NB	2.77	112.09	110.23
18	b3	420	BCR	C15-C14-C13	-2.77	123.36	127.31
15	a5	407	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	a5	414	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	c1	405	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b1	418	BCR	C40-C30-C29	-2.77	97.83	108.91
15	c5	416	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
20	aB	850	LMG	C40-C39-C38	-2.77	100.37	114.42
20	bB	851	LMG	C40-C39-C38	-2.77	100.37	114.42
18	cB	848	BCR	C15-C14-C13	-2.77	123.36	127.31
15	c1	402	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
15	b2	410	CLA	C3B-C4B-NB	-2.77	107.95	110.52
15	b5	416	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
15	c6	410	CLA	CHB-C1B-NB	2.77	127.19	124.26
18	b4	418	BCR	C3-C4-C5	-2.77	109.14	114.08
15	b2	413	CLA	CMB-C2B-C1B	-2.77	121.16	125.37
18	b5	418	BCR	C27-C26-C25	2.77	126.75	122.73
18	cB	846	BCR	C27-C26-C25	2.77	126.75	122.73
15	a6	415	CLA	CHB-C4A-NA	2.77	128.34	124.51
15	bA	803	CLA	CAA-CBA-CGA	-2.77	105.17	113.25
15	a3	410	CLA	CAC-C3C-C2C	2.76	132.26	127.53
15	cB	841	CLA	CHB-C4A-NA	2.76	128.34	124.51
15	aA	818	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
18	aI	103	BCR	C15-C14-C13	-2.76	123.36	127.31
18	a4	419	BCR	C11-C10-C9	-2.76	123.36	127.31
18	bF	202	BCR	C35-C13-C14	-2.76	119.05	122.92
15	aB	824	CLA	CHD-C1D-ND	-2.76	121.91	124.45
18	aB	846	BCR	C40-C30-C25	2.76	114.78	110.30
15	a5	416	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
15	c5	412	CLA	CMB-C2B-C1B	-2.76	121.16	125.37
18	c1	418	BCR	C40-C30-C29	-2.76	97.85	108.91
18	a3	401	BCR	C15-C16-C17	-2.76	117.81	123.47
18	b2	421	BCR	C15-C14-C13	-2.76	123.37	127.31
15	b6	412	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	cB	808	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	c2	422	CLA	C6-C7-C8	-2.76	106.99	115.92
15	b3	405	CLA	C3C-C4C-NC	-2.76	107.47	110.57
15	aA	817	CLA	CHB-C4A-NA	2.76	128.33	124.51
15	cA	811	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	a6	418	CLA	C3A-C2A-C1A	2.76	105.47	101.34
18	aB	848	BCR	C27-C26-C25	2.76	126.74	122.73
18	aF	203	BCR	C7-C8-C9	-2.76	122.06	126.23
15	cB	813	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
15	a6	418	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	cB	846	BCR	C40-C30-C25	2.76	114.78	110.30
18	c6	403	BCR	C15-C14-C13	-2.76	123.37	127.31
18	b3	401	BCR	C15-C16-C17	-2.76	117.82	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	811	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	a4	408	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	aB	816	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
15	b3	421	CLA	C6-C5-C3	-2.76	106.22	113.45
15	aA	840	CLA	O2D-CGD-CBD	2.76	116.17	111.27
15	a5	416	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	b5	414	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	bA	845	CLA	CHB-C1B-NB	2.76	127.18	124.26
15	cA	829	CLA	O2D-CGD-CBD	2.76	116.17	111.27
19	cA	852	LHG	C20-C19-C18	-2.76	100.43	114.42
15	a4	411	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
15	cB	824	CLA	CHD-C1D-ND	-2.76	121.92	124.45
15	aB	808	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	b4	408	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	b6	415	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	cA	844	CLA	CHB-C4A-NA	2.76	128.32	124.51
18	bJ	105	BCR	C7-C8-C9	-2.76	122.07	126.23
19	aA	853	LHG	C20-C19-C18	-2.76	100.44	114.42
15	cA	817	CLA	CHB-C4A-NA	2.76	128.32	124.51
15	aA	829	CLA	O2D-CGD-CBD	2.75	116.16	111.27
15	c4	412	CLA	C2D-C1D-ND	-2.75	108.07	110.10
15	bB	841	CLA	CHB-C4A-NA	2.75	128.32	124.51
15	cA	839	CLA	CHB-C1B-NB	2.75	127.17	124.26
18	b3	401	BCR	C15-C14-C13	-2.75	123.38	127.31
15	bA	833	CLA	CMB-C2B-C1B	-2.75	121.17	125.37
15	c5	416	CLA	CHB-C1B-NB	2.75	127.17	124.26
15	b4	412	CLA	C2D-C1D-ND	-2.75	108.08	110.10
18	aF	202	BCR	C35-C13-C14	-2.75	119.07	122.92
15	a5	407	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b2	409	CLA	C2D-C1D-ND	-2.75	108.08	110.10
15	bA	829	CLA	O2D-CGD-CBD	2.75	116.16	111.27
15	a2	413	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
15	c6	405	CLA	CMB-C2B-C3B	2.75	133.25	126.59
15	a4	412	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
18	a2	421	BCR	C15-C14-C13	-2.75	123.38	127.31
18	c3	420	BCR	C15-C14-C13	-2.75	123.38	127.31
15	a6	405	CLA	CHB-C4A-NA	2.75	128.32	124.51
15	a1	415	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b5	408	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	b1	420	BCR	C35-C13-C14	-2.75	119.07	122.92
15	cA	832	CLA	CHB-C4A-NA	2.75	128.31	124.51
15	aB	813	CLA	CMB-C2B-C1B	-2.75	121.18	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	401	BCR	C7-C8-C9	-2.75	122.08	126.23
15	bB	811	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	b5	416	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
18	c4	419	BCR	C11-C10-C9	-2.75	123.39	127.31
15	aA	832	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	bB	846	BCR	C27-C26-C25	2.75	126.72	122.73
15	c1	409	CLA	C3B-C4B-NB	-2.75	107.97	110.52
15	a4	405	CLA	CHD-C1D-C2D	2.75	131.24	125.48
15	cB	811	CLA	C2A-C1A-CHA	2.75	128.66	123.86
18	cF	204	BCR	C27-C26-C25	2.75	126.72	122.73
18	a4	419	BCR	C15-C16-C17	-2.75	117.85	123.47
15	a2	404	CLA	CHB-C4A-NA	2.75	128.31	124.51
15	a5	403	CLA	CMB-C2B-C3B	2.75	133.24	126.59
15	a2	410	CLA	C3B-C4B-NB	-2.75	107.97	110.52
14	aA	801	CL0	CHB-C4A-NA	2.75	128.31	124.51
15	a1	401	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
15	b1	409	CLA	C3B-C4B-NB	-2.74	107.97	110.52
15	b2	417	CLA	C1-C2-C3	-2.74	122.31	126.75
18	bF	202	BCR	C27-C26-C25	2.74	126.71	122.73
18	a3	401	BCR	C15-C14-C13	-2.74	123.39	127.31
18	a5	418	BCR	C27-C26-C25	2.74	126.71	122.73
15	b1	410	CLA	CAC-C3C-C2C	2.74	132.22	127.53
15	a3	411	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
15	bA	823	CLA	C3B-C4B-NB	-2.74	107.97	110.52
15	a3	416	CLA	CHB-C1B-NB	2.74	127.16	124.26
18	bA	852	BCR	C15-C16-C17	-2.74	117.86	123.47
15	a2	418	CLA	C3A-C2A-C1A	2.74	105.45	101.34
19	bA	854	LHG	C20-C19-C18	-2.74	100.51	114.42
15	bA	811	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	c2	420	BCR	C15-C14-C13	-2.74	123.40	127.31
18	cA	850	BCR	C15-C16-C17	-2.74	117.86	123.47
15	c5	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	b3	410	CLA	CAC-C3C-C2C	2.74	132.22	127.53
15	a5	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	a3	405	CLA	CHD-C1D-ND	-2.74	121.94	124.45
15	a5	412	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
15	b1	405	CLA	CHD-C1D-C2D	2.74	131.23	125.48
15	aA	832	CLA	CHC-C4B-NB	2.74	127.16	124.26
15	b1	403	CLA	CHB-C4A-NA	2.74	128.30	124.51
18	b3	419	BCR	C15-C16-C17	-2.74	117.86	123.47
15	c3	421	CLA	C6-C5-C3	-2.74	106.27	113.45
15	bB	813	CLA	CMB-C2B-C1B	-2.74	121.20	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	816	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
15	c1	408	CLA	CMB-C2B-C3B	2.74	133.22	126.59
15	a5	408	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
15	aB	811	CLA	C2A-C1A-CHA	2.74	128.65	123.86
18	b5	418	BCR	C3-C4-C5	-2.74	109.19	114.08
15	b5	416	CLA	CHB-C1B-NB	2.74	127.15	124.26
15	a3	421	CLA	C6-C5-C3	-2.74	106.28	113.45
15	b6	418	CLA	C3A-C2A-C1A	2.74	105.44	101.34
15	a1	409	CLA	CAC-C3C-C2C	2.74	132.21	127.53
18	cF	205	BCR	C7-C8-C9	-2.74	122.10	126.23
15	cA	832	CLA	CHC-C4B-NB	2.73	127.15	124.26
15	bB	842	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	c5	408	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	a4	408	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	a2	411	CLA	CAC-C3C-C2C	2.73	132.21	127.53
15	bB	811	CLA	C2A-C1A-CHA	2.73	128.64	123.86
15	b1	414	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
15	a6	404	CLA	CMB-C2B-C3B	2.73	133.21	126.59
15	cB	842	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	b6	414	CLA	CAC-C3C-C4C	2.73	128.35	124.81
15	a2	406	CLA	O2D-CGD-CBD	2.73	116.12	111.27
15	cB	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	cA	831	CLA	C2D-C1D-ND	-2.73	108.09	110.10
15	bB	816	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
15	a3	416	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	a4	411	CLA	CHB-C1B-NB	2.73	127.15	124.26
15	b5	407	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	c4	408	CLA	CHB-C4A-NA	2.73	128.29	124.51
15	b4	405	CLA	CHD-C1D-C2D	2.73	131.21	125.48
15	bA	840	CLA	O2D-CGD-CBD	2.73	116.12	111.27
18	aA	851	BCR	C15-C16-C17	-2.73	117.88	123.47
15	aL	202	CLA	CHD-C1D-ND	-2.73	121.95	124.45
15	cA	838	CLA	CHC-C4B-NB	2.73	127.15	124.26
15	a4	412	CLA	C2D-C1D-ND	-2.73	108.09	110.10
15	c4	407	CLA	C2A-C1A-CHA	2.73	128.63	123.86
15	b2	422	CLA	C6-C7-C8	-2.73	107.10	115.92
15	c3	421	CLA	C6-C7-C8	-2.73	107.10	115.92
15	a3	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	a6	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	c3	413	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
15	c5	404	CLA	C1-C2-C3	-2.73	121.33	126.04
15	b6	411	CLA	CMB-C2B-C1B	-2.73	121.22	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	833	CLA	C3B-C4B-NB	-2.73	107.99	110.52
15	c5	408	CLA	CHB-C4A-NA	2.73	128.28	124.51
15	c2	417	CLA	C1-C2-C3	-2.73	122.34	126.75
18	aB	846	BCR	C27-C26-C25	2.73	126.69	122.73
18	aI	103	BCR	C27-C26-C25	2.73	126.69	122.73
18	b1	419	BCR	C8-C9-C10	2.73	123.12	118.94
18	bB	847	BCR	C15-C14-C13	-2.73	123.39	127.30
18	bL	206	BCR	C7-C8-C9	-2.72	122.12	126.23
15	cB	811	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c1	403	CLA	CMB-C2B-C3B	2.72	133.19	126.59
19	bA	854	LHG	C11-C10-C9	-2.72	100.60	114.42
15	b5	403	CLA	CMB-C2B-C3B	2.72	133.19	126.59
15	b5	407	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c5	407	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c5	416	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	a3	412	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	b4	408	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	aA	805	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	c3	416	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
15	b3	411	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	b6	402	BCR	C15-C14-C13	-2.72	123.42	127.31
15	b1	412	CLA	C2D-C1D-ND	-2.72	108.10	110.10
15	b4	407	CLA	C2A-C1A-CHA	2.72	128.62	123.86
15	a1	407	CLA	CMB-C2B-C3B	2.72	133.18	126.59
15	b3	413	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	aB	803	CLA	CHB-C1B-NB	2.72	127.14	124.26
15	a4	404	CLA	CHB-C4A-NA	2.72	128.28	124.51
15	a2	422	CLA	C6-C7-C8	-2.72	107.12	115.92
15	c4	408	CLA	C2D-C1D-ND	-2.72	108.10	110.10
19	aA	853	LHG	C11-C10-C9	-2.72	100.61	114.42
15	c2	404	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	b4	411	CLA	CHB-C1B-NB	2.72	127.14	124.26
18	cB	848	BCR	C27-C26-C25	2.72	126.68	122.73
15	bB	817	CLA	CAC-C3C-C4C	2.72	128.34	124.81
15	bB	826	CLA	CAA-CBA-CGA	-2.72	105.31	113.25
15	a6	411	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	c5	409	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	aA	823	CLA	C3B-C4B-NB	-2.72	107.99	110.52
18	aF	201	BCR	C27-C26-C25	2.72	126.68	122.73
15	a2	417	CLA	C1-C2-C3	-2.72	122.35	126.75
15	bB	807	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
15	a1	403	CLA	CHB-C4A-NA	2.72	128.27	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	405	CLA	CHD-C1D-C2D	2.72	131.18	125.48
15	cB	838	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
15	cA	840	CLA	O2D-CGD-CBD	2.72	116.10	111.27
15	a1	402	CLA	CMB-C2B-C3B	2.72	133.17	126.59
18	bL	201	BCR	C7-C8-C9	-2.72	122.13	126.23
15	aB	826	CLA	CAA-CBA-CGA	-2.72	105.31	113.25
15	b2	409	CLA	CMB-C2B-C3B	2.72	133.17	126.59
15	aA	805	CLA	CMB-C2B-C3B	2.72	133.17	126.59
18	bB	846	BCR	C40-C30-C25	2.72	114.70	110.30
15	c6	412	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
18	a3	419	BCR	C15-C16-C17	-2.72	117.91	123.47
15	b4	416	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	cA	805	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
15	a4	410	CLA	CHB-C4A-NA	2.72	128.27	124.51
15	c6	419	CLA	C3A-C2A-C1A	2.72	105.41	101.34
19	cA	852	LHG	C11-C10-C9	-2.71	100.64	114.42
15	a5	409	CLA	CHB-C4A-NA	2.71	128.27	124.51
15	cA	805	CLA	CMB-C2B-C3B	2.71	133.16	126.59
15	b2	418	CLA	C3A-C2A-C1A	2.71	105.40	101.34
15	aB	837	CLA	CBA-CAA-C2A	2.71	121.87	113.86
15	cA	844	CLA	CHB-C1B-NB	2.71	127.13	124.26
18	a6	402	BCR	C15-C14-C13	-2.71	123.44	127.31
15	b3	416	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	c5	414	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	b6	422	CLA	C16-C15-C13	-2.71	107.15	115.92
15	aB	825	CLA	C2A-C1A-CHA	2.71	128.60	123.86
15	aB	842	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
18	b4	419	BCR	C15-C16-C17	-2.71	117.92	123.47
15	c2	413	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
18	cF	202	BCR	C27-C26-C25	2.71	126.67	122.73
15	c4	405	CLA	CHD-C1D-C2D	2.71	131.17	125.48
15	b4	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	a4	416	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	c6	407	CLA	C3C-C4C-NC	-2.71	107.53	110.57
15	b3	411	CLA	CMB-C2B-C3B	2.71	133.15	126.59
15	b6	404	CLA	CMB-C2B-C3B	2.71	133.15	126.59
15	c3	416	CLA	CHB-C1B-NB	2.71	127.13	124.26
18	a3	401	BCR	C7-C8-C9	-2.71	122.14	126.23
15	a3	402	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	bB	837	CLA	CBA-CAA-C2A	2.71	121.86	113.86
18	b5	419	BCR	C35-C13-C14	-2.71	119.13	122.92
15	c4	404	CLA	CHB-C4A-NA	2.71	128.26	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	819	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
15	b1	408	CLA	CMB-C2B-C3B	2.71	133.15	126.59
18	aA	852	BCR	C27-C26-C25	2.71	126.66	122.73
18	cB	847	BCR	C30-C25-C26	-2.71	118.80	122.61
15	bB	838	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
18	aF	202	BCR	C27-C26-C25	2.71	126.66	122.73
15	aA	808	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	bA	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
15	aA	806	CLA	C3B-C4B-NB	-2.71	108.00	110.52
15	cB	836	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	aB	819	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
15	a6	416	CLA	C2D-C1D-ND	-2.71	108.11	110.10
15	c1	405	CLA	CHD-C1D-C2D	2.71	131.16	125.48
15	aA	845	CLA	CHB-C1B-NB	2.71	127.12	124.26
15	bA	838	CLA	CHC-C4B-NB	2.71	127.12	124.26
15	bA	808	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	b3	410	CLA	CHB-C4A-NA	2.71	128.25	124.51
15	b1	410	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
15	bA	805	CLA	CMB-C2B-C3B	2.71	133.14	126.59
15	a6	422	CLA	C11-C10-C8	-2.70	107.18	115.92
18	bL	205	BCR	C27-C26-C25	2.70	126.66	122.73
15	c1	414	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
15	b3	407	CLA	C2A-C1A-CHA	2.70	128.59	123.86
15	a1	413	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	a2	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	c4	421	CLA	C6-C5-C3	-2.70	106.36	113.45
15	a1	404	CLA	CHD-C1D-C2D	2.70	131.15	125.48
15	b2	411	CLA	CAC-C3C-C2C	2.70	132.15	127.53
18	bA	853	BCR	C27-C26-C25	2.70	126.66	122.73
15	c2	418	CLA	C3A-C2A-C1A	2.70	105.39	101.34
18	cA	847	BCR	C15-C14-C13	-2.70	123.45	127.31
15	cA	833	CLA	CHB-C4A-NA	2.70	128.25	124.51
15	cB	826	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
15	c3	412	CLA	C2D-C1D-ND	-2.70	108.11	110.10
15	c4	416	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
18	b2	420	BCR	C15-C16-C17	-2.70	117.94	123.47
15	a5	417	CLA	C2B-C1B-NB	2.70	112.04	110.23
15	cB	817	CLA	CAC-C3C-C4C	2.70	128.31	124.81
14	bA	801	CL0	CHD-C4C-NC	2.70	128.46	124.20
18	a1	418	BCR	C8-C9-C10	2.70	123.09	118.94
15	a1	415	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
15	c5	407	CLA	CHB-C4A-NA	2.70	128.25	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	805	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
15	a5	416	CLA	CHB-C1B-NB	2.70	127.11	124.26
15	aB	807	CLA	C7-C6-C5	-2.70	106.03	113.36
18	cA	851	BCR	C30-C25-C26	-2.70	118.81	122.61
15	b6	410	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	b1	403	CLA	CMB-C2B-C3B	2.70	133.12	126.59
15	cB	807	CLA	C7-C6-C5	-2.70	106.03	113.36
15	a5	402	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	c3	409	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	cB	837	CLA	CBA-CAA-C2A	2.70	121.83	113.86
15	cB	803	CLA	CHB-C1B-NB	2.70	127.11	124.26
15	bB	807	CLA	C7-C6-C5	-2.70	106.03	113.36
18	c1	419	BCR	C8-C9-C10	2.70	123.08	118.94
15	aB	821	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	a2	415	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
15	b3	409	CLA	CHB-C4A-NA	2.70	128.24	124.51
15	c5	403	CLA	CMB-C2B-C3B	2.70	133.12	126.59
18	c5	419	BCR	C35-C13-C14	-2.70	119.15	122.92
15	aA	820	CLA	C1-C2-C3	-2.70	121.38	126.04
18	cA	851	BCR	C27-C26-C25	2.70	126.64	122.73
15	c1	412	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
18	aB	847	BCR	C15-C14-C13	-2.69	123.44	127.30
18	cB	847	BCR	C15-C14-C13	-2.69	123.44	127.30
18	cL	205	BCR	C27-C26-C25	2.69	126.64	122.73
15	c2	422	CLA	CHA-C1A-NA	-2.69	120.23	126.40
18	bA	849	BCR	C15-C14-C13	-2.69	123.47	127.31
15	c1	414	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	c6	411	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	a3	411	CLA	CMB-C2B-C3B	2.69	133.11	126.59
18	aB	847	BCR	C30-C25-C26	-2.69	118.82	122.61
18	bB	847	BCR	C30-C25-C26	-2.69	118.82	122.61
15	cA	836	CLA	CHC-C4B-NB	2.69	127.11	124.26
15	bB	836	CLA	CHB-C4A-NA	2.69	128.24	124.51
15	c2	411	CLA	CAC-C3C-C2C	2.69	132.13	127.53
15	c5	410	CLA	CAC-C3C-C2C	2.69	132.13	127.53
15	b6	403	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
15	aA	840	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
15	cB	819	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
15	cA	806	CLA	C3B-C4B-NB	-2.69	108.02	110.52
15	cB	835	CLA	O1D-CGD-CBD	2.69	129.99	124.48
15	aB	807	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
18	bB	849	BCR	C27-C26-C25	2.69	126.64	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	803	CLA	CHB-C1B-NB	2.69	127.11	124.26
18	c2	419	BCR	C3-C4-C5	-2.69	109.27	114.08
18	aA	848	BCR	C15-C14-C13	-2.69	123.47	127.31
15	c3	403	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	cA	836	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	aA	817	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	b2	422	CLA	C6-C5-C3	-2.69	106.40	113.45
15	bA	840	CLA	CMB-C2B-C1B	-2.69	121.27	125.37
18	a5	401	BCR	C15-C14-C13	-2.69	123.47	127.31
18	c2	421	BCR	C15-C14-C13	-2.69	123.47	127.31
15	a2	410	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	b3	409	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	a6	409	CLA	CHB-C1B-NB	2.69	127.10	124.26
15	cA	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52
15	b1	410	CLA	CHB-C1B-NB	2.69	127.10	124.26
15	a6	413	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	aB	838	CLA	CMB-C2B-C1B	-2.69	121.28	125.37
15	b2	404	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	bA	853	BCR	C32-C1-C6	2.69	114.66	110.30
15	aA	836	CLA	CHC-C4B-NB	2.69	127.10	124.26
18	a2	420	BCR	C15-C14-C13	-2.69	123.47	127.31
15	b5	410	CLA	CAC-C3C-C2C	2.69	132.12	127.53
15	c3	411	CLA	CHB-C1B-NB	2.69	127.10	124.26
15	bB	803	CLA	C1-C2-C3	-2.69	121.40	126.04
15	b6	412	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	c3	402	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	b2	415	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
15	aA	804	CLA	CMD-C2D-C3D	2.69	133.79	127.61
15	b2	403	CLA	CHB-C4A-NA	2.69	128.22	124.51
18	c3	401	BCR	C7-C8-C9	-2.68	122.18	126.23
15	c3	412	CLA	CMB-C2B-C1B	-2.68	121.28	125.37
15	aB	803	CLA	C1-C2-C3	-2.68	121.40	126.04
15	bB	832	CLA	CHC-C4B-NB	2.68	127.10	124.26
15	c5	410	CLA	CHB-C1B-NB	2.68	127.10	124.26
18	a2	419	BCR	C3-C4-C5	-2.68	109.28	114.08
15	b2	405	CLA	CHD-C1D-C2D	2.68	131.11	125.48
15	c3	408	CLA	CMB-C2B-C3B	2.68	133.09	126.59
15	cA	824	CLA	C3B-C4B-NB	-2.68	108.03	110.52
15	cA	833	CLA	C3B-C4B-NB	-2.68	108.03	110.52
15	b5	402	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	aB	832	CLA	CHC-C4B-NB	2.68	127.10	124.26
18	aA	852	BCR	C32-C1-C6	2.68	114.65	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aF	203	BCR	C27-C26-C25	2.68	126.63	122.73
15	a6	412	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	a2	422	CLA	CHA-C1A-NA	-2.68	120.25	126.40
15	bA	833	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	bB	835	CLA	O1D-CGD-CBD	2.68	129.97	124.48
18	c1	420	BCR	C35-C13-C14	-2.68	119.17	122.92
18	b2	419	BCR	C3-C4-C5	-2.68	109.29	114.08
15	a5	420	CLA	C6-C5-C3	-2.68	106.42	113.45
15	b5	420	CLA	C6-C7-C8	-2.68	107.25	115.92
18	cA	851	BCR	C32-C1-C6	2.68	114.65	110.30
15	a5	410	CLA	CAC-C3C-C2C	2.68	132.12	127.53
15	aB	830	CLA	CMB-C2B-C3B	2.68	133.08	126.59
14	cA	801	CL0	CHD-C4C-NC	2.68	128.43	124.20
15	cB	823	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
18	bJ	105	BCR	C27-C26-C25	2.68	126.62	122.73
18	b1	418	BCR	C27-C26-C25	2.68	126.62	122.73
15	b3	402	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	aB	817	CLA	CAC-C3C-C4C	2.68	128.29	124.81
18	aL	205	BCR	C7-C8-C9	-2.68	122.19	126.23
15	b3	416	CLA	CHB-C1B-NB	2.68	127.09	124.26
15	c2	403	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	aB	849	BCR	C35-C13-C14	-2.68	119.17	122.92
18	a2	420	BCR	C15-C16-C17	-2.68	117.99	123.47
15	cB	810	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
15	cB	832	CLA	CHC-C4B-NB	2.68	127.09	124.26
15	c2	415	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	aB	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	cA	840	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
15	bB	825	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	cB	840	CLA	CAA-CBA-CGA	-2.68	105.43	113.25
15	bB	823	CLA	CMB-C2B-C1B	-2.68	121.29	125.37
15	b6	416	CLA	C2D-C1D-ND	-2.68	108.13	110.10
15	aA	833	CLA	CHB-C4A-NA	2.68	128.21	124.51
18	a5	419	BCR	C35-C13-C14	-2.68	119.17	122.92
15	cB	825	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	c1	405	CLA	C3C-C4C-NC	-2.68	107.57	110.57
18	cF	205	BCR	C27-C26-C25	2.68	126.62	122.73
14	aA	801	CL0	CHD-C4C-NC	2.68	128.42	124.20
15	b5	409	CLA	CHB-C4A-NA	2.68	128.21	124.51
15	a2	405	CLA	CHD-C1D-C2D	2.68	131.09	125.48
15	cB	807	CLA	CHC-C4B-NB	2.68	127.09	124.26
15	a5	420	CLA	C6-C7-C8	-2.68	107.27	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	808	CLA	CHB-C4A-NA	2.68	128.21	124.51
15	a5	407	CLA	C2A-C1A-CHA	2.68	128.54	123.86
15	c2	405	CLA	CHD-C1D-C2D	2.67	131.09	125.48
15	aA	831	CLA	C2D-C1D-ND	-2.67	108.13	110.10
18	c1	418	BCR	C27-C26-C25	2.67	126.61	122.73
15	aB	825	CLA	CMB-C2B-C3B	2.67	133.06	126.59
15	cA	834	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
15	a4	421	CLA	CED-O2D-CGD	2.67	121.98	115.94
15	a3	408	CLA	CMB-C2B-C3B	2.67	133.06	126.59
15	bB	840	CLA	CAA-CBA-CGA	-2.67	105.44	113.25
15	c5	420	CLA	C6-C5-C3	-2.67	106.45	113.45
15	c4	408	CLA	CMB-C2B-C3B	2.67	133.06	126.59
15	bA	844	CLA	C3B-C4B-NB	-2.67	108.04	110.52
15	bA	836	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	b4	404	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	b3	408	CLA	CMB-C2B-C3B	2.67	133.06	126.59
15	b5	407	CLA	C2A-C1A-CHA	2.67	128.53	123.86
15	b5	420	CLA	C6-C5-C3	-2.67	106.45	113.45
15	b6	411	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	cJ	103	BCR	C11-C10-C9	-2.67	123.50	127.31
15	bA	833	CLA	C3B-C4B-NB	-2.67	108.04	110.52
15	aA	836	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	a2	408	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	cA	841	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	cB	825	CLA	CMB-C2B-C3B	2.67	133.05	126.59
15	aA	803	CLA	C1-O2A-CGA	2.67	123.45	116.44
15	a6	411	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
18	cA	847	BCR	C24-C23-C22	-2.67	122.20	126.23
15	a6	415	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	bB	807	CLA	C11-C12-C13	-2.67	107.29	115.92
18	cB	849	BCR	C35-C13-C14	-2.67	119.19	122.92
18	aA	852	BCR	C30-C25-C26	-2.67	118.86	122.61
18	bJ	103	BCR	C11-C10-C9	-2.67	123.50	127.31
15	c5	420	CLA	C6-C7-C8	-2.67	107.30	115.92
15	aA	829	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	b3	405	CLA	CHD-C1D-C2D	2.67	131.07	125.48
15	cB	811	CLA	O2A-C1-C2	-2.67	101.63	108.64
15	b6	415	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	b2	410	CLA	CHB-C4A-NA	2.67	128.20	124.51
15	a3	407	CLA	C2A-C1A-CHA	2.67	128.52	123.86
15	c3	405	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
15	c6	413	CLA	O2D-CGD-O1D	-2.67	118.63	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	407	CLA	C2A-C1A-CHA	2.67	128.52	123.86
15	b2	406	CLA	O2D-CGD-CBD	2.67	116.00	111.27
15	a3	413	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	a6	403	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	cA	804	CLA	CMD-C2D-C3D	2.66	133.74	127.61
15	c6	416	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	bB	830	CLA	CMB-C2B-C3B	2.66	133.04	126.59
15	b1	414	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
15	bA	822	CLA	C3B-C4B-NB	-2.66	108.05	110.52
15	b3	412	CLA	C2D-C1D-ND	-2.66	108.14	110.10
15	aB	811	CLA	O2A-C1-C2	-2.66	101.64	108.64
15	c6	412	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	cB	830	CLA	CMB-C2B-C3B	2.66	133.03	126.59
15	aB	840	CLA	CAA-CBA-CGA	-2.66	105.48	113.25
15	bA	817	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
15	bA	841	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	c3	410	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	cK	101	BCR	C24-C23-C22	-2.66	122.22	126.23
15	c6	412	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
15	cB	803	CLA	C1-C2-C3	-2.66	121.44	126.04
15	aB	823	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
18	b1	401	BCR	C15-C14-C13	-2.66	123.52	127.31
15	cB	807	CLA	C11-C12-C13	-2.66	107.33	115.92
15	cA	815	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	bB	810	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
15	bB	807	CLA	CHC-C4B-NB	2.66	127.07	124.26
15	aA	839	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	b2	420	BCR	C15-C14-C13	-2.66	123.52	127.31
15	cA	803	CLA	C1-O2A-CGA	2.66	123.41	116.44
15	a1	404	CLA	C3C-C4C-NC	-2.66	107.59	110.57
15	a2	422	CLA	C6-C5-C3	-2.66	106.49	113.45
15	b2	422	CLA	CHA-C1A-NA	-2.65	120.32	126.40
15	a4	421	CLA	C6-C5-C3	-2.65	106.50	113.45
15	bA	803	CLA	C1-O2A-CGA	2.65	123.41	116.44
15	bA	804	CLA	CMD-C2D-C3D	2.65	133.72	127.61
15	aB	807	CLA	C11-C12-C13	-2.65	107.34	115.92
15	a1	409	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
18	a1	419	BCR	C24-C23-C22	-2.65	122.23	126.23
15	b2	406	CLA	CAA-C2A-C1A	2.65	120.67	111.97
15	a6	411	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
15	bB	802	CLA	CBA-CAA-C2A	-2.65	106.03	113.86
18	c2	420	BCR	C15-C16-C17	-2.65	118.04	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c5	417	CLA	C2B-C1B-NB	2.65	112.01	110.23
18	c3	401	BCR	C15-C14-C13	-2.65	123.53	127.31
15	cA	820	CLA	C1-C2-C3	-2.65	121.46	126.04
15	a3	415	CLA	C2D-C1D-ND	-2.65	108.15	110.10
15	bB	825	CLA	CMB-C2B-C3B	2.65	133.01	126.59
18	bA	853	BCR	C30-C25-C26	-2.65	118.88	122.61
18	cA	847	BCR	C28-C27-C26	-2.65	109.34	114.08
15	b6	406	CLA	C3C-C4C-NC	-2.65	107.60	110.57
15	bB	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	a2	409	CLA	CMB-C2B-C3B	2.65	133.00	126.59
15	aA	802	CLA	CAA-CBA-CGA	-2.65	105.51	113.25
15	c3	405	CLA	CHD-C1D-C2D	2.65	131.04	125.48
15	aA	814	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	b3	403	CLA	CHB-C4A-NA	2.65	128.18	124.51
15	aB	835	CLA	O1D-CGD-CBD	2.65	129.90	124.48
15	c6	414	CLA	C2D-C1D-ND	-2.65	108.15	110.10
15	aB	802	CLA	CBA-CAA-C2A	-2.65	106.05	113.86
15	bB	811	CLA	O2A-C1-C2	-2.65	101.68	108.64
15	c4	410	CLA	CHB-C4A-NA	2.65	128.17	124.51
15	c4	421	CLA	CED-O2D-CGD	2.65	121.92	115.94
15	b4	412	CLA	CMB-C2B-C1B	-2.65	121.34	125.37
15	bA	824	CLA	C3B-C4B-NB	-2.65	108.06	110.52
15	c6	414	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
15	b6	408	CLA	C2A-C1A-CHA	2.65	128.49	123.86
15	bA	839	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	bA	849	BCR	C28-C27-C26	-2.65	109.35	114.08
18	a1	417	BCR	C27-C26-C25	2.65	126.57	122.73
15	bA	829	CLA	CHB-C4A-NA	2.65	128.17	124.51
15	b2	408	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	c1	420	BCR	C15-C14-C13	-2.65	123.53	127.31
15	aA	838	CLA	CHC-C4B-NB	2.64	127.06	124.26
15	bA	820	CLA	C1-C2-C3	-2.64	121.47	126.04
20	aB	850	LMG	O3-C3-C2	-2.64	104.23	110.35
15	a1	402	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	aA	802	CLA	CMB-C2B-C3B	2.64	132.99	126.59
15	aA	834	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
18	bB	850	BCR	C35-C13-C14	-2.64	119.22	122.92
15	cL	203	CLA	CMB-C2B-C1B	-2.64	121.34	125.37
15	b1	416	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	c6	404	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	c2	408	CLA	C2A-C1A-CHA	2.64	128.48	123.86
15	cA	814	CLA	CHB-C4A-NA	2.64	128.17	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	829	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	a2	406	CLA	CAA-C2A-C1A	2.64	120.63	111.97
15	aA	824	CLA	C3B-C4B-NB	-2.64	108.06	110.52
20	bB	851	LMG	O3-C3-C2	-2.64	104.24	110.35
15	cA	802	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
15	bA	834	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	cB	802	CLA	CBA-CAA-C2A	-2.64	106.07	113.86
15	c1	415	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	c6	413	CLA	CHB-C1B-NB	2.64	127.05	124.26
15	c2	410	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	aB	810	CLA	CMB-C2B-C1B	-2.64	121.35	125.37
15	a6	413	CLA	C2D-C1D-ND	-2.64	108.16	110.10
15	b4	412	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
15	bA	814	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	cA	843	CLA	C3B-C4B-NB	-2.64	108.07	110.52
15	aB	807	CLA	CHC-C4B-NB	2.64	127.05	124.26
15	cB	821	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	a1	413	CLA	CAA-C2A-C3A	-2.64	109.94	116.10
15	c1	403	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	b4	421	CLA	CED-O2D-CGD	2.64	121.90	115.94
15	c4	412	CLA	CMB-C2B-C1B	-2.64	121.35	125.37
15	c6	405	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	bA	806	CLA	C3B-C4B-NB	-2.64	108.07	110.52
15	c4	415	CLA	C2D-C1D-ND	-2.64	108.16	110.10
18	b3	419	BCR	C15-C14-C13	-2.64	123.55	127.31
15	a6	414	CLA	C3C-C4C-NC	-2.64	107.61	110.57
15	c5	402	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	c2	409	CLA	CMB-C2B-C3B	2.63	132.97	126.59
18	aK	101	BCR	C24-C23-C22	-2.63	122.25	126.23
18	bA	848	BCR	C24-C23-C22	-2.63	122.25	126.23
15	b2	413	CLA	CMC-C2C-C3C	2.63	133.27	126.12
18	c5	401	BCR	C15-C14-C13	-2.63	123.55	127.31
15	c4	417	CLA	C2B-C1B-NB	2.63	112.00	110.23
15	c3	407	CLA	C2A-C1A-CHA	2.63	128.47	123.86
15	cF	201	CLA	C2D-C1D-ND	-2.63	108.16	110.10
15	cA	802	CLA	CMB-C2B-C3B	2.63	132.97	126.59
15	a1	409	CLA	CHB-C1B-NB	2.63	127.05	124.26
15	b6	422	CLA	C11-C10-C8	-2.63	107.41	115.92
20	cB	850	LMG	O3-C3-C2	-2.63	104.26	110.35
15	b6	406	CLA	CHD-C1D-C2D	2.63	131.00	125.48
18	b5	419	BCR	C15-C14-C13	-2.63	123.55	127.31
15	c6	417	CLA	C2D-C1D-ND	-2.63	108.16	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	415	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
15	bA	802	CLA	CMB-C2B-C3B	2.63	132.96	126.59
15	bA	802	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
18	aJ	204	BCR	C11-C10-C9	-2.63	123.56	127.31
15	a5	408	CLA	CMB-C2B-C3B	2.63	132.96	126.59
15	b4	408	CLA	CMB-C2B-C3B	2.63	132.96	126.59
15	b2	422	CLA	C3A-C2A-C1A	2.63	105.28	101.34
15	cA	817	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
15	c6	407	CLA	CHD-C1D-C2D	2.63	131.00	125.48
15	a3	412	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
15	c5	408	CLA	CMB-C2B-C3B	2.63	132.96	126.59
15	c3	407	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
18	b1	420	BCR	C15-C14-C13	-2.63	123.56	127.31
15	a6	406	CLA	C3C-C4C-NC	-2.63	107.62	110.57
15	c4	410	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	b3	412	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
15	aA	843	CLA	CHB-C1B-NB	2.63	127.04	124.26
15	b2	406	CLA	CHA-C1A-NA	-2.63	120.38	126.40
15	a4	417	CLA	C2B-C1B-NB	2.63	111.99	110.23
15	cB	832	CLA	CMB-C2B-C3B	2.63	132.95	126.59
18	c5	419	BCR	C15-C14-C13	-2.63	123.56	127.31
15	aB	832	CLA	CMB-C2B-C3B	2.63	132.95	126.59
15	b6	411	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	b3	415	CLA	C2D-C1D-ND	-2.63	108.17	110.10
15	a2	413	CLA	CMC-C2C-C3C	2.63	133.25	126.12
15	b4	410	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
18	aI	103	BCR	C31-C1-C6	2.63	114.56	110.30
15	a1	414	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
15	bB	826	CLA	C2D-C1D-ND	-2.62	108.17	110.10
18	aK	101	BCR	C28-C27-C26	-2.62	109.39	114.08
15	cA	839	CLA	CHB-C4A-NA	2.62	128.14	124.51
15	b6	406	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
18	a1	421	BCR	C7-C8-C9	-2.62	122.27	126.23
18	aA	848	BCR	C28-C27-C26	-2.62	109.39	114.08
15	cA	807	CLA	CMB-C2B-C1B	-2.62	121.37	125.37
18	c1	401	BCR	C15-C14-C13	-2.62	123.57	127.31
15	c2	415	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
15	a2	422	CLA	C3A-C2A-C1A	2.62	105.27	101.34
15	bA	812	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
15	bA	836	CLA	CHC-C4B-NB	2.62	127.03	124.26
15	b5	417	CLA	C2B-C1B-NB	2.62	111.99	110.23
15	a4	412	CLA	O2D-CGD-O1D	-2.62	118.71	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	411	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
15	b4	410	CLA	CAC-C3C-C2C	2.62	132.01	127.53
15	bX	102	CLA	CHB-C1B-NB	2.62	127.03	124.26
15	cA	812	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
15	cB	809	CLA	C3B-C4B-NB	-2.62	108.08	110.52
15	a2	408	CLA	C2A-C1A-CHA	2.62	128.44	123.86
14	cA	801	CL0	C1-C2-C3	-2.62	121.51	126.04
15	a1	406	CLA	C2A-C1A-CHA	2.62	128.44	123.86
15	a6	408	CLA	C2A-C1A-CHA	2.62	128.44	123.86
15	aL	202	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
15	b4	410	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
15	c2	422	CLA	C6-C5-C3	-2.62	106.59	113.45
15	aA	841	CLA	CHB-C4A-NA	2.62	128.13	124.51
18	bA	848	BCR	C28-C27-C26	-2.62	109.40	114.08
18	a5	419	BCR	C15-C14-C13	-2.62	123.58	127.31
18	aA	848	BCR	C24-C23-C22	-2.62	122.28	126.23
15	cA	842	CLA	CHB-C1B-NB	2.62	127.03	124.26
18	cK	101	BCR	C28-C27-C26	-2.62	109.41	114.08
15	aA	815	CLA	CHB-C4A-NA	2.62	128.13	124.51
15	bA	803	CLA	CMB-C2B-C3B	2.62	132.93	126.59
15	aA	805	CLA	C3B-C4B-NB	-2.62	108.09	110.52
15	bA	815	CLA	CHB-C4A-NA	2.62	128.13	124.51
15	bB	817	CLA	C2B-C1B-NB	2.61	111.98	110.23
18	bA	849	BCR	C24-C23-C22	-2.61	122.28	126.23
14	bA	801	CL0	C4-C3-C5	2.61	119.67	115.27
15	c3	409	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
15	b4	421	CLA	C6-C5-C3	-2.61	106.60	113.45
18	bL	205	BCR	C31-C1-C6	2.61	114.54	110.30
14	cA	801	CL0	CGD-CBD-CAD	-2.61	102.27	110.73
15	a6	406	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
15	b2	408	CLA	C2A-C1A-CHA	2.61	128.43	123.86
15	c4	410	CLA	CAC-C3C-C2C	2.61	132.00	127.53
15	a3	403	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	b6	413	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
15	b5	408	CLA	CMB-C2B-C3B	2.61	132.91	126.59
15	a3	405	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
15	c1	410	CLA	CHB-C1B-NB	2.61	127.02	124.26
15	aA	822	CLA	C3B-C4B-NB	-2.61	108.09	110.52
15	a6	406	CLA	CHD-C1D-C2D	2.61	130.96	125.48
18	aB	846	BCR	C39-C30-C25	-2.61	106.06	110.30
15	aX	102	CLA	CHB-C1B-NB	2.61	127.02	124.26
15	a2	411	CLA	CMB-C2B-C1B	-2.61	121.39	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	403	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	b3	417	CLA	C3A-C2A-C1A	2.61	105.25	101.34
15	c2	422	CLA	C3A-C2A-C1A	2.61	105.25	101.34
15	b3	405	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
14	aA	801	CL0	C4-C3-C5	2.61	119.66	115.27
15	c2	406	CLA	O2D-CGD-CBD	2.61	115.91	111.27
15	b6	411	CLA	CAC-C3C-C2C	2.61	131.99	127.53
15	cA	805	CLA	C3B-C4B-NB	-2.61	108.09	110.52
15	c2	406	CLA	CAA-C2A-C1A	2.61	120.53	111.97
15	aA	827	CLA	C3B-C4B-NB	-2.61	108.09	110.52
15	bA	805	CLA	C3B-C4B-NB	-2.61	108.09	110.52
15	b2	411	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	cA	803	CLA	CMB-C2B-C3B	2.61	132.90	126.59
18	c3	419	BCR	C15-C14-C13	-2.61	123.59	127.31
15	c6	415	CLA	C3C-C4C-NC	-2.61	107.65	110.57
15	a4	416	CLA	CHB-C1B-NB	2.61	127.02	124.26
15	cX	102	CLA	CHB-C1B-NB	2.61	127.02	124.26
14	aA	801	CL0	C1-C2-C3	-2.61	121.53	126.04
15	aA	842	CLA	C2D-C1D-ND	-2.61	108.18	110.10
15	b6	413	CLA	C2D-C1D-ND	-2.61	108.18	110.10
15	aA	838	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	a3	407	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
15	aA	844	CLA	C3B-C4B-NB	-2.61	108.10	110.52
14	bA	801	CL0	CGD-CBD-CAD	-2.61	102.29	110.73
15	a3	402	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	c4	401	BCR	C24-C23-C22	-2.61	122.30	126.23
18	cB	845	BCR	C29-C30-C25	2.61	114.49	110.48
15	bA	838	CLA	O2D-CGD-CBD	2.61	115.90	111.27
15	c2	402	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	a4	410	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
18	cM	101	BCR	C33-C5-C6	-2.60	121.60	124.53
14	aA	801	CL0	CGD-CBD-CAD	-2.60	102.30	110.73
15	cA	838	CLA	O2D-CGD-CBD	2.60	115.90	111.27
15	b4	416	CLA	CHB-C1B-NB	2.60	127.01	124.26
18	bB	846	BCR	C39-C30-C25	-2.60	106.08	110.30
15	c1	410	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
15	a4	408	CLA	CMB-C2B-C3B	2.60	132.90	126.59
15	b4	403	CLA	CMB-C2B-C3B	2.60	132.89	126.59
18	c6	421	BCR	C29-C30-C25	2.60	114.49	110.48
15	bA	816	CLA	CMB-C2B-C3B	2.60	132.89	126.59
15	bB	832	CLA	CMB-C2B-C3B	2.60	132.89	126.59
15	aA	822	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c6	409	CLA	C2A-C1A-CHA	2.60	128.41	123.86
15	cB	826	CLA	C2D-C1D-ND	-2.60	108.19	110.10
15	aB	820	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	aA	848	BCR	C11-C10-C9	-2.60	123.60	127.31
15	a2	411	CLA	CHB-C4A-NA	2.60	128.11	124.51
15	c3	405	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
15	aA	807	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
15	bL	203	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
15	b2	410	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	cB	827	CLA	O2A-C1-C2	-2.60	101.80	108.64
15	aB	826	CLA	CMB-C2B-C3B	2.60	132.88	126.59
15	b3	415	CLA	CMB-C2B-C3B	2.60	132.88	126.59
15	bB	837	CLA	CHD-C1D-ND	-2.60	122.07	124.45
15	b6	404	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	a1	404	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
18	bL	201	BCR	C24-C23-C22	-2.60	122.31	126.23
15	aB	827	CLA	O2A-C1-C2	-2.60	101.81	108.64
14	bA	801	CL0	C1-C2-C3	-2.60	121.55	126.04
15	c2	408	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	c1	416	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
15	c4	403	CLA	CHB-C4A-NA	2.60	128.10	124.51
15	c4	412	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	cL	205	BCR	C31-C1-C6	2.59	114.51	110.30
15	cB	833	CLA	O2D-CGD-CBD	2.59	115.88	111.27
15	c5	403	CLA	CHB-C4A-NA	2.59	128.10	124.51
15	b1	407	CLA	C2A-C1A-CHA	2.59	128.40	123.86
15	c6	412	CLA	CAC-C3C-C2C	2.59	131.97	127.53
15	b4	415	CLA	CMB-C2B-C3B	2.59	132.87	126.59
18	a6	420	BCR	C29-C30-C25	2.59	114.47	110.48
15	a4	407	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	bL	206	BCR	C24-C23-C22	-2.59	122.32	126.23
15	a3	410	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
15	c4	403	CLA	CMB-C2B-C3B	2.59	132.87	126.59
15	c2	413	CLA	CMC-C2C-C3C	2.59	133.15	126.12
15	aA	803	CLA	CMB-C2B-C3B	2.59	132.87	126.59
18	c6	421	BCR	C3-C4-C5	-2.59	109.45	114.08
18	a1	419	BCR	C15-C14-C13	-2.59	123.61	127.31
15	b6	422	CLA	O2D-CGD-CBD	2.59	115.87	111.27
15	b5	410	CLA	CHB-C1B-NB	2.59	127.00	124.26
15	c2	411	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
15	a4	417	CLA	CHD-C1D-ND	-2.59	122.07	124.45
15	bB	833	CLA	O2D-CGD-CBD	2.59	115.87	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	414	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	c2	411	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
15	a3	405	CLA	CHD-C1D-C2D	2.59	130.91	125.48
18	aM	101	BCR	C33-C5-C6	-2.59	121.62	124.53
18	bM	101	BCR	C33-C5-C6	-2.59	121.62	124.53
15	cB	817	CLA	C2B-C1B-NB	2.59	111.97	110.23
15	c6	407	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
15	b6	409	CLA	CHB-C1B-NB	2.59	127.00	124.26
15	c2	410	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
15	a6	404	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	c4	409	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
18	cB	846	BCR	C39-C30-C25	-2.59	106.10	110.30
15	a3	411	CLA	CHB-C1B-NB	2.59	127.00	124.26
15	cA	827	CLA	C3B-C4B-NB	-2.59	108.11	110.52
15	bA	822	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
15	cB	831	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	aA	812	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
20	aB	850	LMG	O2-C2-C1	-2.59	103.76	110.05
15	bA	807	CLA	CMB-C2B-C1B	-2.59	121.43	125.37
15	a6	412	CLA	CHB-C1B-NB	2.59	127.00	124.26
18	a1	420	BCR	C15-C14-C13	-2.59	123.62	127.31
19	aA	854	LHG	C11-C10-C9	-2.59	101.30	114.42
15	aB	825	CLA	CHA-C1A-NA	-2.59	120.48	126.40
15	aA	834	CLA	CAA-CBA-CGA	-2.59	105.70	113.25
18	c6	421	BCR	C35-C13-C14	-2.59	119.30	122.92
15	c5	410	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
15	cA	809	CLA	CAA-C2A-C1A	-2.58	103.50	111.97
15	bA	810	CLA	C3B-C4B-NB	-2.58	108.12	110.52
15	aA	819	CLA	CBC-CAC-C3C	2.58	119.56	112.43
15	c3	402	CLA	CHB-C4A-NA	2.58	128.09	124.51
15	bA	819	CLA	CBC-CAC-C3C	2.58	119.55	112.43
15	aB	837	CLA	CHD-C1D-ND	-2.58	122.08	124.45
15	b4	409	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
15	aA	810	CLA	C3B-C4B-NB	-2.58	108.12	110.52
15	aB	809	CLA	C3B-C4B-NB	-2.58	108.12	110.52
15	c1	416	CLA	CHB-C1B-NB	2.58	126.99	124.26
15	cB	825	CLA	CHA-C1A-NA	-2.58	120.48	126.40
15	c2	411	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	aL	205	BCR	C24-C23-C22	-2.58	122.33	126.23
18	bB	845	BCR	C29-C30-C25	2.58	114.46	110.48
15	a3	417	CLA	C3A-C2A-C1A	2.58	105.20	101.34
15	a5	403	CLA	CHB-C4A-NA	2.58	128.08	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
18	aB	845	BCR	C29-C30-C25	2.58	114.45	110.48
18	b6	420	BCR	C3-C4-C5	-2.58	109.47	114.08
15	bA	827	CLA	C3B-C4B-NB	-2.58	108.12	110.52
15	cB	826	CLA	CMB-C2B-C3B	2.58	132.84	126.59
15	cA	822	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
15	aA	809	CLA	CAA-C2A-C1A	-2.58	103.52	111.97
15	b3	410	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
15	c6	412	CLA	CHB-C1B-NB	2.58	126.99	124.26
18	a3	419	BCR	C15-C14-C13	-2.58	123.63	127.31
18	c3	419	BCR	C11-C10-C9	-2.58	123.63	127.31
15	aB	817	CLA	C2B-C1B-NB	2.58	111.96	110.23
15	bB	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	bB	815	CLA	O2D-CGD-CBD	2.58	115.85	111.27
15	cB	818	CLA	O2D-CGD-CBD	2.58	115.85	111.27
19	bA	855	LHG	C11-C10-C9	-2.58	101.33	114.42
15	aA	835	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	b6	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	c3	410	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
15	a4	403	CLA	CMB-C2B-C3B	2.58	132.83	126.59
19	cA	853	LHG	C11-C10-C9	-2.58	101.34	114.42
15	bB	815	CLA	C2D-C1D-ND	-2.58	108.20	110.10
15	cA	819	CLA	CBC-CAC-C3C	2.58	119.53	112.43
15	bB	827	CLA	O2A-C1-C2	-2.58	101.86	108.64
15	bA	834	CLA	CAA-CBA-CGA	-2.58	105.72	113.25
15	cA	816	CLA	CMB-C2B-C3B	2.58	132.83	126.59
15	c2	416	CLA	CMB-C2B-C3B	2.58	132.83	126.59
15	cA	834	CLA	CAA-CBA-CGA	-2.58	105.73	113.25
15	b5	415	CLA	C2D-C1D-ND	-2.58	108.21	110.10
15	aA	816	CLA	CMB-C2B-C3B	2.58	132.83	126.59
15	bA	835	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
15	b3	402	CLA	CHB-C4A-NA	2.58	128.07	124.51
15	c4	416	CLA	CHB-C1B-NB	2.57	126.98	124.26
15	a2	416	CLA	CMB-C2B-C3B	2.57	132.82	126.59
15	b6	422	CLA	CHA-C1A-NA	-2.57	120.50	126.40
15	bA	805	CLA	O2D-CGD-CBD	2.57	115.84	111.27
15	bA	809	CLA	CAA-C2A-C1A	-2.57	103.54	111.97
15	c4	410	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
15	cA	835	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
14	cA	801	CL0	C4-C3-C5	2.57	119.60	115.27
18	b6	420	BCR	C29-C30-C25	2.57	114.44	110.48
15	cA	810	CLA	C3B-C4B-NB	-2.57	108.13	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	807	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	bA	835	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	cB	815	CLA	O2D-CGD-CBD	2.57	115.84	111.27
15	aB	826	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	c1	410	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	bB	809	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	bB	826	CLA	CMB-C2B-C3B	2.57	132.82	126.59
15	aL	201	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	cA	848	BCR	C15-C14-C13	-2.57	123.64	127.31
15	c1	407	CLA	C2A-C1A-CHA	2.57	128.35	123.86
15	a4	405	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	a4	410	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	bB	831	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	b1	405	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	bB	807	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	cA	804	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
15	a5	412	CLA	CMC-C2C-C3C	2.57	133.09	126.12
15	b4	417	CLA	CHD-C1D-ND	-2.57	122.09	124.45
15	c4	409	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
20	cB	850	LMG	O2-C2-C1	-2.57	103.81	110.05
15	a3	409	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
15	bB	818	CLA	O2D-CGD-CBD	2.57	115.83	111.27
15	c5	412	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	cB	820	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	bB	825	CLA	CHA-C1A-NA	-2.57	120.52	126.40
15	cB	837	CLA	CHD-C1D-ND	-2.57	122.09	124.45
18	b5	401	BCR	C15-C14-C13	-2.57	123.65	127.31
15	aA	836	CLA	C3B-C4B-NB	-2.57	108.13	110.52
15	a5	410	CLA	CHB-C1B-NB	2.57	126.97	124.26
15	c6	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	a6	411	CLA	CAC-C3C-C2C	2.57	131.92	127.53
15	b4	415	CLA	C2D-C1D-ND	-2.57	108.21	110.10
15	a4	403	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	aB	807	CLA	CHB-C4A-NA	2.57	128.06	124.51
15	b2	415	CLA	CAA-C2A-C3A	-2.56	110.11	116.10
15	a5	412	CLA	C2D-C1D-ND	-2.56	108.21	110.10
15	bA	838	CLA	C2D-C1D-ND	-2.56	108.21	110.10
18	aJ	205	BCR	C15-C14-C13	-2.56	123.65	127.31
15	bL	202	CLA	CHB-C4A-NA	2.56	128.06	124.51
15	bA	804	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
15	aB	815	CLA	O2D-CGD-CBD	2.56	115.82	111.27
18	bA	849	BCR	C11-C10-C9	-2.56	123.65	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cJ	104	BCR	C15-C14-C13	-2.56	123.65	127.31
15	aA	835	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
15	bA	842	CLA	C2D-C1D-ND	-2.56	108.22	110.10
18	a2	421	BCR	C15-C16-C17	-2.56	118.23	123.47
15	a2	411	CLA	CHB-C1B-NB	2.56	126.97	124.26
15	b2	422	CLA	CHC-C4B-NB	2.56	126.97	124.26
15	aA	804	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
18	a6	420	BCR	C3-C4-C5	-2.56	109.50	114.08
18	cB	849	BCR	C10-C11-C12	-2.56	115.22	123.22
18	cA	847	BCR	C11-C10-C9	-2.56	123.66	127.31
15	c4	407	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
15	a2	402	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	aA	805	CLA	O2D-CGD-CBD	2.56	115.82	111.27
15	bB	831	CLA	CHC-C4B-NB	2.56	126.97	124.26
15	b3	411	CLA	CHB-C1B-NB	2.56	126.97	124.26
20	bB	851	LMG	O2-C2-C1	-2.56	103.83	110.05
15	b4	405	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
15	a2	411	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	bB	812	CLA	CHD-C1D-ND	-2.56	122.10	124.45
15	cB	801	CLA	C2D-C1D-ND	-2.56	108.22	110.10
15	b5	412	CLA	CMC-C2C-C3C	2.56	133.06	126.12
18	a1	419	BCR	C35-C13-C14	-2.56	119.34	122.92
15	b3	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	bB	801	CLA	C2D-C1D-ND	-2.56	108.22	110.10
15	c3	415	CLA	C2D-C1D-ND	-2.56	108.22	110.10
18	bB	850	BCR	C10-C11-C12	-2.56	115.24	123.22
15	cB	819	CLA	CHC-C4B-NB	2.56	126.96	124.26
15	bB	809	CLA	O2D-CGD-CBD	2.56	115.81	111.27
15	b1	408	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	b4	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	a4	415	CLA	CBA-CAA-C2A	2.56	121.41	113.86
15	b2	413	CLA	C1D-ND-C4D	2.55	108.15	106.33
15	aB	818	CLA	O2D-CGD-CBD	2.55	115.81	111.27
15	cA	831	CLA	O2D-CGD-CBD	2.55	115.81	111.27
15	c3	415	CLA	CMB-C2B-C3B	2.55	132.78	126.59
15	a3	415	CLA	CMB-C2B-C3B	2.55	132.77	126.59
15	c6	401	CLA	C11-C10-C8	-2.55	107.66	115.92
15	a3	417	CLA	CHB-C1B-NB	2.55	126.96	124.26
15	bA	845	CLA	CMB-C2B-C1B	-2.55	121.48	125.37
15	cL	202	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	aB	809	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	c3	417	CLA	C3A-C2A-C1A	2.55	105.16	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	405	CLA	CMB-C2B-C1B	-2.55	121.48	125.37
18	bA	850	BCR	C15-C14-C13	-2.55	123.67	127.31
18	b2	421	BCR	C29-C30-C25	2.55	114.41	110.48
15	b6	415	CLA	C3B-C4B-NB	-2.55	108.15	110.52
15	c2	406	CLA	CHA-C1A-NA	-2.55	120.56	126.40
18	aB	849	BCR	C10-C11-C12	-2.55	115.25	123.22
15	cA	835	CLA	CHB-C4A-NA	2.55	128.04	124.51
18	bJ	104	BCR	C15-C14-C13	-2.55	123.67	127.31
15	aB	831	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	b1	402	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	a2	406	CLA	CHA-C1A-NA	-2.55	120.56	126.40
15	bB	819	CLA	CHC-C4B-NB	2.55	126.96	124.26
15	b2	403	CLA	CMB-C2B-C3B	2.55	132.76	126.59
15	aB	833	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	cB	809	CLA	O2D-CGD-CBD	2.55	115.80	111.27
15	b1	406	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
18	c1	418	BCR	C3-C4-C5	-2.55	109.53	114.08
15	cA	809	CLA	C1-C2-C3	-2.55	121.64	126.04
15	bB	823	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	bB	804	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	cF	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	cA	844	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
15	bB	814	CLA	CAC-C3C-C2C	2.55	131.89	127.53
15	a6	403	CLA	CHB-C4A-NA	2.55	128.03	124.51
15	a2	415	CLA	CAA-C2A-C3A	-2.55	110.15	116.10
15	cB	823	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	a2	404	CLA	CHB-C1B-NB	2.55	126.95	124.26
15	b6	417	CLA	C3C-C4C-NC	-2.55	107.72	110.57
15	bB	804	CLA	CMD-C2D-C3D	2.55	133.47	127.61
15	bA	831	CLA	O2D-CGD-CBD	2.55	115.79	111.27
18	bJ	103	BCR	C27-C26-C25	2.55	126.43	122.73
15	aA	831	CLA	O2D-CGD-CBD	2.55	115.79	111.27
15	a5	410	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	a1	414	CLA	CMB-C2B-C3B	2.55	132.75	126.59
15	cB	807	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	a4	410	CLA	CAC-C3C-C2C	2.54	131.88	127.53
15	cA	805	CLA	O2D-CGD-CBD	2.54	115.79	111.27
15	c1	412	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	aA	825	CLA	C3B-C4B-NB	-2.54	108.16	110.52
15	c1	405	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
15	aB	837	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
15	cA	836	CLA	C3B-C4B-NB	-2.54	108.16	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	419	BCR	C11-C10-C9	-2.54	123.68	127.31
15	bB	802	CLA	C6-C5-C3	-2.54	106.79	113.45
15	c5	412	CLA	CMC-C2C-C3C	2.54	133.02	126.12
15	bA	819	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	aB	812	CLA	CHD-C1D-ND	-2.54	122.12	124.45
15	b2	411	CLA	CHB-C1B-NB	2.54	126.95	124.26
15	cB	807	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
15	a6	410	CLA	CHC-C4B-NB	2.54	126.95	124.26
15	a1	411	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	b2	416	CLA	CMB-C2B-C3B	2.54	132.74	126.59
15	b5	412	CLA	C2D-C1D-ND	-2.54	108.23	110.10
15	aA	825	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	bF	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	a3	419	BCR	C11-C10-C9	-2.54	123.69	127.31
15	aB	831	CLA	CHC-C4B-NB	2.54	126.94	124.26
15	c4	405	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
15	bA	815	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	cA	819	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
18	cB	849	BCR	C23-C22-C21	-2.54	115.05	118.94
15	a4	409	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
15	cB	802	CLA	C6-C5-C3	-2.54	106.80	113.45
15	aJ	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	bA	805	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	b1	412	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	b2	402	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	c1	402	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	aB	804	CLA	CMD-C2D-C3D	2.54	133.45	127.61
15	c5	414	CLA	C3B-C4B-NB	-2.54	108.16	110.52
15	aB	814	CLA	CAC-C3C-C2C	2.54	131.87	127.53
18	b1	418	BCR	C3-C4-C5	-2.54	109.55	114.08
15	aB	823	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
15	cB	804	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	cB	814	CLA	CAC-C3C-C2C	2.54	131.87	127.53
15	c1	416	CLA	C3C-C4C-NC	-2.54	107.73	110.57
15	b1	413	CLA	C3B-C4B-NB	-2.54	108.16	110.52
15	a5	415	CLA	C2D-C1D-ND	-2.54	108.23	110.10
15	b2	407	CLA	CHB-C4A-NA	2.54	128.02	124.51
15	aA	815	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
15	aL	202	CLA	CMB-C2B-C3B	2.54	132.73	126.59
15	b5	405	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
15	c1	415	CLA	CMB-C2B-C3B	2.54	132.73	126.59
15	cB	824	CLA	O2D-CGD-O1D	-2.54	118.88	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	819	CLA	CHC-C4B-NB	2.54	126.94	124.26
15	a1	401	CLA	CHC-C4B-NB	2.54	126.94	124.26
15	a3	421	CLA	CHC-C4B-NB	2.54	126.94	124.26
15	a3	414	CLA	C3B-C4B-NB	-2.54	108.16	110.52
18	a6	421	BCR	C15-C14-C13	-2.54	123.69	127.31
15	b3	417	CLA	C2B-C1B-NB	2.53	111.93	110.23
15	a2	417	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
15	cA	825	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
18	b1	401	BCR	C34-C9-C10	-2.53	119.37	122.92
15	c5	415	CLA	C2D-C1D-ND	-2.53	108.24	110.10
15	a2	403	CLA	CMB-C2B-C3B	2.53	132.72	126.59
15	a3	407	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	cJ	101	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	c4	417	CLA	CHD-C1D-ND	-2.53	122.13	124.45
15	bB	837	CLA	CMB-C2B-C1B	-2.53	121.51	125.37
15	c2	417	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	bA	843	CLA	CHB-C1B-NB	2.53	126.94	124.26
15	cB	831	CLA	CHC-C4B-NB	2.53	126.94	124.26
15	c4	407	CLA	CHC-C4B-NB	2.53	126.94	124.26
15	a3	417	CLA	C2B-C1B-NB	2.53	111.93	110.23
15	aB	811	CLA	C1-O2A-CGA	2.53	123.08	116.44
15	bB	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	aA	845	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
15	c6	417	CLA	CBA-CAA-C2A	2.53	121.33	113.86
15	aA	820	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	c6	416	CLA	C3B-C4B-NB	-2.53	108.17	110.52
15	a2	422	CLA	CHC-C4B-NB	2.53	126.94	124.26
15	a1	411	CLA	C1D-ND-C4D	2.53	108.13	106.33
15	cA	838	CLA	C2D-C1D-ND	-2.53	108.24	110.10
15	aA	805	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	aB	810	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	a1	401	CLA	CHB-C4A-NA	2.53	128.01	124.51
15	cL	203	CLA	CMB-C2B-C3B	2.53	132.71	126.59
18	cB	844	BCR	C15-C14-C13	-2.53	123.70	127.31
15	aB	802	CLA	C6-C5-C3	-2.53	106.83	113.45
15	bL	203	CLA	CMB-C2B-C3B	2.53	132.71	126.59
15	b1	411	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	b3	412	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
18	a6	420	BCR	C35-C13-C14	-2.53	119.38	122.92
15	bA	820	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	cJ	103	BCR	C27-C26-C25	2.53	126.40	122.73
18	c2	421	BCR	C29-C30-C25	2.53	114.37	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	407	CLA	CHB-C4A-NA	2.53	128.00	124.51
15	aJ	202	CLA	C3B-C4B-NB	-2.53	108.17	110.52
18	aA	849	BCR	C15-C14-C13	-2.53	123.71	127.31
15	c6	407	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
15	aB	824	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	cB	850	LMG	C38-C37-C36	-2.53	101.61	114.42
15	b4	407	CLA	CHC-C4B-NB	2.52	126.93	124.26
15	a5	405	CLA	CAA-C2A-C3A	-2.52	105.86	112.78
15	b2	411	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
15	a5	405	CLA	CMB-C2B-C1B	-2.52	121.52	125.37
18	aB	849	BCR	C23-C22-C21	-2.52	115.07	118.94
15	cA	820	CLA	C3B-C4B-NB	-2.52	108.17	110.52
15	a2	417	CLA	C2A-C1A-CHA	2.52	128.27	123.86
15	cB	804	CLA	CMD-C2D-C3D	2.52	133.42	127.61
15	a3	410	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
15	b4	414	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
15	bB	801	CLA	CHC-C4B-NB	2.52	126.93	124.26
15	b4	409	CLA	CHB-C1B-NB	2.52	126.93	124.26
15	b6	410	CLA	CHC-C4B-NB	2.52	126.93	124.26
15	aB	801	CLA	C2D-C1D-ND	-2.52	108.24	110.10
18	cA	850	BCR	C15-C14-C13	-2.52	123.71	127.31
18	aJ	204	BCR	C27-C26-C25	2.52	126.39	122.73
18	bB	844	BCR	C15-C14-C13	-2.52	123.71	127.31
15	c1	406	CLA	CHC-C4B-NB	2.52	126.93	124.26
15	bB	811	CLA	C1-O2A-CGA	2.52	123.06	116.44
18	b6	420	BCR	C35-C13-C14	-2.52	119.39	122.92
15	cB	824	CLA	CHB-C1B-NB	2.52	126.93	124.26
15	c3	417	CLA	CHB-C1B-NB	2.52	126.93	124.26
15	a2	410	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	a6	417	CLA	C3C-C4C-NC	-2.52	107.74	110.57
15	c6	416	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
15	cB	811	CLA	C1-O2A-CGA	2.52	123.06	116.44
15	c1	413	CLA	C3B-C4B-NB	-2.52	108.18	110.52
15	b3	416	CLA	C3C-C4C-NC	-2.52	107.74	110.57
18	aB	847	BCR	C38-C26-C27	-2.52	108.77	113.62
15	bJ	101	CLA	C3B-C4B-NB	-2.52	108.18	110.52
18	aL	205	BCR	C15-C16-C17	-2.52	118.31	123.47
15	bA	825	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	cA	815	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
15	b1	405	CLA	C3C-C4C-NC	-2.52	107.75	110.57
15	a6	406	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
15	cB	837	CLA	CMB-C2B-C1B	-2.52	121.53	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	414	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
18	b3	420	BCR	C29-C30-C25	2.52	114.36	110.48
15	aB	828	CLA	C3B-C4B-NB	-2.52	108.18	110.52
15	aB	804	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	bB	847	BCR	C38-C26-C27	-2.52	108.78	113.62
20	aB	850	LMG	C38-C37-C36	-2.52	101.64	114.42
18	aB	844	BCR	C15-C14-C13	-2.52	123.72	127.31
15	bA	827	CLA	CHB-C1B-NB	2.52	126.92	124.26
15	cB	815	CLA	C2D-C1D-ND	-2.52	108.25	110.10
15	cA	826	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	a2	413	CLA	C1D-ND-C4D	2.52	108.12	106.33
15	b6	414	CLA	CAC-C3C-C2C	-2.52	123.22	127.53
18	bA	852	BCR	C15-C14-C13	-2.52	123.72	127.31
15	bB	824	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	bA	825	CLA	C2D-C1D-ND	-2.52	108.25	110.10
18	c3	420	BCR	C35-C13-C14	-2.52	119.40	122.92
20	bB	851	LMG	C38-C37-C36	-2.52	101.65	114.42
15	aA	827	CLA	CHB-C1B-NB	2.52	126.92	124.26
15	c6	418	CLA	C3C-C4C-NC	-2.52	107.75	110.57
18	c6	403	BCR	C1-C6-C5	-2.52	119.07	122.61
15	b2	406	CLA	C3A-C2A-C1A	2.51	105.11	101.34
15	cB	818	CLA	C3B-C4B-NB	-2.51	108.18	110.52
18	aA	851	BCR	C15-C14-C13	-2.51	123.72	127.31
15	b2	410	CLA	CMB-C2B-C1B	-2.51	121.54	125.37
18	bB	850	BCR	C23-C22-C21	-2.51	115.08	118.94
15	c2	413	CLA	C1D-ND-C4D	2.51	108.12	106.33
15	bA	836	CLA	C3B-C4B-NB	-2.51	108.18	110.52
15	b2	416	CLA	C3B-C4B-NB	-2.51	108.18	110.52
15	bA	827	CLA	CMD-C2D-C1D	-2.51	120.28	124.71
15	b2	405	CLA	CHB-C1B-NB	2.51	126.92	124.26
15	aA	825	CLA	C2D-C1D-ND	-2.51	108.25	110.10
15	c6	415	CLA	C2D-C1D-ND	-2.51	108.25	110.10
15	cB	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	a2	422	CLA	C11-C10-C8	-2.51	107.80	115.92
15	b6	410	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
15	b6	407	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	bB	807	CLA	C3B-C4B-NB	-2.51	108.19	110.52
15	c5	405	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
15	aA	818	CLA	C3B-C4B-NB	-2.51	108.19	110.52
15	bB	828	CLA	C3B-C4B-NB	-2.51	108.19	110.52
15	b2	417	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
18	bL	201	BCR	C15-C16-C17	-2.51	118.33	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	815	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
18	b4	401	BCR	C15-C16-C17	-2.51	118.33	123.47
15	cA	807	CLA	O1D-CGD-CBD	2.51	129.62	124.48
15	aA	809	CLA	C1-C2-C3	-2.51	121.70	126.04
15	c3	410	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
18	c5	419	BCR	C29-C30-C25	2.51	114.34	110.48
18	bL	205	BCR	C15-C16-C17	-2.51	118.34	123.47
18	b6	402	BCR	C1-C6-C5	-2.51	119.08	122.61
15	cB	821	CLA	C3B-C4B-NB	-2.51	108.19	110.52
15	a6	411	CLA	CHB-C1B-NB	2.51	126.91	124.26
15	bA	809	CLA	C1-C2-C3	-2.51	121.71	126.04
15	a2	407	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	c6	403	BCR	C15-C16-C17	-2.51	118.34	123.47
15	cA	825	CLA	C3B-C4B-NB	-2.51	108.19	110.52
15	a4	410	CLA	CHB-C1B-NB	2.51	126.91	124.26
15	b3	417	CLA	CHB-C1B-NB	2.51	126.91	124.26
15	cB	801	CLA	CHC-C4B-NB	2.51	126.91	124.26
15	b4	402	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	c5	405	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
18	aM	101	BCR	C7-C8-C9	-2.51	122.45	126.23
15	aA	819	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
18	a6	402	BCR	C1-C6-C5	-2.51	119.08	122.61
15	b2	414	CLA	C2D-C1D-ND	-2.50	108.26	110.10
18	a6	402	BCR	C15-C16-C17	-2.50	118.34	123.47
15	bA	807	CLA	O1D-CGD-CBD	2.50	129.61	124.48
15	c2	417	CLA	C2A-C1A-CHA	2.50	128.24	123.86
15	a2	422	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	cM	101	BCR	C7-C8-C9	-2.50	122.45	126.23
15	b1	416	CLA	C3C-C4C-NC	-2.50	107.76	110.57
15	a2	406	CLA	C3A-C2A-C1A	2.50	105.09	101.34
18	a4	401	BCR	C24-C23-C22	-2.50	122.45	126.23
15	b6	415	CLA	CAA-C2A-C3A	-2.50	110.26	116.10
15	b6	422	CLA	CHA-C4D-ND	2.50	137.74	132.50
18	cB	847	BCR	C38-C26-C27	-2.50	108.81	113.62
15	cA	827	CLA	CHB-C1B-NB	2.50	126.91	124.26
15	c5	416	CLA	C3C-C4C-NC	-2.50	107.76	110.57
18	c4	420	BCR	C29-C30-C25	2.50	114.33	110.48
18	c2	421	BCR	C15-C16-C17	-2.50	118.35	123.47
15	aB	824	CLA	CHC-C4B-NB	2.50	126.91	124.26
15	b1	402	CLA	CHC-C4B-NB	2.50	126.91	124.26
15	b3	408	CLA	CHB-C1B-NB	2.50	126.91	124.26
15	cB	812	CLA	CHD-C1D-ND	-2.50	122.16	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	836	CLA	C2A-C1A-CHA	2.50	128.23	123.86
15	aA	826	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
15	bA	826	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
15	cA	827	CLA	CHB-C4A-NA	2.50	127.97	124.51
15	aB	807	CLA	C3B-C4B-NB	-2.50	108.20	110.52
18	a3	420	BCR	C35-C13-C14	-2.50	119.42	122.92
15	b1	415	CLA	CMB-C2B-C3B	2.50	132.64	126.59
18	aI	101	BCR	C15-C16-C17	-2.50	118.36	123.47
18	bI	101	BCR	C15-C16-C17	-2.50	118.36	123.47
15	aB	823	CLA	C2A-C1A-CHA	2.50	128.22	123.86
15	aB	815	CLA	C2D-C1D-ND	-2.50	108.26	110.10
15	c3	416	CLA	C3C-C4C-NC	-2.50	107.77	110.57
15	c5	408	CLA	CHB-C1B-NB	2.50	126.90	124.26
15	aB	815	CLA	CMB-C2B-C1B	-2.50	121.57	125.37
15	c4	402	CLA	CHB-C4A-NA	2.50	127.96	124.51
15	a6	415	CLA	CAA-C2A-C3A	-2.50	110.27	116.10
20	aB	850	LMG	C42-C41-C40	-2.50	101.75	114.42
20	cB	850	LMG	C42-C41-C40	-2.50	101.75	114.42
15	b4	410	CLA	CHB-C1B-NB	2.50	126.90	124.26
15	aA	827	CLA	CHB-C4A-NA	2.50	127.96	124.51
15	c1	411	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	a5	416	CLA	C3C-C4C-NC	-2.49	107.77	110.57
18	cI	101	BCR	C15-C16-C17	-2.49	118.36	123.47
15	aA	836	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	b5	410	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
15	b3	406	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	bB	836	CLA	C2A-C1A-CHA	2.49	128.22	123.86
18	a3	420	BCR	C29-C30-C25	2.49	114.32	110.48
15	cB	819	CLA	CMB-C2B-C3B	2.49	132.63	126.59
15	aA	825	CLA	CMB-C2B-C1B	-2.49	121.57	125.37
15	bB	807	CLA	CMB-C2B-C1B	-2.49	121.57	125.37
15	c5	405	CLA	CHB-C1B-NB	2.49	126.90	124.26
15	c6	401	CLA	CHA-C1A-NA	-2.49	120.69	126.40
15	cA	827	CLA	CMD-C2D-C1D	-2.49	120.32	124.71
15	b6	416	CLA	CBA-CAA-C2A	2.49	121.22	113.86
15	b2	417	CLA	C2A-C1A-CHA	2.49	128.22	123.86
15	bA	827	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	cB	801	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	aF	203	BCR	C11-C10-C9	-2.49	123.75	127.31
18	b5	419	BCR	C24-C23-C22	-2.49	122.47	126.23
18	aI	103	BCR	C15-C16-C17	-2.49	118.37	123.47
15	cA	805	CLA	CHB-C4A-NA	2.49	127.96	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	420	BCR	C35-C13-C14	-2.49	119.43	122.92
15	bB	823	CLA	C2A-C1A-CHA	2.49	128.22	123.86
15	bB	822	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
20	bB	851	LMG	C42-C41-C40	-2.49	101.78	114.42
15	c3	409	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
18	b4	401	BCR	C24-C23-C22	-2.49	122.47	126.23
15	aB	801	CLA	CHC-C4B-NB	2.49	126.89	124.26
15	b6	412	CLA	CHB-C1B-NB	2.49	126.89	124.26
15	bB	832	CLA	CHB-C4A-NA	2.49	127.95	124.51
15	c6	408	CLA	CHB-C4A-NA	2.49	127.95	124.51
15	a2	405	CLA	CHB-C1B-NB	2.49	126.89	124.26
15	cB	837	CLA	CHB-C1B-NB	2.49	126.89	124.26
15	a5	407	CLA	C3B-C4B-NB	-2.49	108.21	110.52
15	aB	836	CLA	C2A-C1A-CHA	2.49	128.21	123.86
15	c2	409	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	bB	826	CLA	C3C-C4C-NC	-2.49	107.78	110.57
15	aB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	cB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	bB	814	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
15	a1	412	CLA	C3B-C4B-NB	-2.49	108.21	110.52
15	cA	825	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
15	b5	417	CLA	CHD-C1D-ND	-2.49	122.17	124.45
18	bA	852	BCR	C10-C11-C12	-2.49	115.46	123.22
18	bL	206	BCR	C15-C16-C17	-2.49	118.38	123.47
15	c2	406	CLA	C3A-C2A-C1A	2.49	105.06	101.34
15	b2	412	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	cL	204	CLA	O2D-CGD-CBD	2.49	115.69	111.27
15	a4	407	CLA	CHC-C4B-NB	2.49	126.89	124.26
18	b6	421	BCR	C15-C14-C13	-2.49	123.76	127.31
15	a6	416	CLA	CBA-CAA-C2A	2.49	121.20	113.86
15	a4	415	CLA	CMB-C2B-C3B	2.49	132.61	126.59
15	a1	410	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	bA	818	CLA	C3B-C4B-NB	-2.49	108.21	110.52
15	b6	406	CLA	CMB-C2B-C1B	-2.49	121.58	125.37
15	a1	415	CLA	C3C-C4C-NC	-2.49	107.78	110.57
18	b2	421	BCR	C15-C16-C17	-2.48	118.38	123.47
15	aB	832	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	cB	804	CLA	C1C-C2C-C3C	2.48	109.57	106.96
15	cB	816	CLA	CMB-C2B-C3B	2.48	132.61	126.59
15	cB	832	CLA	CHB-C1B-NB	2.48	126.89	124.26
15	b5	415	CLA	CMB-C2B-C3B	2.48	132.60	126.59
15	cB	822	CLA	O2D-CGD-O1D	-2.48	118.98	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	412	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	bL	204	CLA	O2D-CGD-CBD	2.48	115.68	111.27
18	a1	417	BCR	C3-C4-C5	-2.48	109.64	114.08
15	a4	407	CLA	C3B-C4B-NB	-2.48	108.21	110.52
18	b4	420	BCR	C29-C30-C25	2.48	114.30	110.48
15	a1	405	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	a5	408	CLA	CHB-C1B-NB	2.48	126.89	124.26
18	c3	420	BCR	C29-C30-C25	2.48	114.30	110.48
15	c4	414	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
15	c2	412	CLA	C3B-C4B-NB	-2.48	108.21	110.52
18	c1	420	BCR	C24-C23-C22	-2.48	122.49	126.23
15	cB	832	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a6	421	BCR	C24-C23-C22	-2.48	122.49	126.23
15	bB	801	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
15	aB	826	CLA	C3C-C4C-NC	-2.48	107.79	110.57
15	a3	412	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
15	a6	406	CLA	CHB-C1B-NB	2.48	126.88	124.26
15	c3	417	CLA	C2B-C1B-NB	2.48	111.89	110.23
15	cB	833	CLA	C6-C7-C8	-2.48	107.91	115.92
15	bA	811	CLA	CHB-C4A-NA	2.48	127.94	124.51
15	aA	807	CLA	O1D-CGD-CBD	2.48	129.56	124.48
15	bB	816	CLA	CMB-C2B-C3B	2.48	132.59	126.59
18	a1	421	BCR	C15-C14-C13	-2.48	123.77	127.31
15	b3	407	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	aB	806	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
18	cL	205	BCR	C15-C16-C17	-2.48	118.40	123.47
15	aB	819	CLA	CMB-C2B-C3B	2.48	132.59	126.59
15	bA	825	CLA	C3B-C4B-NB	-2.48	108.22	110.52
15	bA	836	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	cB	823	CLA	C2A-C1A-CHA	2.48	128.19	123.86
15	c6	401	CLA	CHA-C4D-ND	2.48	137.68	132.50
15	cB	801	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
15	b1	409	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	a2	421	BCR	C29-C30-C25	2.47	114.29	110.48
15	a3	405	CLA	CHB-C1B-NB	2.47	126.88	124.26
15	aA	827	CLA	CMD-C2D-C1D	-2.47	120.35	124.71
15	c4	415	CLA	CMB-C2B-C3B	2.47	132.58	126.59
18	bJ	105	BCR	C11-C10-C9	-2.47	123.78	127.31
15	c3	417	CLA	CHD-C1D-ND	-2.47	122.18	124.45
15	b6	411	CLA	CHB-C1B-NB	2.47	126.88	124.26
15	c3	408	CLA	CHB-C1B-NB	2.47	126.88	124.26
15	a6	415	CLA	C3B-C4B-NB	-2.47	108.22	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
15	a4	415	CLA	C2D-C1D-ND	-2.47	108.28	110.10
15	c4	415	CLA	CBA-CAA-C2A	2.47	121.16	113.86
15	c2	410	CLA	CMB-C2B-C1B	-2.47	121.60	125.37
15	cB	826	CLA	C3C-C4C-NC	-2.47	107.80	110.57
18	b6	402	BCR	C15-C16-C17	-2.47	118.41	123.47
15	bB	824	CLA	CHC-C4B-NB	2.47	126.87	124.26
15	aB	816	CLA	CMB-C2B-C3B	2.47	132.57	126.59
15	bB	819	CLA	CMB-C2B-C3B	2.47	132.57	126.59
15	a2	413	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	cA	818	CLA	C3B-C4B-NB	-2.47	108.22	110.52
15	c5	407	CLA	C3B-C4B-NB	-2.47	108.22	110.52
15	cA	836	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
18	a4	420	BCR	C29-C30-C25	2.47	114.28	110.48
15	c4	410	CLA	CHB-C1B-NB	2.47	126.87	124.26
15	cB	815	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
15	aB	822	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	a5	414	CLA	C3B-C4B-NB	-2.47	108.22	110.52
15	cA	831	CLA	C3B-C2B-C1B	2.47	110.14	107.16
15	b2	404	CLA	CHB-C1B-NB	2.47	126.87	124.26
15	c2	404	CLA	CHB-C1B-NB	2.47	126.87	124.26
15	bA	829	CLA	C2A-C1A-CHA	2.47	128.18	123.86
15	cA	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	bB	846	BCR	C7-C8-C9	-2.47	122.50	126.23
15	b3	414	CLA	C3B-C4B-NB	-2.47	108.22	110.52
15	b4	415	CLA	C3B-C4B-NB	-2.47	108.22	110.52
14	aA	801	CL0	O2A-CGA-CBA	2.47	119.65	111.91
15	b3	410	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
15	a4	409	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	cA	828	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	b5	410	CLA	C3B-C4B-NB	-2.47	108.23	110.52
15	c5	410	CLA	C3B-C4B-NB	-2.47	108.23	110.52
15	a3	412	CLA	CMC-C2C-C3C	2.47	132.81	126.12
15	c4	408	CLA	CHB-C1B-NB	2.47	126.87	124.26
15	c6	411	CLA	CHC-C4B-NB	2.47	126.87	124.26
15	a2	414	CLA	C2D-C1D-ND	-2.47	108.29	110.10
15	bL	202	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
15	c2	422	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	cF	205	BCR	C11-C10-C9	-2.47	123.79	127.31
15	a2	408	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
15	c3	407	CLA	C3B-C4B-NB	-2.47	108.23	110.52
15	aB	807	CLA	CMB-C2B-C1B	-2.47	121.61	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cA	850	BCR	C10-C11-C12	-2.47	115.52	123.22
15	bA	831	CLA	C3B-C2B-C1B	2.47	110.14	107.16
15	c6	417	CLA	O2A-CGA-O1A	-2.47	117.15	123.30
15	c5	420	CLA	C11-C10-C8	-2.47	107.95	115.92
15	aB	818	CLA	C3B-C4B-NB	-2.47	108.23	110.52
15	b5	414	CLA	C3B-C4B-NB	-2.47	108.23	110.52
18	b5	419	BCR	C29-C30-C25	2.47	114.28	110.48
18	aA	851	BCR	C10-C11-C12	-2.47	115.52	123.22
15	aL	203	CLA	O2D-CGD-CBD	2.46	115.65	111.27
15	bB	833	CLA	C6-C7-C8	-2.46	107.95	115.92
15	a1	409	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
18	bM	101	BCR	C7-C8-C9	-2.46	122.51	126.23
15	a6	413	CLA	CMC-C2C-C3C	2.46	132.81	126.12
15	c4	409	CLA	CHB-C4A-NA	2.46	127.92	124.51
15	b2	408	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	a3	416	CLA	C3C-C4C-NC	-2.46	107.81	110.57
15	b4	412	CLA	C1D-ND-C4D	2.46	108.08	106.33
15	aB	801	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	b6	417	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
15	c2	417	CLA	C3C-C4C-NC	-2.46	107.81	110.57
15	c1	402	CLA	CHC-C4B-NB	2.46	126.86	124.26
15	c4	409	CLA	CHB-C1B-NB	2.46	126.86	124.26
15	a6	410	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
15	c3	412	CLA	CMC-C2C-C3C	2.46	132.80	126.12
15	cF	203	CLA	CMB-C2B-C3B	2.46	132.55	126.59
15	bB	817	CLA	C3B-C2B-C1B	-2.46	104.19	107.16
15	a1	405	CLA	CHC-C4B-NB	2.46	126.86	124.26
15	cB	822	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
15	c5	415	CLA	C3B-C4B-NB	-2.46	108.23	110.52
15	a6	407	CLA	CHB-C4A-NA	2.46	127.92	124.51
18	c4	401	BCR	C15-C16-C17	-2.46	118.43	123.47
15	c2	403	CLA	CMB-C2B-C3B	2.46	132.55	126.59
15	a4	409	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	b5	412	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	aB	833	CLA	C6-C7-C8	-2.46	107.97	115.92
15	bB	837	CLA	CHB-C1B-NB	2.46	126.86	124.26
15	aB	802	CLA	O2D-CGD-CBD	2.46	115.64	111.27
15	aL	201	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	b6	416	CLA	O2A-CGA-O1A	-2.46	117.17	123.30
15	b5	408	CLA	CHB-C1B-NB	2.46	126.86	124.26
15	b6	406	CLA	CHB-C1B-NB	2.46	126.86	124.26
15	bA	841	CLA	C4-C3-C5	2.46	119.41	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cB	846	BCR	C7-C8-C9	-2.46	122.52	126.23
15	b5	416	CLA	C3C-C4C-NC	-2.46	107.81	110.57
15	a5	420	CLA	C11-C10-C8	-2.46	107.97	115.92
15	b4	415	CLA	CBA-CAA-C2A	2.46	121.12	113.86
15	b1	415	CLA	O2A-CGA-O1A	-2.46	117.17	123.30
15	aA	812	CLA	C3B-C4B-NB	-2.46	108.23	110.52
15	cB	828	CLA	C3B-C4B-NB	-2.46	108.23	110.52
15	c3	412	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
15	cB	833	CLA	CHD-C1D-ND	-2.46	122.20	124.45
15	bB	802	CLA	O2D-CGD-CBD	2.46	115.63	111.27
14	bA	801	CL0	O2A-CGA-CBA	2.46	119.62	111.91
15	b3	412	CLA	CMC-C2C-C3C	2.46	132.78	126.12
18	c5	419	BCR	C24-C23-C22	-2.46	122.52	126.23
15	a6	416	CLA	O2A-CGA-O1A	-2.46	117.18	123.30
15	a5	412	CLA	CHA-C1A-NA	-2.46	120.78	126.40
15	c4	412	CLA	CHA-C1A-NA	-2.46	120.78	126.40
15	a5	407	CLA	CHC-C4B-NB	2.46	126.86	124.26
15	bA	841	CLA	CHB-C1B-NB	2.46	126.86	124.26
15	a2	410	CLA	CMB-C2B-C1B	-2.46	121.63	125.37
15	aB	833	CLA	CHD-C1D-ND	-2.45	122.20	124.45
15	cA	825	CLA	C2D-C1D-ND	-2.45	108.30	110.10
15	cK	102	CLA	CHB-C4A-NA	2.45	127.91	124.51
15	c4	406	CLA	CHB-C4A-NA	2.45	127.91	124.51
15	bK	101	CLA	O2A-CGA-O1A	-2.45	117.18	123.30
15	cA	841	CLA	C4-C3-C5	2.45	119.40	115.27
15	b5	415	CLA	CBA-CAA-C2A	2.45	121.11	113.86
15	b1	416	CLA	C2A-C1A-CHA	2.45	128.15	123.86
15	aA	838	CLA	C2D-C1D-ND	-2.45	108.30	110.10
15	b5	407	CLA	C3B-C4B-NB	-2.45	108.24	110.52
15	c1	417	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	aK	102	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	c6	411	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
15	bB	818	CLA	C3B-C4B-NB	-2.45	108.24	110.52
15	a4	405	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	a4	412	CLA	C1D-ND-C4D	2.45	108.08	106.33
18	a2	421	BCR	C3-C4-C5	-2.45	109.70	114.08
15	b5	407	CLA	CHC-C4B-NB	2.45	126.85	124.26
15	cA	835	CLA	C1-C2-C3	-2.45	121.80	126.04
15	aB	801	CLA	CHB-C4A-NA	2.45	127.90	124.51
18	b6	421	BCR	C7-C8-C9	-2.45	122.53	126.23
15	cA	829	CLA	C6-C7-C8	-2.45	108.00	115.92
15	c3	416	CLA	C1C-C2C-C3C	-2.45	104.38	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	806	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
15	b1	416	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	cB	838	CLA	CMB-C2B-C3B	2.45	132.52	126.59
15	a5	412	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
14	cA	801	CL0	O2A-CGA-CBA	2.45	119.60	111.91
15	cK	102	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	c1	415	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
15	c2	405	CLA	CHB-C1B-NB	2.45	126.85	124.26
18	b1	420	BCR	C24-C23-C22	-2.45	122.53	126.23
15	aB	822	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
15	bA	825	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
15	b1	417	CLA	CHB-C1B-NB	2.45	126.85	124.26
18	aA	849	BCR	C30-C25-C26	-2.45	119.17	122.61
15	a1	415	CLA	C2A-C1A-CHA	2.45	128.14	123.86
15	aB	825	CLA	C3B-C4B-NB	-2.45	108.24	110.52
15	bB	821	CLA	C3B-C4B-NB	-2.45	108.24	110.52
15	a1	408	CLA	CHC-C4B-NB	2.45	126.85	124.26
15	cA	841	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	c5	407	CLA	CHC-C4B-NB	2.45	126.85	124.26
18	a5	419	BCR	C29-C30-C25	2.45	114.25	110.48
15	aA	831	CLA	C3B-C2B-C1B	2.45	110.11	107.16
15	c6	414	CLA	CMC-C2C-C3C	2.45	132.76	126.12
15	bB	824	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	c2	411	CLA	CHB-C1B-NB	2.45	126.85	124.26
15	c5	415	CLA	CBA-CAA-C2A	2.45	121.08	113.86
15	cB	802	CLA	O2D-CGD-CBD	2.45	115.61	111.27
15	a5	417	CLA	CHD-C1D-ND	-2.45	122.21	124.45
15	b2	422	CLA	C11-C10-C8	-2.44	108.02	115.92
18	b6	420	BCR	C15-C16-C17	-2.44	118.47	123.47
15	aA	829	CLA	C6-C7-C8	-2.44	108.02	115.92
15	b4	409	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	cL	202	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	b2	417	CLA	C3C-C4C-NC	-2.44	107.83	110.57
15	bA	829	CLA	C6-C7-C8	-2.44	108.02	115.92
15	c1	412	CLA	C1D-ND-C4D	2.44	108.07	106.33
15	aB	824	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	aB	837	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	b2	412	CLA	C3B-C4B-NB	-2.44	108.25	110.52
15	b3	412	CLA	C3B-C4B-NB	-2.44	108.25	110.52
15	cB	825	CLA	C3B-C4B-NB	-2.44	108.25	110.52
15	b5	412	CLA	CHA-C1A-NA	-2.44	120.80	126.40
15	a2	405	CLA	CAA-C2A-C3A	-2.44	106.09	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cF	202	BCR	C1-C6-C5	-2.44	119.17	122.61
18	b6	402	BCR	C24-C23-C22	-2.44	122.55	126.23
15	a1	411	CLA	CMC-C2C-C3C	2.44	132.75	126.12
15	a6	417	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	aB	804	CLA	C1C-C2C-C3C	2.44	109.52	106.96
15	b5	420	CLA	C11-C10-C8	-2.44	108.03	115.92
15	aB	832	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	cB	824	CLA	CHC-C4B-NB	2.44	126.84	124.26
15	c1	408	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	b2	407	CLA	O2A-CGA-O1A	-2.44	117.21	123.30
15	c6	418	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	a6	418	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	bB	822	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
15	b1	410	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
15	bA	835	CLA	C1-C2-C3	-2.44	121.82	126.04
15	bB	842	CLA	CHB-C4A-NA	2.44	127.89	124.51
15	bB	833	CLA	CHD-C1D-ND	-2.44	122.21	124.45
15	cA	829	CLA	C2A-C1A-CHA	2.44	128.12	123.86
15	aA	828	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	aA	841	CLA	C4-C3-C5	2.44	119.37	115.27
15	aJ	201	CLA	CMB-C2B-C3B	2.44	132.49	126.59
15	bB	808	CLA	O2D-CGD-CBD	2.44	115.60	111.27
15	aB	827	CLA	C3B-C4B-NB	-2.44	108.25	110.52
15	cA	807	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
18	aB	846	BCR	C7-C8-C9	-2.44	122.55	126.23
15	bF	201	CLA	CMB-C2B-C3B	2.44	132.49	126.59
15	a4	409	CLA	CHB-C1B-NB	2.44	126.84	124.26
18	c6	421	BCR	C15-C16-C17	-2.44	118.48	123.47
15	cA	823	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
18	c5	401	BCR	C15-C16-C17	-2.44	118.48	123.47
15	bB	814	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
15	cA	815	CLA	C2D-C1D-ND	-2.44	108.31	110.10
15	aA	835	CLA	C1-C2-C3	-2.44	121.83	126.04
18	bA	850	BCR	C30-C25-C26	-2.44	119.18	122.61
18	b2	420	BCR	C27-C26-C25	2.44	126.27	122.73
18	a5	419	BCR	C24-C23-C22	-2.44	122.55	126.23
18	c2	421	BCR	C3-C4-C5	-2.44	109.73	114.08
15	aA	834	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
15	bB	832	CLA	CHB-C1B-NB	2.44	126.84	124.26
15	c1	409	CLA	CHB-C4A-NA	2.44	127.88	124.51
15	c2	405	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
18	bB	849	BCR	C1-C6-C5	-2.43	119.18	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	415	CLA	CMB-C2B-C3B	2.43	132.49	126.59
15	cB	806	CLA	CMB-C2B-C1B	-2.43	121.66	125.37
15	b6	418	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	cA	811	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	c6	407	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	c5	412	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	a6	411	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	bB	804	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	cA	812	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	a2	409	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
18	cM	101	BCR	C24-C23-C22	-2.43	122.56	126.23
15	aA	818	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	cB	814	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
15	aB	817	CLA	C3B-C2B-C1B	-2.43	104.22	107.16
15	bB	804	CLA	C1C-C2C-C3C	2.43	109.51	106.96
15	c4	405	CLA	CHB-C1B-NB	2.43	126.83	124.26
18	b2	421	BCR	C3-C4-C5	-2.43	109.73	114.08
15	bB	801	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	b2	422	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	b4	409	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	b4	407	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	c5	412	CLA	CHA-C1A-NA	-2.43	120.83	126.40
15	b5	406	CLA	O2A-CGA-O1A	-2.43	117.24	123.30
18	b5	401	BCR	C15-C16-C17	-2.43	118.49	123.47
15	a5	405	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	b4	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	c1	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	bA	811	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	c2	413	CLA	CHA-C1A-NA	-2.43	120.83	126.40
15	bK	101	CLA	O2D-CGD-CBD	2.43	115.59	111.27
15	c3	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	bA	823	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	b1	420	BCR	C29-C30-C25	2.43	114.22	110.48
15	c5	415	CLA	CMB-C2B-C3B	2.43	132.47	126.59
15	b2	413	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
15	a2	417	CLA	C3C-C4C-NC	-2.43	107.85	110.57
15	b3	417	CLA	CHD-C1D-ND	-2.43	122.22	124.45
15	c5	417	CLA	CHD-C1D-ND	-2.43	122.22	124.45
15	cA	841	CLA	C3B-C4B-NB	-2.43	108.26	110.52
15	a2	414	CLA	CHC-C4B-NB	2.43	126.83	124.26
15	bK	101	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	a1	421	BCR	C24-C23-C22	-2.43	122.57	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	422	CLA	C11-C10-C8	-2.43	108.07	115.92
15	aA	841	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	b2	405	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
15	a4	402	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	a1	405	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
15	a4	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	aM	101	BCR	C24-C23-C22	-2.43	122.57	126.23
15	aB	808	CLA	O2D-CGD-CBD	2.43	115.58	111.27
15	b4	415	CLA	CHB-C1B-NB	2.43	126.83	124.26
15	a1	408	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	b1	406	CLA	CHB-C4A-NA	2.43	127.87	124.51
15	aA	829	CLA	C2A-C1A-CHA	2.43	128.10	123.86
15	a5	415	CLA	CBA-CAA-C2A	2.43	121.02	113.86
18	c6	402	BCR	C15-C14-C13	-2.43	123.85	127.31
15	cA	804	CLA	C1-C2-C3	-2.42	121.85	126.04
18	b6	421	BCR	C24-C23-C22	-2.42	122.57	126.23
15	aB	842	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	cB	842	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	c3	414	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	bB	815	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
15	a4	415	CLA	CHB-C1B-NB	2.42	126.82	124.26
15	a4	415	CLA	O2A-CGA-O1A	-2.42	117.26	123.30
15	a3	406	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	aB	814	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
15	b2	409	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	cJ	103	BCR	C30-C25-C26	-2.42	119.20	122.61
15	a3	408	CLA	CHB-C1B-NB	2.42	126.82	124.26
15	b4	402	CLA	CHC-C4B-NB	2.42	126.82	124.26
15	b5	405	CLA	CHB-C1B-NB	2.42	126.82	124.26
15	c4	416	CLA	C2A-C1A-CHA	2.42	128.09	123.86
18	cA	848	BCR	C30-C25-C26	-2.42	119.20	122.61
15	a2	412	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
15	bA	828	CLA	CHB-C4A-NA	2.42	127.86	124.51
18	a6	420	BCR	C15-C16-C17	-2.42	118.52	123.47
15	aA	834	CLA	C2D-C1D-ND	-2.42	108.32	110.10
15	b3	416	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
18	aF	201	BCR	C1-C6-C5	-2.42	119.20	122.61
15	aA	841	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	b6	411	CLA	C3B-C4B-NB	-2.42	108.27	110.52
15	bB	838	CLA	CMB-C2B-C3B	2.42	132.45	126.59
15	aB	838	CLA	CMB-C2B-C3B	2.42	132.45	126.59
15	c2	412	CLA	O2D-CGD-O1D	-2.42	119.11	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bJ	103	BCR	C30-C25-C26	-2.42	119.21	122.61
15	b4	412	CLA	CHA-C1A-NA	-2.42	120.86	126.40
15	b6	416	CLA	CMB-C2B-C3B	2.42	132.45	126.59
15	bB	839	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	bB	803	CLA	C2A-C1A-CHA	2.42	128.09	123.86
15	c4	412	CLA	C1D-ND-C4D	2.42	108.05	106.33
15	a6	416	CLA	CMB-C2B-C3B	2.42	132.44	126.59
15	a4	408	CLA	CHB-C1B-NB	2.42	126.82	124.26
15	aA	823	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	aK	102	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	a5	412	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	aL	203	CLA	CHB-C1B-NB	2.42	126.82	124.26
15	cB	815	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
15	b2	406	CLA	C11-C10-C8	-2.42	108.11	115.92
15	c1	412	CLA	CMC-C2C-C3C	2.42	132.68	126.12
15	cB	808	CLA	O2D-CGD-CBD	2.42	115.56	111.27
18	c3	401	BCR	C24-C23-C22	-2.42	122.58	126.23
15	cB	839	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
15	aJ	202	CLA	CAA-CBA-CGA	-2.42	106.10	112.51
15	cA	834	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
18	b1	420	BCR	C3-C4-C5	-2.42	109.76	114.08
15	cB	832	CLA	C2D-C1D-ND	-2.42	108.32	110.10
15	a4	406	CLA	CHC-C4B-NB	2.42	126.81	124.26
15	a6	413	CLA	CHB-C4A-NA	2.42	127.85	124.51
15	bA	807	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
15	a6	422	CLA	CHA-C4D-ND	2.41	137.55	132.50
15	aB	804	CLA	CHC-C1C-NC	2.41	127.87	124.20
15	a3	412	CLA	CHB-C4A-NA	2.41	127.85	124.51
15	c1	406	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
18	c3	420	BCR	C24-C23-C22	-2.41	122.59	126.23
15	c6	417	CLA	CMB-C2B-C3B	2.41	132.43	126.59
18	cA	851	BCR	C1-C6-C5	-2.41	119.22	122.61
15	c5	406	CLA	O2A-CGA-O1A	-2.41	117.29	123.30
15	bB	824	CLA	C3B-C4B-NB	-2.41	108.28	110.52
18	a6	402	BCR	C24-C23-C22	-2.41	122.59	126.23
18	bM	101	BCR	C24-C23-C22	-2.41	122.59	126.23
15	aA	804	CLA	C1-C2-C3	-2.41	121.87	126.04
18	b4	401	BCR	C1-C6-C5	-2.41	119.22	122.61
15	cK	102	CLA	O2D-CGD-CBD	2.41	115.55	111.27
15	aK	102	CLA	O2D-CGD-CBD	2.41	115.55	111.27
18	a2	420	BCR	C27-C26-C25	2.41	126.23	122.73
15	a5	402	CLA	CHC-C4B-NB	2.41	126.81	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	834	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
15	b5	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	c2	414	CLA	C2D-C1D-ND	-2.41	108.33	110.10
15	cB	804	CLA	CHC-C1C-NC	2.41	127.86	124.20
15	aB	803	CLA	C2A-C1A-CHA	2.41	128.07	123.86
18	bA	853	BCR	C1-C6-C5	-2.41	119.22	122.61
15	aB	821	CLA	C3B-C4B-NB	-2.41	108.28	110.52
15	bA	804	CLA	C1-C2-C3	-2.41	121.88	126.04
15	aA	811	CLA	CHB-C1B-NB	2.41	126.81	124.26
15	c4	402	CLA	CHC-C4B-NB	2.41	126.81	124.26
15	a5	406	CLA	O2A-CGA-O1A	-2.41	117.30	123.30
18	b1	401	BCR	C27-C26-C25	2.41	126.23	122.73
18	aJ	204	BCR	C30-C25-C26	-2.41	119.22	122.61
15	a2	418	CLA	C2A-C1A-CHA	2.41	128.07	123.86
15	a3	417	CLA	CHD-C1D-ND	-2.41	122.24	124.45
18	b3	420	BCR	C24-C23-C22	-2.41	122.60	126.23
15	aB	815	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
15	b6	413	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	b2	408	CLA	C3B-C4B-NB	-2.41	108.28	110.52
15	c1	405	CLA	CHB-C1B-NB	2.41	126.80	124.26
15	aA	842	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	cF	201	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	c5	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
15	a2	412	CLA	C3B-C4B-NB	-2.40	108.28	110.52
15	bB	803	CLA	O2D-CGD-CBD	2.40	115.54	111.27
15	bA	842	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	bB	812	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	b6	413	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
15	bB	840	CLA	C2A-C1A-CHA	2.40	128.06	123.86
18	a1	419	BCR	C29-C30-C25	2.40	114.18	110.48
15	b3	405	CLA	CHB-C1B-NB	2.40	126.80	124.26
15	cB	806	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
15	a2	413	CLA	CHA-C1A-NA	-2.40	120.89	126.40
15	bA	841	CLA	C3B-C4B-NB	-2.40	108.28	110.52
18	a3	420	BCR	C24-C23-C22	-2.40	122.60	126.23
18	c4	418	BCR	C7-C8-C9	-2.40	122.60	126.23
18	a1	420	BCR	C34-C9-C10	-2.40	119.56	122.92
18	c1	420	BCR	C29-C30-C25	2.40	114.18	110.48
18	c2	420	BCR	C27-C26-C25	2.40	126.22	122.73
15	a4	402	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	c3	402	CLA	CHC-C4B-NB	2.40	126.80	124.26
18	aA	852	BCR	C1-C6-C5	-2.40	119.23	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	808	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	bB	804	CLA	CHC-C1C-NC	2.40	127.85	124.20
15	c6	414	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
15	aA	813	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
15	c5	411	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
15	b3	409	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
15	a2	408	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	b6	413	CLA	CMC-C2C-C3C	2.40	132.64	126.12
15	b3	421	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	cA	813	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
15	aA	831	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	b1	403	CLA	CHB-C1B-NB	2.40	126.80	124.26
15	c1	416	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	a3	421	CLA	CHA-C4D-ND	2.40	137.52	132.50
15	aA	807	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	b3	406	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
15	b5	415	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	cA	838	CLA	C3B-C4B-NB	-2.40	108.29	110.52
15	b1	409	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	cB	829	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	c3	410	CLA	CHB-C1B-NB	2.40	126.80	124.26
15	a3	416	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
15	b4	416	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	a2	405	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
15	bA	815	CLA	C2D-C1D-ND	-2.40	108.34	110.10
15	b5	409	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	a1	408	CLA	CMB-C2B-C1B	-2.40	121.72	125.37
15	b3	403	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	cB	840	CLA	C2A-C1A-CHA	2.40	128.05	123.86
15	aA	823	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	b1	401	BCR	C7-C8-C9	-2.40	122.61	126.23
15	cB	817	CLA	C3B-C2B-C1B	-2.40	104.27	107.16
18	cI	102	BCR	C16-C15-C14	-2.40	118.57	123.47
15	b4	412	CLA	CMC-C2C-C3C	2.40	132.62	126.12
15	c4	412	CLA	CMC-C2C-C3C	2.40	132.62	126.12
15	bJ	101	CLA	CAA-CBA-CGA	-2.39	106.15	112.51
18	c5	419	BCR	C3-C4-C5	-2.39	109.80	114.08
15	a5	406	CLA	CHB-C4A-NA	2.39	127.82	124.51
18	cI	102	BCR	C16-C17-C18	-2.39	123.89	127.31
15	b4	405	CLA	CHB-C1B-NB	2.39	126.79	124.26
15	aB	803	CLA	O2D-CGD-CBD	2.39	115.52	111.27
18	bL	206	BCR	C15-C14-C13	-2.39	123.90	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a2	406	CLA	O2A-CGA-CBA	-2.39	104.40	111.91
15	bA	813	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
15	aB	806	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
15	aB	840	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	b6	404	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	c3	403	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	c5	415	CLA	O2A-CGA-O1A	-2.39	117.34	123.30
15	a5	416	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
15	c6	419	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	bB	834	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
15	a4	416	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	aA	808	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	a5	410	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	c2	408	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	c4	407	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	cJ	101	CLA	CAA-CBA-CGA	-2.39	106.17	112.51
18	c4	401	BCR	C1-C6-C5	-2.39	119.25	122.61
15	c3	412	CLA	CHA-C1A-NA	-2.39	120.93	126.40
15	bA	818	CLA	CHB-C1B-NB	2.39	126.79	124.26
15	a5	412	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	b4	416	CLA	C3C-C4C-NC	-2.39	107.89	110.57
15	a3	409	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
15	c3	407	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
15	cB	819	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	cA	823	CLA	CHB-C4A-NA	2.39	127.81	124.51
15	b2	413	CLA	CHA-C1A-NA	-2.39	120.93	126.40
15	bA	824	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
15	bB	827	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	cB	827	CLA	C3B-C4B-NB	-2.39	108.30	110.52
15	a3	406	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
15	a4	412	CLA	CHA-C1A-NA	-2.39	120.93	126.40
18	b4	418	BCR	C7-C8-C9	-2.39	122.63	126.23
15	aL	202	CLA	CHB-C1B-NB	2.39	126.78	124.26
15	c2	410	CLA	CHB-C1B-NB	2.39	126.78	124.26
15	cB	834	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
15	a2	402	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
18	aL	205	BCR	C15-C14-C13	-2.39	123.90	127.31
15	cA	843	CLA	CHD-C1D-ND	-2.39	122.26	124.45
18	aA	849	BCR	C38-C26-C27	-2.39	109.03	113.62
15	b5	402	CLA	CHC-C4B-NB	2.39	126.78	124.26
15	cA	818	CLA	CHB-C1B-NB	2.39	126.78	124.26
15	cA	827	CLA	CMB-C2B-C3B	2.39	132.37	126.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	416	CLA	C3C-C4C-NC	-2.39	107.90	110.57
18	bF	202	BCR	C38-C26-C27	-2.39	109.03	113.62
18	a4	401	BCR	C15-C16-C17	-2.38	118.59	123.47
18	c3	419	BCR	C3-C4-C5	-2.38	109.82	114.08
15	a3	415	CLA	CBA-CAA-C2A	2.38	120.90	113.86
15	b2	406	CLA	O2A-CGA-CBA	-2.38	104.42	111.91
15	bA	829	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
15	cA	844	CLA	CAA-CBA-CGA	2.38	120.22	113.25
15	b4	421	CLA	CHA-C4D-ND	2.38	137.49	132.50
15	a1	407	CLA	CHB-C1B-NB	2.38	126.78	124.26
15	cA	831	CLA	CHC-C4B-NB	2.38	126.78	124.26
15	b2	405	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
18	c1	401	BCR	C3-C4-C5	-2.38	109.82	114.08
15	aA	829	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
15	b1	403	CLA	C2A-C1A-CHA	2.38	128.03	123.86
15	cB	803	CLA	C2A-C1A-CHA	2.38	128.03	123.86
18	aI	103	BCR	C39-C30-C25	2.38	114.17	110.30
14	cA	801	CL0	CMB-C2B-C1B	2.38	129.00	125.37
15	b4	414	CLA	C3B-C4B-NB	-2.38	108.30	110.52
15	cB	803	CLA	O2D-CGD-CBD	2.38	115.50	111.27
15	aA	807	CLA	CHB-C1B-NB	2.38	126.78	124.26
15	c3	421	CLA	CHC-C4B-NB	2.38	126.78	124.26
18	aI	101	BCR	C38-C26-C27	-2.38	109.04	113.62
15	b3	415	CLA	O2A-CGA-O1A	-2.38	117.36	123.30
18	cI	101	BCR	C38-C26-C27	-2.38	109.04	113.62
18	a3	401	BCR	C24-C23-C22	-2.38	122.64	126.23
15	aB	839	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
15	bA	827	CLA	CMB-C2B-C3B	2.38	132.36	126.59
15	c5	416	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
18	c6	402	BCR	C27-C26-C25	2.38	126.19	122.73
18	b1	420	BCR	C1-C6-C5	-2.38	119.26	122.61
18	cF	204	BCR	C38-C26-C27	-2.38	109.04	113.62
15	a6	413	CLA	CMB-C2B-C1B	-2.38	121.74	125.37
15	a3	407	CLA	CHC-C4B-NB	2.38	126.78	124.26
18	a1	419	BCR	C15-C16-C17	-2.38	118.60	123.47
15	c4	415	CLA	C3B-C4B-NB	-2.38	108.31	110.52
18	cL	205	BCR	C39-C30-C25	2.38	114.16	110.30
18	bA	850	BCR	C38-C26-C27	-2.38	109.04	113.62
18	bI	102	BCR	C16-C15-C14	-2.38	118.60	123.47
18	b4	420	BCR	C15-C16-C17	-2.38	118.60	123.47
15	aB	808	CLA	CAC-C3C-C4C	2.38	127.90	124.81
15	c3	421	CLA	CHA-C4D-ND	2.38	137.48	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	829	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	cB	845	BCR	C7-C8-C9	-2.38	122.64	126.23
15	c2	407	CLA	O2A-CGA-O1A	-2.38	117.37	123.30
18	b6	401	BCR	C15-C14-C13	-2.38	123.91	127.31
15	aB	832	CLA	C2D-C1D-ND	-2.38	108.35	110.10
15	bA	838	CLA	C3B-C4B-NB	-2.38	108.31	110.52
15	bB	825	CLA	C3B-C4B-NB	-2.38	108.31	110.52
15	cA	831	CLA	C3B-C4B-NB	-2.38	108.31	110.52
18	c1	401	BCR	C27-C26-C25	2.38	126.19	122.73
15	c4	406	CLA	CHC-C4B-NB	2.38	126.78	124.26
15	bB	806	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	cB	812	CLA	CHB-C4A-NA	2.38	127.80	124.51
15	aA	803	CLA	CMD-C2D-C3D	2.38	133.09	127.61
15	a4	414	CLA	C3B-C4B-NB	-2.38	108.31	110.52
15	b6	411	CLA	C1D-ND-C4D	2.38	108.03	106.33
15	c2	418	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	bB	806	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
15	c6	405	CLA	C2A-C1A-CHA	2.38	128.02	123.86
15	bA	825	CLA	CHB-C1B-NB	2.38	126.78	124.26
18	aI	102	BCR	C16-C17-C18	-2.38	123.92	127.31
15	a6	404	CLA	C2A-C1A-CHA	2.38	128.02	123.86
15	bA	812	CLA	C3B-C4B-NB	-2.38	108.31	110.52
18	a3	420	BCR	C15-C16-C17	-2.38	118.60	123.47
15	b3	412	CLA	CHA-C1A-NA	-2.38	120.95	126.40
15	c5	410	CLA	C1D-ND-C4D	2.38	108.02	106.33
15	c6	419	CLA	CHB-C1B-C2B	-2.38	120.52	127.24
15	bA	821	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
18	bI	101	BCR	C38-C26-C27	-2.38	109.05	113.62
15	a5	406	CLA	CHC-C4B-NB	2.38	126.77	124.26
15	aA	845	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	c3	406	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
15	cA	824	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
15	b6	414	CLA	CHC-C1C-NC	2.38	127.81	124.20
15	b6	418	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	cB	814	CLA	CHD-C1D-ND	-2.38	122.27	124.45
18	aI	102	BCR	C16-C15-C14	-2.38	118.61	123.47
15	bA	803	CLA	CMD-C2D-C3D	2.38	133.08	127.61
15	b6	405	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	aB	834	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
15	c6	414	CLA	CHA-C1A-NA	-2.37	120.96	126.40
15	aB	814	CLA	CHD-C1D-ND	-2.37	122.27	124.45
15	aA	824	CLA	O2A-CGA-O1A	-2.37	117.60	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bL	203	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	c5	402	CLA	CHC-C4B-NB	2.37	126.77	124.26
15	aB	804	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	aB	824	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	a1	413	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	a5	409	CLA	CHC-C4B-NB	2.37	126.77	124.26
15	b2	410	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	bA	820	CLA	C2A-C1A-CHA	2.37	128.01	123.86
15	c5	403	CLA	C2A-C1A-CHA	2.37	128.01	123.86
15	a5	415	CLA	C3B-C4B-NB	-2.37	108.31	110.52
15	c1	409	CLA	CHC-C4B-NB	2.37	126.77	124.26
15	a1	407	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	b5	412	CLA	C2A-C1A-CHA	2.37	128.01	123.86
18	b3	419	BCR	C3-C4-C5	-2.37	109.84	114.08
15	a5	411	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	c2	412	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
15	c3	409	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	cA	803	CLA	CMD-C2D-C3D	2.37	133.07	127.61
15	cA	834	CLA	C2D-C1D-ND	-2.37	108.36	110.10
15	b3	412	CLA	C1D-ND-C4D	2.37	108.02	106.33
15	a1	404	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	b1	408	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	b4	406	CLA	CHC-C4B-NB	2.37	126.77	124.26
15	b1	405	CLA	O1D-CGD-CBD	2.37	129.33	124.48
15	aA	821	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
15	c4	413	CLA	C2D-C1D-ND	-2.37	108.36	110.10
14	bA	801	CL0	CMB-C2B-C1B	2.37	128.98	125.37
15	bA	826	CLA	CMB-C2B-C3B	2.37	132.32	126.59
15	b2	403	CLA	C2A-C1A-CHA	2.37	128.00	123.86
15	a1	416	CLA	CHB-C1B-NB	2.37	126.76	124.26
15	bA	831	CLA	CHC-C4B-NB	2.37	126.76	124.26
15	aA	826	CLA	CMB-C2B-C3B	2.37	132.32	126.59
15	b3	421	CLA	CHA-C4D-ND	2.37	137.45	132.50
14	aA	801	CL0	CMB-C2B-C1B	2.37	128.97	125.37
15	aB	806	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
15	aA	825	CLA	CHB-C1B-NB	2.37	126.76	124.26
15	a4	412	CLA	CMC-C2C-C3C	2.37	132.54	126.12
15	a6	408	CLA	C3B-C4B-NB	-2.37	108.32	110.52
15	b1	414	CLA	C3B-C4B-NB	-2.37	108.32	110.52
15	c6	414	CLA	C3B-C4B-NB	-2.37	108.32	110.52
15	c3	410	CLA	C2A-C1A-CHA	2.37	128.00	123.86
18	aA	849	BCR	C11-C10-C9	-2.37	123.93	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a4	401	BCR	C1-C6-C5	-2.37	119.28	122.61
15	cB	806	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
15	bB	805	CLA	CHB-C1B-NB	2.37	126.76	124.26
15	c4	415	CLA	O2A-CGA-O1A	-2.37	117.40	123.30
15	cA	833	CLA	CMB-C2B-C3B	2.37	132.32	126.59
15	aB	828	CLA	CMB-C2B-C1B	-2.37	121.77	125.37
15	bB	819	CLA	C3B-C4B-NB	-2.36	108.32	110.52
18	aF	202	BCR	C38-C26-C27	-2.36	109.07	113.62
18	a1	420	BCR	C3-C4-C5	-2.36	109.86	114.08
15	c6	419	CLA	CHB-C1B-NB	2.36	126.76	124.26
15	bA	823	CLA	CHB-C4A-NA	2.36	127.78	124.51
15	aA	829	CLA	C3B-C4B-NB	-2.36	108.32	110.52
15	aA	838	CLA	C3B-C4B-NB	-2.36	108.32	110.52
15	b6	408	CLA	C3B-C4B-NB	-2.36	108.32	110.52
15	c2	416	CLA	C3B-C4B-NB	-2.36	108.32	110.52
15	a4	416	CLA	C3C-C4C-NC	-2.36	107.92	110.57
15	aA	833	CLA	CMB-C2B-C3B	2.36	132.31	126.59
15	a6	418	CLA	C2A-C1A-CHA	2.36	127.99	123.86
15	aA	844	CLA	CHD-C1D-ND	-2.36	122.28	124.45
18	a6	401	BCR	C15-C14-C13	-2.36	123.94	127.31
18	cA	848	BCR	C38-C26-C27	-2.36	109.08	113.62
18	bB	845	BCR	C7-C8-C9	-2.36	122.66	126.23
15	b1	417	CLA	C3A-C2A-C1A	2.36	104.88	101.34
15	b6	414	CLA	C2D-C1D-ND	-2.36	108.36	110.10
18	a1	420	BCR	C27-C26-C25	2.36	126.16	122.73
15	b4	408	CLA	CHB-C1B-NB	2.36	126.76	124.26
15	cL	204	CLA	CHB-C1B-NB	2.36	126.76	124.26
15	cB	824	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
18	a1	419	BCR	C3-C4-C5	-2.36	109.86	114.08
18	bI	102	BCR	C3-C4-C5	-2.36	109.86	114.08
15	b6	413	CLA	C3B-C4B-NB	-2.36	108.32	110.52
15	c2	406	CLA	O2A-CGA-CBA	-2.36	104.50	111.91
15	a2	418	CLA	CHB-C1B-NB	2.36	126.76	124.26
15	c6	406	CLA	CHB-C1B-NB	2.36	126.76	124.26
15	aA	845	CLA	CAA-CBA-CGA	2.36	120.15	113.25
15	bA	845	CLA	CAA-CBA-CGA	2.36	120.15	113.25
15	b6	418	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
15	a6	411	CLA	C1D-ND-C4D	2.36	108.01	106.33
14	aA	801	CL0	CHB-C1B-NB	-2.36	121.76	124.26
15	a6	422	CLA	CHC-C4B-NB	2.36	126.76	124.26
15	c2	402	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
15	c6	414	CLA	CHB-C4A-NA	2.36	127.78	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	414	CLA	O2A-CGA-O1A	-2.36	117.42	123.30
15	a6	413	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	a6	418	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
15	a6	405	CLA	CHB-C1B-NB	2.36	126.75	124.26
15	c6	412	CLA	C3B-C4B-NB	-2.36	108.33	110.52
16	cA	845	PQN	C21-C20-C18	-2.36	108.29	115.92
15	c3	412	CLA	C1D-ND-C4D	2.36	108.01	106.33
15	cA	826	CLA	CMB-C2B-C3B	2.36	132.30	126.59
15	aB	841	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
15	b3	416	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	b6	418	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	c2	413	CLA	C2A-C1A-CHA	2.36	127.98	123.86
18	a5	401	BCR	C15-C16-C17	-2.36	118.64	123.47
15	a4	421	CLA	CHA-C4D-ND	2.36	137.43	132.50
15	bB	840	CLA	C3B-C4B-NB	-2.36	108.33	110.52
15	c5	413	CLA	C2D-C1D-ND	-2.36	108.37	110.10
18	c1	419	BCR	C27-C26-C25	2.36	126.15	122.73
15	c6	401	CLA	O2D-CGD-CBD	2.36	115.46	111.27
15	aA	807	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	aA	806	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
15	c6	414	CLA	C1D-ND-C4D	2.36	108.01	106.33
15	b4	415	CLA	O2A-CGA-O1A	-2.36	117.43	123.30
15	b5	416	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
15	aA	802	CLA	C11-C10-C8	-2.36	108.30	115.92
15	aB	812	CLA	CHB-C4A-NA	2.36	127.77	124.51
15	a3	402	CLA	CHC-C4B-NB	2.36	126.75	124.26
18	bI	102	BCR	C16-C17-C18	-2.36	123.95	127.31
15	bA	834	CLA	C2D-C1D-ND	-2.36	108.37	110.10
15	c6	418	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	b6	413	CLA	CHA-C1A-NA	-2.36	121.00	126.40
15	b3	410	CLA	C2A-C1A-CHA	2.36	127.98	123.86
15	b2	418	CLA	CHB-C1B-NB	2.35	126.75	124.26
15	c2	402	CLA	CHC-C4B-NB	2.35	126.75	124.26
15	c6	408	CLA	CHC-C4B-NB	2.35	126.75	124.26
15	c5	412	CLA	C2A-C1A-CHA	2.35	127.98	123.86
18	a6	401	BCR	C34-C9-C10	-2.35	119.62	122.92
18	bL	201	BCR	C15-C14-C13	-2.35	123.95	127.31
15	bA	831	CLA	C3B-C4B-NB	-2.35	108.33	110.52
15	b1	410	CLA	C3B-C4B-NB	-2.35	108.33	110.52
15	b2	414	CLA	CHC-C4B-NB	2.35	126.75	124.26
15	b5	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	cB	810	CLA	C2B-C1B-NB	-2.35	108.65	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b6	401	BCR	C27-C26-C25	2.35	126.15	122.73
15	b2	413	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	c1	408	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	c3	412	CLA	C3B-C4B-NB	-2.35	108.33	110.52
16	bA	846	PQN	C21-C20-C18	-2.35	108.31	115.92
15	c2	411	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	a6	413	CLA	C3B-C4B-NB	-2.35	108.33	110.52
18	c6	403	BCR	C24-C23-C22	-2.35	122.68	126.23
15	c1	409	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	b2	416	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	bA	833	CLA	CMB-C2B-C3B	2.35	132.28	126.59
15	a3	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
16	aA	846	PQN	C21-C20-C18	-2.35	108.32	115.92
15	a2	407	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	cB	808	CLA	CAC-C3C-C4C	2.35	127.86	124.81
18	bL	205	BCR	C39-C30-C25	2.35	114.11	110.30
15	bB	841	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	aB	829	CLA	CHC-C4B-NB	2.35	126.75	124.26
15	bA	819	CLA	CHB-C1B-NB	2.35	126.75	124.26
15	b1	406	CLA	CHC-C4B-NB	2.35	126.75	124.26
15	aX	102	CLA	O1A-CGA-CBA	2.35	130.63	123.08
15	aB	821	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	bB	821	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	a5	415	CLA	O2A-CGA-O1A	-2.35	117.44	123.30
15	b1	409	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	bB	814	CLA	CHD-C1D-ND	-2.35	122.29	124.45
15	b2	402	CLA	CHC-C4B-NB	2.35	126.75	124.26
18	cA	848	BCR	C11-C10-C9	-2.35	123.96	127.31
18	aB	845	BCR	C7-C8-C9	-2.35	122.68	126.23
15	a2	413	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	b5	403	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	a4	415	CLA	C3B-C4B-NB	-2.35	108.33	110.52
15	c4	421	CLA	CHA-C4D-ND	2.35	137.41	132.50
15	cA	820	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	c2	418	CLA	CHB-C1B-NB	2.35	126.74	124.26
15	a5	413	CLA	C2D-C1D-ND	-2.35	108.37	110.10
15	a3	412	CLA	CHA-C1A-NA	-2.35	121.02	126.40
15	aB	824	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	cB	828	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	a2	410	CLA	CHB-C1B-NB	2.35	126.74	124.26
15	c5	416	CLA	C2A-C1A-CHA	2.35	127.97	123.86
15	bL	204	CLA	CHB-C4A-NA	2.35	127.76	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b3	401	BCR	C24-C23-C22	-2.35	122.69	126.23
15	c2	416	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
15	cA	831	CLA	CMB-C2B-C3B	2.35	132.27	126.59
15	bA	807	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	bB	839	CLA	C3A-C2A-C1A	2.35	104.86	101.34
15	aA	827	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
15	cB	821	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	c1	405	CLA	CMA-C3A-C2A	-2.35	104.36	113.83
15	cX	102	CLA	O1A-CGA-CBA	2.35	130.62	123.08
15	b3	412	CLA	C2A-C1A-CHA	2.35	127.96	123.86
18	a3	419	BCR	C3-C4-C5	-2.35	109.89	114.08
15	aB	827	CLA	CMB-C2B-C3B	2.35	132.27	126.59
18	b3	419	BCR	C27-C26-C25	2.35	126.14	122.73
15	b3	412	CLA	CHB-C4A-NA	2.35	127.76	124.51
15	bB	817	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	c2	418	CLA	C2A-C1A-CHA	2.35	127.96	123.86
15	cA	827	CLA	CAA-C2A-C3A	-2.35	106.36	112.78
15	b5	415	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
15	aL	203	CLA	CHB-C4A-NA	2.35	127.75	124.51
15	c3	412	CLA	CHB-C4A-NA	2.35	127.75	124.51
18	a4	420	BCR	C15-C16-C17	-2.35	118.67	123.47
15	bB	824	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
15	b1	412	CLA	CMC-C2C-C3C	2.34	132.48	126.12
15	bA	835	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	cB	804	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	c5	411	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	a5	420	CLA	CHA-C1A-NA	-2.34	121.03	126.40
15	b2	416	CLA	CBA-CAA-C2A	2.34	120.78	113.86
15	c3	416	CLA	C2A-C1A-CHA	2.34	127.96	123.86
15	bA	844	CLA	CHD-C1D-ND	-2.34	122.30	124.45
15	bX	102	CLA	O1A-CGA-CBA	2.34	130.61	123.08
15	cA	802	CLA	C11-C10-C8	-2.34	108.34	115.92
15	c6	412	CLA	C1D-ND-C4D	2.34	108.00	106.33
15	bB	808	CLA	CAC-C3C-C4C	2.34	127.85	124.81
15	b6	407	CLA	CHC-C4B-NB	2.34	126.74	124.26
15	a1	409	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	b3	407	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
15	aB	804	CLA	C2C-C1C-NC	-2.34	107.78	109.97
15	bA	827	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
15	bA	802	CLA	C11-C10-C8	-2.34	108.35	115.92
15	cA	806	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
15	cB	841	CLA	CMB-C2B-C1B	-2.34	121.80	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	827	CLA	CMB-C2B-C3B	2.34	132.26	126.59
15	a3	415	CLA	O2A-CGA-O1A	-2.34	117.46	123.30
15	b3	415	CLA	CBA-CAA-C2A	2.34	120.78	113.86
15	c2	404	CLA	CHC-C4B-NB	2.34	126.74	124.26
15	b1	412	CLA	C1D-ND-C4D	2.34	108.00	106.33
18	b6	420	BCR	C24-C23-C22	-2.34	122.70	126.23
15	cA	821	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
14	bA	801	CL0	CHB-C1B-NB	-2.34	121.78	124.26
15	a3	407	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
15	cB	839	CLA	C3A-C2A-C1A	2.34	104.85	101.34
15	aA	820	CLA	C2A-C1A-CHA	2.34	127.95	123.86
15	a1	410	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	cA	808	CLA	C3B-C4B-NB	-2.34	108.34	110.52
18	b5	419	BCR	C15-C16-C17	-2.34	118.68	123.47
18	c1	420	BCR	C15-C16-C17	-2.34	118.68	123.47
15	b6	417	CLA	C2A-C1A-CHA	2.34	127.95	123.86
15	bA	812	CLA	CHB-C1B-NB	2.34	126.73	124.26
15	bB	810	CLA	C2B-C1B-NB	-2.34	108.66	110.23
15	bB	826	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	cB	810	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	c3	411	CLA	C3B-C4B-NB	-2.34	108.34	110.52
15	cA	828	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
15	c2	406	CLA	C11-C10-C8	-2.34	108.36	115.92
15	b5	420	CLA	CHA-C1A-NA	-2.34	121.04	126.40
15	aB	827	CLA	O2D-CGD-CBD	2.34	115.43	111.27
15	cB	804	CLA	C2C-C1C-NC	-2.34	107.78	109.97
18	b1	420	BCR	C15-C16-C17	-2.34	118.68	123.47
14	cA	801	CL0	CHB-C1B-NB	-2.34	121.78	124.26
15	c1	403	CLA	CHB-C1B-NB	2.34	126.73	124.26
15	c5	417	CLA	CHB-C1B-NB	2.34	126.73	124.26
18	bA	850	BCR	C11-C10-C9	-2.34	123.97	127.31
15	a2	418	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
15	a6	417	CLA	C2A-C1A-CHA	2.34	127.95	123.86
15	aA	845	CLA	CMC-C2C-C3C	2.34	132.47	126.12
15	bL	204	CLA	CHB-C1B-NB	2.34	126.73	124.26
18	a1	418	BCR	C27-C26-C25	2.34	126.12	122.73
15	c5	412	CLA	CHB-C4A-NA	2.34	127.74	124.51
18	a5	419	BCR	C3-C4-C5	-2.34	109.90	114.08
15	c1	410	CLA	C3B-C4B-NB	-2.34	108.35	110.52
15	cB	805	CLA	CHB-C1B-NB	2.34	126.73	124.26
15	c3	404	CLA	CHB-C1B-NB	2.34	126.73	124.26
15	bA	842	CLA	O2D-CGD-CBD	2.34	115.42	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	813	CLA	CHB-C4A-NA	2.34	127.74	124.51
15	cA	838	CLA	C1-C2-C3	-2.34	122.00	126.04
15	cA	807	CLA	C2A-C1A-CHA	2.34	127.94	123.86
15	cB	818	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
15	bA	845	CLA	CMC-C2C-C3C	2.34	132.46	126.12
15	a1	404	CLA	CMA-C3A-C2A	-2.33	104.41	113.83
15	c4	414	CLA	C3B-C4B-NB	-2.33	108.35	110.52
15	aA	838	CLA	C1-C2-C3	-2.33	122.00	126.04
15	a4	417	CLA	CMA-C3A-C2A	-2.33	104.41	113.83
15	aA	815	CLA	C2D-C1D-ND	-2.33	108.38	110.10
15	bB	832	CLA	C2D-C1D-ND	-2.33	108.38	110.10
15	cB	834	CLA	C2A-C1A-CHA	2.33	127.94	123.86
15	c6	409	CLA	C3B-C4B-NB	-2.33	108.35	110.52
18	cI	102	BCR	C3-C4-C5	-2.33	109.91	114.08
15	aB	837	CLA	CMB-C2B-C3B	2.33	132.24	126.59
15	bA	831	CLA	CMB-C2B-C3B	2.33	132.24	126.59
15	bA	828	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
18	c1	420	BCR	C3-C4-C5	-2.33	109.91	114.08
15	a5	406	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
15	bA	806	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
15	cB	837	CLA	CMB-C2B-C3B	2.33	132.24	126.59
15	c1	411	CLA	C3B-C4B-NB	-2.33	108.35	110.52
15	c2	405	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
15	bB	828	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
15	c3	415	CLA	CBA-CAA-C2A	2.33	120.75	113.86
15	aA	831	CLA	CMB-C2B-C3B	2.33	132.24	126.59
15	a2	416	CLA	O2A-CGA-O1A	-2.33	117.49	123.30
15	a3	417	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
15	cL	203	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	c2	414	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	cB	827	CLA	O2D-CGD-CBD	2.33	115.41	111.27
18	a4	419	BCR	C27-C26-C25	2.33	126.11	122.73
15	bL	203	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	bB	829	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	b1	405	CLA	CHB-C1B-NB	2.33	126.72	124.26
15	b4	404	CLA	CHB-C1B-NB	2.33	126.72	124.26
15	c2	405	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
15	aL	202	CLA	C3A-C2A-C1A	2.33	104.83	101.34
15	cA	844	CLA	CMC-C2C-C3C	2.33	132.44	126.12
15	cB	827	CLA	CMB-C2B-C3B	2.33	132.23	126.59
15	a5	413	CLA	C3B-C4B-NB	-2.33	108.35	110.52
15	b1	411	CLA	C3B-C4B-NB	-2.33	108.35	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	819	CLA	CHB-C1B-NB	2.33	126.72	124.26
15	cL	204	CLA	CHB-C4A-NA	2.33	127.73	124.51
15	c3	415	CLA	O2A-CGA-O1A	-2.33	117.50	123.30
15	a6	407	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	a2	406	CLA	C11-C10-C8	-2.33	108.39	115.92
15	a3	412	CLA	C1D-ND-C4D	2.33	107.99	106.33
15	bB	827	CLA	CMB-C2B-C3B	2.33	132.23	126.59
15	a3	412	CLA	C2A-C1A-CHA	2.33	127.93	123.86
15	cB	817	CLA	C2A-C1A-CHA	2.33	127.93	123.86
18	c6	421	BCR	C24-C23-C22	-2.33	122.72	126.23
18	b5	401	BCR	C35-C13-C14	-2.33	119.66	122.92
15	aB	819	CLA	C3B-C4B-NB	-2.33	108.36	110.52
15	aB	826	CLA	C3B-C4B-NB	-2.33	108.36	110.52
18	c3	420	BCR	C15-C16-C17	-2.33	118.71	123.47
15	c5	420	CLA	CHA-C1A-NA	-2.33	121.07	126.40
15	b3	402	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	a6	418	CLA	CHD-C1D-ND	-2.33	122.32	124.45
15	b3	407	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	c2	422	CLA	CHC-C4B-NB	2.33	126.72	124.26
15	aA	828	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
15	bA	845	CLA	CHD-C1D-ND	-2.33	122.32	124.45
15	c3	412	CLA	C2A-C1A-CHA	2.32	127.92	123.86
15	cF	203	CLA	CAC-C3C-C4C	2.32	127.83	124.81
15	c6	419	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	b2	412	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
15	bB	827	CLA	O2D-CGD-CBD	2.32	115.40	111.27
15	b3	415	CLA	C3B-C4B-NB	-2.32	108.36	110.52
15	a4	405	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
15	c4	402	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
15	c2	418	CLA	CHB-C1B-C2B	-2.32	120.67	127.24
15	cF	201	CLA	O2D-CGD-CBD	2.32	115.40	111.27
15	a3	403	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	c5	419	BCR	C15-C16-C17	-2.32	118.72	123.47
15	b2	418	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
15	aB	839	CLA	C3A-C2A-C1A	2.32	104.82	101.34
15	b1	417	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
15	cA	844	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	c1	417	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
15	b3	410	CLA	CHB-C1B-NB	2.32	126.72	124.26
15	b4	413	CLA	C2D-C1D-ND	-2.32	108.39	110.10
15	c1	417	CLA	C3A-C2A-C1A	2.32	104.82	101.34
18	b3	420	BCR	C15-C16-C17	-2.32	118.72	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	845	CLA	CMC-C2C-C1C	-2.32	121.50	125.04
15	b5	406	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
15	c4	405	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
15	bA	807	CLA	CHB-C1B-NB	2.32	126.71	124.26
15	b3	404	CLA	CHB-C1B-NB	2.32	126.71	124.26
15	cL	203	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	a5	419	BCR	C15-C16-C17	-2.32	118.72	123.47
15	b6	410	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
15	b5	413	CLA	C2D-C1D-ND	-2.32	108.39	110.10
15	bA	802	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	cA	807	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	c4	419	BCR	C27-C26-C25	2.32	126.10	122.73
15	a2	411	CLA	C2A-C1A-CHA	2.32	127.92	123.86
15	b1	417	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	bI	101	BCR	C1-C6-C5	-2.32	119.35	122.61
15	c6	411	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
15	b2	418	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	cA	825	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	bA	829	CLA	C3B-C4B-NB	-2.32	108.36	110.52
18	a1	419	BCR	C1-C6-C5	-2.32	119.35	122.61
18	b1	419	BCR	C27-C26-C25	2.32	126.10	122.73
15	bB	818	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
15	b2	410	CLA	CHC-C4B-NB	2.32	126.71	124.26
18	b5	419	BCR	C3-C4-C5	-2.32	109.94	114.08
15	aA	825	CLA	CHD-C1D-ND	-2.32	122.32	124.45
15	a4	407	CLA	CHA-C1A-NA	-2.32	121.09	126.40
18	a6	420	BCR	C24-C23-C22	-2.32	122.73	126.23
15	aB	840	CLA	CAC-C3C-C2C	-2.32	123.56	127.53
15	cB	826	CLA	C3B-C4B-NB	-2.32	108.36	110.52
15	c2	408	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
15	bA	838	CLA	C1-C2-C3	-2.32	122.03	126.04
15	c1	412	CLA	CHA-C1A-NA	-2.32	121.09	126.40
15	a5	416	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	b3	417	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	b2	408	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
15	c4	406	CLA	O2A-CGA-O1A	-2.32	117.52	123.30
15	bF	201	CLA	CAC-C3C-C4C	2.32	127.82	124.81
15	a2	416	CLA	C3B-C4B-NB	-2.32	108.37	110.52
15	bB	805	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
15	c1	417	CLA	C2D-C1D-ND	-2.32	108.40	110.10
15	c1	403	CLA	C2A-C1A-CHA	2.32	127.91	123.86
15	aA	802	CLA	CHD-C1D-ND	-2.32	122.33	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a1	411	CLA	CHA-C1A-NA	-2.32	121.09	126.40
15	aB	818	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
15	bB	831	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
15	cB	840	CLA	C3B-C4B-NB	-2.32	108.37	110.52
15	aA	831	CLA	CHC-C4B-NB	2.32	126.71	124.26
15	aA	842	CLA	O2D-CGD-CBD	2.32	115.38	111.27
14	aA	801	CL0	C1-O2A-CGA	2.31	122.52	116.44
15	cB	813	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	bB	837	CLA	CMB-C2B-C3B	2.31	132.19	126.59
15	cB	805	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
18	aB	849	BCR	C16-C15-C14	-2.31	118.73	123.47
15	a1	416	CLA	CHB-C1B-C2B	-2.31	120.70	127.24
15	c2	413	CLA	C3B-C4B-NB	-2.31	108.37	110.52
15	cB	831	CLA	O2A-CGA-O1A	-2.31	117.53	123.30
15	a2	416	CLA	CBA-CAA-C2A	2.31	120.69	113.86
15	b2	418	CLA	CHD-C1D-ND	-2.31	122.33	124.45
15	bB	840	CLA	CAC-C3C-C2C	-2.31	123.57	127.53
18	b4	401	BCR	C15-C14-C13	-2.31	124.01	127.31
18	bF	202	BCR	C34-C9-C10	-2.31	119.68	122.92
15	a2	412	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
15	c1	414	CLA	C3B-C4B-NB	-2.31	108.37	110.52
15	aB	817	CLA	C2A-C1A-CHA	2.31	127.90	123.86
15	aB	805	CLA	CHB-C1B-NB	2.31	126.70	124.26
15	cA	825	CLA	CHB-C1B-NB	2.31	126.70	124.26
15	c3	405	CLA	CHB-C1B-NB	2.31	126.70	124.26
15	b1	415	CLA	C3B-C4B-NB	-2.31	108.37	110.52
14	bA	801	CL0	CMC-C2C-C1C	2.31	128.56	125.04
15	aB	828	CLA	CMB-C2B-C3B	2.31	132.18	126.59
15	aB	805	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
15	bB	831	CLA	O2A-CGA-O1A	-2.31	117.54	123.30
18	c6	402	BCR	C34-C9-C10	-2.31	119.69	122.92
15	aB	840	CLA	C3B-C4B-NB	-2.31	108.37	110.52
15	a3	412	CLA	C3B-C4B-NB	-2.31	108.37	110.52
18	bB	846	BCR	C30-C25-C26	-2.31	119.36	122.61
15	a2	410	CLA	CHC-C4B-NB	2.31	126.70	124.26
15	a3	410	CLA	CHB-C1B-NB	2.31	126.70	124.26
15	c5	406	CLA	CHC-C4B-NB	2.31	126.70	124.26
14	aA	801	CL0	CMC-C2C-C1C	2.31	128.56	125.04
15	bB	828	CLA	CMB-C2B-C3B	2.31	132.18	126.59
15	a2	402	CLA	CHC-C4B-NB	2.31	126.70	124.26
15	a4	404	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	c4	420	BCR	C15-C16-C17	-2.31	118.75	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aJ	204	BCR	C33-C5-C6	-2.31	121.94	124.53
15	a3	415	CLA	C3B-C4B-NB	-2.31	108.37	110.52
15	b2	415	CLA	C3B-C4B-NB	-2.31	108.37	110.52
18	a4	418	BCR	C7-C8-C9	-2.31	122.75	126.23
18	b4	419	BCR	C27-C26-C25	2.31	126.08	122.73
15	b4	409	CLA	CHC-C4B-NB	2.31	126.70	124.26
18	bB	848	BCR	C7-C8-C9	-2.31	122.75	126.23
18	aI	102	BCR	C3-C4-C5	-2.31	109.96	114.08
18	cA	849	BCR	C40-C30-C25	2.31	114.04	110.30
15	b4	407	CLA	CHA-C1A-NA	-2.31	121.12	126.40
15	cF	203	CLA	O2A-CGA-O1A	-2.31	117.55	123.30
15	a2	403	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b1	412	CLA	CHA-C1A-NA	-2.30	121.12	126.40
15	b5	411	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	a5	403	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b2	411	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	b4	412	CLA	C2A-C1A-CHA	2.30	127.89	123.86
15	aA	830	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
15	cB	828	CLA	CMB-C2B-C3B	2.30	132.17	126.59
15	aB	831	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	cB	831	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	a1	416	CLA	C3A-C2A-C1A	2.30	104.79	101.34
15	aB	831	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
15	c4	412	CLA	C2A-C1A-CHA	2.30	127.89	123.86
14	bA	801	CL0	C1-O2A-CGA	2.30	122.48	116.44
15	b4	410	CLA	C2A-C1A-CHA	2.30	127.89	123.86
18	aI	101	BCR	C1-C6-C5	-2.30	119.37	122.61
15	a2	405	CLA	CMA-C3A-C2A	-2.30	104.54	113.83
15	cA	829	CLA	C3B-C4B-NB	-2.30	108.38	110.52
18	a6	401	BCR	C27-C26-C25	2.30	126.07	122.73
15	cB	824	CLA	C3B-C4B-NB	-2.30	108.38	110.52
15	c2	413	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	c1	415	CLA	CBA-CAA-C2A	2.30	120.65	113.86
14	cA	801	CL0	CMC-C2C-C1C	2.30	128.54	125.04
15	b3	405	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
15	c5	412	CLA	C3B-C4B-NB	-2.30	108.38	110.52
18	cF	202	BCR	C40-C30-C25	2.30	114.03	110.30
18	a4	401	BCR	C15-C14-C13	-2.30	124.03	127.31
18	b3	401	BCR	C2-C1-C6	2.30	114.02	110.48
15	a5	412	CLA	C3B-C4B-NB	-2.30	108.38	110.52
15	a6	410	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
18	c2	421	BCR	C35-C13-C14	-2.30	119.70	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	410	CLA	C2A-C1A-CHA	2.30	127.88	123.86
18	cI	101	BCR	C1-C6-C5	-2.30	119.38	122.61
15	bA	837	CLA	O2A-CGA-O1A	-2.30	117.57	123.30
15	aA	814	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
15	a3	410	CLA	C2A-C1A-CHA	2.30	127.88	123.86
15	b5	417	CLA	CHB-C1B-NB	2.30	126.69	124.26
15	a1	414	CLA	CBA-CAA-C2A	2.30	120.64	113.86
18	cB	849	BCR	C16-C15-C14	-2.30	118.77	123.47
15	aB	813	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	aJ	201	CLA	O2A-CGA-O1A	-2.30	117.58	123.30
15	a5	417	CLA	CHB-C1B-NB	2.30	126.69	124.26
15	bA	845	CLA	CMC-C2C-C1C	-2.30	121.54	125.04
15	bA	830	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
15	a1	402	CLA	CHB-C1B-NB	2.30	126.69	124.26
15	bA	838	CLA	CHB-C1B-NB	2.30	126.69	124.26
15	c1	405	CLA	O1D-CGD-CBD	2.30	129.18	124.48
15	c5	406	CLA	CMB-C2B-C1B	-2.29	121.87	125.37
15	c4	407	CLA	CHA-C1A-NA	-2.29	121.14	126.40
15	cA	830	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
18	a4	420	BCR	C3-C4-C5	-2.29	109.98	114.08
15	aA	802	CLA	C4D-C3D-CAD	-2.29	105.39	108.10
18	a5	401	BCR	C35-C13-C14	-2.29	119.71	122.92
15	cA	813	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
15	bB	835	CLA	CAA-C2A-C1A	2.29	119.49	111.97
15	bB	810	CLA	C3B-C4B-NB	-2.29	108.39	110.52
14	cA	801	CL0	C1-O2A-CGA	2.29	122.46	116.44
15	c5	412	CLA	CHC-C1C-NC	2.29	127.68	124.20
18	bB	849	BCR	C40-C30-C25	2.29	114.02	110.30
15	a4	406	CLA	O2A-CGA-O1A	-2.29	117.59	123.30
15	b4	405	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
18	c3	419	BCR	C27-C26-C25	2.29	126.06	122.73
18	cB	846	BCR	C30-C25-C26	-2.29	119.39	122.61
18	c1	420	BCR	C1-C6-C5	-2.29	119.39	122.61
18	c3	401	BCR	C2-C1-C6	2.29	114.01	110.48
18	bB	850	BCR	C30-C25-C26	-2.29	119.39	122.61
15	c4	411	CLA	C3B-C4B-NB	-2.29	108.39	110.52
18	bB	850	BCR	C16-C15-C14	-2.29	118.78	123.47
15	a3	417	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	a5	415	CLA	CHB-C1B-NB	2.29	126.68	124.26
15	c4	417	CLA	CMA-C3A-C2A	-2.29	104.59	113.83
15	bB	815	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	a3	419	BCR	C27-C26-C25	2.29	126.05	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	804	CLA	C2C-C1C-NC	-2.29	107.83	109.97
18	bA	851	BCR	C40-C30-C25	2.29	114.01	110.30
15	aB	810	CLA	C3B-C4B-NB	-2.29	108.39	110.52
15	cB	835	CLA	CAA-C2A-C1A	2.29	119.47	111.97
15	c5	410	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	cB	840	CLA	CHC-C4B-NB	2.29	126.68	124.26
15	bA	818	CLA	CMB-C2B-C3B	2.29	132.13	126.59
15	cA	807	CLA	CHA-C1A-NA	-2.29	121.16	126.40
18	cF	204	BCR	C34-C9-C10	-2.29	119.72	122.92
15	aB	834	CLA	C2A-C1A-CHA	2.29	127.86	123.86
15	aA	819	CLA	CHB-C1B-NB	2.29	126.68	124.26
15	a6	416	CLA	CHB-C1B-NB	2.29	126.68	124.26
15	cB	840	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	b6	401	BCR	C34-C9-C10	-2.29	119.72	122.92
15	a4	413	CLA	C2D-C1D-ND	-2.29	108.42	110.10
15	aB	835	CLA	CAA-C2A-C1A	2.29	119.47	111.97
15	c6	405	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	a6	421	BCR	C7-C8-C9	-2.29	122.78	126.23
15	a3	405	CLA	CMB-C2B-C1B	-2.29	121.89	125.37
15	cB	806	CLA	C2D-C1D-ND	-2.29	108.42	110.10
15	bA	807	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	b4	411	CLA	C3B-C4B-NB	-2.28	108.40	110.52
15	c5	414	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	aB	841	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
15	a1	402	CLA	C2A-C1A-CHA	2.28	127.85	123.86
18	a3	401	BCR	C2-C1-C6	2.28	114.00	110.48
18	cJ	103	BCR	C33-C5-C6	-2.28	121.96	124.53
15	cA	838	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	b4	410	CLA	C3B-C4B-NB	-2.28	108.40	110.52
15	c6	409	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
15	b3	407	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	cB	840	CLA	CAC-C3C-C2C	-2.28	123.62	127.53
15	aA	837	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
15	a6	411	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	b1	412	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	b5	405	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
15	b2	422	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	c4	421	CLA	CHC-C4B-NB	2.28	126.67	124.26
15	b2	405	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
15	c6	415	CLA	CAC-C3C-C4C	2.28	127.77	124.81
15	bB	834	CLA	C2A-C1A-CHA	2.28	127.85	123.86
15	c1	407	CLA	C3B-C4B-NB	-2.28	108.40	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	417	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
15	a2	416	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	b3	403	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	aA	813	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
15	b5	411	CLA	C3B-C4B-NB	-2.28	108.40	110.52
15	a5	414	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	a5	407	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
15	bB	806	CLA	C2D-C1D-ND	-2.28	108.42	110.10
15	c4	415	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	b1	405	CLA	CMA-C3A-C2A	-2.28	104.64	113.83
18	aB	848	BCR	C7-C8-C9	-2.28	122.80	126.23
15	cB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	bB	841	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
15	a3	415	CLA	CHA-C4D-ND	2.28	137.26	132.50
18	aB	846	BCR	C30-C25-C26	-2.28	119.41	122.61
15	bB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	bA	835	CLA	C3C-C4C-NC	-2.28	108.02	110.57
15	c5	404	CLA	CHB-C1B-NB	2.28	126.67	124.26
15	aB	830	CLA	C7-C6-C5	-2.28	107.18	113.36
15	a4	412	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	b4	412	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	a4	402	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
15	b2	402	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
15	b5	413	CLA	C3B-C4B-NB	-2.27	108.41	110.52
15	a1	416	CLA	C2A-C1A-CHA	2.27	127.84	123.86
15	c1	409	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
15	b5	406	CLA	CHC-C4B-NB	2.27	126.66	124.26
15	b4	406	CLA	O2A-CGA-O1A	-2.27	117.63	123.30
18	b4	420	BCR	C3-C4-C5	-2.27	110.02	114.08
15	bA	813	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
15	cA	818	CLA	CMB-C2B-C3B	2.27	132.09	126.59
15	c2	416	CLA	CBA-CAA-C2A	2.27	120.57	113.86
15	aB	815	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	cB	848	BCR	C7-C8-C9	-2.27	122.80	126.23
15	cA	812	CLA	O1D-CGD-CBD	2.27	129.13	124.48
18	b6	419	BCR	C38-C26-C27	-2.27	109.25	113.62
15	aB	840	CLA	CHC-C4B-NB	2.27	126.66	124.26
15	cA	824	CLA	CHB-C1B-NB	2.27	126.66	124.26
15	aA	832	CLA	C1-C2-C3	-2.27	123.08	126.75
15	aA	818	CLA	CMB-C2B-C3B	2.27	132.09	126.59
15	c2	409	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
15	b2	414	CLA	C3B-C4B-NB	-2.27	108.41	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	417	CLA	C2A-C1A-CHA	2.27	127.83	123.86
15	cA	829	CLA	C3A-C2A-C1A	2.27	104.74	101.34
15	a2	415	CLA	C3B-C4B-NB	-2.27	108.41	110.52
15	bB	805	CLA	C3B-C4B-NB	-2.27	108.41	110.52
15	a2	418	CLA	CHD-C1D-ND	-2.27	122.37	124.45
15	c1	416	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
15	aA	840	CLA	CMB-C2B-C3B	2.27	132.09	126.59
15	aA	835	CLA	C3C-C4C-NC	-2.27	108.03	110.57
15	aA	807	CLA	CHA-C1A-NA	-2.27	121.20	126.40
15	b3	415	CLA	CHA-C4D-ND	2.27	137.25	132.50
15	cB	815	CLA	CHB-C1B-NB	2.27	126.66	124.26
15	bF	201	CLA	O2A-CGA-O1A	-2.27	117.64	123.30
18	aA	850	BCR	C40-C30-C25	2.27	113.98	110.30
18	aF	201	BCR	C40-C30-C25	2.27	113.98	110.30
15	bA	814	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
15	a5	405	CLA	CHC-C1C-NC	2.27	127.64	124.20
18	b2	421	BCR	C35-C13-C14	-2.27	119.75	122.92
15	b4	417	CLA	CMA-C3A-C2A	-2.27	104.68	113.83
15	a1	408	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
18	bI	102	BCR	C11-C10-C9	-2.27	124.07	127.31
15	b1	405	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
15	cA	825	CLA	CHC-C4B-NB	2.27	126.66	124.26
15	c4	409	CLA	CHC-C4B-NB	2.27	126.66	124.26
15	cA	844	CLA	CMC-C2C-C1C	-2.27	121.59	125.04
15	a3	402	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
15	c2	403	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	bA	812	CLA	O1D-CGD-CBD	2.27	129.12	124.48
15	bA	823	CLA	CHC-C4B-NB	2.27	126.66	124.26
15	bB	840	CLA	CHB-C1B-NB	2.27	126.66	124.26
15	b3	409	CLA	CHB-C1B-NB	2.27	126.66	124.26
15	bB	817	CLA	CHA-C1A-NA	-2.27	121.21	126.40
18	c4	401	BCR	C15-C14-C13	-2.27	124.08	127.31
15	a4	412	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	b6	411	CLA	C2A-C1A-CHA	2.27	127.82	123.86
15	b5	405	CLA	CHC-C1C-NC	2.26	127.64	124.20
15	a6	408	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
15	a6	404	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	c4	417	CLA	C3A-C2A-C1A	2.26	104.73	101.34
15	aB	801	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
15	a4	405	CLA	CMA-C3A-C2A	-2.26	104.70	113.83
15	bA	803	CLA	C3B-C4B-NB	-2.26	108.42	110.52
15	bA	813	CLA	CHB-C4A-NA	2.26	127.64	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b3	413	CLA	C2D-C1D-ND	-2.26	108.44	110.10
15	aA	812	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	c5	409	CLA	CHC-C4B-NB	2.26	126.65	124.26
15	c3	417	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	cB	849	BCR	C30-C25-C26	-2.26	119.43	122.61
18	bJ	105	BCR	C31-C1-C6	2.26	113.97	110.30
18	bL	201	BCR	C40-C30-C25	2.26	113.97	110.30
15	cB	819	CLA	C4-C3-C5	2.26	119.08	115.27
18	a6	419	BCR	C38-C26-C27	-2.26	109.27	113.62
15	cA	822	CLA	C16-C15-C13	-2.26	108.61	115.92
15	b5	410	CLA	C1D-ND-C4D	2.26	107.94	106.33
15	cA	814	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
15	a3	417	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
15	b5	407	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
15	cB	805	CLA	C3B-C4B-NB	-2.26	108.42	110.52
15	b6	416	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	cA	812	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	cB	805	CLA	CMB-C2B-C3B	2.26	132.06	126.59
15	a6	407	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
15	aA	813	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	aA	829	CLA	C3A-C2A-C1A	2.26	104.73	101.34
15	aB	805	CLA	CMB-C2B-C3B	2.26	132.06	126.59
18	cF	205	BCR	C31-C1-C6	2.26	113.97	110.30
15	b6	408	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
15	aB	830	CLA	CHC-C4B-NB	2.26	126.65	124.26
15	a3	415	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	a4	409	CLA	CHC-C4B-NB	2.26	126.65	124.26
15	cA	839	CLA	C6-C7-C8	-2.26	108.61	115.92
15	b1	409	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
15	c6	412	CLA	C2A-C1A-CHA	2.26	127.81	123.86
15	aA	803	CLA	C3B-C4B-NB	-2.26	108.42	110.52
15	a4	412	CLA	C3B-C4B-NB	-2.26	108.42	110.52
18	cB	847	BCR	C35-C13-C12	2.26	119.59	114.60
15	c3	415	CLA	CHA-C4D-ND	2.26	137.22	132.50
15	bA	825	CLA	CHC-C4B-NB	2.26	126.65	124.26
15	cA	837	CLA	O2A-CGA-O1A	-2.26	117.67	123.30
15	aA	835	CLA	C3B-C4B-NB	-2.26	108.42	110.52
15	c6	410	CLA	C3B-C4B-NB	-2.26	108.42	110.52
18	aB	847	BCR	C35-C13-C12	2.26	119.59	114.60
18	b3	420	BCR	C3-C4-C5	-2.26	110.05	114.08
15	cA	840	CLA	CMB-C2B-C3B	2.26	132.06	126.59
15	cA	802	CLA	CHD-C1D-ND	-2.26	122.38	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	812	CLA	O1D-CGD-CBD	2.26	129.10	124.48
18	aI	102	BCR	C11-C10-C9	-2.26	124.09	127.31
15	b5	409	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
15	bA	829	CLA	C3A-C2A-C1A	2.26	104.72	101.34
15	aB	810	CLA	C2B-C1B-NB	-2.26	108.72	110.23
15	aB	840	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	a3	409	CLA	CHC-C4B-NB	2.26	126.65	124.26
15	b1	409	CLA	CHB-C1B-NB	2.26	126.65	124.26
15	c1	404	CLA	CHB-C1B-NB	2.26	126.65	124.26
18	aL	205	BCR	C40-C30-C25	2.26	113.96	110.30
15	b6	411	CLA	CHA-C1A-NA	-2.26	121.23	126.40
15	bB	805	CLA	CMB-C2B-C3B	2.26	132.05	126.59
15	cA	833	CLA	CHB-C1B-NB	2.26	126.64	124.26
19	cA	852	LHG	O8-C23-O10	-2.26	117.90	123.59
15	bA	840	CLA	CMB-C2B-C3B	2.26	132.05	126.59
15	b5	410	CLA	C2A-C1A-CHA	2.25	127.80	123.86
15	aA	825	CLA	CHC-C4B-NB	2.25	126.64	124.26
15	cB	801	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	a6	411	CLA	CHA-C1A-NA	-2.25	121.23	126.40
15	b3	402	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
18	aF	203	BCR	C31-C1-C6	2.25	113.95	110.30
15	a3	407	CLA	CHA-C1A-NA	-2.25	121.24	126.40
15	c1	415	CLA	C3B-C4B-NB	-2.25	108.42	110.52
15	c4	410	CLA	C3B-C4B-NB	-2.25	108.42	110.52
15	bJ	102	CLA	C2D-C1D-ND	-2.25	108.44	110.10
15	bA	824	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	c2	410	CLA	CHC-C4B-NB	2.25	126.64	124.26
15	c3	407	CLA	CHC-C4B-NB	2.25	126.64	124.26
15	a5	412	CLA	C1D-ND-C4D	2.25	107.94	106.33
15	c5	409	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
18	a2	421	BCR	C24-C23-C22	-2.25	122.83	126.23
15	a5	410	CLA	CMB-C2B-C3B	2.25	132.04	126.59
18	c4	420	BCR	C3-C4-C5	-2.25	110.05	114.08
18	aF	202	BCR	C34-C9-C10	-2.25	119.77	122.92
15	b3	414	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	c4	406	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
18	cJ	104	BCR	C24-C23-C22	-2.25	122.83	126.23
15	cB	817	CLA	CHA-C1A-NA	-2.25	121.24	126.40
18	aB	849	BCR	C30-C25-C26	-2.25	119.44	122.61
15	aB	817	CLA	CHA-C1A-NA	-2.25	121.24	126.40
15	b6	406	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
15	aA	821	CLA	CMC-C2C-C3C	2.25	132.23	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	837	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	cA	823	CLA	CHC-C4B-NB	2.25	126.64	124.26
15	bA	805	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
15	bB	812	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	cB	833	CLA	C16-C17-C18	-2.25	105.38	115.98
15	aA	822	CLA	C16-C15-C13	-2.25	108.64	115.92
15	cA	832	CLA	C1-C2-C3	-2.25	123.11	126.75
15	aB	812	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	bL	204	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	bA	802	CLA	C4D-C3D-CAD	-2.25	105.44	108.10
15	c4	404	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	b3	417	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
15	aB	806	CLA	C2D-C1D-ND	-2.25	108.45	110.10
15	c5	410	CLA	CMB-C2B-C3B	2.25	132.04	126.59
18	bL	206	BCR	C40-C30-C25	2.25	113.95	110.30
18	cM	101	BCR	C16-C15-C14	-2.25	118.87	123.47
15	a5	410	CLA	C1D-ND-C4D	2.25	107.93	106.33
15	a1	411	CLA	C2A-C1A-CHA	2.25	127.79	123.86
15	c4	411	CLA	CHD-C1D-ND	-2.25	122.39	124.45
15	c2	408	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	aA	837	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	a3	409	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	c4	417	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	aL	203	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	c5	417	CLA	CHB-C1B-C2B	-2.25	120.89	127.24
18	b4	419	BCR	C3-C4-C5	-2.25	110.06	114.08
15	a5	411	CLA	C3B-C4B-NB	-2.25	108.43	110.52
15	a2	408	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	cB	803	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
15	cB	812	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
15	aA	833	CLA	CHB-C1B-NB	2.25	126.64	124.26
15	bB	840	CLA	CHC-C4B-NB	2.25	126.64	124.26
18	cA	850	BCR	C27-C26-C25	2.25	126.00	122.73
15	c3	407	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	aB	823	CLA	CMB-C2B-C3B	2.25	132.03	126.59
15	cB	823	CLA	CMB-C2B-C3B	2.25	132.03	126.59
15	bB	819	CLA	C4-C3-C5	2.25	119.05	115.27
15	bA	839	CLA	C6-C7-C8	-2.25	108.65	115.92
15	c3	405	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
19	aA	853	LHG	O8-C23-O10	-2.25	117.92	123.59
18	c4	418	BCR	C38-C26-C27	-2.25	109.30	113.62
15	c1	409	CLA	O2A-CGA-O1A	-2.25	117.92	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	bA	854	LHG	O8-C23-O10	-2.25	117.92	123.59
15	a5	409	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
15	cA	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
15	cB	826	CLA	OBD-CAD-C3D	2.25	133.93	128.52
15	bA	821	CLA	CMC-C2C-C3C	2.25	132.22	126.12
15	aB	803	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
15	a4	406	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
15	aB	819	CLA	C4-C3-C5	2.25	119.05	115.27
15	c1	412	CLA	C2A-C1A-CHA	2.25	127.79	123.86
15	cA	805	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
15	c5	409	CLA	CHB-C1B-NB	2.25	126.63	124.26
15	c6	417	CLA	CHB-C1B-NB	2.25	126.63	124.26
15	aB	804	CLA	CMD-C2D-C1D	-2.25	120.76	124.71
15	cA	821	CLA	CMC-C2C-C3C	2.25	132.21	126.12
15	bB	804	CLA	CMD-C2D-C1D	-2.24	120.76	124.71
18	bB	847	BCR	C35-C13-C12	2.24	119.56	114.60
15	cJ	102	CLA	C2D-C1D-ND	-2.24	108.45	110.10
15	bA	833	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	aJ	201	CLA	CAC-C3C-C4C	2.24	127.72	124.81
15	bB	823	CLA	CMB-C2B-C3B	2.24	132.02	126.59
15	b4	417	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
15	b2	408	CLA	CHA-C1A-NA	-2.24	121.26	126.40
15	bB	826	CLA	OBD-CAD-C3D	2.24	133.92	128.52
15	aA	839	CLA	C6-C7-C8	-2.24	108.67	115.92
15	aB	833	CLA	C16-C17-C18	-2.24	105.41	115.98
18	c5	418	BCR	C7-C8-C9	-2.24	122.84	126.23
15	b1	414	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	cA	837	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	aA	851	BCR	C27-C26-C25	2.24	125.99	122.73
15	aB	805	CLA	C3B-C4B-NB	-2.24	108.43	110.52
15	a4	410	CLA	C3B-C4B-NB	-2.24	108.43	110.52
15	cA	835	CLA	C3B-C4B-NB	-2.24	108.43	110.52
15	bB	830	CLA	CHC-C4B-NB	2.24	126.63	124.26
18	c4	419	BCR	C3-C4-C5	-2.24	110.07	114.08
15	bB	833	CLA	C16-C17-C18	-2.24	105.42	115.98
18	b5	401	BCR	C7-C8-C9	-2.24	122.85	126.23
15	bA	822	CLA	C16-C15-C13	-2.24	108.67	115.92
15	b6	413	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	c5	413	CLA	C3B-C4B-NB	-2.24	108.44	110.52
15	aB	826	CLA	OBD-CAD-C3D	2.24	133.91	128.52
18	cI	102	BCR	C11-C10-C9	-2.24	124.11	127.31
18	bM	101	BCR	C16-C15-C14	-2.24	118.88	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	415	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	cA	807	CLA	C2D-C1D-ND	-2.24	108.45	110.10
18	b5	418	BCR	C7-C8-C9	-2.24	122.85	126.23
15	b3	408	CLA	C3B-C4B-NB	-2.24	108.44	110.52
15	b4	413	CLA	C3B-C4B-NB	-2.24	108.44	110.52
18	bA	852	BCR	C27-C26-C25	2.24	125.98	122.73
15	a2	413	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	a5	417	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
15	b2	411	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	c2	411	CLA	C1D-ND-C4D	2.24	107.93	106.33
15	c6	412	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	c4	416	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	cA	835	CLA	C3C-C4C-NC	-2.24	108.06	110.57
15	a3	403	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	b4	402	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
15	bB	803	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
18	c5	401	BCR	C35-C13-C14	-2.24	119.79	122.92
15	c4	410	CLA	C2A-C1A-CHA	2.24	127.77	123.86
15	aA	838	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	c2	416	CLA	CHB-C1B-NB	2.24	126.63	124.26
15	c5	405	CLA	CHC-C1C-NC	2.24	127.60	124.20
15	a6	410	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
15	c3	417	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
15	aA	833	CLA	CHC-C4B-NB	2.24	126.62	124.26
15	a2	422	CLA	CHB-C1B-NB	2.24	126.62	124.26
15	a6	413	CLA	C1D-ND-C4D	2.24	107.92	106.33
15	aA	805	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
15	a1	414	CLA	CHB-C1B-NB	2.24	126.62	124.26
15	c3	403	CLA	CHB-C1B-NB	2.24	126.62	124.26
15	cB	841	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
18	bJ	103	BCR	C33-C5-C6	-2.24	122.02	124.53
18	aM	101	BCR	C15-C14-C13	-2.24	124.12	127.31
15	bA	825	CLA	CHD-C1D-ND	-2.24	122.40	124.45
18	cM	101	BCR	C27-C26-C25	2.24	125.98	122.73
15	a5	409	CLA	CHB-C1B-NB	2.23	126.62	124.26
18	c2	421	BCR	C24-C23-C22	-2.23	122.86	126.23
18	aM	101	BCR	C16-C15-C14	-2.23	118.90	123.47
18	aI	102	BCR	C27-C26-C25	2.23	125.97	122.73
18	cL	205	BCR	C33-C5-C6	-2.23	122.02	124.53
18	a3	420	BCR	C3-C4-C5	-2.23	110.09	114.08
15	b4	405	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
15	b2	413	CLA	CHC-C1C-NC	2.23	127.59	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	412	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	a5	405	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
15	c1	413	CLA	C2D-C1D-ND	-2.23	108.46	110.10
15	a5	412	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	b5	415	CLA	CHA-C4D-ND	2.23	137.17	132.50
15	a1	404	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
15	b6	410	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
15	cA	803	CLA	C3B-C4B-NB	-2.23	108.44	110.52
15	aA	810	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
15	aA	824	CLA	CHB-C1B-NB	2.23	126.62	124.26
15	bA	832	CLA	C1-C2-C3	-2.23	123.14	126.75
18	c5	401	BCR	C7-C8-C9	-2.23	122.86	126.23
18	aM	101	BCR	C15-C16-C17	-2.23	118.90	123.47
15	a6	409	CLA	C3B-C4B-NB	-2.23	108.44	110.52
15	b5	414	CLA	CHB-C1B-NB	2.23	126.62	124.26
15	c1	405	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
15	aA	826	CLA	CHA-C1A-NA	-2.23	121.29	126.40
15	a4	416	CLA	CHC-C1C-NC	2.23	127.59	124.20
15	a4	421	CLA	CHC-C4B-NB	2.23	126.62	124.26
15	b2	404	CLA	CHC-C4B-NB	2.23	126.62	124.26
15	b5	410	CLA	CMB-C2B-C3B	2.23	131.99	126.59
18	c2	420	BCR	C40-C30-C25	2.23	113.92	110.30
18	bL	205	BCR	C33-C5-C6	-2.23	122.02	124.53
19	bA	854	LHG	C18-C17-C16	-2.23	103.11	114.42
15	cA	826	CLA	CHA-C1A-NA	-2.23	121.29	126.40
15	cA	810	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
18	a2	421	BCR	C35-C13-C14	-2.23	119.80	122.92
15	a4	405	CLA	CHD-C4C-C3C	2.23	128.12	124.84
15	a4	410	CLA	C2A-C1A-CHA	2.23	127.76	123.86
15	c2	415	CLA	C3B-C4B-NB	-2.23	108.45	110.52
19	aA	853	LHG	C18-C17-C16	-2.23	103.11	114.42
18	bM	101	BCR	C27-C26-C25	2.23	125.97	122.73
15	c4	403	CLA	C2A-C1A-CHA	2.23	127.76	123.86
15	cB	818	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	cM	101	BCR	C15-C14-C13	-2.23	124.13	127.31
18	bI	102	BCR	C27-C26-C25	2.23	125.97	122.73
15	b1	417	CLA	C2D-C1D-ND	-2.23	108.46	110.10
15	b2	413	CLA	CHB-C4A-NA	2.23	127.59	124.51
18	b4	418	BCR	C38-C26-C27	-2.23	109.34	113.62
15	cA	807	CLA	CMB-C2B-C3B	2.23	131.98	126.59
15	aA	812	CLA	O2A-C1-C2	-2.23	102.78	108.64
15	b4	406	CLA	CMB-C2B-C1B	-2.23	121.98	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	417	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
15	bA	806	CLA	CAC-C3C-C4C	2.23	127.70	124.81
15	bA	845	CLA	CHC-C4B-NB	2.23	126.61	124.26
15	cB	801	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
15	c2	406	CLA	CED-O2D-CGD	2.23	120.97	115.94
15	bB	809	CLA	C1-C2-C3	-2.23	122.19	126.04
15	c3	408	CLA	C3B-C4B-NB	-2.23	108.45	110.52
15	c3	402	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
19	cA	852	LHG	C18-C17-C16	-2.23	103.13	114.42
15	c5	415	CLA	CHA-C4D-ND	2.22	137.15	132.50
15	a3	409	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
15	a2	405	CLA	CHC-C1C-NC	2.22	127.58	124.20
15	cL	204	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
15	c3	415	CLA	C3B-C4B-NB	-2.22	108.45	110.52
15	b1	415	CLA	CBA-CAA-C2A	2.22	120.43	113.86
15	a6	406	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
15	c3	415	CLA	CHB-C1B-NB	2.22	126.61	124.26
15	a6	413	CLA	C2A-C1A-CHA	2.22	127.75	123.86
15	bA	830	CLA	O2D-CGD-CBD	2.22	115.22	111.27
15	b5	417	CLA	CHB-C1B-C2B	-2.22	120.96	127.24
18	aM	101	BCR	C27-C26-C25	2.22	125.96	122.73
18	cM	101	BCR	C15-C16-C17	-2.22	118.92	123.47
15	aB	818	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	c3	409	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
18	b2	419	BCR	C38-C26-C27	-2.22	109.35	113.62
18	aI	103	BCR	C33-C5-C6	-2.22	122.03	124.53
15	a2	411	CLA	C1D-ND-C4D	2.22	107.91	106.33
15	a2	413	CLA	C3B-C4B-NB	-2.22	108.45	110.52
15	aA	806	CLA	CHC-C4B-NB	2.22	126.61	124.26
15	aB	839	CLA	CHB-C1B-NB	2.22	126.61	124.26
15	a2	404	CLA	CHC-C4B-NB	2.22	126.61	124.26
15	bB	801	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
15	c5	407	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
15	a2	409	CLA	O2A-CGA-O1A	-2.22	117.76	123.30
18	cB	846	BCR	C29-C30-C25	2.22	113.90	110.48
15	bB	838	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	aB	801	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
15	b4	405	CLA	CHC-C1C-NC	2.22	127.57	124.20
15	b4	403	CLA	C2A-C1A-CHA	2.22	127.74	123.86
15	c1	417	CLA	C2A-C1A-CHA	2.22	127.74	123.86
15	c6	414	CLA	C2A-C1A-CHA	2.22	127.74	123.86
18	aJ	205	BCR	C24-C23-C22	-2.22	122.88	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	411	CLA	C3B-C4B-NB	-2.22	108.45	110.52
15	c4	405	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
15	a1	416	CLA	C2D-C1D-ND	-2.22	108.47	110.10
18	b2	421	BCR	C24-C23-C22	-2.22	122.88	126.23
15	aB	818	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
15	bA	803	CLA	O2A-CGA-CBA	2.22	118.88	111.91
15	b1	404	CLA	CHB-C1B-NB	2.22	126.61	124.26
15	b6	409	CLA	C3B-C4B-NB	-2.22	108.45	110.52
15	cA	840	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
15	b6	407	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
15	b1	407	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
15	c6	404	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
15	b4	405	CLA	CHD-C4C-C3C	2.22	128.10	124.84
18	c6	420	BCR	C38-C26-C27	-2.22	109.35	113.62
15	b6	422	CLA	CHC-C4B-NB	2.22	126.61	124.26
15	b3	409	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
15	cB	809	CLA	C1-C2-C3	-2.22	122.21	126.04
15	b2	413	CLA	C3B-C4B-NB	-2.22	108.46	110.52
15	c3	413	CLA	C2D-C1D-ND	-2.22	108.47	110.10
15	bA	810	CLA	CAA-CBA-CGA	-2.22	106.77	113.25
15	cA	812	CLA	O2A-C1-C2	-2.22	102.81	108.64
15	c1	403	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
15	cB	806	CLA	CAC-C3C-C4C	2.22	127.69	124.81
18	a4	401	BCR	C7-C8-C9	-2.22	122.89	126.23
15	cB	804	CLA	CMD-C2D-C1D	-2.22	120.81	124.71
15	b6	416	CLA	CHA-C4D-ND	2.22	137.13	132.50
15	b4	412	CLA	C3B-C4B-NB	-2.22	108.46	110.52
15	c4	413	CLA	C3B-C4B-NB	-2.22	108.46	110.52
15	b3	413	CLA	CHC-C4B-NB	2.22	126.60	124.26
15	c2	408	CLA	CHC-C4B-NB	2.22	126.60	124.26
18	bM	101	BCR	C15-C14-C13	-2.22	124.15	127.31
15	c2	407	CLA	CHC-C4B-NB	2.22	126.60	124.26
18	a4	418	BCR	C38-C26-C27	-2.21	109.36	113.62
15	b2	422	CLA	CHA-C4D-ND	2.21	137.13	132.50
15	bA	814	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	cB	802	CLA	C11-C10-C8	-2.21	108.76	115.92
15	cA	808	CLA	CHC-C4B-NB	2.21	126.60	124.26
15	b2	406	CLA	CED-O2D-CGD	2.21	120.94	115.94
15	a1	414	CLA	C3B-C4B-NB	-2.21	108.46	110.52
15	bA	826	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	c4	412	CLA	CHB-C4A-NA	2.21	127.57	124.51
15	bB	806	CLA	CAC-C3C-C4C	2.21	127.68	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	825	CLA	CMB-C2B-C3B	2.21	131.95	126.59
15	c6	408	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
18	bB	846	BCR	C29-C30-C25	2.21	113.89	110.48
18	bJ	104	BCR	C24-C23-C22	-2.21	122.89	126.23
15	aA	837	CLA	C3B-C4B-NB	-2.21	108.46	110.52
15	c1	405	CLA	C3B-C4B-NB	-2.21	108.46	110.52
15	bA	810	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
15	bB	801	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
18	b2	420	BCR	C40-C30-C25	2.21	113.89	110.30
15	bA	812	CLA	O2A-C1-C2	-2.21	102.82	108.64
15	bA	803	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	aF	201	BCR	C30-C25-C26	-2.21	119.50	122.61
15	c3	405	CLA	CMA-C3A-C2A	-2.21	104.91	113.83
15	a2	405	CLA	CHD-C4C-C3C	2.21	128.09	124.84
18	b2	401	BCR	C24-C23-C22	-2.21	122.89	126.23
18	cK	101	BCR	C7-C8-C9	-2.21	122.89	126.23
15	b1	416	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
15	c4	405	CLA	CHD-C4C-C3C	2.21	128.09	124.84
15	a3	408	CLA	C3B-C4B-NB	-2.21	108.46	110.52
15	b5	412	CLA	C3B-C4B-NB	-2.21	108.46	110.52
18	aB	846	BCR	C29-C30-C25	2.21	113.88	110.48
15	cA	828	CLA	CHD-C4C-NC	2.21	127.69	124.20
15	a6	408	CLA	CHC-C4B-NB	2.21	126.60	124.26
15	b2	416	CLA	CHB-C1B-NB	2.21	126.60	124.26
15	aA	814	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	cB	806	CLA	CMB-C2B-C3B	2.21	131.94	126.59
15	a5	415	CLA	CHA-C4D-ND	2.21	137.12	132.50
18	b4	401	BCR	C7-C8-C9	-2.21	122.90	126.23
18	a3	401	BCR	C16-C15-C14	-2.21	118.95	123.47
15	bA	806	CLA	CHC-C4B-NB	2.21	126.60	124.26
15	b2	408	CLA	CHC-C4B-NB	2.21	126.60	124.26
15	cA	833	CLA	CHC-C4B-NB	2.21	126.60	124.26
15	b4	409	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aA	833	CLA	O2D-CGD-CBD	2.21	115.19	111.27
15	aA	807	CLA	CMB-C2B-C3B	2.21	131.94	126.59
15	b1	413	CLA	C2D-C1D-ND	-2.21	108.48	110.10
15	cB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	bB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aA	845	CLA	CHC-C4B-NB	2.21	126.59	124.26
15	b2	409	CLA	CHB-C1B-NB	2.21	126.59	124.26
15	aB	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aB	802	CLA	C11-C10-C8	-2.21	108.78	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bM	101	BCR	C15-C16-C17	-2.21	118.95	123.47
15	bX	102	CLA	O2A-CGA-O1A	-2.21	117.80	123.30
15	cA	832	CLA	C2D-C1D-ND	-2.21	108.48	110.10
15	aB	806	CLA	CMB-C2B-C3B	2.21	131.94	126.59
15	a2	403	CLA	CHB-C1B-NB	2.21	126.59	124.26
15	b3	409	CLA	CHC-C4B-NB	2.21	126.59	124.26
15	cA	814	CLA	CHB-C1B-NB	2.21	126.59	124.26
15	aA	825	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	aA	840	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	a2	408	CLA	CHC-C4B-NB	2.21	126.59	124.26
15	c5	405	CLA	CMA-C3A-C2A	-2.21	104.93	113.83
15	c4	412	CLA	C3B-C4B-NB	-2.21	108.47	110.52
15	bA	814	CLA	C2A-C1A-CHA	2.21	127.72	123.86
15	cA	802	CLA	C4D-C3D-CAD	-2.21	105.50	108.10
15	aA	810	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
15	b2	403	CLA	CHB-C1B-NB	2.21	126.59	124.26
15	a1	406	CLA	C3B-C4B-NB	-2.21	108.47	110.52
15	c4	417	CLA	C3C-C4C-NC	-2.21	108.10	110.57
15	cB	824	CLA	O2A-CGA-O1A	-2.21	117.80	123.30
15	a3	412	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	b4	416	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	bB	803	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	c4	421	CLA	C11-C10-C8	-2.20	108.79	115.92
15	bA	807	CLA	CMB-C2B-C3B	2.20	131.93	126.59
15	a2	414	CLA	C3B-C4B-NB	-2.20	108.47	110.52
15	cX	102	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
15	cA	803	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
18	cJ	104	BCR	C38-C26-C25	-2.20	122.05	124.53
15	cA	810	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	b2	412	CLA	CHD-C1D-ND	-2.20	122.43	124.45
15	c3	405	CLA	CHC-C1C-NC	2.20	127.55	124.20
15	b6	408	CLA	CHA-C1A-NA	-2.20	121.35	126.40
15	cA	814	CLA	C2A-C1A-CHA	2.20	127.71	123.86
15	aB	809	CLA	C1-C2-C3	-2.20	122.23	126.04
15	cA	814	CLA	CHA-C1A-NA	-2.20	121.35	126.40
18	bA	848	BCR	C7-C8-C9	-2.20	122.91	126.23
15	a4	403	CLA	C2A-C1A-CHA	2.20	127.71	123.86
18	c5	419	BCR	C11-C10-C9	-2.20	124.17	127.31
15	bA	825	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
15	bB	806	CLA	CMB-C2B-C3B	2.20	131.92	126.59
15	bB	802	CLA	C11-C10-C8	-2.20	108.80	115.92
15	a4	417	CLA	CHB-C1B-C2B	-2.20	121.02	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	413	CLA	C3B-C4B-NB	-2.20	108.47	110.52
15	bA	832	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	cA	806	CLA	CHC-C4B-NB	2.20	126.59	124.26
15	c2	409	CLA	CHB-C1B-NB	2.20	126.59	124.26
15	cA	803	CLA	O2A-CGA-CBA	2.20	118.81	111.91
14	cA	801	CL0	C11-C12-C13	-2.20	108.81	115.92
14	aA	801	CL0	C11-C12-C13	-2.20	108.81	115.92
15	aB	827	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	b6	403	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
15	c1	407	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
15	cA	825	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	a1	412	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	aA	814	CLA	C2A-C1A-CHA	2.20	127.70	123.86
15	c4	409	CLA	CMB-C2B-C3B	2.20	131.91	126.59
18	a2	420	BCR	C40-C30-C25	2.20	113.87	110.30
15	a3	414	CLA	CHB-C1B-NB	2.20	126.58	124.26
15	b6	408	CLA	CHC-C4B-NB	2.20	126.58	124.26
15	cA	809	CLA	CHB-C1B-NB	2.20	126.58	124.26
15	bB	839	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
15	cB	827	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
15	bB	839	CLA	CHB-C1B-NB	2.20	126.58	124.26
15	b4	417	CLA	CHB-C1B-NB	2.20	126.58	124.26
15	c3	409	CLA	CHC-C4B-NB	2.20	126.58	124.26
15	cA	837	CLA	C3B-C4B-NB	-2.20	108.48	110.52
15	a1	404	CLA	O1D-CGD-CBD	2.20	128.98	124.48
15	a6	403	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
15	a6	408	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	b1	403	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
15	cF	203	CLA	C3A-C2A-C1A	2.20	104.63	101.34
18	c2	420	BCR	C3-C4-C5	-2.20	110.15	114.08
15	aA	830	CLA	O2D-CGD-CBD	2.20	115.17	111.27
15	aJ	203	CLA	C2D-C1D-ND	-2.20	108.48	110.10
15	aA	803	CLA	O2A-CGA-CBA	2.20	118.80	111.91
15	b6	404	CLA	CHB-C1B-NB	2.20	126.58	124.26
15	a1	416	CLA	CHD-C1D-ND	-2.20	122.44	124.45
15	bB	818	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
15	a6	416	CLA	CHA-C4D-ND	2.20	137.09	132.50
15	a3	405	CLA	CHC-C1C-NC	2.20	127.53	124.20
15	cA	819	CLA	O2D-CGD-CBD	2.20	115.17	111.27
15	cA	806	CLA	CAC-C3C-C4C	2.20	127.66	124.81
15	b2	405	CLA	CHC-C1C-NC	2.19	127.53	124.20
15	bB	827	CLA	O2A-CGA-O1A	-2.19	118.05	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cK	101	BCR	C20-C21-C22	-2.19	124.18	127.31
15	cB	803	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
15	b2	407	CLA	CHC-C4B-NB	2.19	126.58	124.26
18	cF	202	BCR	C30-C25-C26	-2.19	119.52	122.61
15	aB	803	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	bB	804	CLA	O1D-CGD-CBD	2.19	128.97	124.48
18	cB	844	BCR	C7-C8-C9	-2.19	122.92	126.23
15	cA	834	CLA	C7-C6-C5	-2.19	107.40	113.36
15	aB	839	CLA	CAA-CBA-CGA	-2.19	106.84	113.25
15	c6	407	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
15	b1	411	CLA	C2A-C1A-CHA	2.19	127.69	123.86
15	c6	409	CLA	CHA-C1A-NA	-2.19	121.38	126.40
15	b3	415	CLA	CHB-C1B-NB	2.19	126.58	124.26
15	a2	422	CLA	CHA-C4D-ND	2.19	137.09	132.50
14	bA	801	CL0	C11-C12-C13	-2.19	108.83	115.92
15	aB	818	CLA	CGD-CBD-CAD	-2.19	103.63	110.73
15	cB	804	CLA	O1D-CGD-CBD	2.19	128.97	124.48
15	b2	416	CLA	CHA-C4D-ND	2.19	137.08	132.50
15	b5	412	CLA	C1D-ND-C4D	2.19	107.89	106.33
18	c3	419	BCR	C40-C30-C25	2.19	113.85	110.30
15	cA	834	CLA	CMB-C2B-C3B	2.19	131.90	126.59
15	bA	834	CLA	C7-C6-C5	-2.19	107.41	113.36
15	bA	808	CLA	CHC-C4B-NB	2.19	126.58	124.26
15	cA	830	CLA	CHB-C1B-NB	2.19	126.58	124.26
15	cB	820	CLA	CHC-C4B-NB	2.19	126.58	124.26
15	aB	824	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	bA	819	CLA	O2D-CGD-CBD	2.19	115.16	111.27
18	aB	844	BCR	C7-C8-C9	-2.19	122.92	126.23
15	a2	406	CLA	CED-O2D-CGD	2.19	120.89	115.94
15	cA	830	CLA	O2D-CGD-CBD	2.19	115.16	111.27
15	aA	823	CLA	CHC-C4B-NB	2.19	126.58	124.26
15	a1	406	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
18	aK	101	BCR	C20-C21-C22	-2.19	124.18	127.31
15	bB	824	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	b2	408	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	a1	404	CLA	CMA-C3A-C4A	2.19	117.66	111.77
15	bA	836	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	a6	414	CLA	CHC-C1C-NC	2.19	127.53	124.20
15	aA	806	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	bB	801	CLA	CAC-C3C-C4C	2.19	127.65	124.81
15	c1	405	CLA	CMA-C3A-C4A	2.19	117.66	111.77
15	a4	409	CLA	O2A-CGA-O1A	-2.19	118.07	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	839	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
15	bA	816	CLA	C3B-C4B-NB	-2.19	108.48	110.52
15	aB	804	CLA	O1D-CGD-CBD	2.19	128.96	124.48
15	aA	828	CLA	CHD-C4C-NC	2.19	127.65	124.20
18	c6	420	BCR	C15-C16-C17	-2.19	118.99	123.47
15	aA	826	CLA	C7-C6-C5	-2.19	107.41	113.36
15	cB	830	CLA	CHC-C4B-NB	2.19	126.57	124.26
15	bF	201	CLA	C3A-C2A-C1A	2.19	104.62	101.34
15	aB	840	CLA	C1-C2-C3	-2.19	122.26	126.04
18	b1	419	BCR	C15-C14-C13	-2.19	124.19	127.31
15	aX	102	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
15	bX	102	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
15	c5	415	CLA	CHB-C1B-NB	2.19	126.57	124.26
15	c2	405	CLA	CHC-C1C-NC	2.19	127.52	124.20
18	a1	418	BCR	C15-C14-C13	-2.19	124.19	127.31
18	a4	419	BCR	C3-C4-C5	-2.19	110.17	114.08
15	a3	413	CLA	C2D-C1D-ND	-2.19	108.49	110.10
18	aK	101	BCR	C7-C8-C9	-2.19	122.93	126.23
15	b5	402	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
18	aJ	205	BCR	C38-C26-C25	-2.19	122.07	124.53
15	cA	833	CLA	O2D-CGD-CBD	2.19	115.15	111.27
18	a3	418	BCR	C38-C26-C27	-2.19	109.42	113.62
15	bA	840	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	c4	409	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	a2	409	CLA	CHB-C1B-NB	2.19	126.57	124.26
15	c3	414	CLA	CHB-C1B-NB	2.19	126.57	124.26
15	c2	417	CLA	CMD-C2D-C3D	2.19	132.64	127.61
15	cA	825	CLA	CMB-C2B-C3B	2.19	131.88	126.59
15	aA	832	CLA	C2D-C1D-ND	-2.19	108.49	110.10
15	b6	406	CLA	CMA-C3A-C4A	2.19	117.65	111.77
15	a2	408	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
15	a5	402	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
15	c6	411	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
15	a3	404	CLA	CHB-C1B-NB	2.19	126.57	124.26
15	cB	818	CLA	CGD-CBD-CAD	-2.19	103.66	110.73
15	cB	810	CLA	C11-C12-C13	-2.19	108.86	115.92
15	c2	418	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
15	c5	412	CLA	C1D-ND-C4D	2.18	107.89	106.33
15	cA	822	CLA	C2D-C1D-ND	-2.18	108.49	110.10
15	c4	415	CLA	CHA-C4D-ND	2.18	137.07	132.50
15	aA	834	CLA	C7-C6-C5	-2.18	107.43	113.36
15	bA	843	CLA	CBC-CAC-C3C	2.18	118.45	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	404	CLA	CHB-C1B-NB	2.18	126.57	124.26
15	b5	404	CLA	CHB-C1B-NB	2.18	126.57	124.26
15	c6	407	CLA	C3B-C4B-NB	-2.18	108.49	110.52
18	c1	419	BCR	C16-C15-C14	-2.18	119.00	123.47
15	cA	827	CLA	C2D-C1D-ND	-2.18	108.50	110.10
18	b5	419	BCR	C11-C10-C9	-2.18	124.19	127.31
15	b4	405	CLA	CHB-C4A-NA	2.18	127.53	124.51
15	a3	411	CLA	C3B-C4B-NB	-2.18	108.49	110.52
15	a3	405	CLA	CMA-C3A-C2A	-2.18	105.02	113.83
18	b5	401	BCR	C27-C26-C25	2.18	125.90	122.73
18	cI	102	BCR	C27-C26-C25	2.18	125.90	122.73
18	a4	420	BCR	C24-C23-C22	-2.18	122.94	126.23
15	a2	416	CLA	CHA-C4D-ND	2.18	137.06	132.50
15	cB	840	CLA	C1-C2-C3	-2.18	122.27	126.04
15	aL	201	CLA	CHC-C4B-NB	2.18	126.57	124.26
15	c1	414	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	c5	401	BCR	C24-C23-C22	-2.18	122.94	126.23
15	aB	824	CLA	CHB-C4A-NA	2.18	127.53	124.51
15	bX	102	CLA	CMD-C2D-C3D	2.18	132.63	127.61
16	cA	845	PQN	C2M-C2-C3	-2.18	120.84	124.40
15	cB	801	CLA	CAC-C3C-C4C	2.18	127.64	124.81
15	c2	413	CLA	CHC-C1C-NC	2.18	127.51	124.20
15	c3	412	CLA	CHC-C1C-NC	2.18	127.51	124.20
15	a2	413	CLA	CHB-C4A-NA	2.18	127.53	124.51
15	c1	402	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
15	a2	407	CLA	CHC-C4B-NB	2.18	126.56	124.26
18	b1	420	BCR	C11-C10-C9	-2.18	124.20	127.31
15	bA	826	CLA	C7-C6-C5	-2.18	107.44	113.36
18	c3	420	BCR	C3-C4-C5	-2.18	110.19	114.08
15	aX	102	CLA	CMD-C2D-C3D	2.18	132.63	127.61
15	aB	820	CLA	C2D-C1D-ND	-2.18	108.50	110.10
15	aA	808	CLA	CHC-C4B-NB	2.18	126.56	124.26
15	c1	415	CLA	CHB-C1B-NB	2.18	126.56	124.26
15	c2	416	CLA	CHA-C4D-ND	2.18	137.06	132.50
15	aB	820	CLA	CHC-C4B-NB	2.18	126.56	124.26
15	aA	836	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
15	b1	409	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
15	bB	818	CLA	CGD-CBD-CAD	-2.18	103.68	110.73
15	bA	831	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
15	bB	830	CLA	C3B-C2B-C1B	2.18	109.79	107.16
15	b1	405	CLA	C3B-C4B-NB	-2.18	108.50	110.52
15	b4	411	CLA	CHD-C1D-ND	-2.18	122.45	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	833	CLA	CHC-C4B-NB	2.18	126.56	124.26
15	aA	818	CLA	O2D-CGD-CBD	2.18	115.14	111.27
15	bA	840	CLA	C2A-C1A-CHA	2.18	127.67	123.86
15	a3	410	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	bA	834	CLA	CMB-C2B-C3B	2.18	131.86	126.59
15	b6	413	CLA	C2A-C1A-CHA	2.18	127.67	123.86
15	aA	831	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
15	c5	405	CLA	CED-O2D-CGD	-2.18	111.02	115.94
15	cA	826	CLA	C7-C6-C5	-2.18	107.45	113.36
15	cA	842	CLA	CBC-CAC-C3C	2.18	118.43	112.43
18	c3	401	BCR	C16-C15-C14	-2.18	119.02	123.47
15	c2	414	CLA	C3B-C4B-NB	-2.18	108.50	110.52
15	a4	421	CLA	C3A-C2A-C1A	2.18	104.60	101.34
18	bB	849	BCR	C30-C25-C26	-2.18	119.55	122.61
18	aA	848	BCR	C29-C30-C25	2.17	113.83	110.48
15	a1	410	CLA	C2A-C1A-CHA	2.17	127.66	123.86
18	a3	420	BCR	C1-C6-C5	-2.17	119.55	122.61
15	bB	810	CLA	C11-C12-C13	-2.17	108.89	115.92
15	aB	801	CLA	CAC-C3C-C4C	2.17	127.63	124.81
15	b3	411	CLA	C3B-C4B-NB	-2.17	108.50	110.52
15	cA	816	CLA	C3B-C4B-NB	-2.17	108.50	110.52
15	aA	830	CLA	C1-C2-C3	-2.17	122.28	126.04
15	c5	402	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
15	a6	406	CLA	O1D-CGD-CBD	2.17	128.93	124.48
15	cB	839	CLA	CHB-C1B-NB	2.17	126.56	124.26
15	b4	410	CLA	C1D-ND-C4D	2.17	107.88	106.33
15	bA	830	CLA	C1-C2-C3	-2.17	122.28	126.04
15	cA	839	CLA	O1D-CGD-CBD	2.17	128.93	124.48
15	cX	102	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
15	cB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	cA	836	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
18	bA	848	BCR	C20-C21-C22	-2.17	124.21	127.31
15	bB	820	CLA	CHC-C4B-NB	2.17	126.56	124.26
15	aJ	201	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	cA	831	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
15	c6	413	CLA	C2A-C1A-CHA	2.17	127.66	123.86
15	b6	406	CLA	C3B-C4B-NB	-2.17	108.50	110.52
18	c2	401	BCR	C24-C23-C22	-2.17	122.95	126.23
18	c6	403	BCR	C16-C15-C14	-2.17	119.03	123.47
15	c6	417	CLA	CHA-C4D-ND	2.17	137.04	132.50
15	bA	803	CLA	CHC-C4B-NB	2.17	126.56	124.26
15	b4	421	CLA	CHC-C4B-NB	2.17	126.56	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c1	411	CLA	C2A-C1A-CHA	2.17	127.66	123.86
15	c2	408	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
15	bA	825	CLA	CMB-C2B-C3B	2.17	131.85	126.59
15	b4	409	CLA	CMB-C2B-C3B	2.17	131.85	126.59
18	a5	401	BCR	C7-C8-C9	-2.17	122.95	126.23
15	c4	412	CLA	CHC-C1C-NC	2.17	127.50	124.20
15	b1	407	CLA	C3B-C4B-NB	-2.17	108.50	110.52
15	bB	810	CLA	C2A-C1A-CHA	2.17	127.66	123.86
15	a4	417	CLA	CHB-C1B-NB	2.17	126.56	124.26
15	a6	410	CLA	CHB-C1B-NB	2.17	126.56	124.26
15	bA	834	CLA	C1-C2-C3	-2.17	122.29	126.04
15	cB	833	CLA	C3C-C4C-NC	-2.17	108.14	110.57
15	cB	812	CLA	CMB-C2B-C3B	2.17	131.84	126.59
18	aA	850	BCR	C20-C21-C22	-2.17	124.21	127.31
15	bA	833	CLA	O2D-CGD-CBD	2.17	115.12	111.27
18	b3	401	BCR	C16-C15-C14	-2.17	119.03	123.47
15	a6	406	CLA	CMA-C3A-C4A	2.17	117.61	111.77
15	a3	413	CLA	C3B-C4B-NB	-2.17	108.50	110.52
15	bA	807	CLA	C2D-C1D-ND	-2.17	108.50	110.10
15	bA	827	CLA	C2D-C1D-ND	-2.17	108.50	110.10
15	a1	403	CLA	CHB-C1B-NB	2.17	126.55	124.26
15	cX	102	CLA	CMD-C2D-C3D	2.17	132.60	127.61
18	a5	418	BCR	C7-C8-C9	-2.17	122.96	126.23
15	b4	421	CLA	C11-C10-C8	-2.17	108.91	115.92
15	aB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
15	bB	840	CLA	C3A-C2A-C1A	2.17	104.59	101.34
16	aA	846	PQN	C2M-C2-C3	-2.17	120.86	124.40
15	aA	803	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
15	aA	819	CLA	O2D-CGD-CBD	2.17	115.12	111.27
15	bL	202	CLA	CHC-C4B-NB	2.17	126.55	124.26
15	c4	405	CLA	CHB-C4A-NA	2.17	127.51	124.51
15	c5	405	CLA	CHD-C4C-C3C	2.17	128.03	124.84
15	a1	401	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
15	b6	406	CLA	O1D-CGD-CBD	2.17	128.92	124.48
15	a1	413	CLA	CHB-C1B-NB	2.17	126.55	124.26
15	c3	410	CLA	CHA-C1A-NA	-2.17	121.43	126.40
15	aB	833	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	b2	420	BCR	C3-C4-C5	-2.17	110.21	114.08
15	a6	410	CLA	O1D-CGD-CBD	2.17	128.92	124.48
15	bA	814	CLA	CHB-C1B-NB	2.17	126.55	124.26
15	b1	408	CLA	C3C-C4C-NC	-2.17	108.14	110.57
15	bA	828	CLA	CHD-C4C-NC	2.17	127.62	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b2	411	CLA	CHA-C1A-NA	-2.17	121.44	126.40
18	bJ	104	BCR	C38-C26-C25	-2.17	122.09	124.53
15	b3	410	CLA	C1D-ND-C4D	2.17	107.87	106.33
15	aB	812	CLA	CMB-C2B-C3B	2.17	131.84	126.59
18	aL	205	BCR	C27-C26-C25	2.17	125.88	122.73
18	a5	401	BCR	C27-C26-C25	2.17	125.88	122.73
15	cB	830	CLA	C3B-C2B-C1B	2.17	109.78	107.16
18	a6	419	BCR	C15-C16-C17	-2.17	119.04	123.47
15	aA	809	CLA	CHB-C1B-NB	2.17	126.55	124.26
15	c6	415	CLA	CHC-C1C-NC	2.17	127.49	124.20
15	aA	843	CLA	CBC-CAC-C3C	2.17	118.40	112.43
18	c1	419	BCR	C15-C14-C13	-2.17	124.22	127.31
15	cB	836	CLA	CHA-C1A-NA	-2.17	121.44	126.40
15	a5	417	CLA	CMA-C3A-C2A	-2.17	105.09	113.83
15	bA	818	CLA	O2D-CGD-CBD	2.17	115.12	111.27
15	a5	405	CLA	CHB-C4A-NA	2.17	127.51	124.51
15	c5	409	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
15	cL	202	CLA	CHC-C4B-NB	2.17	126.55	124.26
15	b5	417	CLA	CMA-C3A-C2A	-2.16	105.09	113.83
15	b3	405	CLA	CHC-C1C-NC	2.16	127.49	124.20
15	b2	409	CLA	O2A-CGA-O1A	-2.16	117.90	123.30
15	a4	417	CLA	C3A-C2A-C1A	2.16	104.58	101.34
15	b5	407	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	a3	421	CLA	C16-C15-C13	-2.16	108.92	115.92
15	aA	834	CLA	CMB-C2B-C3B	2.16	131.83	126.59
15	a2	418	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
15	b2	405	CLA	CHD-C4C-C3C	2.16	128.02	124.84
15	a1	408	CLA	CHB-C1B-NB	2.16	126.55	124.26
15	cA	844	CLA	CHC-C4B-NB	2.16	126.55	124.26
15	cK	102	CLA	CHB-C1B-NB	2.16	126.55	124.26
15	c4	421	CLA	C3A-C2A-C1A	2.16	104.58	101.34
18	bL	201	BCR	C38-C26-C27	-2.16	109.46	113.62
18	bL	206	BCR	C38-C26-C27	-2.16	109.46	113.62
18	c5	401	BCR	C27-C26-C25	2.16	125.87	122.73
15	aA	816	CLA	C3B-C4B-NB	-2.16	108.51	110.52
15	bA	837	CLA	C3B-C4B-NB	-2.16	108.51	110.52
15	cB	822	CLA	C3B-C4B-NB	-2.16	108.51	110.52
18	c6	402	BCR	C40-C30-C25	2.16	113.81	110.30
15	bB	818	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	bA	806	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
15	bA	839	CLA	O1D-CGD-CBD	2.16	128.91	124.48
15	b2	417	CLA	CMD-C2D-C3D	2.16	132.59	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b4	417	CLA	C3A-C2A-C1A	2.16	104.58	101.34
18	a2	419	BCR	C38-C26-C27	-2.16	109.46	113.62
18	cA	849	BCR	C20-C21-C22	-2.16	124.22	127.31
15	aB	810	CLA	C11-C12-C13	-2.16	108.93	115.92
15	bB	824	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
15	c4	408	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
15	b6	413	CLA	CHC-C1C-NC	2.16	127.48	124.20
18	cA	847	BCR	C29-C30-C25	2.16	113.81	110.48
18	cA	850	BCR	C8-C7-C6	-2.16	121.13	127.20
15	a5	410	CLA	CHA-C1A-NA	-2.16	121.45	126.40
15	b3	412	CLA	CHC-C1C-NC	2.16	127.48	124.20
15	aB	838	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	c3	406	CLA	CHC-C4B-NB	2.16	126.54	124.26
15	cB	830	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
15	c5	405	CLA	C3B-C4B-NB	-2.16	108.51	110.52
15	c5	417	CLA	C3A-C2A-C1A	2.16	104.57	101.34
15	aB	824	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
15	cA	840	CLA	C2A-C1A-CHA	2.16	127.64	123.86
15	a4	409	CLA	CMB-C2B-C3B	2.16	131.82	126.59
15	bB	824	CLA	CHB-C4A-NA	2.16	127.50	124.51
15	aA	826	CLA	C3B-C4B-NB	-2.16	108.51	110.52
15	cB	824	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
15	aA	840	CLA	C2A-C1A-CHA	2.16	127.63	123.86
15	a2	408	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
15	a2	412	CLA	C2A-C1A-CHA	2.16	127.63	123.86
15	a2	411	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	aK	102	CLA	CHB-C1B-NB	2.16	126.54	124.26
18	a5	419	BCR	C11-C10-C9	-2.16	124.23	127.31
18	cF	205	BCR	C3-C4-C5	-2.16	110.22	114.08
15	c6	407	CLA	O1D-CGD-CBD	2.16	128.90	124.48
18	b3	419	BCR	C40-C30-C25	2.16	113.80	110.30
15	c2	413	CLA	CHB-C4A-NA	2.16	127.50	124.51
15	bB	830	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
15	a4	405	CLA	CHC-C1C-NC	2.16	127.47	124.20
15	bB	833	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
15	c2	411	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	c4	410	CLA	C1D-ND-C4D	2.16	107.87	106.33
15	aB	822	CLA	CHC-C4B-NB	2.16	126.54	124.26
15	a6	414	CLA	CHC-C4B-NB	2.16	126.54	124.26
15	bA	835	CLA	CHC-C4B-NB	2.16	126.54	124.26
15	b5	409	CLA	CHB-C1B-NB	2.16	126.54	124.26
15	cA	811	CLA	CHC-C4B-NB	2.16	126.54	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	405	CLA	CHD-C4C-C3C	2.16	128.01	124.84
15	cB	829	CLA	C3B-C4B-NB	-2.16	108.52	110.52
15	cB	811	CLA	CAC-C3C-C4C	2.16	127.61	124.81
15	cA	805	CLA	CAA-C2A-C1A	-2.16	104.91	111.97
15	aX	102	CLA	CMB-C2B-C1B	-2.16	122.09	125.37
15	c1	409	CLA	CHB-C1B-NB	2.16	126.54	124.26
15	aA	805	CLA	CAA-C2A-C1A	-2.16	104.91	111.97
18	bJ	105	BCR	C3-C4-C5	-2.16	110.23	114.08
15	c2	408	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
15	cB	820	CLA	C2D-C1D-ND	-2.15	108.52	110.10
18	c4	401	BCR	C7-C8-C9	-2.15	122.98	126.23
15	b4	417	CLA	C3C-C4C-NC	-2.15	108.16	110.57
15	aA	803	CLA	CMD-C2D-C1D	-2.15	120.92	124.71
15	a4	402	CLA	C3B-C4B-NB	-2.15	108.52	110.52
15	bA	805	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
18	aF	203	BCR	C3-C4-C5	-2.15	110.23	114.08
15	aB	830	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
15	cB	836	CLA	CBC-CAC-C3C	2.15	118.37	112.43
15	bB	822	CLA	CHC-C4B-NB	2.15	126.54	124.26
15	c2	422	CLA	CHB-C1B-NB	2.15	126.54	124.26
15	a4	421	CLA	C11-C10-C8	-2.15	108.96	115.92
18	aL	205	BCR	C38-C26-C27	-2.15	109.48	113.62
15	b4	421	CLA	C3A-C2A-C1A	2.15	104.56	101.34
18	b5	401	BCR	C24-C23-C22	-2.15	122.98	126.23
15	a6	412	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	c6	407	CLA	CMA-C3A-C4A	2.15	117.56	111.77
15	bB	812	CLA	CMB-C2B-C3B	2.15	131.80	126.59
15	cB	824	CLA	CMB-C2B-C3B	2.15	131.80	126.59
15	b5	405	CLA	CHD-C4C-C3C	2.15	128.00	124.84
18	bA	851	BCR	C20-C21-C22	-2.15	124.24	127.31
15	c2	403	CLA	CHB-C1B-NB	2.15	126.53	124.26
15	a4	415	CLA	CHA-C4D-ND	2.15	137.00	132.50
18	a2	420	BCR	C3-C4-C5	-2.15	110.23	114.08
15	aA	830	CLA	C3B-C4B-NB	-2.15	108.52	110.52
15	bA	826	CLA	C3B-C4B-NB	-2.15	108.52	110.52
15	a4	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	c2	412	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	cB	833	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
15	aB	806	CLA	CAC-C3C-C4C	2.15	127.60	124.81
15	bA	803	CLA	CMD-C2D-C1D	-2.15	120.92	124.71
15	b2	407	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
18	aA	851	BCR	C8-C7-C6	-2.15	121.16	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a4	410	CLA	C1D-ND-C4D	2.15	107.86	106.33
15	cB	810	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	aA	817	CLA	CHB-C1B-NB	2.15	126.53	124.26
15	a6	413	CLA	CHC-C1C-NC	2.15	127.47	124.20
15	cB	814	CLA	CHB-C4A-NA	2.15	127.49	124.51
15	bA	843	CLA	O2A-C1-C2	2.15	114.29	108.64
15	a5	407	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	bB	836	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	a6	401	BCR	C40-C30-C25	2.15	113.79	110.30
15	aA	839	CLA	O1D-CGD-CBD	2.15	128.88	124.48
15	cA	838	CLA	C2A-C1A-CHA	2.15	127.62	123.86
15	a4	411	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	aF	201	BCR	C24-C23-C22	-2.15	122.99	126.23
18	a6	420	BCR	C7-C8-C9	-2.15	122.99	126.23
15	a5	420	CLA	O2D-CGD-CBD	2.15	115.09	111.27
15	a1	404	CLA	CHC-C1C-NC	2.15	127.46	124.20
15	c5	420	CLA	O2D-CGD-CBD	2.15	115.09	111.27
15	bA	830	CLA	CHB-C1B-NB	2.15	126.53	124.26
18	b3	418	BCR	C38-C26-C27	-2.15	109.49	113.62
15	b6	411	CLA	CMB-C2B-C3B	2.15	131.79	126.59
15	aA	838	CLA	C2A-C1A-CHA	2.15	127.62	123.86
18	a3	419	BCR	C40-C30-C25	2.15	113.78	110.30
15	cA	830	CLA	C1-C2-C3	-2.15	122.33	126.04
15	b3	405	CLA	CMA-C3A-C2A	-2.15	105.16	113.83
15	bA	822	CLA	C2D-C1D-ND	-2.15	108.52	110.10
15	cL	203	CLA	C2A-C1A-CHA	2.15	127.61	123.86
18	aK	101	BCR	C33-C5-C6	-2.15	122.12	124.53
15	c5	410	CLA	CHA-C1A-NA	-2.15	121.48	126.40
18	bA	852	BCR	C8-C7-C6	-2.15	121.17	127.20
15	a6	416	CLA	C3B-C4B-NB	-2.15	108.52	110.52
15	b2	405	CLA	C3B-C4B-NB	-2.15	108.52	110.52
15	cB	824	CLA	CHB-C4A-NA	2.15	127.48	124.51
15	b3	417	CLA	C2D-C1D-ND	-2.15	108.52	110.10
15	b1	406	CLA	CMB-C2B-C3B	2.15	131.79	126.59
15	b5	405	CLA	CHB-C4A-NA	2.15	127.48	124.51
15	a1	409	CLA	C2A-C1A-CHA	2.15	127.61	123.86
18	cK	101	BCR	C33-C5-C6	-2.15	122.12	124.53
15	b6	410	CLA	CHB-C1B-NB	2.15	126.53	124.26
15	b4	415	CLA	CHA-C4D-ND	2.15	136.99	132.50
15	bA	817	CLA	CHB-C1B-NB	2.15	126.53	124.26
15	c6	409	CLA	CHC-C4B-NB	2.15	126.53	124.26
18	cF	204	BCR	C2-C1-C6	2.14	113.78	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	842	CLA	O2A-C1-C2	2.14	114.27	108.64
15	bA	838	CLA	C2A-C1A-CHA	2.14	127.61	123.86
15	c2	422	CLA	CHA-C4D-ND	2.14	136.99	132.50
18	b6	402	BCR	C16-C15-C14	-2.14	119.08	123.47
15	aB	836	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	cB	822	CLA	CHC-C4B-NB	2.14	126.53	124.26
18	bB	844	BCR	C7-C8-C9	-2.14	123.00	126.23
18	a3	418	BCR	C16-C15-C14	-2.14	119.08	123.47
15	c6	411	CLA	O1D-CGD-CBD	2.14	128.87	124.48
15	a2	417	CLA	CMD-C2D-C3D	2.14	132.54	127.61
15	c5	407	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	aL	202	CLA	C2A-C1A-CHA	2.14	127.61	123.86
15	cA	821	CLA	C2A-C1A-CHA	2.14	127.61	123.86
18	b2	419	BCR	C11-C10-C9	-2.14	124.25	127.31
15	c1	410	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	aA	830	CLA	CHB-C1B-NB	2.14	126.53	124.26
15	b3	406	CLA	CHB-C1B-NB	2.14	126.53	124.26
18	bL	201	BCR	C27-C26-C25	2.14	125.84	122.73
18	bB	850	BCR	C16-C17-C18	-2.14	124.25	127.31
15	cA	806	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
15	c6	417	CLA	C3B-C4B-NB	-2.14	108.53	110.52
15	cA	818	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	bB	840	CLA	C1-C2-C3	-2.14	122.34	126.04
15	b6	415	CLA	CHB-C1B-NB	2.14	126.52	124.26
15	cA	817	CLA	CHB-C1B-NB	2.14	126.52	124.26
15	aA	822	CLA	C2D-C1D-ND	-2.14	108.53	110.10
15	bJ	101	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	c3	405	CLA	CHB-C4A-NA	2.14	127.47	124.51
18	a1	418	BCR	C40-C30-C25	2.14	113.77	110.30
15	aB	830	CLA	C3B-C2B-C1B	2.14	109.75	107.16
16	bA	846	PQN	C2M-C2-C3	-2.14	120.91	124.40
15	aA	806	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
15	b5	410	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	c6	408	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
15	a2	412	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	aF	202	BCR	C2-C1-C6	2.14	113.78	110.48
18	b4	420	BCR	C1-C6-C5	-2.14	119.60	122.61
18	a6	402	BCR	C16-C15-C14	-2.14	119.09	123.47
15	aB	819	CLA	C2A-C1A-CHA	2.14	127.60	123.86
18	b3	401	BCR	C29-C30-C25	2.14	113.78	110.48
16	bA	846	PQN	C14-C13-C15	2.14	118.87	115.27
15	aB	836	CLA	CBC-CAC-C3C	2.14	118.33	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	841	CLA	O2D-CGD-CBD	2.14	115.07	111.27
18	b6	419	BCR	C7-C8-C9	-2.14	123.00	126.23
15	bB	804	CLA	C2A-C1A-CHA	2.14	127.60	123.86
15	aA	843	CLA	O2A-C1-C2	2.14	114.26	108.64
15	b3	410	CLA	CHA-C1A-NA	-2.14	121.50	126.40
18	bL	206	BCR	C27-C26-C25	2.14	125.84	122.73
15	cA	803	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	aF	201	BCR	C32-C1-C2	-2.14	100.35	108.91
15	b4	408	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
15	aA	834	CLA	C1-C2-C3	-2.14	122.34	126.04
18	c3	418	BCR	C1-C6-C5	-2.14	119.60	122.61
18	aB	846	BCR	C35-C13-C14	-2.14	119.93	122.92
15	c3	407	CLA	CMB-C2B-C3B	2.14	131.77	126.59
15	cB	838	CLA	O2D-CGD-CBD	2.14	115.07	111.27
15	a2	407	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
15	a5	409	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	c6	420	BCR	C7-C8-C9	-2.14	123.00	126.23
15	a5	405	CLA	CHD-C4C-C3C	2.14	127.98	124.84
15	cA	803	CLA	CMD-C2D-C1D	-2.14	120.95	124.71
18	b3	420	BCR	C1-C6-C5	-2.14	119.60	122.61
18	c5	418	BCR	C38-C26-C27	-2.14	109.51	113.62
18	cA	849	BCR	C27-C26-C25	2.14	125.83	122.73
18	bA	849	BCR	C29-C30-C25	2.14	113.77	110.48
15	aA	811	CLA	CHC-C4B-NB	2.14	126.52	124.26
15	aB	810	CLA	C2A-C1A-CHA	2.14	127.59	123.86
15	bA	830	CLA	C3B-C4B-NB	-2.14	108.53	110.52
18	aF	201	BCR	C7-C8-C9	-2.14	123.01	126.23
15	a6	411	CLA	CMB-C2B-C3B	2.14	131.76	126.59
15	a1	411	CLA	CHC-C1C-NC	2.14	127.44	124.20
15	aB	841	CLA	O2D-CGD-CBD	2.14	115.06	111.27
15	cA	806	CLA	CMB-C2B-C3B	2.14	131.76	126.59
15	bB	833	CLA	C3C-C4C-NC	-2.14	108.18	110.57
15	a1	402	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
15	bA	821	CLA	C2A-C1A-CHA	2.14	127.59	123.86
15	bB	824	CLA	CMB-C2B-C3B	2.14	131.76	126.59
15	cA	830	CLA	C3B-C4B-NB	-2.14	108.53	110.52
18	bB	849	BCR	C32-C1-C2	-2.14	100.36	108.91
15	aB	834	CLA	CHD-C1D-ND	-2.13	122.49	124.45
15	b3	406	CLA	CHC-C4B-NB	2.13	126.52	124.26
18	b6	419	BCR	C15-C16-C17	-2.13	119.10	123.47
15	c4	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10
15	a6	406	CLA	C3B-C4B-NB	-2.13	108.53	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c3	418	BCR	C16-C15-C14	-2.13	119.10	123.47
15	c6	414	CLA	CHC-C1C-NC	2.13	127.44	124.20
18	cF	202	BCR	C32-C1-C2	-2.13	100.37	108.91
15	a6	407	CLA	CHB-C1B-NB	2.13	126.52	124.26
15	cK	102	CLA	CHC-C4B-NB	2.13	126.52	124.26
15	c6	416	CLA	CHB-C1B-NB	2.13	126.52	124.26
15	a3	407	CLA	CMB-C2B-C3B	2.13	131.76	126.59
18	bA	848	BCR	C33-C5-C6	-2.13	122.13	124.53
18	b1	418	BCR	C15-C14-C13	-2.13	124.27	127.31
15	b6	412	CLA	C2A-C1A-CHA	2.13	127.59	123.86
15	a3	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	a5	401	BCR	C24-C23-C22	-2.13	123.01	126.23
15	c1	405	CLA	CHC-C1C-NC	2.13	127.44	124.20
15	cB	818	CLA	CHD-C1D-ND	-2.13	122.49	124.45
15	b3	407	CLA	CMB-C2B-C3B	2.13	131.75	126.59
15	c3	421	CLA	C16-C15-C13	-2.13	109.03	115.92
18	a4	420	BCR	C1-C6-C5	-2.13	119.61	122.61
15	aB	829	CLA	O2D-CGD-CBD	2.13	115.06	111.27
15	cB	829	CLA	CMB-C2B-C3B	2.13	131.75	126.59
15	a1	404	CLA	C3B-C4B-NB	-2.13	108.54	110.52
15	bB	820	CLA	C2D-C1D-ND	-2.13	108.53	110.10
16	cA	845	PQN	C14-C13-C15	2.13	118.86	115.27
15	a1	404	CLA	CHB-C4A-NA	2.13	127.46	124.51
15	a6	412	CLA	C3B-C4B-NB	-2.13	108.54	110.52
15	c3	413	CLA	CHC-C4B-NB	2.13	126.51	124.26
15	a4	417	CLA	C2D-C1D-ND	-2.13	108.53	110.10
15	a3	417	CLA	C3C-C4C-NC	-2.13	108.18	110.57
15	c5	408	CLA	CAA-CBA-CGA	2.13	118.16	112.51
15	aA	806	CLA	CMB-C2B-C3B	2.13	131.75	126.59
15	cA	834	CLA	C1-C2-C3	-2.13	122.36	126.04
15	c5	417	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
15	aB	838	CLA	O2D-CGD-CBD	2.13	115.05	111.27
15	aA	821	CLA	C2A-C1A-CHA	2.13	127.58	123.86
15	bA	809	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	cF	202	BCR	C24-C23-C22	-2.13	123.02	126.23
15	aB	811	CLA	C7-C6-C5	-2.13	107.58	113.36
15	bB	829	CLA	CMB-C2B-C3B	2.13	131.74	126.59
15	b6	407	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
15	bL	203	CLA	C2A-C1A-CHA	2.13	127.58	123.86
15	aB	808	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	c3	418	BCR	C38-C26-C27	-2.13	109.53	113.62
15	a3	411	CLA	CHD-C1D-ND	-2.13	122.50	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a6	419	BCR	C7-C8-C9	-2.13	123.02	126.23
18	bM	101	BCR	C40-C30-C25	2.13	113.75	110.30
15	b5	408	CLA	CAA-CBA-CGA	2.13	118.16	112.51
18	a3	401	BCR	C29-C30-C25	2.13	113.76	110.48
15	aA	834	CLA	C2A-C1A-CHA	2.13	127.58	123.86
18	cB	849	BCR	C16-C17-C18	-2.13	124.27	127.31
15	cX	102	CLA	O1D-CGD-CBD	2.13	128.84	124.48
15	aA	827	CLA	C2D-C1D-ND	-2.13	108.54	110.10
18	a2	401	BCR	C28-C27-C26	-2.13	110.28	114.08
15	b2	412	CLA	C2A-C1A-CHA	2.13	127.58	123.86
18	c1	418	BCR	C15-C14-C13	-2.13	124.27	127.31
15	aB	824	CLA	CMB-C2B-C3B	2.13	131.74	126.59
15	a2	405	CLA	C3B-C4B-NB	-2.13	108.54	110.52
15	aA	807	CLA	C2D-C1D-ND	-2.13	108.54	110.10
15	bA	806	CLA	CMB-C2B-C3B	2.13	131.74	126.59
18	bB	849	BCR	C7-C8-C9	-2.13	123.02	126.23
15	aA	814	CLA	CHB-C1B-NB	2.13	126.51	124.26
15	a5	407	CLA	CHB-C1B-NB	2.13	126.51	124.26
15	c6	406	CLA	CHC-C4B-NB	2.13	126.51	124.26
15	b2	410	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
15	c3	417	CLA	C3C-C4C-NC	-2.13	108.19	110.57
15	b3	411	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
15	c2	407	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
15	a3	406	CLA	CHC-C4B-NB	2.13	126.51	124.26
15	b2	408	CLA	CHB-C1B-NB	2.13	126.51	124.26
15	c4	403	CLA	CHB-C1B-NB	2.13	126.51	124.26
15	bB	836	CLA	CBC-CAC-C3C	2.13	118.29	112.43
15	a6	407	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
18	b1	419	BCR	C16-C15-C14	-2.13	119.12	123.47
15	bB	811	CLA	CAC-C3C-C4C	2.12	127.57	124.81
15	a1	401	CLA	C3B-C4B-NB	-2.12	108.54	110.52
18	c1	401	BCR	C34-C9-C10	-2.12	119.95	122.92
15	cB	809	CLA	CHC-C4B-NB	2.12	126.51	124.26
15	cB	841	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	cJ	101	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	b4	412	CLA	CHC-C1C-NC	2.12	127.43	124.20
18	a2	401	BCR	C24-C23-C22	-2.12	123.03	126.23
15	b2	413	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a3	405	CLA	CHB-C4A-NA	2.12	127.45	124.51
15	aK	102	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	cK	102	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	c2	412	CLA	C2A-C1A-CHA	2.12	127.57	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cB	846	BCR	C35-C13-C14	-2.12	119.95	122.92
15	cB	830	CLA	O2A-C1-C2	-2.12	103.06	108.64
15	c3	409	CLA	CMB-C2B-C3B	2.12	131.73	126.59
15	cB	838	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
15	bA	803	CLA	O1D-CGD-CBD	2.12	128.83	124.48
15	aB	814	CLA	CHB-C4A-NA	2.12	127.45	124.51
15	aB	829	CLA	C3B-C4B-NB	-2.12	108.55	110.52
15	c1	410	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	aB	833	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a1	407	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	a4	412	CLA	CHC-C1C-NC	2.12	127.42	124.20
18	b4	420	BCR	C24-C23-C22	-2.12	123.03	126.23
15	cA	827	CLA	O2D-CGD-CBD	2.12	115.04	111.27
15	b1	405	CLA	CMA-C3A-C4A	2.12	117.47	111.77
18	b5	418	BCR	C38-C26-C27	-2.12	109.54	113.62
15	aJ	202	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	cJ	101	CLA	C2A-C1A-CHA	2.12	127.57	123.86
15	b6	417	CLA	CMD-C2D-C3D	2.12	132.49	127.61
18	b6	420	BCR	C7-C8-C9	-2.12	123.03	126.23
18	b2	421	BCR	C1-C6-C5	-2.12	119.63	122.61
15	c3	410	CLA	C3B-C4B-NB	-2.12	108.55	110.52
15	cB	829	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
15	aB	805	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
15	cB	838	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	c2	419	BCR	C38-C26-C27	-2.12	109.54	113.62
15	aB	809	CLA	CHC-C4B-NB	2.12	126.50	124.26
15	c6	411	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	c3	401	BCR	C29-C30-C25	2.12	113.74	110.48
18	bB	846	BCR	C35-C13-C14	-2.12	119.95	122.92
15	a4	417	CLA	C3C-C4C-NC	-2.12	108.19	110.57
15	aB	804	CLA	C2A-C1A-CHA	2.12	127.56	123.86
15	aA	823	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	a1	416	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
15	c1	412	CLA	CHC-C1C-NC	2.12	127.42	124.20
18	cF	202	BCR	C7-C8-C9	-2.12	123.03	126.23
15	bB	838	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	aB	829	CLA	CMB-C2B-C3B	2.12	131.72	126.59
15	bA	827	CLA	O2D-CGD-CBD	2.12	115.03	111.27
15	b4	403	CLA	CHB-C1B-NB	2.12	126.50	124.26
15	bB	825	CLA	C2D-C1D-ND	-2.12	108.54	110.10
15	b3	402	CLA	C3B-C4B-NB	-2.12	108.55	110.52
15	c3	413	CLA	C3B-C4B-NB	-2.12	108.55	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	835	CLA	CHC-C4B-NB	2.12	126.50	124.26
18	bF	202	BCR	C2-C1-C6	2.12	113.74	110.48
15	cB	830	CLA	CMC-C2C-C3C	2.12	131.87	126.12
15	b2	413	CLA	CHD-C4C-C3C	2.12	127.95	124.84
15	bA	834	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	bB	845	BCR	C39-C30-C25	2.12	113.73	110.30
15	a5	417	CLA	C3A-C2A-C1A	2.12	104.51	101.34
15	aK	102	CLA	CHC-C4B-NB	2.12	126.50	124.26
15	a4	404	CLA	CHC-C4B-NB	2.12	126.50	124.26
15	a1	411	CLA	C3C-C4C-NC	-2.12	108.20	110.57
15	cA	834	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	bJ	103	BCR	C38-C26-C27	-2.12	109.55	113.62
15	c6	412	CLA	CMB-C2B-C3B	2.12	131.71	126.59
15	bB	830	CLA	CMC-C2C-C3C	2.12	131.86	126.12
18	aJ	204	BCR	C38-C26-C27	-2.12	109.55	113.62
15	bB	808	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
15	c5	407	CLA	O2A-CGA-O1A	-2.12	118.03	123.30
15	b1	410	CLA	C2A-C1A-CHA	2.12	127.56	123.86
15	cA	812	CLA	O1A-CGA-CBA	2.12	131.99	123.73
18	a6	420	BCR	C1-C6-C5	-2.12	119.63	122.61
15	aA	815	CLA	CHD-C1D-ND	-2.12	122.51	124.45
15	bX	102	CLA	O1D-CGD-CBD	2.11	128.81	124.48
18	aM	101	BCR	C16-C17-C18	-2.11	124.29	127.31
15	bB	814	CLA	CHB-C4A-NA	2.11	127.44	124.51
18	b6	401	BCR	C40-C30-C25	2.11	113.73	110.30
18	c5	401	BCR	C40-C30-C25	2.11	113.73	110.30
15	c2	410	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	bB	822	CLA	C3B-C4B-NB	-2.11	108.55	110.52
15	c5	405	CLA	CHB-C4A-NA	2.11	127.44	124.51
18	cM	101	BCR	C40-C30-C25	2.11	113.73	110.30
15	a5	405	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	a2	421	BCR	C1-C6-C5	-2.11	119.64	122.61
15	b1	415	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	a5	401	BCR	C16-C15-C14	-2.11	119.15	123.47
15	aA	815	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
15	a4	416	CLA	C1C-C2C-C3C	-2.11	104.73	106.96
15	cB	804	CLA	C2A-C1A-CHA	2.11	127.55	123.86
18	c3	420	BCR	C1-C6-C5	-2.11	119.64	122.61
15	a1	409	CLA	CHA-C1A-NA	-2.11	121.56	126.40
15	a6	412	CLA	CHD-C1D-ND	-2.11	122.51	124.45
15	b3	411	CLA	CHD-C1D-ND	-2.11	122.51	124.45
15	aB	827	CLA	CAA-C2A-C3A	-2.11	106.99	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c3	408	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
15	a6	422	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	cB	805	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
15	cA	823	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
15	cB	825	CLA	C2D-C1D-ND	-2.11	108.55	110.10
15	aB	830	CLA	O2A-C1-C2	-2.11	103.09	108.64
15	b5	413	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	b3	405	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	aA	850	BCR	C27-C26-C25	2.11	125.80	122.73
18	a6	421	BCR	C2-C3-C4	2.11	116.09	111.38
18	cJ	103	BCR	C38-C26-C27	-2.11	109.56	113.62
15	cB	802	CLA	C2B-C1B-NB	-2.11	108.82	110.23
15	aA	827	CLA	O2D-CGD-CBD	2.11	115.02	111.27
15	cB	829	CLA	O2D-CGD-CBD	2.11	115.02	111.27
15	c1	417	CLA	CHD-C1D-ND	-2.11	122.52	124.45
15	b4	405	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
15	cB	803	CLA	CMD-C2D-C3D	2.11	132.47	127.61
15	c6	418	CLA	CMD-C2D-C3D	2.11	132.47	127.61
15	aA	813	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	bB	830	CLA	CHB-C4A-NA	2.11	127.43	124.51
15	a3	413	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	cA	807	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	bA	808	CLA	O2D-CGD-CBD	2.11	115.02	111.27
14	aA	801	CL0	C2A-C1A-CHA	-2.11	120.17	123.86
15	cA	807	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
15	cB	808	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
15	cB	822	CLA	CMB-C2B-C3B	2.11	131.70	126.59
18	b4	401	BCR	C27-C26-C25	2.11	125.79	122.73
15	aJ	203	CLA	C3B-C4B-NB	-2.11	108.56	110.52
18	b4	420	BCR	C11-C10-C9	-2.11	124.30	127.31
15	aA	803	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	aA	808	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
15	bB	830	CLA	O2A-C1-C2	-2.11	103.09	108.64
18	c4	420	BCR	C1-C6-C5	-2.11	119.64	122.61
15	a3	405	CLA	CMA-C3A-C4A	2.11	117.44	111.77
15	bB	829	CLA	O2D-CGD-CBD	2.11	115.01	111.27
15	bK	101	CLA	C2A-C1A-CHA	2.11	127.55	123.86
15	cB	819	CLA	C2A-C1A-CHA	2.11	127.55	123.86
15	bA	812	CLA	O1A-CGA-CBA	2.11	131.96	123.73
15	aA	803	CLA	O1D-CGD-CBD	2.11	128.80	124.48
15	aB	830	CLA	CMC-C2C-C3C	2.11	131.84	126.12
15	bA	815	CLA	O2A-CGA-O1A	-2.11	118.05	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bL	202	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
15	b3	421	CLA	C16-C15-C13	-2.11	109.11	115.92
15	a4	416	CLA	CMD-C2D-C3D	2.11	132.46	127.61
18	a6	401	BCR	C3-C4-C5	-2.11	110.31	114.08
15	c2	408	CLA	CHB-C1B-NB	2.11	126.49	124.26
15	c4	404	CLA	O1D-CGD-CBD	2.11	128.80	124.48
16	aA	846	PQN	C14-C13-C15	2.11	118.82	115.27
15	c3	403	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
15	aB	838	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
18	aM	101	BCR	C40-C30-C25	2.11	113.72	110.30
15	b1	405	CLA	CHB-C4A-NA	2.11	127.42	124.51
15	bA	811	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	b4	413	CLA	CHC-C4B-NB	2.11	126.49	124.26
15	aX	102	CLA	O1D-CGD-CBD	2.11	128.79	124.48
15	cB	841	CLA	C2A-C1A-CHA	2.11	127.54	123.86
18	bA	851	BCR	C27-C26-C25	2.11	125.79	122.73
15	cA	803	CLA	C11-C12-C13	-2.11	109.11	115.92
15	a5	408	CLA	CAA-CBA-CGA	2.11	118.10	112.51
15	aA	803	CLA	C11-C12-C13	-2.11	109.11	115.92
15	bB	805	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
15	cB	834	CLA	CHD-C1D-ND	-2.11	122.52	124.45
15	cA	815	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
15	aA	812	CLA	O1A-CGA-CBA	2.11	131.95	123.73
15	c6	407	CLA	CHC-C1C-NC	2.11	127.40	124.20
15	c5	411	CLA	C2A-C1A-CHA	2.11	127.54	123.86
15	bB	838	CLA	O2D-CGD-CBD	2.10	115.01	111.27
18	b6	401	BCR	C3-C4-C5	-2.10	110.32	114.08
15	aA	807	CLA	CHC-C4B-NB	2.10	126.48	124.26
15	bA	815	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	a1	417	BCR	C15-C14-C13	-2.10	124.31	127.31
15	a2	411	CLA	C3B-C4B-NB	-2.10	108.56	110.52
15	c2	405	CLA	C3B-C4B-NB	-2.10	108.56	110.52
15	c6	404	CLA	C3B-C4B-NB	-2.10	108.56	110.52
15	b6	405	CLA	CHC-C4B-NB	2.10	126.48	124.26
15	b4	412	CLA	C3C-C4C-NC	-2.10	108.21	110.57
15	bB	819	CLA	C2A-C1A-CHA	2.10	127.54	123.86
14	cA	801	CL0	C2A-C1A-CHA	-2.10	120.18	123.86
15	cB	812	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	bB	822	CLA	CMB-C2B-C3B	2.10	131.68	126.59
15	a2	410	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
15	b4	404	CLA	CHC-C4B-NB	2.10	126.48	124.26
15	cA	803	CLA	O1D-CGD-CBD	2.10	128.79	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	415	CLA	O2D-CGD-CBD	2.10	115.00	111.27
15	bB	841	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	aB	812	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	b2	404	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
15	b1	417	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
18	bB	849	BCR	C24-C23-C22	-2.10	123.06	126.23
15	aA	808	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	b1	419	BCR	C40-C30-C25	2.10	113.71	110.30
15	b1	417	CLA	C3C-C4C-NC	-2.10	108.21	110.57
15	a1	405	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
15	c4	405	CLA	CHC-C1C-NC	2.10	127.39	124.20
18	c1	419	BCR	C40-C30-C25	2.10	113.71	110.30
15	aB	811	CLA	CAC-C3C-C4C	2.10	127.54	124.81
15	bB	803	CLA	CMD-C2D-C3D	2.10	132.45	127.61
15	cB	811	CLA	C7-C6-C5	-2.10	107.65	113.36
15	c3	411	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	a3	406	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
15	c5	403	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	bA	845	CLA	CMB-C2B-C3B	2.10	131.68	126.59
15	cB	827	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	a5	411	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	aA	845	CLA	CMB-C2B-C3B	2.10	131.67	126.59
18	c6	421	BCR	C7-C8-C9	-2.10	123.06	126.23
15	aA	811	CLA	C3B-C4B-NB	-2.10	108.57	110.52
15	a4	408	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
15	c1	412	CLA	C3C-C4C-NC	-2.10	108.22	110.57
15	c2	405	CLA	CMA-C3A-C4A	2.10	117.41	111.77
15	aB	802	CLA	C2B-C1B-NB	-2.10	108.83	110.23
15	bJ	102	CLA	C3B-C4B-NB	-2.10	108.57	110.52
18	cJ	103	BCR	C40-C30-C25	2.10	113.70	110.30
15	a3	421	CLA	C11-C10-C8	-2.10	109.14	115.92
15	bA	803	CLA	C11-C12-C13	-2.10	109.14	115.92
15	c5	417	CLA	C3C-C4C-NC	-2.10	108.22	110.57
15	b1	410	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	aI	101	BCR	C27-C26-C25	2.10	125.78	122.73
15	bK	101	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	b6	401	BCR	C7-C8-C9	-2.10	123.06	126.23
15	b2	418	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
15	a6	403	CLA	C3B-C4B-NB	-2.10	108.57	110.52
15	cA	817	CLA	C3B-C4B-NB	-2.10	108.57	110.52
15	a4	404	CLA	O1D-CGD-CBD	2.10	128.78	124.48
15	aB	827	CLA	C16-C15-C13	-2.10	109.14	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	416	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
15	aB	822	CLA	CMB-C2B-C3B	2.10	131.67	126.59
18	bJ	103	BCR	C40-C30-C25	2.10	113.70	110.30
15	cA	844	CLA	O2D-CGD-CBD	2.10	115.00	111.27
15	a5	404	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	bA	807	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
18	c6	402	BCR	C3-C4-C5	-2.10	110.33	114.08
15	a6	412	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
15	a6	406	CLA	CHC-C1C-NC	2.10	127.38	124.20
15	a3	409	CLA	O1D-CGD-CBD	2.10	128.77	124.48
18	a6	401	BCR	C7-C8-C9	-2.10	123.07	126.23
15	c6	415	CLA	CHD-C1D-C2D	2.10	129.88	125.48
15	cA	808	CLA	O2D-CGD-CBD	2.10	114.99	111.27
18	b2	401	BCR	C28-C27-C26	-2.10	110.33	114.08
18	b6	402	BCR	C28-C27-C26	-2.10	110.33	114.08
18	c6	403	BCR	C28-C27-C26	-2.10	110.33	114.08
18	a1	418	BCR	C16-C15-C14	-2.10	119.18	123.47
15	aJ	202	CLA	O2D-CGD-CBD	2.10	114.99	111.27
15	b3	421	CLA	O2D-CGD-CBD	2.10	114.99	111.27
18	a6	402	BCR	C28-C27-C26	-2.10	110.33	114.08
15	a5	405	CLA	CED-O2D-CGD	-2.10	111.20	115.94
15	a3	410	CLA	C3B-C4B-NB	-2.10	108.57	110.52
15	a3	408	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
18	aF	203	BCR	C15-C16-C17	-2.10	119.18	123.47
15	bA	808	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
18	b3	418	BCR	C16-C15-C14	-2.09	119.18	123.47
15	a5	411	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	bB	827	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
15	bB	829	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
15	a1	408	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
15	b3	413	CLA	C3B-C4B-NB	-2.09	108.57	110.52
15	a2	405	CLA	CMA-C3A-C4A	2.09	117.40	111.77
15	a4	403	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	aB	849	BCR	C16-C17-C18	-2.09	124.32	127.31
15	bB	811	CLA	C7-C6-C5	-2.09	107.67	113.36
15	cA	813	CLA	CHA-C1A-NA	-2.09	121.60	126.40
18	cF	204	BCR	C31-C1-C6	2.09	113.69	110.30
15	cA	844	CLA	CMB-C2B-C3B	2.09	131.66	126.59
15	cK	102	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	a6	412	CLA	CAA-CBA-CGA	2.09	118.06	112.51
15	c1	417	CLA	C3C-C4C-NC	-2.09	108.22	110.57
15	aA	845	CLA	O2D-CGD-CBD	2.09	114.99	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bJ	105	BCR	C15-C16-C17	-2.09	119.19	123.47
15	aA	807	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
15	bB	833	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
18	bM	101	BCR	C16-C17-C18	-2.09	124.33	127.31
18	c4	420	BCR	C11-C10-C9	-2.09	124.33	127.31
15	b5	411	CLA	C2A-C1A-CHA	2.09	127.52	123.86
15	a6	417	CLA	CMD-C2D-C3D	2.09	132.43	127.61
15	c1	417	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
15	b5	405	CLA	CMA-C3A-C4A	2.09	117.39	111.77
15	c3	405	CLA	CMA-C3A-C4A	2.09	117.39	111.77
15	bA	807	CLA	CHC-C4B-NB	2.09	126.47	124.26
18	cM	101	BCR	C16-C17-C18	-2.09	124.33	127.31
15	cA	808	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
15	bJ	101	CLA	C2A-C1A-CHA	2.09	127.51	123.86
15	b5	405	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
15	b3	406	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
15	bA	821	CLA	CHC-C4B-NB	2.09	126.47	124.26
15	c4	406	CLA	CHB-C1B-NB	2.09	126.47	124.26
18	aB	845	BCR	C39-C30-C25	2.09	113.69	110.30
15	b1	414	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
15	b3	417	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	c4	402	CLA	C3B-C4B-NB	-2.09	108.58	110.52
15	b1	412	CLA	CHC-C1C-NC	2.09	127.37	124.20
18	bA	848	BCR	C11-C10-C9	-2.09	124.33	127.31
15	c1	406	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
15	aB	834	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	b5	411	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	cL	202	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	bA	802	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	b4	410	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	bB	829	CLA	C3B-C4B-NB	-2.09	108.58	110.52
15	cA	826	CLA	C3B-C4B-NB	-2.09	108.58	110.52
15	c3	402	CLA	C3B-C4B-NB	-2.09	108.58	110.52
15	aA	808	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
15	bA	823	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	b6	407	CLA	CHB-C1B-NB	2.09	126.47	124.26
15	c6	401	CLA	CHC-C4B-NB	2.09	126.47	124.26
15	a3	412	CLA	C3C-C4C-NC	-2.09	108.23	110.57
15	b5	409	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	c2	417	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
15	bB	812	CLA	CHA-C1A-NA	-2.09	121.62	126.40
18	aK	101	BCR	C29-C30-C25	2.09	113.69	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b6	412	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	c2	421	BCR	C1-C6-C5	-2.09	119.67	122.61
15	b3	409	CLA	CMB-C2B-C3B	2.09	131.64	126.59
18	bF	202	BCR	C23-C22-C21	-2.09	115.74	118.94
15	aB	803	CLA	CMD-C2D-C3D	2.09	132.41	127.61
15	b4	405	CLA	CMA-C3A-C4A	2.09	117.38	111.77
15	b1	404	CLA	O1D-CGD-CBD	2.09	128.75	124.48
18	a1	418	BCR	C7-C8-C9	-2.09	123.08	126.23
19	cX	101	LHG	O8-C23-C24	2.09	121.48	112.38
15	b6	410	CLA	O1D-CGD-CBD	2.09	128.75	124.48
15	bB	803	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	c4	411	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
15	b2	405	CLA	CMA-C3A-C4A	2.09	117.38	111.77
15	bA	811	CLA	C3B-C4B-NB	-2.09	108.58	110.52
15	a3	403	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
15	cA	821	CLA	CHC-C4B-NB	2.09	126.47	124.26
18	a3	418	BCR	C1-C6-C5	-2.09	119.68	122.61
15	cB	803	CLA	C6-C7-C8	-2.09	109.18	115.92
15	b1	406	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
18	cF	205	BCR	C15-C16-C17	-2.09	119.20	123.47
15	bA	813	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	bB	834	CLA	CHD-C1D-ND	-2.08	122.54	124.45
15	a3	406	CLA	CHB-C1B-NB	2.08	126.46	124.26
15	bL	204	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	bB	827	CLA	C16-C15-C13	-2.08	109.18	115.92
15	b5	407	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
15	b5	420	CLA	O2D-CGD-CBD	2.08	114.97	111.27
18	aJ	204	BCR	C40-C30-C25	2.08	113.68	110.30
15	b3	416	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	b6	412	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	b2	408	CLA	CMB-C2B-C3B	2.08	131.63	126.59
15	c3	404	CLA	C2A-C1A-CHA	2.08	127.50	123.86
15	aA	841	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	bA	808	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
18	b3	418	BCR	C7-C8-C9	-2.08	123.09	126.23
15	cB	833	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
15	aK	102	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	cA	841	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	a6	415	CLA	CHB-C1B-NB	2.08	126.46	124.26
15	c4	407	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
15	b3	421	CLA	C11-C10-C8	-2.08	109.19	115.92
15	b3	408	CLA	O2A-CGA-O1A	-2.08	118.11	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a5	405	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
15	aB	841	CLA	C2A-C1A-CHA	2.08	127.50	123.86
18	bF	202	BCR	C31-C1-C6	2.08	113.68	110.30
15	c3	408	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
15	c6	413	CLA	CAA-CBA-CGA	2.08	118.03	112.51
15	aB	814	CLA	O1D-CGD-CBD	2.08	128.74	124.48
15	c6	401	CLA	C16-C15-C13	-2.08	109.19	115.92
15	c5	405	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
18	c4	418	BCR	C1-C6-C5	-2.08	119.68	122.61
15	a2	405	CLA	CHB-C4A-NA	2.08	127.39	124.51
15	cA	802	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	aL	201	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
15	aB	827	CLA	CHC-C4B-NB	2.08	126.46	124.26
15	b2	406	CLA	CHB-C1B-NB	2.08	126.46	124.26
18	b6	420	BCR	C1-C6-C5	-2.08	119.68	122.61
18	c5	401	BCR	C16-C15-C14	-2.08	119.21	123.47
15	c5	405	CLA	O1D-CGD-CBD	2.08	128.74	124.48
15	aB	825	CLA	C2D-C1D-ND	-2.08	108.57	110.10
15	aB	803	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	a4	407	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
15	cA	815	CLA	CHB-C1B-NB	2.08	126.46	124.26
15	cA	808	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
15	c4	405	CLA	CED-O2D-CGD	-2.08	111.23	115.94
15	b1	410	CLA	CMB-C2B-C3B	2.08	131.62	126.59
18	a5	418	BCR	C38-C26-C27	-2.08	109.62	113.62
15	a5	405	CLA	C3B-C4B-NB	-2.08	108.59	110.52
15	aB	833	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
15	c6	413	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
15	a4	405	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
15	a2	406	CLA	CHB-C1B-NB	2.08	126.46	124.26
15	cB	827	CLA	C16-C15-C13	-2.08	109.20	115.92
15	b1	415	CLA	CHA-C4D-ND	2.08	136.85	132.50
15	b6	414	CLA	CHD-C1D-C2D	2.08	129.84	125.48
15	b6	403	CLA	C3B-C4B-NB	-2.08	108.59	110.52
15	b4	407	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
15	a3	407	CLA	CHB-C1B-NB	2.08	126.46	124.26
15	a5	413	CLA	CHC-C4B-NB	2.08	126.46	124.26
15	a6	405	CLA	CHC-C4B-NB	2.08	126.46	124.26
15	aB	803	CLA	C6-C7-C8	-2.08	109.20	115.92
15	a4	405	CLA	CMA-C3A-C4A	2.08	117.36	111.77
15	b5	405	CLA	CED-O2D-CGD	-2.08	111.24	115.94
15	b4	416	CLA	C1C-C2C-C3C	-2.08	104.77	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	aA	846	PQN	C17-C16-C15	-2.08	107.72	113.36
15	b3	410	CLA	C3B-C4B-NB	-2.08	108.59	110.52
18	b1	420	BCR	C16-C15-C14	-2.08	119.22	123.47
15	c4	405	CLA	CMA-C3A-C4A	2.08	117.36	111.77
15	aB	815	CLA	CMB-C2B-C3B	2.08	131.62	126.59
15	a1	405	CLA	CMB-C2B-C3B	2.08	131.62	126.59
19	bX	101	LHG	O8-C23-C24	2.08	121.44	112.38
15	aA	802	CLA	CHA-C1A-NA	-2.08	121.64	126.40
15	b5	420	CLA	O1D-CGD-CBD	2.08	128.73	124.48
15	c5	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
18	aF	202	BCR	C23-C22-C21	-2.08	115.75	118.94
15	b4	409	CLA	O1D-CGD-CBD	2.08	128.73	124.48
15	a3	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
15	bA	841	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
18	aA	851	BCR	C31-C1-C6	2.08	113.67	110.30
15	c4	416	CLA	CMD-C2D-C3D	2.08	132.39	127.61
15	a3	421	CLA	O2D-CGD-CBD	2.08	114.96	111.27
18	c1	419	BCR	C7-C8-C9	-2.08	123.10	126.23
18	a5	401	BCR	C40-C30-C25	2.08	113.67	110.30
15	b5	411	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
15	bB	824	CLA	O1A-CGA-CBA	2.07	129.75	123.08
15	cB	824	CLA	O1A-CGA-CBA	2.07	129.75	123.08
15	aL	203	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
18	c2	419	BCR	C11-C10-C9	-2.07	124.35	127.31
15	c3	421	CLA	C11-C10-C8	-2.07	109.21	115.92
15	a6	405	CLA	C2A-C1A-CHA	2.07	127.49	123.86
15	b3	404	CLA	C2A-C1A-CHA	2.07	127.49	123.86
15	aB	823	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	c3	411	CLA	CHD-C1D-ND	-2.07	122.55	124.45
15	a3	409	CLA	CMB-C2B-C3B	2.07	131.61	126.59
15	b2	410	CLA	CMB-C2B-C3B	2.07	131.61	126.59
18	c1	418	BCR	C16-C15-C14	-2.07	119.23	123.47
15	b4	416	CLA	CMD-C2D-C3D	2.07	132.38	127.61
15	c1	416	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	b4	417	CLA	C2D-C1D-ND	-2.07	108.58	110.10
18	cB	845	BCR	C39-C30-C25	2.07	113.66	110.30
18	c4	420	BCR	C24-C23-C22	-2.07	123.10	126.23
18	a6	421	BCR	C28-C27-C26	-2.07	110.38	114.08
19	aX	101	LHG	O8-C23-C24	2.07	121.42	112.38
15	b3	408	CLA	C3C-C4C-NC	-2.07	108.25	110.57
15	c6	414	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
15	aB	822	CLA	C3B-C4B-NB	-2.07	108.59	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	412	CLA	C3B-C4B-NB	-2.07	108.59	110.52
15	bA	808	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	bB	809	CLA	CHC-C4B-NB	2.07	126.45	124.26
15	cA	808	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	cA	840	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	cB	818	CLA	CHC-C4B-NB	2.07	126.45	124.26
15	c5	403	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	c6	404	CLA	CHC-C4B-NB	2.07	126.45	124.26
15	a4	410	CLA	CHA-C1A-NA	-2.07	121.65	126.40
15	c4	412	CLA	C3C-C4C-NC	-2.07	108.25	110.57
15	b3	403	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	aB	838	CLA	C3B-C4B-NB	-2.07	108.59	110.52
15	bB	815	CLA	CMB-C2B-C3B	2.07	131.60	126.59
15	bA	840	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	cA	835	CLA	CHC-C4B-NB	2.07	126.45	124.26
15	aX	102	CLA	C2A-C1A-CHA	2.07	127.48	123.86
15	b5	409	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
15	aB	824	CLA	O1A-CGA-CBA	2.07	129.73	123.08
15	c1	406	CLA	CMB-C2B-C3B	2.07	131.60	126.59
15	bA	845	CLA	O2D-CGD-CBD	2.07	114.95	111.27
15	b3	408	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
15	cA	815	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	c2	401	BCR	C31-C1-C6	2.07	113.66	110.30
15	bB	803	CLA	C6-C7-C8	-2.07	109.23	115.92
18	a4	401	BCR	C27-C26-C25	2.07	125.73	122.73
15	a1	414	CLA	CHA-C4D-ND	2.07	136.83	132.50
15	cB	830	CLA	CHB-C4A-NA	2.07	127.37	124.51
15	b5	415	CLA	O2D-CGD-CBD	2.07	114.94	111.27
15	b1	406	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	b6	403	CLA	CHC-C4B-NB	2.07	126.45	124.26
15	c3	406	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
18	b1	418	BCR	C1-C6-C5	-2.07	119.70	122.61
15	b5	405	CLA	C3B-C4B-NB	-2.07	108.60	110.52
15	a2	405	CLA	CHA-C4D-ND	2.07	136.83	132.50
15	c3	405	CLA	CHA-C4D-ND	2.07	136.82	132.50
15	bB	814	CLA	O1D-CGD-CBD	2.07	128.72	124.48
18	a4	420	BCR	C11-C10-C9	-2.07	124.36	127.31
15	aA	840	CLA	CHB-C1B-NB	2.07	126.45	124.26
15	a3	405	CLA	C3B-C4B-NB	-2.07	108.60	110.52
15	b2	411	CLA	C3B-C4B-NB	-2.07	108.60	110.52
15	b6	412	CLA	C3B-C4B-NB	-2.07	108.60	110.52
15	bB	802	CLA	C2B-C1B-NB	-2.07	108.85	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	aF	201	BCR	C38-C26-C27	-2.07	109.64	113.62
15	cA	821	CLA	CHC-C1C-NC	2.07	127.34	124.20
15	a2	413	CLA	CHD-C4C-C3C	2.07	127.88	124.84
15	a2	408	CLA	CHB-C1B-NB	2.07	126.44	124.26
15	cB	819	CLA	CHB-C1B-NB	2.07	126.44	124.26
18	bA	852	BCR	C16-C15-C14	-2.07	119.24	123.47
15	a5	405	CLA	O1D-CGD-CBD	2.07	128.71	124.48
14	bA	801	CL0	C2A-C1A-CHA	-2.07	120.25	123.86
15	a6	414	CLA	CHD-C4C-C3C	2.07	127.88	124.84
16	bA	846	PQN	C17-C16-C15	-2.07	107.75	113.36
15	a1	405	CLA	CHB-C1B-NB	2.07	126.44	124.26
18	c6	421	BCR	C1-C6-C5	-2.07	119.70	122.61
18	b1	419	BCR	C7-C8-C9	-2.07	123.11	126.23
18	b5	401	BCR	C16-C15-C14	-2.07	119.24	123.47
15	c4	410	CLA	CHA-C1A-NA	-2.07	121.67	126.40
15	cJ	102	CLA	C3B-C4B-NB	-2.07	108.60	110.52
15	b5	404	CLA	C2A-C1A-CHA	2.07	127.47	123.86
15	bK	101	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	cB	827	CLA	CHC-C4B-NB	2.06	126.44	124.26
15	b1	416	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	aF	202	BCR	C31-C1-C6	2.06	113.65	110.30
15	aA	832	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
18	c2	401	BCR	C28-C27-C26	-2.06	110.39	114.08
15	c6	413	CLA	C3B-C4B-NB	-2.06	108.60	110.52
15	cB	815	CLA	CMB-C2B-C3B	2.06	131.59	126.59
15	b5	403	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
15	aB	829	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
18	b5	419	BCR	C1-C6-C5	-2.06	119.71	122.61
15	cA	832	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
15	b5	416	CLA	CMD-C2D-C3D	2.06	132.36	127.61
15	a3	403	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
15	aA	821	CLA	CHC-C4B-NB	2.06	126.44	124.26
15	bK	101	CLA	CHC-C4B-NB	2.06	126.44	124.26
16	cA	845	PQN	C17-C16-C15	-2.06	107.76	113.36
18	bA	852	BCR	C31-C1-C6	2.06	113.64	110.30
15	c2	403	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
15	a1	406	CLA	CHA-C1A-NA	-2.06	121.67	126.40
18	cF	202	BCR	C38-C26-C27	-2.06	109.65	113.62
15	cA	815	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	bB	818	CLA	CHC-C4B-NB	2.06	126.44	124.26
15	b3	407	CLA	CHB-C1B-NB	2.06	126.44	124.26
15	b5	403	CLA	CHB-C1B-NB	2.06	126.44	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	810	CLA	CAC-C3C-C4C	2.06	127.48	124.81
15	a2	410	CLA	CMB-C2B-C3B	2.06	131.58	126.59
15	b5	417	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	a1	421	BCR	C28-C27-C26	-2.06	110.40	114.08
18	c4	401	BCR	C27-C26-C25	2.06	125.72	122.73
18	aL	205	BCR	C11-C10-C9	-2.06	124.37	127.31
15	c2	404	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
15	c2	411	CLA	C3B-C4B-NB	-2.06	108.60	110.52
15	a5	416	CLA	CMD-C2D-C3D	2.06	132.35	127.61
15	c5	415	CLA	O2D-CGD-CBD	2.06	114.93	111.27
15	b1	405	CLA	CHC-C1C-NC	2.06	127.33	124.20
15	cB	803	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	a3	402	CLA	C3B-C4B-NB	-2.06	108.60	110.52
15	cA	819	CLA	CAC-C3C-C2C	-2.06	124.01	127.53
15	a5	411	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	a3	405	CLA	CHA-C4D-ND	2.06	136.81	132.50
15	bB	810	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	cA	850	BCR	C31-C1-C6	2.06	113.64	110.30
15	b3	403	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	cL	204	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
15	bX	102	CLA	C2A-C1A-CHA	2.06	127.46	123.86
18	cF	204	BCR	C23-C22-C21	-2.06	115.78	118.94
15	c2	410	CLA	CMB-C2B-C3B	2.06	131.57	126.59
15	a3	404	CLA	C2A-C1A-CHA	2.06	127.46	123.86
15	a5	407	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
18	bI	101	BCR	C27-C26-C25	2.06	125.72	122.73
15	bB	834	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	a4	418	BCR	C1-C6-C5	-2.06	119.72	122.61
15	a5	408	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
15	bA	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	b2	409	CLA	CHD-C1D-ND	-2.06	122.56	124.45
15	a1	413	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
15	bA	832	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	bB	823	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	c1	404	CLA	O1D-CGD-CBD	2.06	128.69	124.48
15	aA	808	CLA	O2D-CGD-CBD	2.06	114.92	111.27
15	aA	815	CLA	CHB-C1B-NB	2.06	126.44	124.26
15	c3	406	CLA	CHB-C1B-NB	2.06	126.44	124.26
15	b1	414	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
15	bA	821	CLA	CHC-C1C-NC	2.06	127.32	124.20
18	c5	418	BCR	C15-C16-C17	-2.06	119.26	123.47
15	a4	409	CLA	O1D-CGD-CBD	2.06	128.69	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	405	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
19	cA	852	LHG	C15-C14-C13	-2.06	103.98	114.42
15	c3	416	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	a5	406	CLA	CHB-C1B-NB	2.06	126.43	124.26
15	a6	403	CLA	CHC-C4B-NB	2.06	126.43	124.26
15	c2	406	CLA	CHB-C1B-NB	2.06	126.43	124.26
15	b2	403	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
15	a3	408	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
15	b5	403	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
15	a4	414	CLA	CHB-C1B-NB	2.06	126.43	124.26
15	b2	406	CLA	CHC-C4B-NB	2.06	126.43	124.26
15	c2	406	CLA	CHC-C4B-NB	2.06	126.43	124.26
15	c3	413	CLA	CHB-C1B-NB	2.06	126.43	124.26
15	a6	413	CLA	O2A-CGA-O1A	-2.06	118.18	123.30
15	aA	815	CLA	CHA-C1A-NA	-2.06	121.69	126.40
15	b3	405	CLA	CHA-C4D-ND	2.05	136.80	132.50
15	b1	408	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	c5	409	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
15	a2	413	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	cA	850	BCR	C16-C15-C14	-2.05	119.27	123.47
18	cI	101	BCR	C27-C26-C25	2.05	125.71	122.73
15	b5	417	CLA	C3A-C2A-C1A	2.05	104.42	101.34
15	c4	409	CLA	O1D-CGD-CBD	2.05	128.69	124.48
15	c1	402	CLA	C3B-C4B-NB	-2.05	108.61	110.52
15	aB	808	CLA	C7-C6-C5	-2.05	107.78	113.36
15	c5	411	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	bB	810	CLA	CAC-C3C-C4C	2.05	127.47	124.81
15	cB	807	CLA	CMB-C2B-C3B	2.05	131.56	126.59
15	cB	810	CLA	CAC-C3C-C4C	2.05	127.47	124.81
18	b5	401	BCR	C1-C6-C5	-2.05	119.72	122.61
15	c5	420	CLA	O1D-CGD-CBD	2.05	128.68	124.48
15	cB	841	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	c4	421	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
15	a3	410	CLA	C1D-ND-C4D	2.05	107.79	106.33
18	a1	421	BCR	C34-C9-C10	-2.05	120.05	122.92
15	cB	823	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
15	bB	818	CLA	C2A-C1A-CHA	2.05	127.44	123.86
15	a2	410	CLA	O1D-CGD-CBD	2.05	128.68	124.48
15	c1	407	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	aI	103	BCR	C7-C8-C9	-2.05	123.14	126.23
15	c1	403	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	b6	409	CLA	C3C-C4C-NC	-2.05	108.27	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	819	CLA	CHB-C1B-NB	2.05	126.43	124.26
15	b5	406	CLA	CHB-C1B-NB	2.05	126.43	124.26
19	aA	853	LHG	C15-C14-C13	-2.05	104.02	114.42
18	a5	419	BCR	C1-C6-C5	-2.05	119.73	122.61
15	c3	417	CLA	C2D-C1D-ND	-2.05	108.59	110.10
15	c5	420	CLA	CHA-C4D-ND	2.05	136.78	132.50
18	bB	849	BCR	C38-C26-C27	-2.05	109.68	113.62
15	bB	827	CLA	CHC-C4B-NB	2.05	126.43	124.26
15	a1	409	CLA	CMB-C2B-C3B	2.05	131.55	126.59
15	c1	405	CLA	CHB-C4A-NA	2.05	127.34	124.51
15	a4	415	CLA	O2D-CGD-CBD	2.05	114.91	111.27
15	b4	415	CLA	O2D-CGD-CBD	2.05	114.91	111.27
15	a5	403	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
15	a5	403	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
15	b6	406	CLA	CHC-C1C-NC	2.05	127.31	124.20
15	cA	831	CLA	CMC-C2C-C3C	2.05	131.68	126.12
15	aA	811	CLA	C2D-C1D-ND	-2.05	108.59	110.10
15	c3	411	CLA	C2A-C1A-CHA	2.05	127.44	123.86
15	a4	402	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	a5	420	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	b3	412	CLA	C3C-C4C-NC	-2.05	108.28	110.57
15	aB	819	CLA	CHB-C1B-NB	2.05	126.42	124.26
15	b3	404	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
15	a4	415	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
18	c2	419	BCR	C15-C16-C17	-2.05	119.28	123.47
15	c5	414	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	a1	417	BCR	C1-C6-C5	-2.05	119.73	122.61
15	a4	412	CLA	C3C-C4C-NC	-2.05	108.28	110.57
15	b2	410	CLA	O1D-CGD-CBD	2.05	128.67	124.48
18	bL	206	BCR	C11-C10-C9	-2.05	124.39	127.31
15	c5	405	CLA	CMA-C3A-C4A	2.05	117.27	111.77
15	b4	402	CLA	C3B-C4B-NB	-2.05	108.62	110.52
15	b2	404	CLA	O1D-CGD-CBD	2.05	128.67	124.48
15	b1	405	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
15	c4	402	CLA	O1D-CGD-CBD	2.05	128.67	124.48
18	aK	101	BCR	C11-C10-C9	-2.05	124.39	127.31
18	a1	419	BCR	C11-C10-C9	-2.05	124.39	127.31
15	b1	402	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
15	aA	842	CLA	CHA-C4D-ND	2.05	136.78	132.50
15	c4	415	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
15	b4	406	CLA	CHB-C1B-NB	2.05	126.42	124.26
18	aA	851	BCR	C16-C15-C14	-2.04	119.28	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	808	CLA	C7-C6-C5	-2.04	107.81	113.36
15	c1	411	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	b6	405	CLA	C2A-C1A-CHA	2.04	127.43	123.86
15	b2	417	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
15	a4	406	CLA	CHB-C1B-NB	2.04	126.42	124.26
15	c1	413	CLA	CHB-C1B-NB	2.04	126.42	124.26
15	c3	410	CLA	C1D-ND-C4D	2.04	107.79	106.33
15	cB	814	CLA	O1D-CGD-CBD	2.04	128.67	124.48
18	c3	418	BCR	C7-C8-C9	-2.04	123.15	126.23
18	cK	101	BCR	C29-C30-C25	2.04	113.63	110.48
15	bA	808	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	c5	403	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	c1	420	BCR	C16-C15-C14	-2.04	119.29	123.47
15	b5	405	CLA	O1D-CGD-CBD	2.04	128.66	124.48
19	bA	854	LHG	C15-C14-C13	-2.04	104.06	114.42
15	aA	831	CLA	CMC-C2C-C3C	2.04	131.66	126.12
15	bB	836	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	c6	406	CLA	C2A-C1A-CHA	2.04	127.43	123.86
15	a5	403	CLA	CHB-C1B-NB	2.04	126.42	124.26
15	bA	815	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	bB	845	BCR	C15-C16-C17	-2.04	119.29	123.47
18	a2	419	BCR	C11-C10-C9	-2.04	124.40	127.31
15	b5	405	CLA	CMB-C2B-C3B	2.04	131.53	126.59
18	cB	845	BCR	C15-C16-C17	-2.04	119.29	123.47
15	bB	841	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	b4	414	CLA	CHB-C1B-NB	2.04	126.42	124.26
15	aA	821	CLA	CHC-C1C-NC	2.04	127.30	124.20
15	c2	417	CLA	O2D-CGD-CBD	2.04	114.89	111.27
15	c3	405	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
18	a2	419	BCR	C15-C16-C17	-2.04	119.30	123.47
15	a1	415	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	b6	408	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	cK	101	BCR	C11-C10-C9	-2.04	124.40	127.31
15	aB	841	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	a5	404	CLA	O1D-CGD-CBD	2.04	128.66	124.48
18	c5	419	BCR	C1-C6-C5	-2.04	119.74	122.61
15	cA	829	CLA	C7-C6-C5	-2.04	107.82	113.36
15	cB	810	CLA	CHB-C1B-NB	2.04	126.42	124.26
15	aA	813	CLA	C1-C2-C3	-2.04	122.52	126.04
18	bA	848	BCR	C29-C30-C25	2.04	113.62	110.48
15	a3	405	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
15	c3	403	CLA	O2A-CGA-O1A	-2.04	118.45	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c4	404	CLA	CHC-C4B-NB	2.04	126.42	124.26
15	a3	408	CLA	C3C-C4C-NC	-2.04	108.28	110.57
15	cB	838	CLA	C3B-C4B-NB	-2.04	108.62	110.52
15	cX	102	CLA	C2A-C1A-CHA	2.04	127.42	123.86
15	b2	407	CLA	CMB-C2B-C3B	2.04	131.52	126.59
15	a1	402	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	cB	828	CLA	C2A-C1A-CHA	2.04	127.42	123.86
18	b3	420	BCR	C16-C15-C14	-2.04	119.30	123.47
15	c2	413	CLA	CHD-C4C-C3C	2.04	127.83	124.84
18	aA	850	BCR	C33-C5-C6	-2.04	122.24	124.53
15	a4	413	CLA	CHC-C4B-NB	2.04	126.41	124.26
15	c2	414	CLA	CHB-C1B-NB	2.04	126.41	124.26
15	c5	413	CLA	CHC-C4B-NB	2.04	126.41	124.26
18	cA	849	BCR	C28-C27-C26	-2.04	110.44	114.08
15	a3	404	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	c6	420	BCR	C1-C6-C5	-2.04	119.74	122.61
15	b6	416	CLA	C3B-C4B-NB	-2.04	108.62	110.52
15	cA	811	CLA	C3B-C4B-NB	-2.04	108.62	110.52
15	c2	405	CLA	CHA-C4D-ND	2.04	136.76	132.50
18	c1	418	BCR	C11-C10-C9	-2.04	124.40	127.31
15	a5	405	CLA	CMB-C2B-C3B	2.04	131.52	126.59
18	bA	851	BCR	C33-C5-C6	-2.04	122.24	124.53
15	b2	405	CLA	CHA-C4D-ND	2.04	136.76	132.50
15	c6	405	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
18	cB	849	BCR	C38-C26-C27	-2.04	109.70	113.62
15	cA	802	CLA	C3B-C4B-NB	-2.04	108.63	110.52
15	b6	404	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
15	cB	818	CLA	C2A-C1A-CHA	2.04	127.42	123.86
15	c5	404	CLA	C2A-C1A-CHA	2.04	127.42	123.86
18	b2	419	BCR	C1-C6-C5	-2.04	119.75	122.61
15	aA	819	CLA	CAC-C3C-C2C	-2.04	124.05	127.53
18	aA	850	BCR	C28-C27-C26	-2.04	110.44	114.08
15	a1	406	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	cL	205	BCR	C7-C8-C9	-2.04	123.16	126.23
15	b6	406	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	a1	419	BCR	C16-C15-C14	-2.04	119.30	123.47
15	a2	406	CLA	CHC-C4B-NB	2.04	126.41	124.26
15	c3	409	CLA	O1D-CGD-CBD	2.04	128.65	124.48
18	b5	401	BCR	C40-C30-C25	2.04	113.60	110.30
15	cF	201	CLA	CHA-C4D-ND	2.04	136.76	132.50
15	b1	412	CLA	C3C-C4C-NC	-2.03	108.29	110.57
15	aB	816	CLA	CHC-C4B-NB	2.03	126.41	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bJ	105	BCR	C1-C6-C5	-2.03	119.75	122.61
15	c2	407	CLA	CMB-C2B-C3B	2.03	131.51	126.59
15	bA	829	CLA	C7-C6-C5	-2.03	107.83	113.36
15	b2	405	CLA	CHB-C4A-NA	2.03	127.33	124.51
15	b3	405	CLA	CHB-C4A-NA	2.03	127.33	124.51
15	aB	807	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	cB	824	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	c5	408	CLA	C3B-C4B-NB	-2.03	108.63	110.52
18	c5	401	BCR	C1-C6-C5	-2.03	119.75	122.61
15	bB	812	CLA	CHB-C1B-NB	2.03	126.41	124.26
15	b3	405	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
15	b1	403	CLA	CHA-C1A-NA	-2.03	121.74	126.40
15	cA	806	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	cB	836	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
15	aB	824	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	cA	808	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	a2	419	BCR	C1-C6-C5	-2.03	119.75	122.61
18	bL	201	BCR	C11-C10-C9	-2.03	124.41	127.31
15	c4	413	CLA	CHB-C1B-NB	2.03	126.41	124.26
15	bL	204	CLA	CMB-C2B-C3B	2.03	131.51	126.59
15	c1	407	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
15	b3	409	CLA	O1D-CGD-CBD	2.03	128.64	124.48
15	a3	416	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	cB	807	CLA	C2D-C1D-ND	-2.03	108.61	110.10
15	bB	808	CLA	C7-C6-C5	-2.03	107.84	113.36
15	b5	403	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	b4	402	CLA	O1D-CGD-CBD	2.03	128.64	124.48
18	bL	205	BCR	C7-C8-C9	-2.03	123.17	126.23
18	a5	401	BCR	C1-C6-C5	-2.03	119.75	122.61
18	b3	418	BCR	C1-C6-C5	-2.03	119.75	122.61
18	b2	401	BCR	C31-C1-C6	2.03	113.59	110.30
15	bA	842	CLA	CHA-C4D-ND	2.03	136.75	132.50
18	b6	421	BCR	C28-C27-C26	-2.03	110.45	114.08
15	b6	406	CLA	CHA-C4D-ND	2.03	136.75	132.50
15	c1	410	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	bA	831	CLA	CMC-C2C-C3C	2.03	131.63	126.12
15	c3	421	CLA	O2D-CGD-CBD	2.03	114.88	111.27
18	bF	202	BCR	C33-C5-C6	-2.03	122.25	124.53
15	c2	409	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	b1	407	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	b1	407	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	b1	401	BCR	C40-C30-C25	2.03	113.59	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b1	402	CLA	C3B-C4B-NB	-2.03	108.63	110.52
15	b6	413	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
15	c2	405	CLA	CHB-C4A-NA	2.03	127.32	124.51
18	a3	418	BCR	C7-C8-C9	-2.03	123.17	126.23
15	aB	810	CLA	CHB-C1B-NB	2.03	126.40	124.26
15	aB	818	CLA	CHC-C4B-NB	2.03	126.40	124.26
15	a2	404	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	b6	405	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
18	a5	419	BCR	C16-C15-C14	-2.03	119.32	123.47
15	a6	406	CLA	CHB-C4A-NA	2.03	127.32	124.51
15	a3	417	CLA	CHD-C4C-NC	2.03	127.40	124.20
15	a5	409	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
18	b2	401	BCR	C29-C30-C25	2.03	113.60	110.48
15	a2	407	CLA	CMB-C2B-C3B	2.03	131.50	126.59
15	bB	807	CLA	CMB-C2B-C3B	2.03	131.50	126.59
15	a5	414	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	aL	201	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	a5	418	BCR	C15-C16-C17	-2.03	119.32	123.47
15	aB	818	CLA	C2A-C1A-CHA	2.03	127.40	123.86
15	a3	411	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	aI	101	BCR	C35-C13-C14	-2.03	120.08	122.92
15	a6	404	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
15	b1	411	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
15	aB	828	CLA	C2A-C1A-CHA	2.03	127.40	123.86
15	b5	407	CLA	CHB-C1B-NB	2.03	126.40	124.26
15	aL	203	CLA	CMB-C2B-C3B	2.03	131.50	126.59
18	a6	419	BCR	C1-C6-C5	-2.03	119.76	122.61
15	c6	406	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	bB	828	CLA	C2A-C1A-CHA	2.03	127.40	123.86
18	a2	401	BCR	C29-C30-C25	2.03	113.60	110.48
15	bA	844	CLA	CHC-C4B-NB	2.03	126.40	124.26
15	b3	408	CLA	CHC-C4B-NB	2.03	126.40	124.26
15	cA	843	CLA	CHC-C4B-NB	2.03	126.40	124.26
15	c3	407	CLA	CHB-C1B-NB	2.03	126.40	124.26
15	cF	201	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
18	c6	402	BCR	C7-C8-C9	-2.03	123.17	126.23
15	cB	827	CLA	CHA-C4D-ND	2.03	136.74	132.50
15	c6	407	CLA	CHB-C4A-NA	2.02	127.31	124.51
15	a6	406	CLA	CHA-C4D-ND	2.02	136.73	132.50
15	bA	817	CLA	C3B-C4B-NB	-2.02	108.64	110.52
15	aB	803	CLA	CHC-C4B-NB	2.02	126.40	124.26
15	c1	406	CLA	CHB-C1B-NB	2.02	126.40	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	801	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	aB	836	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
15	a2	417	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
15	aA	829	CLA	C7-C6-C5	-2.02	107.86	113.36
15	aB	807	CLA	CMB-C2B-C3B	2.02	131.49	126.59
18	bA	851	BCR	C28-C27-C26	-2.02	110.46	114.08
15	bL	202	CLA	CHA-C1A-NA	-2.02	121.76	126.40
15	cA	841	CLA	C11-C12-C13	-2.02	109.38	115.92
15	a1	416	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	cB	834	CLA	C3C-C4C-NC	-2.02	108.30	110.57
15	c5	416	CLA	CMD-C2D-C3D	2.02	132.27	127.61
15	c5	405	CLA	CMB-C2B-C3B	2.02	131.49	126.59
15	b3	417	CLA	CHD-C4C-NC	2.02	127.39	124.20
15	b6	417	CLA	O2D-CGD-CBD	2.02	114.86	111.27
15	aB	839	CLA	C7-C6-C5	-2.02	107.87	113.36
18	c1	418	BCR	C7-C8-C9	-2.02	123.18	126.23
15	a3	416	CLA	C3A-C2A-C1A	2.02	104.37	101.34
15	b4	415	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
15	a2	417	CLA	CHD-C4C-NC	-2.02	121.02	124.20
15	cA	811	CLA	C2D-C1D-ND	-2.02	108.61	110.10
15	a1	406	CLA	CHB-C1B-NB	2.02	126.40	124.26
15	a3	413	CLA	CHB-C1B-NB	2.02	126.40	124.26
15	cB	802	CLA	C1D-ND-C4D	-2.02	104.90	106.33
15	b5	404	CLA	O1D-CGD-CBD	2.02	128.62	124.48
15	a5	420	CLA	CHA-C4D-ND	2.02	136.73	132.50
18	a2	401	BCR	C31-C1-C6	2.02	113.58	110.30
15	cB	839	CLA	C7-C6-C5	-2.02	107.87	113.36
15	c6	408	CLA	CHB-C1B-NB	2.02	126.40	124.26
15	cL	202	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	a1	408	CLA	CMB-C2B-C3B	2.02	131.48	126.59
15	a2	411	CLA	CMB-C2B-C3B	2.02	131.48	126.59
18	aB	849	BCR	C38-C26-C27	-2.02	109.73	113.62
15	b5	406	CLA	O1A-CGA-CBA	2.02	129.57	123.08
15	c6	413	CLA	CHD-C1D-ND	-2.02	122.60	124.45
15	aB	838	CLA	CHC-C4B-NB	2.02	126.39	124.26
15	b5	420	CLA	CGD-CBD-CAD	-2.02	104.19	110.73
15	bA	819	CLA	CAC-C3C-C2C	-2.02	124.08	127.53
18	cB	847	BCR	C40-C30-C39	-2.02	102.33	108.53
18	a4	401	BCR	C16-C15-C14	-2.02	119.34	123.47
18	b5	418	BCR	C15-C14-C13	-2.02	124.43	127.31
18	aB	847	BCR	C40-C30-C39	-2.02	102.33	108.53
15	b5	408	CLA	O2A-CGA-O1A	-2.02	118.27	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	839	CLA	C7-C6-C5	-2.02	107.88	113.36
15	c1	415	CLA	CHA-C4D-ND	2.02	136.72	132.50
15	c1	405	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
15	cL	204	CLA	CMB-C2B-C3B	2.02	131.48	126.59
15	b2	403	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	cB	827	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
15	bA	815	CLA	CHB-C1B-NB	2.02	126.39	124.26
15	cB	838	CLA	CHC-C4B-NB	2.02	126.39	124.26
15	b1	404	CLA	C2A-C1A-CHA	2.02	127.39	123.86
15	c2	410	CLA	O1D-CGD-CBD	2.02	128.61	124.48
18	aF	203	BCR	C1-C6-C5	-2.02	119.77	122.61
15	a4	421	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
15	a2	417	CLA	C3A-C2A-C1A	2.02	104.36	101.34
15	bA	812	CLA	CHB-C4A-NA	2.02	127.30	124.51
18	a4	401	BCR	C40-C30-C25	2.02	113.57	110.30
15	a1	404	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
15	aA	825	CLA	O1D-CGD-CBD	2.02	128.61	124.48
15	c6	407	CLA	CHD-C4C-C3C	2.02	127.80	124.84
15	bA	811	CLA	C2D-C1D-ND	-2.02	108.62	110.10
15	b5	417	CLA	C2D-C1D-ND	-2.02	108.62	110.10
15	cB	814	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	a4	410	CLA	CMB-C2B-C3B	2.02	131.47	126.59
15	bA	825	CLA	O1D-CGD-CBD	2.02	128.61	124.48
15	a4	403	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	cA	849	BCR	C33-C5-C6	-2.02	122.27	124.53
18	cF	204	BCR	C33-C5-C6	-2.02	122.27	124.53
15	bA	841	CLA	C11-C12-C13	-2.01	109.41	115.92
15	b6	418	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
15	b6	412	CLA	CAA-CBA-CGA	2.01	117.85	112.51
15	aX	102	CLA	CHA-C1A-NA	-2.01	121.78	126.40
15	bB	814	CLA	CHA-C1A-NA	-2.01	121.78	126.40
18	c1	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	a5	406	CLA	O1A-CGA-CBA	2.01	129.55	123.08
15	bF	201	CLA	C2A-C1A-CHA	2.01	127.38	123.86
15	b2	411	CLA	CMB-C2B-C3B	2.01	131.47	126.59
15	c4	405	CLA	CHA-C4D-ND	2.01	136.71	132.50
15	c5	403	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
15	aB	830	CLA	CHB-C4A-NA	2.01	127.30	124.51
15	c1	404	CLA	CHC-C4B-NB	2.01	126.39	124.26
15	c4	413	CLA	CHC-C4B-NB	2.01	126.39	124.26
18	c1	420	BCR	C11-C10-C9	-2.01	124.44	127.31
15	b3	416	CLA	C3A-C2A-C1A	2.01	104.36	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b5	420	CLA	CHA-C4D-ND	2.01	136.71	132.50
18	c4	419	BCR	C40-C30-C25	2.01	113.56	110.30
15	a4	411	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
15	c5	412	CLA	C3C-C4C-NC	-2.01	108.31	110.57
15	b1	410	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
15	c2	404	CLA	O1D-CGD-CBD	2.01	128.60	124.48
15	aJ	201	CLA	C2A-C1A-CHA	2.01	127.38	123.86
15	c3	412	CLA	C3C-C4C-NC	-2.01	108.31	110.57
15	c6	418	CLA	O2D-CGD-CBD	2.01	114.84	111.27
15	b6	414	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
15	aB	827	CLA	CHA-C4D-ND	2.01	136.71	132.50
15	aB	837	CLA	C1-C2-C3	-2.01	122.56	126.04
15	aA	806	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	bB	850	BCR	C38-C26-C27	-2.01	109.75	113.62
18	bB	847	BCR	C40-C30-C39	-2.01	102.35	108.53
18	a1	420	BCR	C40-C30-C25	2.01	113.56	110.30
15	bA	842	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
15	b6	404	CLA	CHA-C1A-NA	-2.01	121.79	126.40
15	bA	820	CLA	C3A-C2A-C1A	2.01	104.35	101.34
18	c5	419	BCR	C16-C15-C14	-2.01	119.35	123.47
15	c1	410	CLA	CMB-C2B-C3B	2.01	131.46	126.59
15	bB	827	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
18	c5	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	a4	405	CLA	CED-O2D-CGD	-2.01	111.39	115.94
15	bA	837	CLA	O1A-CGA-CBA	2.01	129.54	123.08
15	aA	802	CLA	C3B-C4B-NB	-2.01	108.65	110.52
15	b2	406	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	b4	411	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
15	a1	403	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	a5	420	CLA	CGD-CBD-CAD	-2.01	104.22	110.73
15	cB	822	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	aA	812	CLA	C6-C7-C8	-2.01	109.42	115.92
15	aA	808	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	a4	405	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	cF	203	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	bB	813	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	a1	403	CLA	O1D-CGD-CBD	2.01	128.59	124.48
15	aB	814	CLA	CHA-C1A-NA	-2.01	121.80	126.40
15	c6	405	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	b4	418	BCR	C1-C6-C5	-2.01	119.78	122.61
18	b6	419	BCR	C1-C6-C5	-2.01	119.78	122.61
18	b4	419	BCR	C40-C30-C25	2.01	113.56	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b5	418	BCR	C1-C6-C5	-2.01	119.78	122.61
15	aB	822	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	a6	404	CLA	CHA-C1A-NA	-2.01	121.80	126.40
15	b3	411	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	c1	407	CLA	CHC-C4B-NB	2.01	126.38	124.26
15	c1	408	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	c2	413	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	a1	415	CLA	C3A-C2A-C1A	2.01	104.34	101.34
15	bB	827	CLA	CHA-C4D-ND	2.01	136.70	132.50
15	c3	417	CLA	CHD-C4C-NC	2.01	127.37	124.20
15	aA	842	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
15	b1	405	CLA	CHA-C4D-ND	2.01	136.70	132.50
18	aB	845	BCR	C15-C16-C17	-2.01	119.36	123.47
15	c5	404	CLA	CHC-C4B-NB	2.01	126.38	124.26
15	a1	411	CLA	CHD-C4C-C3C	2.01	127.79	124.84
15	a5	417	CLA	C3C-C4C-NC	-2.01	108.32	110.57
15	c5	408	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
15	cA	812	CLA	CHB-C4A-NA	2.01	127.29	124.51
15	bB	837	CLA	C1-C2-C3	-2.01	122.57	126.04
15	aB	827	CLA	CAA-CBA-CGA	-2.01	107.39	113.25
18	bI	101	BCR	C35-C13-C14	-2.01	120.11	122.92
15	cA	813	CLA	C1-C2-C3	-2.01	122.58	126.04
15	bB	832	CLA	CHA-C1A-NA	-2.01	121.81	126.40
15	b4	421	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
15	c4	405	CLA	C3B-C4B-NB	-2.00	108.66	110.52
18	aF	202	BCR	C40-C30-C25	2.00	113.55	110.30
18	cB	849	BCR	C1-C6-C5	-2.00	119.79	122.61
15	c4	410	CLA	CMB-C2B-C3B	2.00	131.44	126.59
15	a3	415	CLA	CHC-C4B-NB	2.00	126.38	124.26
15	a6	408	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
15	a6	414	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
18	bB	849	BCR	C16-C15-C14	-2.00	119.37	123.47
15	bB	817	CLA	C2D-C1D-ND	-2.00	108.63	110.10
18	a5	418	BCR	C1-C6-C5	-2.00	119.79	122.61
18	c4	401	BCR	C16-C15-C14	-2.00	119.37	123.47
15	cB	814	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
15	c6	410	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	bB	816	CLA	CHC-C4B-NB	2.00	126.38	124.26
15	cA	820	CLA	C3A-C2A-C1A	2.00	104.34	101.34
15	aB	813	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	c5	404	CLA	O1D-CGD-CBD	2.00	128.58	124.48
15	aB	837	CLA	C3C-C4C-NC	-2.00	108.33	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c2	411	CLA	CMB-C2B-C3B	2.00	131.44	126.59
15	a2	404	CLA	O1D-CGD-CBD	2.00	128.58	124.48
15	c3	405	CLA	CHD-C4C-C3C	2.00	127.78	124.84
15	a2	408	CLA	CMB-C2B-C3B	2.00	131.44	126.59
15	aB	812	CLA	CHB-C1B-NB	2.00	126.38	124.26
15	c3	416	CLA	C3A-C2A-C1A	2.00	104.34	101.34
15	bB	822	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
15	aA	845	CLA	CHD-C4C-NC	2.00	127.36	124.20
15	b2	414	CLA	CHB-C4A-NA	2.00	127.28	124.51
15	b2	409	CLA	C3C-C4C-NC	-2.00	108.33	110.57
15	c5	420	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
15	bA	812	CLA	C6-C7-C8	-2.00	109.45	115.92
15	cA	818	CLA	C4-C3-C5	2.00	118.64	115.27
15	cB	813	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

There are no chirality outliers.

All (7649) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	C1A-C2A-CAA-CBA
15	aA	804	CLA	CHA-CBD-CGD-O1D
15	aA	804	CLA	CHA-CBD-CGD-O2D
15	aA	806	CLA	C1A-C2A-CAA-CBA
15	aA	806	CLA	C3A-C2A-CAA-CBA
15	aA	806	CLA	CHA-CBD-CGD-O1D
15	aA	806	CLA	CHA-CBD-CGD-O2D
15	aA	806	CLA	CAD-CBD-CGD-O1D
15	aA	807	CLA	C1A-C2A-CAA-CBA
15	aA	809	CLA	C3A-C2A-CAA-CBA
15	aA	809	CLA	CHA-CBD-CGD-O1D
15	aA	809	CLA	CHA-CBD-CGD-O2D
15	aA	810	CLA	CBD-CGD-O2D-CED
15	aA	811	CLA	C1A-C2A-CAA-CBA
15	aA	811	CLA	C3A-C2A-CAA-CBA
15	aA	811	CLA	C2B-C3B-CAB-CBB
15	aA	811	CLA	C4B-C3B-CAB-CBB
15	aA	811	CLA	CHA-CBD-CGD-O1D
15	aA	811	CLA	CHA-CBD-CGD-O2D
15	aA	811	CLA	CBD-CGD-O2D-CED
15	aA	816	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	816	CLA	CAD-CBD-CGD-O2D
15	aA	817	CLA	C4B-C3B-CAB-CBB
15	aA	819	CLA	C3A-C2A-CAA-CBA
15	aA	820	CLA	C1A-C2A-CAA-CBA
15	aA	820	CLA	C3A-C2A-CAA-CBA
15	aA	820	CLA	CHA-CBD-CGD-O1D
15	aA	820	CLA	CHA-CBD-CGD-O2D
15	aA	821	CLA	C1A-C2A-CAA-CBA
15	aA	821	CLA	C3A-C2A-CAA-CBA
15	aA	821	CLA	C2B-C3B-CAB-CBB
15	aA	821	CLA	C4B-C3B-CAB-CBB
15	aA	824	CLA	CHA-CBD-CGD-O1D
15	aA	824	CLA	CHA-CBD-CGD-O2D
15	aA	824	CLA	C2-C3-C5-C6
15	aA	824	CLA	C4-C3-C5-C6
15	aA	825	CLA	CHA-CBD-CGD-O1D
15	aA	825	CLA	CHA-CBD-CGD-O2D
15	aA	829	CLA	C1A-C2A-CAA-CBA
15	aA	829	CLA	C3A-C2A-CAA-CBA
15	aA	830	CLA	CHA-CBD-CGD-O1D
15	aA	830	CLA	CHA-CBD-CGD-O2D
15	aA	831	CLA	CHA-CBD-CGD-O1D
15	aA	831	CLA	CHA-CBD-CGD-O2D
15	aA	835	CLA	C2B-C3B-CAB-CBB
15	aA	835	CLA	C4B-C3B-CAB-CBB
15	aA	836	CLA	C4B-C3B-CAB-CBB
15	aA	839	CLA	CHA-CBD-CGD-O1D
15	aA	839	CLA	CHA-CBD-CGD-O2D
15	aA	839	CLA	CAD-CBD-CGD-O1D
15	aA	839	CLA	CBD-CGD-O2D-CED
15	aA	842	CLA	C4B-C3B-CAB-CBB
15	aA	842	CLA	CHA-CBD-CGD-O2D
15	aA	842	CLA	CBD-CGD-O2D-CED
15	aA	842	CLA	C2-C3-C5-C6
15	aA	842	CLA	C4-C3-C5-C6
15	aA	843	CLA	C1A-C2A-CAA-CBA
15	aA	844	CLA	C2B-C3B-CAB-CBB
15	aA	844	CLA	C4B-C3B-CAB-CBB
15	aA	845	CLA	CHA-CBD-CGD-O1D
15	aA	845	CLA	CHA-CBD-CGD-O2D
15	aA	845	CLA	CAD-CBD-CGD-O1D
15	aB	801	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	801	CLA	C4B-C3B-CAB-CBB
15	aB	801	CLA	C4-C3-C5-C6
15	aB	802	CLA	CHA-CBD-CGD-O1D
15	aB	802	CLA	CHA-CBD-CGD-O2D
15	aB	802	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	C2-C3-C5-C6
15	aB	803	CLA	C4-C3-C5-C6
15	aB	806	CLA	C1A-C2A-CAA-CBA
15	aB	806	CLA	C3A-C2A-CAA-CBA
15	aB	806	CLA	CHA-CBD-CGD-O1D
15	aB	806	CLA	CHA-CBD-CGD-O2D
15	aB	806	CLA	C6-C7-C8-C9
15	aB	809	CLA	C4B-C3B-CAB-CBB
15	aB	810	CLA	C1A-C2A-CAA-CBA
15	aB	810	CLA	C3A-C2A-CAA-CBA
15	aB	811	CLA	C2B-C3B-CAB-CBB
15	aB	811	CLA	C4B-C3B-CAB-CBB
15	aB	812	CLA	CBD-CGD-O2D-CED
15	aB	814	CLA	C1A-C2A-CAA-CBA
15	aB	814	CLA	C3A-C2A-CAA-CBA
15	aB	814	CLA	CHA-CBD-CGD-O1D
15	aB	814	CLA	CHA-CBD-CGD-O2D
15	aB	816	CLA	CHA-CBD-CGD-O1D
15	aB	816	CLA	CHA-CBD-CGD-O2D
15	aB	817	CLA	C1A-C2A-CAA-CBA
15	aB	819	CLA	C1A-C2A-CAA-CBA
15	aB	819	CLA	C3A-C2A-CAA-CBA
15	aB	821	CLA	C1A-C2A-CAA-CBA
15	aB	821	CLA	C3A-C2A-CAA-CBA
15	aB	825	CLA	C2-C3-C5-C6
15	aB	825	CLA	C4-C3-C5-C6
15	aB	826	CLA	C1A-C2A-CAA-CBA
15	aB	827	CLA	C1A-C2A-CAA-CBA
15	aB	827	CLA	C3A-C2A-CAA-CBA
15	aB	827	CLA	C11-C10-C8-C7
15	aB	828	CLA	CBD-CGD-O2D-CED
15	aB	829	CLA	C1A-C2A-CAA-CBA
15	aB	829	CLA	C3A-C2A-CAA-CBA
15	aB	829	CLA	CHA-CBD-CGD-O1D
15	aB	829	CLA	CHA-CBD-CGD-O2D
15	aB	831	CLA	C1A-C2A-CAA-CBA
15	aB	831	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	831	CLA	C2B-C3B-CAB-CBB
15	aB	831	CLA	C4B-C3B-CAB-CBB
15	aB	834	CLA	C1A-C2A-CAA-CBA
15	aB	834	CLA	CBD-CGD-O2D-CED
15	aB	835	CLA	C1A-C2A-CAA-CBA
15	aB	835	CLA	C3A-C2A-CAA-CBA
15	aB	835	CLA	C2B-C3B-CAB-CBB
15	aB	835	CLA	C4B-C3B-CAB-CBB
15	aB	837	CLA	CHA-CBD-CGD-O1D
15	aB	837	CLA	CHA-CBD-CGD-O2D
15	aB	840	CLA	C1A-C2A-CAA-CBA
15	aB	840	CLA	C3A-C2A-CAA-CBA
15	aJ	201	CLA	C4B-C3B-CAB-CBB
15	aJ	201	CLA	CAD-CBD-CGD-O1D
15	aJ	201	CLA	CAD-CBD-CGD-O2D
15	aJ	201	CLA	CBD-CGD-O2D-CED
15	aJ	202	CLA	CHA-CBD-CGD-O1D
15	aJ	202	CLA	CAD-CBD-CGD-O1D
15	aJ	202	CLA	CAD-CBD-CGD-O2D
15	aJ	202	CLA	CBD-CGD-O2D-CED
15	aK	102	CLA	C2B-C3B-CAB-CBB
15	aK	102	CLA	C4B-C3B-CAB-CBB
15	aL	201	CLA	C1A-C2A-CAA-CBA
15	aL	201	CLA	C3A-C2A-CAA-CBA
15	aL	201	CLA	C4B-C3B-CAB-CBB
15	aL	202	CLA	C2A-CAA-CBA-CGA
15	a1	403	CLA	C4B-C3B-CAB-CBB
15	a1	407	CLA	C1A-C2A-CAA-CBA
15	a1	407	CLA	CBD-CGD-O2D-CED
15	a1	409	CLA	C2B-C3B-CAB-CBB
15	a1	409	CLA	C4B-C3B-CAB-CBB
15	a1	410	CLA	C1A-C2A-CAA-CBA
15	a1	413	CLA	CBD-CGD-O2D-CED
15	a1	414	CLA	C2B-C3B-CAB-CBB
15	a1	414	CLA	C4B-C3B-CAB-CBB
15	a1	414	CLA	CBD-CGD-O2D-CED
15	a1	415	CLA	C1A-C2A-CAA-CBA
15	a1	415	CLA	C3A-C2A-CAA-CBA
15	a1	415	CLA	C2A-CAA-CBA-CGA
15	a1	415	CLA	CBD-CGD-O2D-CED
15	a1	416	CLA	C4B-C3B-CAB-CBB
15	a2	404	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a2	406	CLA	C1A-C2A-CAA-CBA
15	a2	406	CLA	CBD-CGD-O2D-CED
15	a2	406	CLA	C11-C12-C13-C14
15	a2	409	CLA	C1A-C2A-CAA-CBA
15	a2	409	CLA	CBD-CGD-O2D-CED
15	a2	411	CLA	C2B-C3B-CAB-CBB
15	a2	411	CLA	C4B-C3B-CAB-CBB
15	a2	412	CLA	C1A-C2A-CAA-CBA
15	a2	413	CLA	CBD-CGD-O2D-CED
15	a2	415	CLA	C4B-C3B-CAB-CBB
15	a2	415	CLA	CBD-CGD-O2D-CED
15	a2	416	CLA	C2B-C3B-CAB-CBB
15	a2	416	CLA	C4B-C3B-CAB-CBB
15	a2	416	CLA	CBD-CGD-O2D-CED
15	a2	417	CLA	C1A-C2A-CAA-CBA
15	a2	417	CLA	C3A-C2A-CAA-CBA
15	a2	417	CLA	C2A-CAA-CBA-CGA
15	a2	417	CLA	CBD-CGD-O2D-CED
15	a2	418	CLA	C4B-C3B-CAB-CBB
15	a2	422	CLA	C1A-C2A-CAA-CBA
15	a2	422	CLA	CBD-CGD-O2D-CED
15	a3	404	CLA	C4B-C3B-CAB-CBB
15	a3	408	CLA	C1A-C2A-CAA-CBA
15	a3	408	CLA	CBD-CGD-O2D-CED
15	a3	410	CLA	C2B-C3B-CAB-CBB
15	a3	410	CLA	C4B-C3B-CAB-CBB
15	a3	411	CLA	C1A-C2A-CAA-CBA
15	a3	412	CLA	CBD-CGD-O2D-CED
15	a3	414	CLA	C4B-C3B-CAB-CBB
15	a3	414	CLA	CBD-CGD-O2D-CED
15	a3	415	CLA	C2B-C3B-CAB-CBB
15	a3	415	CLA	C4B-C3B-CAB-CBB
15	a3	415	CLA	CBD-CGD-O2D-CED
15	a3	416	CLA	C1A-C2A-CAA-CBA
15	a3	416	CLA	C3A-C2A-CAA-CBA
15	a3	416	CLA	C2A-CAA-CBA-CGA
15	a3	416	CLA	CBD-CGD-O2D-CED
15	a3	417	CLA	C4B-C3B-CAB-CBB
15	a3	417	CLA	CBD-CGD-O2D-CED
15	a3	421	CLA	C1A-C2A-CAA-CBA
15	a3	421	CLA	CBD-CGD-O2D-CED
15	a4	404	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	408	CLA	CBD-CGD-O2D-CED
15	a4	410	CLA	C2B-C3B-CAB-CBB
15	a4	410	CLA	C4B-C3B-CAB-CBB
15	a4	411	CLA	C1A-C2A-CAA-CBA
15	a4	414	CLA	CBD-CGD-O2D-CED
15	a4	415	CLA	C2B-C3B-CAB-CBB
15	a4	415	CLA	C4B-C3B-CAB-CBB
15	a4	415	CLA	CBD-CGD-O2D-CED
15	a4	416	CLA	C1A-C2A-CAA-CBA
15	a4	416	CLA	C3A-C2A-CAA-CBA
15	a4	416	CLA	C2A-CAA-CBA-CGA
15	a4	416	CLA	C2B-C3B-CAB-CBB
15	a4	416	CLA	C4B-C3B-CAB-CBB
15	a4	416	CLA	CBD-CGD-O2D-CED
15	a4	417	CLA	C4B-C3B-CAB-CBB
15	a4	417	CLA	CBD-CGD-O2D-CED
15	a4	421	CLA	C1A-C2A-CAA-CBA
15	a4	421	CLA	CBD-CGD-O2D-CED
15	a5	404	CLA	C4B-C3B-CAB-CBB
15	a5	408	CLA	C1A-C2A-CAA-CBA
15	a5	408	CLA	CBD-CGD-O2D-CED
15	a5	410	CLA	C2B-C3B-CAB-CBB
15	a5	410	CLA	C4B-C3B-CAB-CBB
15	a5	411	CLA	C1A-C2A-CAA-CBA
15	a5	414	CLA	CBD-CGD-O2D-CED
15	a5	415	CLA	C2B-C3B-CAB-CBB
15	a5	415	CLA	C4B-C3B-CAB-CBB
15	a5	415	CLA	CBD-CGD-O2D-CED
15	a5	416	CLA	C1A-C2A-CAA-CBA
15	a5	416	CLA	C3A-C2A-CAA-CBA
15	a5	416	CLA	C2A-CAA-CBA-CGA
15	a5	416	CLA	C2B-C3B-CAB-CBB
15	a5	416	CLA	C4B-C3B-CAB-CBB
15	a5	416	CLA	CBD-CGD-O2D-CED
15	a5	417	CLA	C4B-C3B-CAB-CBB
15	a5	417	CLA	CBD-CGD-O2D-CED
15	a5	420	CLA	CBD-CGD-O2D-CED
15	a6	405	CLA	C2B-C3B-CAB-CBB
15	a6	405	CLA	C4B-C3B-CAB-CBB
15	a6	406	CLA	CBD-CGD-O2D-CED
15	a6	409	CLA	CBD-CGD-O2D-CED
15	a6	411	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	411	CLA	C4B-C3B-CAB-CBB
15	a6	412	CLA	C1A-C2A-CAA-CBA
15	a6	415	CLA	C4B-C3B-CAB-CBB
15	a6	415	CLA	CBD-CGD-O2D-CED
15	a6	416	CLA	C2B-C3B-CAB-CBB
15	a6	416	CLA	C4B-C3B-CAB-CBB
15	a6	416	CLA	CBD-CGD-O2D-CED
15	a6	417	CLA	C1A-C2A-CAA-CBA
15	a6	417	CLA	C3A-C2A-CAA-CBA
15	a6	417	CLA	C2A-CAA-CBA-CGA
15	a6	417	CLA	CBD-CGD-O2D-CED
15	a6	418	CLA	C4B-C3B-CAB-CBB
15	a6	422	CLA	CBD-CGD-O2D-CED
15	bA	803	CLA	CBA-CGA-O2A-C1
15	bA	803	CLA	O1A-CGA-O2A-C1
15	bA	804	CLA	C1A-C2A-CAA-CBA
15	bA	804	CLA	CHA-CBD-CGD-O1D
15	bA	804	CLA	CHA-CBD-CGD-O2D
15	bA	806	CLA	C1A-C2A-CAA-CBA
15	bA	806	CLA	C3A-C2A-CAA-CBA
15	bA	806	CLA	CHA-CBD-CGD-O1D
15	bA	806	CLA	CHA-CBD-CGD-O2D
15	bA	806	CLA	CAD-CBD-CGD-O1D
15	bA	807	CLA	C1A-C2A-CAA-CBA
15	bA	809	CLA	C3A-C2A-CAA-CBA
15	bA	809	CLA	CHA-CBD-CGD-O1D
15	bA	809	CLA	CHA-CBD-CGD-O2D
15	bA	810	CLA	CBD-CGD-O2D-CED
15	bA	811	CLA	C1A-C2A-CAA-CBA
15	bA	811	CLA	C3A-C2A-CAA-CBA
15	bA	811	CLA	C2B-C3B-CAB-CBB
15	bA	811	CLA	C4B-C3B-CAB-CBB
15	bA	811	CLA	CHA-CBD-CGD-O1D
15	bA	811	CLA	CHA-CBD-CGD-O2D
15	bA	811	CLA	CBD-CGD-O2D-CED
15	bA	816	CLA	CAD-CBD-CGD-O1D
15	bA	816	CLA	CAD-CBD-CGD-O2D
15	bA	817	CLA	C4B-C3B-CAB-CBB
15	bA	819	CLA	C3A-C2A-CAA-CBA
15	bA	820	CLA	C1A-C2A-CAA-CBA
15	bA	820	CLA	C3A-C2A-CAA-CBA
15	bA	820	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	820	CLA	CHA-CBD-CGD-O2D
15	bA	821	CLA	C1A-C2A-CAA-CBA
15	bA	821	CLA	C3A-C2A-CAA-CBA
15	bA	821	CLA	C2B-C3B-CAB-CBB
15	bA	821	CLA	C4B-C3B-CAB-CBB
15	bA	824	CLA	CHA-CBD-CGD-O1D
15	bA	824	CLA	CHA-CBD-CGD-O2D
15	bA	824	CLA	C2-C3-C5-C6
15	bA	824	CLA	C4-C3-C5-C6
15	bA	825	CLA	CHA-CBD-CGD-O1D
15	bA	825	CLA	CHA-CBD-CGD-O2D
15	bA	829	CLA	C1A-C2A-CAA-CBA
15	bA	829	CLA	C3A-C2A-CAA-CBA
15	bA	830	CLA	CHA-CBD-CGD-O1D
15	bA	830	CLA	CHA-CBD-CGD-O2D
15	bA	831	CLA	CHA-CBD-CGD-O1D
15	bA	831	CLA	CHA-CBD-CGD-O2D
15	bA	835	CLA	C2B-C3B-CAB-CBB
15	bA	835	CLA	C4B-C3B-CAB-CBB
15	bA	836	CLA	C4B-C3B-CAB-CBB
15	bA	839	CLA	CHA-CBD-CGD-O1D
15	bA	839	CLA	CHA-CBD-CGD-O2D
15	bA	839	CLA	CAD-CBD-CGD-O1D
15	bA	839	CLA	CBD-CGD-O2D-CED
15	bA	842	CLA	C4B-C3B-CAB-CBB
15	bA	842	CLA	CHA-CBD-CGD-O2D
15	bA	842	CLA	CBD-CGD-O2D-CED
15	bA	842	CLA	C2-C3-C5-C6
15	bA	842	CLA	C4-C3-C5-C6
15	bA	843	CLA	C1A-C2A-CAA-CBA
15	bA	844	CLA	C2B-C3B-CAB-CBB
15	bA	844	CLA	C4B-C3B-CAB-CBB
15	bA	845	CLA	CHA-CBD-CGD-O1D
15	bA	845	CLA	CHA-CBD-CGD-O2D
15	bA	845	CLA	CAD-CBD-CGD-O1D
15	bB	801	CLA	C2B-C3B-CAB-CBB
15	bB	801	CLA	C4B-C3B-CAB-CBB
15	bB	801	CLA	C4-C3-C5-C6
15	bB	802	CLA	CHA-CBD-CGD-O1D
15	bB	802	CLA	CHA-CBD-CGD-O2D
15	bB	802	CLA	CBD-CGD-O2D-CED
15	bB	803	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	803	CLA	C4-C3-C5-C6
15	bB	806	CLA	C1A-C2A-CAA-CBA
15	bB	806	CLA	C3A-C2A-CAA-CBA
15	bB	806	CLA	CHA-CBD-CGD-O1D
15	bB	806	CLA	CHA-CBD-CGD-O2D
15	bB	806	CLA	C6-C7-C8-C9
15	bB	809	CLA	C4B-C3B-CAB-CBB
15	bB	810	CLA	C1A-C2A-CAA-CBA
15	bB	810	CLA	C3A-C2A-CAA-CBA
15	bB	811	CLA	C2B-C3B-CAB-CBB
15	bB	811	CLA	C4B-C3B-CAB-CBB
15	bB	812	CLA	CBD-CGD-O2D-CED
15	bB	814	CLA	C1A-C2A-CAA-CBA
15	bB	814	CLA	C3A-C2A-CAA-CBA
15	bB	814	CLA	CHA-CBD-CGD-O1D
15	bB	814	CLA	CHA-CBD-CGD-O2D
15	bB	816	CLA	CHA-CBD-CGD-O1D
15	bB	816	CLA	CHA-CBD-CGD-O2D
15	bB	817	CLA	C1A-C2A-CAA-CBA
15	bB	819	CLA	C1A-C2A-CAA-CBA
15	bB	819	CLA	C3A-C2A-CAA-CBA
15	bB	821	CLA	C1A-C2A-CAA-CBA
15	bB	821	CLA	C3A-C2A-CAA-CBA
15	bB	825	CLA	C2-C3-C5-C6
15	bB	825	CLA	C4-C3-C5-C6
15	bB	826	CLA	C1A-C2A-CAA-CBA
15	bB	827	CLA	C1A-C2A-CAA-CBA
15	bB	827	CLA	C3A-C2A-CAA-CBA
15	bB	827	CLA	C11-C10-C8-C7
15	bB	828	CLA	CBD-CGD-O2D-CED
15	bB	829	CLA	C1A-C2A-CAA-CBA
15	bB	829	CLA	C3A-C2A-CAA-CBA
15	bB	829	CLA	CHA-CBD-CGD-O1D
15	bB	829	CLA	CHA-CBD-CGD-O2D
15	bB	831	CLA	C1A-C2A-CAA-CBA
15	bB	831	CLA	C3A-C2A-CAA-CBA
15	bB	831	CLA	C2B-C3B-CAB-CBB
15	bB	831	CLA	C4B-C3B-CAB-CBB
15	bB	834	CLA	C1A-C2A-CAA-CBA
15	bB	834	CLA	CBD-CGD-O2D-CED
15	bB	835	CLA	C1A-C2A-CAA-CBA
15	bB	835	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	835	CLA	C2B-C3B-CAB-CBB
15	bB	835	CLA	C4B-C3B-CAB-CBB
15	bB	837	CLA	CHA-CBD-CGD-O1D
15	bB	837	CLA	CHA-CBD-CGD-O2D
15	bB	840	CLA	C1A-C2A-CAA-CBA
15	bB	840	CLA	C3A-C2A-CAA-CBA
15	bF	201	CLA	C4B-C3B-CAB-CBB
15	bF	201	CLA	CAD-CBD-CGD-O1D
15	bF	201	CLA	CAD-CBD-CGD-O2D
15	bF	201	CLA	CBD-CGD-O2D-CED
15	bJ	101	CLA	CHA-CBD-CGD-O1D
15	bJ	101	CLA	CAD-CBD-CGD-O1D
15	bJ	101	CLA	CAD-CBD-CGD-O2D
15	bJ	101	CLA	CBD-CGD-O2D-CED
15	bK	101	CLA	C2B-C3B-CAB-CBB
15	bK	101	CLA	C4B-C3B-CAB-CBB
15	bL	202	CLA	C1A-C2A-CAA-CBA
15	bL	202	CLA	C3A-C2A-CAA-CBA
15	bL	202	CLA	C4B-C3B-CAB-CBB
15	bL	203	CLA	C2A-CAA-CBA-CGA
15	b1	404	CLA	C4B-C3B-CAB-CBB
15	b1	408	CLA	C1A-C2A-CAA-CBA
15	b1	408	CLA	CBD-CGD-O2D-CED
15	b1	410	CLA	C2B-C3B-CAB-CBB
15	b1	410	CLA	C4B-C3B-CAB-CBB
15	b1	411	CLA	C1A-C2A-CAA-CBA
15	b1	414	CLA	CBD-CGD-O2D-CED
15	b1	415	CLA	C2B-C3B-CAB-CBB
15	b1	415	CLA	C4B-C3B-CAB-CBB
15	b1	415	CLA	CBD-CGD-O2D-CED
15	b1	416	CLA	C1A-C2A-CAA-CBA
15	b1	416	CLA	C3A-C2A-CAA-CBA
15	b1	416	CLA	C2A-CAA-CBA-CGA
15	b1	416	CLA	C2B-C3B-CAB-CBB
15	b1	416	CLA	C4B-C3B-CAB-CBB
15	b1	416	CLA	CBD-CGD-O2D-CED
15	b1	417	CLA	C4B-C3B-CAB-CBB
15	b2	404	CLA	C2B-C3B-CAB-CBB
15	b2	404	CLA	C4B-C3B-CAB-CBB
15	b2	406	CLA	C1A-C2A-CAA-CBA
15	b2	406	CLA	CBD-CGD-O2D-CED
15	b2	406	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	409	CLA	C1A-C2A-CAA-CBA
15	b2	409	CLA	CBD-CGD-O2D-CED
15	b2	411	CLA	C2B-C3B-CAB-CBB
15	b2	411	CLA	C4B-C3B-CAB-CBB
15	b2	412	CLA	C1A-C2A-CAA-CBA
15	b2	413	CLA	CBD-CGD-O2D-CED
15	b2	415	CLA	C4B-C3B-CAB-CBB
15	b2	415	CLA	CBD-CGD-O2D-CED
15	b2	416	CLA	C2B-C3B-CAB-CBB
15	b2	416	CLA	C4B-C3B-CAB-CBB
15	b2	416	CLA	CBD-CGD-O2D-CED
15	b2	417	CLA	C1A-C2A-CAA-CBA
15	b2	417	CLA	C3A-C2A-CAA-CBA
15	b2	417	CLA	C2A-CAA-CBA-CGA
15	b2	417	CLA	CBD-CGD-O2D-CED
15	b2	418	CLA	C4B-C3B-CAB-CBB
15	b2	422	CLA	C1A-C2A-CAA-CBA
15	b2	422	CLA	CBD-CGD-O2D-CED
15	b3	404	CLA	C4B-C3B-CAB-CBB
15	b3	408	CLA	C1A-C2A-CAA-CBA
15	b3	408	CLA	CBD-CGD-O2D-CED
15	b3	410	CLA	C2B-C3B-CAB-CBB
15	b3	410	CLA	C4B-C3B-CAB-CBB
15	b3	411	CLA	C1A-C2A-CAA-CBA
15	b3	412	CLA	CBD-CGD-O2D-CED
15	b3	414	CLA	C4B-C3B-CAB-CBB
15	b3	414	CLA	CBD-CGD-O2D-CED
15	b3	415	CLA	C2B-C3B-CAB-CBB
15	b3	415	CLA	C4B-C3B-CAB-CBB
15	b3	415	CLA	CBD-CGD-O2D-CED
15	b3	416	CLA	C1A-C2A-CAA-CBA
15	b3	416	CLA	C3A-C2A-CAA-CBA
15	b3	416	CLA	C2A-CAA-CBA-CGA
15	b3	416	CLA	CBD-CGD-O2D-CED
15	b3	417	CLA	C4B-C3B-CAB-CBB
15	b3	417	CLA	CBD-CGD-O2D-CED
15	b3	421	CLA	C1A-C2A-CAA-CBA
15	b3	421	CLA	CBD-CGD-O2D-CED
15	b4	404	CLA	C4B-C3B-CAB-CBB
15	b4	408	CLA	CBD-CGD-O2D-CED
15	b4	410	CLA	C2B-C3B-CAB-CBB
15	b4	410	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b4	411	CLA	C1A-C2A-CAA-CBA
15	b4	414	CLA	CBD-CGD-O2D-CED
15	b4	415	CLA	C2B-C3B-CAB-CBB
15	b4	415	CLA	C4B-C3B-CAB-CBB
15	b4	415	CLA	CBD-CGD-O2D-CED
15	b4	416	CLA	C1A-C2A-CAA-CBA
15	b4	416	CLA	C3A-C2A-CAA-CBA
15	b4	416	CLA	C2A-CAA-CBA-CGA
15	b4	416	CLA	C2B-C3B-CAB-CBB
15	b4	416	CLA	C4B-C3B-CAB-CBB
15	b4	416	CLA	CBD-CGD-O2D-CED
15	b4	417	CLA	C4B-C3B-CAB-CBB
15	b4	417	CLA	CBD-CGD-O2D-CED
15	b4	421	CLA	C1A-C2A-CAA-CBA
15	b4	421	CLA	CBD-CGD-O2D-CED
15	b5	404	CLA	C2B-C3B-CAB-CBB
15	b5	404	CLA	C4B-C3B-CAB-CBB
15	b5	408	CLA	C1A-C2A-CAA-CBA
15	b5	408	CLA	CBD-CGD-O2D-CED
15	b5	410	CLA	C2B-C3B-CAB-CBB
15	b5	410	CLA	C4B-C3B-CAB-CBB
15	b5	411	CLA	C1A-C2A-CAA-CBA
15	b5	414	CLA	CBD-CGD-O2D-CED
15	b5	415	CLA	C2B-C3B-CAB-CBB
15	b5	415	CLA	C4B-C3B-CAB-CBB
15	b5	415	CLA	CBD-CGD-O2D-CED
15	b5	416	CLA	C1A-C2A-CAA-CBA
15	b5	416	CLA	C3A-C2A-CAA-CBA
15	b5	416	CLA	C2A-CAA-CBA-CGA
15	b5	416	CLA	C2B-C3B-CAB-CBB
15	b5	416	CLA	C4B-C3B-CAB-CBB
15	b5	416	CLA	CBD-CGD-O2D-CED
15	b5	417	CLA	C4B-C3B-CAB-CBB
15	b5	417	CLA	CBD-CGD-O2D-CED
15	b5	420	CLA	CBD-CGD-O2D-CED
15	b6	405	CLA	C2B-C3B-CAB-CBB
15	b6	405	CLA	C4B-C3B-CAB-CBB
15	b6	406	CLA	CBD-CGD-O2D-CED
15	b6	409	CLA	C1A-C2A-CAA-CBA
15	b6	409	CLA	CBD-CGD-O2D-CED
15	b6	411	CLA	C2B-C3B-CAB-CBB
15	b6	411	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	412	CLA	C1A-C2A-CAA-CBA
15	b6	415	CLA	CBD-CGD-O2D-CED
15	b6	416	CLA	C2B-C3B-CAB-CBB
15	b6	416	CLA	C4B-C3B-CAB-CBB
15	b6	416	CLA	CBD-CGD-O2D-CED
15	b6	417	CLA	C1A-C2A-CAA-CBA
15	b6	417	CLA	C3A-C2A-CAA-CBA
15	b6	417	CLA	C2A-CAA-CBA-CGA
15	b6	417	CLA	CBD-CGD-O2D-CED
15	b6	418	CLA	C4B-C3B-CAB-CBB
15	b6	422	CLA	CBD-CGD-O2D-CED
15	cA	803	CLA	CBA-CGA-O2A-C1
15	cA	803	CLA	O1A-CGA-O2A-C1
15	cA	804	CLA	C1A-C2A-CAA-CBA
15	cA	804	CLA	CHA-CBD-CGD-O1D
15	cA	804	CLA	CHA-CBD-CGD-O2D
15	cA	806	CLA	C1A-C2A-CAA-CBA
15	cA	806	CLA	C3A-C2A-CAA-CBA
15	cA	806	CLA	CHA-CBD-CGD-O1D
15	cA	806	CLA	CHA-CBD-CGD-O2D
15	cA	806	CLA	CAD-CBD-CGD-O1D
15	cA	807	CLA	C1A-C2A-CAA-CBA
15	cA	809	CLA	C3A-C2A-CAA-CBA
15	cA	809	CLA	CHA-CBD-CGD-O1D
15	cA	809	CLA	CHA-CBD-CGD-O2D
15	cA	810	CLA	CBD-CGD-O2D-CED
15	cA	811	CLA	C1A-C2A-CAA-CBA
15	cA	811	CLA	C3A-C2A-CAA-CBA
15	cA	811	CLA	C2B-C3B-CAB-CBB
15	cA	811	CLA	C4B-C3B-CAB-CBB
15	cA	811	CLA	CHA-CBD-CGD-O1D
15	cA	811	CLA	CHA-CBD-CGD-O2D
15	cA	811	CLA	CBD-CGD-O2D-CED
15	cA	816	CLA	CAD-CBD-CGD-O1D
15	cA	816	CLA	CAD-CBD-CGD-O2D
15	cA	817	CLA	C4B-C3B-CAB-CBB
15	cA	819	CLA	C3A-C2A-CAA-CBA
15	cA	820	CLA	C1A-C2A-CAA-CBA
15	cA	820	CLA	C3A-C2A-CAA-CBA
15	cA	820	CLA	CHA-CBD-CGD-O1D
15	cA	820	CLA	CHA-CBD-CGD-O2D
15	cA	821	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	821	CLA	C3A-C2A-CAA-CBA
15	cA	821	CLA	C2B-C3B-CAB-CBB
15	cA	821	CLA	C4B-C3B-CAB-CBB
15	cA	824	CLA	CHA-CBD-CGD-O1D
15	cA	824	CLA	CHA-CBD-CGD-O2D
15	cA	824	CLA	C2-C3-C5-C6
15	cA	824	CLA	C4-C3-C5-C6
15	cA	825	CLA	CHA-CBD-CGD-O1D
15	cA	825	CLA	CHA-CBD-CGD-O2D
15	cA	829	CLA	C1A-C2A-CAA-CBA
15	cA	829	CLA	C3A-C2A-CAA-CBA
15	cA	830	CLA	CHA-CBD-CGD-O1D
15	cA	830	CLA	CHA-CBD-CGD-O2D
15	cA	831	CLA	CHA-CBD-CGD-O1D
15	cA	831	CLA	CHA-CBD-CGD-O2D
15	cA	835	CLA	C2B-C3B-CAB-CBB
15	cA	835	CLA	C4B-C3B-CAB-CBB
15	cA	836	CLA	C4B-C3B-CAB-CBB
15	cA	839	CLA	CHA-CBD-CGD-O1D
15	cA	839	CLA	CHA-CBD-CGD-O2D
15	cA	839	CLA	CAD-CBD-CGD-O1D
15	cA	839	CLA	CBD-CGD-O2D-CED
15	cA	842	CLA	C1A-C2A-CAA-CBA
15	cA	843	CLA	C2B-C3B-CAB-CBB
15	cA	843	CLA	C4B-C3B-CAB-CBB
15	cA	844	CLA	CHA-CBD-CGD-O1D
15	cA	844	CLA	CHA-CBD-CGD-O2D
15	cA	844	CLA	CAD-CBD-CGD-O1D
15	cB	801	CLA	C2B-C3B-CAB-CBB
15	cB	801	CLA	C4B-C3B-CAB-CBB
15	cB	801	CLA	C4-C3-C5-C6
15	cB	802	CLA	CHA-CBD-CGD-O1D
15	cB	802	CLA	CHA-CBD-CGD-O2D
15	cB	802	CLA	CBD-CGD-O2D-CED
15	cB	803	CLA	C2-C3-C5-C6
15	cB	803	CLA	C4-C3-C5-C6
15	cB	806	CLA	C1A-C2A-CAA-CBA
15	cB	806	CLA	C3A-C2A-CAA-CBA
15	cB	806	CLA	CHA-CBD-CGD-O1D
15	cB	806	CLA	CHA-CBD-CGD-O2D
15	cB	806	CLA	C6-C7-C8-C9
15	cB	809	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	810	CLA	C1A-C2A-CAA-CBA
15	cB	810	CLA	C3A-C2A-CAA-CBA
15	cB	811	CLA	C2B-C3B-CAB-CBB
15	cB	811	CLA	C4B-C3B-CAB-CBB
15	cB	812	CLA	CBD-CGD-O2D-CED
15	cB	814	CLA	C1A-C2A-CAA-CBA
15	cB	814	CLA	C3A-C2A-CAA-CBA
15	cB	814	CLA	CHA-CBD-CGD-O1D
15	cB	814	CLA	CHA-CBD-CGD-O2D
15	cB	816	CLA	CHA-CBD-CGD-O1D
15	cB	816	CLA	CHA-CBD-CGD-O2D
15	cB	817	CLA	C1A-C2A-CAA-CBA
15	cB	819	CLA	C1A-C2A-CAA-CBA
15	cB	819	CLA	C3A-C2A-CAA-CBA
15	cB	821	CLA	C1A-C2A-CAA-CBA
15	cB	821	CLA	C3A-C2A-CAA-CBA
15	cB	825	CLA	CHA-CBD-CGD-O2D
15	cB	825	CLA	C2-C3-C5-C6
15	cB	825	CLA	C4-C3-C5-C6
15	cB	826	CLA	C1A-C2A-CAA-CBA
15	cB	827	CLA	C1A-C2A-CAA-CBA
15	cB	827	CLA	C3A-C2A-CAA-CBA
15	cB	827	CLA	C11-C10-C8-C7
15	cB	828	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	C1A-C2A-CAA-CBA
15	cB	829	CLA	C3A-C2A-CAA-CBA
15	cB	829	CLA	CHA-CBD-CGD-O1D
15	cB	829	CLA	CHA-CBD-CGD-O2D
15	cB	831	CLA	C1A-C2A-CAA-CBA
15	cB	831	CLA	C3A-C2A-CAA-CBA
15	cB	831	CLA	C2B-C3B-CAB-CBB
15	cB	831	CLA	C4B-C3B-CAB-CBB
15	cB	834	CLA	C1A-C2A-CAA-CBA
15	cB	834	CLA	CBD-CGD-O2D-CED
15	cB	835	CLA	C1A-C2A-CAA-CBA
15	cB	835	CLA	C3A-C2A-CAA-CBA
15	cB	835	CLA	C2B-C3B-CAB-CBB
15	cB	835	CLA	C4B-C3B-CAB-CBB
15	cB	837	CLA	CHA-CBD-CGD-O1D
15	cB	837	CLA	CHA-CBD-CGD-O2D
15	cB	840	CLA	C1A-C2A-CAA-CBA
15	cB	840	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cF	201	CLA	C4B-C3B-CAB-CBB
15	cF	201	CLA	CHA-CBD-CGD-O2D
15	cF	201	CLA	CBD-CGD-O2D-CED
15	cF	201	CLA	C2-C3-C5-C6
15	cF	201	CLA	C4-C3-C5-C6
15	cF	203	CLA	C4B-C3B-CAB-CBB
15	cF	203	CLA	CAD-CBD-CGD-O1D
15	cF	203	CLA	CAD-CBD-CGD-O2D
15	cF	203	CLA	CBD-CGD-O2D-CED
15	cJ	101	CLA	CHA-CBD-CGD-O1D
15	cJ	101	CLA	CAD-CBD-CGD-O1D
15	cJ	101	CLA	CAD-CBD-CGD-O2D
15	cJ	101	CLA	CBD-CGD-O2D-CED
15	cK	102	CLA	C2B-C3B-CAB-CBB
15	cK	102	CLA	C4B-C3B-CAB-CBB
15	cL	202	CLA	C1A-C2A-CAA-CBA
15	cL	202	CLA	C3A-C2A-CAA-CBA
15	cL	202	CLA	C4B-C3B-CAB-CBB
15	cL	203	CLA	C2A-CAA-CBA-CGA
15	c1	404	CLA	C4B-C3B-CAB-CBB
15	c1	408	CLA	C1A-C2A-CAA-CBA
15	c1	408	CLA	CBD-CGD-O2D-CED
15	c1	410	CLA	C2B-C3B-CAB-CBB
15	c1	410	CLA	C4B-C3B-CAB-CBB
15	c1	411	CLA	C1A-C2A-CAA-CBA
15	c1	414	CLA	CBD-CGD-O2D-CED
15	c1	415	CLA	C2B-C3B-CAB-CBB
15	c1	415	CLA	C4B-C3B-CAB-CBB
15	c1	415	CLA	CBD-CGD-O2D-CED
15	c1	416	CLA	C1A-C2A-CAA-CBA
15	c1	416	CLA	C3A-C2A-CAA-CBA
15	c1	416	CLA	C2A-CAA-CBA-CGA
15	c1	416	CLA	C4B-C3B-CAB-CBB
15	c1	416	CLA	CBD-CGD-O2D-CED
15	c1	417	CLA	C4B-C3B-CAB-CBB
15	c2	404	CLA	C2B-C3B-CAB-CBB
15	c2	404	CLA	C4B-C3B-CAB-CBB
15	c2	406	CLA	C1A-C2A-CAA-CBA
15	c2	406	CLA	CBD-CGD-O2D-CED
15	c2	406	CLA	C11-C12-C13-C14
15	c2	409	CLA	C1A-C2A-CAA-CBA
15	c2	409	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	411	CLA	C2B-C3B-CAB-CBB
15	c2	411	CLA	C4B-C3B-CAB-CBB
15	c2	412	CLA	C1A-C2A-CAA-CBA
15	c2	415	CLA	C4B-C3B-CAB-CBB
15	c2	415	CLA	CBD-CGD-O2D-CED
15	c2	416	CLA	C2B-C3B-CAB-CBB
15	c2	416	CLA	C4B-C3B-CAB-CBB
15	c2	416	CLA	CBD-CGD-O2D-CED
15	c2	417	CLA	C1A-C2A-CAA-CBA
15	c2	417	CLA	C3A-C2A-CAA-CBA
15	c2	417	CLA	C2A-CAA-CBA-CGA
15	c2	417	CLA	CBD-CGD-O2D-CED
15	c2	418	CLA	C4B-C3B-CAB-CBB
15	c2	422	CLA	C1A-C2A-CAA-CBA
15	c2	422	CLA	CBD-CGD-O2D-CED
15	c3	404	CLA	C4B-C3B-CAB-CBB
15	c3	408	CLA	C1A-C2A-CAA-CBA
15	c3	408	CLA	CBD-CGD-O2D-CED
15	c3	410	CLA	C2B-C3B-CAB-CBB
15	c3	410	CLA	C4B-C3B-CAB-CBB
15	c3	411	CLA	C1A-C2A-CAA-CBA
15	c3	414	CLA	C4B-C3B-CAB-CBB
15	c3	414	CLA	CBD-CGD-O2D-CED
15	c3	415	CLA	C2B-C3B-CAB-CBB
15	c3	415	CLA	C4B-C3B-CAB-CBB
15	c3	415	CLA	CBD-CGD-O2D-CED
15	c3	416	CLA	C1A-C2A-CAA-CBA
15	c3	416	CLA	C3A-C2A-CAA-CBA
15	c3	416	CLA	C2A-CAA-CBA-CGA
15	c3	416	CLA	CBD-CGD-O2D-CED
15	c3	417	CLA	C4B-C3B-CAB-CBB
15	c3	417	CLA	CBD-CGD-O2D-CED
15	c3	421	CLA	C1A-C2A-CAA-CBA
15	c3	421	CLA	CBD-CGD-O2D-CED
15	c4	404	CLA	C4B-C3B-CAB-CBB
15	c4	408	CLA	CBD-CGD-O2D-CED
15	c4	410	CLA	C2B-C3B-CAB-CBB
15	c4	410	CLA	C4B-C3B-CAB-CBB
15	c4	411	CLA	C1A-C2A-CAA-CBA
15	c4	414	CLA	CBD-CGD-O2D-CED
15	c4	415	CLA	C2B-C3B-CAB-CBB
15	c4	415	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	415	CLA	CBD-CGD-O2D-CED
15	c4	416	CLA	C1A-C2A-CAA-CBA
15	c4	416	CLA	C3A-C2A-CAA-CBA
15	c4	416	CLA	C2A-CAA-CBA-CGA
15	c4	416	CLA	C2B-C3B-CAB-CBB
15	c4	416	CLA	C4B-C3B-CAB-CBB
15	c4	416	CLA	CBD-CGD-O2D-CED
15	c4	417	CLA	C4B-C3B-CAB-CBB
15	c4	417	CLA	CBD-CGD-O2D-CED
15	c4	421	CLA	C1A-C2A-CAA-CBA
15	c4	421	CLA	CBD-CGD-O2D-CED
15	c4	421	CLA	C11-C12-C13-C14
15	c5	404	CLA	C4B-C3B-CAB-CBB
15	c5	408	CLA	C1A-C2A-CAA-CBA
15	c5	408	CLA	CBD-CGD-O2D-CED
15	c5	410	CLA	C2B-C3B-CAB-CBB
15	c5	410	CLA	C4B-C3B-CAB-CBB
15	c5	411	CLA	C1A-C2A-CAA-CBA
15	c5	414	CLA	CBD-CGD-O2D-CED
15	c5	415	CLA	C2B-C3B-CAB-CBB
15	c5	415	CLA	C4B-C3B-CAB-CBB
15	c5	416	CLA	C1A-C2A-CAA-CBA
15	c5	416	CLA	C3A-C2A-CAA-CBA
15	c5	416	CLA	C2A-CAA-CBA-CGA
15	c5	416	CLA	C2B-C3B-CAB-CBB
15	c5	416	CLA	C4B-C3B-CAB-CBB
15	c5	416	CLA	CBD-CGD-O2D-CED
15	c5	417	CLA	C4B-C3B-CAB-CBB
15	c5	417	CLA	CBD-CGD-O2D-CED
15	c5	420	CLA	CBD-CGD-O2D-CED
15	c6	401	CLA	CBD-CGD-O2D-CED
15	c6	401	CLA	C11-C12-C13-C14
15	c6	406	CLA	C2B-C3B-CAB-CBB
15	c6	406	CLA	C4B-C3B-CAB-CBB
15	c6	410	CLA	C1A-C2A-CAA-CBA
15	c6	410	CLA	CBD-CGD-O2D-CED
15	c6	412	CLA	C2B-C3B-CAB-CBB
15	c6	412	CLA	C4B-C3B-CAB-CBB
15	c6	413	CLA	C1A-C2A-CAA-CBA
15	c6	416	CLA	CBD-CGD-O2D-CED
15	c6	417	CLA	C2B-C3B-CAB-CBB
15	c6	417	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c6	417	CLA	CBD-CGD-O2D-CED
15	c6	418	CLA	C1A-C2A-CAA-CBA
15	c6	418	CLA	C3A-C2A-CAA-CBA
15	c6	418	CLA	C2A-CAA-CBA-CGA
15	c6	418	CLA	CBD-CGD-O2D-CED
15	c6	419	CLA	C4B-C3B-CAB-CBB
18	aA	848	BCR	C11-C12-C13-C35
18	aA	848	BCR	C20-C21-C22-C23
18	aA	848	BCR	C20-C21-C22-C37
18	aA	848	BCR	C22-C23-C24-C25
18	aA	848	BCR	C23-C24-C25-C30
18	aA	849	BCR	C1-C6-C7-C8
18	aA	849	BCR	C6-C7-C8-C9
18	aA	849	BCR	C7-C8-C9-C10
18	aA	849	BCR	C7-C8-C9-C34
18	aA	849	BCR	C16-C17-C18-C36
18	aA	849	BCR	C37-C22-C23-C24
18	aA	850	BCR	C1-C6-C7-C8
18	aA	850	BCR	C6-C7-C8-C9
18	aA	850	BCR	C7-C8-C9-C34
18	aA	850	BCR	C17-C18-C19-C20
18	aA	850	BCR	C21-C22-C23-C24
18	aA	850	BCR	C22-C23-C24-C25
18	aA	851	BCR	C1-C6-C7-C8
18	aA	851	BCR	C20-C21-C22-C37
18	aA	851	BCR	C21-C22-C23-C24
18	aA	851	BCR	C37-C22-C23-C24
18	aA	851	BCR	C23-C24-C25-C30
18	aA	852	BCR	C7-C8-C9-C10
18	aA	852	BCR	C11-C10-C9-C8
18	aA	852	BCR	C11-C12-C13-C35
18	aA	852	BCR	C16-C17-C18-C19
18	aA	852	BCR	C18-C19-C20-C21
18	aA	852	BCR	C20-C21-C22-C23
18	aA	852	BCR	C20-C21-C22-C37
18	aA	852	BCR	C21-C22-C23-C24
18	aB	844	BCR	C1-C6-C7-C8
18	aB	844	BCR	C7-C8-C9-C10
18	aB	844	BCR	C37-C22-C23-C24
18	aB	845	BCR	C11-C12-C13-C35
18	aB	845	BCR	C21-C22-C23-C24
18	aB	846	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aB	846	BCR	C11-C12-C13-C35
18	aB	846	BCR	C37-C22-C23-C24
18	aB	847	BCR	C16-C17-C18-C36
18	aB	847	BCR	C36-C18-C19-C20
18	aB	847	BCR	C18-C19-C20-C21
18	aB	847	BCR	C20-C21-C22-C23
18	aB	847	BCR	C20-C21-C22-C37
18	aB	848	BCR	C1-C6-C7-C8
18	aB	848	BCR	C7-C8-C9-C10
18	aB	848	BCR	C7-C8-C9-C34
18	aB	848	BCR	C20-C21-C22-C23
18	aB	848	BCR	C37-C22-C23-C24
18	aB	848	BCR	C22-C23-C24-C25
18	aB	848	BCR	C23-C24-C25-C30
18	aB	849	BCR	C1-C6-C7-C8
18	aB	849	BCR	C20-C21-C22-C37
18	aB	849	BCR	C22-C23-C24-C25
18	aF	201	BCR	C7-C8-C9-C34
18	aF	201	BCR	C11-C12-C13-C35
18	aF	201	BCR	C14-C15-C16-C17
18	aF	201	BCR	C21-C22-C23-C24
18	aF	201	BCR	C37-C22-C23-C24
18	aF	202	BCR	C7-C8-C9-C10
18	aF	202	BCR	C12-C13-C14-C15
18	aF	202	BCR	C37-C22-C23-C24
18	aF	203	BCR	C7-C8-C9-C10
18	aF	203	BCR	C7-C8-C9-C34
18	aF	203	BCR	C23-C24-C25-C30
18	aI	101	BCR	C6-C7-C8-C9
18	aI	101	BCR	C7-C8-C9-C34
18	aI	101	BCR	C20-C21-C22-C23
18	aI	101	BCR	C21-C22-C23-C24
18	aI	101	BCR	C37-C22-C23-C24
18	aI	102	BCR	C7-C8-C9-C10
18	aI	102	BCR	C20-C21-C22-C23
18	aI	102	BCR	C20-C21-C22-C37
18	aI	103	BCR	C1-C6-C7-C8
18	aI	103	BCR	C7-C8-C9-C34
18	aI	103	BCR	C37-C22-C23-C24
18	aI	103	BCR	C23-C24-C25-C26
18	aJ	204	BCR	C11-C12-C13-C14
18	aJ	204	BCR	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aJ	204	BCR	C16-C17-C18-C36
18	aJ	205	BCR	C1-C6-C7-C8
18	aJ	205	BCR	C6-C7-C8-C9
18	aJ	205	BCR	C7-C8-C9-C34
18	aJ	205	BCR	C11-C10-C9-C8
18	aJ	205	BCR	C37-C22-C23-C24
18	aK	101	BCR	C1-C6-C7-C8
18	aK	101	BCR	C6-C7-C8-C9
18	aK	101	BCR	C7-C8-C9-C10
18	aK	101	BCR	C7-C8-C9-C34
18	aK	101	BCR	C37-C22-C23-C24
18	aL	205	BCR	C1-C6-C7-C8
18	aL	205	BCR	C7-C8-C9-C34
18	aL	205	BCR	C11-C12-C13-C35
18	aL	205	BCR	C37-C22-C23-C24
18	aM	101	BCR	C7-C8-C9-C34
18	aM	101	BCR	C20-C21-C22-C23
18	aM	101	BCR	C20-C21-C22-C37
18	a1	417	BCR	C1-C6-C7-C8
18	a1	417	BCR	C7-C8-C9-C10
18	a1	418	BCR	C7-C8-C9-C34
18	a1	418	BCR	C19-C20-C21-C22
18	a1	418	BCR	C21-C22-C23-C24
18	a1	419	BCR	C1-C6-C7-C8
18	a1	419	BCR	C6-C7-C8-C9
18	a1	419	BCR	C7-C8-C9-C34
18	a1	419	BCR	C11-C12-C13-C35
18	a1	419	BCR	C22-C23-C24-C25
18	a1	420	BCR	C1-C6-C7-C8
18	a1	420	BCR	C7-C8-C9-C10
18	a1	420	BCR	C21-C22-C23-C24
18	a1	421	BCR	C1-C6-C7-C8
18	a1	421	BCR	C6-C7-C8-C9
18	a1	421	BCR	C7-C8-C9-C10
18	a1	421	BCR	C22-C23-C24-C25
18	a2	401	BCR	C6-C7-C8-C9
18	a2	401	BCR	C7-C8-C9-C10
18	a2	401	BCR	C7-C8-C9-C34
18	a2	401	BCR	C11-C12-C13-C35
18	a2	401	BCR	C22-C23-C24-C25
18	a2	419	BCR	C1-C6-C7-C8
18	a2	419	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a2	419	BCR	C23-C24-C25-C30
18	a2	420	BCR	C7-C8-C9-C10
18	a2	420	BCR	C21-C22-C23-C24
18	a2	421	BCR	C1-C6-C7-C8
18	a2	421	BCR	C6-C7-C8-C9
18	a2	421	BCR	C7-C8-C9-C34
18	a2	421	BCR	C20-C21-C22-C37
18	a2	421	BCR	C22-C23-C24-C25
18	a3	401	BCR	C1-C6-C7-C8
18	a3	401	BCR	C6-C7-C8-C9
18	a3	401	BCR	C7-C8-C9-C10
18	a3	401	BCR	C7-C8-C9-C34
18	a3	401	BCR	C10-C11-C12-C13
18	a3	401	BCR	C11-C12-C13-C35
18	a3	401	BCR	C22-C23-C24-C25
18	a3	418	BCR	C1-C6-C7-C8
18	a3	418	BCR	C7-C8-C9-C10
18	a3	418	BCR	C23-C24-C25-C30
18	a3	419	BCR	C1-C6-C7-C8
18	a3	419	BCR	C19-C20-C21-C22
18	a3	419	BCR	C21-C22-C23-C24
18	a3	420	BCR	C1-C6-C7-C8
18	a3	420	BCR	C6-C7-C8-C9
18	a3	420	BCR	C7-C8-C9-C34
18	a3	420	BCR	C11-C12-C13-C35
18	a3	420	BCR	C22-C23-C24-C25
18	a4	401	BCR	C6-C7-C8-C9
18	a4	401	BCR	C7-C8-C9-C10
18	a4	401	BCR	C7-C8-C9-C34
18	a4	401	BCR	C10-C11-C12-C13
18	a4	401	BCR	C11-C12-C13-C35
18	a4	401	BCR	C22-C23-C24-C25
18	a4	418	BCR	C1-C6-C7-C8
18	a4	418	BCR	C7-C8-C9-C10
18	a4	418	BCR	C23-C24-C25-C30
18	a4	419	BCR	C1-C6-C7-C8
18	a4	419	BCR	C21-C22-C23-C24
18	a4	420	BCR	C1-C6-C7-C8
18	a4	420	BCR	C6-C7-C8-C9
18	a4	420	BCR	C7-C8-C9-C34
18	a4	420	BCR	C11-C12-C13-C35
18	a4	420	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a5	401	BCR	C6-C7-C8-C9
18	a5	401	BCR	C7-C8-C9-C10
18	a5	401	BCR	C7-C8-C9-C34
18	a5	401	BCR	C10-C11-C12-C13
18	a5	401	BCR	C11-C12-C13-C35
18	a5	401	BCR	C22-C23-C24-C25
18	a5	418	BCR	C1-C6-C7-C8
18	a5	418	BCR	C7-C8-C9-C10
18	a5	418	BCR	C23-C24-C25-C30
18	a5	419	BCR	C1-C6-C7-C8
18	a5	419	BCR	C6-C7-C8-C9
18	a5	419	BCR	C7-C8-C9-C34
18	a5	419	BCR	C11-C12-C13-C35
18	a5	419	BCR	C22-C23-C24-C25
18	a6	401	BCR	C1-C6-C7-C8
18	a6	401	BCR	C7-C8-C9-C10
18	a6	401	BCR	C19-C20-C21-C22
18	a6	401	BCR	C21-C22-C23-C24
18	a6	402	BCR	C6-C7-C8-C9
18	a6	402	BCR	C7-C8-C9-C10
18	a6	402	BCR	C7-C8-C9-C34
18	a6	402	BCR	C10-C11-C12-C13
18	a6	402	BCR	C22-C23-C24-C25
18	a6	419	BCR	C1-C6-C7-C8
18	a6	419	BCR	C7-C8-C9-C10
18	a6	419	BCR	C23-C24-C25-C30
18	a6	420	BCR	C1-C6-C7-C8
18	a6	420	BCR	C6-C7-C8-C9
18	a6	420	BCR	C7-C8-C9-C34
18	a6	420	BCR	C11-C12-C13-C35
18	a6	420	BCR	C20-C21-C22-C37
18	a6	420	BCR	C22-C23-C24-C25
18	a6	421	BCR	C1-C6-C7-C8
18	a6	421	BCR	C6-C7-C8-C9
18	a6	421	BCR	C7-C8-C9-C10
18	a6	421	BCR	C7-C8-C9-C34
18	a6	421	BCR	C10-C11-C12-C13
18	a6	421	BCR	C22-C23-C24-C25
18	bA	848	BCR	C1-C6-C7-C8
18	bA	848	BCR	C6-C7-C8-C9
18	bA	848	BCR	C7-C8-C9-C10
18	bA	848	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bA	848	BCR	C37-C22-C23-C24
18	bA	849	BCR	C11-C12-C13-C35
18	bA	849	BCR	C20-C21-C22-C23
18	bA	849	BCR	C20-C21-C22-C37
18	bA	849	BCR	C22-C23-C24-C25
18	bA	849	BCR	C23-C24-C25-C30
18	bA	850	BCR	C1-C6-C7-C8
18	bA	850	BCR	C6-C7-C8-C9
18	bA	850	BCR	C7-C8-C9-C10
18	bA	850	BCR	C7-C8-C9-C34
18	bA	850	BCR	C16-C17-C18-C36
18	bA	850	BCR	C37-C22-C23-C24
18	bA	851	BCR	C1-C6-C7-C8
18	bA	851	BCR	C6-C7-C8-C9
18	bA	851	BCR	C7-C8-C9-C34
18	bA	851	BCR	C17-C18-C19-C20
18	bA	851	BCR	C21-C22-C23-C24
18	bA	851	BCR	C22-C23-C24-C25
18	bA	852	BCR	C1-C6-C7-C8
18	bA	852	BCR	C20-C21-C22-C37
18	bA	852	BCR	C21-C22-C23-C24
18	bA	852	BCR	C37-C22-C23-C24
18	bA	852	BCR	C23-C24-C25-C30
18	bA	853	BCR	C7-C8-C9-C10
18	bA	853	BCR	C11-C10-C9-C8
18	bA	853	BCR	C11-C12-C13-C35
18	bA	853	BCR	C16-C17-C18-C19
18	bA	853	BCR	C18-C19-C20-C21
18	bA	853	BCR	C20-C21-C22-C23
18	bA	853	BCR	C20-C21-C22-C37
18	bA	853	BCR	C21-C22-C23-C24
18	bB	844	BCR	C1-C6-C7-C8
18	bB	844	BCR	C7-C8-C9-C10
18	bB	844	BCR	C37-C22-C23-C24
18	bB	845	BCR	C11-C12-C13-C35
18	bB	845	BCR	C21-C22-C23-C24
18	bB	846	BCR	C1-C6-C7-C8
18	bB	846	BCR	C11-C12-C13-C35
18	bB	846	BCR	C37-C22-C23-C24
18	bB	847	BCR	C16-C17-C18-C36
18	bB	847	BCR	C36-C18-C19-C20
18	bB	847	BCR	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bB	847	BCR	C20-C21-C22-C23
18	bB	847	BCR	C20-C21-C22-C37
18	bB	848	BCR	C1-C6-C7-C8
18	bB	848	BCR	C7-C8-C9-C10
18	bB	848	BCR	C7-C8-C9-C34
18	bB	848	BCR	C20-C21-C22-C23
18	bB	848	BCR	C37-C22-C23-C24
18	bB	848	BCR	C22-C23-C24-C25
18	bB	848	BCR	C23-C24-C25-C30
18	bB	849	BCR	C7-C8-C9-C34
18	bB	849	BCR	C11-C12-C13-C35
18	bB	849	BCR	C14-C15-C16-C17
18	bB	849	BCR	C21-C22-C23-C24
18	bB	849	BCR	C37-C22-C23-C24
18	bB	850	BCR	C1-C6-C7-C8
18	bB	850	BCR	C20-C21-C22-C37
18	bB	850	BCR	C22-C23-C24-C25
18	bF	202	BCR	C7-C8-C9-C10
18	bF	202	BCR	C12-C13-C14-C15
18	bF	202	BCR	C37-C22-C23-C24
18	bI	101	BCR	C6-C7-C8-C9
18	bI	101	BCR	C7-C8-C9-C34
18	bI	101	BCR	C20-C21-C22-C23
18	bI	101	BCR	C21-C22-C23-C24
18	bI	101	BCR	C37-C22-C23-C24
18	bI	102	BCR	C7-C8-C9-C10
18	bI	102	BCR	C20-C21-C22-C23
18	bI	102	BCR	C20-C21-C22-C37
18	bJ	103	BCR	C11-C12-C13-C14
18	bJ	103	BCR	C12-C13-C14-C15
18	bJ	103	BCR	C16-C17-C18-C36
18	bJ	104	BCR	C1-C6-C7-C8
18	bJ	104	BCR	C6-C7-C8-C9
18	bJ	104	BCR	C7-C8-C9-C34
18	bJ	104	BCR	C11-C10-C9-C8
18	bJ	104	BCR	C37-C22-C23-C24
18	bJ	105	BCR	C7-C8-C9-C10
18	bJ	105	BCR	C7-C8-C9-C34
18	bJ	105	BCR	C23-C24-C25-C30
18	bL	201	BCR	C1-C6-C7-C8
18	bL	201	BCR	C7-C8-C9-C34
18	bL	201	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bL	201	BCR	C37-C22-C23-C24
18	bL	205	BCR	C1-C6-C7-C8
18	bL	205	BCR	C7-C8-C9-C34
18	bL	205	BCR	C37-C22-C23-C24
18	bL	205	BCR	C23-C24-C25-C26
18	bL	206	BCR	C1-C6-C7-C8
18	bL	206	BCR	C7-C8-C9-C34
18	bL	206	BCR	C11-C12-C13-C35
18	bL	206	BCR	C37-C22-C23-C24
18	bM	101	BCR	C7-C8-C9-C34
18	bM	101	BCR	C20-C21-C22-C23
18	bM	101	BCR	C20-C21-C22-C37
18	b1	401	BCR	C1-C6-C7-C8
18	b1	401	BCR	C11-C10-C9-C34
18	b1	401	BCR	C19-C20-C21-C22
18	b1	401	BCR	C21-C22-C23-C24
18	b1	418	BCR	C1-C6-C7-C8
18	b1	418	BCR	C7-C8-C9-C10
18	b1	419	BCR	C7-C8-C9-C34
18	b1	419	BCR	C19-C20-C21-C22
18	b1	419	BCR	C21-C22-C23-C24
18	b1	420	BCR	C1-C6-C7-C8
18	b1	420	BCR	C6-C7-C8-C9
18	b1	420	BCR	C7-C8-C9-C34
18	b1	420	BCR	C11-C12-C13-C35
18	b1	420	BCR	C22-C23-C24-C25
18	b2	401	BCR	C6-C7-C8-C9
18	b2	401	BCR	C7-C8-C9-C10
18	b2	401	BCR	C7-C8-C9-C34
18	b2	401	BCR	C11-C12-C13-C35
18	b2	401	BCR	C22-C23-C24-C25
18	b2	419	BCR	C1-C6-C7-C8
18	b2	419	BCR	C7-C8-C9-C10
18	b2	419	BCR	C23-C24-C25-C30
18	b2	420	BCR	C1-C6-C7-C8
18	b2	420	BCR	C7-C8-C9-C10
18	b2	420	BCR	C21-C22-C23-C24
18	b2	421	BCR	C1-C6-C7-C8
18	b2	421	BCR	C6-C7-C8-C9
18	b2	421	BCR	C7-C8-C9-C34
18	b2	421	BCR	C20-C21-C22-C37
18	b2	421	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b3	401	BCR	C1-C6-C7-C8
18	b3	401	BCR	C6-C7-C8-C9
18	b3	401	BCR	C7-C8-C9-C10
18	b3	401	BCR	C7-C8-C9-C34
18	b3	401	BCR	C10-C11-C12-C13
18	b3	401	BCR	C11-C12-C13-C35
18	b3	401	BCR	C22-C23-C24-C25
18	b3	418	BCR	C1-C6-C7-C8
18	b3	418	BCR	C7-C8-C9-C10
18	b3	418	BCR	C23-C24-C25-C30
18	b3	419	BCR	C1-C6-C7-C8
18	b3	419	BCR	C19-C20-C21-C22
18	b3	419	BCR	C21-C22-C23-C24
18	b3	420	BCR	C1-C6-C7-C8
18	b3	420	BCR	C6-C7-C8-C9
18	b3	420	BCR	C7-C8-C9-C34
18	b3	420	BCR	C11-C12-C13-C35
18	b3	420	BCR	C22-C23-C24-C25
18	b4	401	BCR	C6-C7-C8-C9
18	b4	401	BCR	C7-C8-C9-C10
18	b4	401	BCR	C7-C8-C9-C34
18	b4	401	BCR	C10-C11-C12-C13
18	b4	401	BCR	C11-C12-C13-C35
18	b4	401	BCR	C22-C23-C24-C25
18	b4	418	BCR	C1-C6-C7-C8
18	b4	418	BCR	C7-C8-C9-C10
18	b4	418	BCR	C23-C24-C25-C30
18	b4	419	BCR	C1-C6-C7-C8
18	b4	419	BCR	C21-C22-C23-C24
18	b4	420	BCR	C1-C6-C7-C8
18	b4	420	BCR	C6-C7-C8-C9
18	b4	420	BCR	C7-C8-C9-C34
18	b4	420	BCR	C11-C12-C13-C35
18	b4	420	BCR	C22-C23-C24-C25
18	b5	401	BCR	C6-C7-C8-C9
18	b5	401	BCR	C7-C8-C9-C10
18	b5	401	BCR	C7-C8-C9-C34
18	b5	401	BCR	C10-C11-C12-C13
18	b5	401	BCR	C11-C12-C13-C35
18	b5	401	BCR	C22-C23-C24-C25
18	b5	418	BCR	C1-C6-C7-C8
18	b5	418	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b5	418	BCR	C23-C24-C25-C30
18	b5	419	BCR	C1-C6-C7-C8
18	b5	419	BCR	C6-C7-C8-C9
18	b5	419	BCR	C7-C8-C9-C34
18	b5	419	BCR	C11-C12-C13-C35
18	b5	419	BCR	C20-C21-C22-C37
18	b6	401	BCR	C1-C6-C7-C8
18	b6	401	BCR	C7-C8-C9-C10
18	b6	401	BCR	C19-C20-C21-C22
18	b6	401	BCR	C21-C22-C23-C24
18	b6	402	BCR	C6-C7-C8-C9
18	b6	402	BCR	C7-C8-C9-C10
18	b6	402	BCR	C7-C8-C9-C34
18	b6	402	BCR	C10-C11-C12-C13
18	b6	402	BCR	C22-C23-C24-C25
18	b6	419	BCR	C1-C6-C7-C8
18	b6	419	BCR	C7-C8-C9-C10
18	b6	419	BCR	C23-C24-C25-C30
18	b6	420	BCR	C1-C6-C7-C8
18	b6	420	BCR	C6-C7-C8-C9
18	b6	420	BCR	C7-C8-C9-C34
18	b6	420	BCR	C11-C12-C13-C35
18	b6	420	BCR	C22-C23-C24-C25
18	b6	421	BCR	C1-C6-C7-C8
18	b6	421	BCR	C6-C7-C8-C9
18	b6	421	BCR	C7-C8-C9-C10
18	b6	421	BCR	C7-C8-C9-C34
18	b6	421	BCR	C10-C11-C12-C13
18	b6	421	BCR	C22-C23-C24-C25
18	cA	847	BCR	C11-C12-C13-C35
18	cA	847	BCR	C20-C21-C22-C23
18	cA	847	BCR	C20-C21-C22-C37
18	cA	847	BCR	C22-C23-C24-C25
18	cA	847	BCR	C23-C24-C25-C30
18	cA	848	BCR	C1-C6-C7-C8
18	cA	848	BCR	C6-C7-C8-C9
18	cA	848	BCR	C7-C8-C9-C10
18	cA	848	BCR	C7-C8-C9-C34
18	cA	848	BCR	C16-C17-C18-C36
18	cA	848	BCR	C37-C22-C23-C24
18	cA	849	BCR	C1-C6-C7-C8
18	cA	849	BCR	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cA	849	BCR	C7-C8-C9-C34
18	cA	849	BCR	C17-C18-C19-C20
18	cA	849	BCR	C21-C22-C23-C24
18	cA	849	BCR	C22-C23-C24-C25
18	cA	850	BCR	C1-C6-C7-C8
18	cA	850	BCR	C20-C21-C22-C37
18	cA	850	BCR	C21-C22-C23-C24
18	cA	850	BCR	C37-C22-C23-C24
18	cA	850	BCR	C23-C24-C25-C30
18	cA	851	BCR	C7-C8-C9-C10
18	cA	851	BCR	C11-C10-C9-C8
18	cA	851	BCR	C11-C12-C13-C35
18	cA	851	BCR	C16-C17-C18-C19
18	cA	851	BCR	C18-C19-C20-C21
18	cA	851	BCR	C20-C21-C22-C23
18	cA	851	BCR	C20-C21-C22-C37
18	cA	851	BCR	C21-C22-C23-C24
18	cB	844	BCR	C1-C6-C7-C8
18	cB	844	BCR	C7-C8-C9-C10
18	cB	844	BCR	C37-C22-C23-C24
18	cB	845	BCR	C11-C12-C13-C35
18	cB	845	BCR	C21-C22-C23-C24
18	cB	846	BCR	C1-C6-C7-C8
18	cB	846	BCR	C11-C12-C13-C35
18	cB	846	BCR	C37-C22-C23-C24
18	cB	847	BCR	C16-C17-C18-C36
18	cB	847	BCR	C36-C18-C19-C20
18	cB	847	BCR	C18-C19-C20-C21
18	cB	847	BCR	C20-C21-C22-C23
18	cB	847	BCR	C20-C21-C22-C37
18	cB	848	BCR	C1-C6-C7-C8
18	cB	848	BCR	C7-C8-C9-C10
18	cB	848	BCR	C7-C8-C9-C34
18	cB	848	BCR	C20-C21-C22-C23
18	cB	848	BCR	C37-C22-C23-C24
18	cB	848	BCR	C22-C23-C24-C25
18	cB	848	BCR	C23-C24-C25-C30
18	cB	849	BCR	C1-C6-C7-C8
18	cB	849	BCR	C20-C21-C22-C37
18	cB	849	BCR	C22-C23-C24-C25
18	cF	202	BCR	C7-C8-C9-C34
18	cF	202	BCR	C11-C12-C13-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cF	202	BCR	C14-C15-C16-C17
18	cF	202	BCR	C21-C22-C23-C24
18	cF	202	BCR	C37-C22-C23-C24
18	cF	204	BCR	C7-C8-C9-C10
18	cF	204	BCR	C12-C13-C14-C15
18	cF	204	BCR	C37-C22-C23-C24
18	cF	205	BCR	C7-C8-C9-C10
18	cF	205	BCR	C7-C8-C9-C34
18	cF	205	BCR	C23-C24-C25-C30
18	cI	101	BCR	C6-C7-C8-C9
18	cI	101	BCR	C7-C8-C9-C34
18	cI	101	BCR	C20-C21-C22-C23
18	cI	101	BCR	C21-C22-C23-C24
18	cI	101	BCR	C37-C22-C23-C24
18	cI	102	BCR	C7-C8-C9-C10
18	cI	102	BCR	C20-C21-C22-C23
18	cI	102	BCR	C20-C21-C22-C37
18	cJ	103	BCR	C11-C12-C13-C14
18	cJ	103	BCR	C12-C13-C14-C15
18	cJ	103	BCR	C16-C17-C18-C36
18	cJ	104	BCR	C1-C6-C7-C8
18	cJ	104	BCR	C6-C7-C8-C9
18	cJ	104	BCR	C7-C8-C9-C34
18	cJ	104	BCR	C11-C10-C9-C8
18	cJ	104	BCR	C37-C22-C23-C24
18	cK	101	BCR	C1-C6-C7-C8
18	cK	101	BCR	C6-C7-C8-C9
18	cK	101	BCR	C7-C8-C9-C10
18	cK	101	BCR	C7-C8-C9-C34
18	cK	101	BCR	C37-C22-C23-C24
18	cL	205	BCR	C1-C6-C7-C8
18	cL	205	BCR	C7-C8-C9-C34
18	cL	205	BCR	C37-C22-C23-C24
18	cL	205	BCR	C23-C24-C25-C26
18	cM	101	BCR	C7-C8-C9-C34
18	cM	101	BCR	C20-C21-C22-C23
18	cM	101	BCR	C20-C21-C22-C37
18	c1	401	BCR	C11-C10-C9-C34
18	c1	401	BCR	C21-C22-C23-C24
18	c1	418	BCR	C1-C6-C7-C8
18	c1	418	BCR	C7-C8-C9-C10
18	c1	419	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c1	419	BCR	C21-C22-C23-C24
18	c1	420	BCR	C1-C6-C7-C8
18	c1	420	BCR	C6-C7-C8-C9
18	c1	420	BCR	C7-C8-C9-C34
18	c1	420	BCR	C11-C12-C13-C35
18	c1	420	BCR	C22-C23-C24-C25
18	c2	401	BCR	C6-C7-C8-C9
18	c2	401	BCR	C7-C8-C9-C10
18	c2	401	BCR	C7-C8-C9-C34
18	c2	401	BCR	C11-C12-C13-C35
18	c2	401	BCR	C22-C23-C24-C25
18	c2	419	BCR	C1-C6-C7-C8
18	c2	419	BCR	C7-C8-C9-C10
18	c2	419	BCR	C23-C24-C25-C30
18	c2	420	BCR	C7-C8-C9-C10
18	c2	420	BCR	C21-C22-C23-C24
18	c2	421	BCR	C1-C6-C7-C8
18	c2	421	BCR	C6-C7-C8-C9
18	c2	421	BCR	C7-C8-C9-C34
18	c2	421	BCR	C20-C21-C22-C37
18	c2	421	BCR	C22-C23-C24-C25
18	c3	401	BCR	C1-C6-C7-C8
18	c3	401	BCR	C6-C7-C8-C9
18	c3	401	BCR	C7-C8-C9-C10
18	c3	401	BCR	C7-C8-C9-C34
18	c3	401	BCR	C10-C11-C12-C13
18	c3	401	BCR	C11-C12-C13-C35
18	c3	401	BCR	C22-C23-C24-C25
18	c3	418	BCR	C1-C6-C7-C8
18	c3	418	BCR	C7-C8-C9-C10
18	c3	418	BCR	C23-C24-C25-C30
18	c3	419	BCR	C1-C6-C7-C8
18	c3	419	BCR	C19-C20-C21-C22
18	c3	419	BCR	C21-C22-C23-C24
18	c3	420	BCR	C1-C6-C7-C8
18	c3	420	BCR	C6-C7-C8-C9
18	c3	420	BCR	C7-C8-C9-C34
18	c3	420	BCR	C11-C12-C13-C35
18	c3	420	BCR	C22-C23-C24-C25
18	c4	401	BCR	C6-C7-C8-C9
18	c4	401	BCR	C7-C8-C9-C10
18	c4	401	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c4	401	BCR	C10-C11-C12-C13
18	c4	401	BCR	C11-C12-C13-C35
18	c4	401	BCR	C22-C23-C24-C25
18	c4	418	BCR	C1-C6-C7-C8
18	c4	418	BCR	C7-C8-C9-C10
18	c4	418	BCR	C23-C24-C25-C30
18	c4	419	BCR	C1-C6-C7-C8
18	c4	419	BCR	C21-C22-C23-C24
18	c4	420	BCR	C1-C6-C7-C8
18	c4	420	BCR	C6-C7-C8-C9
18	c4	420	BCR	C7-C8-C9-C34
18	c4	420	BCR	C11-C12-C13-C35
18	c4	420	BCR	C22-C23-C24-C25
18	c5	401	BCR	C6-C7-C8-C9
18	c5	401	BCR	C7-C8-C9-C10
18	c5	401	BCR	C7-C8-C9-C34
18	c5	401	BCR	C10-C11-C12-C13
18	c5	401	BCR	C11-C12-C13-C35
18	c5	401	BCR	C22-C23-C24-C25
18	c5	418	BCR	C1-C6-C7-C8
18	c5	418	BCR	C7-C8-C9-C10
18	c5	418	BCR	C23-C24-C25-C30
18	c5	419	BCR	C1-C6-C7-C8
18	c5	419	BCR	C6-C7-C8-C9
18	c5	419	BCR	C7-C8-C9-C34
18	c5	419	BCR	C11-C12-C13-C35
18	c5	419	BCR	C22-C23-C24-C25
18	c6	402	BCR	C1-C6-C7-C8
18	c6	402	BCR	C7-C8-C9-C10
18	c6	402	BCR	C19-C20-C21-C22
18	c6	402	BCR	C21-C22-C23-C24
18	c6	403	BCR	C6-C7-C8-C9
18	c6	403	BCR	C7-C8-C9-C10
18	c6	403	BCR	C7-C8-C9-C34
18	c6	403	BCR	C10-C11-C12-C13
18	c6	403	BCR	C22-C23-C24-C25
18	c6	420	BCR	C1-C6-C7-C8
18	c6	420	BCR	C7-C8-C9-C10
18	c6	420	BCR	C23-C24-C25-C30
18	c6	421	BCR	C1-C6-C7-C8
18	c6	421	BCR	C6-C7-C8-C9
18	c6	421	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c6	421	BCR	C11-C12-C13-C35
18	c6	421	BCR	C22-C23-C24-C25
19	aA	853	LHG	C3-O3-P-O5
19	aA	854	LHG	C1-C2-C3-O3
19	aA	854	LHG	C3-O3-P-O5
19	aA	854	LHG	C4-O6-P-O5
19	aX	101	LHG	O1-C1-C2-C3
19	aX	101	LHG	C3-O3-P-O4
19	aX	101	LHG	C3-O3-P-O5
19	bA	854	LHG	C3-O3-P-O5
19	bA	855	LHG	C1-C2-C3-O3
19	bA	855	LHG	C3-O3-P-O5
19	bX	101	LHG	O1-C1-C2-C3
19	bX	101	LHG	C3-O3-P-O4
19	bX	101	LHG	C3-O3-P-O5
19	cA	852	LHG	C3-O3-P-O5
19	cA	853	LHG	C1-C2-C3-O3
19	cA	853	LHG	C3-O3-P-O5
19	cX	101	LHG	O1-C1-C2-C3
19	cX	101	LHG	C3-O3-P-O4
19	cX	101	LHG	C3-O3-P-O5
15	aA	845	CLA	C4C-C3C-CAC-CBC
15	a1	409	CLA	C4C-C3C-CAC-CBC
15	a2	411	CLA	C4C-C3C-CAC-CBC
15	a3	410	CLA	C4C-C3C-CAC-CBC
15	a4	410	CLA	C4C-C3C-CAC-CBC
15	a5	410	CLA	C4C-C3C-CAC-CBC
15	a6	411	CLA	C4C-C3C-CAC-CBC
15	bA	845	CLA	C4C-C3C-CAC-CBC
15	b1	410	CLA	C4C-C3C-CAC-CBC
15	b2	411	CLA	C4C-C3C-CAC-CBC
15	b3	410	CLA	C4C-C3C-CAC-CBC
15	b4	410	CLA	C4C-C3C-CAC-CBC
15	b5	410	CLA	C4C-C3C-CAC-CBC
15	b6	411	CLA	C4C-C3C-CAC-CBC
15	cA	844	CLA	C4C-C3C-CAC-CBC
15	c1	410	CLA	C4C-C3C-CAC-CBC
15	c2	411	CLA	C4C-C3C-CAC-CBC
15	c4	410	CLA	C4C-C3C-CAC-CBC
15	c5	410	CLA	C4C-C3C-CAC-CBC
15	c6	412	CLA	C4C-C3C-CAC-CBC
15	aX	102	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	405	CLA	O1D-CGD-O2D-CED
15	a2	407	CLA	O1D-CGD-O2D-CED
15	a2	422	CLA	O1D-CGD-O2D-CED
15	a3	406	CLA	O1D-CGD-O2D-CED
15	a4	406	CLA	O1D-CGD-O2D-CED
15	a4	421	CLA	O1D-CGD-O2D-CED
15	a5	406	CLA	O1D-CGD-O2D-CED
15	a6	407	CLA	O1D-CGD-O2D-CED
15	a6	422	CLA	O1D-CGD-O2D-CED
15	bX	102	CLA	O1D-CGD-O2D-CED
15	b1	406	CLA	O1D-CGD-O2D-CED
15	b2	407	CLA	O1D-CGD-O2D-CED
15	b2	422	CLA	O1D-CGD-O2D-CED
15	b3	406	CLA	O1D-CGD-O2D-CED
15	b4	406	CLA	O1D-CGD-O2D-CED
15	b4	421	CLA	O1D-CGD-O2D-CED
15	b5	406	CLA	O1D-CGD-O2D-CED
15	b6	407	CLA	O1D-CGD-O2D-CED
15	cX	102	CLA	O1D-CGD-O2D-CED
15	c1	406	CLA	O1D-CGD-O2D-CED
15	c2	407	CLA	O1D-CGD-O2D-CED
15	c2	422	CLA	O1D-CGD-O2D-CED
15	c3	406	CLA	O1D-CGD-O2D-CED
15	c4	406	CLA	O1D-CGD-O2D-CED
15	c4	421	CLA	O1D-CGD-O2D-CED
15	c5	406	CLA	O1D-CGD-O2D-CED
15	c6	408	CLA	O1D-CGD-O2D-CED
15	aA	845	CLA	C2C-C3C-CAC-CBC
15	a1	409	CLA	C2C-C3C-CAC-CBC
15	a2	411	CLA	C2C-C3C-CAC-CBC
15	a3	410	CLA	C2C-C3C-CAC-CBC
15	a4	410	CLA	C2C-C3C-CAC-CBC
15	a5	410	CLA	C2C-C3C-CAC-CBC
15	a6	411	CLA	C2C-C3C-CAC-CBC
15	bA	845	CLA	C2C-C3C-CAC-CBC
15	b1	410	CLA	C2C-C3C-CAC-CBC
15	b2	411	CLA	C2C-C3C-CAC-CBC
15	b3	410	CLA	C2C-C3C-CAC-CBC
15	b4	410	CLA	C2C-C3C-CAC-CBC
15	b5	410	CLA	C2C-C3C-CAC-CBC
15	b6	411	CLA	C2C-C3C-CAC-CBC
15	cA	844	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	410	CLA	C2C-C3C-CAC-CBC
15	c2	411	CLA	C2C-C3C-CAC-CBC
15	c3	410	CLA	C4C-C3C-CAC-CBC
15	c4	410	CLA	C2C-C3C-CAC-CBC
15	c5	410	CLA	C2C-C3C-CAC-CBC
15	c6	412	CLA	C2C-C3C-CAC-CBC
15	aA	811	CLA	O1D-CGD-O2D-CED
15	aA	839	CLA	O1D-CGD-O2D-CED
15	a1	415	CLA	O1D-CGD-O2D-CED
15	a2	406	CLA	O1D-CGD-O2D-CED
15	a2	417	CLA	O1D-CGD-O2D-CED
15	a3	416	CLA	O1D-CGD-O2D-CED
15	a4	416	CLA	O1D-CGD-O2D-CED
15	a5	416	CLA	O1D-CGD-O2D-CED
15	a6	417	CLA	O1D-CGD-O2D-CED
15	bA	811	CLA	O1D-CGD-O2D-CED
15	bA	839	CLA	O1D-CGD-O2D-CED
15	b1	416	CLA	O1D-CGD-O2D-CED
15	b2	406	CLA	O1D-CGD-O2D-CED
15	b2	417	CLA	O1D-CGD-O2D-CED
15	b3	416	CLA	O1D-CGD-O2D-CED
15	b4	416	CLA	O1D-CGD-O2D-CED
15	b5	416	CLA	O1D-CGD-O2D-CED
15	b6	417	CLA	O1D-CGD-O2D-CED
15	b6	422	CLA	O1D-CGD-O2D-CED
15	cA	811	CLA	O1D-CGD-O2D-CED
15	cA	839	CLA	O1D-CGD-O2D-CED
15	cB	835	CLA	O1D-CGD-O2D-CED
15	c1	416	CLA	O1D-CGD-O2D-CED
15	c2	406	CLA	O1D-CGD-O2D-CED
15	c2	417	CLA	O1D-CGD-O2D-CED
15	c3	416	CLA	O1D-CGD-O2D-CED
15	c4	416	CLA	O1D-CGD-O2D-CED
15	c5	416	CLA	O1D-CGD-O2D-CED
15	c6	401	CLA	O1D-CGD-O2D-CED
15	c6	418	CLA	O1D-CGD-O2D-CED
15	aA	802	CLA	CBD-CGD-O2D-CED
15	aA	812	CLA	CBD-CGD-O2D-CED
15	aA	829	CLA	CBD-CGD-O2D-CED
15	aA	838	CLA	CBD-CGD-O2D-CED
15	aA	840	CLA	CBD-CGD-O2D-CED
15	aA	841	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	845	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	CBD-CGD-O2D-CED
15	aB	804	CLA	CBD-CGD-O2D-CED
15	aB	815	CLA	CBD-CGD-O2D-CED
15	aB	816	CLA	CBD-CGD-O2D-CED
15	aB	821	CLA	CBD-CGD-O2D-CED
15	aB	825	CLA	CBD-CGD-O2D-CED
15	aB	835	CLA	CBD-CGD-O2D-CED
15	aB	836	CLA	CBD-CGD-O2D-CED
15	aB	840	CLA	CBD-CGD-O2D-CED
15	aX	102	CLA	CBD-CGD-O2D-CED
15	a1	402	CLA	CBD-CGD-O2D-CED
15	a1	403	CLA	CBD-CGD-O2D-CED
15	a1	404	CLA	CBD-CGD-O2D-CED
15	a1	405	CLA	CBD-CGD-O2D-CED
15	a1	411	CLA	CBD-CGD-O2D-CED
15	a1	416	CLA	CBD-CGD-O2D-CED
15	a2	403	CLA	CBD-CGD-O2D-CED
15	a2	404	CLA	CBD-CGD-O2D-CED
15	a2	405	CLA	CBD-CGD-O2D-CED
15	a2	407	CLA	CBD-CGD-O2D-CED
15	a2	418	CLA	CBD-CGD-O2D-CED
15	a3	403	CLA	CBD-CGD-O2D-CED
15	a3	404	CLA	CBD-CGD-O2D-CED
15	a3	405	CLA	CBD-CGD-O2D-CED
15	a3	406	CLA	CBD-CGD-O2D-CED
15	a4	403	CLA	CBD-CGD-O2D-CED
15	a4	404	CLA	CBD-CGD-O2D-CED
15	a4	405	CLA	CBD-CGD-O2D-CED
15	a4	406	CLA	CBD-CGD-O2D-CED
15	a4	412	CLA	CBD-CGD-O2D-CED
15	a5	403	CLA	CBD-CGD-O2D-CED
15	a5	404	CLA	CBD-CGD-O2D-CED
15	a5	405	CLA	CBD-CGD-O2D-CED
15	a5	406	CLA	CBD-CGD-O2D-CED
15	a5	412	CLA	CBD-CGD-O2D-CED
15	a6	404	CLA	CBD-CGD-O2D-CED
15	a6	405	CLA	CBD-CGD-O2D-CED
15	a6	407	CLA	CBD-CGD-O2D-CED
15	a6	413	CLA	CBD-CGD-O2D-CED
15	a6	418	CLA	CBD-CGD-O2D-CED
15	bA	802	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	812	CLA	CBD-CGD-O2D-CED
15	bA	829	CLA	CBD-CGD-O2D-CED
15	bA	838	CLA	CBD-CGD-O2D-CED
15	bA	840	CLA	CBD-CGD-O2D-CED
15	bA	841	CLA	CBD-CGD-O2D-CED
15	bA	845	CLA	CBD-CGD-O2D-CED
15	bB	803	CLA	CBD-CGD-O2D-CED
15	bB	804	CLA	CBD-CGD-O2D-CED
15	bB	815	CLA	CBD-CGD-O2D-CED
15	bB	816	CLA	CBD-CGD-O2D-CED
15	bB	821	CLA	CBD-CGD-O2D-CED
15	bB	825	CLA	CBD-CGD-O2D-CED
15	bB	835	CLA	CBD-CGD-O2D-CED
15	bB	836	CLA	CBD-CGD-O2D-CED
15	bB	840	CLA	CBD-CGD-O2D-CED
15	bX	102	CLA	CBD-CGD-O2D-CED
15	b1	403	CLA	CBD-CGD-O2D-CED
15	b1	404	CLA	CBD-CGD-O2D-CED
15	b1	405	CLA	CBD-CGD-O2D-CED
15	b1	406	CLA	CBD-CGD-O2D-CED
15	b1	412	CLA	CBD-CGD-O2D-CED
15	b1	417	CLA	CBD-CGD-O2D-CED
15	b2	403	CLA	CBD-CGD-O2D-CED
15	b2	404	CLA	CBD-CGD-O2D-CED
15	b2	405	CLA	CBD-CGD-O2D-CED
15	b2	407	CLA	CBD-CGD-O2D-CED
15	b2	418	CLA	CBD-CGD-O2D-CED
15	b3	403	CLA	CBD-CGD-O2D-CED
15	b3	404	CLA	CBD-CGD-O2D-CED
15	b3	405	CLA	CBD-CGD-O2D-CED
15	b3	406	CLA	CBD-CGD-O2D-CED
15	b4	403	CLA	CBD-CGD-O2D-CED
15	b4	404	CLA	CBD-CGD-O2D-CED
15	b4	405	CLA	CBD-CGD-O2D-CED
15	b4	406	CLA	CBD-CGD-O2D-CED
15	b4	412	CLA	CBD-CGD-O2D-CED
15	b5	403	CLA	CBD-CGD-O2D-CED
15	b5	404	CLA	CBD-CGD-O2D-CED
15	b5	405	CLA	CBD-CGD-O2D-CED
15	b5	406	CLA	CBD-CGD-O2D-CED
15	b5	412	CLA	CBD-CGD-O2D-CED
15	b6	404	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	405	CLA	CBD-CGD-O2D-CED
15	b6	407	CLA	CBD-CGD-O2D-CED
15	b6	413	CLA	CBD-CGD-O2D-CED
15	b6	418	CLA	CBD-CGD-O2D-CED
15	cA	802	CLA	CBD-CGD-O2D-CED
15	cA	812	CLA	CBD-CGD-O2D-CED
15	cA	829	CLA	CBD-CGD-O2D-CED
15	cA	838	CLA	CBD-CGD-O2D-CED
15	cA	840	CLA	CBD-CGD-O2D-CED
15	cA	841	CLA	CBD-CGD-O2D-CED
15	cA	844	CLA	CBD-CGD-O2D-CED
15	cB	803	CLA	CBD-CGD-O2D-CED
15	cB	804	CLA	CBD-CGD-O2D-CED
15	cB	815	CLA	CBD-CGD-O2D-CED
15	cB	816	CLA	CBD-CGD-O2D-CED
15	cB	821	CLA	CBD-CGD-O2D-CED
15	cB	825	CLA	CBD-CGD-O2D-CED
15	cB	835	CLA	CBD-CGD-O2D-CED
15	cB	836	CLA	CBD-CGD-O2D-CED
15	cB	840	CLA	CBD-CGD-O2D-CED
15	cX	102	CLA	CBD-CGD-O2D-CED
15	c1	403	CLA	CBD-CGD-O2D-CED
15	c1	404	CLA	CBD-CGD-O2D-CED
15	c1	405	CLA	CBD-CGD-O2D-CED
15	c1	406	CLA	CBD-CGD-O2D-CED
15	c1	412	CLA	CBD-CGD-O2D-CED
15	c1	417	CLA	CBD-CGD-O2D-CED
15	c2	403	CLA	CBD-CGD-O2D-CED
15	c2	404	CLA	CBD-CGD-O2D-CED
15	c2	405	CLA	CBD-CGD-O2D-CED
15	c2	407	CLA	CBD-CGD-O2D-CED
15	c2	413	CLA	CBD-CGD-O2D-CED
15	c2	418	CLA	CBD-CGD-O2D-CED
15	c3	403	CLA	CBD-CGD-O2D-CED
15	c3	404	CLA	CBD-CGD-O2D-CED
15	c3	405	CLA	CBD-CGD-O2D-CED
15	c3	406	CLA	CBD-CGD-O2D-CED
15	c3	412	CLA	CBD-CGD-O2D-CED
15	c4	403	CLA	CBD-CGD-O2D-CED
15	c4	404	CLA	CBD-CGD-O2D-CED
15	c4	405	CLA	CBD-CGD-O2D-CED
15	c4	406	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	412	CLA	CBD-CGD-O2D-CED
15	c5	403	CLA	CBD-CGD-O2D-CED
15	c5	404	CLA	CBD-CGD-O2D-CED
15	c5	405	CLA	CBD-CGD-O2D-CED
15	c5	406	CLA	CBD-CGD-O2D-CED
15	c5	412	CLA	CBD-CGD-O2D-CED
15	c5	415	CLA	CBD-CGD-O2D-CED
15	c6	405	CLA	CBD-CGD-O2D-CED
15	c6	406	CLA	CBD-CGD-O2D-CED
15	c6	407	CLA	CBD-CGD-O2D-CED
15	c6	408	CLA	CBD-CGD-O2D-CED
15	c6	414	CLA	CBD-CGD-O2D-CED
15	c6	419	CLA	CBD-CGD-O2D-CED
15	c3	410	CLA	C2C-C3C-CAC-CBC
15	aA	842	CLA	O1D-CGD-O2D-CED
15	aB	804	CLA	O1D-CGD-O2D-CED
15	aB	835	CLA	O1D-CGD-O2D-CED
15	aJ	201	CLA	O1D-CGD-O2D-CED
15	a1	411	CLA	O1D-CGD-O2D-CED
15	a2	415	CLA	O1D-CGD-O2D-CED
15	a3	408	CLA	O1D-CGD-O2D-CED
15	a3	414	CLA	O1D-CGD-O2D-CED
15	a3	421	CLA	O1D-CGD-O2D-CED
15	a4	414	CLA	O1D-CGD-O2D-CED
15	a5	414	CLA	O1D-CGD-O2D-CED
15	a5	420	CLA	O1D-CGD-O2D-CED
15	a6	413	CLA	O1D-CGD-O2D-CED
15	a6	415	CLA	O1D-CGD-O2D-CED
15	bA	842	CLA	O1D-CGD-O2D-CED
15	bB	804	CLA	O1D-CGD-O2D-CED
15	bB	835	CLA	O1D-CGD-O2D-CED
15	bF	201	CLA	O1D-CGD-O2D-CED
15	b1	412	CLA	O1D-CGD-O2D-CED
15	b3	414	CLA	O1D-CGD-O2D-CED
15	b3	421	CLA	O1D-CGD-O2D-CED
15	b4	414	CLA	O1D-CGD-O2D-CED
15	b5	420	CLA	O1D-CGD-O2D-CED
15	b6	413	CLA	O1D-CGD-O2D-CED
15	b6	415	CLA	O1D-CGD-O2D-CED
15	cB	804	CLA	O1D-CGD-O2D-CED
15	cF	201	CLA	O1D-CGD-O2D-CED
15	cF	203	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	412	CLA	O1D-CGD-O2D-CED
15	c2	415	CLA	O1D-CGD-O2D-CED
15	c3	414	CLA	O1D-CGD-O2D-CED
15	c3	421	CLA	O1D-CGD-O2D-CED
15	c4	414	CLA	O1D-CGD-O2D-CED
15	c5	414	CLA	O1D-CGD-O2D-CED
15	c5	420	CLA	O1D-CGD-O2D-CED
15	c6	414	CLA	O1D-CGD-O2D-CED
15	c6	416	CLA	O1D-CGD-O2D-CED
15	aA	810	CLA	O1D-CGD-O2D-CED
15	aB	802	CLA	O1D-CGD-O2D-CED
15	aB	815	CLA	O1D-CGD-O2D-CED
15	aB	825	CLA	O1D-CGD-O2D-CED
15	aB	834	CLA	O1D-CGD-O2D-CED
15	aJ	202	CLA	O1D-CGD-O2D-CED
15	a1	407	CLA	O1D-CGD-O2D-CED
15	a1	413	CLA	O1D-CGD-O2D-CED
15	a1	416	CLA	O1D-CGD-O2D-CED
15	a2	413	CLA	O1D-CGD-O2D-CED
15	a2	418	CLA	O1D-CGD-O2D-CED
15	a3	412	CLA	O1D-CGD-O2D-CED
15	a3	417	CLA	O1D-CGD-O2D-CED
15	a4	412	CLA	O1D-CGD-O2D-CED
15	a4	415	CLA	O1D-CGD-O2D-CED
15	a4	417	CLA	O1D-CGD-O2D-CED
15	a5	408	CLA	O1D-CGD-O2D-CED
15	a5	412	CLA	O1D-CGD-O2D-CED
15	a5	415	CLA	O1D-CGD-O2D-CED
15	a5	417	CLA	O1D-CGD-O2D-CED
15	a6	409	CLA	O1D-CGD-O2D-CED
15	a6	418	CLA	O1D-CGD-O2D-CED
15	bA	810	CLA	O1D-CGD-O2D-CED
15	bB	802	CLA	O1D-CGD-O2D-CED
15	bB	815	CLA	O1D-CGD-O2D-CED
15	bB	825	CLA	O1D-CGD-O2D-CED
15	bB	834	CLA	O1D-CGD-O2D-CED
15	bJ	101	CLA	O1D-CGD-O2D-CED
15	b1	414	CLA	O1D-CGD-O2D-CED
15	b1	417	CLA	O1D-CGD-O2D-CED
15	b2	413	CLA	O1D-CGD-O2D-CED
15	b2	415	CLA	O1D-CGD-O2D-CED
15	b2	416	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	418	CLA	O1D-CGD-O2D-CED
15	b3	408	CLA	O1D-CGD-O2D-CED
15	b3	412	CLA	O1D-CGD-O2D-CED
15	b3	417	CLA	O1D-CGD-O2D-CED
15	b4	412	CLA	O1D-CGD-O2D-CED
15	b4	415	CLA	O1D-CGD-O2D-CED
15	b4	417	CLA	O1D-CGD-O2D-CED
15	b5	408	CLA	O1D-CGD-O2D-CED
15	b5	412	CLA	O1D-CGD-O2D-CED
15	b5	414	CLA	O1D-CGD-O2D-CED
15	b5	415	CLA	O1D-CGD-O2D-CED
15	b5	417	CLA	O1D-CGD-O2D-CED
15	b6	409	CLA	O1D-CGD-O2D-CED
15	b6	418	CLA	O1D-CGD-O2D-CED
15	cA	810	CLA	O1D-CGD-O2D-CED
15	cB	802	CLA	O1D-CGD-O2D-CED
15	cB	815	CLA	O1D-CGD-O2D-CED
15	cB	825	CLA	O1D-CGD-O2D-CED
15	cB	834	CLA	O1D-CGD-O2D-CED
15	cJ	101	CLA	O1D-CGD-O2D-CED
15	c1	408	CLA	O1D-CGD-O2D-CED
15	c1	414	CLA	O1D-CGD-O2D-CED
15	c1	417	CLA	O1D-CGD-O2D-CED
15	c2	413	CLA	O1D-CGD-O2D-CED
15	c2	416	CLA	O1D-CGD-O2D-CED
15	c2	418	CLA	O1D-CGD-O2D-CED
15	c3	408	CLA	O1D-CGD-O2D-CED
15	c3	412	CLA	O1D-CGD-O2D-CED
15	c3	417	CLA	O1D-CGD-O2D-CED
15	c4	412	CLA	O1D-CGD-O2D-CED
15	c4	415	CLA	O1D-CGD-O2D-CED
15	c4	417	CLA	O1D-CGD-O2D-CED
15	c5	408	CLA	O1D-CGD-O2D-CED
15	c5	412	CLA	O1D-CGD-O2D-CED
15	c5	415	CLA	O1D-CGD-O2D-CED
15	c5	417	CLA	O1D-CGD-O2D-CED
15	c6	410	CLA	O1D-CGD-O2D-CED
15	c6	419	CLA	O1D-CGD-O2D-CED
15	aA	819	CLA	CBD-CGD-O2D-CED
15	aA	820	CLA	CBD-CGD-O2D-CED
15	aA	835	CLA	CBD-CGD-O2D-CED
15	aB	809	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	832	CLA	CBD-CGD-O2D-CED
15	aB	839	CLA	CBD-CGD-O2D-CED
15	a1	401	CLA	CBD-CGD-O2D-CED
15	a1	406	CLA	CBD-CGD-O2D-CED
15	a2	402	CLA	CBD-CGD-O2D-CED
15	a2	408	CLA	CBD-CGD-O2D-CED
15	a3	402	CLA	CBD-CGD-O2D-CED
15	a3	407	CLA	CBD-CGD-O2D-CED
15	a4	402	CLA	CBD-CGD-O2D-CED
15	a4	407	CLA	CBD-CGD-O2D-CED
15	a5	402	CLA	CBD-CGD-O2D-CED
15	a5	407	CLA	CBD-CGD-O2D-CED
15	a6	403	CLA	CBD-CGD-O2D-CED
15	a6	408	CLA	CBD-CGD-O2D-CED
15	bA	819	CLA	CBD-CGD-O2D-CED
15	bA	820	CLA	CBD-CGD-O2D-CED
15	bA	835	CLA	CBD-CGD-O2D-CED
15	bB	809	CLA	CBD-CGD-O2D-CED
15	bB	832	CLA	CBD-CGD-O2D-CED
15	bB	839	CLA	CBD-CGD-O2D-CED
15	b1	402	CLA	CBD-CGD-O2D-CED
15	b1	407	CLA	CBD-CGD-O2D-CED
15	b2	402	CLA	CBD-CGD-O2D-CED
15	b2	408	CLA	CBD-CGD-O2D-CED
15	b3	402	CLA	CBD-CGD-O2D-CED
15	b3	407	CLA	CBD-CGD-O2D-CED
15	b4	402	CLA	CBD-CGD-O2D-CED
15	b4	407	CLA	CBD-CGD-O2D-CED
15	b5	402	CLA	CBD-CGD-O2D-CED
15	b5	407	CLA	CBD-CGD-O2D-CED
15	b6	403	CLA	CBD-CGD-O2D-CED
15	b6	408	CLA	CBD-CGD-O2D-CED
15	cA	819	CLA	CBD-CGD-O2D-CED
15	cA	820	CLA	CBD-CGD-O2D-CED
15	cA	835	CLA	CBD-CGD-O2D-CED
15	cB	809	CLA	CBD-CGD-O2D-CED
15	cB	832	CLA	CBD-CGD-O2D-CED
15	cB	839	CLA	CBD-CGD-O2D-CED
15	c1	402	CLA	CBD-CGD-O2D-CED
15	c1	407	CLA	CBD-CGD-O2D-CED
15	c2	402	CLA	CBD-CGD-O2D-CED
15	c2	408	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	402	CLA	CBD-CGD-O2D-CED
15	c3	407	CLA	CBD-CGD-O2D-CED
15	c4	402	CLA	CBD-CGD-O2D-CED
15	c4	407	CLA	CBD-CGD-O2D-CED
15	c5	402	CLA	CBD-CGD-O2D-CED
15	c5	407	CLA	CBD-CGD-O2D-CED
15	c6	404	CLA	CBD-CGD-O2D-CED
15	c6	409	CLA	CBD-CGD-O2D-CED
15	aA	806	CLA	O1A-CGA-O2A-C1
15	aB	817	CLA	O1A-CGA-O2A-C1
15	a3	416	CLA	O1A-CGA-O2A-C1
15	a4	416	CLA	O1A-CGA-O2A-C1
15	a5	416	CLA	O1A-CGA-O2A-C1
15	a6	417	CLA	O1A-CGA-O2A-C1
15	bA	806	CLA	O1A-CGA-O2A-C1
15	bB	817	CLA	O1A-CGA-O2A-C1
15	b1	416	CLA	O1A-CGA-O2A-C1
15	b2	417	CLA	O1A-CGA-O2A-C1
15	b3	416	CLA	O1A-CGA-O2A-C1
15	b4	416	CLA	O1A-CGA-O2A-C1
15	b5	416	CLA	O1A-CGA-O2A-C1
15	b6	417	CLA	O1A-CGA-O2A-C1
15	cA	806	CLA	O1A-CGA-O2A-C1
15	cB	817	CLA	O1A-CGA-O2A-C1
15	c1	416	CLA	O1A-CGA-O2A-C1
15	c2	417	CLA	O1A-CGA-O2A-C1
15	c3	416	CLA	O1A-CGA-O2A-C1
15	c4	416	CLA	O1A-CGA-O2A-C1
15	c5	416	CLA	O1A-CGA-O2A-C1
15	c6	418	CLA	O1A-CGA-O2A-C1
15	a2	409	CLA	O1D-CGD-O2D-CED
15	a2	416	CLA	O1D-CGD-O2D-CED
15	a4	408	CLA	O1D-CGD-O2D-CED
15	b1	408	CLA	O1D-CGD-O2D-CED
15	b2	409	CLA	O1D-CGD-O2D-CED
15	b4	408	CLA	O1D-CGD-O2D-CED
15	c1	415	CLA	O1D-CGD-O2D-CED
15	c2	409	CLA	O1D-CGD-O2D-CED
15	c4	408	CLA	O1D-CGD-O2D-CED
15	aB	812	CLA	O1D-CGD-O2D-CED
15	a1	414	CLA	O1D-CGD-O2D-CED
15	a3	415	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	812	CLA	O1D-CGD-O2D-CED
15	b1	415	CLA	O1D-CGD-O2D-CED
15	b3	415	CLA	O1D-CGD-O2D-CED
15	cB	812	CLA	O1D-CGD-O2D-CED
15	c3	415	CLA	O1D-CGD-O2D-CED
15	aB	828	CLA	O1D-CGD-O2D-CED
15	a6	406	CLA	O1D-CGD-O2D-CED
15	a6	416	CLA	O1D-CGD-O2D-CED
15	bB	828	CLA	O1D-CGD-O2D-CED
15	b6	406	CLA	O1D-CGD-O2D-CED
15	b6	416	CLA	O1D-CGD-O2D-CED
15	cB	828	CLA	O1D-CGD-O2D-CED
15	c6	407	CLA	O1D-CGD-O2D-CED
15	c6	417	CLA	O1D-CGD-O2D-CED
15	a1	415	CLA	O1A-CGA-O2A-C1
15	a2	417	CLA	O1A-CGA-O2A-C1
15	aA	841	CLA	O1D-CGD-O2D-CED
15	bA	841	CLA	O1D-CGD-O2D-CED
15	cA	841	CLA	O1D-CGD-O2D-CED
15	aA	803	CLA	C3-C5-C6-C7
15	aA	806	CLA	C3-C5-C6-C7
15	aA	809	CLA	C3-C5-C6-C7
15	aA	810	CLA	C3-C5-C6-C7
15	aB	807	CLA	C3-C5-C6-C7
15	aB	810	CLA	C3-C5-C6-C7
15	aB	811	CLA	C3-C5-C6-C7
15	aB	828	CLA	C3-C5-C6-C7
15	aB	839	CLA	C3-C5-C6-C7
15	a1	409	CLA	C3-C5-C6-C7
15	a2	411	CLA	C3-C5-C6-C7
15	a3	410	CLA	C3-C5-C6-C7
15	a5	410	CLA	C3-C5-C6-C7
15	a6	411	CLA	C3-C5-C6-C7
15	bA	803	CLA	C3-C5-C6-C7
15	bA	806	CLA	C3-C5-C6-C7
15	bA	809	CLA	C3-C5-C6-C7
15	bA	810	CLA	C3-C5-C6-C7
15	bA	827	CLA	C3-C5-C6-C7
15	bB	807	CLA	C3-C5-C6-C7
15	bB	810	CLA	C3-C5-C6-C7
15	bB	811	CLA	C3-C5-C6-C7
15	bB	828	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	839	CLA	C3-C5-C6-C7
15	b1	410	CLA	C3-C5-C6-C7
15	b2	411	CLA	C3-C5-C6-C7
15	b3	410	CLA	C3-C5-C6-C7
15	b5	410	CLA	C3-C5-C6-C7
15	b6	411	CLA	C3-C5-C6-C7
15	cA	803	CLA	C3-C5-C6-C7
15	cA	806	CLA	C3-C5-C6-C7
15	cA	809	CLA	C3-C5-C6-C7
15	cA	810	CLA	C3-C5-C6-C7
15	cA	827	CLA	C3-C5-C6-C7
15	cB	807	CLA	C3-C5-C6-C7
15	cB	810	CLA	C3-C5-C6-C7
15	cB	811	CLA	C3-C5-C6-C7
15	cB	828	CLA	C3-C5-C6-C7
15	cB	839	CLA	C3-C5-C6-C7
15	c2	411	CLA	C3-C5-C6-C7
15	c3	410	CLA	C3-C5-C6-C7
15	c5	410	CLA	C3-C5-C6-C7
15	c6	412	CLA	C3-C5-C6-C7
15	aA	806	CLA	CBA-CGA-O2A-C1
15	aA	840	CLA	CBA-CGA-O2A-C1
15	aB	817	CLA	CBA-CGA-O2A-C1
15	bA	806	CLA	CBA-CGA-O2A-C1
15	bA	840	CLA	CBA-CGA-O2A-C1
15	bB	817	CLA	CBA-CGA-O2A-C1
15	cA	806	CLA	CBA-CGA-O2A-C1
15	cA	840	CLA	CBA-CGA-O2A-C1
15	cB	817	CLA	CBA-CGA-O2A-C1
15	a2	405	CLA	O1D-CGD-O2D-CED
15	a4	404	CLA	O1D-CGD-O2D-CED
15	b2	405	CLA	O1D-CGD-O2D-CED
15	c2	405	CLA	O1D-CGD-O2D-CED
15	c4	405	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	CBD-CGD-O2D-CED
15	bA	825	CLA	CBD-CGD-O2D-CED
15	cA	825	CLA	CBD-CGD-O2D-CED
15	cB	837	CLA	CBD-CGD-O2D-CED
15	b5	405	CLA	O1D-CGD-O2D-CED
15	aA	843	CLA	C4-C3-C5-C6
15	a1	416	CLA	C4-C3-C5-C6
15	a5	417	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	843	CLA	C4-C3-C5-C6
15	b1	417	CLA	C4-C3-C5-C6
15	b5	417	CLA	C4-C3-C5-C6
15	cA	842	CLA	C4-C3-C5-C6
15	c1	417	CLA	C4-C3-C5-C6
15	aB	801	CLA	C2-C3-C5-C6
15	bB	801	CLA	C2-C3-C5-C6
15	cB	801	CLA	C2-C3-C5-C6
15	aB	820	CLA	CBD-CGD-O2D-CED
15	aB	837	CLA	CBD-CGD-O2D-CED
15	bB	820	CLA	CBD-CGD-O2D-CED
15	bB	837	CLA	CBD-CGD-O2D-CED
15	cB	820	CLA	CBD-CGD-O2D-CED
15	aA	802	CLA	C2A-CAA-CBA-CGA
15	aA	830	CLA	C2A-CAA-CBA-CGA
15	aA	832	CLA	C2A-CAA-CBA-CGA
15	aA	845	CLA	C2A-CAA-CBA-CGA
15	aB	801	CLA	C2A-CAA-CBA-CGA
15	aB	803	CLA	C2A-CAA-CBA-CGA
15	aB	825	CLA	C2A-CAA-CBA-CGA
15	aB	828	CLA	C2A-CAA-CBA-CGA
15	aB	839	CLA	C2A-CAA-CBA-CGA
15	a1	401	CLA	C2A-CAA-CBA-CGA
15	a2	402	CLA	C2A-CAA-CBA-CGA
15	a3	402	CLA	C2A-CAA-CBA-CGA
15	a4	402	CLA	C2A-CAA-CBA-CGA
15	a5	402	CLA	C2A-CAA-CBA-CGA
15	a6	403	CLA	C2A-CAA-CBA-CGA
15	bA	802	CLA	C2A-CAA-CBA-CGA
15	bA	830	CLA	C2A-CAA-CBA-CGA
15	bA	832	CLA	C2A-CAA-CBA-CGA
15	bA	845	CLA	C2A-CAA-CBA-CGA
15	bB	801	CLA	C2A-CAA-CBA-CGA
15	bB	803	CLA	C2A-CAA-CBA-CGA
15	bB	825	CLA	C2A-CAA-CBA-CGA
15	bB	828	CLA	C2A-CAA-CBA-CGA
15	bB	839	CLA	C2A-CAA-CBA-CGA
15	b1	402	CLA	C2A-CAA-CBA-CGA
15	b2	402	CLA	C2A-CAA-CBA-CGA
15	b3	402	CLA	C2A-CAA-CBA-CGA
15	b4	402	CLA	C2A-CAA-CBA-CGA
15	b5	402	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	403	CLA	C2A-CAA-CBA-CGA
15	b6	422	CLA	C2A-CAA-CBA-CGA
15	cA	802	CLA	C2A-CAA-CBA-CGA
15	cA	830	CLA	C2A-CAA-CBA-CGA
15	cA	832	CLA	C2A-CAA-CBA-CGA
15	cA	844	CLA	C2A-CAA-CBA-CGA
15	cB	801	CLA	C2A-CAA-CBA-CGA
15	cB	803	CLA	C2A-CAA-CBA-CGA
15	cB	825	CLA	C2A-CAA-CBA-CGA
15	cB	828	CLA	C2A-CAA-CBA-CGA
15	cB	839	CLA	C2A-CAA-CBA-CGA
15	c1	402	CLA	C2A-CAA-CBA-CGA
15	c2	402	CLA	C2A-CAA-CBA-CGA
15	c3	402	CLA	C2A-CAA-CBA-CGA
15	c4	402	CLA	C2A-CAA-CBA-CGA
15	c5	402	CLA	C2A-CAA-CBA-CGA
15	c6	401	CLA	C2A-CAA-CBA-CGA
15	c6	404	CLA	C2A-CAA-CBA-CGA
15	aA	820	CLA	O1A-CGA-O2A-C1
15	bA	820	CLA	O1A-CGA-O2A-C1
15	cA	820	CLA	O1A-CGA-O2A-C1
15	a5	405	CLA	O1D-CGD-O2D-CED
15	b4	405	CLA	O1D-CGD-O2D-CED
15	c5	405	CLA	O1D-CGD-O2D-CED
15	aA	813	CLA	C3-C5-C6-C7
15	aA	827	CLA	C3-C5-C6-C7
15	aB	809	CLA	C3-C5-C6-C7
15	aB	817	CLA	C3-C5-C6-C7
15	a4	410	CLA	C3-C5-C6-C7
15	bA	813	CLA	C3-C5-C6-C7
15	bB	809	CLA	C3-C5-C6-C7
15	bB	817	CLA	C3-C5-C6-C7
15	b4	410	CLA	C3-C5-C6-C7
15	cA	813	CLA	C3-C5-C6-C7
15	cB	809	CLA	C3-C5-C6-C7
15	cB	817	CLA	C3-C5-C6-C7
15	c1	410	CLA	C3-C5-C6-C7
15	c4	410	CLA	C3-C5-C6-C7
15	aA	809	CLA	CBA-CGA-O2A-C1
15	aA	820	CLA	CBA-CGA-O2A-C1
15	aA	836	CLA	CBA-CGA-O2A-C1
15	aB	819	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	821	CLA	CBA-CGA-O2A-C1
15	aL	201	CLA	CBA-CGA-O2A-C1
15	a1	415	CLA	CBA-CGA-O2A-C1
15	a2	417	CLA	CBA-CGA-O2A-C1
15	a3	416	CLA	CBA-CGA-O2A-C1
15	a4	416	CLA	CBA-CGA-O2A-C1
15	a5	416	CLA	CBA-CGA-O2A-C1
15	a6	417	CLA	CBA-CGA-O2A-C1
15	bA	809	CLA	CBA-CGA-O2A-C1
15	bA	820	CLA	CBA-CGA-O2A-C1
15	bA	836	CLA	CBA-CGA-O2A-C1
15	bB	819	CLA	CBA-CGA-O2A-C1
15	bB	821	CLA	CBA-CGA-O2A-C1
15	bL	202	CLA	CBA-CGA-O2A-C1
15	b1	416	CLA	CBA-CGA-O2A-C1
15	b2	417	CLA	CBA-CGA-O2A-C1
15	b3	416	CLA	CBA-CGA-O2A-C1
15	b4	416	CLA	CBA-CGA-O2A-C1
15	b5	416	CLA	CBA-CGA-O2A-C1
15	b6	417	CLA	CBA-CGA-O2A-C1
15	cA	809	CLA	CBA-CGA-O2A-C1
15	cA	820	CLA	CBA-CGA-O2A-C1
15	cA	836	CLA	CBA-CGA-O2A-C1
15	cB	819	CLA	CBA-CGA-O2A-C1
15	cB	821	CLA	CBA-CGA-O2A-C1
15	cL	202	CLA	CBA-CGA-O2A-C1
15	c1	416	CLA	CBA-CGA-O2A-C1
15	c2	417	CLA	CBA-CGA-O2A-C1
15	c3	416	CLA	CBA-CGA-O2A-C1
15	c4	416	CLA	CBA-CGA-O2A-C1
15	c5	416	CLA	CBA-CGA-O2A-C1
15	c6	418	CLA	CBA-CGA-O2A-C1
15	aA	829	CLA	O1D-CGD-O2D-CED
15	a4	405	CLA	O1D-CGD-O2D-CED
15	bA	829	CLA	O1D-CGD-O2D-CED
15	b4	404	CLA	O1D-CGD-O2D-CED
15	b6	405	CLA	O1D-CGD-O2D-CED
15	c4	404	CLA	O1D-CGD-O2D-CED
15	aA	840	CLA	O1D-CGD-O2D-CED
15	aB	840	CLA	O1D-CGD-O2D-CED
15	a1	402	CLA	O1D-CGD-O2D-CED
15	a1	403	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a4	403	CLA	O1D-CGD-O2D-CED
15	a5	404	CLA	O1D-CGD-O2D-CED
15	a6	405	CLA	O1D-CGD-O2D-CED
15	bA	840	CLA	O1D-CGD-O2D-CED
15	bB	840	CLA	O1D-CGD-O2D-CED
15	b1	404	CLA	O1D-CGD-O2D-CED
15	b1	405	CLA	O1D-CGD-O2D-CED
15	b3	404	CLA	O1D-CGD-O2D-CED
15	b3	405	CLA	O1D-CGD-O2D-CED
15	cA	829	CLA	O1D-CGD-O2D-CED
15	cA	840	CLA	O1D-CGD-O2D-CED
15	cB	840	CLA	O1D-CGD-O2D-CED
15	c1	404	CLA	O1D-CGD-O2D-CED
15	c1	405	CLA	O1D-CGD-O2D-CED
15	c3	404	CLA	O1D-CGD-O2D-CED
15	c3	405	CLA	O1D-CGD-O2D-CED
15	c5	404	CLA	O1D-CGD-O2D-CED
15	c6	406	CLA	O1D-CGD-O2D-CED
15	aA	813	CLA	O1A-CGA-O2A-C1
15	aA	838	CLA	O1A-CGA-O2A-C1
15	aB	819	CLA	O1A-CGA-O2A-C1
15	aL	201	CLA	O1A-CGA-O2A-C1
15	bA	813	CLA	O1A-CGA-O2A-C1
15	bA	838	CLA	O1A-CGA-O2A-C1
15	bB	819	CLA	O1A-CGA-O2A-C1
15	bL	202	CLA	O1A-CGA-O2A-C1
15	cA	813	CLA	O1A-CGA-O2A-C1
15	cA	838	CLA	O1A-CGA-O2A-C1
15	cB	819	CLA	O1A-CGA-O2A-C1
15	cL	202	CLA	O1A-CGA-O2A-C1
15	a1	404	CLA	O1D-CGD-O2D-CED
15	a2	404	CLA	O1D-CGD-O2D-CED
15	a3	404	CLA	O1D-CGD-O2D-CED
15	a3	405	CLA	O1D-CGD-O2D-CED
15	b2	404	CLA	O1D-CGD-O2D-CED
15	b5	403	CLA	O1D-CGD-O2D-CED
15	b5	404	CLA	O1D-CGD-O2D-CED
15	c2	404	CLA	O1D-CGD-O2D-CED
18	aJ	204	BCR	C9-C10-C11-C12
18	a1	420	BCR	C19-C20-C21-C22
18	a1	421	BCR	C9-C10-C11-C12
18	a2	401	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a2	420	BCR	C19-C20-C21-C22
18	a3	401	BCR	C9-C10-C11-C12
18	a4	419	BCR	C19-C20-C21-C22
18	a6	402	BCR	C9-C10-C11-C12
18	bJ	103	BCR	C9-C10-C11-C12
18	b2	401	BCR	C9-C10-C11-C12
18	b2	420	BCR	C19-C20-C21-C22
18	b3	401	BCR	C9-C10-C11-C12
18	b4	419	BCR	C19-C20-C21-C22
18	b6	402	BCR	C9-C10-C11-C12
18	cJ	103	BCR	C9-C10-C11-C12
18	c1	401	BCR	C19-C20-C21-C22
18	c2	401	BCR	C9-C10-C11-C12
18	c2	420	BCR	C19-C20-C21-C22
18	c3	401	BCR	C9-C10-C11-C12
18	c4	419	BCR	C19-C20-C21-C22
18	c6	403	BCR	C9-C10-C11-C12
15	aA	805	CLA	CBD-CGD-O2D-CED
15	aA	830	CLA	CBD-CGD-O2D-CED
15	aB	814	CLA	CBD-CGD-O2D-CED
15	a1	408	CLA	CBD-CGD-O2D-CED
15	a2	410	CLA	CBD-CGD-O2D-CED
15	a6	410	CLA	CBD-CGD-O2D-CED
15	bA	805	CLA	CBD-CGD-O2D-CED
15	bA	830	CLA	CBD-CGD-O2D-CED
15	bB	814	CLA	CBD-CGD-O2D-CED
15	b1	409	CLA	CBD-CGD-O2D-CED
15	b2	410	CLA	CBD-CGD-O2D-CED
15	b6	410	CLA	CBD-CGD-O2D-CED
15	cA	805	CLA	CBD-CGD-O2D-CED
15	cA	830	CLA	CBD-CGD-O2D-CED
15	cB	814	CLA	CBD-CGD-O2D-CED
15	c1	409	CLA	CBD-CGD-O2D-CED
15	c2	410	CLA	CBD-CGD-O2D-CED
15	c4	409	CLA	CBD-CGD-O2D-CED
15	aA	838	CLA	O1D-CGD-O2D-CED
15	aB	816	CLA	O1D-CGD-O2D-CED
15	aB	821	CLA	O1D-CGD-O2D-CED
15	a5	403	CLA	O1D-CGD-O2D-CED
15	a6	404	CLA	O1D-CGD-O2D-CED
15	bA	838	CLA	O1D-CGD-O2D-CED
15	bB	816	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	821	CLA	O1D-CGD-O2D-CED
15	b1	403	CLA	O1D-CGD-O2D-CED
15	b4	403	CLA	O1D-CGD-O2D-CED
15	b6	404	CLA	O1D-CGD-O2D-CED
15	cA	838	CLA	O1D-CGD-O2D-CED
15	cB	816	CLA	O1D-CGD-O2D-CED
15	cB	821	CLA	O1D-CGD-O2D-CED
15	c1	403	CLA	O1D-CGD-O2D-CED
15	c4	403	CLA	O1D-CGD-O2D-CED
15	c5	403	CLA	O1D-CGD-O2D-CED
15	c6	405	CLA	O1D-CGD-O2D-CED
19	aA	854	LHG	O2-C2-C3-O3
19	bA	855	LHG	O2-C2-C3-O3
19	cA	853	LHG	O2-C2-C3-O3
15	aA	802	CLA	C3-C5-C6-C7
15	bA	802	CLA	C3-C5-C6-C7
15	bA	836	CLA	C3-C5-C6-C7
15	cA	802	CLA	C3-C5-C6-C7
15	aA	813	CLA	CBA-CGA-O2A-C1
15	aA	838	CLA	CBA-CGA-O2A-C1
15	bA	813	CLA	CBA-CGA-O2A-C1
15	bA	838	CLA	CBA-CGA-O2A-C1
15	cA	813	CLA	CBA-CGA-O2A-C1
15	cA	838	CLA	CBA-CGA-O2A-C1
15	aA	836	CLA	O1A-CGA-O2A-C1
15	aA	840	CLA	O1A-CGA-O2A-C1
15	aB	821	CLA	O1A-CGA-O2A-C1
15	bA	836	CLA	O1A-CGA-O2A-C1
15	bA	840	CLA	O1A-CGA-O2A-C1
15	cA	836	CLA	O1A-CGA-O2A-C1
15	cA	840	CLA	O1A-CGA-O2A-C1
15	aA	845	CLA	O1D-CGD-O2D-CED
15	a3	403	CLA	O1D-CGD-O2D-CED
15	bA	845	CLA	O1D-CGD-O2D-CED
15	cA	844	CLA	O1D-CGD-O2D-CED
15	c2	403	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	CBD-CGD-O2D-CED
15	a4	409	CLA	CBD-CGD-O2D-CED
15	bL	204	CLA	CBD-CGD-O2D-CED
15	b4	409	CLA	CBD-CGD-O2D-CED
15	b5	409	CLA	CBD-CGD-O2D-CED
15	cL	204	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c6	411	CLA	CBD-CGD-O2D-CED
15	b3	403	CLA	O1D-CGD-O2D-CED
15	c3	403	CLA	O1D-CGD-O2D-CED
15	bB	821	CLA	O1A-CGA-O2A-C1
15	cB	821	CLA	O1A-CGA-O2A-C1
15	aA	802	CLA	O1D-CGD-O2D-CED
15	aA	812	CLA	O1D-CGD-O2D-CED
15	aA	835	CLA	O1D-CGD-O2D-CED
15	a2	403	CLA	O1D-CGD-O2D-CED
15	bA	802	CLA	O1D-CGD-O2D-CED
15	bA	812	CLA	O1D-CGD-O2D-CED
15	cA	802	CLA	O1D-CGD-O2D-CED
15	cA	812	CLA	O1D-CGD-O2D-CED
15	cA	835	CLA	O1D-CGD-O2D-CED
15	aB	807	CLA	CBD-CGD-O2D-CED
15	bB	807	CLA	CBD-CGD-O2D-CED
15	cB	807	CLA	CBD-CGD-O2D-CED
15	aA	826	CLA	C3-C5-C6-C7
15	aA	836	CLA	C3-C5-C6-C7
15	aB	833	CLA	C3-C5-C6-C7
15	bA	826	CLA	C3-C5-C6-C7
15	bB	833	CLA	C3-C5-C6-C7
15	cA	826	CLA	C3-C5-C6-C7
15	cA	836	CLA	C3-C5-C6-C7
15	cB	833	CLA	C3-C5-C6-C7
15	bA	835	CLA	O1D-CGD-O2D-CED
15	aB	814	CLA	C2C-C3C-CAC-CBC
15	cB	814	CLA	C2C-C3C-CAC-CBC
15	aA	809	CLA	O1A-CGA-O2A-C1
15	bB	814	CLA	C2C-C3C-CAC-CBC
20	aB	850	LMG	O6-C5-C6-O5
20	bB	851	LMG	O6-C5-C6-O5
20	cB	850	LMG	O6-C5-C6-O5
15	aA	818	CLA	C4-C3-C5-C6
15	aB	819	CLA	C4-C3-C5-C6
15	bA	818	CLA	C4-C3-C5-C6
15	bB	819	CLA	C4-C3-C5-C6
15	b4	417	CLA	C4-C3-C5-C6
15	cA	818	CLA	C4-C3-C5-C6
15	cB	819	CLA	C4-C3-C5-C6
15	c5	417	CLA	C4-C3-C5-C6
15	aA	818	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	819	CLA	C2-C3-C5-C6
15	bA	818	CLA	C2-C3-C5-C6
15	bB	819	CLA	C2-C3-C5-C6
15	cA	818	CLA	C2-C3-C5-C6
15	cB	819	CLA	C2-C3-C5-C6
15	aA	844	CLA	C2A-CAA-CBA-CGA
15	aB	832	CLA	C2A-CAA-CBA-CGA
15	bA	844	CLA	C2A-CAA-CBA-CGA
15	bB	832	CLA	C2A-CAA-CBA-CGA
15	cA	843	CLA	C2A-CAA-CBA-CGA
15	cB	832	CLA	C2A-CAA-CBA-CGA
15	aB	809	CLA	O1D-CGD-O2D-CED
15	bB	809	CLA	O1D-CGD-O2D-CED
15	b2	403	CLA	O1D-CGD-O2D-CED
15	cB	809	CLA	O1D-CGD-O2D-CED
15	bA	809	CLA	O1A-CGA-O2A-C1
15	cA	809	CLA	O1A-CGA-O2A-C1
20	aB	850	LMG	O6-C1-O1-C7
20	bB	851	LMG	O6-C1-O1-C7
20	cB	850	LMG	O6-C1-O1-C7
15	aB	801	CLA	CBA-CGA-O2A-C1
15	a3	417	CLA	CBA-CGA-O2A-C1
15	bB	801	CLA	CBA-CGA-O2A-C1
15	b3	417	CLA	CBA-CGA-O2A-C1
15	cB	801	CLA	CBA-CGA-O2A-C1
15	aA	809	CLA	CBD-CGD-O2D-CED
15	aA	834	CLA	CBD-CGD-O2D-CED
15	bA	809	CLA	CBD-CGD-O2D-CED
15	b2	411	CLA	CBD-CGD-O2D-CED
15	cA	809	CLA	CBD-CGD-O2D-CED
15	cA	834	CLA	CBD-CGD-O2D-CED
15	c5	409	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	O1D-CGD-O2D-CED
15	bB	803	CLA	O1D-CGD-O2D-CED
15	cB	803	CLA	O1D-CGD-O2D-CED
15	aB	836	CLA	O1D-CGD-O2D-CED
15	a4	402	CLA	O1D-CGD-O2D-CED
15	a6	403	CLA	O1D-CGD-O2D-CED
15	bB	836	CLA	O1D-CGD-O2D-CED
15	b4	402	CLA	O1D-CGD-O2D-CED
15	b6	403	CLA	O1D-CGD-O2D-CED
15	cB	836	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	402	CLA	O1D-CGD-O2D-CED
15	c4	402	CLA	O1D-CGD-O2D-CED
15	c6	404	CLA	O1D-CGD-O2D-CED
15	aA	822	CLA	CBD-CGD-O2D-CED
15	a2	411	CLA	CBD-CGD-O2D-CED
15	a5	409	CLA	CBD-CGD-O2D-CED
15	bA	822	CLA	CBD-CGD-O2D-CED
15	bA	834	CLA	CBD-CGD-O2D-CED
15	cA	822	CLA	CBD-CGD-O2D-CED
15	b2	402	CLA	O1D-CGD-O2D-CED
15	b5	402	CLA	O1D-CGD-O2D-CED
15	c5	402	CLA	O1D-CGD-O2D-CED
19	aX	101	LHG	C1-C2-C3-O3
19	bX	101	LHG	C1-C2-C3-O3
19	cX	101	LHG	C1-C2-C3-O3
15	aB	801	CLA	O1A-CGA-O2A-C1
15	a3	417	CLA	O1A-CGA-O2A-C1
15	bB	801	CLA	O1A-CGA-O2A-C1
15	b3	417	CLA	O1A-CGA-O2A-C1
15	cB	801	CLA	O1A-CGA-O2A-C1
15	a5	402	CLA	O1D-CGD-O2D-CED
15	a5	407	CLA	O1D-CGD-O2D-CED
15	b5	407	CLA	O1D-CGD-O2D-CED
15	c5	407	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	CBA-CGA-O2A-C1
15	aA	833	CLA	CBA-CGA-O2A-C1
15	aB	832	CLA	CBA-CGA-O2A-C1
15	a1	416	CLA	CBA-CGA-O2A-C1
15	a2	418	CLA	CBA-CGA-O2A-C1
15	a4	417	CLA	CBA-CGA-O2A-C1
15	a5	417	CLA	CBA-CGA-O2A-C1
15	a6	418	CLA	CBA-CGA-O2A-C1
15	bA	825	CLA	CBA-CGA-O2A-C1
15	bA	833	CLA	CBA-CGA-O2A-C1
15	bB	832	CLA	CBA-CGA-O2A-C1
15	b1	417	CLA	CBA-CGA-O2A-C1
15	b2	418	CLA	CBA-CGA-O2A-C1
15	b4	417	CLA	CBA-CGA-O2A-C1
15	b5	417	CLA	CBA-CGA-O2A-C1
15	b6	418	CLA	CBA-CGA-O2A-C1
15	cA	825	CLA	CBA-CGA-O2A-C1
15	cA	833	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	832	CLA	CBA-CGA-O2A-C1
15	c1	417	CLA	CBA-CGA-O2A-C1
15	c2	418	CLA	CBA-CGA-O2A-C1
15	c3	417	CLA	CBA-CGA-O2A-C1
15	c4	417	CLA	CBA-CGA-O2A-C1
15	c5	417	CLA	CBA-CGA-O2A-C1
15	c6	419	CLA	CBA-CGA-O2A-C1
18	a6	421	BCR	C9-C10-C11-C12
18	b6	421	BCR	C9-C10-C11-C12
15	aB	807	CLA	C8-C10-C11-C12
15	bB	807	CLA	C8-C10-C11-C12
20	aB	850	LMG	C4-C5-C6-O5
20	bB	851	LMG	C4-C5-C6-O5
20	cB	850	LMG	C4-C5-C6-O5
15	aA	802	CLA	C10-C11-C12-C13
15	aA	821	CLA	C5-C6-C7-C8
15	aB	814	CLA	C8-C10-C11-C12
15	bA	802	CLA	C10-C11-C12-C13
15	bA	821	CLA	C5-C6-C7-C8
15	bB	814	CLA	C8-C10-C11-C12
15	cA	802	CLA	C10-C11-C12-C13
15	cA	821	CLA	C5-C6-C7-C8
15	cB	807	CLA	C8-C10-C11-C12
15	cB	814	CLA	C8-C10-C11-C12
15	aA	845	CLA	C3-C5-C6-C7
15	bA	845	CLA	C3-C5-C6-C7
15	cA	844	CLA	C3-C5-C6-C7
15	aA	833	CLA	O1A-CGA-O2A-C1
15	a2	418	CLA	O1A-CGA-O2A-C1
15	a6	418	CLA	O1A-CGA-O2A-C1
15	bA	833	CLA	O1A-CGA-O2A-C1
15	b2	418	CLA	O1A-CGA-O2A-C1
15	b6	418	CLA	O1A-CGA-O2A-C1
15	cA	833	CLA	O1A-CGA-O2A-C1
15	c2	418	CLA	O1A-CGA-O2A-C1
15	c3	417	CLA	O1A-CGA-O2A-C1
15	c6	419	CLA	O1A-CGA-O2A-C1
15	aB	827	CLA	C4-C3-C5-C6
15	a3	417	CLA	C4-C3-C5-C6
15	a4	417	CLA	C4-C3-C5-C6
15	a6	418	CLA	C4-C3-C5-C6
15	bB	827	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	418	CLA	C4-C3-C5-C6
15	b6	418	CLA	C4-C3-C5-C6
15	cB	827	CLA	C4-C3-C5-C6
15	c2	418	CLA	C4-C3-C5-C6
15	c3	417	CLA	C4-C3-C5-C6
15	c4	417	CLA	C4-C3-C5-C6
15	c6	419	CLA	C4-C3-C5-C6
15	aA	843	CLA	C2-C3-C5-C6
15	bA	843	CLA	C2-C3-C5-C6
15	b1	417	CLA	C2-C3-C5-C6
15	cA	842	CLA	C2-C3-C5-C6
15	aA	804	CLA	C11-C12-C13-C14
15	aA	806	CLA	C6-C7-C8-C9
15	aA	807	CLA	C6-C7-C8-C9
15	aA	812	CLA	C14-C13-C15-C16
15	aA	821	CLA	C11-C12-C13-C14
15	aA	828	CLA	C6-C7-C8-C9
15	aA	834	CLA	C6-C7-C8-C9
15	aA	843	CLA	C11-C10-C8-C9
15	aB	807	CLA	C14-C13-C15-C16
15	aB	819	CLA	C6-C7-C8-C9
15	a1	402	CLA	C6-C7-C8-C9
15	a2	403	CLA	C6-C7-C8-C9
15	a2	422	CLA	C11-C12-C13-C14
15	a3	403	CLA	C6-C7-C8-C9
15	a3	421	CLA	C11-C12-C13-C14
15	a4	403	CLA	C6-C7-C8-C9
15	a4	421	CLA	C11-C12-C13-C14
15	a5	403	CLA	C6-C7-C8-C9
15	a5	420	CLA	C11-C12-C13-C14
15	a6	404	CLA	C6-C7-C8-C9
15	a6	422	CLA	C11-C12-C13-C14
15	bA	804	CLA	C11-C12-C13-C14
15	bA	806	CLA	C6-C7-C8-C9
15	bA	807	CLA	C6-C7-C8-C9
15	bA	812	CLA	C14-C13-C15-C16
15	bA	821	CLA	C11-C12-C13-C14
15	bA	828	CLA	C6-C7-C8-C9
15	bA	834	CLA	C6-C7-C8-C9
15	bA	843	CLA	C11-C10-C8-C9
15	bB	807	CLA	C14-C13-C15-C16
15	bB	819	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b1	403	CLA	C6-C7-C8-C9
15	b2	403	CLA	C6-C7-C8-C9
15	b2	422	CLA	C11-C12-C13-C14
15	b3	403	CLA	C6-C7-C8-C9
15	b3	421	CLA	C11-C12-C13-C14
15	b4	403	CLA	C6-C7-C8-C9
15	b4	421	CLA	C11-C12-C13-C14
15	b5	403	CLA	C6-C7-C8-C9
15	b5	420	CLA	C11-C12-C13-C14
15	b6	404	CLA	C6-C7-C8-C9
15	b6	422	CLA	C11-C12-C13-C14
15	cA	804	CLA	C11-C12-C13-C14
15	cA	806	CLA	C6-C7-C8-C9
15	cA	807	CLA	C6-C7-C8-C9
15	cA	812	CLA	C14-C13-C15-C16
15	cA	821	CLA	C11-C12-C13-C14
15	cA	828	CLA	C6-C7-C8-C9
15	cA	834	CLA	C6-C7-C8-C9
15	cA	842	CLA	C11-C10-C8-C9
15	cB	807	CLA	C14-C13-C15-C16
15	cB	819	CLA	C6-C7-C8-C9
15	c1	403	CLA	C6-C7-C8-C9
15	c2	403	CLA	C6-C7-C8-C9
15	c2	422	CLA	C11-C12-C13-C14
15	c3	403	CLA	C6-C7-C8-C9
15	c3	421	CLA	C11-C12-C13-C14
15	c4	403	CLA	C6-C7-C8-C9
15	c5	403	CLA	C6-C7-C8-C9
15	c5	420	CLA	C11-C12-C13-C14
15	c6	405	CLA	C6-C7-C8-C9
15	aB	832	CLA	O1D-CGD-O2D-CED
15	aB	839	CLA	O1D-CGD-O2D-CED
15	a2	402	CLA	O1D-CGD-O2D-CED
15	a3	402	CLA	O1D-CGD-O2D-CED
15	a6	408	CLA	O1D-CGD-O2D-CED
15	bB	832	CLA	O1D-CGD-O2D-CED
15	bB	839	CLA	O1D-CGD-O2D-CED
15	b1	402	CLA	O1D-CGD-O2D-CED
15	b3	402	CLA	O1D-CGD-O2D-CED
15	b3	407	CLA	O1D-CGD-O2D-CED
15	b6	408	CLA	O1D-CGD-O2D-CED
15	cB	832	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	839	CLA	O1D-CGD-O2D-CED
15	c3	402	CLA	O1D-CGD-O2D-CED
15	c3	407	CLA	O1D-CGD-O2D-CED
15	c6	409	CLA	O1D-CGD-O2D-CED
15	aA	814	CLA	CBD-CGD-O2D-CED
15	b3	409	CLA	CBD-CGD-O2D-CED
15	cA	814	CLA	CBD-CGD-O2D-CED
18	aA	852	BCR	C7-C8-C9-C34
18	aA	852	BCR	C37-C22-C23-C24
18	aB	844	BCR	C7-C8-C9-C34
18	aI	102	BCR	C7-C8-C9-C34
18	aI	102	BCR	C11-C12-C13-C35
18	a1	417	BCR	C7-C8-C9-C34
18	a1	421	BCR	C7-C8-C9-C34
18	a2	419	BCR	C7-C8-C9-C34
18	a2	420	BCR	C7-C8-C9-C34
18	a2	421	BCR	C11-C12-C13-C35
18	a3	418	BCR	C7-C8-C9-C34
18	a3	419	BCR	C7-C8-C9-C34
18	a4	418	BCR	C7-C8-C9-C34
18	a4	419	BCR	C7-C8-C9-C34
18	a5	418	BCR	C7-C8-C9-C34
18	a6	402	BCR	C11-C12-C13-C35
18	a6	419	BCR	C7-C8-C9-C34
18	bA	853	BCR	C7-C8-C9-C34
18	bA	853	BCR	C37-C22-C23-C24
18	bB	844	BCR	C7-C8-C9-C34
18	bI	102	BCR	C7-C8-C9-C34
18	bI	102	BCR	C11-C12-C13-C35
18	b1	418	BCR	C7-C8-C9-C34
18	b2	419	BCR	C7-C8-C9-C34
18	b2	420	BCR	C7-C8-C9-C34
18	b2	421	BCR	C11-C12-C13-C35
18	b3	418	BCR	C7-C8-C9-C34
18	b3	419	BCR	C7-C8-C9-C34
18	b4	418	BCR	C7-C8-C9-C34
18	b4	419	BCR	C7-C8-C9-C34
18	b5	418	BCR	C7-C8-C9-C34
18	b6	419	BCR	C7-C8-C9-C34
18	cA	851	BCR	C7-C8-C9-C34
18	cA	851	BCR	C37-C22-C23-C24
18	cB	844	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cI	102	BCR	C7-C8-C9-C34
18	cI	102	BCR	C11-C12-C13-C35
18	c1	418	BCR	C7-C8-C9-C34
18	c1	419	BCR	C7-C8-C9-C34
18	c2	419	BCR	C7-C8-C9-C34
18	c2	420	BCR	C7-C8-C9-C34
18	c2	421	BCR	C11-C12-C13-C35
18	c3	418	BCR	C7-C8-C9-C34
18	c3	419	BCR	C7-C8-C9-C34
18	c4	418	BCR	C7-C8-C9-C34
18	c4	419	BCR	C7-C8-C9-C34
18	c5	418	BCR	C7-C8-C9-C34
18	c6	403	BCR	C11-C12-C13-C35
18	c6	420	BCR	C7-C8-C9-C34
18	aB	844	BCR	C21-C22-C23-C24
18	aI	103	BCR	C7-C8-C9-C10
18	aI	103	BCR	C21-C22-C23-C24
18	aL	205	BCR	C7-C8-C9-C10
18	a1	418	BCR	C7-C8-C9-C10
18	a3	419	BCR	C7-C8-C9-C10
18	a4	419	BCR	C7-C8-C9-C10
18	bB	844	BCR	C21-C22-C23-C24
18	bL	201	BCR	C7-C8-C9-C10
18	bL	205	BCR	C7-C8-C9-C10
18	bL	205	BCR	C21-C22-C23-C24
18	bL	206	BCR	C7-C8-C9-C10
18	b1	401	BCR	C7-C8-C9-C10
18	b1	419	BCR	C7-C8-C9-C10
18	b3	419	BCR	C7-C8-C9-C10
18	b4	419	BCR	C7-C8-C9-C10
18	cB	844	BCR	C21-C22-C23-C24
18	cL	205	BCR	C7-C8-C9-C10
18	cL	205	BCR	C21-C22-C23-C24
18	c1	401	BCR	C7-C8-C9-C10
18	c1	419	BCR	C7-C8-C9-C10
18	c3	419	BCR	C7-C8-C9-C10
18	c4	419	BCR	C7-C8-C9-C10
15	bA	819	CLA	O1D-CGD-O2D-CED
15	c1	402	CLA	O1D-CGD-O2D-CED
15	a4	417	CLA	O1A-CGA-O2A-C1
15	a5	417	CLA	O1A-CGA-O2A-C1
15	b4	417	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b5	417	CLA	O1A-CGA-O2A-C1
15	c4	417	CLA	O1A-CGA-O2A-C1
15	c5	417	CLA	O1A-CGA-O2A-C1
15	aA	828	CLA	C10-C11-C12-C13
15	aA	843	CLA	C10-C11-C12-C13
15	bA	828	CLA	C10-C11-C12-C13
15	bA	843	CLA	C10-C11-C12-C13
15	cA	828	CLA	C10-C11-C12-C13
15	cA	842	CLA	C10-C11-C12-C13
15	aA	819	CLA	O1D-CGD-O2D-CED
15	cA	819	CLA	O1D-CGD-O2D-CED
15	c4	407	CLA	O1D-CGD-O2D-CED
15	a3	409	CLA	CBD-CGD-O2D-CED
15	bA	814	CLA	CBD-CGD-O2D-CED
15	bB	826	CLA	CBD-CGD-O2D-CED
15	cB	826	CLA	CBD-CGD-O2D-CED
15	c2	411	CLA	CBD-CGD-O2D-CED
15	a4	407	CLA	O1D-CGD-O2D-CED
15	b4	407	CLA	O1D-CGD-O2D-CED
15	aA	828	CLA	C3-C5-C6-C7
15	aA	839	CLA	C3-C5-C6-C7
15	bA	828	CLA	C3-C5-C6-C7
15	bA	839	CLA	C3-C5-C6-C7
15	cA	828	CLA	C3-C5-C6-C7
15	cA	839	CLA	C3-C5-C6-C7
14	aA	801	CL0	C8-C10-C11-C12
14	bA	801	CL0	C8-C10-C11-C12
14	cA	801	CL0	C8-C10-C11-C12
15	aB	804	CLA	C10-C11-C12-C13
15	aB	814	CLA	C10-C11-C12-C13
15	aB	836	CLA	C8-C10-C11-C12
15	bB	804	CLA	C10-C11-C12-C13
15	bB	814	CLA	C10-C11-C12-C13
15	bB	819	CLA	C5-C6-C7-C8
15	bB	836	CLA	C8-C10-C11-C12
15	cA	829	CLA	C15-C16-C17-C18
15	cB	804	CLA	C10-C11-C12-C13
15	cB	814	CLA	C10-C11-C12-C13
15	cB	819	CLA	C5-C6-C7-C8
15	a1	401	CLA	O1D-CGD-O2D-CED
15	a3	407	CLA	O1D-CGD-O2D-CED
15	b1	407	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	826	CLA	CBD-CGD-O2D-CED
15	c2	408	CLA	O1D-CGD-O2D-CED
15	aA	804	CLA	C10-C11-C12-C13
15	aA	809	CLA	C15-C16-C17-C18
15	aA	810	CLA	C5-C6-C7-C8
15	aA	829	CLA	C15-C16-C17-C18
15	aA	839	CLA	C8-C10-C11-C12
15	aA	843	CLA	C8-C10-C11-C12
15	aA	843	CLA	C13-C15-C16-C17
15	aB	807	CLA	C13-C15-C16-C17
15	aB	815	CLA	C5-C6-C7-C8
15	aB	819	CLA	C5-C6-C7-C8
15	aB	829	CLA	C5-C6-C7-C8
15	bA	804	CLA	C10-C11-C12-C13
15	bA	809	CLA	C15-C16-C17-C18
15	bA	810	CLA	C5-C6-C7-C8
15	bA	839	CLA	C8-C10-C11-C12
15	bA	843	CLA	C8-C10-C11-C12
15	bA	843	CLA	C13-C15-C16-C17
15	bB	807	CLA	C13-C15-C16-C17
15	bB	815	CLA	C5-C6-C7-C8
15	bB	829	CLA	C5-C6-C7-C8
15	cA	804	CLA	C10-C11-C12-C13
15	cA	809	CLA	C15-C16-C17-C18
15	cA	810	CLA	C5-C6-C7-C8
15	cA	839	CLA	C8-C10-C11-C12
15	cA	842	CLA	C8-C10-C11-C12
15	cA	842	CLA	C13-C15-C16-C17
15	cB	807	CLA	C13-C15-C16-C17
15	cB	815	CLA	C5-C6-C7-C8
15	cB	829	CLA	C5-C6-C7-C8
15	cB	836	CLA	C8-C10-C11-C12
15	aA	820	CLA	O1D-CGD-O2D-CED
15	cA	820	CLA	O1D-CGD-O2D-CED
15	a1	416	CLA	O1A-CGA-O2A-C1
15	c1	417	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	CBD-CGD-O2D-CED
15	bA	804	CLA	CBD-CGD-O2D-CED
15	b6	411	CLA	CBD-CGD-O2D-CED
15	cA	804	CLA	CBD-CGD-O2D-CED
15	a2	408	CLA	O1D-CGD-O2D-CED
15	bA	820	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	408	CLA	O1D-CGD-O2D-CED
15	aB	810	CLA	C5-C6-C7-C8
15	a3	402	CLA	C15-C16-C17-C18
15	a5	402	CLA	C15-C16-C17-C18
15	bA	829	CLA	C15-C16-C17-C18
15	bB	810	CLA	C5-C6-C7-C8
15	b3	402	CLA	C15-C16-C17-C18
15	b5	402	CLA	C15-C16-C17-C18
15	cB	810	CLA	C5-C6-C7-C8
15	c3	402	CLA	C15-C16-C17-C18
15	c5	402	CLA	C15-C16-C17-C18
16	aA	846	PQN	C23-C25-C26-C27
16	bA	846	PQN	C23-C25-C26-C27
16	cA	845	PQN	C23-C25-C26-C27
15	a1	406	CLA	O1D-CGD-O2D-CED
15	c1	407	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	C10-C11-C12-C13
15	a4	402	CLA	C15-C16-C17-C18
15	bL	204	CLA	C10-C11-C12-C13
15	b4	402	CLA	C15-C16-C17-C18
15	cL	204	CLA	C10-C11-C12-C13
15	c1	402	CLA	C15-C16-C17-C18
15	c4	402	CLA	C15-C16-C17-C18
19	aA	854	LHG	C7-C8-C9-C10
19	bA	855	LHG	C7-C8-C9-C10
19	cA	853	LHG	C7-C8-C9-C10
15	aB	833	CLA	CBD-CGD-O2D-CED
15	a6	411	CLA	CBD-CGD-O2D-CED
15	bB	833	CLA	CBD-CGD-O2D-CED
15	cB	833	CLA	CBD-CGD-O2D-CED
15	c3	410	CLA	CBD-CGD-O2D-CED
15	c6	412	CLA	CBD-CGD-O2D-CED
15	aB	809	CLA	C13-C15-C16-C17
15	bA	812	CLA	C15-C16-C17-C18
15	bB	809	CLA	C13-C15-C16-C17
15	b1	402	CLA	C15-C16-C17-C18
15	cA	812	CLA	C15-C16-C17-C18
15	cB	809	CLA	C13-C15-C16-C17
15	aA	810	CLA	C11-C10-C8-C7
15	aA	831	CLA	C11-C10-C8-C7
15	aA	843	CLA	C11-C10-C8-C7
15	aB	833	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	840	CLA	C12-C13-C15-C16
15	a4	403	CLA	C6-C7-C8-C10
15	bA	810	CLA	C11-C10-C8-C7
15	bA	831	CLA	C11-C10-C8-C7
15	bA	843	CLA	C11-C10-C8-C7
15	bB	833	CLA	C11-C12-C13-C15
15	bB	840	CLA	C12-C13-C15-C16
15	b4	403	CLA	C6-C7-C8-C10
15	cA	810	CLA	C11-C10-C8-C7
15	cA	831	CLA	C11-C10-C8-C7
15	cA	842	CLA	C11-C10-C8-C7
15	cB	833	CLA	C11-C12-C13-C15
15	cB	840	CLA	C12-C13-C15-C16
15	c4	403	CLA	C6-C7-C8-C10
16	aB	843	PQN	C17-C18-C20-C21
16	bB	843	PQN	C17-C18-C20-C21
16	cB	843	PQN	C17-C18-C20-C21
15	aB	832	CLA	O1A-CGA-O2A-C1
15	bB	832	CLA	O1A-CGA-O2A-C1
15	b1	417	CLA	O1A-CGA-O2A-C1
15	cB	832	CLA	O1A-CGA-O2A-C1
18	aA	852	BCR	C13-C14-C15-C16
18	aA	852	BCR	C15-C16-C17-C18
18	a1	417	BCR	C19-C20-C21-C22
18	a2	419	BCR	C19-C20-C21-C22
18	a3	418	BCR	C19-C20-C21-C22
18	a4	418	BCR	C19-C20-C21-C22
18	a5	401	BCR	C9-C10-C11-C12
18	a5	418	BCR	C19-C20-C21-C22
18	bA	853	BCR	C13-C14-C15-C16
18	bA	853	BCR	C15-C16-C17-C18
18	b1	418	BCR	C19-C20-C21-C22
18	b3	418	BCR	C19-C20-C21-C22
18	b4	418	BCR	C19-C20-C21-C22
18	b5	401	BCR	C9-C10-C11-C12
18	b5	418	BCR	C19-C20-C21-C22
18	cA	851	BCR	C13-C14-C15-C16
18	cA	851	BCR	C15-C16-C17-C18
18	c1	418	BCR	C19-C20-C21-C22
18	c2	419	BCR	C19-C20-C21-C22
18	c3	418	BCR	C19-C20-C21-C22
18	c4	418	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c5	401	BCR	C9-C10-C11-C12
18	c5	418	BCR	C19-C20-C21-C22
15	aA	810	CLA	C2A-CAA-CBA-CGA
15	aA	825	CLA	C2A-CAA-CBA-CGA
15	aB	805	CLA	C2A-CAA-CBA-CGA
15	aB	840	CLA	C2A-CAA-CBA-CGA
15	a1	403	CLA	C2A-CAA-CBA-CGA
15	a2	404	CLA	C2A-CAA-CBA-CGA
15	a3	404	CLA	C2A-CAA-CBA-CGA
15	a4	404	CLA	C2A-CAA-CBA-CGA
15	a5	404	CLA	C2A-CAA-CBA-CGA
15	a6	405	CLA	C2A-CAA-CBA-CGA
15	bA	810	CLA	C2A-CAA-CBA-CGA
15	bA	825	CLA	C2A-CAA-CBA-CGA
15	bB	805	CLA	C2A-CAA-CBA-CGA
15	bB	840	CLA	C2A-CAA-CBA-CGA
15	b1	404	CLA	C2A-CAA-CBA-CGA
15	b2	404	CLA	C2A-CAA-CBA-CGA
15	b3	404	CLA	C2A-CAA-CBA-CGA
15	b4	404	CLA	C2A-CAA-CBA-CGA
15	b5	404	CLA	C2A-CAA-CBA-CGA
15	b6	405	CLA	C2A-CAA-CBA-CGA
15	cA	810	CLA	C2A-CAA-CBA-CGA
15	cA	825	CLA	C2A-CAA-CBA-CGA
15	cB	805	CLA	C2A-CAA-CBA-CGA
15	cB	840	CLA	C2A-CAA-CBA-CGA
15	c1	404	CLA	C2A-CAA-CBA-CGA
15	c2	404	CLA	C2A-CAA-CBA-CGA
15	c3	404	CLA	C2A-CAA-CBA-CGA
15	c4	404	CLA	C2A-CAA-CBA-CGA
15	c5	404	CLA	C2A-CAA-CBA-CGA
15	c6	406	CLA	C2A-CAA-CBA-CGA
15	aA	812	CLA	C15-C16-C17-C18
15	aA	827	CLA	C8-C10-C11-C12
15	aA	828	CLA	C13-C15-C16-C17
15	aB	804	CLA	C15-C16-C17-C18
15	aB	811	CLA	C15-C16-C17-C18
15	aB	839	CLA	C8-C10-C11-C12
15	a1	401	CLA	C15-C16-C17-C18
15	a2	402	CLA	C15-C16-C17-C18
15	a6	403	CLA	C15-C16-C17-C18
15	bA	827	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	828	CLA	C13-C15-C16-C17
15	bB	804	CLA	C15-C16-C17-C18
15	bB	811	CLA	C15-C16-C17-C18
15	bB	839	CLA	C8-C10-C11-C12
15	b2	402	CLA	C15-C16-C17-C18
15	b6	403	CLA	C15-C16-C17-C18
15	cA	827	CLA	C8-C10-C11-C12
15	cA	828	CLA	C13-C15-C16-C17
15	cB	804	CLA	C15-C16-C17-C18
15	cB	811	CLA	C15-C16-C17-C18
15	cB	839	CLA	C8-C10-C11-C12
15	c2	402	CLA	C15-C16-C17-C18
15	aB	814	CLA	C4C-C3C-CAC-CBC
15	bB	814	CLA	C4C-C3C-CAC-CBC
15	cB	814	CLA	C4C-C3C-CAC-CBC
18	b5	419	BCR	C22-C23-C24-C25
15	aA	825	CLA	O1A-CGA-O2A-C1
15	bA	825	CLA	O1A-CGA-O2A-C1
15	cA	825	CLA	O1A-CGA-O2A-C1
15	aA	832	CLA	CBD-CGD-O2D-CED
15	aB	801	CLA	CBD-CGD-O2D-CED
15	bA	832	CLA	CBD-CGD-O2D-CED
15	bB	801	CLA	CBD-CGD-O2D-CED
15	b3	410	CLA	CBD-CGD-O2D-CED
15	cA	832	CLA	CBD-CGD-O2D-CED
15	cB	801	CLA	CBD-CGD-O2D-CED
15	c3	409	CLA	CBD-CGD-O2D-CED
15	aB	803	CLA	C13-C15-C16-C17
15	bB	803	CLA	C13-C15-C16-C17
15	cB	803	CLA	C13-C15-C16-C17
15	c6	401	CLA	C10-C11-C12-C13
18	aA	850	BCR	C18-C19-C20-C21
18	aB	844	BCR	C18-C19-C20-C21
18	aF	203	BCR	C18-C19-C20-C21
18	aJ	204	BCR	C18-C19-C20-C21
18	a1	418	BCR	C10-C11-C12-C13
18	a1	419	BCR	C10-C11-C12-C13
18	a1	420	BCR	C10-C11-C12-C13
18	a1	420	BCR	C18-C19-C20-C21
18	a1	421	BCR	C10-C11-C12-C13
18	a1	421	BCR	C18-C19-C20-C21
18	a2	401	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a2	401	BCR	C18-C19-C20-C21
18	a2	420	BCR	C10-C11-C12-C13
18	a2	421	BCR	C10-C11-C12-C13
18	a3	401	BCR	C18-C19-C20-C21
18	a3	419	BCR	C10-C11-C12-C13
18	a3	420	BCR	C10-C11-C12-C13
18	a4	401	BCR	C18-C19-C20-C21
18	a4	419	BCR	C18-C19-C20-C21
18	a4	420	BCR	C10-C11-C12-C13
18	a5	401	BCR	C18-C19-C20-C21
18	a5	419	BCR	C10-C11-C12-C13
18	a6	401	BCR	C10-C11-C12-C13
18	a6	402	BCR	C18-C19-C20-C21
18	a6	420	BCR	C10-C11-C12-C13
18	a6	421	BCR	C18-C19-C20-C21
18	bA	851	BCR	C18-C19-C20-C21
18	bB	844	BCR	C18-C19-C20-C21
18	bJ	103	BCR	C18-C19-C20-C21
18	bJ	105	BCR	C18-C19-C20-C21
18	b1	401	BCR	C10-C11-C12-C13
18	b1	401	BCR	C18-C19-C20-C21
18	b1	419	BCR	C10-C11-C12-C13
18	b1	420	BCR	C10-C11-C12-C13
18	b2	401	BCR	C18-C19-C20-C21
18	b2	420	BCR	C10-C11-C12-C13
18	b2	421	BCR	C10-C11-C12-C13
18	b3	401	BCR	C18-C19-C20-C21
18	b3	419	BCR	C10-C11-C12-C13
18	b3	420	BCR	C10-C11-C12-C13
18	b4	401	BCR	C18-C19-C20-C21
18	b4	419	BCR	C18-C19-C20-C21
18	b4	420	BCR	C10-C11-C12-C13
18	b5	401	BCR	C18-C19-C20-C21
18	b5	419	BCR	C10-C11-C12-C13
18	b6	401	BCR	C10-C11-C12-C13
18	b6	402	BCR	C18-C19-C20-C21
18	b6	420	BCR	C10-C11-C12-C13
18	b6	421	BCR	C18-C19-C20-C21
18	cA	849	BCR	C18-C19-C20-C21
18	cB	844	BCR	C18-C19-C20-C21
18	cJ	103	BCR	C18-C19-C20-C21
18	c1	401	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c1	401	BCR	C18-C19-C20-C21
18	c1	419	BCR	C10-C11-C12-C13
18	c1	420	BCR	C10-C11-C12-C13
18	c2	401	BCR	C18-C19-C20-C21
18	c2	420	BCR	C10-C11-C12-C13
18	c2	421	BCR	C10-C11-C12-C13
18	c3	401	BCR	C18-C19-C20-C21
18	c3	419	BCR	C10-C11-C12-C13
18	c3	420	BCR	C10-C11-C12-C13
18	c4	401	BCR	C18-C19-C20-C21
18	c4	419	BCR	C18-C19-C20-C21
18	c4	420	BCR	C10-C11-C12-C13
18	c5	401	BCR	C18-C19-C20-C21
18	c5	419	BCR	C10-C11-C12-C13
18	c6	402	BCR	C10-C11-C12-C13
18	c6	403	BCR	C18-C19-C20-C21
18	c6	421	BCR	C10-C11-C12-C13
19	aX	101	LHG	O2-C2-C3-O3
19	bX	101	LHG	O2-C2-C3-O3
19	cX	101	LHG	O2-C2-C3-O3
15	aA	803	CLA	C15-C16-C17-C18
15	aA	807	CLA	C15-C16-C17-C18
15	aB	834	CLA	C5-C6-C7-C8
15	a3	402	CLA	C8-C10-C11-C12
15	a6	403	CLA	C8-C10-C11-C12
15	bA	803	CLA	C15-C16-C17-C18
15	bA	807	CLA	C15-C16-C17-C18
15	bB	834	CLA	C5-C6-C7-C8
15	b1	402	CLA	C8-C10-C11-C12
15	b6	403	CLA	C8-C10-C11-C12
15	cA	803	CLA	C15-C16-C17-C18
15	cA	807	CLA	C15-C16-C17-C18
15	cB	834	CLA	C5-C6-C7-C8
15	c1	402	CLA	C8-C10-C11-C12
15	c4	402	CLA	C8-C10-C11-C12
15	c6	404	CLA	C8-C10-C11-C12
15	c6	404	CLA	C15-C16-C17-C18
15	a3	410	CLA	CBD-CGD-O2D-CED
15	aB	826	CLA	CBA-CGA-O2A-C1
15	bB	826	CLA	CBA-CGA-O2A-C1
15	cB	826	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	825	CLA	C8-C10-C11-C12
15	aB	837	CLA	C13-C15-C16-C17
15	a2	422	CLA	C10-C11-C12-C13
15	a6	422	CLA	C10-C11-C12-C13
15	bA	803	CLA	C8-C10-C11-C12
15	bA	825	CLA	C8-C10-C11-C12
15	bB	837	CLA	C13-C15-C16-C17
15	b2	422	CLA	C10-C11-C12-C13
15	b6	422	CLA	C10-C11-C12-C13
15	cA	803	CLA	C8-C10-C11-C12
15	cA	825	CLA	C8-C10-C11-C12
15	cB	837	CLA	C13-C15-C16-C17
15	c2	422	CLA	C10-C11-C12-C13
15	bA	826	CLA	CBD-CGD-O2D-CED
15	aA	829	CLA	C5-C6-C7-C8
15	aB	802	CLA	C8-C10-C11-C12
15	aB	806	CLA	C15-C16-C17-C18
15	aB	815	CLA	C15-C16-C17-C18
15	aB	833	CLA	C10-C11-C12-C13
15	a2	406	CLA	C10-C11-C12-C13
15	a3	421	CLA	C10-C11-C12-C13
15	a4	402	CLA	C8-C10-C11-C12
15	a4	421	CLA	C10-C11-C12-C13
15	a5	402	CLA	C8-C10-C11-C12
15	a5	420	CLA	C10-C11-C12-C13
15	bB	802	CLA	C8-C10-C11-C12
15	bB	806	CLA	C15-C16-C17-C18
15	bB	815	CLA	C15-C16-C17-C18
15	bB	833	CLA	C10-C11-C12-C13
15	b3	402	CLA	C8-C10-C11-C12
15	b4	402	CLA	C8-C10-C11-C12
15	b4	421	CLA	C10-C11-C12-C13
15	b5	402	CLA	C8-C10-C11-C12
15	cB	802	CLA	C8-C10-C11-C12
15	cB	806	CLA	C15-C16-C17-C18
15	cB	815	CLA	C15-C16-C17-C18
15	cB	833	CLA	C10-C11-C12-C13
15	c3	402	CLA	C8-C10-C11-C12
15	c3	421	CLA	C10-C11-C12-C13
15	c4	421	CLA	C10-C11-C12-C13
15	c5	402	CLA	C8-C10-C11-C12
19	aA	854	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	aA	854	LHG	C4-O6-P-O3
19	aX	101	LHG	C3-O3-P-O6
19	bA	855	LHG	C3-O3-P-O6
19	bA	855	LHG	C4-O6-P-O3
19	bX	101	LHG	C3-O3-P-O6
19	cA	853	LHG	C3-O3-P-O6
19	cX	101	LHG	C3-O3-P-O6
15	aB	814	CLA	C3-C5-C6-C7
15	bB	814	CLA	C3-C5-C6-C7
15	cB	814	CLA	C3-C5-C6-C7
15	aB	837	CLA	O1D-CGD-O2D-CED
15	bB	837	CLA	O1D-CGD-O2D-CED
15	cB	837	CLA	O1D-CGD-O2D-CED
15	aA	826	CLA	CBD-CGD-O2D-CED
15	cA	826	CLA	CBD-CGD-O2D-CED
15	aB	828	CLA	C10-C11-C12-C13
15	bA	829	CLA	C5-C6-C7-C8
15	bB	828	CLA	C10-C11-C12-C13
15	b2	406	CLA	C10-C11-C12-C13
15	b3	421	CLA	C10-C11-C12-C13
15	b5	420	CLA	C10-C11-C12-C13
15	cA	829	CLA	C5-C6-C7-C8
15	cB	828	CLA	C10-C11-C12-C13
15	c2	406	CLA	C10-C11-C12-C13
15	c5	420	CLA	C10-C11-C12-C13
15	a2	418	CLA	C4-C3-C5-C6
15	b3	417	CLA	C4-C3-C5-C6
15	a1	416	CLA	C2-C3-C5-C6
15	c1	417	CLA	C2-C3-C5-C6
15	aA	829	CLA	C13-C15-C16-C17
15	a1	401	CLA	C8-C10-C11-C12
15	bA	829	CLA	C13-C15-C16-C17
15	cA	829	CLA	C13-C15-C16-C17
16	aB	843	PQN	C25-C26-C27-C28
16	bB	843	PQN	C25-C26-C27-C28
16	cB	843	PQN	C25-C26-C27-C28
15	aA	813	CLA	C2A-CAA-CBA-CGA
15	aA	816	CLA	C2A-CAA-CBA-CGA
15	aA	823	CLA	C2A-CAA-CBA-CGA
15	bA	813	CLA	C2A-CAA-CBA-CGA
15	bA	816	CLA	C2A-CAA-CBA-CGA
15	bA	823	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	813	CLA	C2A-CAA-CBA-CGA
15	cA	816	CLA	C2A-CAA-CBA-CGA
15	cA	823	CLA	C2A-CAA-CBA-CGA
15	aB	801	CLA	C3-C5-C6-C7
15	aB	819	CLA	C3-C5-C6-C7
15	bB	801	CLA	C3-C5-C6-C7
15	bB	819	CLA	C3-C5-C6-C7
15	cB	801	CLA	C3-C5-C6-C7
15	cB	819	CLA	C3-C5-C6-C7
15	aA	821	CLA	CBA-CGA-O2A-C1
15	aB	818	CLA	CBA-CGA-O2A-C1
15	a1	401	CLA	CBA-CGA-O2A-C1
15	a3	402	CLA	CBA-CGA-O2A-C1
15	bA	821	CLA	CBA-CGA-O2A-C1
15	bB	818	CLA	CBA-CGA-O2A-C1
15	cA	821	CLA	CBA-CGA-O2A-C1
15	cB	818	CLA	CBA-CGA-O2A-C1
15	c2	402	CLA	CBA-CGA-O2A-C1
15	c5	410	CLA	CBA-CGA-O2A-C1
15	aB	803	CLA	C8-C10-C11-C12
15	aB	814	CLA	C13-C15-C16-C17
15	bB	803	CLA	C8-C10-C11-C12
15	bB	814	CLA	C13-C15-C16-C17
15	b2	402	CLA	C8-C10-C11-C12
15	cB	803	CLA	C8-C10-C11-C12
15	cB	814	CLA	C13-C15-C16-C17
15	aA	810	CLA	C13-C15-C16-C17
15	aA	826	CLA	C5-C6-C7-C8
15	aB	815	CLA	C8-C10-C11-C12
15	a2	402	CLA	C8-C10-C11-C12
15	bA	810	CLA	C13-C15-C16-C17
15	bA	826	CLA	C5-C6-C7-C8
15	bB	815	CLA	C8-C10-C11-C12
15	cA	810	CLA	C13-C15-C16-C17
15	cA	826	CLA	C5-C6-C7-C8
15	cA	841	CLA	C5-C6-C7-C8
15	c2	402	CLA	C8-C10-C11-C12
18	a4	401	BCR	C9-C10-C11-C12
18	a6	419	BCR	C19-C20-C21-C22
18	b2	419	BCR	C19-C20-C21-C22
18	b4	401	BCR	C9-C10-C11-C12
18	b6	419	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c4	401	BCR	C9-C10-C11-C12
18	c6	420	BCR	C19-C20-C21-C22
15	aA	841	CLA	C5-C6-C7-C8
15	bA	841	CLA	C5-C6-C7-C8
15	cB	815	CLA	C8-C10-C11-C12
18	aA	848	BCR	C16-C17-C18-C36
18	aA	849	BCR	C20-C21-C22-C37
18	aA	850	BCR	C20-C21-C22-C37
18	aA	852	BCR	C16-C17-C18-C36
18	aB	845	BCR	C16-C17-C18-C36
18	aB	845	BCR	C20-C21-C22-C37
18	aF	201	BCR	C16-C17-C18-C36
18	aF	201	BCR	C20-C21-C22-C37
18	aF	202	BCR	C35-C13-C14-C15
18	aF	202	BCR	C16-C17-C18-C36
18	aF	203	BCR	C16-C17-C18-C36
18	aI	101	BCR	C16-C17-C18-C36
18	aI	102	BCR	C16-C17-C18-C36
18	aI	103	BCR	C20-C21-C22-C37
18	aJ	204	BCR	C35-C13-C14-C15
18	aJ	204	BCR	C20-C21-C22-C37
18	a1	417	BCR	C16-C17-C18-C36
18	a1	418	BCR	C20-C21-C22-C37
18	a1	419	BCR	C20-C21-C22-C37
18	a1	420	BCR	C11-C10-C9-C34
18	a1	420	BCR	C20-C21-C22-C37
18	a2	419	BCR	C20-C21-C22-C37
18	a2	420	BCR	C20-C21-C22-C37
18	a3	419	BCR	C20-C21-C22-C37
18	a3	420	BCR	C20-C21-C22-C37
18	a4	419	BCR	C20-C21-C22-C37
18	a4	420	BCR	C20-C21-C22-C37
18	a5	419	BCR	C20-C21-C22-C37
18	a6	401	BCR	C11-C10-C9-C34
18	a6	401	BCR	C20-C21-C22-C37
18	a6	419	BCR	C16-C17-C18-C36
18	bA	849	BCR	C16-C17-C18-C36
18	bA	850	BCR	C20-C21-C22-C37
18	bA	851	BCR	C20-C21-C22-C37
18	bA	853	BCR	C16-C17-C18-C36
18	bB	845	BCR	C16-C17-C18-C36
18	bB	845	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bB	849	BCR	C16-C17-C18-C36
18	bB	849	BCR	C20-C21-C22-C37
18	bF	202	BCR	C35-C13-C14-C15
18	bF	202	BCR	C16-C17-C18-C36
18	bI	101	BCR	C16-C17-C18-C36
18	bI	102	BCR	C16-C17-C18-C36
18	bJ	103	BCR	C35-C13-C14-C15
18	bJ	103	BCR	C20-C21-C22-C37
18	bJ	105	BCR	C16-C17-C18-C36
18	bL	205	BCR	C20-C21-C22-C37
18	b1	401	BCR	C20-C21-C22-C37
18	b1	418	BCR	C16-C17-C18-C36
18	b1	419	BCR	C20-C21-C22-C37
18	b1	420	BCR	C20-C21-C22-C37
18	b2	419	BCR	C20-C21-C22-C37
18	b2	420	BCR	C20-C21-C22-C37
18	b3	419	BCR	C20-C21-C22-C37
18	b3	420	BCR	C20-C21-C22-C37
18	b4	419	BCR	C20-C21-C22-C37
18	b4	420	BCR	C20-C21-C22-C37
18	b6	401	BCR	C11-C10-C9-C34
18	b6	401	BCR	C20-C21-C22-C37
18	b6	419	BCR	C16-C17-C18-C36
18	b6	420	BCR	C20-C21-C22-C37
18	cA	847	BCR	C16-C17-C18-C36
18	cA	848	BCR	C20-C21-C22-C37
18	cA	849	BCR	C20-C21-C22-C37
18	cA	851	BCR	C16-C17-C18-C36
18	cB	845	BCR	C16-C17-C18-C36
18	cB	845	BCR	C20-C21-C22-C37
18	cF	202	BCR	C16-C17-C18-C36
18	cF	202	BCR	C20-C21-C22-C37
18	cF	204	BCR	C35-C13-C14-C15
18	cF	204	BCR	C16-C17-C18-C36
18	cF	205	BCR	C16-C17-C18-C36
18	cI	101	BCR	C16-C17-C18-C36
18	cI	102	BCR	C16-C17-C18-C36
18	cJ	103	BCR	C35-C13-C14-C15
18	cJ	103	BCR	C20-C21-C22-C37
18	cL	205	BCR	C20-C21-C22-C37
18	c1	401	BCR	C20-C21-C22-C37
18	c1	418	BCR	C16-C17-C18-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c1	419	BCR	C20-C21-C22-C37
18	c1	420	BCR	C20-C21-C22-C37
18	c2	420	BCR	C20-C21-C22-C37
18	c3	419	BCR	C20-C21-C22-C37
18	c3	420	BCR	C20-C21-C22-C37
18	c4	418	BCR	C20-C21-C22-C37
18	c4	419	BCR	C20-C21-C22-C37
18	c4	420	BCR	C20-C21-C22-C37
18	c5	419	BCR	C20-C21-C22-C37
18	c6	402	BCR	C11-C10-C9-C34
18	c6	402	BCR	C20-C21-C22-C37
18	c6	420	BCR	C16-C17-C18-C36
18	c6	421	BCR	C20-C21-C22-C37
19	aA	854	LHG	C9-C10-C11-C12
19	bA	854	LHG	C26-C27-C28-C29
19	bA	855	LHG	C9-C10-C11-C12
19	cA	852	LHG	C26-C27-C28-C29
19	cA	853	LHG	C9-C10-C11-C12
15	aA	825	CLA	O1D-CGD-O2D-CED
15	aB	814	CLA	O1D-CGD-O2D-CED
15	bA	825	CLA	O1D-CGD-O2D-CED
15	bB	814	CLA	O1D-CGD-O2D-CED
15	cA	825	CLA	O1D-CGD-O2D-CED
15	cB	814	CLA	O1D-CGD-O2D-CED
15	aB	802	CLA	C16-C17-C18-C19
15	bB	802	CLA	C16-C17-C18-C19
15	cB	802	CLA	C16-C17-C18-C19
16	aB	843	PQN	C26-C27-C28-C29
16	bB	843	PQN	C26-C27-C28-C29
16	cB	843	PQN	C26-C27-C28-C29
15	aB	814	CLA	CBA-CGA-O2A-C1
15	a1	409	CLA	CBA-CGA-O2A-C1
15	a2	402	CLA	CBA-CGA-O2A-C1
15	a4	402	CLA	CBA-CGA-O2A-C1
15	a5	410	CLA	CBA-CGA-O2A-C1
15	bB	814	CLA	CBA-CGA-O2A-C1
15	b2	402	CLA	CBA-CGA-O2A-C1
15	b3	402	CLA	CBA-CGA-O2A-C1
15	b3	410	CLA	CBA-CGA-O2A-C1
15	b4	402	CLA	CBA-CGA-O2A-C1
15	b5	410	CLA	CBA-CGA-O2A-C1
15	cB	814	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	402	CLA	CBA-CGA-O2A-C1
15	c3	402	CLA	CBA-CGA-O2A-C1
15	c4	402	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C26-C27-C28-C29
15	cB	820	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	O9-C7-O7-C5
19	bA	854	LHG	O9-C7-O7-C5
19	cA	852	LHG	O9-C7-O7-C5
15	cB	836	CLA	C5-C6-C7-C8
15	aB	820	CLA	O1D-CGD-O2D-CED
15	bB	820	CLA	O1D-CGD-O2D-CED
15	aB	809	CLA	C8-C10-C11-C12
15	bB	809	CLA	C8-C10-C11-C12
15	bB	836	CLA	C5-C6-C7-C8
15	cB	809	CLA	C8-C10-C11-C12
15	aA	843	CLA	C3-C5-C6-C7
15	bA	843	CLA	C3-C5-C6-C7
15	cA	842	CLA	C3-C5-C6-C7
18	aA	849	BCR	C11-C10-C9-C8
18	aA	849	BCR	C16-C17-C18-C19
18	aA	850	BCR	C11-C10-C9-C8
18	aA	851	BCR	C20-C21-C22-C23
18	aA	852	BCR	C12-C13-C14-C15
18	aB	846	BCR	C20-C21-C22-C23
18	aB	848	BCR	C12-C13-C14-C15
18	aB	849	BCR	C20-C21-C22-C23
18	aF	201	BCR	C20-C21-C22-C23
18	aI	101	BCR	C16-C17-C18-C19
18	aJ	204	BCR	C16-C17-C18-C19
18	aJ	204	BCR	C20-C21-C22-C23
18	aJ	205	BCR	C16-C17-C18-C19
18	aL	205	BCR	C12-C13-C14-C15
18	aM	101	BCR	C11-C10-C9-C8
18	aM	101	BCR	C16-C17-C18-C19
18	a1	419	BCR	C20-C21-C22-C23
18	a3	420	BCR	C20-C21-C22-C23
18	a4	420	BCR	C20-C21-C22-C23
18	a5	419	BCR	C20-C21-C22-C23
18	bA	850	BCR	C11-C10-C9-C8
18	bA	850	BCR	C16-C17-C18-C19
18	bA	851	BCR	C11-C10-C9-C8
18	bA	852	BCR	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bA	853	BCR	C12-C13-C14-C15
18	bB	846	BCR	C20-C21-C22-C23
18	bB	848	BCR	C12-C13-C14-C15
18	bB	849	BCR	C20-C21-C22-C23
18	bB	850	BCR	C20-C21-C22-C23
18	bI	101	BCR	C16-C17-C18-C19
18	bJ	103	BCR	C16-C17-C18-C19
18	bJ	103	BCR	C20-C21-C22-C23
18	bJ	104	BCR	C16-C17-C18-C19
18	bL	201	BCR	C12-C13-C14-C15
18	bL	206	BCR	C12-C13-C14-C15
18	bM	101	BCR	C11-C10-C9-C8
18	bM	101	BCR	C16-C17-C18-C19
18	b1	420	BCR	C20-C21-C22-C23
18	b2	421	BCR	C20-C21-C22-C23
18	b5	419	BCR	C20-C21-C22-C23
18	b6	420	BCR	C20-C21-C22-C23
18	cA	848	BCR	C11-C10-C9-C8
18	cA	848	BCR	C16-C17-C18-C19
18	cA	849	BCR	C11-C10-C9-C8
18	cA	850	BCR	C20-C21-C22-C23
18	cA	851	BCR	C12-C13-C14-C15
18	cB	846	BCR	C20-C21-C22-C23
18	cB	848	BCR	C12-C13-C14-C15
18	cB	849	BCR	C20-C21-C22-C23
18	cF	202	BCR	C20-C21-C22-C23
18	cI	101	BCR	C16-C17-C18-C19
18	cJ	103	BCR	C16-C17-C18-C19
18	cJ	103	BCR	C20-C21-C22-C23
18	cJ	104	BCR	C16-C17-C18-C19
18	cM	101	BCR	C11-C10-C9-C8
18	cM	101	BCR	C16-C17-C18-C19
18	c1	420	BCR	C20-C21-C22-C23
18	c2	421	BCR	C20-C21-C22-C23
18	c3	420	BCR	C20-C21-C22-C23
18	c5	419	BCR	C20-C21-C22-C23
20	aB	850	LMG	C2-C1-O1-C7
20	bB	851	LMG	C2-C1-O1-C7
20	cB	850	LMG	C2-C1-O1-C7
15	a3	410	CLA	CBA-CGA-O2A-C1
15	b1	402	CLA	CBA-CGA-O2A-C1
15	b1	410	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	410	CLA	CBA-CGA-O2A-C1
15	c3	410	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C18-C19-C20-C21
19	aA	853	LHG	C28-C29-C30-C31
19	bA	854	LHG	C28-C29-C30-C31
19	cA	852	LHG	C28-C29-C30-C31
15	aA	814	CLA	C10-C11-C12-C13
15	aB	836	CLA	C5-C6-C7-C8
15	bA	814	CLA	C10-C11-C12-C13
15	cA	814	CLA	C10-C11-C12-C13
15	aL	203	CLA	C16-C17-C18-C20
15	bL	204	CLA	C16-C17-C18-C20
15	cL	204	CLA	C16-C17-C18-C20
15	a1	408	CLA	O1D-CGD-O2D-CED
15	b1	409	CLA	O1D-CGD-O2D-CED
15	c1	409	CLA	O1D-CGD-O2D-CED
15	aB	808	CLA	C4-C3-C5-C6
15	a2	404	CLA	C4-C3-C5-C6
15	a5	404	CLA	C4-C3-C5-C6
15	a6	405	CLA	C4-C3-C5-C6
15	bB	808	CLA	C4-C3-C5-C6
15	b1	404	CLA	C4-C3-C5-C6
15	b2	404	CLA	C4-C3-C5-C6
15	b3	404	CLA	C4-C3-C5-C6
15	cB	808	CLA	C4-C3-C5-C6
15	c3	404	CLA	C4-C3-C5-C6
15	c5	404	CLA	C4-C3-C5-C6
15	bB	804	CLA	C2C-C3C-CAC-CBC
15	cB	804	CLA	C2C-C3C-CAC-CBC
19	bA	854	LHG	C18-C19-C20-C21
19	cA	852	LHG	C18-C19-C20-C21
15	a5	417	CLA	C2-C3-C5-C6
15	b5	417	CLA	C2-C3-C5-C6
15	c5	417	CLA	C2-C3-C5-C6
15	aA	821	CLA	C6-C7-C8-C9
15	aA	822	CLA	C14-C13-C15-C16
15	aA	829	CLA	C11-C10-C8-C9
15	aB	814	CLA	C14-C13-C15-C16
15	aB	827	CLA	C6-C7-C8-C9
15	aB	833	CLA	C14-C13-C15-C16
15	a3	402	CLA	C14-C13-C15-C16
15	a4	402	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	402	CLA	C14-C13-C15-C16
15	bA	821	CLA	C6-C7-C8-C9
15	bA	822	CLA	C14-C13-C15-C16
15	bA	829	CLA	C11-C10-C8-C9
15	bB	814	CLA	C14-C13-C15-C16
15	bB	827	CLA	C6-C7-C8-C9
15	bB	833	CLA	C14-C13-C15-C16
15	b3	402	CLA	C14-C13-C15-C16
15	b4	402	CLA	C14-C13-C15-C16
15	b5	402	CLA	C14-C13-C15-C16
15	cA	821	CLA	C6-C7-C8-C9
15	cA	822	CLA	C14-C13-C15-C16
15	cA	829	CLA	C11-C10-C8-C9
15	cB	814	CLA	C14-C13-C15-C16
15	cB	827	CLA	C6-C7-C8-C9
15	cB	833	CLA	C14-C13-C15-C16
15	c1	402	CLA	C14-C13-C15-C16
15	c3	402	CLA	C14-C13-C15-C16
15	c4	402	CLA	C14-C13-C15-C16
15	c5	402	CLA	C14-C13-C15-C16
15	cB	810	CLA	CBD-CGD-O2D-CED
15	aA	813	CLA	C5-C6-C7-C8
15	bA	813	CLA	C5-C6-C7-C8
15	cA	813	CLA	C5-C6-C7-C8
15	aB	804	CLA	C2A-CAA-CBA-CGA
15	a6	422	CLA	C2A-CAA-CBA-CGA
18	aF	202	BCR	C7-C8-C9-C34
18	a1	420	BCR	C7-C8-C9-C34
18	a6	401	BCR	C7-C8-C9-C34
18	bF	202	BCR	C7-C8-C9-C34
18	b6	401	BCR	C7-C8-C9-C34
18	cF	204	BCR	C7-C8-C9-C34
18	c6	402	BCR	C7-C8-C9-C34
15	aB	804	CLA	C2C-C3C-CAC-CBC
20	aB	850	LMG	C17-C18-C19-C20
20	bB	851	LMG	C17-C18-C19-C20
18	aM	101	BCR	C7-C8-C9-C10
18	a1	419	BCR	C7-C8-C9-C10
18	a2	421	BCR	C7-C8-C9-C10
18	a3	420	BCR	C7-C8-C9-C10
18	a4	420	BCR	C7-C8-C9-C10
18	a5	419	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a6	420	BCR	C7-C8-C9-C10
18	bM	101	BCR	C7-C8-C9-C10
18	b1	420	BCR	C7-C8-C9-C10
18	b2	421	BCR	C7-C8-C9-C10
18	b3	420	BCR	C7-C8-C9-C10
18	b4	420	BCR	C7-C8-C9-C10
18	b5	419	BCR	C7-C8-C9-C10
18	b6	420	BCR	C7-C8-C9-C10
18	cM	101	BCR	C7-C8-C9-C10
18	c1	420	BCR	C7-C8-C9-C10
18	c2	421	BCR	C7-C8-C9-C10
18	c3	420	BCR	C7-C8-C9-C10
18	c4	420	BCR	C7-C8-C9-C10
18	c5	419	BCR	C7-C8-C9-C10
18	c6	421	BCR	C7-C8-C9-C10
15	aB	830	CLA	C13-C15-C16-C17
15	bB	830	CLA	C13-C15-C16-C17
15	cB	830	CLA	C13-C15-C16-C17
20	cB	850	LMG	C17-C18-C19-C20
15	aB	810	CLA	CBD-CGD-O2D-CED
15	bB	810	CLA	CBD-CGD-O2D-CED
19	aA	853	LHG	C23-C24-C25-C26
19	bA	854	LHG	C23-C24-C25-C26
19	cA	852	LHG	C23-C24-C25-C26
15	aA	810	CLA	C4B-C3B-CAB-CBB
15	aA	812	CLA	C4B-C3B-CAB-CBB
15	aA	814	CLA	C4B-C3B-CAB-CBB
15	aA	815	CLA	C4B-C3B-CAB-CBB
15	aA	839	CLA	C4B-C3B-CAB-CBB
15	aA	841	CLA	C4B-C3B-CAB-CBB
15	aB	817	CLA	C4B-C3B-CAB-CBB
15	aB	821	CLA	C4B-C3B-CAB-CBB
15	aB	839	CLA	C4B-C3B-CAB-CBB
15	aB	841	CLA	C4B-C3B-CAB-CBB
15	aJ	203	CLA	C4B-C3B-CAB-CBB
15	a1	412	CLA	C4B-C3B-CAB-CBB
15	a1	413	CLA	C4B-C3B-CAB-CBB
15	a2	406	CLA	C4B-C3B-CAB-CBB
15	a2	422	CLA	C4B-C3B-CAB-CBB
15	a3	421	CLA	C4B-C3B-CAB-CBB
15	a4	414	CLA	C4B-C3B-CAB-CBB
15	a4	421	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	413	CLA	C4B-C3B-CAB-CBB
15	a5	414	CLA	C4B-C3B-CAB-CBB
15	a6	417	CLA	C4B-C3B-CAB-CBB
15	a6	422	CLA	C4B-C3B-CAB-CBB
15	bA	810	CLA	C4B-C3B-CAB-CBB
15	bA	812	CLA	C4B-C3B-CAB-CBB
15	bA	814	CLA	C4B-C3B-CAB-CBB
15	bA	815	CLA	C4B-C3B-CAB-CBB
15	bA	839	CLA	C4B-C3B-CAB-CBB
15	bA	841	CLA	C4B-C3B-CAB-CBB
15	bB	817	CLA	C4B-C3B-CAB-CBB
15	bB	821	CLA	C4B-C3B-CAB-CBB
15	bB	839	CLA	C4B-C3B-CAB-CBB
15	bB	841	CLA	C4B-C3B-CAB-CBB
15	bJ	102	CLA	C4B-C3B-CAB-CBB
15	b1	413	CLA	C4B-C3B-CAB-CBB
15	b1	414	CLA	C4B-C3B-CAB-CBB
15	b2	406	CLA	C4B-C3B-CAB-CBB
15	b2	414	CLA	C4B-C3B-CAB-CBB
15	b2	422	CLA	C4B-C3B-CAB-CBB
15	b3	421	CLA	C4B-C3B-CAB-CBB
15	b4	414	CLA	C4B-C3B-CAB-CBB
15	b4	421	CLA	C4B-C3B-CAB-CBB
15	b5	413	CLA	C4B-C3B-CAB-CBB
15	b5	414	CLA	C4B-C3B-CAB-CBB
15	b6	415	CLA	C4B-C3B-CAB-CBB
15	b6	417	CLA	C4B-C3B-CAB-CBB
15	b6	422	CLA	C4B-C3B-CAB-CBB
15	cA	810	CLA	C4B-C3B-CAB-CBB
15	cA	812	CLA	C4B-C3B-CAB-CBB
15	cA	814	CLA	C4B-C3B-CAB-CBB
15	cA	815	CLA	C4B-C3B-CAB-CBB
15	cA	839	CLA	C4B-C3B-CAB-CBB
15	cA	841	CLA	C4B-C3B-CAB-CBB
15	cB	817	CLA	C4B-C3B-CAB-CBB
15	cB	821	CLA	C4B-C3B-CAB-CBB
15	cB	839	CLA	C4B-C3B-CAB-CBB
15	cB	841	CLA	C4B-C3B-CAB-CBB
15	cJ	102	CLA	C4B-C3B-CAB-CBB
15	c1	413	CLA	C4B-C3B-CAB-CBB
15	c1	414	CLA	C4B-C3B-CAB-CBB
15	c2	406	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c2	422	CLA	C4B-C3B-CAB-CBB
15	c3	421	CLA	C4B-C3B-CAB-CBB
15	c4	414	CLA	C4B-C3B-CAB-CBB
15	c4	421	CLA	C4B-C3B-CAB-CBB
15	c5	414	CLA	C4B-C3B-CAB-CBB
15	c5	420	CLA	C4B-C3B-CAB-CBB
15	c6	401	CLA	C4B-C3B-CAB-CBB
15	c6	416	CLA	C4B-C3B-CAB-CBB
15	c6	418	CLA	C4B-C3B-CAB-CBB
15	aB	828	CLA	C16-C17-C18-C19
15	aL	203	CLA	C16-C17-C18-C19
15	bB	828	CLA	C16-C17-C18-C19
15	bL	204	CLA	C16-C17-C18-C19
15	cB	828	CLA	C16-C17-C18-C19
15	cL	204	CLA	C16-C17-C18-C19
15	aA	841	CLA	C8-C10-C11-C12
15	bA	841	CLA	C8-C10-C11-C12
15	cA	841	CLA	C8-C10-C11-C12
20	aB	850	LMG	C40-C41-C42-C43
20	bB	851	LMG	C40-C41-C42-C43
20	cB	850	LMG	C40-C41-C42-C43
15	aB	829	CLA	CBD-CGD-O2D-CED
15	bB	829	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	CBD-CGD-O2D-CED
15	c4	411	CLA	CBD-CGD-O2D-CED
15	c4	409	CLA	O1D-CGD-O2D-CED
19	bA	854	LHG	C32-C33-C34-C35
19	cA	852	LHG	C32-C33-C34-C35
15	aA	821	CLA	O1A-CGA-O2A-C1
15	bA	821	CLA	O1A-CGA-O2A-C1
15	cA	821	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	C32-C33-C34-C35
15	aA	824	CLA	CBA-CGA-O2A-C1
15	a2	411	CLA	CBA-CGA-O2A-C1
15	a4	410	CLA	CBA-CGA-O2A-C1
15	a6	403	CLA	CBA-CGA-O2A-C1
15	a6	411	CLA	CBA-CGA-O2A-C1
15	bA	824	CLA	CBA-CGA-O2A-C1
15	b2	411	CLA	CBA-CGA-O2A-C1
15	b4	410	CLA	CBA-CGA-O2A-C1
15	b6	403	CLA	CBA-CGA-O2A-C1
15	b6	411	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	824	CLA	CBA-CGA-O2A-C1
15	c2	411	CLA	CBA-CGA-O2A-C1
15	c4	410	CLA	CBA-CGA-O2A-C1
15	c6	412	CLA	CBA-CGA-O2A-C1
20	aB	850	LMG	C34-C35-C36-C37
20	bB	851	LMG	C34-C35-C36-C37
20	cB	850	LMG	C34-C35-C36-C37
15	a2	410	CLA	O1D-CGD-O2D-CED
15	bA	830	CLA	O1D-CGD-O2D-CED
15	b2	410	CLA	O1D-CGD-O2D-CED
15	b6	410	CLA	O1D-CGD-O2D-CED
15	cA	830	CLA	O1D-CGD-O2D-CED
15	aA	804	CLA	C3A-C2A-CAA-CBA
15	aA	805	CLA	C3A-C2A-CAA-CBA
15	aA	842	CLA	C3A-C2A-CAA-CBA
15	a1	410	CLA	C3A-C2A-CAA-CBA
15	a1	411	CLA	C3A-C2A-CAA-CBA
15	a2	412	CLA	C3A-C2A-CAA-CBA
15	a3	411	CLA	C3A-C2A-CAA-CBA
15	a4	411	CLA	C3A-C2A-CAA-CBA
15	a5	411	CLA	C3A-C2A-CAA-CBA
15	a6	412	CLA	C3A-C2A-CAA-CBA
15	a6	413	CLA	C3A-C2A-CAA-CBA
15	bA	804	CLA	C3A-C2A-CAA-CBA
15	bA	805	CLA	C3A-C2A-CAA-CBA
15	bA	842	CLA	C3A-C2A-CAA-CBA
15	b1	411	CLA	C3A-C2A-CAA-CBA
15	b2	412	CLA	C3A-C2A-CAA-CBA
15	b3	411	CLA	C3A-C2A-CAA-CBA
15	b4	411	CLA	C3A-C2A-CAA-CBA
15	b5	411	CLA	C3A-C2A-CAA-CBA
15	b6	412	CLA	C3A-C2A-CAA-CBA
15	b6	413	CLA	C3A-C2A-CAA-CBA
15	cA	804	CLA	C3A-C2A-CAA-CBA
15	cA	805	CLA	C3A-C2A-CAA-CBA
15	cF	201	CLA	C3A-C2A-CAA-CBA
15	c1	411	CLA	C3A-C2A-CAA-CBA
15	c2	412	CLA	C3A-C2A-CAA-CBA
15	c3	411	CLA	C3A-C2A-CAA-CBA
15	c4	411	CLA	C3A-C2A-CAA-CBA
15	c5	411	CLA	C3A-C2A-CAA-CBA
15	c6	413	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aL	202	CLA	C10-C11-C12-C13
15	bL	203	CLA	C10-C11-C12-C13
15	cL	203	CLA	C10-C11-C12-C13
18	aA	850	BCR	C19-C20-C21-C22
18	bA	851	BCR	C19-C20-C21-C22
18	cA	849	BCR	C19-C20-C21-C22
15	aA	830	CLA	O1D-CGD-O2D-CED
15	a4	409	CLA	O1D-CGD-O2D-CED
15	a6	410	CLA	O1D-CGD-O2D-CED
15	b4	409	CLA	O1D-CGD-O2D-CED
15	c2	410	CLA	O1D-CGD-O2D-CED
15	a1	401	CLA	O1A-CGA-O2A-C1
15	a2	402	CLA	O1A-CGA-O2A-C1
15	a3	402	CLA	O1A-CGA-O2A-C1
15	c1	402	CLA	O1A-CGA-O2A-C1
15	c2	402	CLA	O1A-CGA-O2A-C1
15	aA	814	CLA	C11-C12-C13-C14
15	aA	814	CLA	C11-C12-C13-C15
15	aB	806	CLA	C16-C17-C18-C19
15	bA	814	CLA	C11-C12-C13-C14
15	bA	814	CLA	C11-C12-C13-C15
15	bB	806	CLA	C16-C17-C18-C19
15	cA	814	CLA	C11-C12-C13-C14
15	cA	814	CLA	C11-C12-C13-C15
15	cB	806	CLA	C16-C17-C18-C19
16	aB	843	PQN	C26-C27-C28-C30
16	bB	843	PQN	C26-C27-C28-C30
16	cB	843	PQN	C26-C27-C28-C30
15	b5	409	CLA	O1D-CGD-O2D-CED
15	aB	818	CLA	CBD-CGD-O2D-CED
15	a5	410	CLA	CBD-CGD-O2D-CED
15	bB	818	CLA	CBD-CGD-O2D-CED
15	b5	410	CLA	CBD-CGD-O2D-CED
15	cB	818	CLA	CBD-CGD-O2D-CED
15	c3	411	CLA	CBD-CGD-O2D-CED
15	c5	410	CLA	CBD-CGD-O2D-CED
20	aB	850	LMG	C19-C20-C21-C22
20	bB	851	LMG	C19-C20-C21-C22
20	cB	850	LMG	C19-C20-C21-C22
18	aA	852	BCR	C14-C15-C16-C17
18	bA	853	BCR	C14-C15-C16-C17
18	cA	851	BCR	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	814	CLA	O1D-CGD-O2D-CED
15	bA	814	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	O1A-CGA-O2A-C1
15	c3	402	CLA	O1A-CGA-O2A-C1
15	a1	403	CLA	C4-C3-C5-C6
15	a3	404	CLA	C4-C3-C5-C6
15	a4	404	CLA	C4-C3-C5-C6
15	b4	404	CLA	C4-C3-C5-C6
15	b5	404	CLA	C4-C3-C5-C6
15	b6	405	CLA	C4-C3-C5-C6
15	c1	404	CLA	C4-C3-C5-C6
15	c2	404	CLA	C4-C3-C5-C6
15	c4	404	CLA	C4-C3-C5-C6
15	c6	406	CLA	C4-C3-C5-C6
15	aB	815	CLA	CBA-CGA-O2A-C1
15	bB	815	CLA	CBA-CGA-O2A-C1
15	cB	815	CLA	CBA-CGA-O2A-C1
15	c6	404	CLA	CBA-CGA-O2A-C1
15	aB	808	CLA	C2-C3-C5-C6
15	aB	827	CLA	C2-C3-C5-C6
15	a1	403	CLA	C2-C3-C5-C6
15	a3	404	CLA	C2-C3-C5-C6
15	a4	404	CLA	C2-C3-C5-C6
15	bB	808	CLA	C2-C3-C5-C6
15	bB	827	CLA	C2-C3-C5-C6
15	b4	417	CLA	C2-C3-C5-C6
15	cB	808	CLA	C2-C3-C5-C6
15	cB	827	CLA	C2-C3-C5-C6
15	c1	404	CLA	C2-C3-C5-C6
15	c2	404	CLA	C2-C3-C5-C6
15	c4	404	CLA	C2-C3-C5-C6
15	c6	406	CLA	C2-C3-C5-C6
15	cA	814	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	CBD-CGD-O2D-CED
15	c6	411	CLA	O1D-CGD-O2D-CED
15	bB	804	CLA	C2A-CAA-CBA-CGA
15	cB	804	CLA	C2A-CAA-CBA-CGA
19	aX	101	LHG	O1-C1-C2-O2
19	bX	101	LHG	O1-C1-C2-O2
19	cX	101	LHG	O1-C1-C2-O2
15	aB	809	CLA	C5-C6-C7-C8
15	bB	809	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a3	410	CLA	O1A-CGA-O2A-C1
15	a4	402	CLA	O1A-CGA-O2A-C1
15	b1	410	CLA	O1A-CGA-O2A-C1
15	b2	402	CLA	O1A-CGA-O2A-C1
15	b3	402	CLA	O1A-CGA-O2A-C1
15	b4	402	CLA	O1A-CGA-O2A-C1
15	aB	802	CLA	C16-C17-C18-C20
15	bB	802	CLA	C16-C17-C18-C20
15	cB	802	CLA	C16-C17-C18-C20
15	aA	809	CLA	C2B-C3B-CAB-CBB
15	aA	810	CLA	C2B-C3B-CAB-CBB
15	aA	812	CLA	C2B-C3B-CAB-CBB
15	aA	814	CLA	C2B-C3B-CAB-CBB
15	aA	815	CLA	C2B-C3B-CAB-CBB
15	aA	817	CLA	C2B-C3B-CAB-CBB
15	aA	836	CLA	C2B-C3B-CAB-CBB
15	aA	839	CLA	C2B-C3B-CAB-CBB
15	aA	842	CLA	C2B-C3B-CAB-CBB
15	aB	809	CLA	C2B-C3B-CAB-CBB
15	aB	817	CLA	C2B-C3B-CAB-CBB
15	aB	839	CLA	C2B-C3B-CAB-CBB
15	aB	841	CLA	C2B-C3B-CAB-CBB
15	aJ	201	CLA	C2B-C3B-CAB-CBB
15	aJ	203	CLA	C2B-C3B-CAB-CBB
15	aL	201	CLA	C2B-C3B-CAB-CBB
15	a1	403	CLA	C2B-C3B-CAB-CBB
15	a1	412	CLA	C2B-C3B-CAB-CBB
15	a1	413	CLA	C2B-C3B-CAB-CBB
15	a2	404	CLA	C2B-C3B-CAB-CBB
15	a2	406	CLA	C2B-C3B-CAB-CBB
15	a2	415	CLA	C2B-C3B-CAB-CBB
15	a2	422	CLA	C2B-C3B-CAB-CBB
15	a3	404	CLA	C2B-C3B-CAB-CBB
15	a3	414	CLA	C2B-C3B-CAB-CBB
15	a3	421	CLA	C2B-C3B-CAB-CBB
15	a4	404	CLA	C2B-C3B-CAB-CBB
15	a4	414	CLA	C2B-C3B-CAB-CBB
15	a4	421	CLA	C2B-C3B-CAB-CBB
15	a5	404	CLA	C2B-C3B-CAB-CBB
15	a5	414	CLA	C2B-C3B-CAB-CBB
15	a5	420	CLA	C2B-C3B-CAB-CBB
15	a6	415	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	422	CLA	C2B-C3B-CAB-CBB
15	bA	809	CLA	C2B-C3B-CAB-CBB
15	bA	810	CLA	C2B-C3B-CAB-CBB
15	bA	812	CLA	C2B-C3B-CAB-CBB
15	bA	814	CLA	C2B-C3B-CAB-CBB
15	bA	815	CLA	C2B-C3B-CAB-CBB
15	bA	817	CLA	C2B-C3B-CAB-CBB
15	bA	836	CLA	C2B-C3B-CAB-CBB
15	bA	839	CLA	C2B-C3B-CAB-CBB
15	bA	842	CLA	C2B-C3B-CAB-CBB
15	bB	809	CLA	C2B-C3B-CAB-CBB
15	bB	817	CLA	C2B-C3B-CAB-CBB
15	bB	839	CLA	C2B-C3B-CAB-CBB
15	bB	841	CLA	C2B-C3B-CAB-CBB
15	bF	201	CLA	C2B-C3B-CAB-CBB
15	bJ	102	CLA	C2B-C3B-CAB-CBB
15	bL	202	CLA	C2B-C3B-CAB-CBB
15	b1	404	CLA	C2B-C3B-CAB-CBB
15	b1	413	CLA	C2B-C3B-CAB-CBB
15	b1	414	CLA	C2B-C3B-CAB-CBB
15	b2	406	CLA	C2B-C3B-CAB-CBB
15	b2	415	CLA	C2B-C3B-CAB-CBB
15	b2	422	CLA	C2B-C3B-CAB-CBB
15	b3	404	CLA	C2B-C3B-CAB-CBB
15	b3	414	CLA	C2B-C3B-CAB-CBB
15	b3	421	CLA	C2B-C3B-CAB-CBB
15	b4	404	CLA	C2B-C3B-CAB-CBB
15	b4	414	CLA	C2B-C3B-CAB-CBB
15	b4	421	CLA	C2B-C3B-CAB-CBB
15	b5	414	CLA	C2B-C3B-CAB-CBB
15	b5	420	CLA	C2B-C3B-CAB-CBB
15	b6	415	CLA	C2B-C3B-CAB-CBB
15	b6	422	CLA	C2B-C3B-CAB-CBB
15	cA	809	CLA	C2B-C3B-CAB-CBB
15	cA	810	CLA	C2B-C3B-CAB-CBB
15	cA	812	CLA	C2B-C3B-CAB-CBB
15	cA	814	CLA	C2B-C3B-CAB-CBB
15	cA	815	CLA	C2B-C3B-CAB-CBB
15	cA	817	CLA	C2B-C3B-CAB-CBB
15	cA	836	CLA	C2B-C3B-CAB-CBB
15	cA	839	CLA	C2B-C3B-CAB-CBB
15	cB	809	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	817	CLA	C2B-C3B-CAB-CBB
15	cB	839	CLA	C2B-C3B-CAB-CBB
15	cB	841	CLA	C2B-C3B-CAB-CBB
15	cF	201	CLA	C2B-C3B-CAB-CBB
15	cF	203	CLA	C2B-C3B-CAB-CBB
15	cJ	102	CLA	C2B-C3B-CAB-CBB
15	cL	202	CLA	C2B-C3B-CAB-CBB
15	c1	404	CLA	C2B-C3B-CAB-CBB
15	c1	413	CLA	C2B-C3B-CAB-CBB
15	c1	414	CLA	C2B-C3B-CAB-CBB
15	c1	416	CLA	C2B-C3B-CAB-CBB
15	c2	406	CLA	C2B-C3B-CAB-CBB
15	c2	415	CLA	C2B-C3B-CAB-CBB
15	c2	422	CLA	C2B-C3B-CAB-CBB
15	c3	404	CLA	C2B-C3B-CAB-CBB
15	c3	414	CLA	C2B-C3B-CAB-CBB
15	c3	421	CLA	C2B-C3B-CAB-CBB
15	c4	404	CLA	C2B-C3B-CAB-CBB
15	c4	414	CLA	C2B-C3B-CAB-CBB
15	c4	421	CLA	C2B-C3B-CAB-CBB
15	c5	404	CLA	C2B-C3B-CAB-CBB
15	c5	414	CLA	C2B-C3B-CAB-CBB
15	c5	420	CLA	C2B-C3B-CAB-CBB
15	c6	401	CLA	C2B-C3B-CAB-CBB
15	c6	416	CLA	C2B-C3B-CAB-CBB
15	cB	809	CLA	C5-C6-C7-C8
15	aL	202	CLA	C3-C5-C6-C7
15	a1	408	CLA	C3-C5-C6-C7
15	a3	409	CLA	C3-C5-C6-C7
15	bL	203	CLA	C3-C5-C6-C7
15	b1	409	CLA	C3-C5-C6-C7
15	b6	410	CLA	C3-C5-C6-C7
15	cL	203	CLA	C3-C5-C6-C7
15	c1	409	CLA	C3-C5-C6-C7
15	a1	409	CLA	O1A-CGA-O2A-C1
15	a5	410	CLA	O1A-CGA-O2A-C1
15	b1	402	CLA	O1A-CGA-O2A-C1
15	b3	410	CLA	O1A-CGA-O2A-C1
15	b5	410	CLA	O1A-CGA-O2A-C1
15	c3	410	CLA	O1A-CGA-O2A-C1
15	c4	402	CLA	O1A-CGA-O2A-C1
15	c5	410	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	806	CLA	C2-C1-O2A-CGA
15	aA	843	CLA	C2-C1-O2A-CGA
15	bA	806	CLA	C2-C1-O2A-CGA
15	bA	843	CLA	C2-C1-O2A-CGA
15	cA	806	CLA	C2-C1-O2A-CGA
15	cA	842	CLA	C2-C1-O2A-CGA
15	aB	829	CLA	C13-C15-C16-C17
15	bB	829	CLA	C13-C15-C16-C17
15	cB	829	CLA	C13-C15-C16-C17
15	a2	411	CLA	O1A-CGA-O2A-C1
15	a6	403	CLA	O1A-CGA-O2A-C1
15	b6	403	CLA	O1A-CGA-O2A-C1
15	c4	410	CLA	O1A-CGA-O2A-C1
15	c6	404	CLA	O1A-CGA-O2A-C1
15	b1	410	CLA	CBD-CGD-O2D-CED
15	a5	409	CLA	C3-C5-C6-C7
15	a6	410	CLA	C3-C5-C6-C7
15	b3	409	CLA	C3-C5-C6-C7
15	c3	409	CLA	C3-C5-C6-C7
15	c5	409	CLA	C3-C5-C6-C7
18	aA	848	BCR	C1-C6-C7-C8
18	aA	848	BCR	C5-C6-C7-C8
18	aA	848	BCR	C23-C24-C25-C26
18	aA	849	BCR	C5-C6-C7-C8
18	aA	850	BCR	C5-C6-C7-C8
18	aA	850	BCR	C23-C24-C25-C26
18	aA	850	BCR	C23-C24-C25-C30
18	aA	851	BCR	C5-C6-C7-C8
18	aA	851	BCR	C23-C24-C25-C26
18	aB	844	BCR	C5-C6-C7-C8
18	aB	844	BCR	C23-C24-C25-C26
18	aB	844	BCR	C23-C24-C25-C30
18	aB	845	BCR	C5-C6-C7-C8
18	aB	846	BCR	C5-C6-C7-C8
18	aB	848	BCR	C5-C6-C7-C8
18	aB	848	BCR	C23-C24-C25-C26
18	aB	849	BCR	C5-C6-C7-C8
18	aF	202	BCR	C1-C6-C7-C8
18	aF	202	BCR	C5-C6-C7-C8
18	aF	203	BCR	C23-C24-C25-C26
18	aI	103	BCR	C5-C6-C7-C8
18	aI	103	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	aJ	204	BCR	C1-C6-C7-C8
18	aJ	204	BCR	C5-C6-C7-C8
18	aJ	205	BCR	C5-C6-C7-C8
18	aJ	205	BCR	C23-C24-C25-C26
18	aJ	205	BCR	C23-C24-C25-C30
18	aK	101	BCR	C5-C6-C7-C8
18	aL	205	BCR	C5-C6-C7-C8
18	aM	101	BCR	C1-C6-C7-C8
18	aM	101	BCR	C5-C6-C7-C8
18	a1	417	BCR	C5-C6-C7-C8
18	a1	417	BCR	C23-C24-C25-C26
18	a1	417	BCR	C23-C24-C25-C30
18	a1	418	BCR	C1-C6-C7-C8
18	a1	418	BCR	C5-C6-C7-C8
18	a1	419	BCR	C5-C6-C7-C8
18	a1	419	BCR	C23-C24-C25-C26
18	a1	419	BCR	C23-C24-C25-C30
18	a1	420	BCR	C5-C6-C7-C8
18	a1	421	BCR	C5-C6-C7-C8
18	a2	419	BCR	C5-C6-C7-C8
18	a2	419	BCR	C23-C24-C25-C26
18	a2	420	BCR	C1-C6-C7-C8
18	a2	420	BCR	C5-C6-C7-C8
18	a2	421	BCR	C5-C6-C7-C8
18	a2	421	BCR	C23-C24-C25-C26
18	a2	421	BCR	C23-C24-C25-C30
18	a3	401	BCR	C5-C6-C7-C8
18	a3	418	BCR	C5-C6-C7-C8
18	a3	418	BCR	C23-C24-C25-C26
18	a3	419	BCR	C5-C6-C7-C8
18	a3	420	BCR	C5-C6-C7-C8
18	a3	420	BCR	C23-C24-C25-C26
18	a3	420	BCR	C23-C24-C25-C30
18	a4	418	BCR	C5-C6-C7-C8
18	a4	418	BCR	C23-C24-C25-C26
18	a4	419	BCR	C5-C6-C7-C8
18	a4	420	BCR	C5-C6-C7-C8
18	a4	420	BCR	C23-C24-C25-C26
18	a4	420	BCR	C23-C24-C25-C30
18	a5	418	BCR	C5-C6-C7-C8
18	a5	418	BCR	C23-C24-C25-C26
18	a5	419	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a5	419	BCR	C23-C24-C25-C26
18	a5	419	BCR	C23-C24-C25-C30
18	a6	401	BCR	C5-C6-C7-C8
18	a6	419	BCR	C5-C6-C7-C8
18	a6	419	BCR	C23-C24-C25-C26
18	a6	420	BCR	C5-C6-C7-C8
18	a6	420	BCR	C23-C24-C25-C26
18	a6	420	BCR	C23-C24-C25-C30
18	a6	421	BCR	C5-C6-C7-C8
18	bA	848	BCR	C5-C6-C7-C8
18	bA	849	BCR	C1-C6-C7-C8
18	bA	849	BCR	C5-C6-C7-C8
18	bA	849	BCR	C23-C24-C25-C26
18	bA	850	BCR	C5-C6-C7-C8
18	bA	851	BCR	C5-C6-C7-C8
18	bA	851	BCR	C23-C24-C25-C26
18	bA	851	BCR	C23-C24-C25-C30
18	bA	852	BCR	C5-C6-C7-C8
18	bA	852	BCR	C23-C24-C25-C26
18	bB	844	BCR	C5-C6-C7-C8
18	bB	844	BCR	C23-C24-C25-C26
18	bB	844	BCR	C23-C24-C25-C30
18	bB	845	BCR	C5-C6-C7-C8
18	bB	846	BCR	C5-C6-C7-C8
18	bB	848	BCR	C5-C6-C7-C8
18	bB	848	BCR	C23-C24-C25-C26
18	bB	850	BCR	C5-C6-C7-C8
18	bF	202	BCR	C1-C6-C7-C8
18	bF	202	BCR	C5-C6-C7-C8
18	bJ	103	BCR	C1-C6-C7-C8
18	bJ	103	BCR	C5-C6-C7-C8
18	bJ	104	BCR	C5-C6-C7-C8
18	bJ	104	BCR	C23-C24-C25-C26
18	bJ	104	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C23-C24-C25-C26
18	bL	201	BCR	C5-C6-C7-C8
18	bL	205	BCR	C5-C6-C7-C8
18	bL	205	BCR	C23-C24-C25-C30
18	bL	206	BCR	C5-C6-C7-C8
18	bM	101	BCR	C1-C6-C7-C8
18	bM	101	BCR	C5-C6-C7-C8
18	b1	401	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b1	418	BCR	C5-C6-C7-C8
18	b1	418	BCR	C23-C24-C25-C26
18	b1	418	BCR	C23-C24-C25-C30
18	b1	419	BCR	C1-C6-C7-C8
18	b1	419	BCR	C5-C6-C7-C8
18	b1	420	BCR	C23-C24-C25-C26
18	b1	420	BCR	C23-C24-C25-C30
18	b2	419	BCR	C5-C6-C7-C8
18	b2	419	BCR	C23-C24-C25-C26
18	b2	420	BCR	C5-C6-C7-C8
18	b2	421	BCR	C5-C6-C7-C8
18	b2	421	BCR	C23-C24-C25-C26
18	b2	421	BCR	C23-C24-C25-C30
18	b3	401	BCR	C5-C6-C7-C8
18	b3	418	BCR	C5-C6-C7-C8
18	b3	418	BCR	C23-C24-C25-C26
18	b3	419	BCR	C5-C6-C7-C8
18	b3	420	BCR	C5-C6-C7-C8
18	b3	420	BCR	C23-C24-C25-C26
18	b3	420	BCR	C23-C24-C25-C30
18	b4	418	BCR	C5-C6-C7-C8
18	b4	418	BCR	C23-C24-C25-C26
18	b4	419	BCR	C5-C6-C7-C8
18	b4	420	BCR	C5-C6-C7-C8
18	b4	420	BCR	C23-C24-C25-C26
18	b4	420	BCR	C23-C24-C25-C30
18	b5	418	BCR	C5-C6-C7-C8
18	b5	418	BCR	C23-C24-C25-C26
18	b5	419	BCR	C5-C6-C7-C8
18	b5	419	BCR	C23-C24-C25-C26
18	b5	419	BCR	C23-C24-C25-C30
18	b6	401	BCR	C5-C6-C7-C8
18	b6	419	BCR	C5-C6-C7-C8
18	b6	419	BCR	C23-C24-C25-C26
18	b6	420	BCR	C5-C6-C7-C8
18	b6	420	BCR	C23-C24-C25-C26
18	b6	420	BCR	C23-C24-C25-C30
18	b6	421	BCR	C5-C6-C7-C8
18	cA	847	BCR	C1-C6-C7-C8
18	cA	847	BCR	C5-C6-C7-C8
18	cA	847	BCR	C23-C24-C25-C26
18	cA	848	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cA	849	BCR	C5-C6-C7-C8
18	cA	849	BCR	C23-C24-C25-C26
18	cA	849	BCR	C23-C24-C25-C30
18	cA	850	BCR	C5-C6-C7-C8
18	cA	850	BCR	C23-C24-C25-C26
18	cB	844	BCR	C5-C6-C7-C8
18	cB	844	BCR	C23-C24-C25-C26
18	cB	844	BCR	C23-C24-C25-C30
18	cB	845	BCR	C5-C6-C7-C8
18	cB	846	BCR	C5-C6-C7-C8
18	cB	848	BCR	C5-C6-C7-C8
18	cB	848	BCR	C23-C24-C25-C26
18	cB	849	BCR	C5-C6-C7-C8
18	cF	204	BCR	C1-C6-C7-C8
18	cF	204	BCR	C5-C6-C7-C8
18	cF	205	BCR	C23-C24-C25-C26
18	cJ	103	BCR	C1-C6-C7-C8
18	cJ	103	BCR	C5-C6-C7-C8
18	cJ	104	BCR	C5-C6-C7-C8
18	cJ	104	BCR	C23-C24-C25-C26
18	cJ	104	BCR	C23-C24-C25-C30
18	cK	101	BCR	C5-C6-C7-C8
18	cL	205	BCR	C5-C6-C7-C8
18	cL	205	BCR	C23-C24-C25-C30
18	cM	101	BCR	C1-C6-C7-C8
18	cM	101	BCR	C5-C6-C7-C8
18	c1	401	BCR	C1-C6-C7-C8
18	c1	418	BCR	C5-C6-C7-C8
18	c1	418	BCR	C23-C24-C25-C26
18	c1	418	BCR	C23-C24-C25-C30
18	c1	419	BCR	C1-C6-C7-C8
18	c1	419	BCR	C5-C6-C7-C8
18	c1	420	BCR	C5-C6-C7-C8
18	c1	420	BCR	C23-C24-C25-C26
18	c1	420	BCR	C23-C24-C25-C30
18	c2	419	BCR	C5-C6-C7-C8
18	c2	419	BCR	C23-C24-C25-C26
18	c2	420	BCR	C1-C6-C7-C8
18	c2	420	BCR	C5-C6-C7-C8
18	c2	421	BCR	C5-C6-C7-C8
18	c2	421	BCR	C23-C24-C25-C26
18	c2	421	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c3	401	BCR	C5-C6-C7-C8
18	c3	418	BCR	C5-C6-C7-C8
18	c3	418	BCR	C23-C24-C25-C26
18	c3	419	BCR	C5-C6-C7-C8
18	c3	420	BCR	C5-C6-C7-C8
18	c3	420	BCR	C23-C24-C25-C26
18	c3	420	BCR	C23-C24-C25-C30
18	c4	418	BCR	C5-C6-C7-C8
18	c4	418	BCR	C23-C24-C25-C26
18	c4	419	BCR	C5-C6-C7-C8
18	c4	420	BCR	C5-C6-C7-C8
18	c4	420	BCR	C23-C24-C25-C26
18	c4	420	BCR	C23-C24-C25-C30
18	c5	418	BCR	C5-C6-C7-C8
18	c5	418	BCR	C23-C24-C25-C26
18	c5	419	BCR	C5-C6-C7-C8
18	c5	419	BCR	C23-C24-C25-C26
18	c5	419	BCR	C23-C24-C25-C30
18	c6	402	BCR	C5-C6-C7-C8
18	c6	403	BCR	C23-C24-C25-C26
18	c6	420	BCR	C5-C6-C7-C8
18	c6	420	BCR	C23-C24-C25-C26
18	c6	421	BCR	C5-C6-C7-C8
18	c6	421	BCR	C23-C24-C25-C26
18	c6	421	BCR	C23-C24-C25-C30
15	b5	402	CLA	CBA-CGA-O2A-C1
15	c5	402	CLA	CBA-CGA-O2A-C1
15	aA	806	CLA	C8-C10-C11-C12
15	aA	822	CLA	C8-C10-C11-C12
15	aB	837	CLA	C15-C16-C17-C18
15	a2	403	CLA	C13-C15-C16-C17
15	a4	402	CLA	C13-C15-C16-C17
15	bA	806	CLA	C8-C10-C11-C12
15	bA	822	CLA	C8-C10-C11-C12
15	bB	837	CLA	C15-C16-C17-C18
15	b2	403	CLA	C13-C15-C16-C17
15	cA	806	CLA	C8-C10-C11-C12
15	cA	822	CLA	C8-C10-C11-C12
15	cB	837	CLA	C15-C16-C17-C18
15	c2	403	CLA	C13-C15-C16-C17
15	aA	825	CLA	C11-C12-C13-C14
15	bA	825	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	825	CLA	C11-C12-C13-C14
15	cA	805	CLA	O1D-CGD-O2D-CED
15	aA	824	CLA	O1A-CGA-O2A-C1
15	aB	818	CLA	O1A-CGA-O2A-C1
15	a4	410	CLA	O1A-CGA-O2A-C1
15	a6	411	CLA	O1A-CGA-O2A-C1
15	bA	824	CLA	O1A-CGA-O2A-C1
15	bB	818	CLA	O1A-CGA-O2A-C1
15	b2	411	CLA	O1A-CGA-O2A-C1
15	b4	410	CLA	O1A-CGA-O2A-C1
15	b6	411	CLA	O1A-CGA-O2A-C1
15	cA	824	CLA	O1A-CGA-O2A-C1
15	cB	818	CLA	O1A-CGA-O2A-C1
15	c2	411	CLA	O1A-CGA-O2A-C1
15	aA	835	CLA	C5-C6-C7-C8
15	a5	402	CLA	C13-C15-C16-C17
15	bA	835	CLA	C5-C6-C7-C8
15	b4	402	CLA	C13-C15-C16-C17
15	cA	835	CLA	C5-C6-C7-C8
15	c3	403	CLA	C13-C15-C16-C17
15	c4	402	CLA	C13-C15-C16-C17
15	c5	402	CLA	C13-C15-C16-C17
15	aA	805	CLA	O1D-CGD-O2D-CED
15	bA	805	CLA	O1D-CGD-O2D-CED
15	aA	821	CLA	C4-C3-C5-C6
15	aB	836	CLA	C4-C3-C5-C6
15	bA	821	CLA	C4-C3-C5-C6
15	bB	836	CLA	C4-C3-C5-C6
15	cA	821	CLA	C4-C3-C5-C6
15	cB	836	CLA	C4-C3-C5-C6
15	aA	802	CLA	C11-C10-C8-C7
15	aA	803	CLA	C6-C7-C8-C10
15	aA	804	CLA	C11-C12-C13-C15
15	aA	806	CLA	C6-C7-C8-C10
15	aA	809	CLA	C6-C7-C8-C10
15	aA	822	CLA	C12-C13-C15-C16
15	aB	807	CLA	C12-C13-C15-C16
15	aB	814	CLA	C12-C13-C15-C16
15	aB	819	CLA	C6-C7-C8-C10
15	aB	827	CLA	C6-C7-C8-C10
15	aB	828	CLA	C11-C12-C13-C15
15	aB	834	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	836	CLA	C2-C3-C5-C6
15	aB	840	CLA	C11-C12-C13-C15
15	a1	402	CLA	C6-C7-C8-C10
15	a2	403	CLA	C6-C7-C8-C10
15	a2	404	CLA	C2-C3-C5-C6
15	a3	402	CLA	C12-C13-C15-C16
15	a3	403	CLA	C6-C7-C8-C10
15	a4	402	CLA	C12-C13-C15-C16
15	a4	417	CLA	C2-C3-C5-C6
15	a5	402	CLA	C12-C13-C15-C16
15	a5	403	CLA	C6-C7-C8-C10
15	a5	404	CLA	C2-C3-C5-C6
15	a6	404	CLA	C6-C7-C8-C10
15	a6	405	CLA	C2-C3-C5-C6
15	bA	802	CLA	C11-C10-C8-C7
15	bA	803	CLA	C6-C7-C8-C10
15	bA	804	CLA	C11-C12-C13-C15
15	bA	806	CLA	C6-C7-C8-C10
15	bA	809	CLA	C6-C7-C8-C10
15	bA	822	CLA	C12-C13-C15-C16
15	bB	807	CLA	C12-C13-C15-C16
15	bB	814	CLA	C11-C10-C8-C7
15	bB	814	CLA	C12-C13-C15-C16
15	bB	819	CLA	C6-C7-C8-C10
15	bB	827	CLA	C6-C7-C8-C10
15	bB	828	CLA	C11-C12-C13-C15
15	bB	834	CLA	C6-C7-C8-C10
15	bB	836	CLA	C2-C3-C5-C6
15	bB	840	CLA	C11-C12-C13-C15
15	b1	403	CLA	C6-C7-C8-C10
15	b1	404	CLA	C2-C3-C5-C6
15	b2	403	CLA	C6-C7-C8-C10
15	b2	404	CLA	C2-C3-C5-C6
15	b3	402	CLA	C12-C13-C15-C16
15	b3	403	CLA	C6-C7-C8-C10
15	b3	404	CLA	C2-C3-C5-C6
15	b4	402	CLA	C12-C13-C15-C16
15	b4	404	CLA	C2-C3-C5-C6
15	b5	402	CLA	C12-C13-C15-C16
15	b5	403	CLA	C6-C7-C8-C10
15	b5	404	CLA	C2-C3-C5-C6
15	b6	404	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b6	405	CLA	C2-C3-C5-C6
15	cA	802	CLA	C11-C10-C8-C7
15	cA	803	CLA	C6-C7-C8-C10
15	cA	804	CLA	C11-C12-C13-C15
15	cA	806	CLA	C6-C7-C8-C10
15	cA	809	CLA	C6-C7-C8-C10
15	cA	822	CLA	C12-C13-C15-C16
15	cB	807	CLA	C12-C13-C15-C16
15	cB	814	CLA	C11-C10-C8-C7
15	cB	814	CLA	C12-C13-C15-C16
15	cB	819	CLA	C6-C7-C8-C10
15	cB	827	CLA	C6-C7-C8-C10
15	cB	828	CLA	C11-C12-C13-C15
15	cB	834	CLA	C6-C7-C8-C10
15	cB	836	CLA	C2-C3-C5-C6
15	cB	840	CLA	C11-C12-C13-C15
15	c1	403	CLA	C6-C7-C8-C10
15	c2	403	CLA	C6-C7-C8-C10
15	c3	402	CLA	C12-C13-C15-C16
15	c3	403	CLA	C6-C7-C8-C10
15	c3	404	CLA	C2-C3-C5-C6
15	c4	402	CLA	C12-C13-C15-C16
15	c4	417	CLA	C2-C3-C5-C6
15	c5	402	CLA	C12-C13-C15-C16
15	c5	403	CLA	C6-C7-C8-C10
15	c5	404	CLA	C2-C3-C5-C6
15	c6	405	CLA	C6-C7-C8-C10
15	c6	419	CLA	C2-C3-C5-C6
15	aB	814	CLA	O1A-CGA-O2A-C1
15	aB	815	CLA	O1A-CGA-O2A-C1
15	bB	814	CLA	O1A-CGA-O2A-C1
15	bB	815	CLA	O1A-CGA-O2A-C1
15	cB	814	CLA	O1A-CGA-O2A-C1
15	cB	815	CLA	O1A-CGA-O2A-C1
15	c6	412	CLA	O1A-CGA-O2A-C1
15	a3	402	CLA	C13-C15-C16-C17
15	a4	403	CLA	C13-C15-C16-C17
15	b3	402	CLA	C13-C15-C16-C17
15	b5	402	CLA	C13-C15-C16-C17
15	c4	403	CLA	C13-C15-C16-C17
15	c5	403	CLA	C13-C15-C16-C17
18	aA	848	BCR	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bA	849	BCR	C15-C16-C17-C18
18	cA	847	BCR	C15-C16-C17-C18
15	a1	409	CLA	CBD-CGD-O2D-CED
15	a3	411	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	C16-C17-C18-C20
15	bB	806	CLA	C16-C17-C18-C20
15	cB	806	CLA	C16-C17-C18-C20
15	aA	809	CLA	O1D-CGD-O2D-CED
15	aL	203	CLA	O1D-CGD-O2D-CED
15	bA	809	CLA	O1D-CGD-O2D-CED
15	bL	204	CLA	O1D-CGD-O2D-CED
15	cA	809	CLA	O1D-CGD-O2D-CED
19	aX	101	LHG	O9-C7-O7-C5
19	bX	101	LHG	O9-C7-O7-C5
19	cX	101	LHG	O9-C7-O7-C5
15	aB	820	CLA	CBA-CGA-O2A-C1
15	aB	834	CLA	CBA-CGA-O2A-C1
15	a5	402	CLA	CBA-CGA-O2A-C1
15	bB	820	CLA	CBA-CGA-O2A-C1
15	bB	834	CLA	CBA-CGA-O2A-C1
15	cB	820	CLA	CBA-CGA-O2A-C1
15	cB	834	CLA	CBA-CGA-O2A-C1
15	aA	809	CLA	C2A-CAA-CBA-CGA
15	aA	814	CLA	C2A-CAA-CBA-CGA
15	aB	813	CLA	C2A-CAA-CBA-CGA
15	aB	831	CLA	C2A-CAA-CBA-CGA
15	aB	835	CLA	C2A-CAA-CBA-CGA
15	aL	203	CLA	C2A-CAA-CBA-CGA
15	bA	809	CLA	C2A-CAA-CBA-CGA
15	bA	814	CLA	C2A-CAA-CBA-CGA
15	bB	813	CLA	C2A-CAA-CBA-CGA
15	bB	831	CLA	C2A-CAA-CBA-CGA
15	bB	835	CLA	C2A-CAA-CBA-CGA
15	bL	204	CLA	C2A-CAA-CBA-CGA
15	cA	809	CLA	C2A-CAA-CBA-CGA
15	cA	814	CLA	C2A-CAA-CBA-CGA
15	cB	813	CLA	C2A-CAA-CBA-CGA
15	cB	831	CLA	C2A-CAA-CBA-CGA
15	cB	835	CLA	C2A-CAA-CBA-CGA
15	cL	204	CLA	C2A-CAA-CBA-CGA
15	cL	204	CLA	O1D-CGD-O2D-CED
15	aB	804	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	403	CLA	C13-C15-C16-C17
15	bB	804	CLA	C13-C15-C16-C17
15	b1	402	CLA	C13-C15-C16-C17
15	b3	403	CLA	C13-C15-C16-C17
15	b4	403	CLA	C13-C15-C16-C17
15	b5	403	CLA	C13-C15-C16-C17
15	cB	804	CLA	C13-C15-C16-C17
15	c5	402	CLA	O1A-CGA-O2A-C1
15	c5	409	CLA	O1D-CGD-O2D-CED
15	a3	403	CLA	C13-C15-C16-C17
15	c3	402	CLA	C13-C15-C16-C17
15	bB	825	CLA	C3-C5-C6-C7
15	b5	409	CLA	C3-C5-C6-C7
15	c6	411	CLA	C3-C5-C6-C7
18	aF	201	BCR	C22-C23-C24-C25
18	bB	849	BCR	C22-C23-C24-C25
18	cF	202	BCR	C22-C23-C24-C25
15	aA	822	CLA	C16-C17-C18-C19
15	bA	822	CLA	C16-C17-C18-C19
15	cA	822	CLA	C16-C17-C18-C19
15	c1	403	CLA	C13-C15-C16-C17
15	aB	807	CLA	O1D-CGD-O2D-CED
15	a5	409	CLA	O1D-CGD-O2D-CED
15	bB	807	CLA	O1D-CGD-O2D-CED
15	b2	411	CLA	O1D-CGD-O2D-CED
15	cB	807	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	C8-C7-O7-C5
19	bA	854	LHG	C8-C7-O7-C5
19	cA	852	LHG	C8-C7-O7-C5
18	aB	848	BCR	C10-C11-C12-C13
18	a5	418	BCR	C18-C19-C20-C21
18	bB	848	BCR	C10-C11-C12-C13
18	b2	401	BCR	C10-C11-C12-C13
18	b5	418	BCR	C18-C19-C20-C21
18	cB	848	BCR	C10-C11-C12-C13
18	cF	205	BCR	C18-C19-C20-C21
15	a6	403	CLA	C13-C15-C16-C17
15	b6	403	CLA	C13-C15-C16-C17
15	c1	402	CLA	C13-C15-C16-C17
15	c6	404	CLA	C13-C15-C16-C17
15	aB	811	CLA	CBD-CGD-O2D-CED
15	bB	811	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	833	CLA	CBD-CGD-O2D-CED
15	cB	811	CLA	CBD-CGD-O2D-CED
15	aB	825	CLA	C3-C5-C6-C7
15	cB	825	CLA	C3-C5-C6-C7
19	aA	853	LHG	O7-C5-C6-O8
19	bA	854	LHG	O7-C5-C6-O8
19	cA	852	LHG	O7-C5-C6-O8
15	bA	833	CLA	CBD-CGD-O2D-CED
15	b5	402	CLA	O1A-CGA-O2A-C1
15	a1	401	CLA	C13-C15-C16-C17
15	a1	402	CLA	C13-C15-C16-C17
15	b1	403	CLA	C13-C15-C16-C17
15	b2	402	CLA	C13-C15-C16-C17
15	aA	821	CLA	C2-C3-C5-C6
15	a2	418	CLA	C2-C3-C5-C6
15	a3	417	CLA	C2-C3-C5-C6
15	a6	418	CLA	C2-C3-C5-C6
15	bA	821	CLA	C2-C3-C5-C6
15	b2	418	CLA	C2-C3-C5-C6
15	b3	417	CLA	C2-C3-C5-C6
15	b6	418	CLA	C2-C3-C5-C6
15	cA	821	CLA	C2-C3-C5-C6
15	c2	418	CLA	C2-C3-C5-C6
15	c3	417	CLA	C2-C3-C5-C6
15	aA	802	CLA	C11-C10-C8-C9
15	aA	822	CLA	C11-C10-C8-C9
15	aA	831	CLA	C11-C10-C8-C9
15	aA	835	CLA	C14-C13-C15-C16
15	aB	828	CLA	C11-C12-C13-C14
15	aB	837	CLA	C6-C7-C8-C9
15	aB	840	CLA	C11-C12-C13-C14
15	aB	840	CLA	C14-C13-C15-C16
15	bA	802	CLA	C11-C10-C8-C9
15	bA	822	CLA	C11-C10-C8-C9
15	bA	831	CLA	C11-C10-C8-C9
15	bA	835	CLA	C14-C13-C15-C16
15	bB	828	CLA	C11-C12-C13-C14
15	bB	837	CLA	C6-C7-C8-C9
15	bB	840	CLA	C11-C12-C13-C14
15	bB	840	CLA	C14-C13-C15-C16
15	cA	802	CLA	C11-C10-C8-C9
15	cA	822	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	831	CLA	C11-C10-C8-C9
15	cA	835	CLA	C14-C13-C15-C16
15	cB	828	CLA	C11-C12-C13-C14
15	cB	837	CLA	C6-C7-C8-C9
15	cB	840	CLA	C11-C12-C13-C14
15	cB	840	CLA	C14-C13-C15-C16
16	aA	846	PQN	C19-C18-C20-C21
16	bA	846	PQN	C19-C18-C20-C21
16	cA	845	PQN	C19-C18-C20-C21
15	aA	824	CLA	CBD-CGD-O2D-CED
15	aA	833	CLA	CBD-CGD-O2D-CED
15	a2	410	CLA	C3-C5-C6-C7
15	a5	402	CLA	C3-C5-C6-C7
15	b5	402	CLA	C3-C5-C6-C7
15	c2	410	CLA	C3-C5-C6-C7
15	c5	402	CLA	C3-C5-C6-C7
15	cA	834	CLA	O1D-CGD-O2D-CED
15	aA	803	CLA	C2A-CAA-CBA-CGA
15	aA	819	CLA	C2A-CAA-CBA-CGA
15	aA	821	CLA	C2A-CAA-CBA-CGA
15	bA	803	CLA	C2A-CAA-CBA-CGA
15	bA	819	CLA	C2A-CAA-CBA-CGA
15	bA	821	CLA	C2A-CAA-CBA-CGA
15	cA	803	CLA	C2A-CAA-CBA-CGA
15	cA	819	CLA	C2A-CAA-CBA-CGA
15	cA	821	CLA	C2A-CAA-CBA-CGA
18	a1	421	BCR	C11-C12-C13-C35
18	a6	421	BCR	C11-C12-C13-C35
15	aA	834	CLA	O1D-CGD-O2D-CED
15	aB	826	CLA	O1D-CGD-O2D-CED
15	a2	411	CLA	O1D-CGD-O2D-CED
15	bA	834	CLA	O1D-CGD-O2D-CED
15	bB	826	CLA	O1D-CGD-O2D-CED
15	cB	826	CLA	O1D-CGD-O2D-CED
15	c2	402	CLA	C13-C15-C16-C17
15	cA	824	CLA	CBD-CGD-O2D-CED
19	cA	852	LHG	C27-C28-C29-C30
15	a5	402	CLA	O1A-CGA-O2A-C1
15	aA	805	CLA	C1A-C2A-CAA-CBA
15	aA	809	CLA	C1A-C2A-CAA-CBA
15	aA	810	CLA	C1A-C2A-CAA-CBA
15	aA	812	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	819	CLA	C1A-C2A-CAA-CBA
15	aA	822	CLA	C1A-C2A-CAA-CBA
15	aA	831	CLA	C1A-C2A-CAA-CBA
15	aA	833	CLA	C1A-C2A-CAA-CBA
15	aA	835	CLA	C1A-C2A-CAA-CBA
15	aA	836	CLA	C1A-C2A-CAA-CBA
15	aA	845	CLA	C1A-C2A-CAA-CBA
15	aB	815	CLA	C1A-C2A-CAA-CBA
15	aB	830	CLA	C1A-C2A-CAA-CBA
15	aB	833	CLA	C1A-C2A-CAA-CBA
15	aK	102	CLA	C1A-C2A-CAA-CBA
15	a1	401	CLA	C1A-C2A-CAA-CBA
15	a1	404	CLA	C1A-C2A-CAA-CBA
15	a1	411	CLA	C1A-C2A-CAA-CBA
15	a2	402	CLA	C1A-C2A-CAA-CBA
15	a2	413	CLA	C1A-C2A-CAA-CBA
15	a3	402	CLA	C1A-C2A-CAA-CBA
15	a3	405	CLA	C1A-C2A-CAA-CBA
15	a4	402	CLA	C1A-C2A-CAA-CBA
15	a4	408	CLA	C1A-C2A-CAA-CBA
15	a4	412	CLA	C1A-C2A-CAA-CBA
15	a5	402	CLA	C1A-C2A-CAA-CBA
15	a5	405	CLA	C1A-C2A-CAA-CBA
15	a5	412	CLA	C1A-C2A-CAA-CBA
15	a5	420	CLA	C1A-C2A-CAA-CBA
15	a6	403	CLA	C1A-C2A-CAA-CBA
15	a6	406	CLA	C1A-C2A-CAA-CBA
15	a6	409	CLA	C1A-C2A-CAA-CBA
15	a6	413	CLA	C1A-C2A-CAA-CBA
15	a6	422	CLA	C1A-C2A-CAA-CBA
15	bA	805	CLA	C1A-C2A-CAA-CBA
15	bA	809	CLA	C1A-C2A-CAA-CBA
15	bA	810	CLA	C1A-C2A-CAA-CBA
15	bA	812	CLA	C1A-C2A-CAA-CBA
15	bA	819	CLA	C1A-C2A-CAA-CBA
15	bA	822	CLA	C1A-C2A-CAA-CBA
15	bA	831	CLA	C1A-C2A-CAA-CBA
15	bA	833	CLA	C1A-C2A-CAA-CBA
15	bA	835	CLA	C1A-C2A-CAA-CBA
15	bA	836	CLA	C1A-C2A-CAA-CBA
15	bA	845	CLA	C1A-C2A-CAA-CBA
15	bB	815	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	830	CLA	C1A-C2A-CAA-CBA
15	bB	833	CLA	C1A-C2A-CAA-CBA
15	bK	101	CLA	C1A-C2A-CAA-CBA
15	b1	402	CLA	C1A-C2A-CAA-CBA
15	b1	405	CLA	C1A-C2A-CAA-CBA
15	b1	412	CLA	C1A-C2A-CAA-CBA
15	b2	402	CLA	C1A-C2A-CAA-CBA
15	b2	405	CLA	C1A-C2A-CAA-CBA
15	b2	413	CLA	C1A-C2A-CAA-CBA
15	b3	402	CLA	C1A-C2A-CAA-CBA
15	b3	405	CLA	C1A-C2A-CAA-CBA
15	b4	402	CLA	C1A-C2A-CAA-CBA
15	b4	408	CLA	C1A-C2A-CAA-CBA
15	b4	412	CLA	C1A-C2A-CAA-CBA
15	b5	402	CLA	C1A-C2A-CAA-CBA
15	b5	405	CLA	C1A-C2A-CAA-CBA
15	b5	412	CLA	C1A-C2A-CAA-CBA
15	b5	420	CLA	C1A-C2A-CAA-CBA
15	b6	403	CLA	C1A-C2A-CAA-CBA
15	b6	406	CLA	C1A-C2A-CAA-CBA
15	b6	413	CLA	C1A-C2A-CAA-CBA
15	cA	805	CLA	C1A-C2A-CAA-CBA
15	cA	809	CLA	C1A-C2A-CAA-CBA
15	cA	810	CLA	C1A-C2A-CAA-CBA
15	cA	812	CLA	C1A-C2A-CAA-CBA
15	cA	819	CLA	C1A-C2A-CAA-CBA
15	cA	822	CLA	C1A-C2A-CAA-CBA
15	cA	831	CLA	C1A-C2A-CAA-CBA
15	cA	833	CLA	C1A-C2A-CAA-CBA
15	cA	835	CLA	C1A-C2A-CAA-CBA
15	cA	836	CLA	C1A-C2A-CAA-CBA
15	cA	844	CLA	C1A-C2A-CAA-CBA
15	cB	815	CLA	C1A-C2A-CAA-CBA
15	cB	830	CLA	C1A-C2A-CAA-CBA
15	cB	833	CLA	C1A-C2A-CAA-CBA
15	cK	102	CLA	C1A-C2A-CAA-CBA
15	c1	402	CLA	C1A-C2A-CAA-CBA
15	c1	405	CLA	C1A-C2A-CAA-CBA
15	c1	412	CLA	C1A-C2A-CAA-CBA
15	c2	402	CLA	C1A-C2A-CAA-CBA
15	c2	405	CLA	C1A-C2A-CAA-CBA
15	c2	413	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	402	CLA	C1A-C2A-CAA-CBA
15	c3	405	CLA	C1A-C2A-CAA-CBA
15	c4	402	CLA	C1A-C2A-CAA-CBA
15	c4	405	CLA	C1A-C2A-CAA-CBA
15	c4	408	CLA	C1A-C2A-CAA-CBA
15	c4	412	CLA	C1A-C2A-CAA-CBA
15	c5	402	CLA	C1A-C2A-CAA-CBA
15	c5	405	CLA	C1A-C2A-CAA-CBA
15	c5	412	CLA	C1A-C2A-CAA-CBA
15	c5	420	CLA	C1A-C2A-CAA-CBA
15	c6	404	CLA	C1A-C2A-CAA-CBA
15	c6	407	CLA	C1A-C2A-CAA-CBA
15	c6	414	CLA	C1A-C2A-CAA-CBA
19	aA	853	LHG	C27-C28-C29-C30
19	bA	854	LHG	C27-C28-C29-C30
20	aB	850	LMG	C31-C32-C33-C34
20	bB	851	LMG	C31-C32-C33-C34
20	cB	850	LMG	C31-C32-C33-C34
15	a2	402	CLA	C13-C15-C16-C17
19	cA	853	LHG	C4-O6-P-O3
19	aA	853	LHG	C17-C18-C19-C20
15	bA	824	CLA	CBD-CGD-O2D-CED
15	aA	804	CLA	O1D-CGD-O2D-CED
15	b3	409	CLA	O1D-CGD-O2D-CED
19	bA	854	LHG	C17-C18-C19-C20
19	cA	852	LHG	C17-C18-C19-C20
15	aB	807	CLA	C15-C16-C17-C18
15	aB	840	CLA	C13-C15-C16-C17
15	bB	840	CLA	C13-C15-C16-C17
15	cB	807	CLA	C15-C16-C17-C18
15	cB	840	CLA	C13-C15-C16-C17
15	bA	804	CLA	O1D-CGD-O2D-CED
15	cA	804	CLA	O1D-CGD-O2D-CED
15	a3	409	CLA	O1D-CGD-O2D-CED
15	bB	807	CLA	C15-C16-C17-C18
15	aA	822	CLA	C16-C17-C18-C20
15	bA	822	CLA	C16-C17-C18-C20
15	cA	822	CLA	C16-C17-C18-C20
15	b2	410	CLA	C3-C5-C6-C7
15	aA	820	CLA	C8-C10-C11-C12
15	bA	820	CLA	C8-C10-C11-C12
15	cA	820	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b2	404	CLA	CBA-CGA-O2A-C1
15	bA	836	CLA	C5-C6-C7-C8
19	aA	854	LHG	C11-C10-C9-C8
19	bA	855	LHG	C11-C10-C9-C8
19	cA	853	LHG	C11-C10-C9-C8
15	aA	822	CLA	C5-C6-C7-C8
15	cA	822	CLA	C5-C6-C7-C8
15	aA	836	CLA	C5-C6-C7-C8
15	cA	836	CLA	C5-C6-C7-C8
15	aB	834	CLA	O1A-CGA-O2A-C1
15	a6	422	CLA	O1A-CGA-O2A-C1
15	bB	834	CLA	O1A-CGA-O2A-C1
15	cB	834	CLA	O1A-CGA-O2A-C1
15	aA	810	CLA	C15-C16-C17-C18
15	bA	810	CLA	C15-C16-C17-C18
15	aB	822	CLA	C2A-CAA-CBA-CGA
15	bB	822	CLA	C2A-CAA-CBA-CGA
15	cB	822	CLA	C2A-CAA-CBA-CGA
15	aA	803	CLA	C16-C17-C18-C20
15	bA	803	CLA	C16-C17-C18-C20
15	cA	803	CLA	C16-C17-C18-C20
15	aA	822	CLA	O1D-CGD-O2D-CED
15	bA	822	CLA	O1D-CGD-O2D-CED
15	bA	826	CLA	O1D-CGD-O2D-CED
15	cA	822	CLA	O1D-CGD-O2D-CED
15	a6	403	CLA	C3-C5-C6-C7
15	b6	403	CLA	C3-C5-C6-C7
15	c4	402	CLA	C3-C5-C6-C7
15	c6	404	CLA	C3-C5-C6-C7
15	cA	826	CLA	O1D-CGD-O2D-CED
15	bA	822	CLA	C5-C6-C7-C8
15	cA	810	CLA	C15-C16-C17-C18
20	aB	850	LMG	C35-C36-C37-C38
20	bB	851	LMG	C35-C36-C37-C38
15	aA	826	CLA	O1D-CGD-O2D-CED
15	c2	411	CLA	O1D-CGD-O2D-CED
20	cB	850	LMG	C35-C36-C37-C38
15	b6	412	CLA	CBD-CGD-O2D-CED
15	aA	831	CLA	C5-C6-C7-C8
15	bA	831	CLA	C5-C6-C7-C8
15	bL	202	CLA	C13-C15-C16-C17
15	cA	831	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cL	202	CLA	C13-C15-C16-C17
19	aA	854	LHG	C10-C11-C12-C13
19	bA	855	LHG	C10-C11-C12-C13
19	cA	853	LHG	C10-C11-C12-C13
15	c4	409	CLA	C3-C5-C6-C7
15	aL	201	CLA	C13-C15-C16-C17
15	a6	412	CLA	CBD-CGD-O2D-CED
15	aB	828	CLA	CAA-CBA-CGA-O2A
15	bB	828	CLA	CAA-CBA-CGA-O2A
15	cB	828	CLA	CAA-CBA-CGA-O2A
15	c3	410	CLA	O1D-CGD-O2D-CED
15	aA	829	CLA	C10-C11-C12-C13
15	bA	829	CLA	C10-C11-C12-C13
15	cA	829	CLA	C10-C11-C12-C13
18	aB	848	BCR	C20-C21-C22-C37
18	aB	849	BCR	C11-C10-C9-C34
18	aI	101	BCR	C20-C21-C22-C37
18	a2	401	BCR	C20-C21-C22-C37
18	a2	419	BCR	C16-C17-C18-C36
18	a3	418	BCR	C20-C21-C22-C37
18	a4	418	BCR	C20-C21-C22-C37
18	bB	848	BCR	C20-C21-C22-C37
18	bB	850	BCR	C11-C10-C9-C34
18	bI	101	BCR	C20-C21-C22-C37
18	b2	419	BCR	C16-C17-C18-C36
18	b4	418	BCR	C20-C21-C22-C37
18	cB	848	BCR	C20-C21-C22-C37
18	cB	849	BCR	C11-C10-C9-C34
18	cI	101	BCR	C20-C21-C22-C37
18	c2	401	BCR	C20-C21-C22-C37
18	c2	419	BCR	C16-C17-C18-C36
18	c2	419	BCR	C20-C21-C22-C37
18	c5	418	BCR	C20-C21-C22-C37
15	bB	826	CLA	O1A-CGA-O2A-C1
15	aB	828	CLA	C4-C3-C5-C6
15	bB	828	CLA	C4-C3-C5-C6
15	cB	828	CLA	C4-C3-C5-C6
20	bB	851	LMG	C39-C40-C41-C42
15	aA	812	CLA	CBA-CGA-O2A-C1
15	c2	404	CLA	CBA-CGA-O2A-C1
20	aB	850	LMG	C39-C40-C41-C42
15	a4	410	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bK	101	CLA	CBD-CGD-O2D-CED
15	b3	411	CLA	CBD-CGD-O2D-CED
15	cK	102	CLA	CBD-CGD-O2D-CED
15	c4	410	CLA	CBD-CGD-O2D-CED
15	aA	843	CLA	C15-C16-C17-C18
15	cA	842	CLA	C15-C16-C17-C18
20	cB	850	LMG	C39-C40-C41-C42
15	aB	826	CLA	O1A-CGA-O2A-C1
15	cB	826	CLA	O1A-CGA-O2A-C1
15	aB	821	CLA	C2A-CAA-CBA-CGA
15	bB	821	CLA	C2A-CAA-CBA-CGA
15	cB	821	CLA	C2A-CAA-CBA-CGA
15	bA	843	CLA	C15-C16-C17-C18
15	b5	403	CLA	C8-C10-C11-C12
15	a6	411	CLA	O1D-CGD-O2D-CED
15	b3	410	CLA	O1D-CGD-O2D-CED
15	c3	409	CLA	O1D-CGD-O2D-CED
15	aK	102	CLA	CBD-CGD-O2D-CED
15	a4	402	CLA	C3-C5-C6-C7
15	b4	402	CLA	C3-C5-C6-C7
15	b6	411	CLA	O1D-CGD-O2D-CED
15	c6	412	CLA	O1D-CGD-O2D-CED
15	aA	810	CLA	C8-C10-C11-C12
15	aB	828	CLA	C8-C10-C11-C12
15	bB	828	CLA	C8-C10-C11-C12
15	cB	828	CLA	C8-C10-C11-C12
16	aA	846	PQN	C20-C21-C22-C23
16	bA	846	PQN	C20-C21-C22-C23
16	cA	845	PQN	C20-C21-C22-C23
15	aB	828	CLA	CBA-CGA-O2A-C1
15	a2	404	CLA	CBA-CGA-O2A-C1
15	bA	812	CLA	CBA-CGA-O2A-C1
15	bB	828	CLA	CBA-CGA-O2A-C1
15	cA	812	CLA	CBA-CGA-O2A-C1
15	cB	828	CLA	CBA-CGA-O2A-C1
15	aB	820	CLA	O1A-CGA-O2A-C1
15	bB	820	CLA	O1A-CGA-O2A-C1
15	cB	820	CLA	O1A-CGA-O2A-C1
15	a3	410	CLA	O1D-CGD-O2D-CED
15	b4	410	CLA	CBD-CGD-O2D-CED
15	a5	403	CLA	C8-C10-C11-C12
15	bA	810	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	810	CLA	C8-C10-C11-C12
16	aB	843	PQN	C18-C20-C21-C22
16	bB	843	PQN	C18-C20-C21-C22
16	cB	843	PQN	C18-C20-C21-C22
20	aB	850	LMG	C15-C16-C17-C18
20	bB	851	LMG	C15-C16-C17-C18
20	cB	850	LMG	C15-C16-C17-C18
15	b2	404	CLA	O1A-CGA-O2A-C1
15	aA	818	CLA	C6-C7-C8-C9
15	a1	402	CLA	C8-C10-C11-C12
15	a3	403	CLA	C8-C10-C11-C12
15	b1	403	CLA	C8-C10-C11-C12
15	b3	403	CLA	C8-C10-C11-C12
15	c1	403	CLA	C8-C10-C11-C12
15	c5	403	CLA	C8-C10-C11-C12
18	aB	846	BCR	C12-C13-C14-C15
18	a2	421	BCR	C20-C21-C22-C23
18	a6	420	BCR	C20-C21-C22-C23
18	bB	846	BCR	C12-C13-C14-C15
18	b3	420	BCR	C20-C21-C22-C23
18	b4	420	BCR	C20-C21-C22-C23
18	cB	846	BCR	C12-C13-C14-C15
18	c4	420	BCR	C20-C21-C22-C23
18	c6	421	BCR	C20-C21-C22-C23
15	bA	818	CLA	C6-C7-C8-C9
15	cA	818	CLA	C6-C7-C8-C9
19	aX	101	LHG	O7-C5-C6-O8
19	bX	101	LHG	O7-C5-C6-O8
19	cX	101	LHG	O7-C5-C6-O8
15	aA	812	CLA	C5-C6-C7-C8
15	a6	404	CLA	C8-C10-C11-C12
15	cA	812	CLA	C5-C6-C7-C8
15	c2	404	CLA	O1A-CGA-O2A-C1
15	aA	806	CLA	C15-C16-C17-C18
15	bA	806	CLA	C15-C16-C17-C18
15	bA	812	CLA	C5-C6-C7-C8
15	cA	806	CLA	C15-C16-C17-C18
15	c3	403	CLA	C8-C10-C11-C12
15	aA	806	CLA	C11-C12-C13-C15
15	aA	810	CLA	C11-C12-C13-C15
15	aA	812	CLA	C12-C13-C15-C16
15	aA	821	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	821	CLA	C11-C12-C13-C15
15	aA	822	CLA	C11-C10-C8-C7
15	aA	826	CLA	C12-C13-C15-C16
15	aA	827	CLA	C12-C13-C15-C16
15	aA	829	CLA	C11-C12-C13-C15
15	aA	830	CLA	C12-C13-C15-C16
15	aA	834	CLA	C6-C7-C8-C10
15	aA	834	CLA	C12-C13-C15-C16
15	aA	835	CLA	C12-C13-C15-C16
15	aA	841	CLA	C6-C7-C8-C10
15	aB	804	CLA	C12-C13-C15-C16
15	aB	806	CLA	C11-C10-C8-C7
15	aB	814	CLA	C11-C10-C8-C7
15	aB	815	CLA	C11-C10-C8-C7
15	aB	827	CLA	C11-C12-C13-C15
15	aB	828	CLA	C2-C3-C5-C6
15	aB	833	CLA	C6-C7-C8-C10
15	aB	837	CLA	C6-C7-C8-C10
15	aL	202	CLA	C11-C12-C13-C15
15	a1	402	CLA	C11-C12-C13-C15
15	a2	403	CLA	C11-C12-C13-C15
15	a2	406	CLA	C11-C12-C13-C15
15	a2	422	CLA	C11-C12-C13-C15
15	a3	421	CLA	C11-C12-C13-C15
15	a4	403	CLA	C11-C10-C8-C7
15	a4	421	CLA	C11-C12-C13-C15
15	a5	403	CLA	C11-C10-C8-C7
15	a5	420	CLA	C11-C12-C13-C15
15	a6	404	CLA	C11-C12-C13-C15
15	a6	422	CLA	C11-C12-C13-C15
15	bA	806	CLA	C11-C12-C13-C15
15	bA	810	CLA	C11-C12-C13-C15
15	bA	812	CLA	C12-C13-C15-C16
15	bA	821	CLA	C6-C7-C8-C10
15	bA	821	CLA	C11-C12-C13-C15
15	bA	822	CLA	C11-C10-C8-C7
15	bA	826	CLA	C12-C13-C15-C16
15	bA	827	CLA	C12-C13-C15-C16
15	bA	829	CLA	C11-C12-C13-C15
15	bA	830	CLA	C12-C13-C15-C16
15	bA	834	CLA	C6-C7-C8-C10
15	bA	834	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	835	CLA	C12-C13-C15-C16
15	bA	841	CLA	C6-C7-C8-C10
15	bB	804	CLA	C12-C13-C15-C16
15	bB	806	CLA	C11-C10-C8-C7
15	bB	815	CLA	C11-C10-C8-C7
15	bB	827	CLA	C11-C12-C13-C15
15	bB	828	CLA	C2-C3-C5-C6
15	bB	833	CLA	C6-C7-C8-C10
15	bB	837	CLA	C6-C7-C8-C10
15	bL	203	CLA	C11-C12-C13-C15
15	b1	403	CLA	C11-C10-C8-C7
15	b1	403	CLA	C11-C12-C13-C15
15	b2	403	CLA	C11-C12-C13-C15
15	b2	406	CLA	C11-C12-C13-C15
15	b2	422	CLA	C11-C12-C13-C15
15	b3	421	CLA	C11-C12-C13-C15
15	b4	403	CLA	C11-C10-C8-C7
15	b4	403	CLA	C11-C12-C13-C15
15	b4	421	CLA	C11-C12-C13-C15
15	b5	403	CLA	C11-C10-C8-C7
15	b5	420	CLA	C11-C12-C13-C15
15	b6	404	CLA	C11-C12-C13-C15
15	b6	422	CLA	C11-C12-C13-C15
15	cA	806	CLA	C11-C12-C13-C15
15	cA	810	CLA	C11-C12-C13-C15
15	cA	812	CLA	C12-C13-C15-C16
15	cA	821	CLA	C6-C7-C8-C10
15	cA	821	CLA	C11-C12-C13-C15
15	cA	822	CLA	C11-C10-C8-C7
15	cA	826	CLA	C12-C13-C15-C16
15	cA	827	CLA	C12-C13-C15-C16
15	cA	829	CLA	C11-C12-C13-C15
15	cA	830	CLA	C12-C13-C15-C16
15	cA	834	CLA	C6-C7-C8-C10
15	cA	834	CLA	C12-C13-C15-C16
15	cA	835	CLA	C12-C13-C15-C16
15	cA	841	CLA	C6-C7-C8-C10
15	cB	804	CLA	C12-C13-C15-C16
15	cB	806	CLA	C11-C10-C8-C7
15	cB	815	CLA	C11-C10-C8-C7
15	cB	827	CLA	C11-C12-C13-C15
15	cB	828	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	833	CLA	C6-C7-C8-C10
15	cB	837	CLA	C6-C7-C8-C10
15	cL	203	CLA	C11-C12-C13-C15
15	c1	402	CLA	C12-C13-C15-C16
15	c1	403	CLA	C11-C12-C13-C15
15	c2	403	CLA	C11-C12-C13-C15
15	c2	406	CLA	C11-C12-C13-C15
15	c2	422	CLA	C11-C12-C13-C15
15	c3	421	CLA	C11-C12-C13-C15
15	c4	403	CLA	C11-C10-C8-C7
15	c4	421	CLA	C11-C12-C13-C15
15	c5	403	CLA	C11-C10-C8-C7
15	c5	420	CLA	C11-C12-C13-C15
15	c6	401	CLA	C11-C12-C13-C15
15	c6	405	CLA	C11-C12-C13-C15
16	aA	846	PQN	C17-C18-C20-C21
16	bA	846	PQN	C17-C18-C20-C21
16	cA	845	PQN	C17-C18-C20-C21
15	a2	404	CLA	O1A-CGA-O2A-C1
15	aA	806	CLA	C11-C12-C13-C14
15	aA	810	CLA	C11-C12-C13-C14
15	aA	834	CLA	C14-C13-C15-C16
15	aA	841	CLA	C6-C7-C8-C9
15	aB	803	CLA	C14-C13-C15-C16
15	aB	804	CLA	C14-C13-C15-C16
15	aB	806	CLA	C11-C10-C8-C9
15	aB	811	CLA	C6-C7-C8-C9
15	aB	814	CLA	C11-C10-C8-C9
15	aB	820	CLA	C11-C10-C8-C9
15	aB	827	CLA	C11-C12-C13-C14
15	aB	833	CLA	C6-C7-C8-C9
15	aB	833	CLA	C11-C10-C8-C9
15	aB	837	CLA	C11-C12-C13-C14
15	aL	202	CLA	C6-C7-C8-C9
15	aL	202	CLA	C11-C12-C13-C14
15	a1	401	CLA	C11-C10-C8-C9
15	a1	401	CLA	C14-C13-C15-C16
15	a1	402	CLA	C11-C12-C13-C14
15	a2	402	CLA	C11-C10-C8-C9
15	a2	403	CLA	C11-C12-C13-C14
15	a3	402	CLA	C11-C10-C8-C9
15	a4	402	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	402	CLA	C11-C10-C8-C9
15	a6	403	CLA	C11-C10-C8-C9
15	a6	404	CLA	C11-C12-C13-C14
15	bA	806	CLA	C11-C12-C13-C14
15	bA	810	CLA	C11-C12-C13-C14
15	bA	834	CLA	C14-C13-C15-C16
15	bA	841	CLA	C6-C7-C8-C9
15	bB	803	CLA	C14-C13-C15-C16
15	bB	804	CLA	C14-C13-C15-C16
15	bB	806	CLA	C11-C10-C8-C9
15	bB	811	CLA	C6-C7-C8-C9
15	bB	814	CLA	C11-C10-C8-C9
15	bB	820	CLA	C11-C10-C8-C9
15	bB	827	CLA	C11-C12-C13-C14
15	bB	833	CLA	C6-C7-C8-C9
15	bB	833	CLA	C11-C10-C8-C9
15	bB	837	CLA	C11-C12-C13-C14
15	bL	203	CLA	C6-C7-C8-C9
15	bL	203	CLA	C11-C12-C13-C14
15	b1	402	CLA	C11-C10-C8-C9
15	b1	402	CLA	C14-C13-C15-C16
15	b1	403	CLA	C11-C12-C13-C14
15	b2	402	CLA	C11-C10-C8-C9
15	b2	403	CLA	C11-C12-C13-C14
15	b3	402	CLA	C11-C10-C8-C9
15	b4	402	CLA	C11-C10-C8-C9
15	b5	402	CLA	C11-C10-C8-C9
15	b6	403	CLA	C11-C10-C8-C9
15	b6	404	CLA	C11-C12-C13-C14
15	cA	806	CLA	C11-C12-C13-C14
15	cA	810	CLA	C11-C12-C13-C14
15	cA	834	CLA	C14-C13-C15-C16
15	cA	841	CLA	C6-C7-C8-C9
15	cB	803	CLA	C14-C13-C15-C16
15	cB	804	CLA	C14-C13-C15-C16
15	cB	806	CLA	C11-C10-C8-C9
15	cB	811	CLA	C6-C7-C8-C9
15	cB	814	CLA	C11-C10-C8-C9
15	cB	820	CLA	C11-C10-C8-C9
15	cB	827	CLA	C11-C12-C13-C14
15	cB	833	CLA	C6-C7-C8-C9
15	cB	833	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	837	CLA	C11-C12-C13-C14
15	cL	203	CLA	C6-C7-C8-C9
15	cL	203	CLA	C11-C12-C13-C14
15	c1	402	CLA	C11-C10-C8-C9
15	c1	403	CLA	C11-C12-C13-C14
15	c2	402	CLA	C11-C10-C8-C9
15	c3	402	CLA	C11-C10-C8-C9
15	c4	402	CLA	C11-C10-C8-C9
15	c5	402	CLA	C11-C10-C8-C9
15	c5	403	CLA	C11-C12-C13-C14
15	c6	404	CLA	C11-C10-C8-C9
15	c6	405	CLA	C11-C12-C13-C14
15	a4	411	CLA	CBD-CGD-O2D-CED
15	c6	413	CLA	CBD-CGD-O2D-CED
15	a1	403	CLA	CBA-CGA-O2A-C1
15	a3	404	CLA	CBA-CGA-O2A-C1
15	a5	404	CLA	CBA-CGA-O2A-C1
15	a6	422	CLA	CBA-CGA-O2A-C1
15	b1	404	CLA	CBA-CGA-O2A-C1
15	b3	404	CLA	CBA-CGA-O2A-C1
15	b5	404	CLA	CBA-CGA-O2A-C1
15	c1	404	CLA	CBA-CGA-O2A-C1
15	c3	404	CLA	CBA-CGA-O2A-C1
15	c5	404	CLA	CBA-CGA-O2A-C1
15	b6	404	CLA	C8-C10-C11-C12
15	c6	405	CLA	C8-C10-C11-C12
18	aB	849	BCR	C11-C12-C13-C35
18	bB	850	BCR	C11-C12-C13-C35
18	b6	402	BCR	C11-C12-C13-C35
18	cB	849	BCR	C11-C12-C13-C35
15	aA	830	CLA	C15-C16-C17-C18
15	bA	830	CLA	C15-C16-C17-C18
15	aB	823	CLA	C6-C7-C8-C10
15	a2	422	CLA	C16-C17-C18-C19
15	bB	823	CLA	C6-C7-C8-C10
15	b2	422	CLA	C16-C17-C18-C19
15	cB	823	CLA	C6-C7-C8-C10
15	c2	422	CLA	C16-C17-C18-C19
15	aA	805	CLA	C11-C12-C13-C14
15	bA	805	CLA	C11-C12-C13-C14
15	bA	819	CLA	C2C-C3C-CAC-CBC
15	cA	805	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	819	CLA	C2C-C3C-CAC-CBC
15	a1	401	CLA	C3-C5-C6-C7
15	a2	402	CLA	C3-C5-C6-C7
15	a4	409	CLA	C3-C5-C6-C7
15	b1	402	CLA	C3-C5-C6-C7
15	b2	402	CLA	C3-C5-C6-C7
15	b4	409	CLA	C3-C5-C6-C7
15	c2	402	CLA	C3-C5-C6-C7
15	aB	801	CLA	O1D-CGD-O2D-CED
15	cB	801	CLA	O1D-CGD-O2D-CED
15	aB	819	CLA	C10-C11-C12-C13
15	aB	829	CLA	C10-C11-C12-C13
15	a4	403	CLA	C8-C10-C11-C12
15	bB	819	CLA	C10-C11-C12-C13
15	bB	829	CLA	C10-C11-C12-C13
15	cB	819	CLA	C10-C11-C12-C13
15	cB	829	CLA	C10-C11-C12-C13
15	aA	841	CLA	CBA-CGA-O2A-C1
15	aB	830	CLA	CBA-CGA-O2A-C1
15	a4	404	CLA	CBA-CGA-O2A-C1
15	a6	405	CLA	CBA-CGA-O2A-C1
15	bA	841	CLA	CBA-CGA-O2A-C1
15	bB	830	CLA	CBA-CGA-O2A-C1
15	b4	404	CLA	CBA-CGA-O2A-C1
15	b6	405	CLA	CBA-CGA-O2A-C1
15	cA	841	CLA	CBA-CGA-O2A-C1
15	cB	830	CLA	CBA-CGA-O2A-C1
15	c4	404	CLA	CBA-CGA-O2A-C1
15	c6	406	CLA	CBA-CGA-O2A-C1
15	bB	801	CLA	O1D-CGD-O2D-CED
15	aA	819	CLA	C2C-C3C-CAC-CBC
15	cA	830	CLA	C15-C16-C17-C18
18	aA	849	BCR	C22-C23-C24-C25
18	bA	850	BCR	C22-C23-C24-C25
18	cA	848	BCR	C22-C23-C24-C25
15	bB	805	CLA	CBD-CGD-O2D-CED
15	b4	411	CLA	CBD-CGD-O2D-CED
15	cB	805	CLA	CBD-CGD-O2D-CED
15	aA	809	CLA	C4B-C3B-CAB-CBB
15	aA	825	CLA	C4B-C3B-CAB-CBB
15	aA	832	CLA	C4B-C3B-CAB-CBB
15	aB	802	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	808	CLA	C4B-C3B-CAB-CBB
15	aB	820	CLA	C4B-C3B-CAB-CBB
15	aB	834	CLA	C4B-C3B-CAB-CBB
15	aB	842	CLA	C4B-C3B-CAB-CBB
15	aJ	202	CLA	C4B-C3B-CAB-CBB
15	aX	102	CLA	C4B-C3B-CAB-CBB
15	a1	415	CLA	C4B-C3B-CAB-CBB
15	a2	414	CLA	C4B-C3B-CAB-CBB
15	a3	413	CLA	C4B-C3B-CAB-CBB
15	a3	416	CLA	C4B-C3B-CAB-CBB
15	a4	413	CLA	C4B-C3B-CAB-CBB
15	a5	420	CLA	C4B-C3B-CAB-CBB
15	a6	414	CLA	C4B-C3B-CAB-CBB
15	bA	809	CLA	C4B-C3B-CAB-CBB
15	bA	825	CLA	C4B-C3B-CAB-CBB
15	bA	832	CLA	C4B-C3B-CAB-CBB
15	bB	802	CLA	C4B-C3B-CAB-CBB
15	bB	808	CLA	C4B-C3B-CAB-CBB
15	bB	820	CLA	C4B-C3B-CAB-CBB
15	bB	834	CLA	C4B-C3B-CAB-CBB
15	bB	842	CLA	C4B-C3B-CAB-CBB
15	bJ	101	CLA	C4B-C3B-CAB-CBB
15	bX	102	CLA	C4B-C3B-CAB-CBB
15	b3	413	CLA	C4B-C3B-CAB-CBB
15	b3	416	CLA	C4B-C3B-CAB-CBB
15	b4	413	CLA	C4B-C3B-CAB-CBB
15	b5	420	CLA	C4B-C3B-CAB-CBB
15	b6	414	CLA	C4B-C3B-CAB-CBB
15	cA	809	CLA	C4B-C3B-CAB-CBB
15	cA	825	CLA	C4B-C3B-CAB-CBB
15	cA	832	CLA	C4B-C3B-CAB-CBB
15	cB	802	CLA	C4B-C3B-CAB-CBB
15	cB	808	CLA	C4B-C3B-CAB-CBB
15	cB	820	CLA	C4B-C3B-CAB-CBB
15	cB	834	CLA	C4B-C3B-CAB-CBB
15	cB	842	CLA	C4B-C3B-CAB-CBB
15	cJ	101	CLA	C4B-C3B-CAB-CBB
15	cX	102	CLA	C4B-C3B-CAB-CBB
15	c2	414	CLA	C4B-C3B-CAB-CBB
15	c3	413	CLA	C4B-C3B-CAB-CBB
15	c3	416	CLA	C4B-C3B-CAB-CBB
15	c4	413	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c5	413	CLA	C4B-C3B-CAB-CBB
15	c6	415	CLA	C4B-C3B-CAB-CBB
15	aA	826	CLA	C8-C10-C11-C12
15	aB	833	CLA	C13-C15-C16-C17
15	bA	826	CLA	C8-C10-C11-C12
15	bB	833	CLA	C13-C15-C16-C17
15	cA	826	CLA	C8-C10-C11-C12
15	cB	833	CLA	C13-C15-C16-C17
15	c1	402	CLA	C3-C5-C6-C7
19	aA	853	LHG	C34-C35-C36-C37
19	bA	854	LHG	C34-C35-C36-C37
19	cA	852	LHG	C34-C35-C36-C37
15	aA	814	CLA	CBA-CGA-O2A-C1
15	bA	814	CLA	CBA-CGA-O2A-C1
18	aI	102	BCR	C18-C19-C20-C21
18	cI	102	BCR	C18-C19-C20-C21
15	aA	820	CLA	C13-C15-C16-C17
15	aB	801	CLA	C8-C10-C11-C12
15	bA	820	CLA	C13-C15-C16-C17
15	bB	801	CLA	C8-C10-C11-C12
15	cA	820	CLA	C13-C15-C16-C17
15	cB	801	CLA	C8-C10-C11-C12
15	aA	820	CLA	C4-C3-C5-C6
15	aA	828	CLA	C4-C3-C5-C6
15	bA	820	CLA	C4-C3-C5-C6
15	bA	828	CLA	C4-C3-C5-C6
15	cA	820	CLA	C4-C3-C5-C6
15	cA	828	CLA	C4-C3-C5-C6
15	a5	410	CLA	O1D-CGD-O2D-CED
15	c3	402	CLA	C3-C5-C6-C7
15	c5	410	CLA	O1D-CGD-O2D-CED
15	aA	831	CLA	CBA-CGA-O2A-C1
15	aA	845	CLA	CBA-CGA-O2A-C1
15	bA	831	CLA	CBA-CGA-O2A-C1
15	bA	845	CLA	CBA-CGA-O2A-C1
15	cA	814	CLA	CBA-CGA-O2A-C1
15	cA	831	CLA	CBA-CGA-O2A-C1
15	cA	844	CLA	CBA-CGA-O2A-C1
15	aA	802	CLA	C3A-C2A-CAA-CBA
15	aA	807	CLA	C3A-C2A-CAA-CBA
15	aA	837	CLA	C3A-C2A-CAA-CBA
15	aA	843	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	817	CLA	C3A-C2A-CAA-CBA
15	aB	818	CLA	C3A-C2A-CAA-CBA
15	aB	826	CLA	C3A-C2A-CAA-CBA
15	a2	406	CLA	C3A-C2A-CAA-CBA
15	a2	413	CLA	C3A-C2A-CAA-CBA
15	a3	412	CLA	C3A-C2A-CAA-CBA
15	a3	421	CLA	C3A-C2A-CAA-CBA
15	a4	412	CLA	C3A-C2A-CAA-CBA
15	a5	412	CLA	C3A-C2A-CAA-CBA
15	bA	802	CLA	C3A-C2A-CAA-CBA
15	bA	807	CLA	C3A-C2A-CAA-CBA
15	bA	837	CLA	C3A-C2A-CAA-CBA
15	bA	843	CLA	C3A-C2A-CAA-CBA
15	bB	817	CLA	C3A-C2A-CAA-CBA
15	bB	818	CLA	C3A-C2A-CAA-CBA
15	bB	826	CLA	C3A-C2A-CAA-CBA
15	b1	412	CLA	C3A-C2A-CAA-CBA
15	b2	406	CLA	C3A-C2A-CAA-CBA
15	b2	413	CLA	C3A-C2A-CAA-CBA
15	b3	412	CLA	C3A-C2A-CAA-CBA
15	b3	421	CLA	C3A-C2A-CAA-CBA
15	b4	412	CLA	C3A-C2A-CAA-CBA
15	b5	412	CLA	C3A-C2A-CAA-CBA
15	cA	802	CLA	C3A-C2A-CAA-CBA
15	cA	807	CLA	C3A-C2A-CAA-CBA
15	cA	837	CLA	C3A-C2A-CAA-CBA
15	cA	842	CLA	C3A-C2A-CAA-CBA
15	cA	843	CLA	C3A-C2A-CAA-CBA
15	cB	817	CLA	C3A-C2A-CAA-CBA
15	cB	818	CLA	C3A-C2A-CAA-CBA
15	cB	826	CLA	C3A-C2A-CAA-CBA
15	c1	412	CLA	C3A-C2A-CAA-CBA
15	c2	406	CLA	C3A-C2A-CAA-CBA
15	c2	413	CLA	C3A-C2A-CAA-CBA
15	c3	412	CLA	C3A-C2A-CAA-CBA
15	c3	421	CLA	C3A-C2A-CAA-CBA
15	c4	412	CLA	C3A-C2A-CAA-CBA
15	c5	412	CLA	C3A-C2A-CAA-CBA
15	c6	414	CLA	C3A-C2A-CAA-CBA
15	b5	410	CLA	O1D-CGD-O2D-CED
18	aL	205	BCR	C15-C16-C17-C18
18	bL	201	BCR	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bL	206	BCR	C15-C16-C17-C18
15	aB	805	CLA	CBD-CGD-O2D-CED
15	aB	827	CLA	C8-C10-C11-C12
15	cB	827	CLA	C8-C10-C11-C12
15	aB	829	CLA	CBA-CGA-O2A-C1
15	bB	829	CLA	CBA-CGA-O2A-C1
15	cB	829	CLA	CBA-CGA-O2A-C1
19	bA	854	LHG	C24-C25-C26-C27
15	a6	404	CLA	C13-C15-C16-C17
15	bB	827	CLA	C8-C10-C11-C12
15	b4	403	CLA	C8-C10-C11-C12
15	c4	403	CLA	C8-C10-C11-C12
15	c6	405	CLA	C13-C15-C16-C17
19	aX	101	LHG	C4-C5-C6-O8
19	bX	101	LHG	C4-C5-C6-O8
19	cX	101	LHG	C4-C5-C6-O8
15	c1	411	CLA	CBD-CGD-O2D-CED
15	aA	836	CLA	C6-C7-C8-C9
15	bA	836	CLA	C6-C7-C8-C9
15	cA	836	CLA	C6-C7-C8-C9
19	aA	853	LHG	C24-C25-C26-C27
19	aA	853	LHG	C30-C31-C32-C33
19	cA	852	LHG	C24-C25-C26-C27
19	cA	852	LHG	C30-C31-C32-C33
19	bA	854	LHG	C30-C31-C32-C33
15	b6	404	CLA	C13-C15-C16-C17
18	bB	848	BCR	C14-C15-C16-C17
18	cB	848	BCR	C14-C15-C16-C17
15	a3	402	CLA	C3-C5-C6-C7
15	b3	402	CLA	C3-C5-C6-C7
16	aB	843	PQN	C13-C15-C16-C17
16	bB	843	PQN	C13-C15-C16-C17
16	cB	843	PQN	C13-C15-C16-C17
15	bA	805	CLA	C8-C10-C11-C12
15	cA	805	CLA	C8-C10-C11-C12
15	aA	841	CLA	C4-C3-C5-C6
15	bA	841	CLA	C4-C3-C5-C6
15	cA	841	CLA	C4-C3-C5-C6
15	aB	807	CLA	C16-C17-C18-C19
15	bB	807	CLA	C16-C17-C18-C19
15	cB	807	CLA	C16-C17-C18-C19
15	aA	828	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	828	CLA	C2-C3-C5-C6
15	cA	828	CLA	C2-C3-C5-C6
15	c4	411	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	C8-C10-C11-C12
15	aA	812	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	O10-C23-O8-C6
19	bA	854	LHG	O10-C23-O8-C6
15	aB	810	CLA	C2A-CAA-CBA-CGA
15	bB	810	CLA	C2A-CAA-CBA-CGA
15	cB	810	CLA	C2A-CAA-CBA-CGA
15	bB	808	CLA	C8-C10-C11-C12
15	cB	808	CLA	C8-C10-C11-C12
20	aB	850	LMG	C30-C31-C32-C33
20	bB	851	LMG	C30-C31-C32-C33
15	aA	829	CLA	CBA-CGA-O2A-C1
15	bA	829	CLA	CBA-CGA-O2A-C1
15	cA	829	CLA	CBA-CGA-O2A-C1
20	cB	850	LMG	C30-C31-C32-C33
15	a1	409	CLA	O1D-CGD-O2D-CED
15	b1	410	CLA	O1D-CGD-O2D-CED
15	c1	410	CLA	O1D-CGD-O2D-CED
15	a1	403	CLA	O1A-CGA-O2A-C1
15	a3	404	CLA	O1A-CGA-O2A-C1
15	a5	404	CLA	O1A-CGA-O2A-C1
15	bA	812	CLA	O1A-CGA-O2A-C1
15	b3	404	CLA	O1A-CGA-O2A-C1
15	b5	404	CLA	O1A-CGA-O2A-C1
15	cA	812	CLA	O1A-CGA-O2A-C1
15	c3	404	CLA	O1A-CGA-O2A-C1
19	cA	852	LHG	O10-C23-O8-C6
20	aB	850	LMG	C28-C29-C30-C31
20	cB	850	LMG	C28-C29-C30-C31
15	aA	803	CLA	C16-C17-C18-C19
15	bA	803	CLA	C16-C17-C18-C19
15	cA	803	CLA	C16-C17-C18-C19
15	cB	823	CLA	C6-C7-C8-C9
15	aB	808	CLA	C8-C10-C11-C12
15	bB	806	CLA	CAA-CBA-CGA-O2A
15	c3	411	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	C2B-C3B-CAB-CBB
15	aA	832	CLA	C2B-C3B-CAB-CBB
15	aB	802	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	820	CLA	C2B-C3B-CAB-CBB
15	aB	821	CLA	C2B-C3B-CAB-CBB
15	aB	834	CLA	C2B-C3B-CAB-CBB
15	a2	414	CLA	C2B-C3B-CAB-CBB
15	a4	413	CLA	C2B-C3B-CAB-CBB
15	a5	413	CLA	C2B-C3B-CAB-CBB
15	a6	414	CLA	C2B-C3B-CAB-CBB
15	a6	417	CLA	C2B-C3B-CAB-CBB
15	bA	825	CLA	C2B-C3B-CAB-CBB
15	bA	832	CLA	C2B-C3B-CAB-CBB
15	bB	802	CLA	C2B-C3B-CAB-CBB
15	bB	820	CLA	C2B-C3B-CAB-CBB
15	bB	821	CLA	C2B-C3B-CAB-CBB
15	bB	834	CLA	C2B-C3B-CAB-CBB
15	b2	414	CLA	C2B-C3B-CAB-CBB
15	b4	413	CLA	C2B-C3B-CAB-CBB
15	b5	413	CLA	C2B-C3B-CAB-CBB
15	b6	414	CLA	C2B-C3B-CAB-CBB
15	b6	417	CLA	C2B-C3B-CAB-CBB
15	cA	825	CLA	C2B-C3B-CAB-CBB
15	cA	832	CLA	C2B-C3B-CAB-CBB
15	cB	802	CLA	C2B-C3B-CAB-CBB
15	cB	820	CLA	C2B-C3B-CAB-CBB
15	cB	821	CLA	C2B-C3B-CAB-CBB
15	cB	834	CLA	C2B-C3B-CAB-CBB
15	c2	414	CLA	C2B-C3B-CAB-CBB
15	c4	413	CLA	C2B-C3B-CAB-CBB
15	c5	413	CLA	C2B-C3B-CAB-CBB
15	c6	415	CLA	C2B-C3B-CAB-CBB
15	c6	418	CLA	C2B-C3B-CAB-CBB
15	aB	828	CLA	O1A-CGA-O2A-C1
15	a6	405	CLA	O1A-CGA-O2A-C1
15	bB	828	CLA	O1A-CGA-O2A-C1
15	b1	404	CLA	O1A-CGA-O2A-C1
15	cB	828	CLA	O1A-CGA-O2A-C1
15	c1	404	CLA	O1A-CGA-O2A-C1
15	c5	404	CLA	O1A-CGA-O2A-C1
15	c6	406	CLA	O1A-CGA-O2A-C1
20	bB	851	LMG	C28-C29-C30-C31
15	a1	410	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	CAA-CBA-CGA-O2A
15	cB	806	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	823	CLA	C6-C7-C8-C9
15	bB	823	CLA	C6-C7-C8-C9
15	c5	420	CLA	C16-C17-C18-C19
15	aA	825	CLA	C2-C1-O2A-CGA
15	aA	827	CLA	C2-C1-O2A-CGA
15	aB	803	CLA	C2-C1-O2A-CGA
15	bA	825	CLA	C2-C1-O2A-CGA
15	bA	827	CLA	C2-C1-O2A-CGA
15	bB	803	CLA	C2-C1-O2A-CGA
15	cA	825	CLA	C2-C1-O2A-CGA
15	cA	827	CLA	C2-C1-O2A-CGA
15	cB	803	CLA	C2-C1-O2A-CGA
15	aA	820	CLA	C2-C3-C5-C6
15	bA	820	CLA	C2-C3-C5-C6
15	cA	820	CLA	C2-C3-C5-C6
20	aB	850	LMG	C16-C17-C18-C19
20	bB	851	LMG	C41-C42-C43-C44
20	cB	850	LMG	C16-C17-C18-C19
15	b4	404	CLA	O1A-CGA-O2A-C1
15	b6	405	CLA	O1A-CGA-O2A-C1
15	aA	803	CLA	C10-C11-C12-C13
15	bA	803	CLA	C10-C11-C12-C13
15	cA	803	CLA	C10-C11-C12-C13
15	aA	805	CLA	C11-C10-C8-C9
15	aA	820	CLA	C11-C12-C13-C14
15	aA	826	CLA	C14-C13-C15-C16
15	aA	827	CLA	C14-C13-C15-C16
15	aA	830	CLA	C14-C13-C15-C16
15	aA	839	CLA	C6-C7-C8-C9
15	aA	843	CLA	C11-C12-C13-C14
15	aB	808	CLA	C11-C10-C8-C9
15	aB	814	CLA	C6-C7-C8-C9
15	aB	828	CLA	C14-C13-C15-C16
15	aB	829	CLA	C14-C13-C15-C16
15	aB	833	CLA	C11-C12-C13-C14
15	a3	403	CLA	C11-C12-C13-C14
15	a4	403	CLA	C11-C12-C13-C14
15	a5	403	CLA	C11-C12-C13-C14
15	a6	403	CLA	C14-C13-C15-C16
15	bA	805	CLA	C11-C10-C8-C9
15	bA	820	CLA	C11-C12-C13-C14
15	bA	826	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	827	CLA	C14-C13-C15-C16
15	bA	830	CLA	C14-C13-C15-C16
15	bA	839	CLA	C6-C7-C8-C9
15	bA	843	CLA	C11-C12-C13-C14
15	bB	808	CLA	C11-C10-C8-C9
15	bB	814	CLA	C6-C7-C8-C9
15	bB	828	CLA	C14-C13-C15-C16
15	bB	829	CLA	C14-C13-C15-C16
15	bB	833	CLA	C11-C12-C13-C14
15	b3	403	CLA	C11-C12-C13-C14
15	b4	403	CLA	C11-C12-C13-C14
15	b5	403	CLA	C11-C12-C13-C14
15	b6	403	CLA	C14-C13-C15-C16
15	cA	805	CLA	C11-C10-C8-C9
15	cA	820	CLA	C11-C12-C13-C14
15	cA	826	CLA	C14-C13-C15-C16
15	cA	827	CLA	C14-C13-C15-C16
15	cA	830	CLA	C14-C13-C15-C16
15	cA	839	CLA	C6-C7-C8-C9
15	cA	842	CLA	C11-C12-C13-C14
15	cB	808	CLA	C11-C10-C8-C9
15	cB	814	CLA	C6-C7-C8-C9
15	cB	828	CLA	C14-C13-C15-C16
15	cB	829	CLA	C14-C13-C15-C16
15	cB	833	CLA	C11-C12-C13-C14
15	c2	403	CLA	C11-C12-C13-C14
15	c3	403	CLA	C11-C12-C13-C14
15	c4	403	CLA	C11-C12-C13-C14
15	c6	404	CLA	C14-C13-C15-C16
20	aB	850	LMG	C41-C42-C43-C44
20	bB	851	LMG	C16-C17-C18-C19
20	cB	850	LMG	C41-C42-C43-C44
15	aA	806	CLA	C10-C11-C12-C13
19	aX	101	LHG	C2-C3-O3-P
19	bX	101	LHG	C2-C3-O3-P
19	cX	101	LHG	C2-C3-O3-P
15	c4	404	CLA	O1A-CGA-O2A-C1
15	aA	820	CLA	C16-C17-C18-C20
15	aB	817	CLA	C6-C7-C8-C10
15	a5	420	CLA	C16-C17-C18-C19
15	bA	820	CLA	C16-C17-C18-C20
15	bB	817	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b5	420	CLA	C16-C17-C18-C19
15	cA	820	CLA	C16-C17-C18-C20
15	cB	817	CLA	C6-C7-C8-C10
15	aA	820	CLA	C3-C5-C6-C7
15	bA	820	CLA	C3-C5-C6-C7
15	b2	403	CLA	C3-C5-C6-C7
15	cA	820	CLA	C3-C5-C6-C7
18	aA	852	BCR	C5-C6-C7-C8
18	aA	852	BCR	C23-C24-C25-C26
18	aA	852	BCR	C23-C24-C25-C30
18	aB	845	BCR	C1-C6-C7-C8
18	aB	846	BCR	C23-C24-C25-C26
18	aB	847	BCR	C23-C24-C25-C30
18	aB	849	BCR	C23-C24-C25-C26
18	aB	849	BCR	C23-C24-C25-C30
18	aF	201	BCR	C23-C24-C25-C26
18	aF	203	BCR	C5-C6-C7-C8
18	aI	102	BCR	C23-C24-C25-C30
18	aM	101	BCR	C23-C24-C25-C26
18	aM	101	BCR	C23-C24-C25-C30
18	a1	418	BCR	C23-C24-C25-C26
18	a1	420	BCR	C23-C24-C25-C26
18	a1	421	BCR	C23-C24-C25-C26
18	a1	421	BCR	C23-C24-C25-C30
18	a2	401	BCR	C23-C24-C25-C26
18	a2	401	BCR	C23-C24-C25-C30
18	a2	420	BCR	C23-C24-C25-C30
18	a3	401	BCR	C23-C24-C25-C26
18	a3	401	BCR	C23-C24-C25-C30
18	a3	419	BCR	C23-C24-C25-C26
18	a4	401	BCR	C1-C6-C7-C8
18	a4	401	BCR	C5-C6-C7-C8
18	a4	401	BCR	C23-C24-C25-C26
18	a4	401	BCR	C23-C24-C25-C30
18	a4	419	BCR	C23-C24-C25-C26
18	a5	401	BCR	C1-C6-C7-C8
18	a5	401	BCR	C5-C6-C7-C8
18	a5	401	BCR	C23-C24-C25-C26
18	a6	401	BCR	C23-C24-C25-C26
18	a6	402	BCR	C23-C24-C25-C26
18	a6	402	BCR	C23-C24-C25-C30
18	a6	421	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a6	421	BCR	C23-C24-C25-C30
18	bA	853	BCR	C5-C6-C7-C8
18	bA	853	BCR	C23-C24-C25-C26
18	bA	853	BCR	C23-C24-C25-C30
18	bB	845	BCR	C1-C6-C7-C8
18	bB	846	BCR	C23-C24-C25-C26
18	bB	847	BCR	C23-C24-C25-C30
18	bB	849	BCR	C23-C24-C25-C26
18	bB	850	BCR	C23-C24-C25-C26
18	bB	850	BCR	C23-C24-C25-C30
18	bI	102	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C5-C6-C7-C8
18	bM	101	BCR	C23-C24-C25-C26
18	bM	101	BCR	C23-C24-C25-C30
18	b1	401	BCR	C23-C24-C25-C26
18	b1	419	BCR	C23-C24-C25-C26
18	b1	420	BCR	C5-C6-C7-C8
18	b2	401	BCR	C23-C24-C25-C26
18	b2	401	BCR	C23-C24-C25-C30
18	b2	420	BCR	C23-C24-C25-C30
18	b3	401	BCR	C23-C24-C25-C30
18	b3	419	BCR	C23-C24-C25-C26
18	b4	401	BCR	C1-C6-C7-C8
18	b4	401	BCR	C5-C6-C7-C8
18	b4	401	BCR	C23-C24-C25-C26
18	b4	401	BCR	C23-C24-C25-C30
18	b4	419	BCR	C23-C24-C25-C26
18	b5	401	BCR	C1-C6-C7-C8
18	b5	401	BCR	C5-C6-C7-C8
18	b5	401	BCR	C23-C24-C25-C26
18	b6	401	BCR	C23-C24-C25-C26
18	b6	402	BCR	C23-C24-C25-C26
18	b6	402	BCR	C23-C24-C25-C30
18	b6	421	BCR	C23-C24-C25-C26
18	b6	421	BCR	C23-C24-C25-C30
18	cA	851	BCR	C5-C6-C7-C8
18	cA	851	BCR	C23-C24-C25-C26
18	cA	851	BCR	C23-C24-C25-C30
18	cB	845	BCR	C1-C6-C7-C8
18	cB	846	BCR	C23-C24-C25-C26
18	cB	847	BCR	C23-C24-C25-C30
18	cB	849	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cB	849	BCR	C23-C24-C25-C30
18	cF	202	BCR	C23-C24-C25-C26
18	cF	205	BCR	C5-C6-C7-C8
18	cI	102	BCR	C23-C24-C25-C30
18	cM	101	BCR	C23-C24-C25-C26
18	cM	101	BCR	C23-C24-C25-C30
18	c1	401	BCR	C5-C6-C7-C8
18	c1	401	BCR	C23-C24-C25-C26
18	c1	419	BCR	C23-C24-C25-C26
18	c2	401	BCR	C23-C24-C25-C26
18	c2	401	BCR	C23-C24-C25-C30
18	c2	420	BCR	C23-C24-C25-C26
18	c2	420	BCR	C23-C24-C25-C30
18	c3	401	BCR	C23-C24-C25-C26
18	c3	401	BCR	C23-C24-C25-C30
18	c3	419	BCR	C23-C24-C25-C26
18	c4	401	BCR	C1-C6-C7-C8
18	c4	401	BCR	C5-C6-C7-C8
18	c4	401	BCR	C23-C24-C25-C26
18	c4	401	BCR	C23-C24-C25-C30
18	c4	419	BCR	C23-C24-C25-C26
18	c5	401	BCR	C1-C6-C7-C8
18	c5	401	BCR	C5-C6-C7-C8
18	c5	401	BCR	C23-C24-C25-C26
18	c6	402	BCR	C23-C24-C25-C26
18	c6	403	BCR	C23-C24-C25-C30
15	bA	806	CLA	C10-C11-C12-C13
15	b2	403	CLA	C8-C10-C11-C12
15	aA	829	CLA	CAA-CBA-CGA-O2A
15	bA	829	CLA	CAA-CBA-CGA-O2A
15	cA	829	CLA	CAA-CBA-CGA-O2A
18	b1	401	BCR	C7-C8-C9-C34
18	b6	421	BCR	C11-C12-C13-C35
15	a4	404	CLA	O1A-CGA-O2A-C1
18	aB	847	BCR	C35-C13-C14-C15
18	aB	849	BCR	C21-C22-C23-C24
18	a4	401	BCR	C11-C12-C13-C14
18	bB	847	BCR	C35-C13-C14-C15
18	bB	850	BCR	C21-C22-C23-C24
18	b4	401	BCR	C11-C12-C13-C14
18	cB	847	BCR	C35-C13-C14-C15
18	cB	849	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	827	CLA	C5-C6-C7-C8
15	aB	807	CLA	C5-C6-C7-C8
15	aB	815	CLA	C10-C11-C12-C13
15	aB	828	CLA	C5-C6-C7-C8
15	a2	403	CLA	C8-C10-C11-C12
15	bA	827	CLA	C5-C6-C7-C8
15	bB	807	CLA	C5-C6-C7-C8
15	bB	815	CLA	C10-C11-C12-C13
15	bB	828	CLA	C5-C6-C7-C8
15	cA	827	CLA	C5-C6-C7-C8
15	cB	807	CLA	C5-C6-C7-C8
15	cB	815	CLA	C10-C11-C12-C13
15	cB	828	CLA	C5-C6-C7-C8
18	aB	848	BCR	C14-C15-C16-C17
18	aF	203	BCR	C14-C15-C16-C17
18	bJ	105	BCR	C14-C15-C16-C17
18	cF	205	BCR	C14-C15-C16-C17
15	cA	806	CLA	C10-C11-C12-C13
15	aB	828	CLA	C16-C17-C18-C20
15	bB	828	CLA	C16-C17-C18-C20
15	cB	828	CLA	C16-C17-C18-C20
15	cB	833	CLA	O1D-CGD-O2D-CED
15	aB	833	CLA	O1D-CGD-O2D-CED
15	a3	411	CLA	O1D-CGD-O2D-CED
15	bB	833	CLA	O1D-CGD-O2D-CED
15	c2	403	CLA	C8-C10-C11-C12
15	aB	829	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	C11-C10-C8-C7
15	aA	807	CLA	C6-C7-C8-C10
15	aA	807	CLA	C12-C13-C15-C16
15	aA	828	CLA	C11-C10-C8-C7
15	aA	829	CLA	C11-C10-C8-C7
15	aA	839	CLA	C6-C7-C8-C10
15	aA	839	CLA	C12-C13-C15-C16
15	aB	803	CLA	C12-C13-C15-C16
15	aB	809	CLA	C11-C10-C8-C7
15	aB	820	CLA	C11-C10-C8-C7
15	aB	829	CLA	C12-C13-C15-C16
15	aB	833	CLA	C11-C10-C8-C7
15	aB	833	CLA	C12-C13-C15-C16
15	aB	837	CLA	C11-C12-C13-C15
15	aB	840	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	401	CLA	C11-C10-C8-C7
15	a1	401	CLA	C12-C13-C15-C16
15	a1	402	CLA	C11-C10-C8-C7
15	a2	402	CLA	C11-C10-C8-C7
15	a2	403	CLA	C11-C10-C8-C7
15	a3	402	CLA	C11-C10-C8-C7
15	a3	403	CLA	C11-C10-C8-C7
15	a4	402	CLA	C11-C10-C8-C7
15	a4	403	CLA	C11-C12-C13-C15
15	a5	402	CLA	C11-C10-C8-C7
15	a5	403	CLA	C11-C12-C13-C15
15	a6	403	CLA	C11-C10-C8-C7
15	a6	404	CLA	C11-C10-C8-C7
15	bA	805	CLA	C11-C10-C8-C7
15	bA	807	CLA	C6-C7-C8-C10
15	bA	807	CLA	C12-C13-C15-C16
15	bA	828	CLA	C11-C10-C8-C7
15	bA	829	CLA	C11-C10-C8-C7
15	bA	839	CLA	C6-C7-C8-C10
15	bA	839	CLA	C12-C13-C15-C16
15	bB	803	CLA	C12-C13-C15-C16
15	bB	809	CLA	C11-C10-C8-C7
15	bB	820	CLA	C11-C10-C8-C7
15	bB	829	CLA	C12-C13-C15-C16
15	bB	833	CLA	C11-C10-C8-C7
15	bB	833	CLA	C12-C13-C15-C16
15	bB	837	CLA	C11-C12-C13-C15
15	bB	840	CLA	C11-C10-C8-C7
15	b1	402	CLA	C11-C10-C8-C7
15	b2	402	CLA	C11-C10-C8-C7
15	b2	403	CLA	C11-C10-C8-C7
15	b3	402	CLA	C11-C10-C8-C7
15	b3	403	CLA	C11-C10-C8-C7
15	b4	402	CLA	C11-C10-C8-C7
15	b5	402	CLA	C11-C10-C8-C7
15	b5	403	CLA	C11-C12-C13-C15
15	b6	403	CLA	C11-C10-C8-C7
15	b6	404	CLA	C11-C10-C8-C7
15	cA	805	CLA	C11-C10-C8-C7
15	cA	807	CLA	C6-C7-C8-C10
15	cA	807	CLA	C12-C13-C15-C16
15	cA	828	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	829	CLA	C11-C10-C8-C7
15	cA	839	CLA	C6-C7-C8-C10
15	cA	839	CLA	C12-C13-C15-C16
15	cB	803	CLA	C12-C13-C15-C16
15	cB	809	CLA	C11-C10-C8-C7
15	cB	820	CLA	C11-C10-C8-C7
15	cB	829	CLA	C12-C13-C15-C16
15	cB	833	CLA	C11-C10-C8-C7
15	cB	833	CLA	C12-C13-C15-C16
15	cB	837	CLA	C11-C12-C13-C15
15	cB	840	CLA	C11-C10-C8-C7
15	c1	402	CLA	C11-C10-C8-C7
15	c1	403	CLA	C11-C10-C8-C7
15	c2	402	CLA	C11-C10-C8-C7
15	c2	403	CLA	C11-C10-C8-C7
15	c3	402	CLA	C11-C10-C8-C7
15	c3	403	CLA	C11-C10-C8-C7
15	c4	402	CLA	C11-C10-C8-C7
15	c4	403	CLA	C11-C12-C13-C15
15	c5	402	CLA	C11-C10-C8-C7
15	c5	403	CLA	C11-C12-C13-C15
15	c6	404	CLA	C11-C10-C8-C7
15	c6	405	CLA	C11-C10-C8-C7
15	b6	412	CLA	O1D-CGD-O2D-CED
15	cB	829	CLA	O1D-CGD-O2D-CED
15	bA	821	CLA	C10-C11-C12-C13
15	cA	821	CLA	C10-C11-C12-C13
18	aB	845	BCR	C19-C20-C21-C22
18	bB	845	BCR	C19-C20-C21-C22
18	cB	845	BCR	C19-C20-C21-C22
15	a6	422	CLA	C16-C17-C18-C20
15	aA	809	CLA	C13-C15-C16-C17
15	aA	821	CLA	C10-C11-C12-C13
15	aA	839	CLA	C10-C11-C12-C13
15	aB	837	CLA	C5-C6-C7-C8
15	bA	839	CLA	C10-C11-C12-C13
15	bB	837	CLA	C5-C6-C7-C8
15	cA	809	CLA	C13-C15-C16-C17
15	cA	839	CLA	C10-C11-C12-C13
15	cB	837	CLA	C5-C6-C7-C8
15	aA	841	CLA	C2A-CAA-CBA-CGA
15	bA	841	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	841	CLA	C2A-CAA-CBA-CGA
15	bA	809	CLA	C13-C15-C16-C17
18	aF	202	BCR	C20-C21-C22-C37
18	aI	101	BCR	C11-C10-C9-C34
18	aL	205	BCR	C16-C17-C18-C36
18	a1	421	BCR	C11-C10-C9-C34
18	a1	421	BCR	C20-C21-C22-C37
18	a3	418	BCR	C16-C17-C18-C36
18	a4	418	BCR	C16-C17-C18-C36
18	a5	401	BCR	C35-C13-C14-C15
18	a5	418	BCR	C16-C17-C18-C36
18	a5	418	BCR	C20-C21-C22-C37
18	a6	402	BCR	C20-C21-C22-C37
18	a6	419	BCR	C20-C21-C22-C37
18	bF	202	BCR	C20-C21-C22-C37
18	bI	101	BCR	C11-C10-C9-C34
18	bL	201	BCR	C16-C17-C18-C36
18	bL	206	BCR	C16-C17-C18-C36
18	b1	418	BCR	C20-C21-C22-C37
18	b2	401	BCR	C20-C21-C22-C37
18	b3	401	BCR	C35-C13-C14-C15
18	b3	418	BCR	C16-C17-C18-C36
18	b3	418	BCR	C20-C21-C22-C37
18	b5	401	BCR	C35-C13-C14-C15
18	b5	418	BCR	C16-C17-C18-C36
18	b5	418	BCR	C20-C21-C22-C37
18	b6	402	BCR	C20-C21-C22-C37
18	b6	419	BCR	C20-C21-C22-C37
18	cF	204	BCR	C20-C21-C22-C37
18	cI	101	BCR	C11-C10-C9-C34
18	c3	418	BCR	C16-C17-C18-C36
18	c3	418	BCR	C20-C21-C22-C37
18	c5	401	BCR	C35-C13-C14-C15
18	c6	403	BCR	C20-C21-C22-C37
18	c6	420	BCR	C20-C21-C22-C37
15	a2	403	CLA	C3-C5-C6-C7
15	c2	403	CLA	C3-C5-C6-C7
15	cB	807	CLA	C16-C17-C18-C20
15	aA	806	CLA	C13-C15-C16-C17
15	bA	806	CLA	C13-C15-C16-C17
15	aA	817	CLA	CBA-CGA-O2A-C1
15	bA	817	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	817	CLA	CBA-CGA-O2A-C1
15	bB	829	CLA	O1D-CGD-O2D-CED
15	aB	825	CLA	C5-C6-C7-C8
15	bB	825	CLA	C5-C6-C7-C8
15	cB	825	CLA	C5-C6-C7-C8
15	cB	810	CLA	O1D-CGD-O2D-CED
15	aB	806	CLA	C13-C15-C16-C17
15	bB	806	CLA	C13-C15-C16-C17
15	cA	806	CLA	C13-C15-C16-C17
15	cB	806	CLA	C13-C15-C16-C17
15	aA	802	CLA	CAD-CBD-CGD-O2D
15	aA	806	CLA	CAD-CBD-CGD-O2D
15	aA	813	CLA	CAD-CBD-CGD-O2D
15	aA	818	CLA	CAD-CBD-CGD-O2D
15	aA	827	CLA	CAD-CBD-CGD-O2D
15	aB	811	CLA	CAD-CBD-CGD-O2D
15	aB	830	CLA	CAD-CBD-CGD-O2D
15	aB	838	CLA	CAD-CBD-CGD-O2D
15	aB	840	CLA	CAD-CBD-CGD-O2D
15	a1	409	CLA	CAD-CBD-CGD-O2D
15	a2	411	CLA	CAD-CBD-CGD-O2D
15	a2	412	CLA	CAD-CBD-CGD-O2D
15	a3	410	CLA	CAD-CBD-CGD-O2D
15	a4	405	CLA	CAD-CBD-CGD-O2D
15	a4	410	CLA	CAD-CBD-CGD-O2D
15	a5	410	CLA	CAD-CBD-CGD-O2D
15	a5	411	CLA	CAD-CBD-CGD-O2D
15	bA	802	CLA	CAD-CBD-CGD-O2D
15	bA	806	CLA	CAD-CBD-CGD-O2D
15	bA	813	CLA	CAD-CBD-CGD-O2D
15	bA	818	CLA	CAD-CBD-CGD-O2D
15	bA	827	CLA	CAD-CBD-CGD-O2D
15	bB	811	CLA	CAD-CBD-CGD-O2D
15	bB	830	CLA	CAD-CBD-CGD-O2D
15	bB	838	CLA	CAD-CBD-CGD-O2D
15	bB	840	CLA	CAD-CBD-CGD-O2D
15	b1	410	CLA	CAD-CBD-CGD-O2D
15	b2	411	CLA	CAD-CBD-CGD-O2D
15	b2	412	CLA	CAD-CBD-CGD-O2D
15	b3	410	CLA	CAD-CBD-CGD-O2D
15	b3	411	CLA	CAD-CBD-CGD-O2D
15	b4	405	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b4	410	CLA	CAD-CBD-CGD-O2D
15	b5	410	CLA	CAD-CBD-CGD-O2D
15	b5	411	CLA	CAD-CBD-CGD-O2D
15	b6	411	CLA	CAD-CBD-CGD-O2D
15	cA	802	CLA	CAD-CBD-CGD-O2D
15	cA	806	CLA	CAD-CBD-CGD-O2D
15	cA	813	CLA	CAD-CBD-CGD-O2D
15	cA	818	CLA	CAD-CBD-CGD-O2D
15	cA	827	CLA	CAD-CBD-CGD-O2D
15	cB	811	CLA	CAD-CBD-CGD-O2D
15	cB	830	CLA	CAD-CBD-CGD-O2D
15	cB	838	CLA	CAD-CBD-CGD-O2D
15	cB	840	CLA	CAD-CBD-CGD-O2D
15	c1	410	CLA	CAD-CBD-CGD-O2D
15	c2	411	CLA	CAD-CBD-CGD-O2D
15	c2	412	CLA	CAD-CBD-CGD-O2D
15	c3	410	CLA	CAD-CBD-CGD-O2D
15	c4	405	CLA	CAD-CBD-CGD-O2D
15	c4	410	CLA	CAD-CBD-CGD-O2D
15	c5	410	CLA	CAD-CBD-CGD-O2D
15	c5	411	CLA	CAD-CBD-CGD-O2D
15	a6	412	CLA	O1D-CGD-O2D-CED
15	bB	810	CLA	O1D-CGD-O2D-CED
15	aA	825	CLA	C5-C6-C7-C8
15	aA	830	CLA	C10-C11-C12-C13
15	bA	825	CLA	C5-C6-C7-C8
15	bA	830	CLA	C10-C11-C12-C13
15	cA	825	CLA	C5-C6-C7-C8
15	cA	830	CLA	C10-C11-C12-C13
15	aB	810	CLA	O1D-CGD-O2D-CED
15	bA	833	CLA	O1D-CGD-O2D-CED
18	aI	102	BCR	C22-C23-C24-C25
18	bI	102	BCR	C22-C23-C24-C25
18	b3	418	BCR	C22-C23-C24-C25
18	cI	102	BCR	C22-C23-C24-C25
15	aB	830	CLA	O1A-CGA-O2A-C1
15	aB	808	CLA	CBA-CGA-O2A-C1
15	bB	808	CLA	CBA-CGA-O2A-C1
15	cB	808	CLA	CBA-CGA-O2A-C1
15	cA	833	CLA	O1D-CGD-O2D-CED
15	aB	807	CLA	C16-C17-C18-C20
15	bB	807	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	aB	850	LMG	O1-C7-C8-C9
20	bB	851	LMG	O1-C7-C8-C9
20	cB	850	LMG	O1-C7-C8-C9
15	bB	817	CLA	CBD-CGD-O2D-CED
15	cB	817	CLA	CBD-CGD-O2D-CED
15	bB	830	CLA	O1A-CGA-O2A-C1
15	cB	830	CLA	O1A-CGA-O2A-C1
15	c6	401	CLA	O1A-CGA-O2A-C1
15	aA	802	CLA	C13-C15-C16-C17
15	aA	807	CLA	C10-C11-C12-C13
15	bA	802	CLA	C13-C15-C16-C17
15	bA	807	CLA	C10-C11-C12-C13
15	cA	802	CLA	C13-C15-C16-C17
15	cA	807	CLA	C10-C11-C12-C13
15	aL	203	CLA	CAA-CBA-CGA-O2A
15	bL	204	CLA	CAA-CBA-CGA-O2A
15	cL	204	CLA	CAA-CBA-CGA-O2A
18	bI	102	BCR	C18-C19-C20-C21
15	aB	817	CLA	CBD-CGD-O2D-CED
15	cB	829	CLA	O1A-CGA-O2A-C1
15	aB	817	CLA	C6-C7-C8-C9
15	a5	420	CLA	C16-C17-C18-C20
15	bB	817	CLA	C6-C7-C8-C9
15	b5	409	CLA	C16-C17-C18-C19
15	b5	420	CLA	C16-C17-C18-C20
15	cB	817	CLA	C6-C7-C8-C9
15	c5	409	CLA	C16-C17-C18-C19
15	c5	420	CLA	C16-C17-C18-C20
15	c6	411	CLA	C16-C17-C18-C19
15	aA	833	CLA	O1D-CGD-O2D-CED
15	aA	805	CLA	CHA-CBD-CGD-O1D
15	aA	805	CLA	CHA-CBD-CGD-O2D
15	aA	814	CLA	CHA-CBD-CGD-O1D
15	aA	814	CLA	CHA-CBD-CGD-O2D
15	aA	828	CLA	CHA-CBD-CGD-O1D
15	aA	835	CLA	CHA-CBD-CGD-O1D
15	aA	835	CLA	CHA-CBD-CGD-O2D
15	aA	837	CLA	CHA-CBD-CGD-O1D
15	aA	837	CLA	CHA-CBD-CGD-O2D
15	aA	838	CLA	CHA-CBD-CGD-O1D
15	aA	842	CLA	CHA-CBD-CGD-O1D
15	aB	808	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	815	CLA	CHA-CBD-CGD-O1D
15	aB	815	CLA	CHA-CBD-CGD-O2D
15	aB	825	CLA	CHA-CBD-CGD-O1D
15	aB	825	CLA	CHA-CBD-CGD-O2D
15	aB	826	CLA	CHA-CBD-CGD-O1D
15	aB	827	CLA	CHA-CBD-CGD-O1D
15	aB	836	CLA	CHA-CBD-CGD-O1D
15	aB	836	CLA	CHA-CBD-CGD-O2D
15	aJ	202	CLA	CHA-CBD-CGD-O2D
15	aK	102	CLA	CHA-CBD-CGD-O1D
15	aL	201	CLA	CHA-CBD-CGD-O1D
15	aL	201	CLA	CHA-CBD-CGD-O2D
15	aX	102	CLA	CHA-CBD-CGD-O1D
15	aX	102	CLA	CHA-CBD-CGD-O2D
15	a1	406	CLA	CHA-CBD-CGD-O1D
15	a1	406	CLA	CHA-CBD-CGD-O2D
15	a1	411	CLA	CHA-CBD-CGD-O1D
15	a1	415	CLA	CHA-CBD-CGD-O1D
15	a1	415	CLA	CHA-CBD-CGD-O2D
15	a2	408	CLA	CHA-CBD-CGD-O1D
15	a2	408	CLA	CHA-CBD-CGD-O2D
15	a2	413	CLA	CHA-CBD-CGD-O1D
15	a2	417	CLA	CHA-CBD-CGD-O1D
15	a2	417	CLA	CHA-CBD-CGD-O2D
15	a2	422	CLA	CHA-CBD-CGD-O1D
15	a3	407	CLA	CHA-CBD-CGD-O1D
15	a3	407	CLA	CHA-CBD-CGD-O2D
15	a3	412	CLA	CHA-CBD-CGD-O1D
15	a3	416	CLA	CHA-CBD-CGD-O1D
15	a3	416	CLA	CHA-CBD-CGD-O2D
15	a4	407	CLA	CHA-CBD-CGD-O1D
15	a4	407	CLA	CHA-CBD-CGD-O2D
15	a4	412	CLA	CHA-CBD-CGD-O1D
15	a4	416	CLA	CHA-CBD-CGD-O1D
15	a4	416	CLA	CHA-CBD-CGD-O2D
15	a5	407	CLA	CHA-CBD-CGD-O1D
15	a5	407	CLA	CHA-CBD-CGD-O2D
15	a5	412	CLA	CHA-CBD-CGD-O1D
15	a5	416	CLA	CHA-CBD-CGD-O1D
15	a5	416	CLA	CHA-CBD-CGD-O2D
15	a6	408	CLA	CHA-CBD-CGD-O1D
15	a6	408	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	413	CLA	CHA-CBD-CGD-O1D
15	a6	413	CLA	CHA-CBD-CGD-O2D
15	a6	417	CLA	CHA-CBD-CGD-O1D
15	a6	417	CLA	CHA-CBD-CGD-O2D
15	bA	803	CLA	CHA-CBD-CGD-O2D
15	bA	805	CLA	CHA-CBD-CGD-O1D
15	bA	805	CLA	CHA-CBD-CGD-O2D
15	bA	814	CLA	CHA-CBD-CGD-O1D
15	bA	814	CLA	CHA-CBD-CGD-O2D
15	bA	828	CLA	CHA-CBD-CGD-O1D
15	bA	835	CLA	CHA-CBD-CGD-O1D
15	bA	835	CLA	CHA-CBD-CGD-O2D
15	bA	837	CLA	CHA-CBD-CGD-O1D
15	bA	837	CLA	CHA-CBD-CGD-O2D
15	bA	838	CLA	CHA-CBD-CGD-O1D
15	bA	842	CLA	CHA-CBD-CGD-O1D
15	bB	808	CLA	CHA-CBD-CGD-O1D
15	bB	815	CLA	CHA-CBD-CGD-O1D
15	bB	815	CLA	CHA-CBD-CGD-O2D
15	bB	825	CLA	CHA-CBD-CGD-O1D
15	bB	825	CLA	CHA-CBD-CGD-O2D
15	bB	826	CLA	CHA-CBD-CGD-O1D
15	bB	827	CLA	CHA-CBD-CGD-O1D
15	bB	836	CLA	CHA-CBD-CGD-O1D
15	bB	836	CLA	CHA-CBD-CGD-O2D
15	bJ	101	CLA	CHA-CBD-CGD-O2D
15	bK	101	CLA	CHA-CBD-CGD-O1D
15	bL	202	CLA	CHA-CBD-CGD-O1D
15	bL	202	CLA	CHA-CBD-CGD-O2D
15	bX	102	CLA	CHA-CBD-CGD-O1D
15	bX	102	CLA	CHA-CBD-CGD-O2D
15	b1	407	CLA	CHA-CBD-CGD-O1D
15	b1	407	CLA	CHA-CBD-CGD-O2D
15	b1	412	CLA	CHA-CBD-CGD-O1D
15	b1	416	CLA	CHA-CBD-CGD-O1D
15	b1	416	CLA	CHA-CBD-CGD-O2D
15	b2	408	CLA	CHA-CBD-CGD-O1D
15	b2	408	CLA	CHA-CBD-CGD-O2D
15	b2	413	CLA	CHA-CBD-CGD-O1D
15	b2	417	CLA	CHA-CBD-CGD-O1D
15	b2	417	CLA	CHA-CBD-CGD-O2D
15	b3	407	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b3	407	CLA	CHA-CBD-CGD-O2D
15	b3	412	CLA	CHA-CBD-CGD-O1D
15	b3	416	CLA	CHA-CBD-CGD-O1D
15	b3	416	CLA	CHA-CBD-CGD-O2D
15	b4	407	CLA	CHA-CBD-CGD-O1D
15	b4	407	CLA	CHA-CBD-CGD-O2D
15	b4	412	CLA	CHA-CBD-CGD-O1D
15	b4	416	CLA	CHA-CBD-CGD-O1D
15	b4	416	CLA	CHA-CBD-CGD-O2D
15	b5	407	CLA	CHA-CBD-CGD-O1D
15	b5	407	CLA	CHA-CBD-CGD-O2D
15	b5	412	CLA	CHA-CBD-CGD-O1D
15	b5	416	CLA	CHA-CBD-CGD-O1D
15	b5	416	CLA	CHA-CBD-CGD-O2D
15	b6	408	CLA	CHA-CBD-CGD-O1D
15	b6	408	CLA	CHA-CBD-CGD-O2D
15	b6	413	CLA	CHA-CBD-CGD-O1D
15	b6	413	CLA	CHA-CBD-CGD-O2D
15	b6	417	CLA	CHA-CBD-CGD-O1D
15	b6	417	CLA	CHA-CBD-CGD-O2D
15	cA	803	CLA	CHA-CBD-CGD-O2D
15	cA	805	CLA	CHA-CBD-CGD-O1D
15	cA	805	CLA	CHA-CBD-CGD-O2D
15	cA	814	CLA	CHA-CBD-CGD-O1D
15	cA	814	CLA	CHA-CBD-CGD-O2D
15	cA	828	CLA	CHA-CBD-CGD-O1D
15	cA	835	CLA	CHA-CBD-CGD-O1D
15	cA	835	CLA	CHA-CBD-CGD-O2D
15	cA	837	CLA	CHA-CBD-CGD-O1D
15	cA	837	CLA	CHA-CBD-CGD-O2D
15	cA	838	CLA	CHA-CBD-CGD-O1D
15	cB	808	CLA	CHA-CBD-CGD-O1D
15	cB	815	CLA	CHA-CBD-CGD-O1D
15	cB	815	CLA	CHA-CBD-CGD-O2D
15	cB	825	CLA	CHA-CBD-CGD-O1D
15	cB	826	CLA	CHA-CBD-CGD-O1D
15	cB	827	CLA	CHA-CBD-CGD-O1D
15	cB	836	CLA	CHA-CBD-CGD-O1D
15	cB	836	CLA	CHA-CBD-CGD-O2D
15	cF	201	CLA	CHA-CBD-CGD-O1D
15	cJ	101	CLA	CHA-CBD-CGD-O2D
15	cK	102	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cL	202	CLA	CHA-CBD-CGD-O1D
15	cL	202	CLA	CHA-CBD-CGD-O2D
15	cX	102	CLA	CHA-CBD-CGD-O1D
15	cX	102	CLA	CHA-CBD-CGD-O2D
15	c1	407	CLA	CHA-CBD-CGD-O1D
15	c1	407	CLA	CHA-CBD-CGD-O2D
15	c1	412	CLA	CHA-CBD-CGD-O1D
15	c1	416	CLA	CHA-CBD-CGD-O1D
15	c1	416	CLA	CHA-CBD-CGD-O2D
15	c2	408	CLA	CHA-CBD-CGD-O1D
15	c2	408	CLA	CHA-CBD-CGD-O2D
15	c2	413	CLA	CHA-CBD-CGD-O1D
15	c2	417	CLA	CHA-CBD-CGD-O1D
15	c2	417	CLA	CHA-CBD-CGD-O2D
15	c2	422	CLA	CHA-CBD-CGD-O1D
15	c3	407	CLA	CHA-CBD-CGD-O1D
15	c3	407	CLA	CHA-CBD-CGD-O2D
15	c3	412	CLA	CHA-CBD-CGD-O1D
15	c3	416	CLA	CHA-CBD-CGD-O1D
15	c3	416	CLA	CHA-CBD-CGD-O2D
15	c4	407	CLA	CHA-CBD-CGD-O1D
15	c4	407	CLA	CHA-CBD-CGD-O2D
15	c4	412	CLA	CHA-CBD-CGD-O1D
15	c4	416	CLA	CHA-CBD-CGD-O1D
15	c4	416	CLA	CHA-CBD-CGD-O2D
15	c5	407	CLA	CHA-CBD-CGD-O1D
15	c5	407	CLA	CHA-CBD-CGD-O2D
15	c5	412	CLA	CHA-CBD-CGD-O1D
15	c5	416	CLA	CHA-CBD-CGD-O1D
15	c5	416	CLA	CHA-CBD-CGD-O2D
15	c6	401	CLA	CHA-CBD-CGD-O1D
15	c6	409	CLA	CHA-CBD-CGD-O1D
15	c6	409	CLA	CHA-CBD-CGD-O2D
15	c6	414	CLA	CHA-CBD-CGD-O1D
15	c6	414	CLA	CHA-CBD-CGD-O2D
15	c6	418	CLA	CHA-CBD-CGD-O1D
15	c6	418	CLA	CHA-CBD-CGD-O2D
15	a4	410	CLA	O1D-CGD-O2D-CED
15	a4	403	CLA	C3-C5-C6-C7
15	b4	403	CLA	C3-C5-C6-C7
15	aA	814	CLA	O1A-CGA-O2A-C1
15	aA	829	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	831	CLA	O1A-CGA-O2A-C1
15	aB	829	CLA	O1A-CGA-O2A-C1
15	bA	814	CLA	O1A-CGA-O2A-C1
15	bA	829	CLA	O1A-CGA-O2A-C1
15	bA	831	CLA	O1A-CGA-O2A-C1
15	bB	829	CLA	O1A-CGA-O2A-C1
15	cA	829	CLA	O1A-CGA-O2A-C1
15	cA	831	CLA	O1A-CGA-O2A-C1
18	aB	845	BCR	C11-C10-C9-C8
18	aF	202	BCR	C11-C10-C9-C8
18	bB	845	BCR	C11-C10-C9-C8
18	bF	202	BCR	C11-C10-C9-C8
18	cB	845	BCR	C11-C10-C9-C8
18	cF	204	BCR	C11-C10-C9-C8
15	bA	832	CLA	O1D-CGD-O2D-CED
15	cA	832	CLA	O1D-CGD-O2D-CED
15	cA	814	CLA	O1A-CGA-O2A-C1
15	aA	833	CLA	C16-C17-C18-C19
15	a5	409	CLA	C16-C17-C18-C19
15	bA	833	CLA	C16-C17-C18-C19
15	cA	833	CLA	C16-C17-C18-C19
15	c4	409	CLA	C16-C17-C18-C19
15	aA	832	CLA	O1D-CGD-O2D-CED
15	b4	410	CLA	O1D-CGD-O2D-CED
15	c4	410	CLA	O1D-CGD-O2D-CED
15	c6	413	CLA	O1D-CGD-O2D-CED
15	b1	411	CLA	CBD-CGD-O2D-CED
15	aA	807	CLA	C14-C13-C15-C16
15	aA	828	CLA	C11-C10-C8-C9
15	aA	839	CLA	C14-C13-C15-C16
15	aA	841	CLA	C11-C10-C8-C9
15	aB	802	CLA	C11-C12-C13-C14
15	aB	827	CLA	C11-C10-C8-C9
15	aB	840	CLA	C11-C10-C8-C9
15	a2	402	CLA	C14-C13-C15-C16
15	bA	807	CLA	C14-C13-C15-C16
15	bA	839	CLA	C14-C13-C15-C16
15	bA	841	CLA	C11-C10-C8-C9
15	bB	802	CLA	C11-C12-C13-C14
15	bB	827	CLA	C11-C10-C8-C9
15	bB	840	CLA	C11-C10-C8-C9
15	b2	402	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	807	CLA	C14-C13-C15-C16
15	cA	828	CLA	C11-C10-C8-C9
15	cA	839	CLA	C14-C13-C15-C16
15	cA	841	CLA	C11-C10-C8-C9
15	cB	802	CLA	C11-C12-C13-C14
15	cB	827	CLA	C11-C10-C8-C9
15	cB	840	CLA	C11-C10-C8-C9
15	c2	402	CLA	C14-C13-C15-C16
15	bA	824	CLA	O1D-CGD-O2D-CED
15	cA	844	CLA	O1A-CGA-O2A-C1
15	aA	824	CLA	O1D-CGD-O2D-CED
15	cA	824	CLA	O1D-CGD-O2D-CED
15	aB	814	CLA	C2A-CAA-CBA-CGA
15	bB	814	CLA	C2A-CAA-CBA-CGA
15	cB	814	CLA	C2A-CAA-CBA-CGA
15	aB	811	CLA	O1D-CGD-O2D-CED
15	c1	411	CLA	O1D-CGD-O2D-CED
15	aA	845	CLA	O1A-CGA-O2A-C1
15	bA	845	CLA	O1A-CGA-O2A-C1
15	b6	422	CLA	O1A-CGA-O2A-C1
18	c1	401	BCR	C7-C8-C9-C34
15	a1	410	CLA	O1D-CGD-O2D-CED
15	aA	841	CLA	C10-C11-C12-C13
15	bA	841	CLA	C10-C11-C12-C13
15	cA	802	CLA	C15-C16-C17-C18
18	c4	401	BCR	C11-C12-C13-C14
15	b1	403	CLA	C3-C5-C6-C7
15	c4	403	CLA	C3-C5-C6-C7
20	cB	850	LMG	C38-C39-C40-C41
15	aA	813	CLA	C1A-C2A-CAA-CBA
15	aA	827	CLA	C1A-C2A-CAA-CBA
15	aA	832	CLA	C1A-C2A-CAA-CBA
15	aA	844	CLA	C1A-C2A-CAA-CBA
15	aB	812	CLA	C1A-C2A-CAA-CBA
15	aB	813	CLA	C1A-C2A-CAA-CBA
15	aB	818	CLA	C1A-C2A-CAA-CBA
15	a2	405	CLA	C1A-C2A-CAA-CBA
15	a3	412	CLA	C1A-C2A-CAA-CBA
15	a4	405	CLA	C1A-C2A-CAA-CBA
15	a5	413	CLA	C1A-C2A-CAA-CBA
15	a6	414	CLA	C1A-C2A-CAA-CBA
15	bA	813	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	827	CLA	C1A-C2A-CAA-CBA
15	bA	844	CLA	C1A-C2A-CAA-CBA
15	bB	812	CLA	C1A-C2A-CAA-CBA
15	bB	813	CLA	C1A-C2A-CAA-CBA
15	bB	818	CLA	C1A-C2A-CAA-CBA
15	b3	412	CLA	C1A-C2A-CAA-CBA
15	b4	405	CLA	C1A-C2A-CAA-CBA
15	b5	413	CLA	C1A-C2A-CAA-CBA
15	b6	414	CLA	C1A-C2A-CAA-CBA
15	cA	813	CLA	C1A-C2A-CAA-CBA
15	cA	827	CLA	C1A-C2A-CAA-CBA
15	cA	832	CLA	C1A-C2A-CAA-CBA
15	cA	843	CLA	C1A-C2A-CAA-CBA
15	cB	812	CLA	C1A-C2A-CAA-CBA
15	cB	813	CLA	C1A-C2A-CAA-CBA
15	cB	818	CLA	C1A-C2A-CAA-CBA
15	c3	412	CLA	C1A-C2A-CAA-CBA
15	c5	413	CLA	C1A-C2A-CAA-CBA
15	c6	415	CLA	C1A-C2A-CAA-CBA
15	a1	408	CLA	C16-C17-C18-C19
15	b1	409	CLA	C16-C17-C18-C19
15	b2	410	CLA	C16-C17-C18-C19
15	b4	409	CLA	C16-C17-C18-C19
15	b6	410	CLA	C16-C17-C18-C19
15	b6	422	CLA	C16-C17-C18-C20
15	c1	409	CLA	C16-C17-C18-C19
15	aA	802	CLA	C15-C16-C17-C18
15	bA	802	CLA	C15-C16-C17-C18
15	cA	841	CLA	C10-C11-C12-C13
20	aB	850	LMG	C38-C39-C40-C41
20	bB	851	LMG	C38-C39-C40-C41
15	bB	811	CLA	O1D-CGD-O2D-CED
15	b3	411	CLA	O1D-CGD-O2D-CED
15	cB	805	CLA	O1D-CGD-O2D-CED
15	cB	811	CLA	O1D-CGD-O2D-CED
15	bA	817	CLA	O1A-CGA-O2A-C1
19	aA	853	LHG	C3-O3-P-O6
19	bA	854	LHG	C3-O3-P-O6
19	cA	852	LHG	C3-O3-P-O6
15	aB	805	CLA	O1D-CGD-O2D-CED
15	a4	411	CLA	O1D-CGD-O2D-CED
15	bB	805	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	840	CLA	C2C-C3C-CAC-CBC
15	bB	840	CLA	C2C-C3C-CAC-CBC
15	cB	840	CLA	C2C-C3C-CAC-CBC
15	aA	825	CLA	C3-C5-C6-C7
15	bA	825	CLA	C3-C5-C6-C7
15	cA	825	CLA	C3-C5-C6-C7
15	aA	817	CLA	O1A-CGA-O2A-C1
15	cA	817	CLA	O1A-CGA-O2A-C1
15	cA	841	CLA	O1A-CGA-O2A-C1
15	aA	819	CLA	C4B-C3B-CAB-CBB
15	aA	824	CLA	C4B-C3B-CAB-CBB
15	aA	828	CLA	C4B-C3B-CAB-CBB
15	aB	840	CLA	C4B-C3B-CAB-CBB
15	bA	819	CLA	C4B-C3B-CAB-CBB
15	bA	824	CLA	C4B-C3B-CAB-CBB
15	bA	828	CLA	C4B-C3B-CAB-CBB
15	bB	840	CLA	C4B-C3B-CAB-CBB
15	cA	819	CLA	C4B-C3B-CAB-CBB
15	cA	824	CLA	C4B-C3B-CAB-CBB
15	cA	828	CLA	C4B-C3B-CAB-CBB
15	cB	840	CLA	C4B-C3B-CAB-CBB
19	aA	854	LHG	C3-O3-P-O4
19	bA	855	LHG	C3-O3-P-O4
19	bA	855	LHG	C4-O6-P-O5
19	cA	853	LHG	C3-O3-P-O4
19	cA	853	LHG	C4-O6-P-O5
15	a4	409	CLA	C16-C17-C18-C19
15	a6	410	CLA	C16-C17-C18-C19
15	aB	806	CLA	CBA-CGA-O2A-C1
15	bB	806	CLA	CBA-CGA-O2A-C1
15	cB	806	CLA	CBA-CGA-O2A-C1
15	aA	841	CLA	O1A-CGA-O2A-C1
15	bA	841	CLA	O1A-CGA-O2A-C1
15	aA	822	CLA	C3-C5-C6-C7
15	bA	822	CLA	C3-C5-C6-C7
15	cA	822	CLA	C3-C5-C6-C7
15	c1	403	CLA	C3-C5-C6-C7
15	b4	411	CLA	O1D-CGD-O2D-CED
20	aB	850	LMG	C32-C33-C34-C35
20	bB	851	LMG	C32-C33-C34-C35
15	aA	833	CLA	C16-C17-C18-C20
15	bA	833	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	833	CLA	C16-C17-C18-C20
20	cB	850	LMG	C32-C33-C34-C35
15	aA	814	CLA	CAD-CBD-CGD-O1D
15	aA	838	CLA	CAD-CBD-CGD-O1D
15	aB	803	CLA	CAD-CBD-CGD-O1D
15	aB	806	CLA	CAD-CBD-CGD-O1D
15	aB	814	CLA	CAD-CBD-CGD-O1D
15	aB	836	CLA	CAD-CBD-CGD-O1D
15	aL	201	CLA	CAD-CBD-CGD-O1D
15	a1	411	CLA	CAD-CBD-CGD-O1D
15	a2	413	CLA	CAD-CBD-CGD-O1D
15	a3	412	CLA	CAD-CBD-CGD-O1D
15	a4	412	CLA	CAD-CBD-CGD-O1D
15	a5	412	CLA	CAD-CBD-CGD-O1D
15	a5	415	CLA	CAD-CBD-CGD-O1D
15	a6	413	CLA	CAD-CBD-CGD-O1D
15	bA	814	CLA	CAD-CBD-CGD-O1D
15	bA	838	CLA	CAD-CBD-CGD-O1D
15	bB	803	CLA	CAD-CBD-CGD-O1D
15	bB	806	CLA	CAD-CBD-CGD-O1D
15	bB	814	CLA	CAD-CBD-CGD-O1D
15	bB	836	CLA	CAD-CBD-CGD-O1D
15	bL	202	CLA	CAD-CBD-CGD-O1D
15	b1	412	CLA	CAD-CBD-CGD-O1D
15	b2	413	CLA	CAD-CBD-CGD-O1D
15	b3	412	CLA	CAD-CBD-CGD-O1D
15	b4	412	CLA	CAD-CBD-CGD-O1D
15	b5	412	CLA	CAD-CBD-CGD-O1D
15	b5	415	CLA	CAD-CBD-CGD-O1D
15	b6	413	CLA	CAD-CBD-CGD-O1D
15	cA	814	CLA	CAD-CBD-CGD-O1D
15	cA	815	CLA	CAD-CBD-CGD-O1D
15	cA	838	CLA	CAD-CBD-CGD-O1D
15	cB	803	CLA	CAD-CBD-CGD-O1D
15	cB	806	CLA	CAD-CBD-CGD-O1D
15	cB	814	CLA	CAD-CBD-CGD-O1D
15	cB	836	CLA	CAD-CBD-CGD-O1D
15	cL	202	CLA	CAD-CBD-CGD-O1D
15	c1	412	CLA	CAD-CBD-CGD-O1D
15	c2	413	CLA	CAD-CBD-CGD-O1D
15	c3	412	CLA	CAD-CBD-CGD-O1D
15	c4	412	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c5	412	CLA	CAD-CBD-CGD-O1D
15	c5	415	CLA	CAD-CBD-CGD-O1D
15	c6	414	CLA	CAD-CBD-CGD-O1D
15	aB	810	CLA	C13-C15-C16-C17
15	bB	810	CLA	C13-C15-C16-C17
15	cB	810	CLA	C13-C15-C16-C17
15	aB	806	CLA	O1A-CGA-O2A-C1
15	bB	806	CLA	O1A-CGA-O2A-C1
15	cB	806	CLA	O1A-CGA-O2A-C1
15	a1	402	CLA	C3-C5-C6-C7
15	a3	403	CLA	C3-C5-C6-C7
15	b3	403	CLA	C3-C5-C6-C7
15	c3	403	CLA	C3-C5-C6-C7
15	aA	832	CLA	CBA-CGA-O2A-C1
15	bA	832	CLA	CBA-CGA-O2A-C1
15	cA	832	CLA	CBA-CGA-O2A-C1
15	aA	835	CLA	C16-C17-C18-C20
15	a3	409	CLA	C16-C17-C18-C19
15	bA	835	CLA	C16-C17-C18-C20
15	b3	409	CLA	C16-C17-C18-C19
15	cA	835	CLA	C16-C17-C18-C20
15	c2	410	CLA	C16-C17-C18-C19
15	c3	409	CLA	C16-C17-C18-C19
15	c6	401	CLA	C16-C17-C18-C20
15	aA	820	CLA	C11-C12-C13-C15
15	aA	825	CLA	C11-C10-C8-C7
15	aA	828	CLA	C6-C7-C8-C10
15	aA	841	CLA	C11-C10-C8-C7
15	aA	844	CLA	C3A-C2A-CAA-CBA
15	aB	814	CLA	C6-C7-C8-C10
15	aB	834	CLA	C3A-C2A-CAA-CBA
15	aB	837	CLA	C12-C13-C15-C16
15	aB	839	CLA	C11-C12-C13-C15
15	aL	203	CLA	C6-C7-C8-C10
15	a3	403	CLA	C11-C12-C13-C15
15	bA	820	CLA	C11-C12-C13-C15
15	bA	825	CLA	C11-C10-C8-C7
15	bA	828	CLA	C6-C7-C8-C10
15	bA	841	CLA	C11-C10-C8-C7
15	bA	844	CLA	C3A-C2A-CAA-CBA
15	bB	814	CLA	C6-C7-C8-C10
15	bB	834	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	837	CLA	C12-C13-C15-C16
15	bB	839	CLA	C11-C12-C13-C15
15	bL	204	CLA	C6-C7-C8-C10
15	b3	403	CLA	C11-C12-C13-C15
15	cA	820	CLA	C11-C12-C13-C15
15	cA	825	CLA	C11-C10-C8-C7
15	cA	828	CLA	C6-C7-C8-C10
15	cA	841	CLA	C11-C10-C8-C7
15	cB	814	CLA	C6-C7-C8-C10
15	cB	834	CLA	C3A-C2A-CAA-CBA
15	cB	837	CLA	C12-C13-C15-C16
15	cB	839	CLA	C11-C12-C13-C15
15	cL	204	CLA	C6-C7-C8-C10
15	c3	403	CLA	C11-C12-C13-C15
20	cB	850	LMG	C36-C37-C38-C39
20	aB	850	LMG	C36-C37-C38-C39
20	bB	851	LMG	C36-C37-C38-C39
20	aB	850	LMG	O1-C7-C8-O7
20	bB	851	LMG	O1-C7-C8-O7
20	cB	850	LMG	O1-C7-C8-O7
15	b1	411	CLA	O1D-CGD-O2D-CED
15	aB	818	CLA	O1D-CGD-O2D-CED
15	cB	818	CLA	O1D-CGD-O2D-CED
19	aA	853	LHG	C11-C10-C9-C8
19	bA	854	LHG	C11-C10-C9-C8
15	aA	834	CLA	C4-C3-C5-C6
15	bA	834	CLA	C4-C3-C5-C6
15	cA	834	CLA	C4-C3-C5-C6
19	cA	852	LHG	C11-C10-C9-C8
15	aA	806	CLA	C11-C10-C8-C9
15	aA	810	CLA	C11-C10-C8-C9
15	aA	829	CLA	C11-C12-C13-C14
15	aA	829	CLA	C14-C13-C15-C16
15	aA	833	CLA	C11-C10-C8-C9
15	aB	808	CLA	C11-C12-C13-C14
15	aB	809	CLA	C11-C10-C8-C9
15	aB	837	CLA	C14-C13-C15-C16
15	a2	403	CLA	C11-C10-C8-C9
15	bA	806	CLA	C11-C10-C8-C9
15	bA	810	CLA	C11-C10-C8-C9
15	bA	828	CLA	C11-C10-C8-C9
15	bA	829	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	829	CLA	C14-C13-C15-C16
15	bA	833	CLA	C11-C10-C8-C9
15	bB	808	CLA	C11-C12-C13-C14
15	bB	809	CLA	C11-C10-C8-C9
15	bB	837	CLA	C14-C13-C15-C16
15	cA	806	CLA	C11-C10-C8-C9
15	cA	810	CLA	C11-C10-C8-C9
15	cA	829	CLA	C11-C12-C13-C14
15	cA	829	CLA	C14-C13-C15-C16
15	cA	833	CLA	C11-C10-C8-C9
15	cB	808	CLA	C11-C12-C13-C14
15	cB	809	CLA	C11-C10-C8-C9
15	cB	837	CLA	C14-C13-C15-C16
16	aB	843	PQN	C19-C18-C20-C21
16	bB	843	PQN	C19-C18-C20-C21
16	cB	843	PQN	C19-C18-C20-C21
15	bB	818	CLA	O1D-CGD-O2D-CED
18	aK	101	BCR	C22-C23-C24-C25
18	aL	205	BCR	C6-C7-C8-C9
18	a3	418	BCR	C22-C23-C24-C25
18	a6	419	BCR	C22-C23-C24-C25
18	bA	848	BCR	C22-C23-C24-C25
18	bL	201	BCR	C6-C7-C8-C9
18	bL	206	BCR	C6-C7-C8-C9
18	b2	419	BCR	C22-C23-C24-C25
18	b6	419	BCR	C22-C23-C24-C25
18	cK	101	BCR	C22-C23-C24-C25
18	c6	420	BCR	C22-C23-C24-C25
15	cA	834	CLA	O1A-CGA-O2A-C1
15	c5	403	CLA	C3-C5-C6-C7
15	c6	405	CLA	C3-C5-C6-C7
15	a6	422	CLA	C16-C17-C18-C19
15	aA	834	CLA	O1A-CGA-O2A-C1
15	bA	834	CLA	O1A-CGA-O2A-C1
15	a5	403	CLA	C3-C5-C6-C7
15	aB	815	CLA	C16-C17-C18-C20
15	bB	815	CLA	C16-C17-C18-C20
15	cB	815	CLA	C16-C17-C18-C20
15	aA	807	CLA	C2B-C3B-CAB-CBB
15	aA	808	CLA	C2B-C3B-CAB-CBB
15	aA	822	CLA	C2B-C3B-CAB-CBB
15	aA	823	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	824	CLA	C2B-C3B-CAB-CBB
15	aA	841	CLA	C2B-C3B-CAB-CBB
15	aB	808	CLA	C2B-C3B-CAB-CBB
15	aB	842	CLA	C2B-C3B-CAB-CBB
15	aJ	202	CLA	C2B-C3B-CAB-CBB
15	aL	202	CLA	C2B-C3B-CAB-CBB
15	aX	102	CLA	C2B-C3B-CAB-CBB
15	a3	413	CLA	C2B-C3B-CAB-CBB
15	bA	807	CLA	C2B-C3B-CAB-CBB
15	bA	808	CLA	C2B-C3B-CAB-CBB
15	bA	822	CLA	C2B-C3B-CAB-CBB
15	bA	823	CLA	C2B-C3B-CAB-CBB
15	bA	824	CLA	C2B-C3B-CAB-CBB
15	bA	841	CLA	C2B-C3B-CAB-CBB
15	bB	808	CLA	C2B-C3B-CAB-CBB
15	bB	842	CLA	C2B-C3B-CAB-CBB
15	bJ	101	CLA	C2B-C3B-CAB-CBB
15	bX	102	CLA	C2B-C3B-CAB-CBB
15	b3	413	CLA	C2B-C3B-CAB-CBB
15	cA	807	CLA	C2B-C3B-CAB-CBB
15	cA	808	CLA	C2B-C3B-CAB-CBB
15	cA	822	CLA	C2B-C3B-CAB-CBB
15	cA	823	CLA	C2B-C3B-CAB-CBB
15	cA	824	CLA	C2B-C3B-CAB-CBB
15	cA	841	CLA	C2B-C3B-CAB-CBB
15	cB	808	CLA	C2B-C3B-CAB-CBB
15	cB	842	CLA	C2B-C3B-CAB-CBB
15	cJ	101	CLA	C2B-C3B-CAB-CBB
15	cL	203	CLA	C2B-C3B-CAB-CBB
15	cX	102	CLA	C2B-C3B-CAB-CBB
15	c3	413	CLA	C2B-C3B-CAB-CBB
18	c4	418	BCR	C16-C17-C18-C36
15	bA	832	CLA	O1A-CGA-O2A-C1
15	cA	832	CLA	O1A-CGA-O2A-C1
15	aA	820	CLA	C16-C17-C18-C19
15	a2	410	CLA	C16-C17-C18-C19
15	bA	820	CLA	C16-C17-C18-C19
15	cA	820	CLA	C16-C17-C18-C19
15	aA	823	CLA	C1-C2-C3-C4
15	aB	832	CLA	C1-C2-C3-C4
15	bA	823	CLA	C1-C2-C3-C4
15	bB	832	CLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	823	CLA	C1-C2-C3-C4
15	cB	832	CLA	C1-C2-C3-C4
15	aA	832	CLA	O1A-CGA-O2A-C1
15	a6	404	CLA	C3-C5-C6-C7
15	bB	806	CLA	C3-C5-C6-C7
15	b5	403	CLA	C3-C5-C6-C7
15	b6	404	CLA	C3-C5-C6-C7
15	cB	806	CLA	C3-C5-C6-C7
15	aA	829	CLA	C2A-CAA-CBA-CGA
15	a1	409	CLA	C2A-CAA-CBA-CGA
15	a5	410	CLA	C2A-CAA-CBA-CGA
15	bA	829	CLA	C2A-CAA-CBA-CGA
15	b5	410	CLA	C2A-CAA-CBA-CGA
15	cA	829	CLA	C2A-CAA-CBA-CGA
15	c1	410	CLA	C2A-CAA-CBA-CGA
15	c5	410	CLA	C2A-CAA-CBA-CGA
15	aA	814	CLA	C2-C1-O2A-CGA
15	aA	841	CLA	C2-C1-O2A-CGA
15	aB	807	CLA	C2-C1-O2A-CGA
15	aB	829	CLA	C2-C1-O2A-CGA
15	bA	814	CLA	C2-C1-O2A-CGA
15	bA	841	CLA	C2-C1-O2A-CGA
15	bB	807	CLA	C2-C1-O2A-CGA
15	bB	829	CLA	C2-C1-O2A-CGA
15	cA	814	CLA	C2-C1-O2A-CGA
15	cA	841	CLA	C2-C1-O2A-CGA
15	cB	807	CLA	C2-C1-O2A-CGA
15	cB	829	CLA	C2-C1-O2A-CGA
15	aB	802	CLA	CAA-CBA-CGA-O2A
15	bB	802	CLA	CAA-CBA-CGA-O2A
15	cB	802	CLA	CAA-CBA-CGA-O2A
15	cB	808	CLA	O1A-CGA-O2A-C1
15	aB	806	CLA	C3-C5-C6-C7
15	aA	834	CLA	CBA-CGA-O2A-C1
15	bA	834	CLA	CBA-CGA-O2A-C1
15	cA	834	CLA	CBA-CGA-O2A-C1
15	c6	401	CLA	CBA-CGA-O2A-C1
18	cI	101	BCR	C9-C10-C11-C12
15	aB	808	CLA	O1A-CGA-O2A-C1
15	bB	808	CLA	O1A-CGA-O2A-C1
15	b6	404	CLA	O1A-CGA-O2A-C1
15	cA	834	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	822	CLA	C4-C3-C5-C6
15	cA	822	CLA	C4-C3-C5-C6
18	aA	849	BCR	C23-C24-C25-C26
18	aA	852	BCR	C1-C6-C7-C8
18	aB	847	BCR	C23-C24-C25-C26
18	aI	102	BCR	C23-C24-C25-C26
18	aL	205	BCR	C23-C24-C25-C26
18	a1	418	BCR	C23-C24-C25-C30
18	a1	420	BCR	C23-C24-C25-C30
18	a2	420	BCR	C23-C24-C25-C26
18	a3	419	BCR	C23-C24-C25-C30
18	a4	419	BCR	C23-C24-C25-C30
18	a5	401	BCR	C23-C24-C25-C30
18	a6	401	BCR	C23-C24-C25-C30
18	a6	402	BCR	C1-C6-C7-C8
18	bA	850	BCR	C23-C24-C25-C26
18	bA	853	BCR	C1-C6-C7-C8
18	bB	847	BCR	C23-C24-C25-C26
18	bI	102	BCR	C23-C24-C25-C26
18	bL	201	BCR	C23-C24-C25-C26
18	bL	206	BCR	C23-C24-C25-C26
18	b1	401	BCR	C23-C24-C25-C30
18	b1	419	BCR	C23-C24-C25-C30
18	b2	420	BCR	C23-C24-C25-C26
18	b3	401	BCR	C23-C24-C25-C26
18	b3	419	BCR	C23-C24-C25-C30
18	b4	419	BCR	C23-C24-C25-C30
18	b5	401	BCR	C23-C24-C25-C30
18	b6	401	BCR	C23-C24-C25-C30
18	b6	402	BCR	C1-C6-C7-C8
18	cA	848	BCR	C23-C24-C25-C26
18	cA	851	BCR	C1-C6-C7-C8
18	cB	847	BCR	C23-C24-C25-C26
18	cI	102	BCR	C23-C24-C25-C26
18	c1	401	BCR	C23-C24-C25-C30
18	c1	419	BCR	C23-C24-C25-C30
18	c3	419	BCR	C23-C24-C25-C30
18	c4	419	BCR	C23-C24-C25-C30
18	c5	401	BCR	C23-C24-C25-C30
18	c6	402	BCR	C23-C24-C25-C30
18	c6	403	BCR	C1-C6-C7-C8
15	aA	834	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	834	CLA	C16-C17-C18-C20
15	bA	822	CLA	C15-C16-C17-C18
15	cA	822	CLA	C15-C16-C17-C18
15	b1	410	CLA	C2A-CAA-CBA-CGA
18	aF	203	BCR	C16-C17-C18-C19
18	bJ	105	BCR	C16-C17-C18-C19
18	cF	205	BCR	C16-C17-C18-C19
19	aA	854	LHG	O7-C5-C6-O8
19	bA	855	LHG	O7-C5-C6-O8
19	cA	853	LHG	O7-C5-C6-O8
15	aA	822	CLA	C15-C16-C17-C18
19	aA	853	LHG	C11-C12-C13-C14
19	bA	854	LHG	C11-C12-C13-C14
19	cA	852	LHG	C11-C12-C13-C14
15	b6	404	CLA	CBA-CGA-O2A-C1
19	aA	853	LHG	C4-C5-C6-O8
19	aA	854	LHG	C4-C5-C6-O8
19	bA	854	LHG	C4-C5-C6-O8
19	bA	855	LHG	C4-C5-C6-O8
19	cA	852	LHG	C4-C5-C6-O8
19	cA	853	LHG	C4-C5-C6-O8
14	aA	801	CL0	C12-C13-C15-C16
14	bA	801	CL0	C12-C13-C15-C16
14	cA	801	CL0	C12-C13-C15-C16
15	aA	841	CLA	C2-C3-C5-C6
15	aB	828	CLA	C12-C13-C15-C16
15	a2	402	CLA	C12-C13-C15-C16
15	a6	403	CLA	C12-C13-C15-C16
15	bA	841	CLA	C2-C3-C5-C6
15	bB	828	CLA	C12-C13-C15-C16
15	b1	402	CLA	C12-C13-C15-C16
15	b2	402	CLA	C12-C13-C15-C16
15	b6	403	CLA	C12-C13-C15-C16
15	cA	841	CLA	C2-C3-C5-C6
15	cB	828	CLA	C12-C13-C15-C16
15	c2	402	CLA	C12-C13-C15-C16
15	c6	404	CLA	C12-C13-C15-C16
15	aB	815	CLA	C11-C10-C8-C9
15	a1	402	CLA	C11-C10-C8-C9
15	a3	403	CLA	C11-C10-C8-C9
15	a5	403	CLA	C11-C10-C8-C9
15	a6	404	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	815	CLA	C11-C10-C8-C9
15	bB	839	CLA	C11-C12-C13-C14
15	b1	403	CLA	C11-C10-C8-C9
15	b2	403	CLA	C11-C10-C8-C9
15	b3	403	CLA	C11-C10-C8-C9
15	b4	403	CLA	C11-C10-C8-C9
15	b5	403	CLA	C11-C10-C8-C9
15	b6	404	CLA	C11-C10-C8-C9
15	cB	815	CLA	C11-C10-C8-C9
15	cB	839	CLA	C11-C12-C13-C14
15	c1	403	CLA	C11-C10-C8-C9
15	c2	403	CLA	C11-C10-C8-C9
15	c3	403	CLA	C11-C10-C8-C9
15	c5	403	CLA	C11-C10-C8-C9
15	c6	405	CLA	C11-C10-C8-C9
15	aB	810	CLA	C8-C10-C11-C12
18	aF	203	BCR	C15-C16-C17-C18
18	aI	101	BCR	C9-C10-C11-C12
18	aL	205	BCR	C9-C10-C11-C12
18	bI	101	BCR	C9-C10-C11-C12
18	bJ	105	BCR	C15-C16-C17-C18
18	bL	201	BCR	C9-C10-C11-C12
18	bL	206	BCR	C9-C10-C11-C12
18	cF	205	BCR	C15-C16-C17-C18
15	aA	835	CLA	C16-C17-C18-C19
15	bA	835	CLA	C16-C17-C18-C19
15	cA	835	CLA	C16-C17-C18-C19
16	aB	843	PQN	C23-C25-C26-C27
16	bB	843	PQN	C23-C25-C26-C27
16	cB	843	PQN	C23-C25-C26-C27
15	bB	810	CLA	C8-C10-C11-C12
15	cB	810	CLA	C8-C10-C11-C12
15	a6	404	CLA	O1A-CGA-O2A-C1
15	c6	405	CLA	O1A-CGA-O2A-C1
15	b2	422	CLA	C16-C17-C18-C20
15	b6	422	CLA	C16-C17-C18-C19
15	c2	422	CLA	C16-C17-C18-C20
15	b3	403	CLA	CBA-CGA-O2A-C1
19	aA	854	LHG	C2-C3-O3-P
19	bA	855	LHG	C2-C3-O3-P
19	cA	853	LHG	C2-C3-O3-P
15	bA	822	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	822	CLA	C2-C3-C5-C6
15	aA	834	CLA	C2-C3-C5-C6
15	bA	822	CLA	C2-C3-C5-C6
15	bA	834	CLA	C2-C3-C5-C6
15	cA	822	CLA	C2-C3-C5-C6
15	cA	834	CLA	C2-C3-C5-C6
15	aA	834	CLA	C16-C17-C18-C19
15	a2	422	CLA	C16-C17-C18-C20
15	bA	834	CLA	C16-C17-C18-C19
15	cA	834	CLA	C16-C17-C18-C19
15	aB	833	CLA	CBA-CGA-O2A-C1
15	a2	403	CLA	CBA-CGA-O2A-C1
15	a3	403	CLA	CBA-CGA-O2A-C1
15	a6	404	CLA	CBA-CGA-O2A-C1
15	bB	833	CLA	CBA-CGA-O2A-C1
15	b2	403	CLA	CBA-CGA-O2A-C1
15	b4	403	CLA	CBA-CGA-O2A-C1
15	cB	833	CLA	CBA-CGA-O2A-C1
15	c2	403	CLA	CBA-CGA-O2A-C1
15	c6	405	CLA	CBA-CGA-O2A-C1
15	a4	403	CLA	O1A-CGA-O2A-C1
15	aB	835	CLA	CAA-CBA-CGA-O2A
15	bB	835	CLA	CAA-CBA-CGA-O2A
15	cB	835	CLA	CAA-CBA-CGA-O2A
14	aA	801	CL0	CAA-CBA-CGA-O2A
14	bA	801	CL0	CAA-CBA-CGA-O2A
14	cA	801	CL0	CAA-CBA-CGA-O2A
15	cA	803	CLA	O1D-CGD-O2D-CED
18	a5	418	BCR	C22-C23-C24-C25
15	a3	403	CLA	O1A-CGA-O2A-C1
15	a4	403	CLA	CBA-CGA-O2A-C1
15	c3	403	CLA	CBA-CGA-O2A-C1
15	aA	808	CLA	C4B-C3B-CAB-CBB
15	aA	823	CLA	C4B-C3B-CAB-CBB
15	aB	810	CLA	C4B-C3B-CAB-CBB
15	aL	202	CLA	C4B-C3B-CAB-CBB
15	aL	203	CLA	C4B-C3B-CAB-CBB
15	a2	408	CLA	C4B-C3B-CAB-CBB
15	a3	407	CLA	C4B-C3B-CAB-CBB
15	a4	407	CLA	C4B-C3B-CAB-CBB
15	a5	407	CLA	C4B-C3B-CAB-CBB
15	bA	808	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	823	CLA	C4B-C3B-CAB-CBB
15	bB	810	CLA	C4B-C3B-CAB-CBB
15	bL	203	CLA	C4B-C3B-CAB-CBB
15	bL	204	CLA	C4B-C3B-CAB-CBB
15	b5	407	CLA	C4B-C3B-CAB-CBB
15	cA	808	CLA	C4B-C3B-CAB-CBB
15	cA	823	CLA	C4B-C3B-CAB-CBB
15	cB	810	CLA	C4B-C3B-CAB-CBB
15	cL	203	CLA	C4B-C3B-CAB-CBB
15	cL	204	CLA	C4B-C3B-CAB-CBB
15	c2	408	CLA	C4B-C3B-CAB-CBB
15	c3	407	CLA	C4B-C3B-CAB-CBB
15	c5	407	CLA	C4B-C3B-CAB-CBB
15	bB	808	CLA	C2A-CAA-CBA-CGA
15	cB	808	CLA	C2A-CAA-CBA-CGA
18	aB	847	BCR	C15-C16-C17-C18
18	bB	847	BCR	C15-C16-C17-C18
18	cB	847	BCR	C15-C16-C17-C18
20	cB	850	LMG	C29-C30-C31-C32
18	a1	418	BCR	C18-C19-C20-C21
18	a4	419	BCR	C10-C11-C12-C13
18	b1	419	BCR	C18-C19-C20-C21
18	b4	419	BCR	C10-C11-C12-C13
18	c1	419	BCR	C18-C19-C20-C21
18	c2	401	BCR	C10-C11-C12-C13
18	c2	420	BCR	C18-C19-C20-C21
18	c3	418	BCR	C18-C19-C20-C21
18	c4	419	BCR	C10-C11-C12-C13
18	c5	418	BCR	C18-C19-C20-C21
15	a2	403	CLA	O1A-CGA-O2A-C1
15	b2	403	CLA	O1A-CGA-O2A-C1
15	b4	403	CLA	O1A-CGA-O2A-C1
15	c2	403	CLA	O1A-CGA-O2A-C1
15	aB	818	CLA	C10-C11-C12-C13
15	bB	818	CLA	C10-C11-C12-C13
15	cB	818	CLA	C10-C11-C12-C13
20	aB	850	LMG	C29-C30-C31-C32
20	bB	851	LMG	C29-C30-C31-C32
15	aB	809	CLA	C4-C3-C5-C6
15	bB	809	CLA	C4-C3-C5-C6
15	cB	809	CLA	C4-C3-C5-C6
15	aB	833	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	833	CLA	O1A-CGA-O2A-C1
15	b3	403	CLA	O1A-CGA-O2A-C1
15	c3	403	CLA	O1A-CGA-O2A-C1
15	aA	809	CLA	C8-C10-C11-C12
15	aB	802	CLA	C15-C16-C17-C18
15	a5	410	CLA	C13-C15-C16-C17
15	bA	809	CLA	C8-C10-C11-C12
15	bB	802	CLA	C15-C16-C17-C18
15	c2	416	CLA	CAA-CBA-CGA-O1A
15	aA	808	CLA	C2-C1-O2A-CGA
15	aA	812	CLA	C2-C1-O2A-CGA
15	aA	829	CLA	C2-C1-O2A-CGA
15	bA	808	CLA	C2-C1-O2A-CGA
15	bA	812	CLA	C2-C1-O2A-CGA
15	bA	829	CLA	C2-C1-O2A-CGA
15	cA	808	CLA	C2-C1-O2A-CGA
15	cA	812	CLA	C2-C1-O2A-CGA
15	cA	829	CLA	C2-C1-O2A-CGA
15	cA	809	CLA	C8-C10-C11-C12
15	cB	802	CLA	C15-C16-C17-C18
15	c6	411	CLA	C16-C17-C18-C20
15	cB	833	CLA	O1A-CGA-O2A-C1
15	a2	416	CLA	CAA-CBA-CGA-O1A
15	a5	415	CLA	CAA-CBA-CGA-O1A
15	bB	835	CLA	CAA-CBA-CGA-O1A
15	cB	835	CLA	CAA-CBA-CGA-O1A
15	aA	837	CLA	C2A-CAA-CBA-CGA
15	aB	808	CLA	C2A-CAA-CBA-CGA
15	aX	102	CLA	C2A-CAA-CBA-CGA
15	a2	411	CLA	C2A-CAA-CBA-CGA
15	a3	410	CLA	C2A-CAA-CBA-CGA
15	a4	410	CLA	C2A-CAA-CBA-CGA
15	a6	411	CLA	C2A-CAA-CBA-CGA
15	bA	837	CLA	C2A-CAA-CBA-CGA
15	bX	102	CLA	C2A-CAA-CBA-CGA
15	b2	411	CLA	C2A-CAA-CBA-CGA
15	b3	410	CLA	C2A-CAA-CBA-CGA
15	b4	410	CLA	C2A-CAA-CBA-CGA
15	b6	411	CLA	C2A-CAA-CBA-CGA
15	cA	837	CLA	C2A-CAA-CBA-CGA
15	cX	102	CLA	C2A-CAA-CBA-CGA
15	c2	411	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c3	410	CLA	C2A-CAA-CBA-CGA
15	c4	410	CLA	C2A-CAA-CBA-CGA
15	c6	412	CLA	C2A-CAA-CBA-CGA
15	cA	818	CLA	C5-C6-C7-C8
15	aB	828	CLA	CAA-CBA-CGA-O1A
15	bB	828	CLA	CAA-CBA-CGA-O1A
15	cB	828	CLA	CAA-CBA-CGA-O1A
15	bA	803	CLA	O1D-CGD-O2D-CED
15	aA	818	CLA	C5-C6-C7-C8
15	bA	818	CLA	C5-C6-C7-C8
15	aB	835	CLA	CAA-CBA-CGA-O1A
15	a3	415	CLA	CAA-CBA-CGA-O1A
15	c3	415	CLA	CAA-CBA-CGA-O1A
15	c4	409	CLA	C16-C17-C18-C20
18	aA	852	BCR	C19-C20-C21-C22
18	bA	853	BCR	C19-C20-C21-C22
18	cA	851	BCR	C19-C20-C21-C22
15	a3	410	CLA	C13-C15-C16-C17
15	aA	803	CLA	O1D-CGD-O2D-CED
15	aB	824	CLA	CAA-CBA-CGA-O1A
15	bB	824	CLA	CAA-CBA-CGA-O1A
15	cB	824	CLA	CAA-CBA-CGA-O1A
15	aA	809	CLA	C6-C7-C8-C9
15	aB	815	CLA	C11-C12-C13-C14
15	aB	839	CLA	C11-C12-C13-C14
15	a4	403	CLA	C11-C10-C8-C9
15	bA	809	CLA	C6-C7-C8-C9
15	bB	815	CLA	C11-C12-C13-C14
15	cA	809	CLA	C6-C7-C8-C9
15	cB	815	CLA	C11-C12-C13-C14
15	c4	403	CLA	C11-C10-C8-C9
20	aB	850	LMG	C13-C14-C15-C16
20	bB	851	LMG	C13-C14-C15-C16
20	cB	850	LMG	C13-C14-C15-C16
15	b5	415	CLA	CAA-CBA-CGA-O1A
15	b3	410	CLA	C13-C15-C16-C17
18	aA	852	BCR	C11-C10-C9-C34
18	aB	846	BCR	C11-C10-C9-C34
18	aB	846	BCR	C20-C21-C22-C37
18	aB	849	BCR	C35-C13-C14-C15
18	a1	417	BCR	C20-C21-C22-C37
18	a6	421	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bA	853	BCR	C11-C10-C9-C34
18	bB	846	BCR	C11-C10-C9-C34
18	bB	846	BCR	C20-C21-C22-C37
18	bB	850	BCR	C35-C13-C14-C15
18	b6	421	BCR	C20-C21-C22-C37
18	cA	851	BCR	C11-C10-C9-C34
18	cB	846	BCR	C11-C10-C9-C34
18	cB	846	BCR	C20-C21-C22-C37
18	cB	849	BCR	C35-C13-C14-C15
18	c3	401	BCR	C35-C13-C14-C15
18	c5	418	BCR	C16-C17-C18-C36
15	a6	416	CLA	CAA-CBA-CGA-O1A
15	bB	831	CLA	CAA-CBA-CGA-O1A
15	b5	415	CLA	CAA-CBA-CGA-O2A
15	b6	416	CLA	CAA-CBA-CGA-O1A
15	cB	831	CLA	CAA-CBA-CGA-O1A
15	c5	415	CLA	CAA-CBA-CGA-O1A
15	c5	415	CLA	CAA-CBA-CGA-O2A
15	aA	809	CLA	C16-C17-C18-C20
15	aB	815	CLA	C16-C17-C18-C19
15	bA	809	CLA	C16-C17-C18-C20
15	bB	815	CLA	C16-C17-C18-C19
15	b2	406	CLA	C16-C17-C18-C19
15	cA	809	CLA	C16-C17-C18-C20
15	cB	815	CLA	C16-C17-C18-C19
15	aA	806	CLA	O2A-C1-C2-C3
15	bA	806	CLA	O2A-C1-C2-C3
15	cA	806	CLA	O2A-C1-C2-C3
15	c4	403	CLA	CBA-CGA-O2A-C1
15	aB	831	CLA	CAA-CBA-CGA-O1A
15	aK	102	CLA	CAA-CBA-CGA-O1A
15	a3	415	CLA	CAA-CBA-CGA-O2A
15	a4	415	CLA	CAA-CBA-CGA-O1A
15	bK	101	CLA	CAA-CBA-CGA-O1A
15	b4	415	CLA	CAA-CBA-CGA-O1A
15	c4	415	CLA	CAA-CBA-CGA-O1A
20	aB	850	LMG	C33-C34-C35-C36
20	bB	851	LMG	C33-C34-C35-C36
20	cB	850	LMG	C33-C34-C35-C36
18	aF	201	BCR	C7-C8-C9-C10
18	aL	205	BCR	C21-C22-C23-C24
18	bB	849	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	bL	201	BCR	C21-C22-C23-C24
18	bL	206	BCR	C21-C22-C23-C24
18	cF	202	BCR	C7-C8-C9-C10
15	a1	414	CLA	CAA-CBA-CGA-O1A
15	a2	416	CLA	CAA-CBA-CGA-O2A
15	a5	415	CLA	CAA-CBA-CGA-O2A
15	b1	415	CLA	CAA-CBA-CGA-O1A
15	b1	415	CLA	CAA-CBA-CGA-O2A
15	b2	416	CLA	CAA-CBA-CGA-O1A
15	b2	416	CLA	CAA-CBA-CGA-O2A
15	b3	415	CLA	CAA-CBA-CGA-O1A
15	cB	824	CLA	CAA-CBA-CGA-O2A
15	cK	102	CLA	CAA-CBA-CGA-O1A
15	aA	802	CLA	C1A-C2A-CAA-CBA
15	aA	808	CLA	C1A-C2A-CAA-CBA
15	aA	817	CLA	C1A-C2A-CAA-CBA
15	aA	825	CLA	C1A-C2A-CAA-CBA
15	aA	837	CLA	C1A-C2A-CAA-CBA
15	aA	842	CLA	C1A-C2A-CAA-CBA
15	aB	811	CLA	C1A-C2A-CAA-CBA
15	aB	838	CLA	C1A-C2A-CAA-CBA
15	a1	403	CLA	C1A-C2A-CAA-CBA
15	a1	412	CLA	C1A-C2A-CAA-CBA
15	a3	404	CLA	C1A-C2A-CAA-CBA
15	a4	404	CLA	C1A-C2A-CAA-CBA
15	bA	802	CLA	C1A-C2A-CAA-CBA
15	bA	808	CLA	C1A-C2A-CAA-CBA
15	bA	817	CLA	C1A-C2A-CAA-CBA
15	bA	825	CLA	C1A-C2A-CAA-CBA
15	bA	832	CLA	C1A-C2A-CAA-CBA
15	bA	837	CLA	C1A-C2A-CAA-CBA
15	bA	842	CLA	C1A-C2A-CAA-CBA
15	bB	811	CLA	C1A-C2A-CAA-CBA
15	bB	838	CLA	C1A-C2A-CAA-CBA
15	b1	413	CLA	C1A-C2A-CAA-CBA
15	b4	413	CLA	C1A-C2A-CAA-CBA
15	cA	802	CLA	C1A-C2A-CAA-CBA
15	cA	808	CLA	C1A-C2A-CAA-CBA
15	cA	817	CLA	C1A-C2A-CAA-CBA
15	cA	825	CLA	C1A-C2A-CAA-CBA
15	cA	837	CLA	C1A-C2A-CAA-CBA
15	cB	811	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	838	CLA	C1A-C2A-CAA-CBA
15	cF	201	CLA	C1A-C2A-CAA-CBA
15	c1	404	CLA	C1A-C2A-CAA-CBA
15	c1	413	CLA	C1A-C2A-CAA-CBA
15	c4	413	CLA	C1A-C2A-CAA-CBA
15	aA	802	CLA	C6-C7-C8-C10
15	aA	829	CLA	C12-C13-C15-C16
15	aA	833	CLA	C6-C7-C8-C10
15	aB	802	CLA	C11-C12-C13-C15
15	bA	802	CLA	C6-C7-C8-C10
15	bA	829	CLA	C12-C13-C15-C16
15	bA	833	CLA	C6-C7-C8-C10
15	bB	802	CLA	C11-C12-C13-C15
15	cA	802	CLA	C6-C7-C8-C10
15	cA	829	CLA	C12-C13-C15-C16
15	cA	833	CLA	C6-C7-C8-C10
15	cB	802	CLA	C11-C12-C13-C15
15	aB	824	CLA	CAA-CBA-CGA-O2A
15	bB	824	CLA	CAA-CBA-CGA-O2A
15	b3	415	CLA	CAA-CBA-CGA-O2A
15	a1	414	CLA	CAA-CBA-CGA-O2A
15	b2	409	CLA	CAA-CBA-CGA-O2A
15	b3	408	CLA	CAA-CBA-CGA-O2A
15	b6	409	CLA	CAA-CBA-CGA-O2A
15	c1	415	CLA	CAA-CBA-CGA-O1A
15	c5	408	CLA	CAA-CBA-CGA-O2A
15	c6	410	CLA	CAA-CBA-CGA-O2A
15	c6	417	CLA	CAA-CBA-CGA-O1A
15	aL	201	CLA	C8-C10-C11-C12
15	bL	202	CLA	C8-C10-C11-C12
15	cA	833	CLA	C5-C6-C7-C8
15	cB	814	CLA	C5-C6-C7-C8
15	cL	202	CLA	C8-C10-C11-C12
15	aA	835	CLA	C2A-CAA-CBA-CGA
15	aB	829	CLA	C2A-CAA-CBA-CGA
15	a2	418	CLA	C2A-CAA-CBA-CGA
15	bA	835	CLA	C2A-CAA-CBA-CGA
15	bB	829	CLA	C2A-CAA-CBA-CGA
15	cA	835	CLA	C2A-CAA-CBA-CGA
15	cB	829	CLA	C2A-CAA-CBA-CGA
15	c2	418	CLA	C2A-CAA-CBA-CGA
15	bB	814	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b5	410	CLA	C13-C15-C16-C17
15	c5	410	CLA	C13-C15-C16-C17
15	aA	823	CLA	CAA-CBA-CGA-O2A
15	aB	833	CLA	CAA-CBA-CGA-O2A
15	bA	823	CLA	CAA-CBA-CGA-O2A
15	bB	833	CLA	CAA-CBA-CGA-O2A
15	cA	823	CLA	CAA-CBA-CGA-O2A
15	cB	833	CLA	CAA-CBA-CGA-O2A
15	a3	408	CLA	CAA-CBA-CGA-O2A
15	a6	409	CLA	CAA-CBA-CGA-O2A
15	c1	415	CLA	CAA-CBA-CGA-O2A
15	c2	409	CLA	CAA-CBA-CGA-O2A
15	aA	833	CLA	C5-C6-C7-C8
15	aB	814	CLA	C5-C6-C7-C8
15	bA	830	CLA	C5-C6-C7-C8
15	bA	833	CLA	C5-C6-C7-C8
15	bL	204	CLA	C13-C15-C16-C17
15	b2	411	CLA	C13-C15-C16-C17
15	aB	809	CLA	CBA-CGA-O2A-C1
15	a4	409	CLA	C16-C17-C18-C20
15	a6	410	CLA	C16-C17-C18-C20
15	b4	409	CLA	C16-C17-C18-C20
15	b5	409	CLA	C16-C17-C18-C20
15	b6	410	CLA	C16-C17-C18-C20
15	aL	203	CLA	C13-C15-C16-C17
15	a1	407	CLA	CAA-CBA-CGA-O1A
15	a2	409	CLA	CAA-CBA-CGA-O2A
15	a4	408	CLA	CAA-CBA-CGA-O2A
15	a5	408	CLA	CAA-CBA-CGA-O2A
15	b1	408	CLA	CAA-CBA-CGA-O2A
15	b5	408	CLA	CAA-CBA-CGA-O2A
15	c3	408	CLA	CAA-CBA-CGA-O2A
15	aA	830	CLA	C5-C6-C7-C8
15	cA	830	CLA	C5-C6-C7-C8
15	cL	204	CLA	C13-C15-C16-C17
15	c3	410	CLA	C13-C15-C16-C17
15	aA	819	CLA	C2B-C3B-CAB-CBB
15	aA	828	CLA	C2B-C3B-CAB-CBB
15	aB	810	CLA	C2B-C3B-CAB-CBB
15	aB	836	CLA	C2B-C3B-CAB-CBB
15	aB	840	CLA	C2B-C3B-CAB-CBB
15	aL	203	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	415	CLA	C2B-C3B-CAB-CBB
15	a2	408	CLA	C2B-C3B-CAB-CBB
15	a3	416	CLA	C2B-C3B-CAB-CBB
15	a4	407	CLA	C2B-C3B-CAB-CBB
15	a5	407	CLA	C2B-C3B-CAB-CBB
15	bA	819	CLA	C2B-C3B-CAB-CBB
15	bA	828	CLA	C2B-C3B-CAB-CBB
15	bB	810	CLA	C2B-C3B-CAB-CBB
15	bB	836	CLA	C2B-C3B-CAB-CBB
15	bB	840	CLA	C2B-C3B-CAB-CBB
15	bL	203	CLA	C2B-C3B-CAB-CBB
15	bL	204	CLA	C2B-C3B-CAB-CBB
15	b3	416	CLA	C2B-C3B-CAB-CBB
15	b4	407	CLA	C2B-C3B-CAB-CBB
15	b5	407	CLA	C2B-C3B-CAB-CBB
15	cA	819	CLA	C2B-C3B-CAB-CBB
15	cA	828	CLA	C2B-C3B-CAB-CBB
15	cB	810	CLA	C2B-C3B-CAB-CBB
15	cB	836	CLA	C2B-C3B-CAB-CBB
15	cB	840	CLA	C2B-C3B-CAB-CBB
15	cL	204	CLA	C2B-C3B-CAB-CBB
15	c2	408	CLA	C2B-C3B-CAB-CBB
15	c3	416	CLA	C2B-C3B-CAB-CBB
15	c4	407	CLA	C2B-C3B-CAB-CBB
15	c5	407	CLA	C2B-C3B-CAB-CBB
15	bB	809	CLA	CBA-CGA-O2A-C1
15	b1	408	CLA	CAA-CBA-CGA-O1A
15	b4	408	CLA	CAA-CBA-CGA-O2A
15	c1	408	CLA	CAA-CBA-CGA-O1A
15	c4	403	CLA	O1A-CGA-O2A-C1
15	c5	409	CLA	C16-C17-C18-C20
18	aB	846	BCR	C11-C10-C9-C8
18	bB	846	BCR	C11-C10-C9-C8
18	cB	846	BCR	C11-C10-C9-C8
15	a2	411	CLA	C13-C15-C16-C17
15	a4	408	CLA	CAA-CBA-CGA-O1A
15	a4	415	CLA	CAA-CBA-CGA-O2A
15	a6	416	CLA	CAA-CBA-CGA-O2A
15	b4	415	CLA	CAA-CBA-CGA-O2A
15	b6	416	CLA	CAA-CBA-CGA-O2A
15	c3	415	CLA	CAA-CBA-CGA-O2A
15	c4	408	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	415	CLA	CAA-CBA-CGA-O2A
15	c6	417	CLA	CAA-CBA-CGA-O2A
15	a5	403	CLA	O1A-CGA-O2A-C1
15	a5	403	CLA	CBA-CGA-O2A-C1
15	cB	809	CLA	CBA-CGA-O2A-C1
15	b2	418	CLA	C2A-CAA-CBA-CGA
20	aB	850	LMG	C42-C43-C44-C45
20	bB	851	LMG	C42-C43-C44-C45
20	cB	850	LMG	C42-C43-C44-C45
18	aF	201	BCR	C13-C14-C15-C16
18	aJ	204	BCR	C13-C14-C15-C16
18	bB	849	BCR	C13-C14-C15-C16
18	bJ	103	BCR	C13-C14-C15-C16
18	cF	202	BCR	C13-C14-C15-C16
18	cJ	103	BCR	C13-C14-C15-C16
15	c2	416	CLA	CAA-CBA-CGA-O2A
18	a2	419	BCR	C22-C23-C24-C25
18	c2	419	BCR	C22-C23-C24-C25
18	c3	418	BCR	C22-C23-C24-C25
15	a5	409	CLA	C16-C17-C18-C20
15	c4	421	CLA	C16-C17-C18-C20
15	b5	403	CLA	O1A-CGA-O2A-C1
15	a1	407	CLA	CAA-CBA-CGA-O2A
15	c1	408	CLA	CAA-CBA-CGA-O2A
15	c4	408	CLA	CAA-CBA-CGA-O1A
15	aA	839	CLA	C4-C3-C5-C6
15	aB	811	CLA	C4-C3-C5-C6
15	aB	837	CLA	C4-C3-C5-C6
15	bA	839	CLA	C4-C3-C5-C6
15	bB	811	CLA	C4-C3-C5-C6
15	bB	837	CLA	C4-C3-C5-C6
15	cA	839	CLA	C4-C3-C5-C6
15	cB	811	CLA	C4-C3-C5-C6
15	cB	837	CLA	C4-C3-C5-C6
15	bB	809	CLA	C2-C3-C5-C6
15	c5	403	CLA	O1A-CGA-O2A-C1
18	a2	420	BCR	C18-C19-C20-C21
15	a2	409	CLA	CAA-CBA-CGA-O1A
15	a3	408	CLA	CAA-CBA-CGA-O1A
15	b3	408	CLA	CAA-CBA-CGA-O1A
15	b5	408	CLA	CAA-CBA-CGA-O1A
15	cB	831	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c5	408	CLA	CAA-CBA-CGA-O1A
15	aA	805	CLA	CAA-CBA-CGA-O2A
15	cA	805	CLA	CAA-CBA-CGA-O2A
15	a5	408	CLA	CAA-CBA-CGA-O1A
15	a6	409	CLA	CAA-CBA-CGA-O1A
15	b2	409	CLA	CAA-CBA-CGA-O1A
15	b4	408	CLA	CAA-CBA-CGA-O1A
15	b6	409	CLA	CAA-CBA-CGA-O1A
15	c2	409	CLA	CAA-CBA-CGA-O1A
15	bA	826	CLA	C15-C16-C17-C18
15	cA	826	CLA	C15-C16-C17-C18
15	b2	410	CLA	C16-C17-C18-C20
18	aA	849	BCR	C23-C24-C25-C30
18	aB	845	BCR	C23-C24-C25-C26
18	aB	845	BCR	C23-C24-C25-C30
18	aB	846	BCR	C23-C24-C25-C30
18	aF	201	BCR	C23-C24-C25-C30
18	aF	202	BCR	C23-C24-C25-C30
18	aF	203	BCR	C1-C6-C7-C8
18	aI	101	BCR	C23-C24-C25-C30
18	aI	102	BCR	C1-C6-C7-C8
18	aJ	204	BCR	C23-C24-C25-C26
18	aJ	204	BCR	C23-C24-C25-C30
18	aK	101	BCR	C23-C24-C25-C30
18	aL	205	BCR	C23-C24-C25-C30
18	a2	401	BCR	C1-C6-C7-C8
18	a6	402	BCR	C5-C6-C7-C8
18	bA	848	BCR	C23-C24-C25-C30
18	bA	850	BCR	C23-C24-C25-C30
18	bB	845	BCR	C23-C24-C25-C26
18	bB	845	BCR	C23-C24-C25-C30
18	bB	846	BCR	C23-C24-C25-C30
18	bB	849	BCR	C23-C24-C25-C30
18	bF	202	BCR	C23-C24-C25-C30
18	bI	101	BCR	C23-C24-C25-C30
18	bI	102	BCR	C1-C6-C7-C8
18	bJ	103	BCR	C23-C24-C25-C26
18	bJ	103	BCR	C23-C24-C25-C30
18	bJ	105	BCR	C1-C6-C7-C8
18	bL	201	BCR	C23-C24-C25-C30
18	bL	206	BCR	C23-C24-C25-C30
18	b2	401	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	cA	848	BCR	C23-C24-C25-C30
18	cB	845	BCR	C23-C24-C25-C26
18	cB	845	BCR	C23-C24-C25-C30
18	cB	846	BCR	C23-C24-C25-C30
18	cF	202	BCR	C23-C24-C25-C30
18	cF	204	BCR	C23-C24-C25-C30
18	cF	205	BCR	C1-C6-C7-C8
18	cI	101	BCR	C23-C24-C25-C30
18	cI	102	BCR	C1-C6-C7-C8
18	cJ	103	BCR	C23-C24-C25-C26
18	cJ	103	BCR	C23-C24-C25-C30
18	cK	101	BCR	C23-C24-C25-C30
18	c2	401	BCR	C1-C6-C7-C8
18	c6	403	BCR	C5-C6-C7-C8
15	aA	826	CLA	C15-C16-C17-C18
15	bA	805	CLA	CAA-CBA-CGA-O2A
15	aB	831	CLA	CAA-CBA-CGA-O2A
15	aK	102	CLA	CAA-CBA-CGA-O2A
15	bB	831	CLA	CAA-CBA-CGA-O2A
15	bK	101	CLA	CAA-CBA-CGA-O2A
15	cK	102	CLA	CAA-CBA-CGA-O2A
15	aA	810	CLA	C4-C3-C5-C6
15	bA	810	CLA	C4-C3-C5-C6
15	cA	810	CLA	C4-C3-C5-C6
18	aB	846	BCR	C7-C8-C9-C10
18	bB	846	BCR	C7-C8-C9-C10
18	cB	846	BCR	C7-C8-C9-C10
15	aA	812	CLA	C13-C15-C16-C17
15	bA	812	CLA	C13-C15-C16-C17
15	cA	812	CLA	C13-C15-C16-C17
15	c2	411	CLA	C13-C15-C16-C17
15	aB	809	CLA	C2-C3-C5-C6
15	cB	809	CLA	C2-C3-C5-C6
15	aB	841	CLA	CAA-CBA-CGA-O2A
15	bB	841	CLA	CAA-CBA-CGA-O2A
15	cB	841	CLA	CAA-CBA-CGA-O2A
15	c6	410	CLA	CAA-CBA-CGA-O1A
15	b5	403	CLA	CBA-CGA-O2A-C1
15	cA	819	CLA	CAA-CBA-CGA-O2A
15	b4	421	CLA	C16-C17-C18-C20
15	aA	835	CLA	C13-C15-C16-C17
15	aB	820	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	835	CLA	C13-C15-C16-C17
15	bB	820	CLA	C13-C15-C16-C17
15	cA	835	CLA	C13-C15-C16-C17
15	cB	806	CLA	C10-C11-C12-C13
15	cK	102	CLA	O1D-CGD-O2D-CED
15	aA	844	CLA	CAA-CBA-CGA-O2A
15	a1	406	CLA	CAA-CBA-CGA-O2A
15	bA	844	CLA	CAA-CBA-CGA-O2A
15	b1	407	CLA	CAA-CBA-CGA-O2A
15	cA	843	CLA	CAA-CBA-CGA-O2A
15	aB	816	CLA	C2A-CAA-CBA-CGA
15	aB	824	CLA	C2A-CAA-CBA-CGA
15	a6	418	CLA	C2A-CAA-CBA-CGA
15	bB	824	CLA	C2A-CAA-CBA-CGA
15	b6	418	CLA	C2A-CAA-CBA-CGA
15	cB	816	CLA	C2A-CAA-CBA-CGA
15	cB	824	CLA	C2A-CAA-CBA-CGA
15	c6	419	CLA	C2A-CAA-CBA-CGA
15	cB	820	CLA	C13-C15-C16-C17
15	aA	819	CLA	CAA-CBA-CGA-O2A
15	bA	819	CLA	CAA-CBA-CGA-O2A
15	c5	403	CLA	CBA-CGA-O2A-C1
15	aB	813	CLA	CAA-CBA-CGA-O1A
15	aB	841	CLA	CAA-CBA-CGA-O1A
15	a1	411	CLA	CAA-CBA-CGA-O2A
15	bB	813	CLA	CAA-CBA-CGA-O1A
15	bB	841	CLA	CAA-CBA-CGA-O1A
15	b4	407	CLA	CAA-CBA-CGA-O2A
15	cB	813	CLA	CAA-CBA-CGA-O1A
15	cB	841	CLA	CAA-CBA-CGA-O1A
15	c1	407	CLA	CAA-CBA-CGA-O2A
15	c3	408	CLA	CAA-CBA-CGA-O1A
15	c5	407	CLA	CAA-CBA-CGA-O2A
15	aA	822	CLA	C4B-C3B-CAB-CBB
15	a1	406	CLA	C4B-C3B-CAB-CBB
15	a6	408	CLA	C4B-C3B-CAB-CBB
15	bA	822	CLA	C4B-C3B-CAB-CBB
15	b1	407	CLA	C4B-C3B-CAB-CBB
15	b2	408	CLA	C4B-C3B-CAB-CBB
15	b3	407	CLA	C4B-C3B-CAB-CBB
15	b4	407	CLA	C4B-C3B-CAB-CBB
15	b6	408	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	822	CLA	C4B-C3B-CAB-CBB
15	c1	407	CLA	C4B-C3B-CAB-CBB
15	c4	407	CLA	C4B-C3B-CAB-CBB
15	c6	409	CLA	C4B-C3B-CAB-CBB
15	a4	421	CLA	C16-C17-C18-C20
15	bK	101	CLA	O1D-CGD-O2D-CED
15	aA	830	CLA	CAA-CBA-CGA-O2A
15	bA	830	CLA	CAA-CBA-CGA-O2A
15	cA	830	CLA	CAA-CBA-CGA-O2A
15	aA	802	CLA	C4-C3-C5-C6
15	aB	818	CLA	C4-C3-C5-C6
15	bA	802	CLA	C4-C3-C5-C6
15	bB	818	CLA	C4-C3-C5-C6
15	cA	802	CLA	C4-C3-C5-C6
15	cB	818	CLA	C4-C3-C5-C6
15	a1	401	CLA	C6-C7-C8-C10
15	a4	402	CLA	C6-C7-C8-C10
15	a5	402	CLA	C6-C7-C8-C10
15	a6	403	CLA	C6-C7-C8-C10
15	b1	402	CLA	C6-C7-C8-C10
15	b2	402	CLA	C6-C7-C8-C10
15	b4	402	CLA	C6-C7-C8-C10
15	b5	402	CLA	C6-C7-C8-C10
15	b6	403	CLA	C6-C7-C8-C10
15	c1	402	CLA	C6-C7-C8-C10
15	c3	402	CLA	C6-C7-C8-C10
15	c4	402	CLA	C6-C7-C8-C10
15	c5	402	CLA	C6-C7-C8-C10
15	c6	404	CLA	C6-C7-C8-C10
15	c4	407	CLA	CAA-CBA-CGA-O2A
15	b6	422	CLA	CBA-CGA-O2A-C1
15	cB	827	CLA	CBD-CGD-O2D-CED
15	aB	806	CLA	C10-C11-C12-C13
15	bB	806	CLA	C10-C11-C12-C13
18	aM	101	BCR	C15-C16-C17-C18
18	bM	101	BCR	C15-C16-C17-C18
18	cM	101	BCR	C15-C16-C17-C18
15	c2	418	CLA	CAA-CBA-CGA-O2A
15	c5	417	CLA	CAA-CBA-CGA-O2A
15	c6	419	CLA	CAA-CBA-CGA-O2A
15	aB	827	CLA	CBD-CGD-O2D-CED
15	bB	827	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	407	CLA	CAA-CBA-CGA-O2A
15	a1	402	CLA	O1A-CGA-O2A-C1
15	aK	102	CLA	O1D-CGD-O2D-CED
15	a4	407	CLA	CAA-CBA-CGA-O2A
15	b1	412	CLA	CAA-CBA-CGA-O2A
15	b5	407	CLA	CAA-CBA-CGA-O2A
15	c1	412	CLA	CAA-CBA-CGA-O2A
15	a2	418	CLA	CAA-CBA-CGA-O2A
15	a5	417	CLA	CAA-CBA-CGA-O2A
15	a6	418	CLA	CAA-CBA-CGA-O2A
15	b5	417	CLA	CAA-CBA-CGA-O2A
15	b6	418	CLA	CAA-CBA-CGA-O2A
15	c3	417	CLA	CAA-CBA-CGA-O2A
15	c4	417	CLA	CAA-CBA-CGA-O2A
15	a3	417	CLA	C2A-CAA-CBA-CGA
15	bB	816	CLA	C2A-CAA-CBA-CGA
15	c2	406	CLA	C16-C17-C18-C19
15	c6	401	CLA	C16-C17-C18-C19
15	aA	811	CLA	CAA-CBA-CGA-O2A
15	bA	811	CLA	CAA-CBA-CGA-O2A
15	b3	407	CLA	CAA-CBA-CGA-O2A
15	cA	811	CLA	CAA-CBA-CGA-O2A
18	aB	845	BCR	C11-C10-C9-C34
18	aB	846	BCR	C16-C17-C18-C36
18	bB	845	BCR	C11-C10-C9-C34
18	bB	846	BCR	C16-C17-C18-C36
18	b4	418	BCR	C16-C17-C18-C36
18	cB	845	BCR	C11-C10-C9-C34
18	cB	846	BCR	C16-C17-C18-C36
15	a3	417	CLA	CAA-CBA-CGA-O2A
15	a4	417	CLA	CAA-CBA-CGA-O2A
15	b1	417	CLA	CAA-CBA-CGA-O2A
15	b3	417	CLA	CAA-CBA-CGA-O2A
15	b4	417	CLA	CAA-CBA-CGA-O2A
15	c6	401	CLA	CAA-CBA-CGA-O2A
15	aA	830	CLA	C4-C3-C5-C6
15	bA	830	CLA	C4-C3-C5-C6
15	cA	830	CLA	C4-C3-C5-C6
16	aB	843	PQN	C14-C13-C15-C16
16	cB	843	PQN	C14-C13-C15-C16
15	b5	412	CLA	CAA-CBA-CGA-O2A
15	c3	407	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	809	CLA	C16-C17-C18-C19
15	bA	809	CLA	C16-C17-C18-C19
15	cA	809	CLA	C16-C17-C18-C19
15	a1	416	CLA	CAA-CBA-CGA-O2A
14	aA	801	CL0	C11-C12-C13-C14
14	bA	801	CL0	C11-C12-C13-C14
14	cA	801	CL0	C11-C12-C13-C14
15	aA	803	CLA	C6-C7-C8-C9
15	aA	826	CLA	C11-C10-C8-C9
15	aA	833	CLA	C6-C7-C8-C9
15	aB	810	CLA	C11-C10-C8-C9
15	aB	834	CLA	C6-C7-C8-C9
15	aL	203	CLA	C6-C7-C8-C9
15	a2	402	CLA	C6-C7-C8-C9
15	a3	402	CLA	C6-C7-C8-C9
15	bA	803	CLA	C6-C7-C8-C9
15	bA	826	CLA	C11-C10-C8-C9
15	bA	833	CLA	C6-C7-C8-C9
15	bB	810	CLA	C11-C10-C8-C9
15	bB	834	CLA	C6-C7-C8-C9
15	bL	204	CLA	C6-C7-C8-C9
15	cA	803	CLA	C6-C7-C8-C9
15	cA	826	CLA	C11-C10-C8-C9
15	cA	833	CLA	C6-C7-C8-C9
15	cB	810	CLA	C11-C10-C8-C9
15	cB	834	CLA	C6-C7-C8-C9
15	cL	204	CLA	C6-C7-C8-C9
15	a3	407	CLA	CAA-CBA-CGA-O2A
15	a5	412	CLA	CAA-CBA-CGA-O2A
15	b2	408	CLA	CAA-CBA-CGA-O2A
15	c2	408	CLA	CAA-CBA-CGA-O2A
15	aA	824	CLA	C3A-C2A-CAA-CBA
15	aA	827	CLA	C3A-C2A-CAA-CBA
15	aB	828	CLA	C3A-C2A-CAA-CBA
15	aL	202	CLA	C3A-C2A-CAA-CBA
15	a2	422	CLA	C3A-C2A-CAA-CBA
15	bA	824	CLA	C3A-C2A-CAA-CBA
15	bA	827	CLA	C3A-C2A-CAA-CBA
15	bB	828	CLA	C3A-C2A-CAA-CBA
15	bL	203	CLA	C3A-C2A-CAA-CBA
15	b2	422	CLA	C3A-C2A-CAA-CBA
15	cA	824	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cA	827	CLA	C3A-C2A-CAA-CBA
15	cB	828	CLA	C3A-C2A-CAA-CBA
15	cL	203	CLA	C3A-C2A-CAA-CBA
15	c2	422	CLA	C3A-C2A-CAA-CBA
15	b2	418	CLA	CAA-CBA-CGA-O2A
15	c1	417	CLA	CAA-CBA-CGA-O2A
15	aA	811	CLA	CAA-CBA-CGA-O1A
15	aA	844	CLA	CAA-CBA-CGA-O1A
15	a1	406	CLA	CAA-CBA-CGA-O1A
15	a2	408	CLA	CAA-CBA-CGA-O2A
15	a4	412	CLA	CAA-CBA-CGA-O2A
15	bA	844	CLA	CAA-CBA-CGA-O1A
15	b1	407	CLA	CAA-CBA-CGA-O1A
15	cA	843	CLA	CAA-CBA-CGA-O1A
15	c5	412	CLA	CAA-CBA-CGA-O2A
15	c6	409	CLA	CAA-CBA-CGA-O2A
15	aA	822	CLA	CAD-CBD-CGD-O2D
15	aA	823	CLA	CAD-CBD-CGD-O2D
15	aA	839	CLA	CAD-CBD-CGD-O2D
15	aA	845	CLA	CAD-CBD-CGD-O2D
15	aB	819	CLA	CAD-CBD-CGD-O2D
15	aB	823	CLA	CAD-CBD-CGD-O2D
15	aB	833	CLA	CAD-CBD-CGD-O2D
15	aB	834	CLA	CAD-CBD-CGD-O2D
15	a1	401	CLA	CAD-CBD-CGD-O2D
15	a1	408	CLA	CAD-CBD-CGD-O2D
15	a1	412	CLA	CAD-CBD-CGD-O2D
15	a2	402	CLA	CAD-CBD-CGD-O2D
15	a2	405	CLA	CAD-CBD-CGD-O2D
15	a2	406	CLA	CAD-CBD-CGD-O2D
15	a2	414	CLA	CAD-CBD-CGD-O2D
15	a3	402	CLA	CAD-CBD-CGD-O2D
15	a3	404	CLA	CAD-CBD-CGD-O2D
15	a3	411	CLA	CAD-CBD-CGD-O2D
15	a4	402	CLA	CAD-CBD-CGD-O2D
15	a4	411	CLA	CAD-CBD-CGD-O2D
15	a4	413	CLA	CAD-CBD-CGD-O2D
15	a4	421	CLA	CAD-CBD-CGD-O2D
15	a5	402	CLA	CAD-CBD-CGD-O2D
15	a5	405	CLA	CAD-CBD-CGD-O2D
15	a5	409	CLA	CAD-CBD-CGD-O2D
15	a5	420	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a6	403	CLA	CAD-CBD-CGD-O2D
15	a6	411	CLA	CAD-CBD-CGD-O2D
15	a6	414	CLA	CAD-CBD-CGD-O2D
15	a6	422	CLA	CAD-CBD-CGD-O2D
15	bA	822	CLA	CAD-CBD-CGD-O2D
15	bA	823	CLA	CAD-CBD-CGD-O2D
15	bA	839	CLA	CAD-CBD-CGD-O2D
15	bA	845	CLA	CAD-CBD-CGD-O2D
15	bB	819	CLA	CAD-CBD-CGD-O2D
15	bB	823	CLA	CAD-CBD-CGD-O2D
15	bB	833	CLA	CAD-CBD-CGD-O2D
15	bB	834	CLA	CAD-CBD-CGD-O2D
15	b1	402	CLA	CAD-CBD-CGD-O2D
15	b1	404	CLA	CAD-CBD-CGD-O2D
15	b1	409	CLA	CAD-CBD-CGD-O2D
15	b1	411	CLA	CAD-CBD-CGD-O2D
15	b1	413	CLA	CAD-CBD-CGD-O2D
15	b2	402	CLA	CAD-CBD-CGD-O2D
15	b2	405	CLA	CAD-CBD-CGD-O2D
15	b3	402	CLA	CAD-CBD-CGD-O2D
15	b4	402	CLA	CAD-CBD-CGD-O2D
15	b4	409	CLA	CAD-CBD-CGD-O2D
15	b4	411	CLA	CAD-CBD-CGD-O2D
15	b4	413	CLA	CAD-CBD-CGD-O2D
15	b4	421	CLA	CAD-CBD-CGD-O2D
15	b5	402	CLA	CAD-CBD-CGD-O2D
15	b5	405	CLA	CAD-CBD-CGD-O2D
15	b5	409	CLA	CAD-CBD-CGD-O2D
15	b5	420	CLA	CAD-CBD-CGD-O2D
15	b6	403	CLA	CAD-CBD-CGD-O2D
15	b6	414	CLA	CAD-CBD-CGD-O2D
15	cA	822	CLA	CAD-CBD-CGD-O2D
15	cA	823	CLA	CAD-CBD-CGD-O2D
15	cA	839	CLA	CAD-CBD-CGD-O2D
15	cA	844	CLA	CAD-CBD-CGD-O2D
15	cB	819	CLA	CAD-CBD-CGD-O2D
15	cB	823	CLA	CAD-CBD-CGD-O2D
15	cB	833	CLA	CAD-CBD-CGD-O2D
15	cB	834	CLA	CAD-CBD-CGD-O2D
15	c1	402	CLA	CAD-CBD-CGD-O2D
15	c1	409	CLA	CAD-CBD-CGD-O2D
15	c1	411	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c1	413	CLA	CAD-CBD-CGD-O2D
15	c2	402	CLA	CAD-CBD-CGD-O2D
15	c2	406	CLA	CAD-CBD-CGD-O2D
15	c2	414	CLA	CAD-CBD-CGD-O2D
15	c3	402	CLA	CAD-CBD-CGD-O2D
15	c3	411	CLA	CAD-CBD-CGD-O2D
15	c3	413	CLA	CAD-CBD-CGD-O2D
15	c4	402	CLA	CAD-CBD-CGD-O2D
15	c4	413	CLA	CAD-CBD-CGD-O2D
15	c4	421	CLA	CAD-CBD-CGD-O2D
15	c5	402	CLA	CAD-CBD-CGD-O2D
15	c5	405	CLA	CAD-CBD-CGD-O2D
15	c5	409	CLA	CAD-CBD-CGD-O2D
15	c5	420	CLA	CAD-CBD-CGD-O2D
15	c6	404	CLA	CAD-CBD-CGD-O2D
15	c6	412	CLA	CAD-CBD-CGD-O2D
15	c6	415	CLA	CAD-CBD-CGD-O2D
15	b3	417	CLA	C2A-CAA-CBA-CGA
15	aB	806	CLA	C2-C1-O2A-CGA
15	bB	806	CLA	C2-C1-O2A-CGA
15	cB	806	CLA	C2-C1-O2A-CGA
15	a6	408	CLA	CAA-CBA-CGA-O2A
15	bA	811	CLA	CAA-CBA-CGA-O1A
15	b6	408	CLA	CAA-CBA-CGA-O2A
15	cA	811	CLA	CAA-CBA-CGA-O1A
15	aA	809	CLA	CAA-CBA-CGA-O2A
15	bA	809	CLA	CAA-CBA-CGA-O2A
15	cA	809	CLA	CAA-CBA-CGA-O2A
18	b5	418	BCR	C22-C23-C24-C25
18	c5	418	BCR	C22-C23-C24-C25
15	aB	814	CLA	C4-C3-C5-C6
15	bB	814	CLA	C4-C3-C5-C6
15	cB	814	CLA	C4-C3-C5-C6
16	bB	843	PQN	C14-C13-C15-C16
15	b1	409	CLA	C16-C17-C18-C20
15	a5	407	CLA	CAA-CBA-CGA-O1A
15	c2	413	CLA	CAA-CBA-CGA-O2A
15	c6	414	CLA	CAA-CBA-CGA-O2A
15	aA	810	CLA	C2-C3-C5-C6
15	aB	811	CLA	C2-C3-C5-C6
15	aB	818	CLA	C2-C3-C5-C6
15	aB	837	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	810	CLA	C2-C3-C5-C6
15	bB	811	CLA	C2-C3-C5-C6
15	bB	818	CLA	C2-C3-C5-C6
15	bB	837	CLA	C2-C3-C5-C6
15	cA	810	CLA	C2-C3-C5-C6
15	cB	811	CLA	C2-C3-C5-C6
15	cB	818	CLA	C2-C3-C5-C6
15	cB	837	CLA	C2-C3-C5-C6
15	aA	806	CLA	CAA-CBA-CGA-O2A
15	aB	807	CLA	CAA-CBA-CGA-O2A
15	bA	806	CLA	CAA-CBA-CGA-O2A
15	bB	807	CLA	CAA-CBA-CGA-O2A
15	cA	806	CLA	CAA-CBA-CGA-O2A
15	cB	807	CLA	CAA-CBA-CGA-O2A
18	aA	852	BCR	C11-C12-C13-C14
18	aB	845	BCR	C11-C12-C13-C14
18	aJ	205	BCR	C21-C22-C23-C24
18	bA	853	BCR	C11-C12-C13-C14
18	bB	845	BCR	C11-C12-C13-C14
18	bJ	104	BCR	C21-C22-C23-C24
18	cA	851	BCR	C11-C12-C13-C14
18	cB	845	BCR	C11-C12-C13-C14
18	cJ	104	BCR	C21-C22-C23-C24
15	a2	408	CLA	CAA-CBA-CGA-O1A
15	a3	407	CLA	CAA-CBA-CGA-O1A
15	a3	412	CLA	CAA-CBA-CGA-O2A
15	b3	412	CLA	CAA-CBA-CGA-O2A
15	b6	413	CLA	CAA-CBA-CGA-O2A
15	c1	407	CLA	CAA-CBA-CGA-O1A
15	c5	407	CLA	CAA-CBA-CGA-O1A
15	aA	818	CLA	C3-C5-C6-C7
15	bA	818	CLA	C3-C5-C6-C7
15	bB	806	CLA	CAA-CBA-CGA-O1A
15	cB	806	CLA	CAA-CBA-CGA-O1A
15	a2	413	CLA	CAA-CBA-CGA-O2A
15	a6	413	CLA	CAA-CBA-CGA-O2A
15	b2	408	CLA	CAA-CBA-CGA-O1A
15	b2	413	CLA	CAA-CBA-CGA-O2A
15	b4	412	CLA	CAA-CBA-CGA-O2A
15	c3	407	CLA	CAA-CBA-CGA-O1A
15	c3	412	CLA	CAA-CBA-CGA-O2A
15	c4	412	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	O2A-C1-C2-C3
15	aA	827	CLA	O2A-C1-C2-C3
15	aA	829	CLA	O2A-C1-C2-C3
15	aB	805	CLA	O2A-C1-C2-C3
15	aB	825	CLA	O2A-C1-C2-C3
15	a2	410	CLA	O2A-C1-C2-C3
15	bA	803	CLA	O2A-C1-C2-C3
15	bA	827	CLA	O2A-C1-C2-C3
15	bA	829	CLA	O2A-C1-C2-C3
15	bB	805	CLA	O2A-C1-C2-C3
15	bB	825	CLA	O2A-C1-C2-C3
15	b2	410	CLA	O2A-C1-C2-C3
15	cA	803	CLA	O2A-C1-C2-C3
15	cA	827	CLA	O2A-C1-C2-C3
15	cA	829	CLA	O2A-C1-C2-C3
15	cB	805	CLA	O2A-C1-C2-C3
15	cB	825	CLA	O2A-C1-C2-C3
15	c4	409	CLA	O2A-C1-C2-C3
15	c3	417	CLA	C2A-CAA-CBA-CGA
15	aB	806	CLA	CAA-CBA-CGA-O1A
15	b1	417	CLA	C3-C5-C6-C7
15	cA	818	CLA	C3-C5-C6-C7
15	aA	837	CLA	CAA-CBA-CGA-O2A
15	a1	411	CLA	CAA-CBA-CGA-O1A
15	a2	413	CLA	CAA-CBA-CGA-O1A
15	a4	407	CLA	CAA-CBA-CGA-O1A
15	a6	408	CLA	CAA-CBA-CGA-O1A
15	a6	413	CLA	CAA-CBA-CGA-O1A
15	bA	837	CLA	CAA-CBA-CGA-O2A
15	b2	413	CLA	CAA-CBA-CGA-O1A
15	b3	407	CLA	CAA-CBA-CGA-O1A
15	b4	407	CLA	CAA-CBA-CGA-O1A
15	b5	407	CLA	CAA-CBA-CGA-O1A
15	b6	408	CLA	CAA-CBA-CGA-O1A
15	b6	413	CLA	CAA-CBA-CGA-O1A
15	cA	837	CLA	CAA-CBA-CGA-O2A
15	c1	412	CLA	CAA-CBA-CGA-O1A
15	c2	408	CLA	CAA-CBA-CGA-O1A
15	c4	407	CLA	CAA-CBA-CGA-O1A
15	c6	409	CLA	CAA-CBA-CGA-O1A
15	aB	839	CLA	C13-C15-C16-C17
15	c2	418	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	408	CLA	C16-C17-C18-C20
14	aA	801	CL0	CHA-CBD-CGD-O1D
14	aA	801	CL0	CHA-CBD-CGD-O2D
14	bA	801	CL0	CHA-CBD-CGD-O1D
14	bA	801	CL0	CHA-CBD-CGD-O2D
14	cA	801	CL0	CHA-CBD-CGD-O1D
14	cA	801	CL0	CHA-CBD-CGD-O2D
15	aA	803	CLA	CHA-CBD-CGD-O1D
15	aA	803	CLA	CHA-CBD-CGD-O2D
15	aA	815	CLA	CHA-CBD-CGD-O1D
15	aA	828	CLA	CHA-CBD-CGD-O2D
15	aA	838	CLA	CHA-CBD-CGD-O2D
15	aB	804	CLA	CHA-CBD-CGD-O1D
15	aB	804	CLA	CHA-CBD-CGD-O2D
15	aB	805	CLA	CHA-CBD-CGD-O1D
15	aB	808	CLA	CHA-CBD-CGD-O2D
15	aB	810	CLA	CHA-CBD-CGD-O1D
15	aB	810	CLA	CHA-CBD-CGD-O2D
15	aB	811	CLA	CHA-CBD-CGD-O2D
15	aB	821	CLA	CHA-CBD-CGD-O1D
15	aB	821	CLA	CHA-CBD-CGD-O2D
15	aB	824	CLA	CHA-CBD-CGD-O1D
15	aB	824	CLA	CHA-CBD-CGD-O2D
15	aB	826	CLA	CHA-CBD-CGD-O2D
15	aB	827	CLA	CHA-CBD-CGD-O2D
15	aB	831	CLA	CHA-CBD-CGD-O2D
15	aJ	201	CLA	CHA-CBD-CGD-O1D
15	aJ	201	CLA	CHA-CBD-CGD-O2D
15	aK	102	CLA	CHA-CBD-CGD-O2D
15	aL	203	CLA	CHA-CBD-CGD-O1D
15	aL	203	CLA	CHA-CBD-CGD-O2D
15	a1	402	CLA	CHA-CBD-CGD-O2D
15	a1	403	CLA	CHA-CBD-CGD-O1D
15	a1	405	CLA	CHA-CBD-CGD-O1D
15	a1	405	CLA	CHA-CBD-CGD-O2D
15	a1	411	CLA	CHA-CBD-CGD-O2D
15	a2	403	CLA	CHA-CBD-CGD-O2D
15	a2	404	CLA	CHA-CBD-CGD-O1D
15	a2	407	CLA	CHA-CBD-CGD-O1D
15	a2	407	CLA	CHA-CBD-CGD-O2D
15	a2	413	CLA	CHA-CBD-CGD-O2D
15	a3	406	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a3	406	CLA	CHA-CBD-CGD-O2D
15	a3	412	CLA	CHA-CBD-CGD-O2D
15	a4	403	CLA	CHA-CBD-CGD-O2D
15	a4	404	CLA	CHA-CBD-CGD-O1D
15	a4	406	CLA	CHA-CBD-CGD-O1D
15	a4	406	CLA	CHA-CBD-CGD-O2D
15	a4	412	CLA	CHA-CBD-CGD-O2D
15	a5	403	CLA	CHA-CBD-CGD-O2D
15	a5	404	CLA	CHA-CBD-CGD-O1D
15	a5	406	CLA	CHA-CBD-CGD-O1D
15	a5	406	CLA	CHA-CBD-CGD-O2D
15	a5	412	CLA	CHA-CBD-CGD-O2D
15	a6	404	CLA	CHA-CBD-CGD-O2D
15	a6	405	CLA	CHA-CBD-CGD-O1D
15	a6	407	CLA	CHA-CBD-CGD-O1D
15	a6	407	CLA	CHA-CBD-CGD-O2D
15	bA	803	CLA	CHA-CBD-CGD-O1D
15	bA	815	CLA	CHA-CBD-CGD-O1D
15	bA	828	CLA	CHA-CBD-CGD-O2D
15	bA	838	CLA	CHA-CBD-CGD-O2D
15	bB	804	CLA	CHA-CBD-CGD-O1D
15	bB	804	CLA	CHA-CBD-CGD-O2D
15	bB	805	CLA	CHA-CBD-CGD-O1D
15	bB	808	CLA	CHA-CBD-CGD-O2D
15	bB	810	CLA	CHA-CBD-CGD-O1D
15	bB	810	CLA	CHA-CBD-CGD-O2D
15	bB	811	CLA	CHA-CBD-CGD-O2D
15	bB	821	CLA	CHA-CBD-CGD-O1D
15	bB	821	CLA	CHA-CBD-CGD-O2D
15	bB	824	CLA	CHA-CBD-CGD-O1D
15	bB	824	CLA	CHA-CBD-CGD-O2D
15	bB	826	CLA	CHA-CBD-CGD-O2D
15	bB	827	CLA	CHA-CBD-CGD-O2D
15	bB	831	CLA	CHA-CBD-CGD-O2D
15	bF	201	CLA	CHA-CBD-CGD-O1D
15	bF	201	CLA	CHA-CBD-CGD-O2D
15	bK	101	CLA	CHA-CBD-CGD-O2D
15	bL	204	CLA	CHA-CBD-CGD-O1D
15	bL	204	CLA	CHA-CBD-CGD-O2D
15	b1	403	CLA	CHA-CBD-CGD-O2D
15	b1	404	CLA	CHA-CBD-CGD-O1D
15	b1	406	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b1	406	CLA	CHA-CBD-CGD-O2D
15	b1	412	CLA	CHA-CBD-CGD-O2D
15	b2	403	CLA	CHA-CBD-CGD-O2D
15	b2	404	CLA	CHA-CBD-CGD-O1D
15	b2	407	CLA	CHA-CBD-CGD-O1D
15	b2	407	CLA	CHA-CBD-CGD-O2D
15	b2	413	CLA	CHA-CBD-CGD-O2D
15	b3	406	CLA	CHA-CBD-CGD-O1D
15	b3	406	CLA	CHA-CBD-CGD-O2D
15	b3	412	CLA	CHA-CBD-CGD-O2D
15	b4	403	CLA	CHA-CBD-CGD-O2D
15	b4	404	CLA	CHA-CBD-CGD-O1D
15	b4	406	CLA	CHA-CBD-CGD-O1D
15	b4	406	CLA	CHA-CBD-CGD-O2D
15	b4	412	CLA	CHA-CBD-CGD-O2D
15	b5	403	CLA	CHA-CBD-CGD-O2D
15	b5	404	CLA	CHA-CBD-CGD-O1D
15	b5	406	CLA	CHA-CBD-CGD-O1D
15	b5	406	CLA	CHA-CBD-CGD-O2D
15	b5	412	CLA	CHA-CBD-CGD-O2D
15	b6	404	CLA	CHA-CBD-CGD-O2D
15	b6	405	CLA	CHA-CBD-CGD-O1D
15	b6	407	CLA	CHA-CBD-CGD-O1D
15	b6	407	CLA	CHA-CBD-CGD-O2D
15	b6	422	CLA	CHA-CBD-CGD-O1D
15	cA	803	CLA	CHA-CBD-CGD-O1D
15	cA	815	CLA	CHA-CBD-CGD-O1D
15	cA	828	CLA	CHA-CBD-CGD-O2D
15	cA	838	CLA	CHA-CBD-CGD-O2D
15	cB	804	CLA	CHA-CBD-CGD-O1D
15	cB	804	CLA	CHA-CBD-CGD-O2D
15	cB	805	CLA	CHA-CBD-CGD-O1D
15	cB	808	CLA	CHA-CBD-CGD-O2D
15	cB	810	CLA	CHA-CBD-CGD-O1D
15	cB	810	CLA	CHA-CBD-CGD-O2D
15	cB	811	CLA	CHA-CBD-CGD-O2D
15	cB	821	CLA	CHA-CBD-CGD-O1D
15	cB	821	CLA	CHA-CBD-CGD-O2D
15	cB	824	CLA	CHA-CBD-CGD-O1D
15	cB	824	CLA	CHA-CBD-CGD-O2D
15	cB	826	CLA	CHA-CBD-CGD-O2D
15	cB	827	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	831	CLA	CHA-CBD-CGD-O2D
15	cF	203	CLA	CHA-CBD-CGD-O1D
15	cF	203	CLA	CHA-CBD-CGD-O2D
15	cK	102	CLA	CHA-CBD-CGD-O2D
15	cL	204	CLA	CHA-CBD-CGD-O1D
15	cL	204	CLA	CHA-CBD-CGD-O2D
15	c1	403	CLA	CHA-CBD-CGD-O2D
15	c1	404	CLA	CHA-CBD-CGD-O1D
15	c1	406	CLA	CHA-CBD-CGD-O1D
15	c1	406	CLA	CHA-CBD-CGD-O2D
15	c1	412	CLA	CHA-CBD-CGD-O2D
15	c2	403	CLA	CHA-CBD-CGD-O2D
15	c2	404	CLA	CHA-CBD-CGD-O1D
15	c2	407	CLA	CHA-CBD-CGD-O1D
15	c2	407	CLA	CHA-CBD-CGD-O2D
15	c2	413	CLA	CHA-CBD-CGD-O2D
15	c3	406	CLA	CHA-CBD-CGD-O1D
15	c3	406	CLA	CHA-CBD-CGD-O2D
15	c3	412	CLA	CHA-CBD-CGD-O2D
15	c4	403	CLA	CHA-CBD-CGD-O2D
15	c4	406	CLA	CHA-CBD-CGD-O1D
15	c4	406	CLA	CHA-CBD-CGD-O2D
15	c4	412	CLA	CHA-CBD-CGD-O2D
15	c5	403	CLA	CHA-CBD-CGD-O2D
15	c5	404	CLA	CHA-CBD-CGD-O1D
15	c5	406	CLA	CHA-CBD-CGD-O1D
15	c5	406	CLA	CHA-CBD-CGD-O2D
15	c5	412	CLA	CHA-CBD-CGD-O2D
15	c6	405	CLA	CHA-CBD-CGD-O2D
15	c6	406	CLA	CHA-CBD-CGD-O1D
15	c6	408	CLA	CHA-CBD-CGD-O1D
15	c6	408	CLA	CHA-CBD-CGD-O2D
15	bB	839	CLA	C13-C15-C16-C17
15	b2	418	CLA	C5-C6-C7-C8
15	cB	839	CLA	C13-C15-C16-C17
15	a3	412	CLA	CAA-CBA-CGA-O1A
15	b4	412	CLA	CAA-CBA-CGA-O1A
15	cA	837	CLA	CAA-CBA-CGA-O1A
15	c3	412	CLA	CAA-CBA-CGA-O1A
15	c6	414	CLA	CAA-CBA-CGA-O1A
15	aB	821	CLA	CAA-CBA-CGA-O2A
15	bB	821	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a1	402	CLA	CBA-CGA-O2A-C1
15	bB	808	CLA	C3-C5-C6-C7
15	aA	837	CLA	CAA-CBA-CGA-O1A
15	a4	412	CLA	CAA-CBA-CGA-O1A
15	bA	837	CLA	CAA-CBA-CGA-O1A
15	b3	412	CLA	CAA-CBA-CGA-O1A
15	c2	413	CLA	CAA-CBA-CGA-O1A
15	c4	412	CLA	CAA-CBA-CGA-O1A
15	c5	412	CLA	CAA-CBA-CGA-O1A
15	aB	823	CLA	CAA-CBA-CGA-O2A
15	a6	422	CLA	CAA-CBA-CGA-O2A
15	bB	823	CLA	CAA-CBA-CGA-O2A
15	cB	821	CLA	CAA-CBA-CGA-O2A
15	b1	403	CLA	O1A-CGA-O2A-C1
15	b1	412	CLA	CAA-CBA-CGA-O1A
15	c1	403	CLA	O1A-CGA-O2A-C1
15	aA	824	CLA	CAA-CBA-CGA-O2A
15	bA	824	CLA	CAA-CBA-CGA-O2A
15	bB	834	CLA	CAA-CBA-CGA-O2A
15	cA	824	CLA	CAA-CBA-CGA-O2A
15	cB	823	CLA	CAA-CBA-CGA-O2A
15	cB	834	CLA	CAA-CBA-CGA-O2A
15	c1	409	CLA	C16-C17-C18-C20
15	a2	418	CLA	C5-C6-C7-C8
15	cA	819	CLA	C5-C6-C7-C8
15	aB	808	CLA	C3-C5-C6-C7
15	cB	808	CLA	C3-C5-C6-C7
15	aB	834	CLA	CAA-CBA-CGA-O2A
15	b6	422	CLA	CAA-CBA-CGA-O2A
15	aB	806	CLA	C4-C3-C5-C6
15	bB	806	CLA	C4-C3-C5-C6
15	cB	806	CLA	C4-C3-C5-C6
15	aA	819	CLA	C5-C6-C7-C8
15	bA	819	CLA	C5-C6-C7-C8
15	bB	807	CLA	CAA-CBA-CGA-O1A
15	aB	806	CLA	C6-C7-C8-C10
15	aL	201	CLA	C2-C3-C5-C6
15	a2	402	CLA	C6-C7-C8-C10
15	a3	402	CLA	C6-C7-C8-C10
15	bB	806	CLA	C6-C7-C8-C10
15	bL	202	CLA	C2-C3-C5-C6
15	b3	402	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b3	421	CLA	C12-C13-C15-C16
15	cB	806	CLA	C6-C7-C8-C10
15	cL	202	CLA	C2-C3-C5-C6
15	c2	402	CLA	C6-C7-C8-C10
15	c2	410	CLA	C16-C17-C18-C20
15	a4	410	CLA	C13-C15-C16-C17
15	c4	410	CLA	C13-C15-C16-C17
15	b5	412	CLA	CAA-CBA-CGA-O1A
15	aA	802	CLA	C6-C7-C8-C9
15	aA	825	CLA	C11-C10-C8-C9
15	aL	201	CLA	C11-C10-C8-C9
15	a1	401	CLA	C6-C7-C8-C9
15	a3	421	CLA	C14-C13-C15-C16
15	a4	402	CLA	C6-C7-C8-C9
15	a5	402	CLA	C6-C7-C8-C9
15	a6	403	CLA	C6-C7-C8-C9
15	bA	802	CLA	C6-C7-C8-C9
15	bA	825	CLA	C11-C10-C8-C9
15	bL	202	CLA	C11-C10-C8-C9
15	b1	402	CLA	C6-C7-C8-C9
15	b2	402	CLA	C6-C7-C8-C9
15	b3	402	CLA	C6-C7-C8-C9
15	b3	421	CLA	C14-C13-C15-C16
15	b4	402	CLA	C6-C7-C8-C9
15	b5	402	CLA	C6-C7-C8-C9
15	b6	403	CLA	C6-C7-C8-C9
15	cA	802	CLA	C6-C7-C8-C9
15	cA	825	CLA	C11-C10-C8-C9
15	cL	202	CLA	C11-C10-C8-C9
15	c1	402	CLA	C6-C7-C8-C9
15	c2	402	CLA	C6-C7-C8-C9
15	c3	402	CLA	C6-C7-C8-C9
15	c3	421	CLA	C14-C13-C15-C16
15	c4	402	CLA	C6-C7-C8-C9
15	c5	402	CLA	C6-C7-C8-C9
15	c6	404	CLA	C6-C7-C8-C9
15	cB	807	CLA	CAA-CBA-CGA-O1A
18	aA	848	BCR	C19-C20-C21-C22
18	bA	849	BCR	C19-C20-C21-C22
18	cA	847	BCR	C19-C20-C21-C22
15	a1	406	CLA	C2B-C3B-CAB-CBB
15	c1	407	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a5	417	CLA	CAA-CBA-CGA-O1A
15	a3	417	CLA	C3-C5-C6-C7
15	cA	807	CLA	C3-C5-C6-C7
15	c3	417	CLA	C3-C5-C6-C7
15	a5	412	CLA	CAA-CBA-CGA-O1A
15	aA	806	CLA	CAA-CBA-CGA-O1A
15	aB	807	CLA	CAA-CBA-CGA-O1A
15	bA	806	CLA	CAA-CBA-CGA-O1A
15	cA	806	CLA	CAA-CBA-CGA-O1A
15	c5	417	CLA	CAA-CBA-CGA-O1A
15	aB	804	CLA	C4C-C3C-CAC-CBC
15	cB	804	CLA	C4C-C3C-CAC-CBC
15	aA	807	CLA	C3-C5-C6-C7
15	bA	807	CLA	C3-C5-C6-C7
15	c4	417	CLA	CAA-CBA-CGA-O1A
15	a5	410	CLA	C5-C6-C7-C8
15	a5	410	CLA	C8-C10-C11-C12
15	b4	410	CLA	C5-C6-C7-C8
15	b6	411	CLA	C5-C6-C7-C8
15	aA	829	CLA	C4-C3-C5-C6
15	bA	829	CLA	C4-C3-C5-C6
15	cA	829	CLA	C4-C3-C5-C6
15	bB	804	CLA	C4C-C3C-CAC-CBC
15	b1	403	CLA	CBA-CGA-O2A-C1
15	c1	403	CLA	CBA-CGA-O2A-C1
15	aB	810	CLA	C15-C16-C17-C18
15	a4	410	CLA	C5-C6-C7-C8
15	bB	810	CLA	C15-C16-C17-C18
15	cB	810	CLA	C15-C16-C17-C18
15	c6	412	CLA	C5-C6-C7-C8
15	b6	418	CLA	C3-C5-C6-C7
15	aA	803	CLA	C1A-C2A-CAA-CBA
15	aA	814	CLA	C1A-C2A-CAA-CBA
15	aA	824	CLA	C1A-C2A-CAA-CBA
15	aA	830	CLA	C1A-C2A-CAA-CBA
15	aB	816	CLA	C1A-C2A-CAA-CBA
15	aB	822	CLA	C1A-C2A-CAA-CBA
15	aB	828	CLA	C1A-C2A-CAA-CBA
15	aL	202	CLA	C1A-C2A-CAA-CBA
15	a2	404	CLA	C1A-C2A-CAA-CBA
15	a3	413	CLA	C1A-C2A-CAA-CBA
15	a4	413	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	803	CLA	C1A-C2A-CAA-CBA
15	bA	814	CLA	C1A-C2A-CAA-CBA
15	bA	824	CLA	C1A-C2A-CAA-CBA
15	bA	830	CLA	C1A-C2A-CAA-CBA
15	bB	816	CLA	C1A-C2A-CAA-CBA
15	bB	822	CLA	C1A-C2A-CAA-CBA
15	bB	828	CLA	C1A-C2A-CAA-CBA
15	bL	203	CLA	C1A-C2A-CAA-CBA
15	b1	404	CLA	C1A-C2A-CAA-CBA
15	b2	414	CLA	C1A-C2A-CAA-CBA
15	b3	404	CLA	C1A-C2A-CAA-CBA
15	b3	413	CLA	C1A-C2A-CAA-CBA
15	b4	404	CLA	C1A-C2A-CAA-CBA
15	cA	803	CLA	C1A-C2A-CAA-CBA
15	cA	814	CLA	C1A-C2A-CAA-CBA
15	cA	824	CLA	C1A-C2A-CAA-CBA
15	cA	830	CLA	C1A-C2A-CAA-CBA
15	cB	816	CLA	C1A-C2A-CAA-CBA
15	cB	822	CLA	C1A-C2A-CAA-CBA
15	cB	828	CLA	C1A-C2A-CAA-CBA
15	cL	203	CLA	C1A-C2A-CAA-CBA
15	c2	414	CLA	C1A-C2A-CAA-CBA
15	c3	404	CLA	C1A-C2A-CAA-CBA
15	c3	413	CLA	C1A-C2A-CAA-CBA
15	c4	404	CLA	C1A-C2A-CAA-CBA
15	a2	406	CLA	C16-C17-C18-C19
15	a4	417	CLA	CAA-CBA-CGA-O1A
15	b5	417	CLA	CAA-CBA-CGA-O1A
15	c6	419	CLA	CAA-CBA-CGA-O1A
20	bB	851	LMG	C21-C22-C23-C24
20	cB	850	LMG	C21-C22-C23-C24
15	aB	832	CLA	C2-C1-O2A-CGA
15	bB	832	CLA	C2-C1-O2A-CGA
15	cB	832	CLA	C2-C1-O2A-CGA
20	aB	850	LMG	C21-C22-C23-C24
15	a1	409	CLA	C8-C10-C11-C12
15	a2	418	CLA	CAA-CBA-CGA-O1A
15	a6	418	CLA	CAA-CBA-CGA-O1A
15	b1	417	CLA	CAA-CBA-CGA-O1A
15	b4	417	CLA	CAA-CBA-CGA-O1A
15	b6	418	CLA	CAA-CBA-CGA-O1A
15	c2	418	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c6	401	CLA	CAA-CBA-CGA-O1A
15	aB	813	CLA	CAA-CBA-CGA-O2A
15	bB	813	CLA	CAA-CBA-CGA-O2A
15	cB	813	CLA	CAA-CBA-CGA-O2A
15	aB	817	CLA	C2A-CAA-CBA-CGA
15	bB	817	CLA	C2A-CAA-CBA-CGA
15	cB	817	CLA	C2A-CAA-CBA-CGA
15	aB	821	CLA	CAA-CBA-CGA-O1A
15	a3	417	CLA	CAA-CBA-CGA-O1A
15	bB	821	CLA	CAA-CBA-CGA-O1A
15	b3	417	CLA	CAA-CBA-CGA-O1A
15	b6	422	CLA	CAA-CBA-CGA-O1A
15	cB	821	CLA	CAA-CBA-CGA-O1A
15	c1	417	CLA	CAA-CBA-CGA-O1A
15	c3	417	CLA	CAA-CBA-CGA-O1A
15	bB	830	CLA	C15-C16-C17-C18
15	b5	410	CLA	C5-C6-C7-C8
15	c1	410	CLA	C8-C10-C11-C12
15	bF	201	CLA	CAA-CBA-CGA-O2A
15	b1	410	CLA	C8-C10-C11-C12
16	aA	846	PQN	C25-C26-C27-C28
15	a6	418	CLA	C3-C5-C6-C7
15	b3	417	CLA	C3-C5-C6-C7
15	c6	419	CLA	C3-C5-C6-C7
15	a1	416	CLA	CAA-CBA-CGA-O1A
15	aJ	201	CLA	CAA-CBA-CGA-O2A
15	cF	203	CLA	CAA-CBA-CGA-O2A
15	aB	830	CLA	C15-C16-C17-C18
15	cB	830	CLA	C15-C16-C17-C18
16	bA	846	PQN	C25-C26-C27-C28
16	cA	845	PQN	C25-C26-C27-C28
15	aA	807	CLA	C4B-C3B-CAB-CBB
15	aB	836	CLA	C4B-C3B-CAB-CBB
15	bA	807	CLA	C4B-C3B-CAB-CBB
15	bB	836	CLA	C4B-C3B-CAB-CBB
15	cA	807	CLA	C4B-C3B-CAB-CBB
15	cB	836	CLA	C4B-C3B-CAB-CBB
15	aA	829	CLA	CAA-CBA-CGA-O1A
15	bA	829	CLA	CAA-CBA-CGA-O1A
15	b2	418	CLA	CAA-CBA-CGA-O1A
15	cA	829	CLA	CAA-CBA-CGA-O1A
15	aA	817	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bA	817	CLA	O2A-C1-C2-C3
15	cA	817	CLA	O2A-C1-C2-C3
15	b2	422	CLA	CAA-CBA-CGA-O2A
15	b4	410	CLA	C13-C15-C16-C17
15	aX	102	CLA	CAA-CBA-CGA-O2A
15	bX	102	CLA	CAA-CBA-CGA-O2A
15	cX	102	CLA	CAA-CBA-CGA-O2A
18	aF	201	BCR	C5-C6-C7-C8
18	aF	202	BCR	C23-C24-C25-C26
18	aK	101	BCR	C23-C24-C25-C26
18	bA	848	BCR	C23-C24-C25-C26
18	bB	849	BCR	C5-C6-C7-C8
18	bF	202	BCR	C23-C24-C25-C26
18	b6	402	BCR	C5-C6-C7-C8
18	cF	202	BCR	C5-C6-C7-C8
18	cF	204	BCR	C23-C24-C25-C26
18	cK	101	BCR	C23-C24-C25-C26
15	aA	820	CLA	C15-C16-C17-C18
15	bA	820	CLA	C15-C16-C17-C18
15	b5	410	CLA	C8-C10-C11-C12
15	cA	820	CLA	C15-C16-C17-C18
15	c4	410	CLA	C5-C6-C7-C8
15	aB	820	CLA	C8-C10-C11-C12
15	cB	820	CLA	C8-C10-C11-C12
15	c3	409	CLA	C16-C17-C18-C20
18	a3	418	BCR	C18-C19-C20-C21
18	a3	419	BCR	C18-C19-C20-C21
18	b2	420	BCR	C18-C19-C20-C21
18	b3	419	BCR	C18-C19-C20-C21
15	aA	809	CLA	CAA-CBA-CGA-O1A
15	bA	809	CLA	CAA-CBA-CGA-O1A
15	bB	817	CLA	O1D-CGD-O2D-CED
15	bB	820	CLA	C8-C10-C11-C12
15	a3	404	CLA	C10-C11-C12-C13
15	cA	809	CLA	CAA-CBA-CGA-O1A
15	aA	804	CLA	C13-C15-C16-C17
15	cA	804	CLA	C13-C15-C16-C17
15	aA	815	CLA	CAD-CBD-CGD-O1D
15	aA	828	CLA	CAD-CBD-CGD-O1D
15	aA	838	CLA	C2-C3-C5-C6
15	aB	815	CLA	CAD-CBD-CGD-O1D
15	aB	827	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	aB	834	CLA	CAD-CBD-CGD-O1D
15	aK	102	CLA	CAD-CBD-CGD-O1D
15	aL	203	CLA	CAD-CBD-CGD-O1D
15	a1	403	CLA	CAD-CBD-CGD-O1D
15	a1	414	CLA	CAD-CBD-CGD-O1D
15	a2	404	CLA	CAD-CBD-CGD-O1D
15	a2	410	CLA	CAD-CBD-CGD-O1D
15	a2	416	CLA	CAD-CBD-CGD-O1D
15	a3	409	CLA	CAD-CBD-CGD-O1D
15	a3	415	CLA	CAD-CBD-CGD-O1D
15	a4	404	CLA	CAD-CBD-CGD-O1D
15	a4	415	CLA	CAD-CBD-CGD-O1D
15	a5	404	CLA	CAD-CBD-CGD-O1D
15	a6	405	CLA	CAD-CBD-CGD-O1D
15	a6	410	CLA	CAD-CBD-CGD-O1D
15	a6	416	CLA	CAD-CBD-CGD-O1D
15	a6	422	CLA	CAD-CBD-CGD-O1D
15	bA	815	CLA	CAD-CBD-CGD-O1D
15	bA	828	CLA	CAD-CBD-CGD-O1D
15	bA	838	CLA	C2-C3-C5-C6
15	bB	815	CLA	CAD-CBD-CGD-O1D
15	bB	827	CLA	CAD-CBD-CGD-O1D
15	bB	834	CLA	CAD-CBD-CGD-O1D
15	bK	101	CLA	CAD-CBD-CGD-O1D
15	bL	204	CLA	CAD-CBD-CGD-O1D
15	b1	404	CLA	CAD-CBD-CGD-O1D
15	b1	415	CLA	CAD-CBD-CGD-O1D
15	b2	404	CLA	CAD-CBD-CGD-O1D
15	b2	410	CLA	CAD-CBD-CGD-O1D
15	b2	416	CLA	CAD-CBD-CGD-O1D
15	b3	404	CLA	CAD-CBD-CGD-O1D
15	b3	409	CLA	CAD-CBD-CGD-O1D
15	b3	415	CLA	CAD-CBD-CGD-O1D
15	b4	404	CLA	CAD-CBD-CGD-O1D
15	b4	415	CLA	CAD-CBD-CGD-O1D
15	b5	404	CLA	CAD-CBD-CGD-O1D
15	b6	405	CLA	CAD-CBD-CGD-O1D
15	b6	410	CLA	CAD-CBD-CGD-O1D
15	b6	416	CLA	CAD-CBD-CGD-O1D
15	b6	422	CLA	CAD-CBD-CGD-O1D
15	cA	828	CLA	CAD-CBD-CGD-O1D
15	cA	838	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	815	CLA	CAD-CBD-CGD-O1D
15	cB	827	CLA	CAD-CBD-CGD-O1D
15	cB	834	CLA	CAD-CBD-CGD-O1D
15	cK	102	CLA	CAD-CBD-CGD-O1D
15	cL	204	CLA	CAD-CBD-CGD-O1D
15	c1	404	CLA	CAD-CBD-CGD-O1D
15	c1	415	CLA	CAD-CBD-CGD-O1D
15	c2	404	CLA	CAD-CBD-CGD-O1D
15	c2	410	CLA	CAD-CBD-CGD-O1D
15	c2	416	CLA	CAD-CBD-CGD-O1D
15	c3	409	CLA	CAD-CBD-CGD-O1D
15	c3	415	CLA	CAD-CBD-CGD-O1D
15	c4	404	CLA	CAD-CBD-CGD-O1D
15	c4	415	CLA	CAD-CBD-CGD-O1D
15	c5	404	CLA	CAD-CBD-CGD-O1D
15	c6	401	CLA	CAD-CBD-CGD-O1D
15	c6	406	CLA	CAD-CBD-CGD-O1D
15	c6	411	CLA	CAD-CBD-CGD-O1D
15	c6	417	CLA	CAD-CBD-CGD-O1D
15	aA	843	CLA	CAA-CBA-CGA-O2A
15	cA	842	CLA	CAA-CBA-CGA-O2A
15	aA	802	CLA	C14-C13-C15-C16
15	a1	409	CLA	C11-C10-C8-C9
15	a4	421	CLA	C14-C13-C15-C16
15	a6	422	CLA	C14-C13-C15-C16
15	bA	802	CLA	C14-C13-C15-C16
15	b4	421	CLA	C14-C13-C15-C16
15	b6	411	CLA	C11-C10-C8-C9
15	b6	422	CLA	C14-C13-C15-C16
15	cA	802	CLA	C14-C13-C15-C16
15	c1	410	CLA	C11-C10-C8-C9
15	aB	817	CLA	O1D-CGD-O2D-CED
15	a6	411	CLA	C5-C6-C7-C8
15	bA	804	CLA	C13-C15-C16-C17
15	c3	404	CLA	C10-C11-C12-C13
15	c5	410	CLA	C5-C6-C7-C8
15	aA	813	CLA	CAA-CBA-CGA-O2A
15	aB	801	CLA	CAA-CBA-CGA-O2A
15	a3	421	CLA	CAA-CBA-CGA-O2A
15	bA	813	CLA	CAA-CBA-CGA-O2A
15	bA	843	CLA	CAA-CBA-CGA-O2A
15	cB	801	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	c4	421	CLA	CAA-CBA-CGA-O2A
15	b3	404	CLA	C8-C10-C11-C12
15	c1	410	CLA	C13-C15-C16-C17
15	bA	824	CLA	CAA-CBA-CGA-O1A
15	a2	422	CLA	CAA-CBA-CGA-O2A
15	a4	421	CLA	CAA-CBA-CGA-O2A
15	b3	421	CLA	CAA-CBA-CGA-O2A
15	b4	421	CLA	CAA-CBA-CGA-O2A
15	b5	420	CLA	CAA-CBA-CGA-O2A
15	cA	813	CLA	CAA-CBA-CGA-O2A
15	c2	422	CLA	CAA-CBA-CGA-O2A
15	c3	421	CLA	CAA-CBA-CGA-O2A
15	c5	420	CLA	CAA-CBA-CGA-O2A
19	aA	854	LHG	O7-C7-C8-C9
15	a1	403	CLA	C8-C10-C11-C12
15	a2	411	CLA	C5-C6-C7-C8
15	aL	201	CLA	C4-C3-C5-C6
15	bL	202	CLA	C4-C3-C5-C6
15	cL	202	CLA	C4-C3-C5-C6
15	aB	814	CLA	C15-C16-C17-C18
15	a6	422	CLA	C13-C15-C16-C17
15	bB	814	CLA	C15-C16-C17-C18
15	cB	814	CLA	C15-C16-C17-C18
15	aA	806	CLA	C11-C10-C8-C7
15	aA	814	CLA	C3A-C2A-CAA-CBA
15	aB	807	CLA	C11-C10-C8-C7
15	aB	808	CLA	C11-C12-C13-C15
15	aB	811	CLA	C11-C10-C8-C7
15	aL	201	CLA	C11-C10-C8-C7
15	a1	409	CLA	C11-C10-C8-C7
15	a3	421	CLA	C12-C13-C15-C16
15	a4	421	CLA	C12-C13-C15-C16
15	bA	806	CLA	C11-C10-C8-C7
15	bA	814	CLA	C3A-C2A-CAA-CBA
15	bB	807	CLA	C11-C10-C8-C7
15	bB	808	CLA	C11-C12-C13-C15
15	bB	811	CLA	C11-C10-C8-C7
15	bL	202	CLA	C11-C10-C8-C7
15	b1	410	CLA	C11-C10-C8-C7
15	b4	421	CLA	C12-C13-C15-C16
15	cA	806	CLA	C11-C10-C8-C7
15	cA	814	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	cB	807	CLA	C11-C10-C8-C7
15	cB	808	CLA	C11-C12-C13-C15
15	cB	811	CLA	C11-C10-C8-C7
15	cL	202	CLA	C11-C10-C8-C7
15	c1	410	CLA	C11-C10-C8-C7
15	c3	421	CLA	C12-C13-C15-C16
15	c4	421	CLA	C12-C13-C15-C16
16	aB	843	PQN	C16-C17-C18-C20
16	bB	843	PQN	C16-C17-C18-C20
16	cB	843	PQN	C16-C17-C18-C20
15	aA	824	CLA	CAA-CBA-CGA-O1A
15	aB	823	CLA	CAA-CBA-CGA-O1A
15	bB	823	CLA	CAA-CBA-CGA-O1A
15	cA	824	CLA	CAA-CBA-CGA-O1A
15	cB	823	CLA	CAA-CBA-CGA-O1A
15	a5	420	CLA	CAA-CBA-CGA-O2A
15	bB	801	CLA	CAA-CBA-CGA-O2A
19	bA	855	LHG	O7-C7-C8-C9
19	cA	853	LHG	O7-C7-C8-C9
15	b2	411	CLA	C5-C6-C7-C8
15	aB	832	CLA	O2A-C1-C2-C3
15	bB	832	CLA	O2A-C1-C2-C3
15	cB	832	CLA	O2A-C1-C2-C3
15	c5	417	CLA	C3-C5-C6-C7
15	b1	404	CLA	C10-C11-C12-C13
18	aK	101	BCR	C21-C22-C23-C24
18	bA	848	BCR	C21-C22-C23-C24
18	cK	101	BCR	C21-C22-C23-C24
15	bF	201	CLA	CAA-CBA-CGA-O1A
18	a6	402	BCR	C15-C16-C17-C18
18	b5	401	BCR	C15-C16-C17-C18
18	b6	402	BCR	C15-C16-C17-C18
15	cB	817	CLA	O1D-CGD-O2D-CED
15	a6	411	CLA	C13-C15-C16-C17
15	b6	411	CLA	C13-C15-C16-C17
15	c1	404	CLA	C8-C10-C11-C12
15	c3	404	CLA	C8-C10-C11-C12
15	aJ	201	CLA	CAA-CBA-CGA-O1A
15	cF	203	CLA	CAA-CBA-CGA-O1A
15	aA	810	CLA	CAA-CBA-CGA-O2A
15	aB	810	CLA	CAA-CBA-CGA-O2A
15	bA	810	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	bB	810	CLA	CAA-CBA-CGA-O2A
15	cA	810	CLA	CAA-CBA-CGA-O2A
15	cB	810	CLA	CAA-CBA-CGA-O2A
15	cB	818	CLA	CAA-CBA-CGA-O2A
15	b1	417	CLA	C5-C6-C7-C8
15	aB	834	CLA	CAA-CBA-CGA-O1A
15	bB	834	CLA	CAA-CBA-CGA-O1A
15	cB	834	CLA	CAA-CBA-CGA-O1A
15	a1	416	CLA	C2A-CAA-CBA-CGA
15	b1	417	CLA	C2A-CAA-CBA-CGA
15	aA	826	CLA	C13-C15-C16-C17
15	a3	417	CLA	C5-C6-C7-C8
15	b1	410	CLA	C13-C15-C16-C17
15	cA	826	CLA	C13-C15-C16-C17
15	b5	417	CLA	C3-C5-C6-C7
15	a6	422	CLA	CAA-CBA-CGA-O1A
15	aB	818	CLA	CAA-CBA-CGA-O2A
15	aB	829	CLA	CAA-CBA-CGA-O2A
15	bA	840	CLA	CAA-CBA-CGA-O2A
15	bB	818	CLA	CAA-CBA-CGA-O2A
15	bB	829	CLA	CAA-CBA-CGA-O2A
15	cA	840	CLA	CAA-CBA-CGA-O2A
15	cB	829	CLA	CAA-CBA-CGA-O2A
15	bA	826	CLA	C13-C15-C16-C17

There are no ring outliers.

660 monomers are involved in 1881 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	818	CLA	2	0
15	b1	411	CLA	1	0
16	aA	846	PQN	3	0
15	a3	402	CLA	9	0
15	c2	405	CLA	1	0
15	bA	838	CLA	1	0
15	aA	835	CLA	5	0
15	a6	415	CLA	1	0
15	bA	808	CLA	2	0
16	cB	843	PQN	3	0
18	b3	401	BCR	1	0
15	aA	837	CLA	1	0
15	bB	825	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b2	403	CLA	5	0
15	cA	831	CLA	5	0
15	cB	835	CLA	2	0
15	a6	411	CLA	3	0
15	cB	833	CLA	9	0
15	cA	815	CLA	2	0
15	bA	842	CLA	3	0
15	bA	815	CLA	1	0
15	b5	417	CLA	6	0
15	a1	413	CLA	1	0
15	c2	415	CLA	1	0
15	c2	413	CLA	3	0
15	aA	840	CLA	2	0
15	bB	828	CLA	5	0
15	c5	405	CLA	1	0
15	c5	409	CLA	3	0
15	a6	412	CLA	1	0
15	cA	810	CLA	6	0
15	c2	411	CLA	4	0
15	a4	421	CLA	7	0
18	a3	419	BCR	2	0
15	aA	836	CLA	3	0
15	b2	402	CLA	8	0
15	aB	841	CLA	1	0
15	b5	402	CLA	9	0
18	b1	418	BCR	3	0
15	aA	834	CLA	5	0
15	cB	810	CLA	4	0
15	aA	818	CLA	1	0
15	b5	403	CLA	4	0
15	b2	415	CLA	1	0
18	c1	419	BCR	4	0
15	b5	415	CLA	8	0
15	a3	417	CLA	5	0
15	bB	841	CLA	1	0
15	aA	838	CLA	1	0
18	b4	419	BCR	3	0
15	b2	417	CLA	6	0
15	bB	817	CLA	4	0
15	a2	418	CLA	4	0
15	c3	416	CLA	4	0
15	b2	410	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	826	CLA	3	0
15	aB	814	CLA	7	0
15	aL	202	CLA	4	0
15	a4	417	CLA	6	0
15	cL	202	CLA	5	0
18	b3	419	BCR	3	0
15	bA	825	CLA	5	0
15	a5	408	CLA	1	0
15	cF	201	CLA	3	0
15	aA	842	CLA	3	0
15	aB	816	CLA	1	0
15	a5	417	CLA	4	0
15	c1	417	CLA	2	0
18	aB	848	BCR	3	0
15	aB	830	CLA	3	0
18	aB	847	BCR	3	0
15	bB	819	CLA	4	0
15	bA	841	CLA	3	0
15	b3	416	CLA	4	0
18	c2	401	BCR	5	0
15	a3	408	CLA	1	0
15	c6	401	CLA	8	0
18	c1	401	BCR	2	0
15	a4	416	CLA	5	0
15	cA	820	CLA	3	0
15	cB	818	CLA	3	0
15	c2	418	CLA	4	0
15	cA	812	CLA	5	0
15	c1	405	CLA	1	0
15	c1	409	CLA	3	0
15	b6	416	CLA	8	0
18	a6	420	BCR	3	0
18	b2	401	BCR	4	0
18	b3	418	BCR	2	0
18	b4	420	BCR	5	0
15	aA	806	CLA	5	0
18	a6	401	BCR	3	0
15	a3	411	CLA	1	0
15	bA	826	CLA	3	0
19	aA	853	LHG	3	0
15	bB	820	CLA	1	0
15	bB	837	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a6	406	CLA	1	0
15	b3	414	CLA	1	0
18	a1	419	BCR	3	0
19	cA	852	LHG	3	0
18	a3	401	BCR	2	0
15	cA	832	CLA	1	0
15	c6	416	CLA	1	0
15	bA	821	CLA	3	0
15	aB	828	CLA	6	0
15	c2	402	CLA	9	0
15	c2	416	CLA	8	0
15	b6	406	CLA	1	0
15	b4	415	CLA	8	0
15	bB	836	CLA	1	0
15	bB	832	CLA	4	0
15	bB	803	CLA	4	0
15	a2	415	CLA	1	0
15	a4	412	CLA	2	0
18	cA	851	BCR	4	0
15	cB	827	CLA	3	0
15	bA	833	CLA	3	0
15	aL	203	CLA	4	0
15	aA	829	CLA	4	0
15	a2	417	CLA	6	0
18	a1	418	BCR	4	0
15	bB	839	CLA	4	0
18	c2	420	BCR	2	0
15	bJ	101	CLA	1	0
15	cA	840	CLA	2	0
18	a4	420	BCR	5	0
15	cA	822	CLA	3	0
18	b5	418	BCR	1	0
18	c4	401	BCR	4	0
15	c5	415	CLA	8	0
15	aA	812	CLA	5	0
14	aA	801	CL0	4	0
15	aB	801	CLA	4	0
15	aA	845	CLA	1	0
18	b3	420	BCR	5	0
15	bL	204	CLA	5	0
15	cA	807	CLA	5	0
15	bB	840	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bB	811	CLA	7	0
15	cL	204	CLA	5	0
18	bA	850	BCR	3	0
15	cA	809	CLA	2	0
15	c5	411	CLA	1	0
15	c4	416	CLA	2	0
18	a6	419	BCR	2	0
15	c6	413	CLA	1	0
15	aA	809	CLA	2	0
15	b4	412	CLA	1	0
18	bA	852	BCR	3	0
15	cB	809	CLA	3	0
15	cA	834	CLA	5	0
15	c6	411	CLA	3	0
15	aA	816	CLA	1	0
15	c2	404	CLA	3	0
15	c5	414	CLA	1	0
15	aB	818	CLA	4	0
18	a2	401	BCR	6	0
15	a1	410	CLA	1	0
18	b6	421	BCR	1	0
15	c3	417	CLA	6	0
15	b1	410	CLA	3	0
15	b4	403	CLA	5	0
15	bA	844	CLA	1	0
15	bB	834	CLA	1	0
19	bA	854	LHG	3	0
15	b6	422	CLA	9	0
15	c6	418	CLA	5	0
18	b6	402	BCR	3	0
15	a3	412	CLA	2	0
15	cA	838	CLA	1	0
15	a3	407	CLA	1	0
18	c6	421	BCR	2	0
15	c3	402	CLA	9	0
15	bB	838	CLA	1	0
18	cM	101	BCR	4	0
15	b5	409	CLA	3	0
15	bB	808	CLA	2	0
15	b6	412	CLA	1	0
15	bA	832	CLA	1	0
18	c6	402	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c4	414	CLA	1	0
15	aB	819	CLA	3	0
18	a1	421	BCR	2	0
15	cB	801	CLA	5	0
15	aB	839	CLA	4	0
18	bJ	104	BCR	5	0
15	c6	405	CLA	4	0
18	aJ	205	BCR	3	0
15	bA	834	CLA	5	0
15	a6	418	CLA	4	0
15	bB	842	CLA	2	0
15	cB	817	CLA	4	0
15	c6	414	CLA	3	0
15	bB	826	CLA	2	0
15	aA	826	CLA	3	0
15	bA	818	CLA	2	0
15	c5	420	CLA	8	0
15	cA	836	CLA	2	0
15	c1	413	CLA	1	0
15	aA	821	CLA	4	0
18	cF	202	BCR	5	0
15	cB	831	CLA	3	0
18	b6	420	BCR	3	0
18	c5	401	BCR	3	0
15	cA	835	CLA	3	0
18	bJ	105	BCR	4	0
15	a5	420	CLA	10	0
15	cA	803	CLA	5	0
18	cI	101	BCR	1	0
15	aB	806	CLA	2	0
15	cA	806	CLA	4	0
18	c1	418	BCR	2	0
14	cA	801	CL0	3	0
15	bB	829	CLA	5	0
15	b4	409	CLA	3	0
15	b4	410	CLA	4	0
18	b6	419	BCR	1	0
15	b3	403	CLA	4	0
15	a3	414	CLA	1	0
15	bB	812	CLA	2	0
18	c1	420	BCR	4	0
15	aB	804	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bB	846	BCR	2	0
15	c3	404	CLA	3	0
18	a3	420	BCR	4	0
15	a4	403	CLA	5	0
15	bB	824	CLA	1	0
15	aB	827	CLA	3	0
15	a5	415	CLA	8	0
15	aB	815	CLA	5	0
15	a5	402	CLA	9	0
15	b5	420	CLA	10	0
18	aF	203	BCR	6	0
15	b5	414	CLA	1	0
15	b4	421	CLA	10	0
15	c5	403	CLA	4	0
15	a5	411	CLA	1	0
18	cB	846	BCR	2	0
15	bB	810	CLA	3	0
15	bA	806	CLA	4	0
18	aL	205	BCR	1	0
15	c1	415	CLA	8	0
15	c3	412	CLA	2	0
18	c4	419	BCR	3	0
18	cB	849	BCR	5	0
18	c3	418	BCR	1	0
15	a2	411	CLA	3	0
14	bA	801	CL0	4	0
15	a1	409	CLA	4	0
15	bA	845	CLA	1	0
15	b6	410	CLA	4	0
15	a5	414	CLA	1	0
15	c3	410	CLA	3	0
15	aA	839	CLA	5	0
15	bB	809	CLA	3	0
15	aB	802	CLA	2	0
15	a1	414	CLA	7	0
15	aJ	202	CLA	1	0
15	a2	405	CLA	1	0
15	b2	411	CLA	3	0
18	bB	845	BCR	3	0
15	bA	813	CLA	2	0
18	c4	418	BCR	1	0
15	b1	414	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c5	412	CLA	3	0
15	bB	833	CLA	4	0
15	bA	810	CLA	6	0
18	a2	419	BCR	1	0
15	bA	827	CLA	4	0
15	b3	408	CLA	1	0
15	a2	416	CLA	8	0
18	bB	844	BCR	3	0
15	a6	417	CLA	5	0
15	b3	410	CLA	4	0
18	cA	848	BCR	3	0
20	bB	851	LMG	1	0
18	bA	853	BCR	4	0
15	bA	809	CLA	2	0
15	a4	410	CLA	4	0
15	c2	412	CLA	2	0
15	cA	842	CLA	11	0
15	cA	805	CLA	2	0
15	c5	404	CLA	3	0
15	aA	807	CLA	5	0
15	c5	408	CLA	1	0
20	cB	850	LMG	1	0
15	bB	816	CLA	1	0
15	b6	417	CLA	4	0
18	cF	204	BCR	5	0
15	b1	405	CLA	1	0
15	c1	414	CLA	1	0
15	c5	410	CLA	4	0
15	c2	417	CLA	6	0
15	c6	404	CLA	9	0
15	c6	410	CLA	1	0
15	a6	416	CLA	8	0
18	b4	418	BCR	1	0
15	a4	408	CLA	1	0
15	a3	416	CLA	4	0
15	c6	419	CLA	4	0
18	cF	205	BCR	8	0
18	a2	420	BCR	3	0
15	a1	401	CLA	9	0
15	c1	403	CLA	4	0
18	a5	419	BCR	5	0
15	c3	414	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aA	820	CLA	2	0
15	a4	411	CLA	1	0
15	aB	833	CLA	8	0
15	c4	417	CLA	5	0
15	cA	830	CLA	1	0
15	a1	402	CLA	4	0
15	bL	203	CLA	4	0
15	c3	421	CLA	6	0
18	cL	205	BCR	3	0
15	b3	409	CLA	3	0
15	cA	821	CLA	4	0
15	b6	403	CLA	9	0
15	cA	837	CLA	1	0
18	aB	844	BCR	2	0
15	b1	402	CLA	9	0
15	bA	829	CLA	6	0
15	b5	408	CLA	1	0
18	aB	849	BCR	4	0
15	aB	831	CLA	2	0
15	a5	403	CLA	4	0
15	b6	405	CLA	3	0
15	aA	814	CLA	2	0
15	b2	406	CLA	16	0
15	b6	409	CLA	1	0
15	bB	821	CLA	2	0
18	c6	420	BCR	2	0
15	c3	415	CLA	7	0
18	a1	417	BCR	4	0
15	bA	835	CLA	6	0
15	cB	803	CLA	2	0
15	aB	821	CLA	2	0
16	bB	843	PQN	4	0
15	cJ	101	CLA	1	0
15	aA	805	CLA	3	0
15	aA	830	CLA	1	0
18	bI	102	BCR	4	0
15	b2	412	CLA	2	0
15	c3	409	CLA	3	0
15	bB	835	CLA	2	0
15	c4	408	CLA	1	0
18	aA	850	BCR	3	0
18	a6	402	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b1	401	BCR	2	0
15	bA	820	CLA	3	0
15	c2	409	CLA	1	0
15	aB	825	CLA	1	0
15	bA	822	CLA	3	0
15	b6	413	CLA	3	0
15	a6	413	CLA	3	0
15	c4	405	CLA	1	0
18	aA	852	BCR	4	0
15	cA	844	CLA	3	0
15	c1	410	CLA	4	0
18	bA	849	BCR	3	0
15	b2	404	CLA	2	0
18	a4	418	BCR	1	0
15	bA	831	CLA	5	0
15	aA	828	CLA	3	0
15	cA	839	CLA	6	0
15	cB	824	CLA	2	0
15	bB	807	CLA	4	0
15	b1	415	CLA	8	0
15	b6	418	CLA	5	0
15	cB	825	CLA	1	0
15	aA	841	CLA	5	0
15	b3	411	CLA	1	0
15	b2	422	CLA	9	0
15	a2	412	CLA	3	0
18	aA	848	BCR	4	0
15	a6	422	CLA	11	0
15	a2	403	CLA	5	0
15	cF	203	CLA	3	0
18	bB	847	BCR	4	0
15	c1	408	CLA	1	0
15	a4	404	CLA	3	0
15	c4	409	CLA	3	0
18	bF	202	BCR	5	0
15	cA	833	CLA	3	0
15	cB	806	CLA	2	0
15	cB	834	CLA	1	0
18	cK	101	BCR	1	0
18	bJ	103	BCR	5	0
15	aA	802	CLA	2	0
15	cA	814	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	812	CLA	5	0
15	b2	405	CLA	1	0
15	aA	822	CLA	4	0
15	a4	405	CLA	1	0
18	b2	419	BCR	3	0
15	b5	411	CLA	1	0
15	a6	409	CLA	1	0
15	bA	816	CLA	1	0
15	a1	415	CLA	5	0
18	bL	205	BCR	3	0
15	b4	402	CLA	9	0
15	a6	403	CLA	9	0
18	b5	419	BCR	5	0
15	aX	102	CLA	2	0
15	a5	405	CLA	1	0
18	c2	419	BCR	1	0
18	c3	401	BCR	1	0
15	cA	829	CLA	4	0
15	bB	827	CLA	3	0
15	a1	411	CLA	2	0
15	cA	808	CLA	2	0
15	cB	837	CLA	5	0
18	a3	418	BCR	1	0
15	c5	417	CLA	4	0
15	aA	819	CLA	1	0
15	a2	413	CLA	3	0
15	b4	404	CLA	3	0
15	b3	402	CLA	9	0
15	c3	408	CLA	1	0
15	a2	409	CLA	1	0
18	aA	849	BCR	2	0
15	a4	402	CLA	9	0
15	bA	828	CLA	3	0
15	cA	804	CLA	8	0
15	cX	102	CLA	2	0
15	a2	410	CLA	3	0
15	b3	415	CLA	7	0
15	aB	824	CLA	1	0
15	b5	405	CLA	1	0
15	c5	402	CLA	9	0
15	c5	416	CLA	5	0
18	a1	420	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	aB	850	LMG	1	0
15	bA	836	CLA	3	0
15	aA	844	CLA	1	0
15	b6	415	CLA	1	0
15	a2	422	CLA	8	0
15	bA	803	CLA	8	0
15	aB	813	CLA	3	0
15	a4	409	CLA	3	0
15	cA	828	CLA	3	0
15	aB	832	CLA	2	0
15	b6	411	CLA	3	0
18	a2	421	BCR	4	0
15	b3	412	CLA	2	0
15	c1	411	CLA	1	0
15	aA	813	CLA	2	0
15	aB	803	CLA	1	0
15	aA	804	CLA	6	0
15	a6	410	CLA	3	0
18	bB	848	BCR	2	0
15	a3	421	CLA	6	0
15	cB	828	CLA	4	0
15	cB	811	CLA	4	0
15	cA	802	CLA	2	0
15	aB	834	CLA	1	0
15	aA	843	CLA	11	0
15	a1	403	CLA	2	0
15	c4	412	CLA	2	0
15	cB	815	CLA	5	0
15	b1	404	CLA	3	0
15	b1	403	CLA	4	0
15	aB	810	CLA	2	0
15	cB	813	CLA	3	0
18	b1	420	BCR	5	0
18	cA	847	BCR	3	0
15	cB	832	CLA	2	0
15	bB	802	CLA	3	0
15	b3	404	CLA	3	0
15	cA	825	CLA	5	0
18	bL	206	BCR	2	0
15	a4	415	CLA	8	0
15	bA	840	CLA	2	0
15	c6	412	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a5	410	CLA	3	0
15	b1	409	CLA	3	0
15	b3	417	CLA	5	0
18	bA	848	BCR	2	0
18	cJ	104	BCR	3	0
15	cA	819	CLA	1	0
15	a3	415	CLA	8	0
15	cA	841	CLA	6	0
15	aB	840	CLA	1	0
15	a4	414	CLA	1	0
18	c4	420	BCR	5	0
15	b3	405	CLA	1	0
15	bA	805	CLA	3	0
15	cB	812	CLA	2	0
15	cB	814	CLA	7	0
15	a3	405	CLA	1	0
15	cB	839	CLA	5	0
15	c6	407	CLA	1	0
15	cA	816	CLA	1	0
15	a1	407	CLA	1	0
18	aJ	204	BCR	5	0
15	a3	410	CLA	4	0
15	aA	815	CLA	2	0
15	cB	804	CLA	4	0
15	bA	802	CLA	1	0
15	aB	807	CLA	2	0
15	cB	816	CLA	1	0
15	aA	808	CLA	2	0
15	cB	830	CLA	3	0
18	bA	851	BCR	2	0
15	c6	417	CLA	8	0
15	cB	841	CLA	1	0
15	c4	415	CLA	9	0
15	b5	410	CLA	4	0
15	aB	829	CLA	5	0
15	bB	830	CLA	3	0
15	b5	416	CLA	5	0
15	cB	840	CLA	2	0
15	c3	405	CLA	1	0
18	b6	401	BCR	3	0
15	a1	404	CLA	1	0
18	aI	102	BCR	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bL	201	BCR	1	0
18	cB	848	BCR	2	0
15	b2	416	CLA	8	0
15	c4	411	CLA	1	0
18	b1	419	BCR	3	0
18	c3	419	BCR	1	0
15	bL	202	CLA	2	0
15	bB	806	CLA	2	0
15	b5	412	CLA	3	0
18	aK	101	BCR	1	0
15	cB	807	CLA	3	0
18	b5	401	BCR	3	0
18	aI	103	BCR	4	0
15	b4	414	CLA	1	0
15	b4	408	CLA	1	0
15	a5	416	CLA	5	0
15	aA	833	CLA	2	0
15	bB	822	CLA	1	0
15	cB	829	CLA	4	0
15	cB	802	CLA	3	0
15	cA	843	CLA	1	0
15	aB	820	CLA	1	0
15	cA	827	CLA	2	0
15	bA	807	CLA	5	0
15	aB	826	CLA	3	0
15	c4	421	CLA	7	0
18	bB	849	BCR	6	0
15	bB	801	CLA	6	0
15	bB	813	CLA	3	0
18	a5	418	BCR	1	0
18	a5	401	BCR	4	0
15	c1	402	CLA	9	0
15	c1	416	CLA	4	0
15	cB	838	CLA	3	0
15	c2	406	CLA	13	0
16	bA	846	PQN	3	0
18	cA	849	BCR	2	0
18	cB	844	BCR	2	0
15	bB	815	CLA	5	0
15	cB	808	CLA	5	0
15	b2	409	CLA	1	0
15	b4	411	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	c3	420	BCR	6	0
15	cB	819	CLA	3	0
18	c5	418	BCR	1	0
15	b2	413	CLA	2	0
15	aA	831	CLA	4	0
15	a5	404	CLA	2	0
16	aB	843	PQN	3	0
15	cB	842	CLA	2	0
15	c1	404	CLA	2	0
18	cA	850	BCR	3	0
15	cB	826	CLA	3	0
15	c2	403	CLA	5	0
15	b3	421	CLA	5	0
15	aA	810	CLA	6	0
15	cB	821	CLA	2	0
15	aJ	201	CLA	4	0
19	aX	101	LHG	1	0
15	a6	404	CLA	4	0
18	aF	202	BCR	7	0
15	aB	812	CLA	2	0
15	aA	825	CLA	5	0
15	c6	406	CLA	3	0
15	bA	819	CLA	1	0
18	a4	401	BCR	4	0
18	aB	846	BCR	1	0
15	aB	837	CLA	8	0
18	c5	419	BCR	5	0
15	bA	843	CLA	10	0
15	a3	404	CLA	3	0
15	a3	403	CLA	4	0
15	c1	412	CLA	2	0
15	c2	410	CLA	2	0
15	bB	814	CLA	8	0
18	b2	420	BCR	3	0
15	aB	811	CLA	10	0
15	a3	409	CLA	2	0
15	bB	818	CLA	4	0
15	bB	804	CLA	4	0
15	b6	404	CLA	4	0
15	b4	417	CLA	5	0
18	b2	421	BCR	4	0
15	c2	422	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a6	421	BCR	1	0
18	bB	850	BCR	5	0
15	c4	402	CLA	8	0
18	bM	101	BCR	4	0
15	aB	809	CLA	3	0
18	cI	102	BCR	3	0
15	c3	411	CLA	1	0
15	a2	406	CLA	11	0
15	c4	403	CLA	4	0
15	a5	409	CLA	3	0
15	b1	417	CLA	4	0
15	bA	814	CLA	1	0
18	aB	845	BCR	3	0
18	aA	851	BCR	2	0
18	aF	201	BCR	3	0
15	bA	839	CLA	5	0
18	b4	401	BCR	3	0
18	cB	847	BCR	2	0
15	bA	837	CLA	1	0
15	aB	835	CLA	2	0
15	b4	405	CLA	1	0
15	bA	804	CLA	8	0
15	b5	404	CLA	3	0
15	c4	404	CLA	2	0
15	aL	201	CLA	3	0
15	a6	405	CLA	2	0
15	aB	838	CLA	3	0
15	a2	402	CLA	9	0
15	aB	808	CLA	5	0
15	a5	412	CLA	3	0
15	c4	410	CLA	4	0
15	a1	416	CLA	2	0
15	b2	418	CLA	4	0
15	cB	820	CLA	1	0
15	cL	203	CLA	3	0
18	cJ	103	BCR	6	0
18	cB	845	BCR	3	0
15	aB	817	CLA	4	0
15	a1	412	CLA	1	0
15	b1	416	CLA	4	0
18	a4	419	BCR	3	0
15	cA	813	CLA	2	0

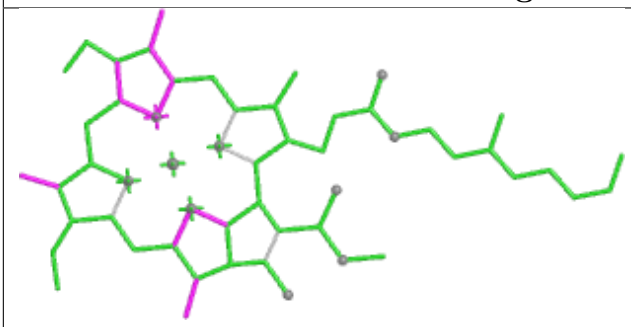
Continued on next page...

Continued from previous page...

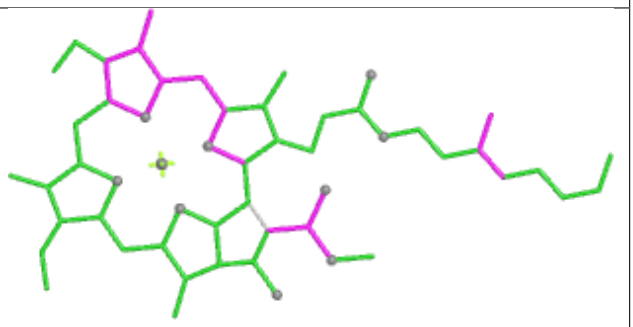
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a1	408	CLA	3	0
15	c3	403	CLA	4	0
15	b1	412	CLA	2	0
15	aB	842	CLA	2	0
16	cA	845	PQN	4	0
15	b4	416	CLA	5	0
15	a2	404	CLA	2	0
15	b1	408	CLA	1	0
18	c2	421	BCR	3	0
18	c6	403	BCR	3	0
18	aM	101	BCR	3	0
15	bB	831	CLA	3	0
15	bF	201	CLA	2	0
15	aA	827	CLA	2	0
15	bX	102	CLA	3	0
15	aA	832	CLA	1	0
15	aA	803	CLA	5	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.

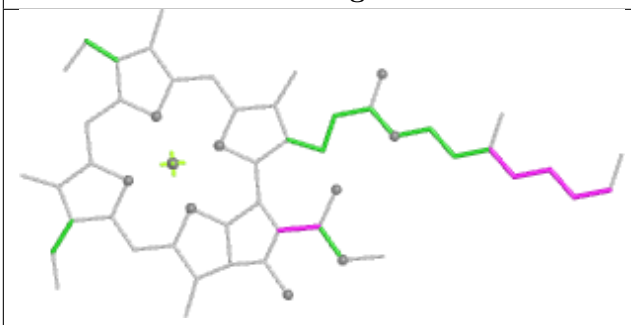
Ligand CLA cA 818



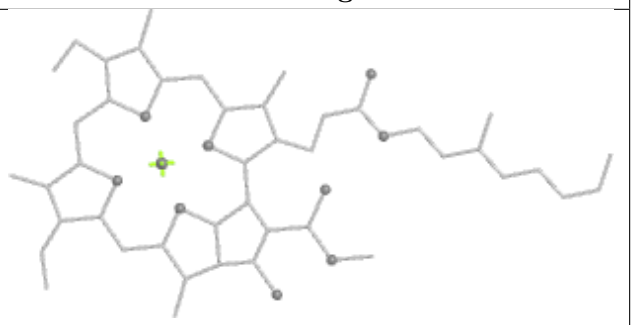
Bond lengths



Bond angles

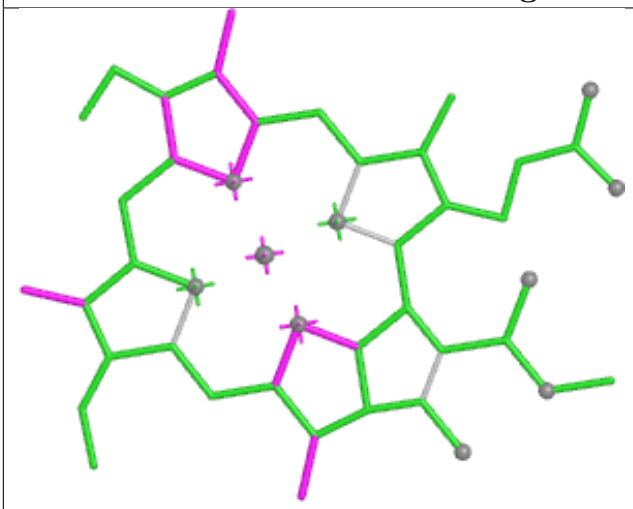


Torsions

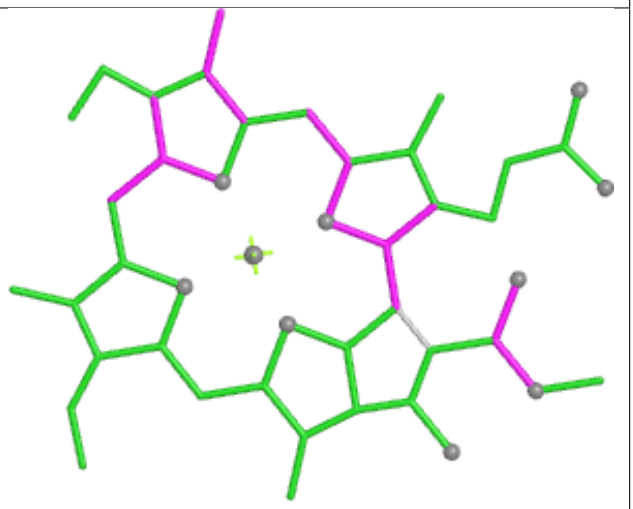


Rings

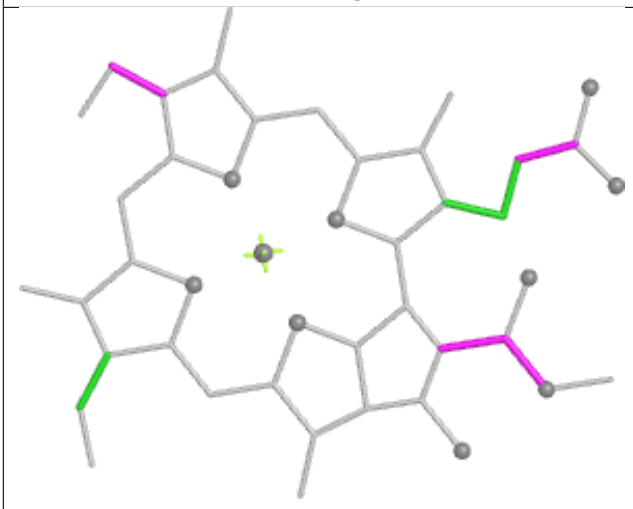
Ligand CLA a4 407



Bond lengths



Bond angles

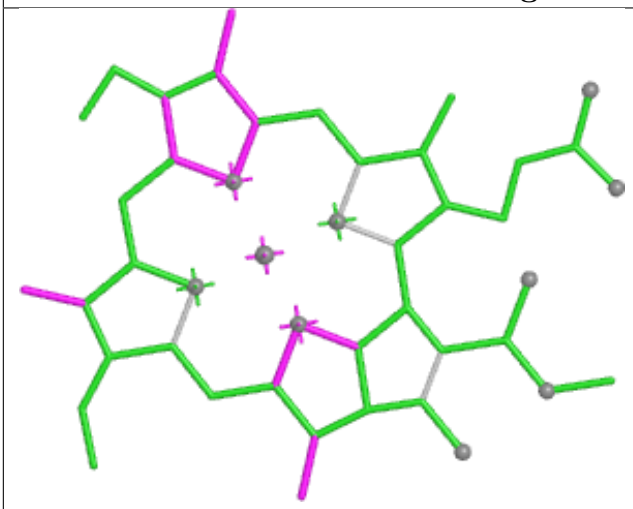


Torsions

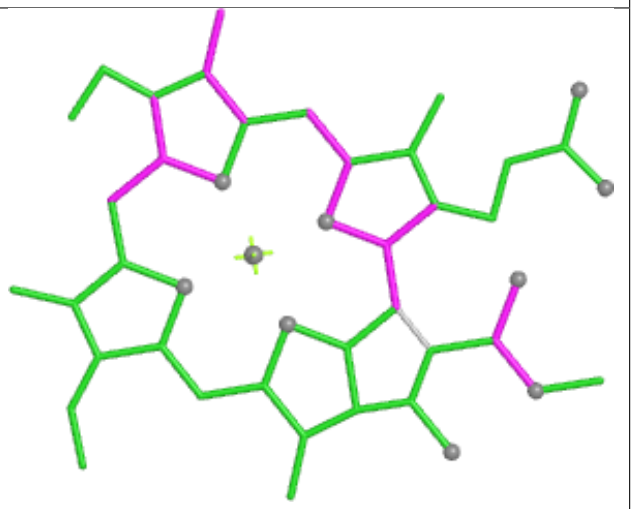


Rings

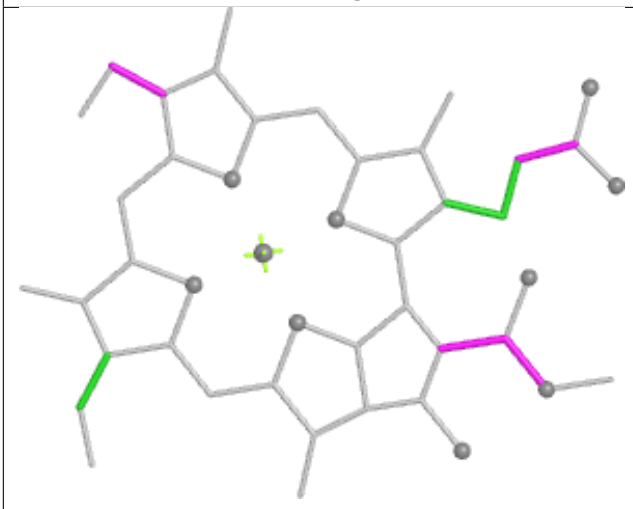
Ligand CLA c4 407



Bond lengths



Bond angles

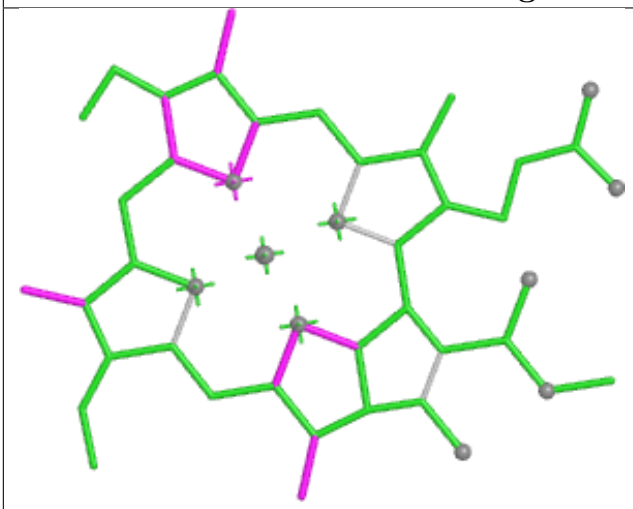


Torsions

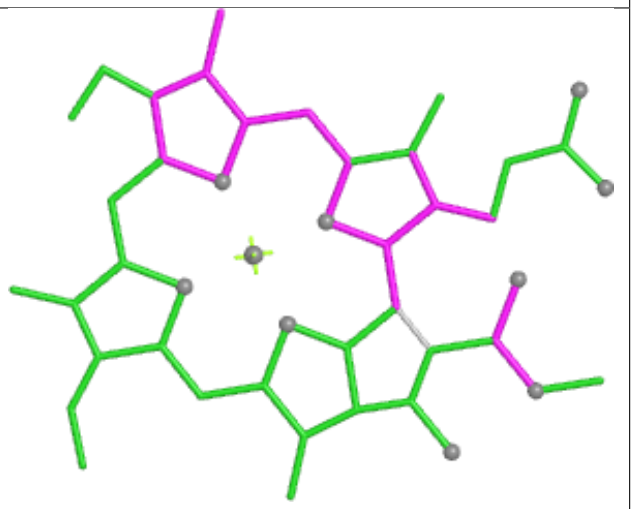


Rings

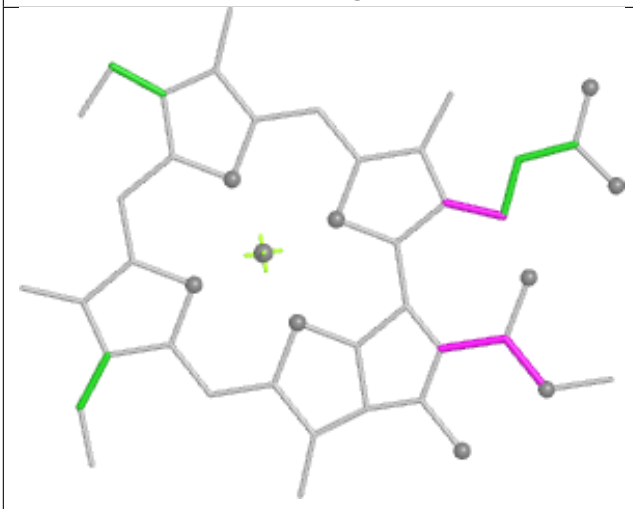
Ligand CLA b1 411



Bond lengths



Bond angles

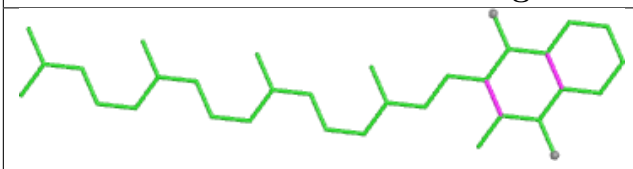


Torsions

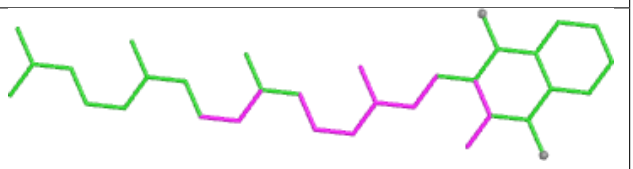


Rings

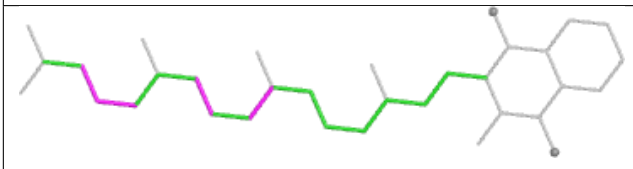
Ligand PQN aA 846



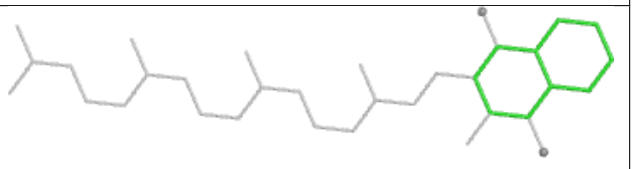
Bond lengths



Bond angles

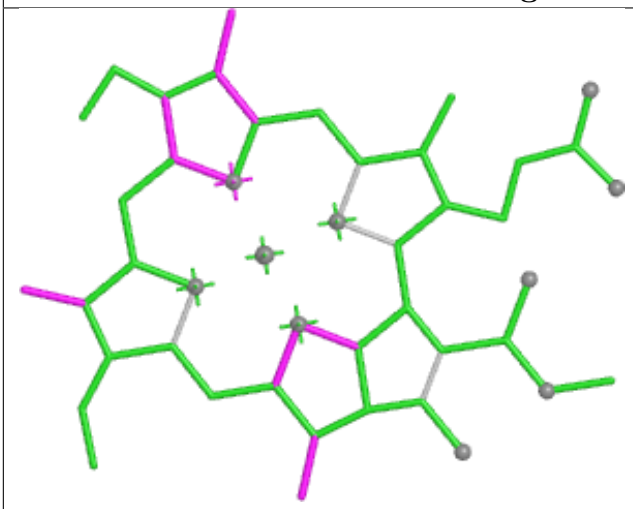


Torsions

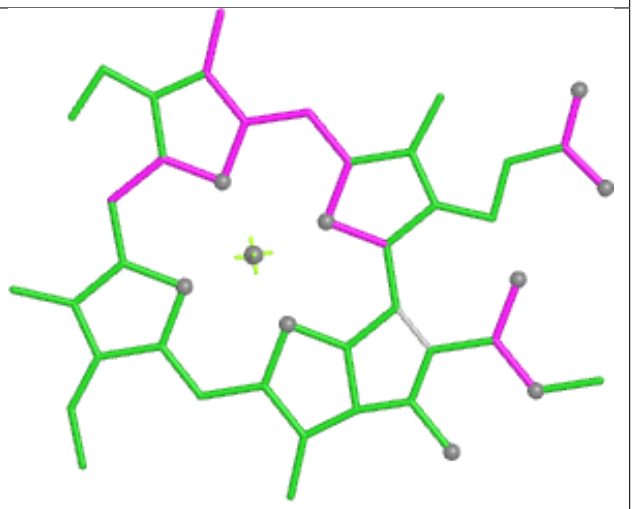


Rings

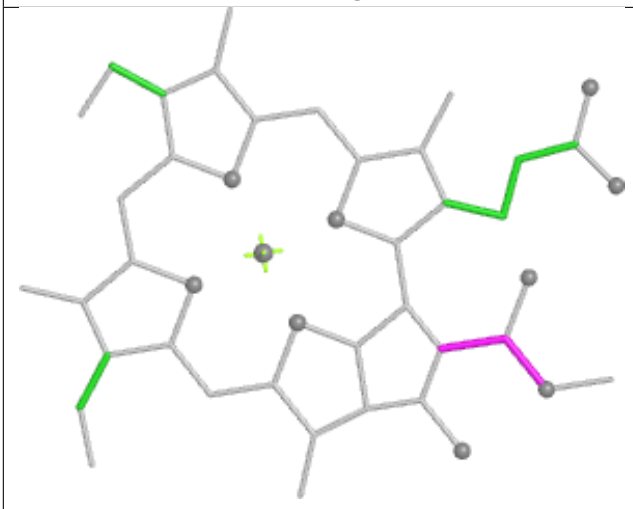
Ligand CLA c3 406



Bond lengths



Bond angles

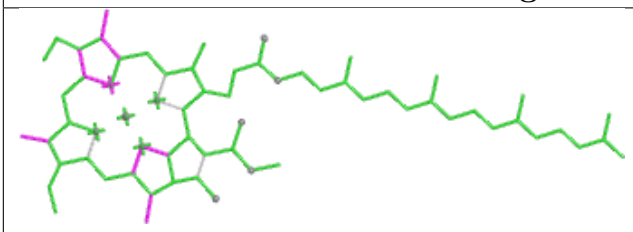


Torsions

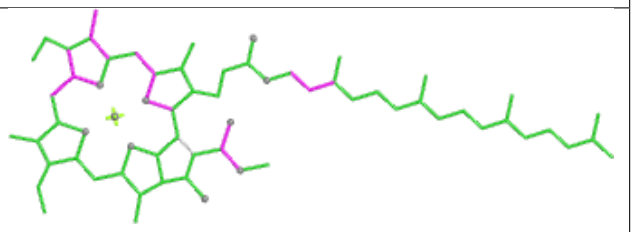


Rings

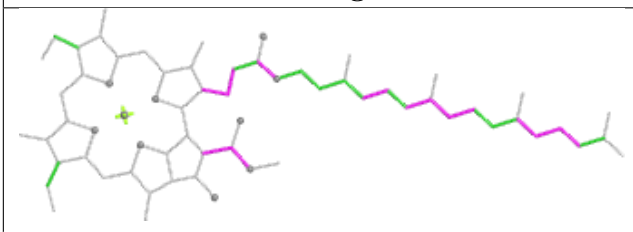
Ligand CLA a3 402



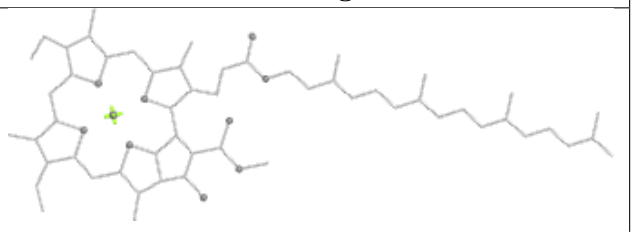
Bond lengths



Bond angles

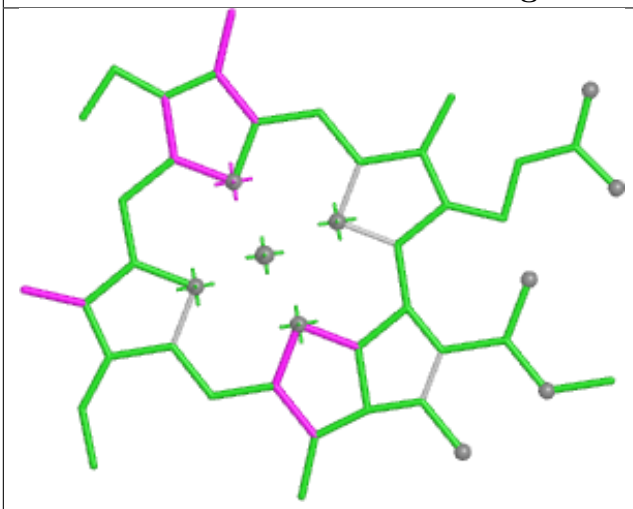


Torsions

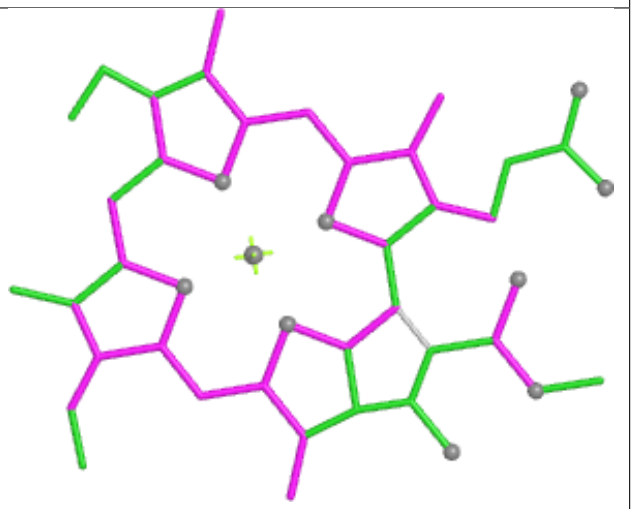


Rings

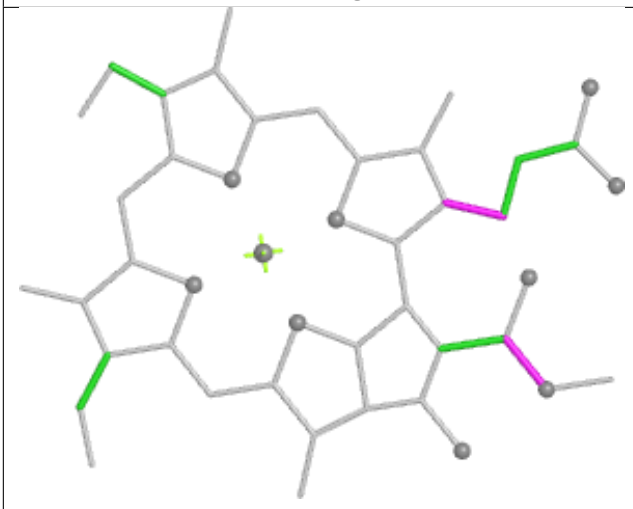
Ligand CLA c2 405



Bond lengths



Bond angles

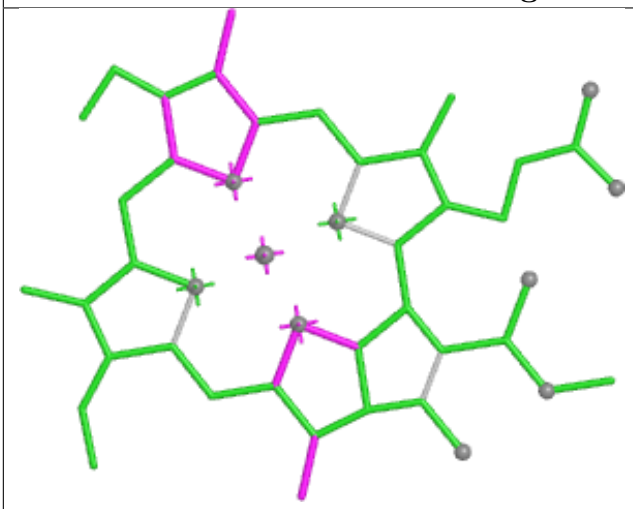


Torsions

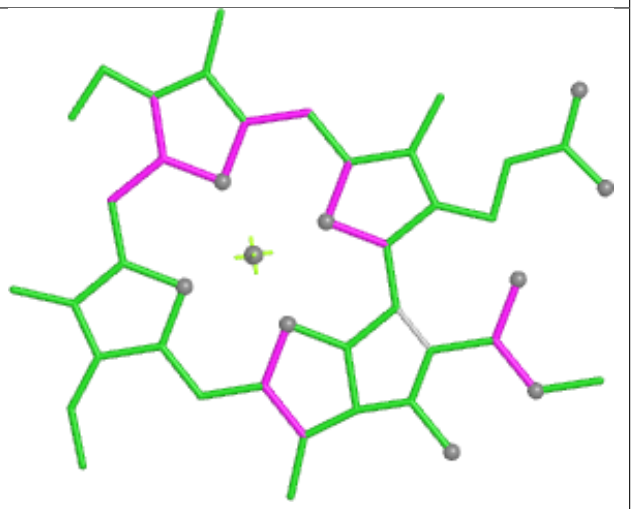


Rings

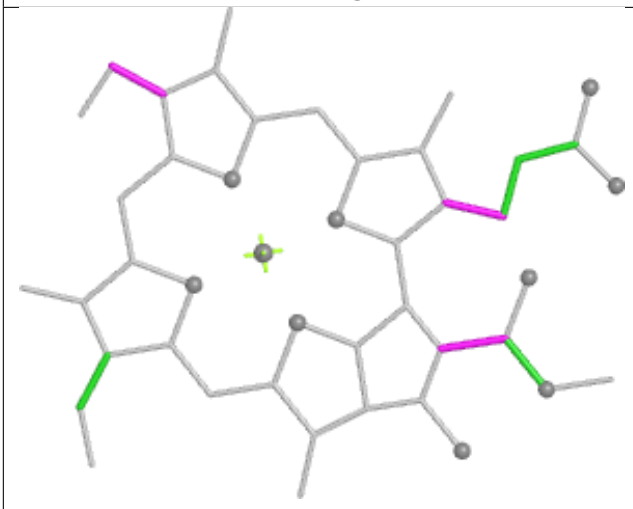
Ligand CLA c2 414



Bond lengths



Bond angles

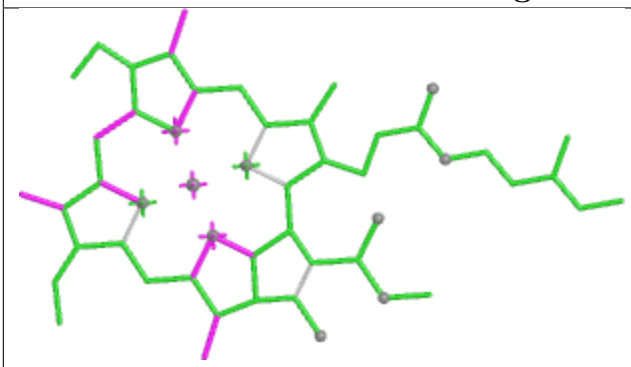


Torsions

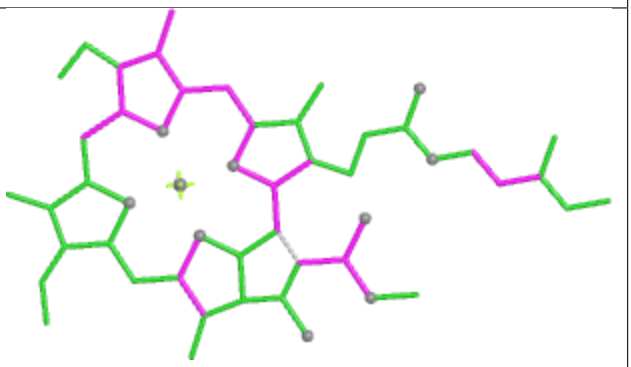


Rings

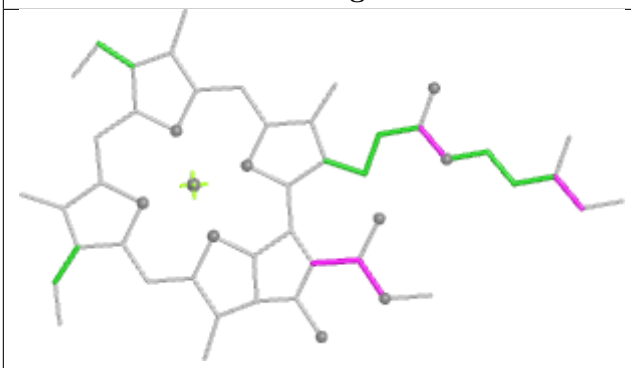
Ligand CLA bA 838



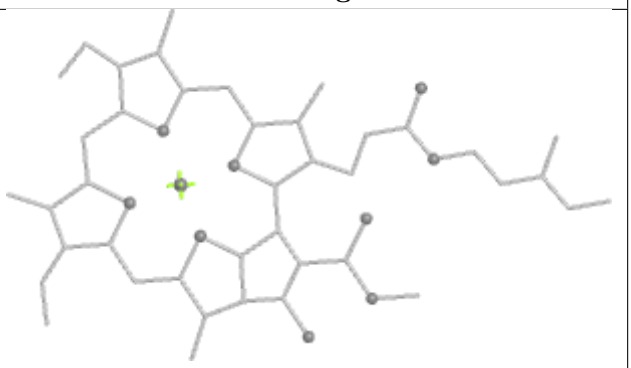
Bond lengths



Bond angles

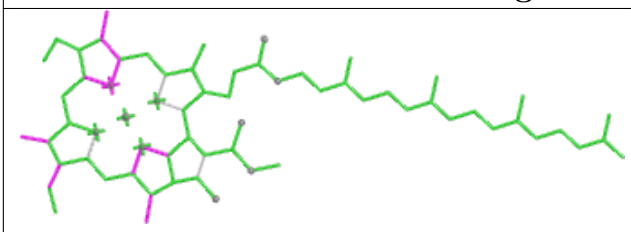


Torsions

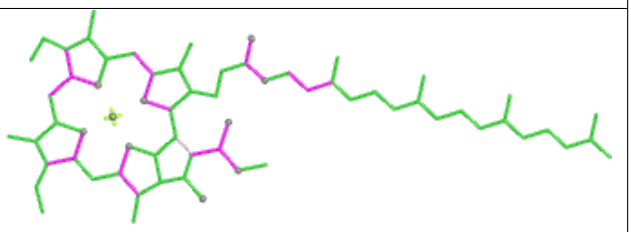


Rings

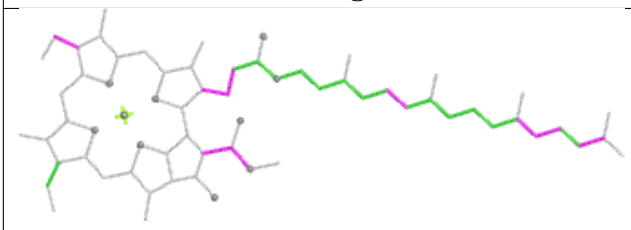
Ligand CLA aA 835



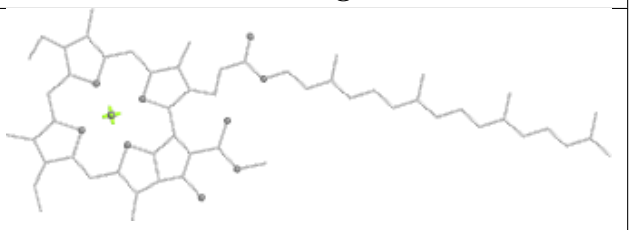
Bond lengths



Bond angles

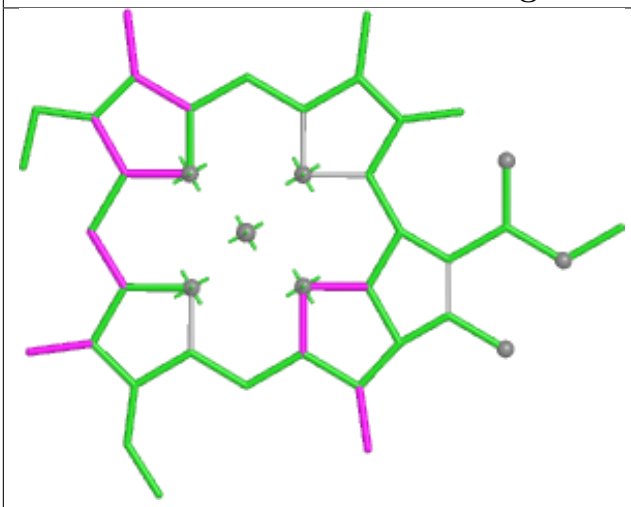


Torsions

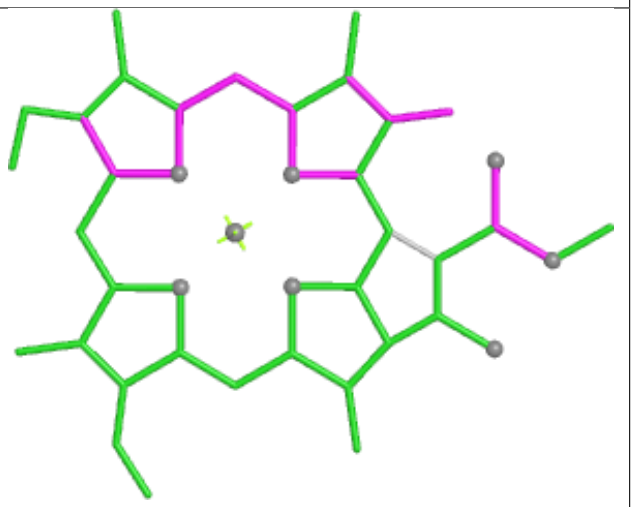


Rings

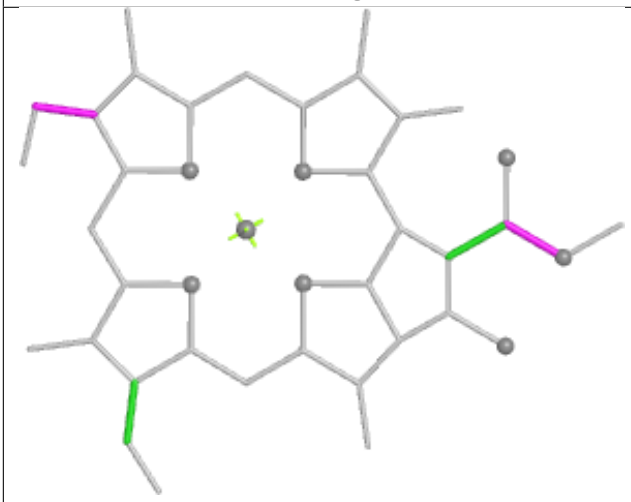
Ligand CLA a6 415



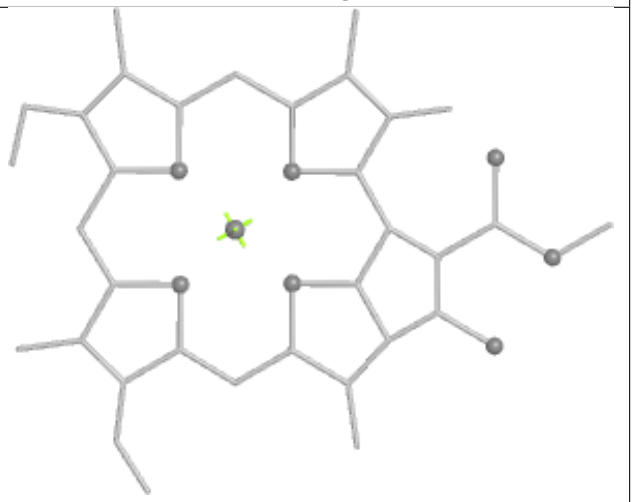
Bond lengths



Bond angles

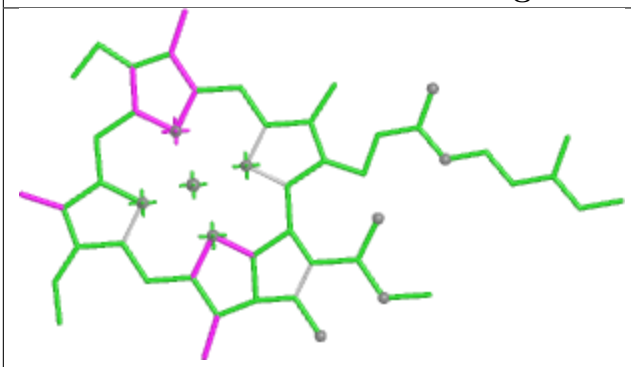


Torsions

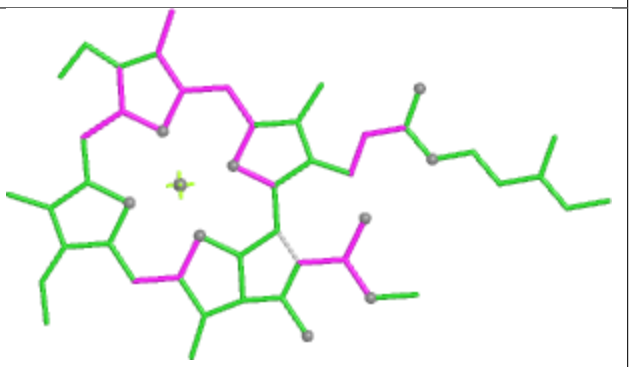


Rings

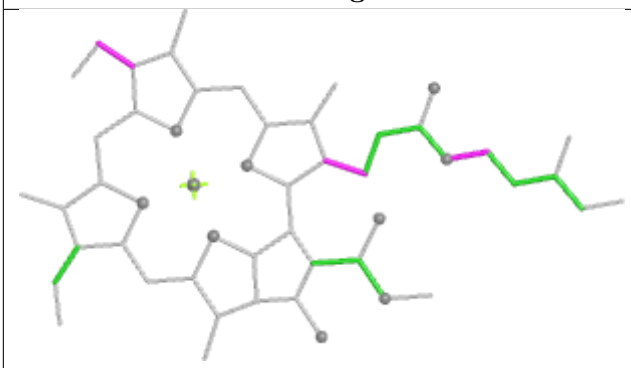
Ligand CLA bA 808



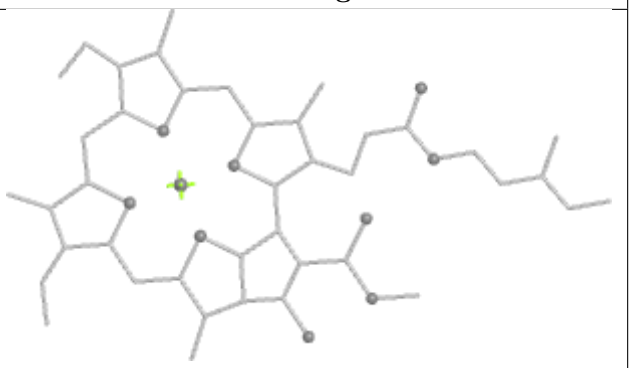
Bond lengths



Bond angles

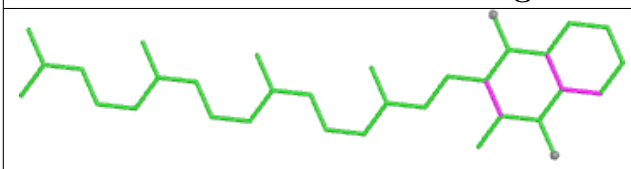


Torsions

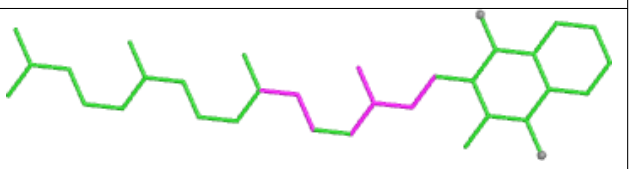


Rings

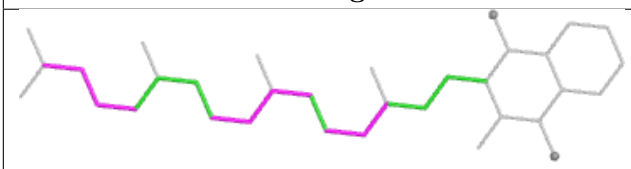
Ligand PQN cB 843



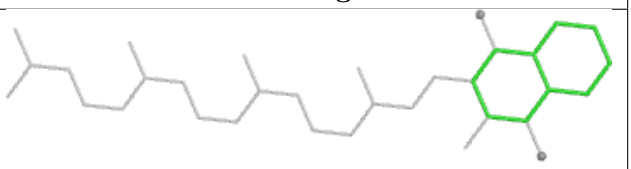
Bond lengths



Bond angles

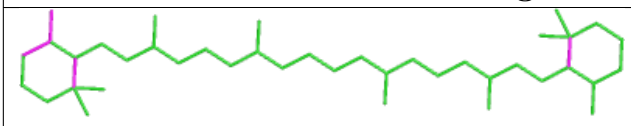


Torsions

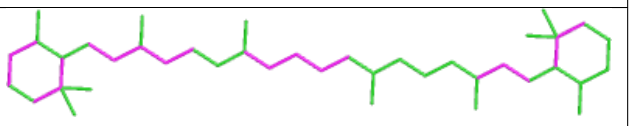


Rings

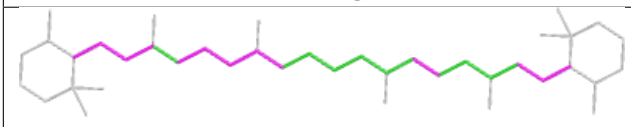
Ligand BCR b3 401



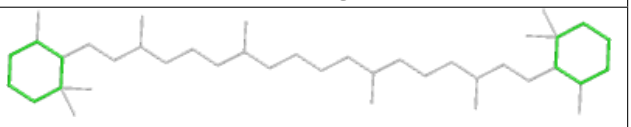
Bond lengths



Bond angles

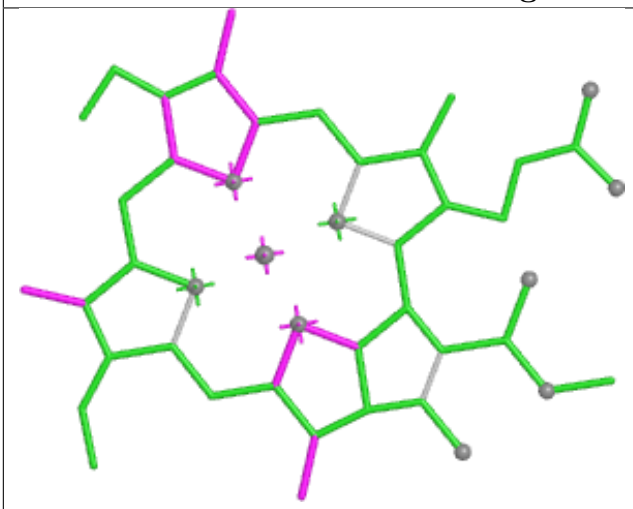


Torsions

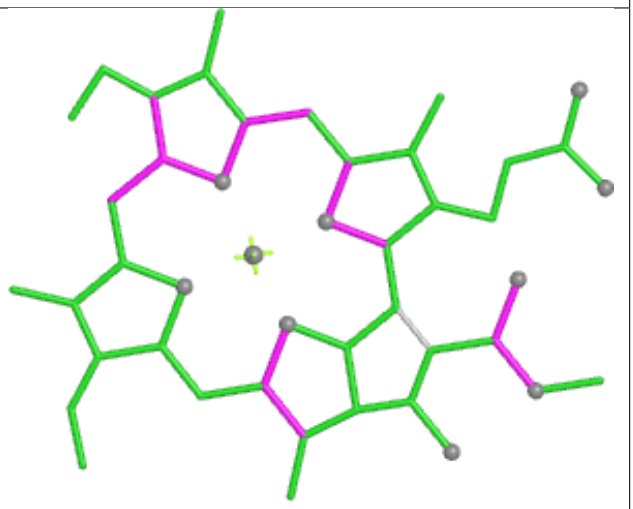


Rings

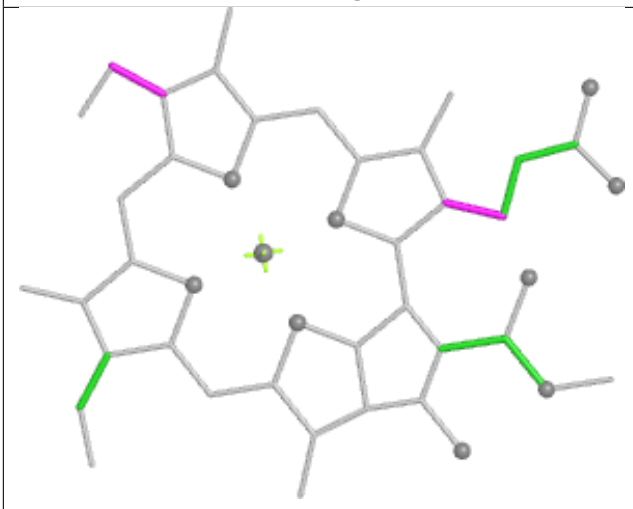
Ligand CLA a3 413



Bond lengths



Bond angles

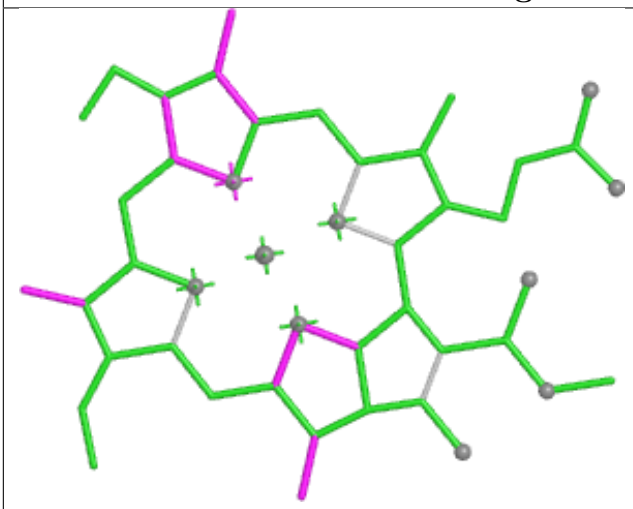


Torsions

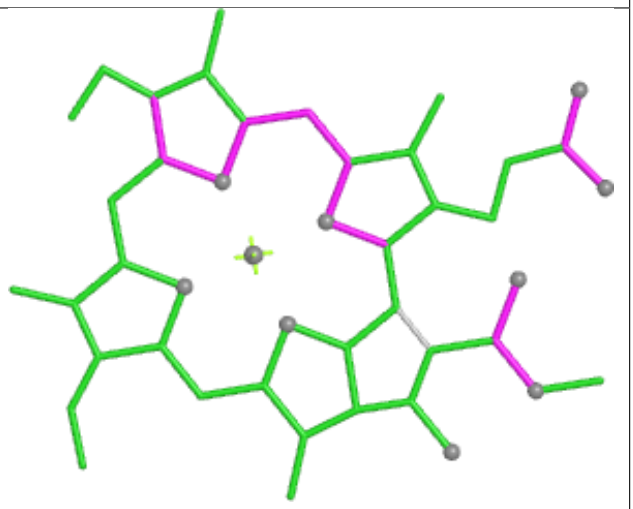


Rings

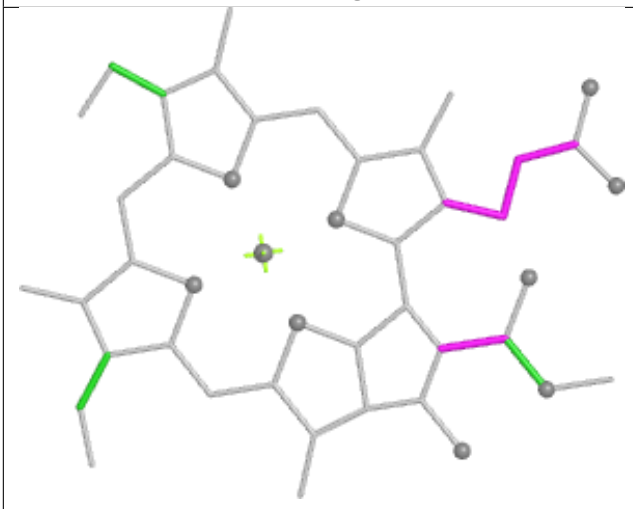
Ligand CLA aA 837



Bond lengths



Bond angles

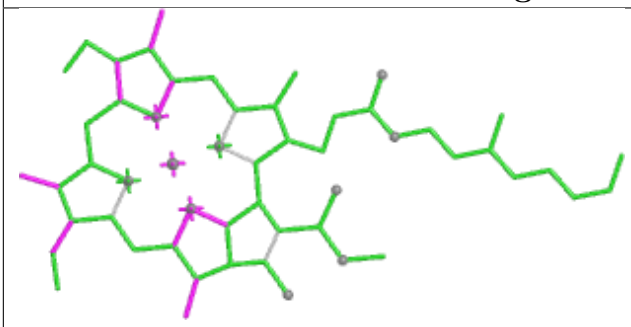


Torsions

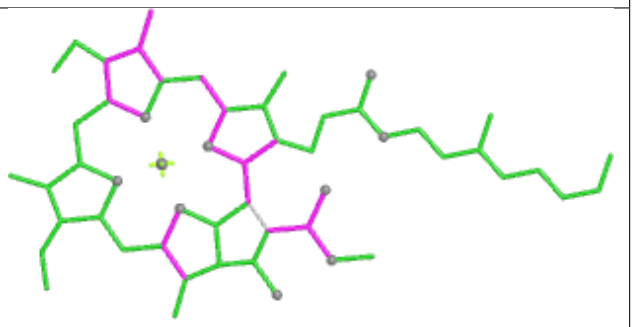


Rings

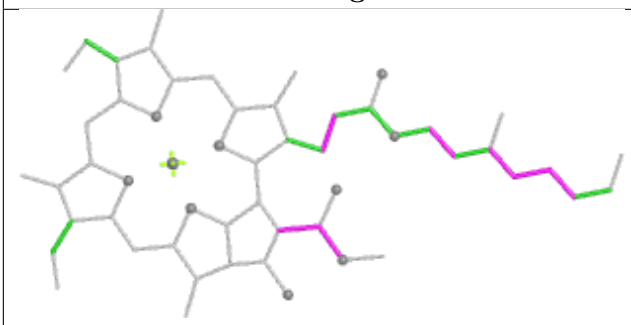
Ligand CLA bB 825



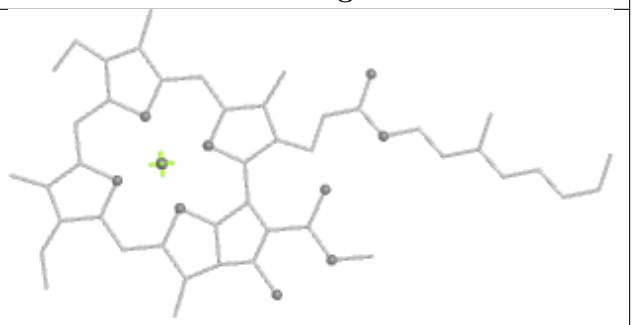
Bond lengths



Bond angles

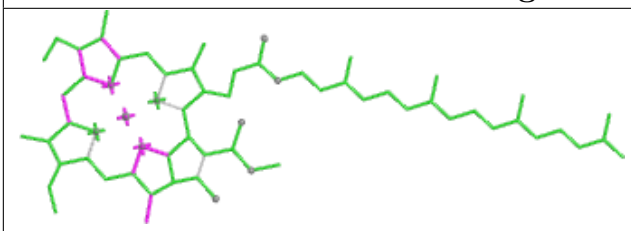


Torsions

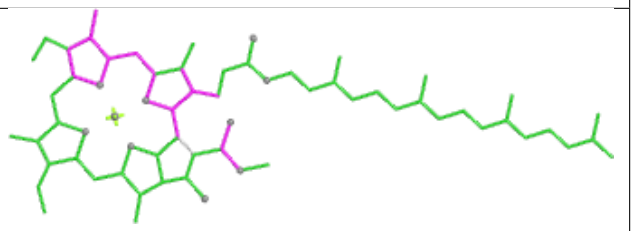


Rings

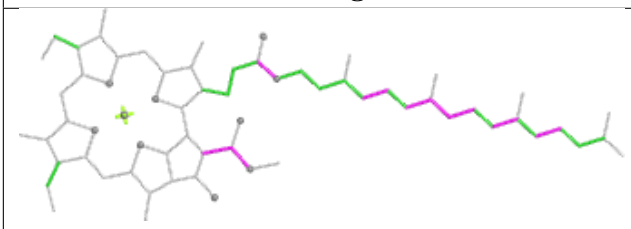
Ligand CLA b2 403



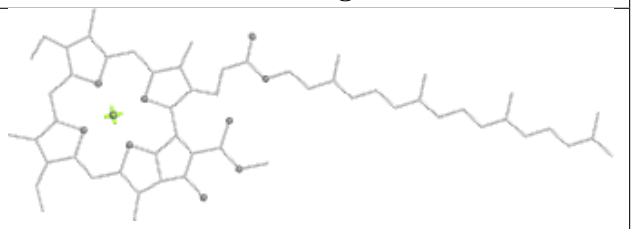
Bond lengths



Bond angles

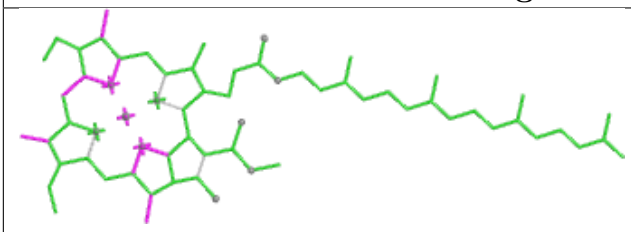


Torsions

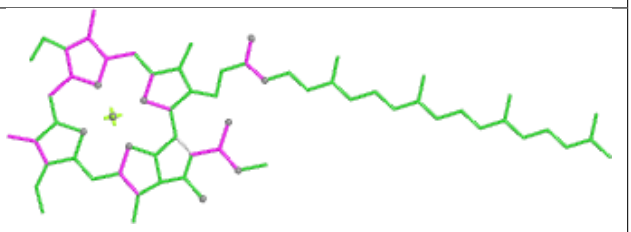


Rings

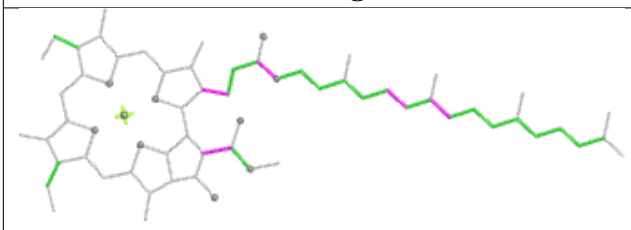
Ligand CLA cA 831



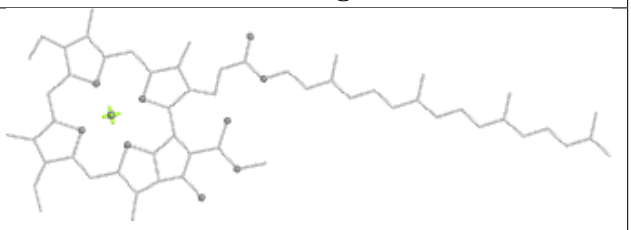
Bond lengths



Bond angles

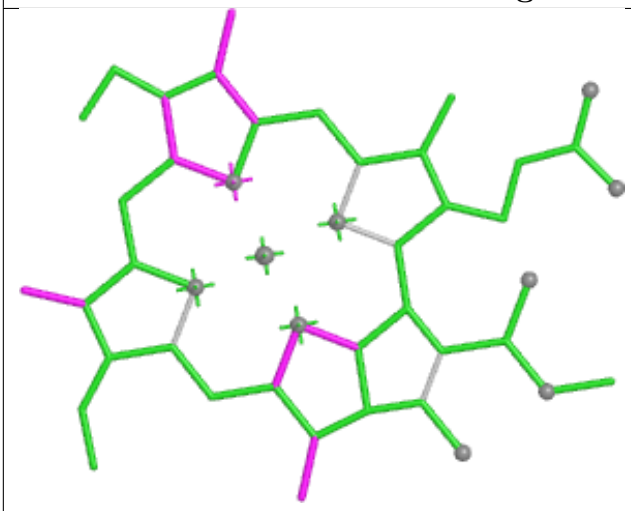


Torsions

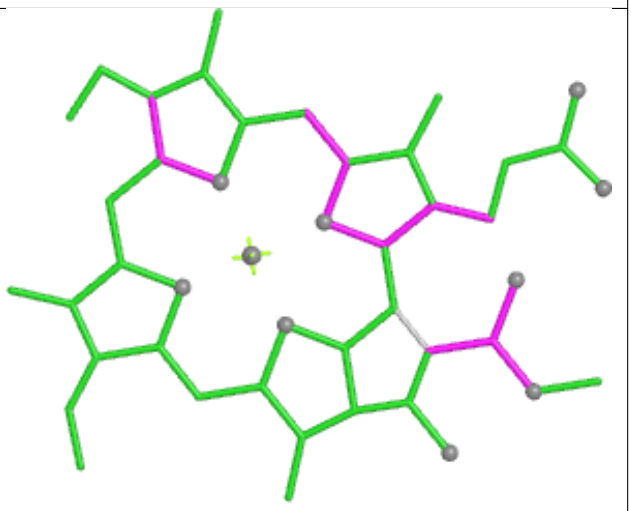


Rings

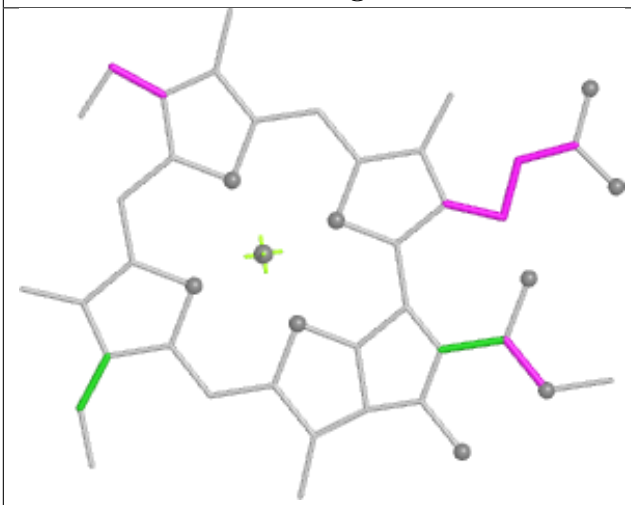
Ligand CLA cB 835



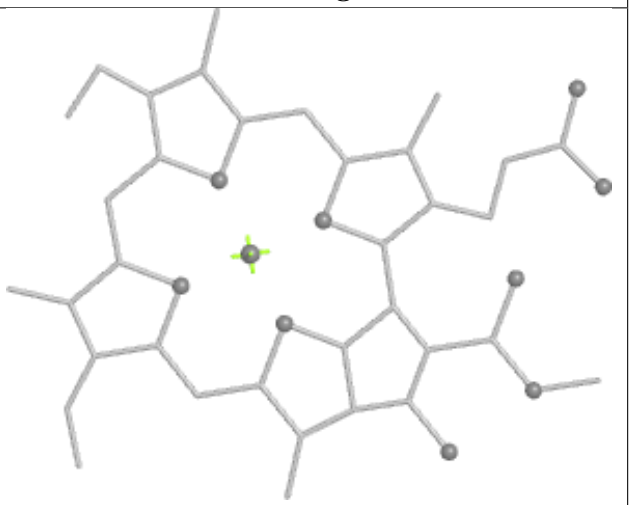
Bond lengths



Bond angles

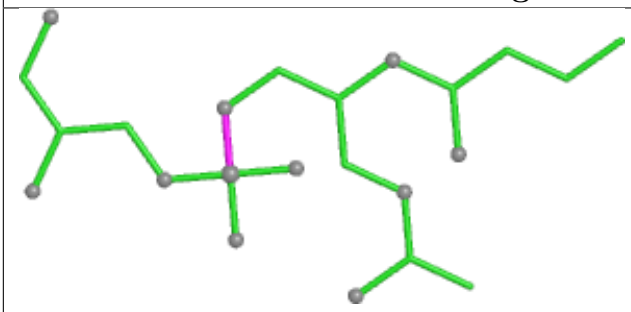


Torsions

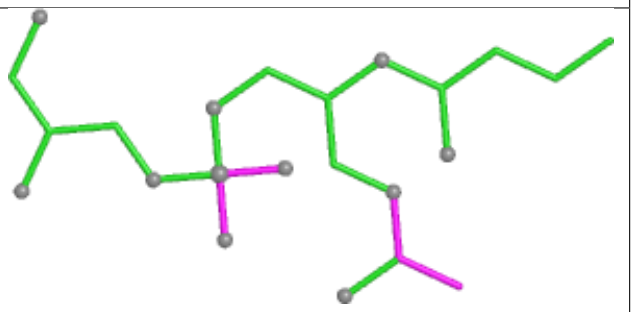


Rings

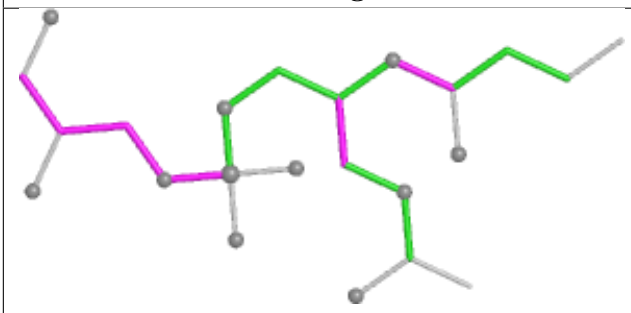
Ligand LHG bX 101



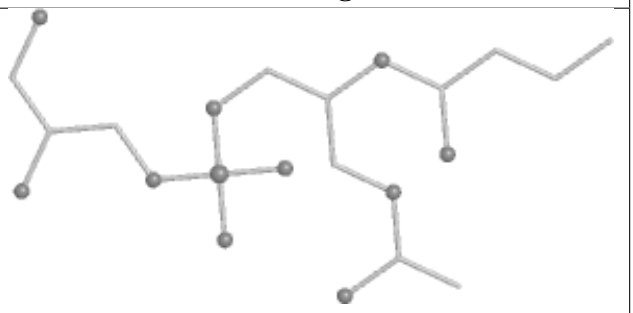
Bond lengths



Bond angles

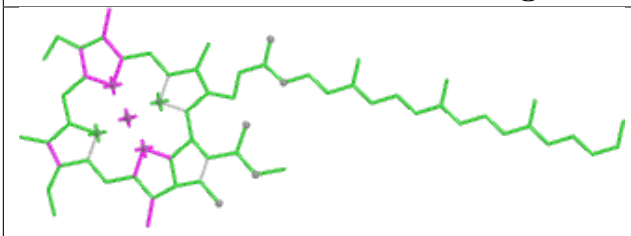


Torsions

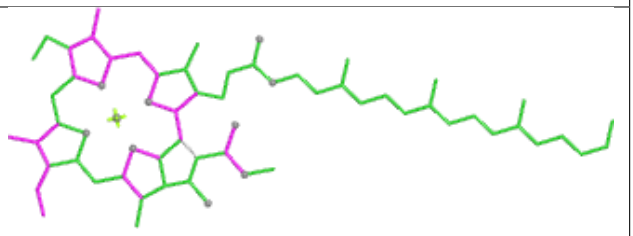


Rings

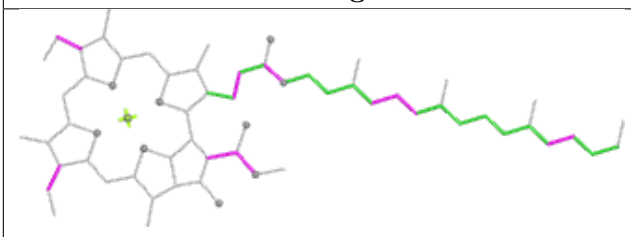
Ligand CLA a6 411



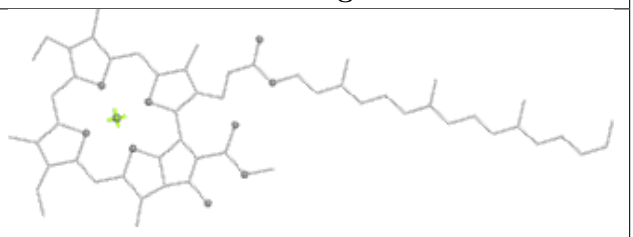
Bond lengths



Bond angles

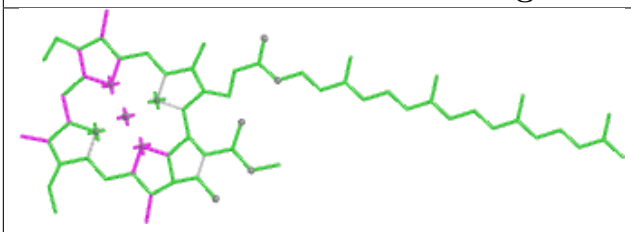


Torsions

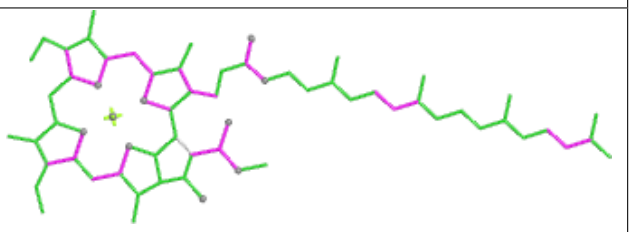


Rings

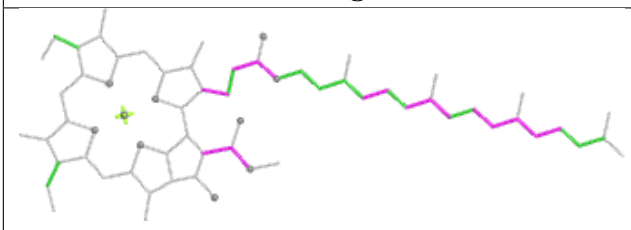
Ligand CLA cB 833



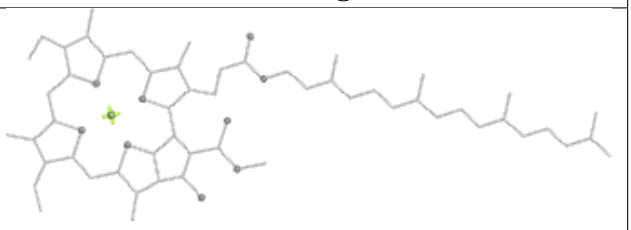
Bond lengths



Bond angles

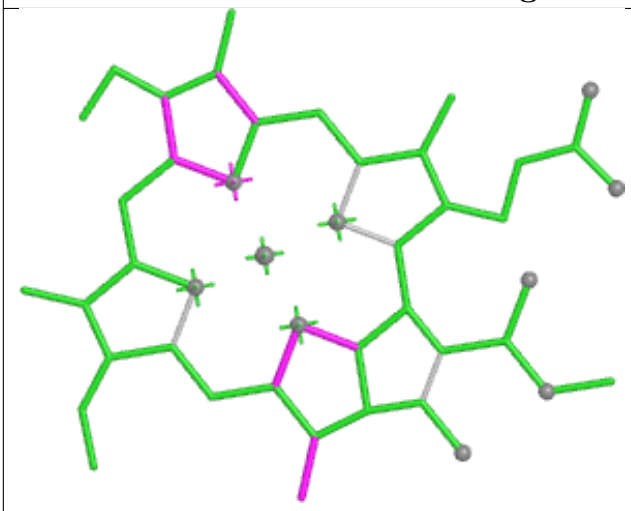


Torsions

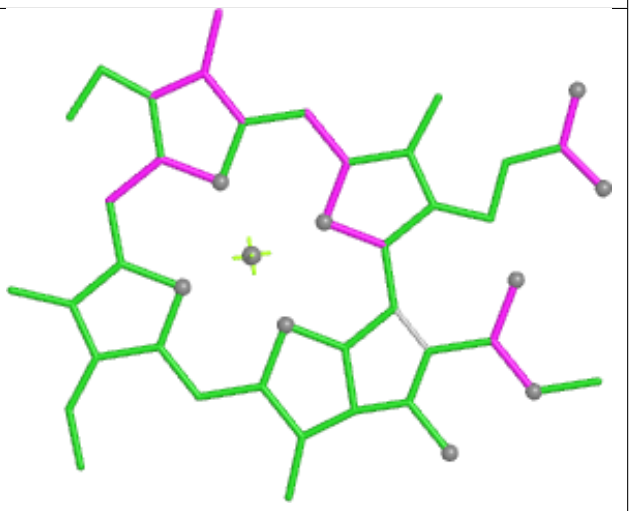


Rings

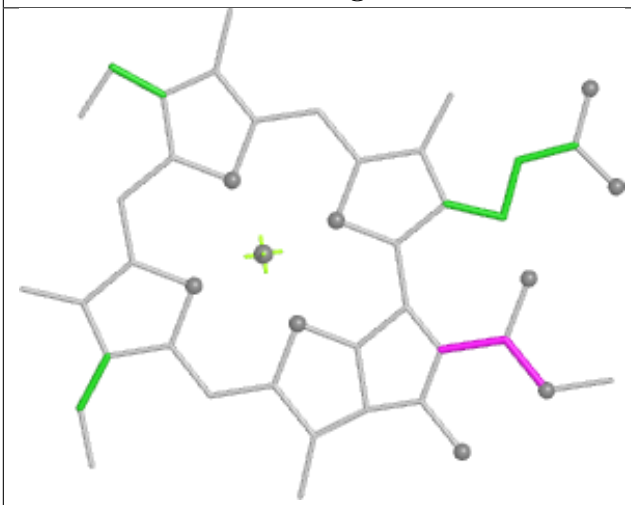
Ligand CLA a2 407



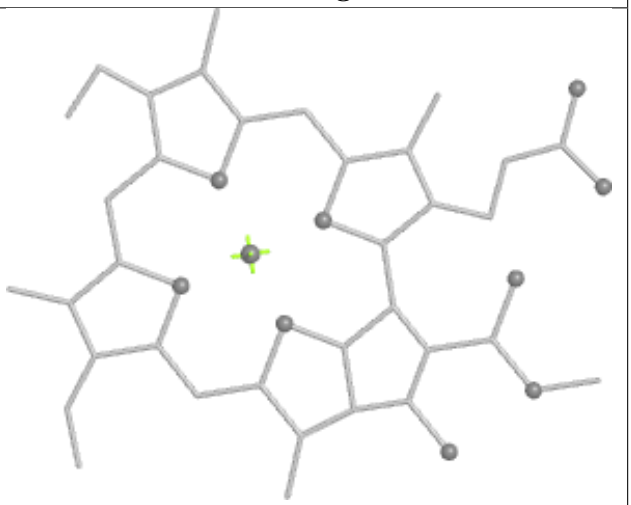
Bond lengths



Bond angles

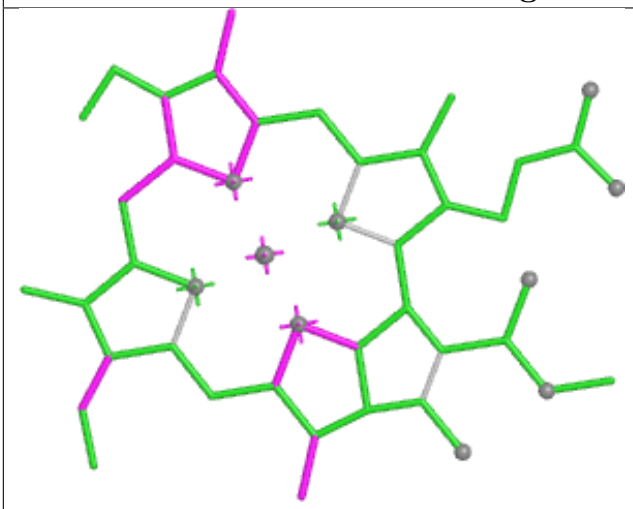


Torsions

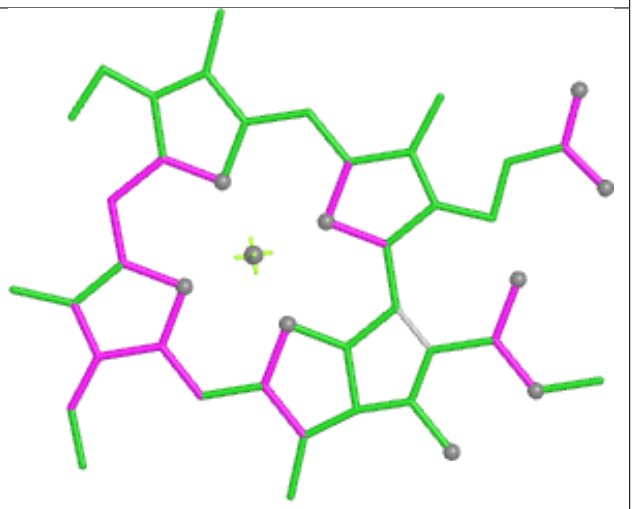


Rings

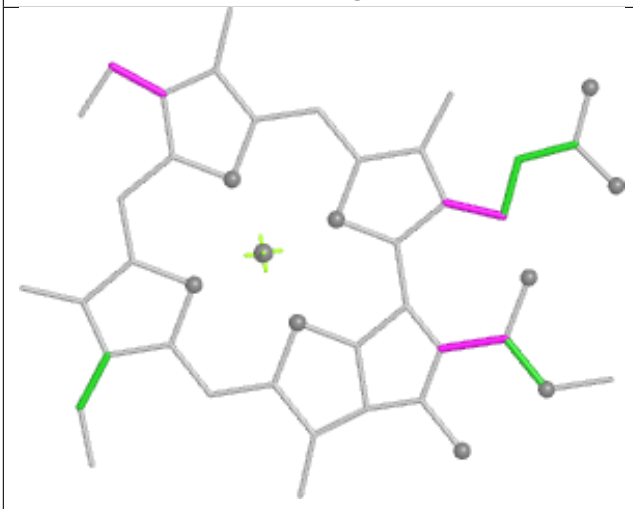
Ligand CLA a6 414



Bond lengths



Bond angles

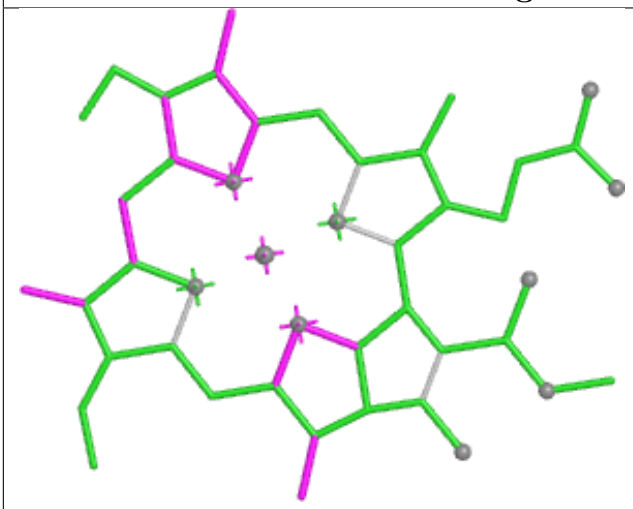


Torsions

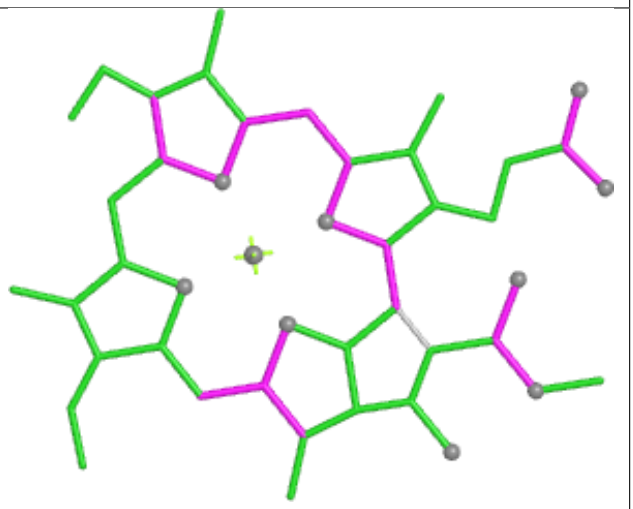


Rings

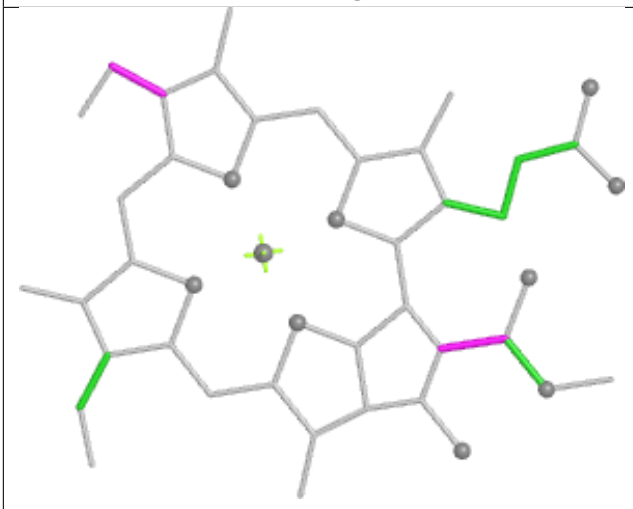
Ligand CLA cA 815



Bond lengths



Bond angles

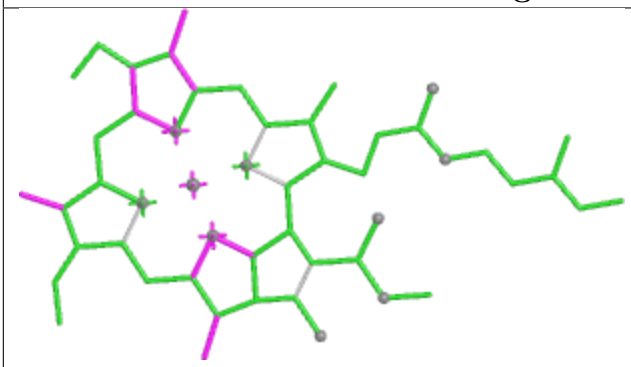


Torsions

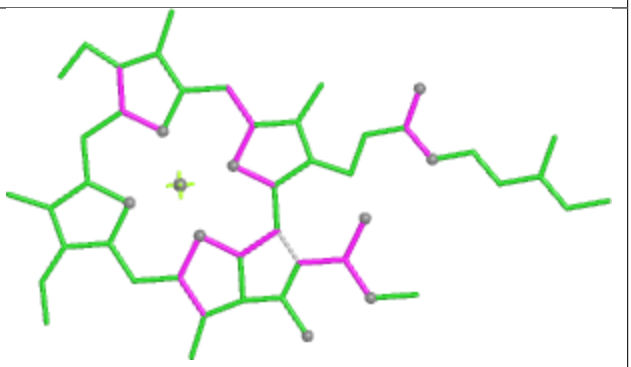


Rings

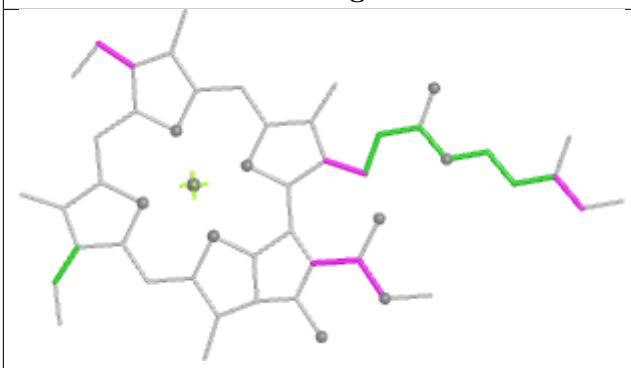
Ligand CLA bA 842



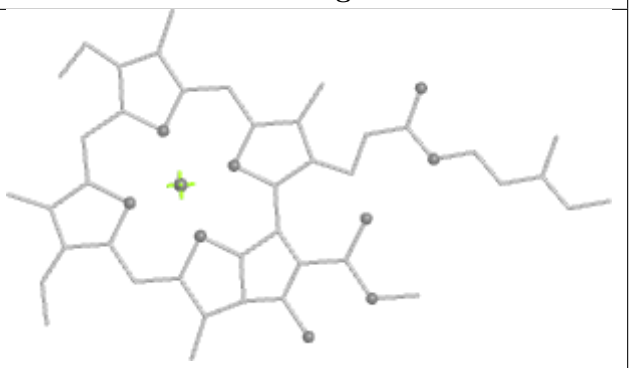
Bond lengths



Bond angles

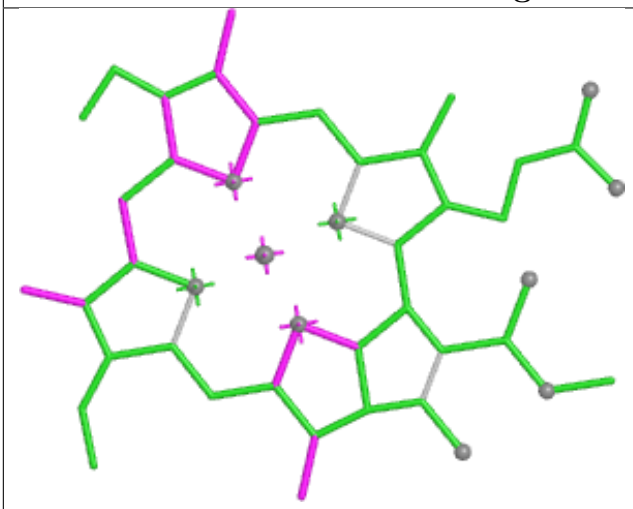


Torsions

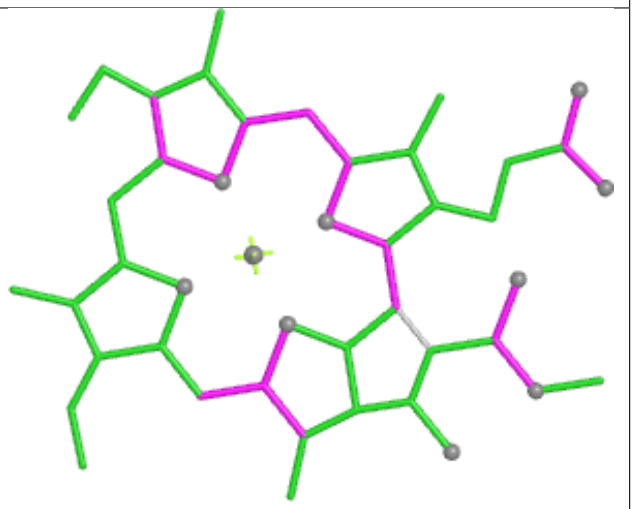


Rings

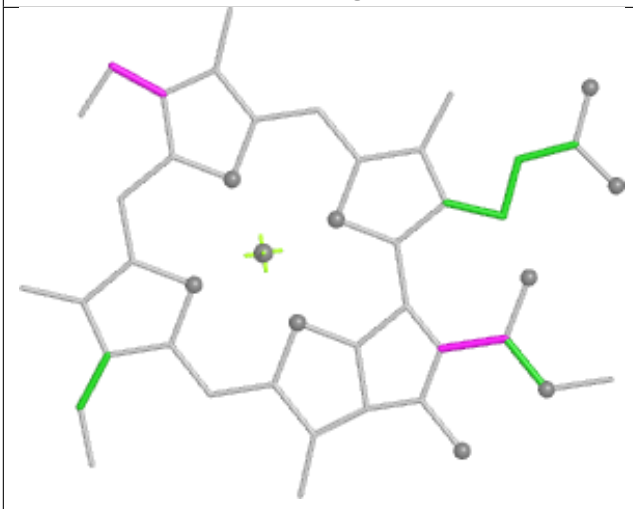
Ligand CLA bA 815



Bond lengths



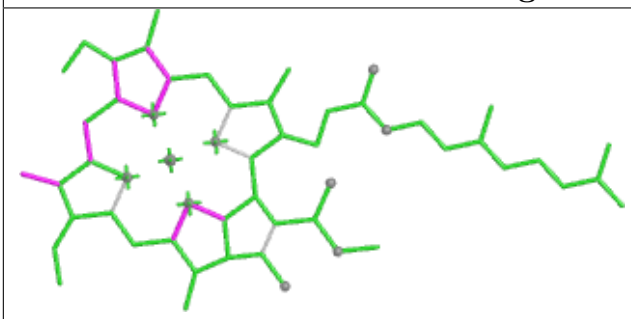
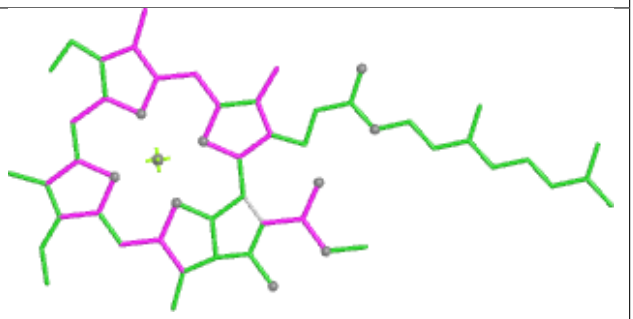
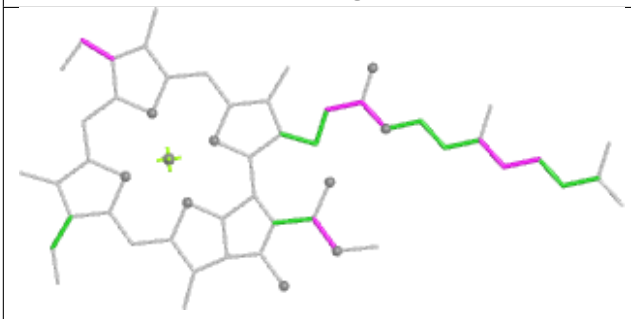
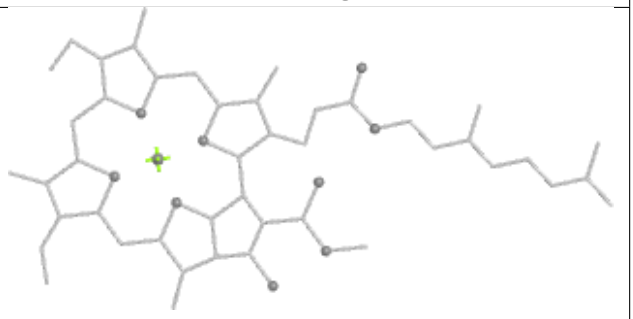
Bond angles



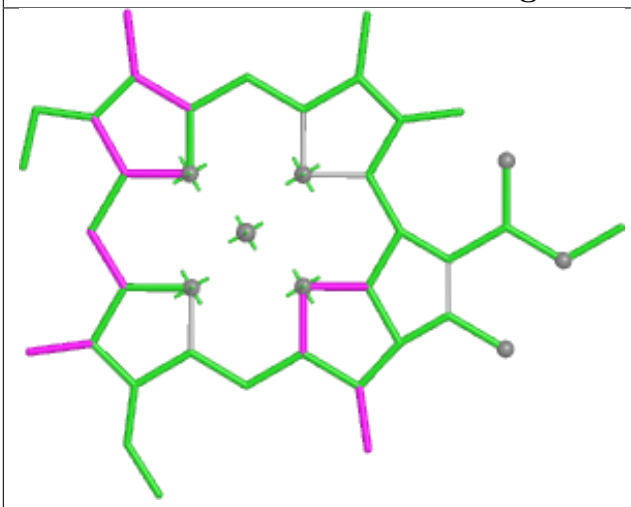
Torsions



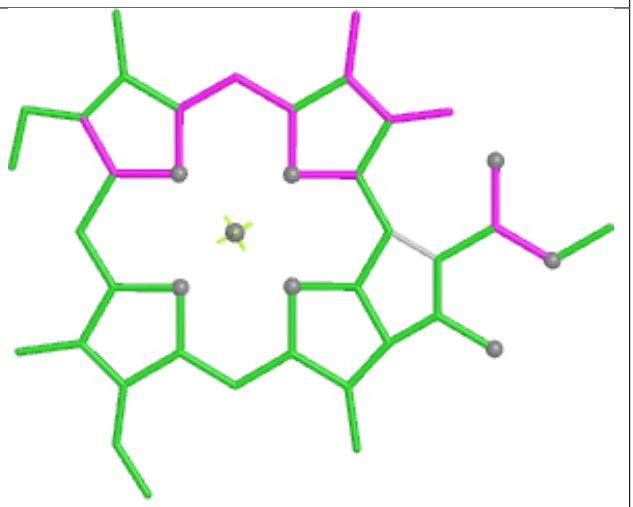
Rings

Ligand CLA b5 417	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

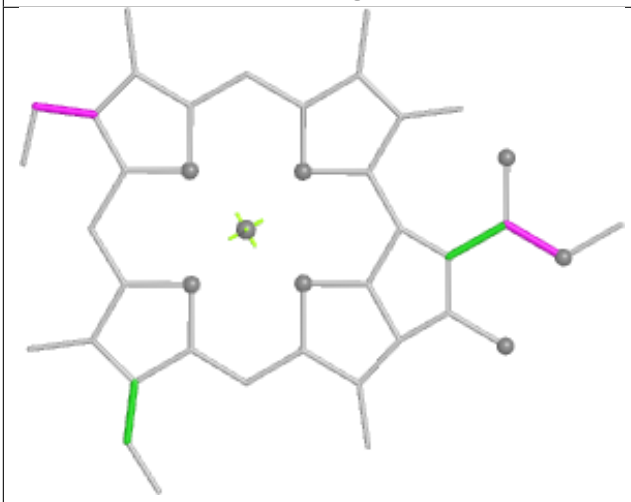
Ligand CLA a1 413



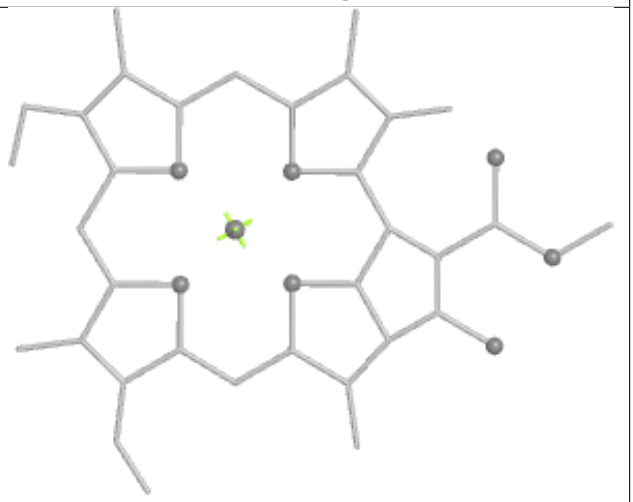
Bond lengths



Bond angles

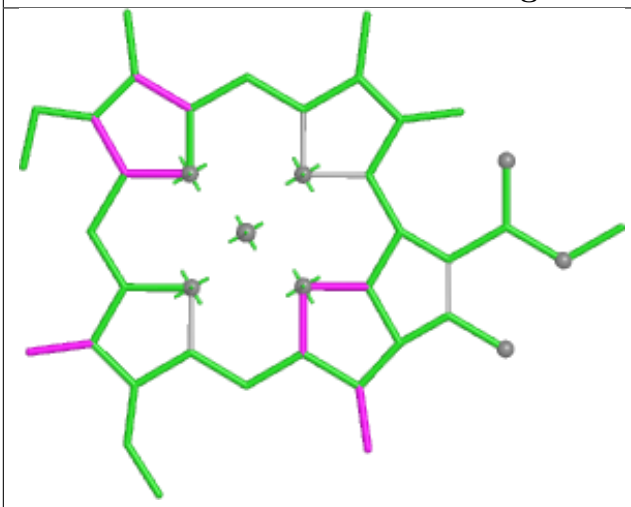


Torsions

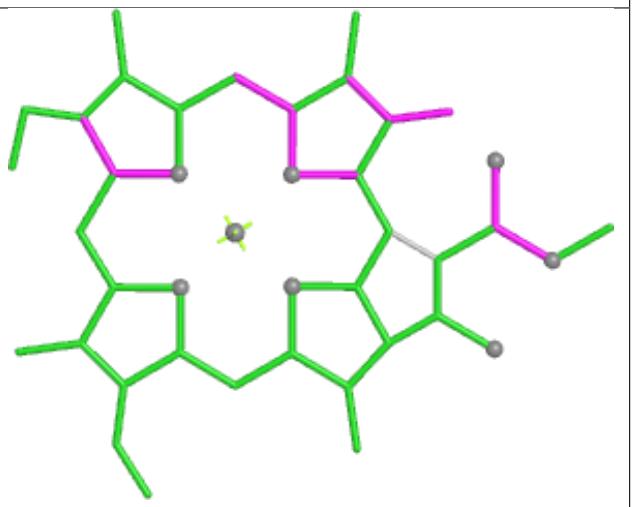


Rings

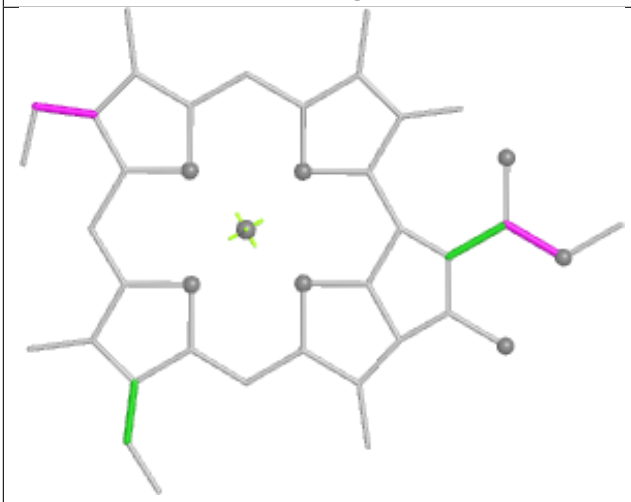
Ligand CLA c2 415



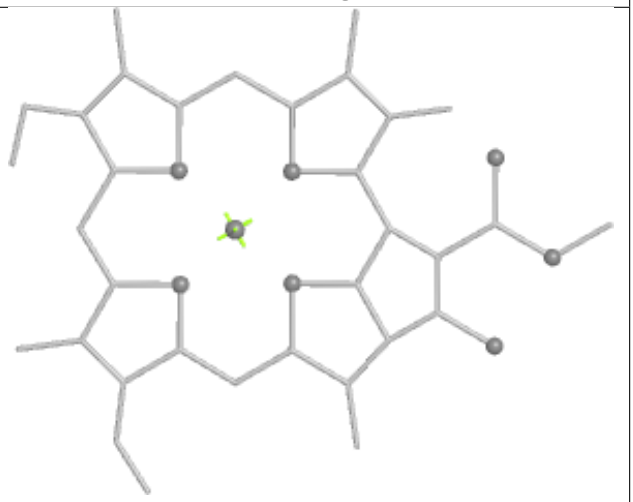
Bond lengths



Bond angles

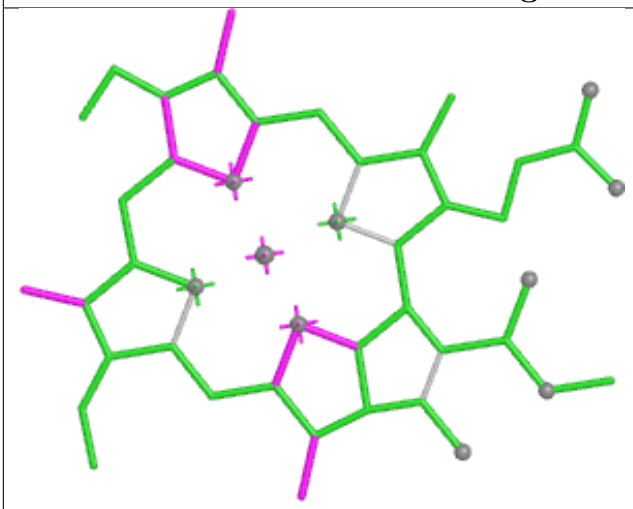


Torsions

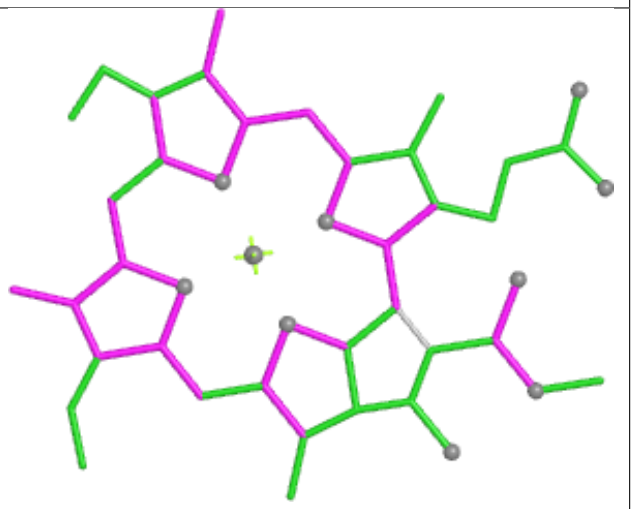


Rings

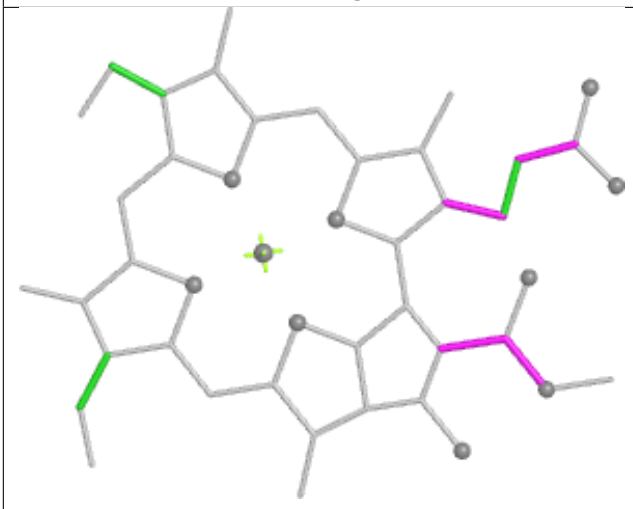
Ligand CLA c2 413



Bond lengths



Bond angles

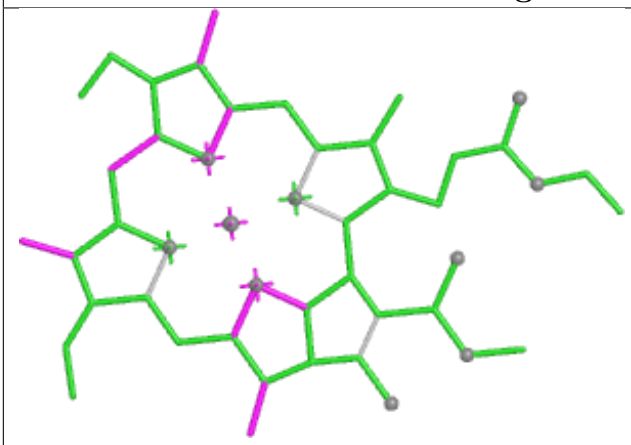


Torsions

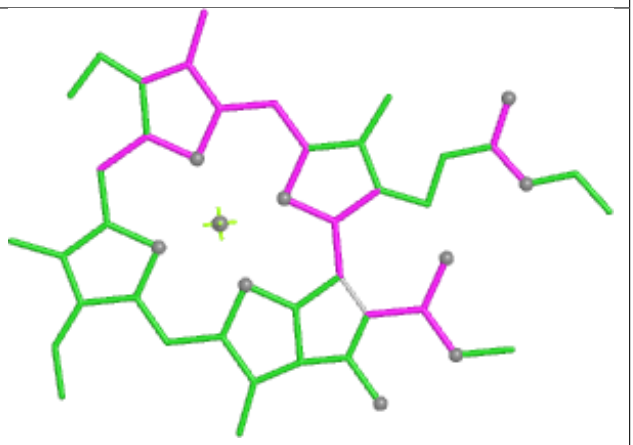


Rings

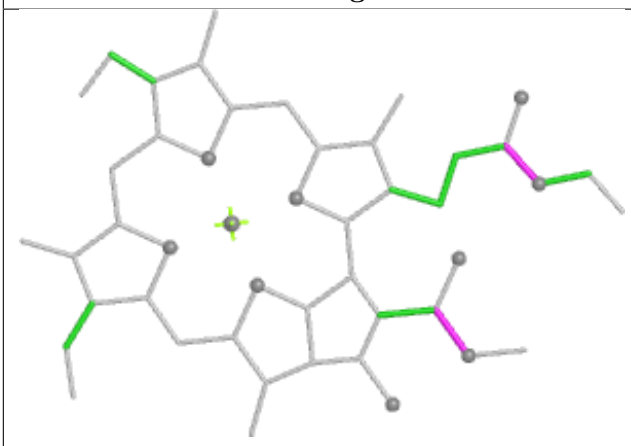
Ligand CLA aA 840



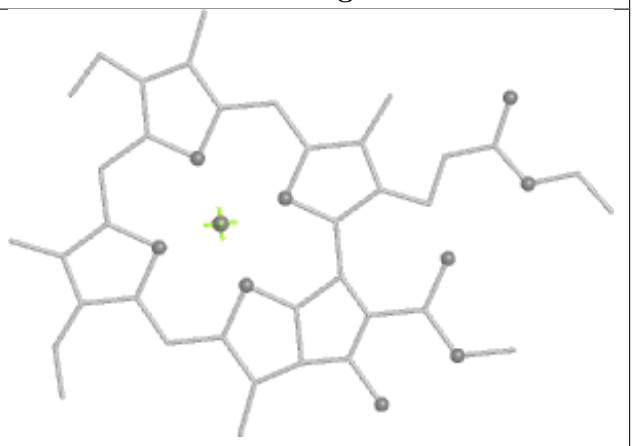
Bond lengths



Bond angles

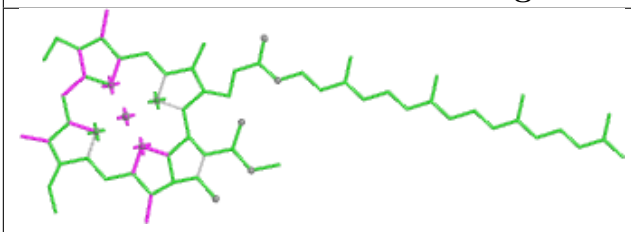


Torsions

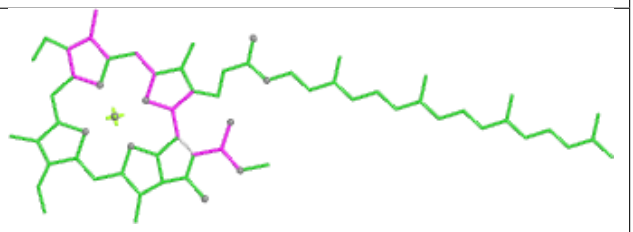


Rings

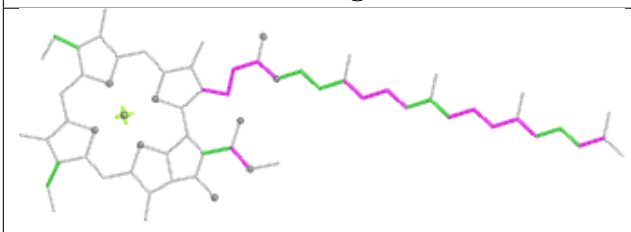
Ligand CLA bB 828



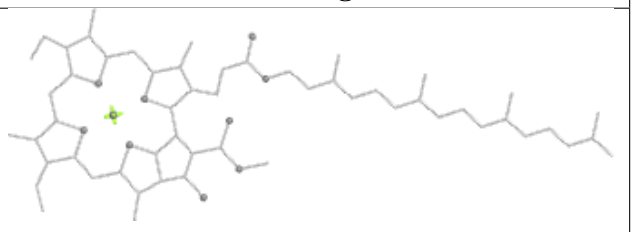
Bond lengths



Bond angles

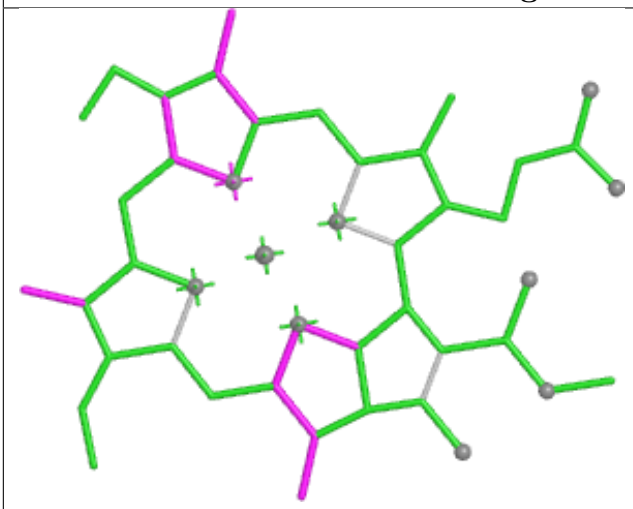


Torsions

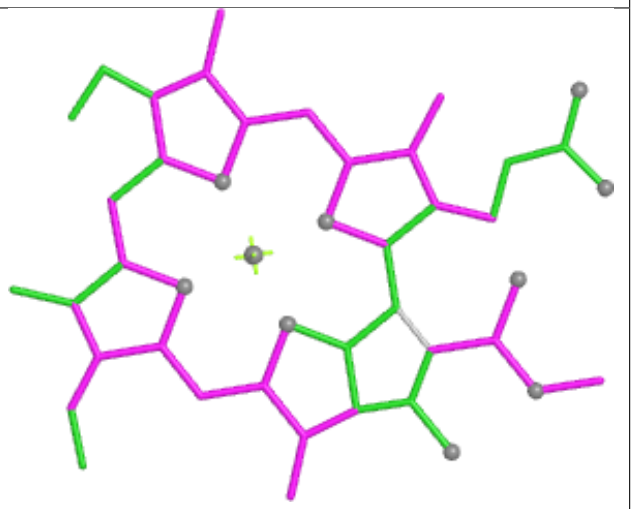


Rings

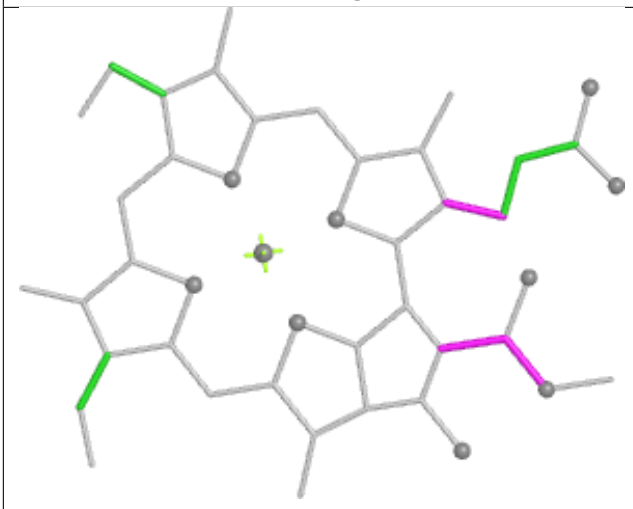
Ligand CLA c5 405



Bond lengths



Bond angles

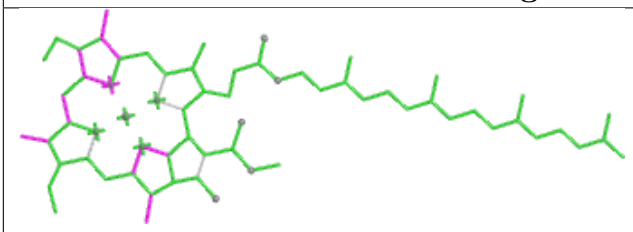


Torsions

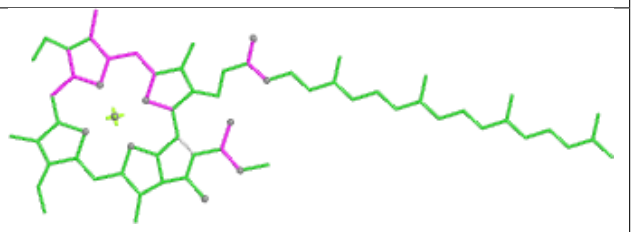


Rings

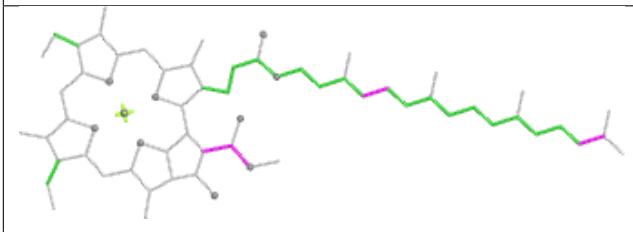
Ligand CLA c5 409



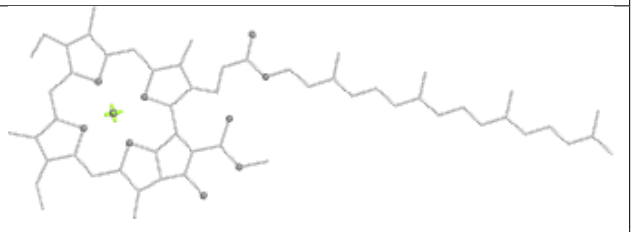
Bond lengths



Bond angles

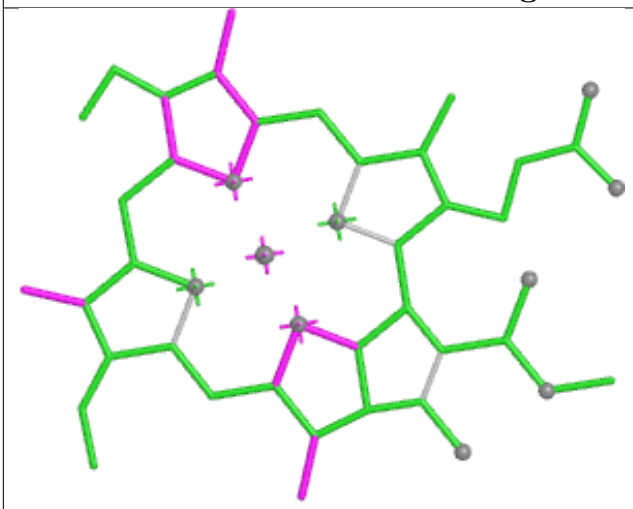


Torsions

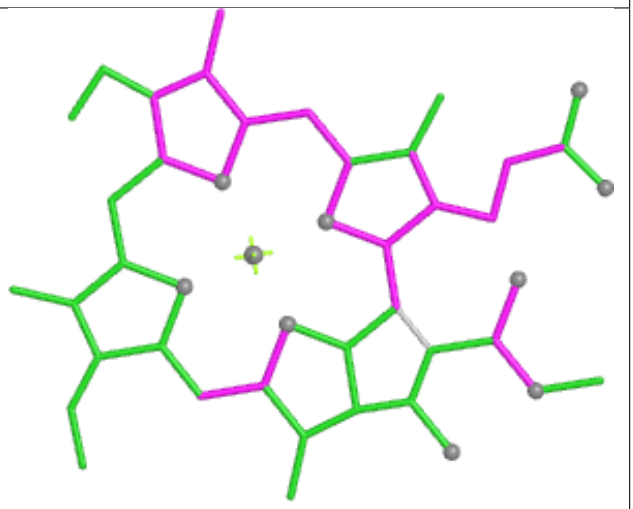


Rings

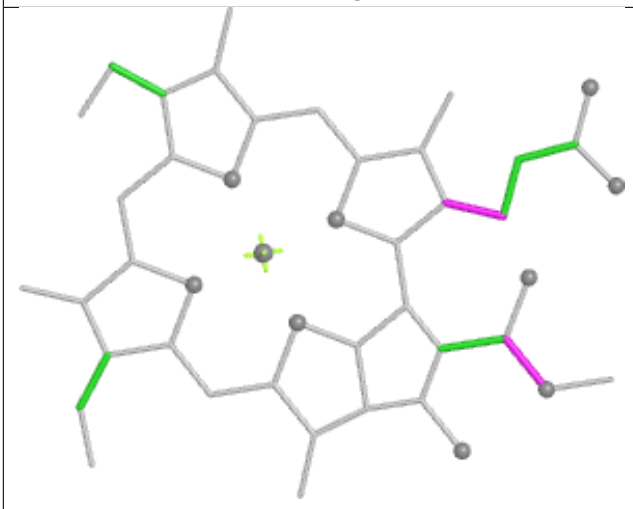
Ligand CLA a6 412



Bond lengths



Bond angles

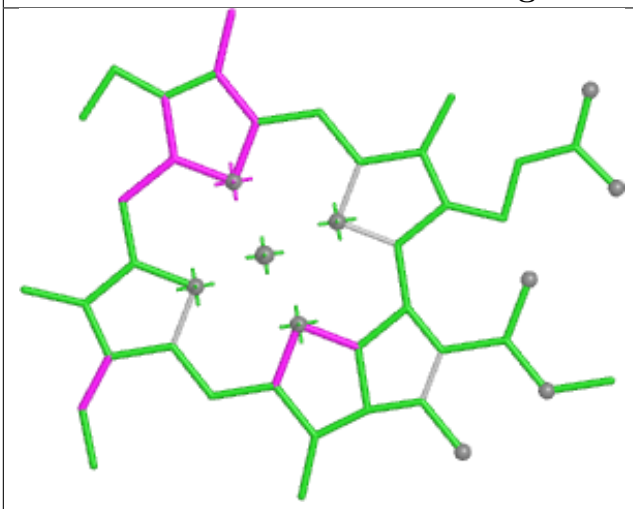


Torsions

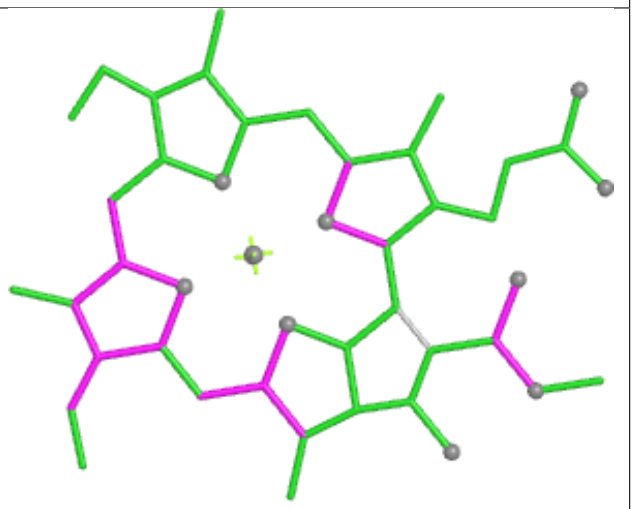


Rings

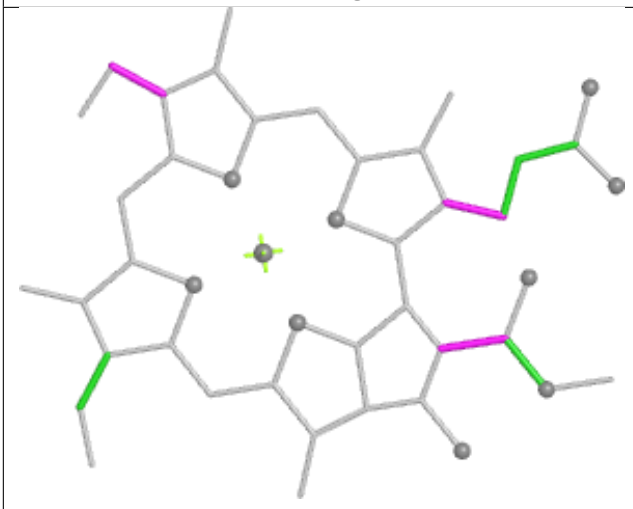
Ligand CLA b6 414



Bond lengths



Bond angles

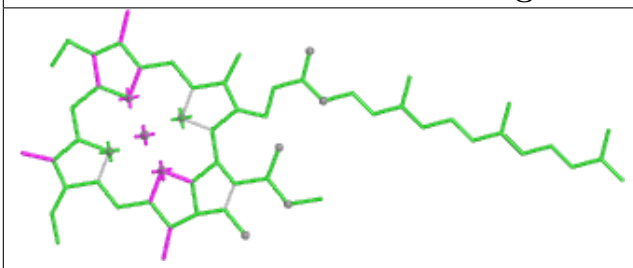


Torsions

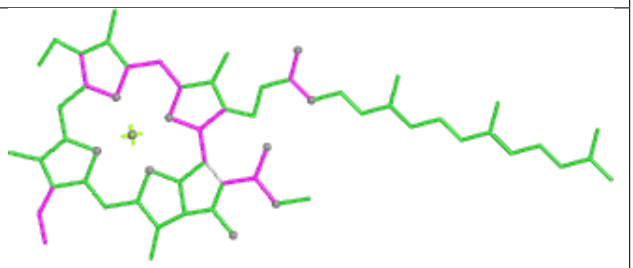


Rings

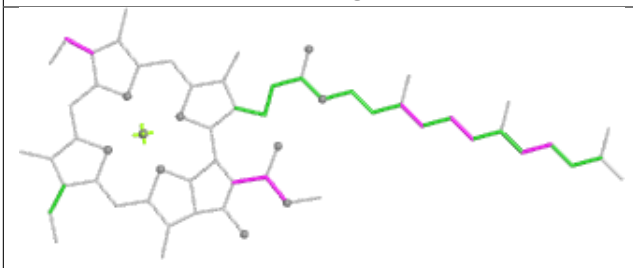
Ligand CLA aB 836



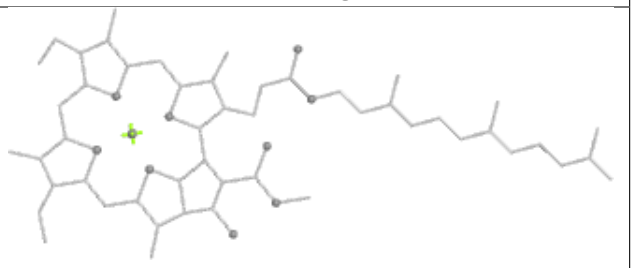
Bond lengths



Bond angles

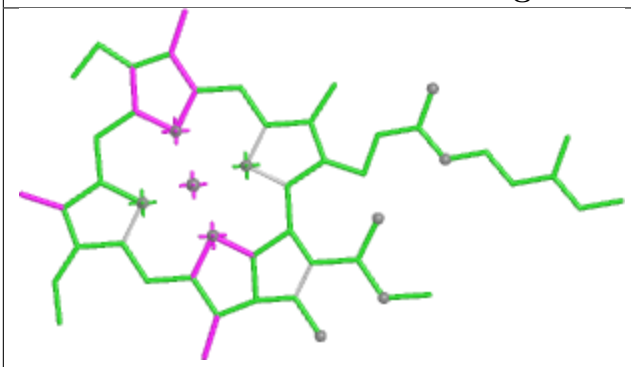


Torsions

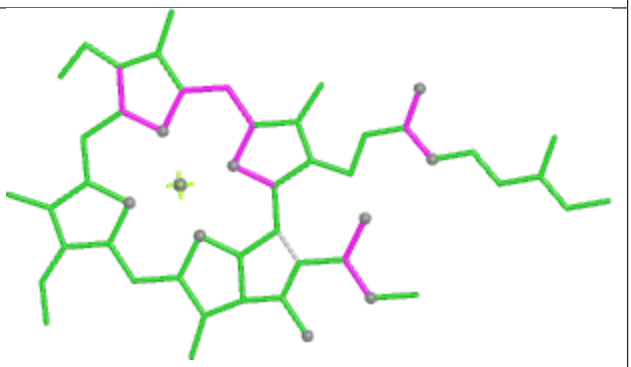


Rings

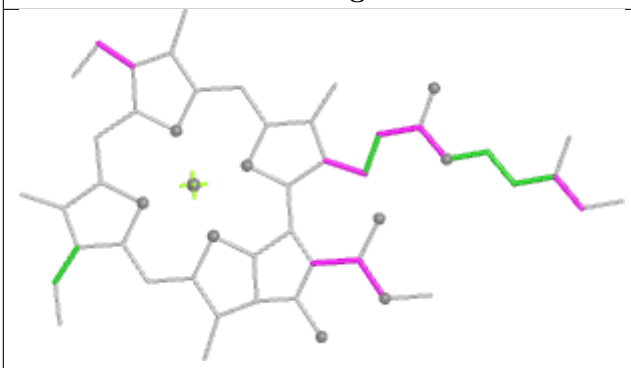
Ligand CLA bA 824



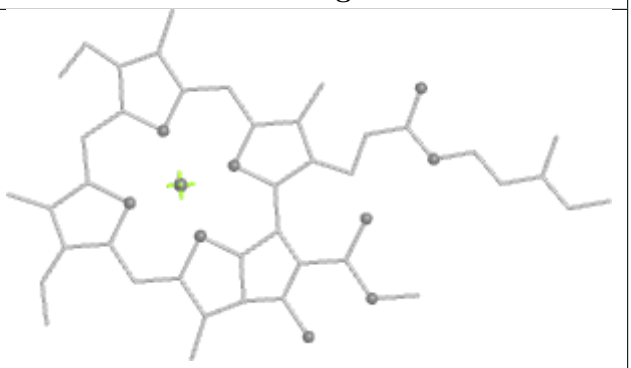
Bond lengths



Bond angles

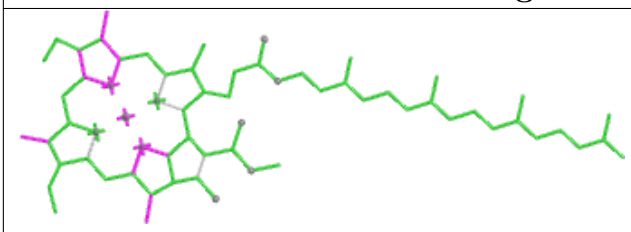


Torsions

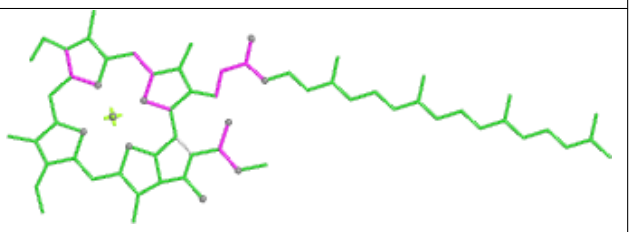


Rings

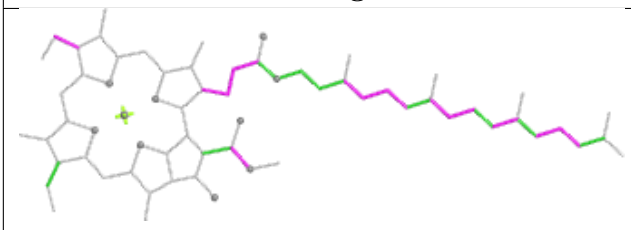
Ligand CLA cA 810



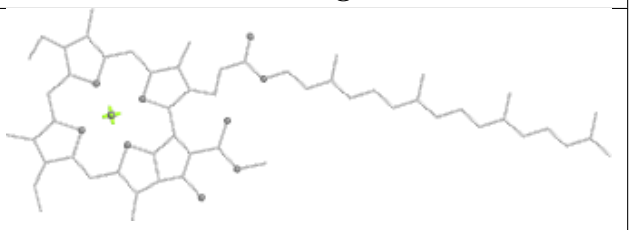
Bond lengths



Bond angles

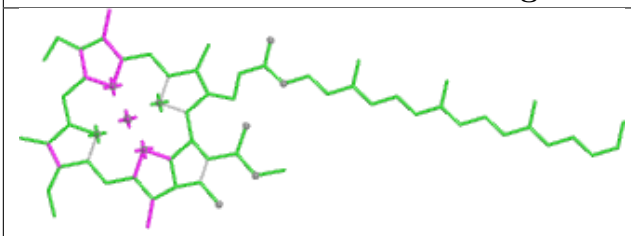


Torsions

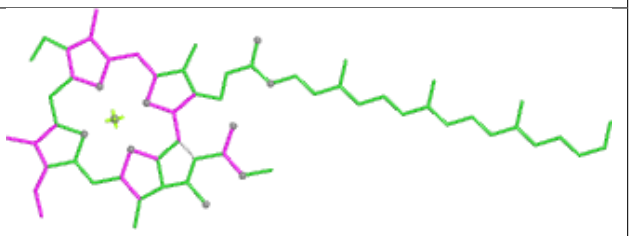


Rings

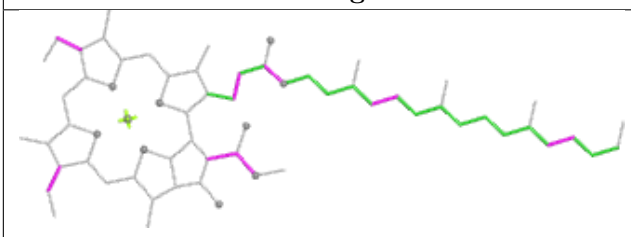
Ligand CLA c2 411



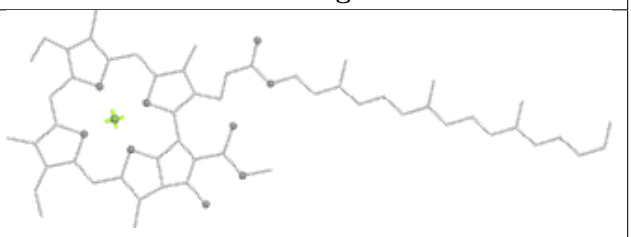
Bond lengths



Bond angles

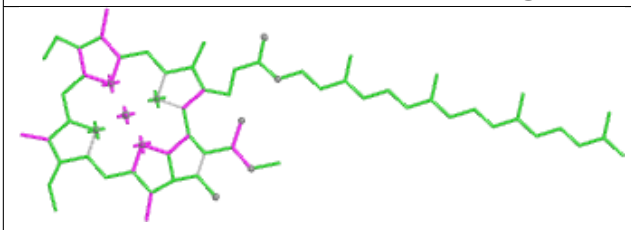


Torsions

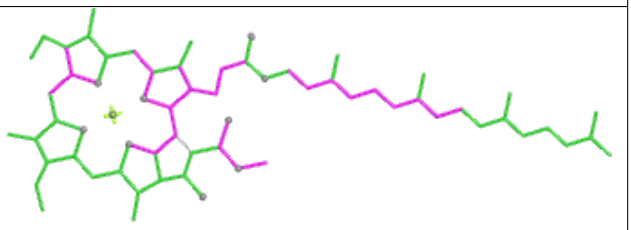


Rings

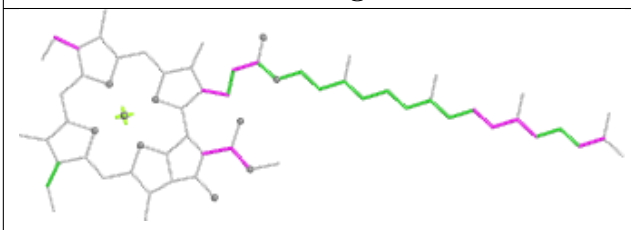
Ligand CLA a4 421



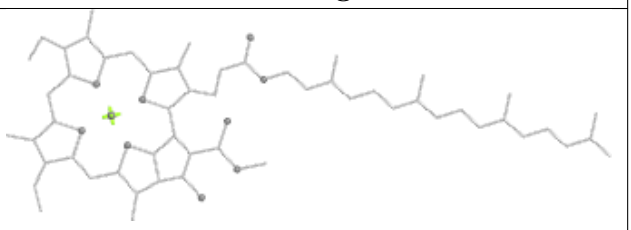
Bond lengths



Bond angles



Torsions

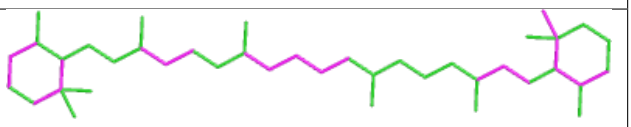


Rings

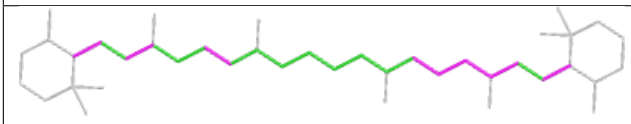
Ligand BCR a3 419



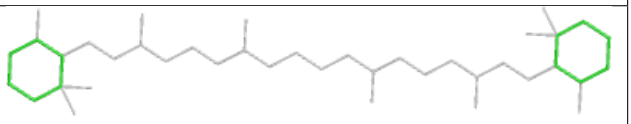
Bond lengths



Bond angles

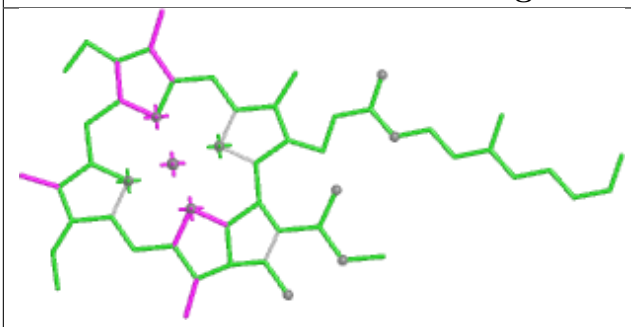


Torsions

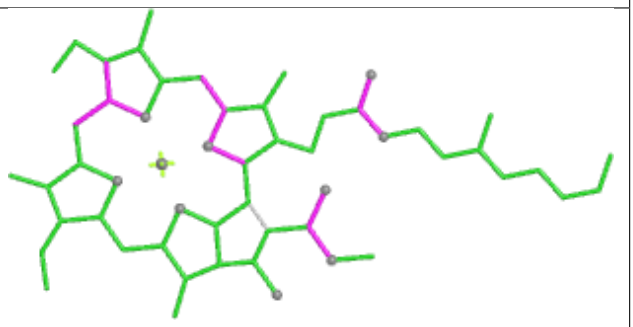


Rings

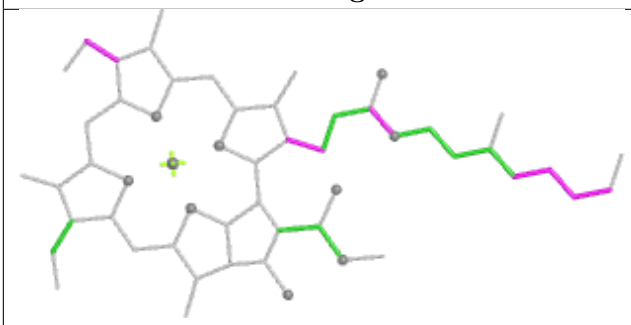
Ligand CLA aA 836



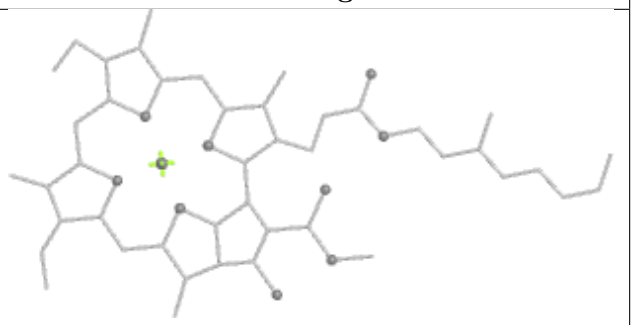
Bond lengths



Bond angles

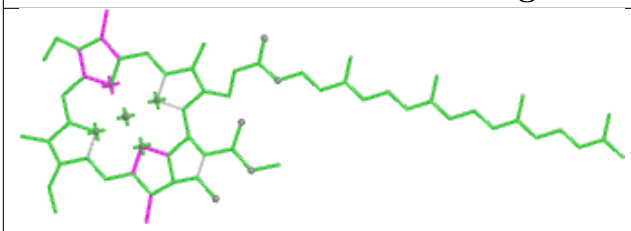


Torsions

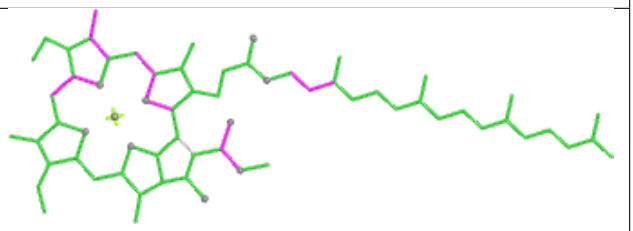


Rings

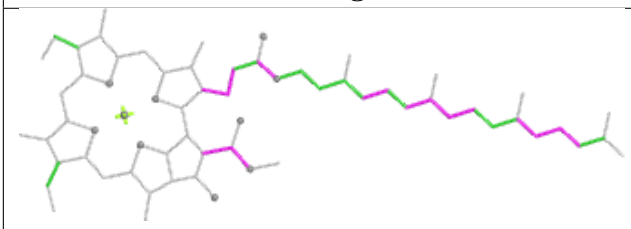
Ligand CLA b2 402



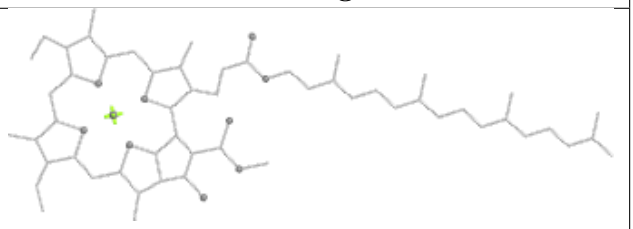
Bond lengths



Bond angles

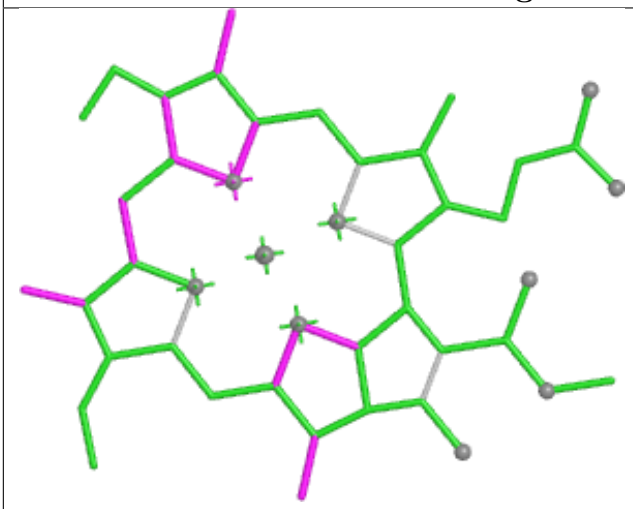


Torsions

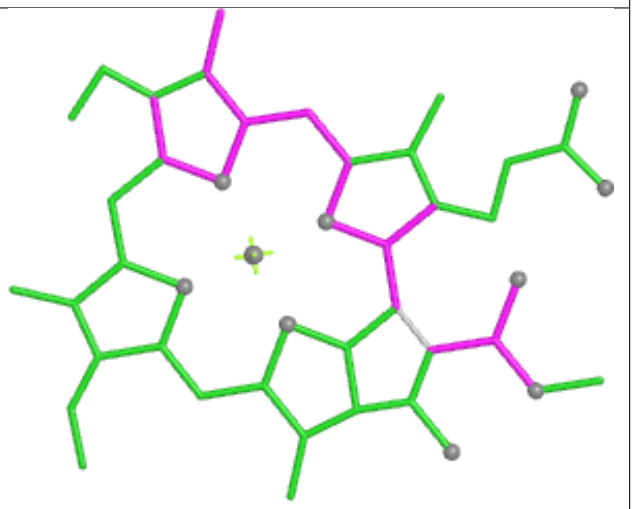


Rings

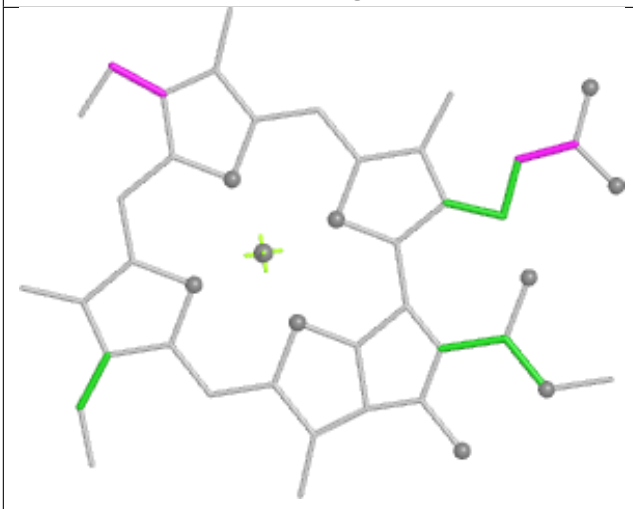
Ligand CLA aB 841



Bond lengths



Bond angles

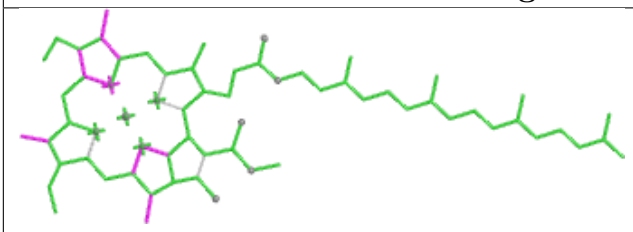


Torsions

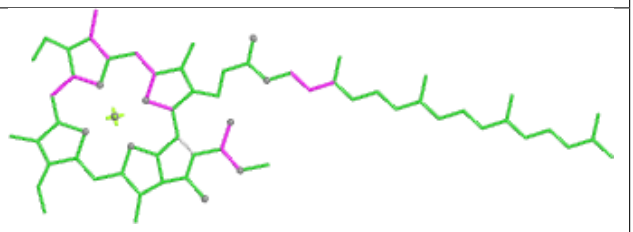


Rings

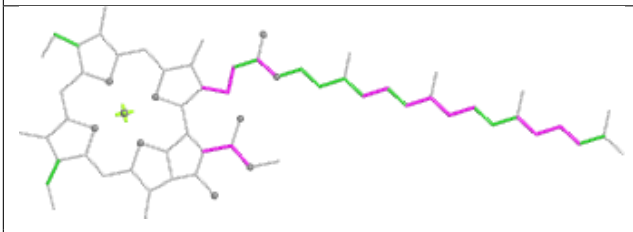
Ligand CLA b5 402



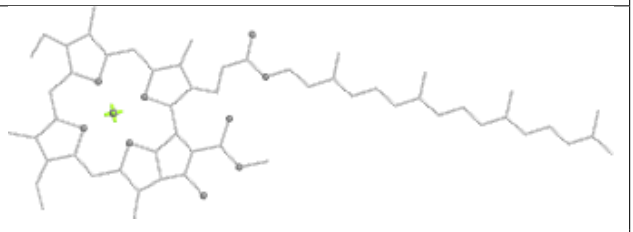
Bond lengths



Bond angles

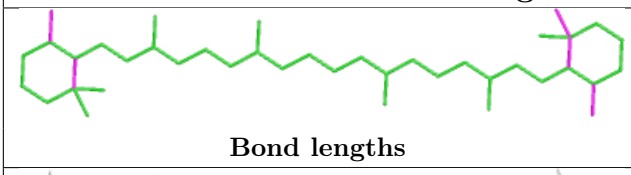


Torsions

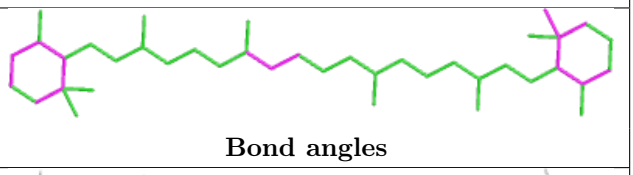


Rings

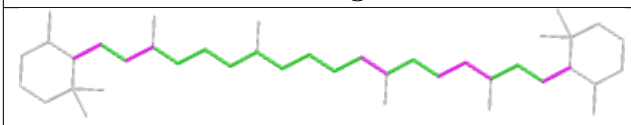
Ligand BCR b1 418



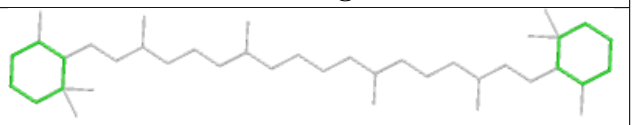
Bond lengths



Bond angles

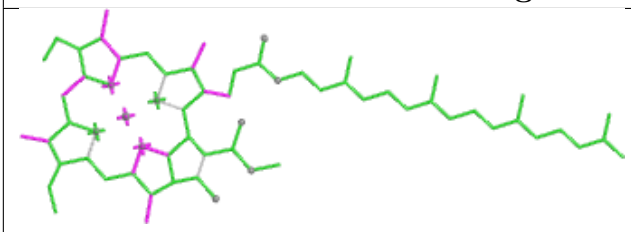


Torsions

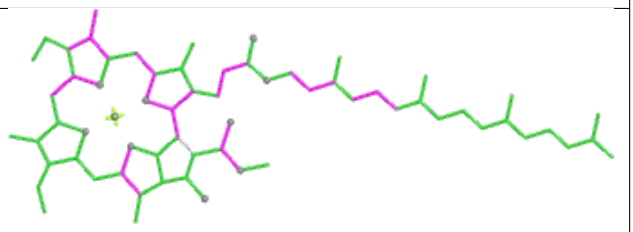


Rings

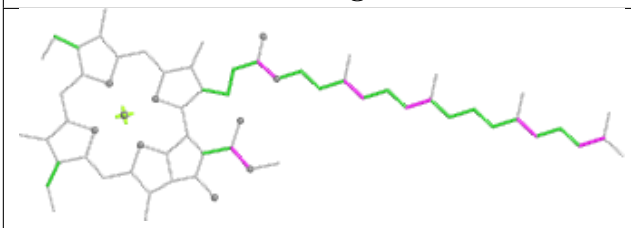
Ligand CLA aA 834



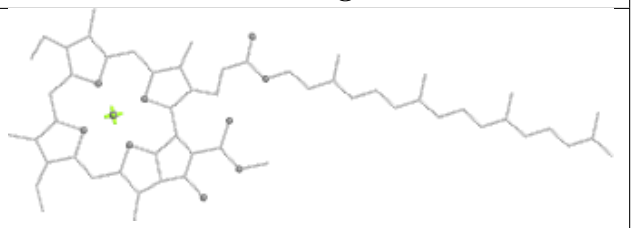
Bond lengths



Bond angles

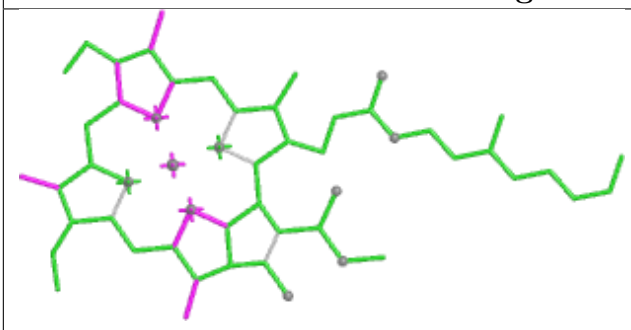


Torsions

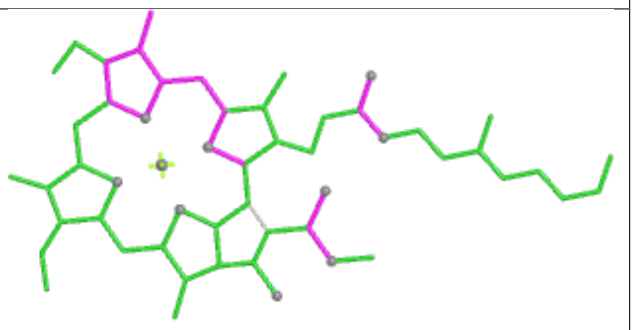


Rings

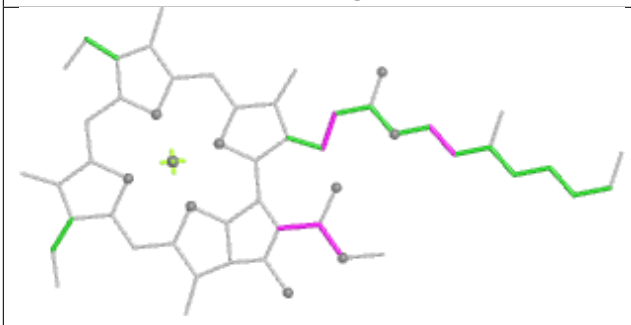
Ligand CLA aB 805



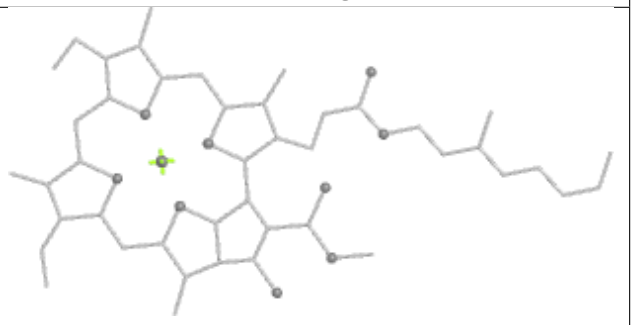
Bond lengths



Bond angles

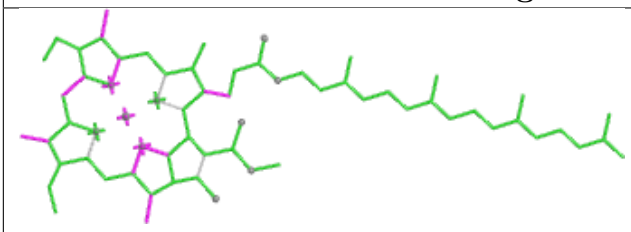


Torsions

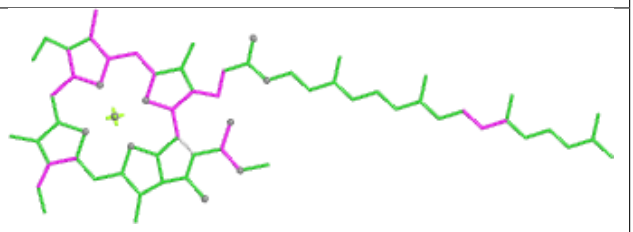


Rings

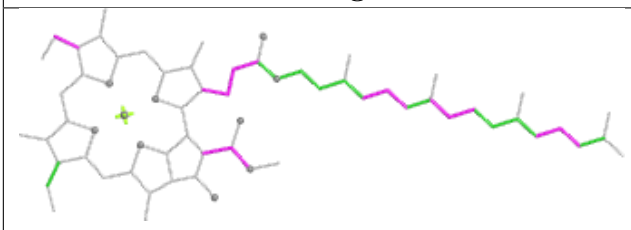
Ligand CLA cB 810



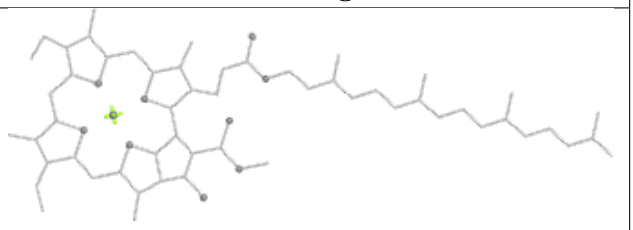
Bond lengths



Bond angles

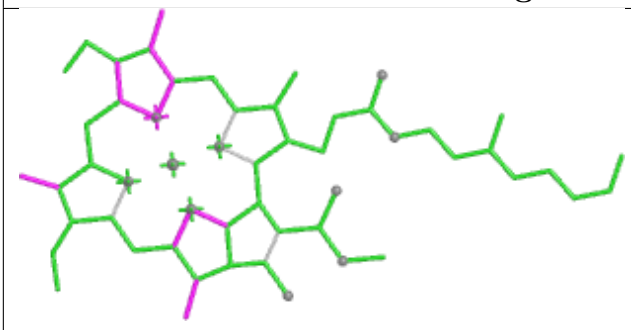


Torsions

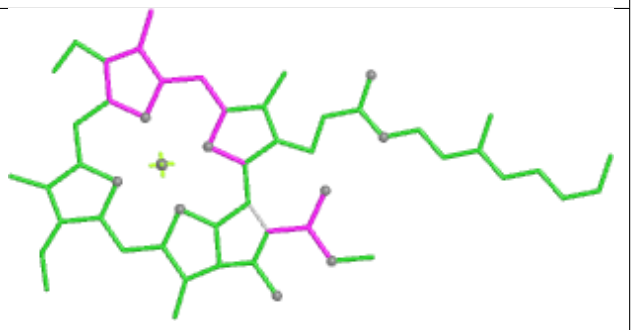


Rings

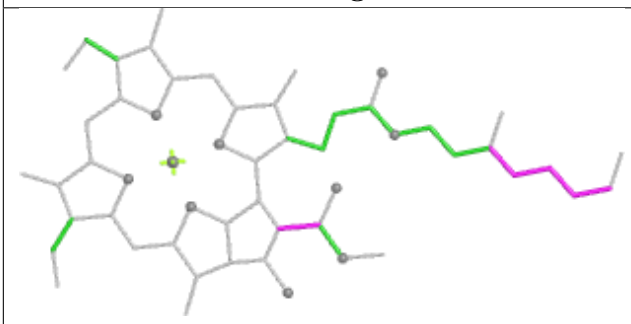
Ligand CLA aA 818



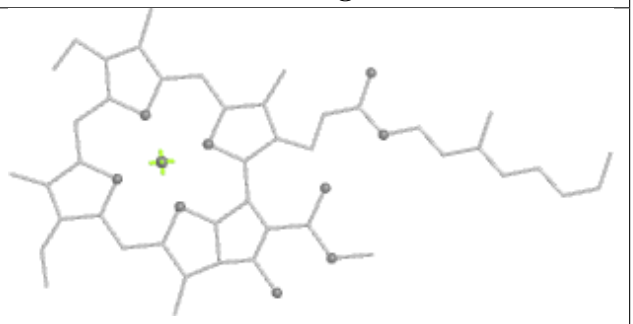
Bond lengths



Bond angles

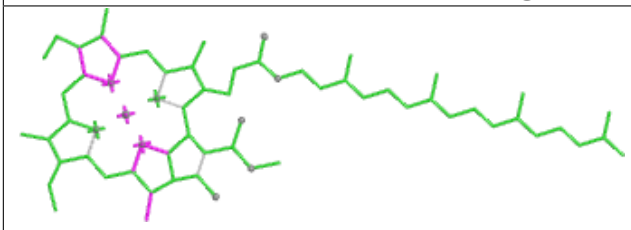


Torsions

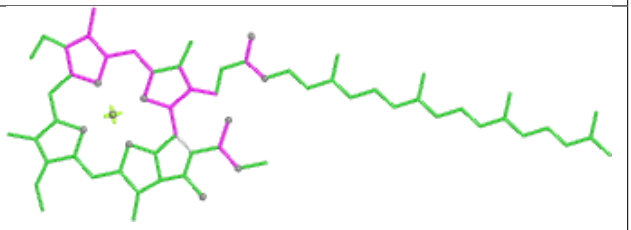


Rings

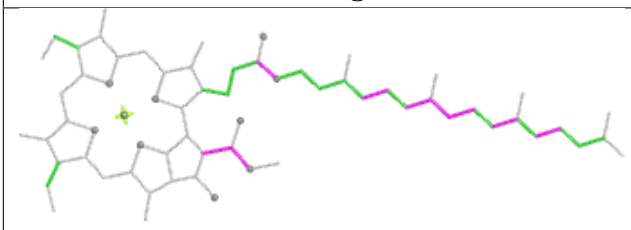
Ligand CLA b5 403



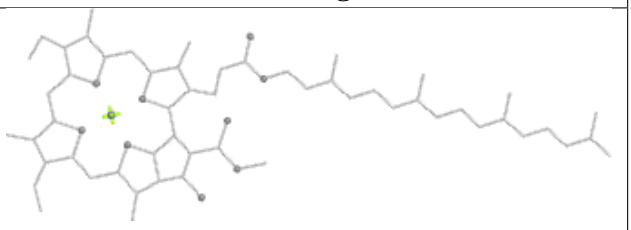
Bond lengths



Bond angles

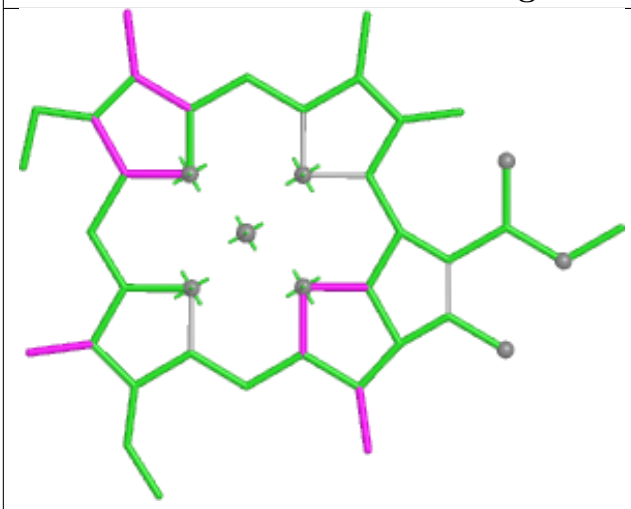


Torsions

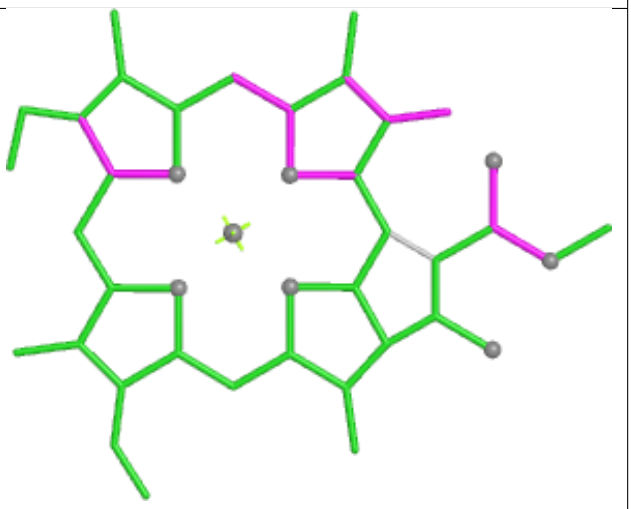


Rings

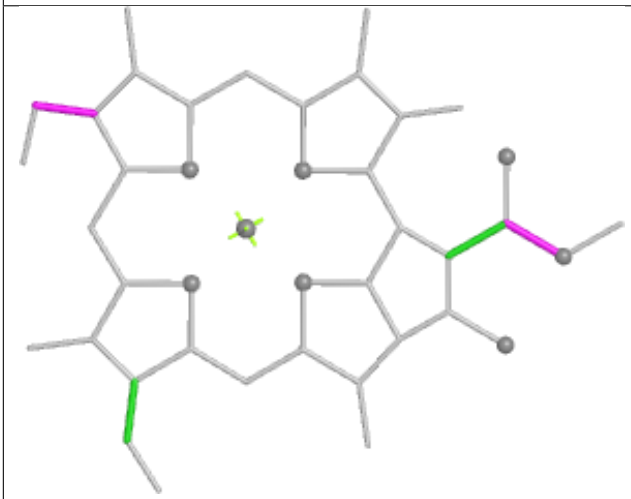
Ligand CLA b2 415



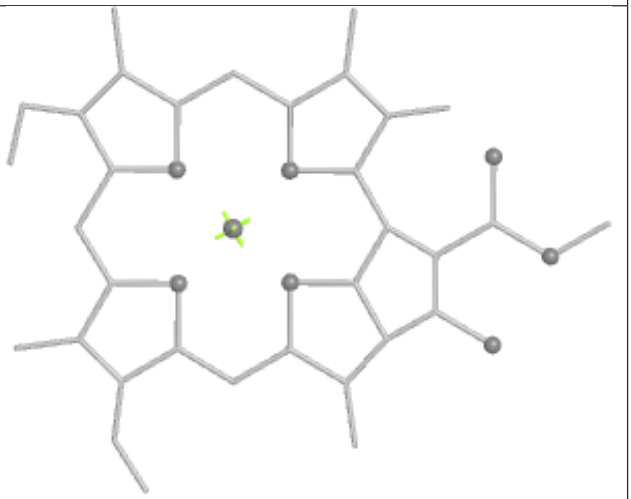
Bond lengths



Bond angles

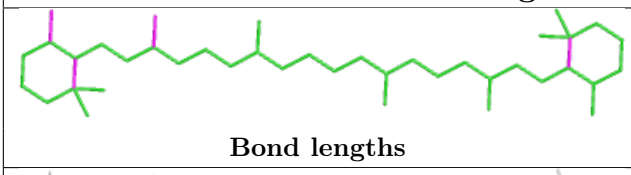


Torsions

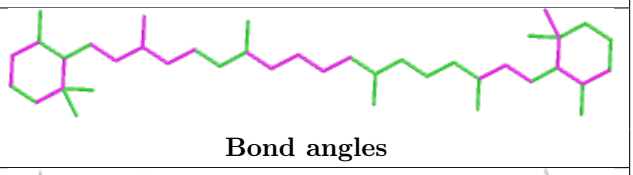


Rings

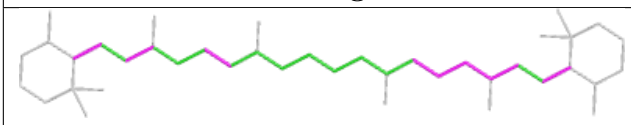
Ligand BCR c1 419



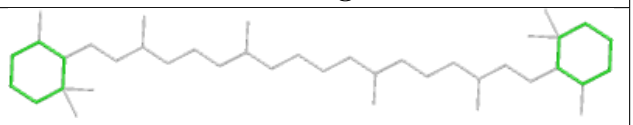
Bond lengths



Bond angles

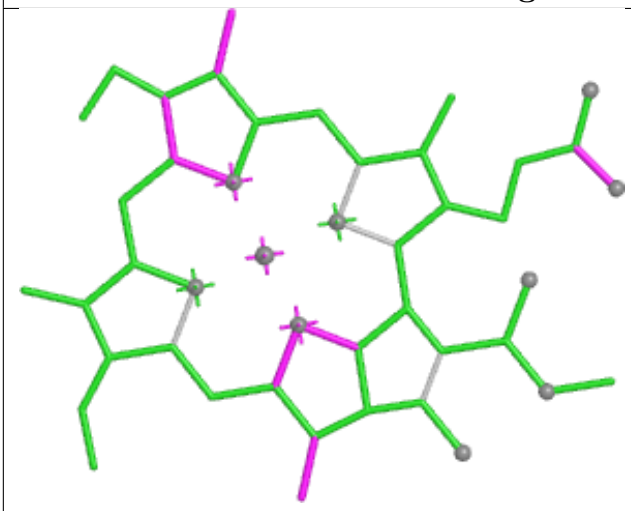


Torsions

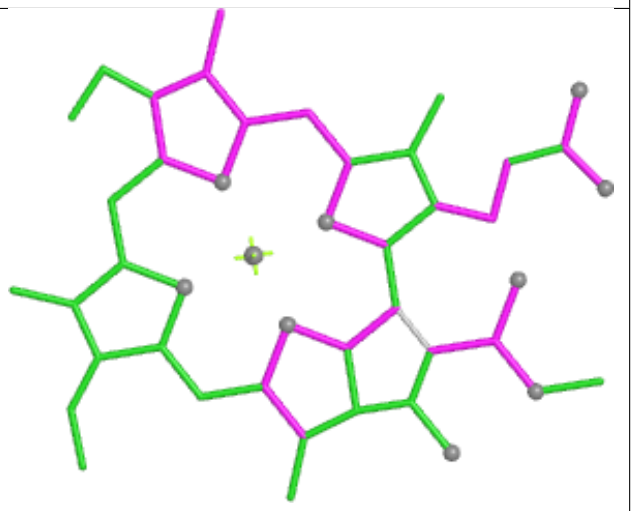


Rings

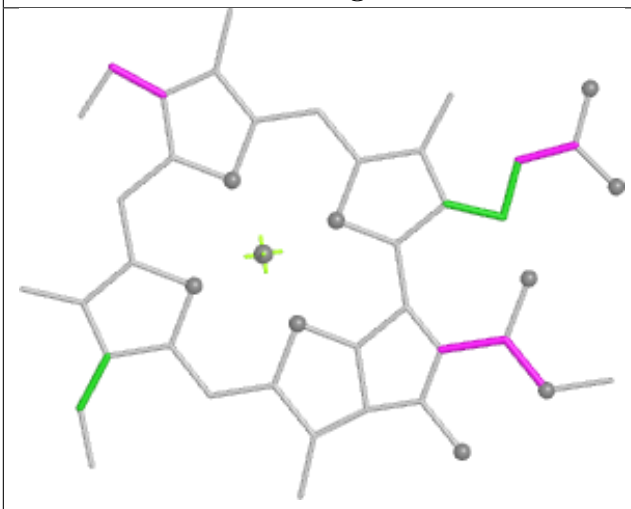
Ligand CLA b5 415



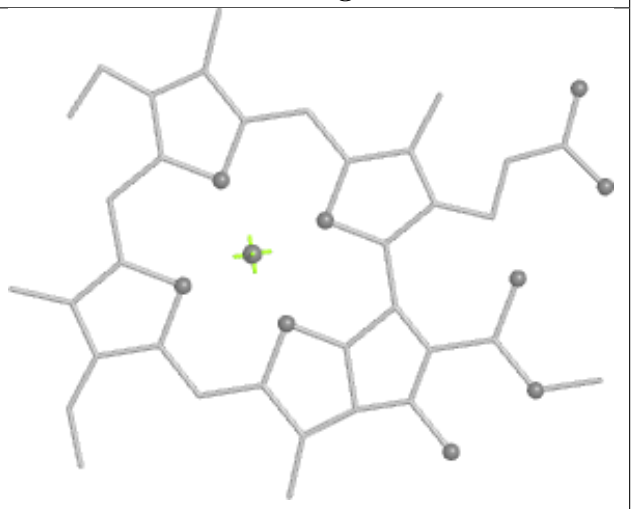
Bond lengths



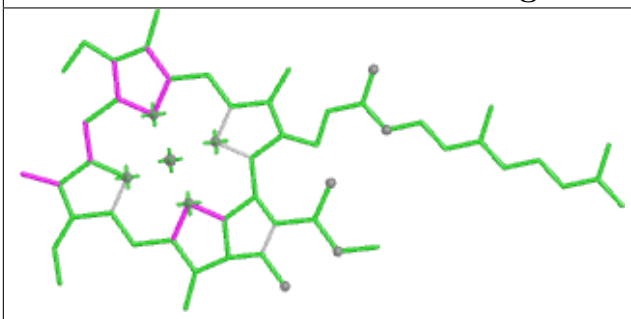
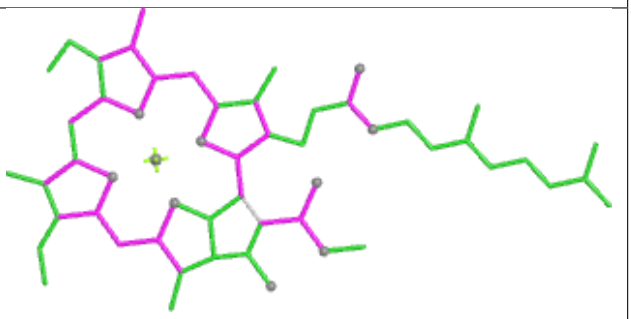
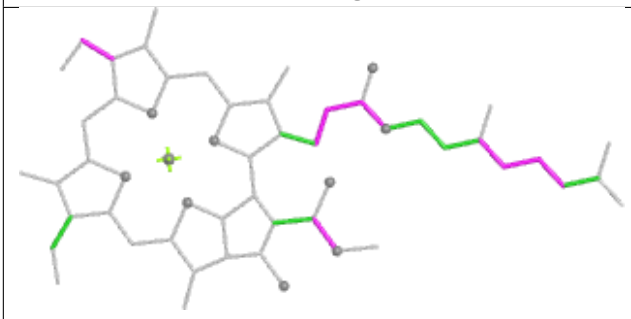
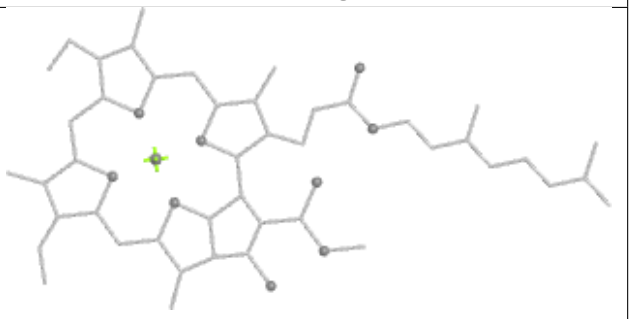
Bond angles

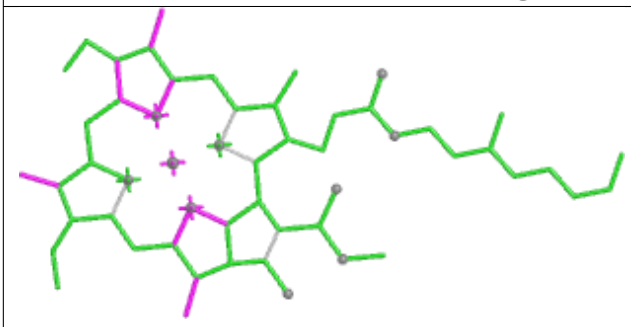
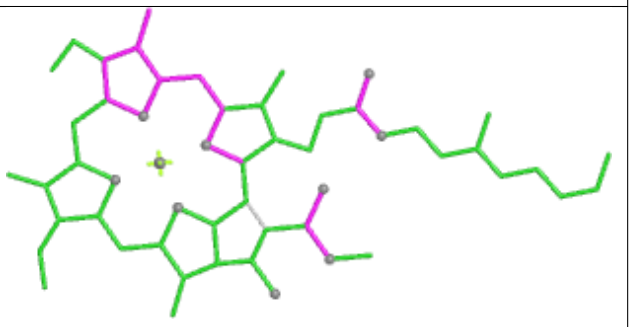
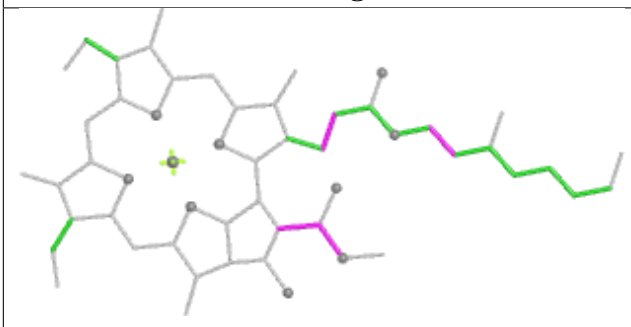
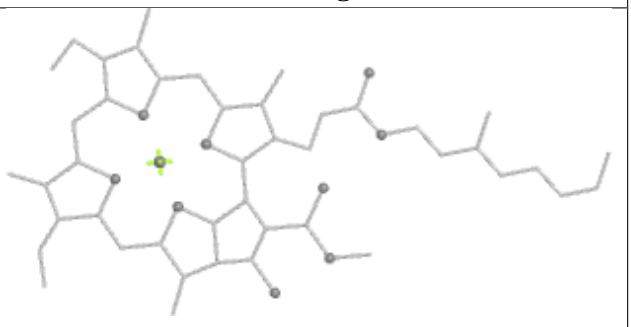


Torsions

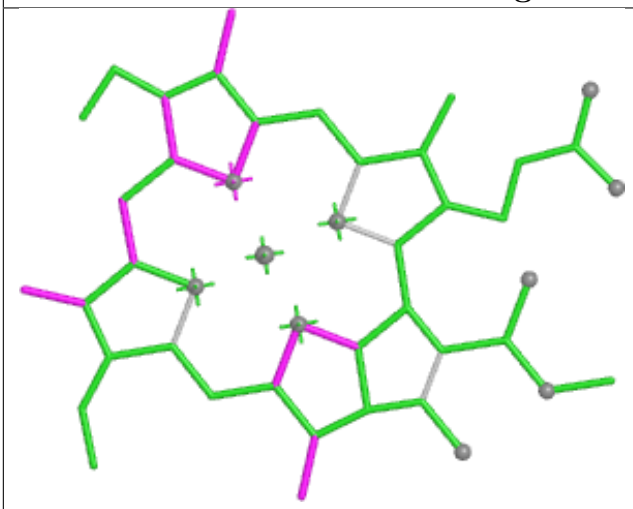


Rings

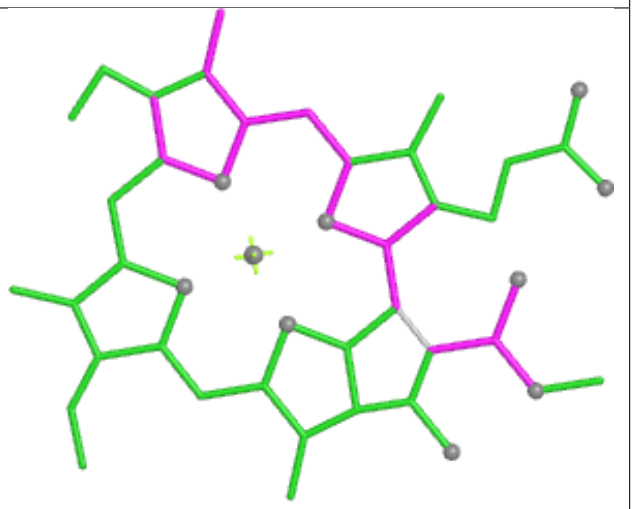
Ligand CLA a3 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

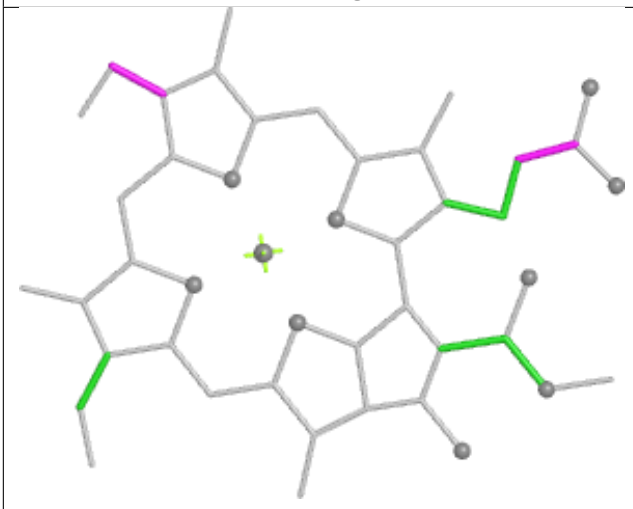
Ligand CLA bB 841



Bond lengths



Bond angles

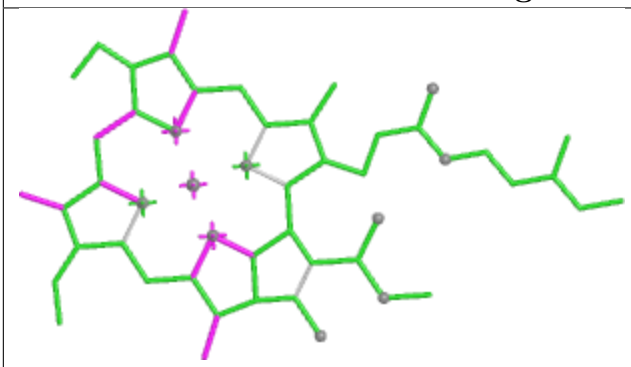


Torsions

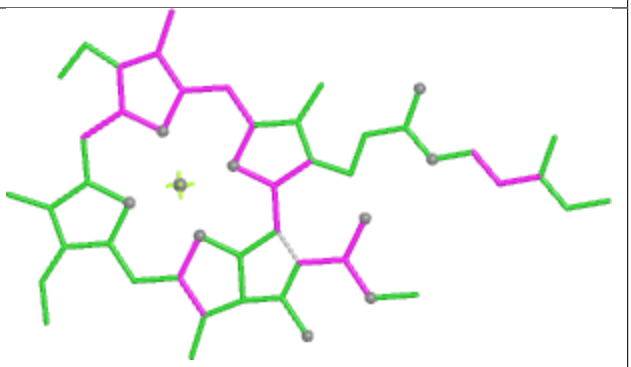


Rings

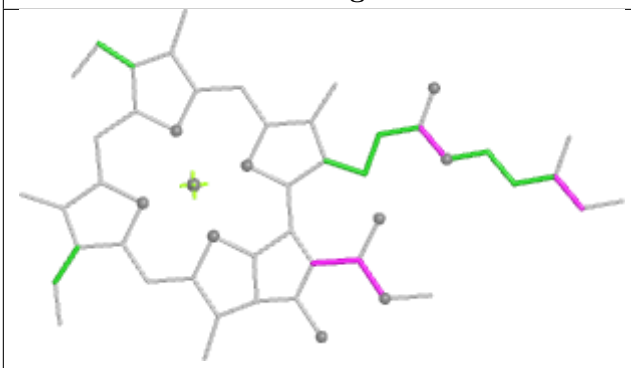
Ligand CLA aA 838



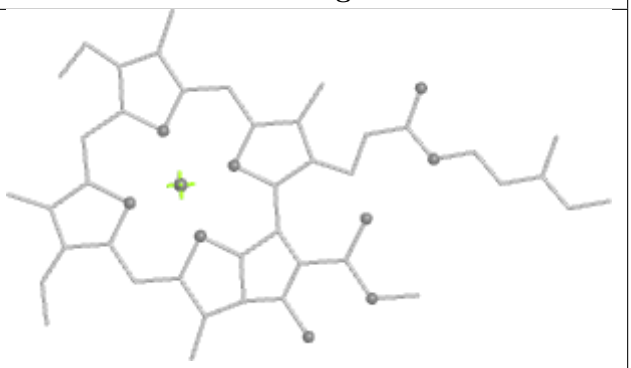
Bond lengths



Bond angles

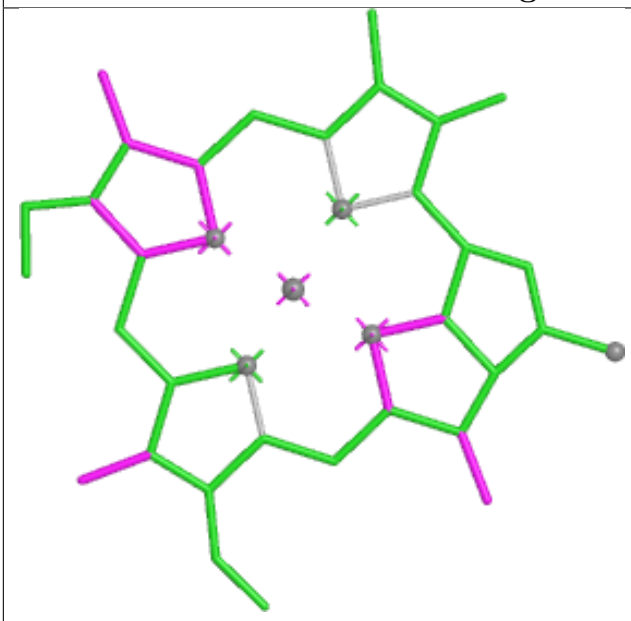


Torsions



Rings

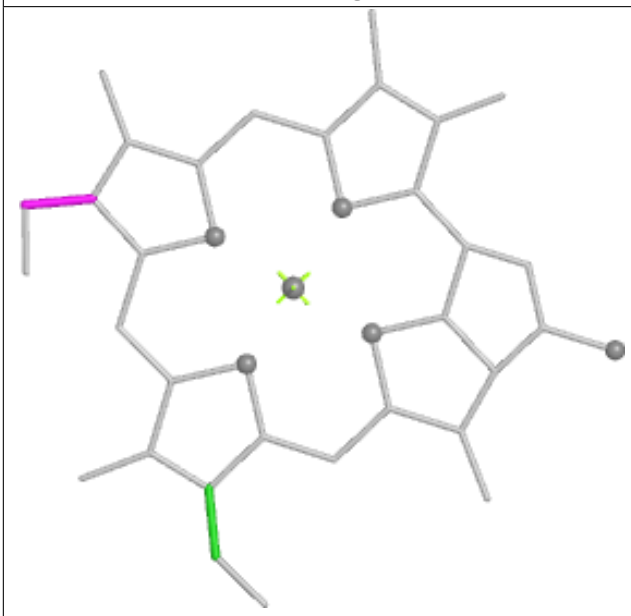
Ligand CLA aJ 203



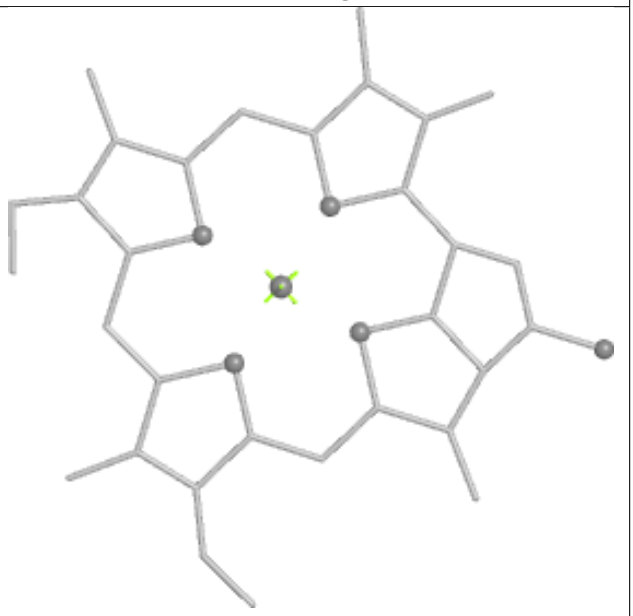
Bond lengths



Bond angles

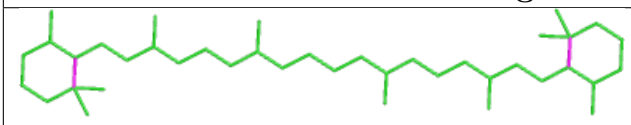


Torsions

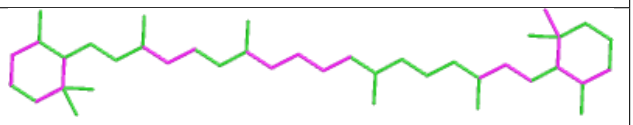


Rings

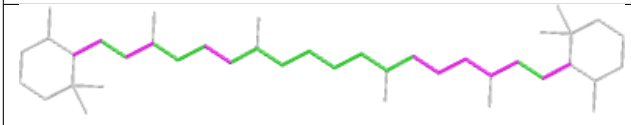
Ligand BCR b4 419



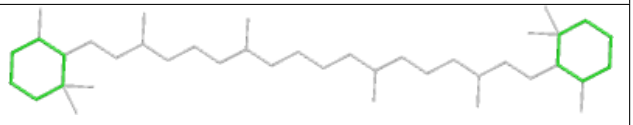
Bond lengths



Bond angles

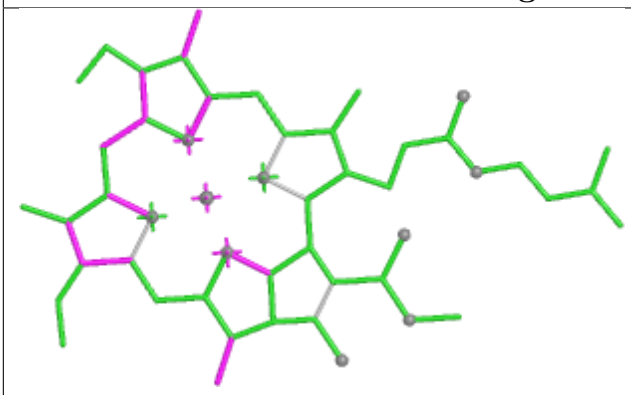


Torsions

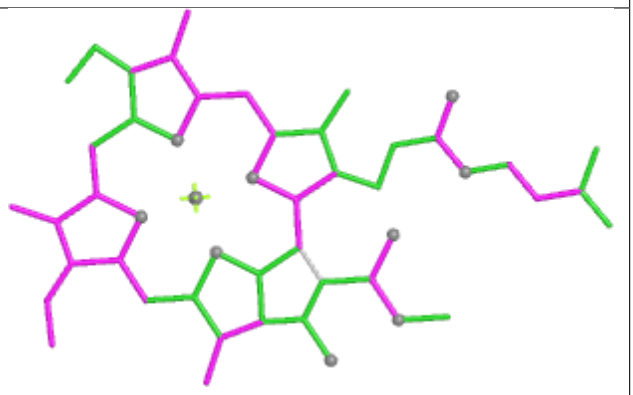


Rings

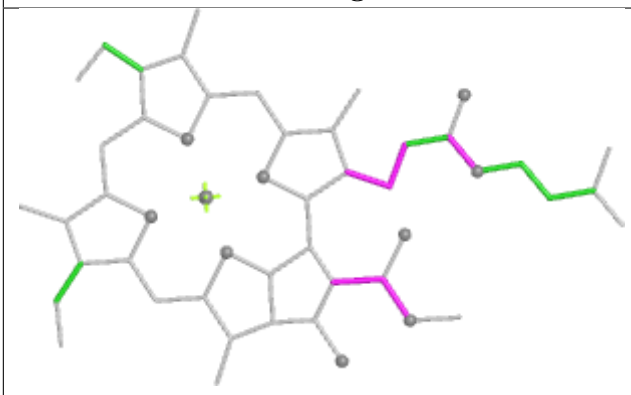
Ligand CLA b2 417



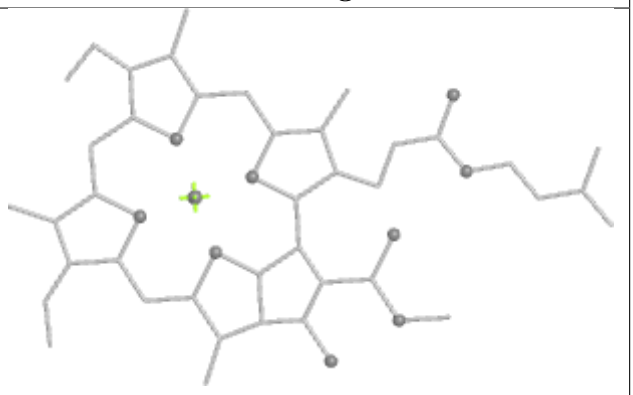
Bond lengths



Bond angles

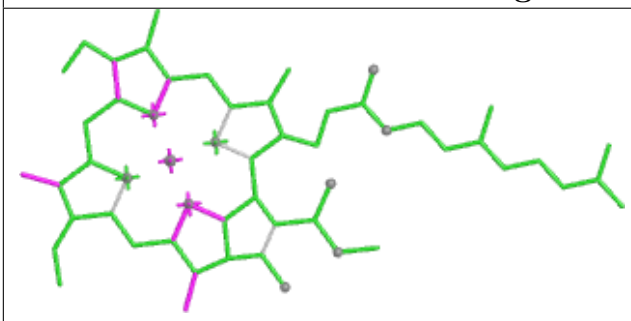


Torsions

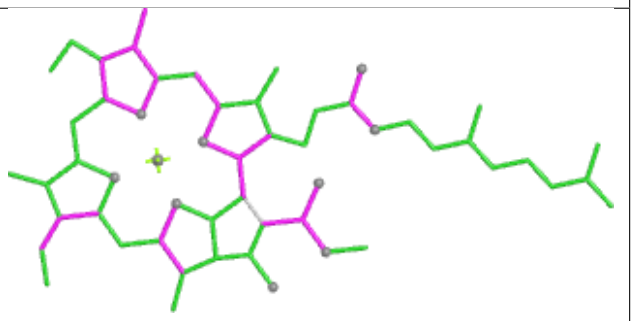


Rings

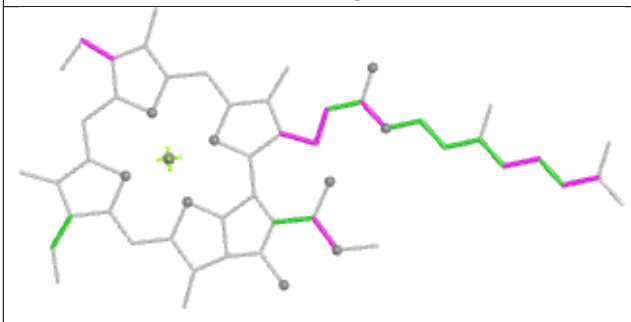
Ligand CLA bB 817



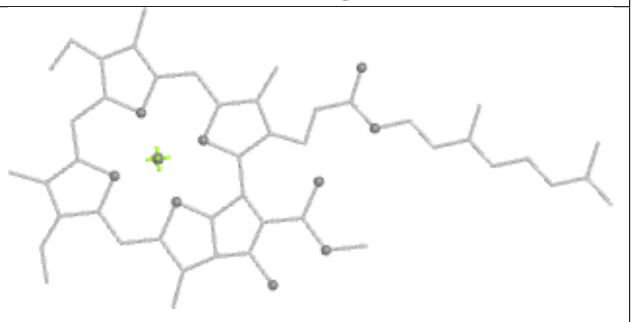
Bond lengths



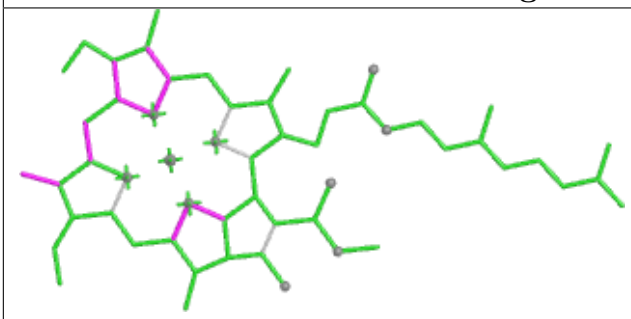
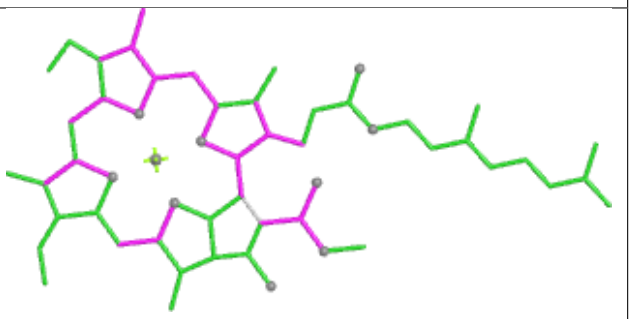
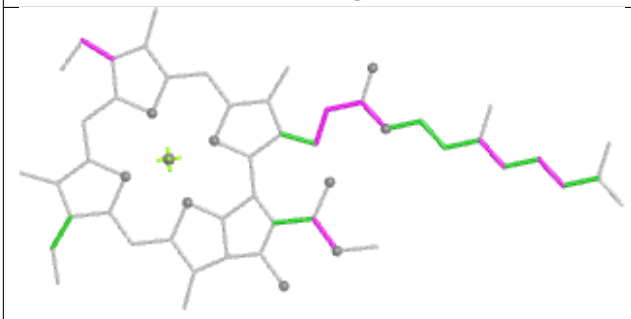
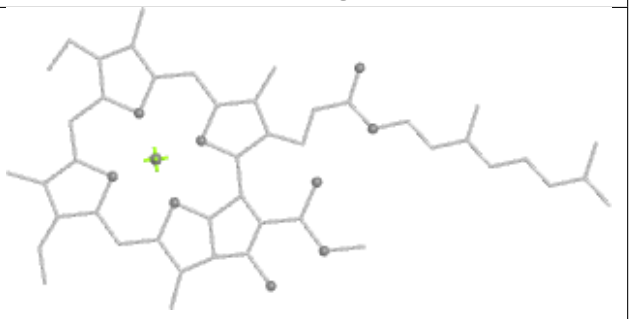
Bond angles

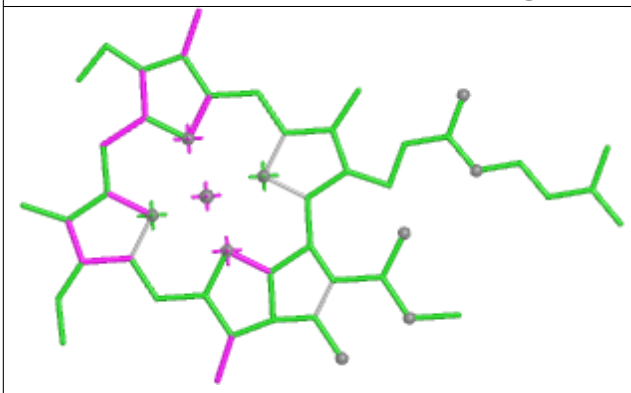
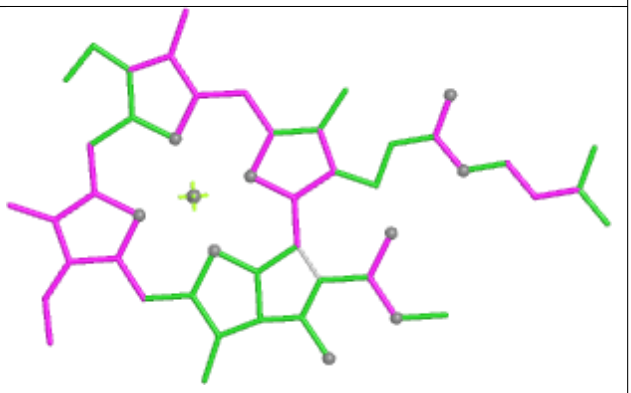
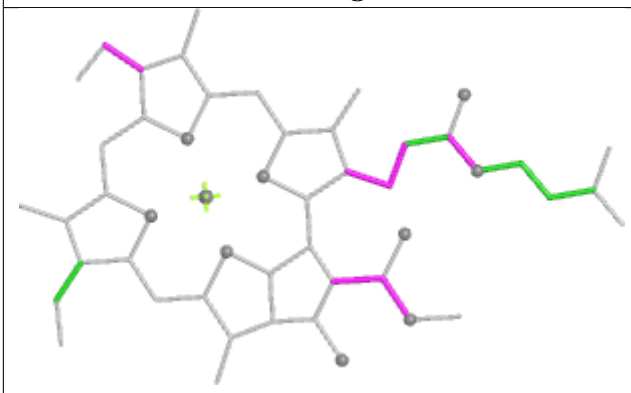
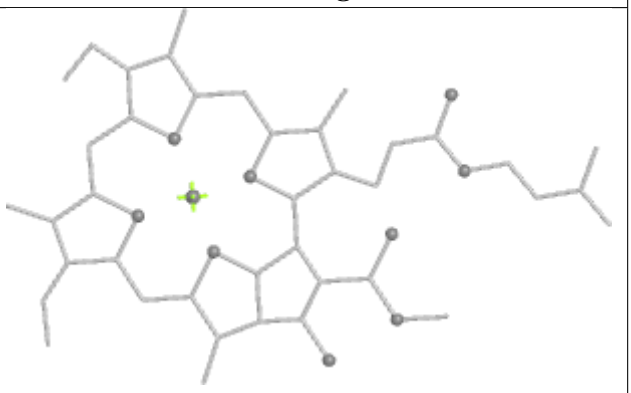


Torsions

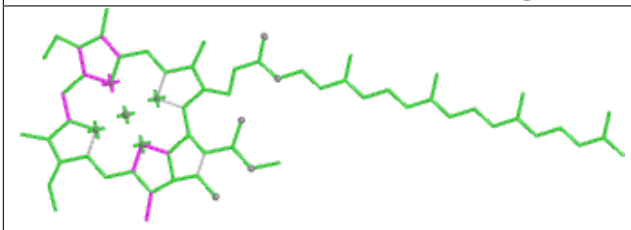


Rings

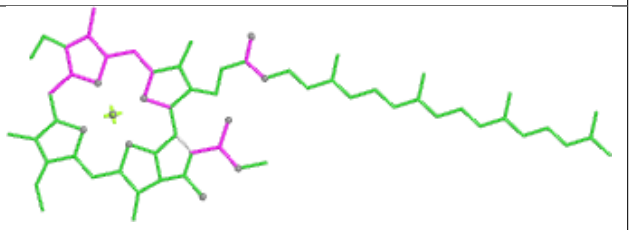
Ligand CLA a2 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c3 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

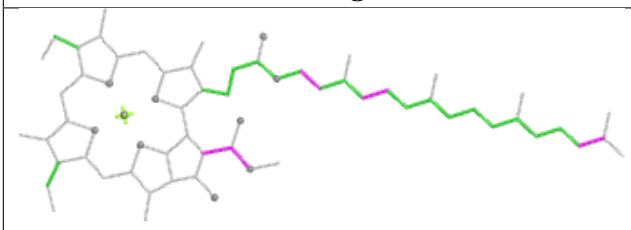
Ligand CLA b2 410



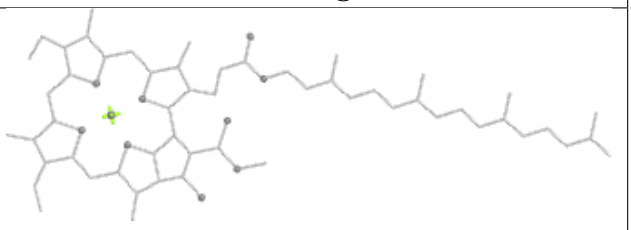
Bond lengths



Bond angles

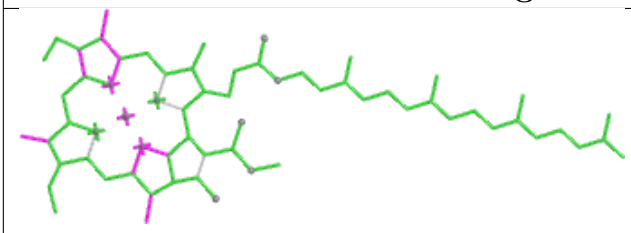


Torsions

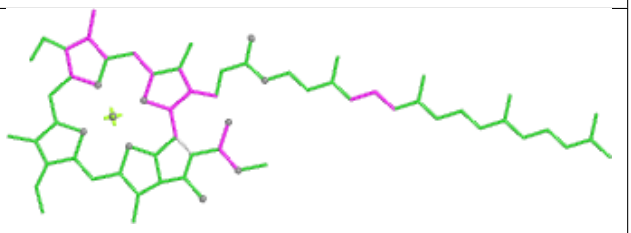


Rings

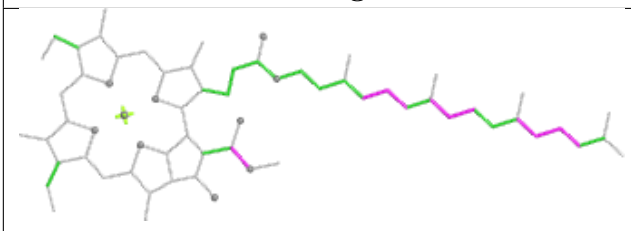
Ligand CLA cA 826



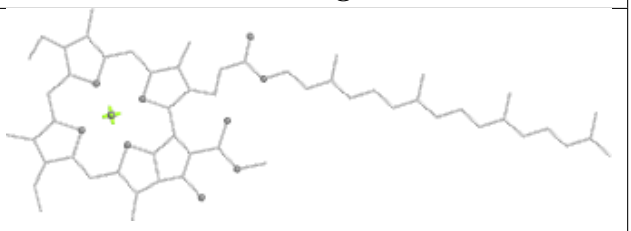
Bond lengths



Bond angles

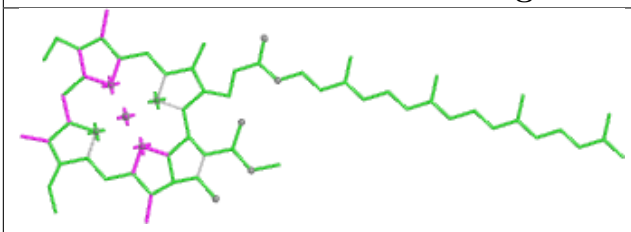


Torsions

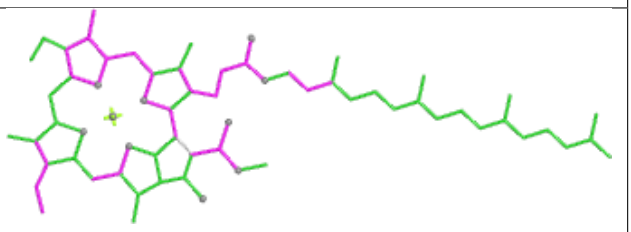


Rings

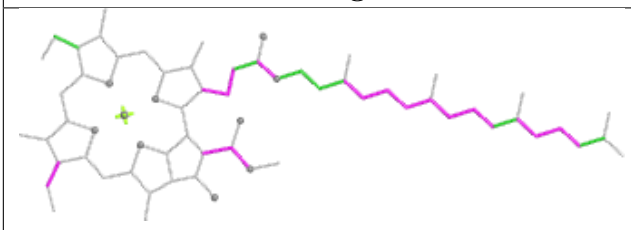
Ligand CLA aB 814



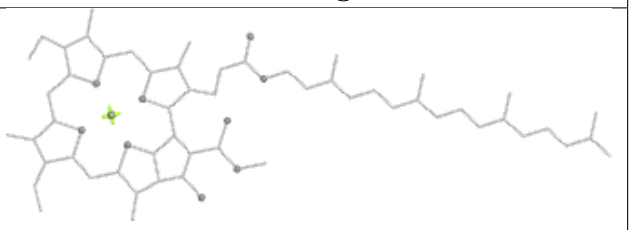
Bond lengths



Bond angles

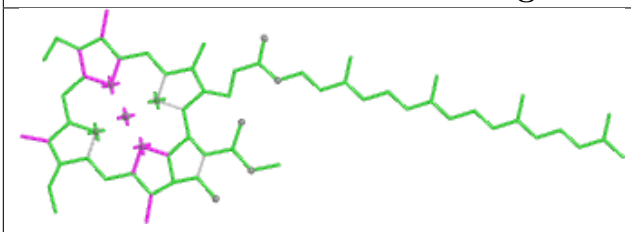


Torsions

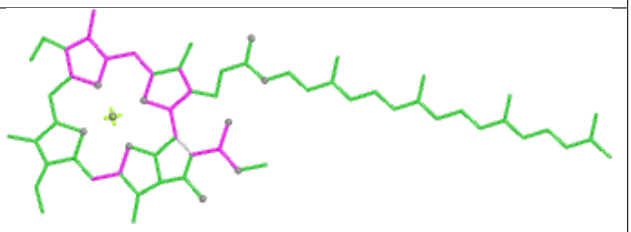


Rings

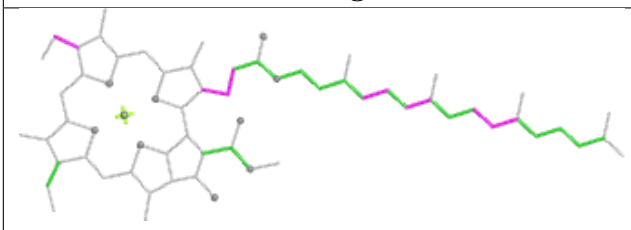
Ligand CLA aL 202



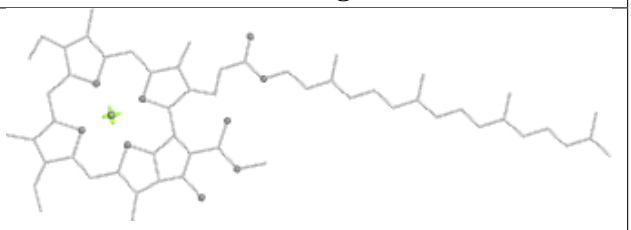
Bond lengths



Bond angles

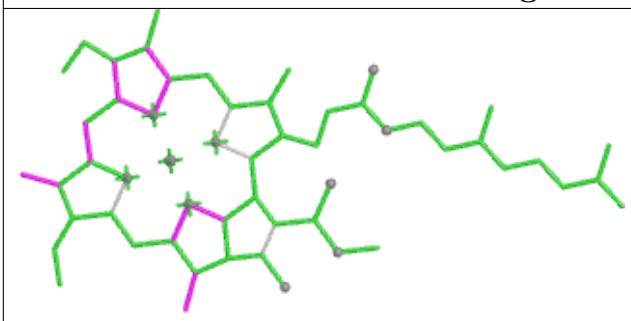


Torsions

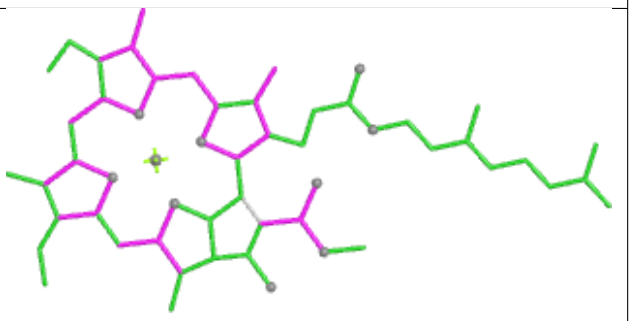


Rings

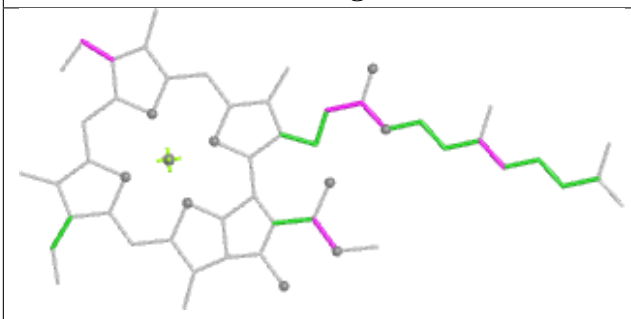
Ligand CLA a4 417



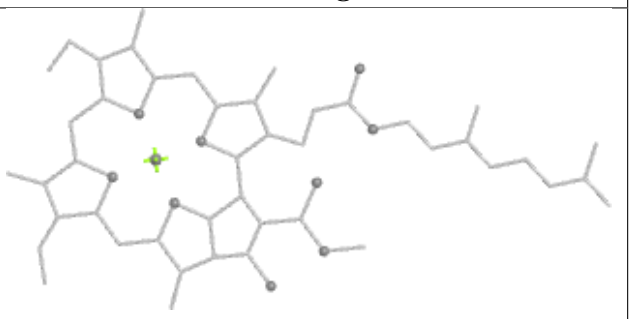
Bond lengths



Bond angles

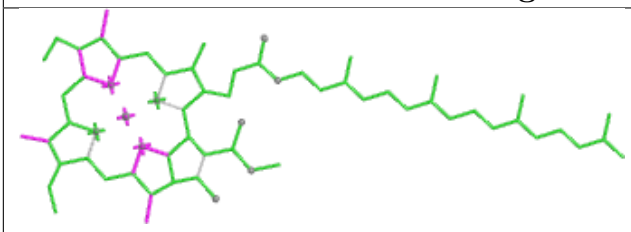


Torsions

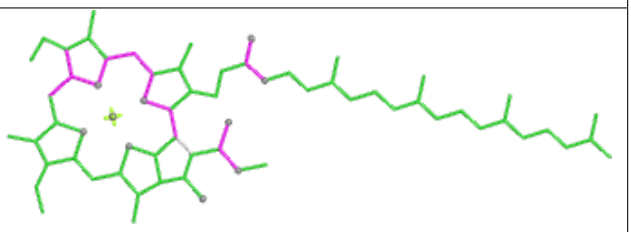


Rings

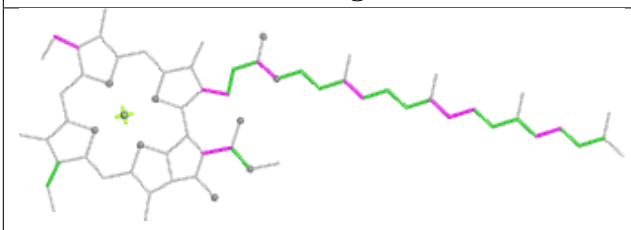
Ligand CLA cL 202



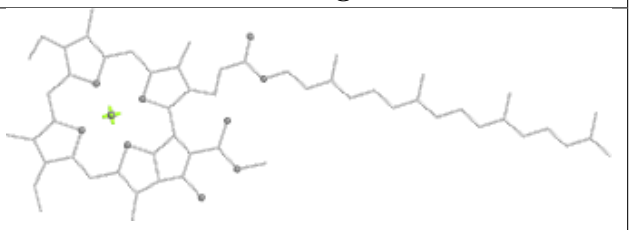
Bond lengths



Bond angles



Torsions

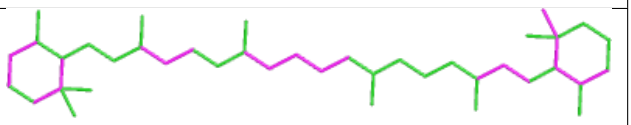


Rings

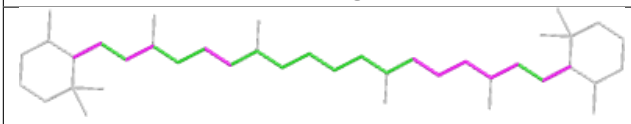
Ligand BCR b3 419



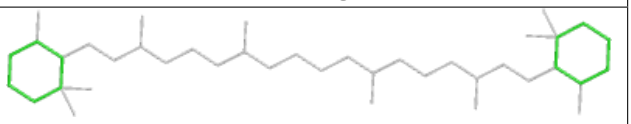
Bond lengths



Bond angles

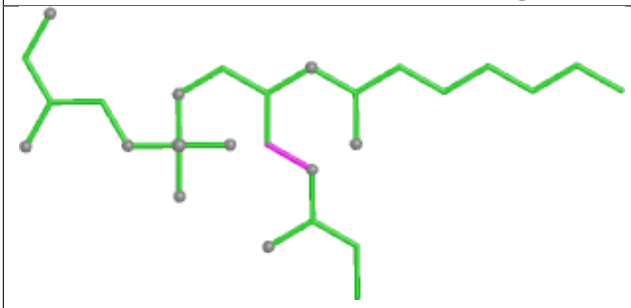


Torsions

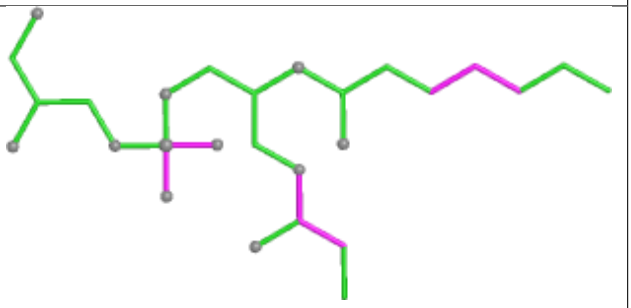


Rings

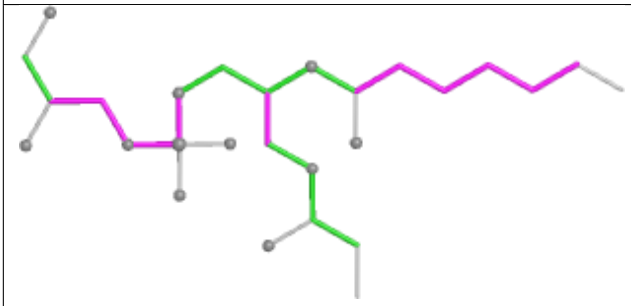
Ligand LHG aA 854



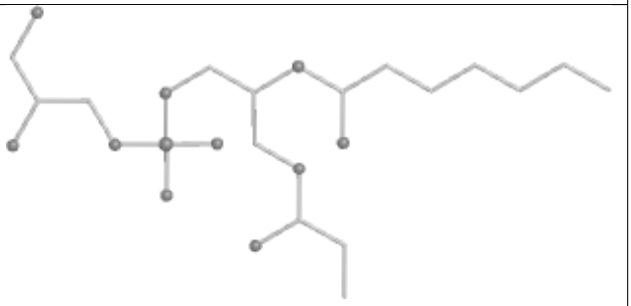
Bond lengths



Bond angles

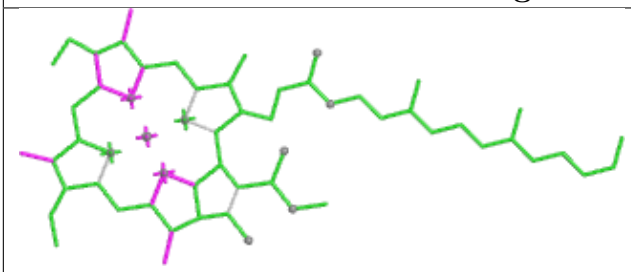


Torsions

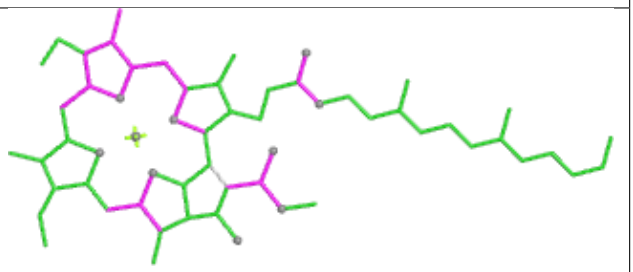


Rings

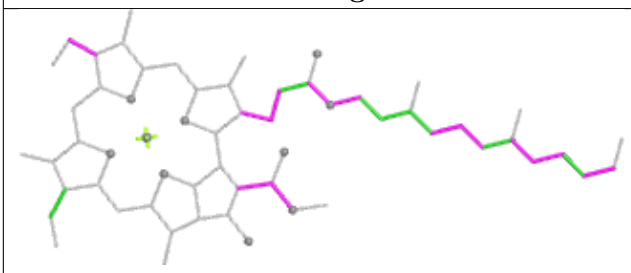
Ligand CLA bA 825



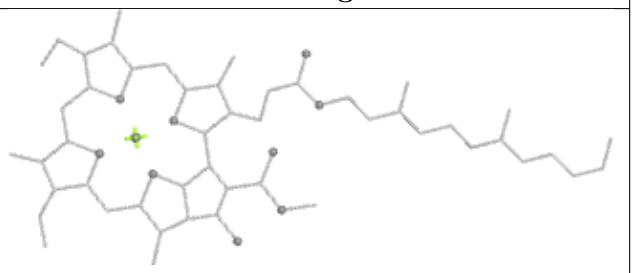
Bond lengths



Bond angles

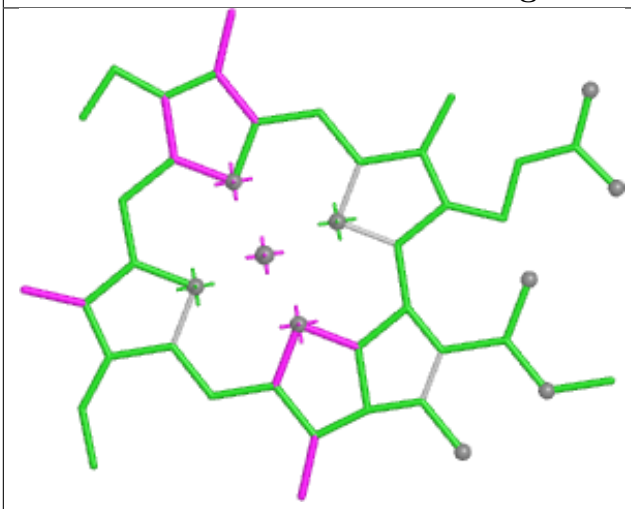


Torsions

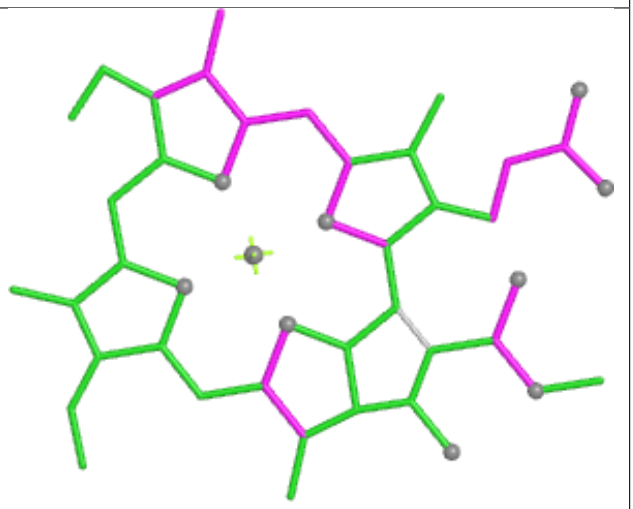


Rings

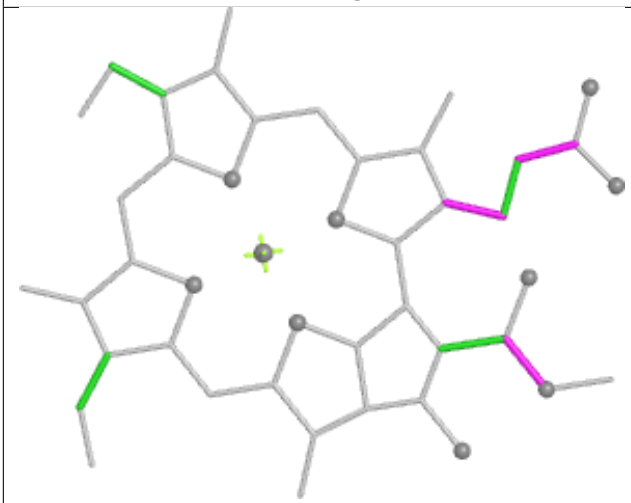
Ligand CLA a5 408



Bond lengths



Bond angles

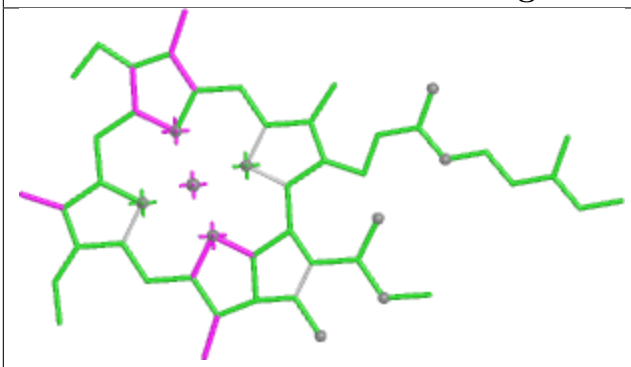


Torsions

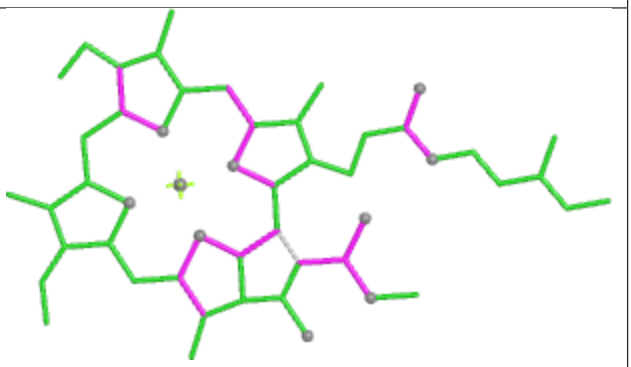


Rings

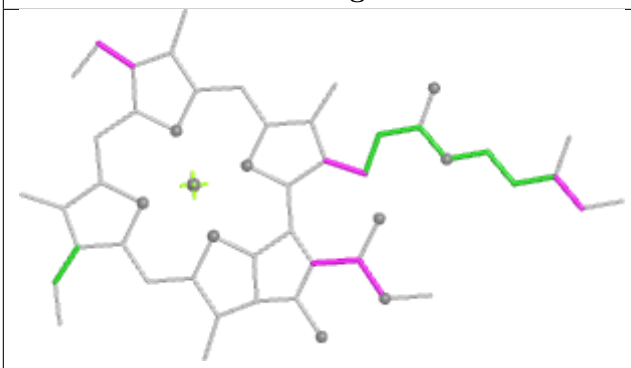
Ligand CLA cF 201



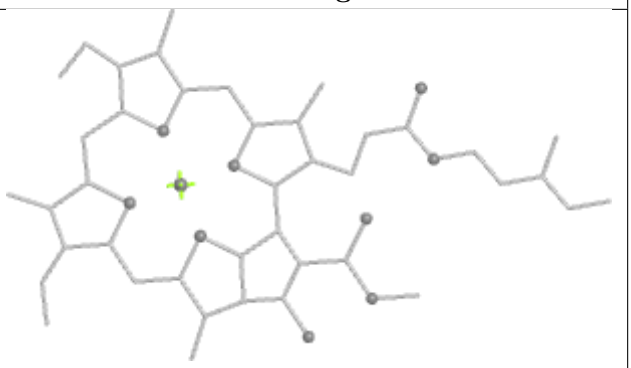
Bond lengths



Bond angles

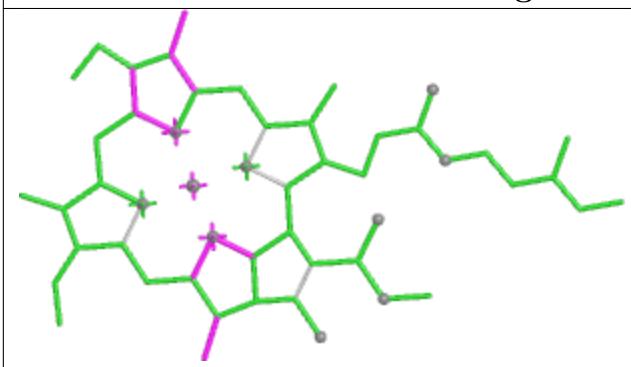


Torsions

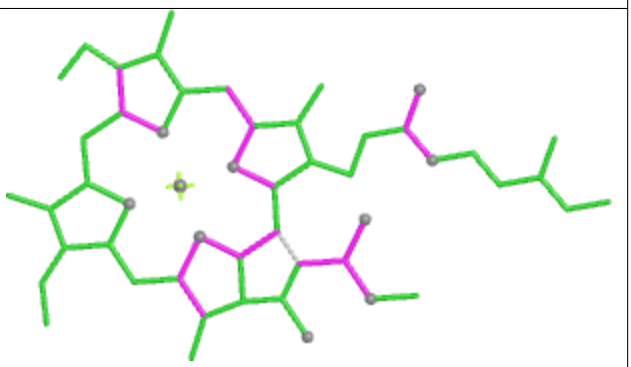


Rings

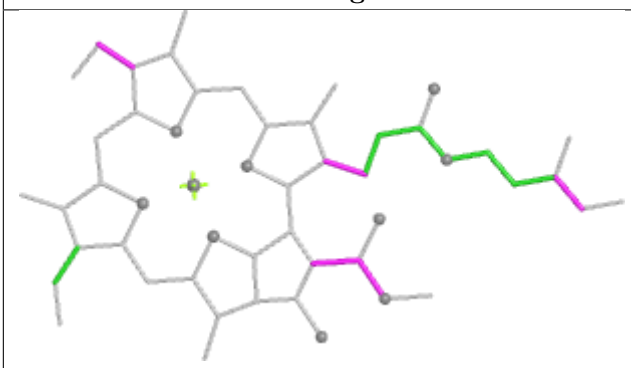
Ligand CLA aA 842



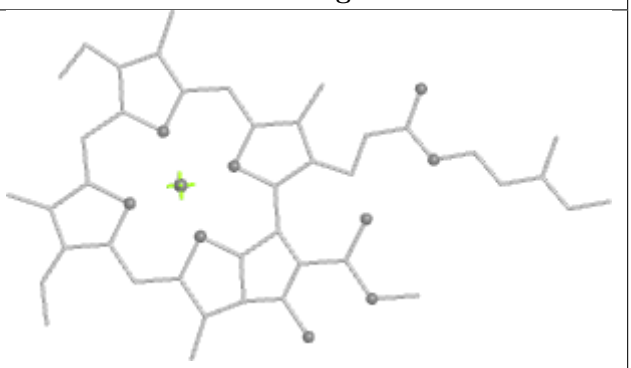
Bond lengths



Bond angles

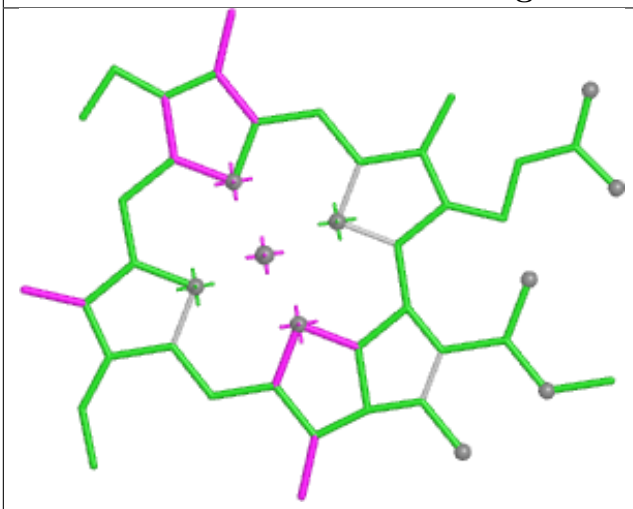


Torsions

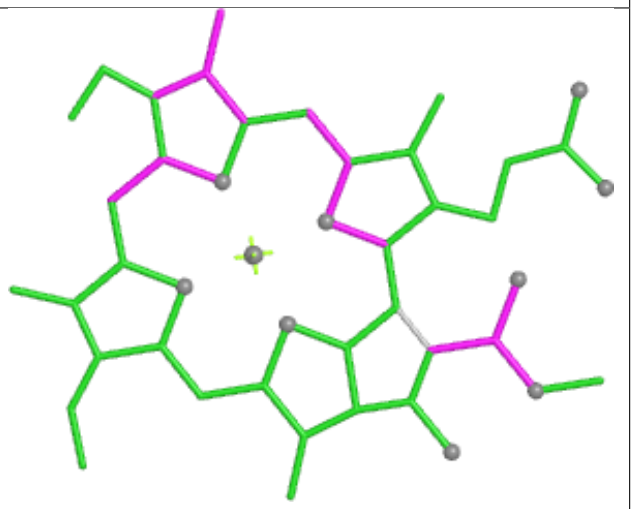


Rings

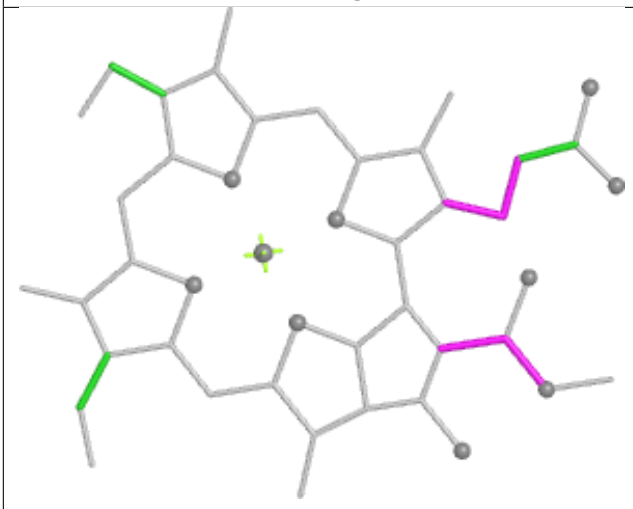
Ligand CLA aB 816



Bond lengths



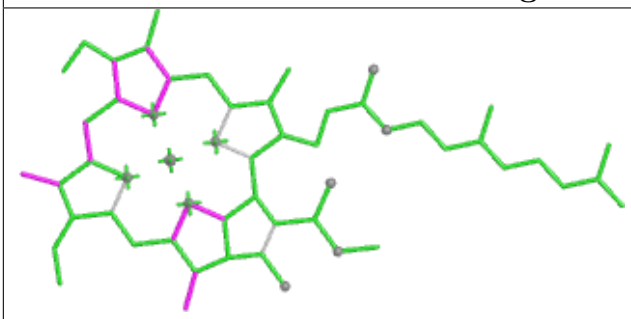
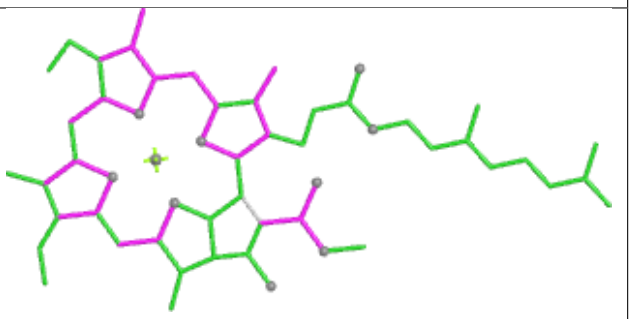
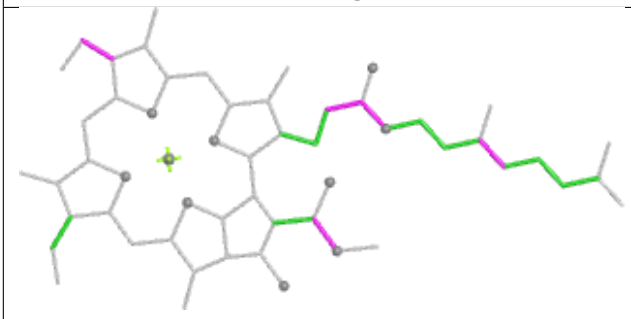
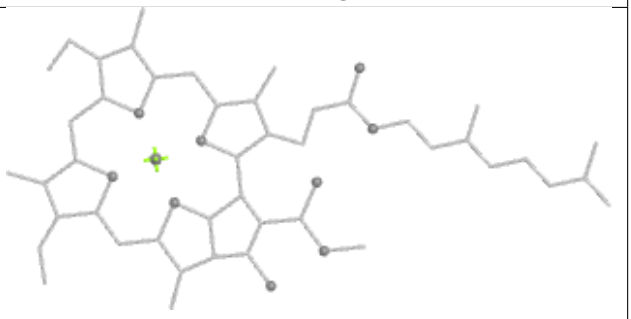
Bond angles

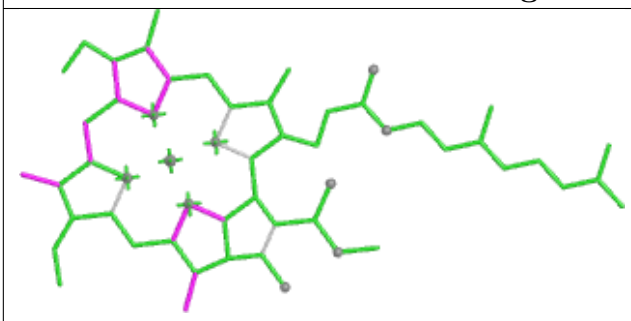
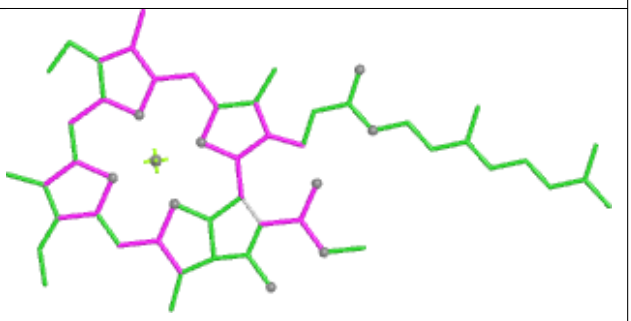
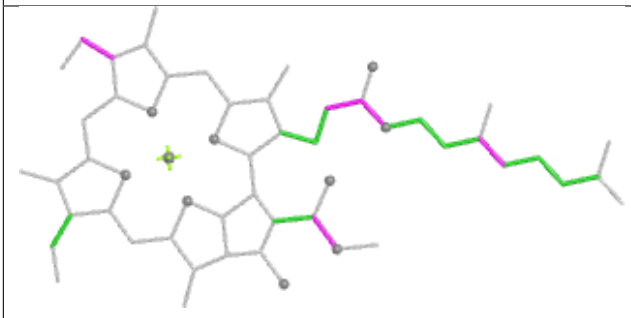
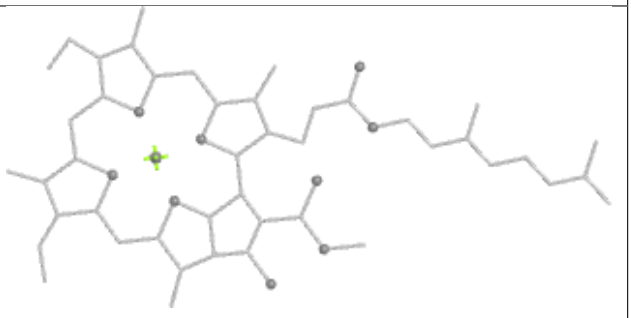


Torsions

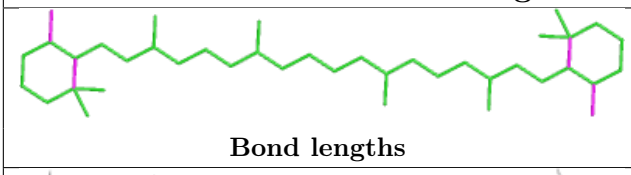


Rings

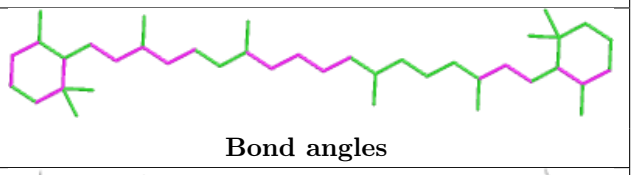
Ligand CLA a5 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c1 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

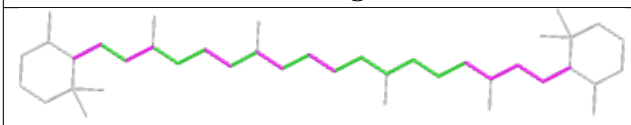
Ligand BCR aB 848



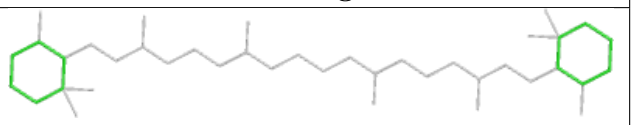
Bond lengths



Bond angles

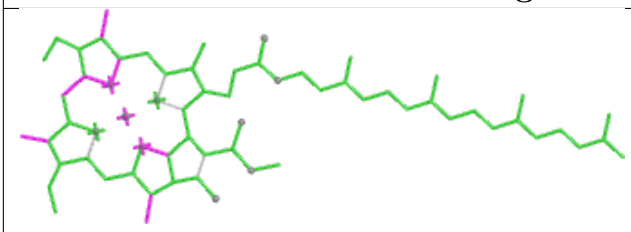


Torsions

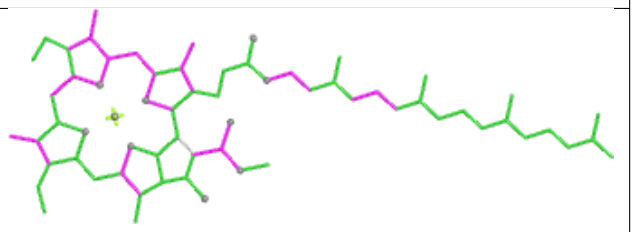


Rings

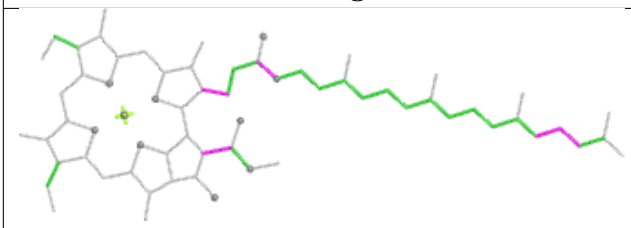
Ligand CLA aB 830



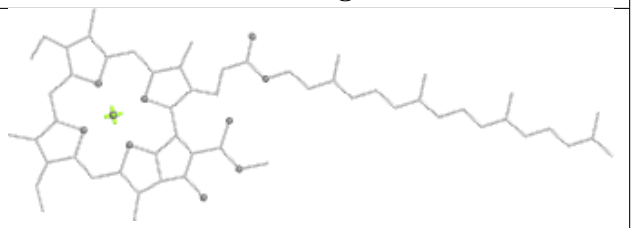
Bond lengths



Bond angles

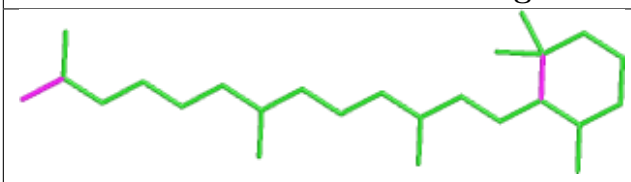


Torsions

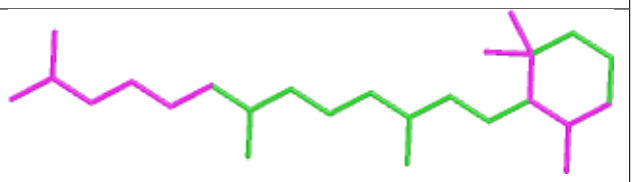


Rings

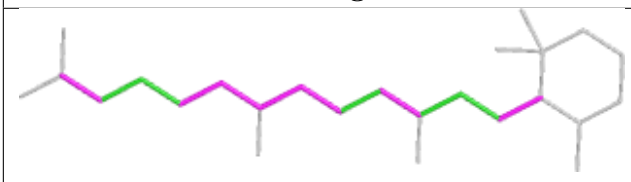
Ligand BCR aB 847



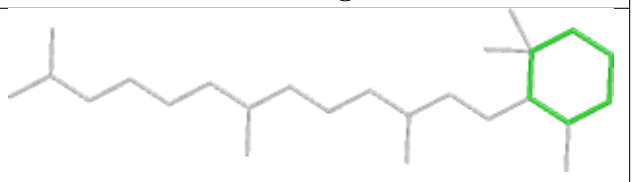
Bond lengths



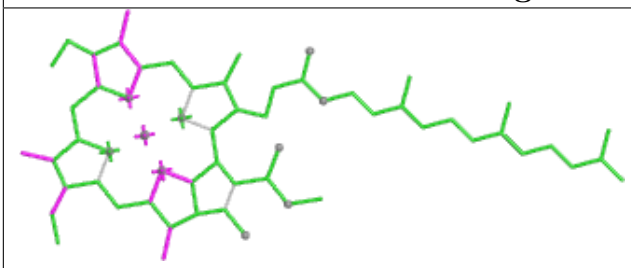
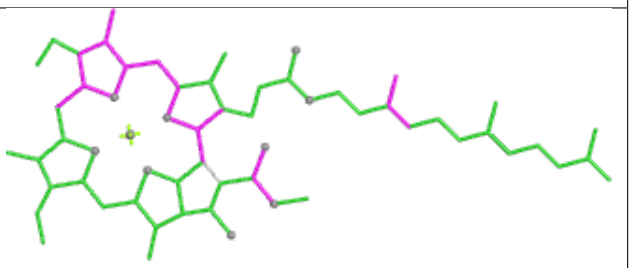
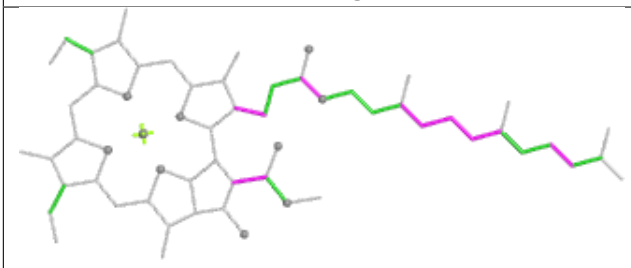
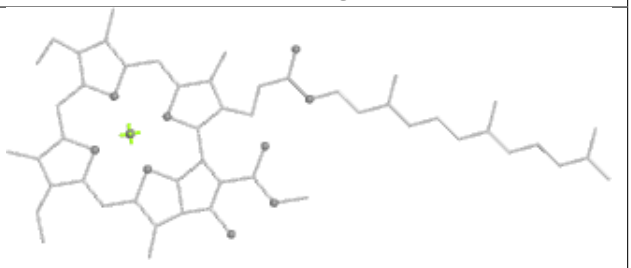
Bond angles

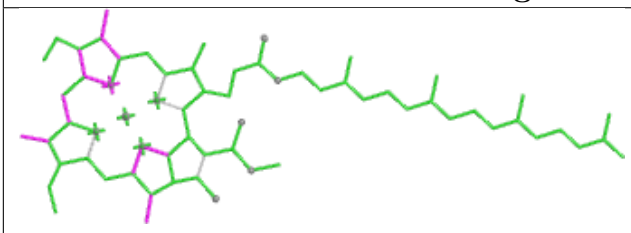
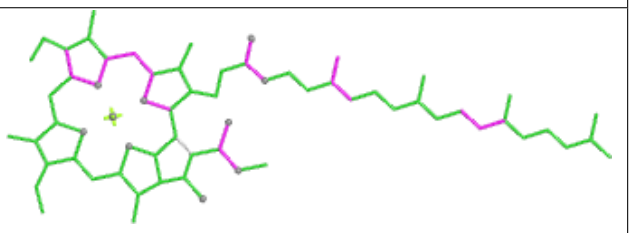
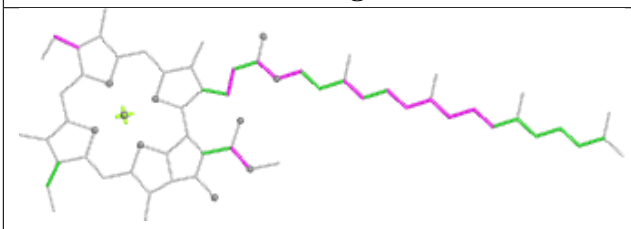
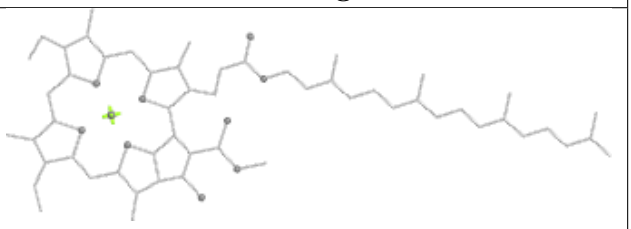


Torsions

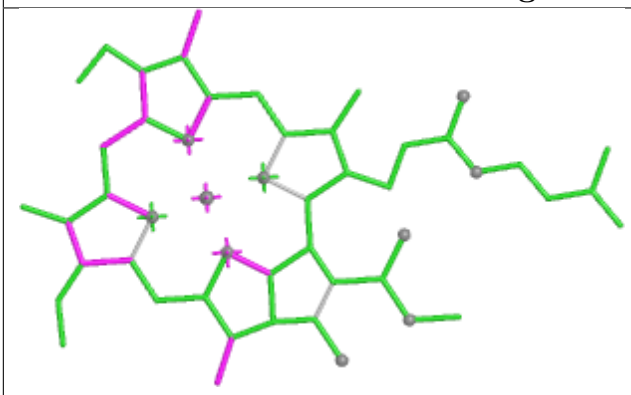


Rings

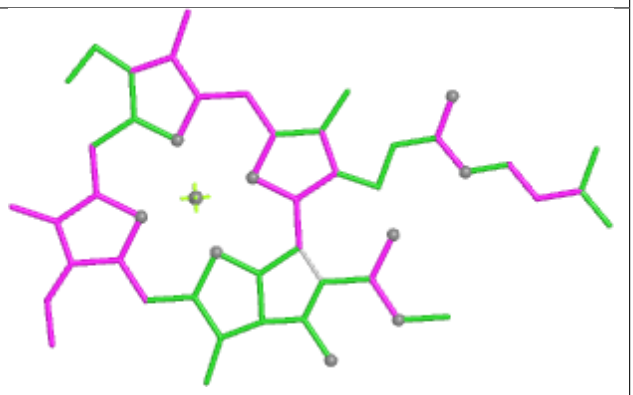
Ligand CLA bB 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

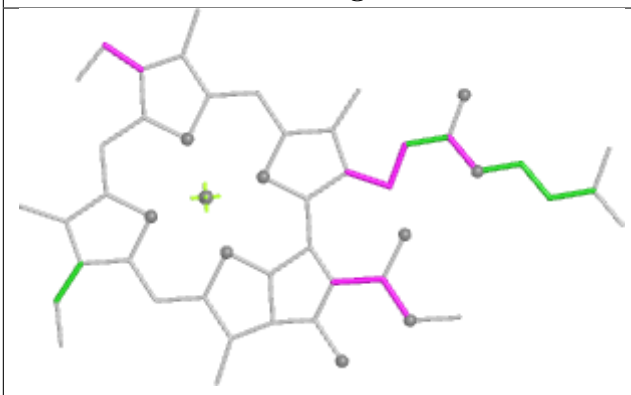
Ligand CLA b3 416



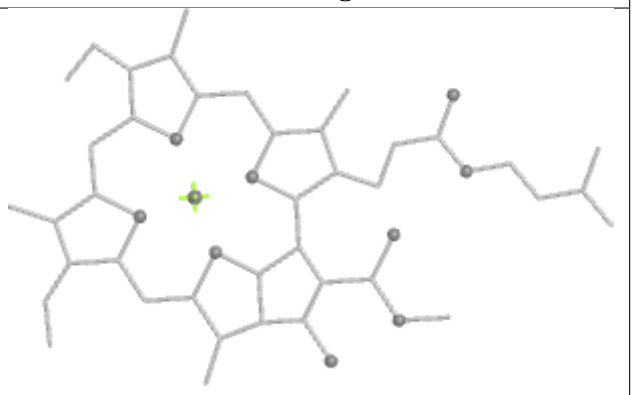
Bond lengths



Bond angles



Torsions

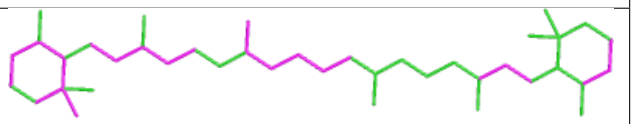


Rings

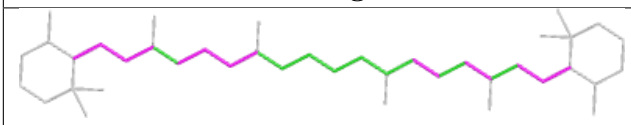
Ligand BCR c2 401



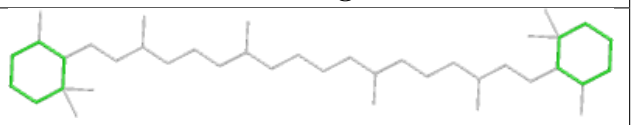
Bond lengths



Bond angles

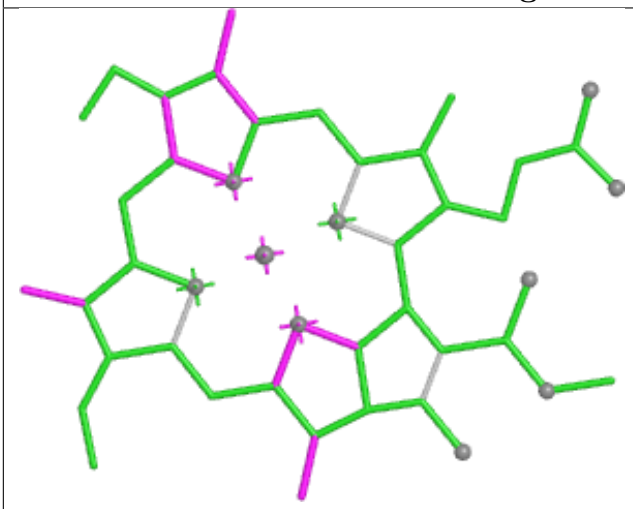


Torsions

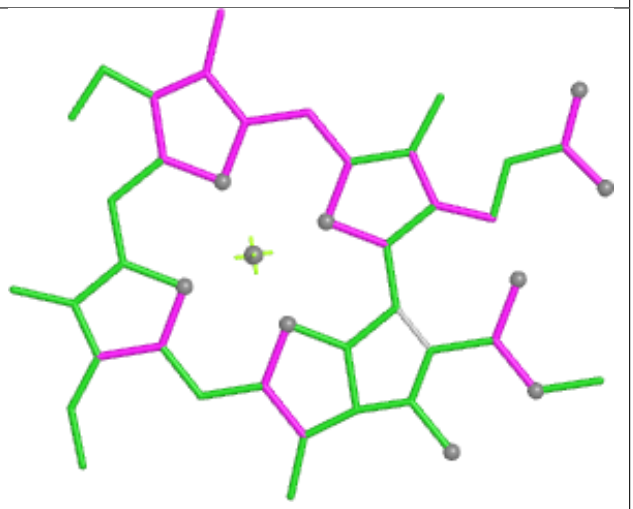


Rings

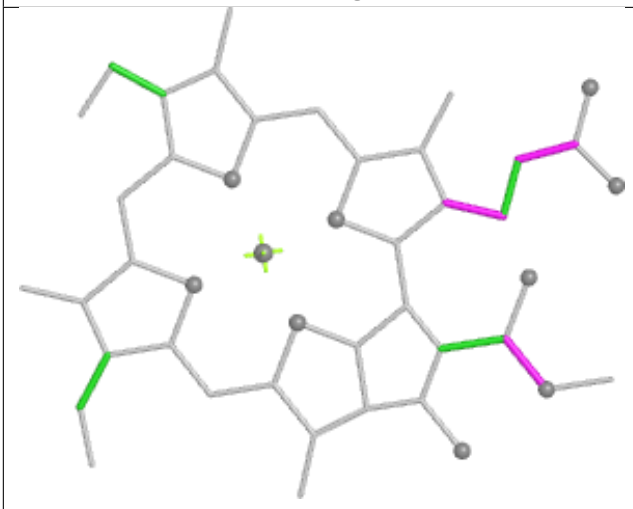
Ligand CLA a3 408



Bond lengths



Bond angles

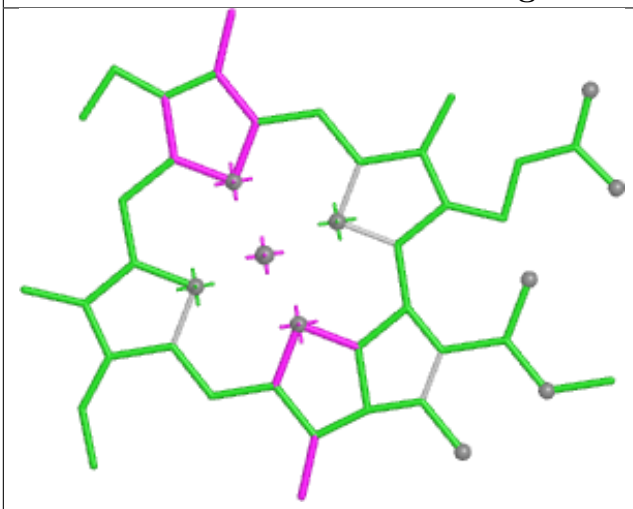


Torsions

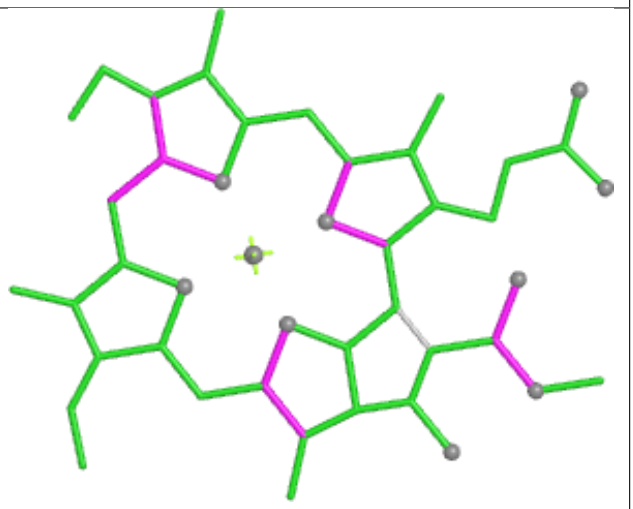


Rings

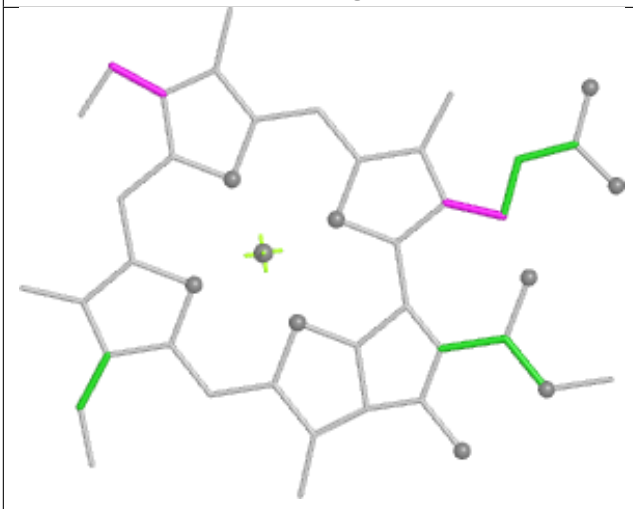
Ligand CLA b3 413



Bond lengths



Bond angles

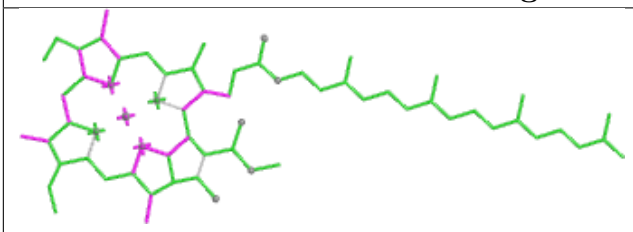


Torsions

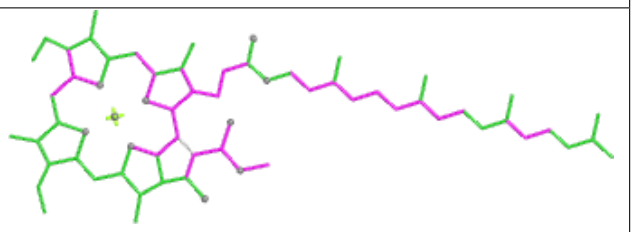


Rings

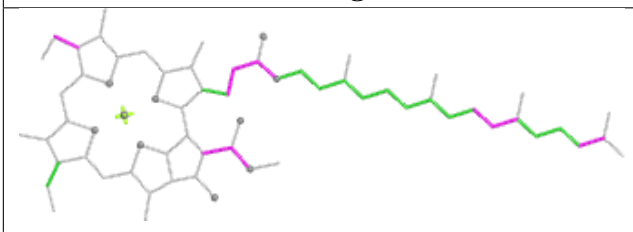
Ligand CLA c6 401



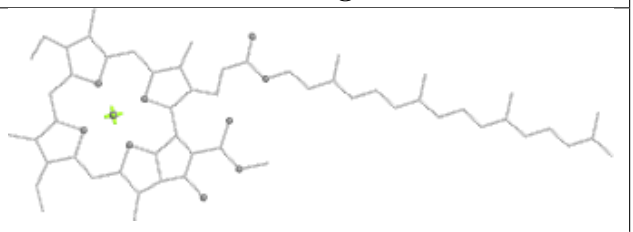
Bond lengths



Bond angles

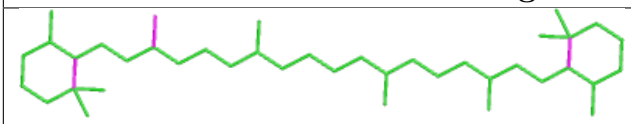


Torsions

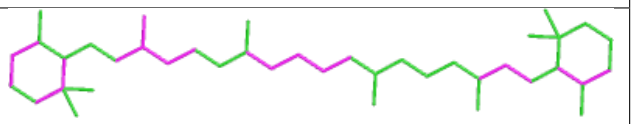


Rings

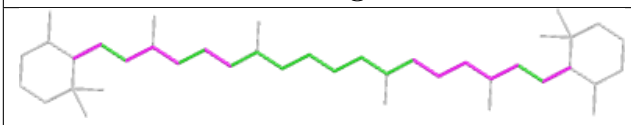
Ligand BCR c1 401



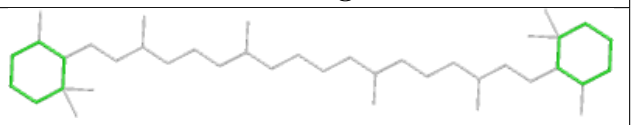
Bond lengths



Bond angles

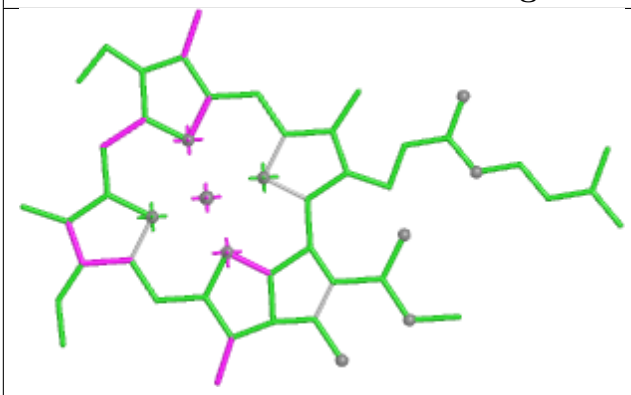


Torsions

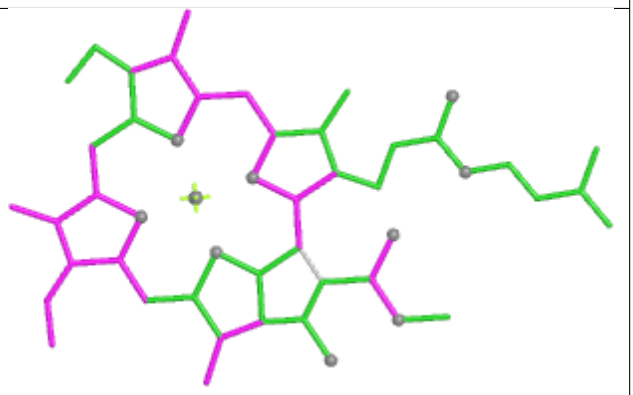


Rings

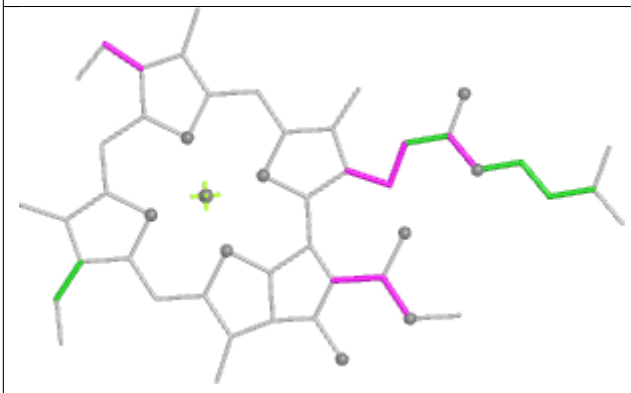
Ligand CLA a4 416



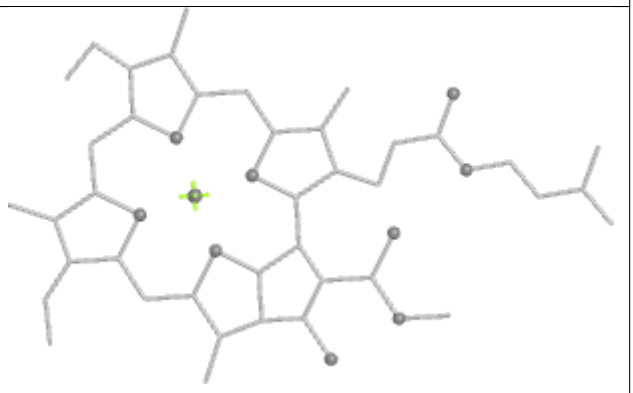
Bond lengths



Bond angles

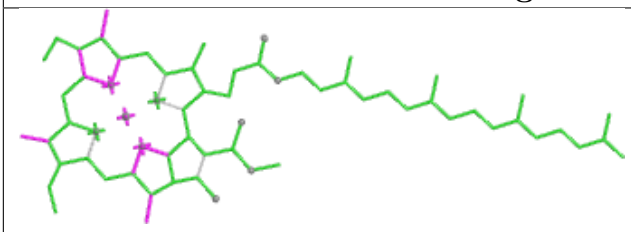


Torsions

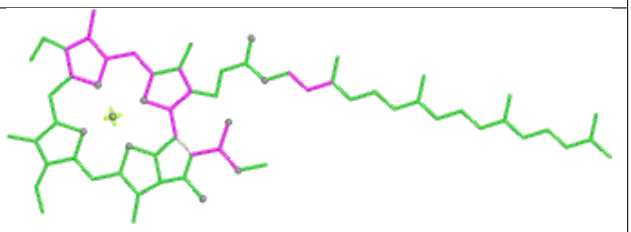


Rings

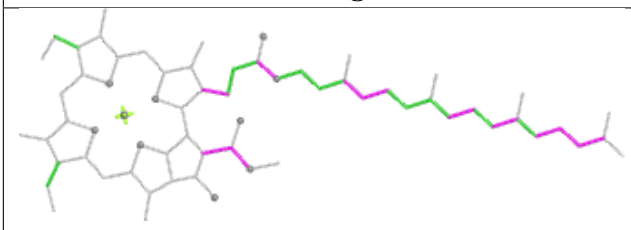
Ligand CLA cA 820



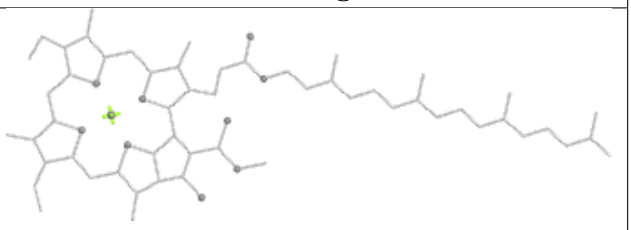
Bond lengths



Bond angles

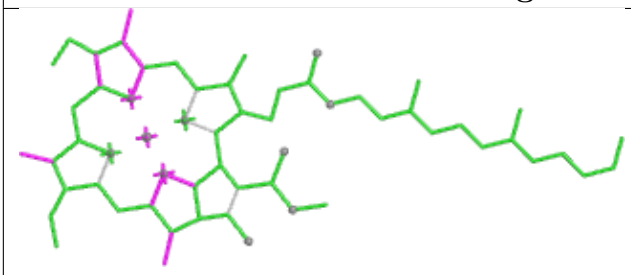


Torsions

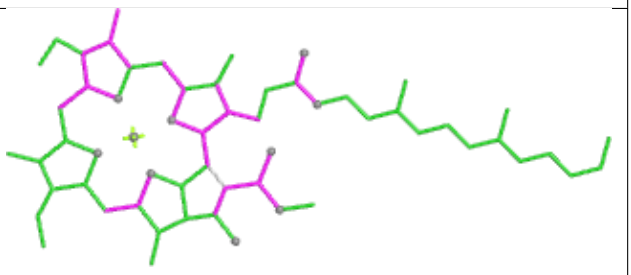


Rings

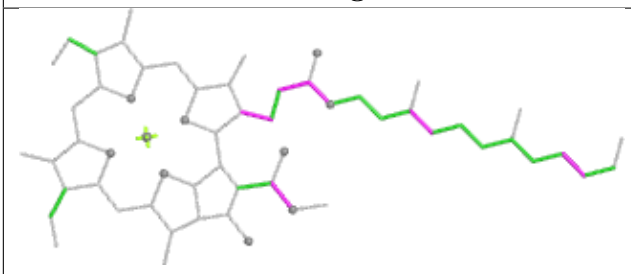
Ligand CLA cB 818



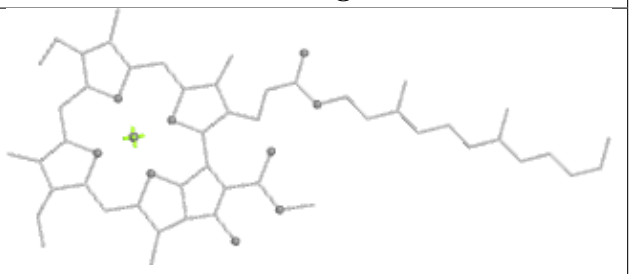
Bond lengths



Bond angles

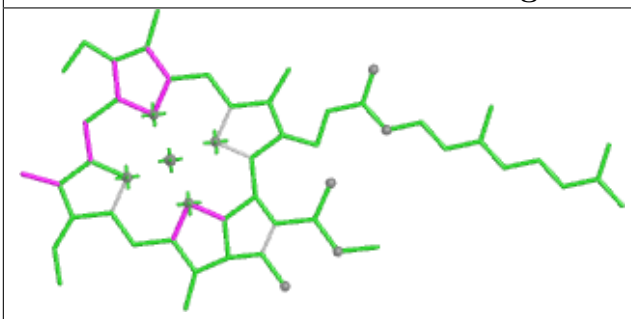


Torsions

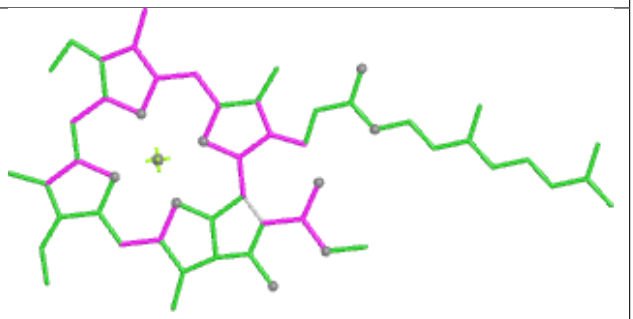


Rings

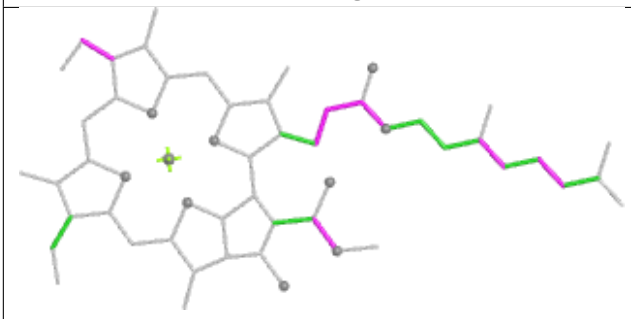
Ligand CLA c2 418



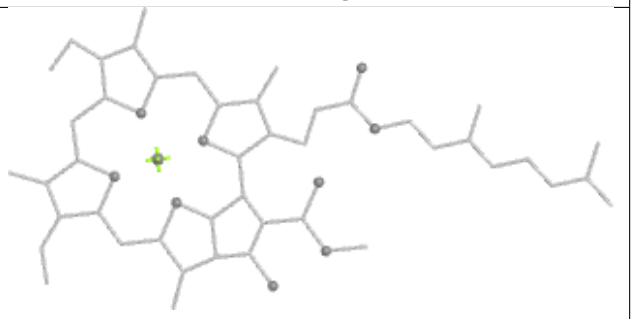
Bond lengths



Bond angles

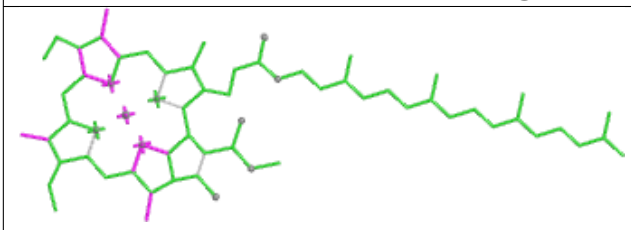


Torsions

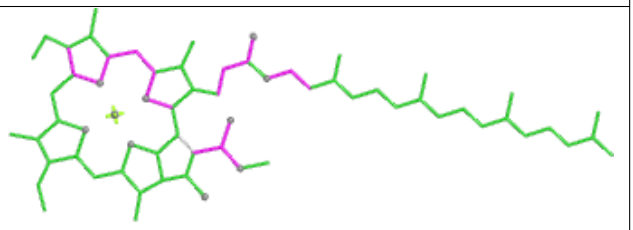


Rings

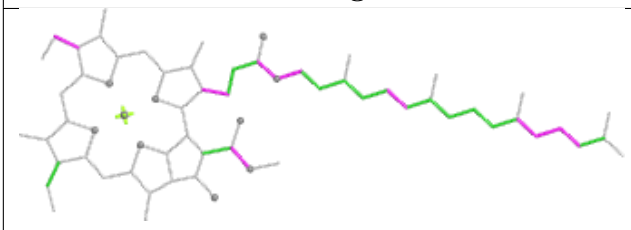
Ligand CLA cA 812



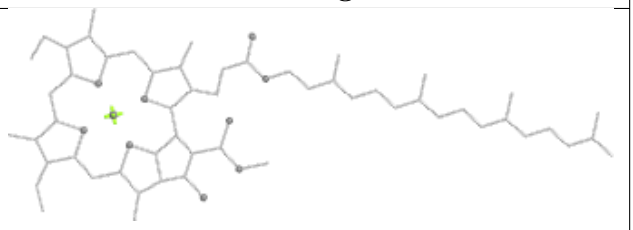
Bond lengths



Bond angles

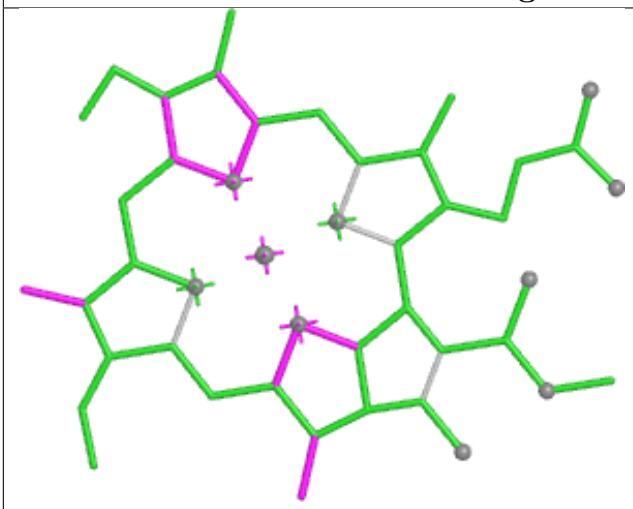


Torsions

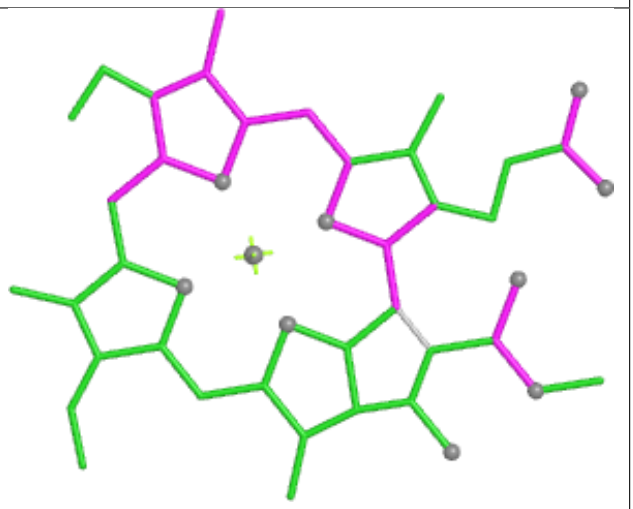


Rings

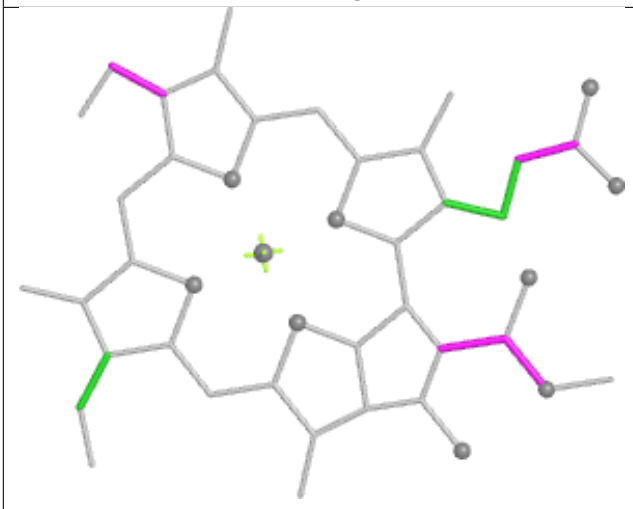
Ligand CLA b2 408



Bond lengths



Bond angles

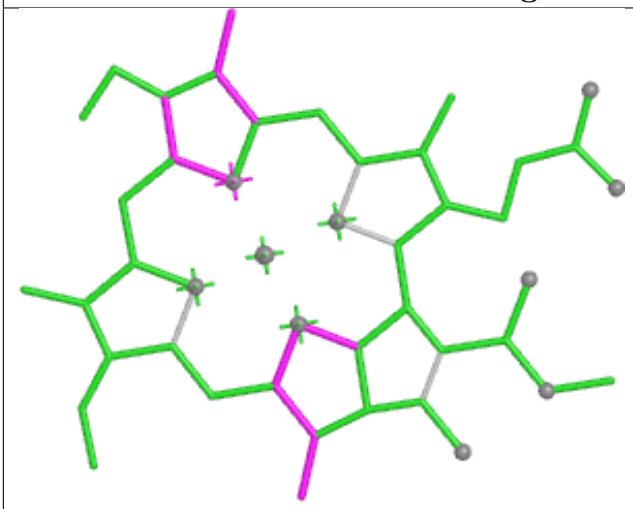


Torsions

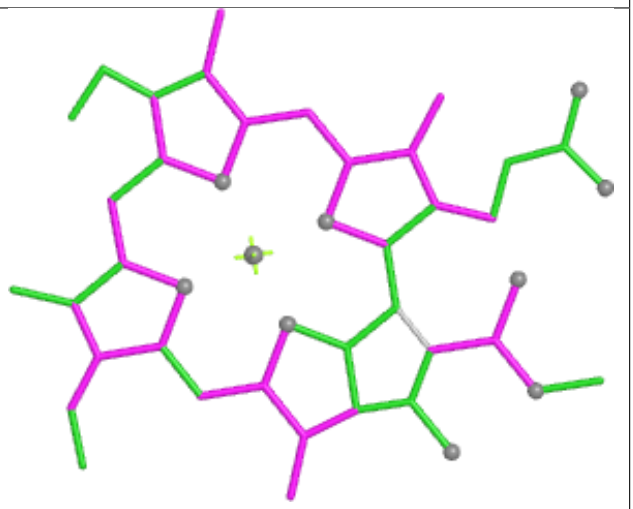


Rings

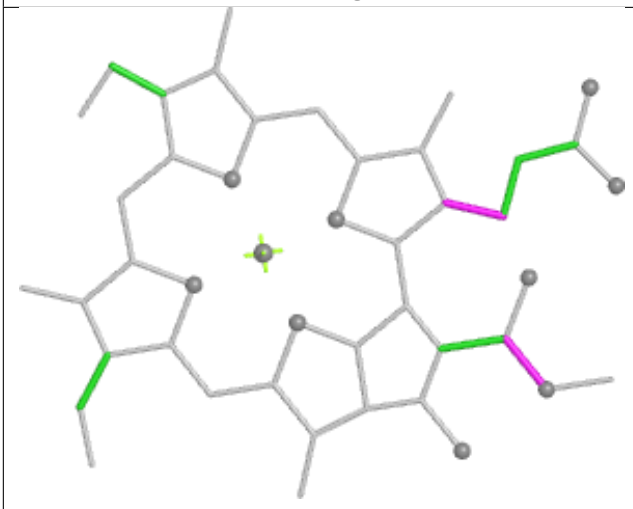
Ligand CLA c1 405



Bond lengths



Bond angles

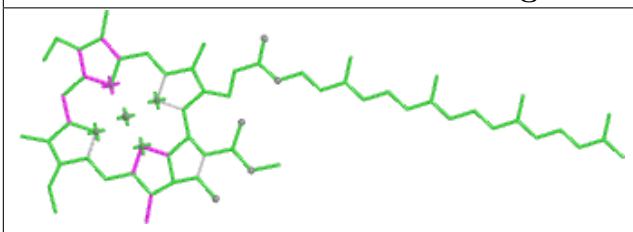


Torsions

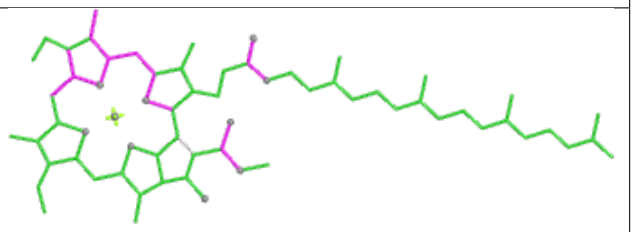


Rings

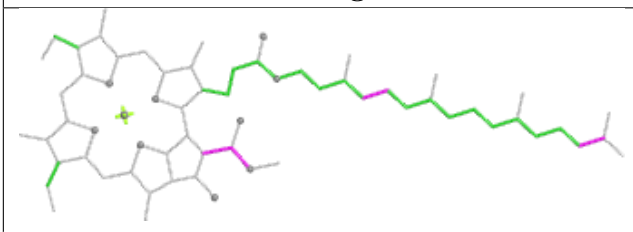
Ligand CLA c1 409



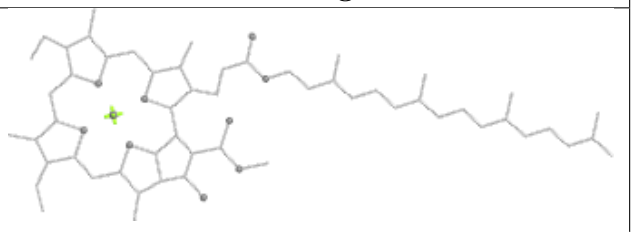
Bond lengths



Bond angles

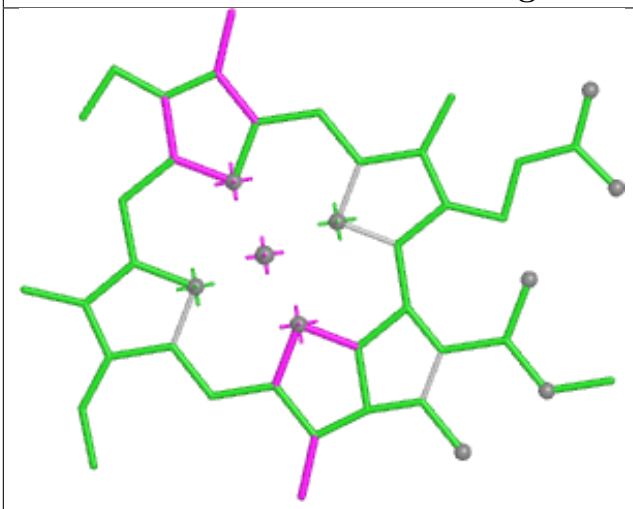


Torsions

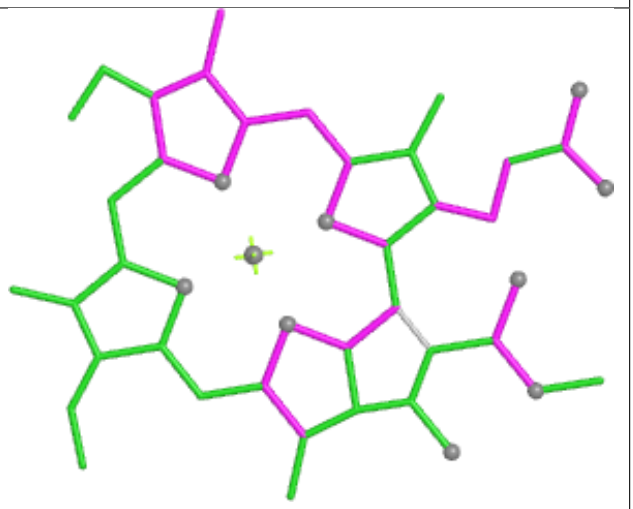


Rings

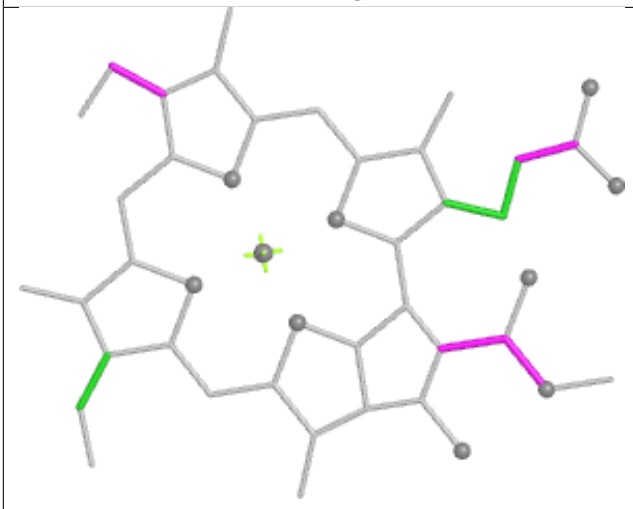
Ligand CLA b6 416



Bond lengths



Bond angles

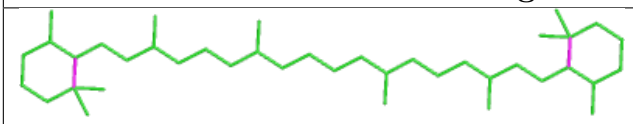


Torsions

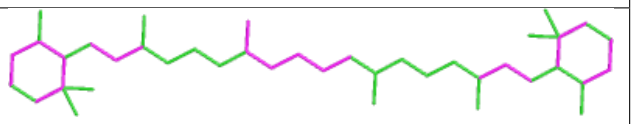


Rings

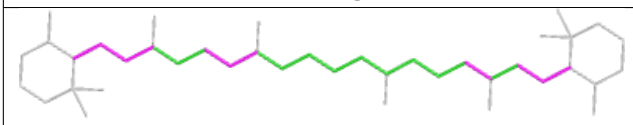
Ligand BCR a6 420



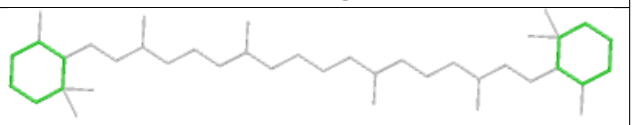
Bond lengths



Bond angles

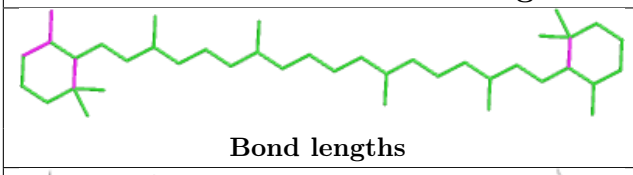


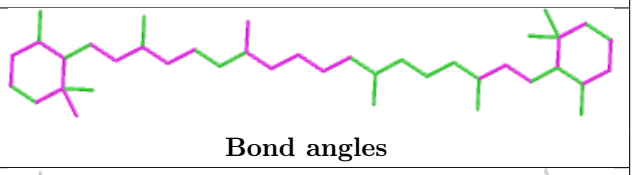
Torsions

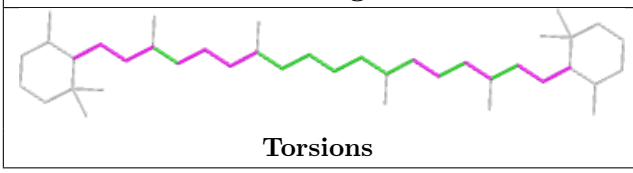


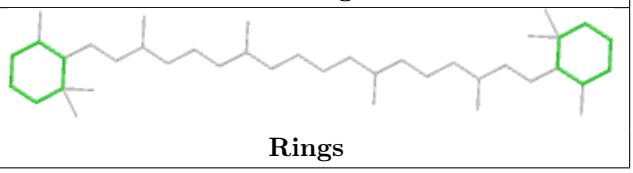
Rings

Ligand BCR b2 401

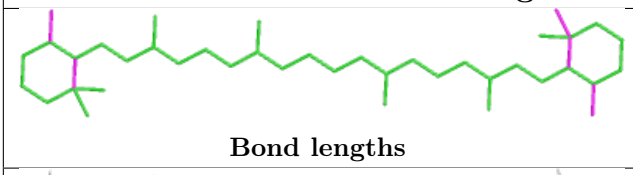

Bond lengths

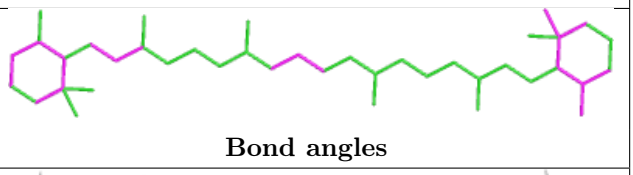

Bond angles


Torsions

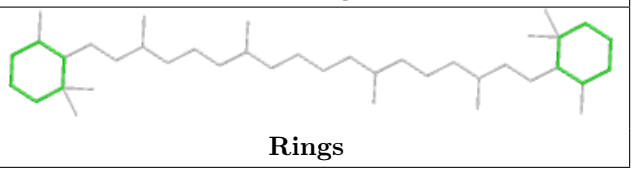

Rings

Ligand BCR b3 418

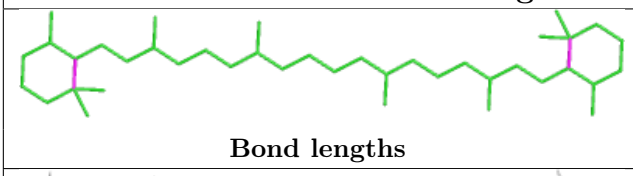

Bond lengths

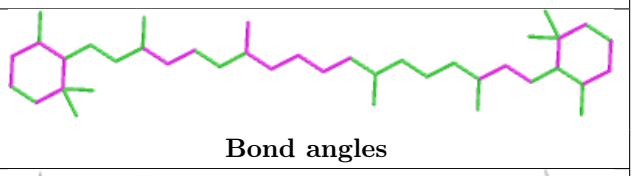

Bond angles

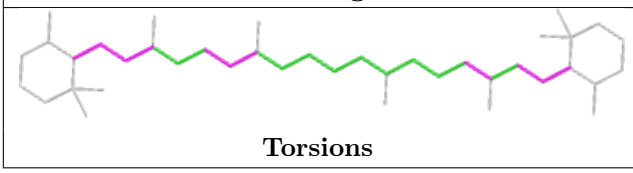

Torsions

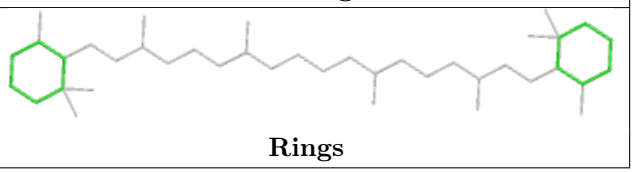

Rings

Ligand BCR b4 420

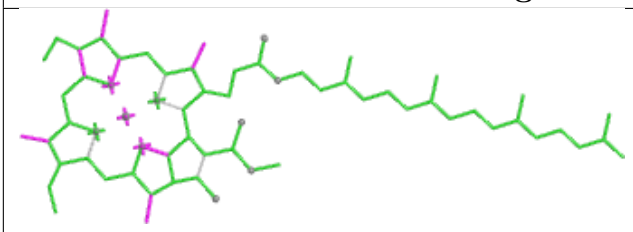

Bond lengths

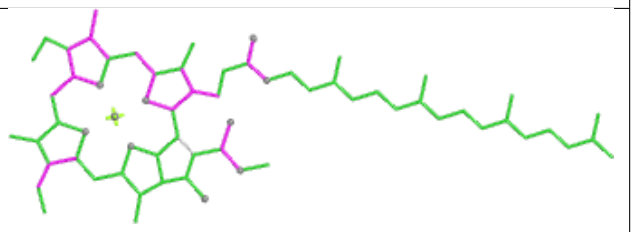

Bond angles

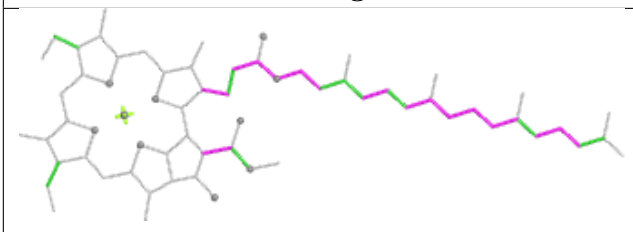

Torsions

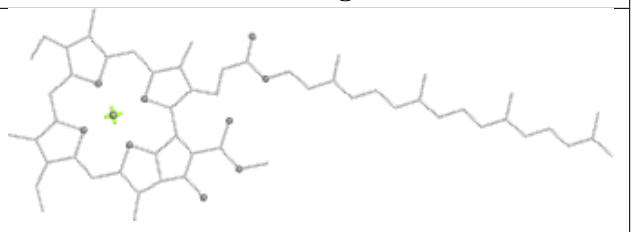

Rings

Ligand CLA aA 806

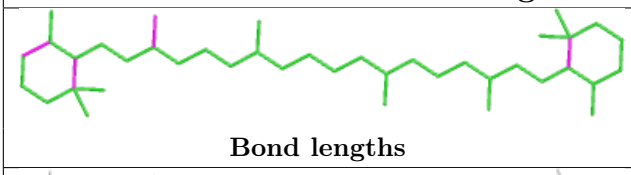

Bond lengths


Bond angles

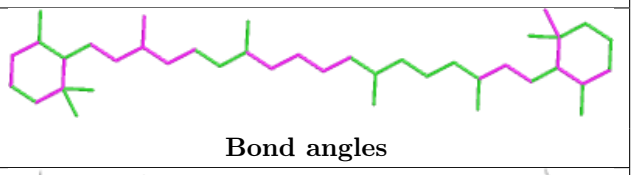

Torsions


Rings

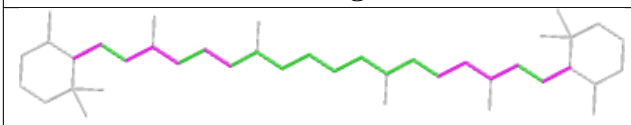
Ligand BCR a6 401



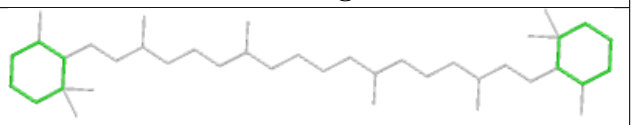
Bond lengths



Bond angles

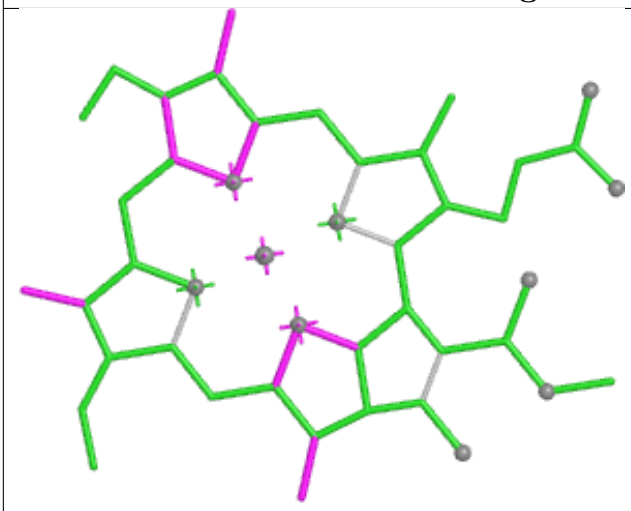


Torsions

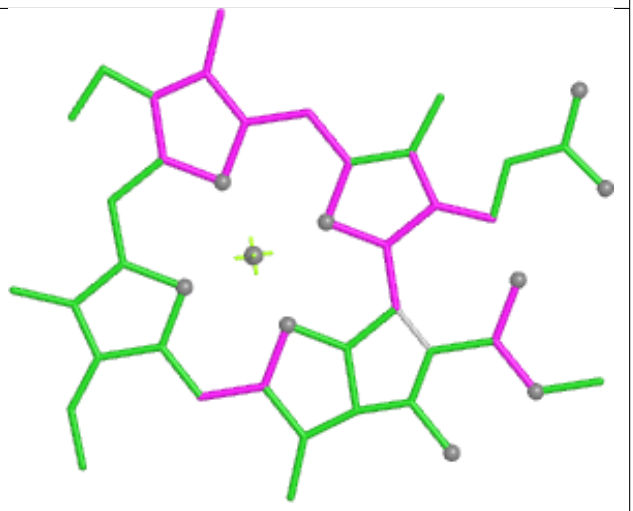


Rings

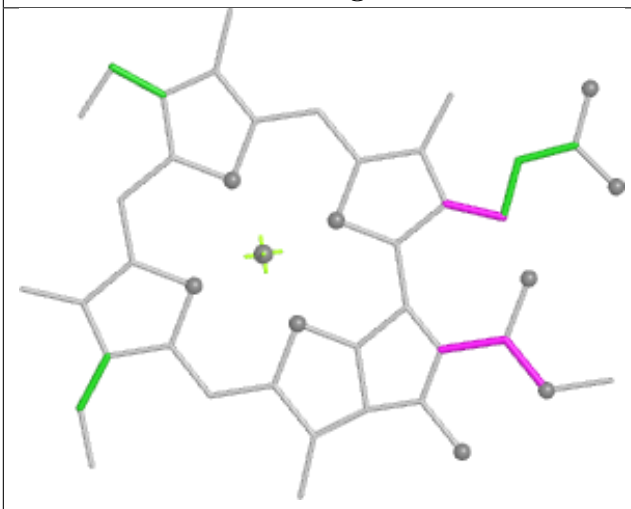
Ligand CLA a3 411



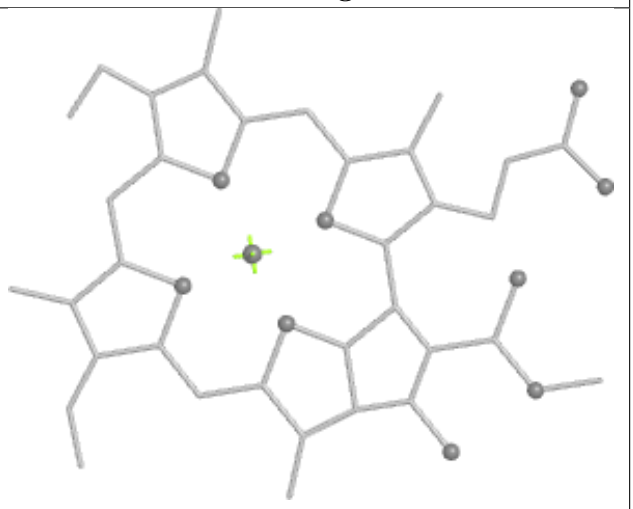
Bond lengths



Bond angles

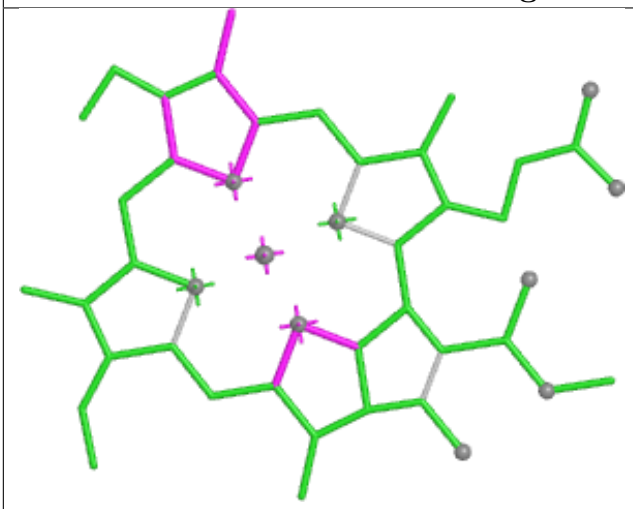


Torsions

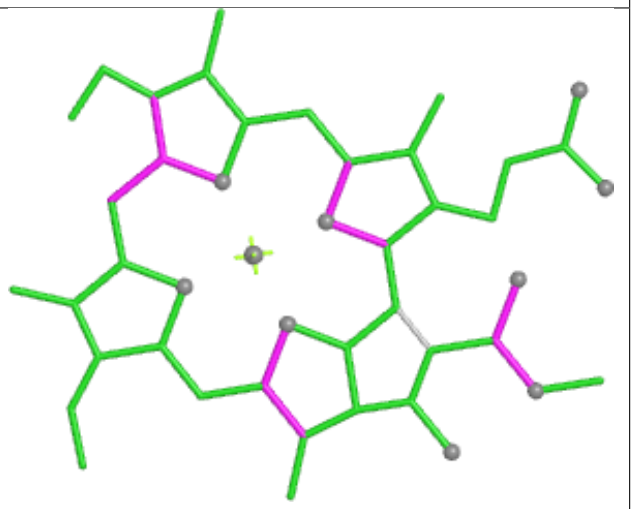


Rings

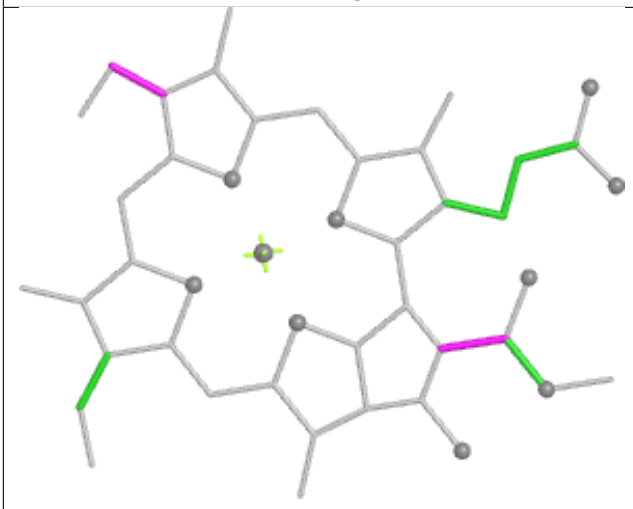
Ligand CLA a2 414



Bond lengths



Bond angles

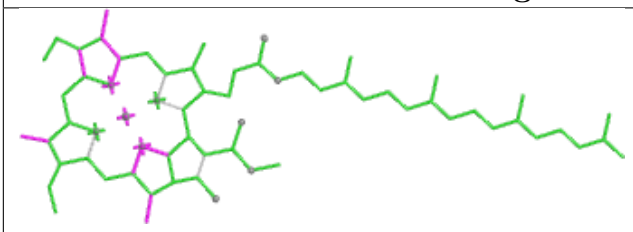


Torsions

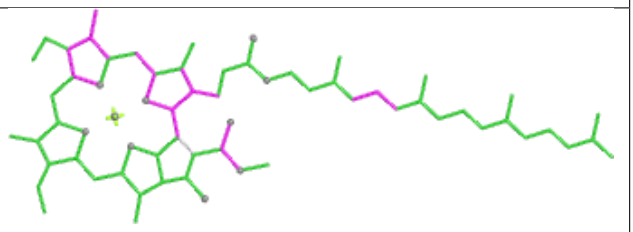


Rings

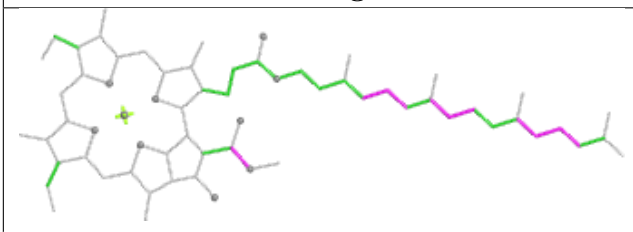
Ligand CLA bA 826



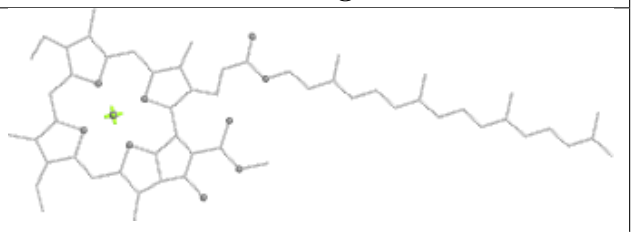
Bond lengths



Bond angles

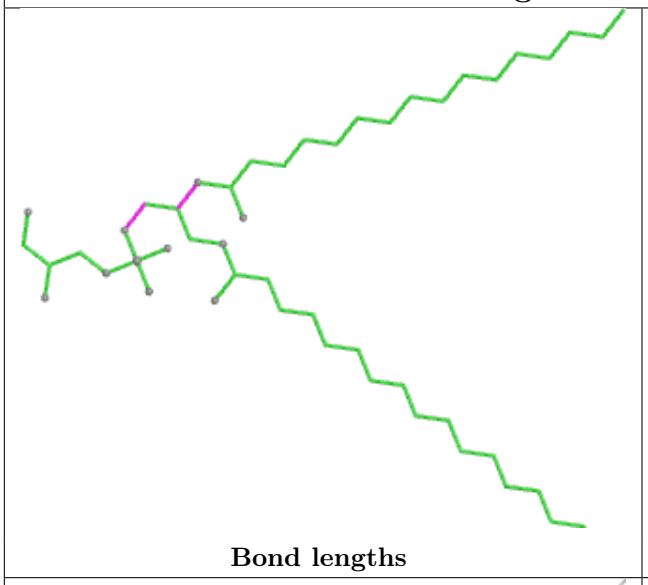


Torsions

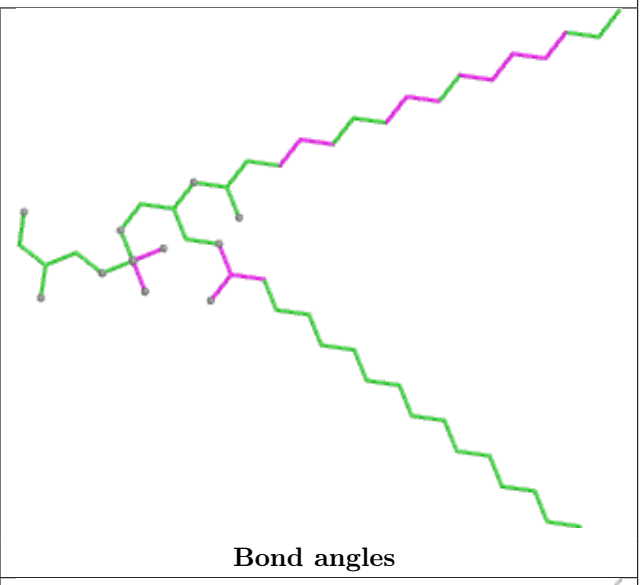


Rings

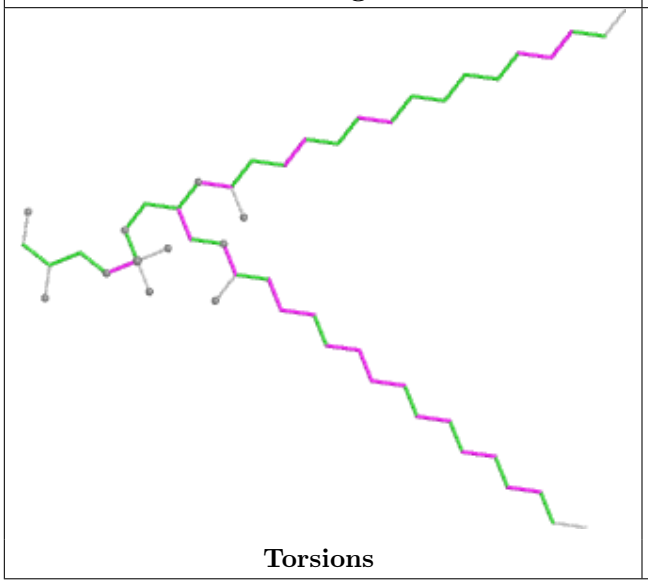
Ligand LHG aA 853



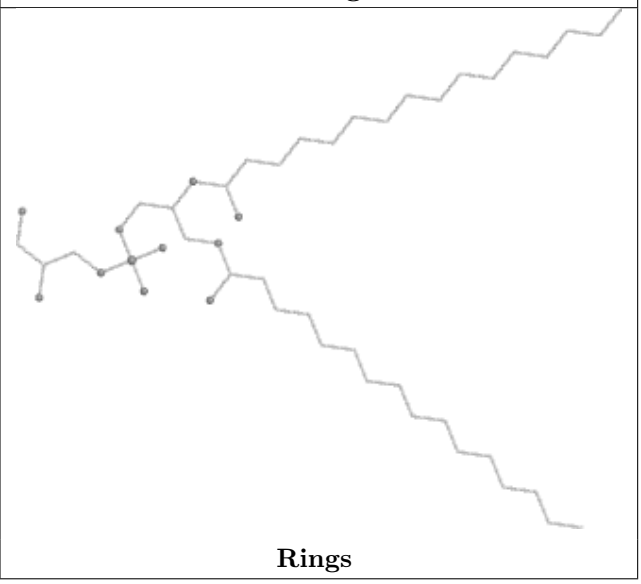
Bond lengths



Bond angles

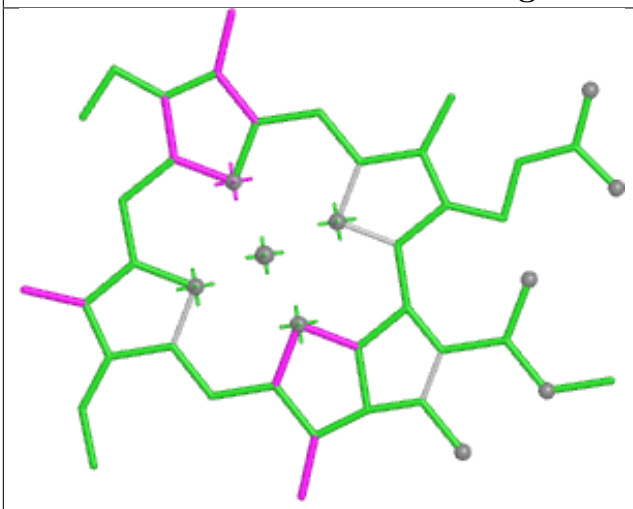


Torsions

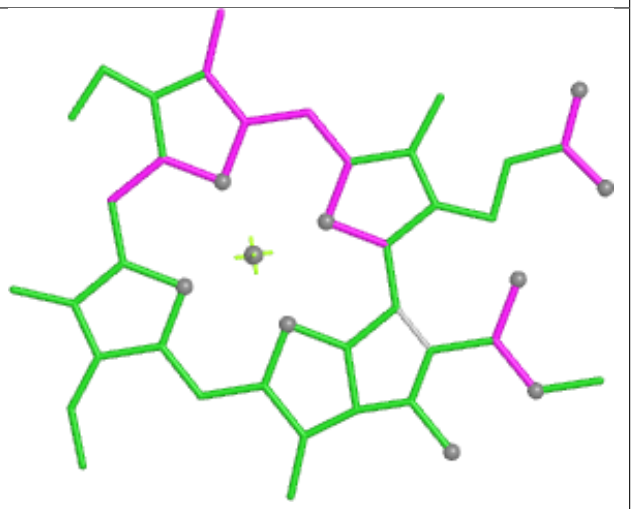


Rings

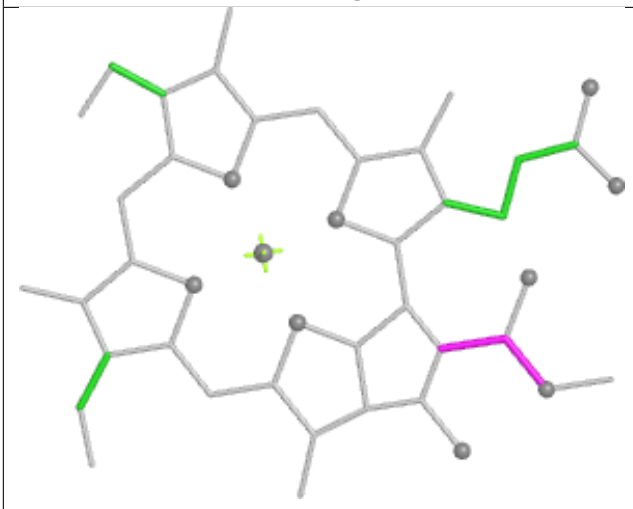
Ligand CLA b3 406



Bond lengths



Bond angles

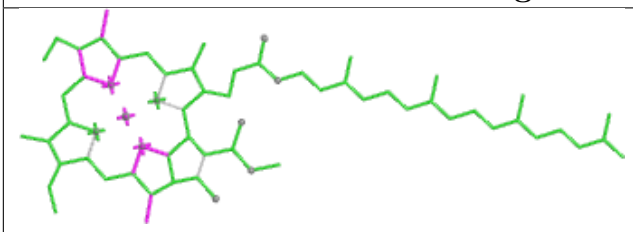


Torsions

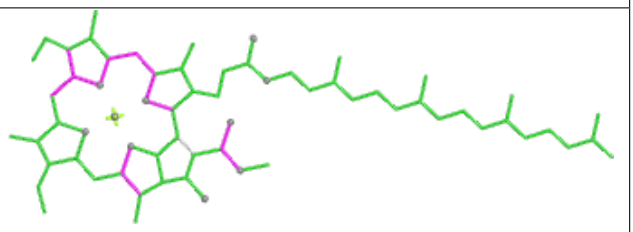


Rings

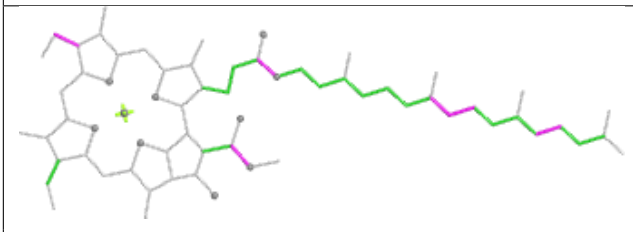
Ligand CLA bB 820



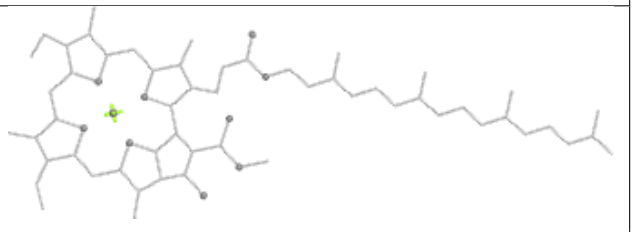
Bond lengths



Bond angles

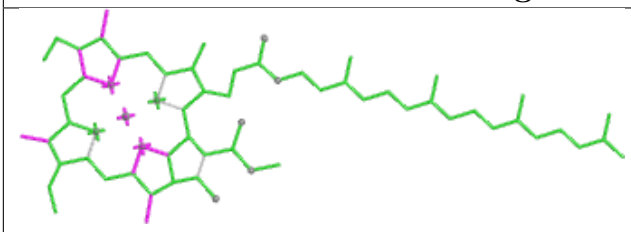


Torsions

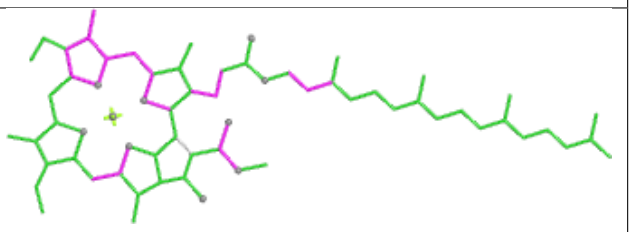


Rings

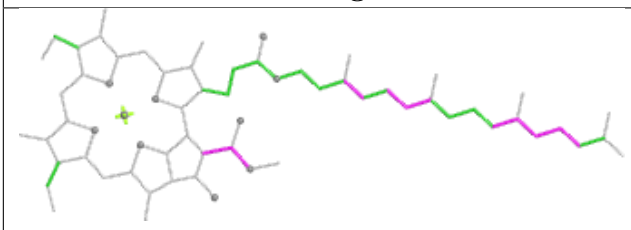
Ligand CLA bB 837



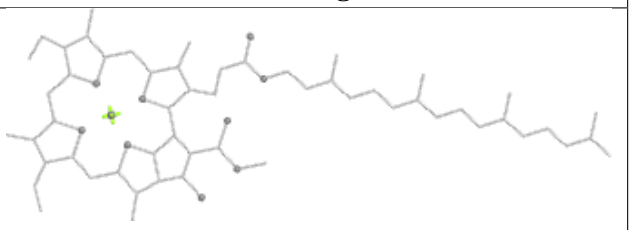
Bond lengths



Bond angles

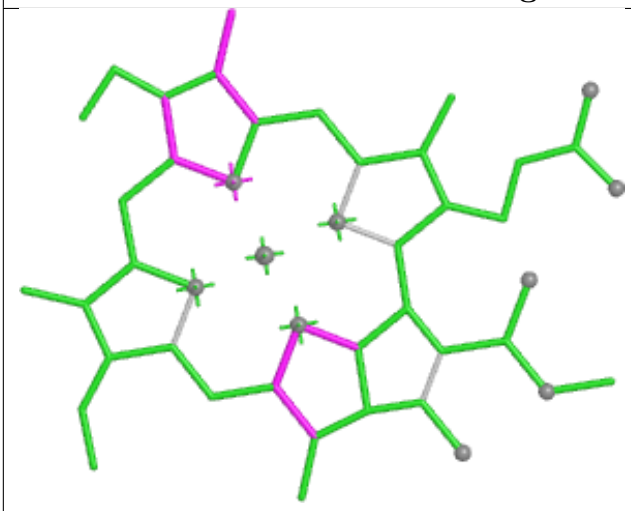


Torsions

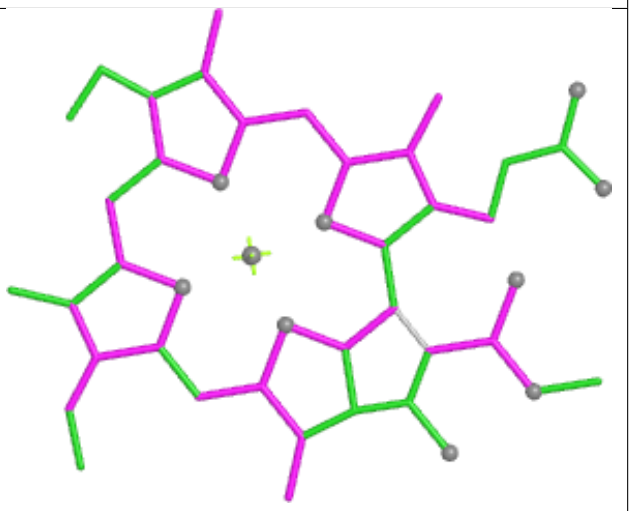


Rings

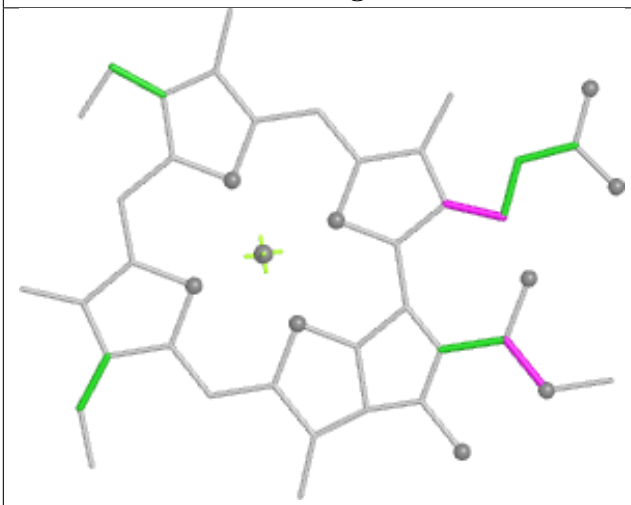
Ligand CLA a6 406



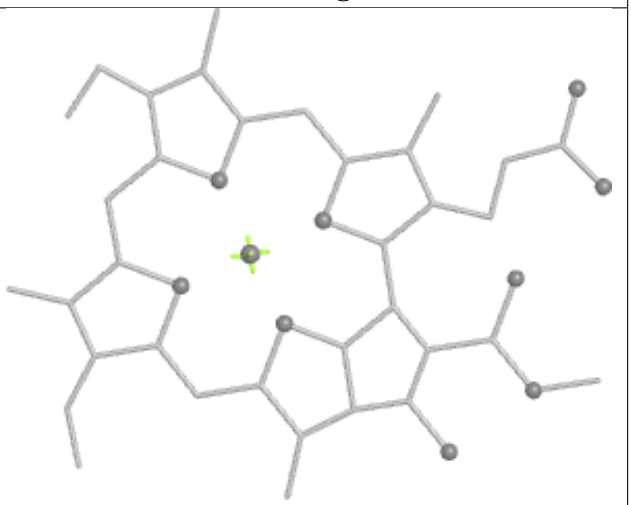
Bond lengths



Bond angles

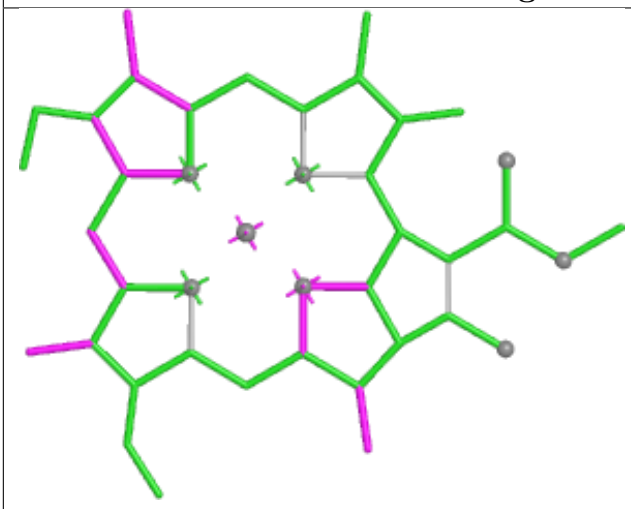


Torsions

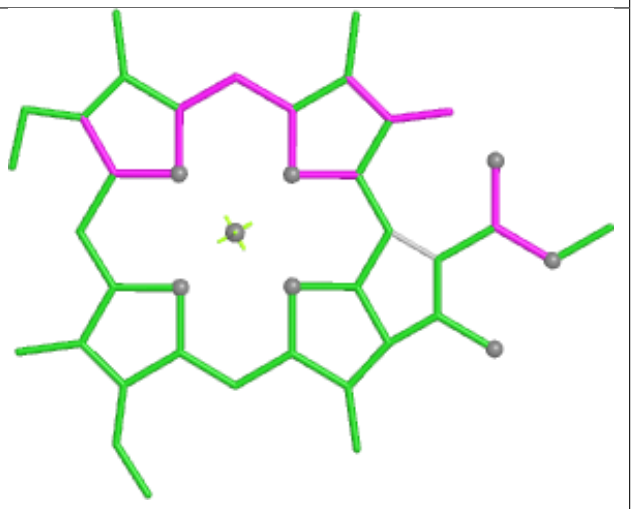


Rings

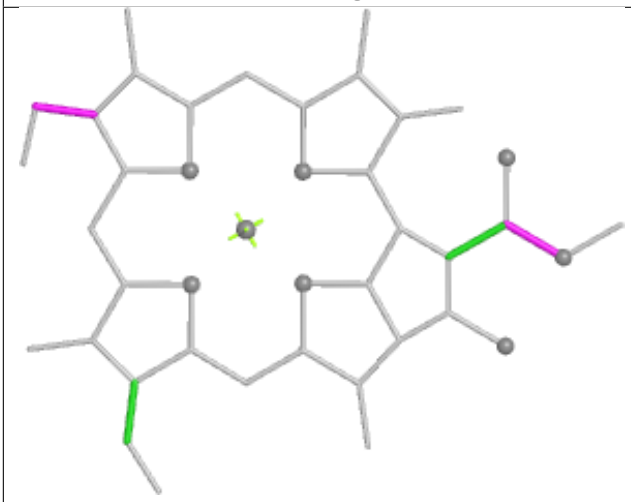
Ligand CLA b3 414



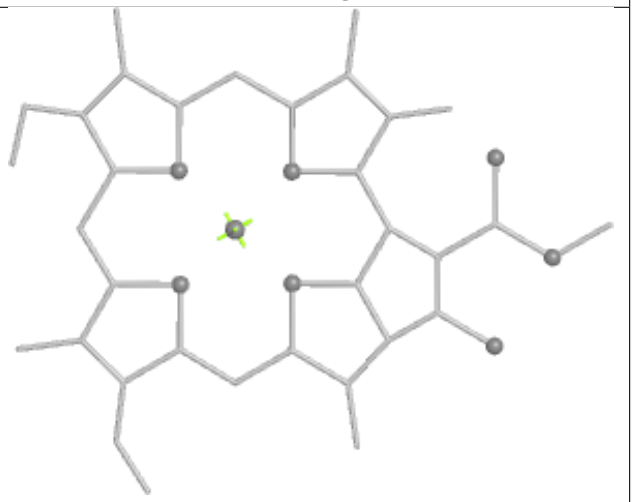
Bond lengths



Bond angles

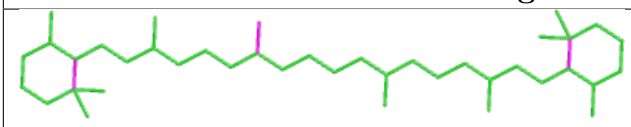


Torsions

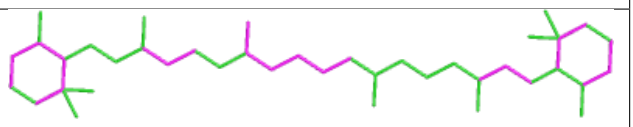


Rings

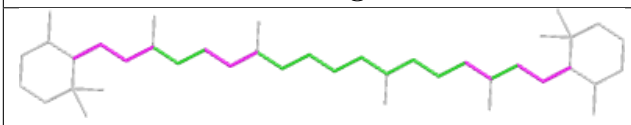
Ligand BCR a1 419



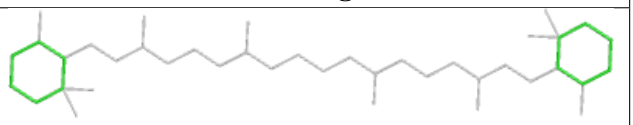
Bond lengths



Bond angles

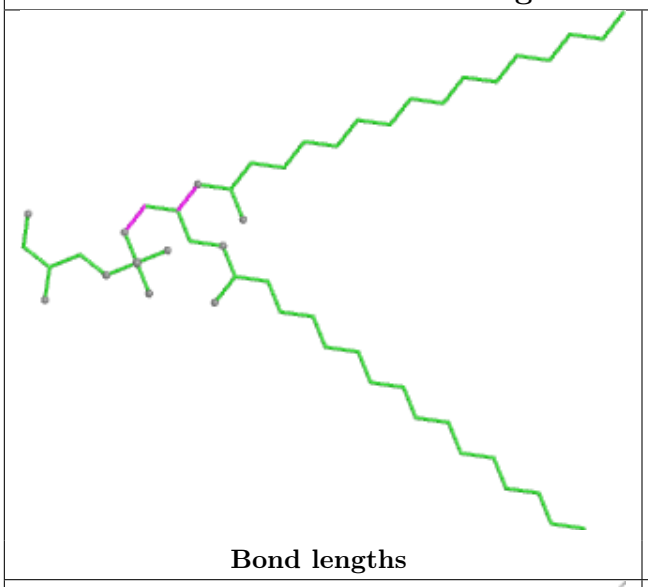


Torsions

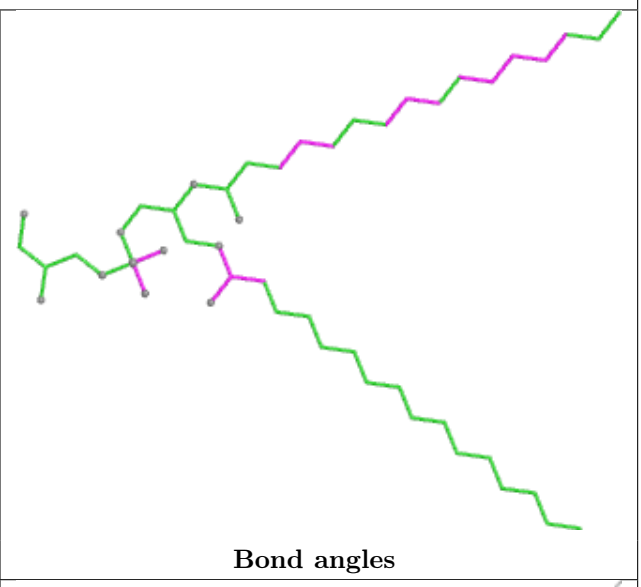


Rings

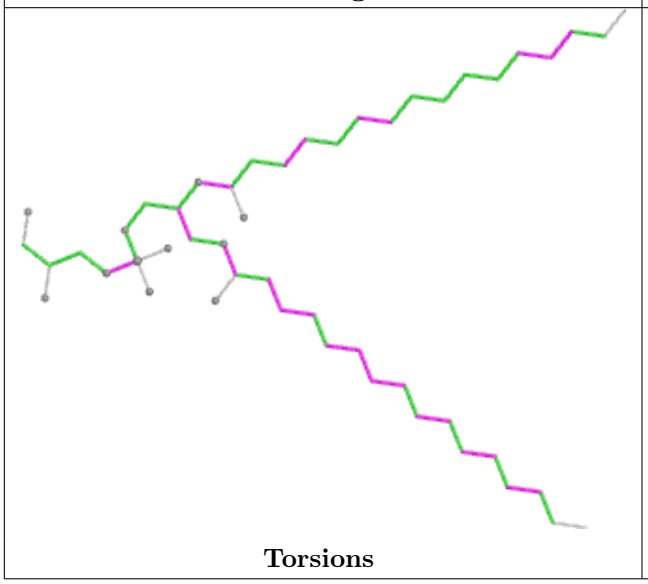
Ligand LHG cA 852



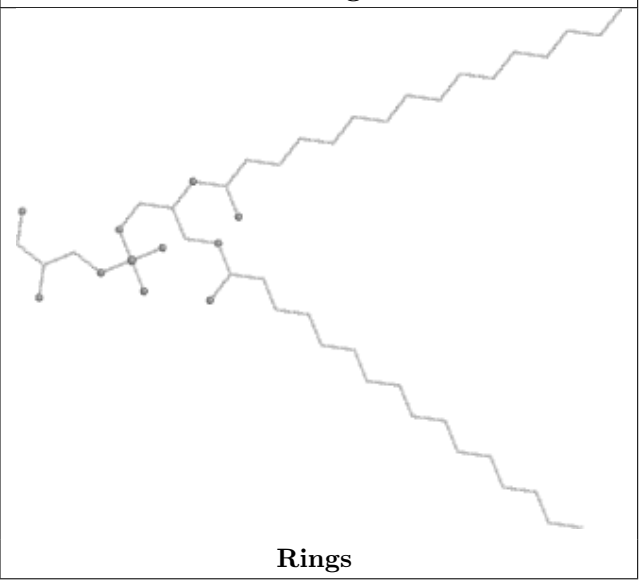
Bond lengths



Bond angles



Torsions

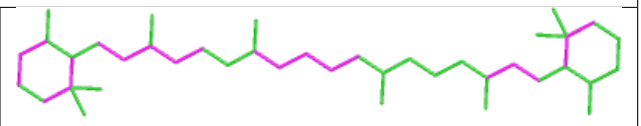


Rings

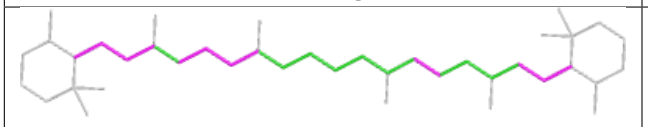
Ligand BCR a3 401



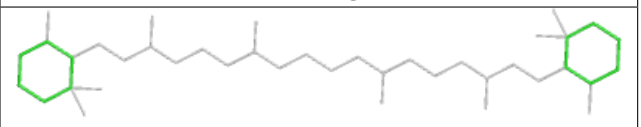
Bond lengths



Bond angles

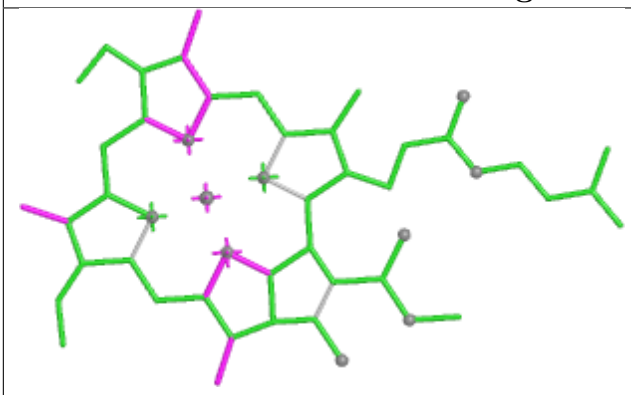


Torsions

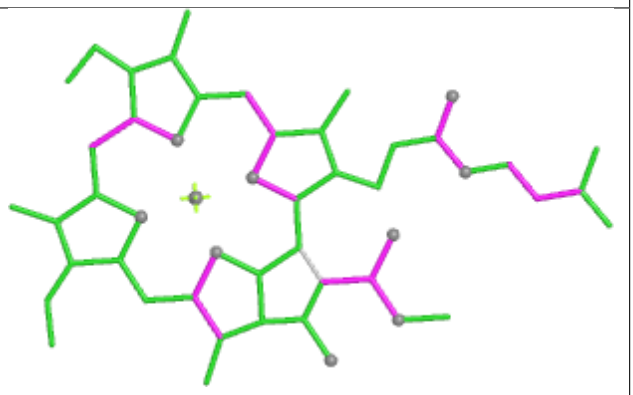


Rings

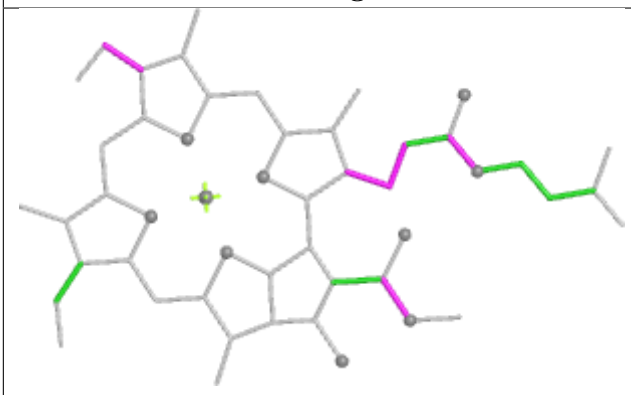
Ligand CLA cA 832



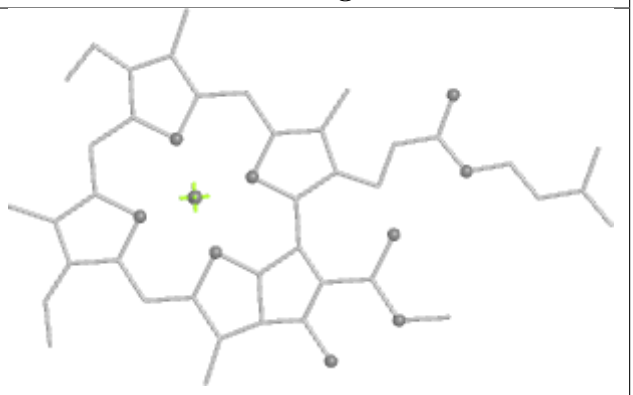
Bond lengths



Bond angles

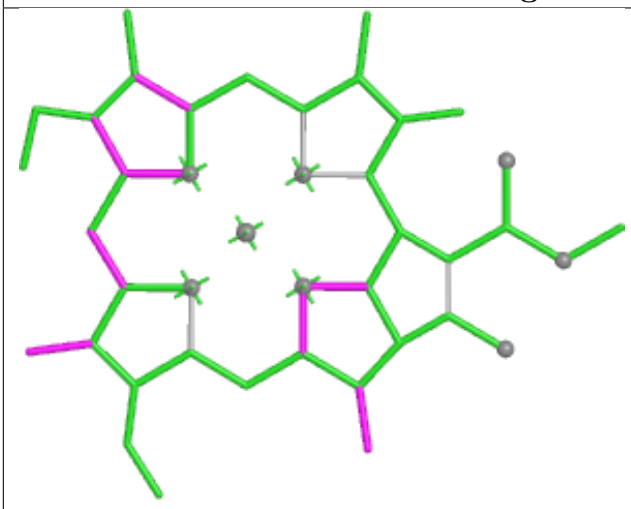


Torsions

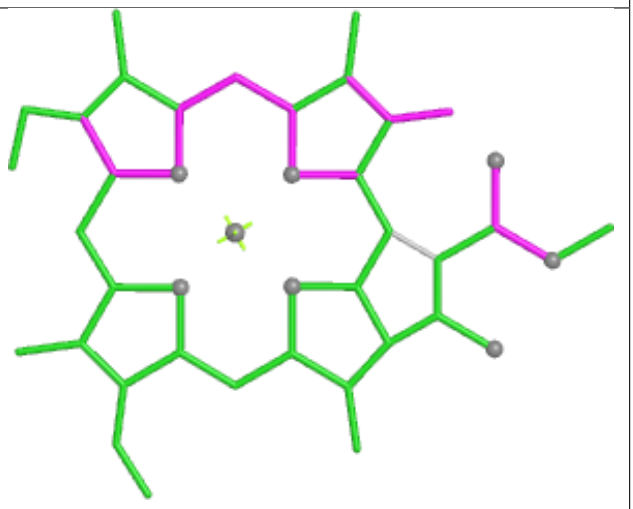


Rings

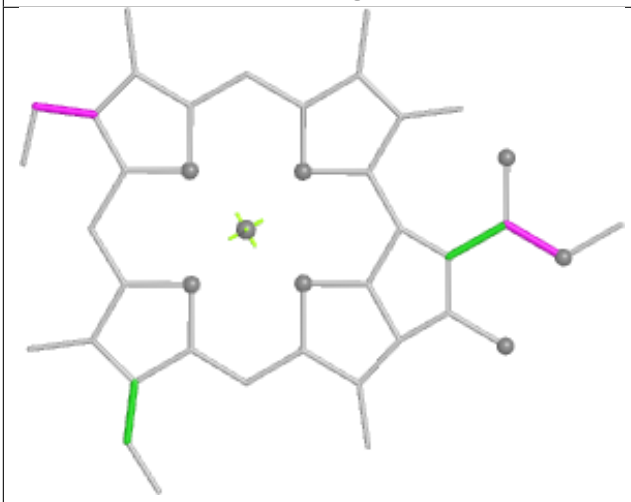
Ligand CLA c6 416



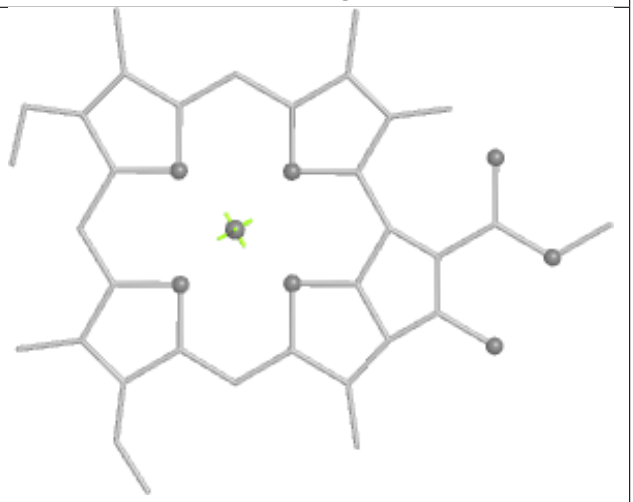
Bond lengths



Bond angles

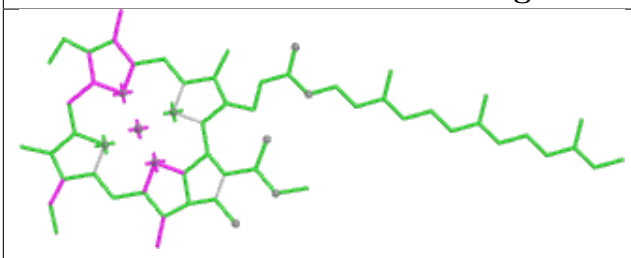


Torsions

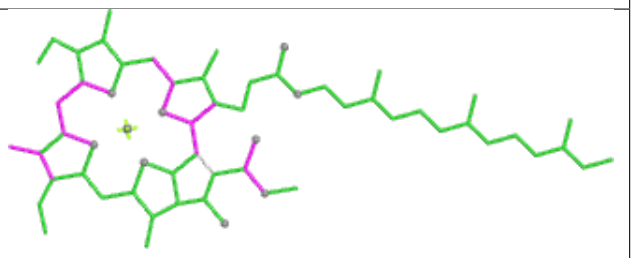


Rings

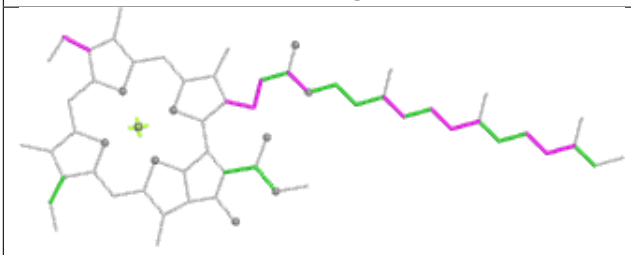
Ligand CLA bA 821



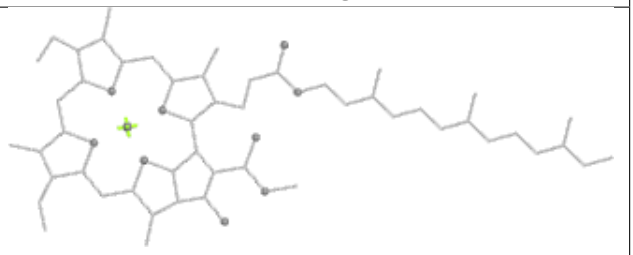
Bond lengths



Bond angles

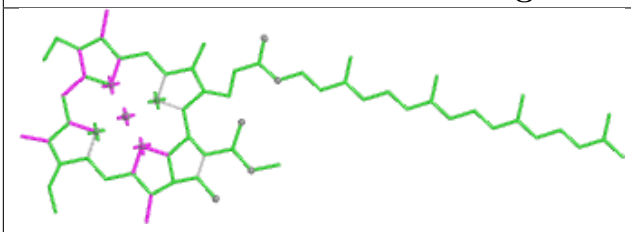


Torsions

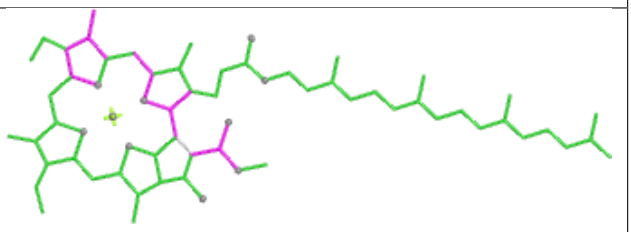


Rings

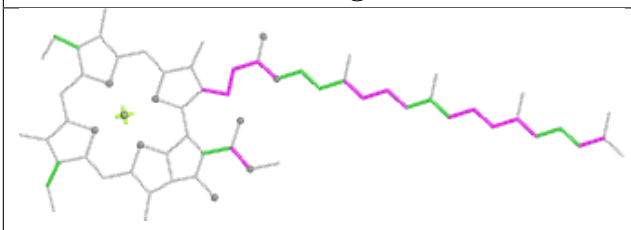
Ligand CLA aB 828



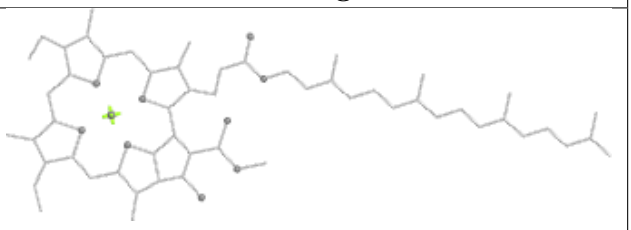
Bond lengths



Bond angles

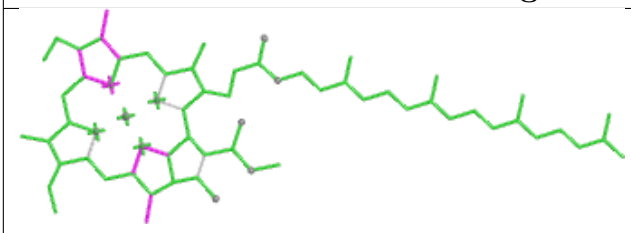


Torsions

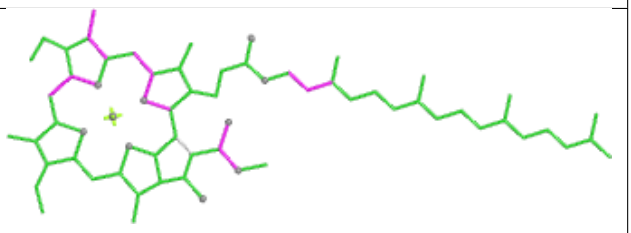


Rings

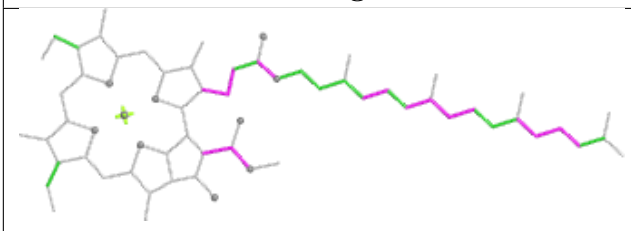
Ligand CLA c2 402



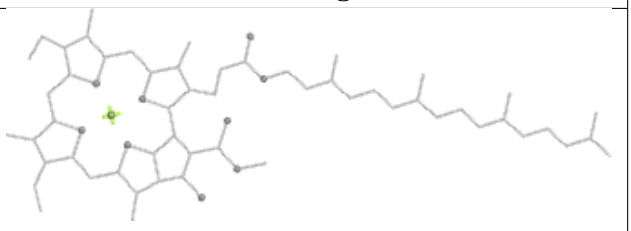
Bond lengths



Bond angles

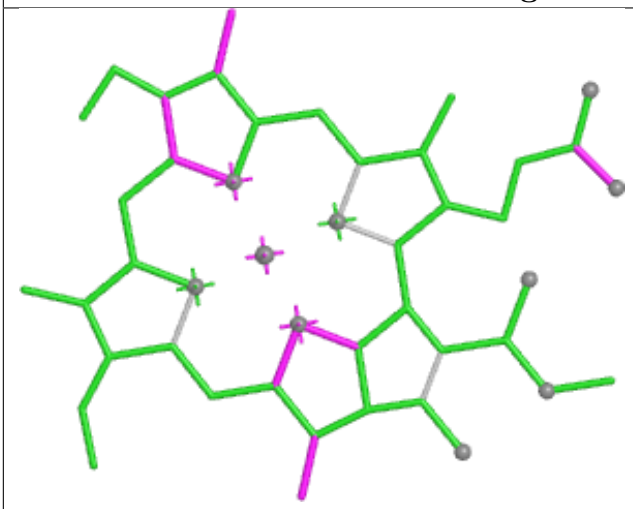


Torsions

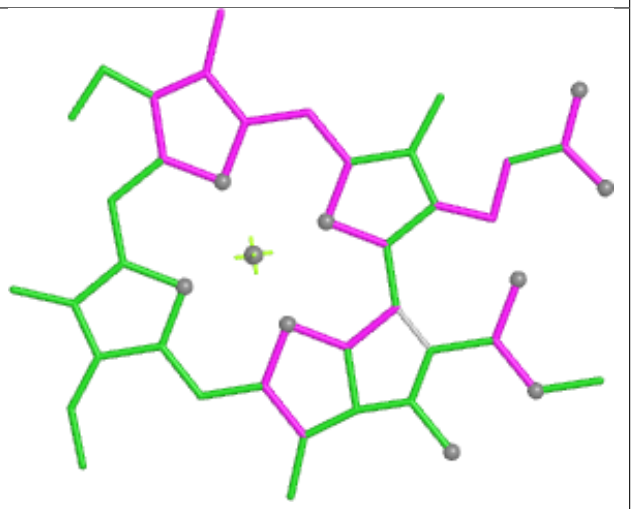


Rings

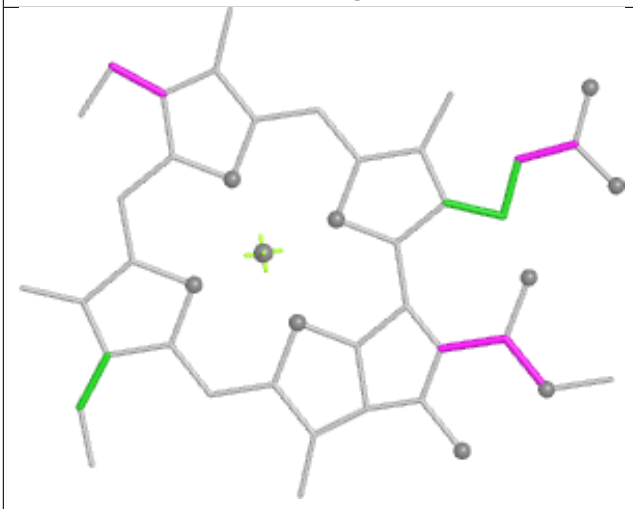
Ligand CLA c2 416



Bond lengths



Bond angles

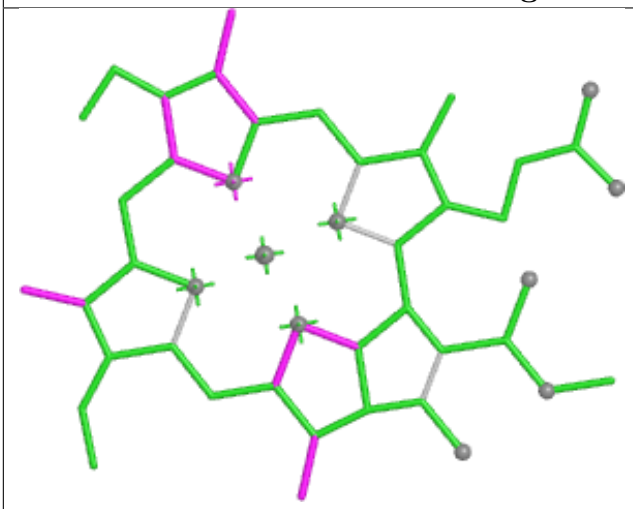


Torsions

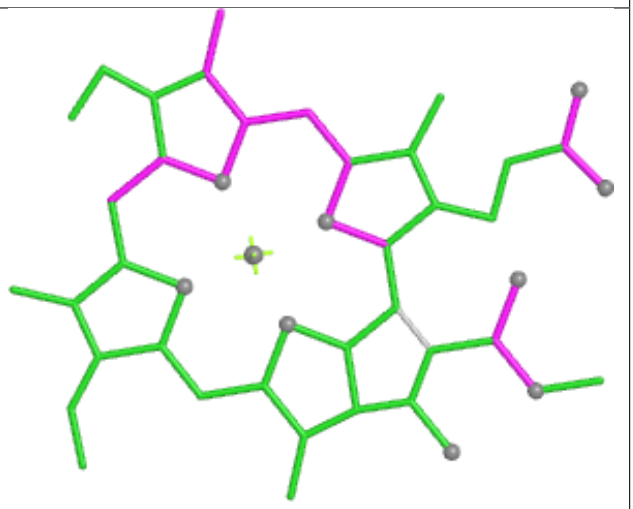


Rings

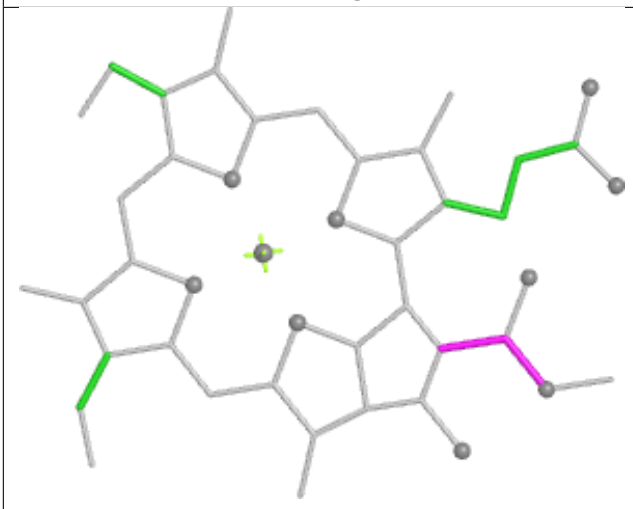
Ligand CLA c6 408



Bond lengths



Bond angles

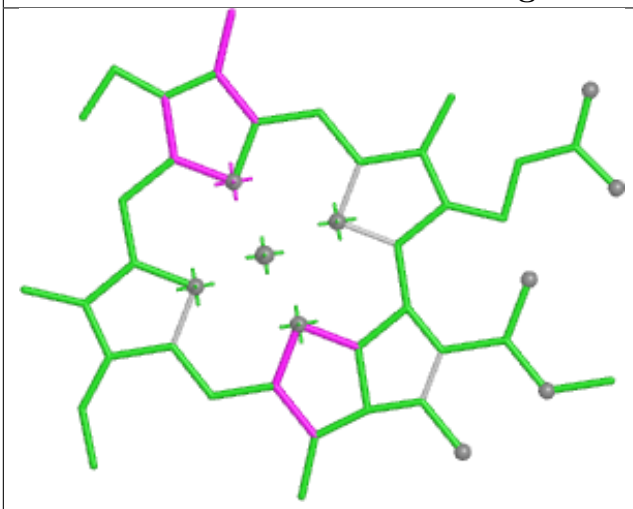


Torsions

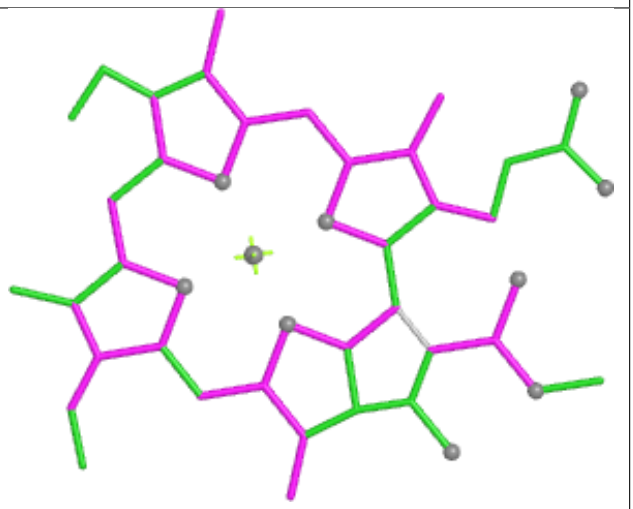


Rings

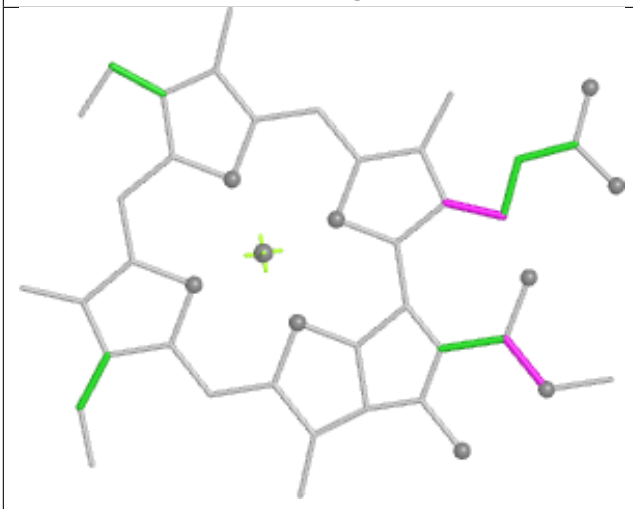
Ligand CLA b6 406



Bond lengths



Bond angles

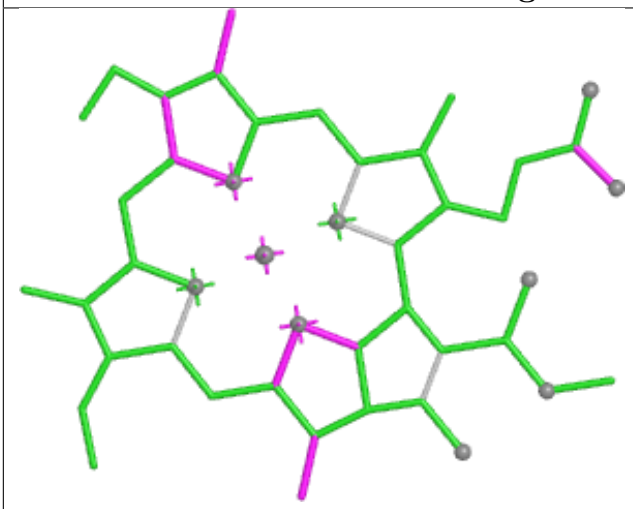


Torsions

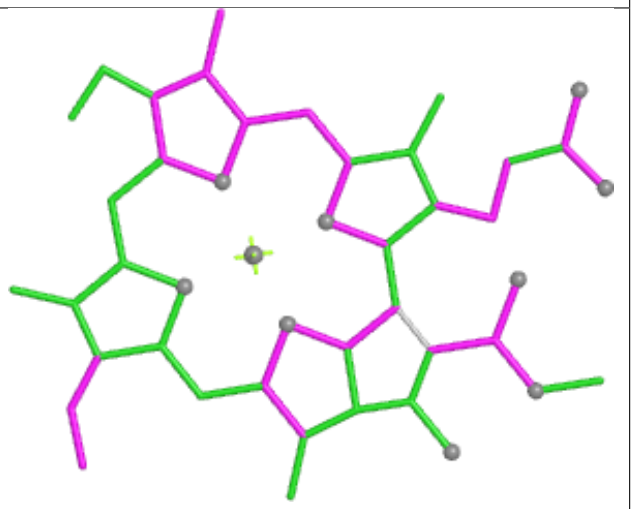


Rings

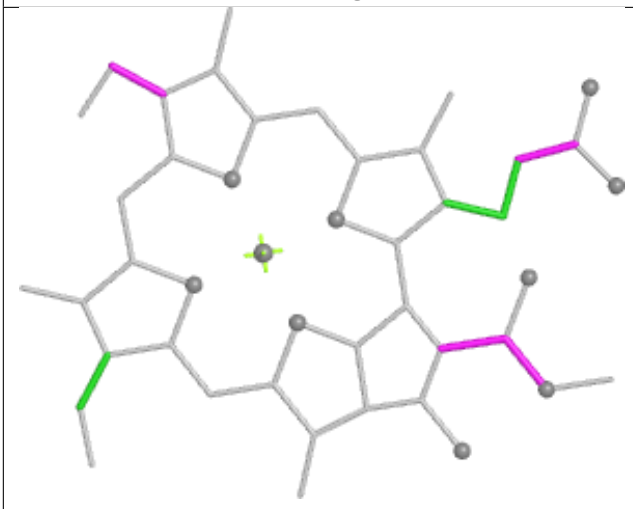
Ligand CLA b4 415



Bond lengths



Bond angles

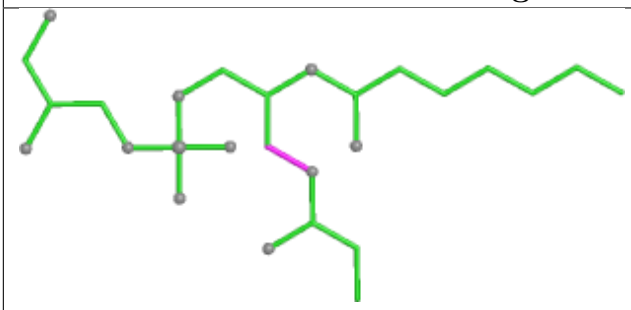


Torsions

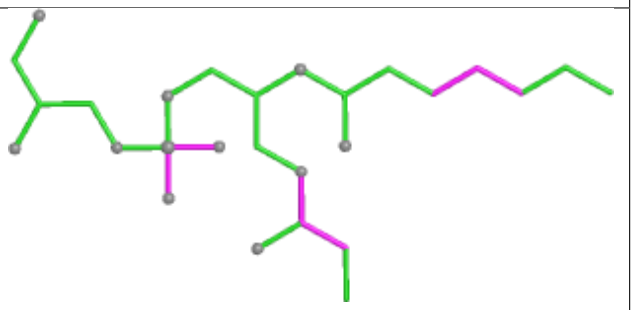


Rings

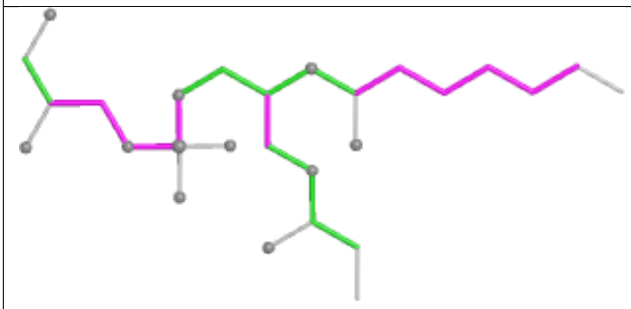
Ligand LHG bA 855



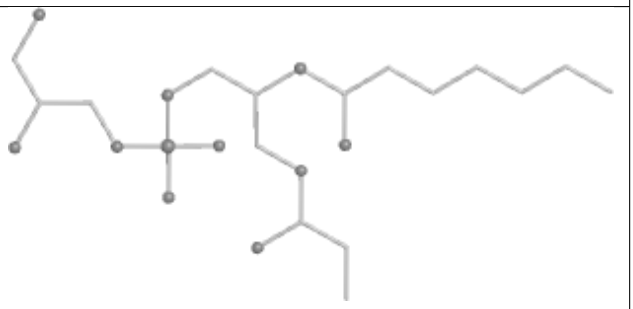
Bond lengths



Bond angles

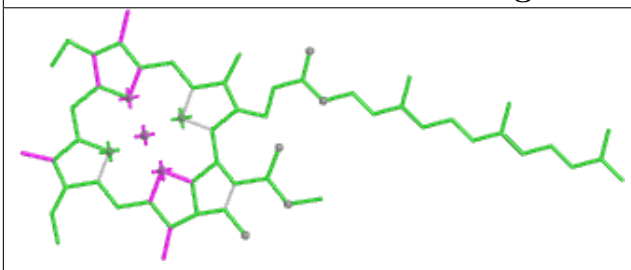


Torsions

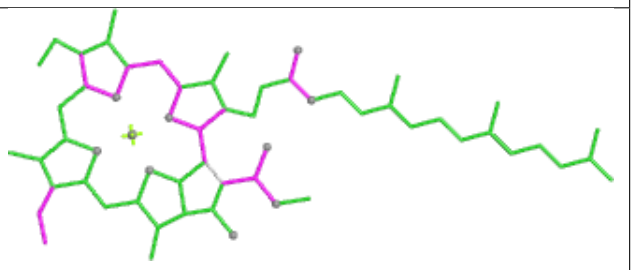


Rings

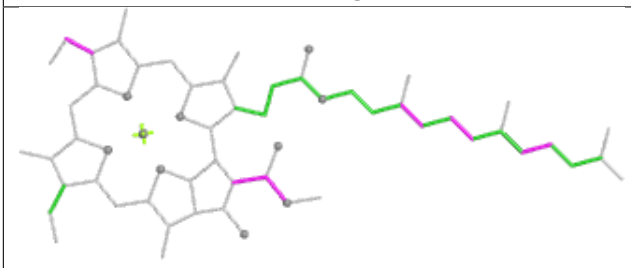
Ligand CLA bB 836



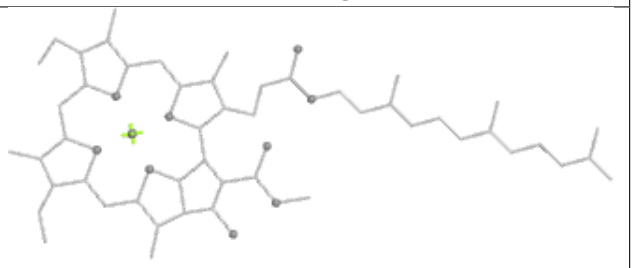
Bond lengths



Bond angles

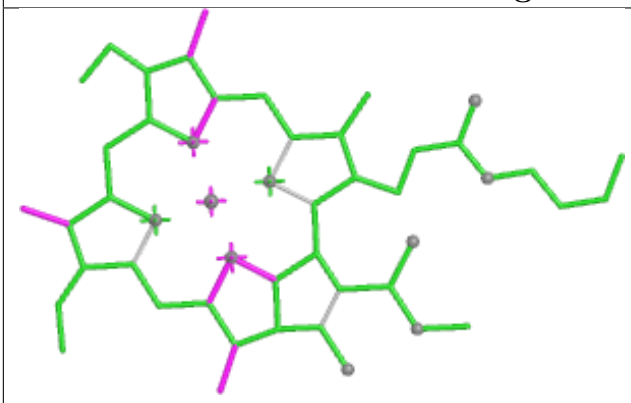


Torsions

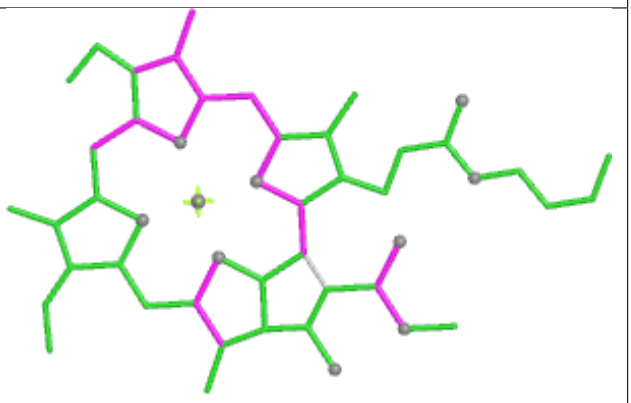


Rings

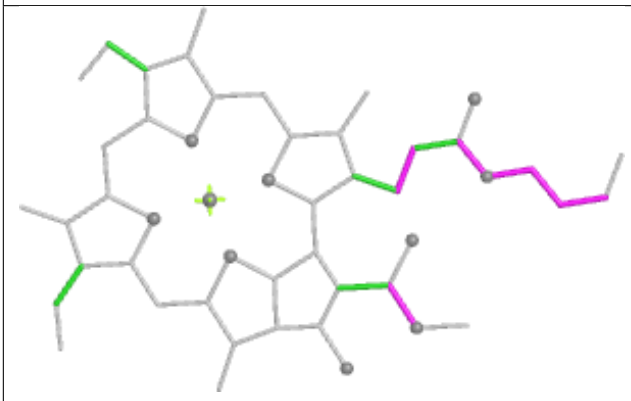
Ligand CLA bB 832



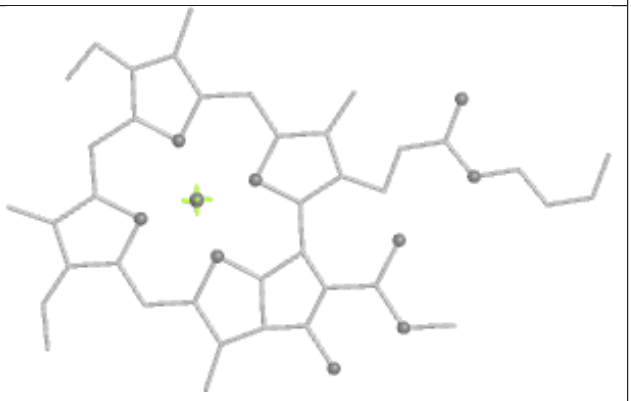
Bond lengths



Bond angles

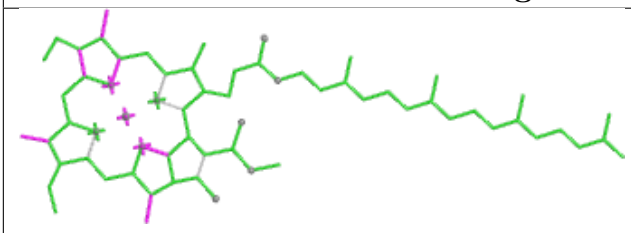


Torsions

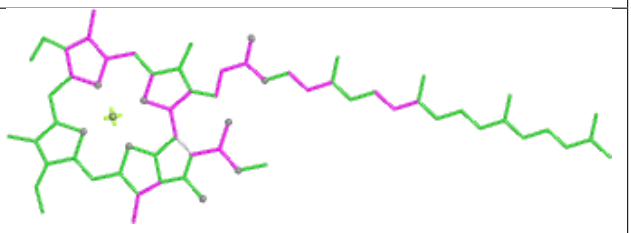


Rings

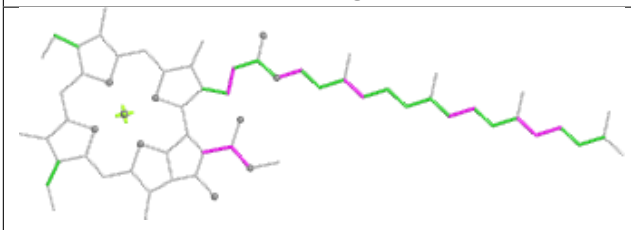
Ligand CLA bB 803



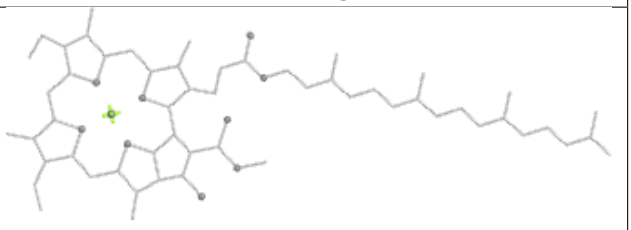
Bond lengths



Bond angles

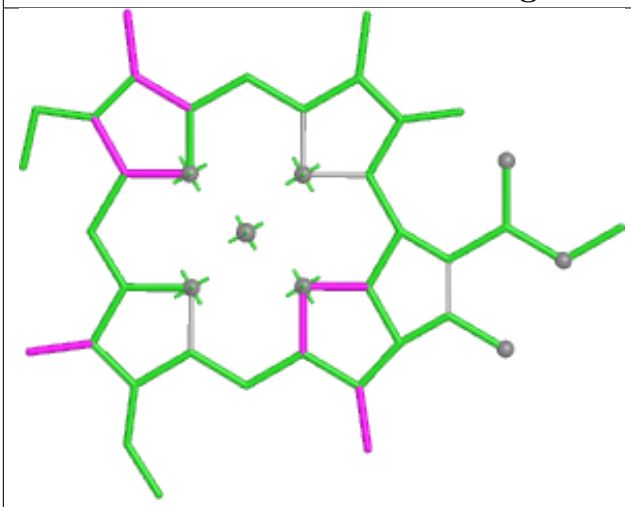


Torsions

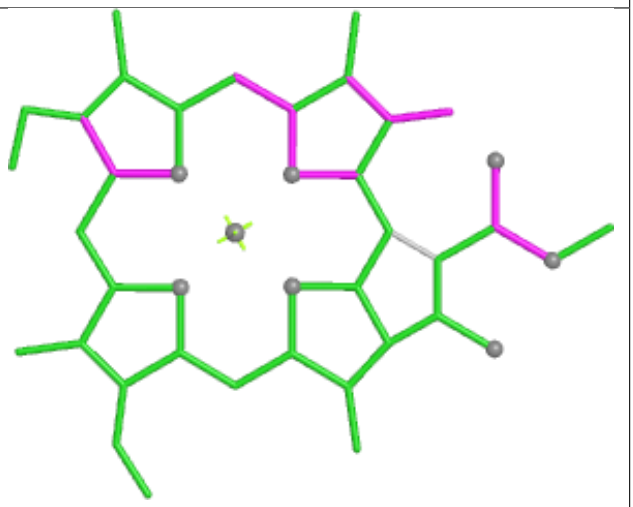


Rings

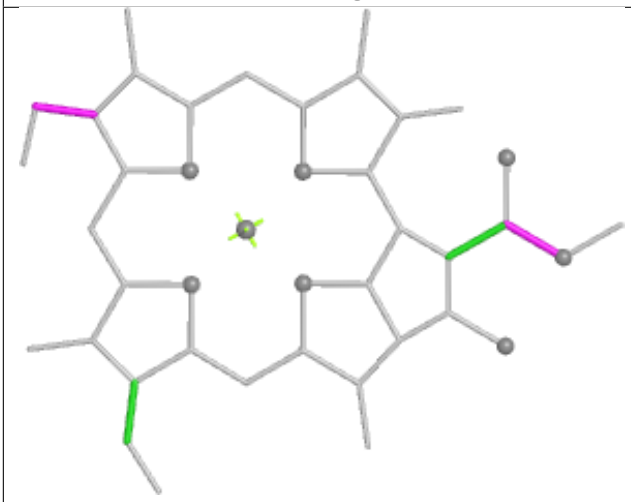
Ligand CLA a2 415



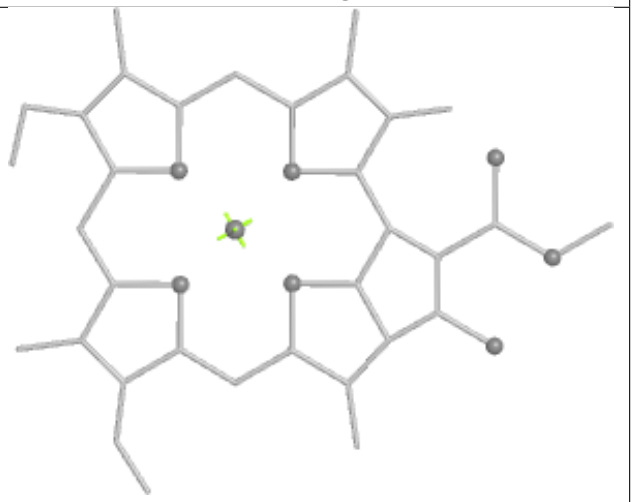
Bond lengths



Bond angles

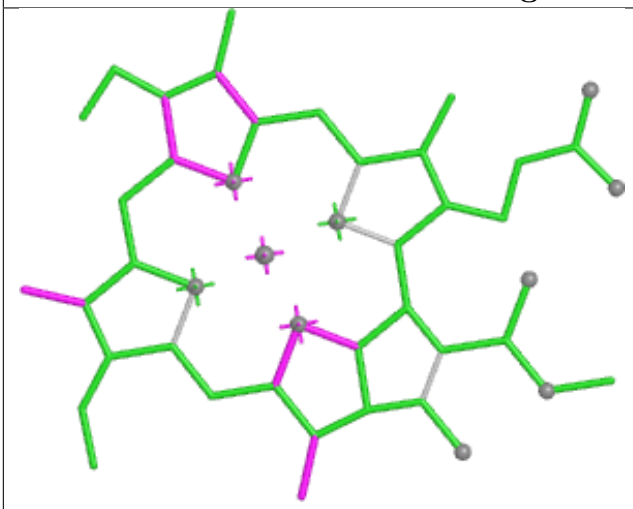


Torsions

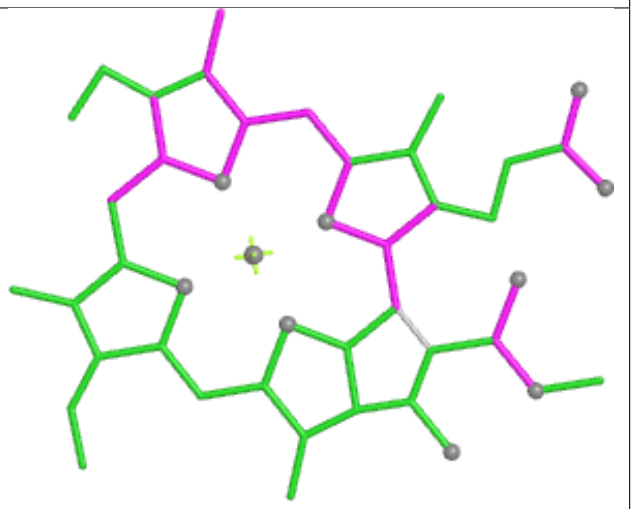


Rings

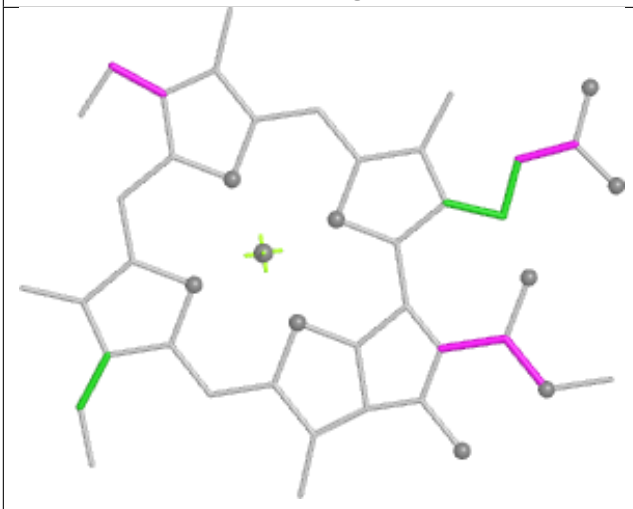
Ligand CLA c2 408



Bond lengths



Bond angles

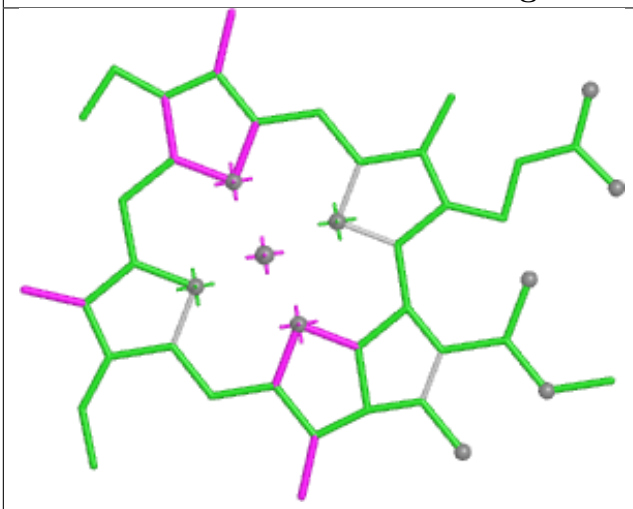


Torsions

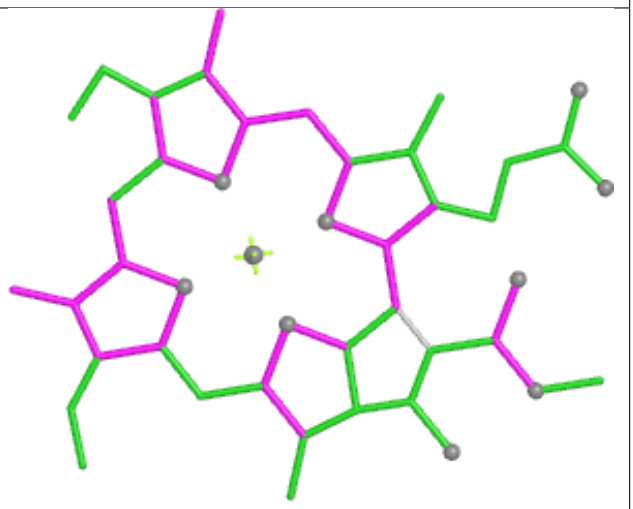


Rings

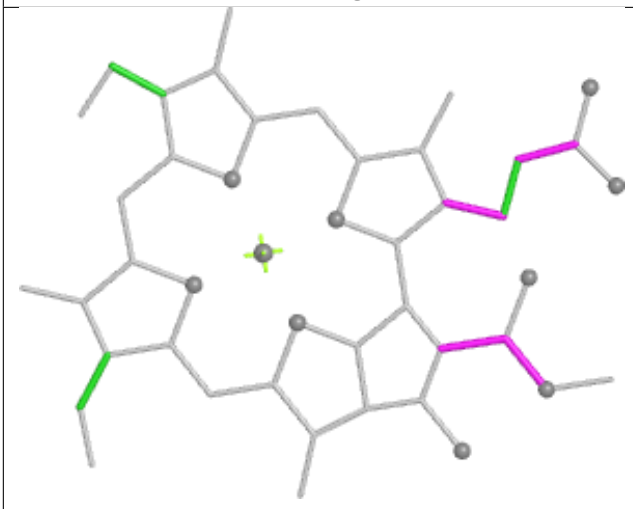
Ligand CLA a4 412



Bond lengths



Bond angles

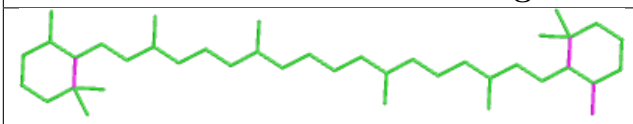


Torsions

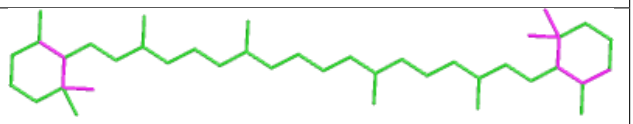


Rings

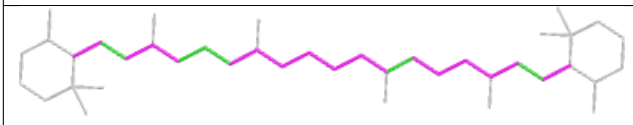
Ligand BCR cA 851



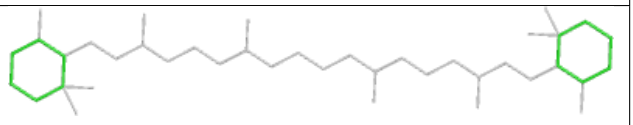
Bond lengths



Bond angles

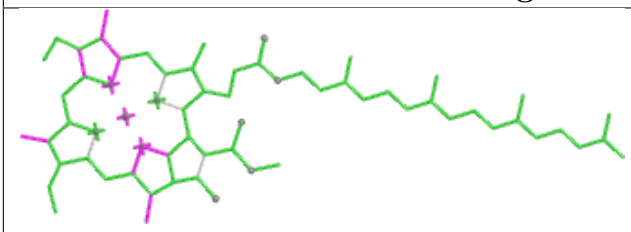


Torsions

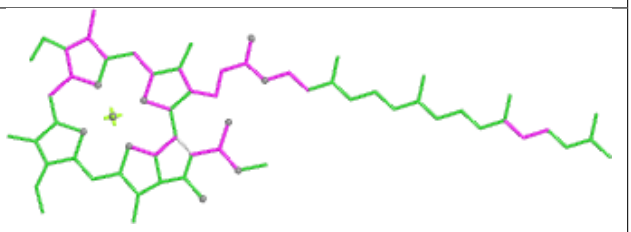


Rings

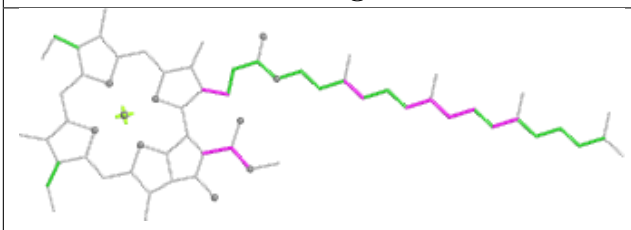
Ligand CLA cB 827



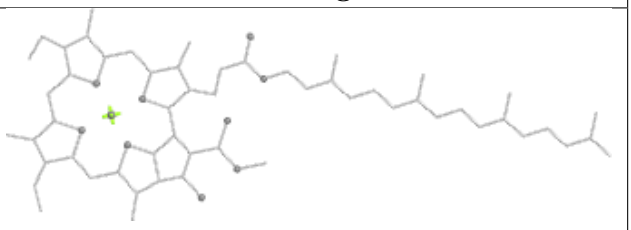
Bond lengths



Bond angles

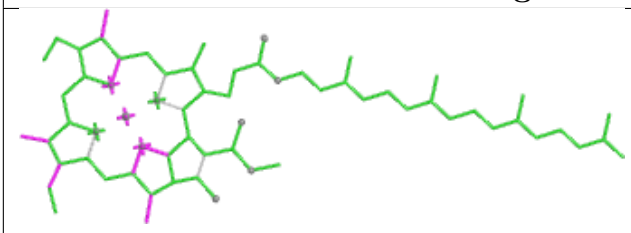


Torsions

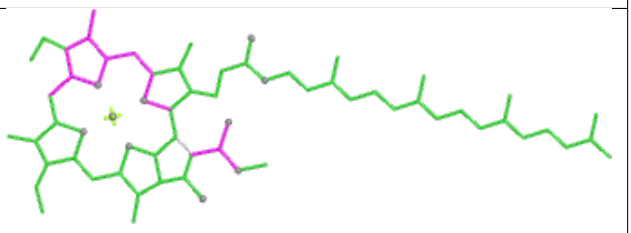


Rings

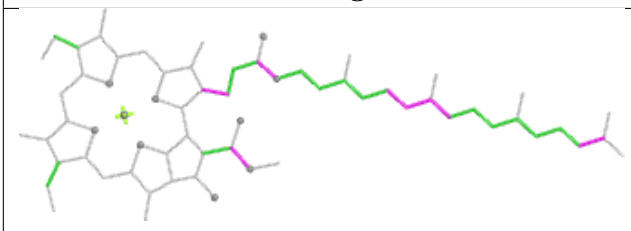
Ligand CLA bA 833



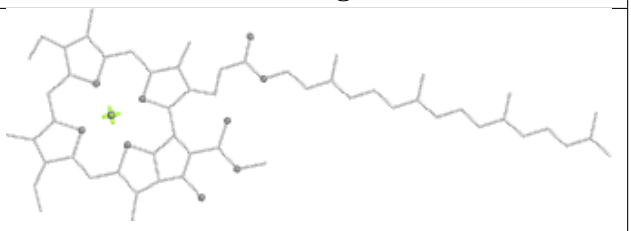
Bond lengths



Bond angles

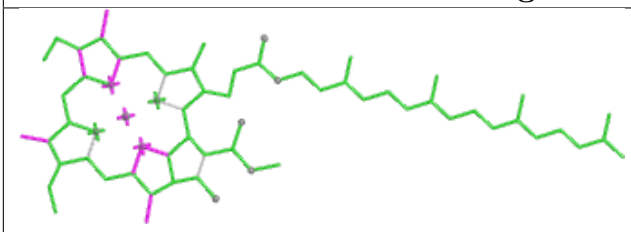


Torsions

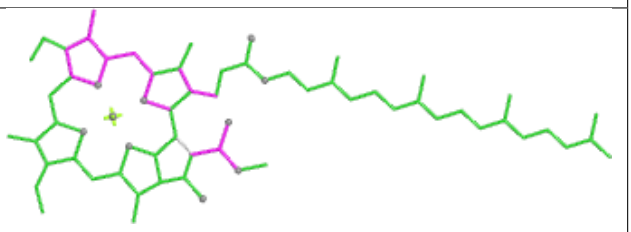


Rings

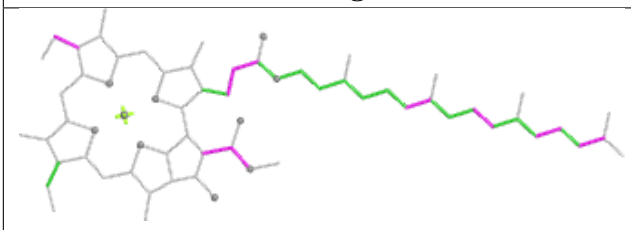
Ligand CLA aL 203



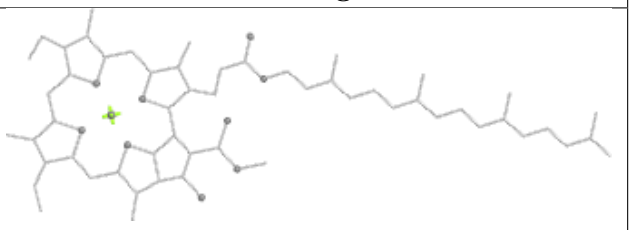
Bond lengths



Bond angles

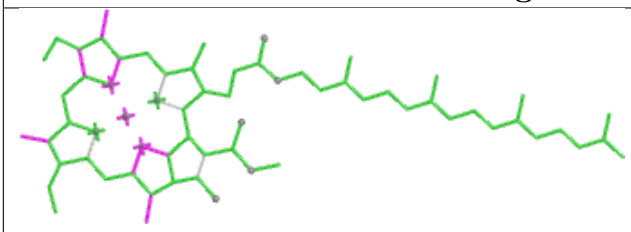


Torsions

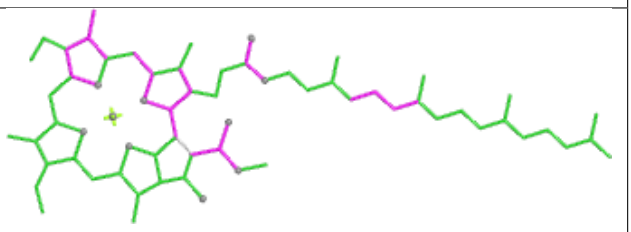


Rings

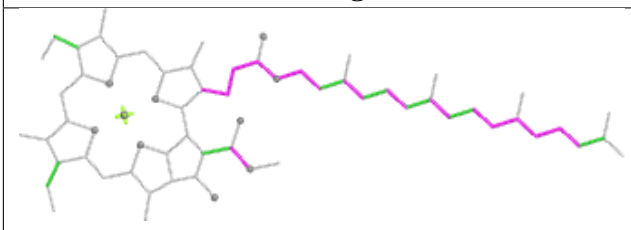
Ligand CLA aA 829



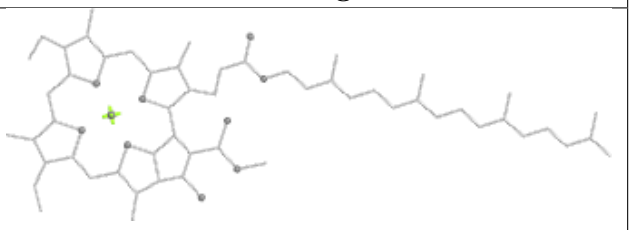
Bond lengths



Bond angles

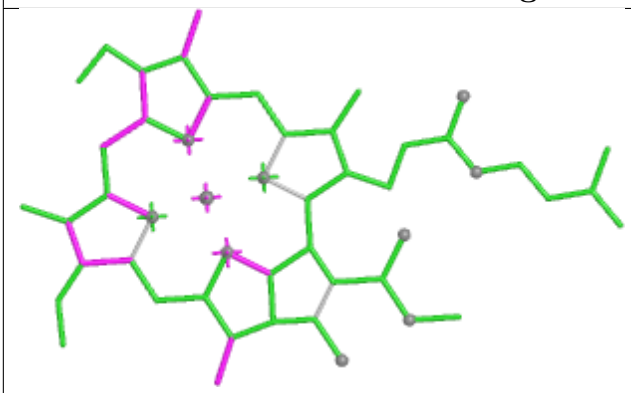


Torsions

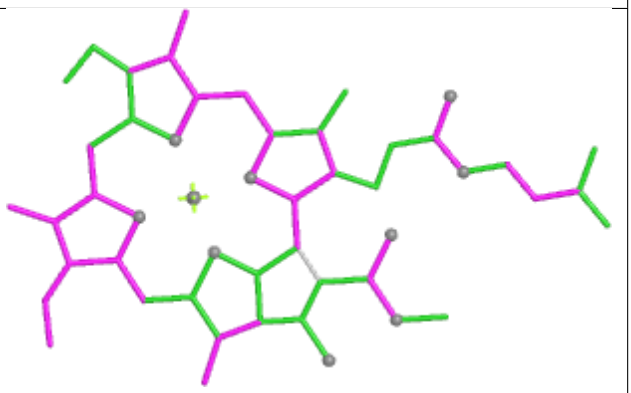


Rings

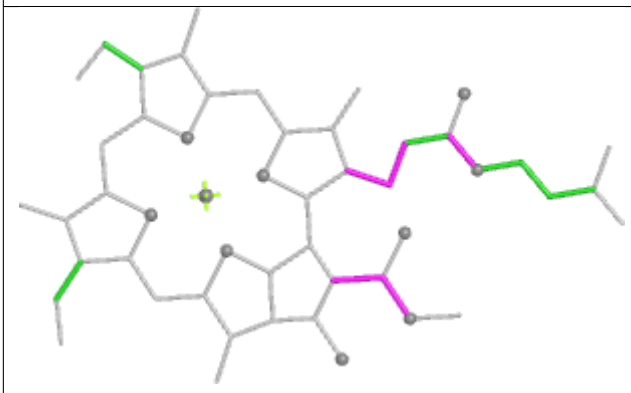
Ligand CLA a2 417



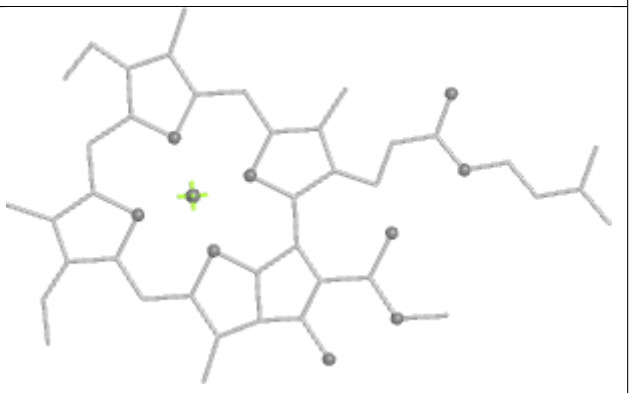
Bond lengths



Bond angles

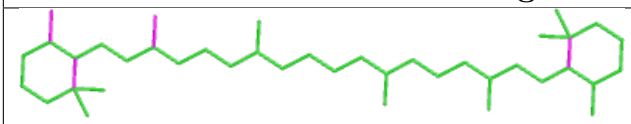


Torsions

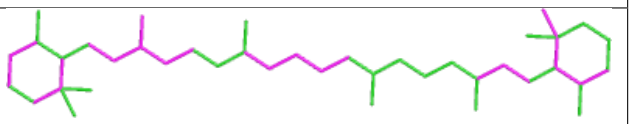


Rings

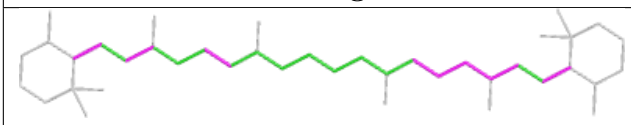
Ligand BCR a1 418



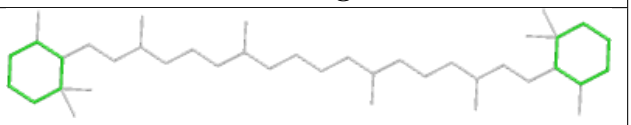
Bond lengths



Bond angles

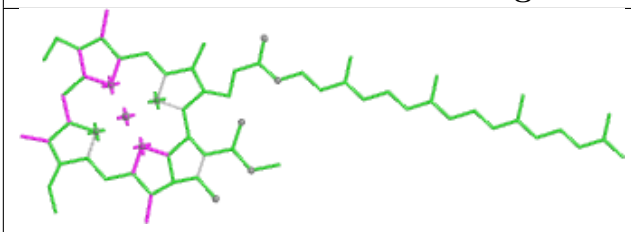


Torsions

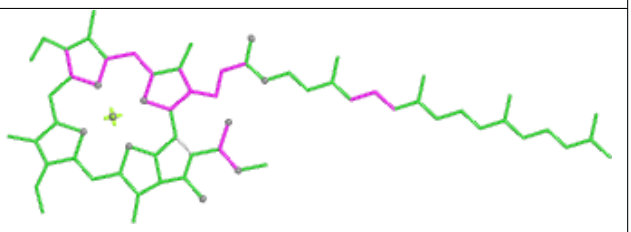


Rings

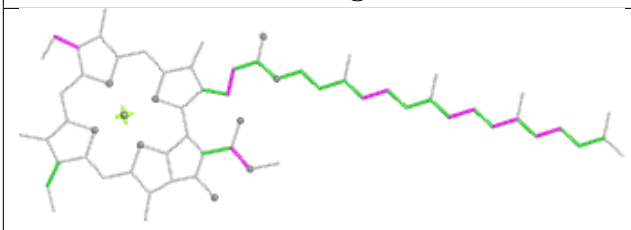
Ligand CLA bB 839



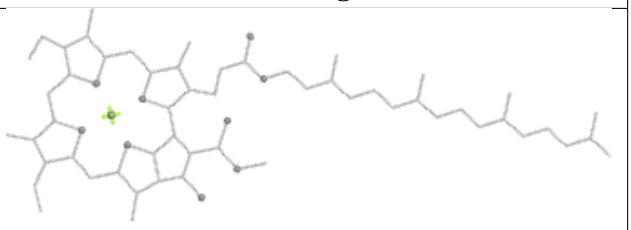
Bond lengths



Bond angles

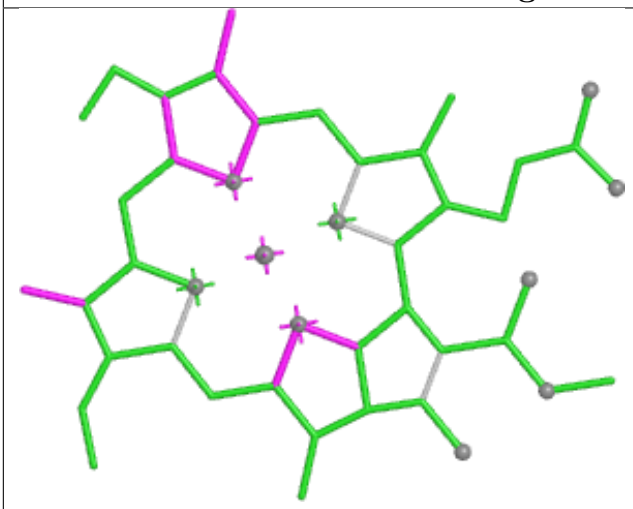


Torsions

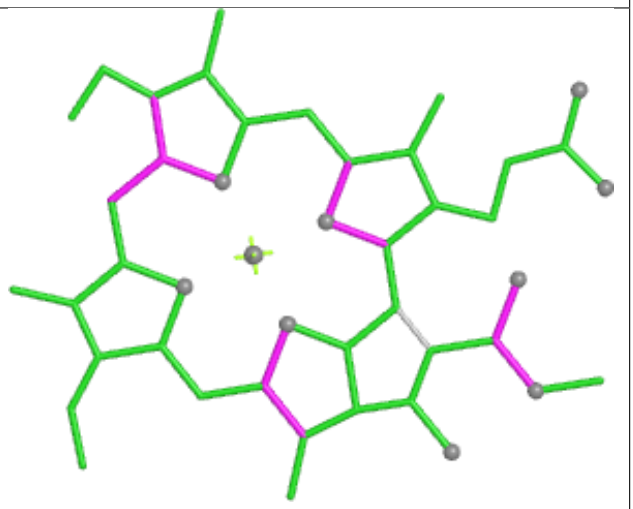


Rings

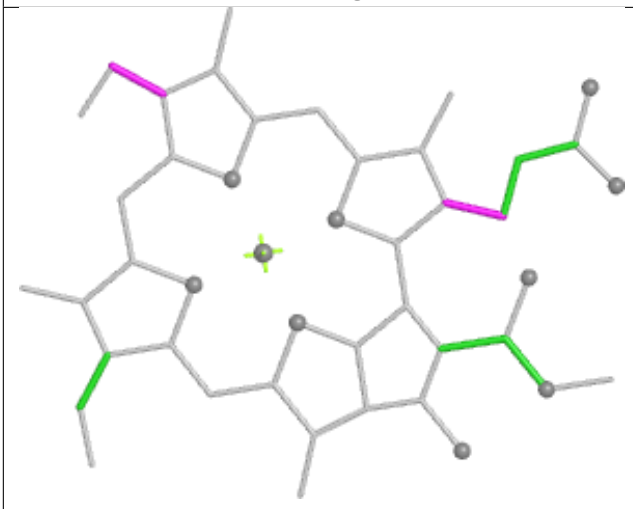
Ligand CLA b5 413



Bond lengths



Bond angles

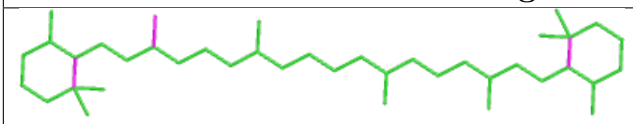


Torsions

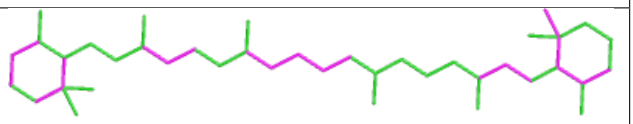


Rings

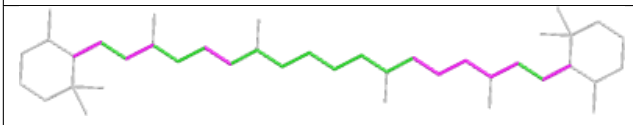
Ligand BCR c2 420



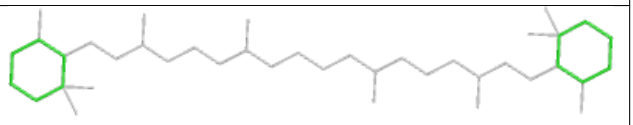
Bond lengths



Bond angles

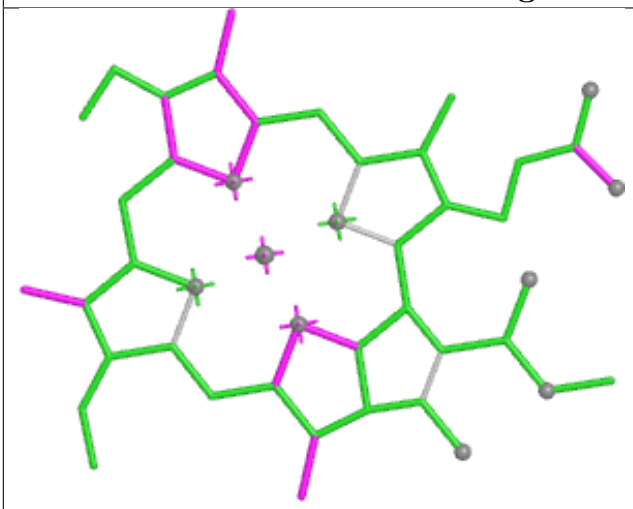


Torsions

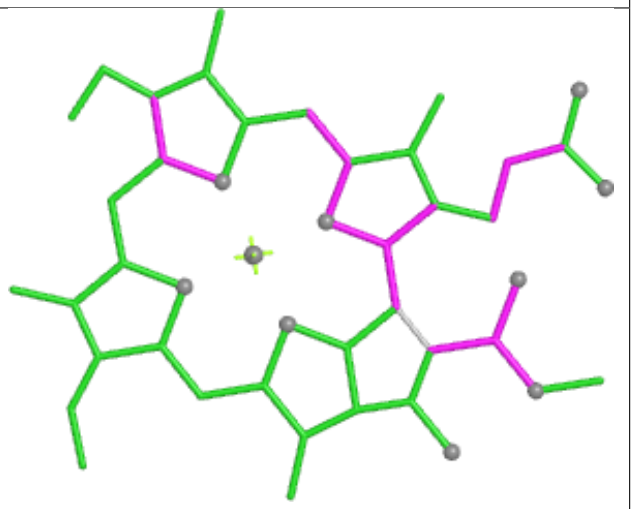


Rings

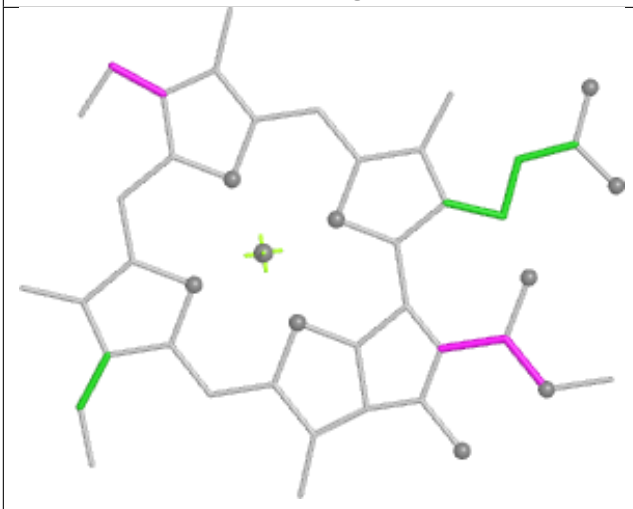
Ligand CLA bJ 101



Bond lengths



Bond angles

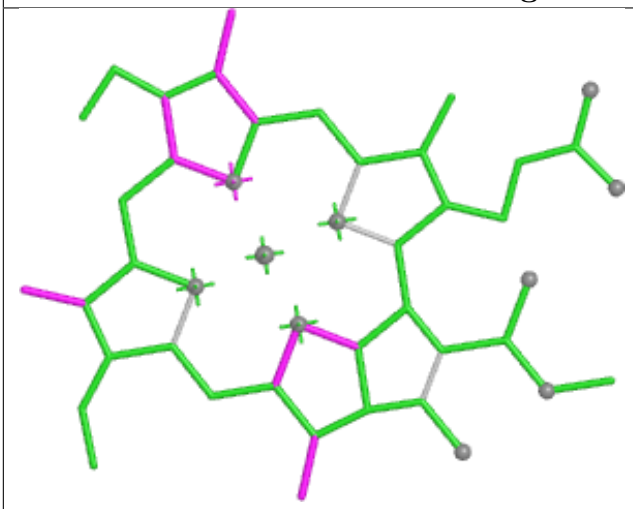


Torsions

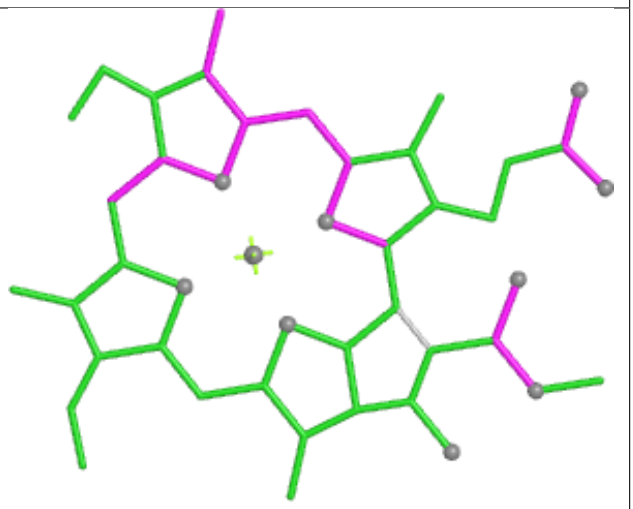


Rings

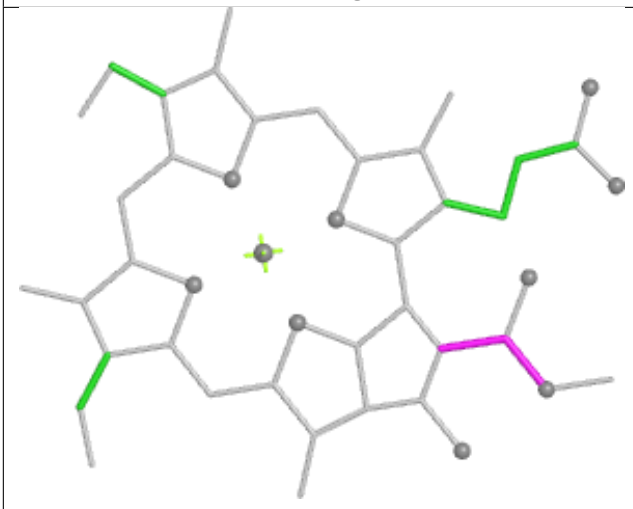
Ligand CLA c4 406



Bond lengths



Bond angles

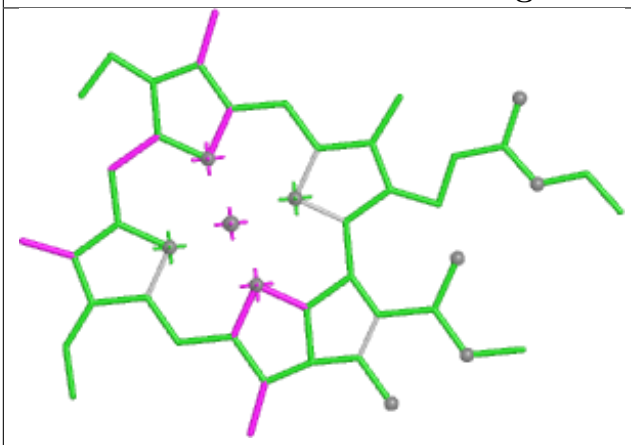


Torsions

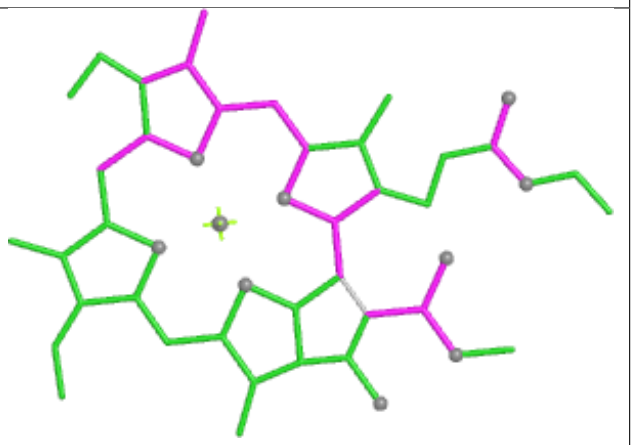


Rings

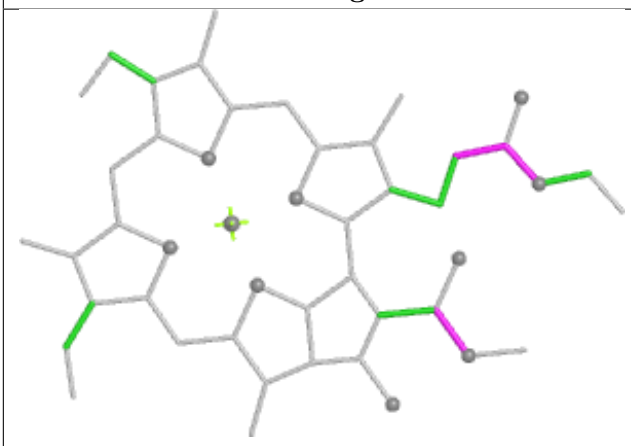
Ligand CLA cA 840



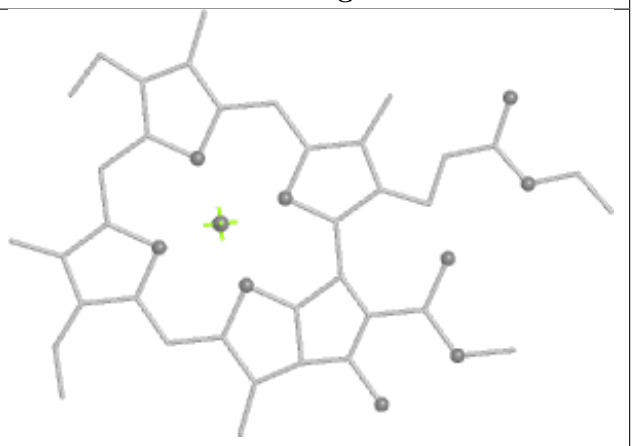
Bond lengths



Bond angles

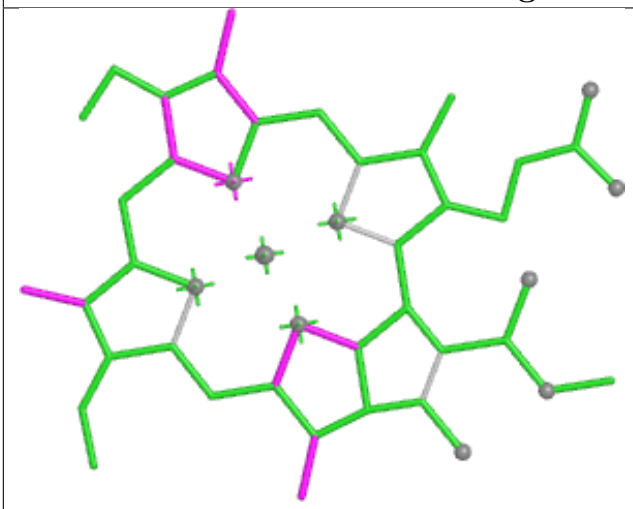


Torsions

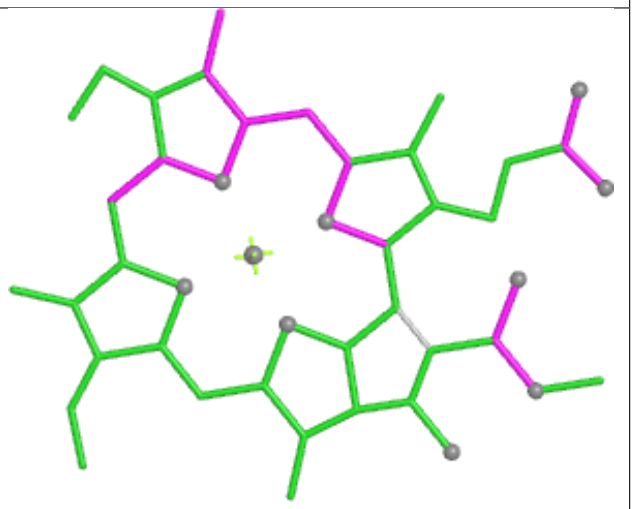


Rings

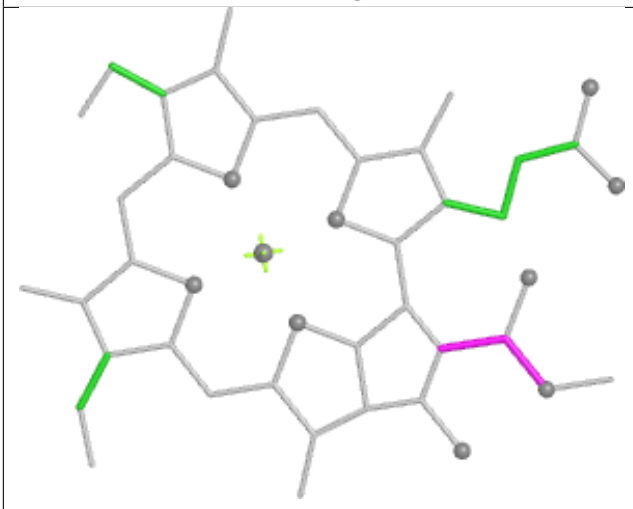
Ligand CLA b6 407



Bond lengths



Bond angles

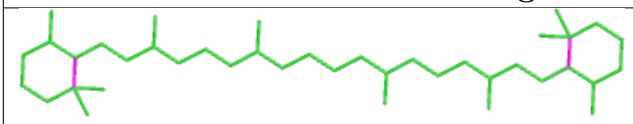


Torsions

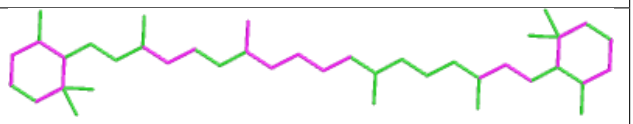


Rings

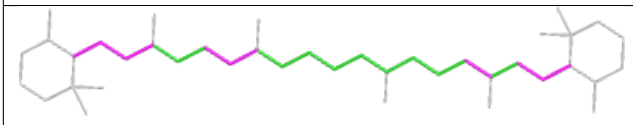
Ligand BCR a4 420



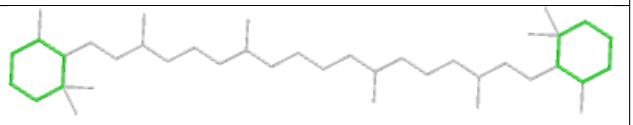
Bond lengths



Bond angles

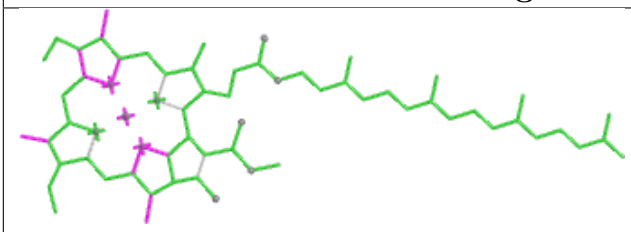


Torsions

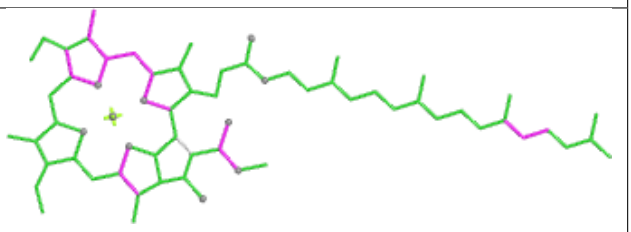


Rings

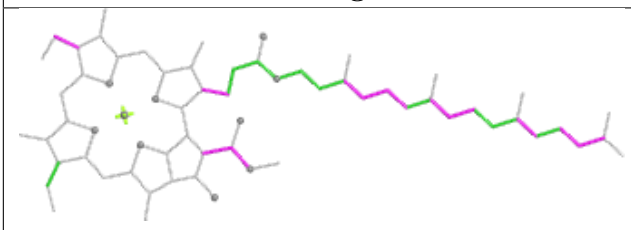
Ligand CLA cA 822



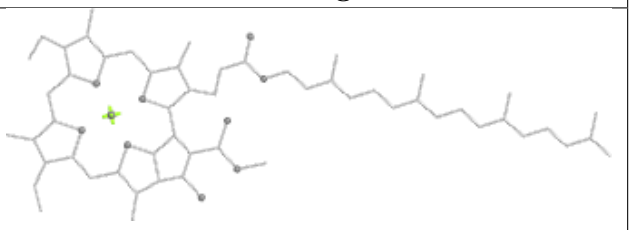
Bond lengths



Bond angles



Torsions

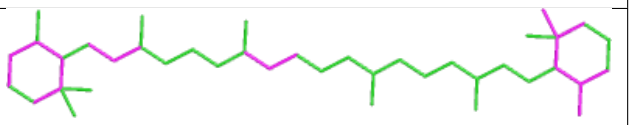


Rings

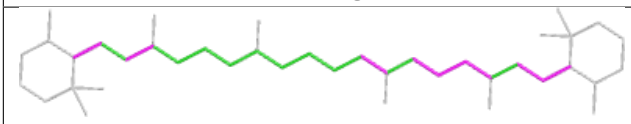
Ligand BCR b5 418



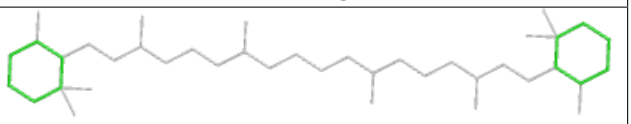
Bond lengths



Bond angles

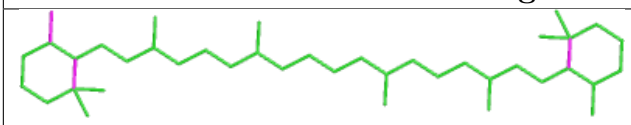


Torsions

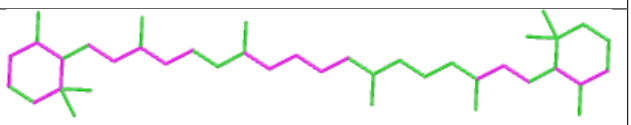


Rings

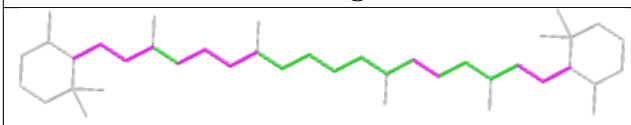
Ligand BCR c4 401



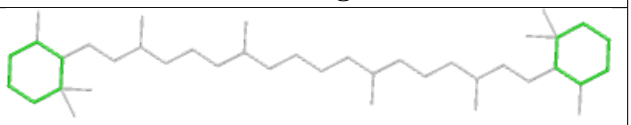
Bond lengths



Bond angles

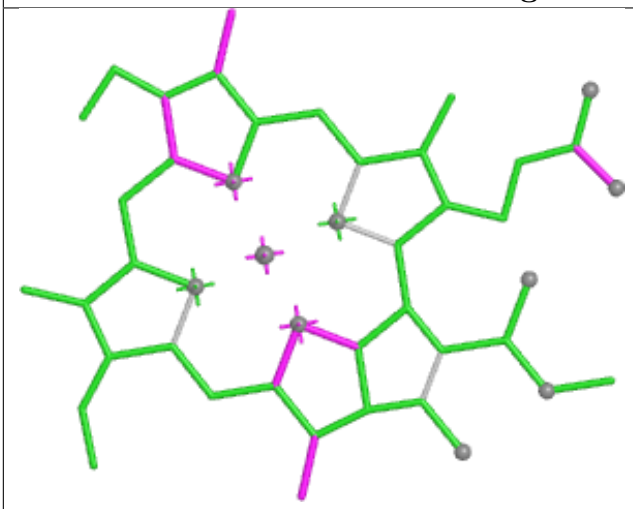


Torsions

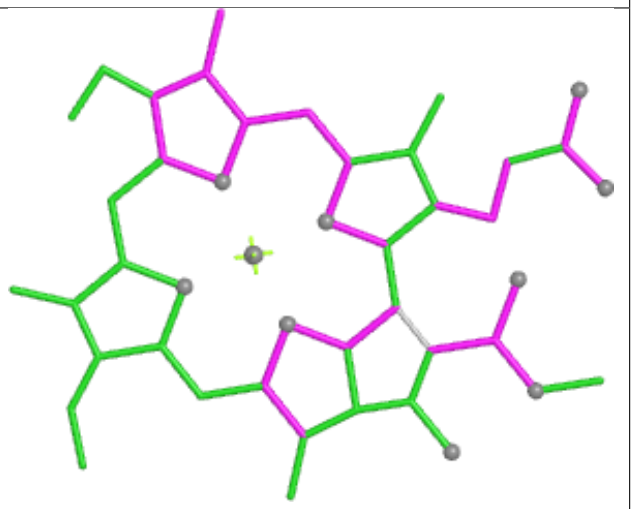


Rings

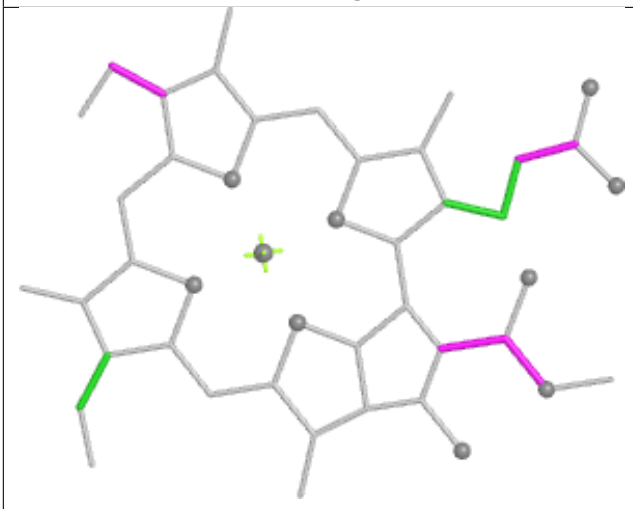
Ligand CLA c5 415



Bond lengths



Bond angles

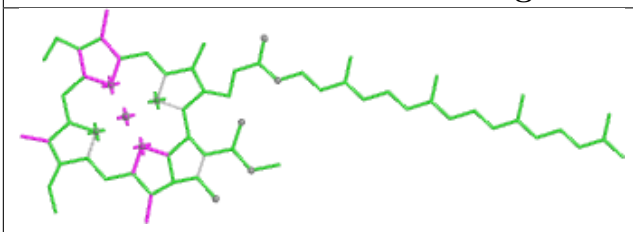


Torsions

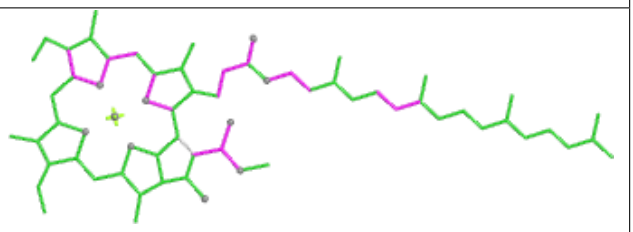


Rings

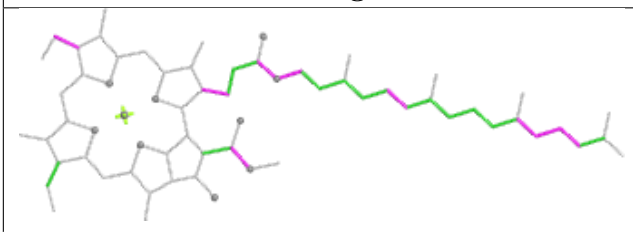
Ligand CLA aA 812



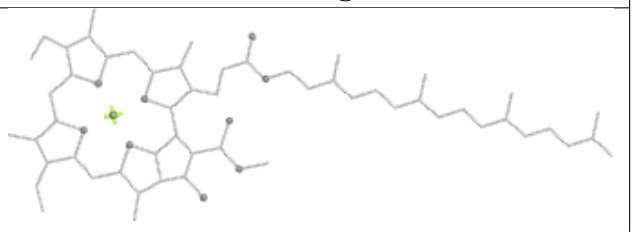
Bond lengths



Bond angles

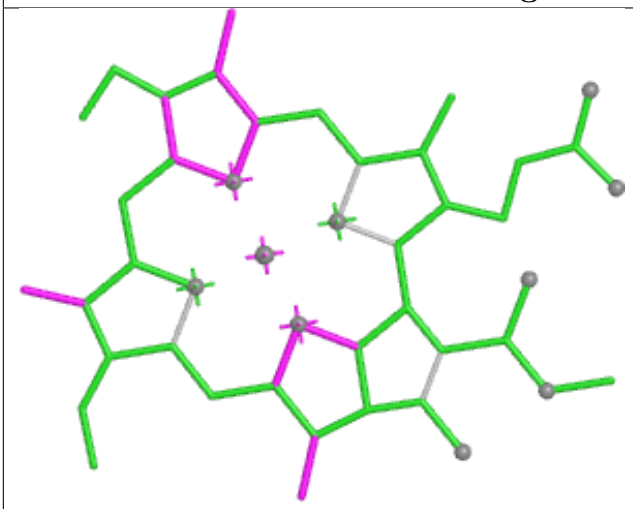


Torsions

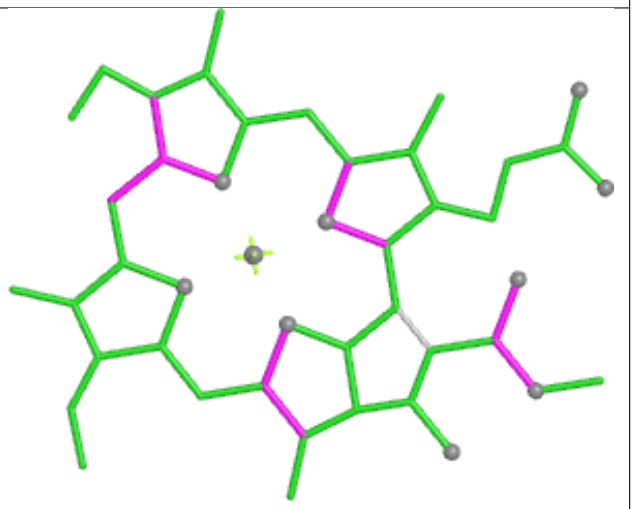


Rings

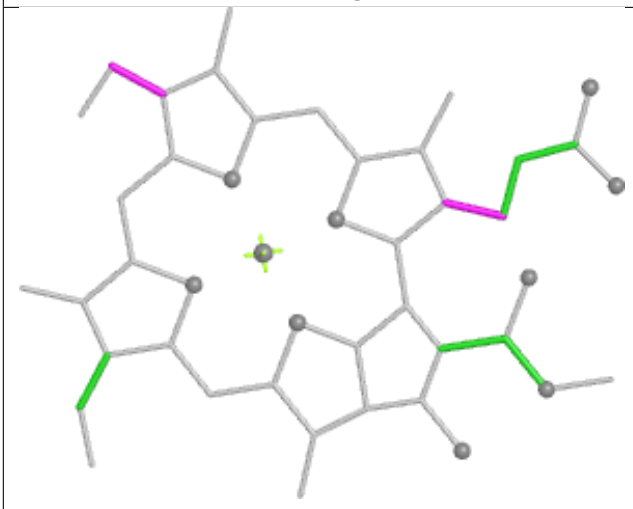
Ligand CLA c5 413



Bond lengths



Bond angles

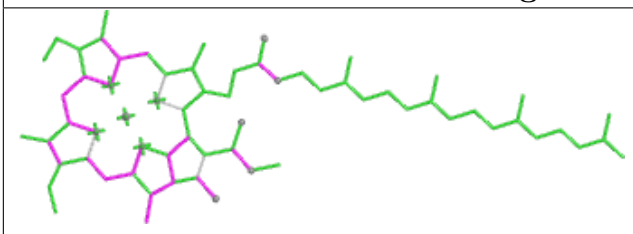


Torsions

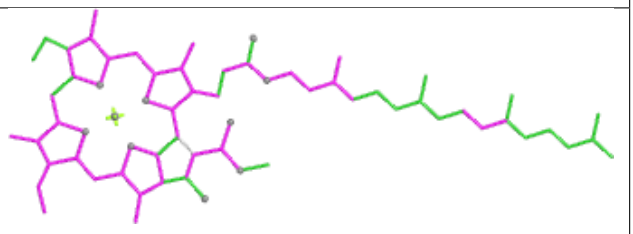


Rings

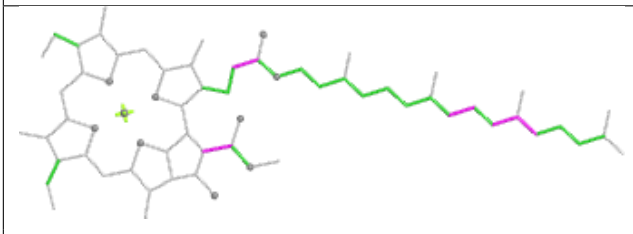
Ligand CL0 aA 801



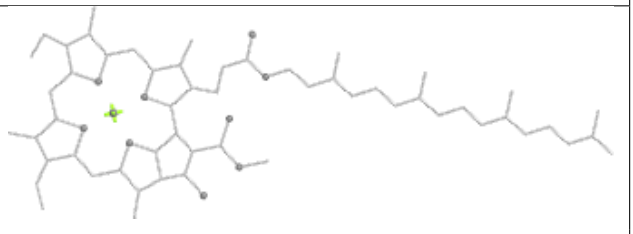
Bond lengths



Bond angles

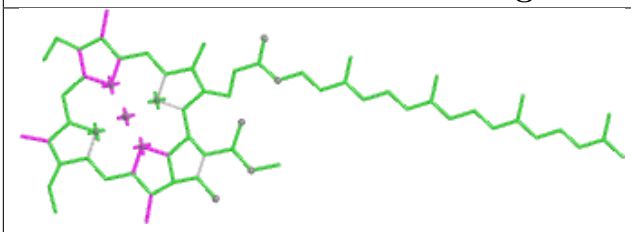


Torsions

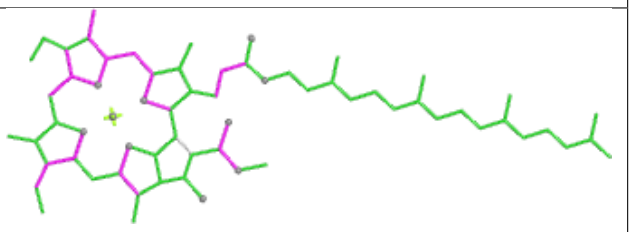


Rings

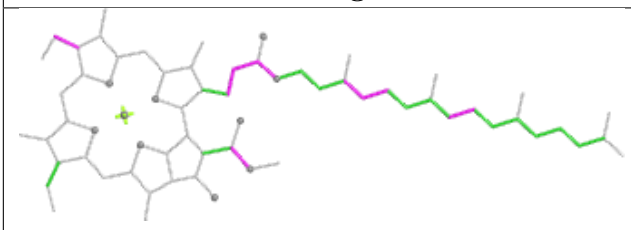
Ligand CLA aB 801



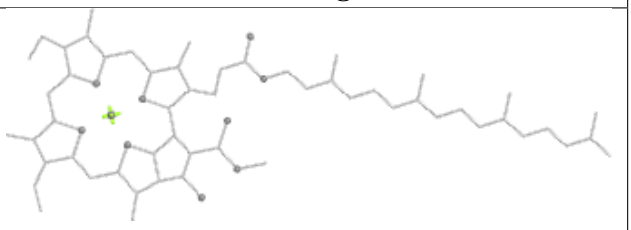
Bond lengths



Bond angles

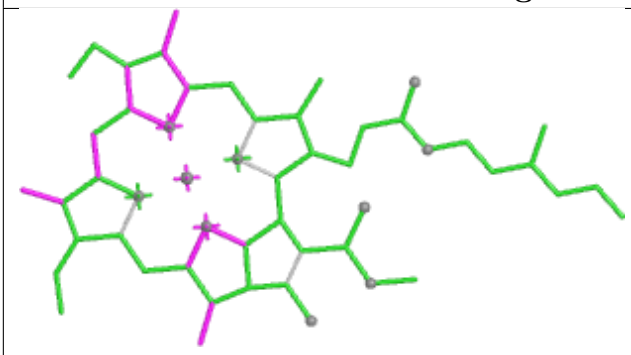


Torsions

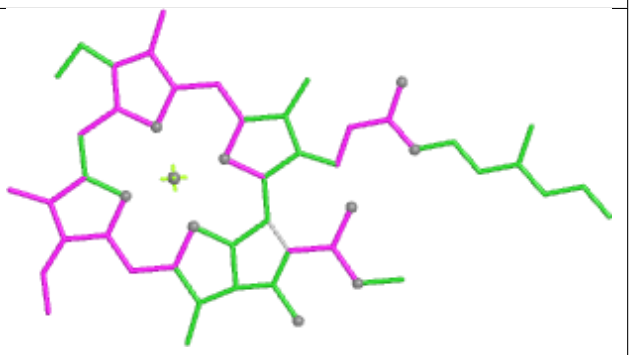


Rings

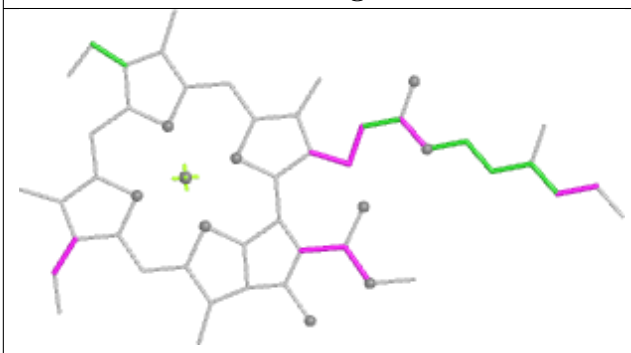
Ligand CLA aA 845



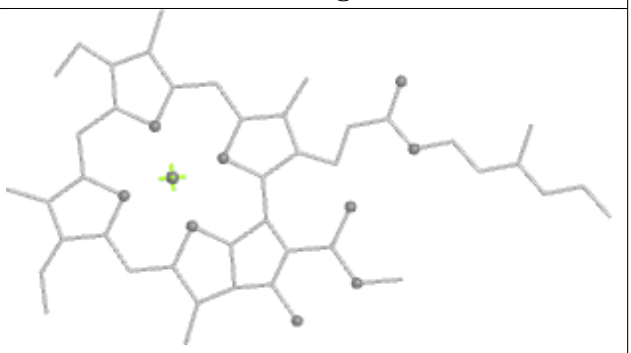
Bond lengths



Bond angles



Torsions

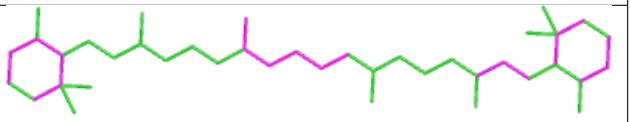


Rings

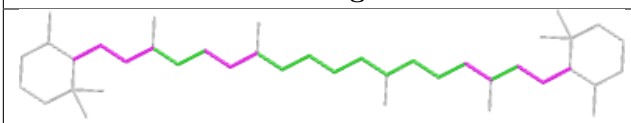
Ligand BCR b3 420



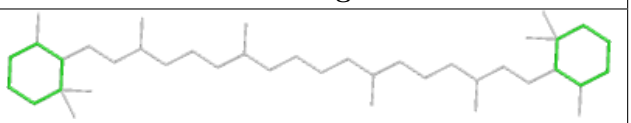
Bond lengths



Bond angles

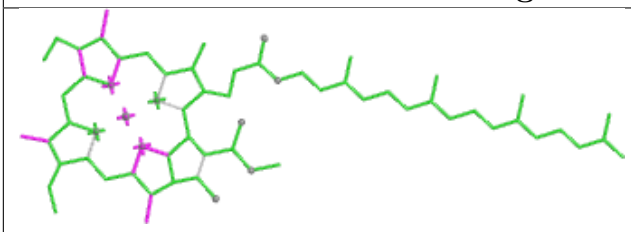


Torsions

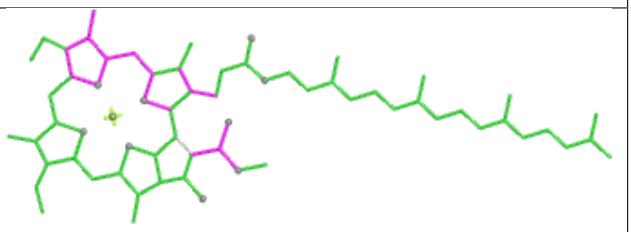


Rings

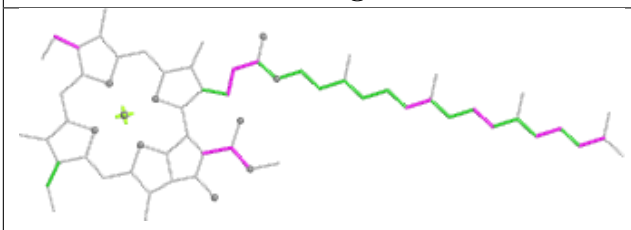
Ligand CLA bL 204



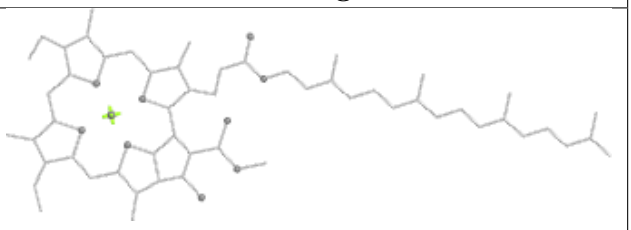
Bond lengths



Bond angles

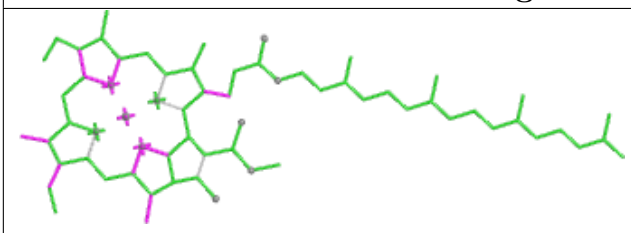


Torsions

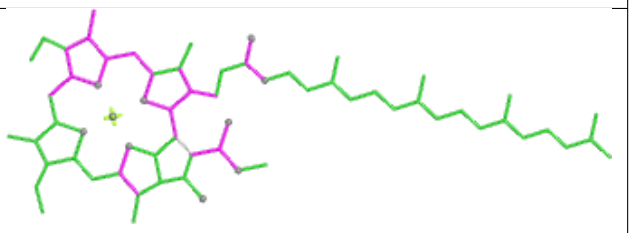


Rings

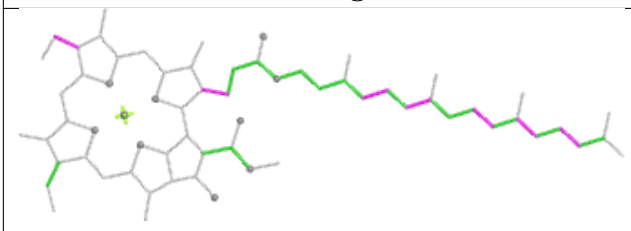
Ligand CLA cA 807



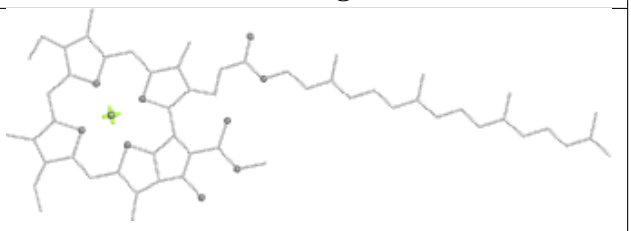
Bond lengths



Bond angles

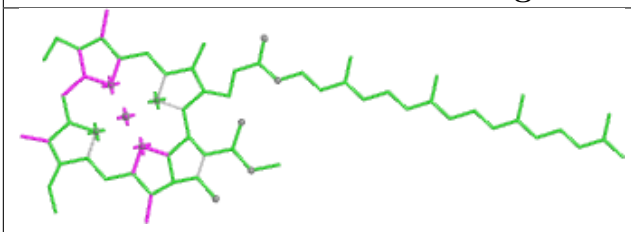


Torsions

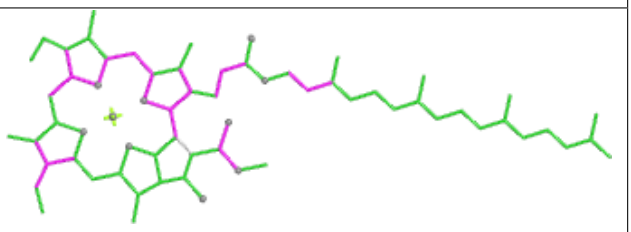


Rings

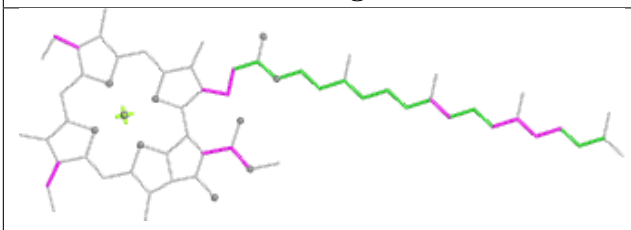
Ligand CLA bB 840



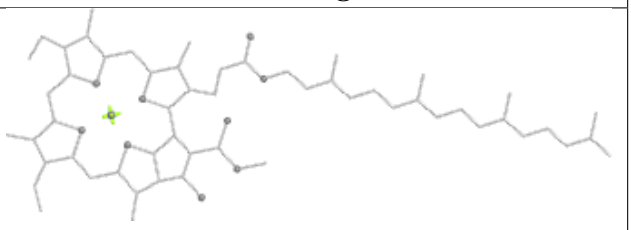
Bond lengths



Bond angles

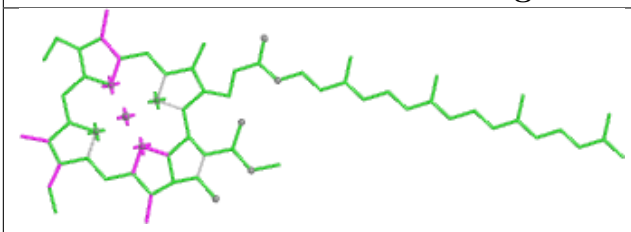


Torsions

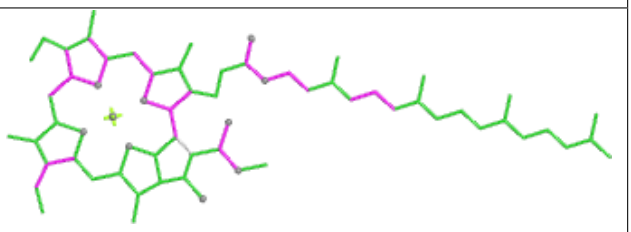


Rings

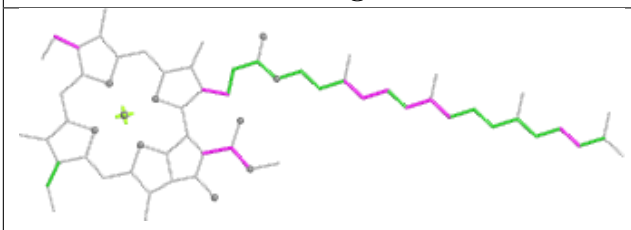
Ligand CLA bB 811



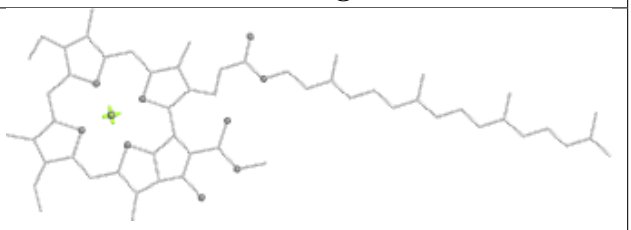
Bond lengths



Bond angles

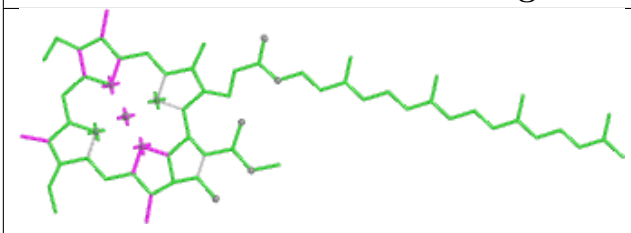


Torsions

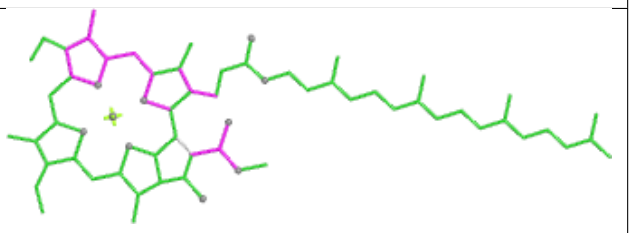


Rings

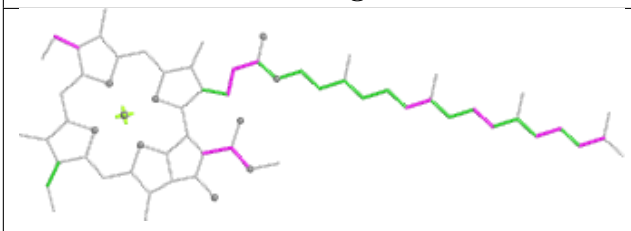
Ligand CLA cL 204



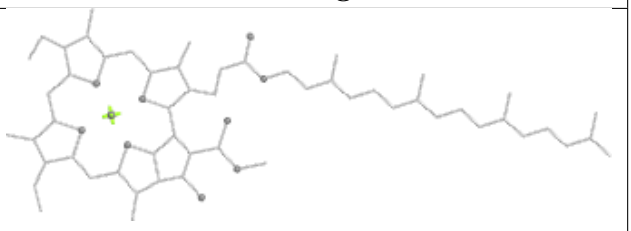
Bond lengths



Bond angles

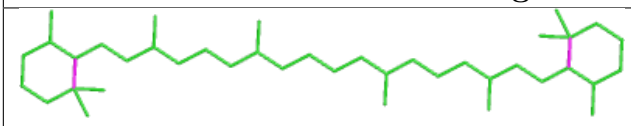


Torsions

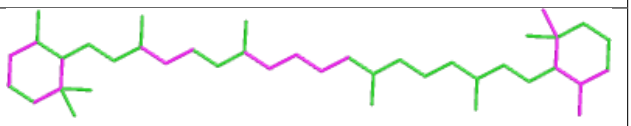


Rings

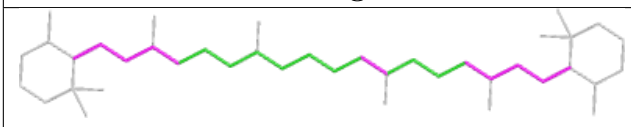
Ligand BCR bA 850



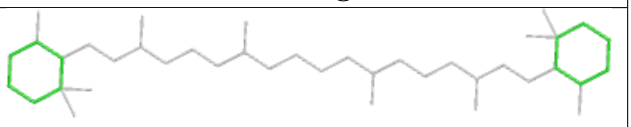
Bond lengths



Bond angles

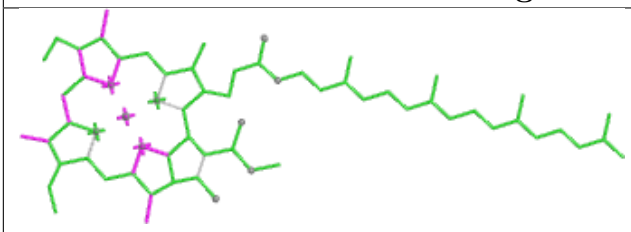


Torsions

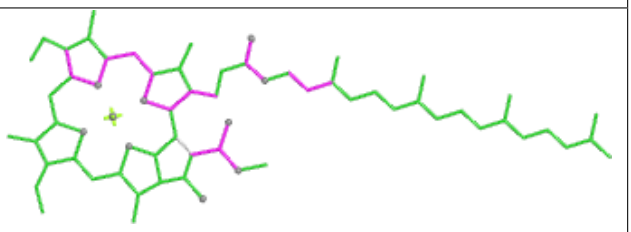


Rings

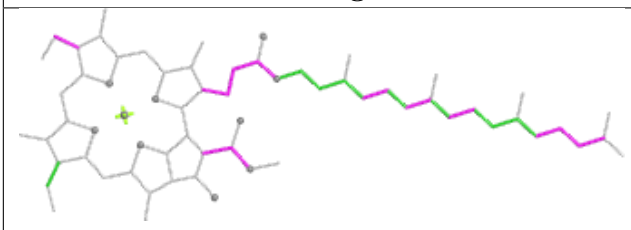
Ligand CLA cA 809



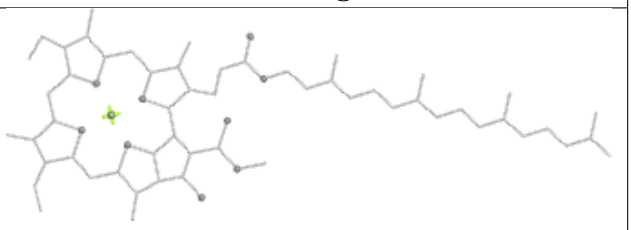
Bond lengths



Bond angles

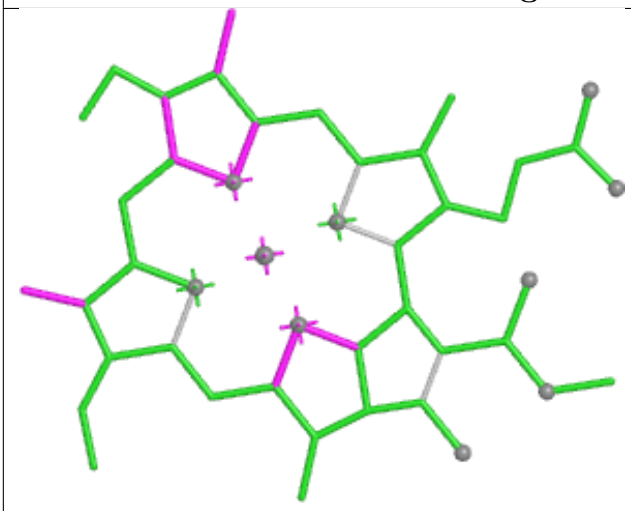


Torsions

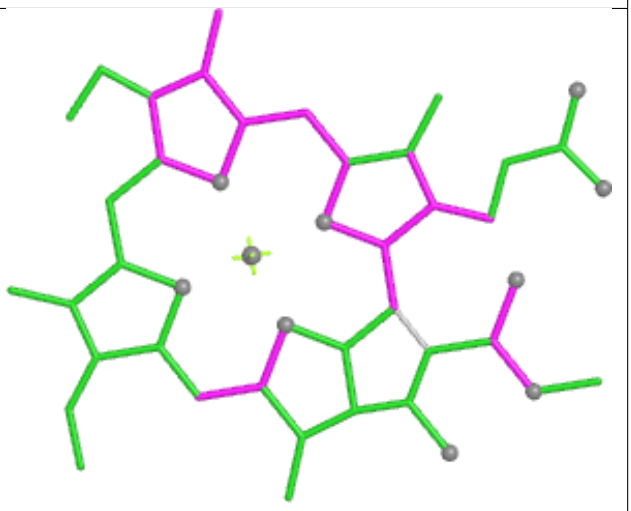


Rings

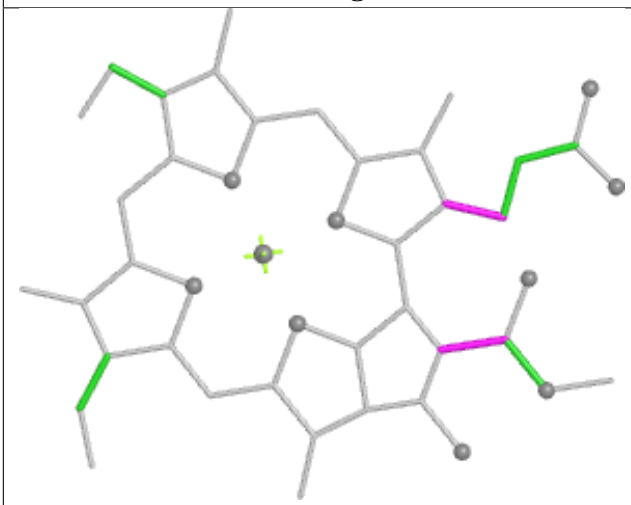
Ligand CLA c5 411



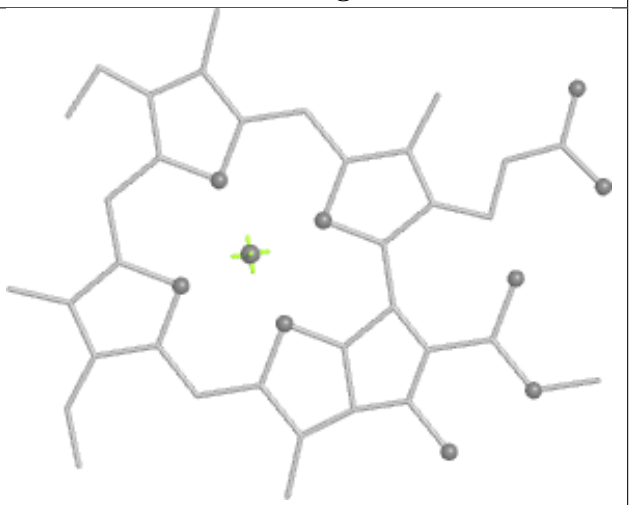
Bond lengths



Bond angles

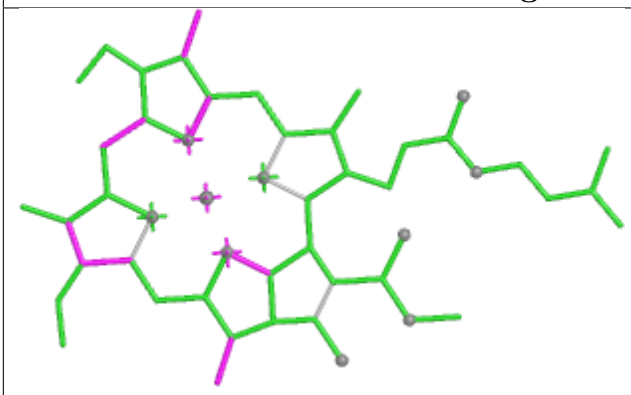


Torsions

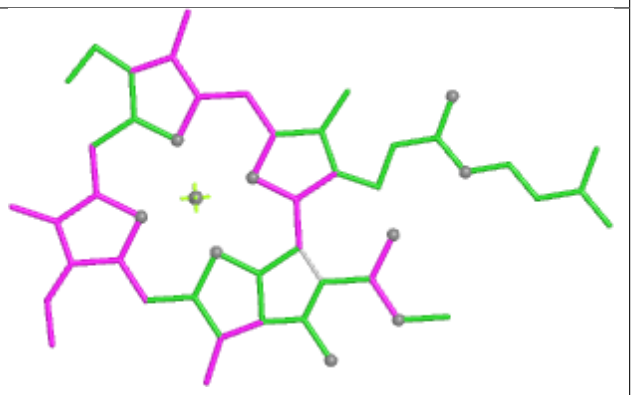


Rings

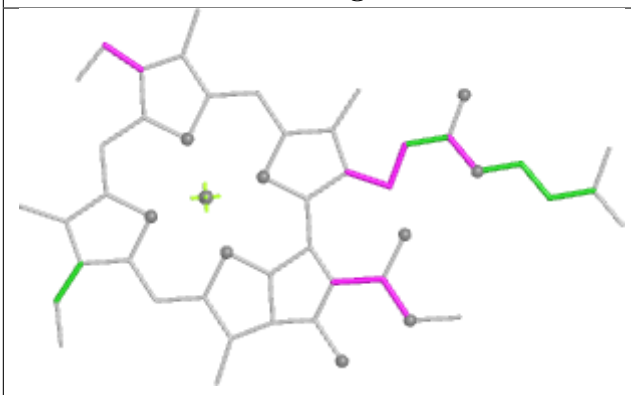
Ligand CLA c4 416



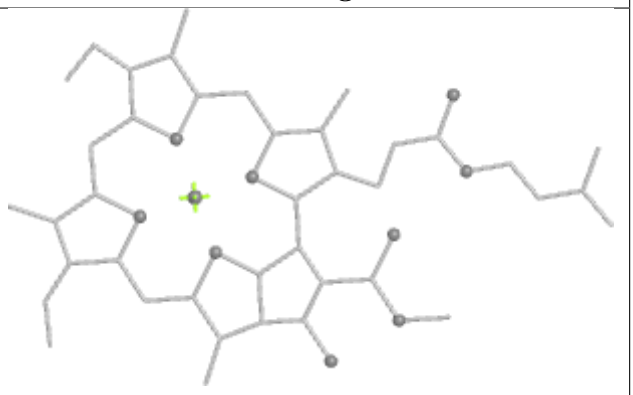
Bond lengths



Bond angles



Torsions

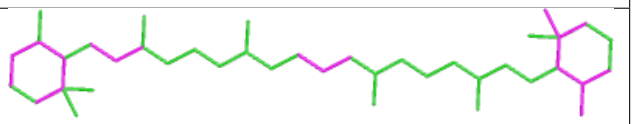


Rings

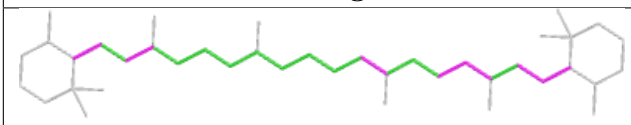
Ligand BCR a6 419



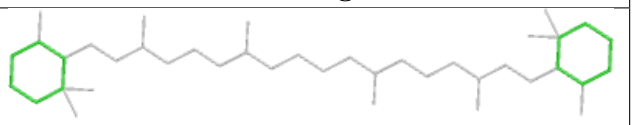
Bond lengths



Bond angles

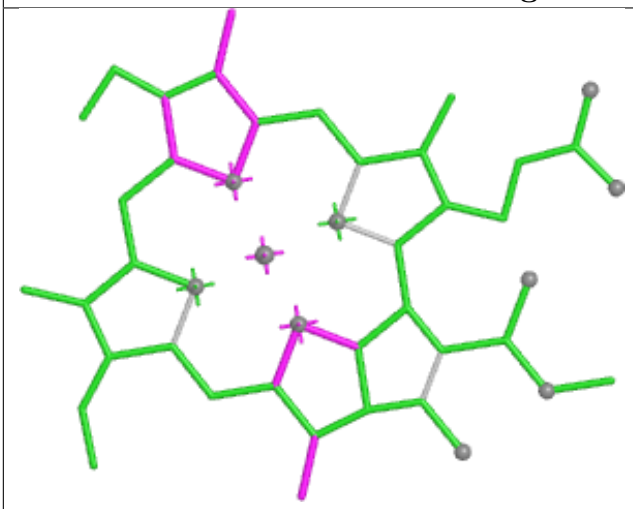


Torsions

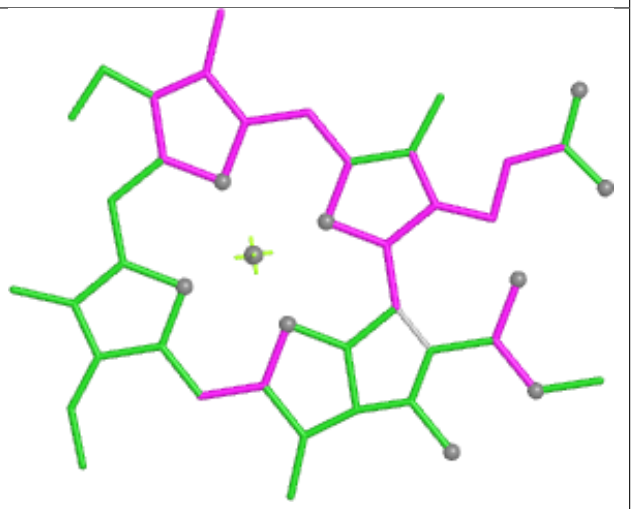


Rings

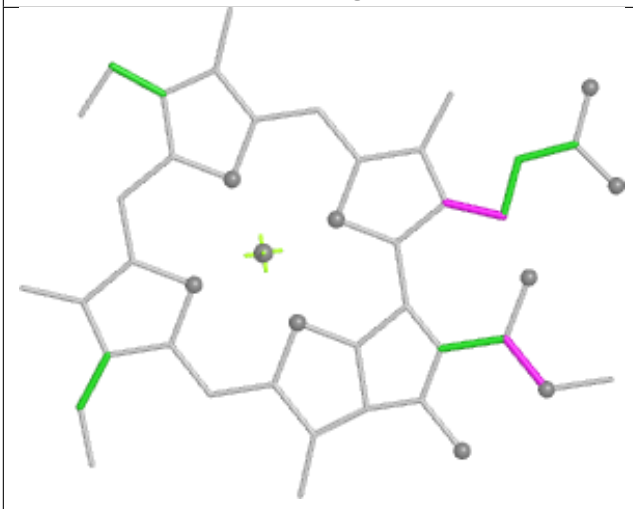
Ligand CLA c6 413



Bond lengths



Bond angles

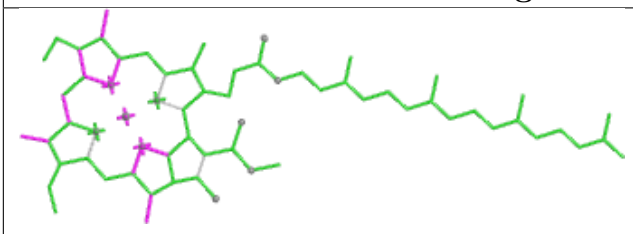


Torsions

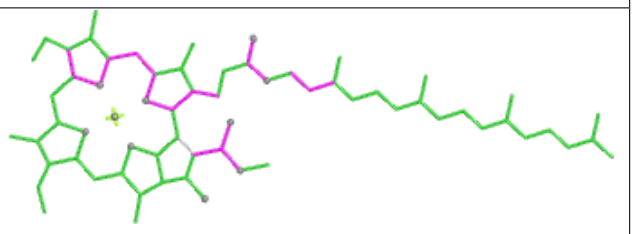


Rings

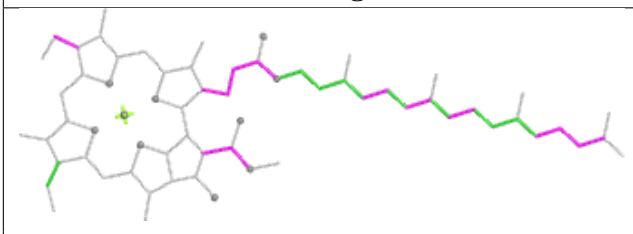
Ligand CLA aA 809



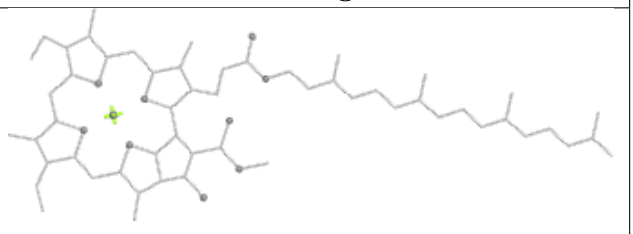
Bond lengths



Bond angles

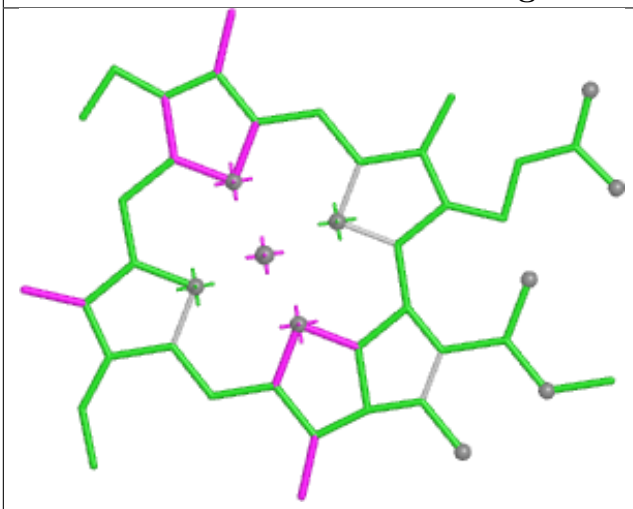


Torsions

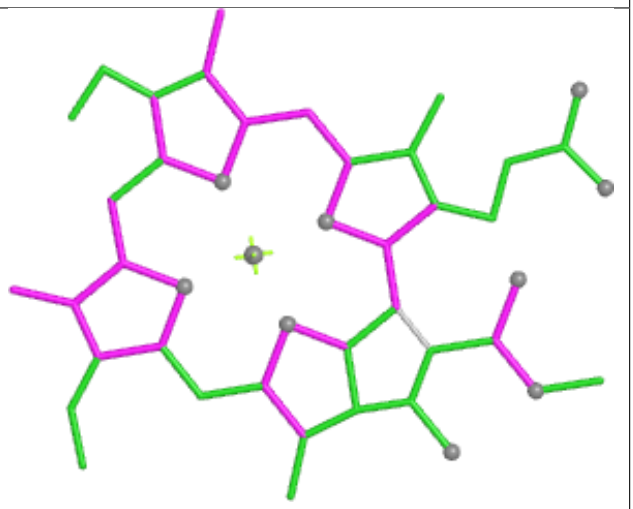


Rings

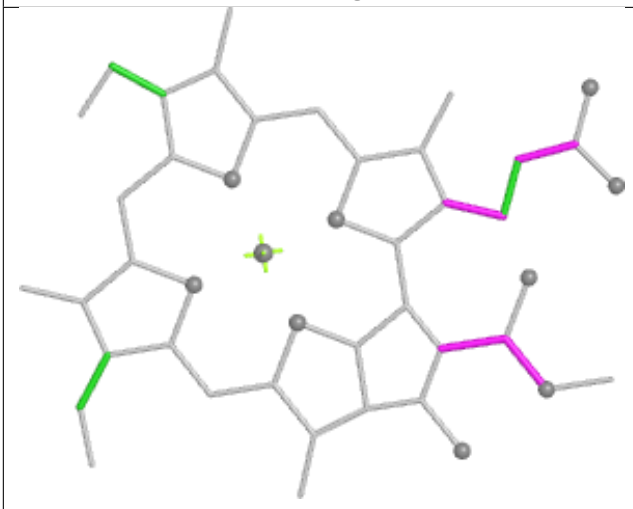
Ligand CLA b4 412



Bond lengths



Bond angles

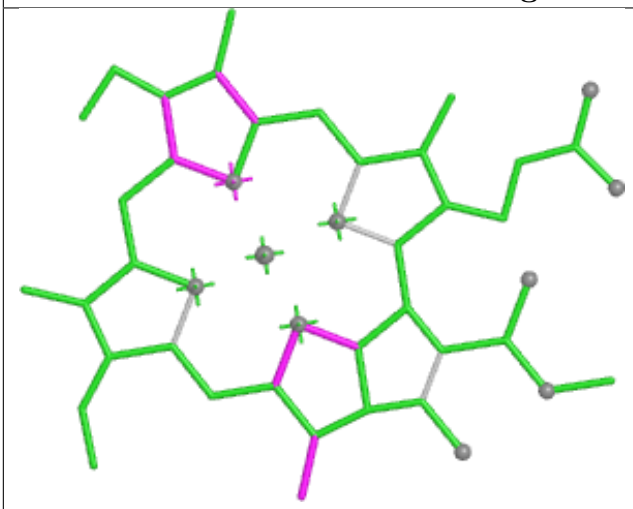


Torsions

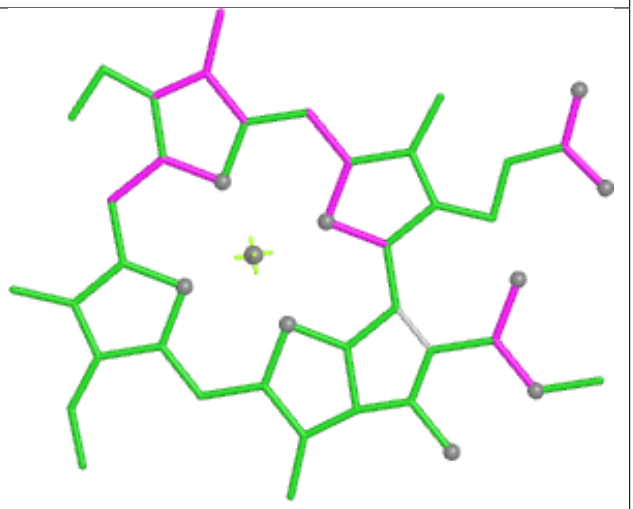


Rings

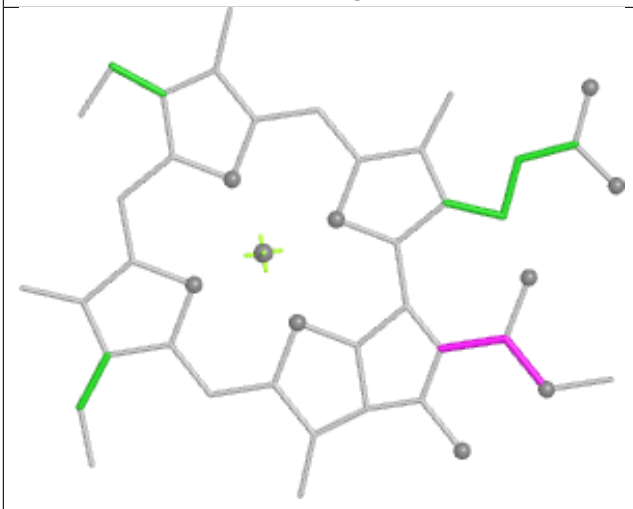
Ligand CLA c2 407



Bond lengths



Bond angles

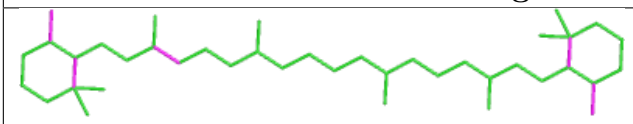


Torsions

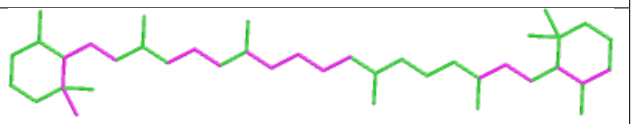


Rings

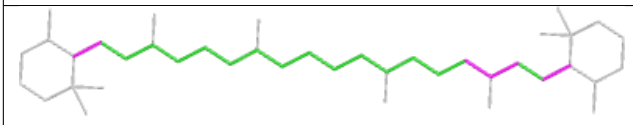
Ligand BCR bA 852



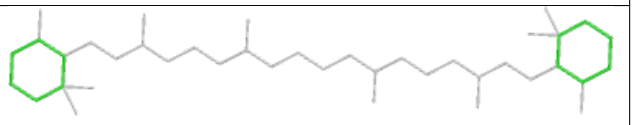
Bond lengths



Bond angles

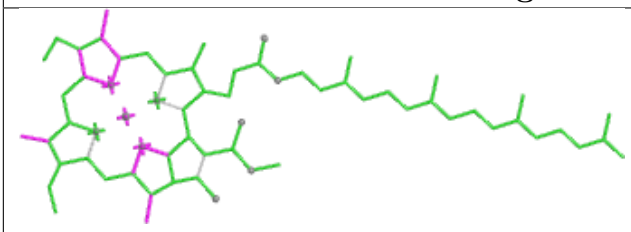


Torsions

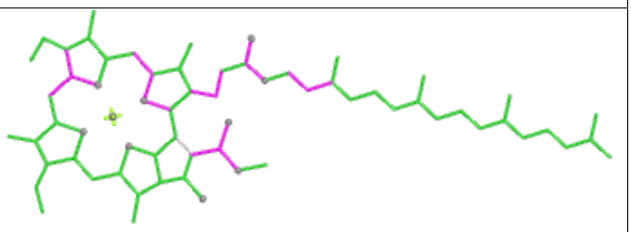


Rings

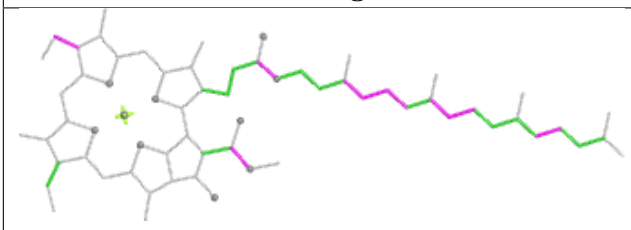
Ligand CLA cB 809



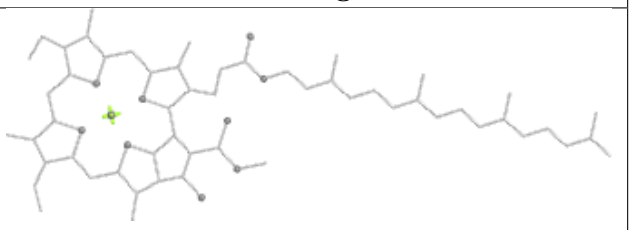
Bond lengths



Bond angles

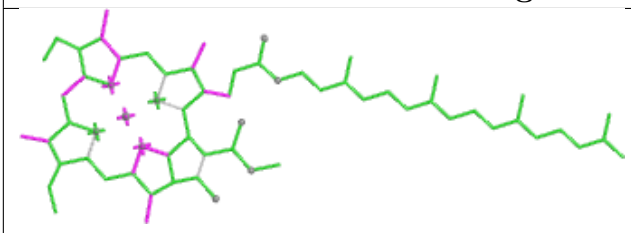


Torsions

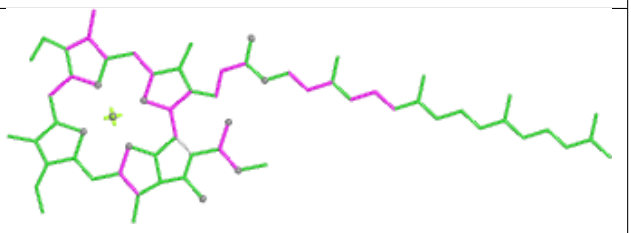


Rings

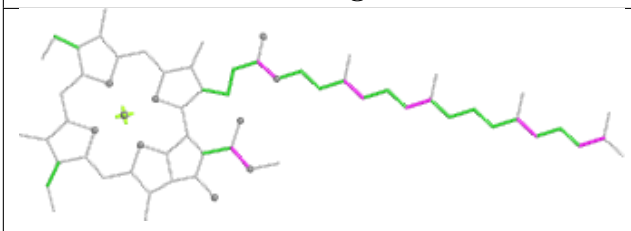
Ligand CLA cA 834



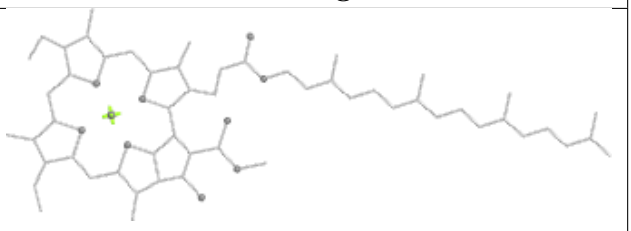
Bond lengths



Bond angles

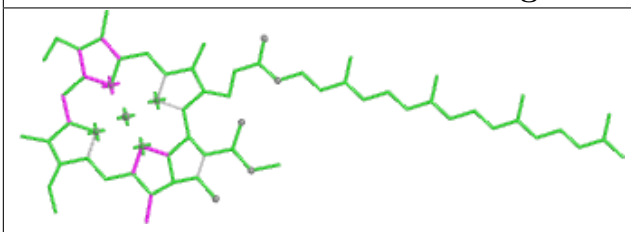


Torsions

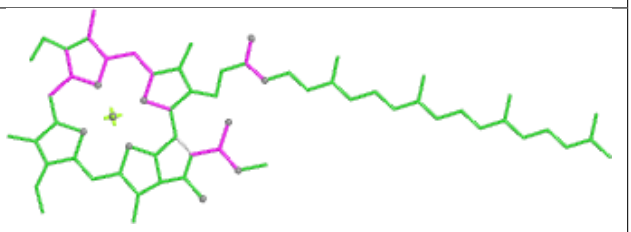


Rings

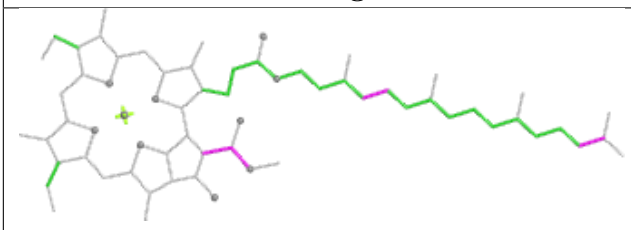
Ligand CLA c6 411



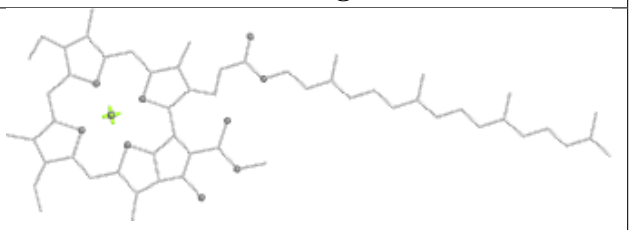
Bond lengths



Bond angles

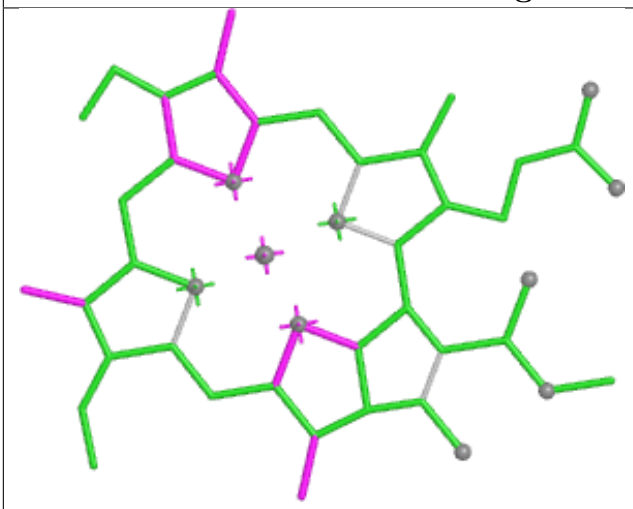


Torsions

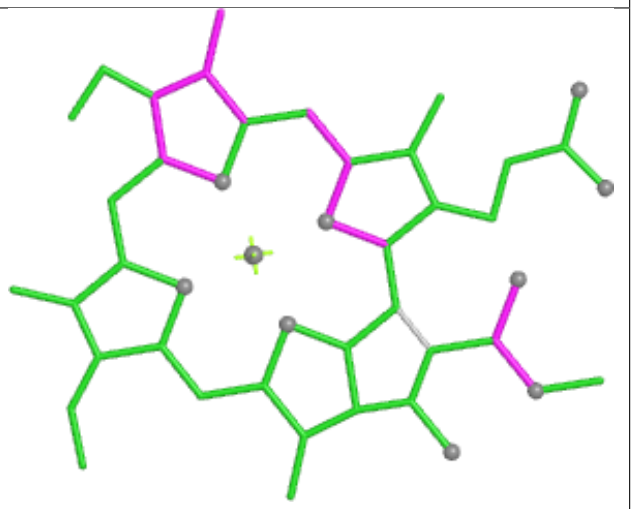


Rings

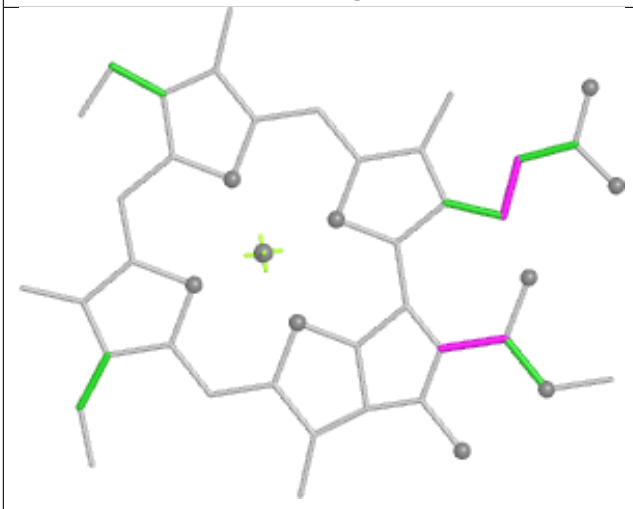
Ligand CLA aA 816



Bond lengths



Bond angles

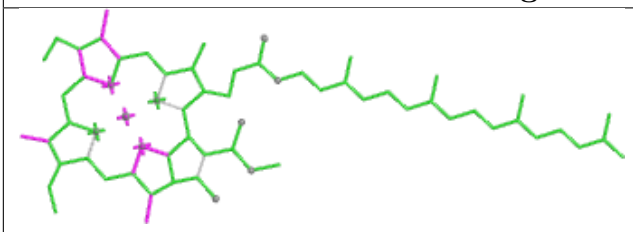


Torsions

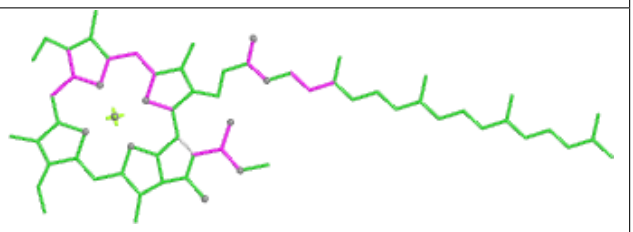


Rings

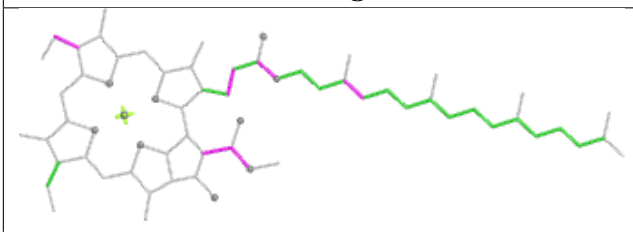
Ligand CLA c2 404



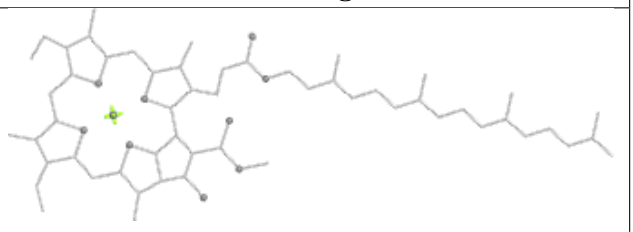
Bond lengths



Bond angles

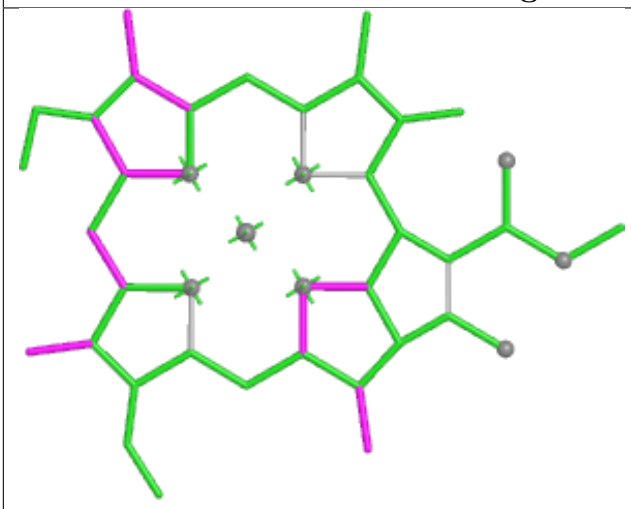


Torsions

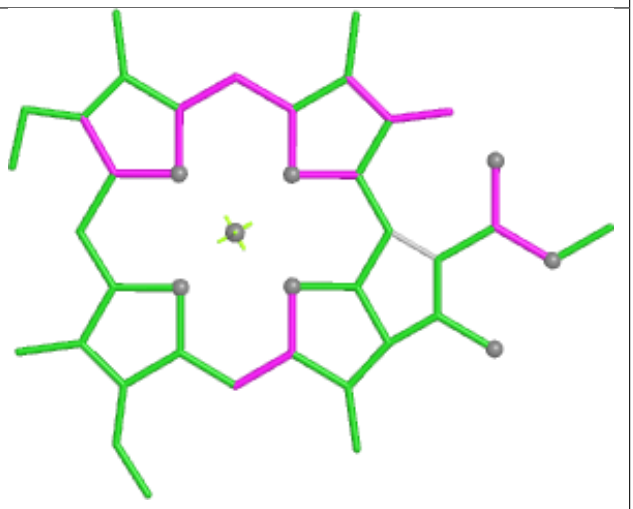


Rings

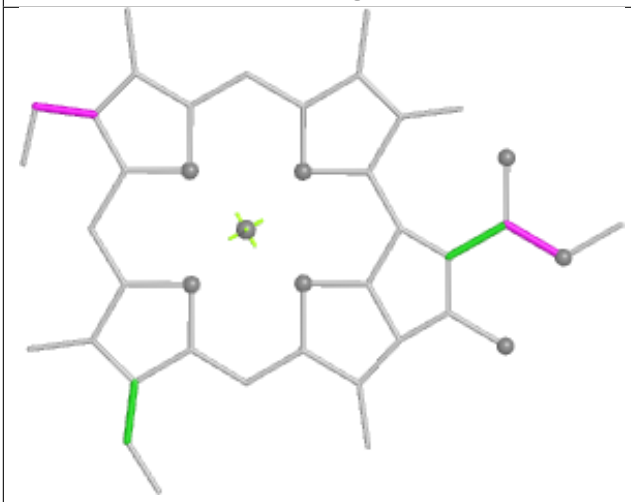
Ligand CLA c5 414



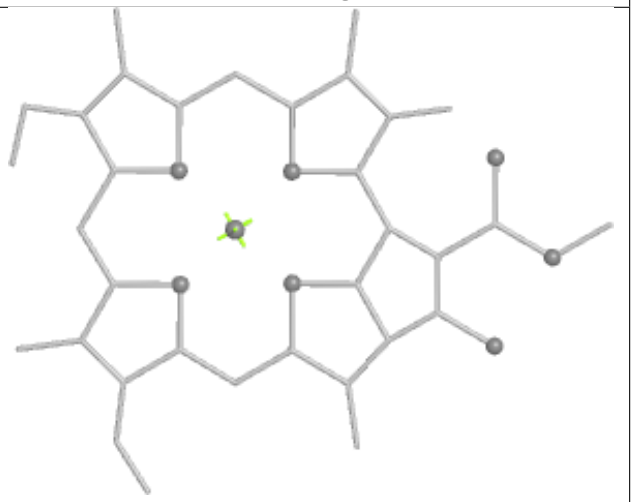
Bond lengths



Bond angles

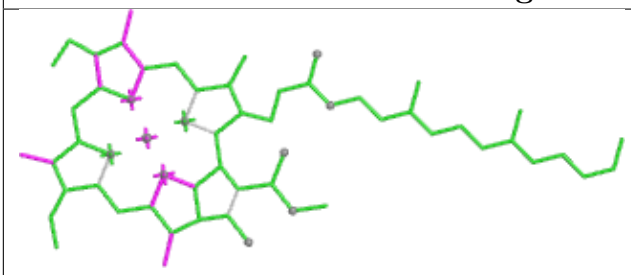


Torsions

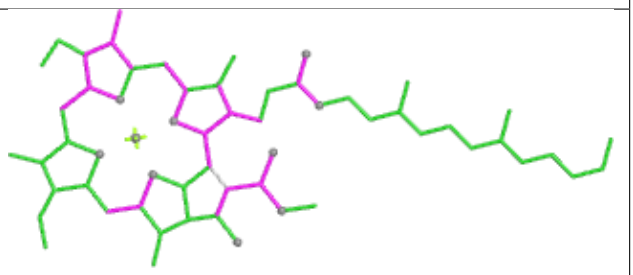


Rings

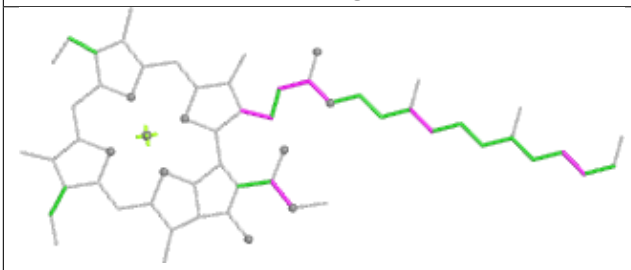
Ligand CLA aB 818



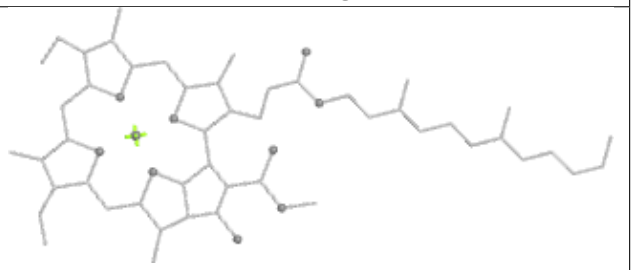
Bond lengths



Bond angles

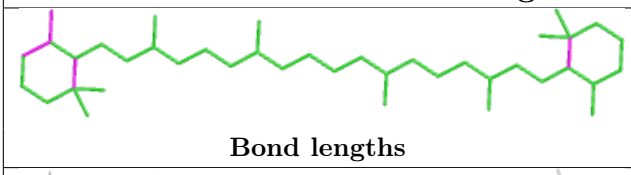


Torsions

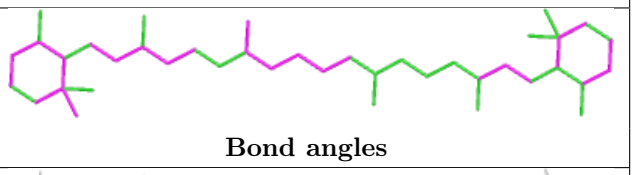


Rings

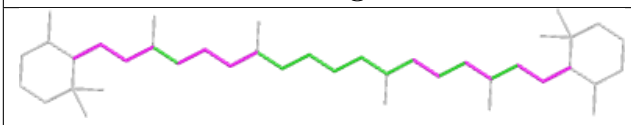
Ligand BCR a2 401



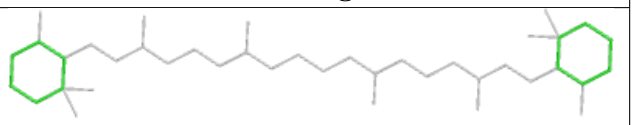
Bond lengths



Bond angles

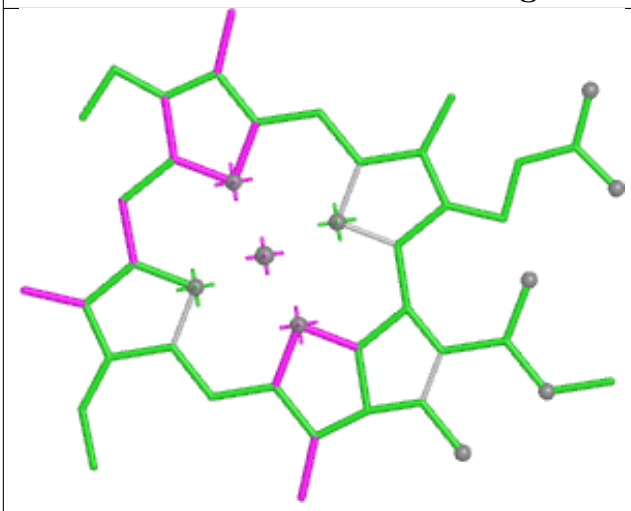


Torsions

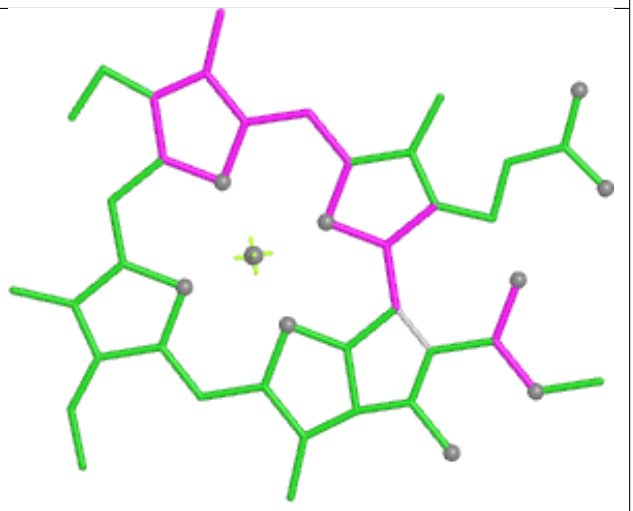


Rings

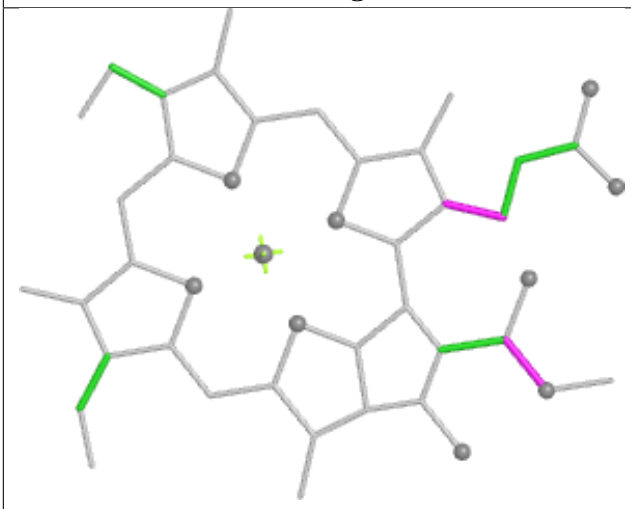
Ligand CLA a1 410



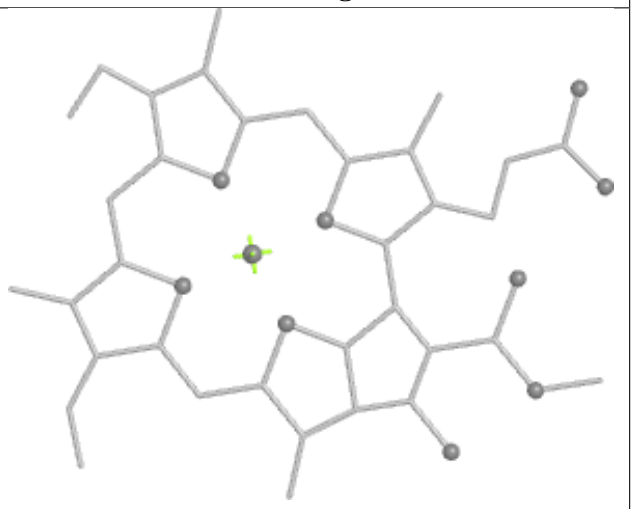
Bond lengths



Bond angles

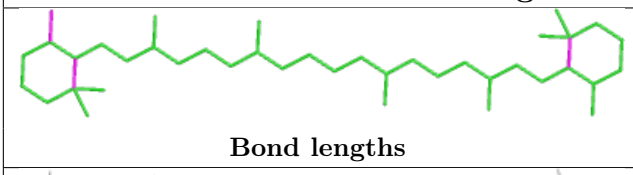


Torsions

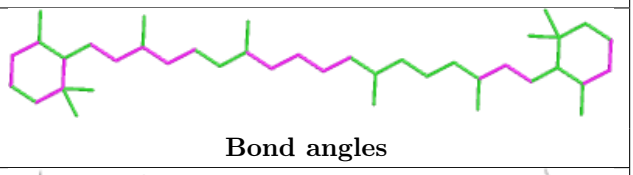


Rings

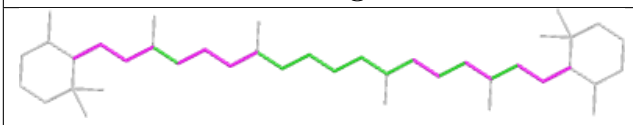
Ligand BCR b6 421



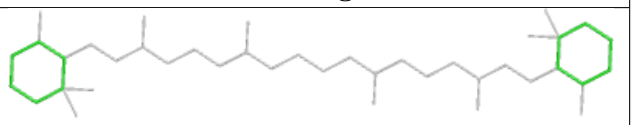
Bond lengths



Bond angles

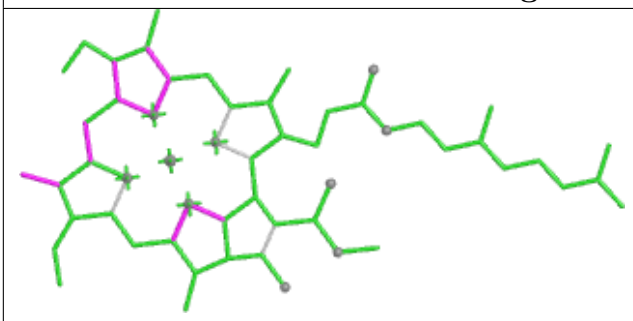


Torsions

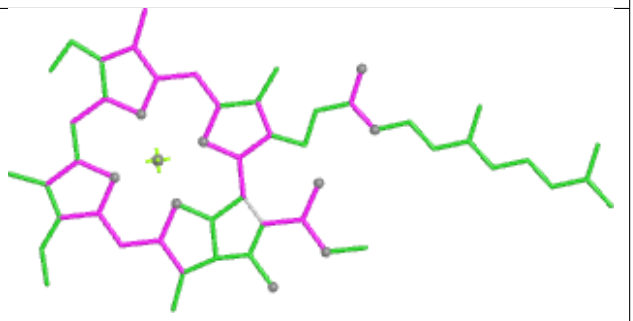


Rings

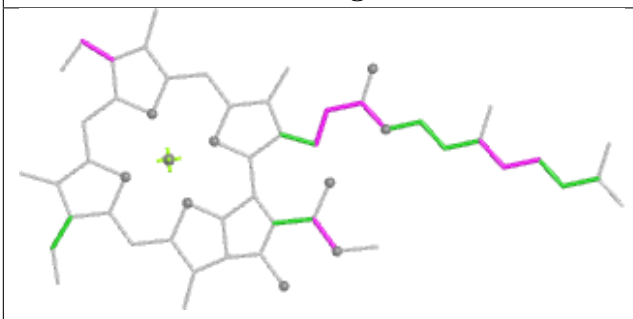
Ligand CLA c3 417



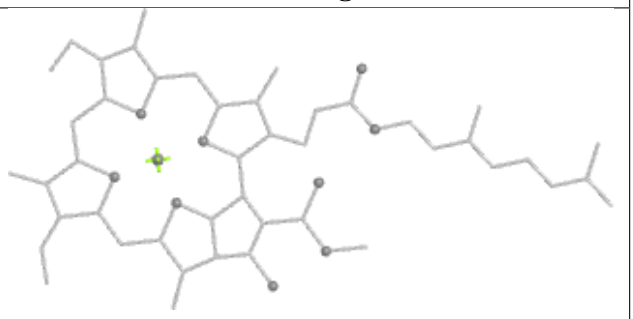
Bond lengths



Bond angles

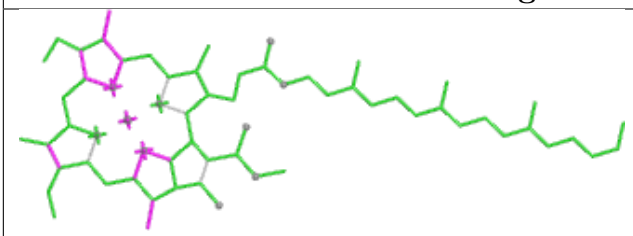


Torsions

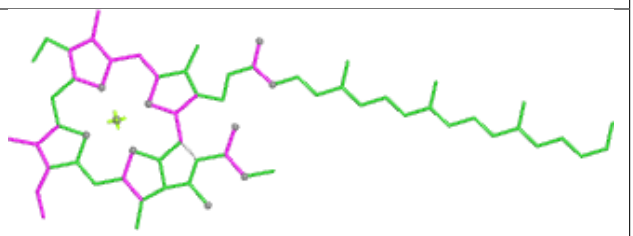


Rings

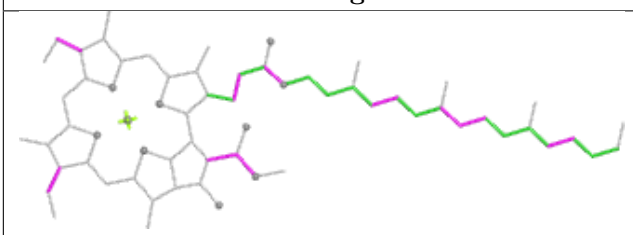
Ligand CLA b1 410



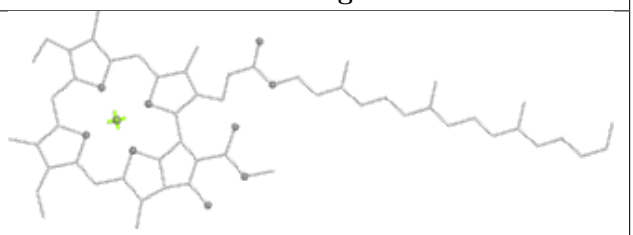
Bond lengths



Bond angles

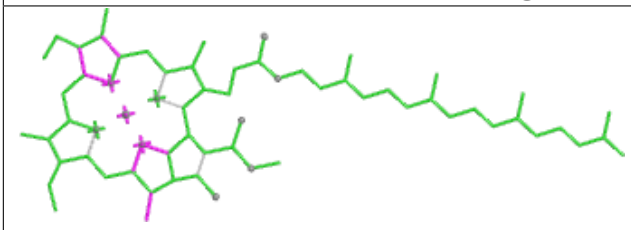


Torsions

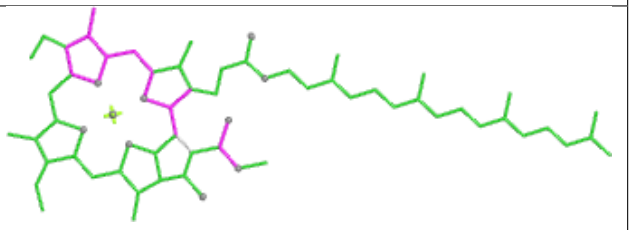


Rings

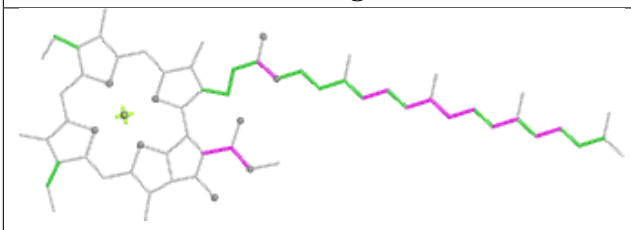
Ligand CLA b4 403



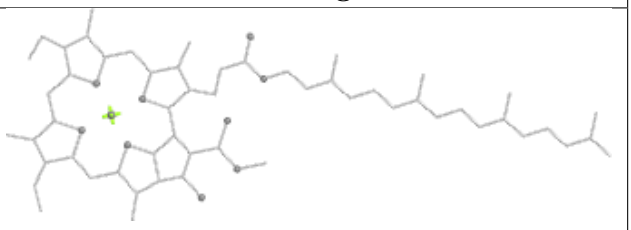
Bond lengths



Bond angles

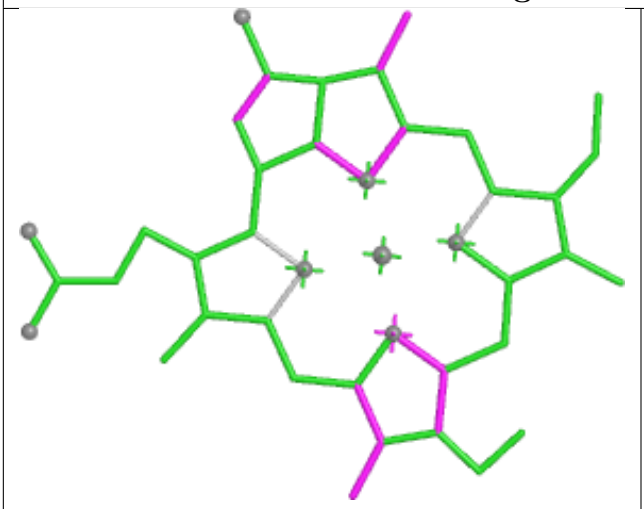


Torsions

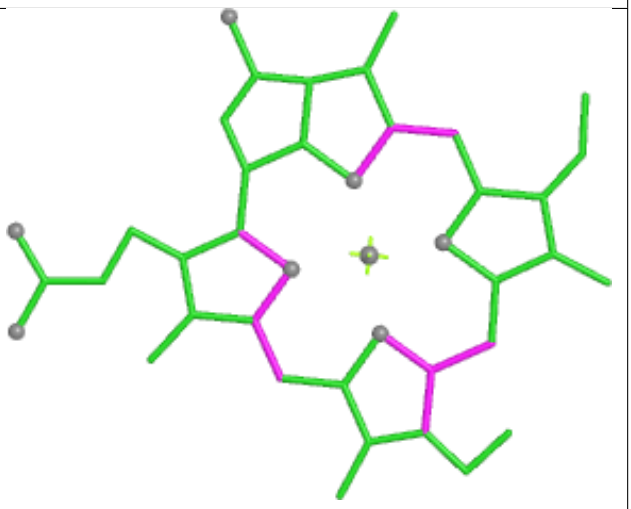


Rings

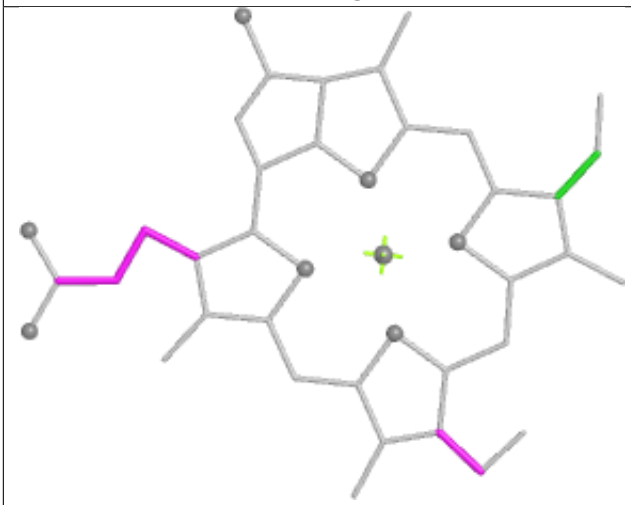
Ligand CLA bA 844



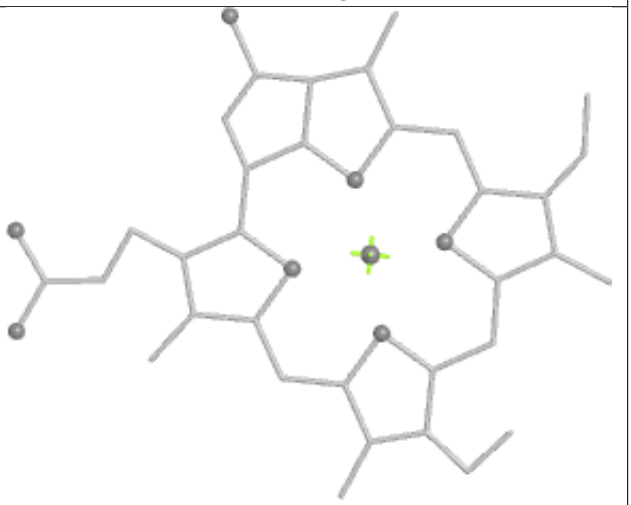
Bond lengths



Bond angles

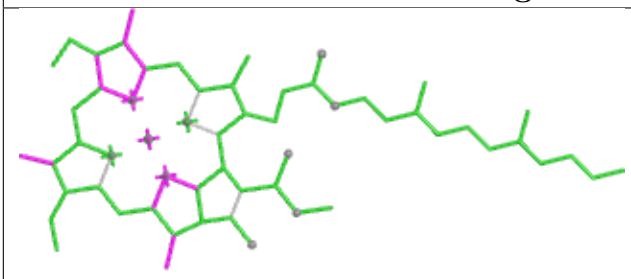


Torsions

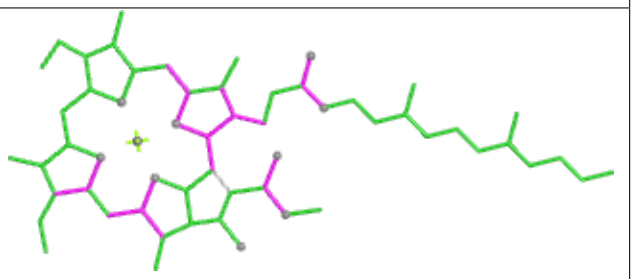


Rings

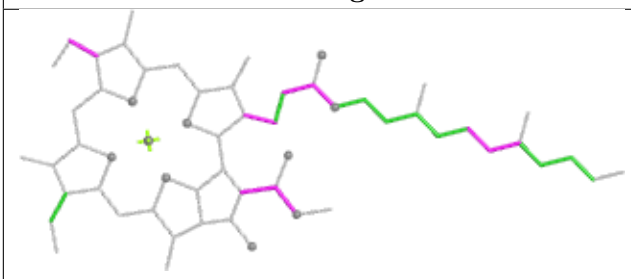
Ligand CLA bB 834



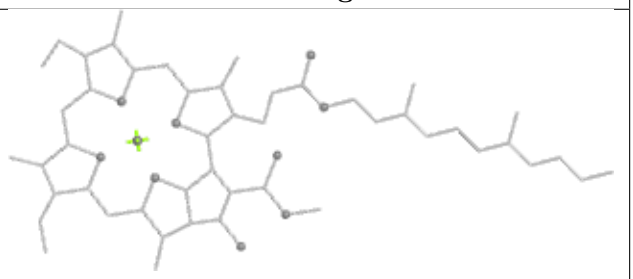
Bond lengths



Bond angles

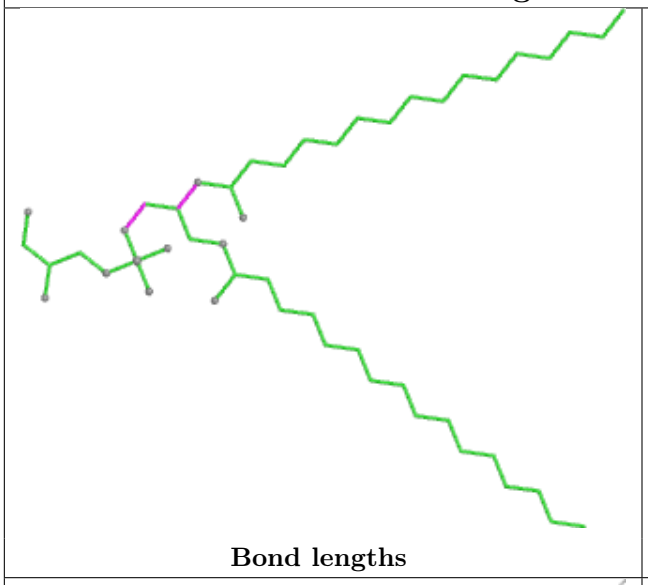


Torsions

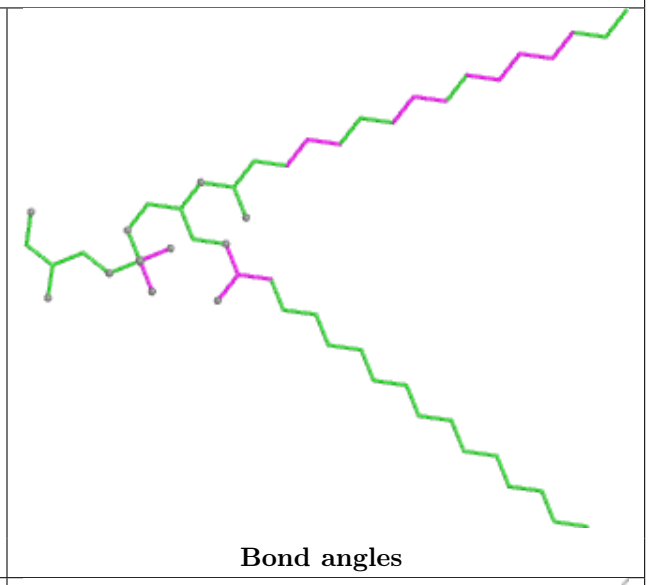


Rings

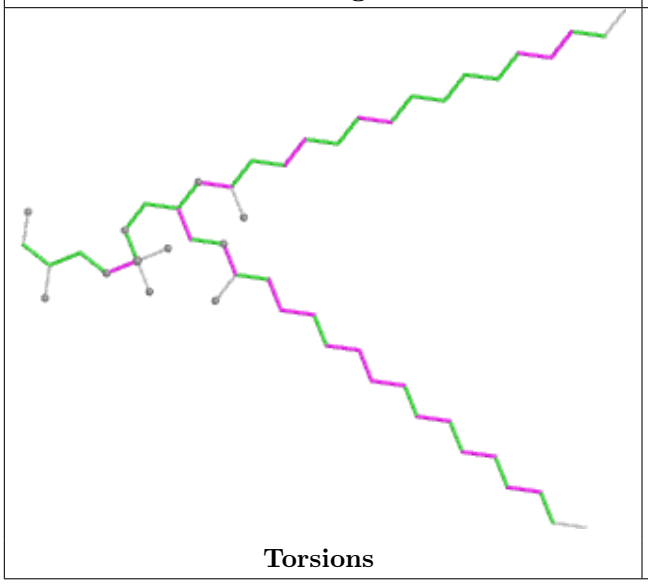
Ligand LHG bA 854



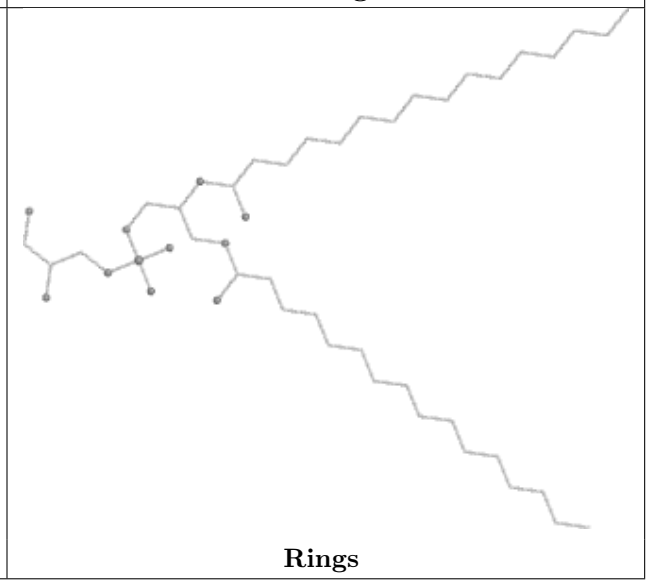
Bond lengths



Bond angles

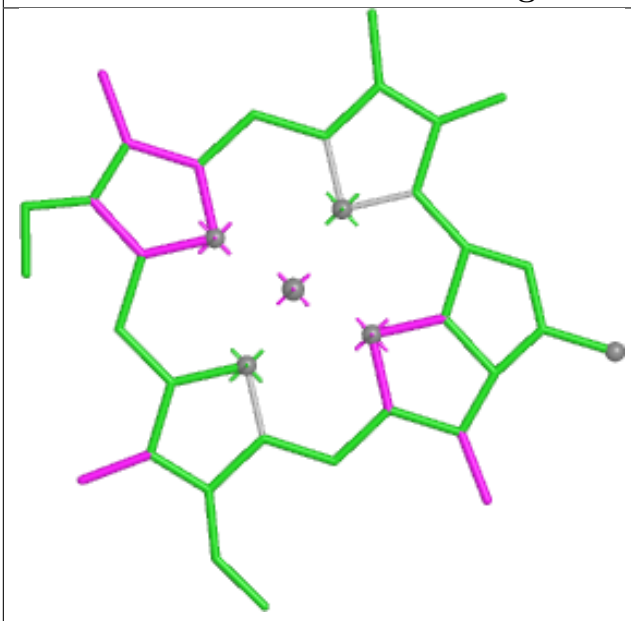


Torsions



Rings

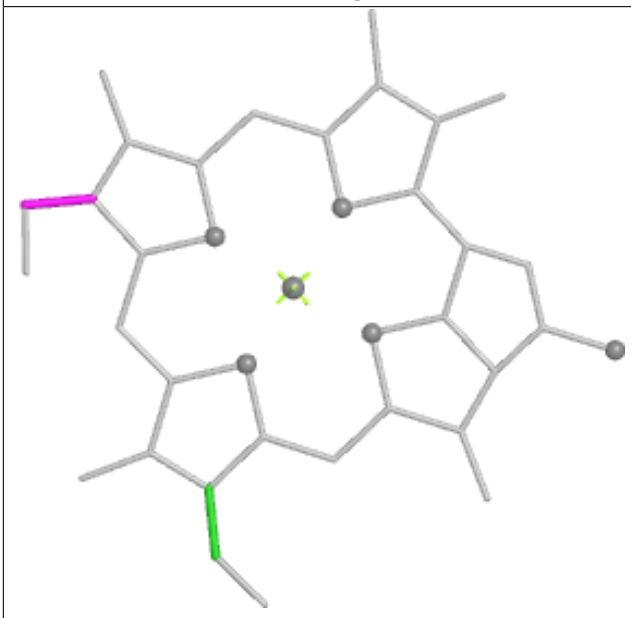
Ligand CLA bJ 102



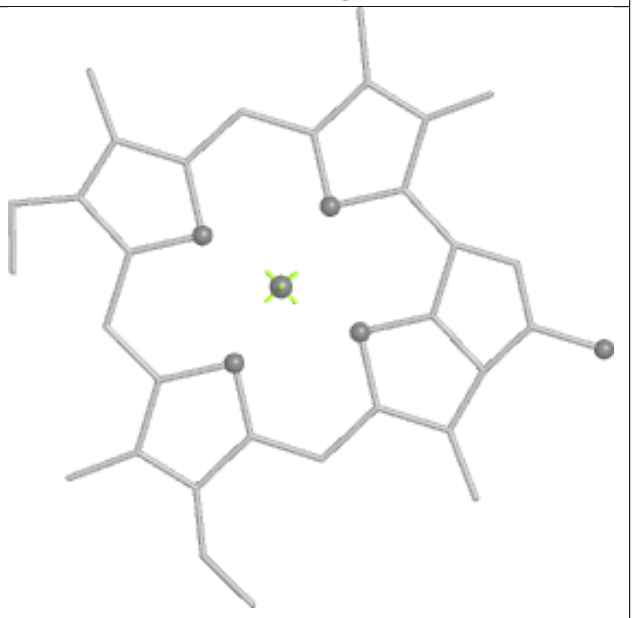
Bond lengths



Bond angles

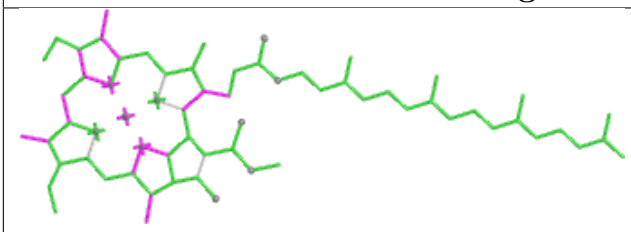


Torsions

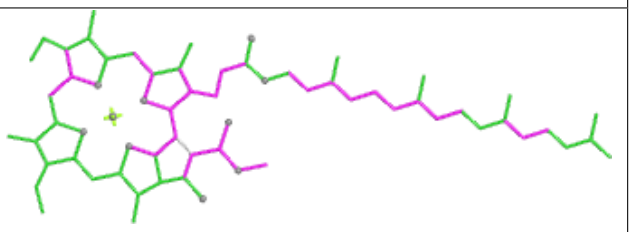


Rings

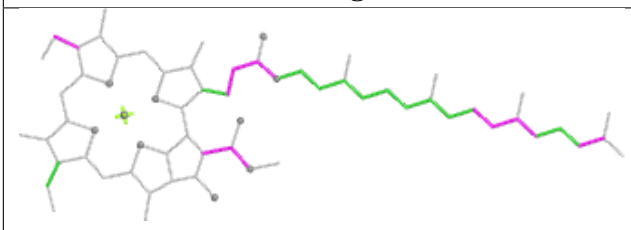
Ligand CLA b6 422



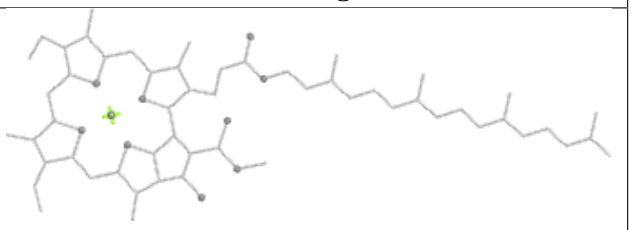
Bond lengths



Bond angles

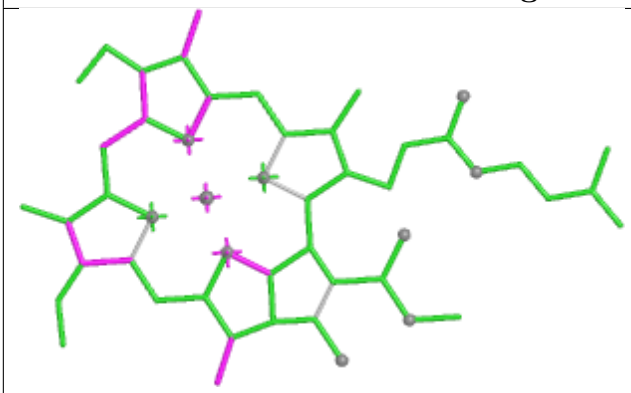


Torsions

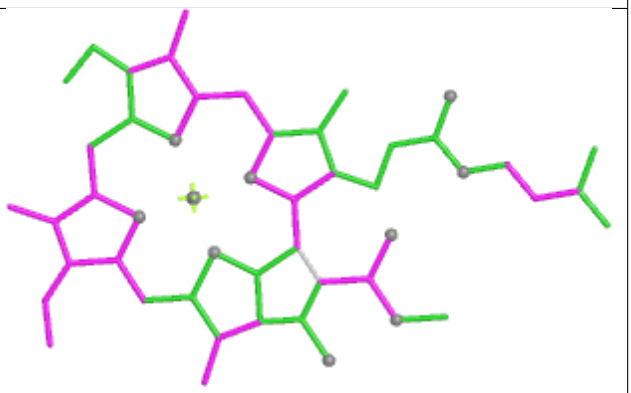


Rings

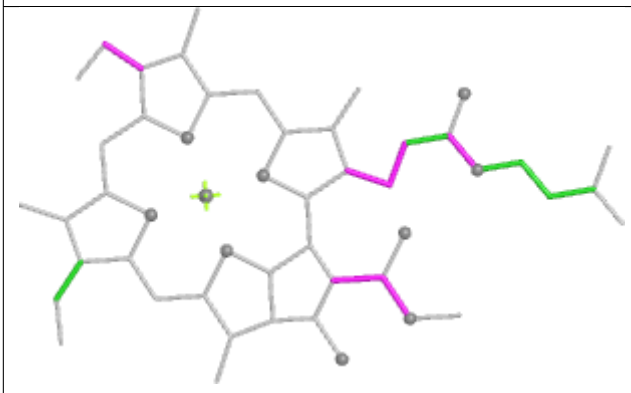
Ligand CLA c6 418



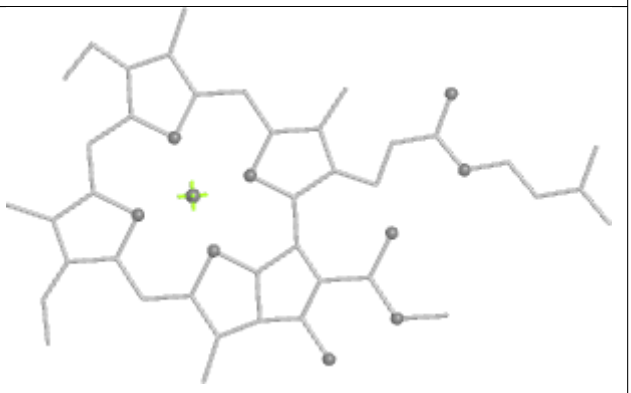
Bond lengths



Bond angles

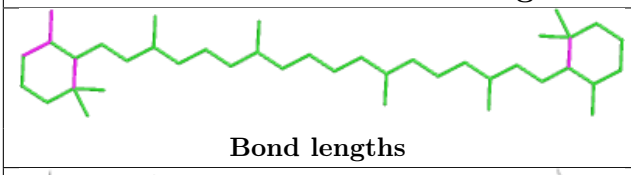


Torsions

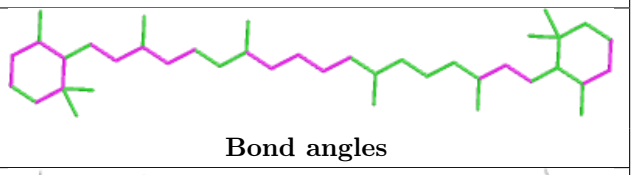


Rings

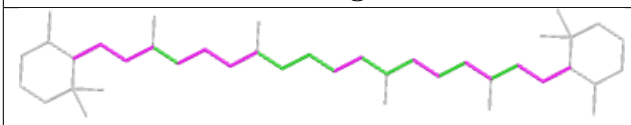
Ligand BCR b6 402



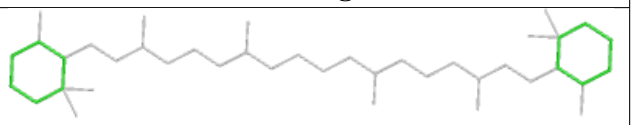
Bond lengths



Bond angles

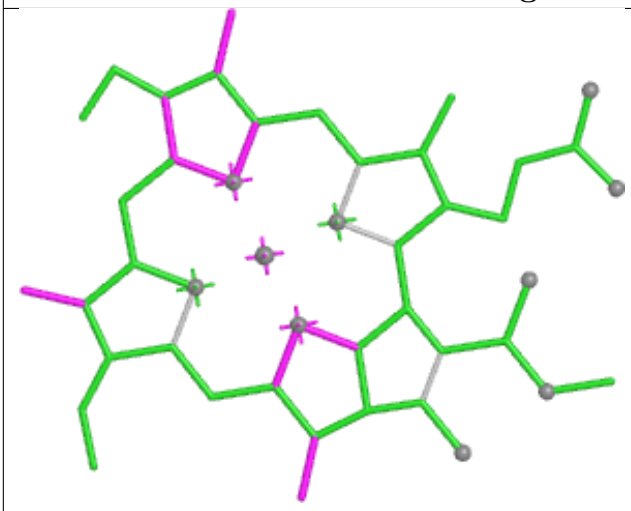


Torsions

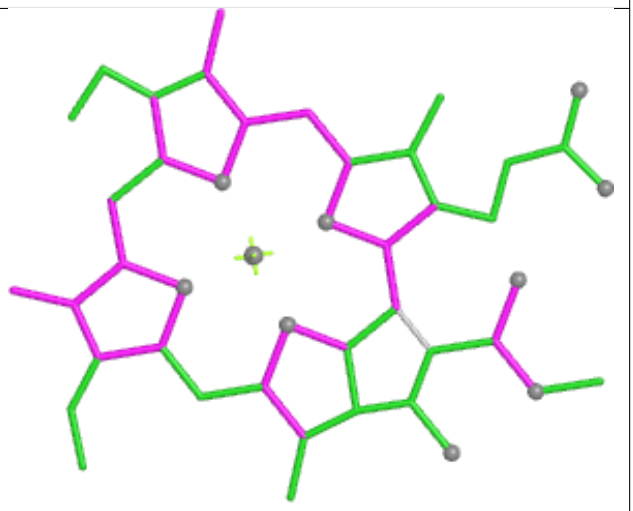


Rings

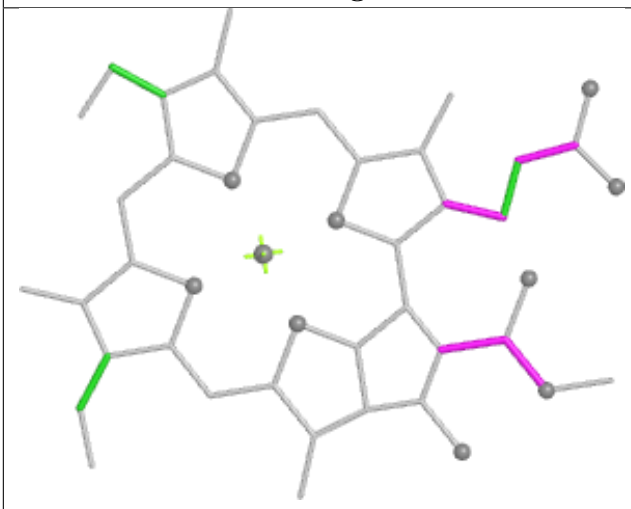
Ligand CLA a3 412



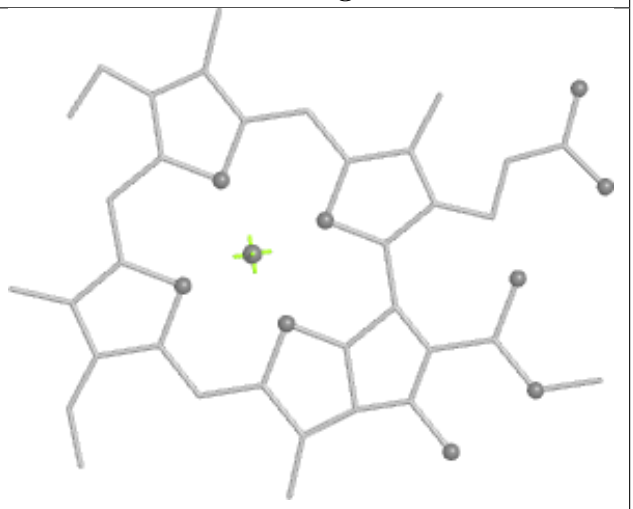
Bond lengths



Bond angles

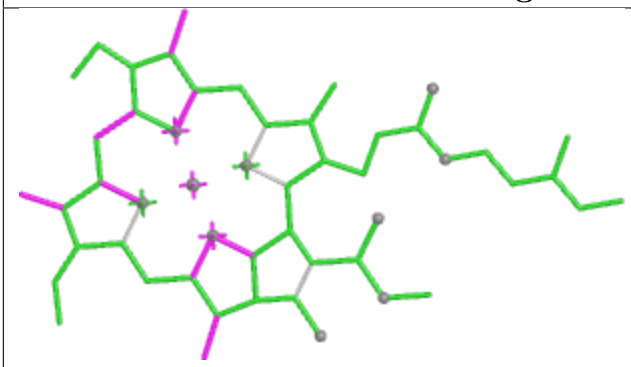


Torsions

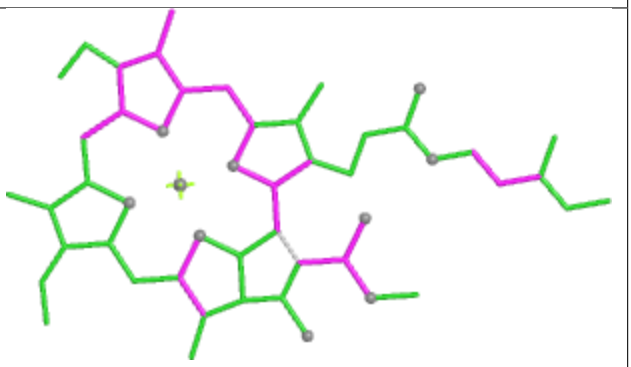


Rings

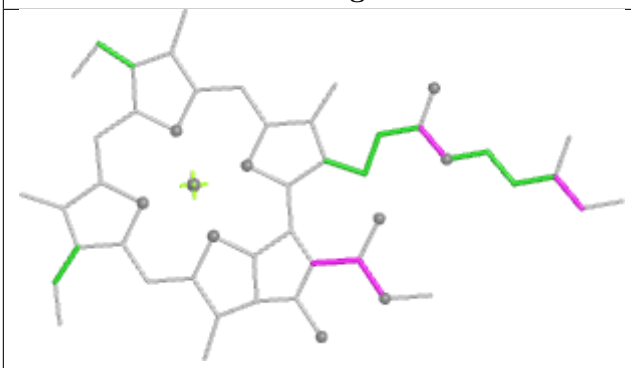
Ligand CLA cA 838



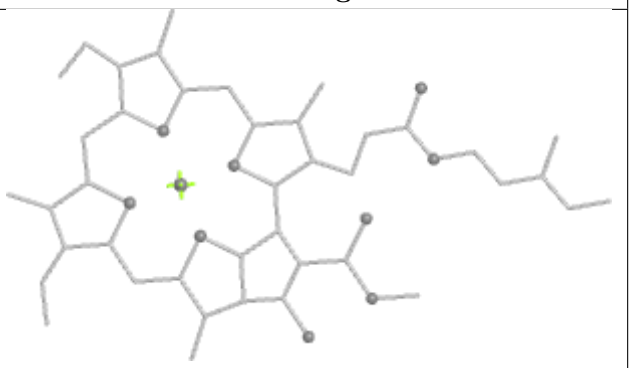
Bond lengths



Bond angles

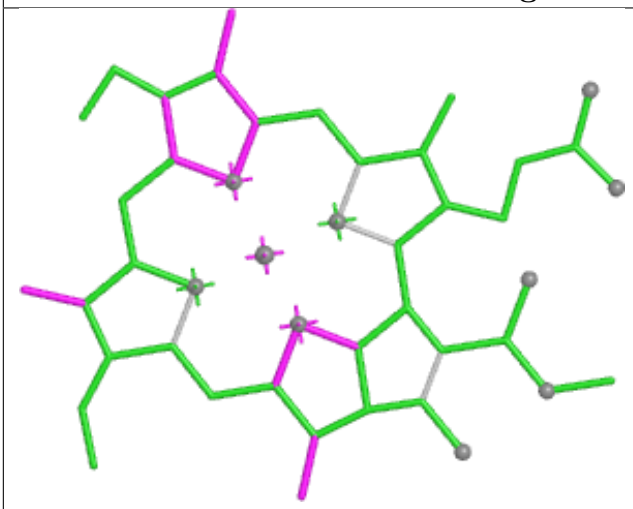


Torsions

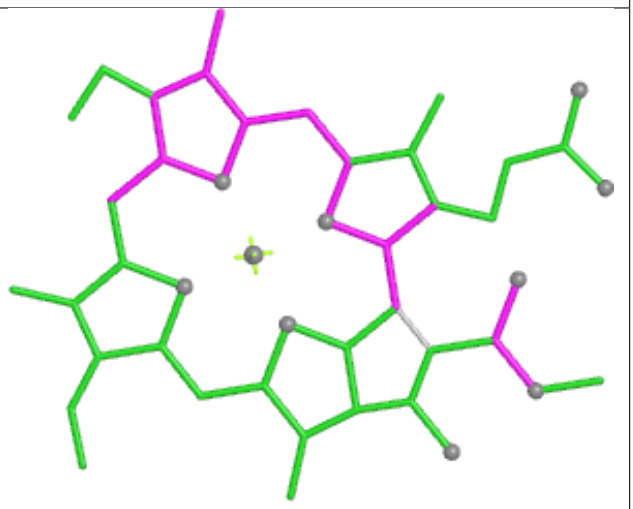


Rings

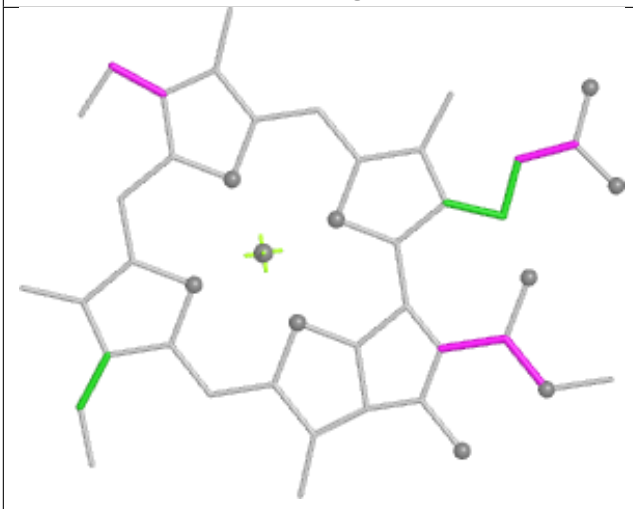
Ligand CLA a3 407



Bond lengths



Bond angles

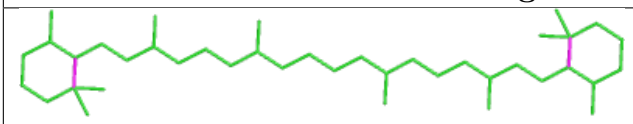


Torsions

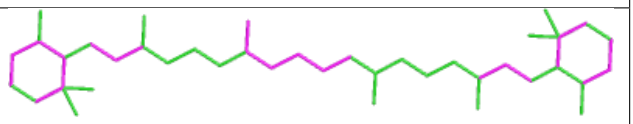


Rings

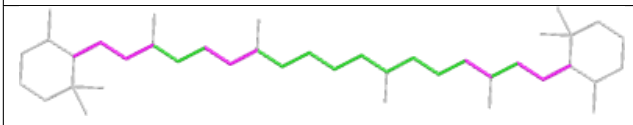
Ligand BCR c6 421



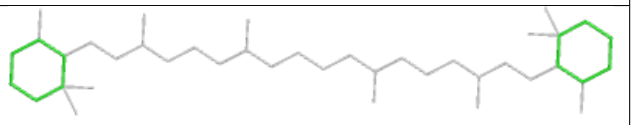
Bond lengths



Bond angles

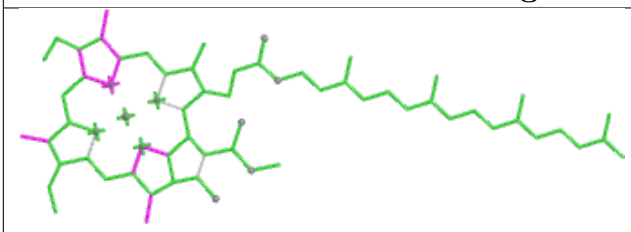


Torsions

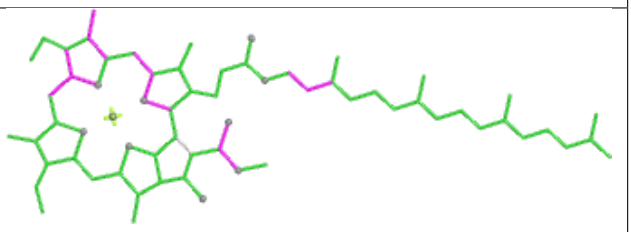


Rings

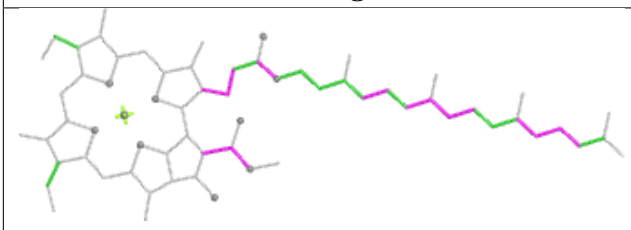
Ligand CLA c3 402



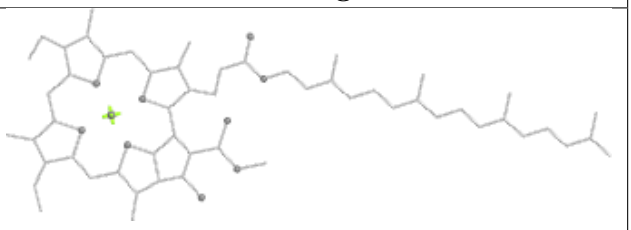
Bond lengths



Bond angles

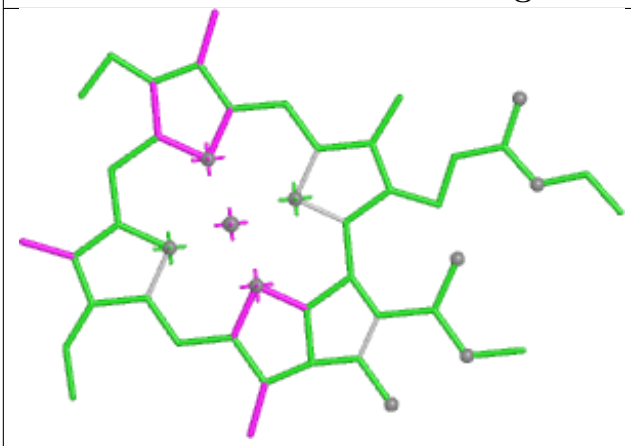


Torsions

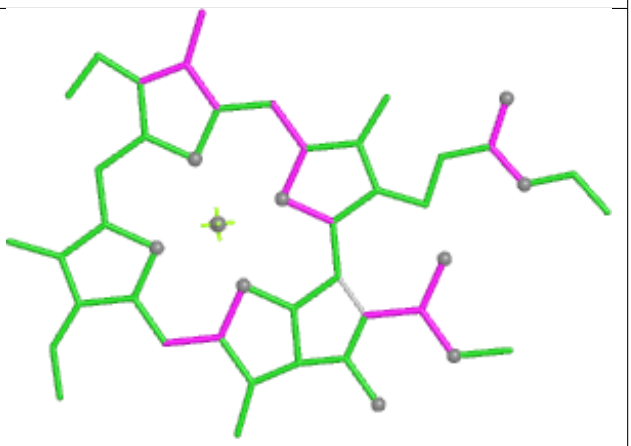


Rings

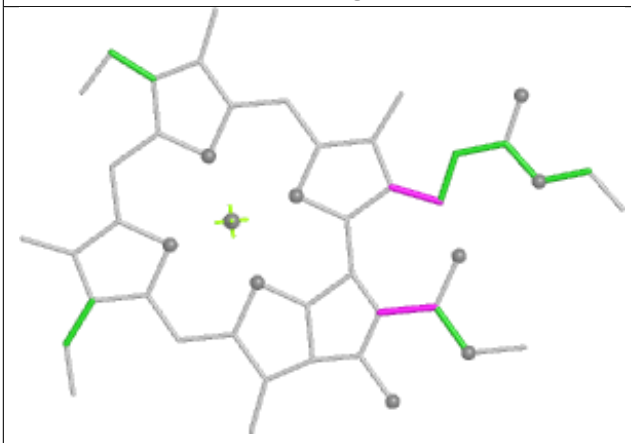
Ligand CLA bB 838



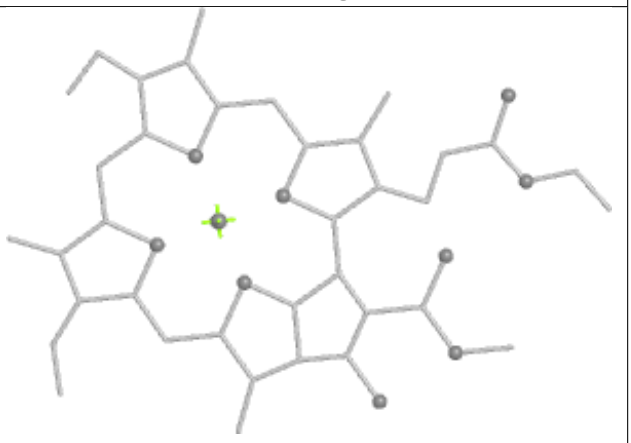
Bond lengths



Bond angles

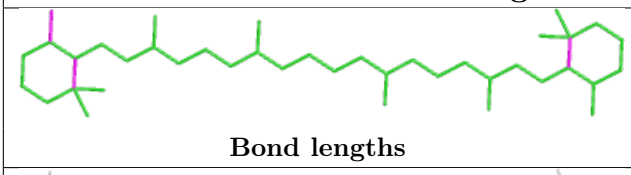


Torsions

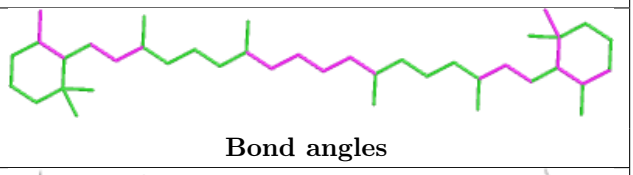


Rings

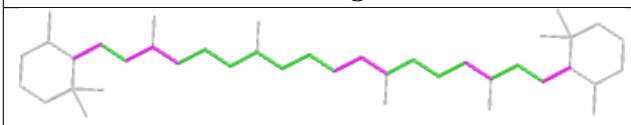
Ligand BCR cM 101



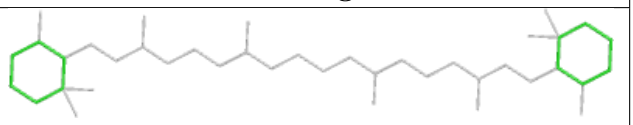
Bond lengths



Bond angles

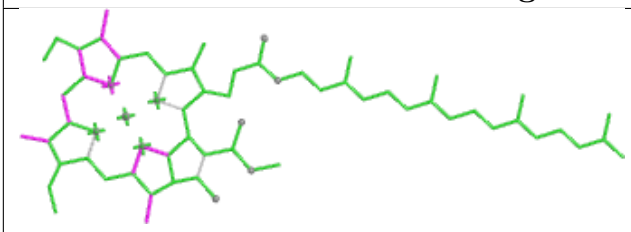


Torsions

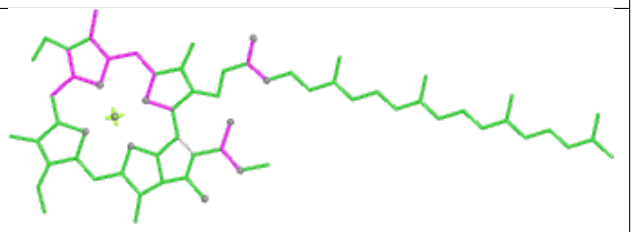


Rings

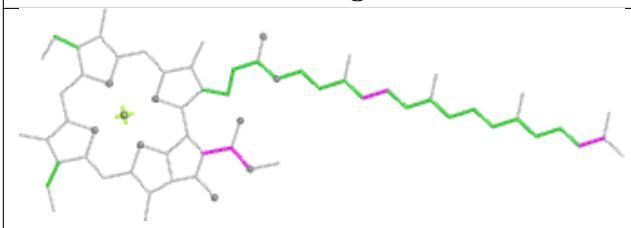
Ligand CLA b5 409



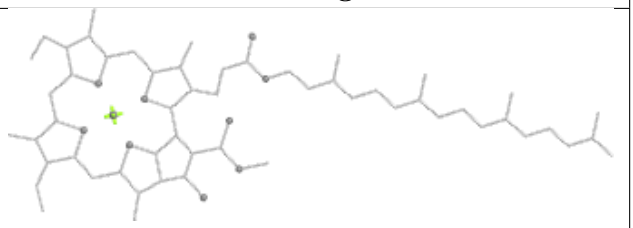
Bond lengths



Bond angles

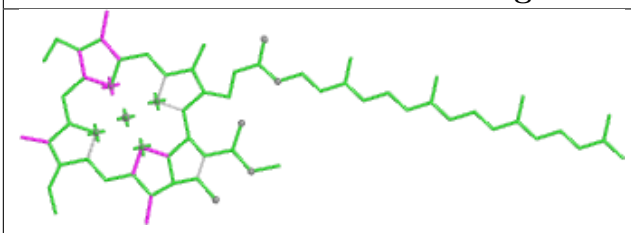


Torsions

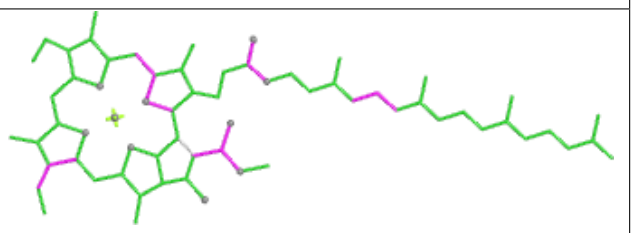


Rings

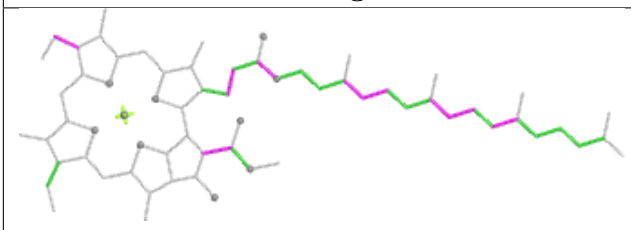
Ligand CLA bB 808



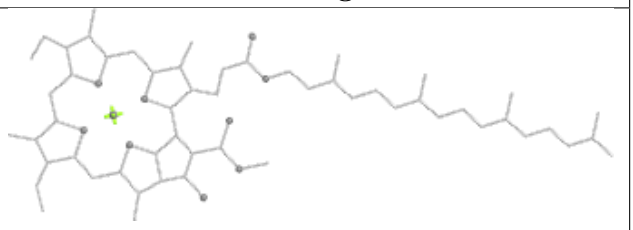
Bond lengths



Bond angles

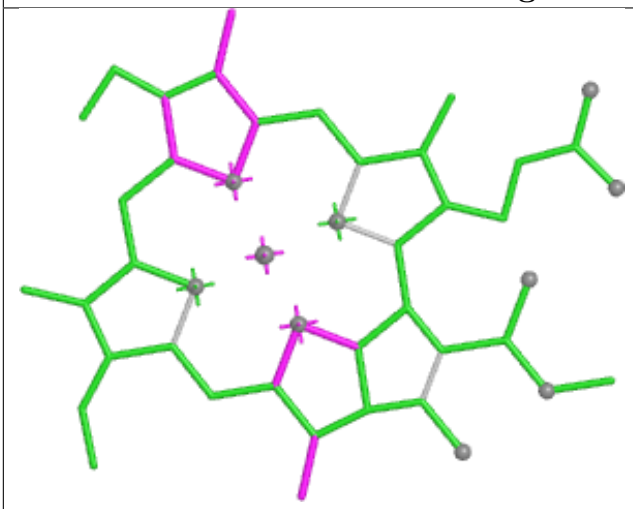


Torsions

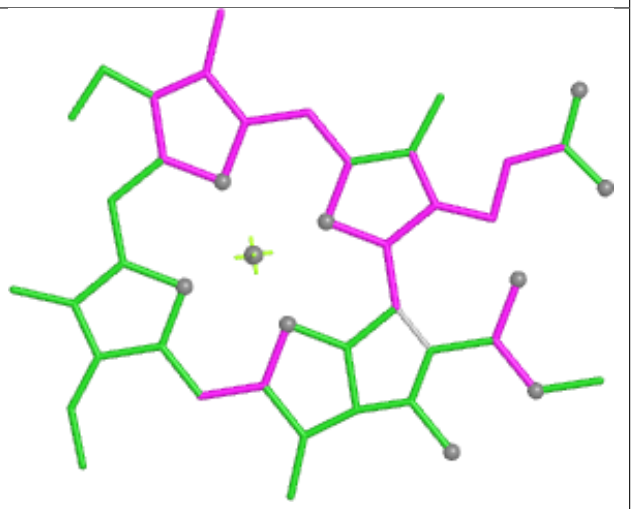


Rings

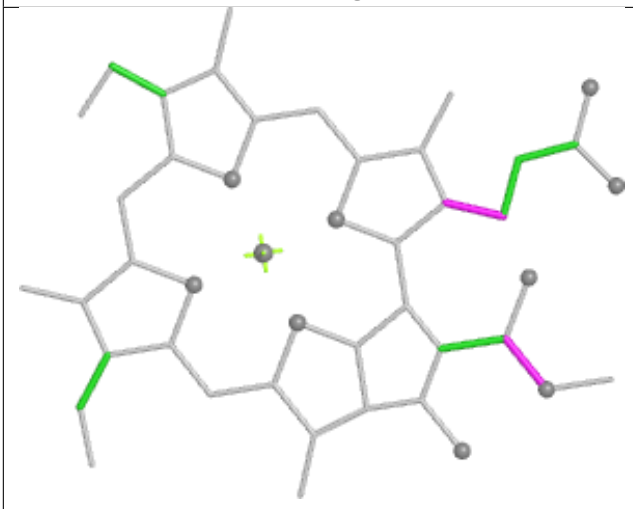
Ligand CLA b6 412



Bond lengths



Bond angles

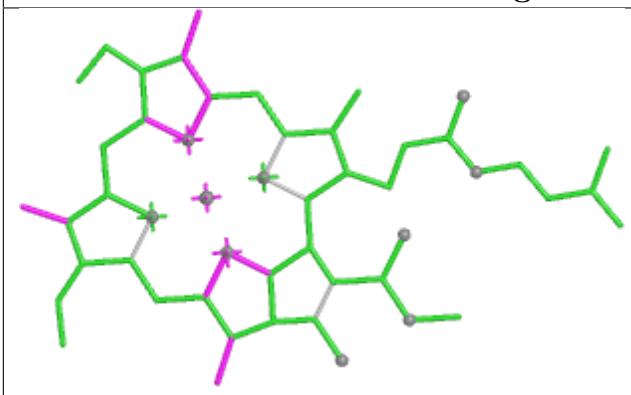


Torsions

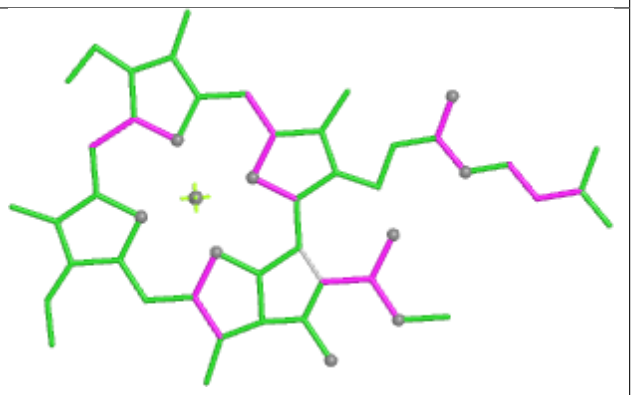


Rings

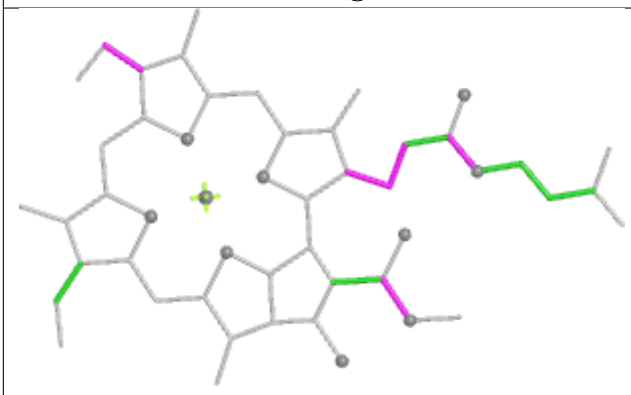
Ligand CLA bA 832



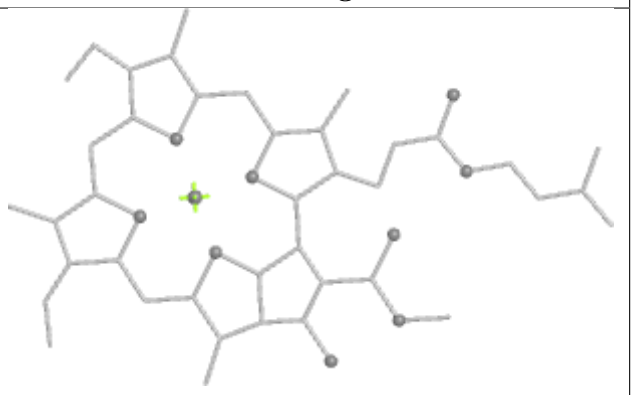
Bond lengths



Bond angles



Torsions

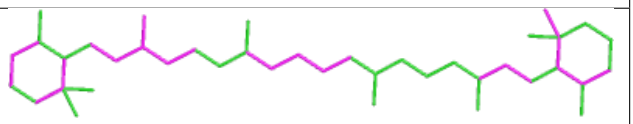


Rings

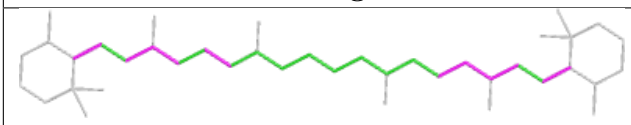
Ligand BCR c6 402



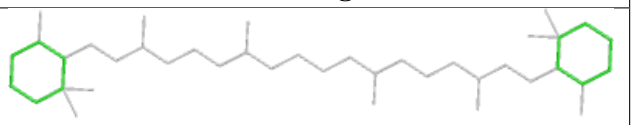
Bond lengths



Bond angles

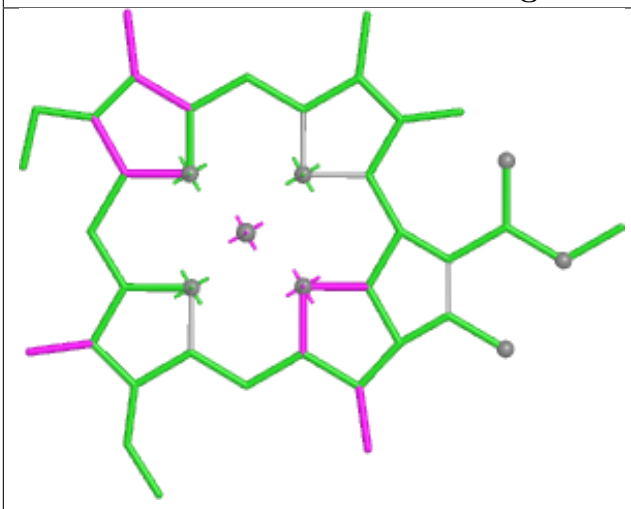


Torsions

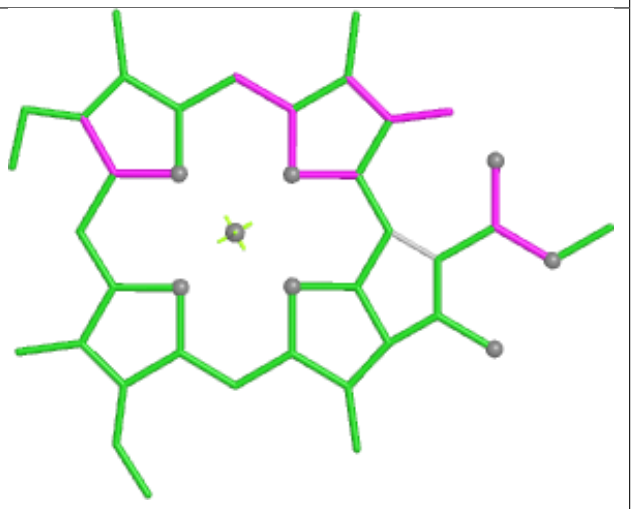


Rings

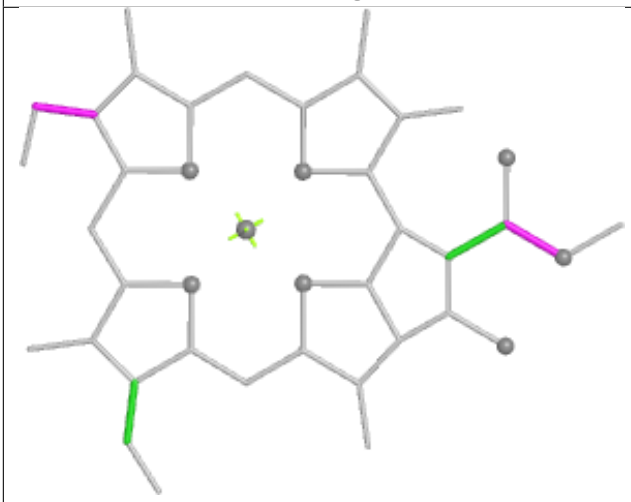
Ligand CLA c4 414



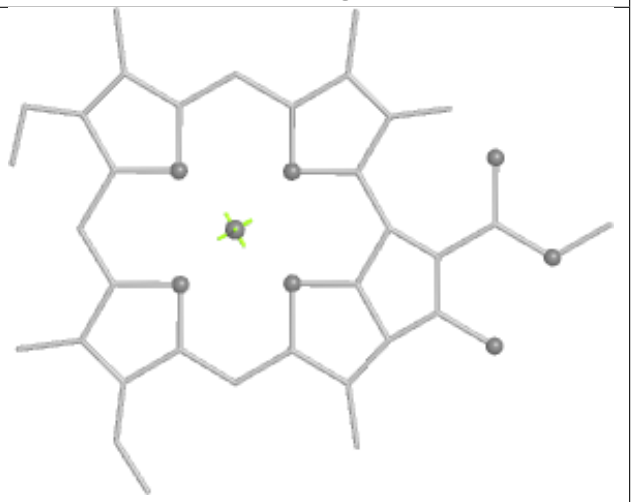
Bond lengths



Bond angles

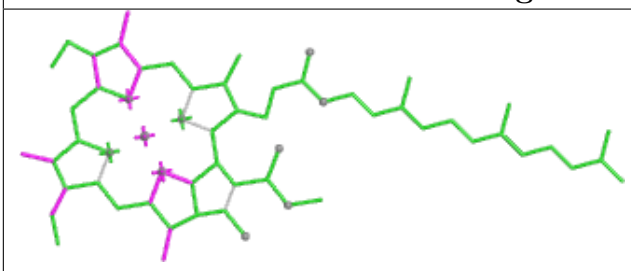


Torsions

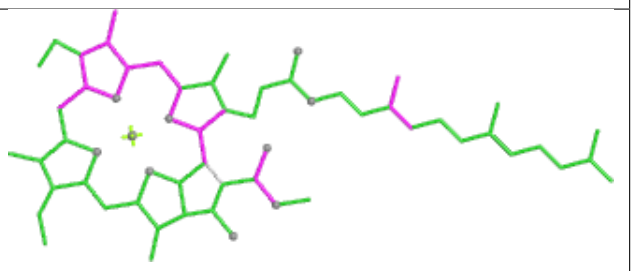


Rings

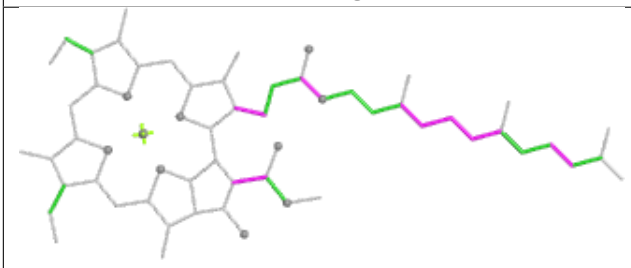
Ligand CLA aB 819



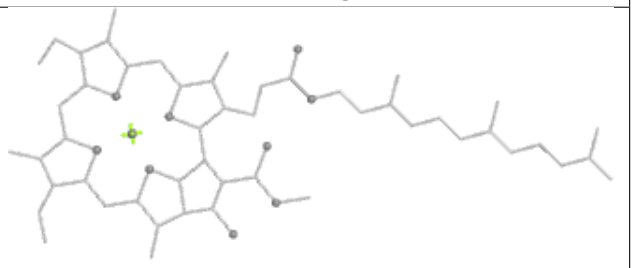
Bond lengths



Bond angles

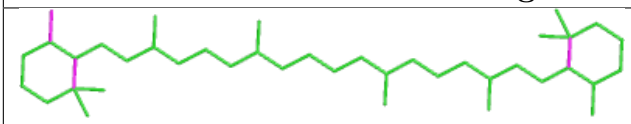


Torsions

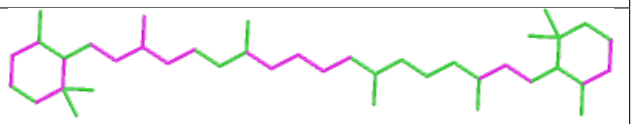


Rings

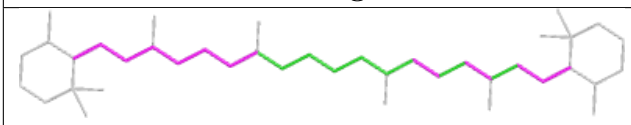
Ligand BCR a1 421



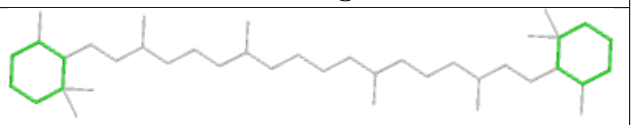
Bond lengths



Bond angles

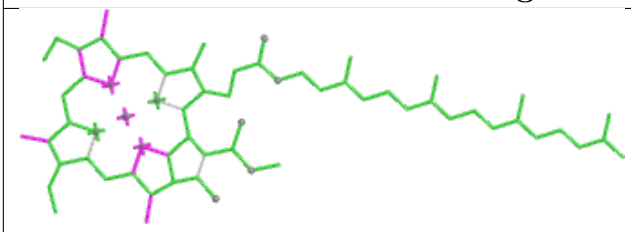


Torsions

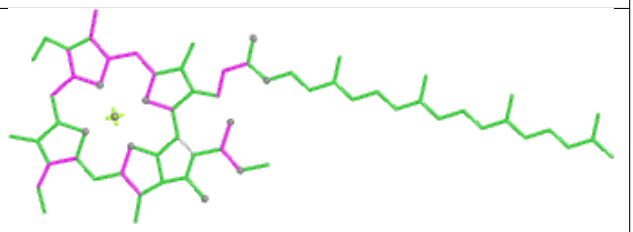


Rings

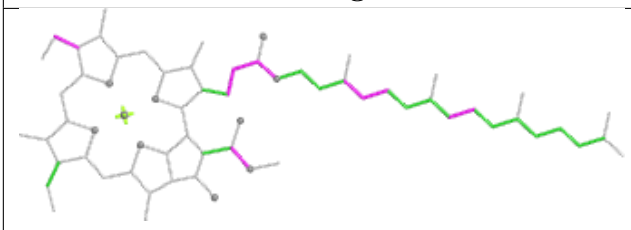
Ligand CLA cB 801



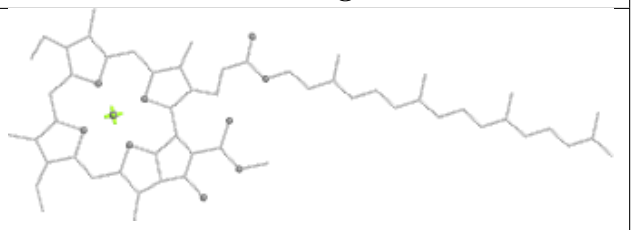
Bond lengths



Bond angles

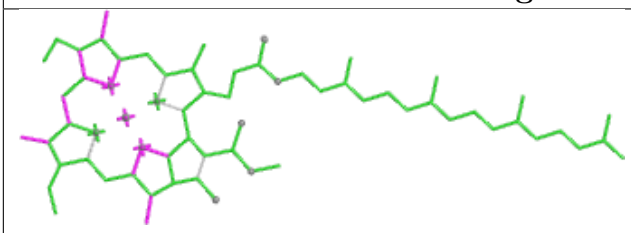


Torsions

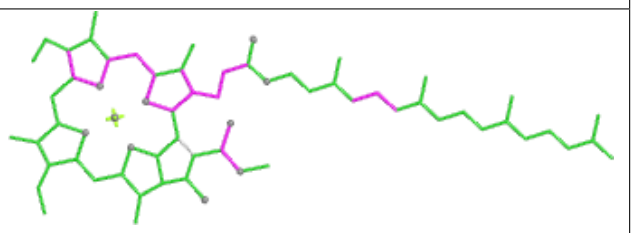


Rings

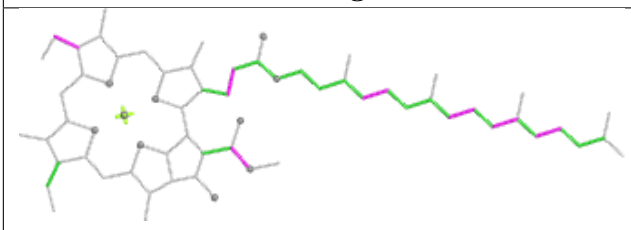
Ligand CLA aB 839



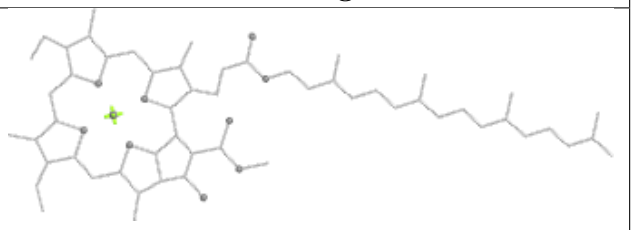
Bond lengths



Bond angles

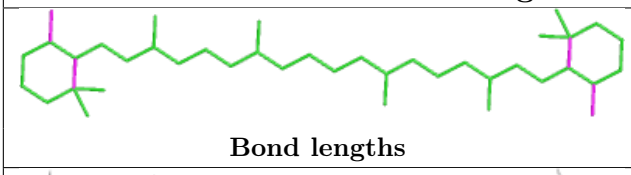


Torsions

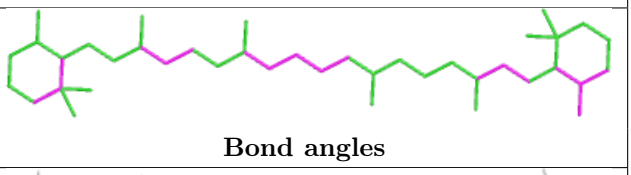


Rings

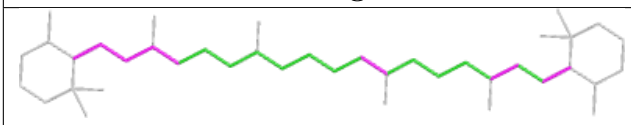
Ligand BCR bJ 104



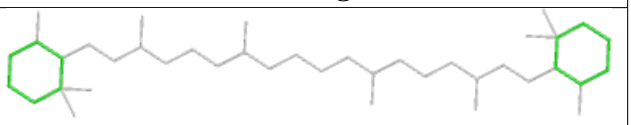
Bond lengths



Bond angles

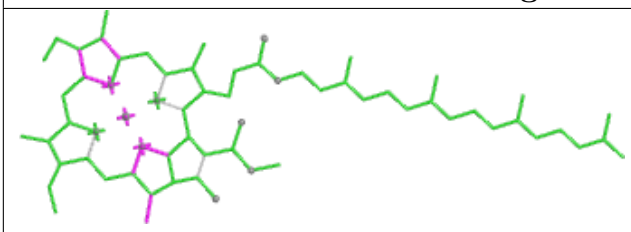


Torsions

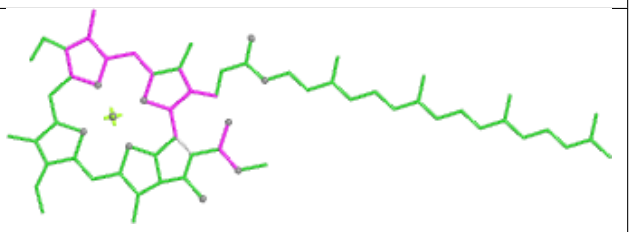


Rings

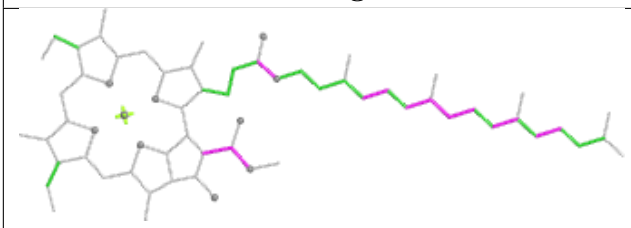
Ligand CLA c6 405



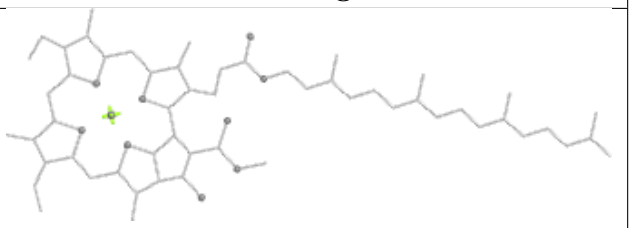
Bond lengths



Bond angles

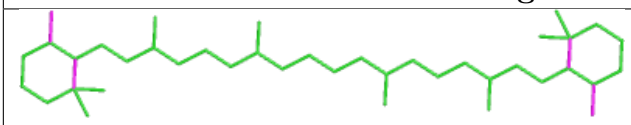


Torsions

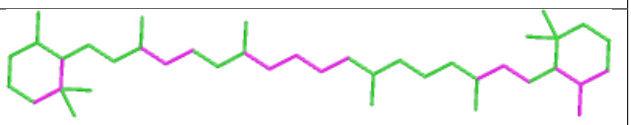


Rings

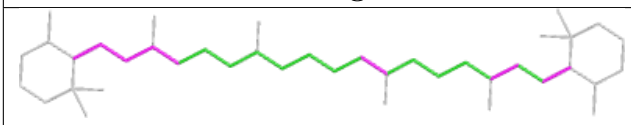
Ligand BCR aJ 205



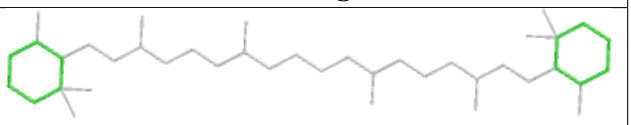
Bond lengths



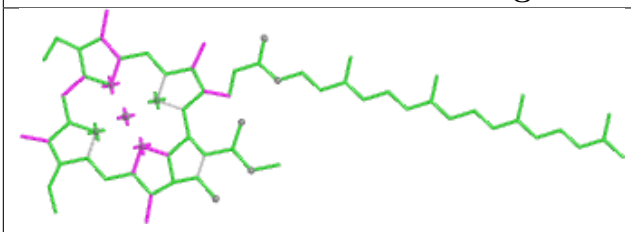
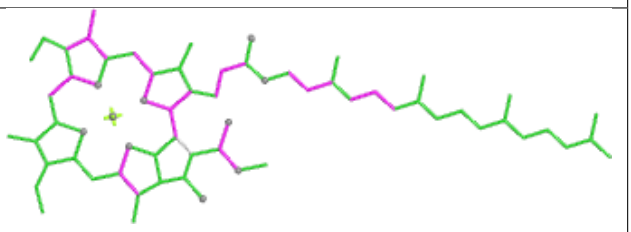
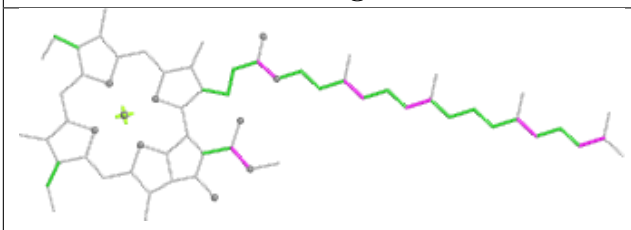
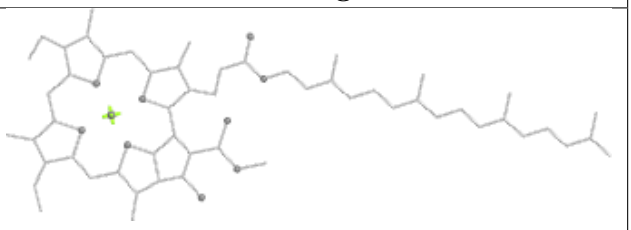
Bond angles

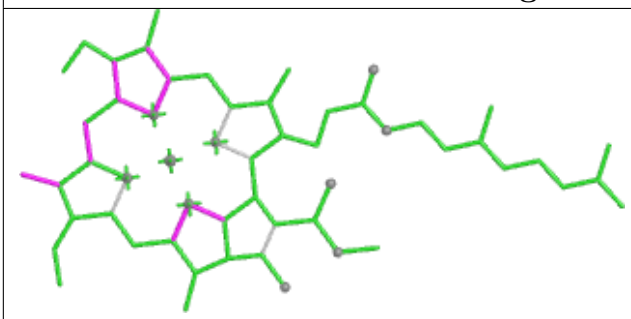
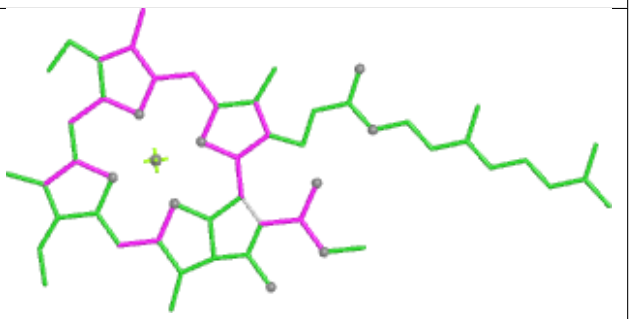
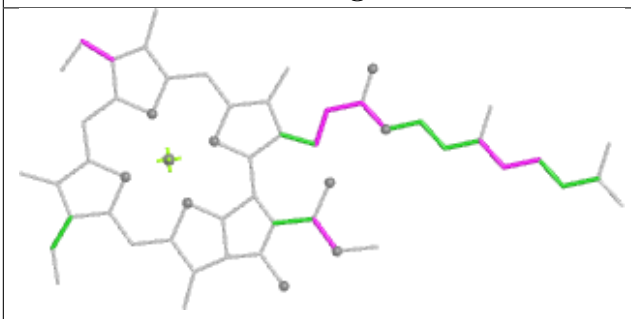
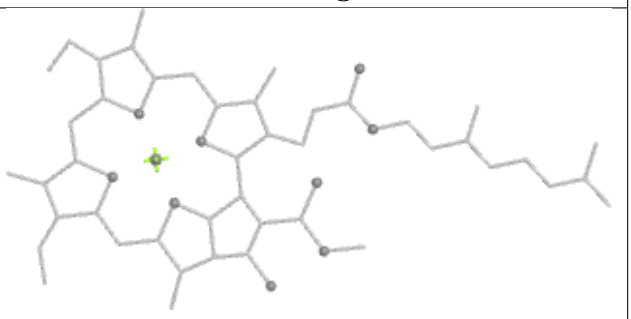


Torsions

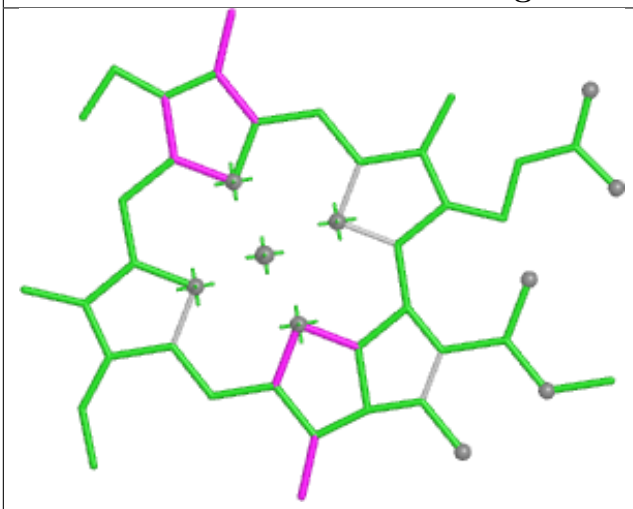


Rings

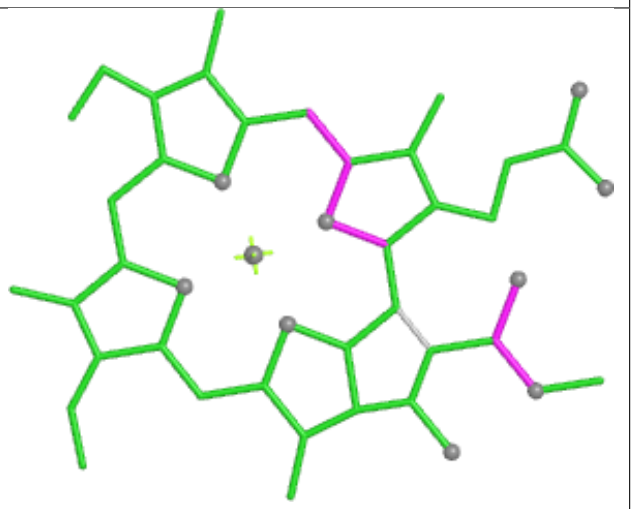
Ligand CLA bA 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a6 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

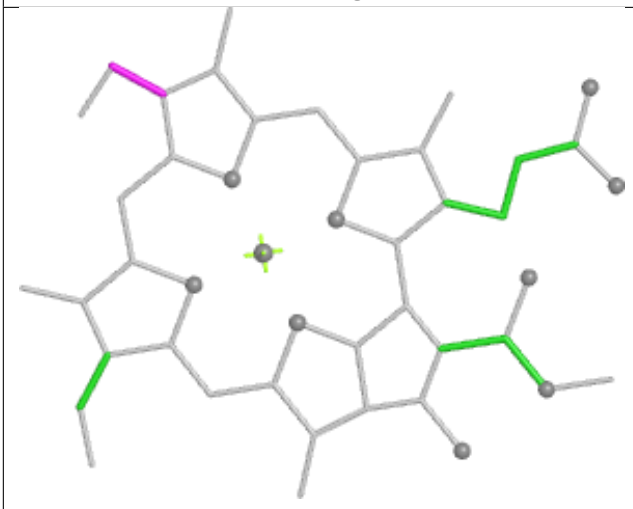
Ligand CLA bB 842



Bond lengths



Bond angles

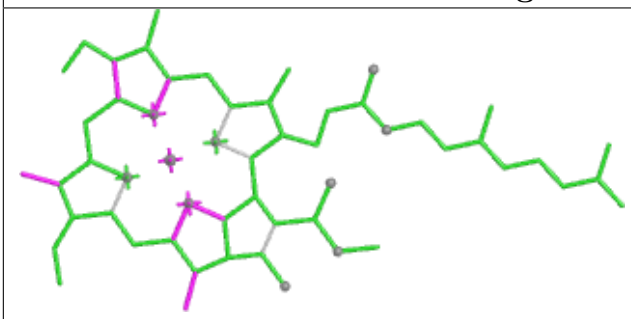


Torsions

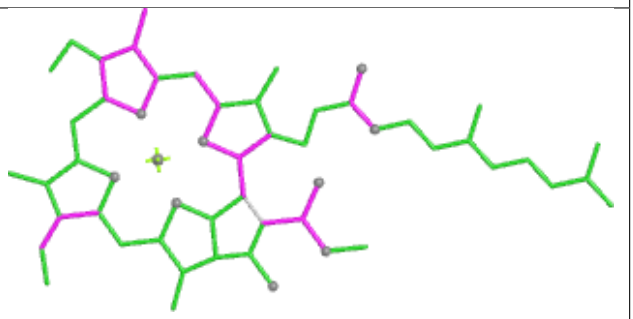


Rings

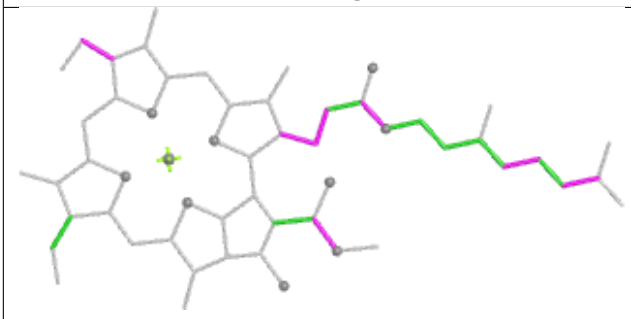
Ligand CLA cB 817



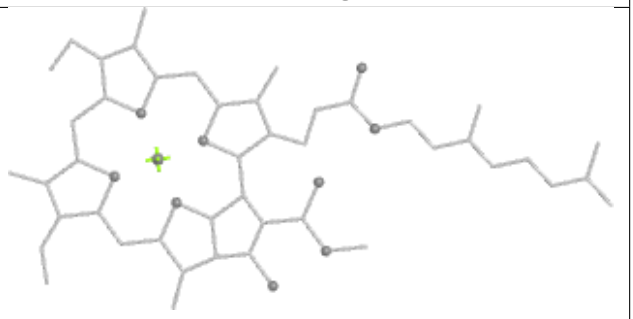
Bond lengths



Bond angles

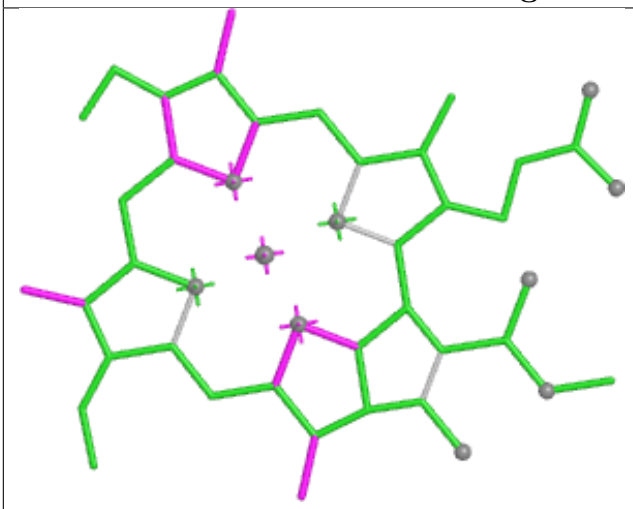


Torsions

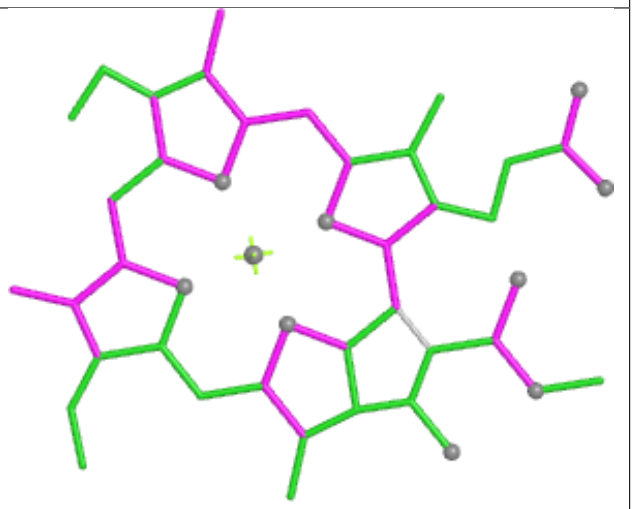


Rings

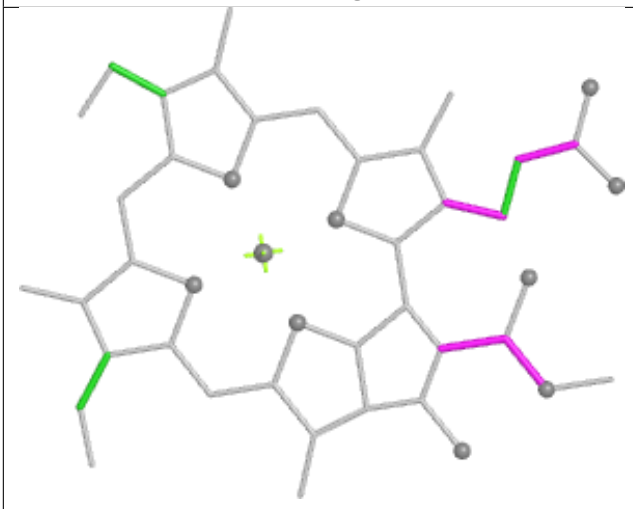
Ligand CLA c6 414



Bond lengths



Bond angles

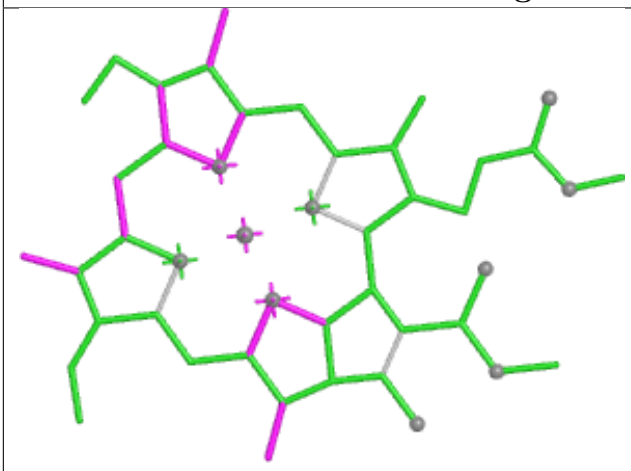


Torsions

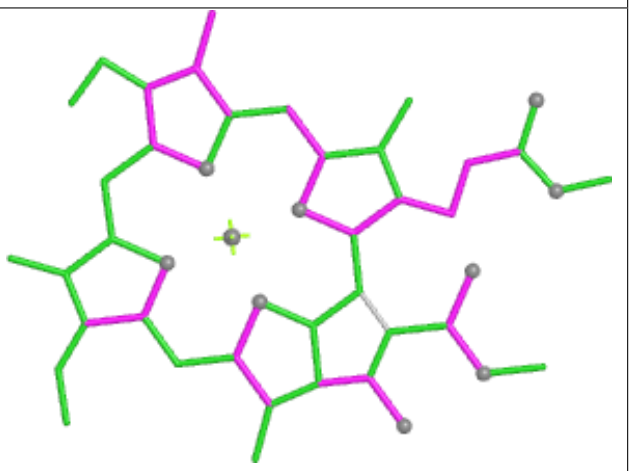


Rings

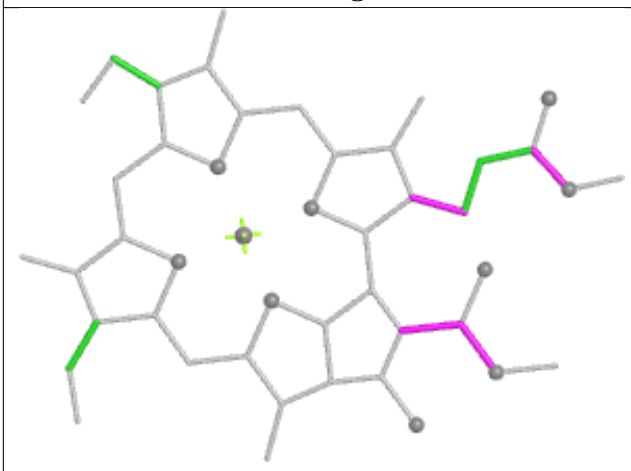
Ligand CLA bB 826



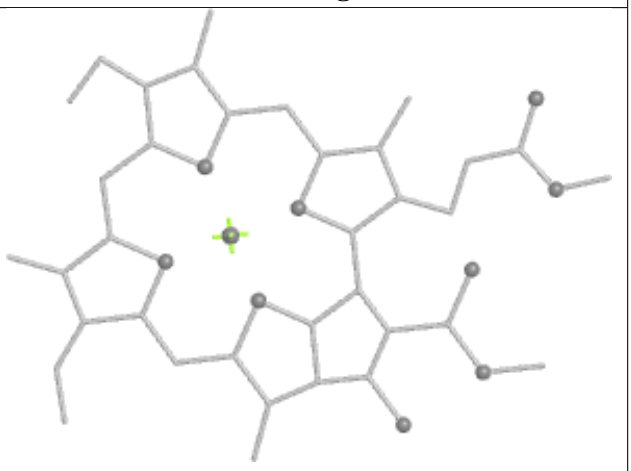
Bond lengths



Bond angles

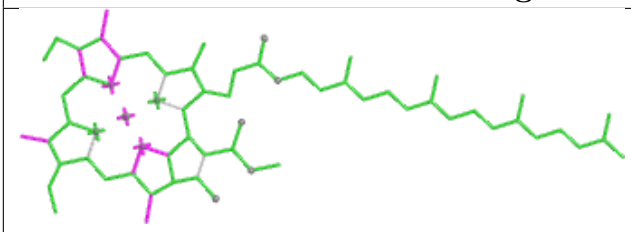


Torsions

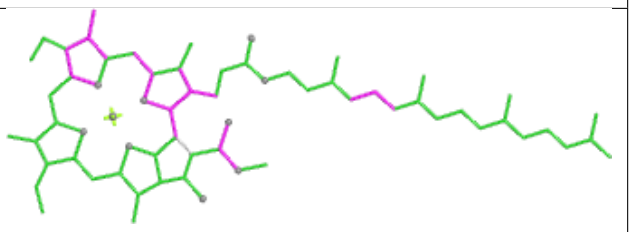


Rings

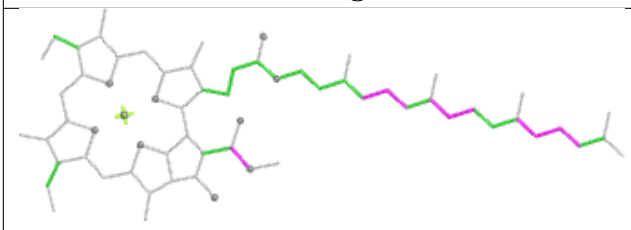
Ligand CLA aA 826



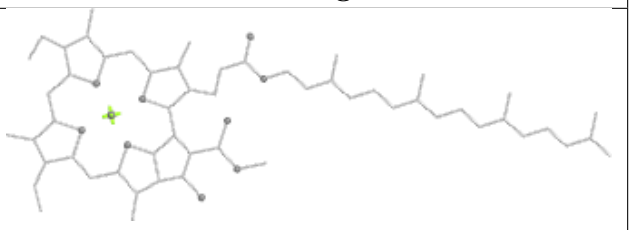
Bond lengths



Bond angles

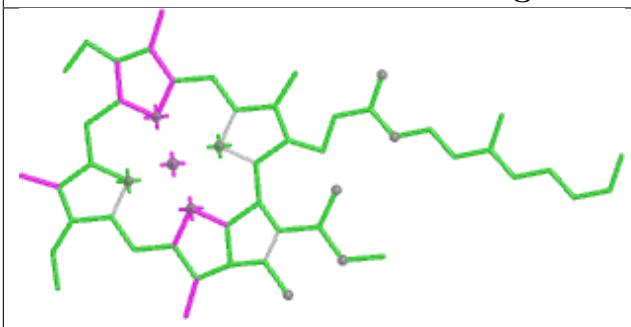


Torsions

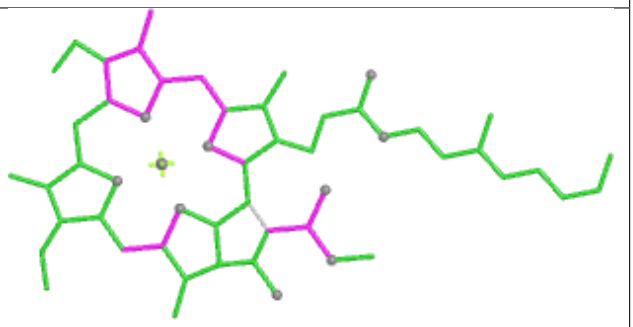


Rings

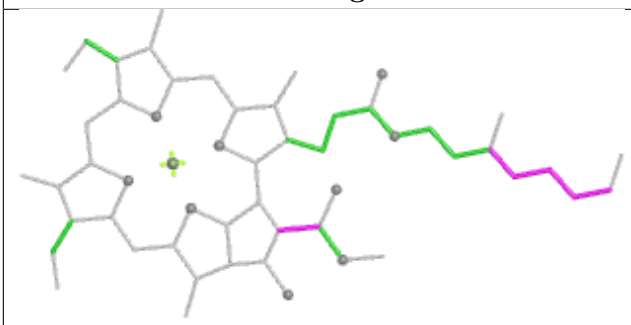
Ligand CLA bA 818



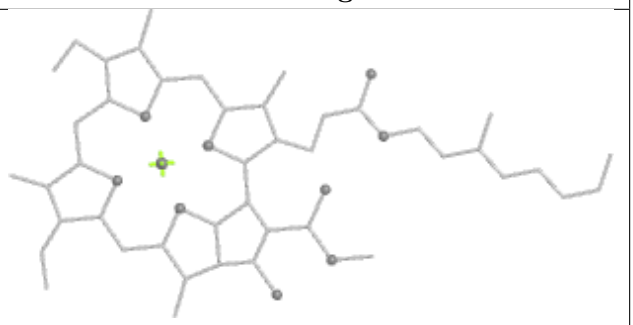
Bond lengths



Bond angles

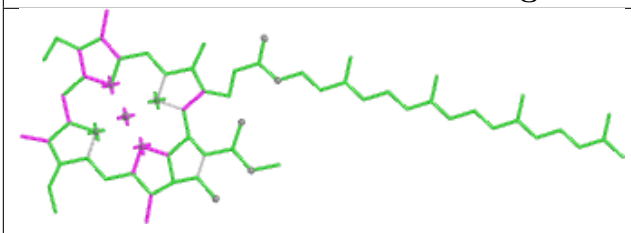


Torsions

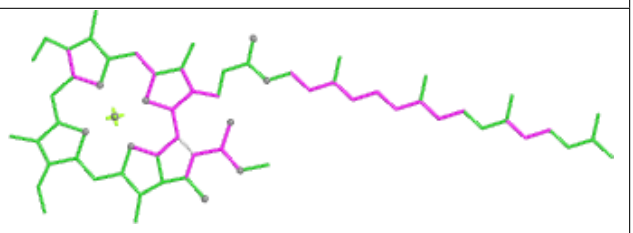


Rings

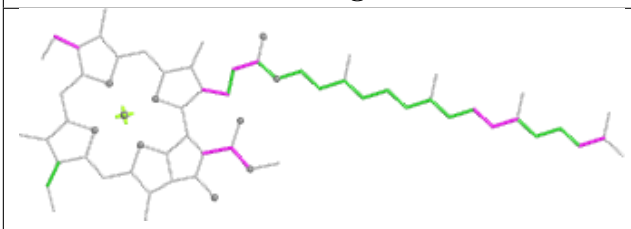
Ligand CLA c5 420



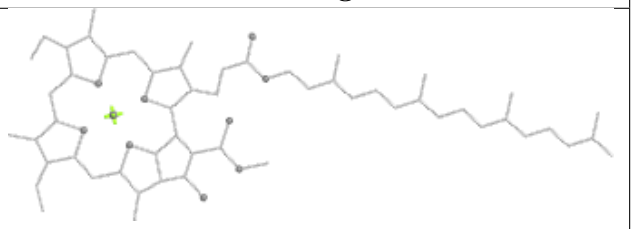
Bond lengths



Bond angles

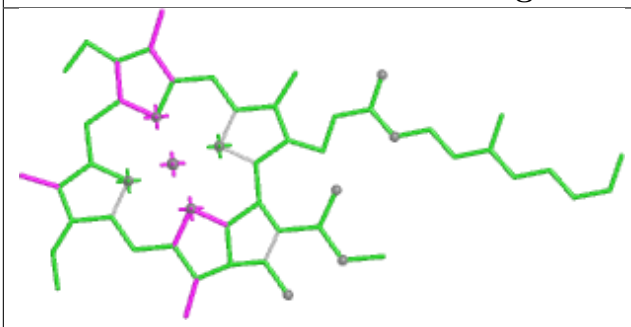


Torsions

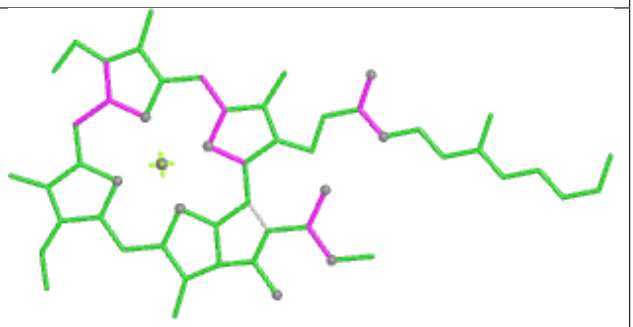


Rings

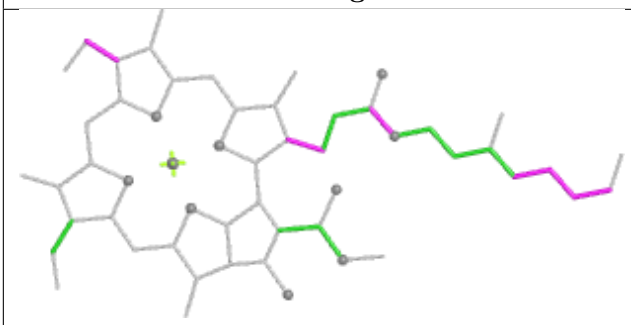
Ligand CLA cA 836



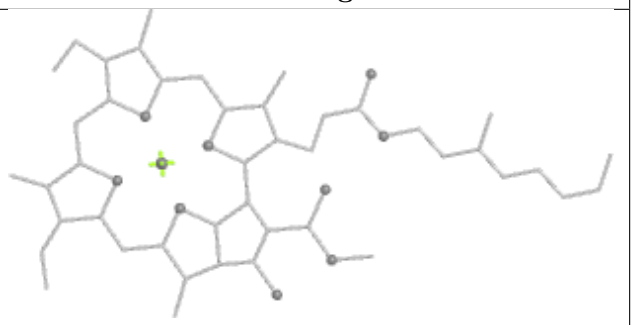
Bond lengths



Bond angles

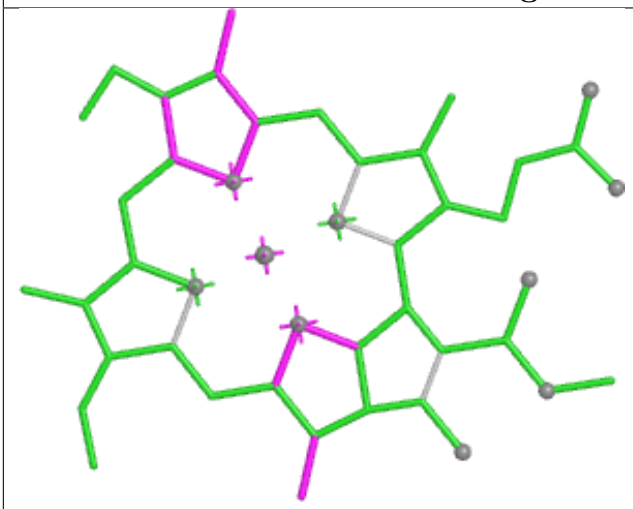


Torsions

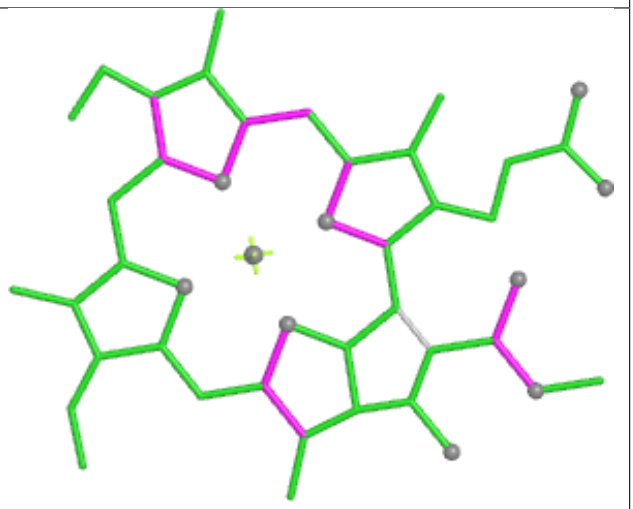


Rings

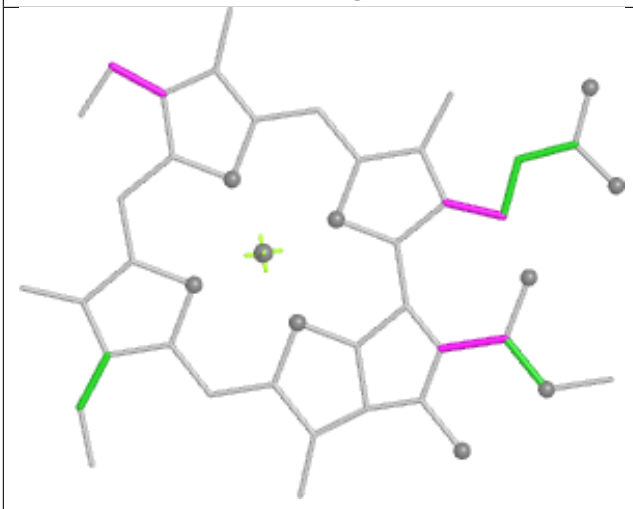
Ligand CLA c1 413



Bond lengths



Bond angles

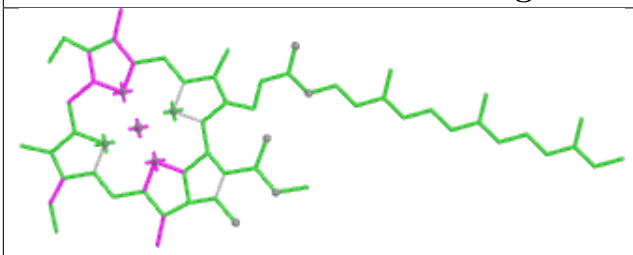


Torsions

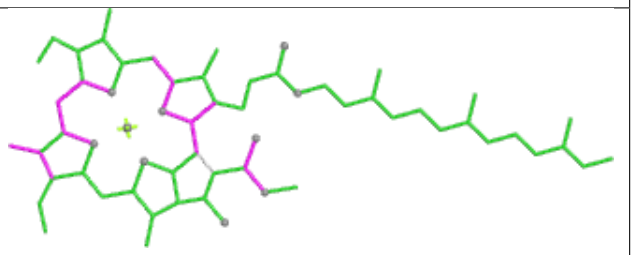


Rings

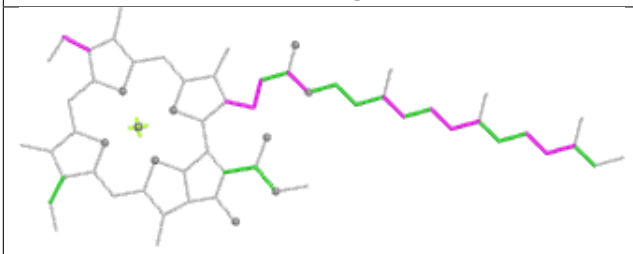
Ligand CLA aA 821



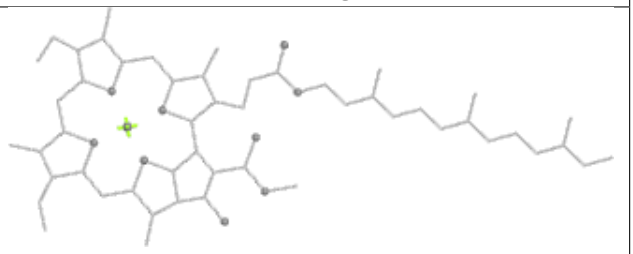
Bond lengths



Bond angles

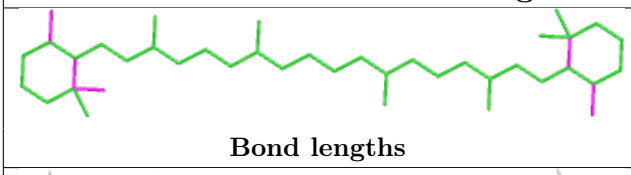


Torsions

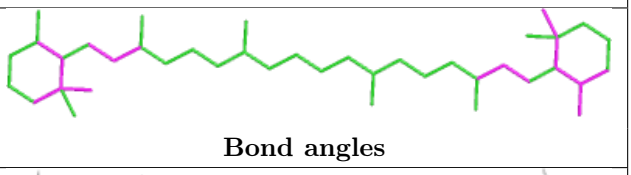


Rings

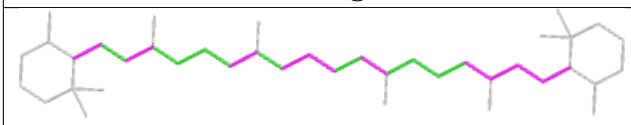
Ligand BCR cF 202



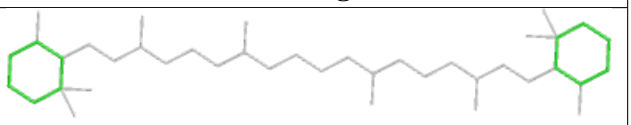
Bond lengths



Bond angles

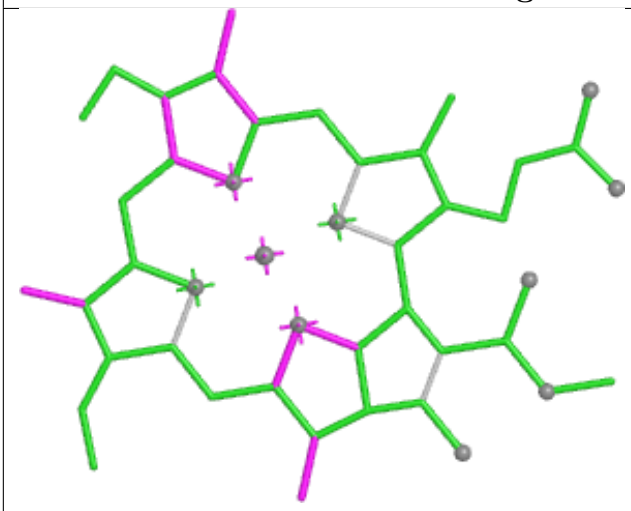


Torsions

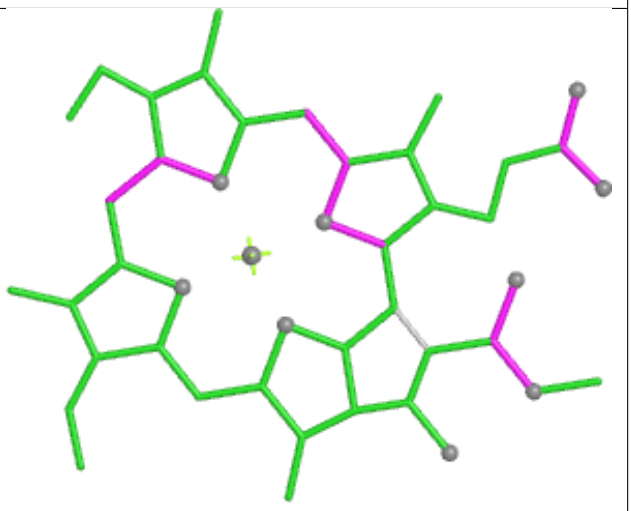


Rings

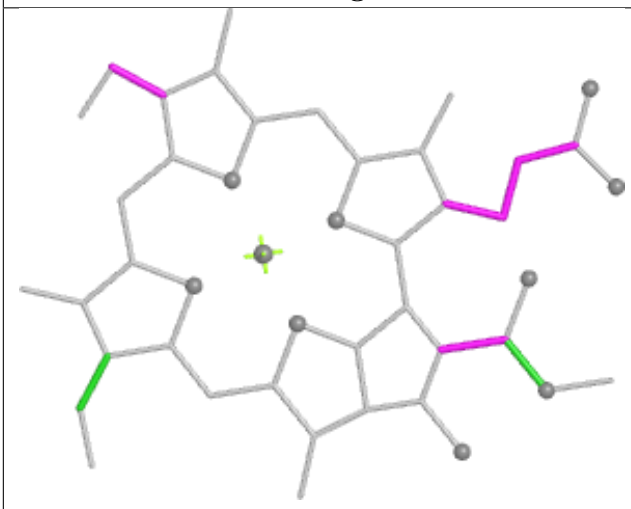
Ligand CLA cB 831



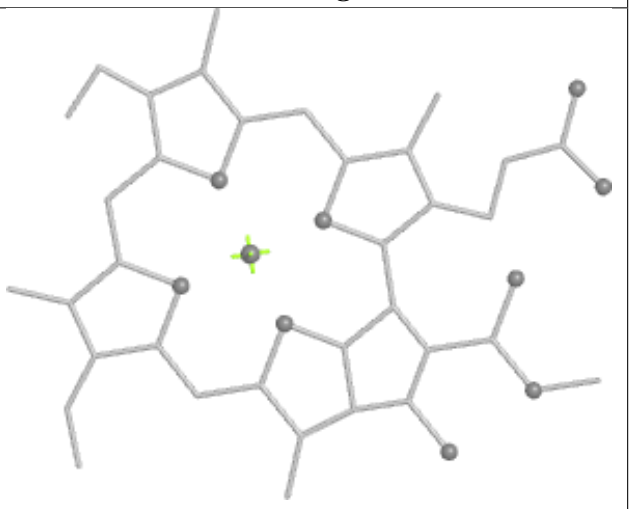
Bond lengths



Bond angles

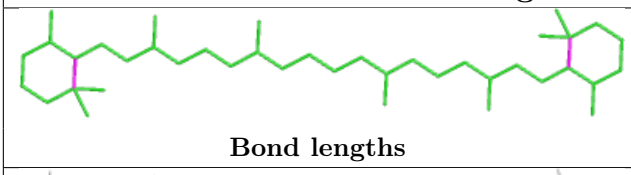


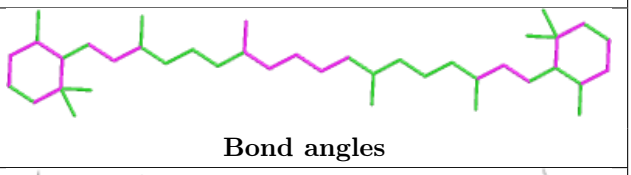
Torsions

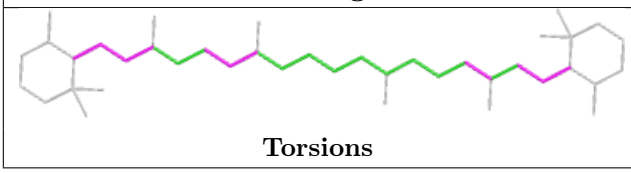


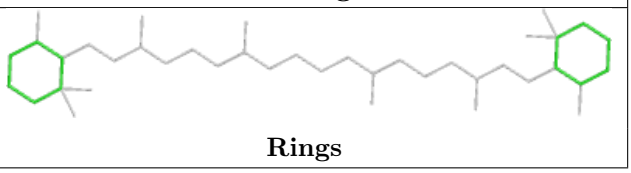
Rings

Ligand BCR b6 420

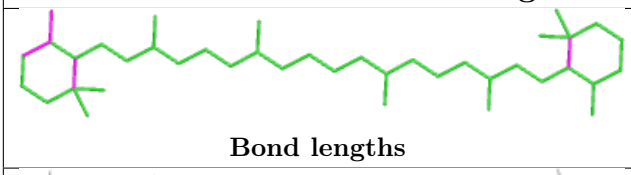

Bond lengths

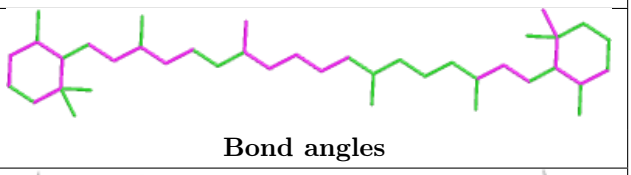

Bond angles

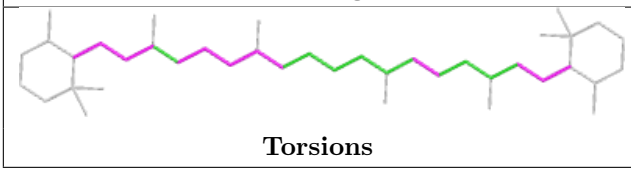

Torsions

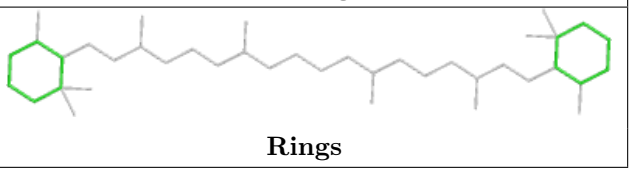

Rings

Ligand BCR c5 401

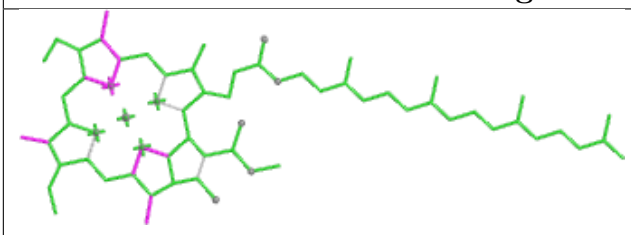

Bond lengths

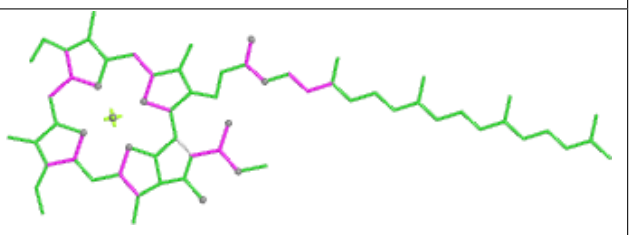

Bond angles

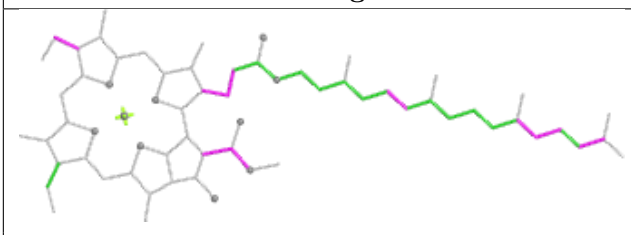

Torsions

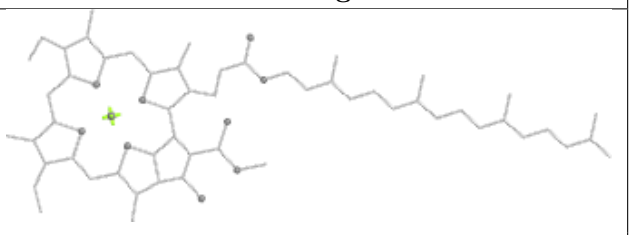

Rings

Ligand CLA cA 835


Bond lengths

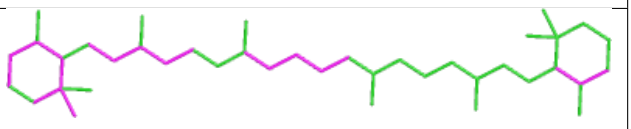

Bond angles

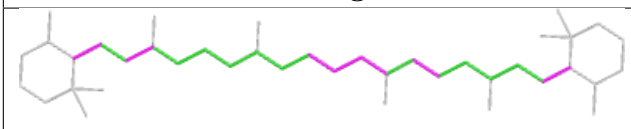

Torsions

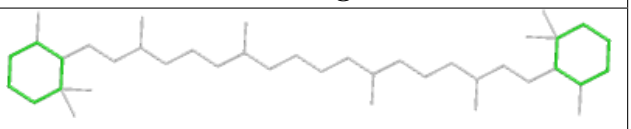

Rings

Ligand BCR bJ 105

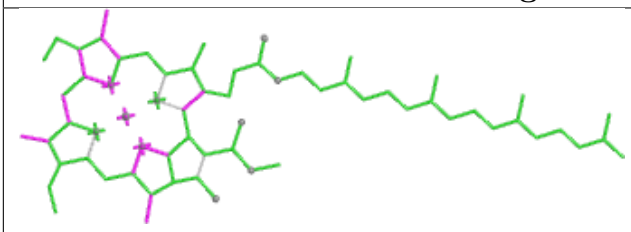

Bond lengths


Bond angles

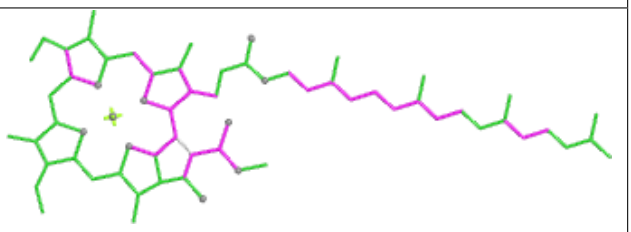

Torsions


Rings

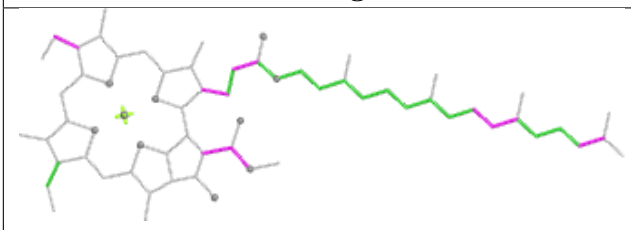
Ligand CLA a5 420



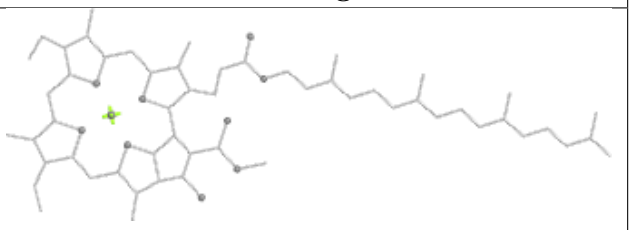
Bond lengths



Bond angles

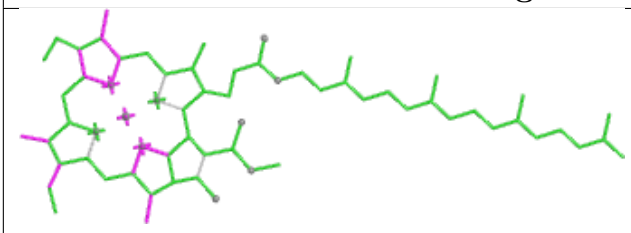


Torsions

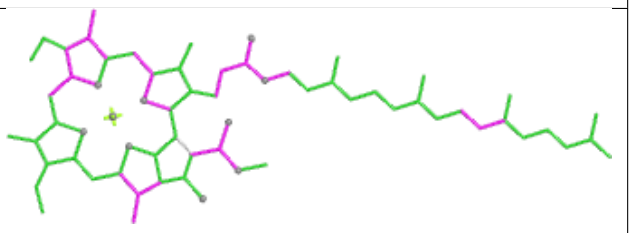


Rings

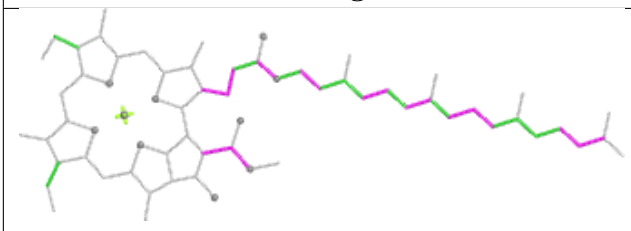
Ligand CLA cA 803



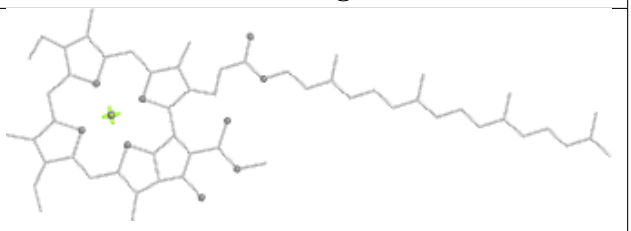
Bond lengths



Bond angles

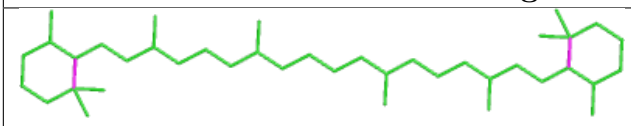


Torsions

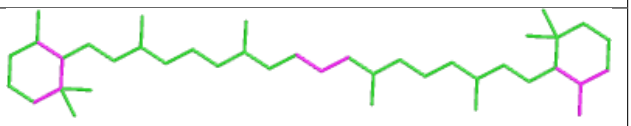


Rings

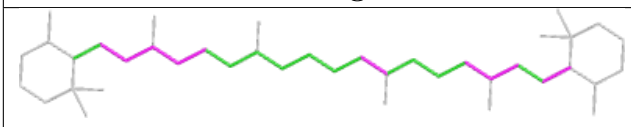
Ligand BCR cI 101



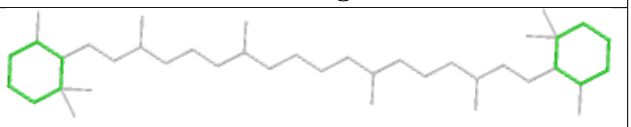
Bond lengths



Bond angles

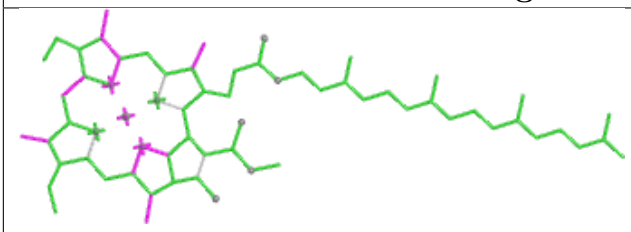


Torsions

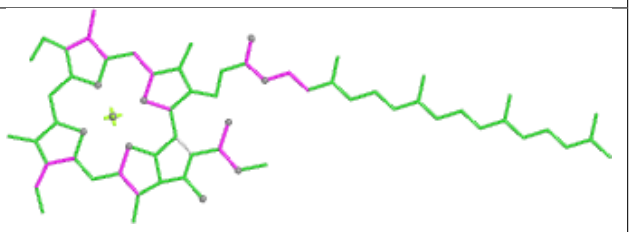


Rings

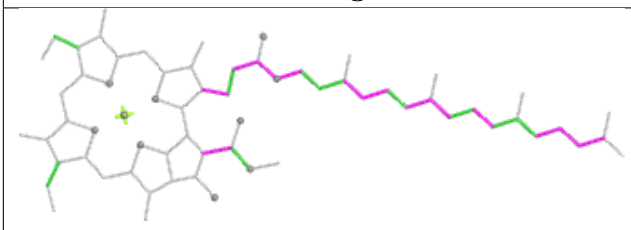
Ligand CLA aB 806



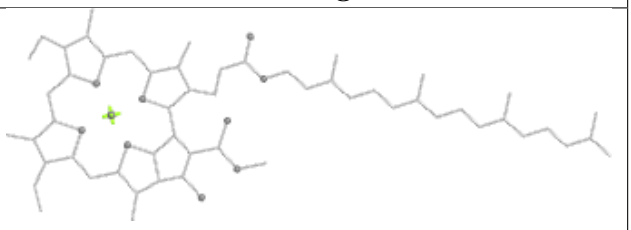
Bond lengths



Bond angles

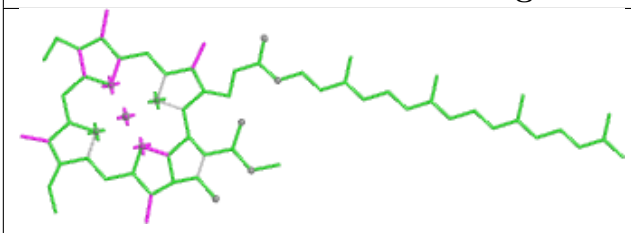


Torsions

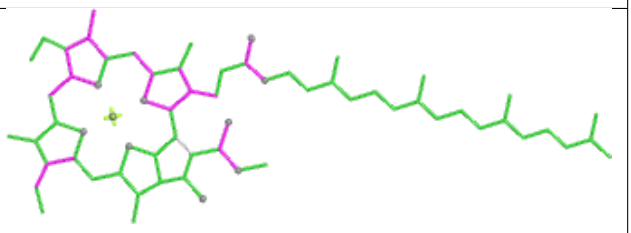


Rings

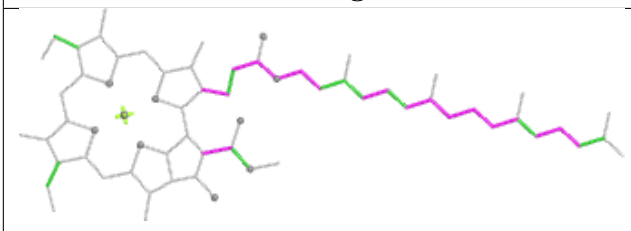
Ligand CLA cA 806



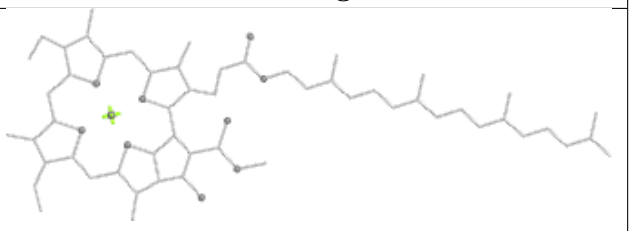
Bond lengths



Bond angles

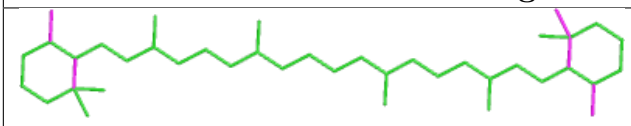


Torsions

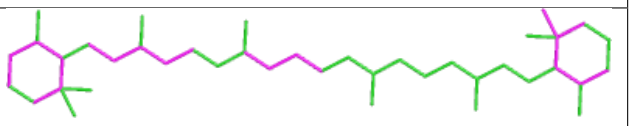


Rings

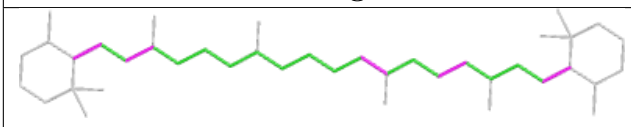
Ligand BCR c1 418



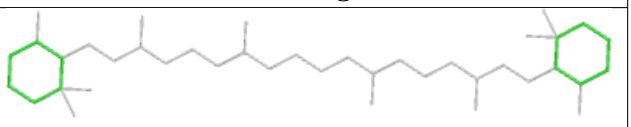
Bond lengths



Bond angles

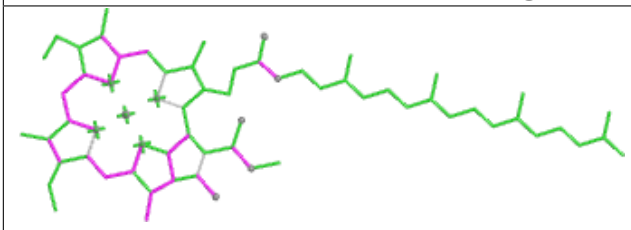


Torsions

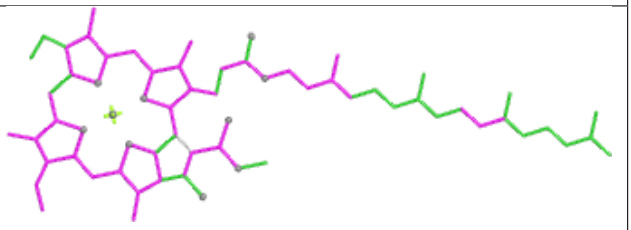


Rings

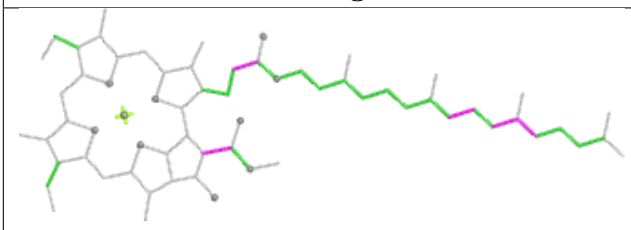
Ligand CL0 cA 801



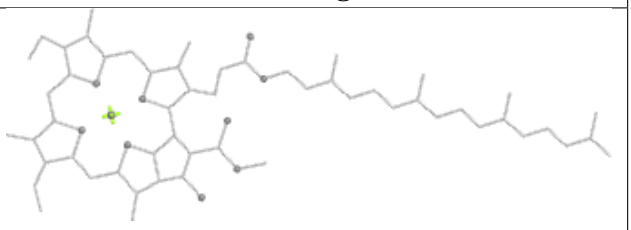
Bond lengths



Bond angles

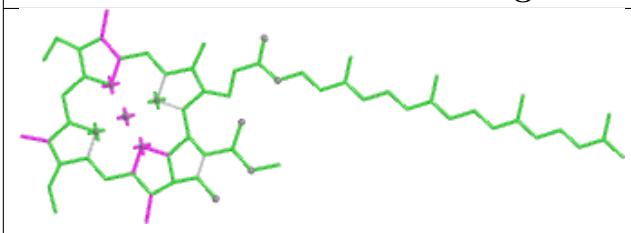


Torsions

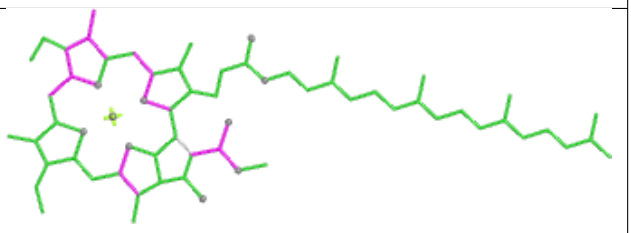


Rings

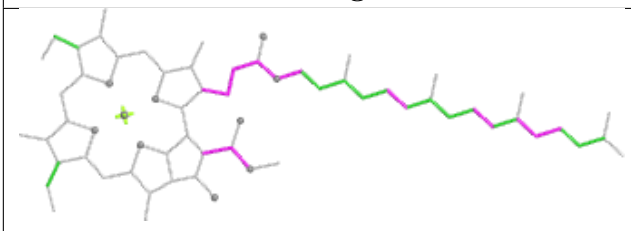
Ligand CLA bB 829



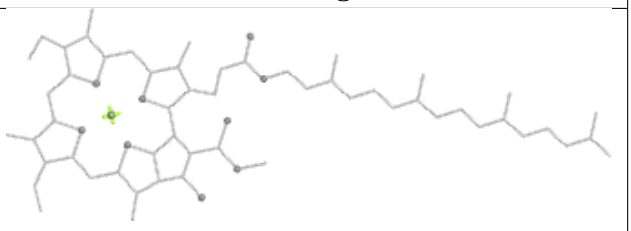
Bond lengths



Bond angles

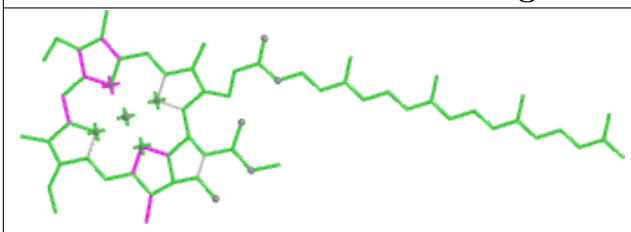


Torsions

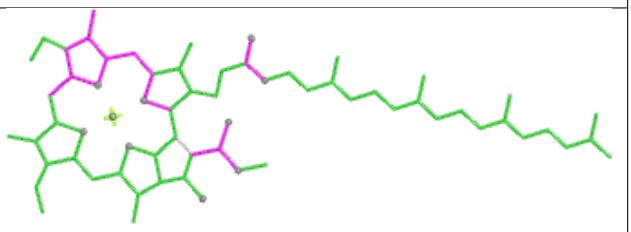


Rings

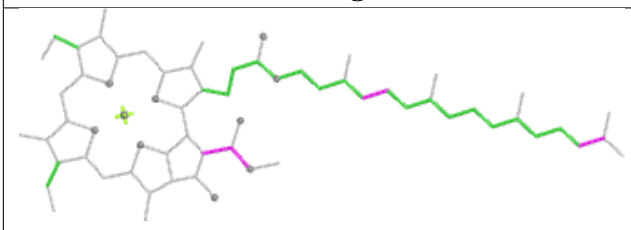
Ligand CLA b4 409



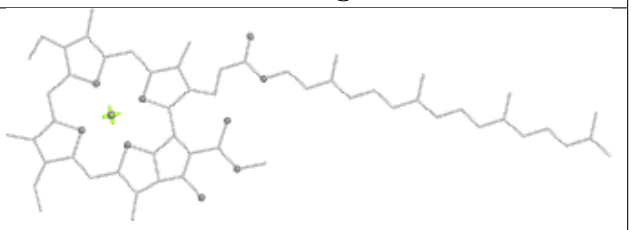
Bond lengths



Bond angles

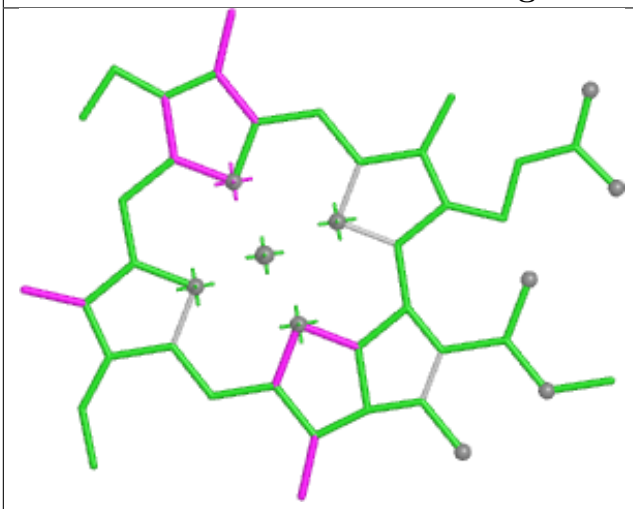


Torsions

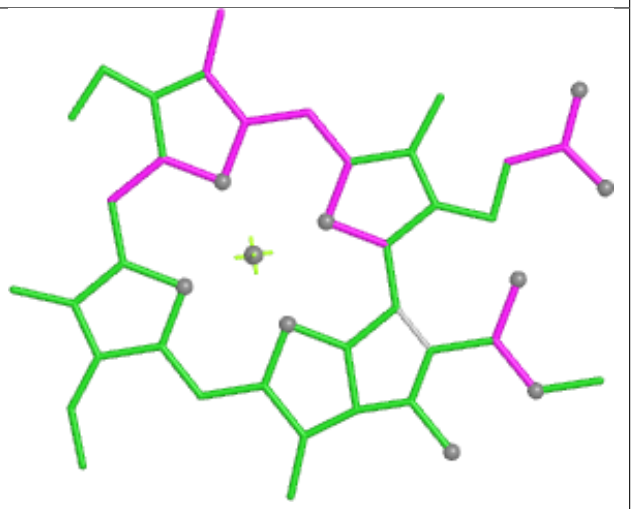


Rings

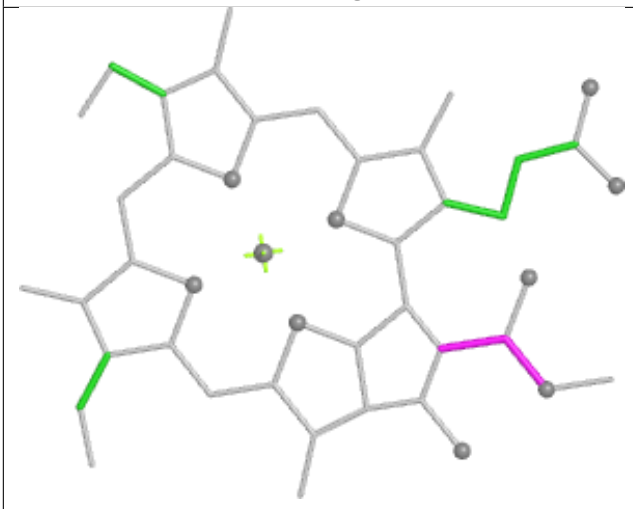
Ligand CLA b5 406



Bond lengths



Bond angles

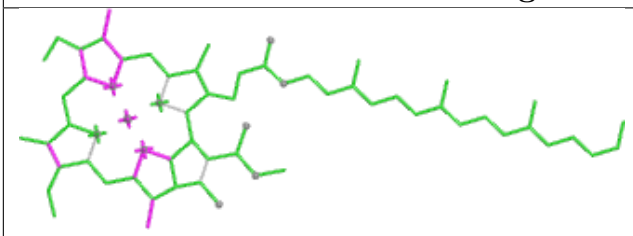


Torsions

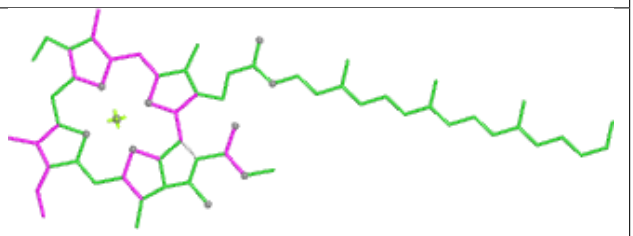


Rings

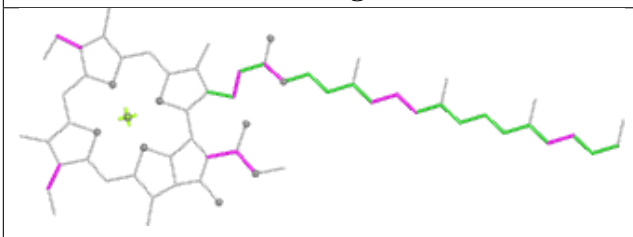
Ligand CLA b4 410



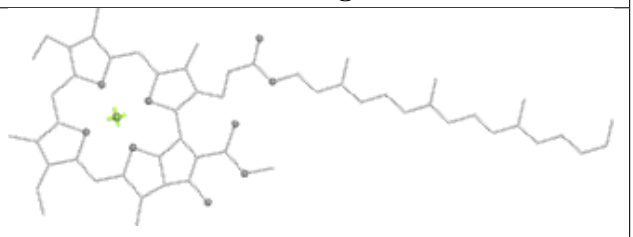
Bond lengths



Bond angles

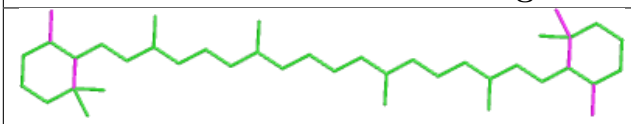


Torsions

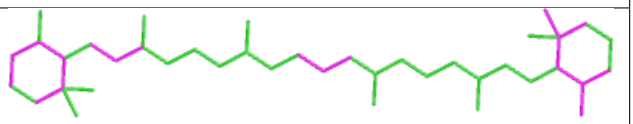


Rings

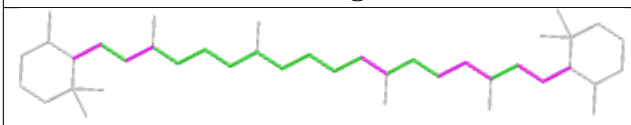
Ligand BCR b6 419



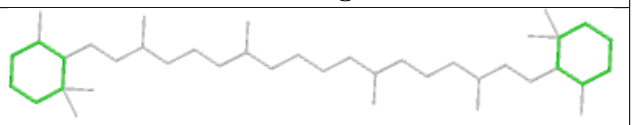
Bond lengths



Bond angles

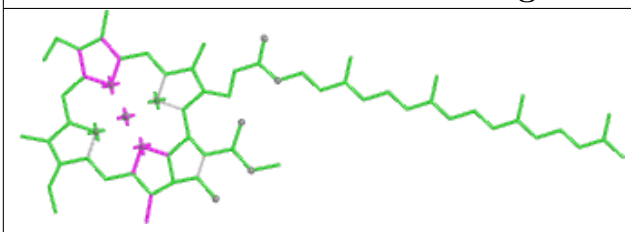


Torsions

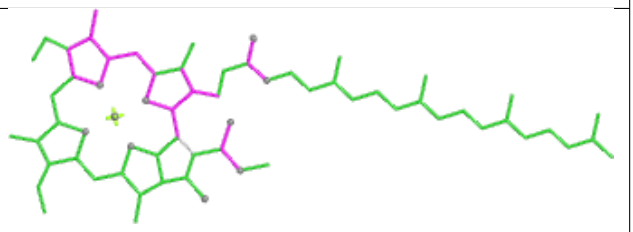


Rings

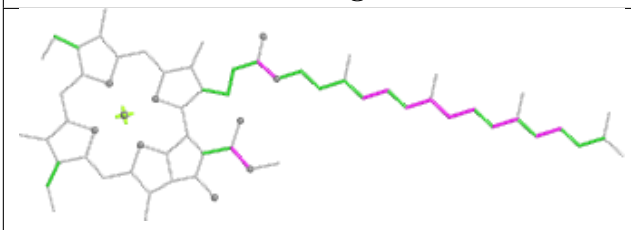
Ligand CLA b3 403



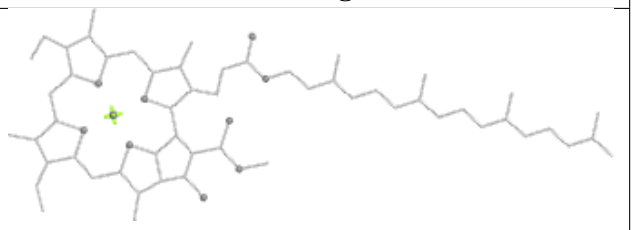
Bond lengths



Bond angles

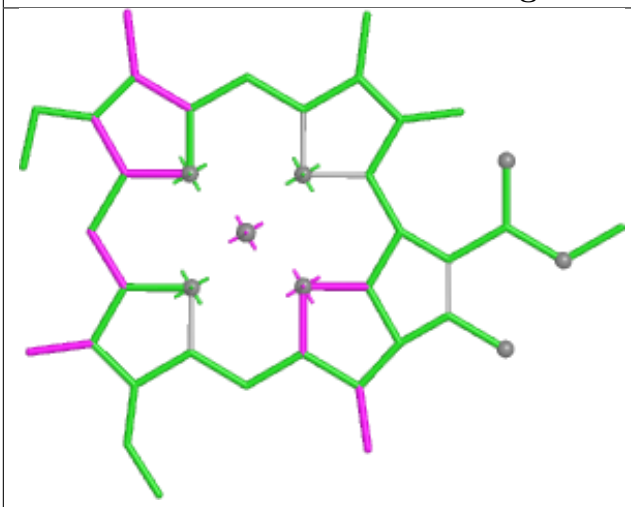


Torsions

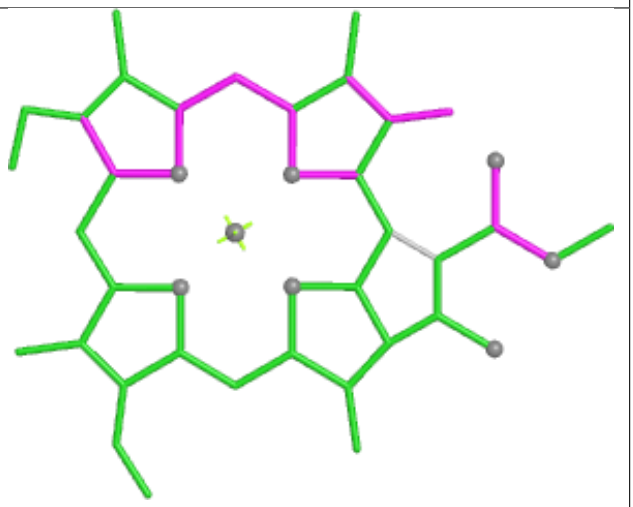


Rings

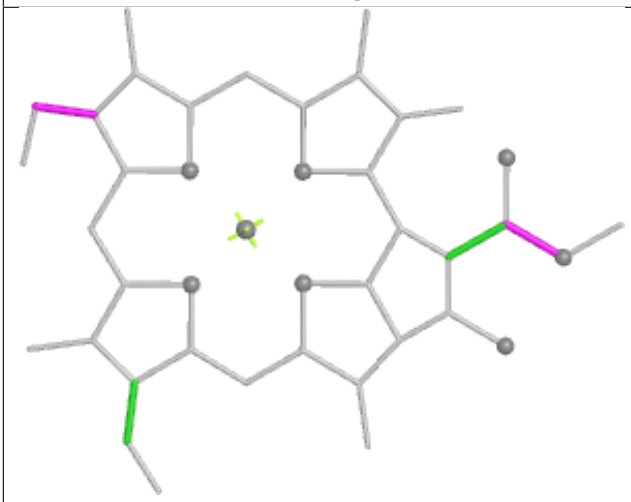
Ligand CLA a3 414



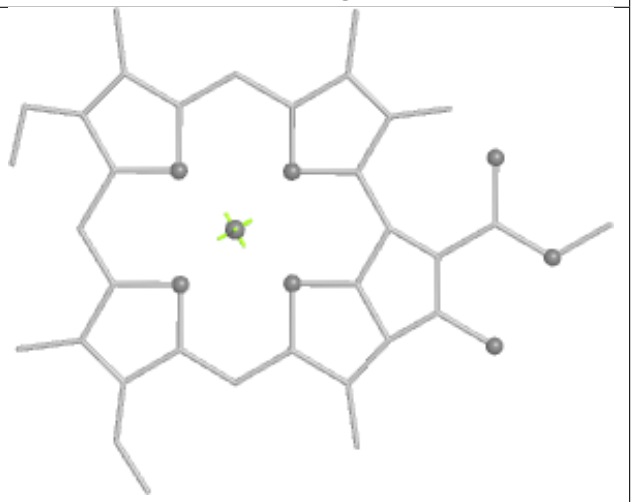
Bond lengths



Bond angles

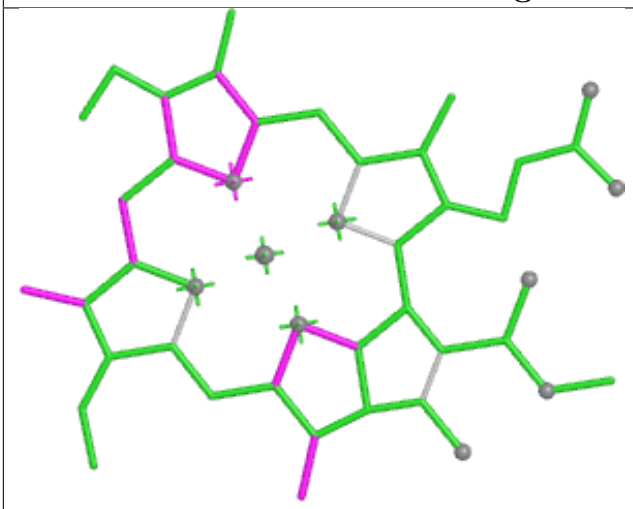


Torsions

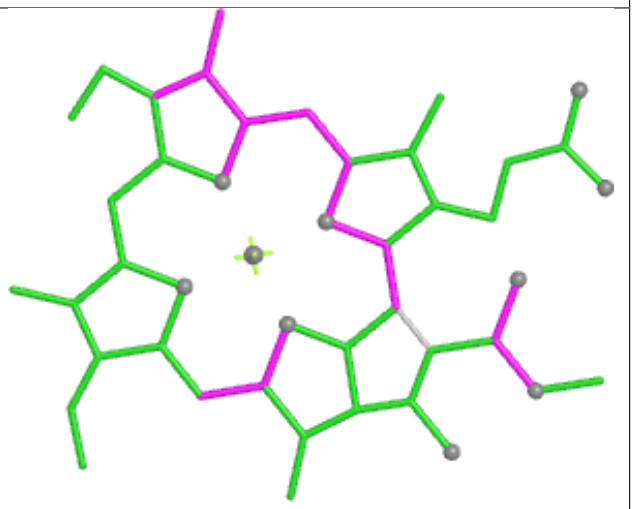


Rings

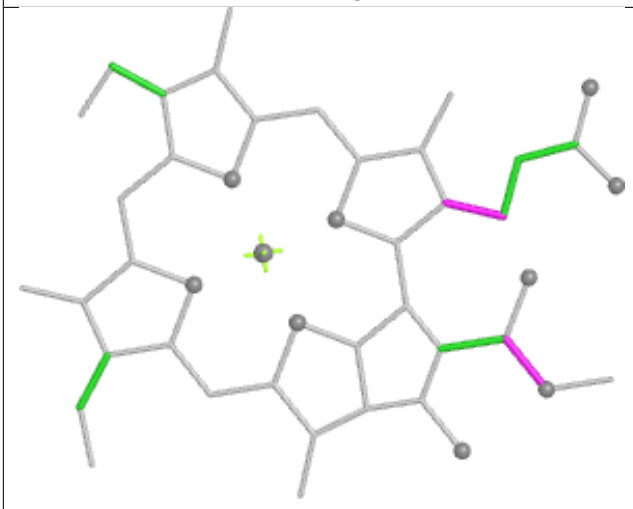
Ligand CLA bB 812



Bond lengths



Bond angles

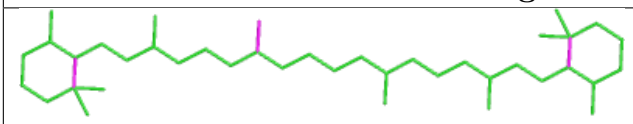


Torsions

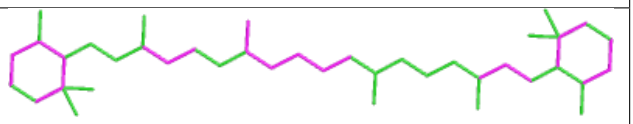


Rings

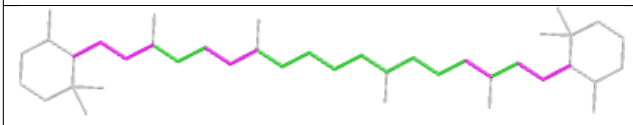
Ligand BCR c1 420



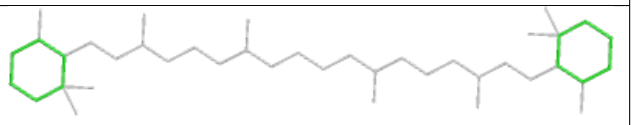
Bond lengths



Bond angles

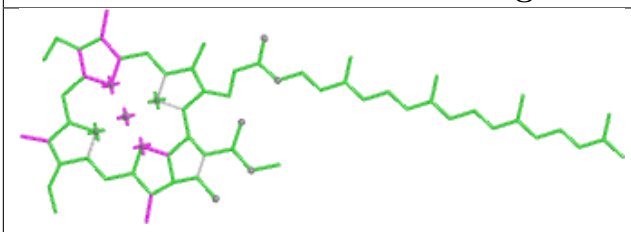


Torsions

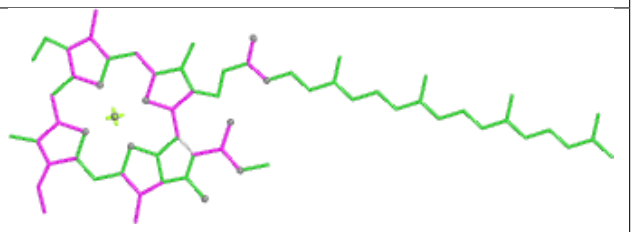


Rings

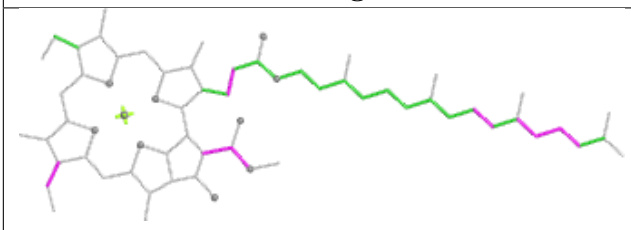
Ligand CLA aB 804



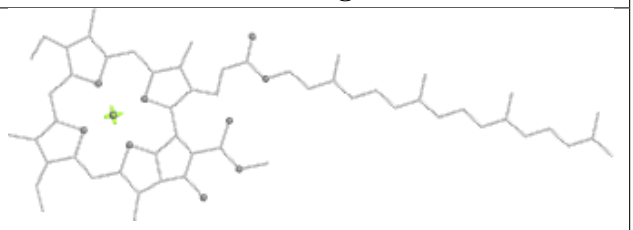
Bond lengths



Bond angles



Torsions

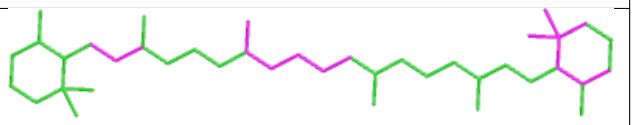


Rings

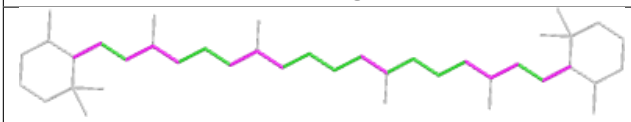
Ligand BCR bB 846



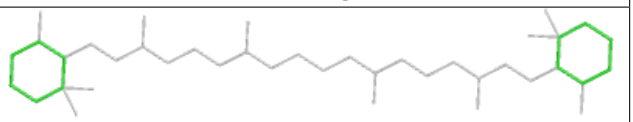
Bond lengths



Bond angles

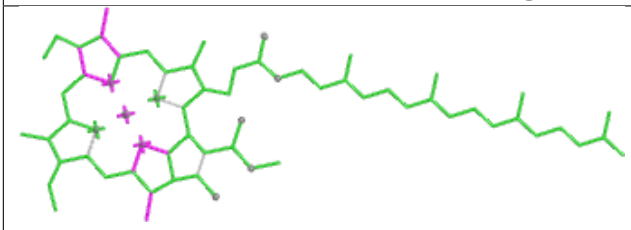


Torsions

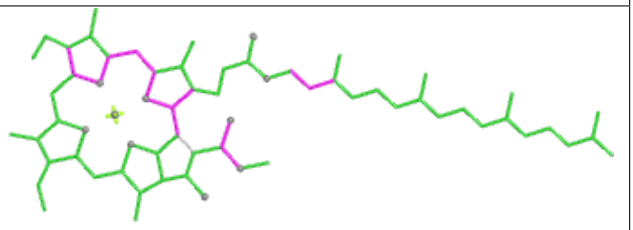


Rings

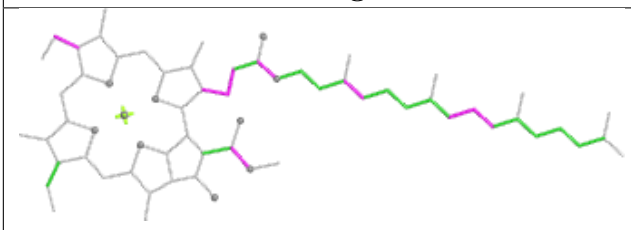
Ligand CLA c3 404



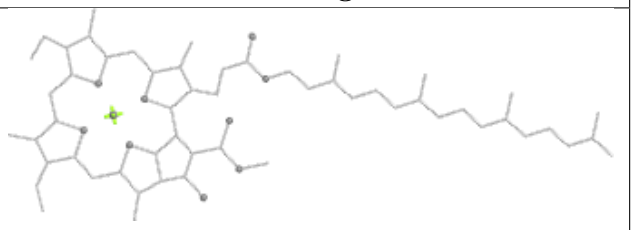
Bond lengths



Bond angles

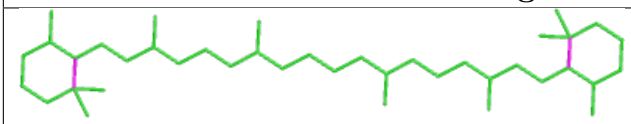


Torsions

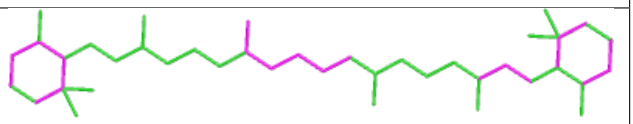


Rings

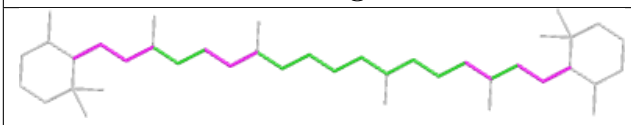
Ligand BCR a3 420



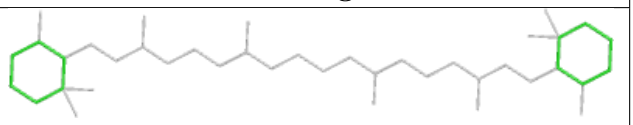
Bond lengths



Bond angles

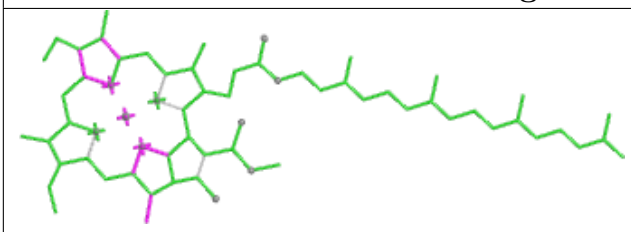


Torsions

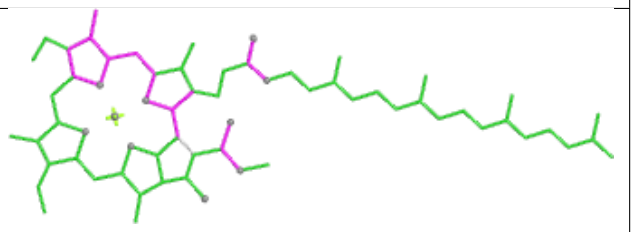


Rings

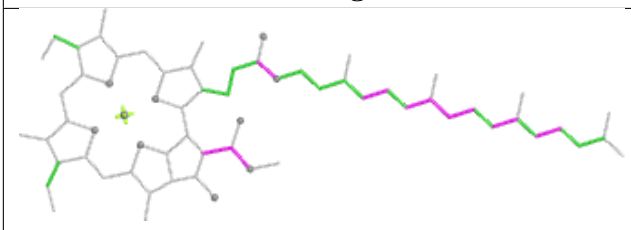
Ligand CLA a4 403



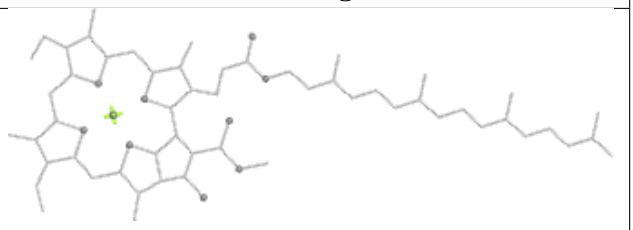
Bond lengths



Bond angles

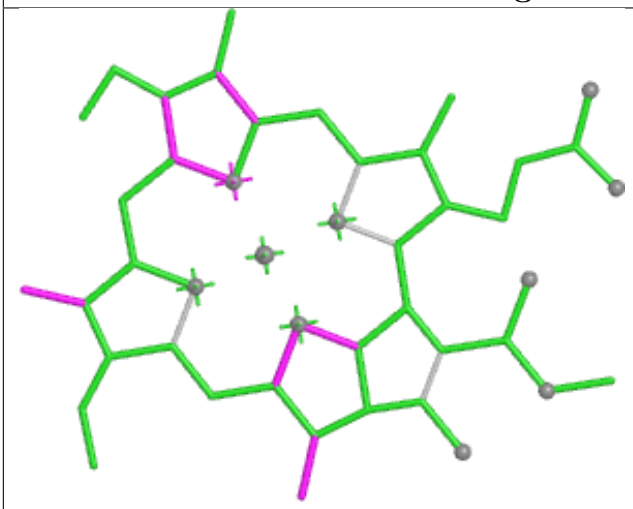


Torsions

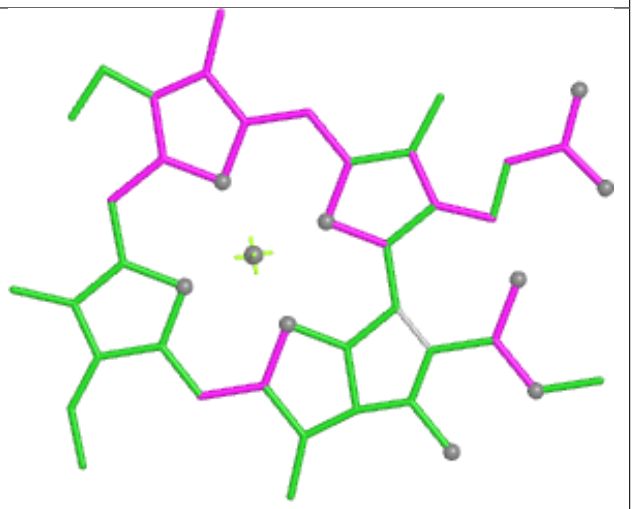


Rings

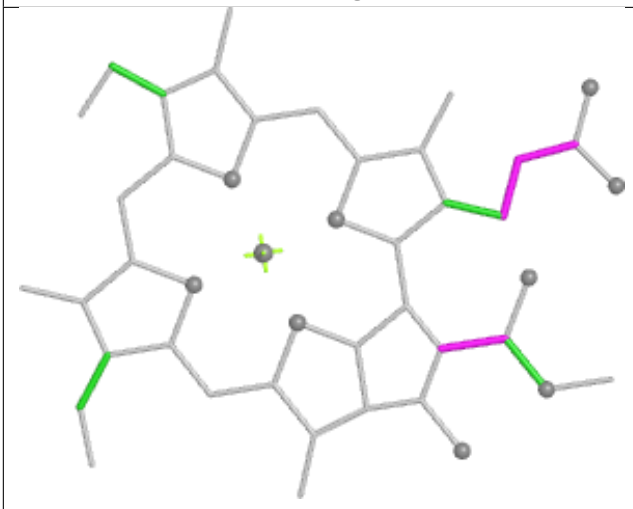
Ligand CLA bB 824



Bond lengths



Bond angles

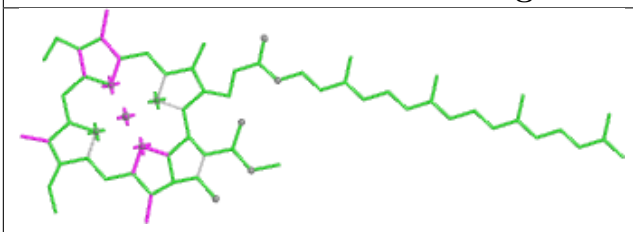


Torsions

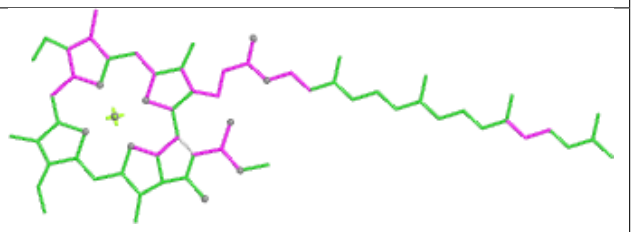


Rings

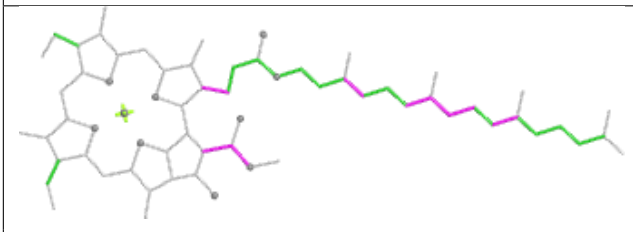
Ligand CLA aB 827



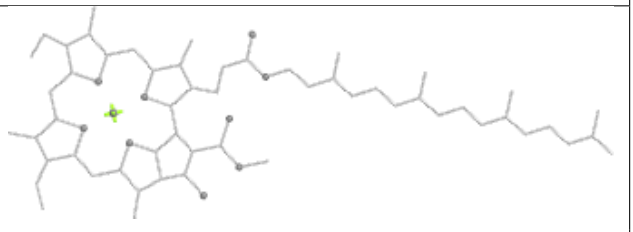
Bond lengths



Bond angles

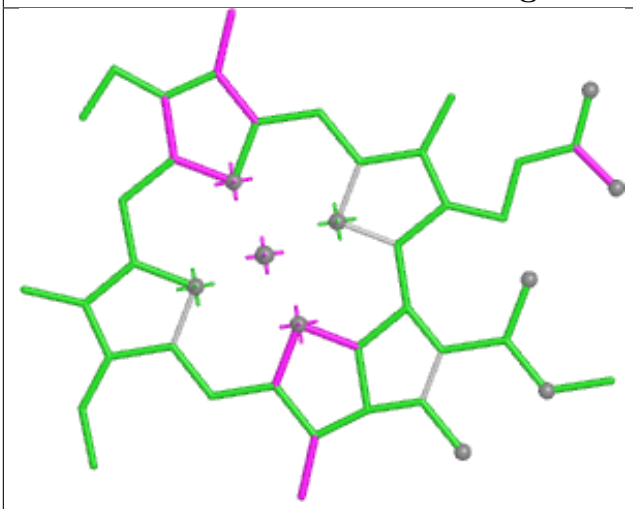


Torsions

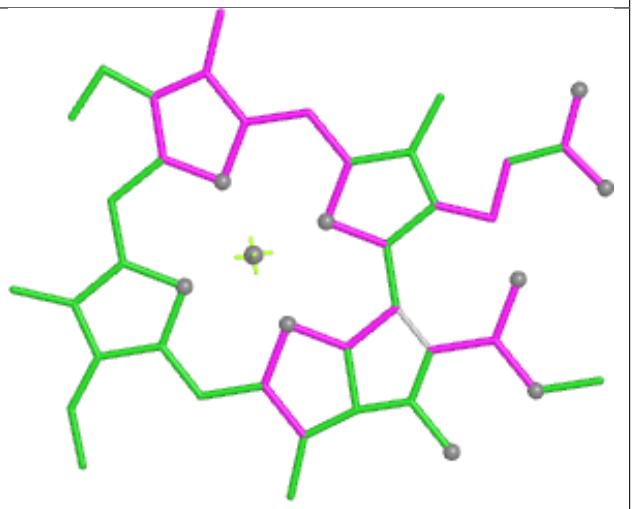


Rings

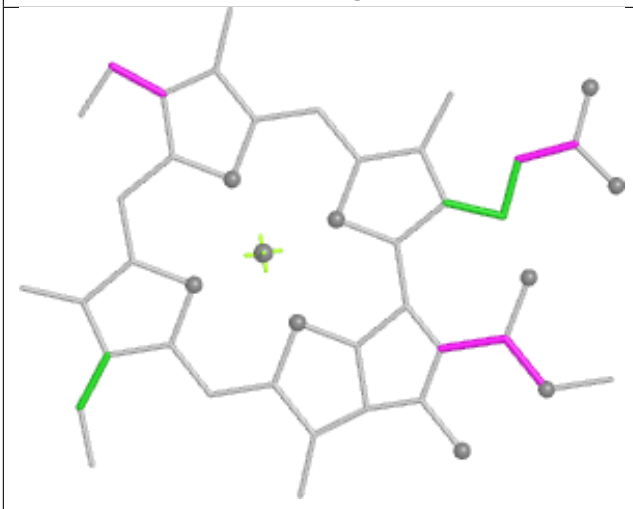
Ligand CLA a5 415



Bond lengths



Bond angles

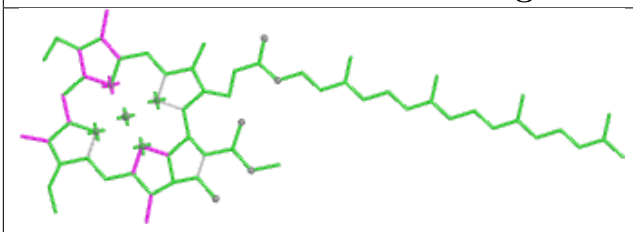


Torsions

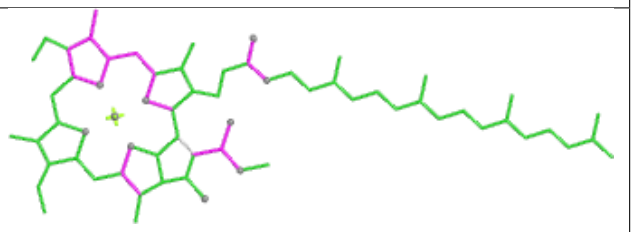


Rings

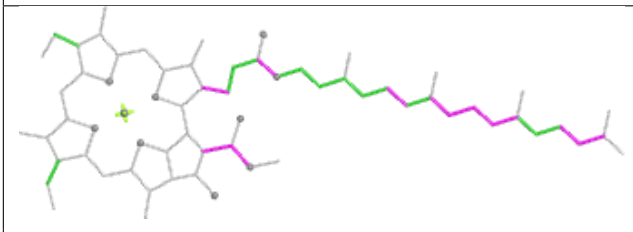
Ligand CLA aB 815



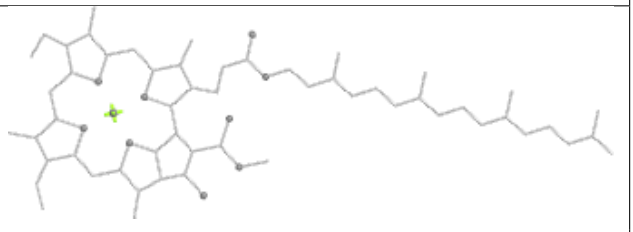
Bond lengths



Bond angles

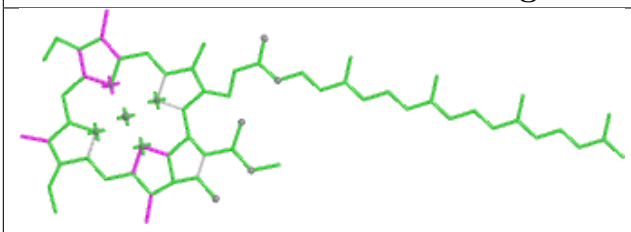


Torsions

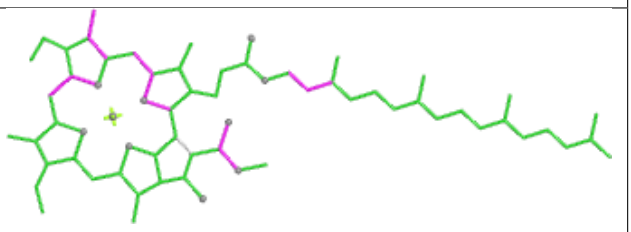


Rings

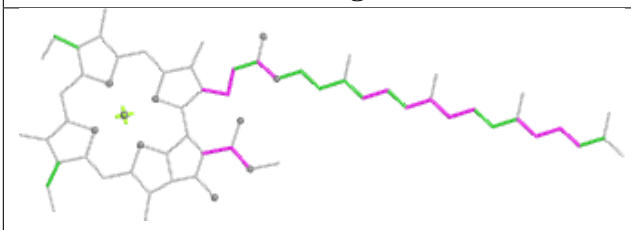
Ligand CLA a5 402



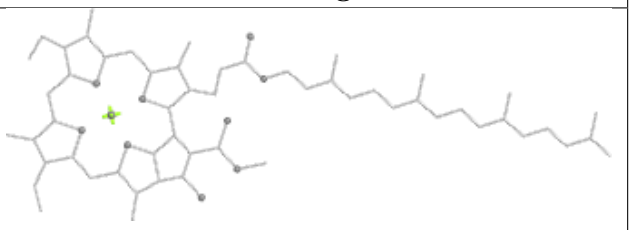
Bond lengths



Bond angles

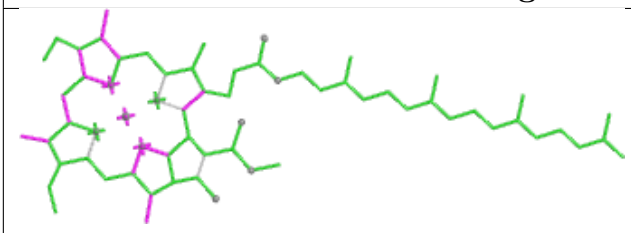


Torsions

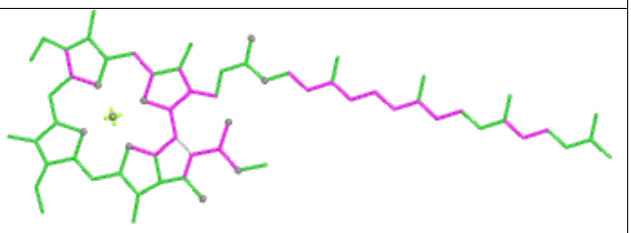


Rings

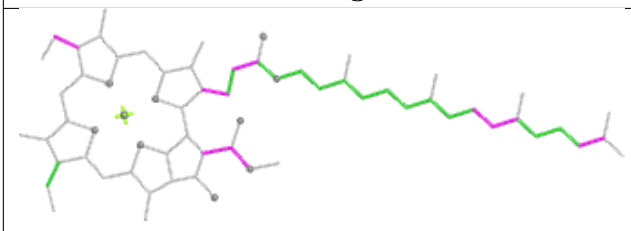
Ligand CLA b5 420



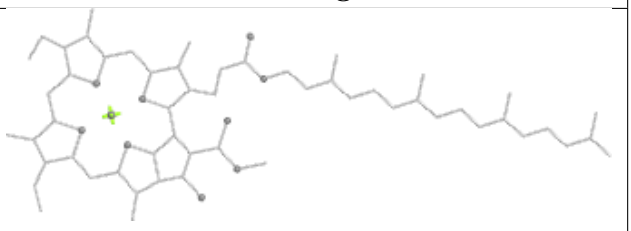
Bond lengths



Bond angles

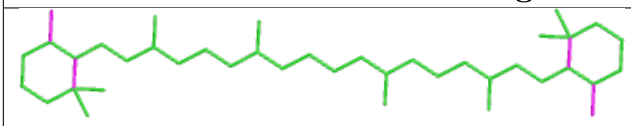


Torsions

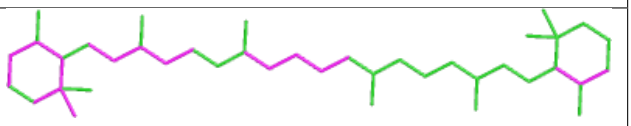


Rings

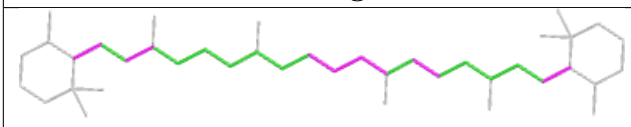
Ligand BCR aF 203



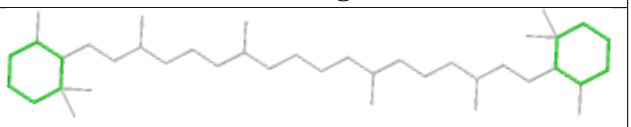
Bond lengths



Bond angles

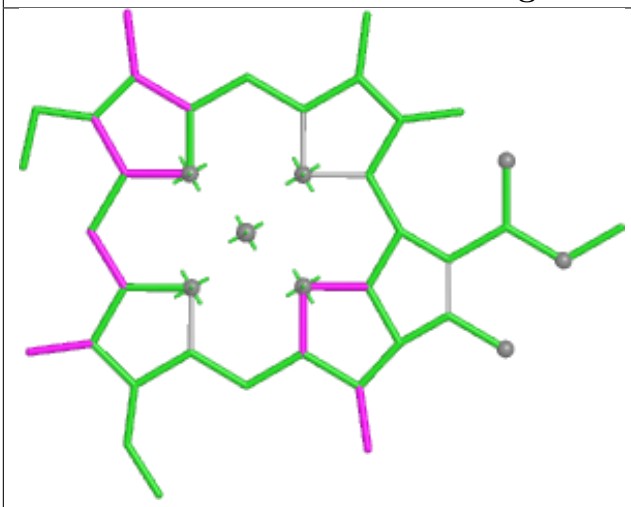


Torsions

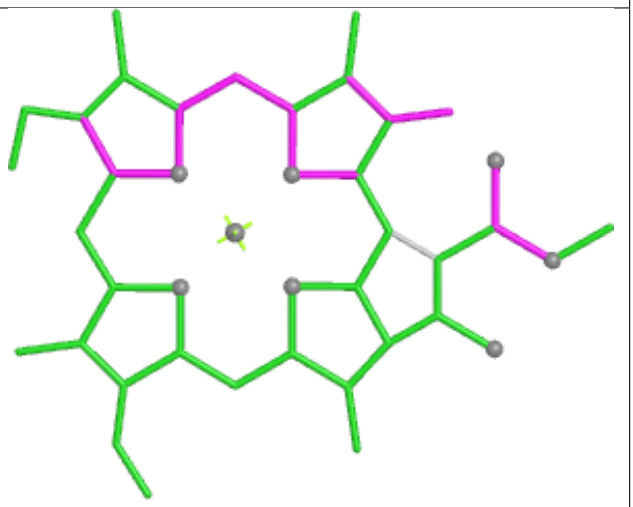


Rings

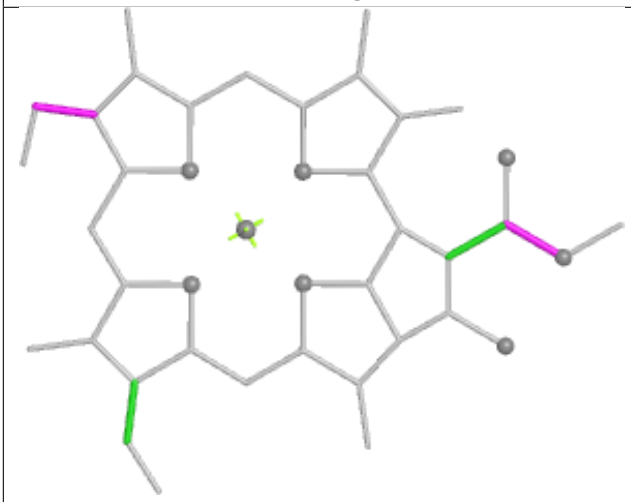
Ligand CLA b5 414



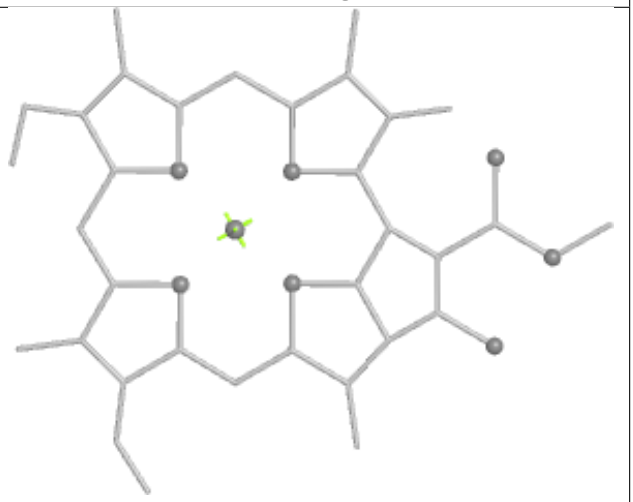
Bond lengths



Bond angles

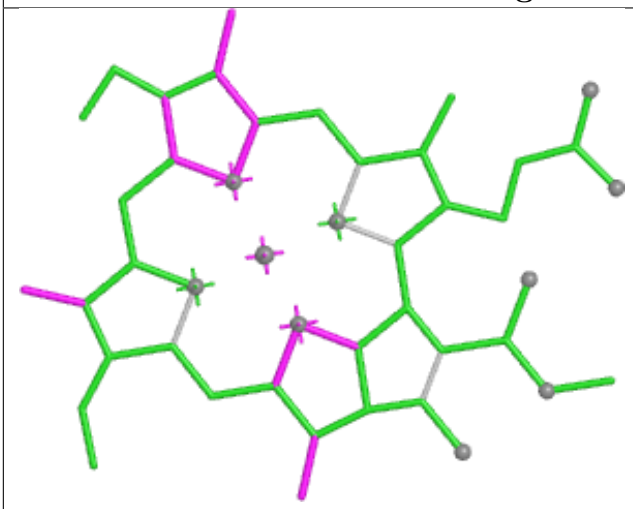


Torsions

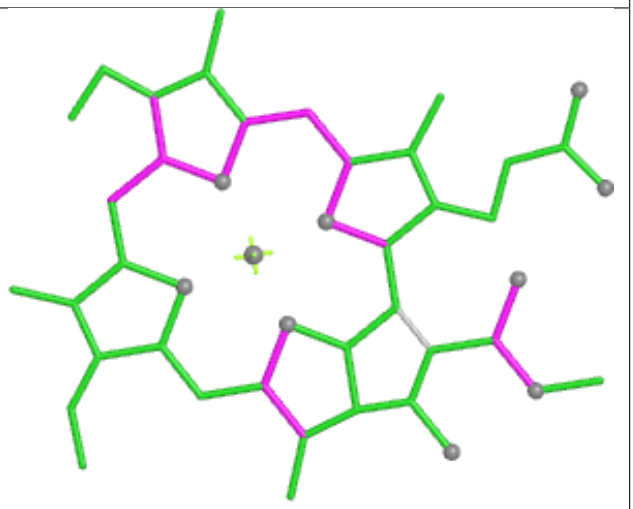


Rings

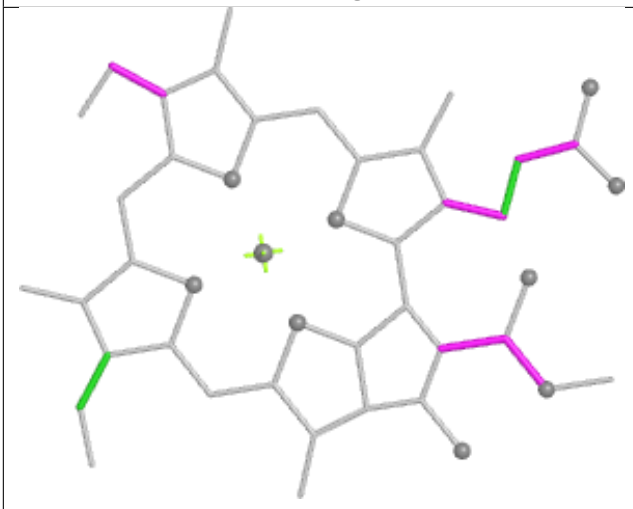
Ligand CLA cA 811



Bond lengths



Bond angles

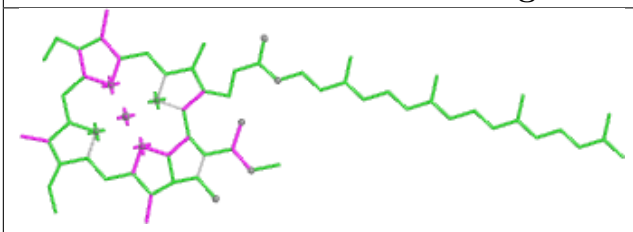


Torsions

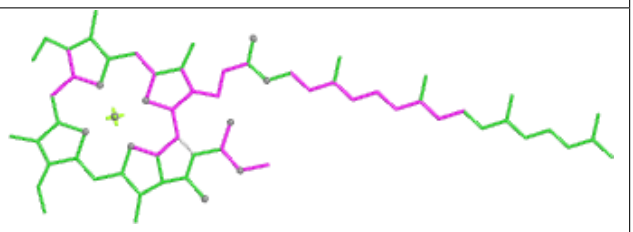


Rings

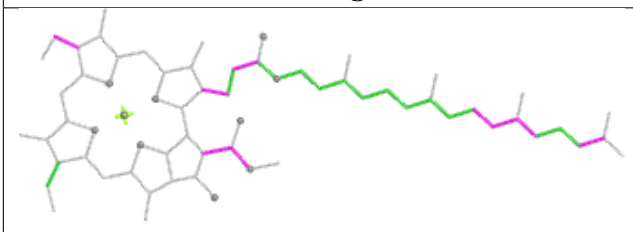
Ligand CLA b4 421



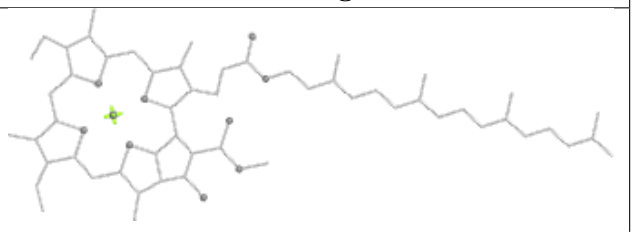
Bond lengths



Bond angles

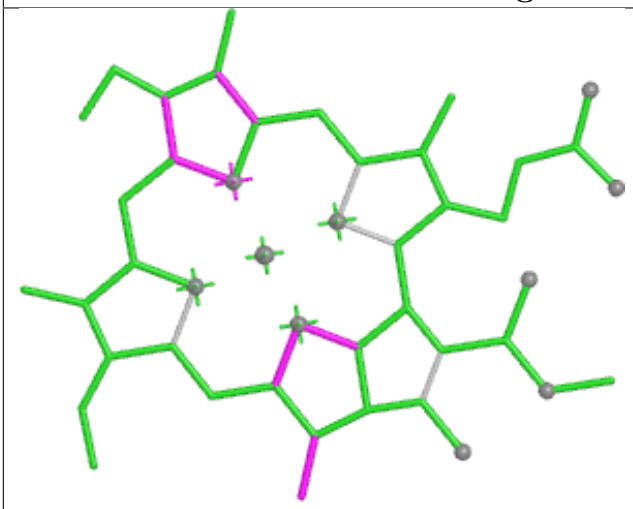


Torsions

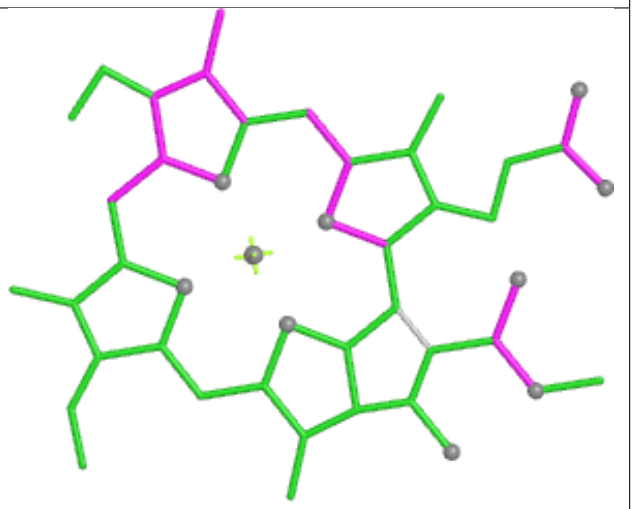


Rings

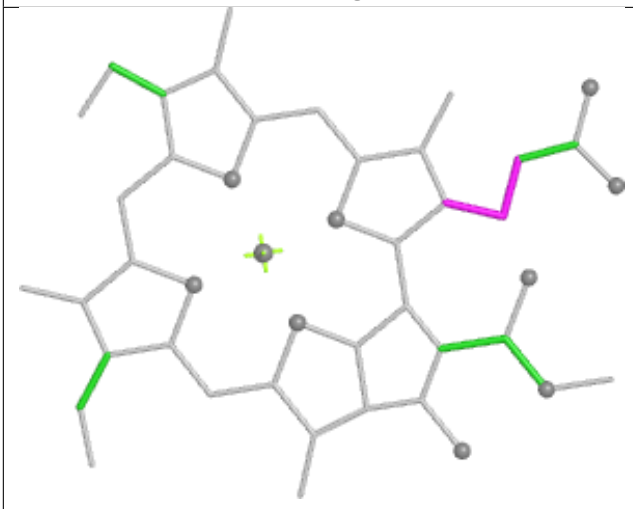
Ligand CLA cB 822



Bond lengths



Bond angles

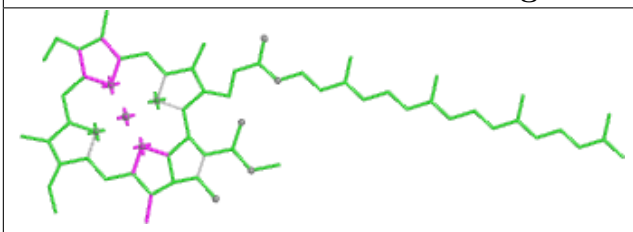


Torsions

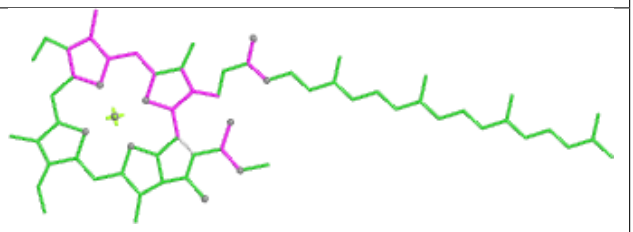


Rings

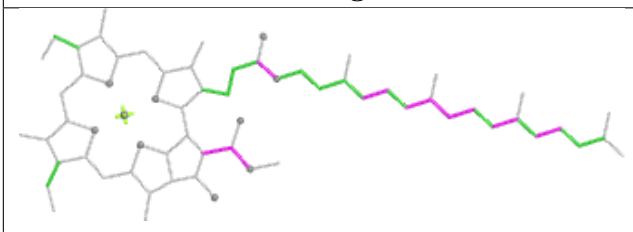
Ligand CLA c5 403



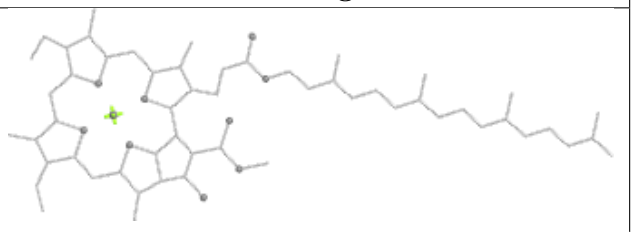
Bond lengths



Bond angles

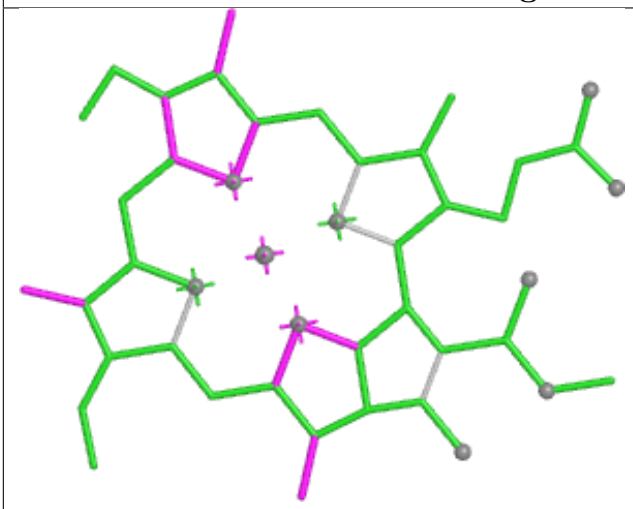


Torsions

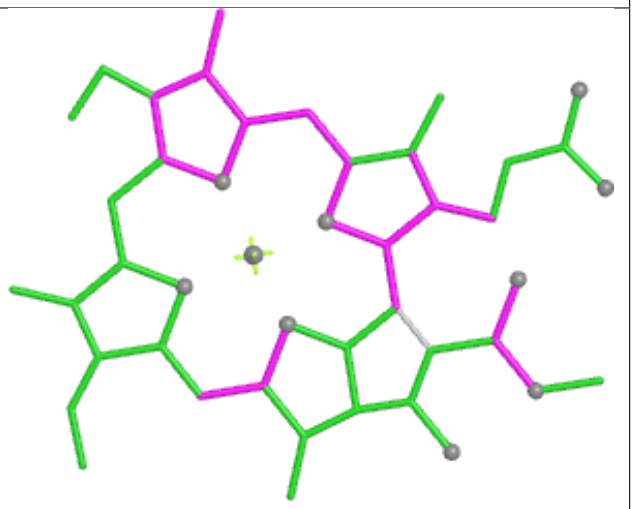


Rings

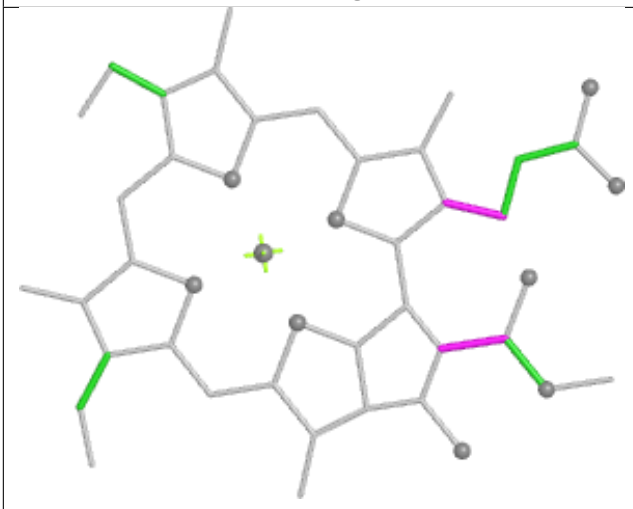
Ligand CLA a5 411



Bond lengths



Bond angles

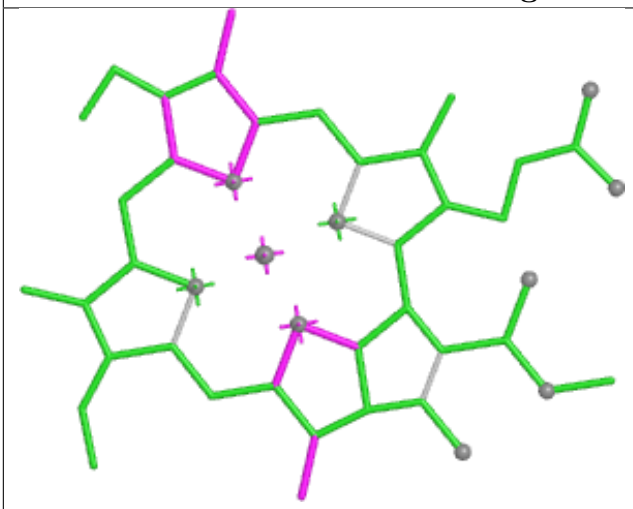


Torsions

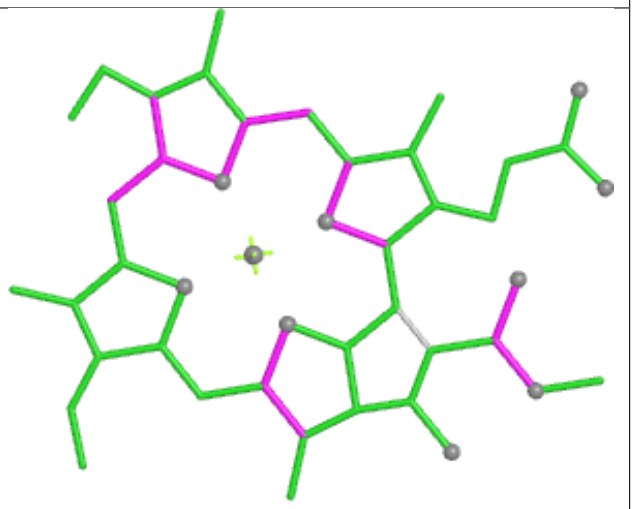


Rings

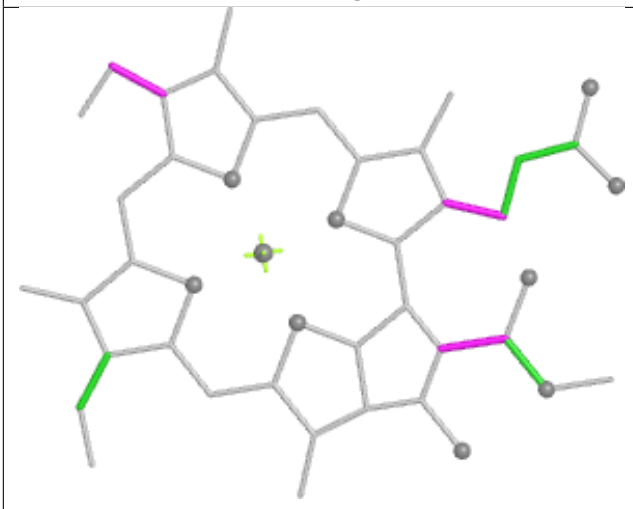
Ligand CLA c3 413



Bond lengths



Bond angles

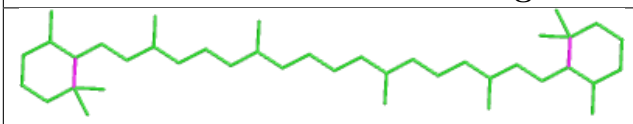


Torsions

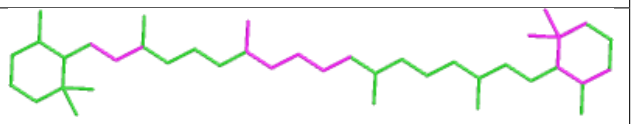


Rings

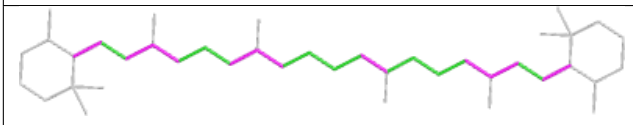
Ligand BCR cB 846



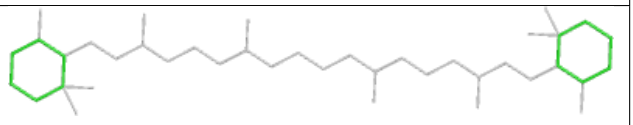
Bond lengths



Bond angles

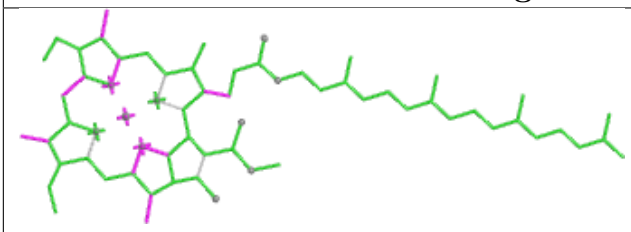


Torsions

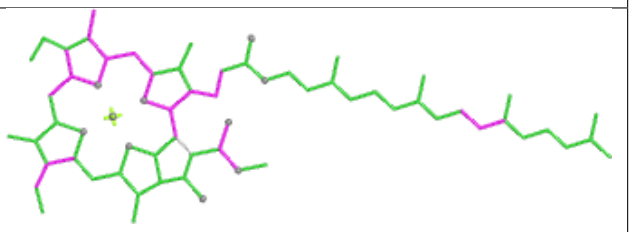


Rings

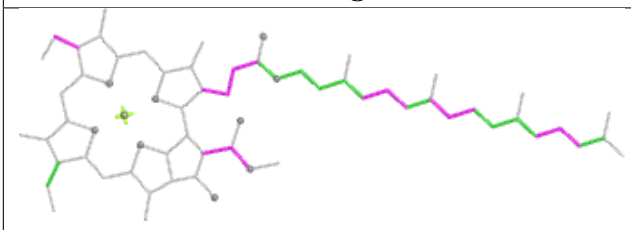
Ligand CLA bB 810



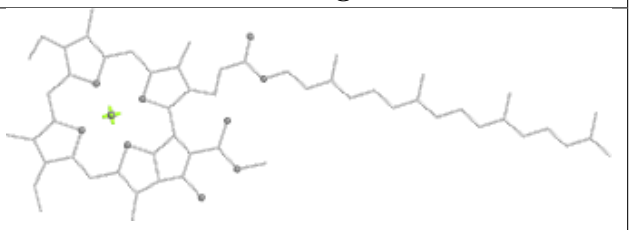
Bond lengths



Bond angles

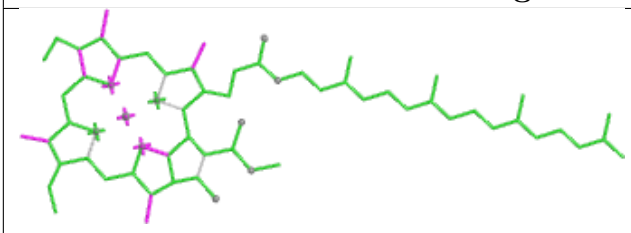


Torsions

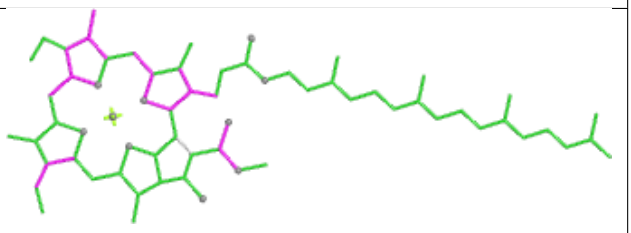


Rings

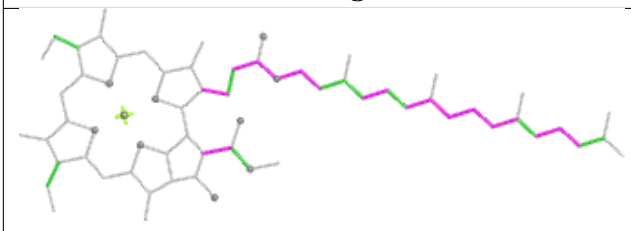
Ligand CLA bA 806



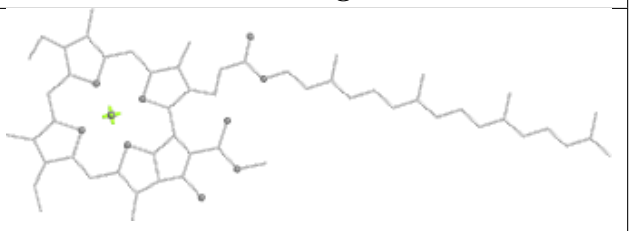
Bond lengths



Bond angles

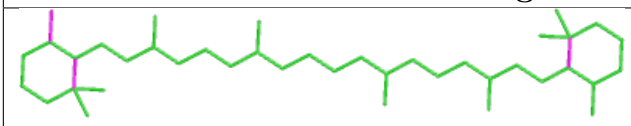


Torsions

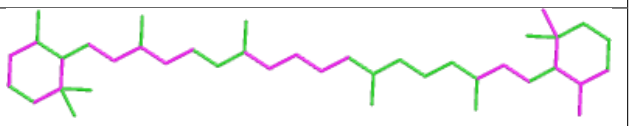


Rings

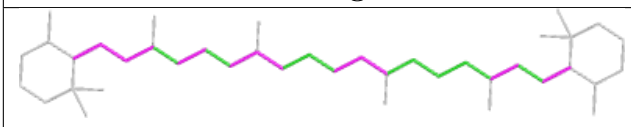
Ligand BCR aL 205



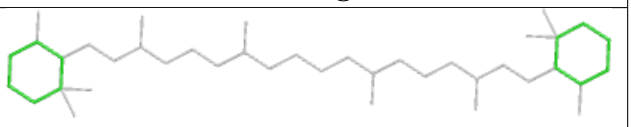
Bond lengths



Bond angles

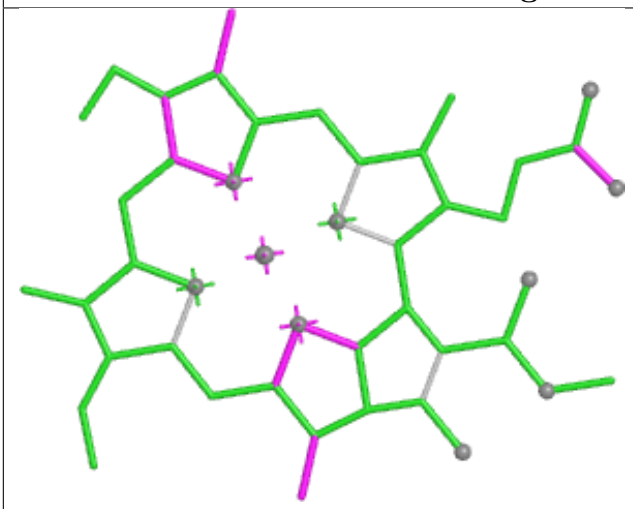


Torsions

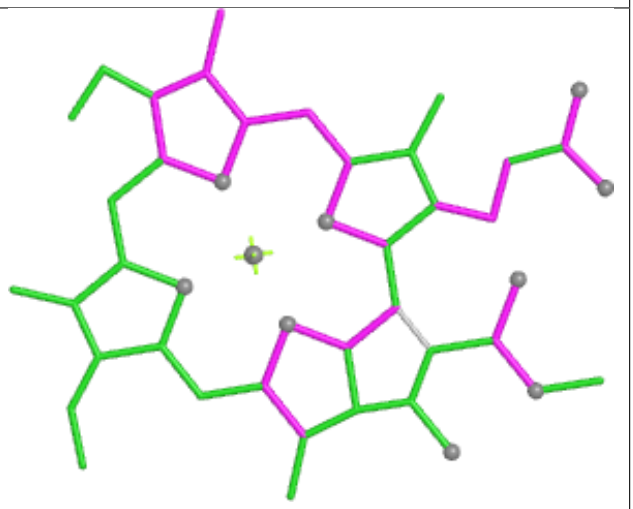


Rings

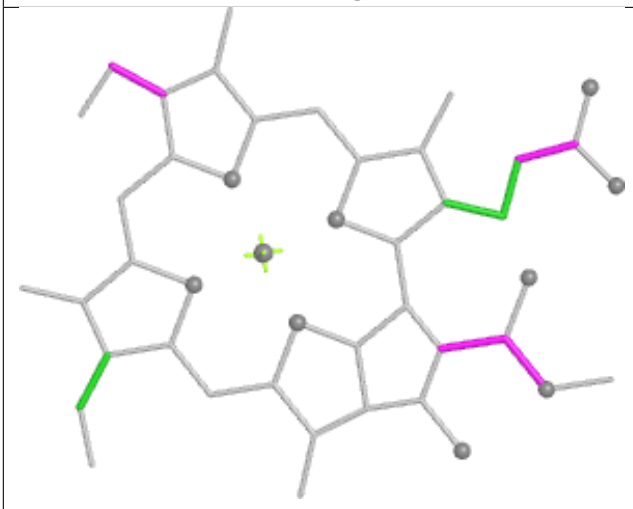
Ligand CLA c1 415



Bond lengths



Bond angles

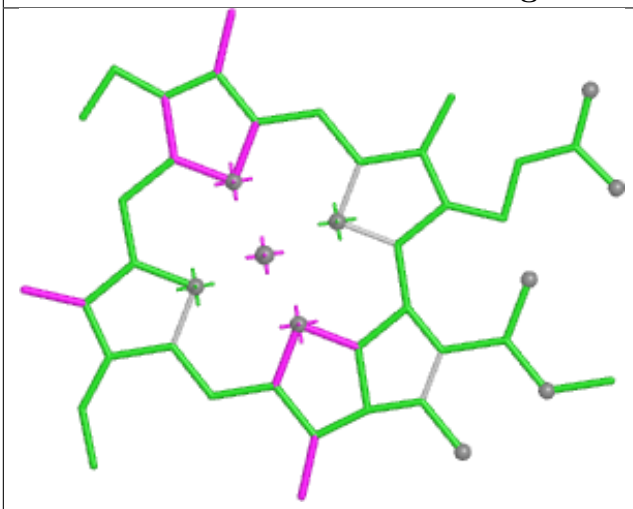


Torsions

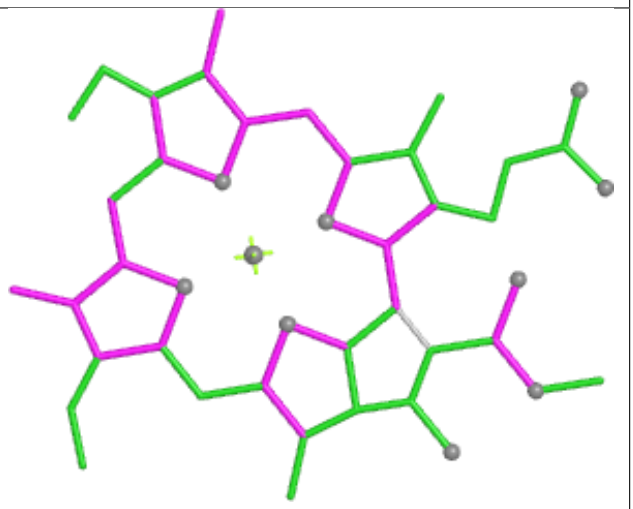


Rings

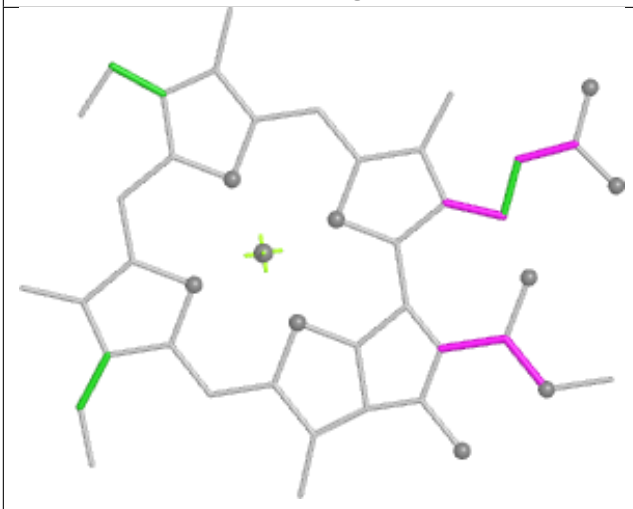
Ligand CLA c3 412



Bond lengths



Bond angles

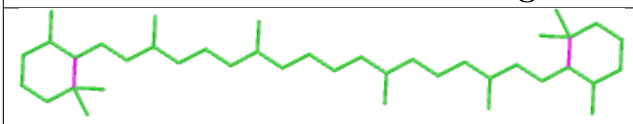


Torsions

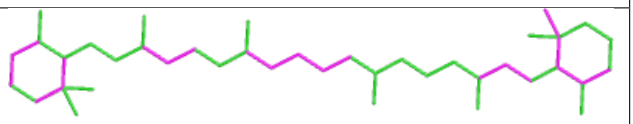


Rings

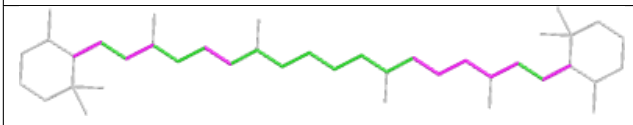
Ligand BCR c4 419



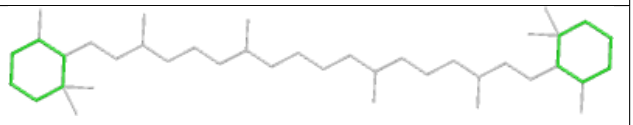
Bond lengths



Bond angles

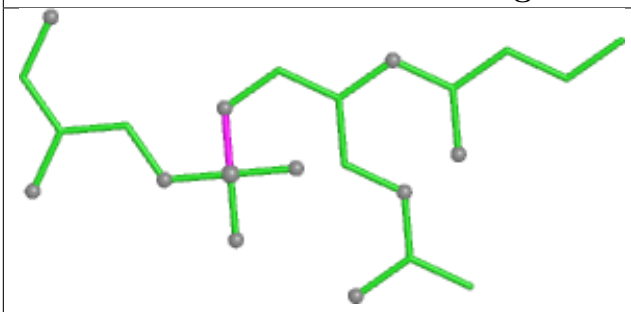


Torsions

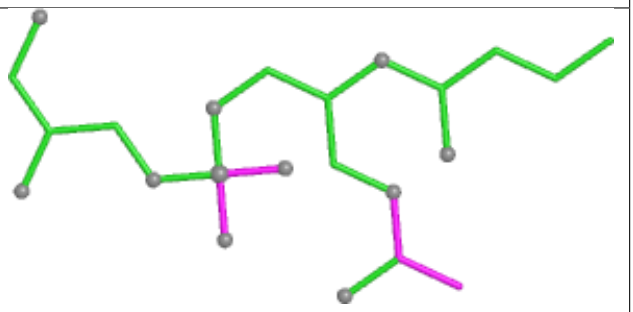


Rings

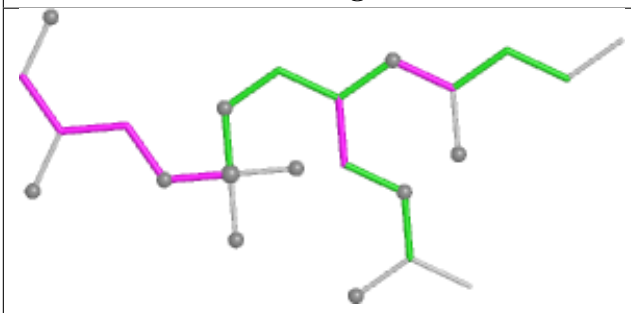
Ligand LHG cX 101



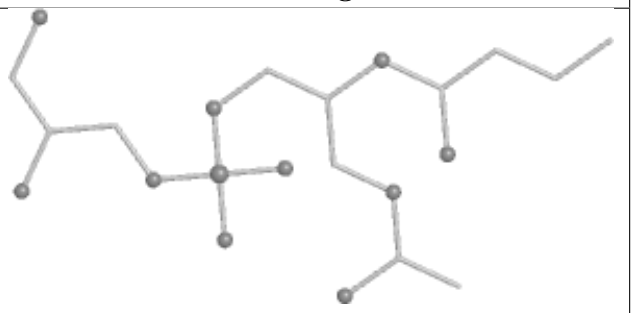
Bond lengths



Bond angles



Torsions

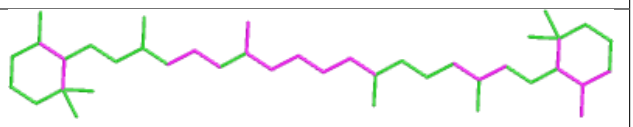


Rings

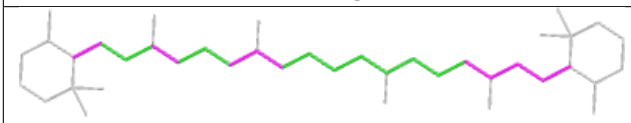
Ligand BCR cB 849



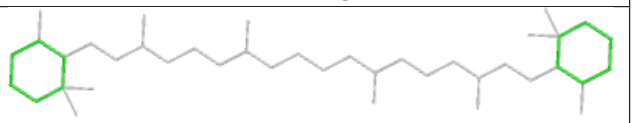
Bond lengths



Bond angles

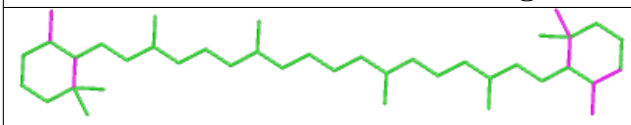


Torsions

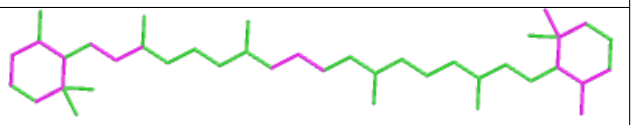


Rings

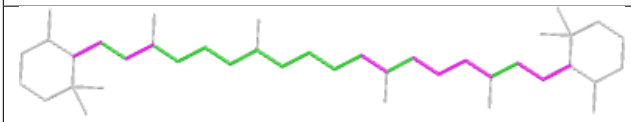
Ligand BCR c3 418



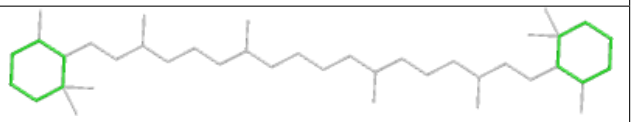
Bond lengths



Bond angles

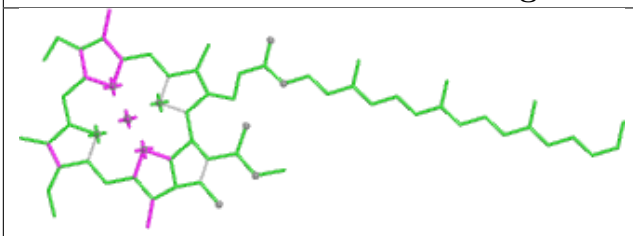


Torsions

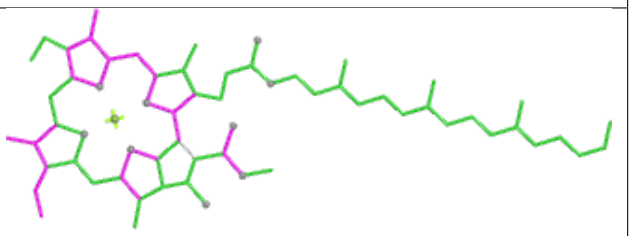


Rings

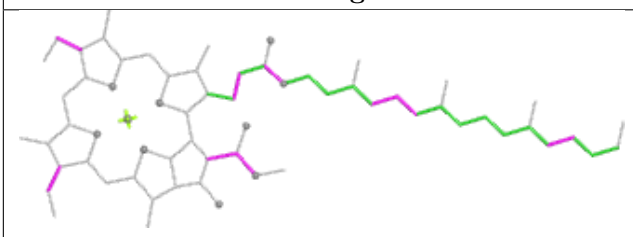
Ligand CLA a2 411



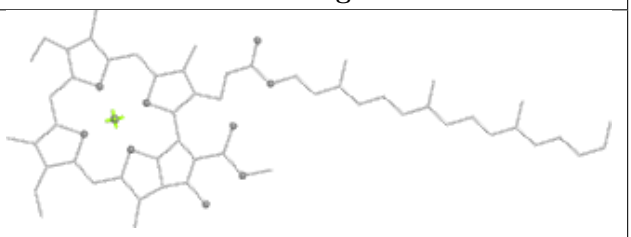
Bond lengths



Bond angles

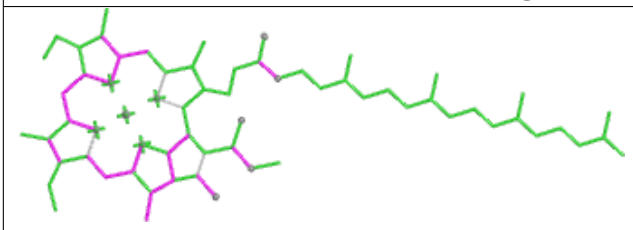


Torsions

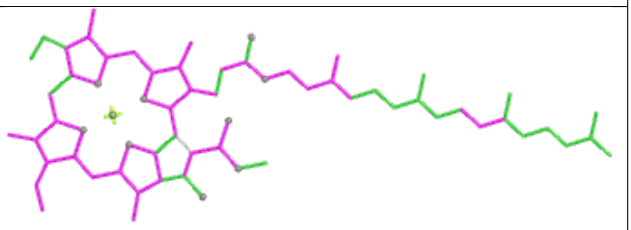


Rings

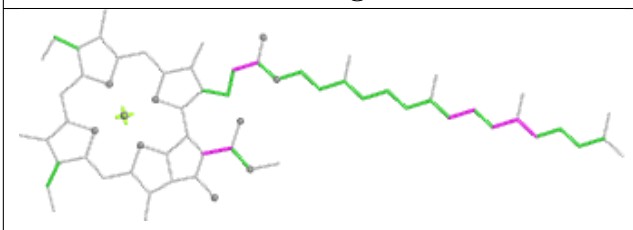
Ligand CL0 bA 801



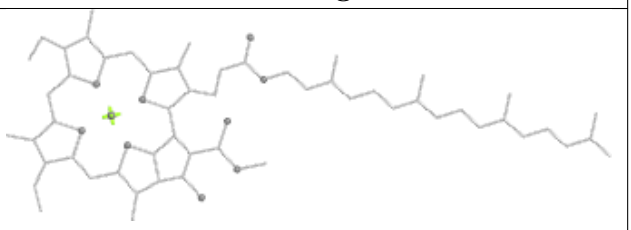
Bond lengths



Bond angles

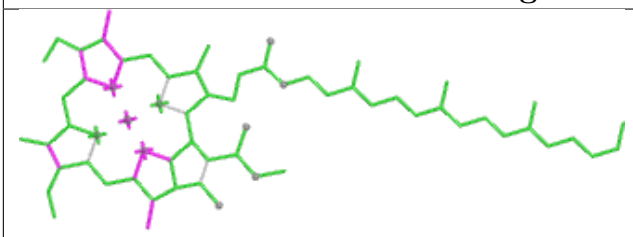


Torsions

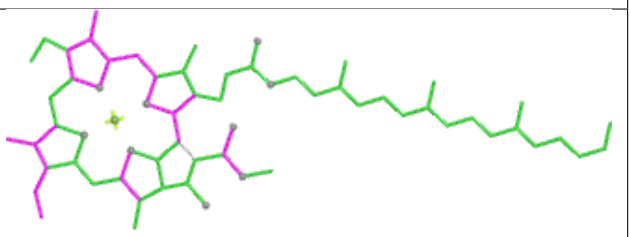


Rings

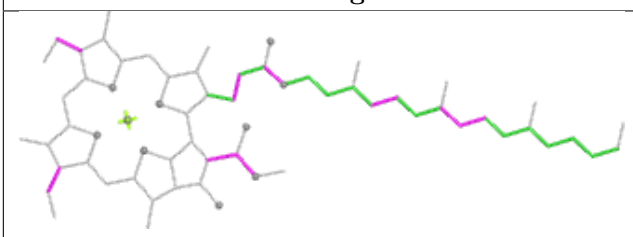
Ligand CLA a1 409



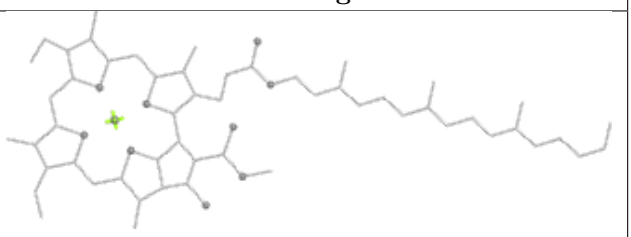
Bond lengths



Bond angles

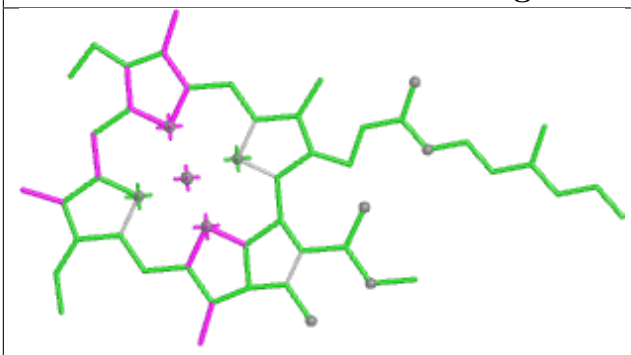


Torsions

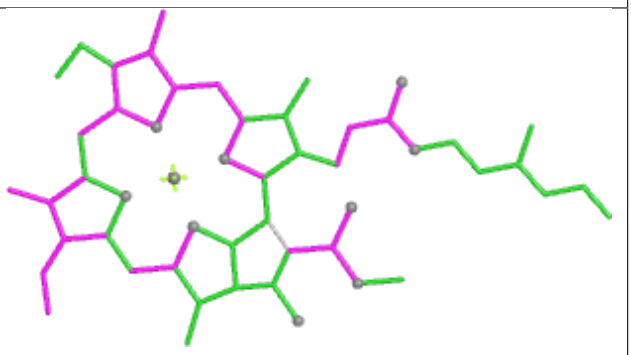


Rings

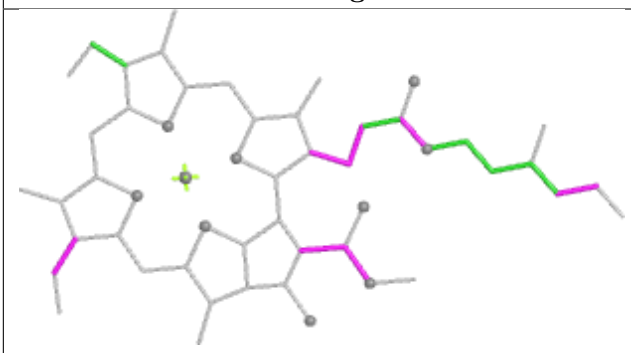
Ligand CLA bA 845



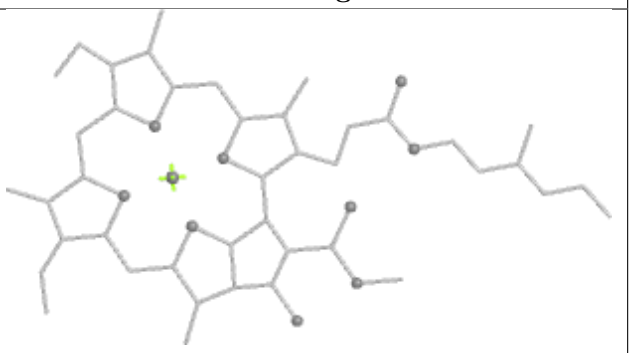
Bond lengths



Bond angles

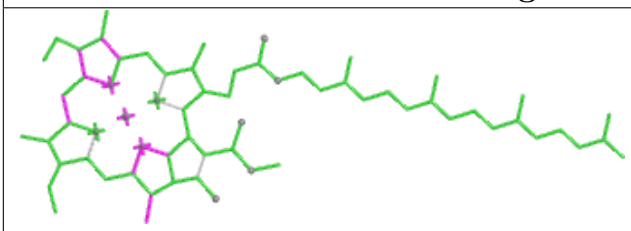


Torsions

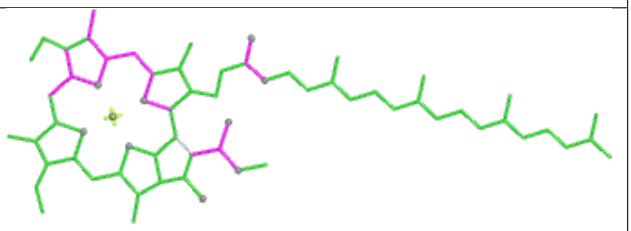


Rings

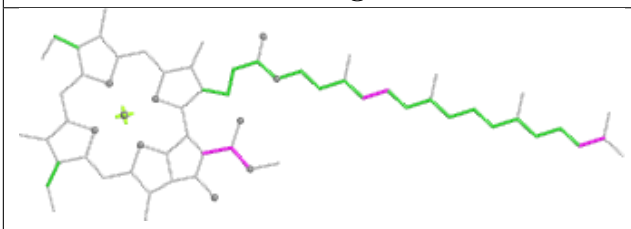
Ligand CLA b6 410



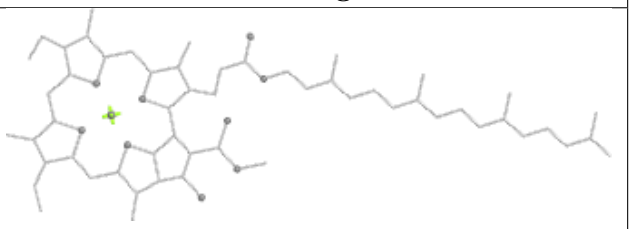
Bond lengths



Bond angles

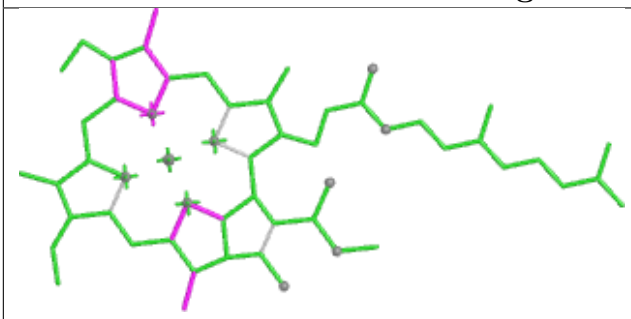


Torsions

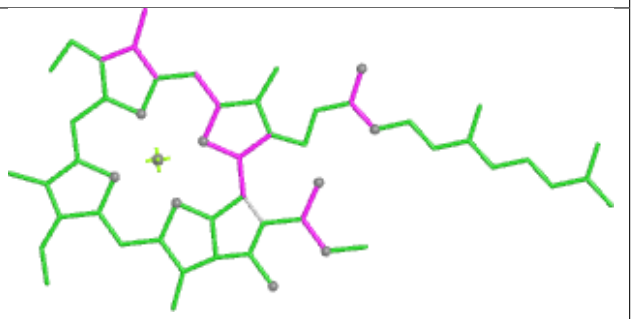


Rings

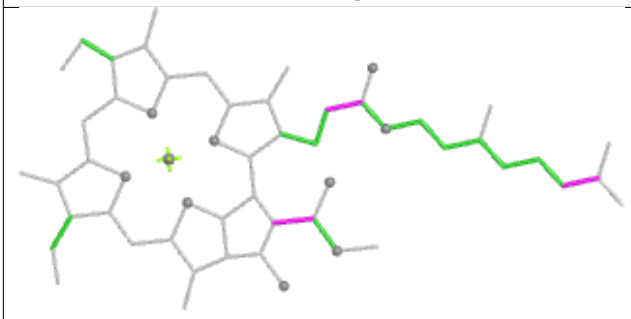
Ligand CLA cB 823



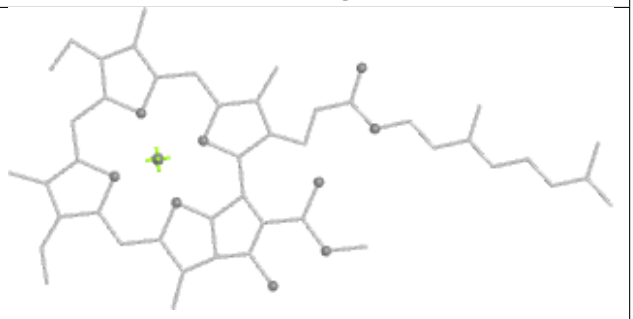
Bond lengths



Bond angles

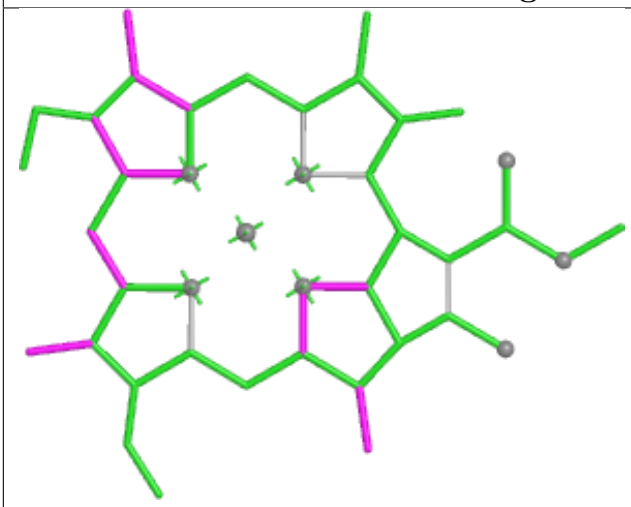


Torsions

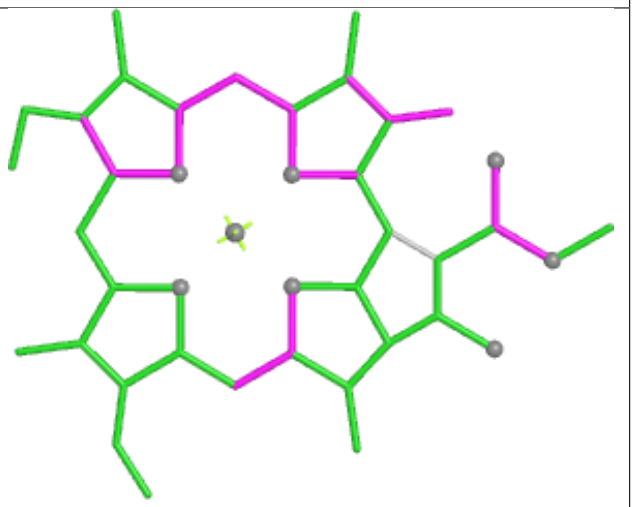


Rings

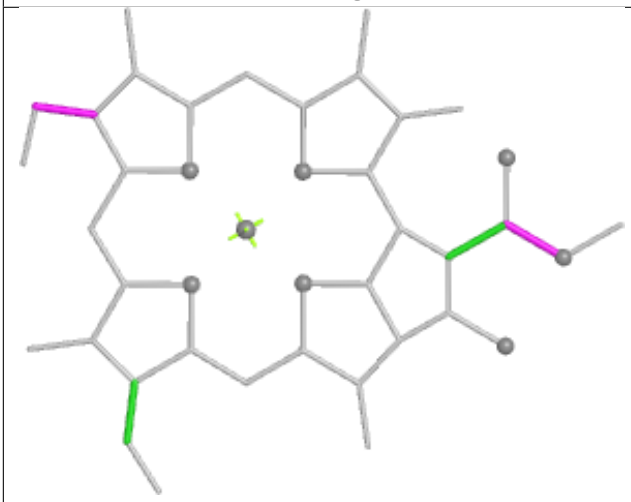
Ligand CLA a5 414



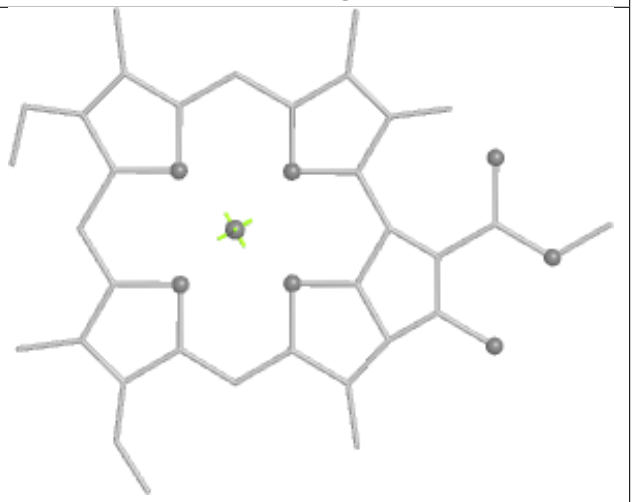
Bond lengths



Bond angles

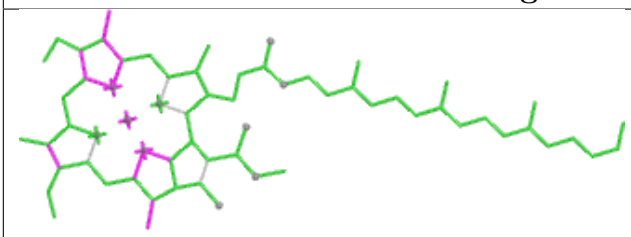


Torsions

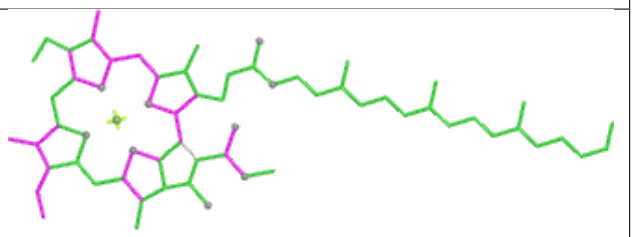


Rings

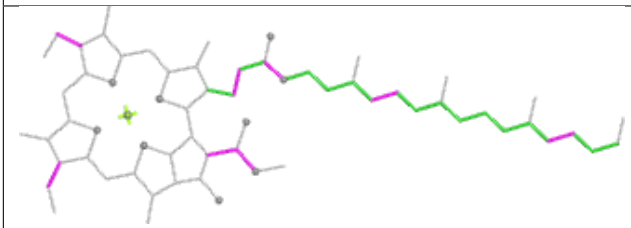
Ligand CLA c3 410



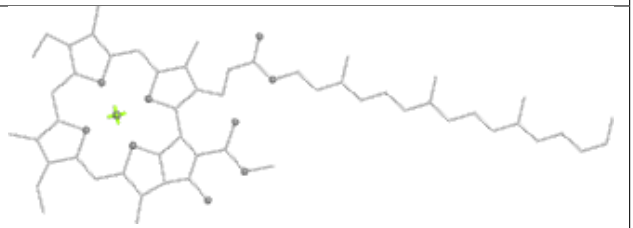
Bond lengths



Bond angles

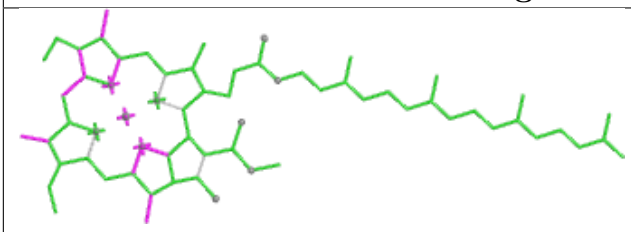


Torsions

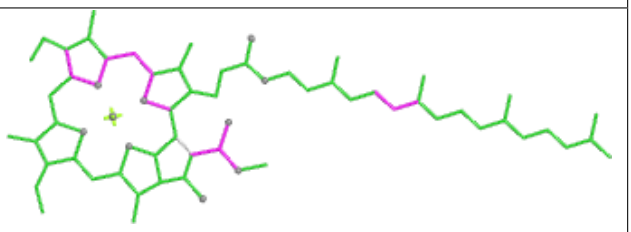


Rings

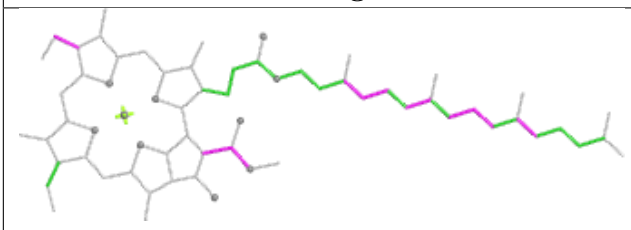
Ligand CLA aA 839



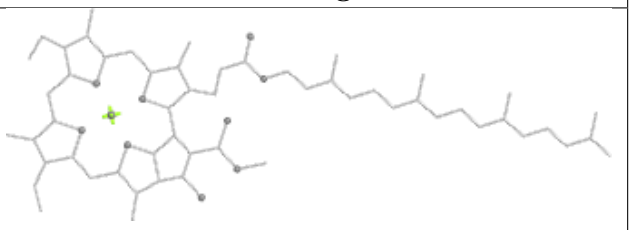
Bond lengths



Bond angles

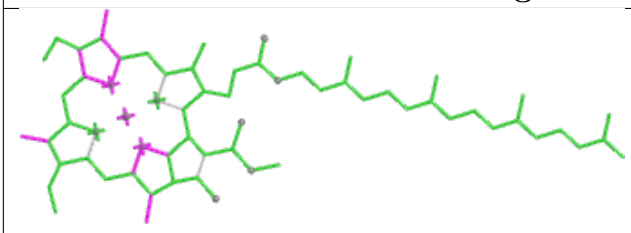


Torsions

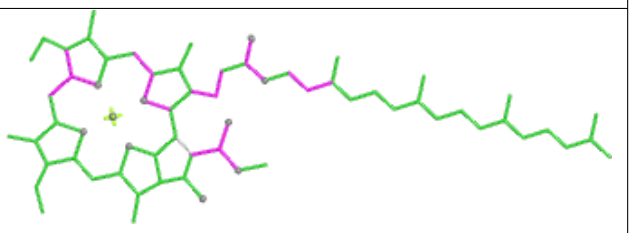


Rings

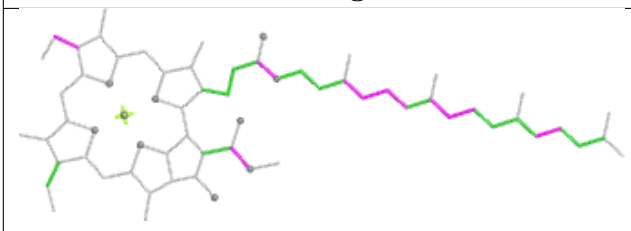
Ligand CLA bB 809



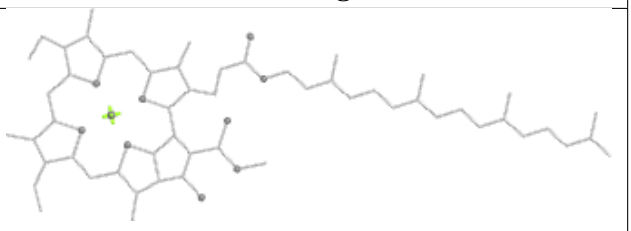
Bond lengths



Bond angles

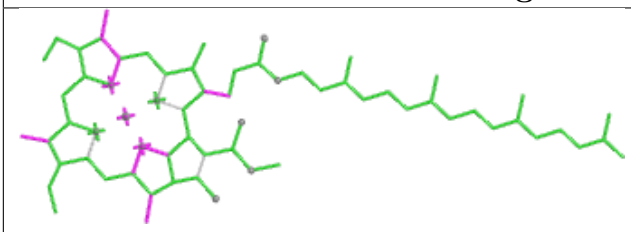


Torsions

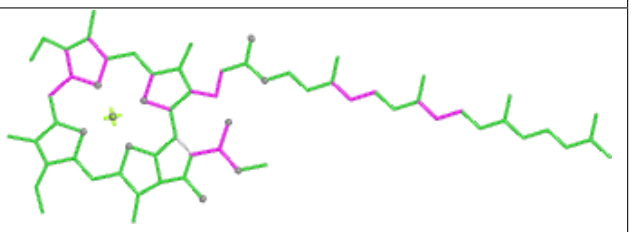


Rings

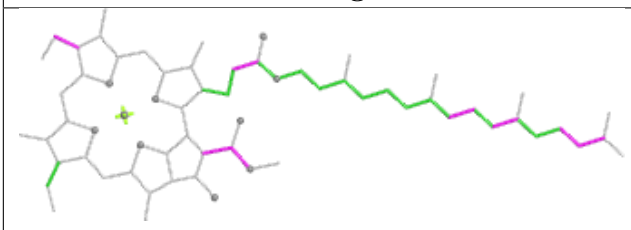
Ligand CLA aB 802



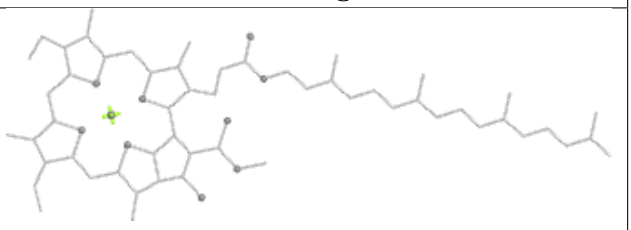
Bond lengths



Bond angles

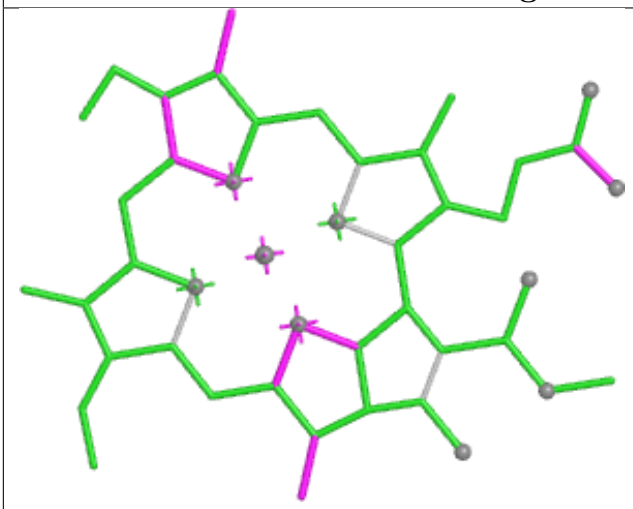


Torsions

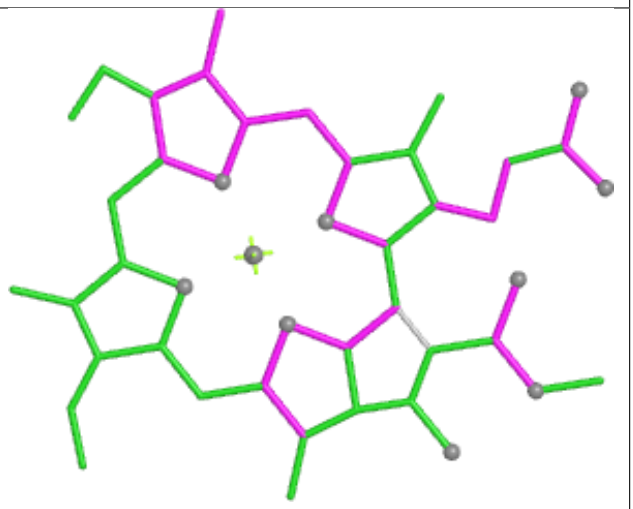


Rings

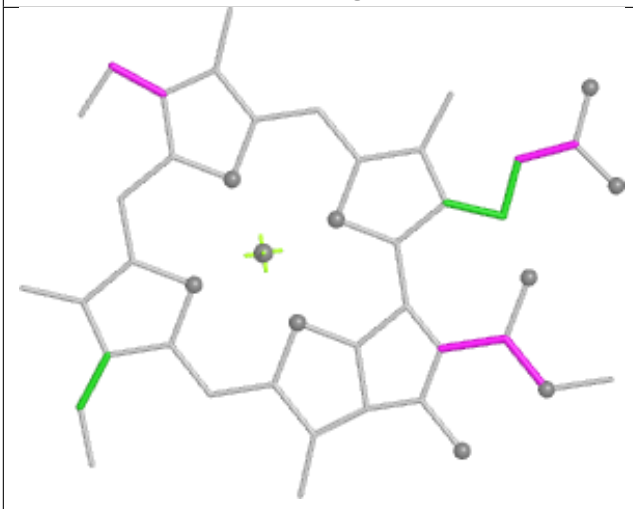
Ligand CLA a1 414



Bond lengths



Bond angles

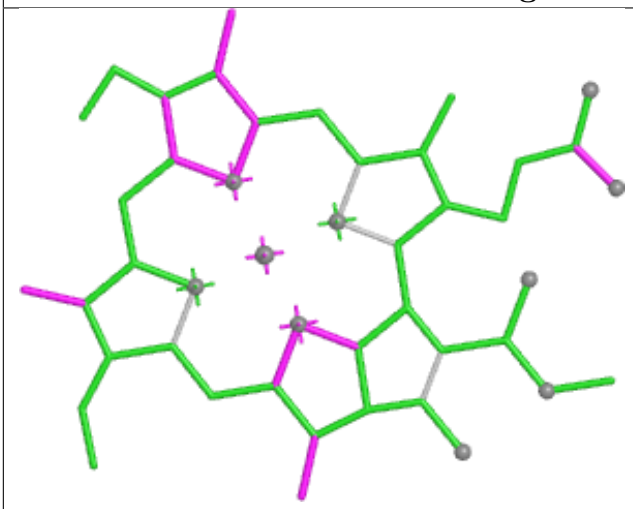


Torsions

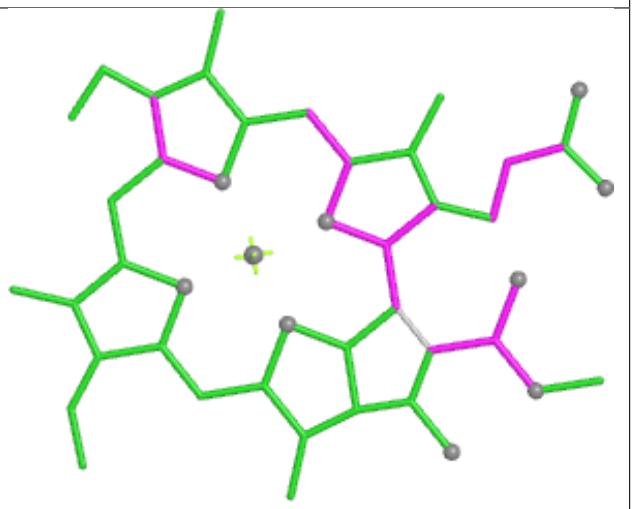


Rings

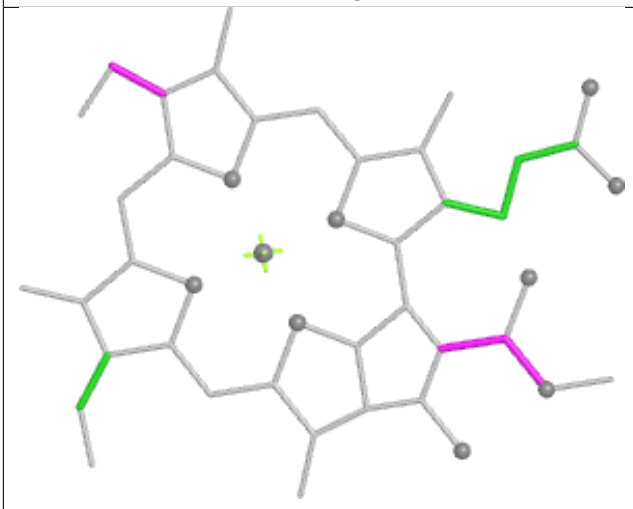
Ligand CLA aJ 202



Bond lengths



Bond angles

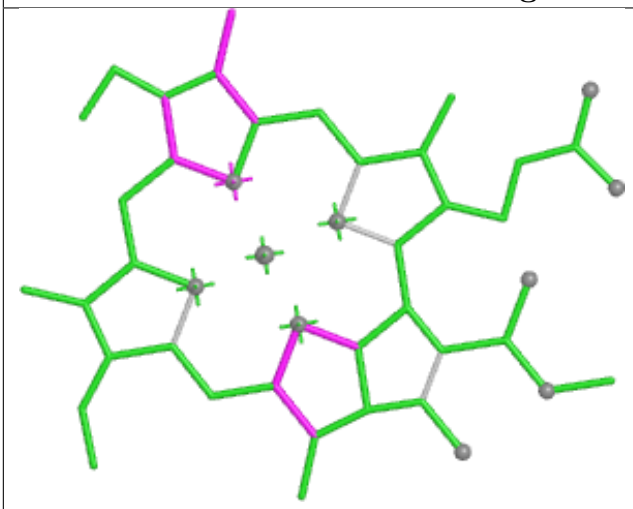


Torsions

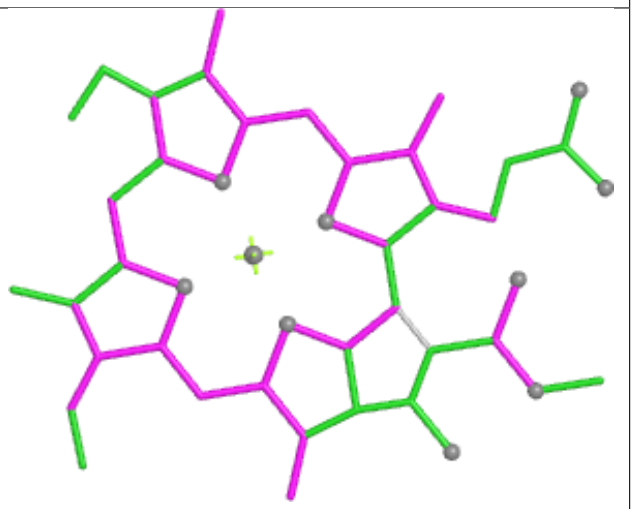


Rings

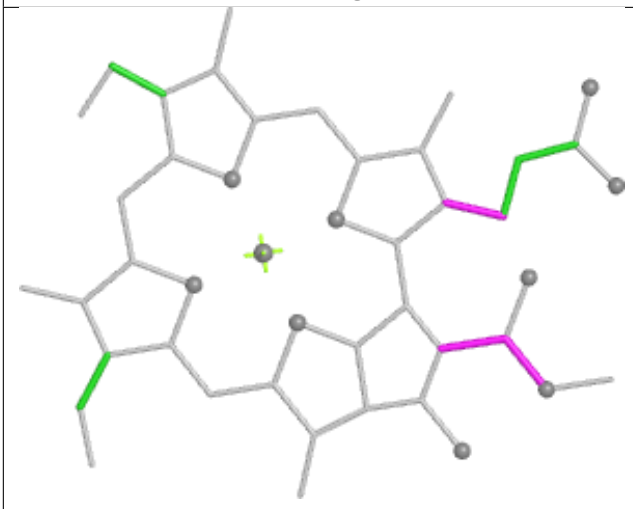
Ligand CLA a2 405



Bond lengths



Bond angles

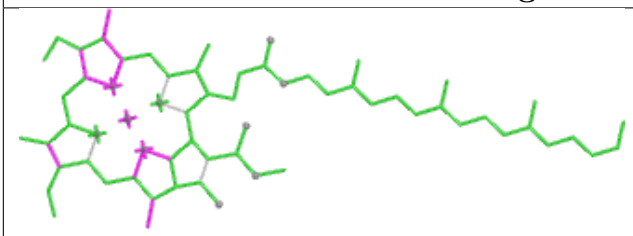


Torsions

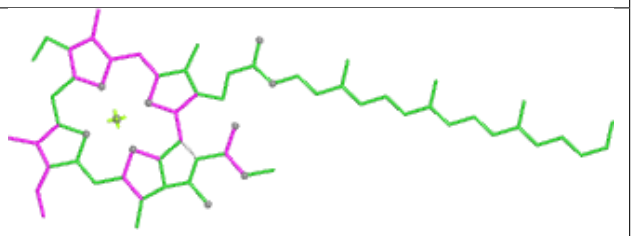


Rings

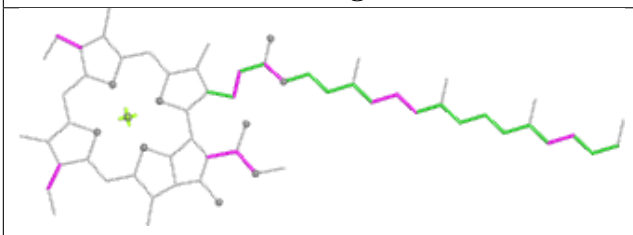
Ligand CLA b2 411



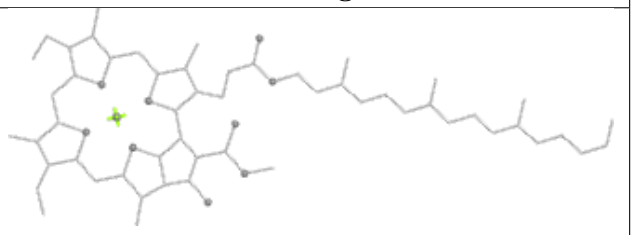
Bond lengths



Bond angles

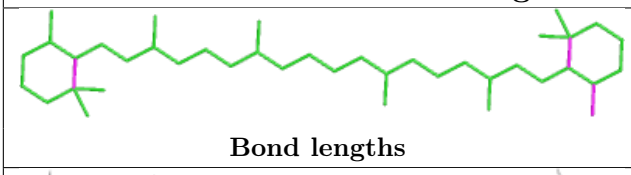


Torsions

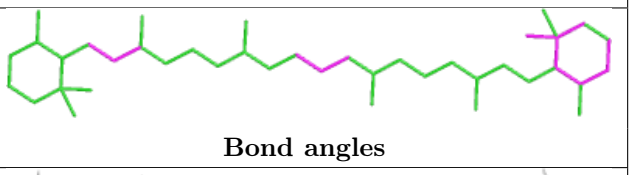


Rings

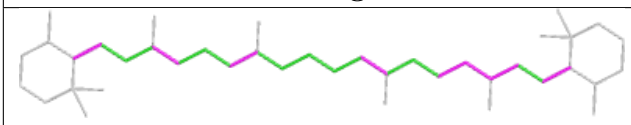
Ligand BCR bB 845



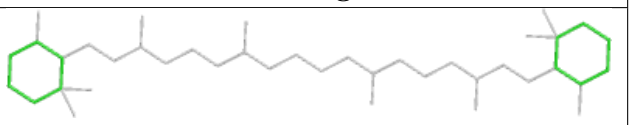
Bond lengths



Bond angles

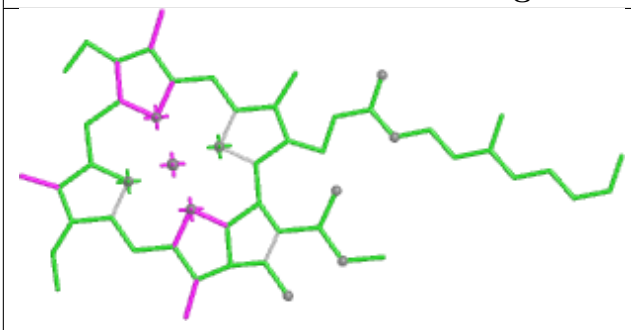


Torsions

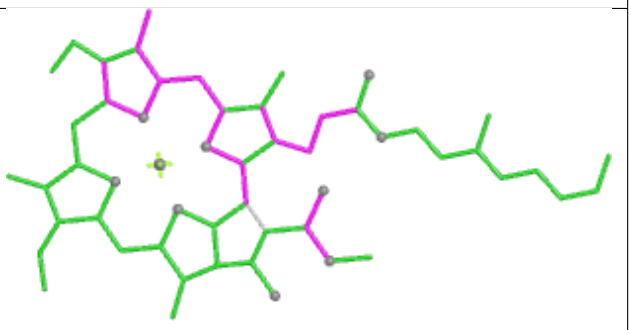


Rings

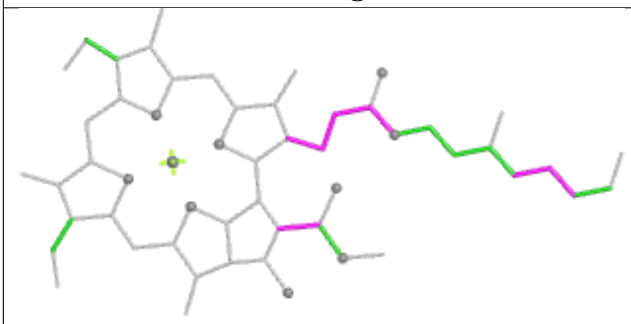
Ligand CLA bA 813



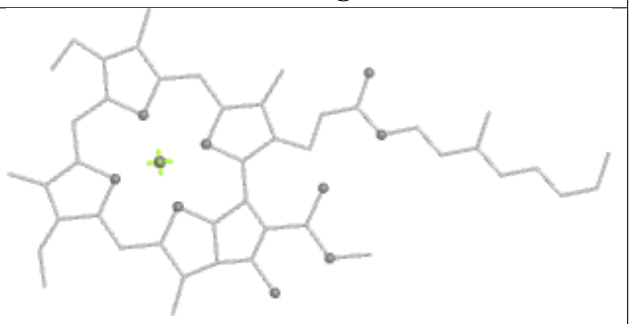
Bond lengths



Bond angles

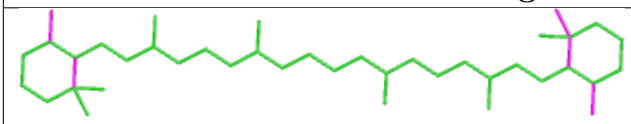


Torsions

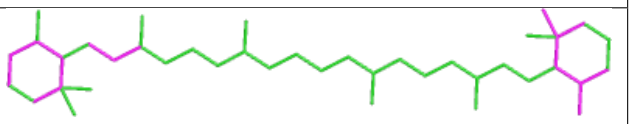


Rings

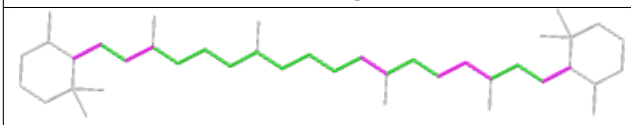
Ligand BCR c4 418



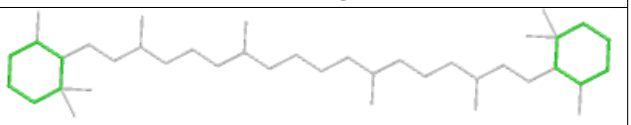
Bond lengths



Bond angles

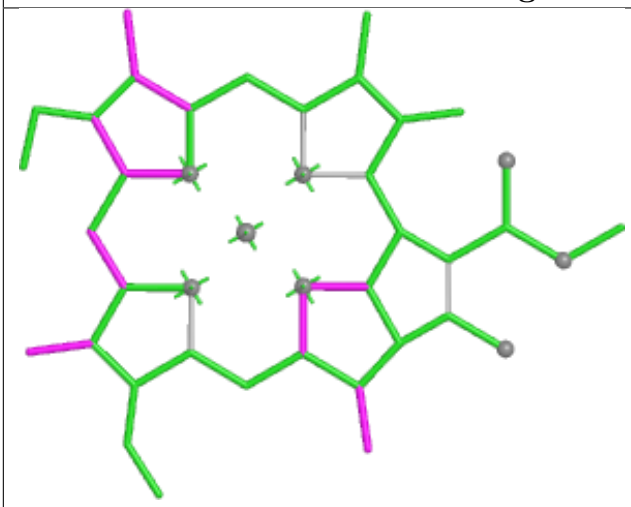


Torsions

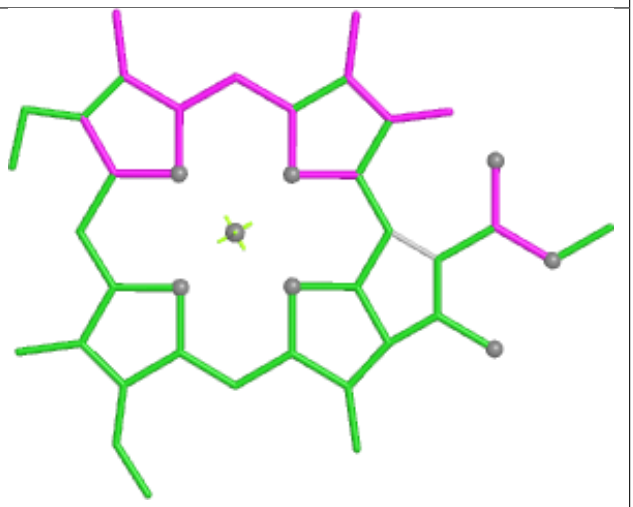


Rings

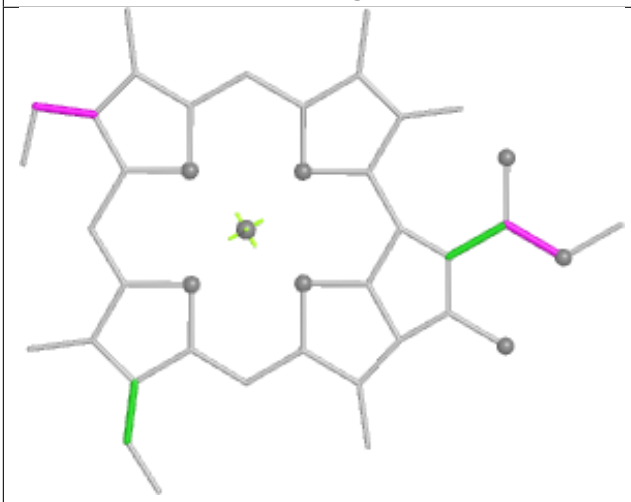
Ligand CLA b1 414



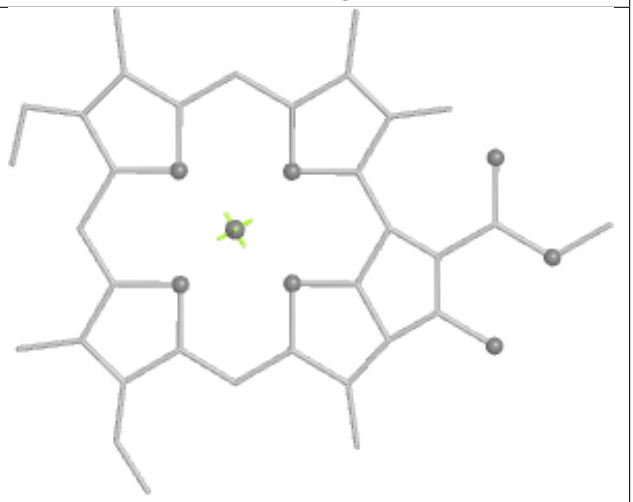
Bond lengths



Bond angles

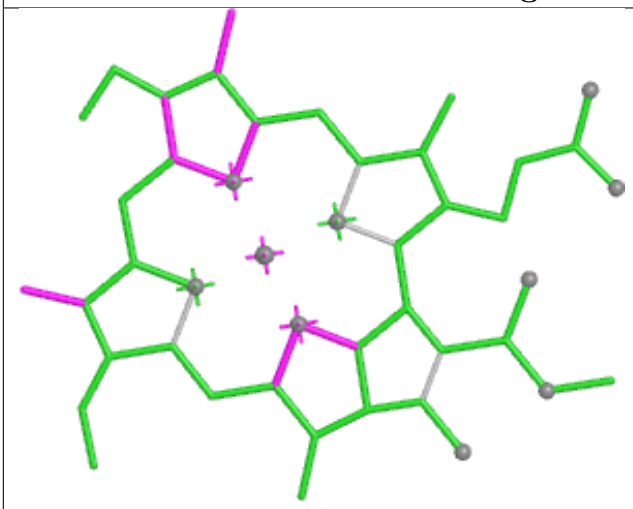


Torsions

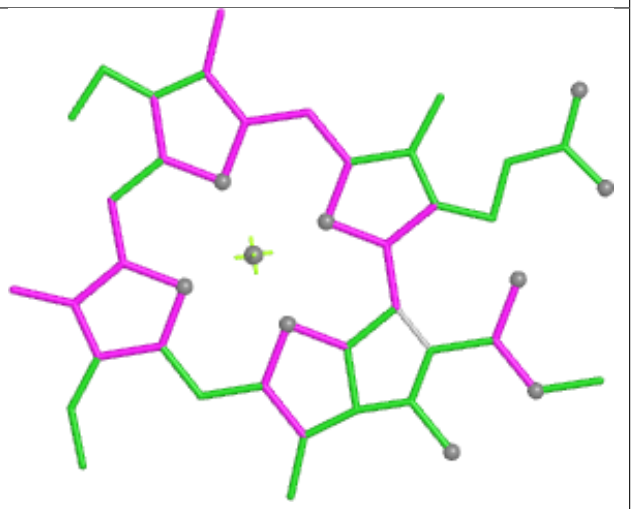


Rings

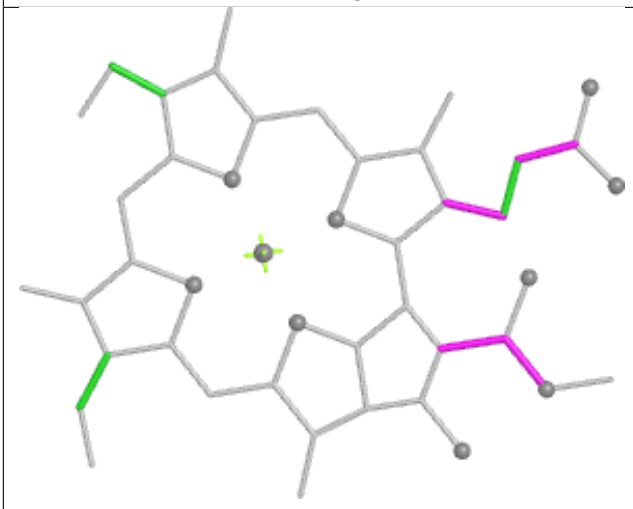
Ligand CLA c5 412



Bond lengths



Bond angles

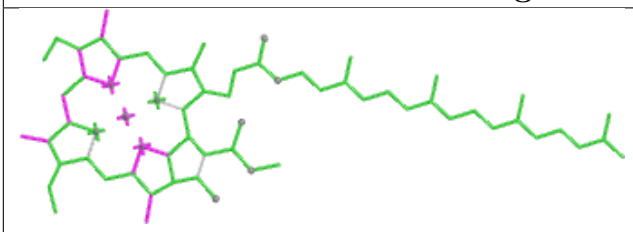


Torsions

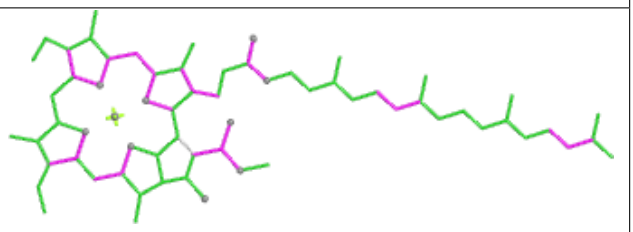


Rings

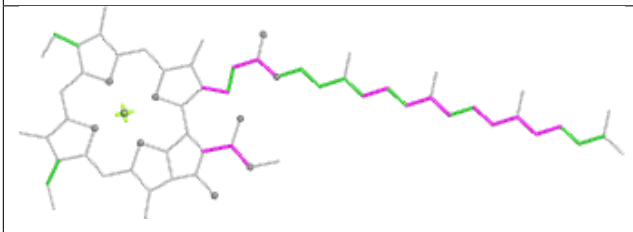
Ligand CLA bB 833



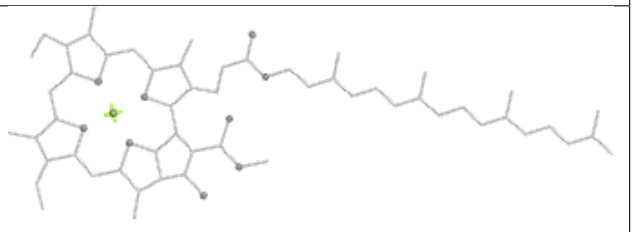
Bond lengths



Bond angles

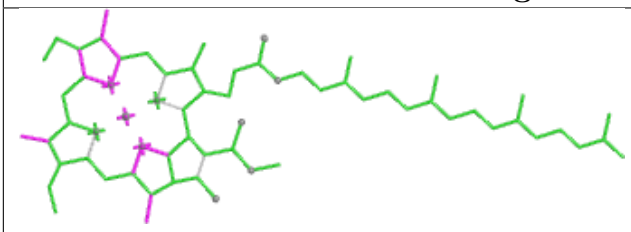


Torsions

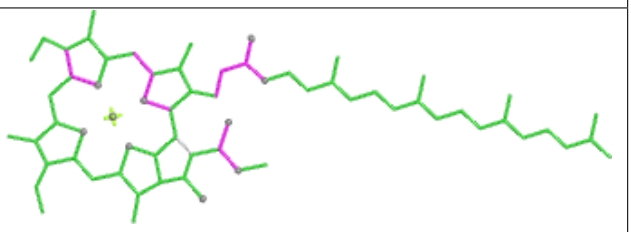


Rings

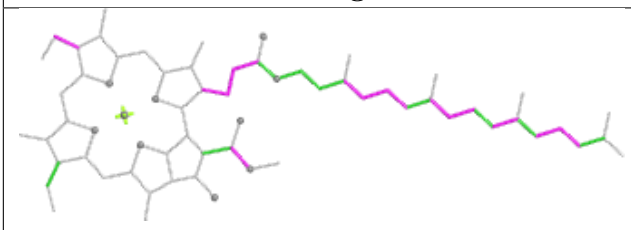
Ligand CLA bA 810



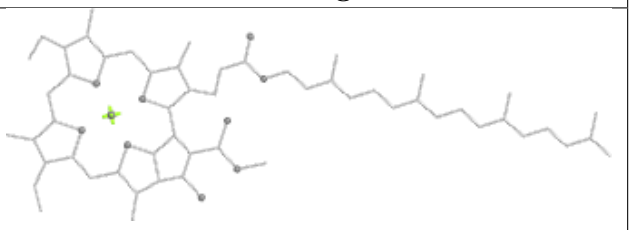
Bond lengths



Bond angles



Torsions

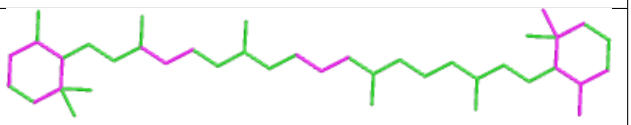


Rings

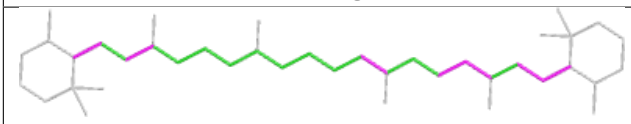
Ligand BCR a2 419



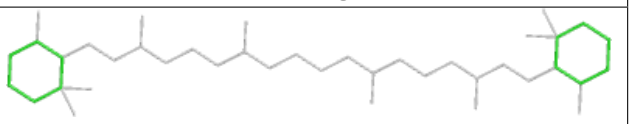
Bond lengths



Bond angles

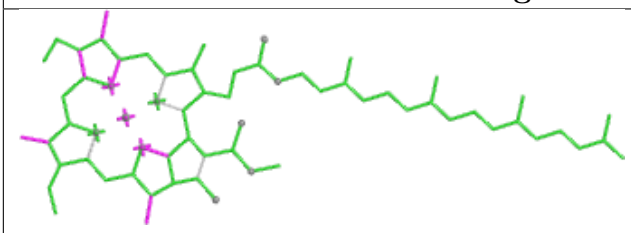


Torsions

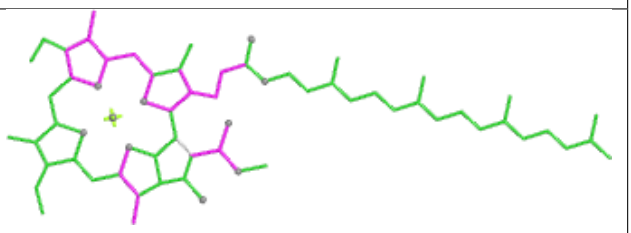


Rings

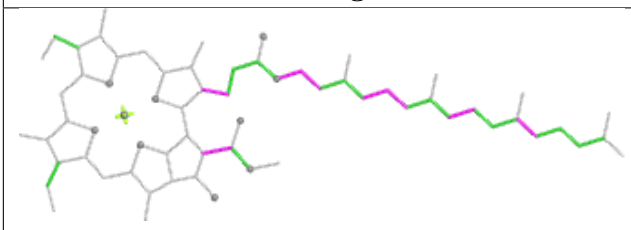
Ligand CLA bA 827



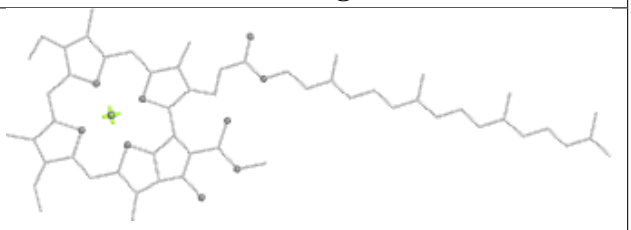
Bond lengths



Bond angles

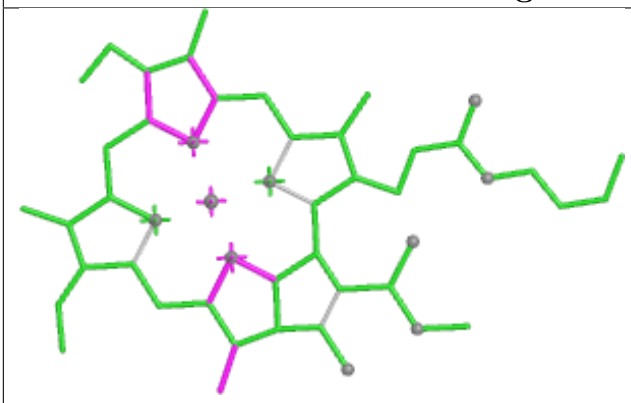


Torsions

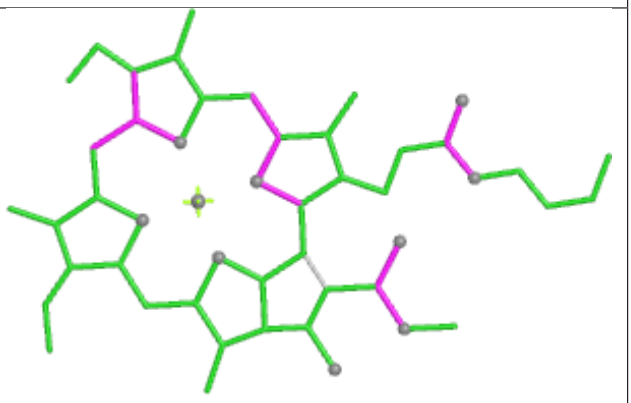


Rings

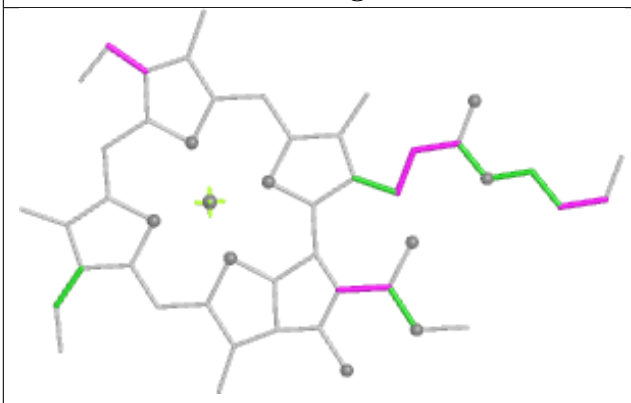
Ligand CLA cA 823



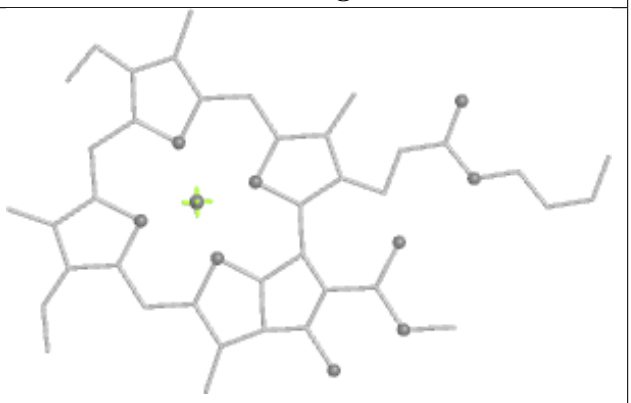
Bond lengths



Bond angles

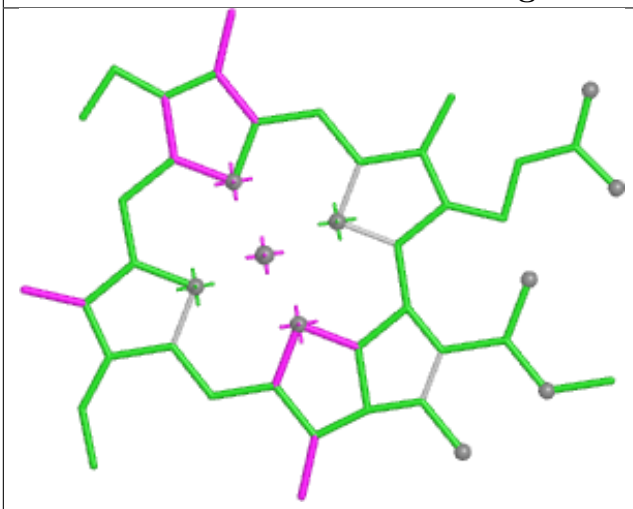


Torsions

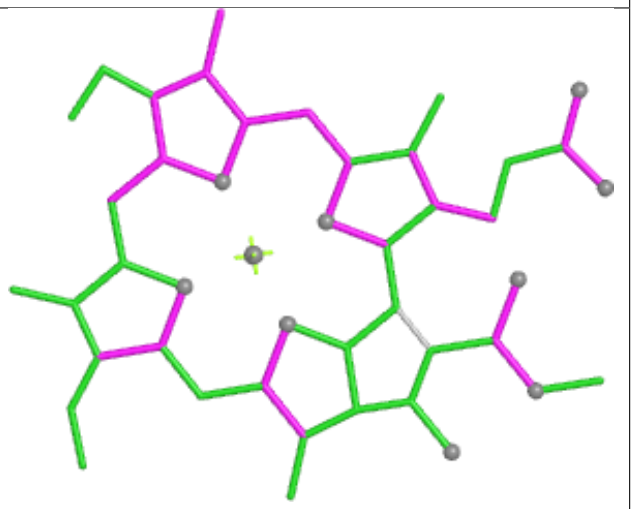


Rings

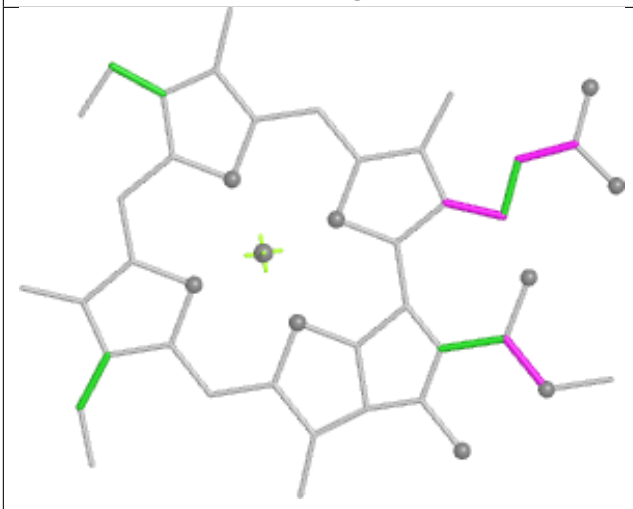
Ligand CLA b3 408



Bond lengths



Bond angles

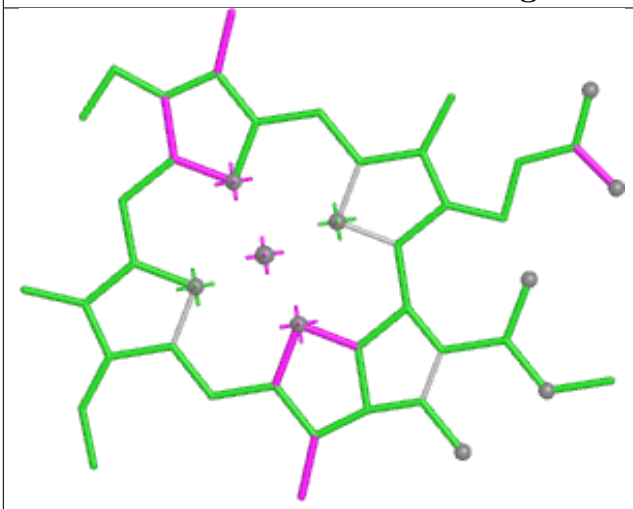


Torsions

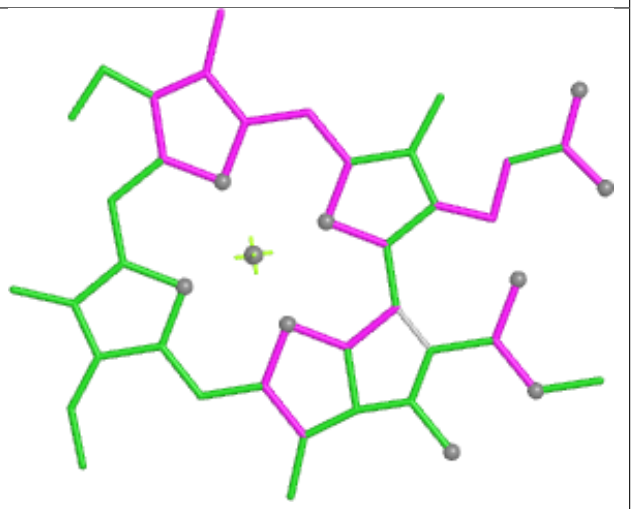


Rings

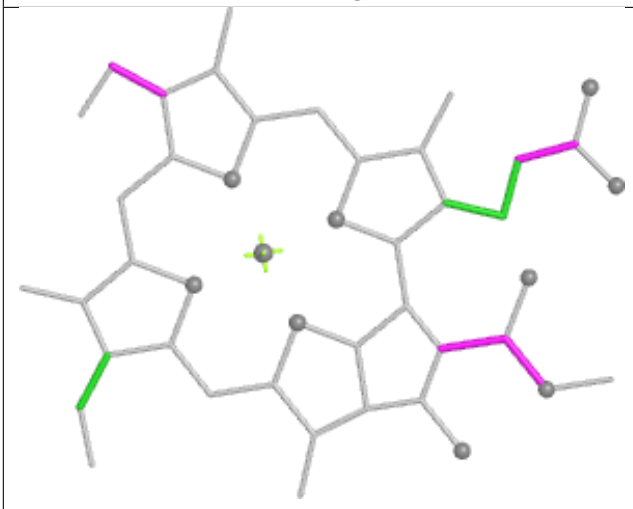
Ligand CLA a2 416



Bond lengths



Bond angles

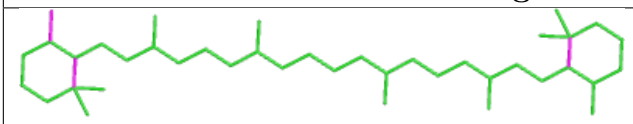


Torsions

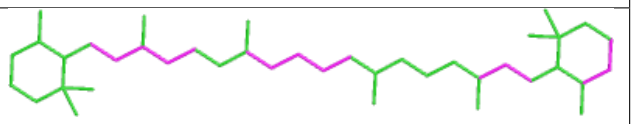


Rings

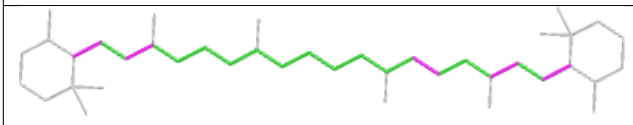
Ligand BCR bB 844



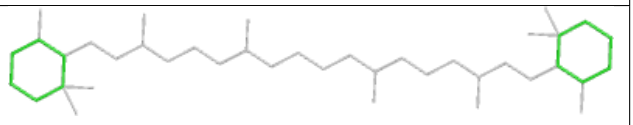
Bond lengths



Bond angles

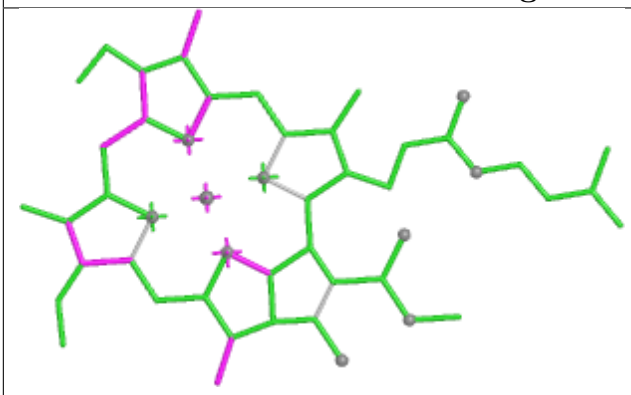


Torsions

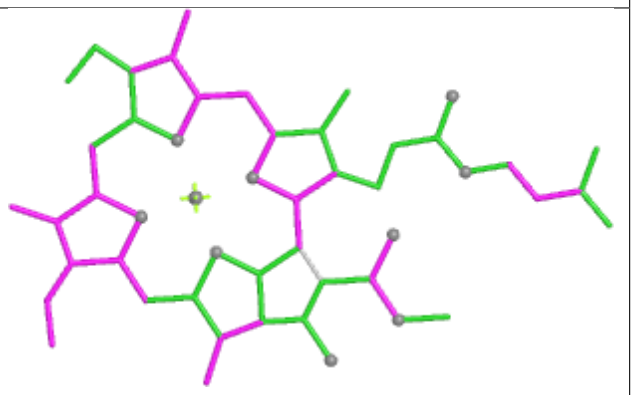


Rings

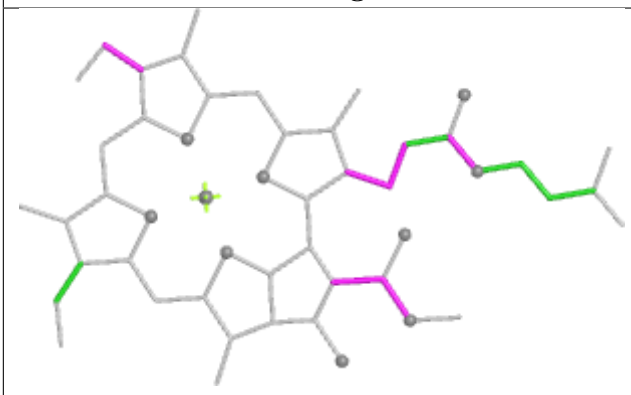
Ligand CLA a6 417



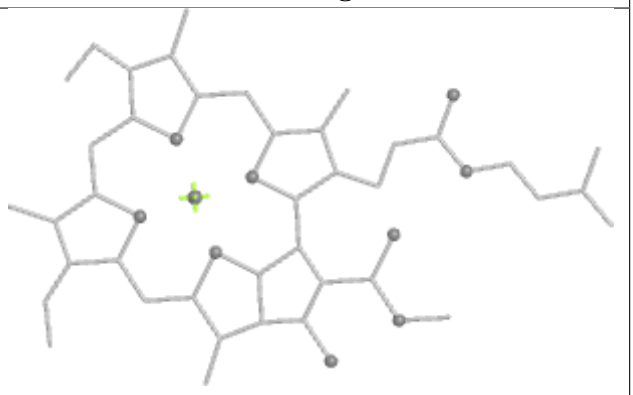
Bond lengths



Bond angles

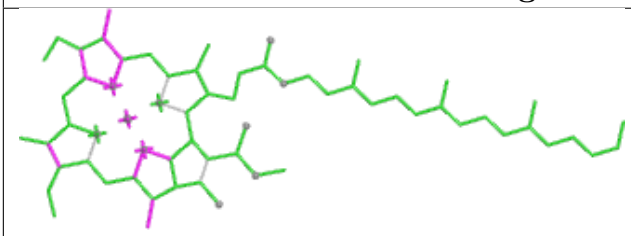


Torsions

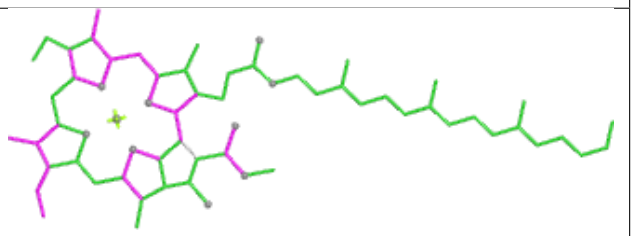


Rings

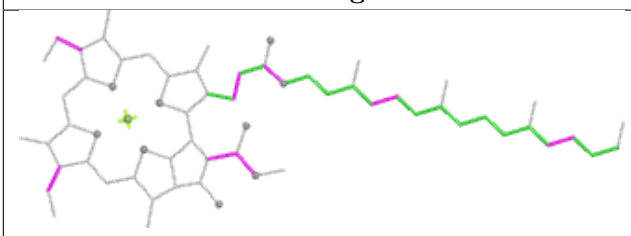
Ligand CLA b3 410



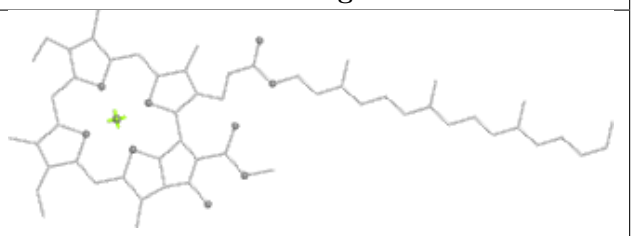
Bond lengths



Bond angles

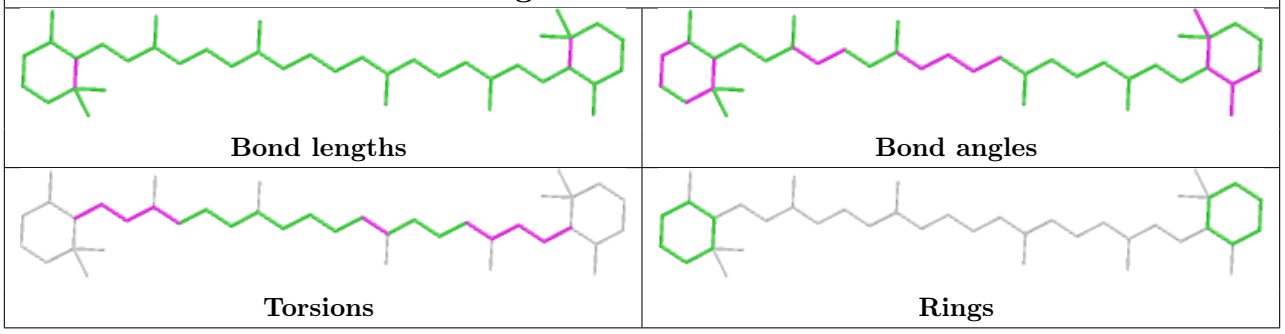


Torsions

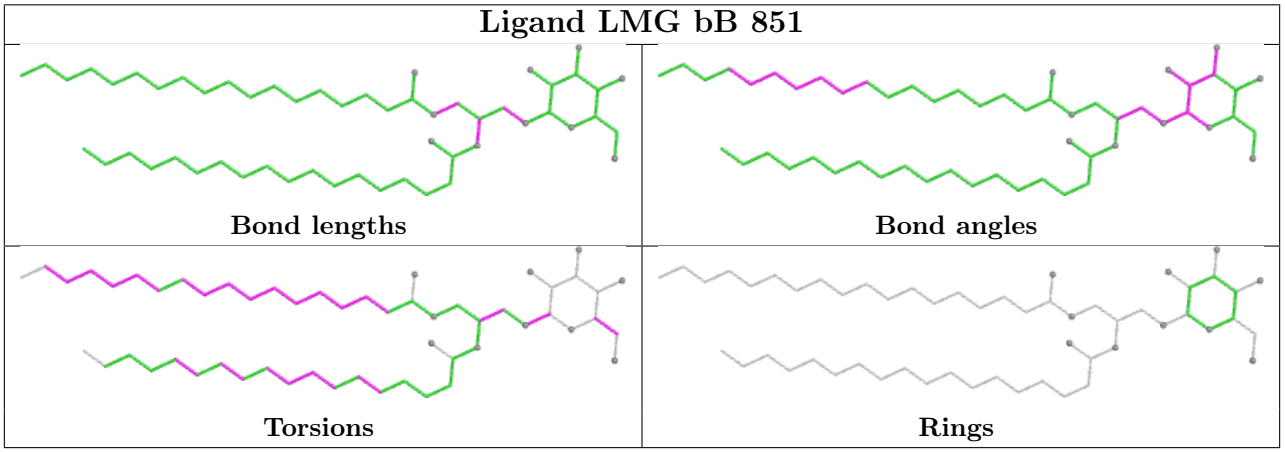


Rings

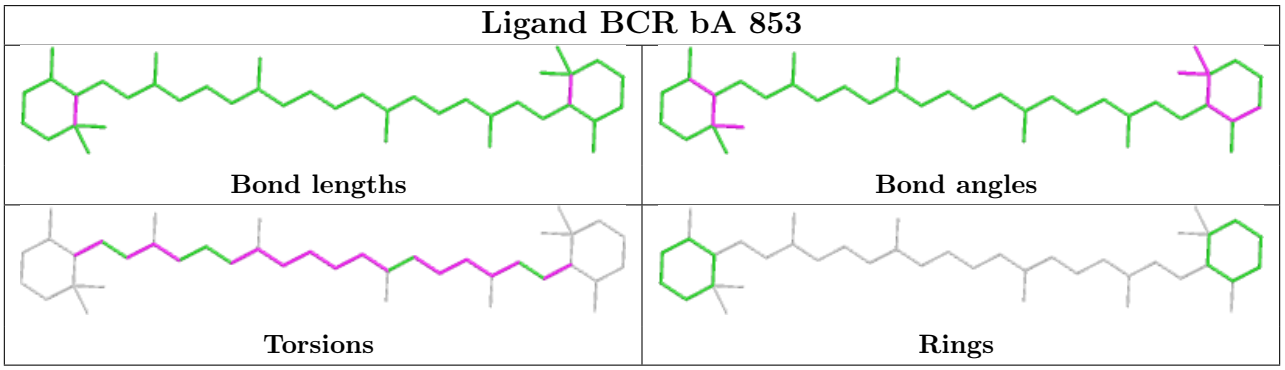
Ligand BCR cA 848



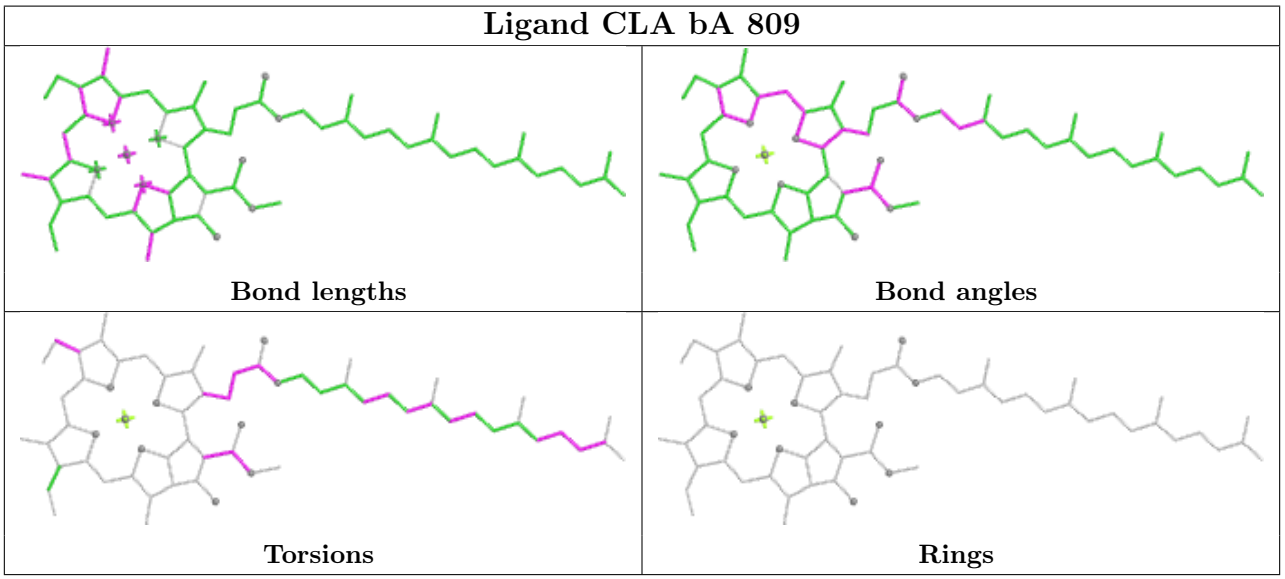
Ligand LMG bB 851

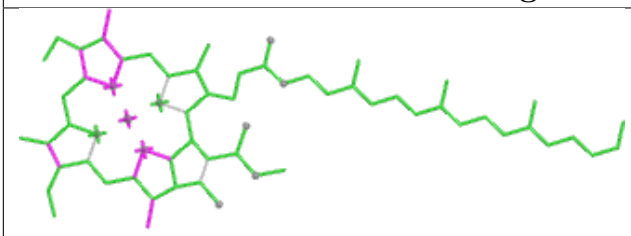
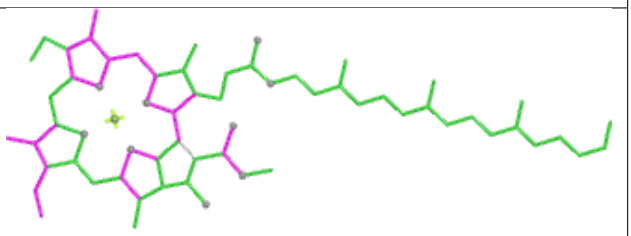
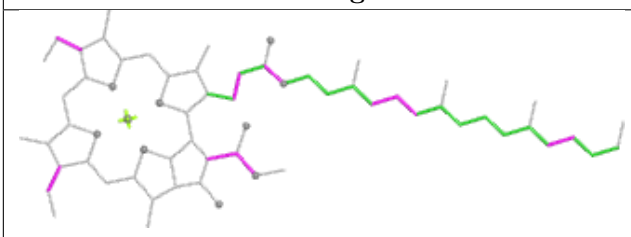
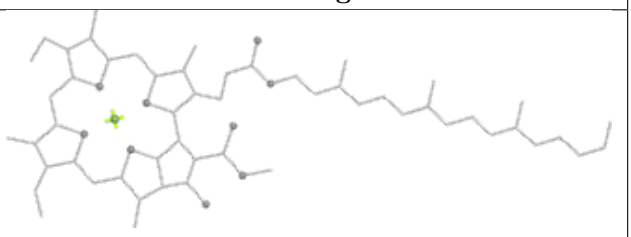


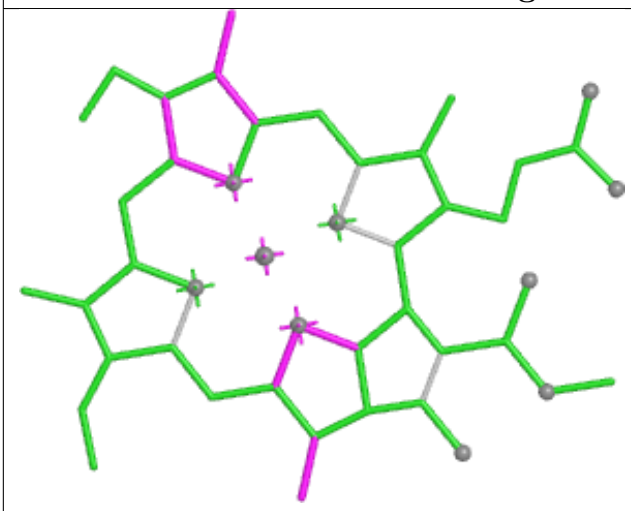
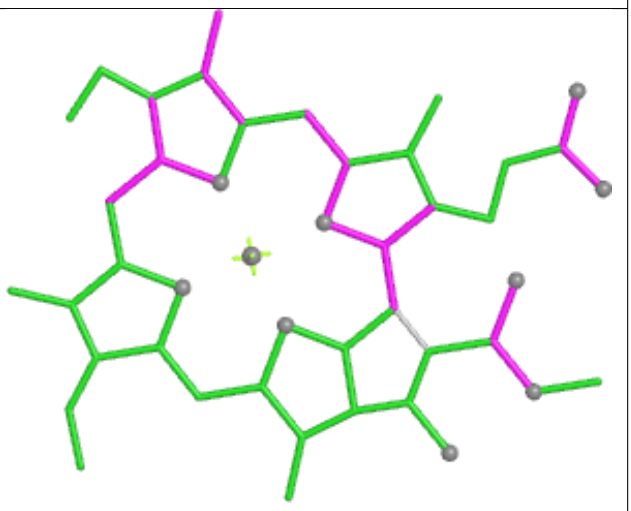
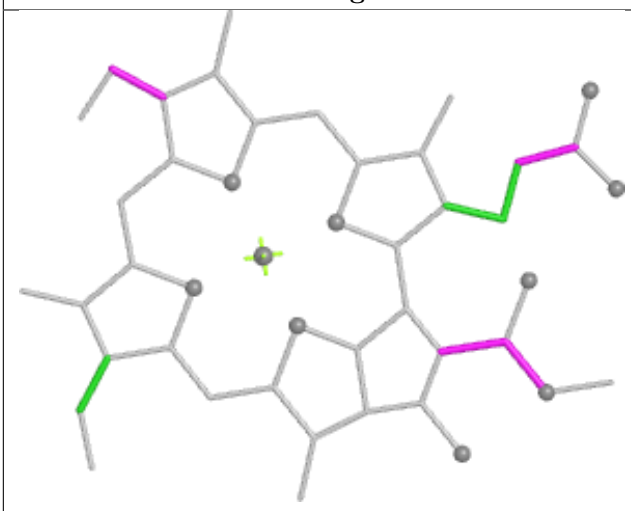
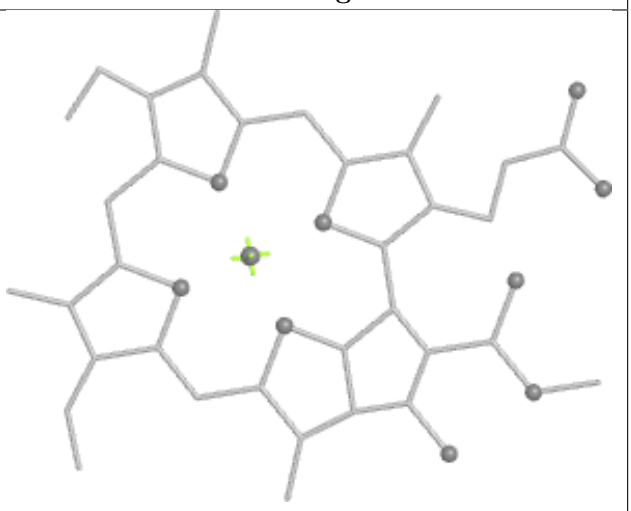
Ligand BCR bA 853



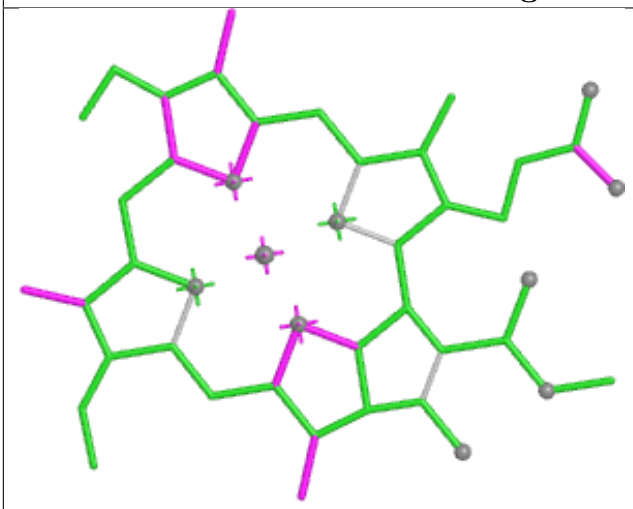
Ligand CLA bA 809



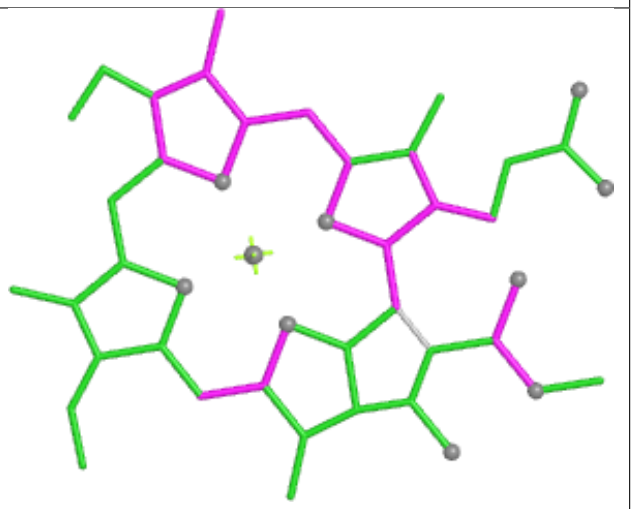
Ligand CLA a4 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b6 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

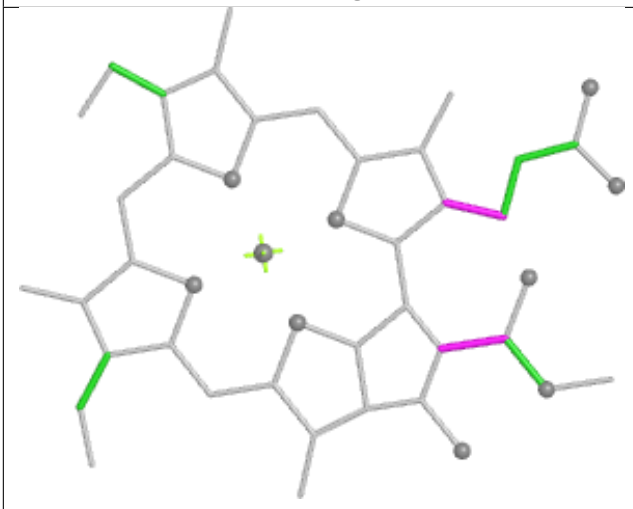
Ligand CLA c2 412



Bond lengths



Bond angles

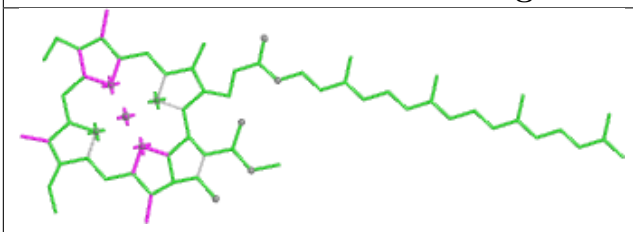


Torsions

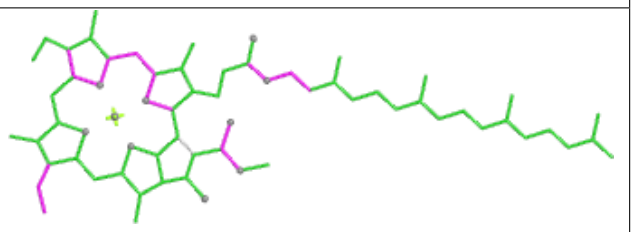


Rings

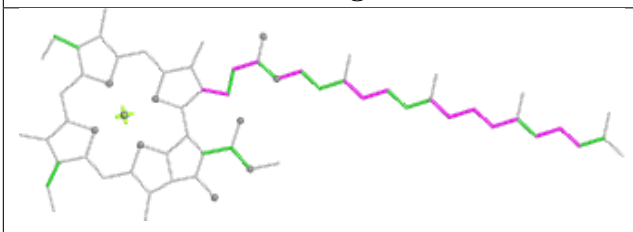
Ligand CLA cA 842



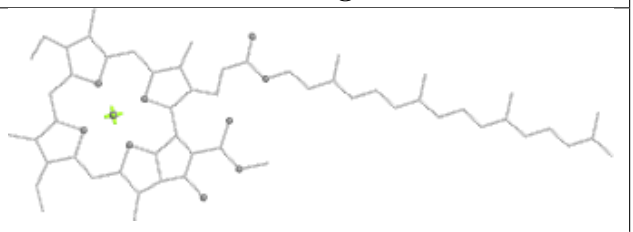
Bond lengths



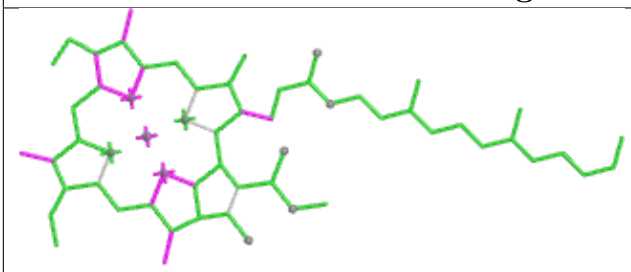
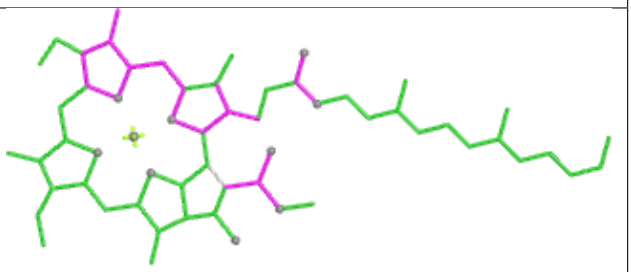
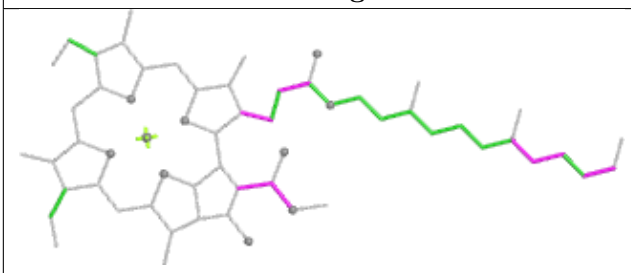
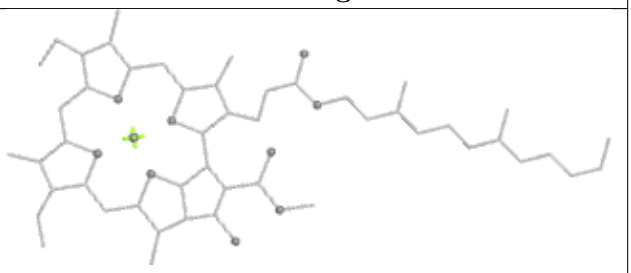
Bond angles

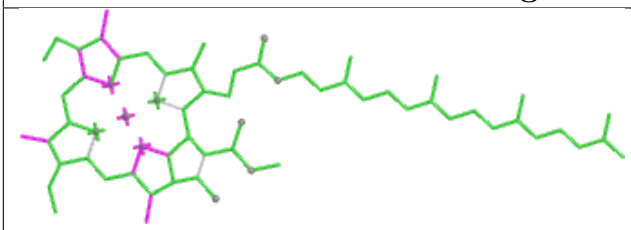
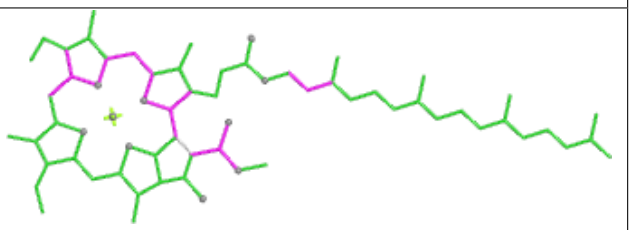
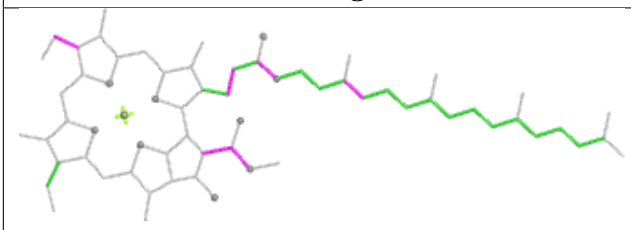
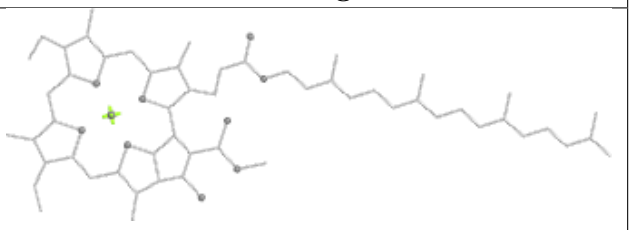


Torsions

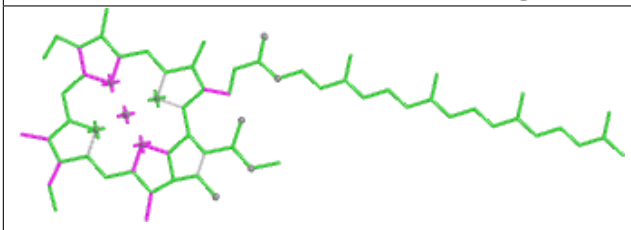


Rings

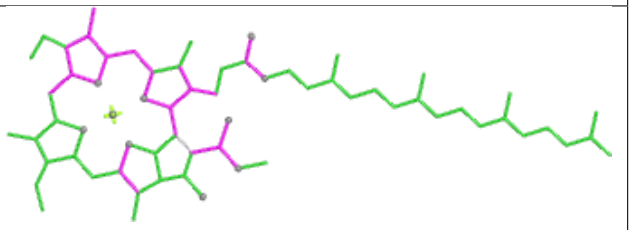
Ligand CLA cA 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c5 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

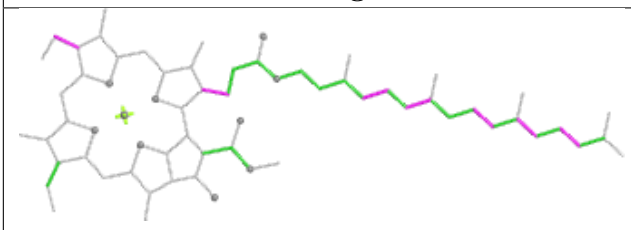
Ligand CLA aA 807



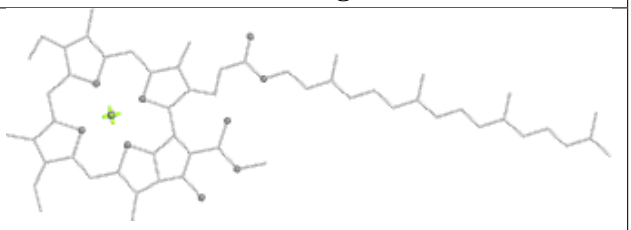
Bond lengths



Bond angles

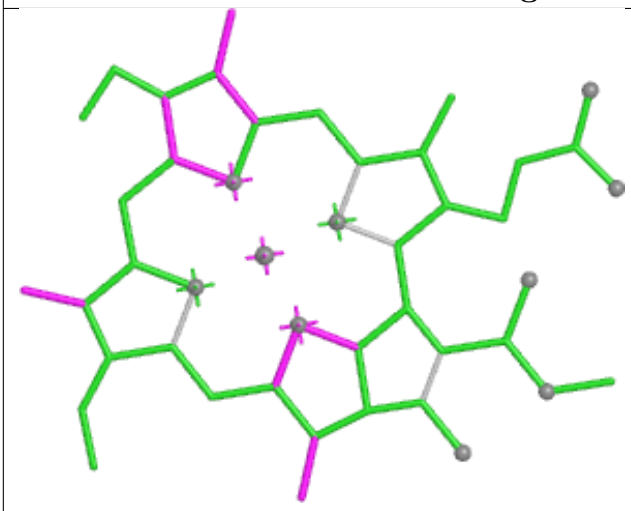


Torsions

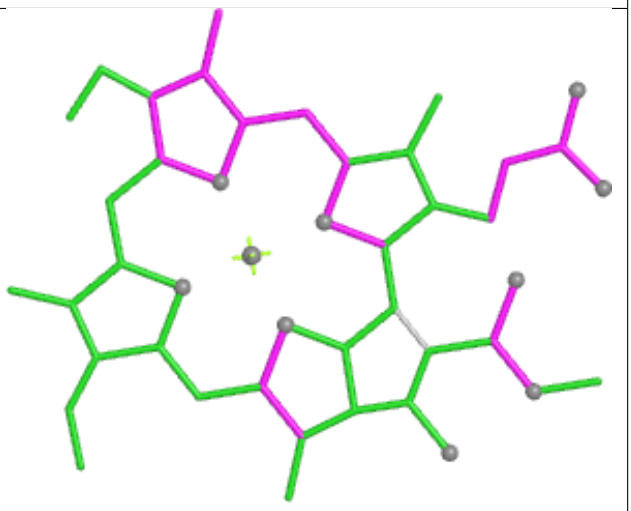


Rings

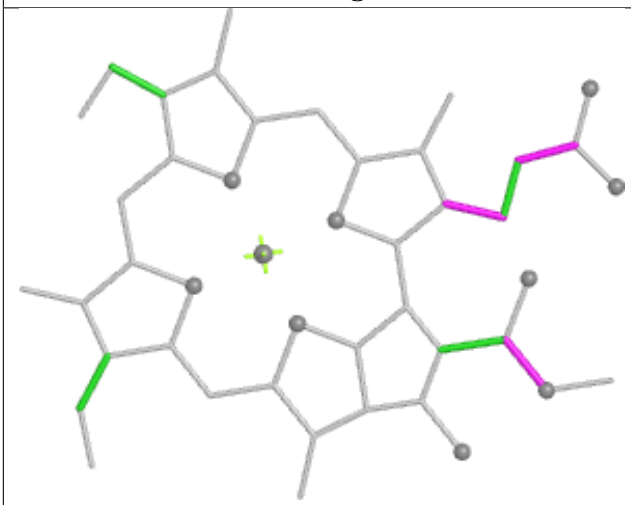
Ligand CLA c5 408



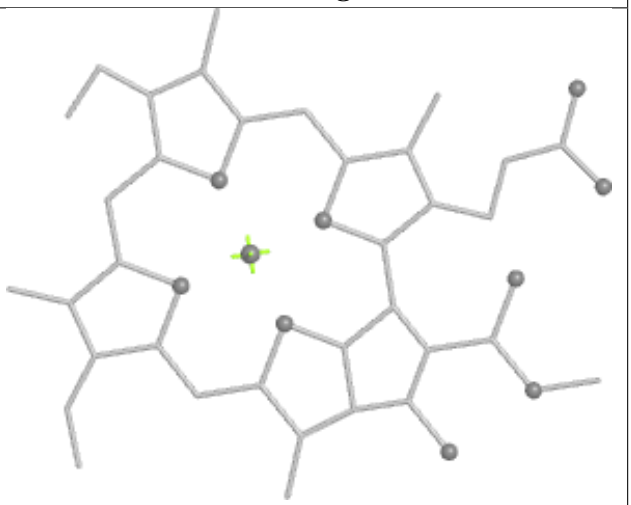
Bond lengths



Bond angles

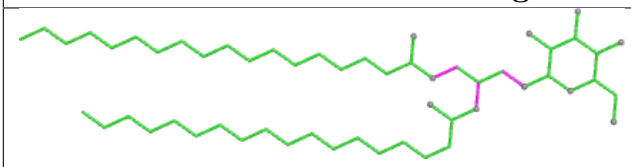


Torsions

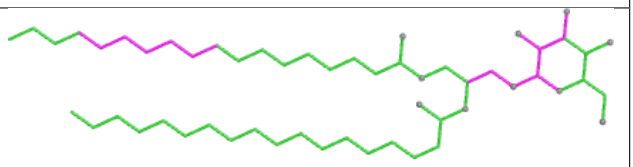


Rings

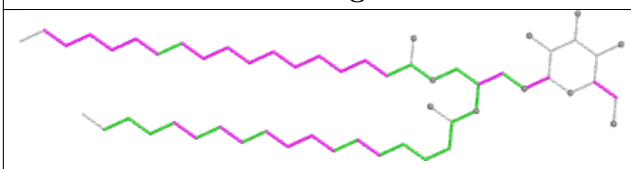
Ligand LMG cB 850



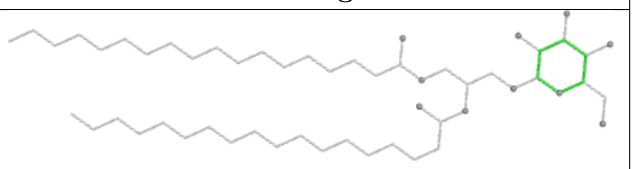
Bond lengths



Bond angles

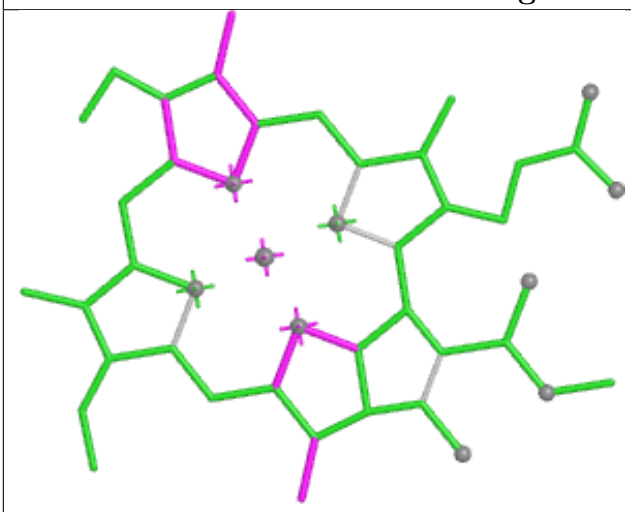


Torsions

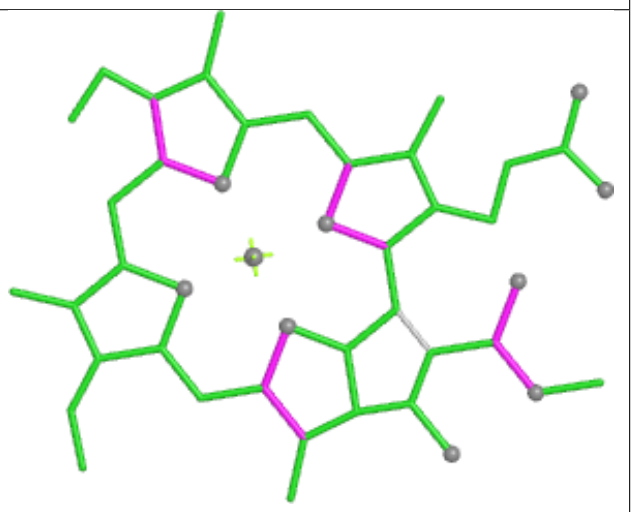


Rings

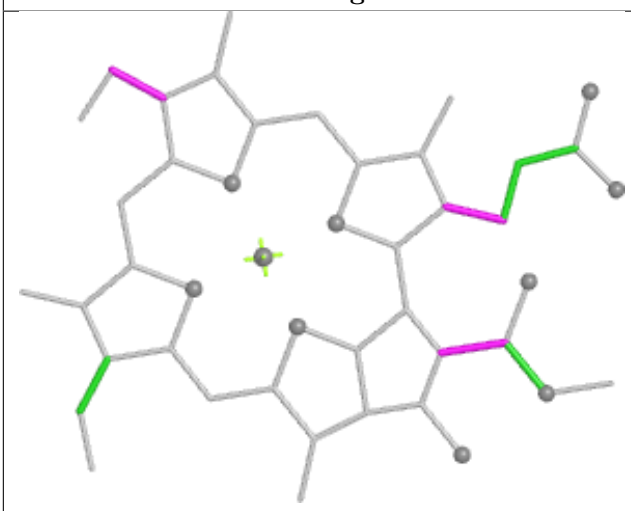
Ligand CLA b1 413



Bond lengths



Bond angles

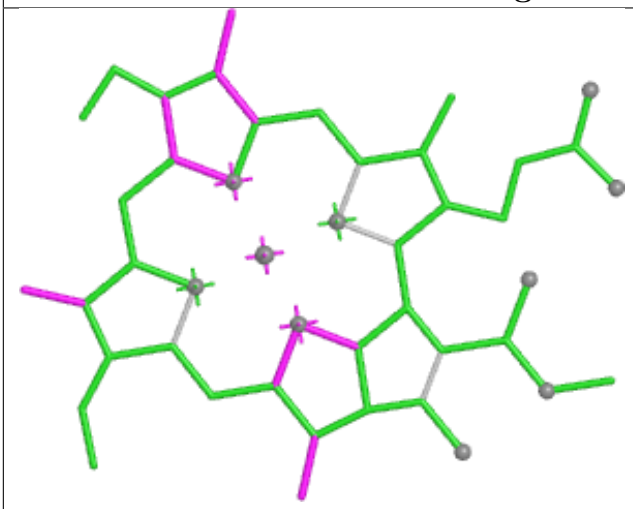


Torsions

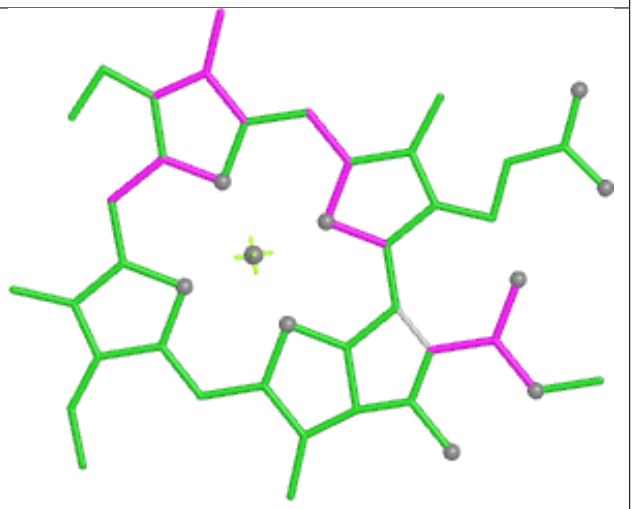


Rings

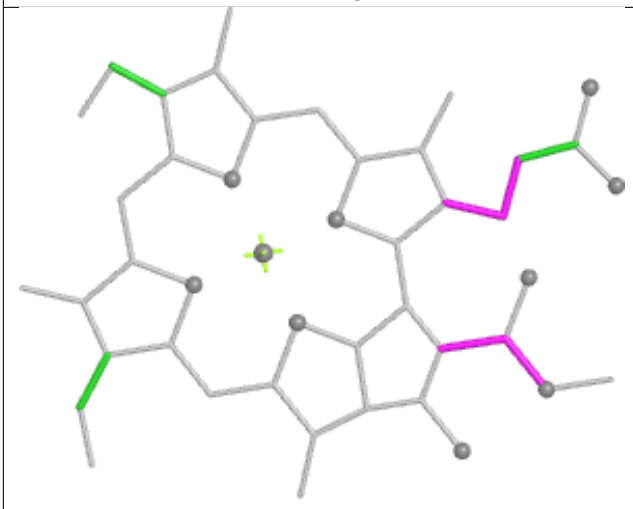
Ligand CLA bB 816



Bond lengths



Bond angles

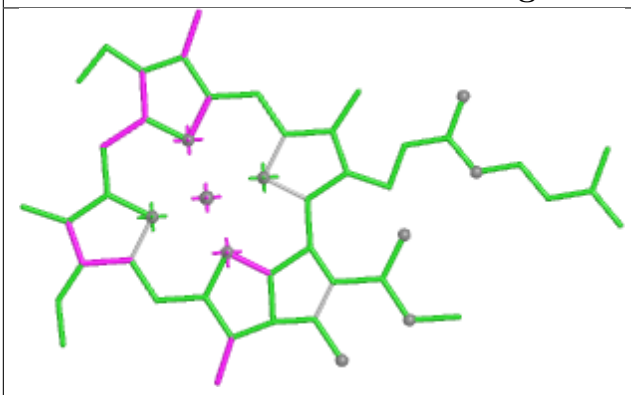


Torsions

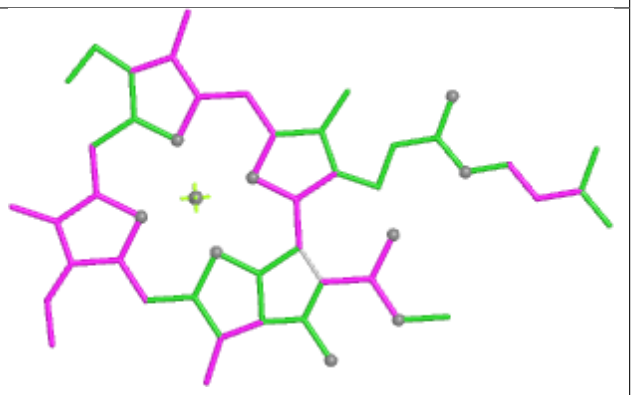


Rings

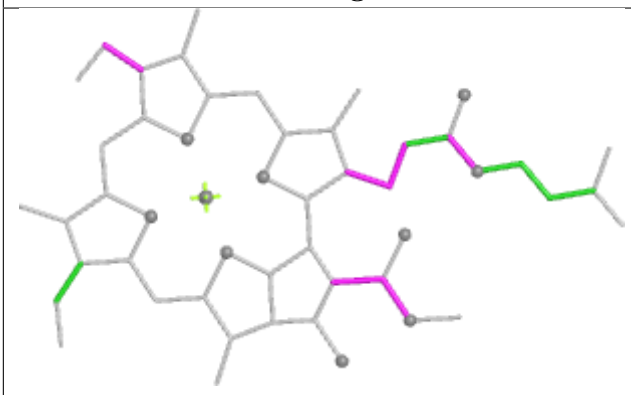
Ligand CLA b6 417



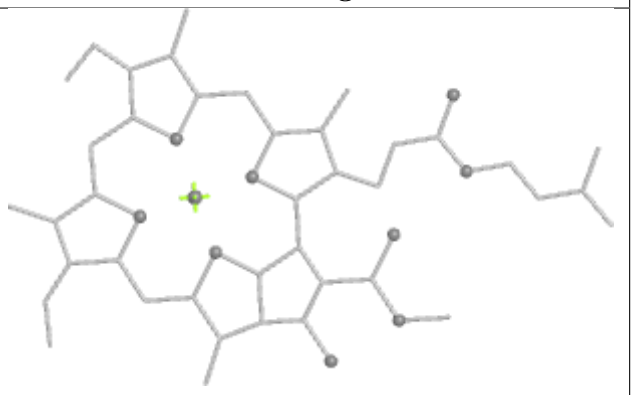
Bond lengths



Bond angles



Torsions

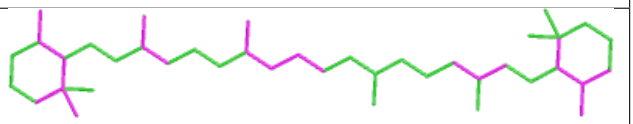


Rings

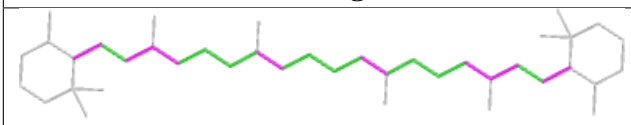
Ligand BCR cF 204



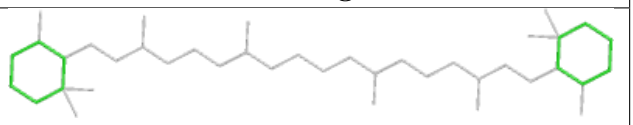
Bond lengths



Bond angles

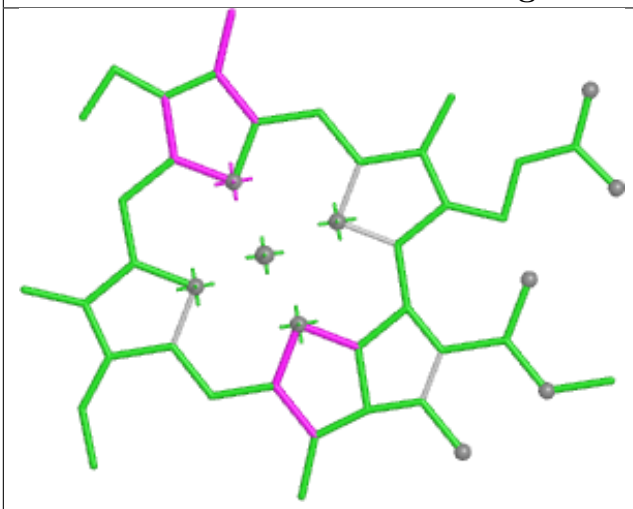


Torsions

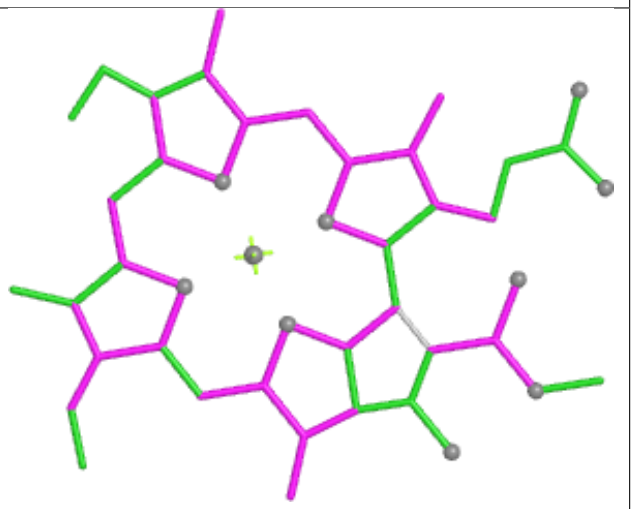


Rings

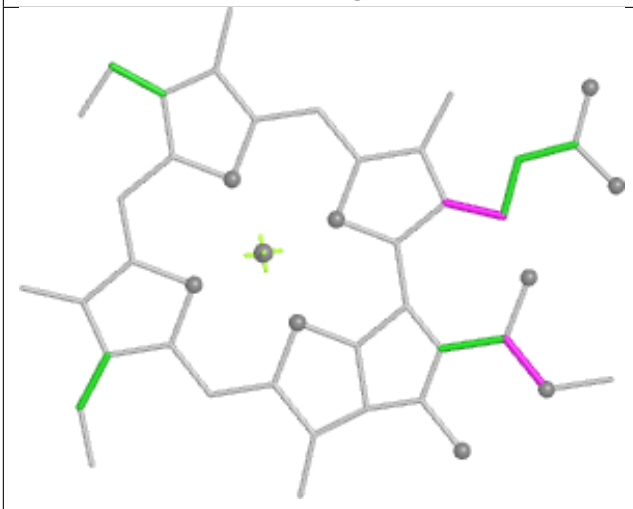
Ligand CLA b1 405



Bond lengths



Bond angles

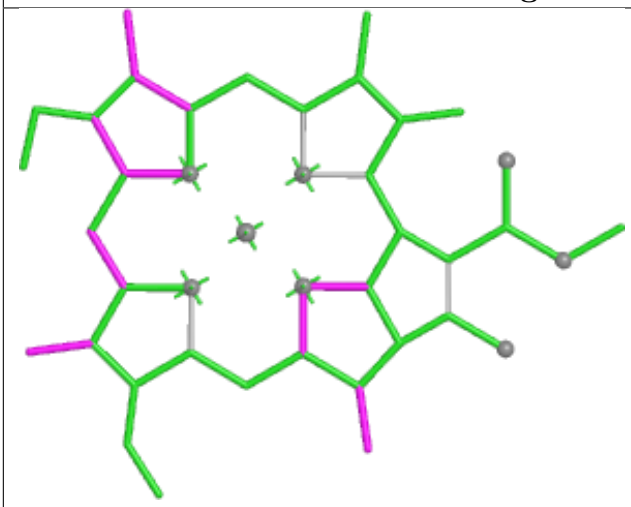


Torsions

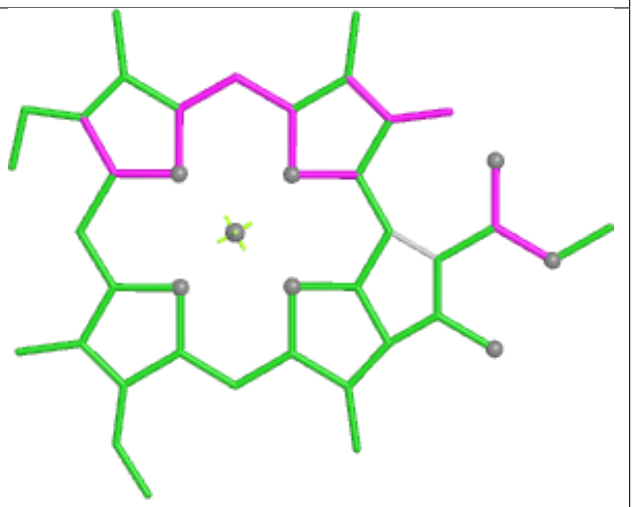


Rings

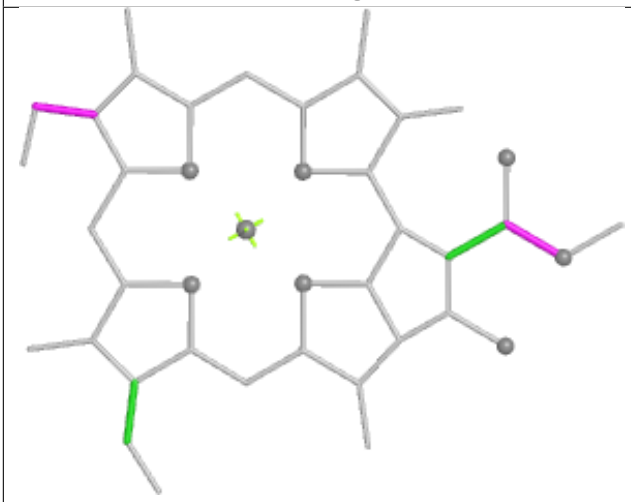
Ligand CLA c1 414



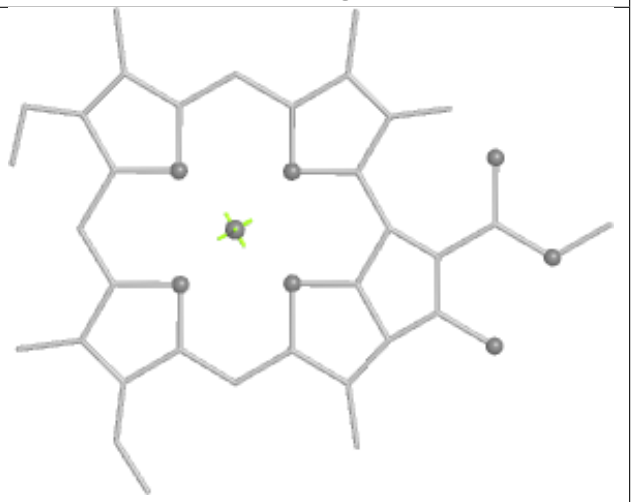
Bond lengths



Bond angles

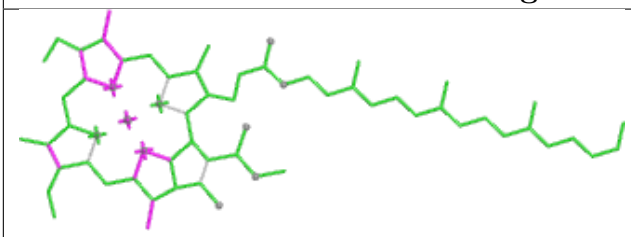


Torsions

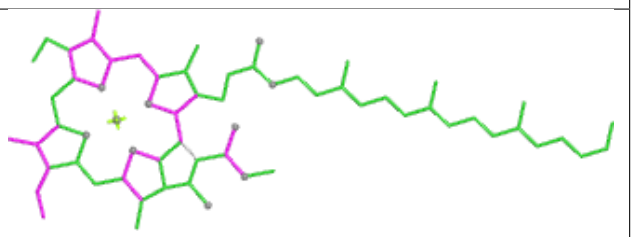


Rings

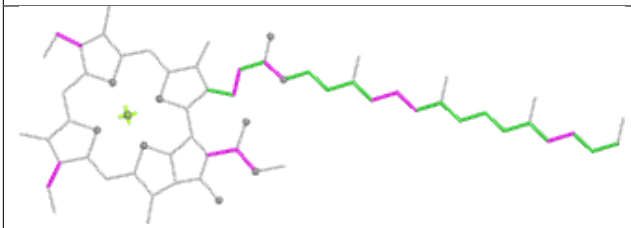
Ligand CLA c5 410



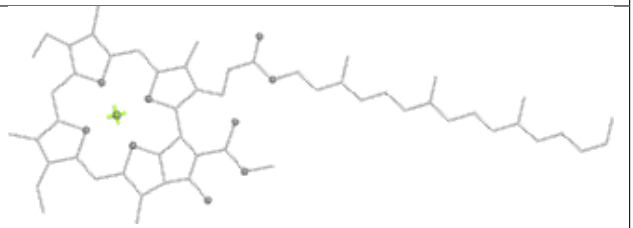
Bond lengths



Bond angles

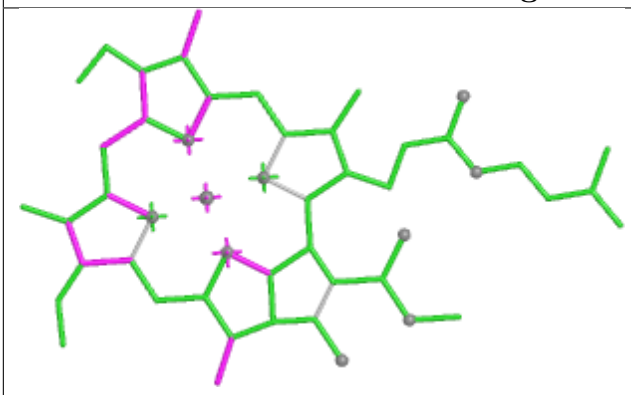


Torsions

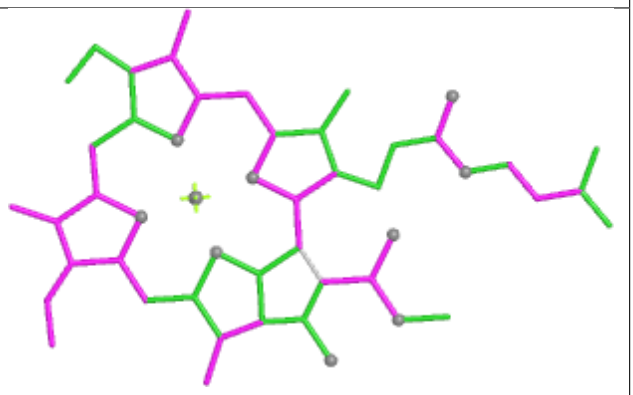


Rings

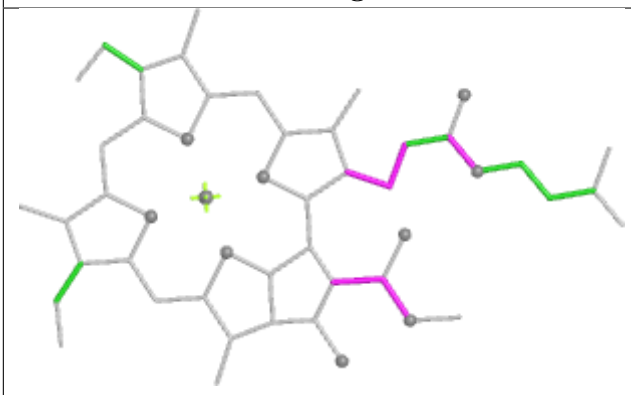
Ligand CLA c2 417



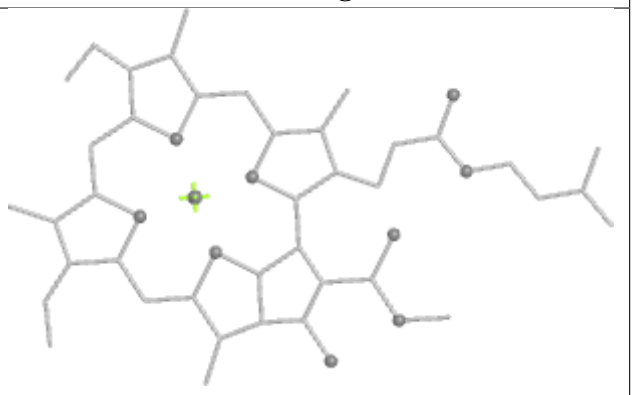
Bond lengths



Bond angles

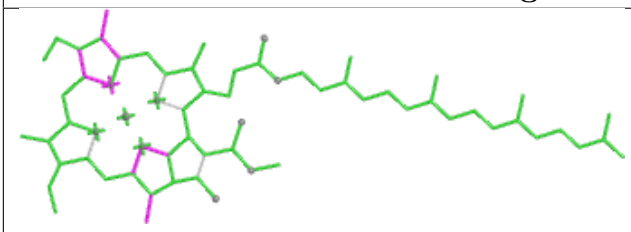


Torsions

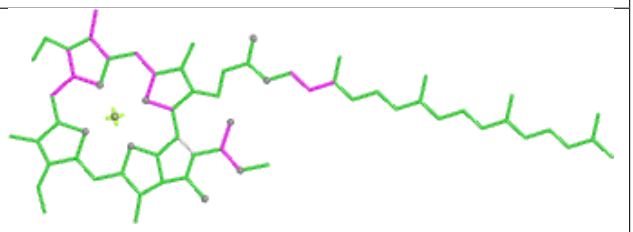


Rings

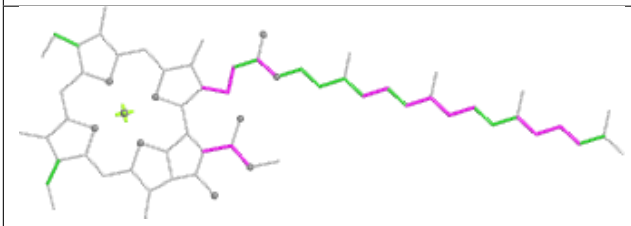
Ligand CLA c6 404



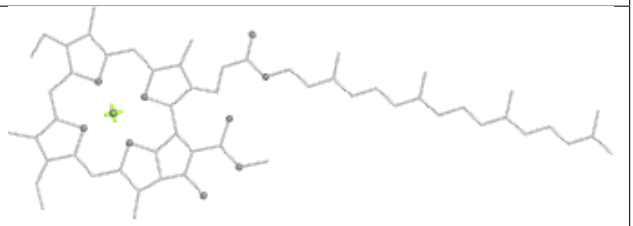
Bond lengths



Bond angles

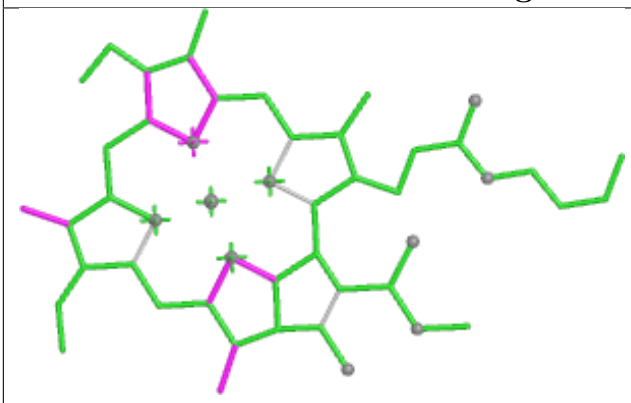


Torsions

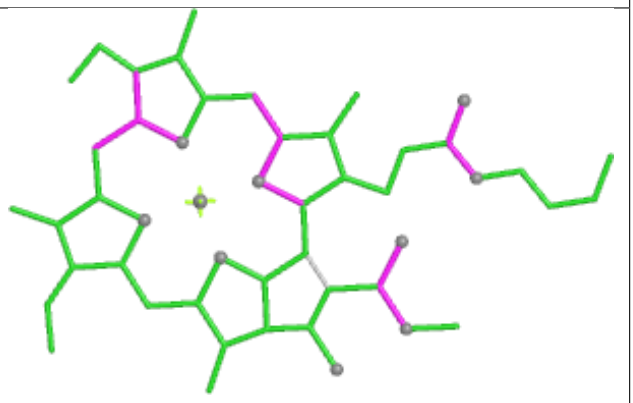


Rings

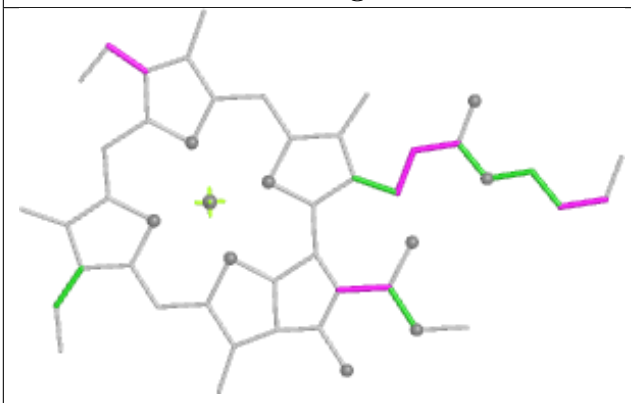
Ligand CLA aA 823



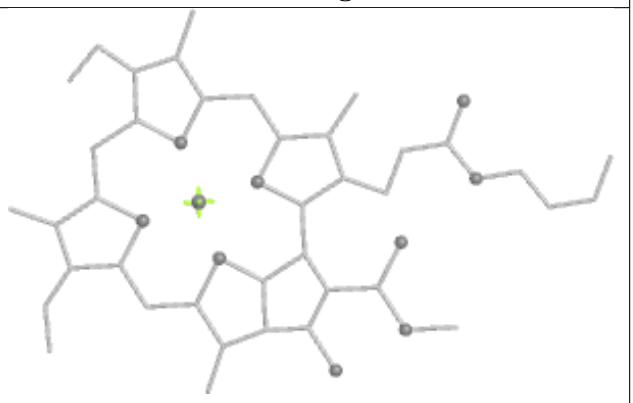
Bond lengths



Bond angles

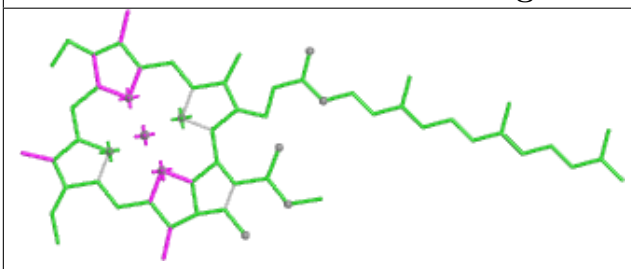


Torsions

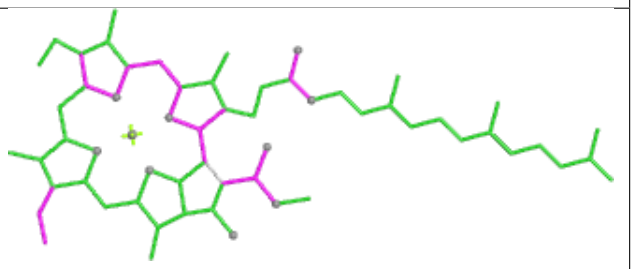


Rings

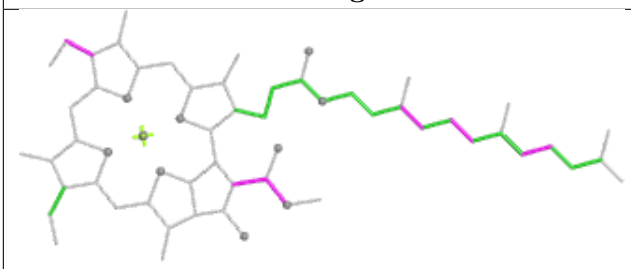
Ligand CLA cB 836



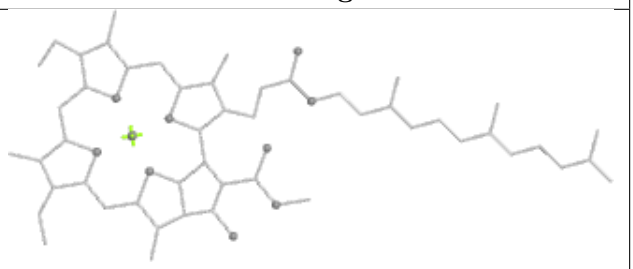
Bond lengths



Bond angles

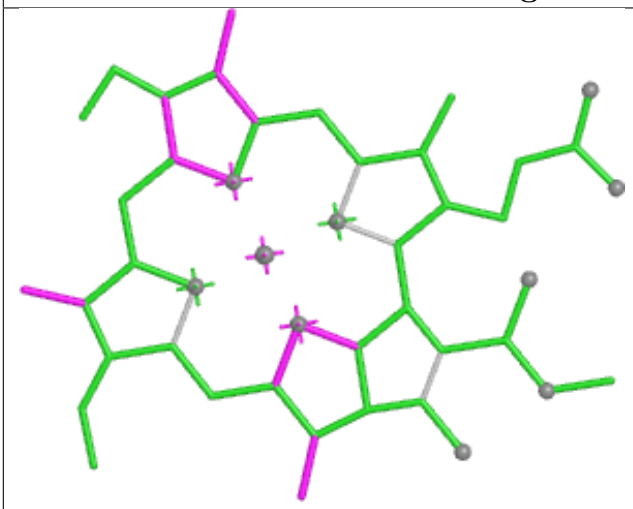


Torsions

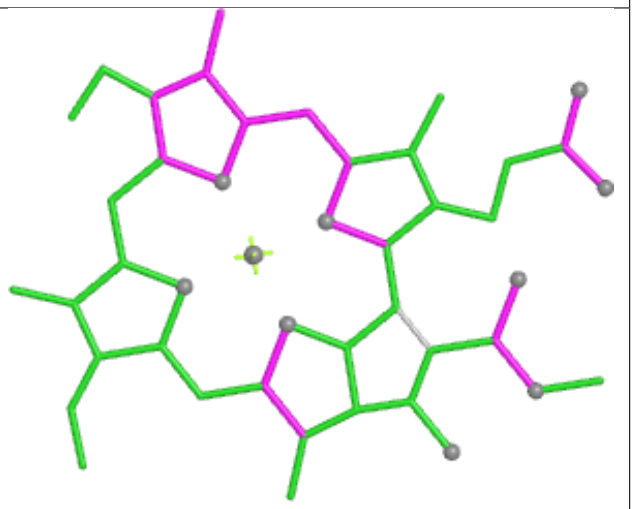


Rings

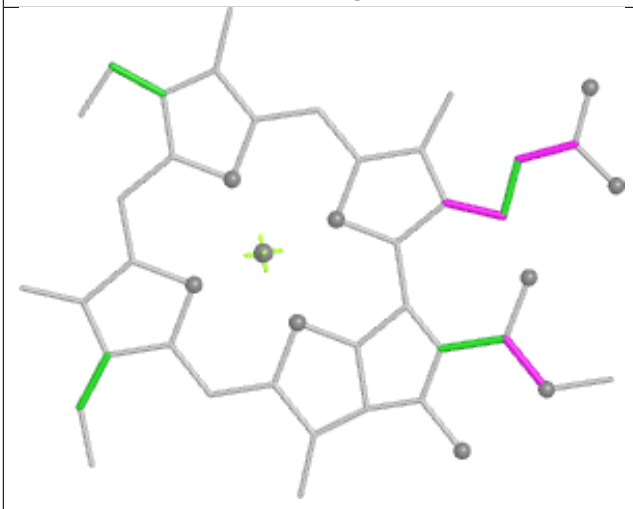
Ligand CLA c6 410



Bond lengths



Bond angles

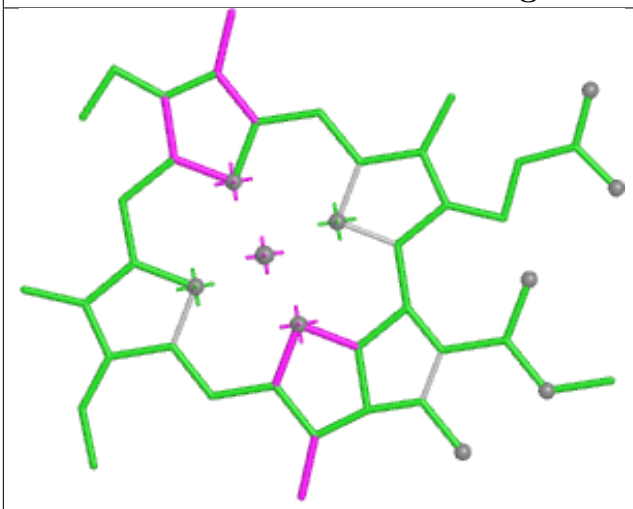


Torsions

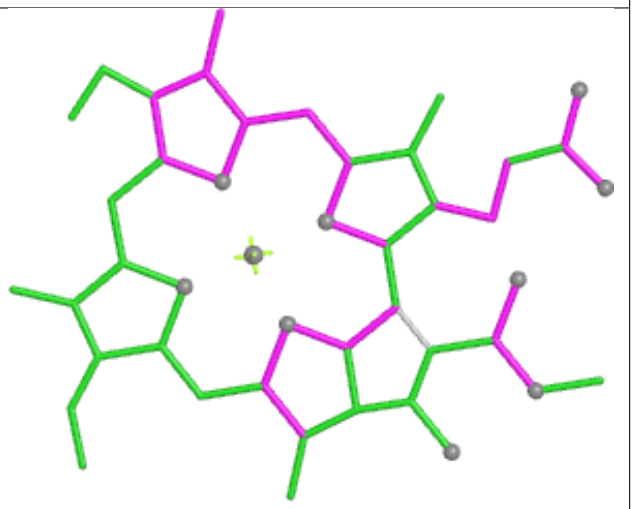


Rings

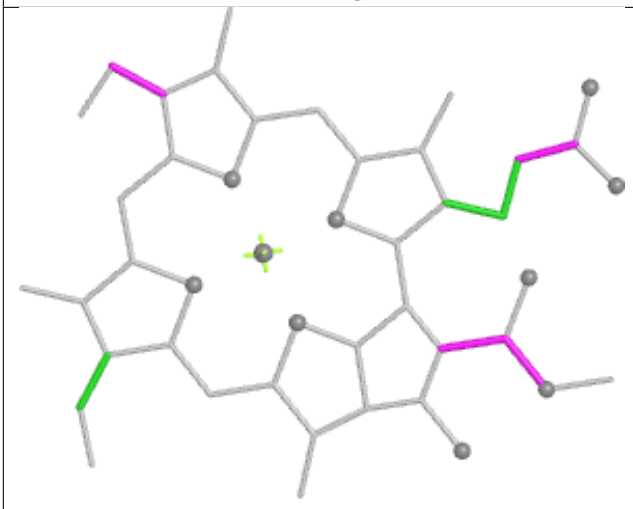
Ligand CLA a6 416



Bond lengths



Bond angles

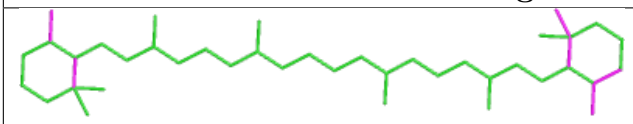


Torsions

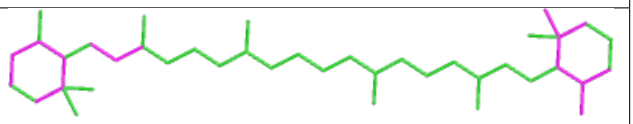


Rings

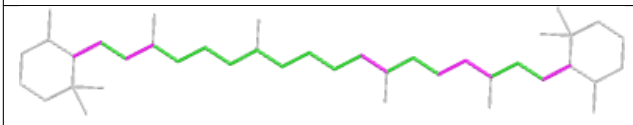
Ligand BCR b4 418



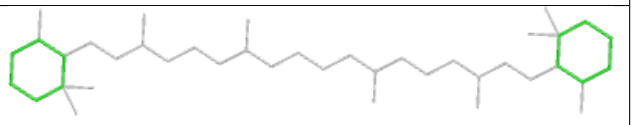
Bond lengths



Bond angles

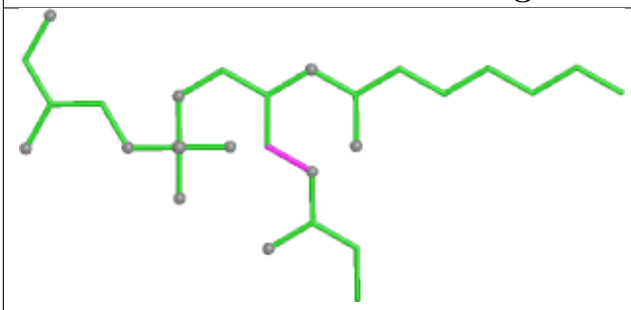


Torsions

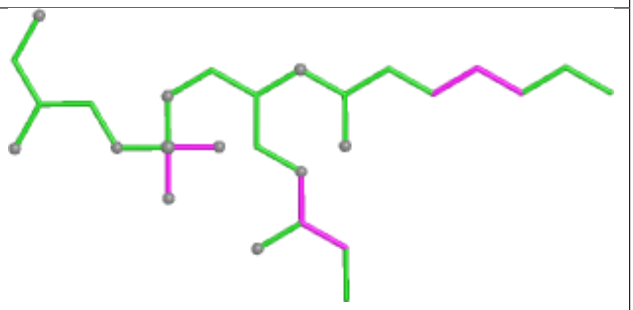


Rings

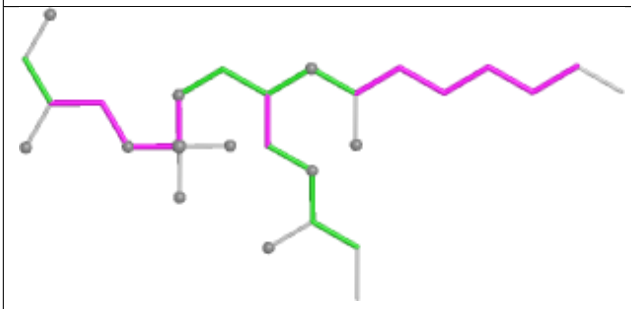
Ligand LHG cA 853



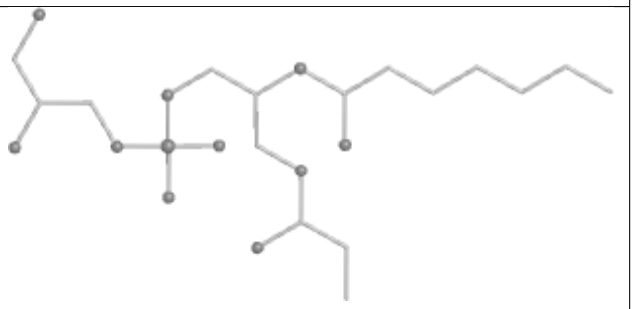
Bond lengths



Bond angles

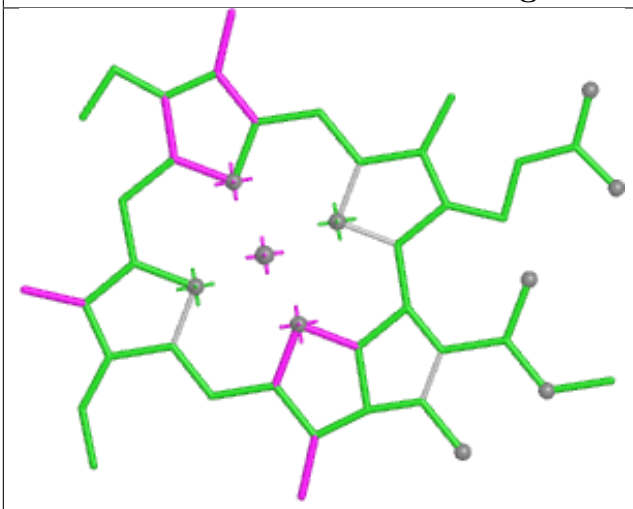


Torsions

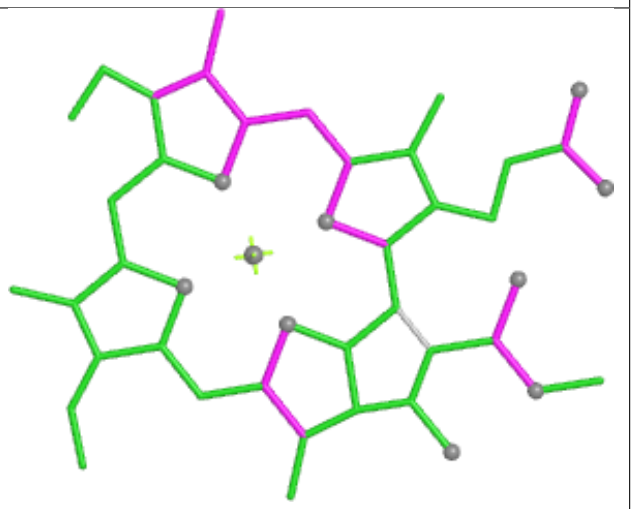


Rings

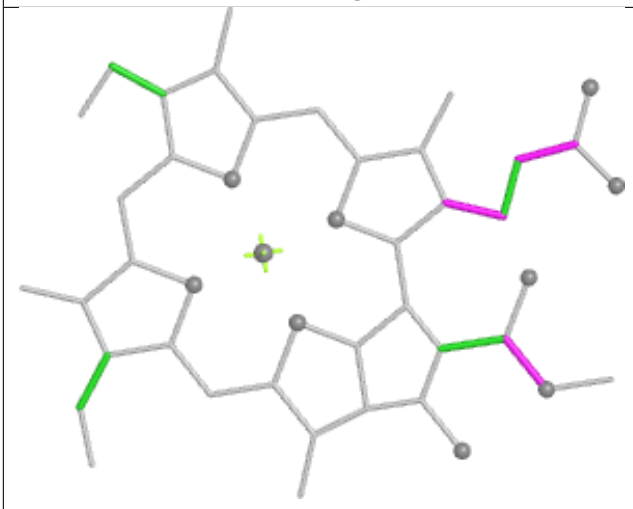
Ligand CLA a4 408



Bond lengths



Bond angles

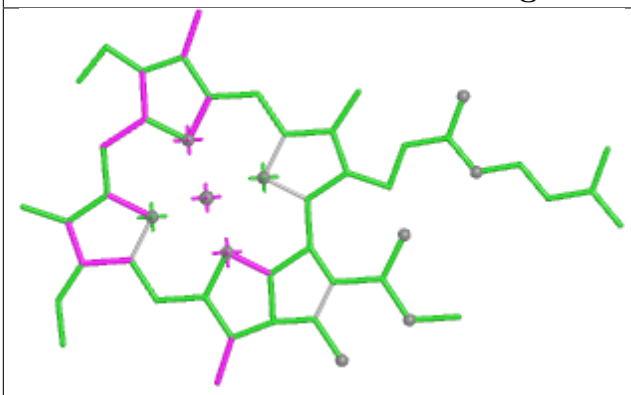


Torsions

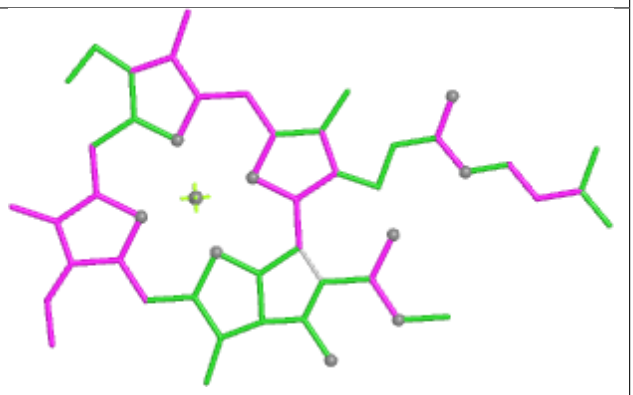


Rings

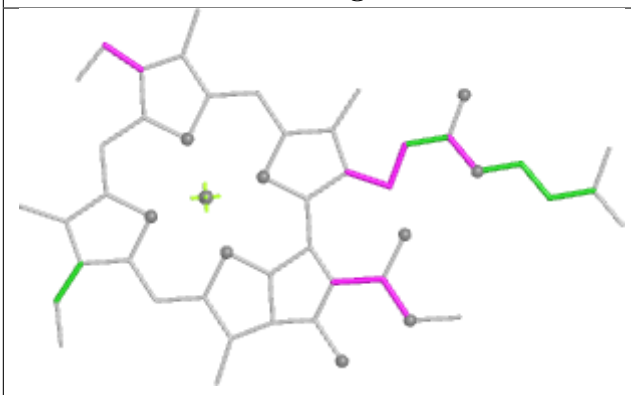
Ligand CLA a3 416



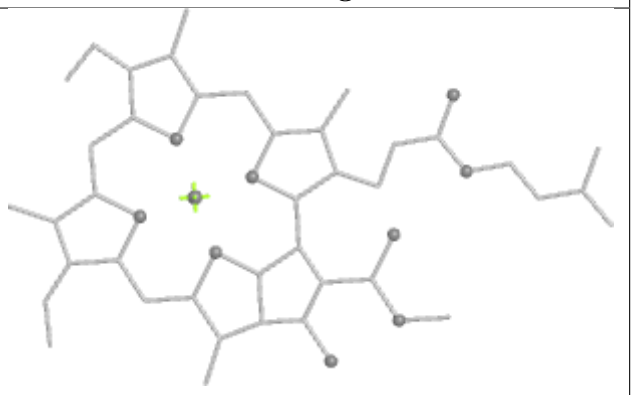
Bond lengths



Bond angles

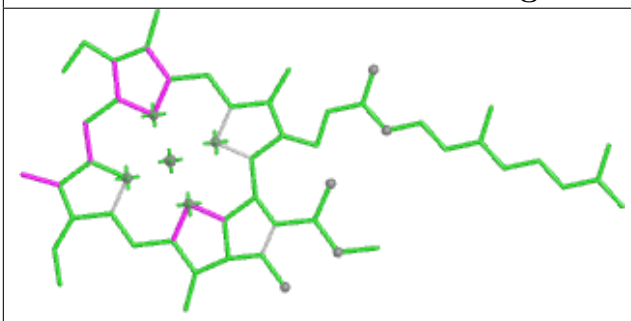


Torsions

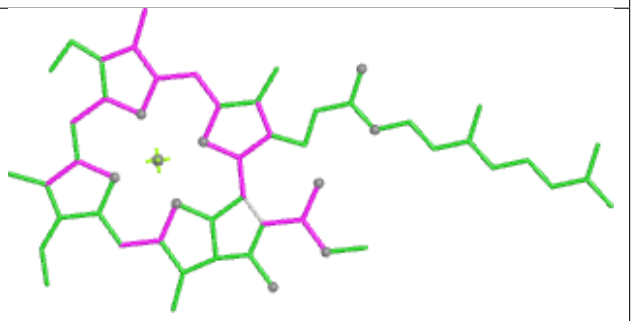


Rings

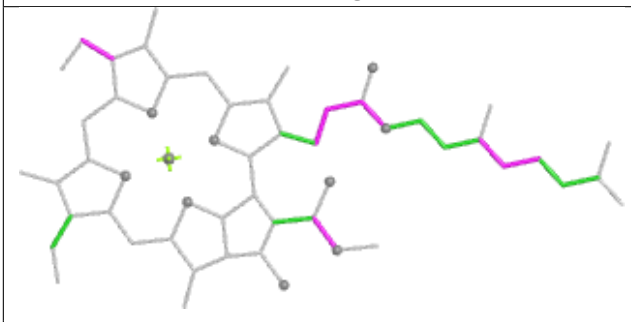
Ligand CLA c6 419



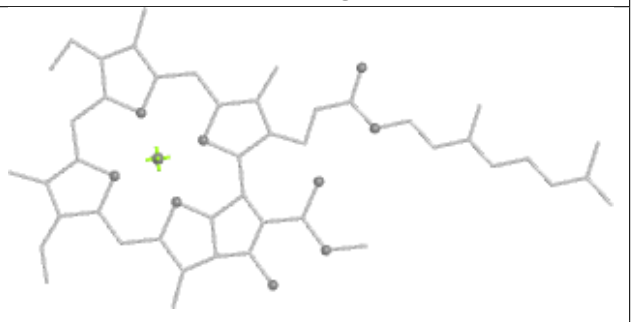
Bond lengths



Bond angles

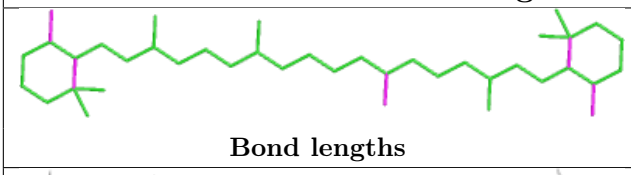


Torsions

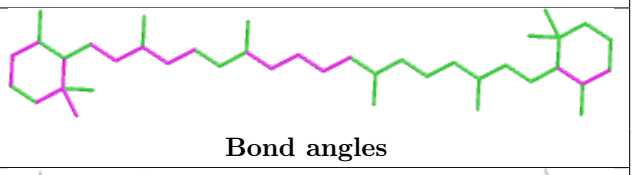


Rings

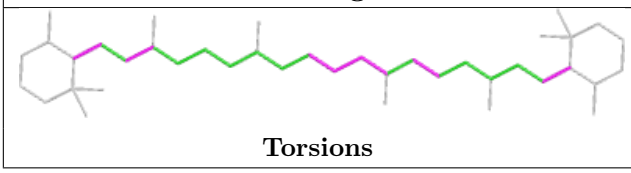
Ligand BCR cF 205



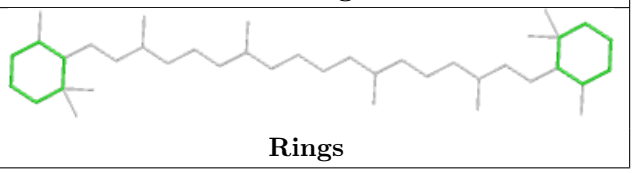
Bond lengths



Bond angles

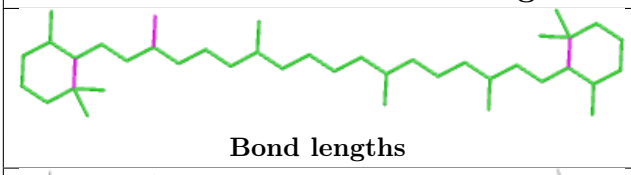


Torsions

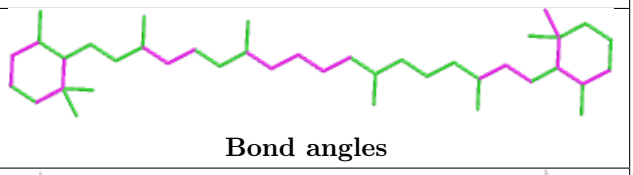


Rings

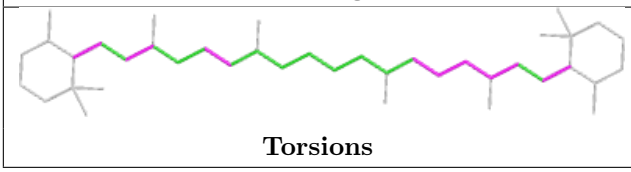
Ligand BCR a2 420



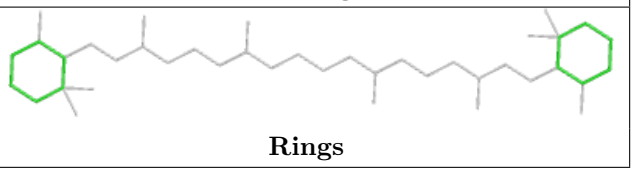
Bond lengths



Bond angles

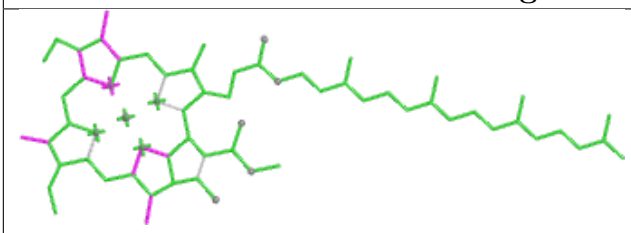


Torsions

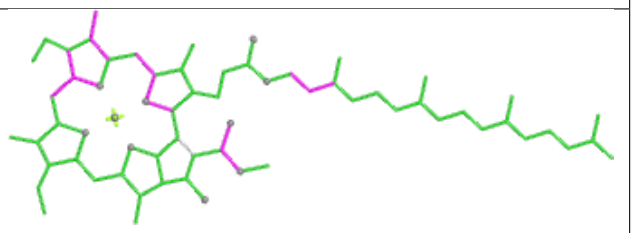


Rings

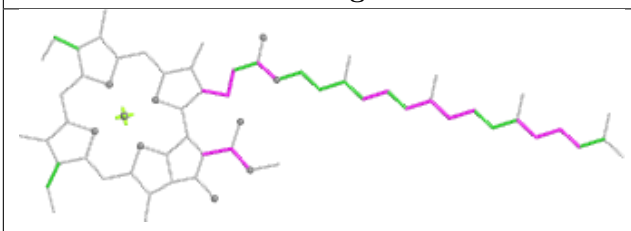
Ligand CLA a1 401



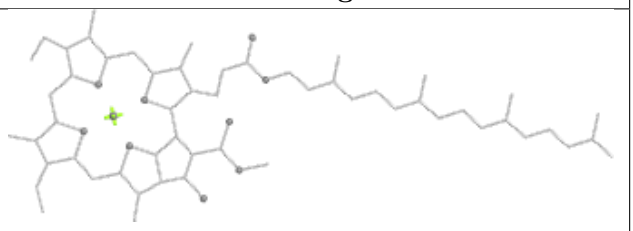
Bond lengths



Bond angles

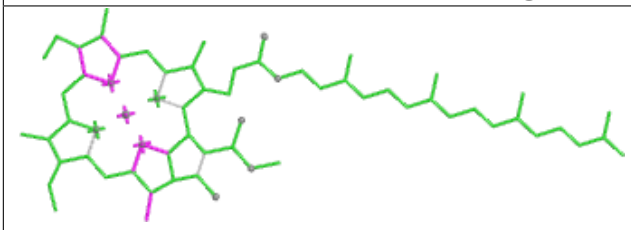


Torsions

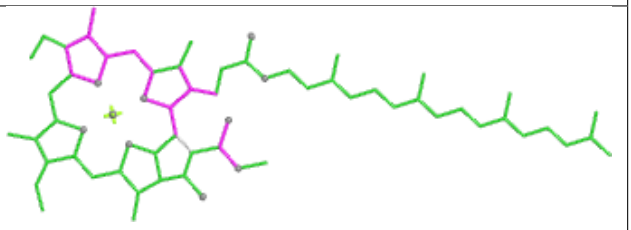


Rings

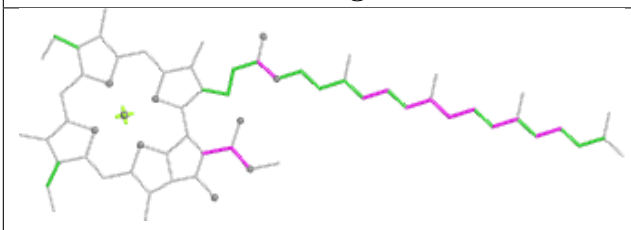
Ligand CLA c1 403



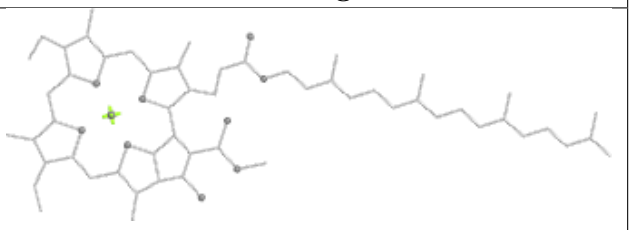
Bond lengths



Bond angles



Torsions

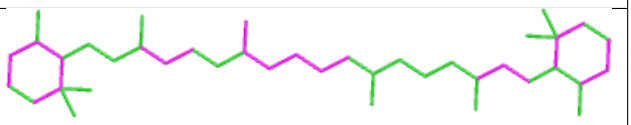


Rings

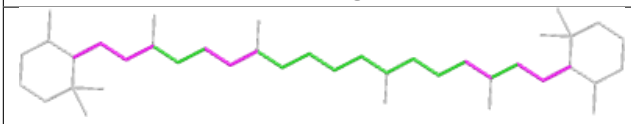
Ligand BCR a5 419



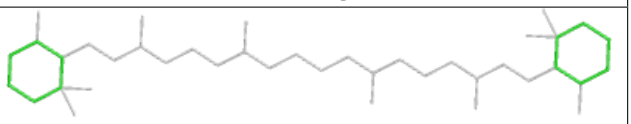
Bond lengths



Bond angles

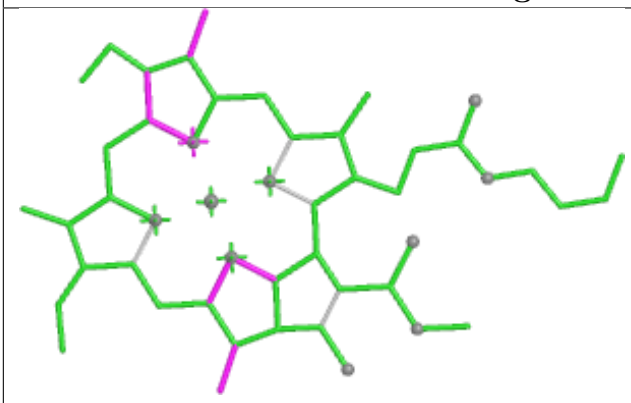


Torsions

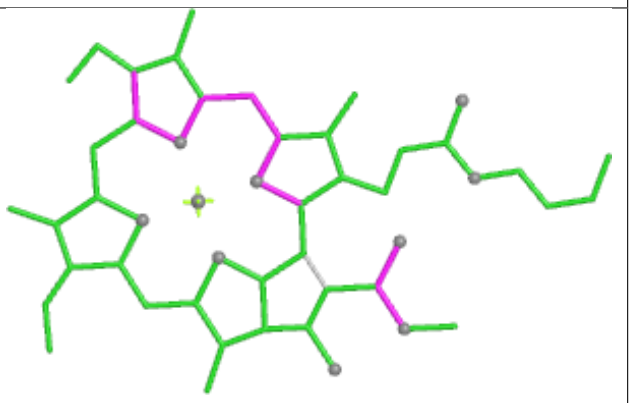


Rings

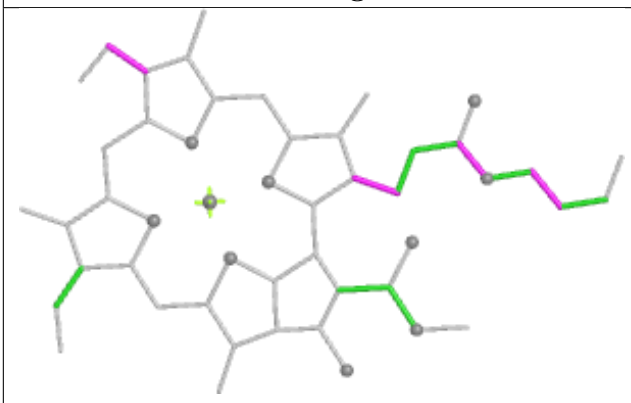
Ligand CLA bA 817



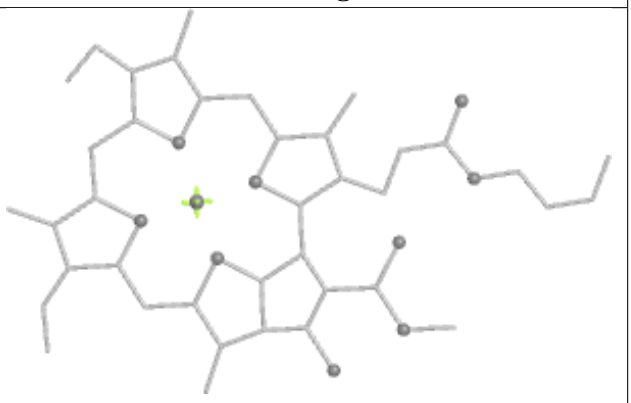
Bond lengths



Bond angles

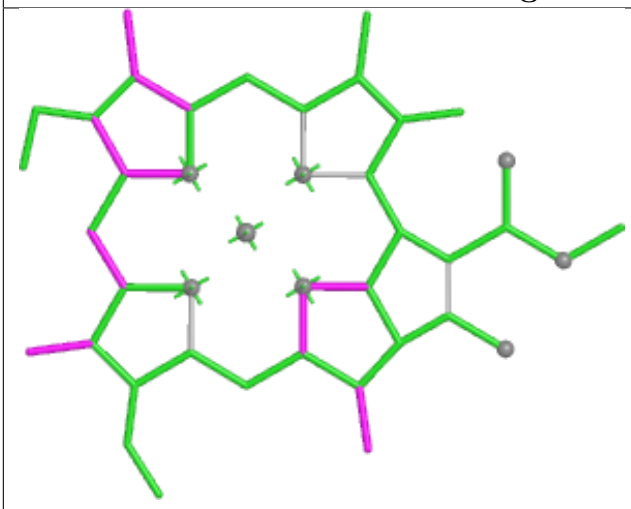


Torsions

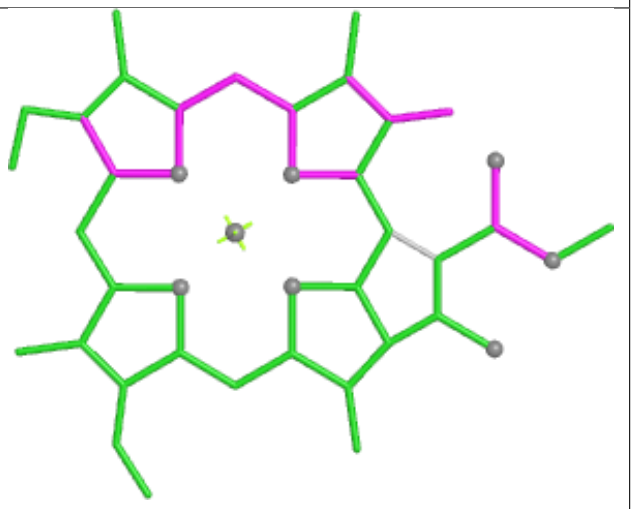


Rings

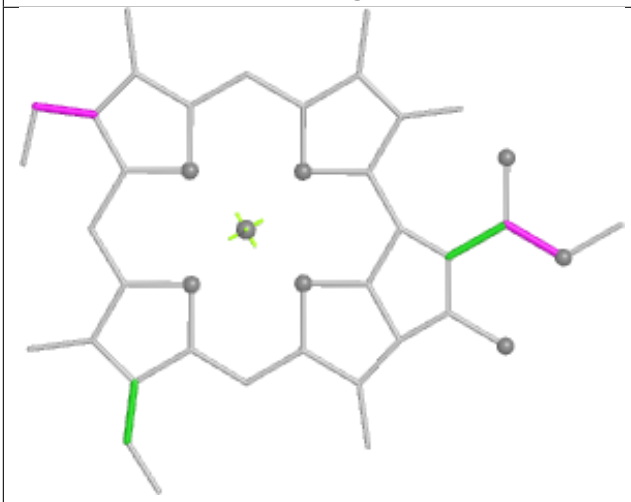
Ligand CLA c3 414



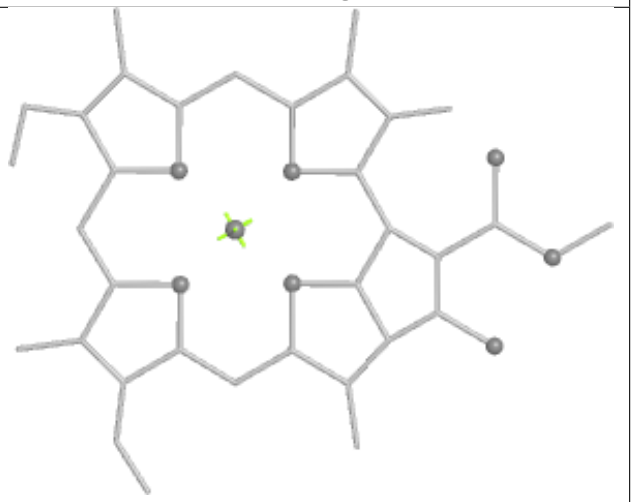
Bond lengths



Bond angles

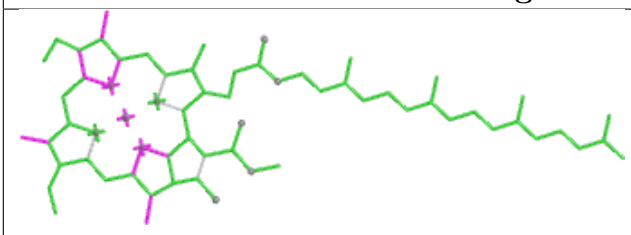


Torsions

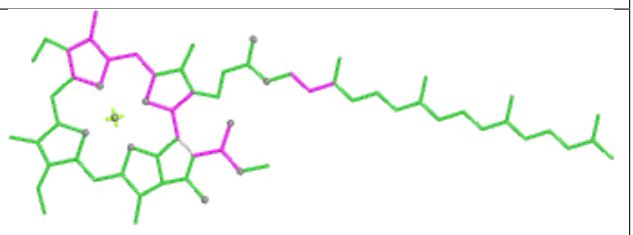


Rings

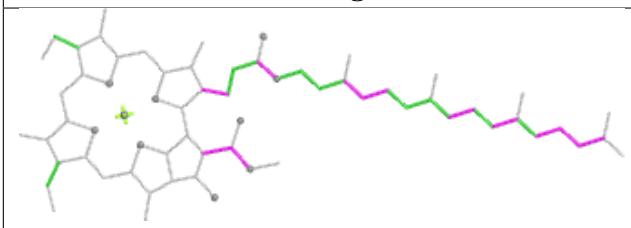
Ligand CLA aA 820



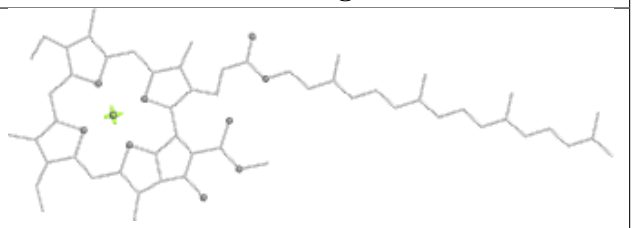
Bond lengths



Bond angles

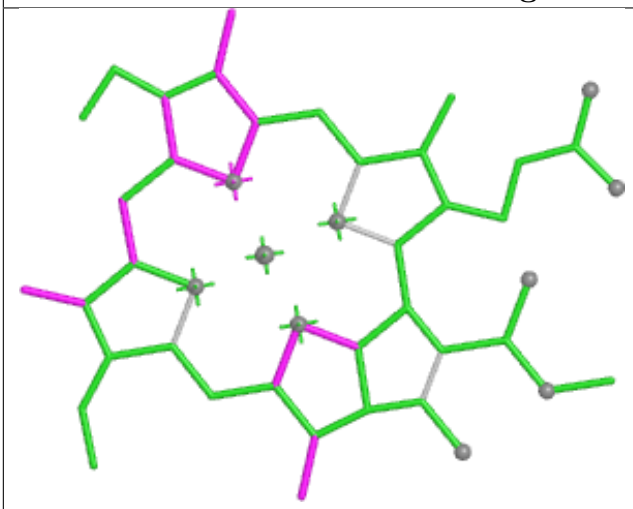


Torsions

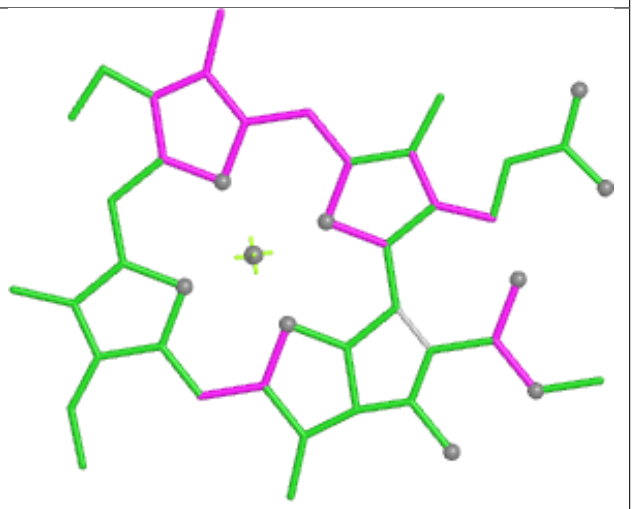


Rings

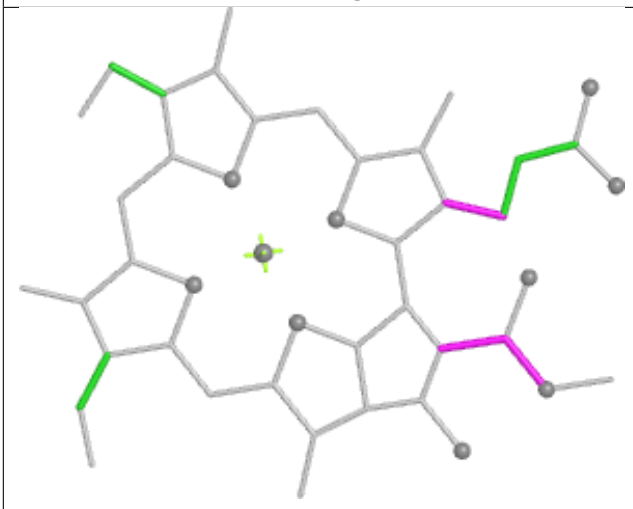
Ligand CLA a4 411



Bond lengths



Bond angles

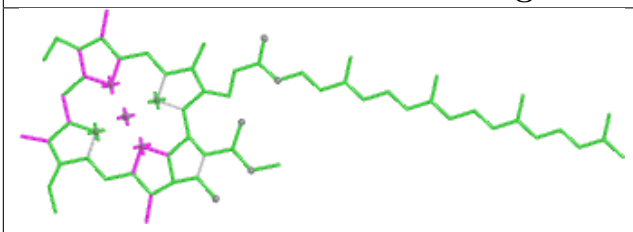


Torsions

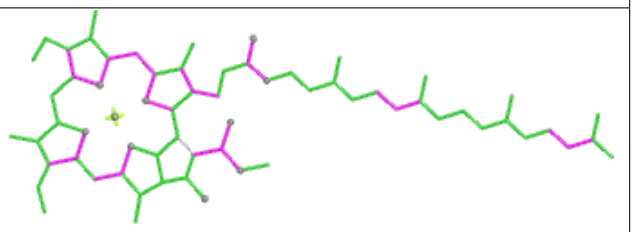


Rings

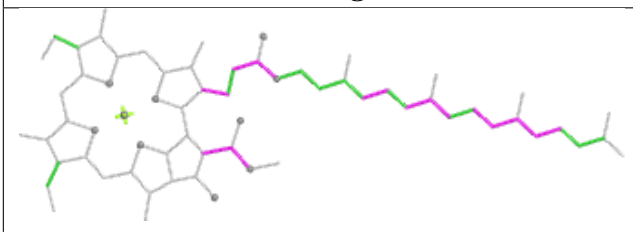
Ligand CLA aB 833



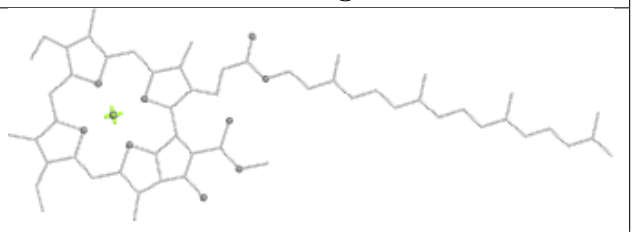
Bond lengths



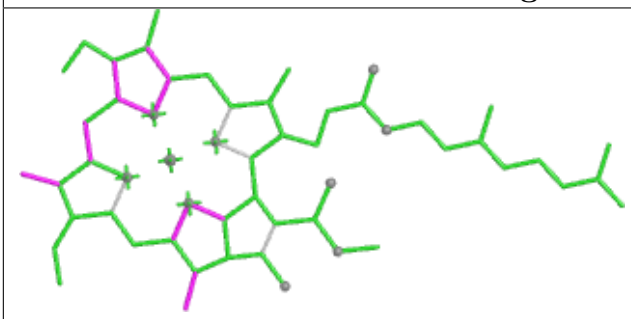
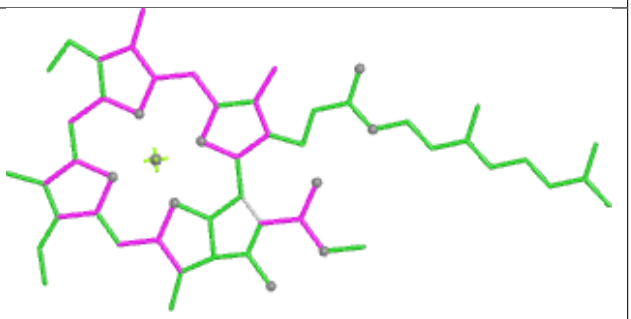
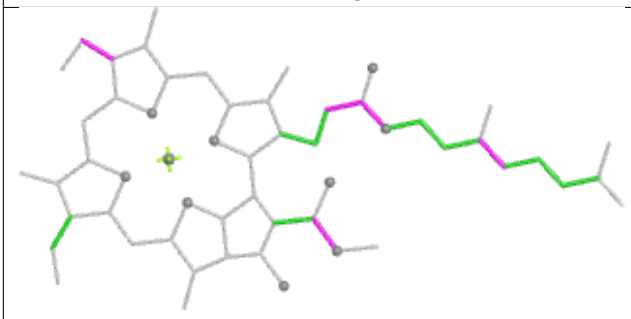
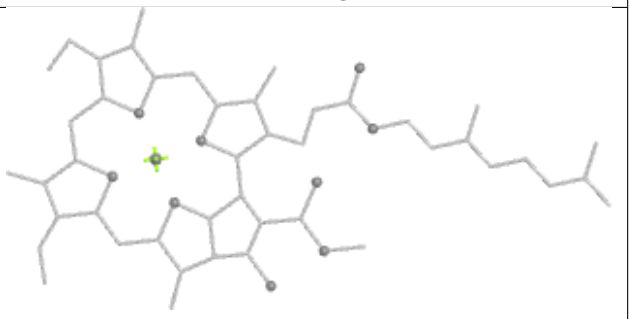
Bond angles

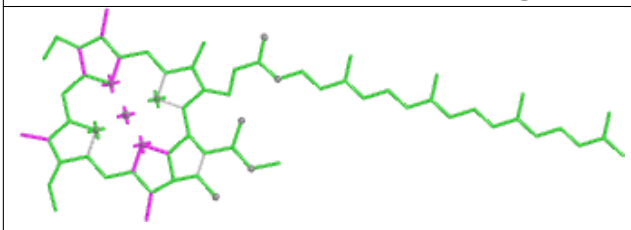
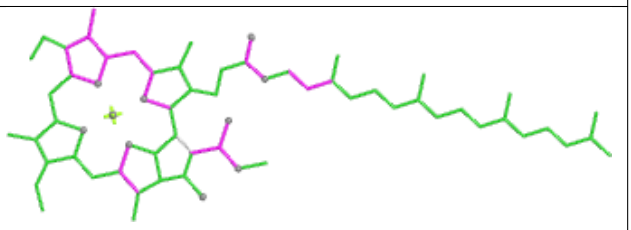
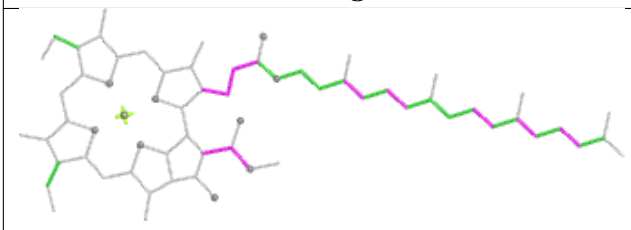
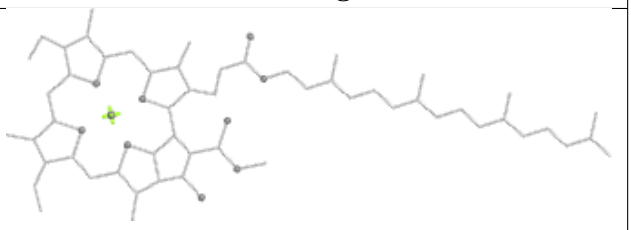


Torsions

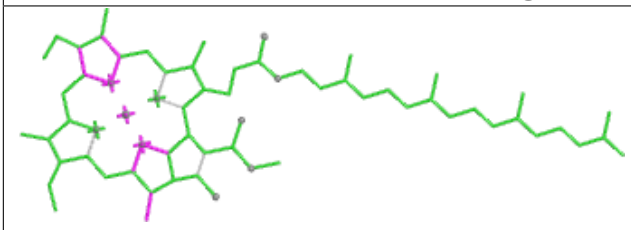


Rings

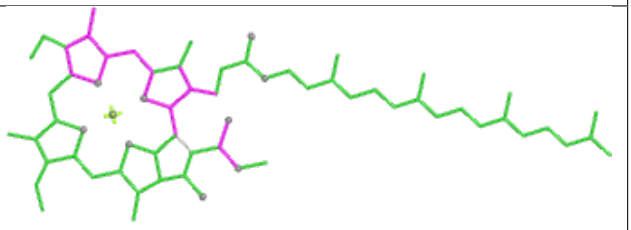
Ligand CLA c4 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cA 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

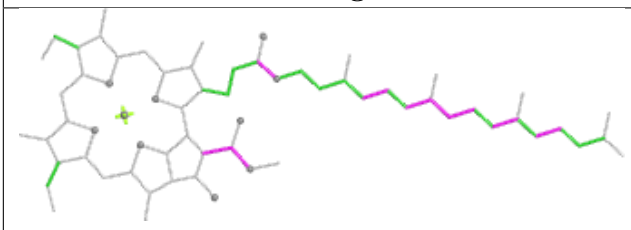
Ligand CLA a1 402



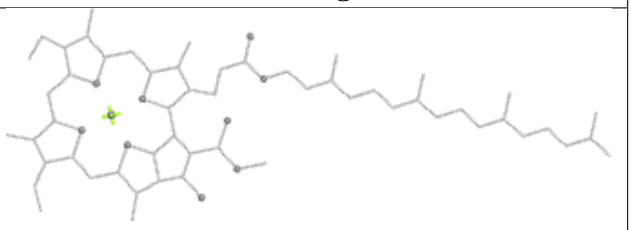
Bond lengths



Bond angles

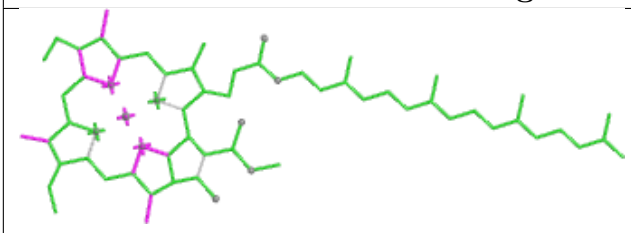


Torsions

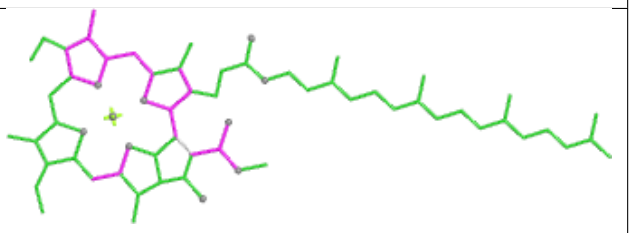


Rings

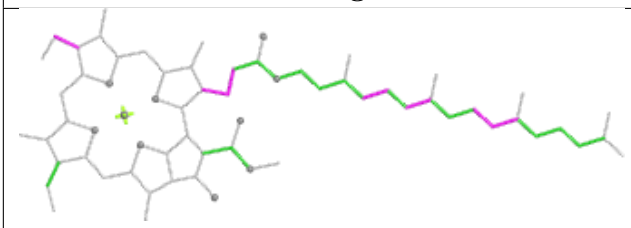
Ligand CLA bL 203



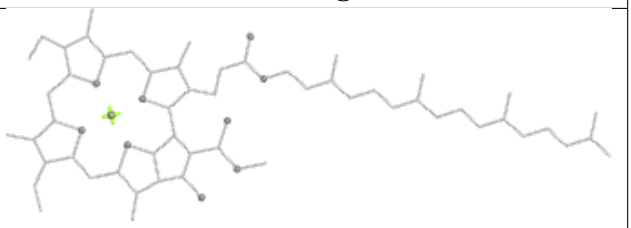
Bond lengths



Bond angles

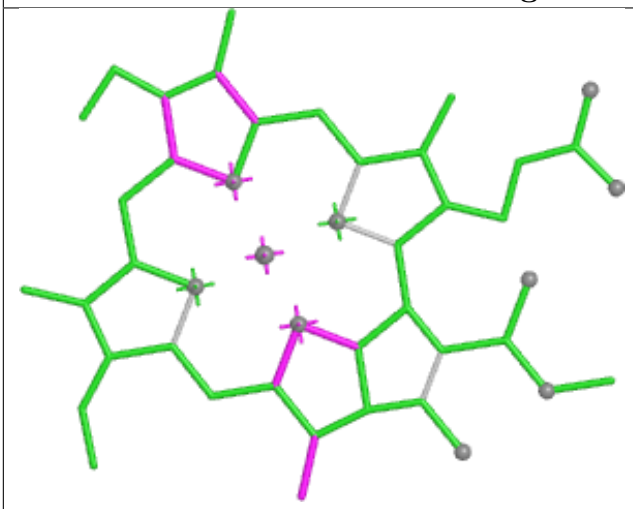


Torsions

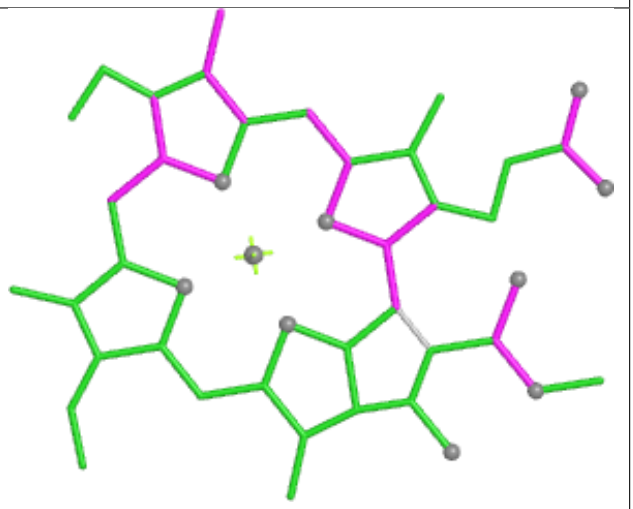


Rings

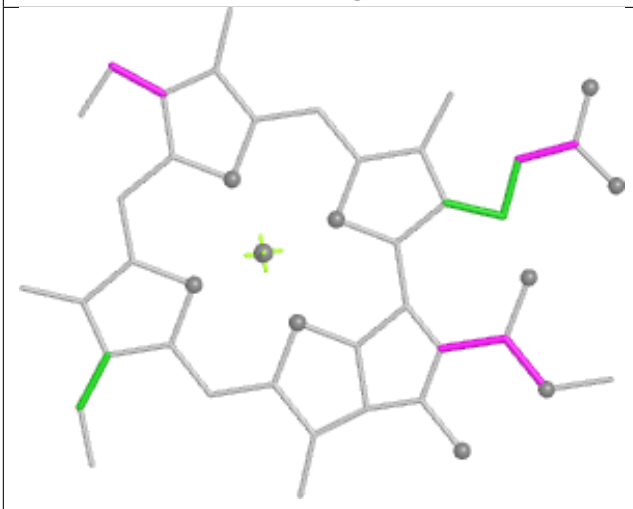
Ligand CLA c5 407



Bond lengths



Bond angles

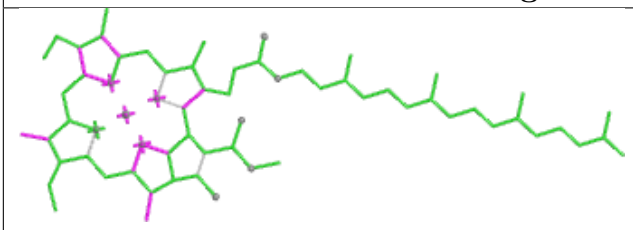


Torsions

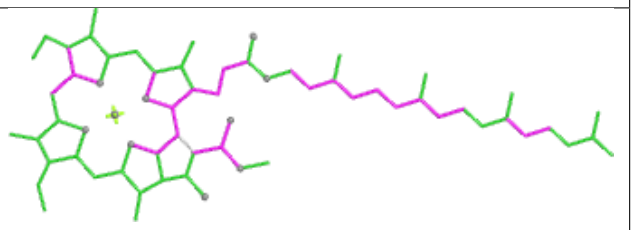


Rings

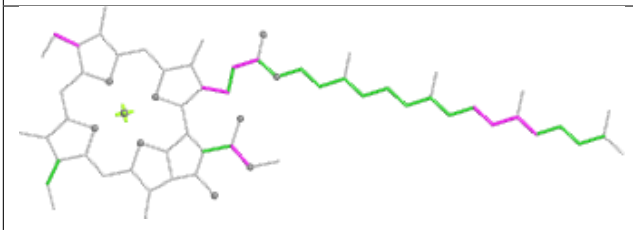
Ligand CLA c3 421



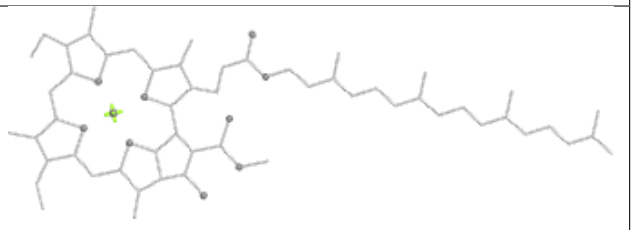
Bond lengths



Bond angles

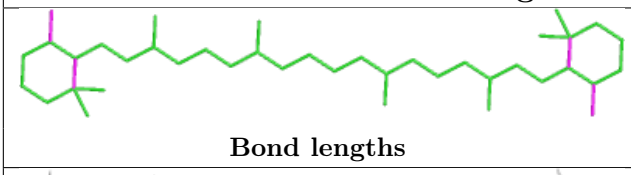


Torsions

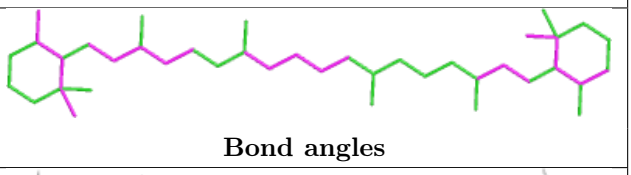


Rings

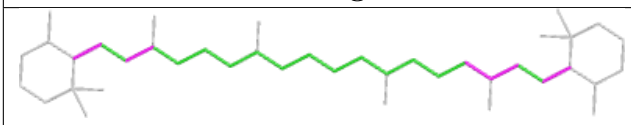
Ligand BCR cL 205



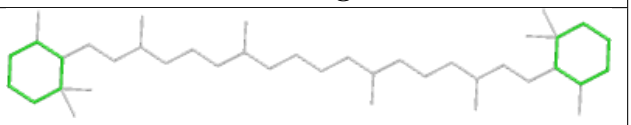
Bond lengths



Bond angles

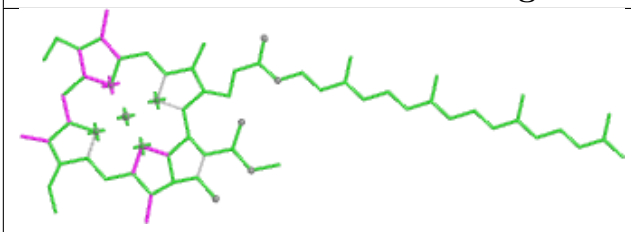


Torsions

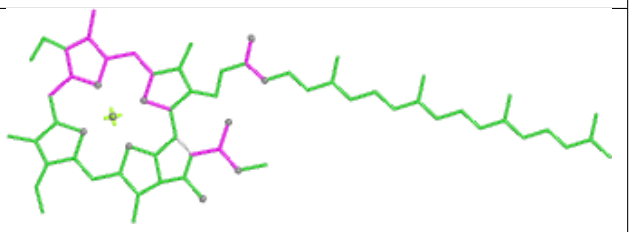


Rings

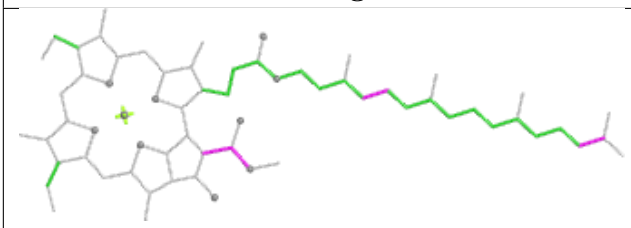
Ligand CLA b3 409



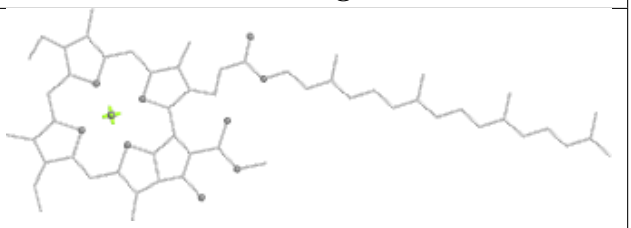
Bond lengths



Bond angles

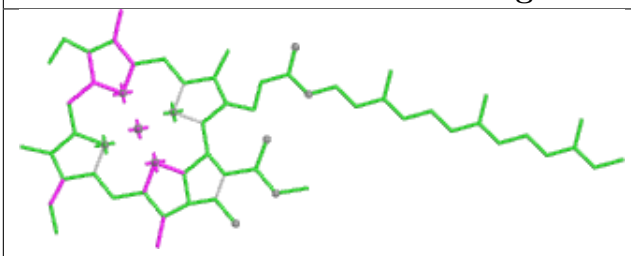


Torsions

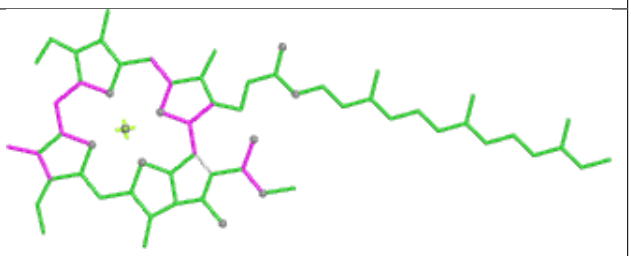


Rings

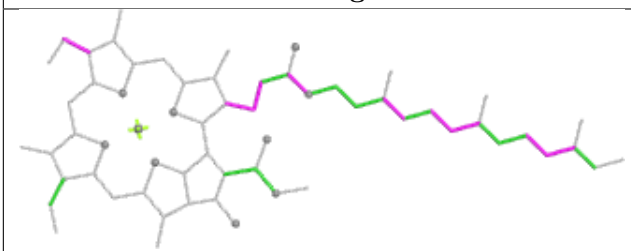
Ligand CLA cA 821



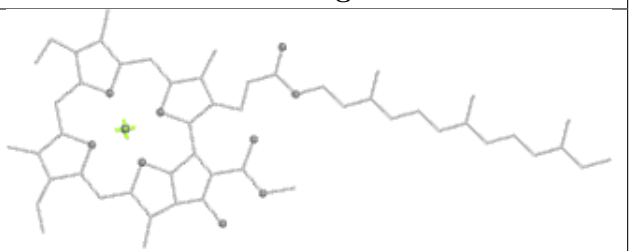
Bond lengths



Bond angles

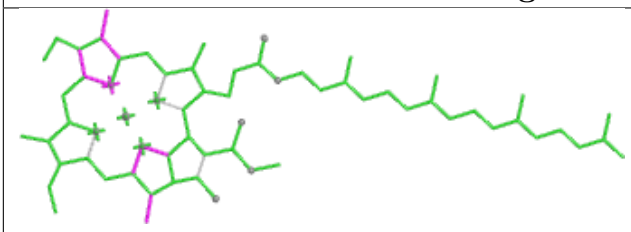


Torsions

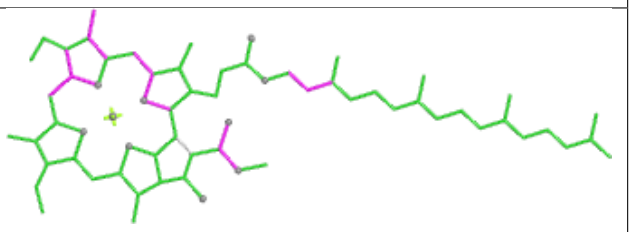


Rings

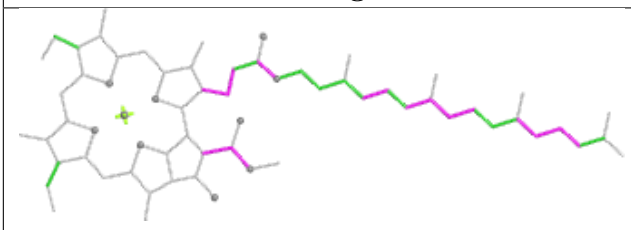
Ligand CLA b6 403



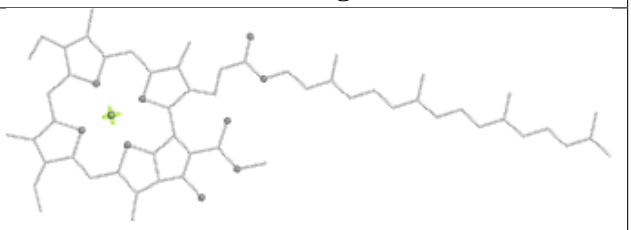
Bond lengths



Bond angles

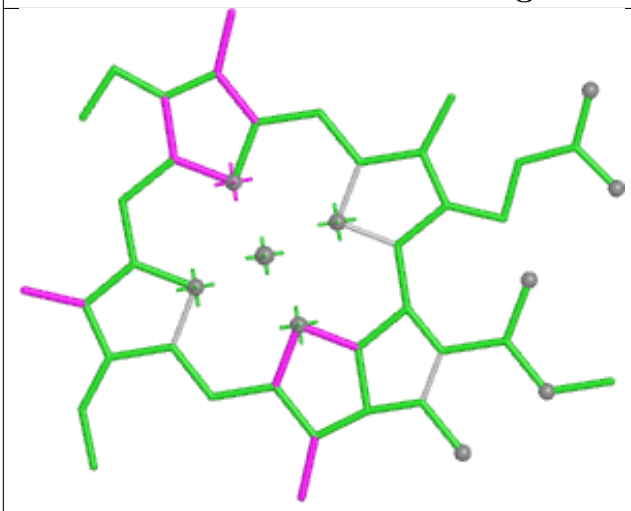


Torsions

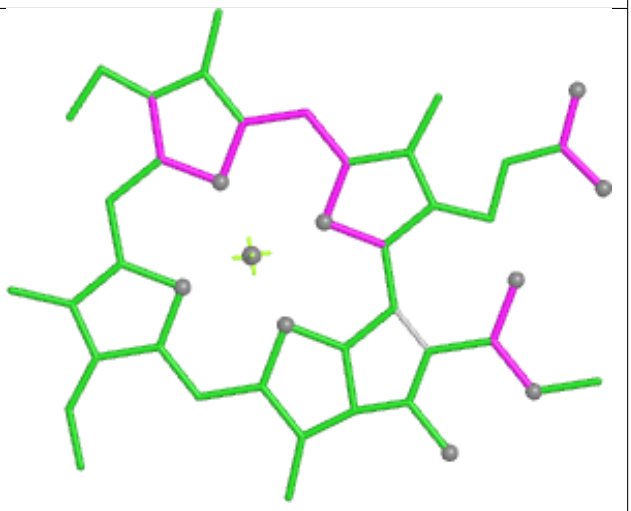


Rings

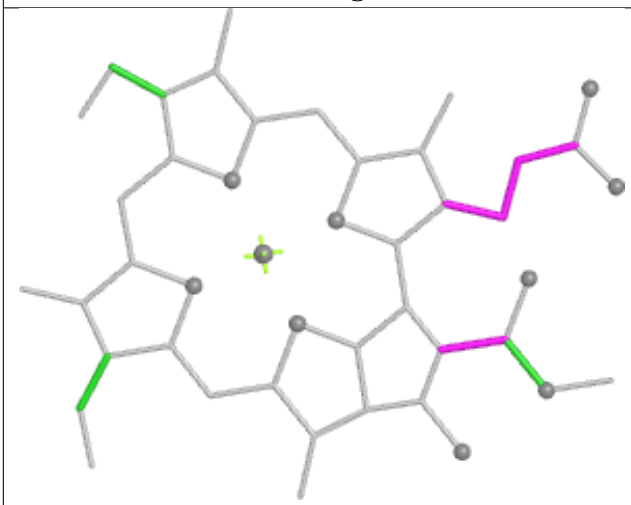
Ligand CLA cA 837



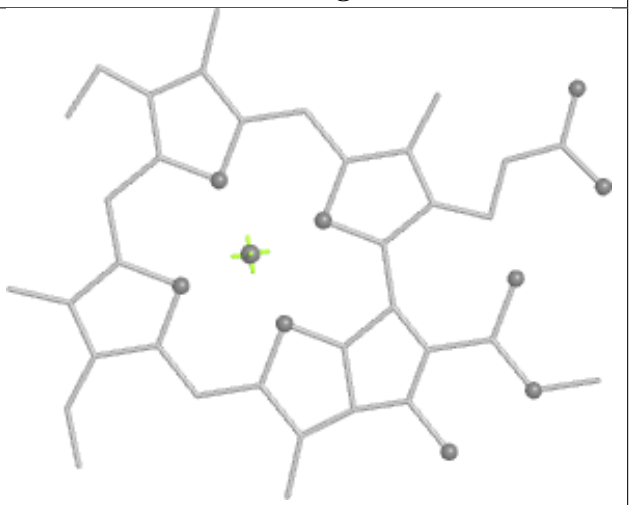
Bond lengths



Bond angles

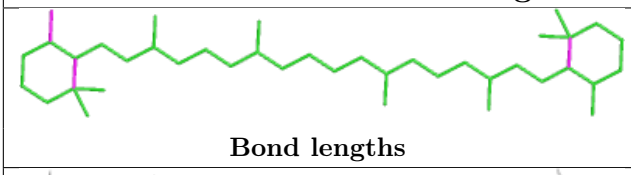


Torsions

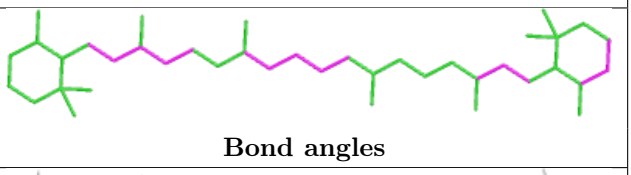


Rings

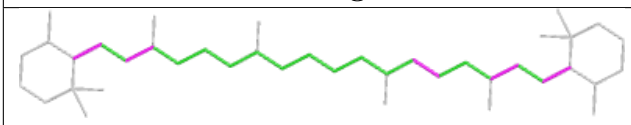
Ligand BCR aB 844



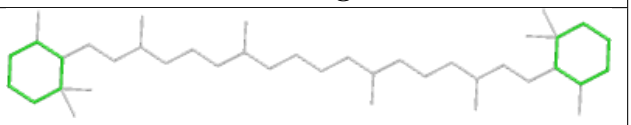
Bond lengths



Bond angles

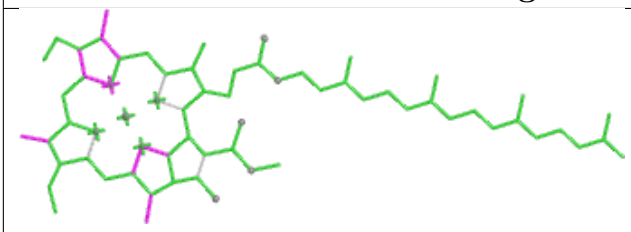


Torsions

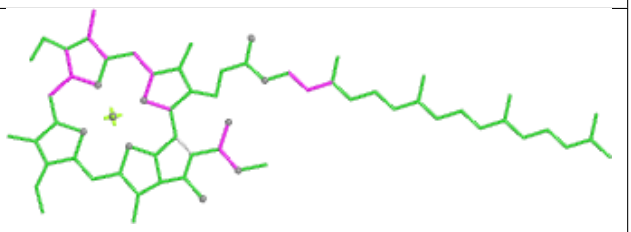


Rings

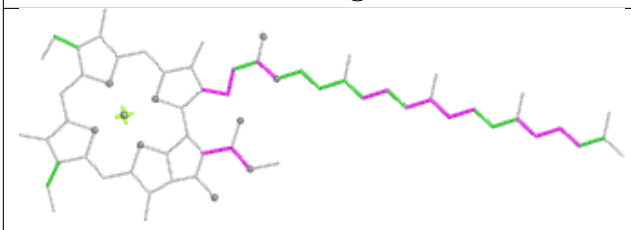
Ligand CLA b1 402



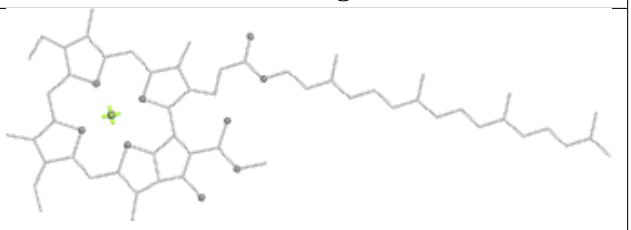
Bond lengths



Bond angles

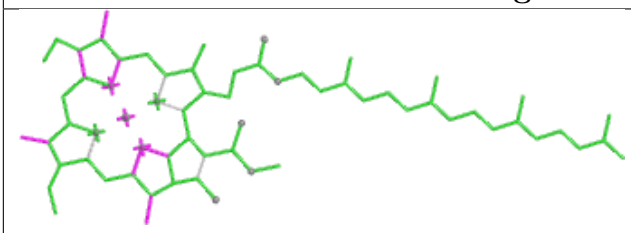


Torsions

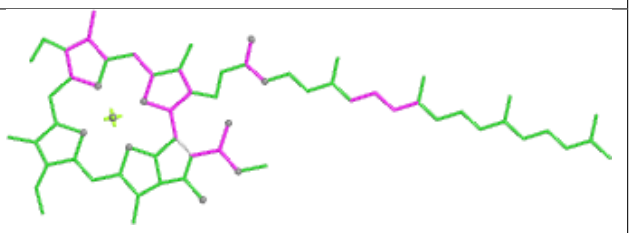


Rings

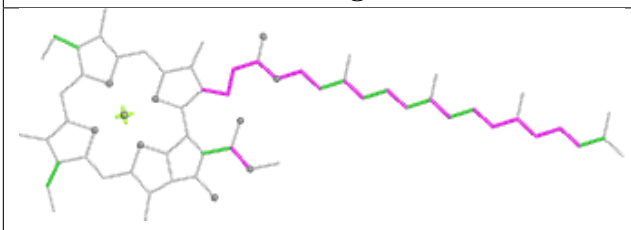
Ligand CLA bA 829



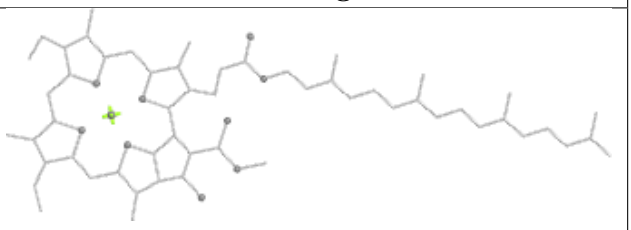
Bond lengths



Bond angles

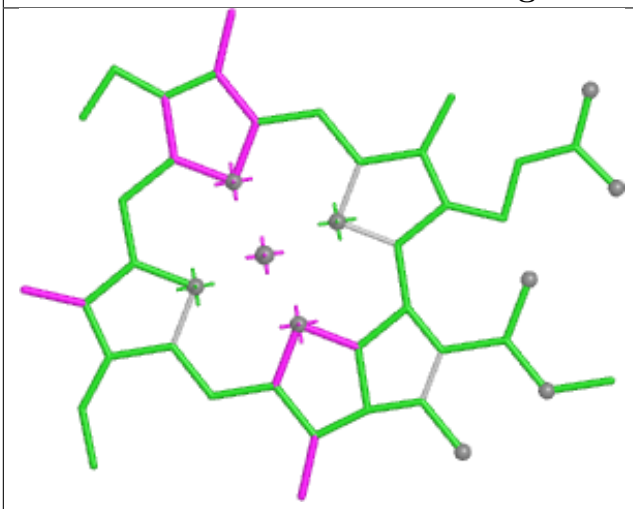


Torsions

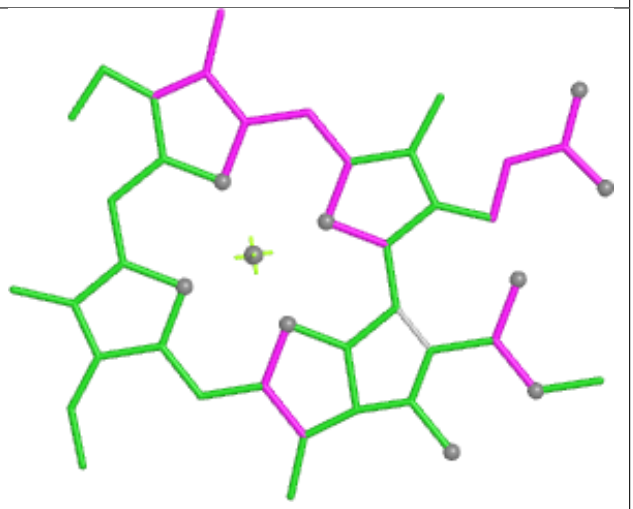


Rings

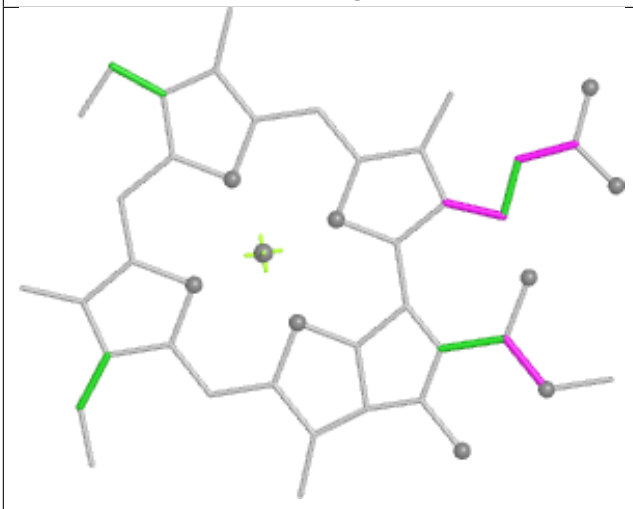
Ligand CLA b5 408



Bond lengths



Bond angles

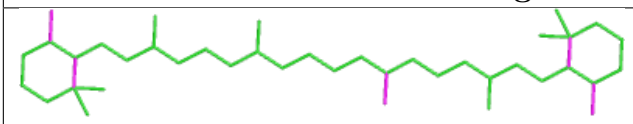


Torsions

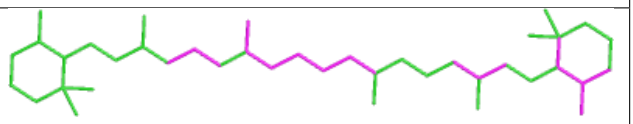


Rings

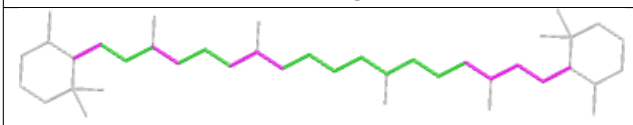
Ligand BCR aB 849



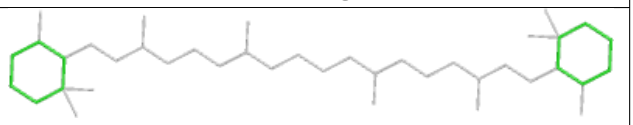
Bond lengths



Bond angles

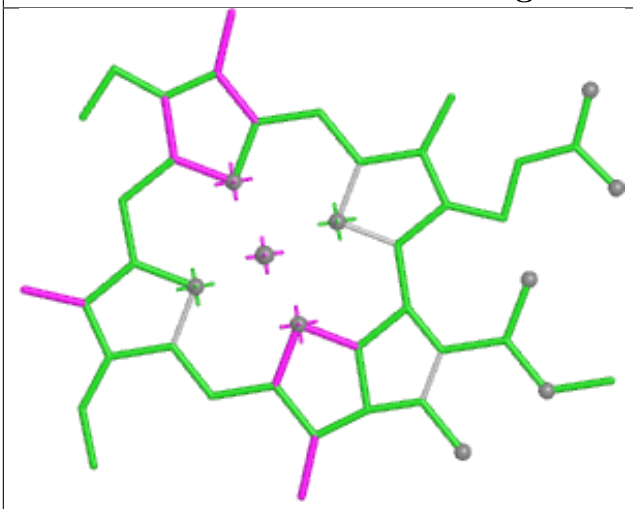


Torsions

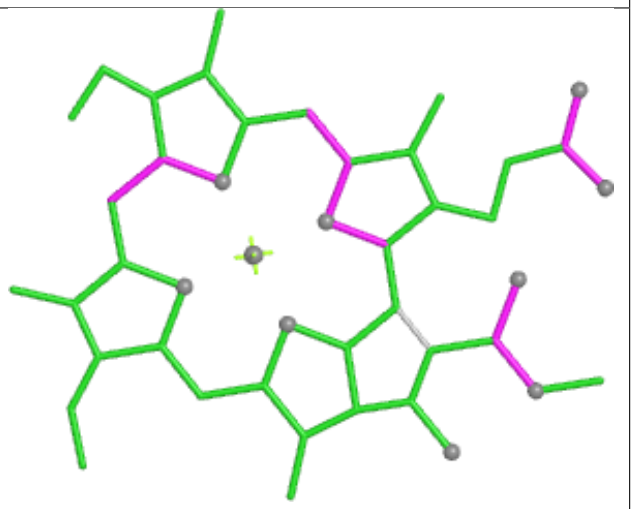


Rings

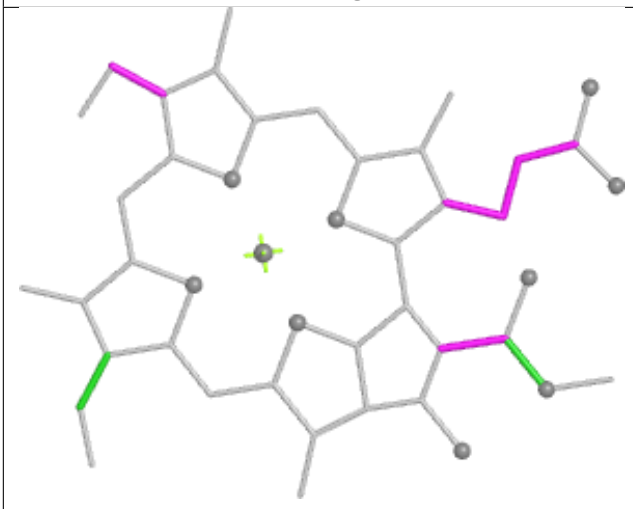
Ligand CLA aB 831



Bond lengths



Bond angles

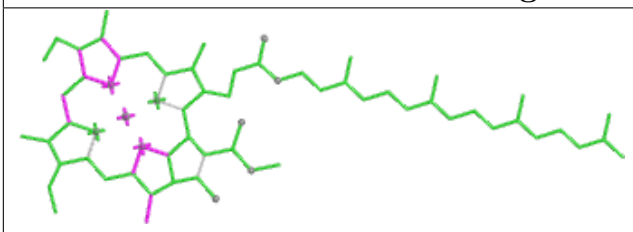


Torsions

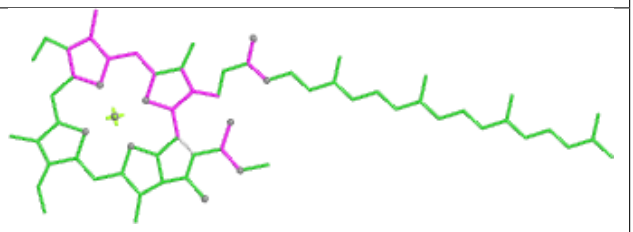


Rings

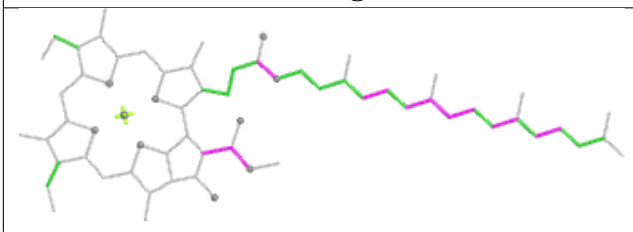
Ligand CLA a5 403



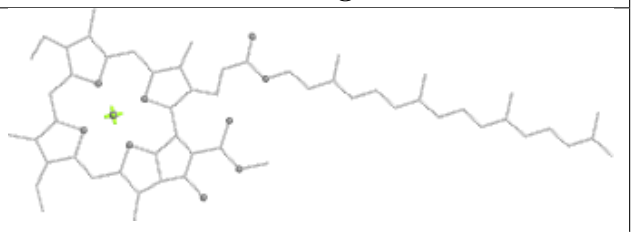
Bond lengths



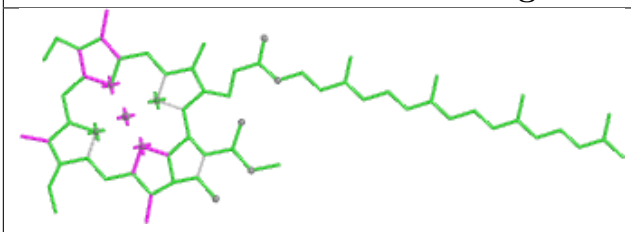
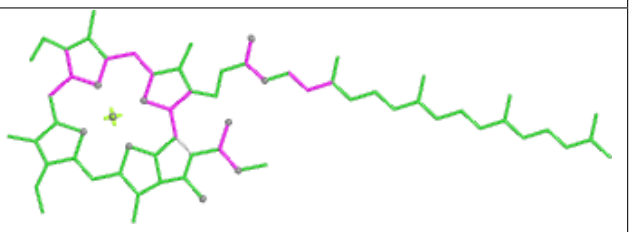
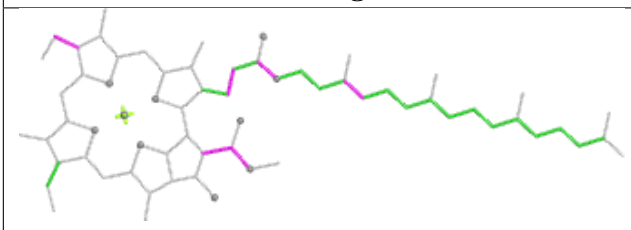
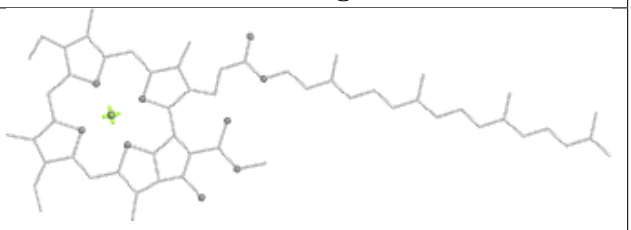
Bond angles

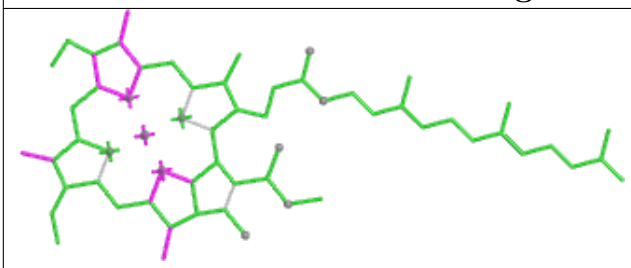
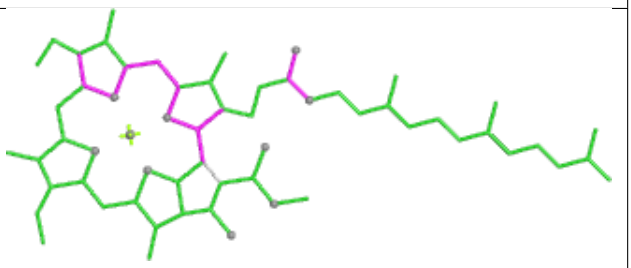
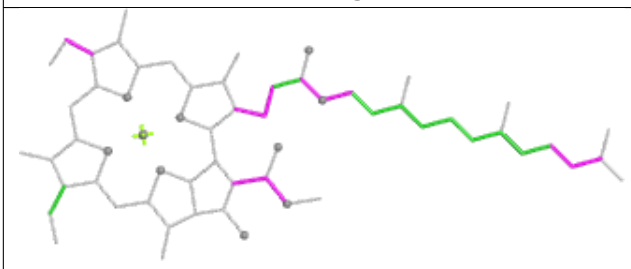
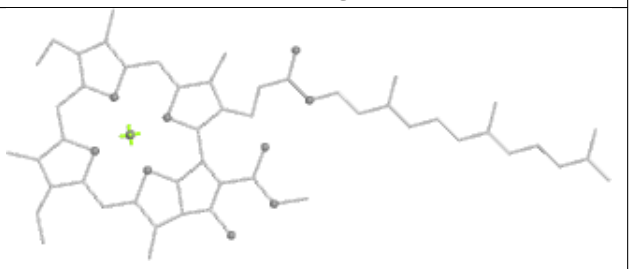


Torsions

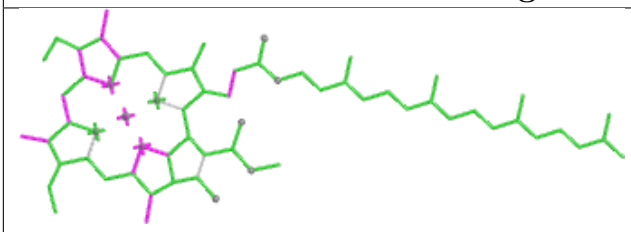


Rings

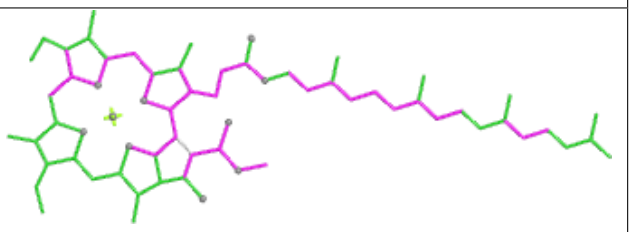
Ligand CLA b6 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

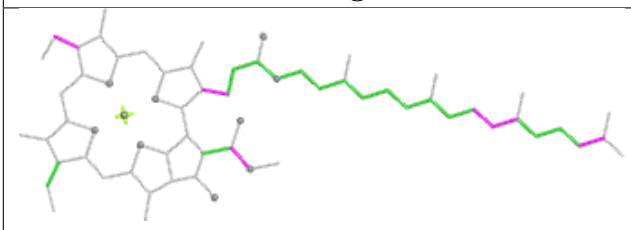
Ligand CLA b2 406



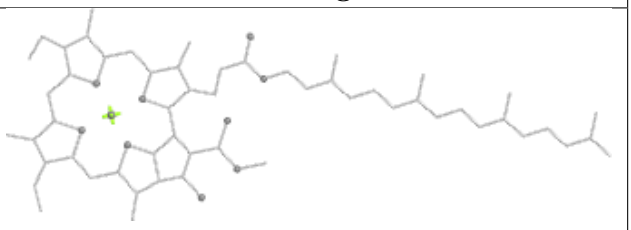
Bond lengths



Bond angles

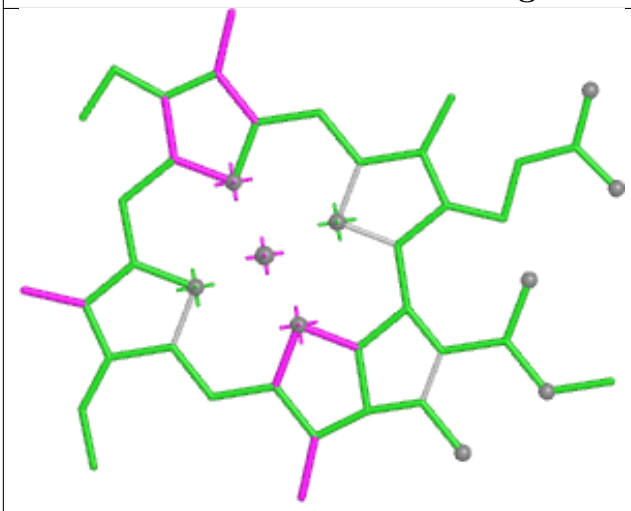


Torsions

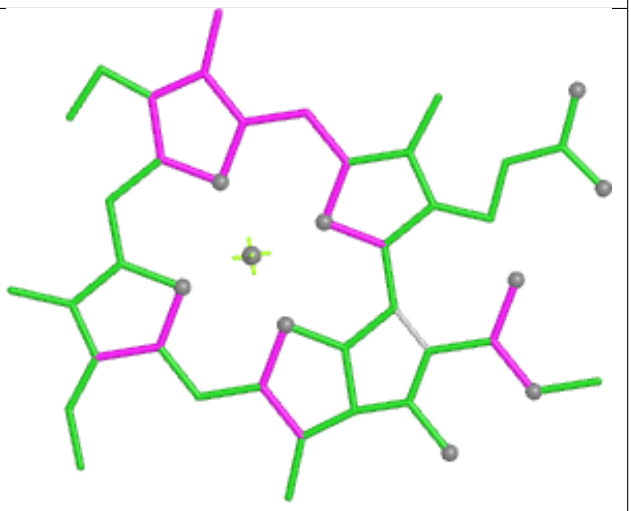


Rings

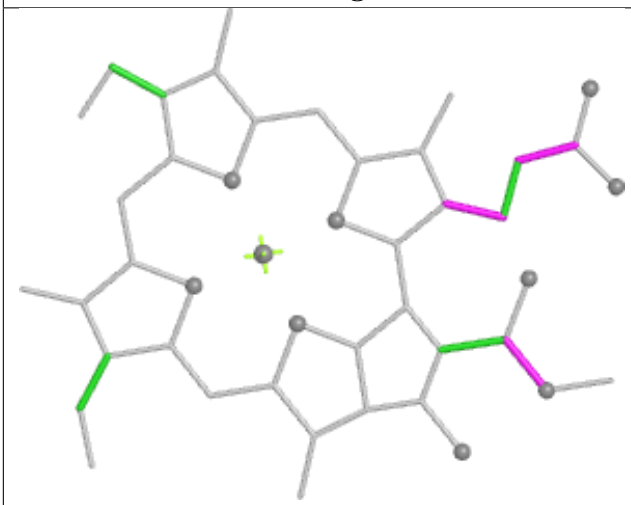
Ligand CLA b6 409



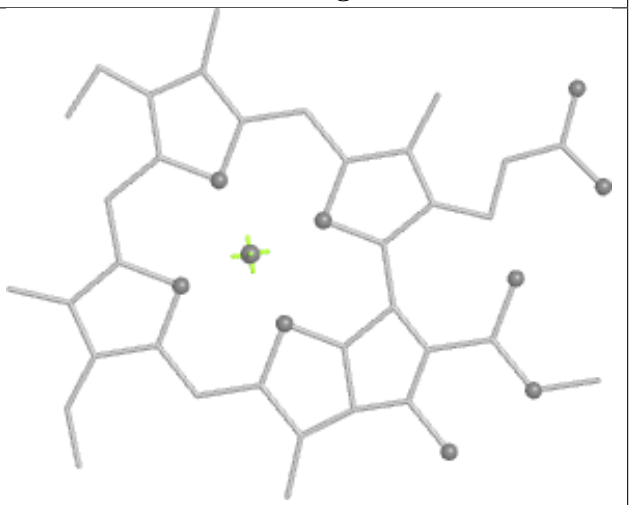
Bond lengths



Bond angles

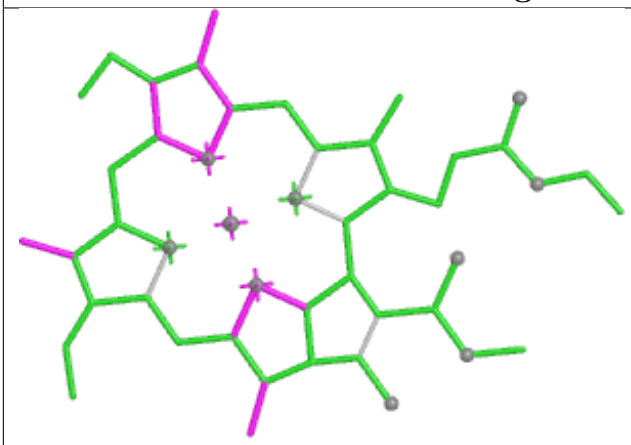


Torsions

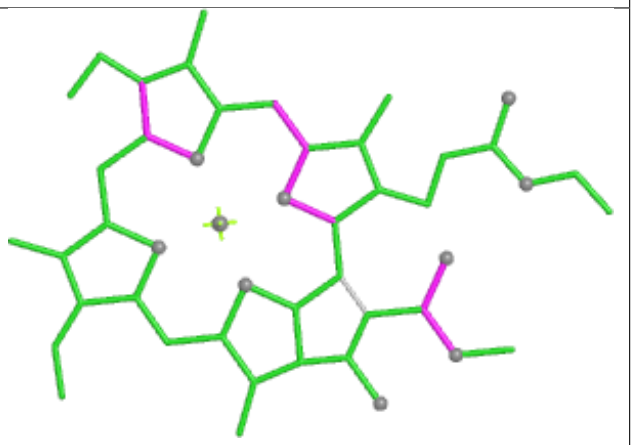


Rings

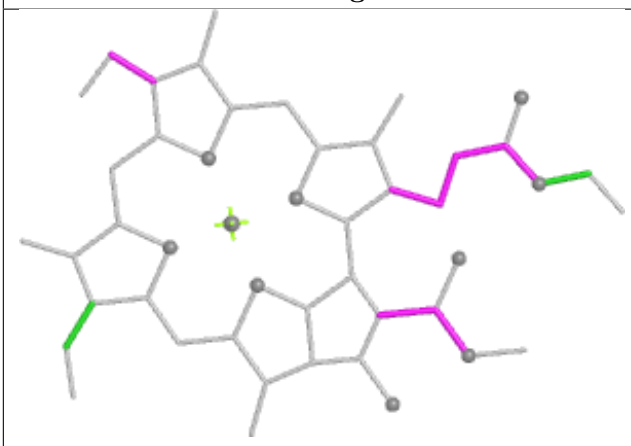
Ligand CLA bB 821



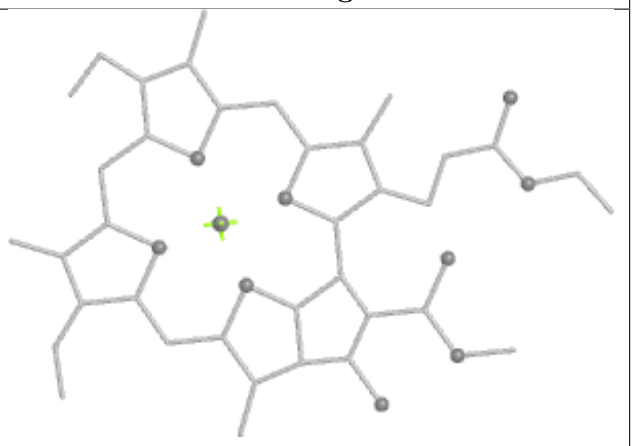
Bond lengths



Bond angles



Torsions

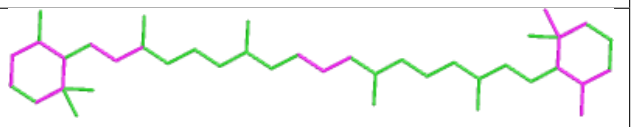


Rings

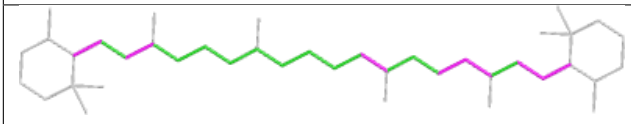
Ligand BCR c6 420



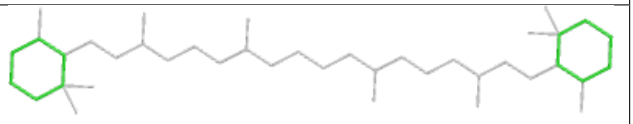
Bond lengths



Bond angles

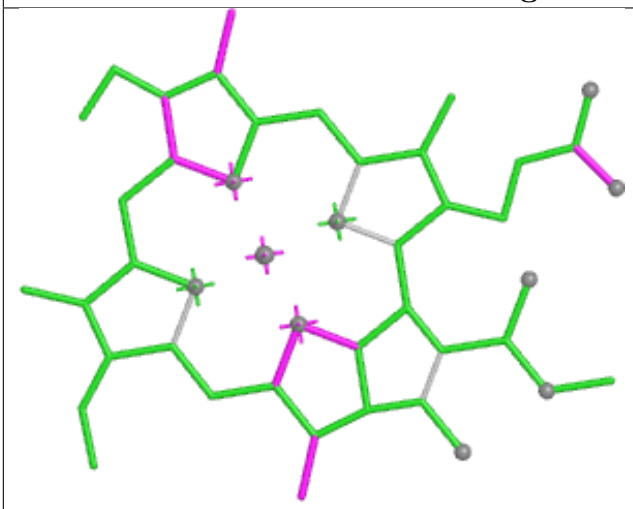


Torsions

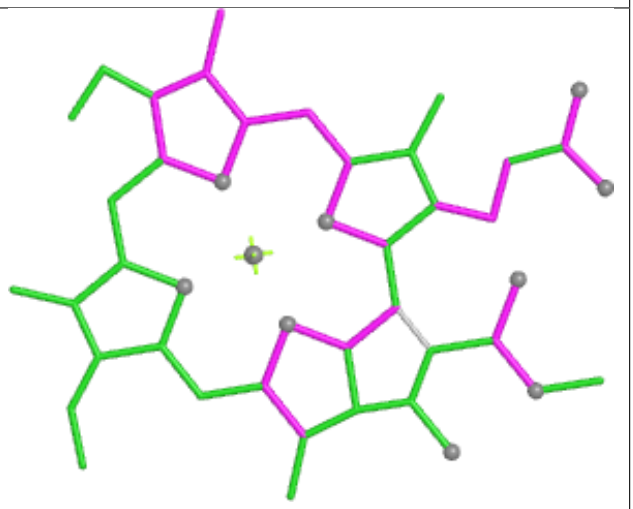


Rings

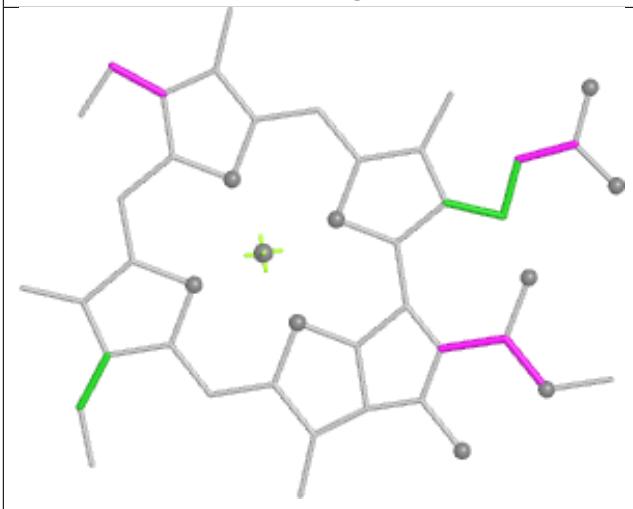
Ligand CLA c3 415



Bond lengths



Bond angles

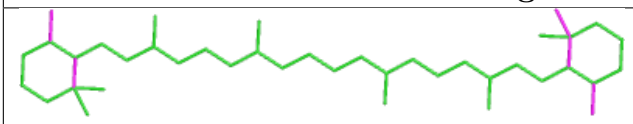


Torsions

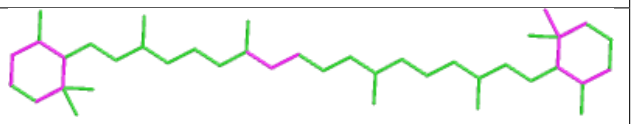


Rings

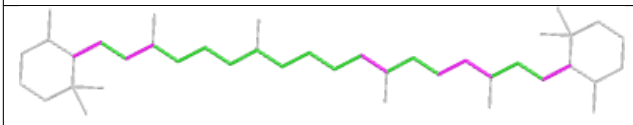
Ligand BCR a1 417



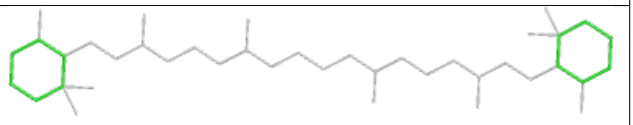
Bond lengths



Bond angles

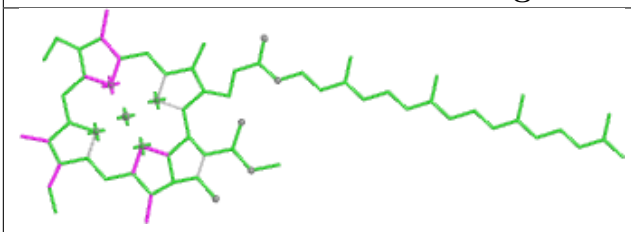


Torsions

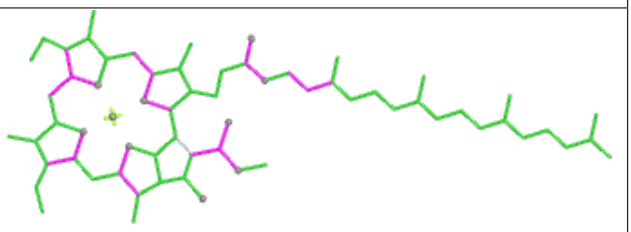


Rings

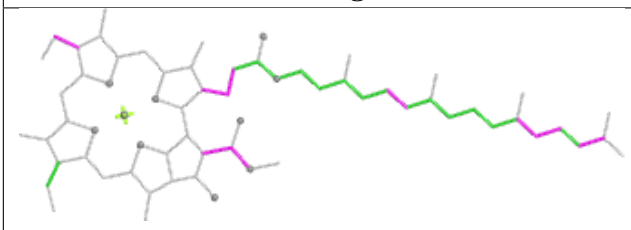
Ligand CLA bA 835



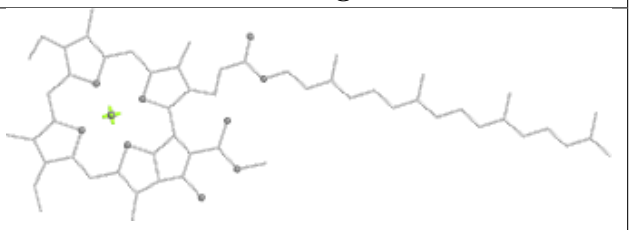
Bond lengths



Bond angles

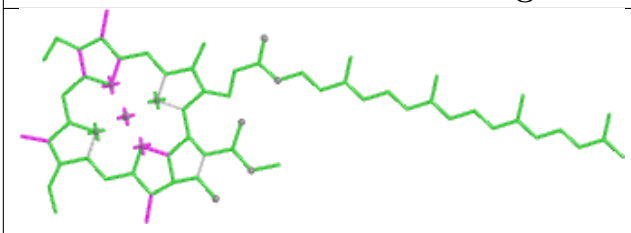


Torsions

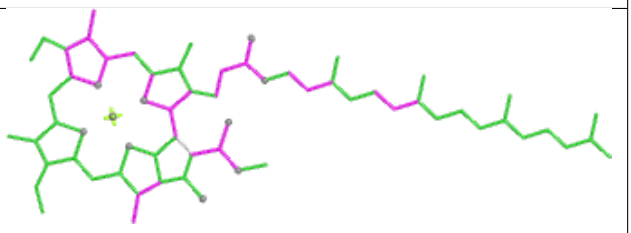


Rings

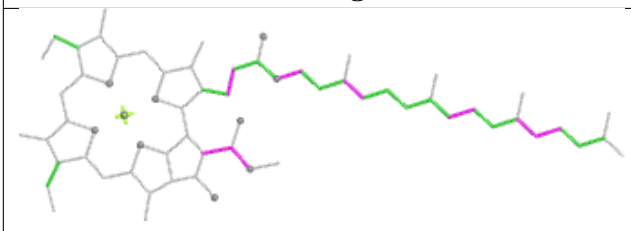
Ligand CLA cB 803



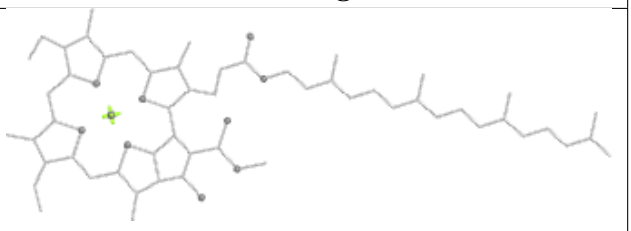
Bond lengths



Bond angles

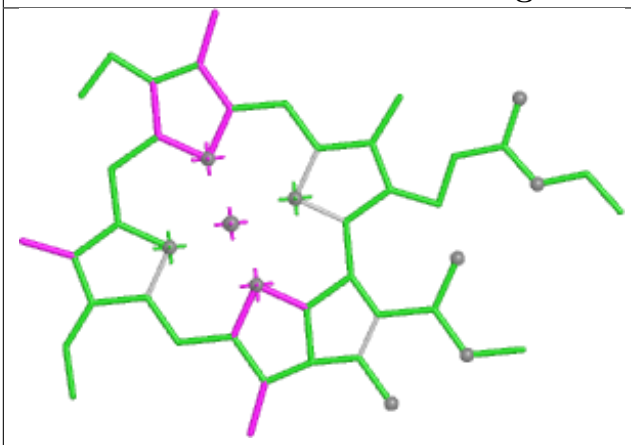


Torsions

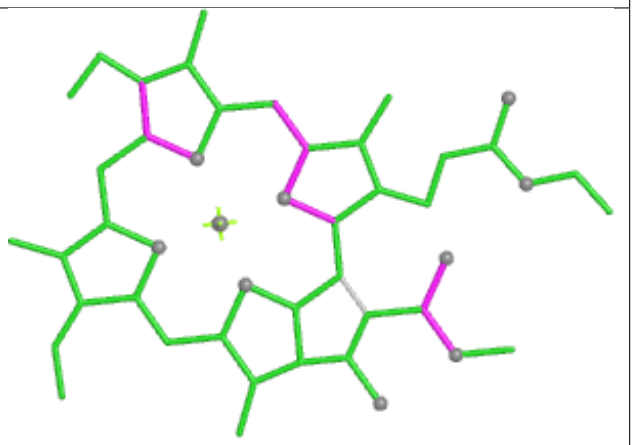


Rings

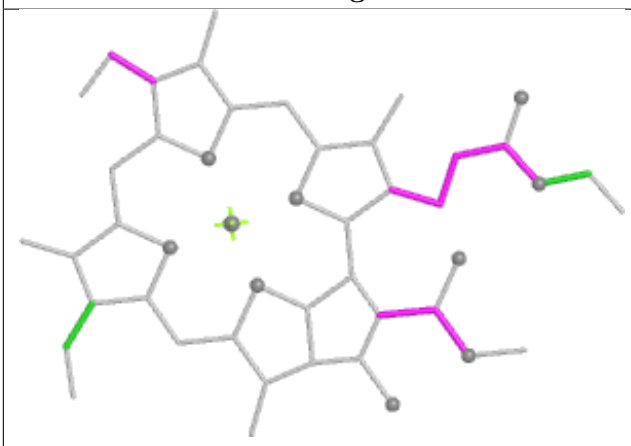
Ligand CLA aB 821



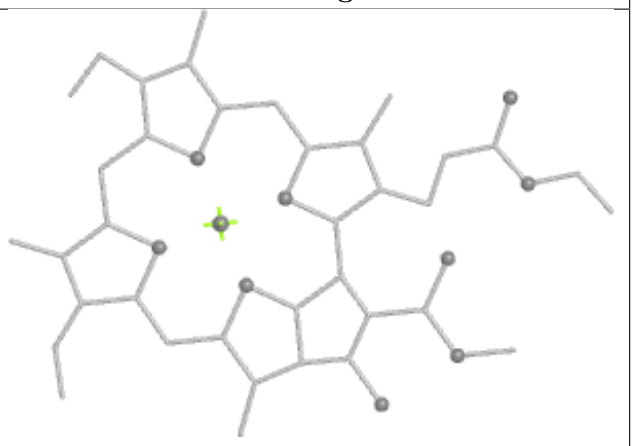
Bond lengths



Bond angles

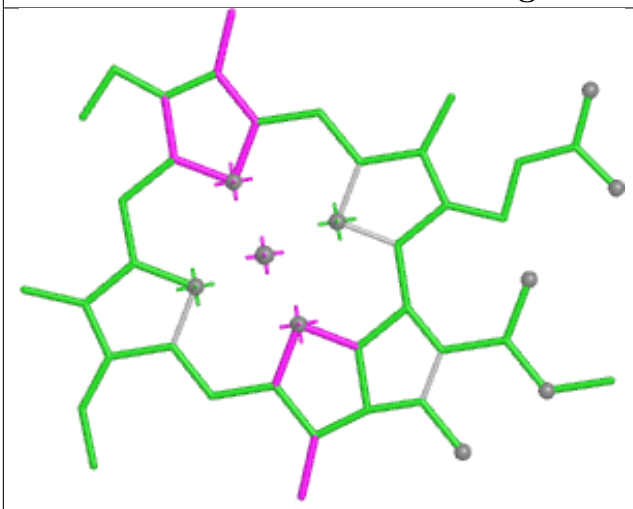


Torsions

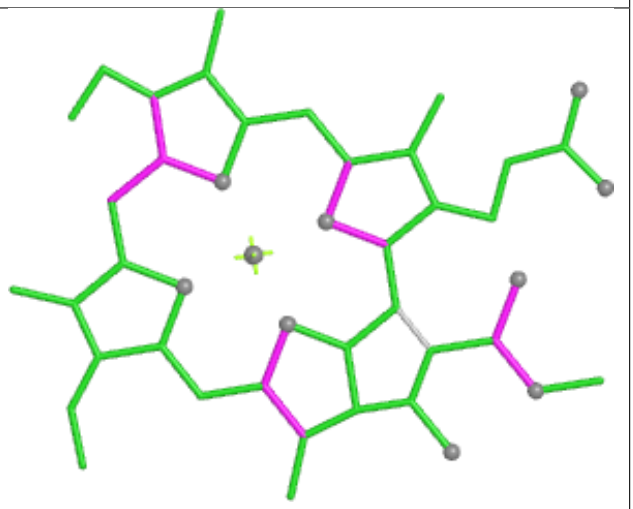


Rings

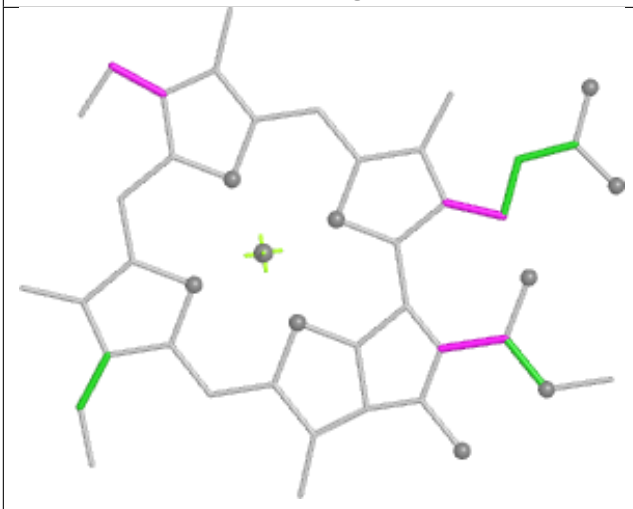
Ligand CLA b4 413



Bond lengths



Bond angles

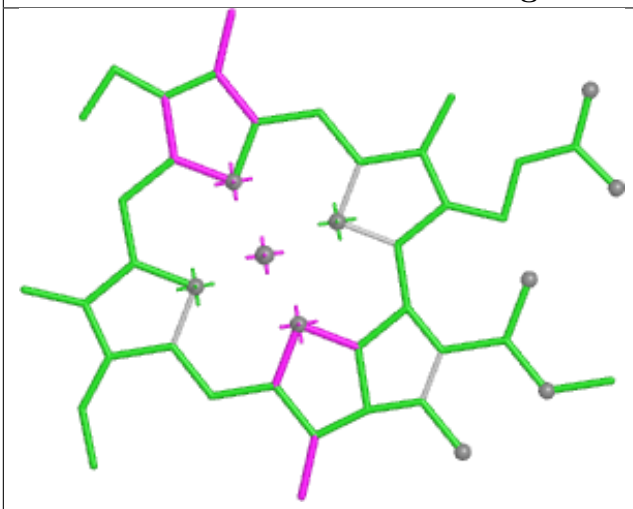


Torsions

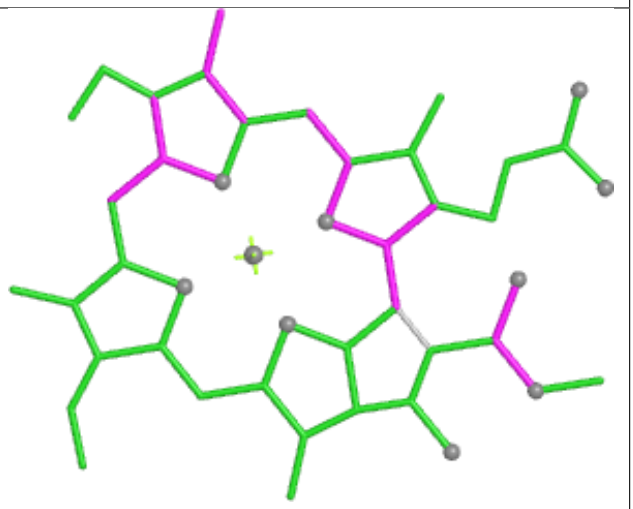


Rings

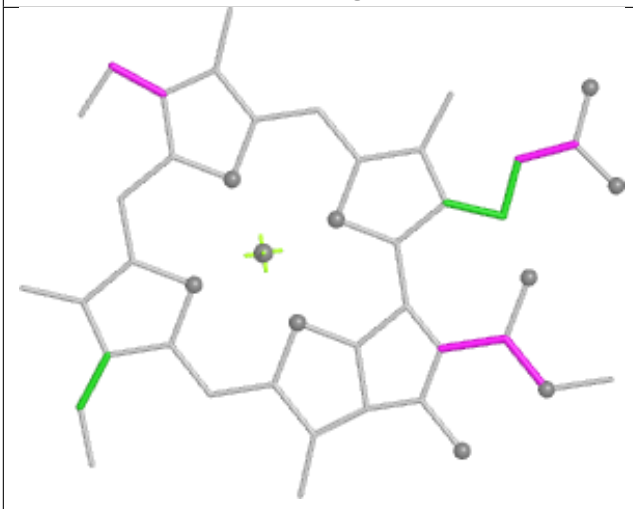
Ligand CLA c6 409



Bond lengths



Bond angles

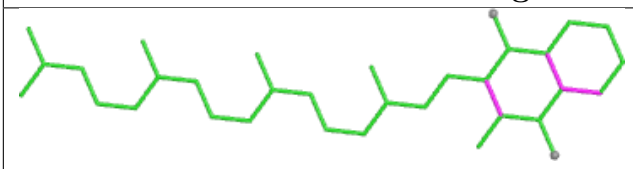


Torsions

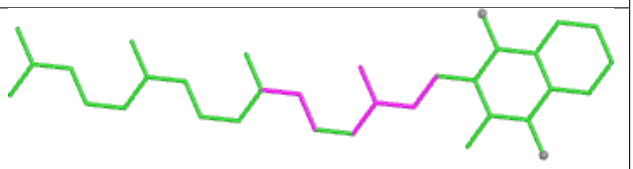


Rings

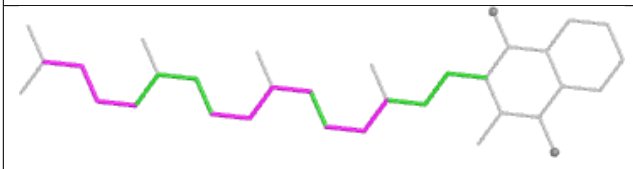
Ligand PQN bB 843



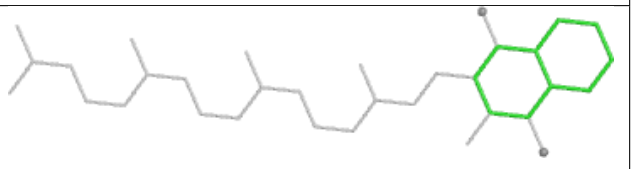
Bond lengths



Bond angles

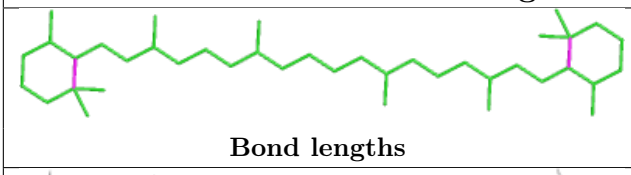


Torsions

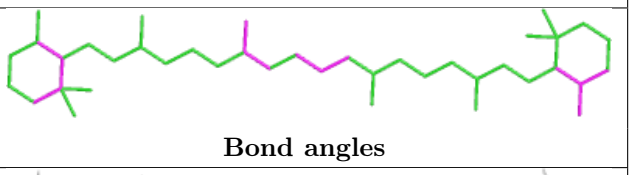


Rings

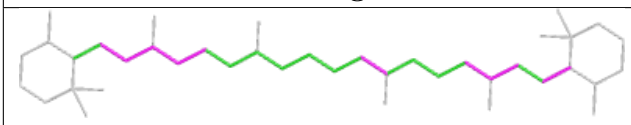
Ligand BCR bI 101



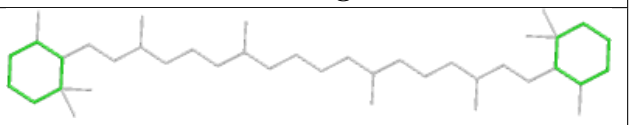
Bond lengths



Bond angles

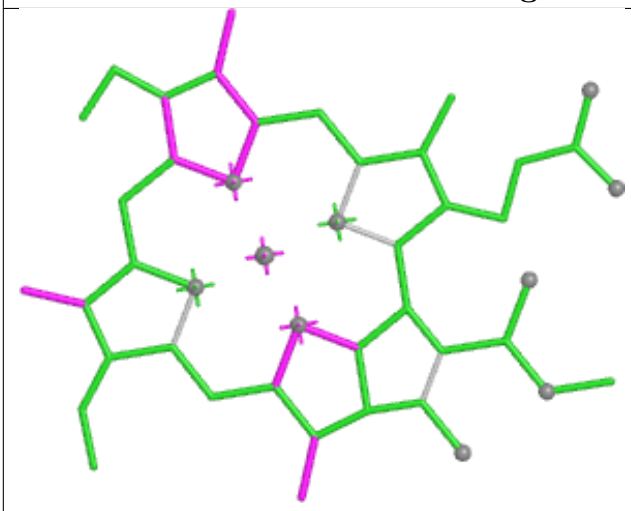


Torsions

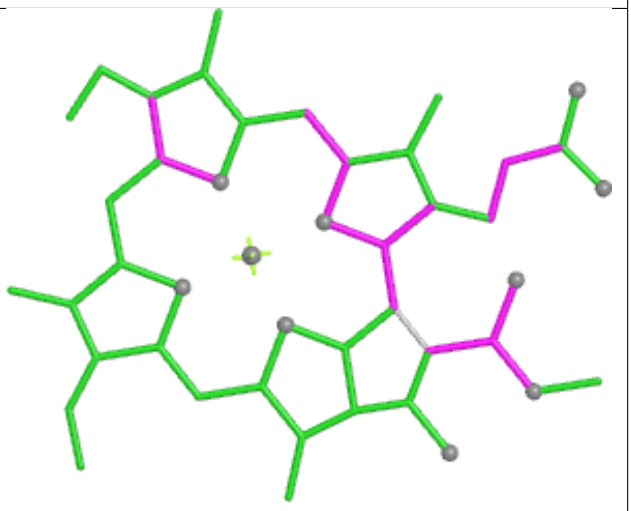


Rings

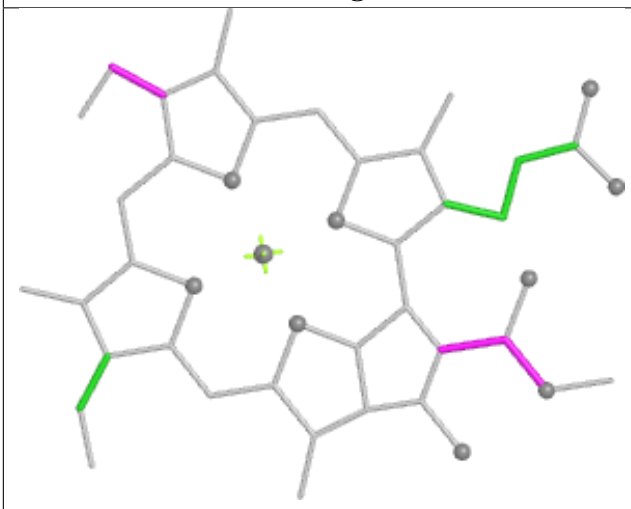
Ligand CLA cJ 101



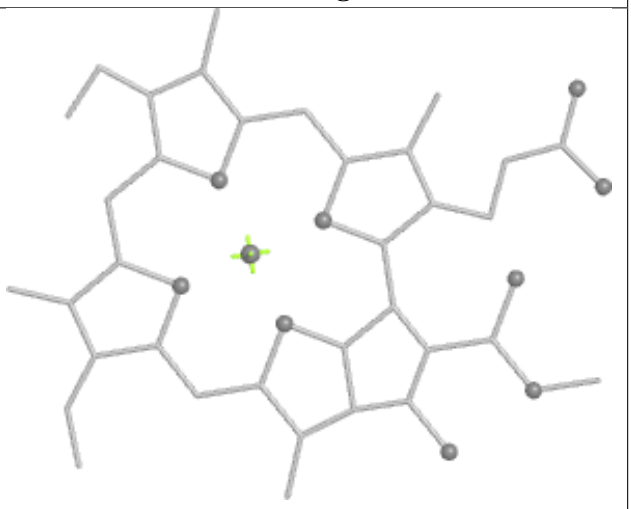
Bond lengths



Bond angles

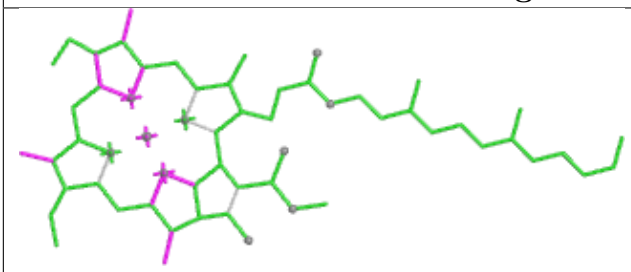


Torsions

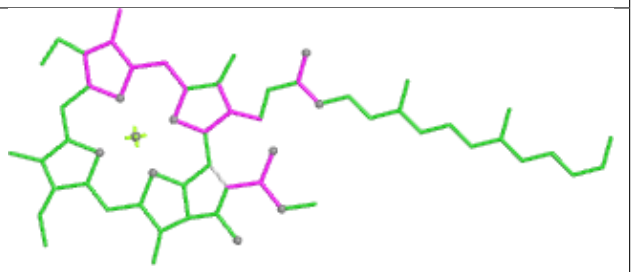


Rings

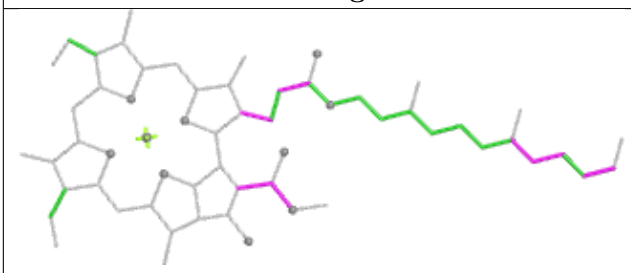
Ligand CLA aA 805



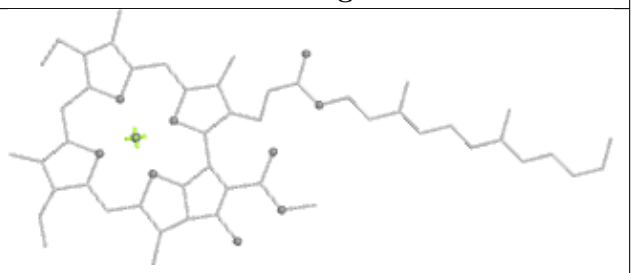
Bond lengths



Bond angles

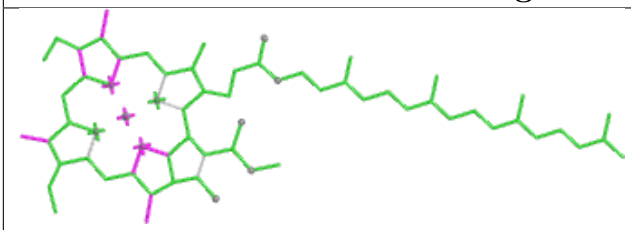


Torsions

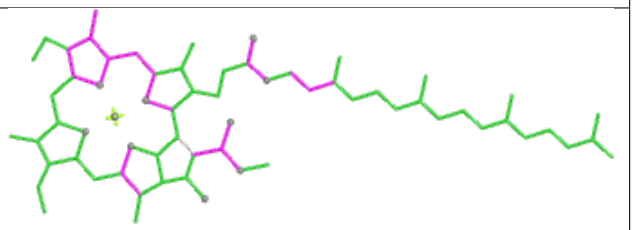


Rings

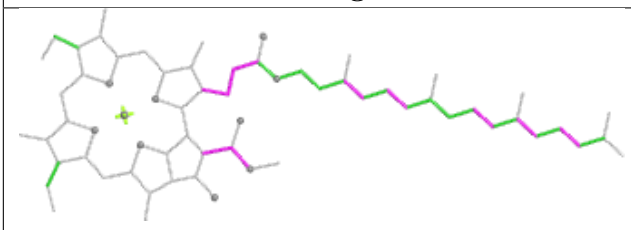
Ligand CLA aA 830



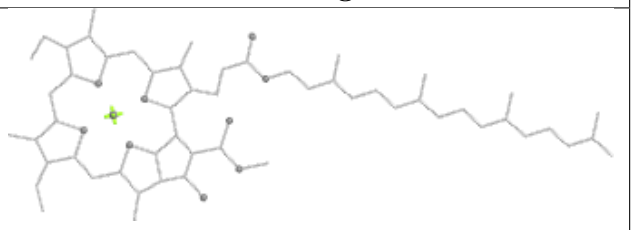
Bond lengths



Bond angles

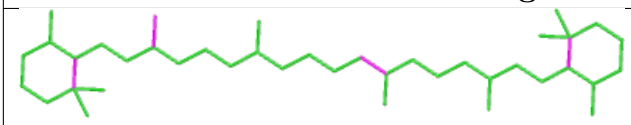


Torsions

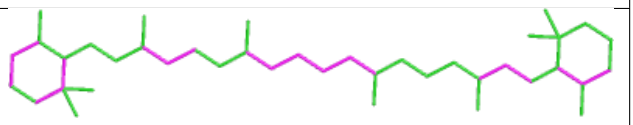


Rings

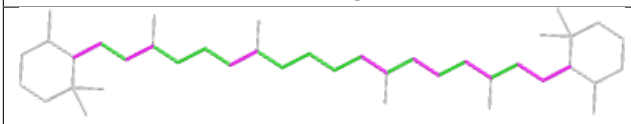
Ligand BCR bI 102



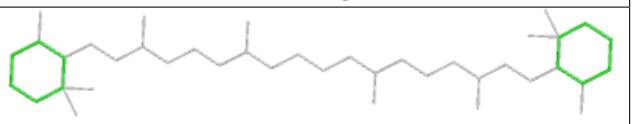
Bond lengths



Bond angles

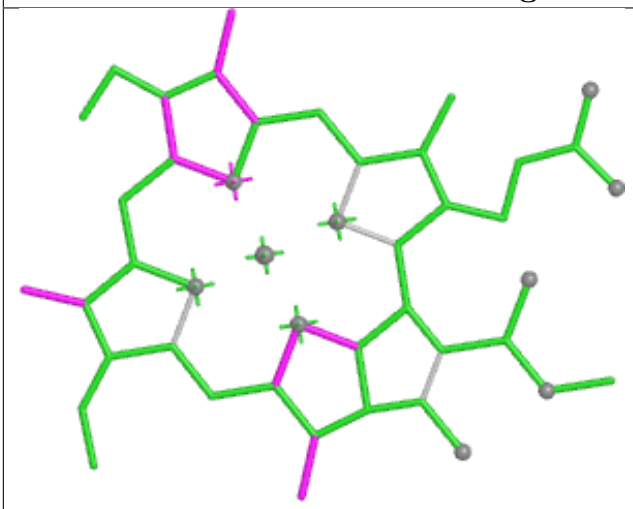


Torsions

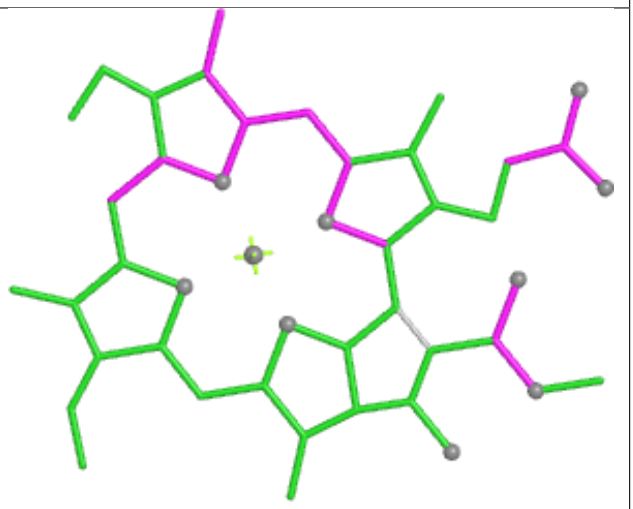


Rings

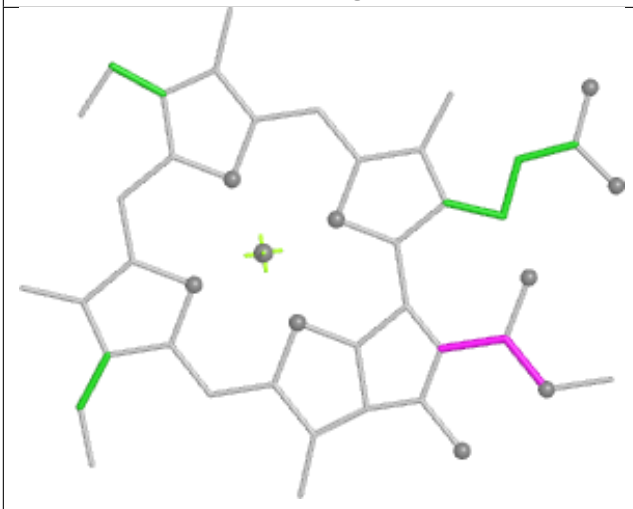
Ligand CLA a5 406



Bond lengths



Bond angles

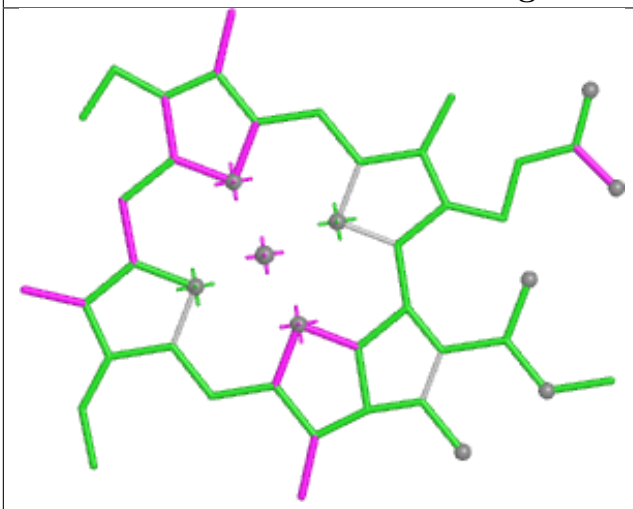


Torsions

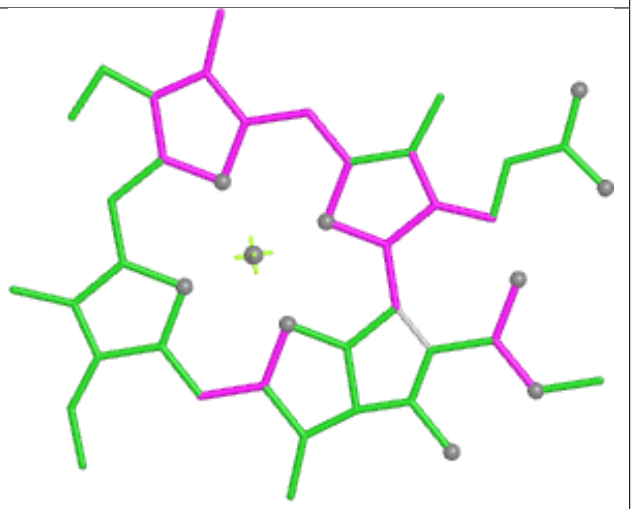


Rings

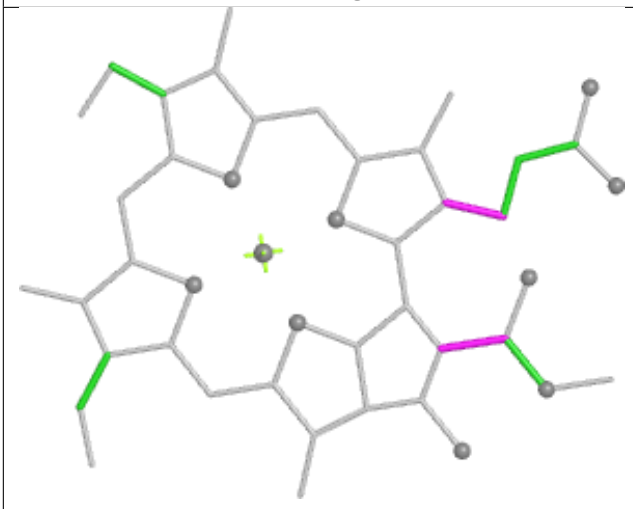
Ligand CLA b2 412



Bond lengths



Bond angles

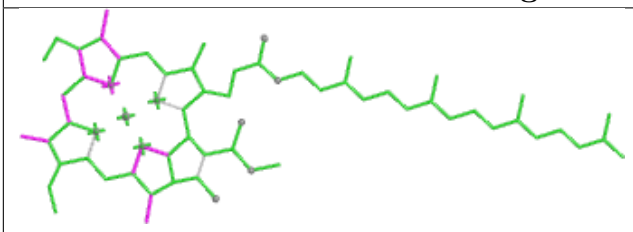


Torsions

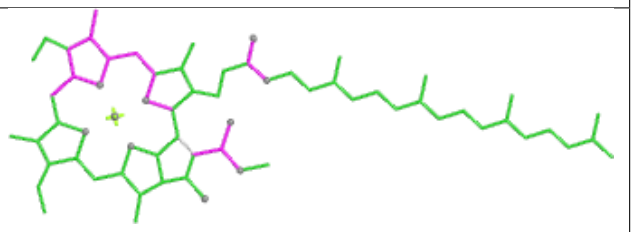


Rings

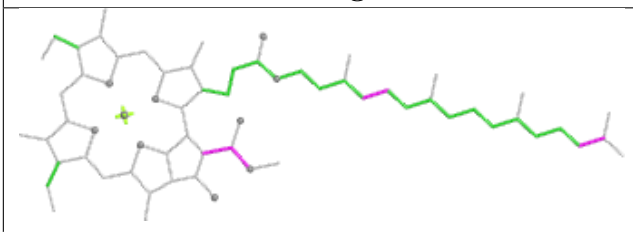
Ligand CLA c3 409



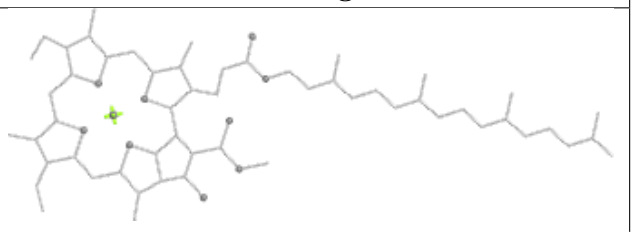
Bond lengths



Bond angles

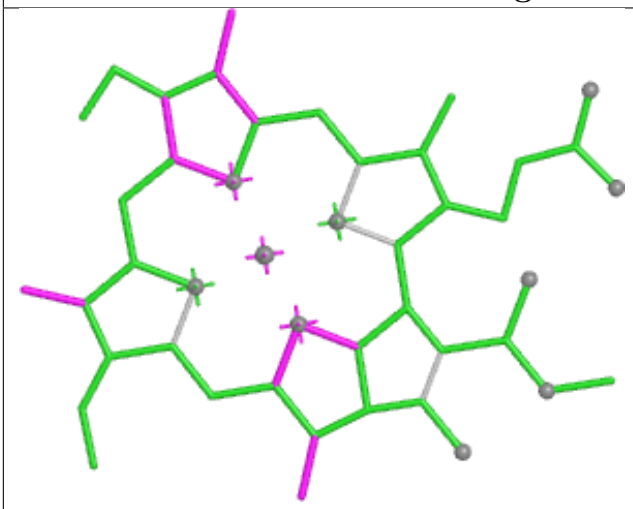


Torsions

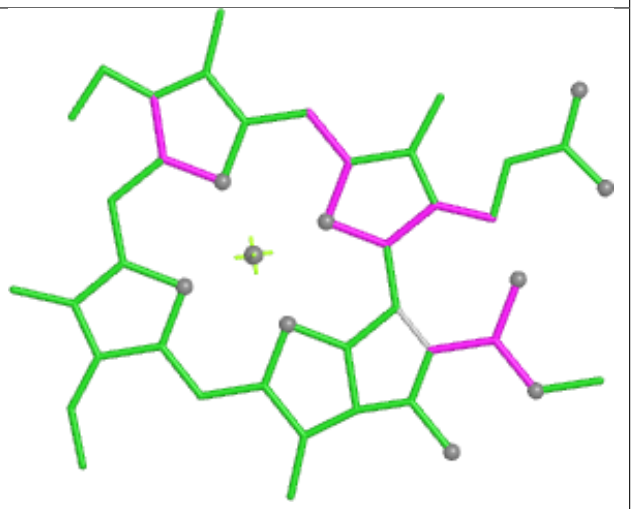


Rings

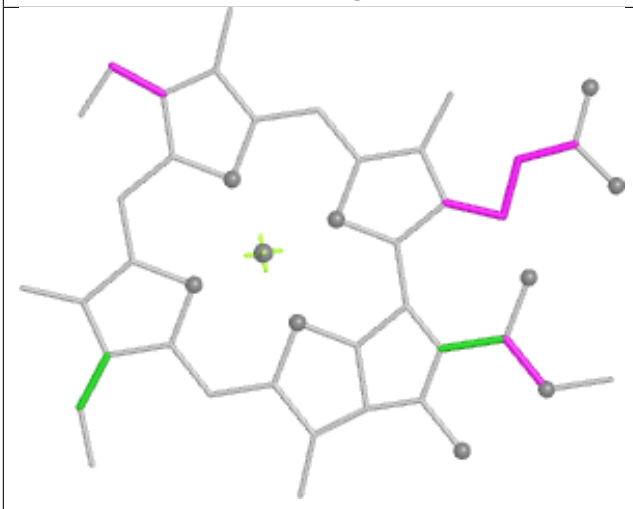
Ligand CLA bB 835



Bond lengths



Bond angles

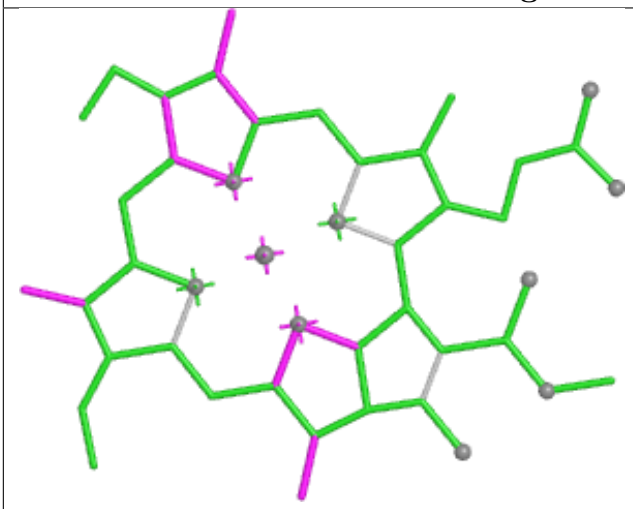


Torsions

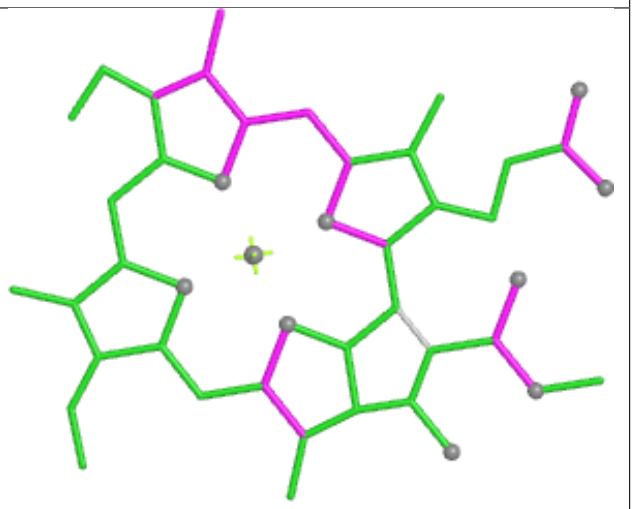


Rings

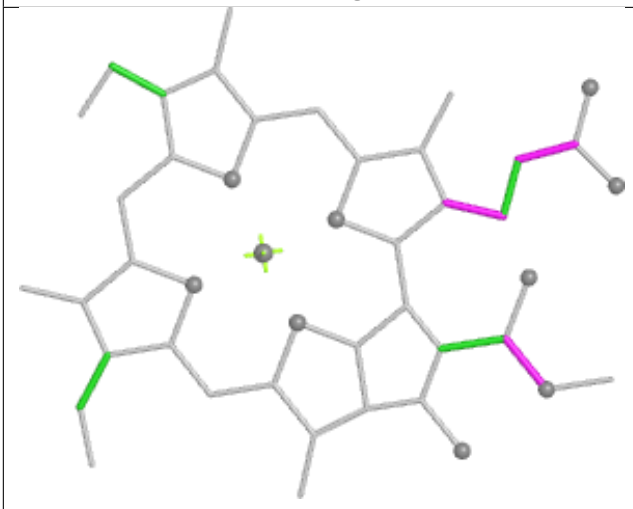
Ligand CLA c4 408



Bond lengths



Bond angles

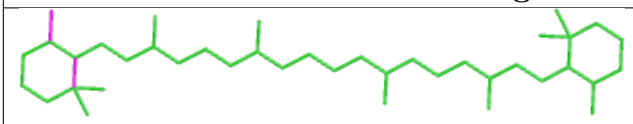


Torsions

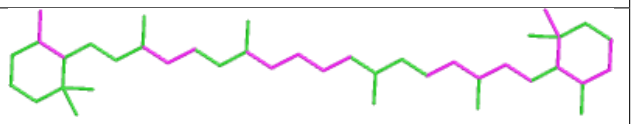


Rings

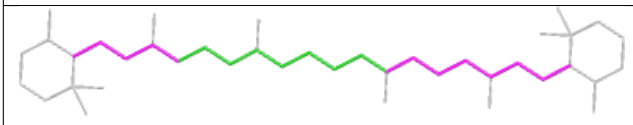
Ligand BCR aA 850



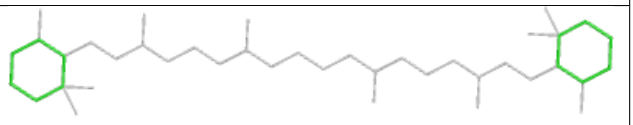
Bond lengths



Bond angles

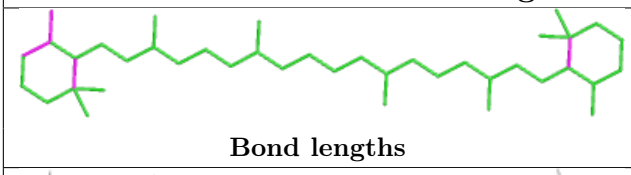


Torsions

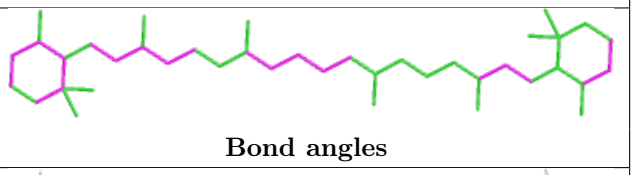


Rings

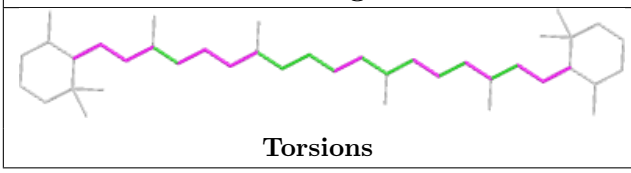
Ligand BCR a6 402



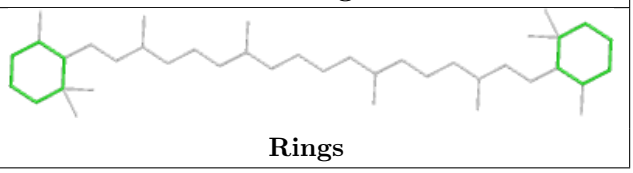
Bond lengths



Bond angles

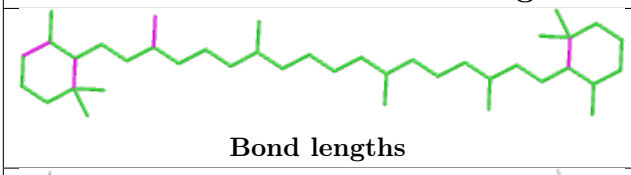


Torsions

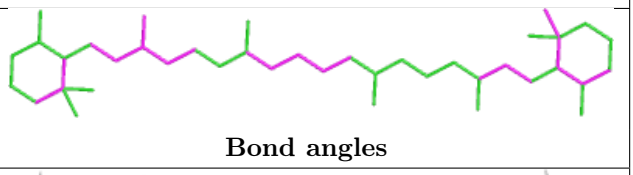


Rings

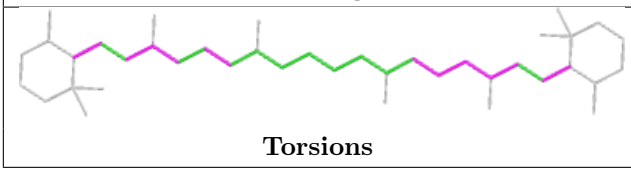
Ligand BCR b1 401



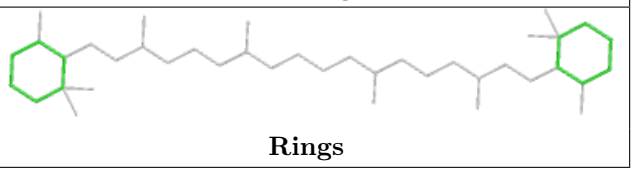
Bond lengths



Bond angles

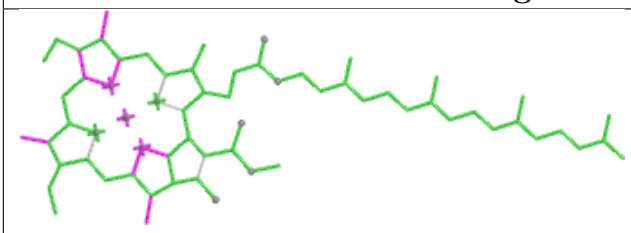


Torsions

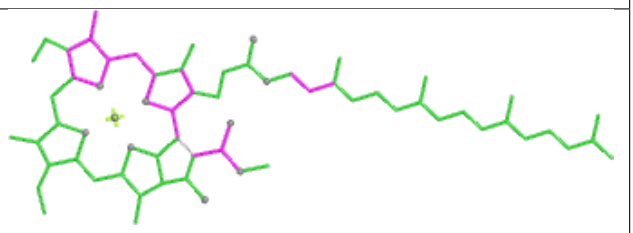


Rings

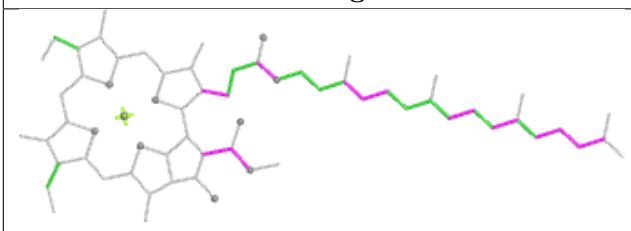
Ligand CLA bA 820



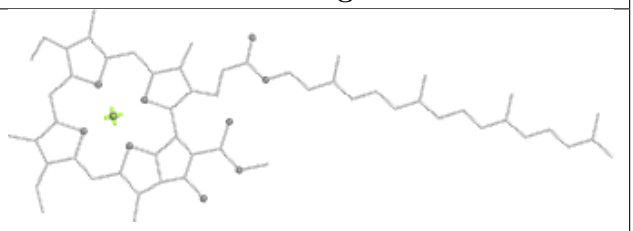
Bond lengths



Bond angles

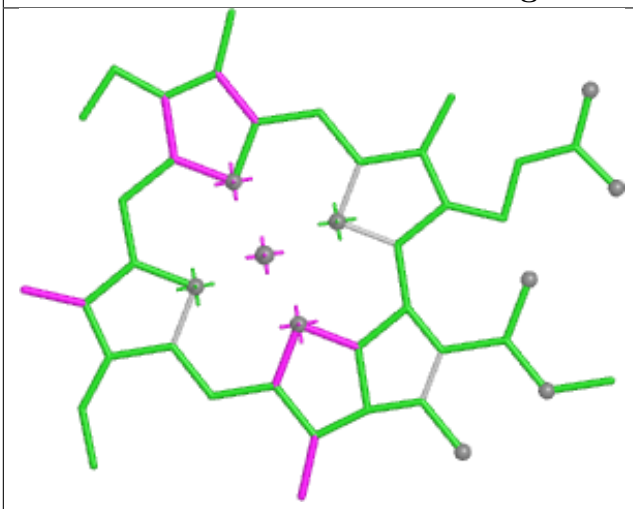


Torsions

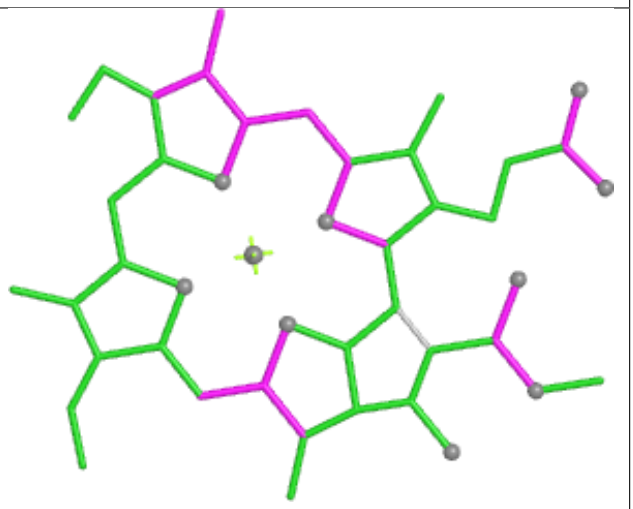


Rings

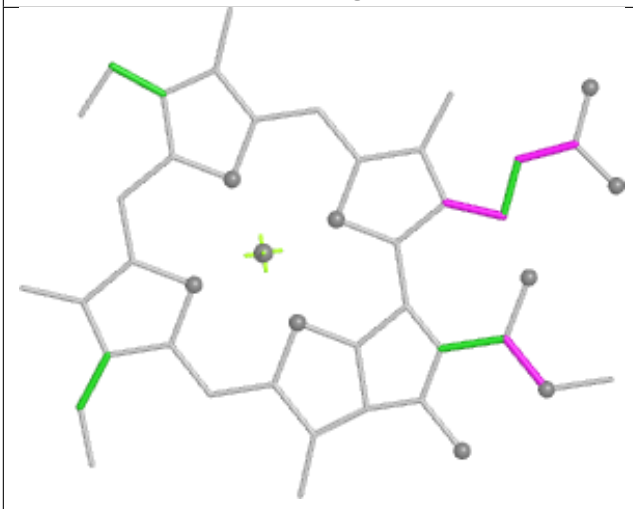
Ligand CLA c2 409



Bond lengths



Bond angles

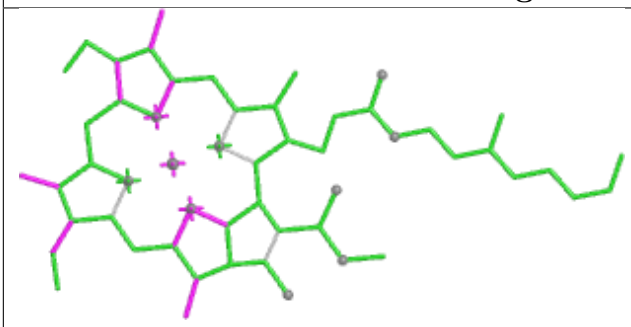


Torsions

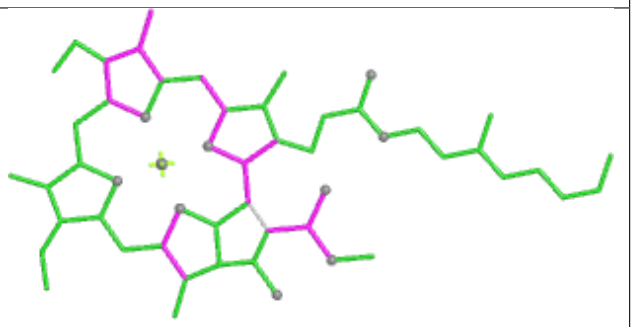


Rings

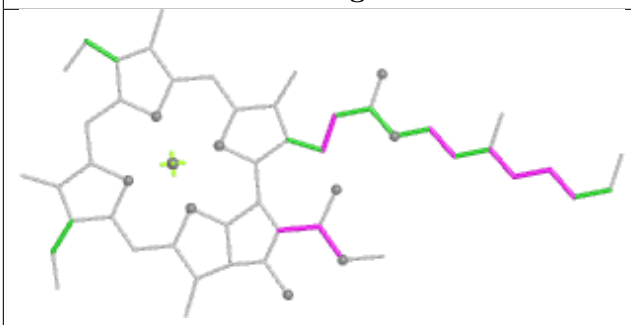
Ligand CLA aB 825



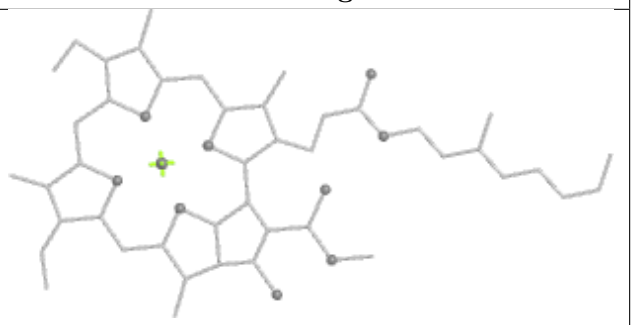
Bond lengths



Bond angles

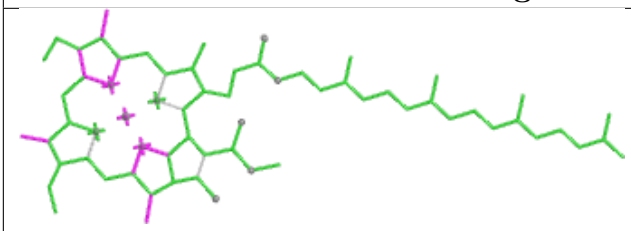


Torsions

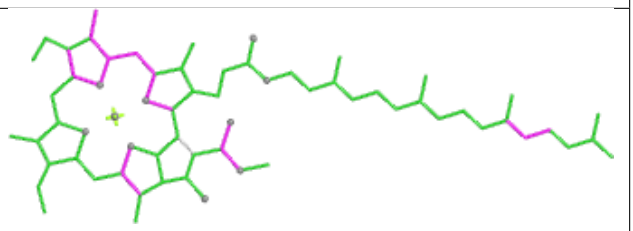


Rings

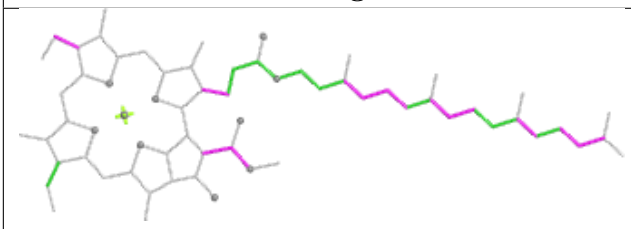
Ligand CLA bA 822



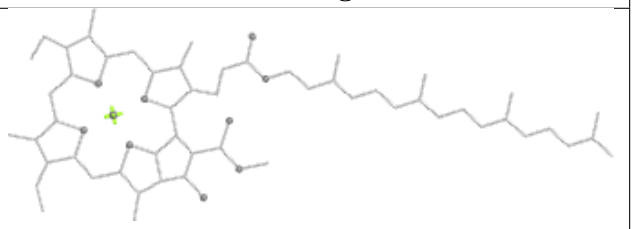
Bond lengths



Bond angles

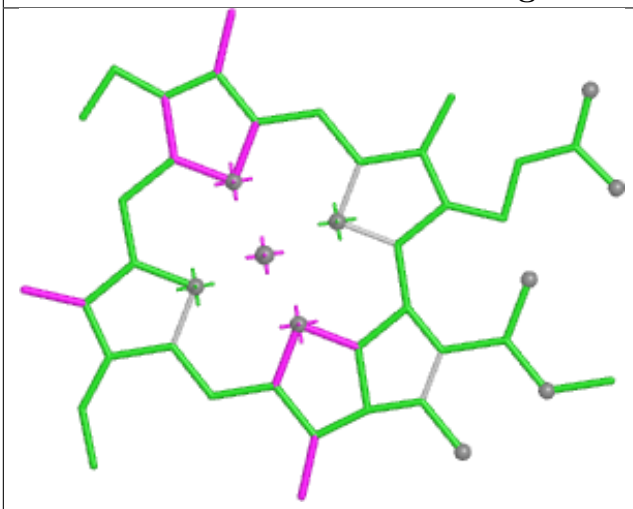


Torsions

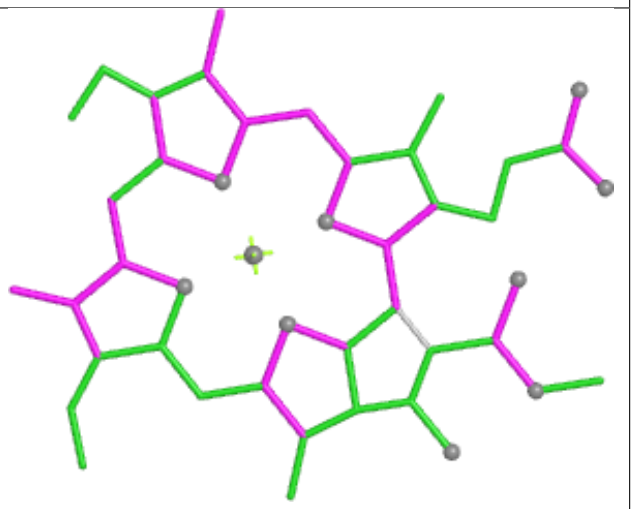


Rings

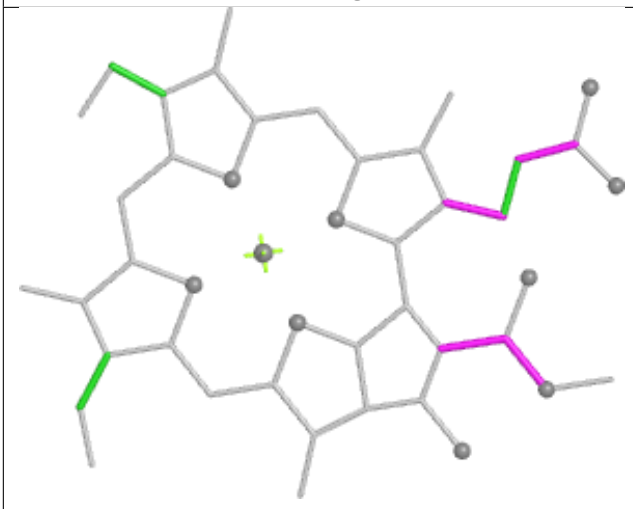
Ligand CLA b6 413



Bond lengths



Bond angles

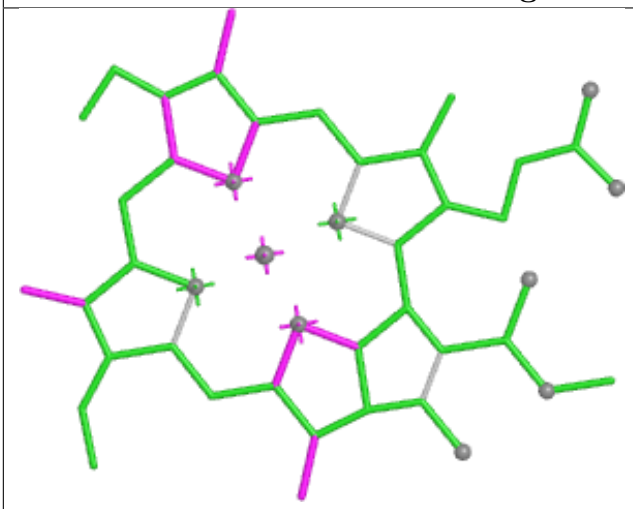


Torsions

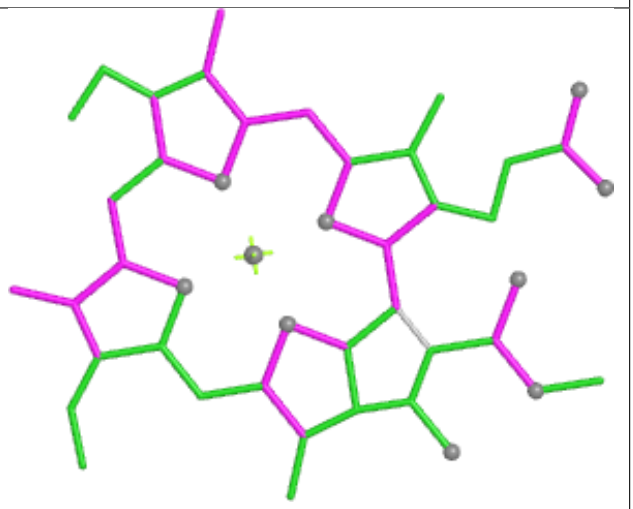


Rings

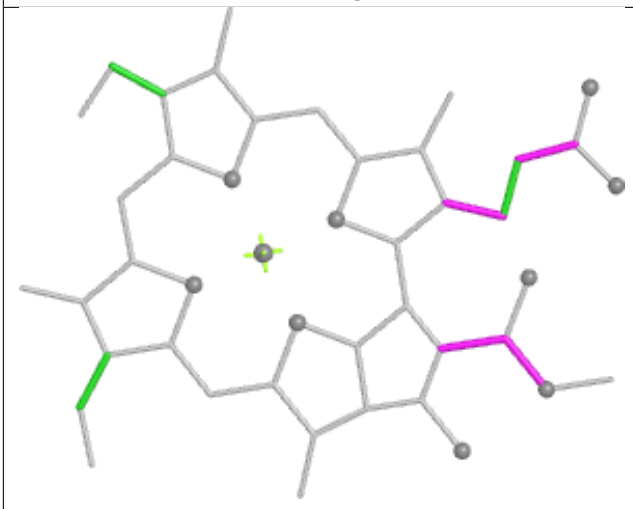
Ligand CLA a6 413



Bond lengths



Bond angles

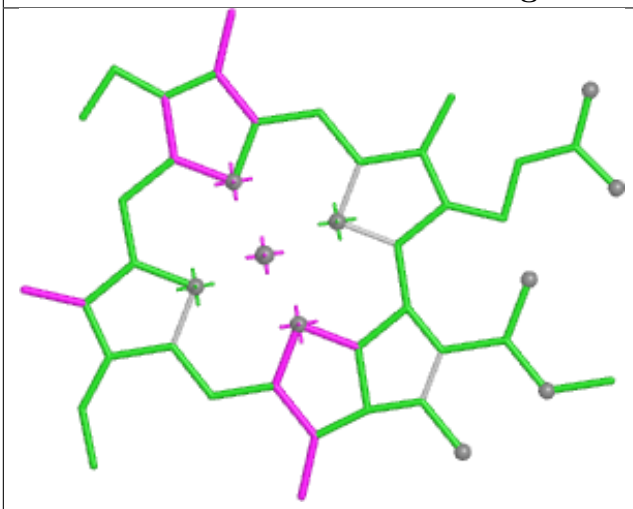


Torsions

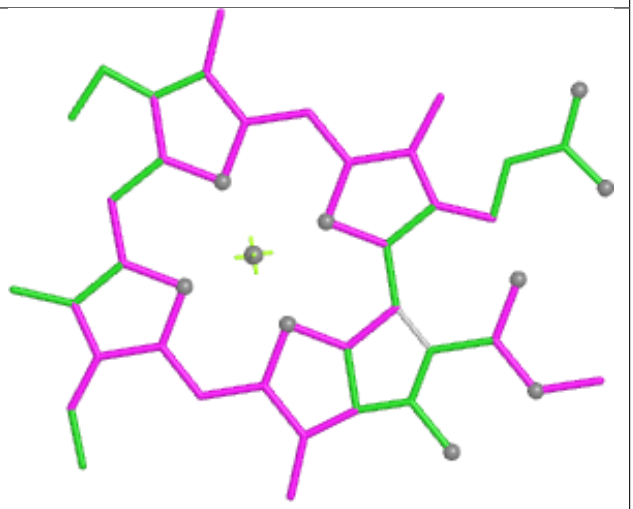


Rings

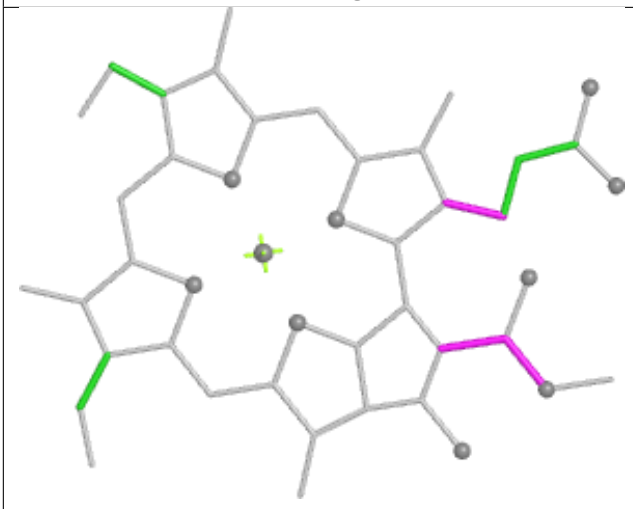
Ligand CLA c4 405



Bond lengths



Bond angles

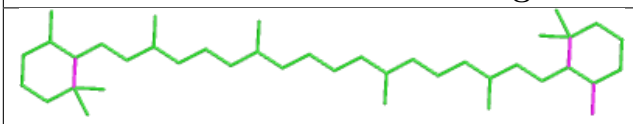


Torsions

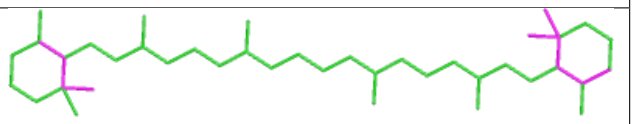


Rings

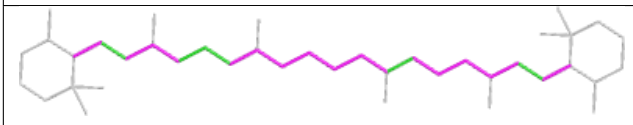
Ligand BCR aA 852



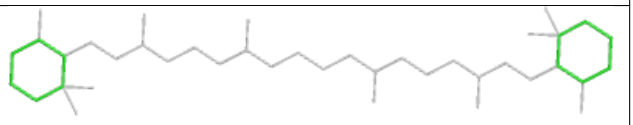
Bond lengths



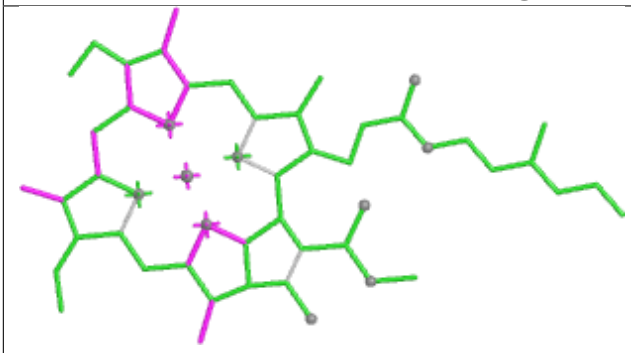
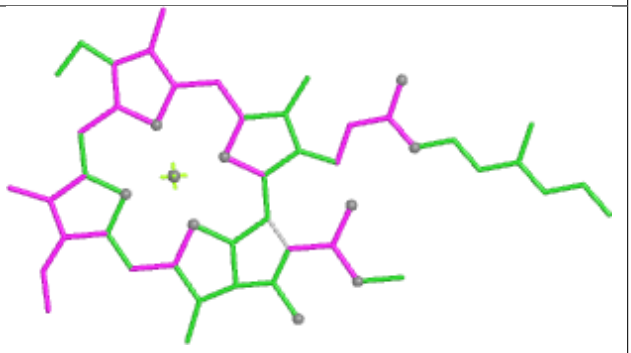
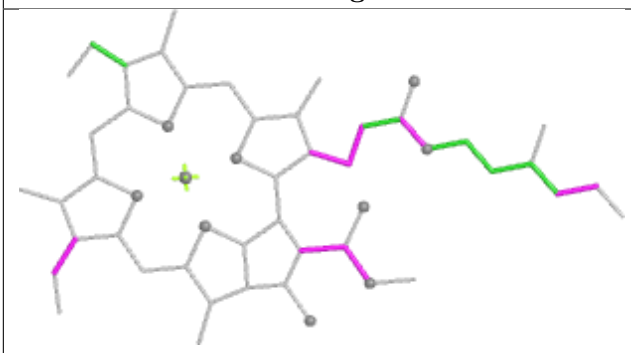
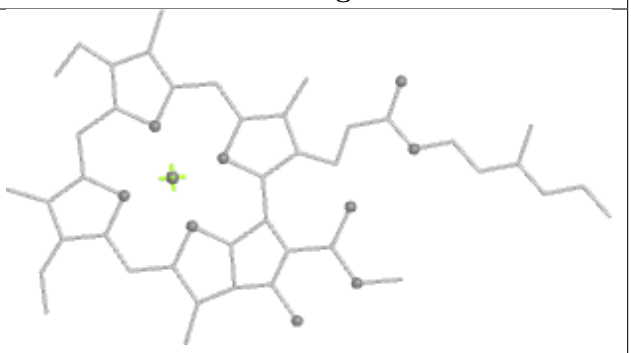
Bond angles

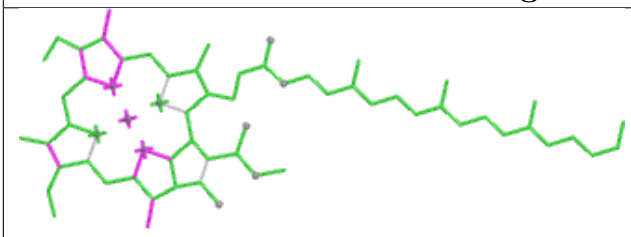
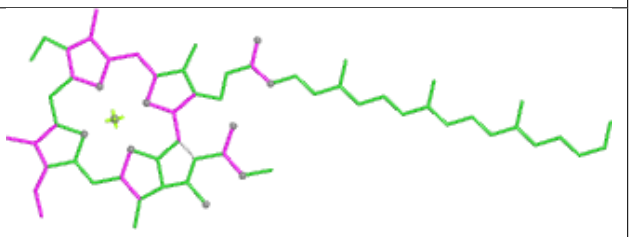
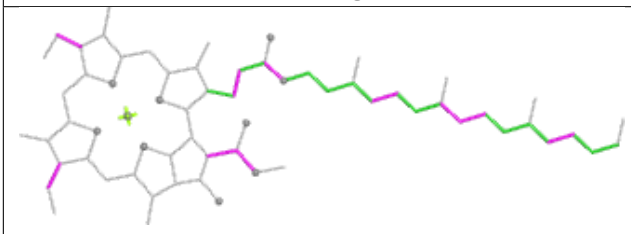
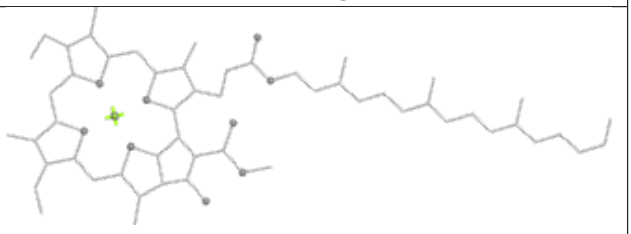


Torsions

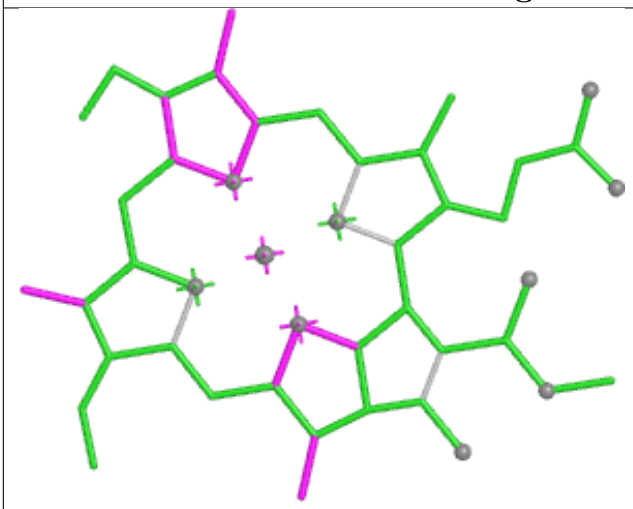


Rings

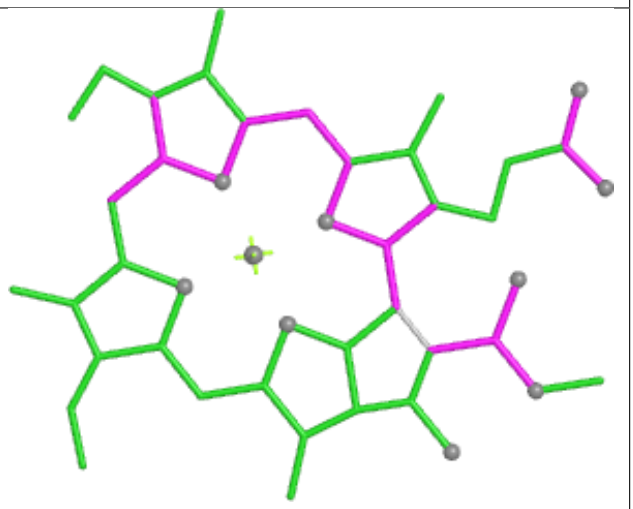
Ligand CLA cA 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c1 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

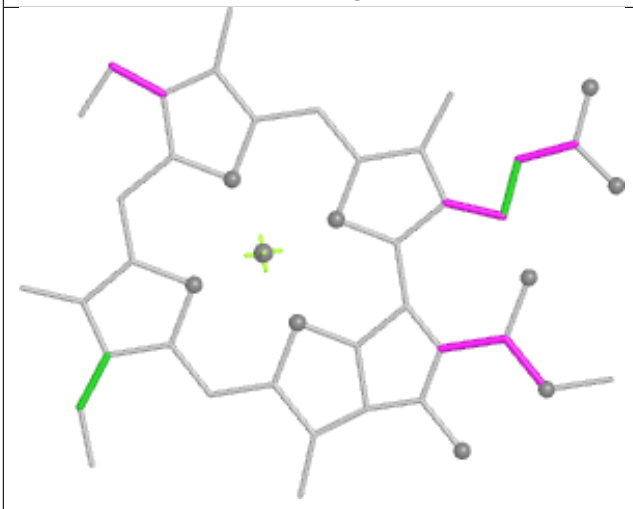
Ligand CLA cK 102



Bond lengths



Bond angles

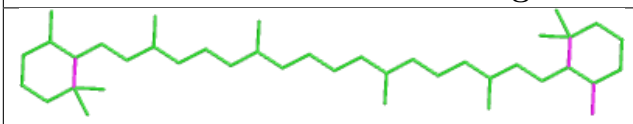


Torsions

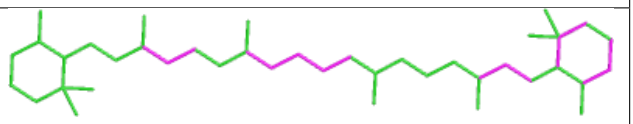


Rings

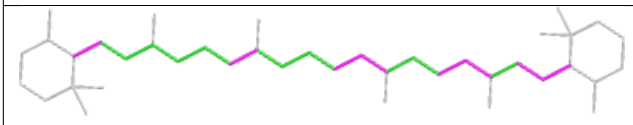
Ligand BCR bA 849



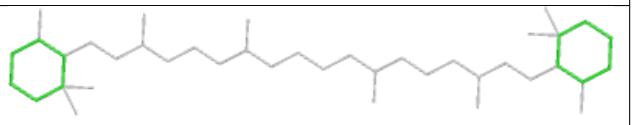
Bond lengths



Bond angles

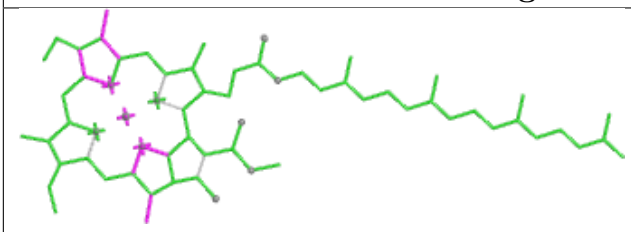


Torsions

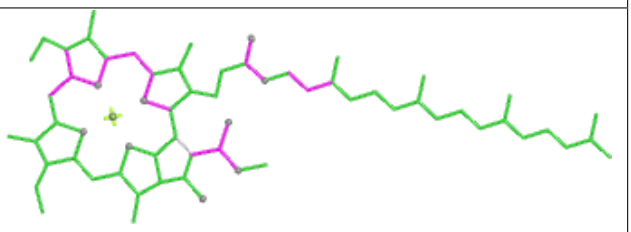


Rings

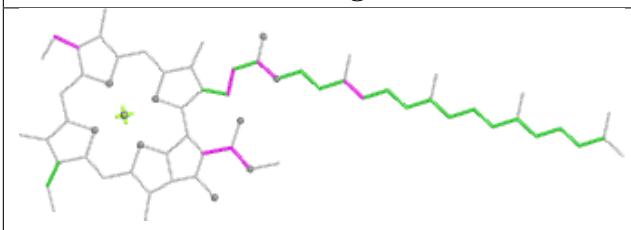
Ligand CLA b2 404



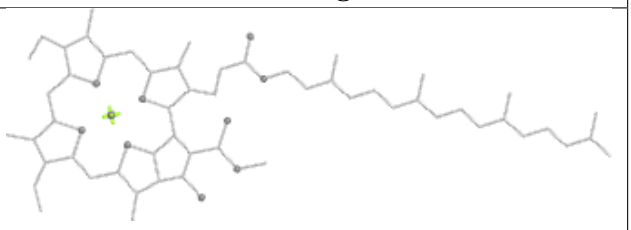
Bond lengths



Bond angles



Torsions

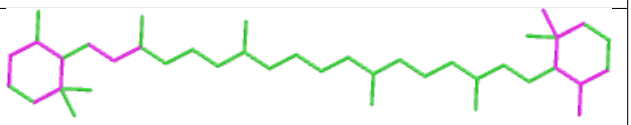


Rings

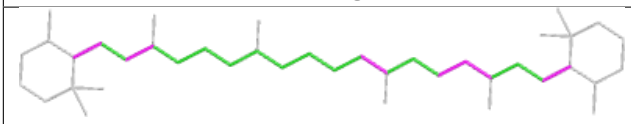
Ligand BCR a4 418



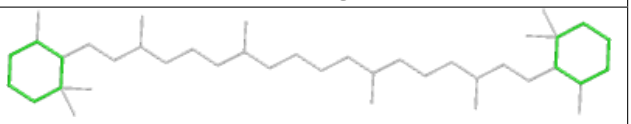
Bond lengths



Bond angles

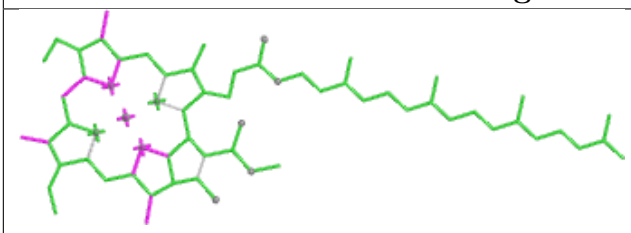


Torsions

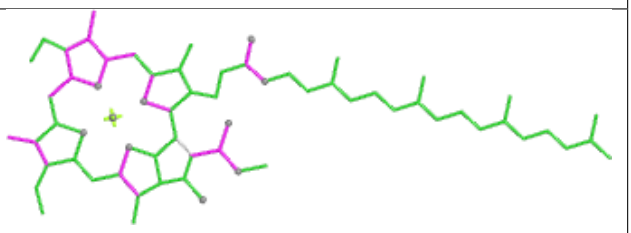


Rings

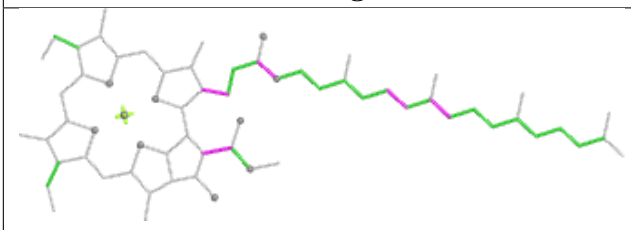
Ligand CLA bA 831



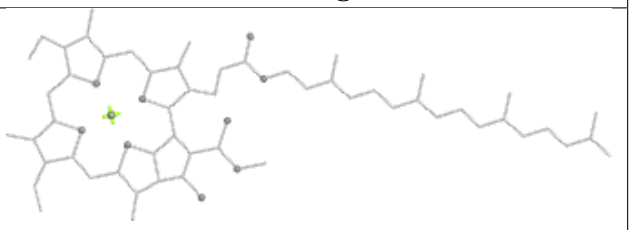
Bond lengths



Bond angles

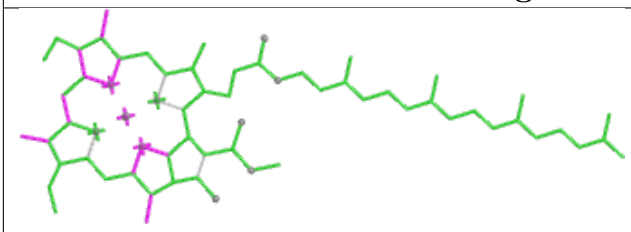


Torsions

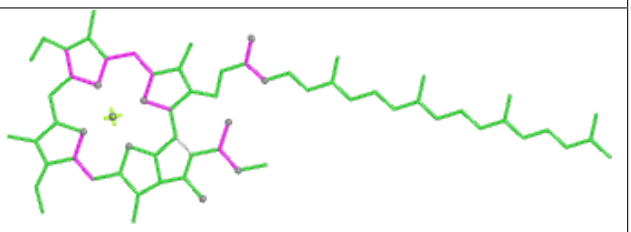


Rings

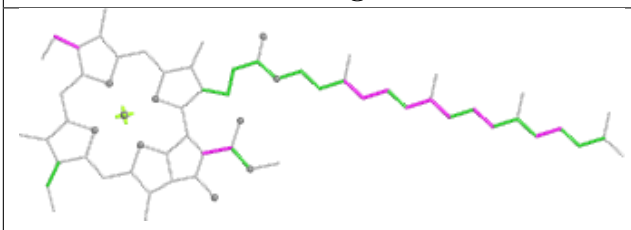
Ligand CLA aA 828



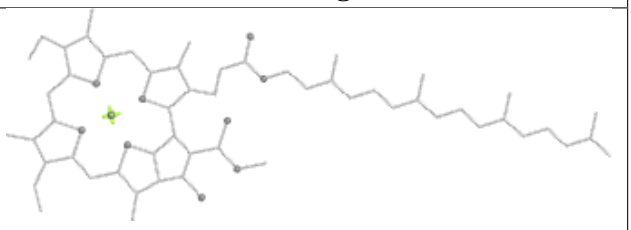
Bond lengths



Bond angles

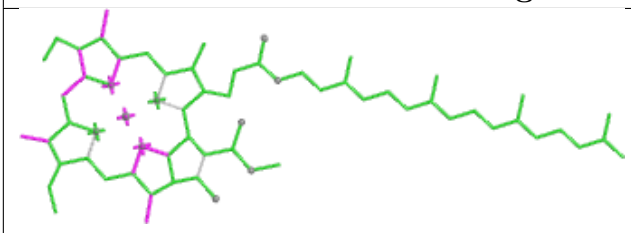


Torsions

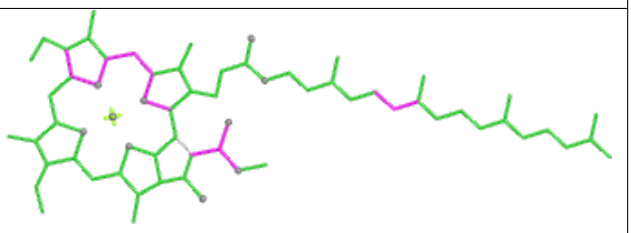


Rings

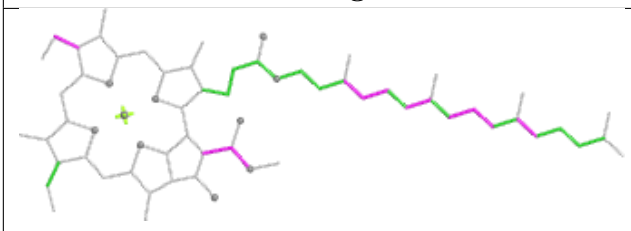
Ligand CLA cA 839



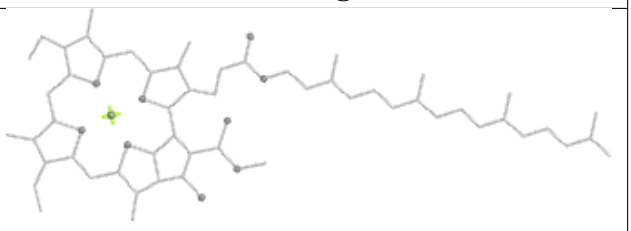
Bond lengths



Bond angles

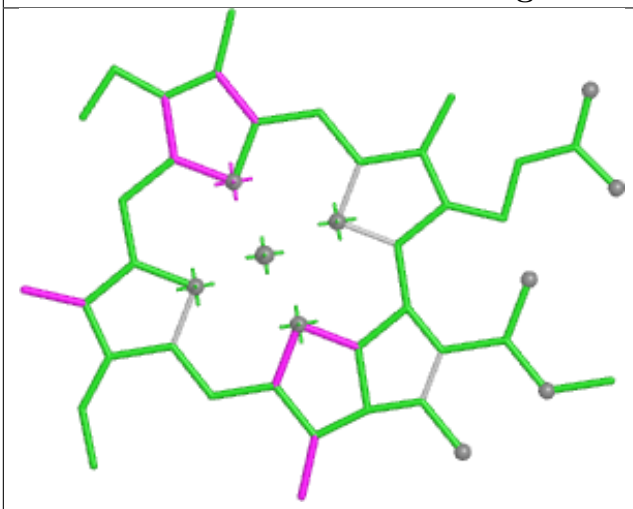


Torsions

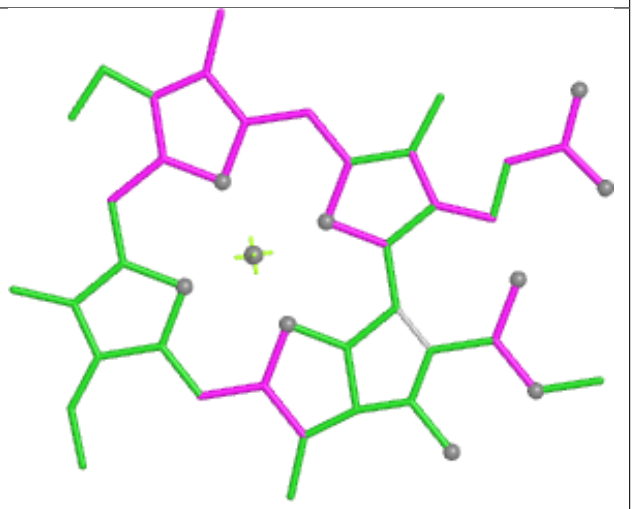


Rings

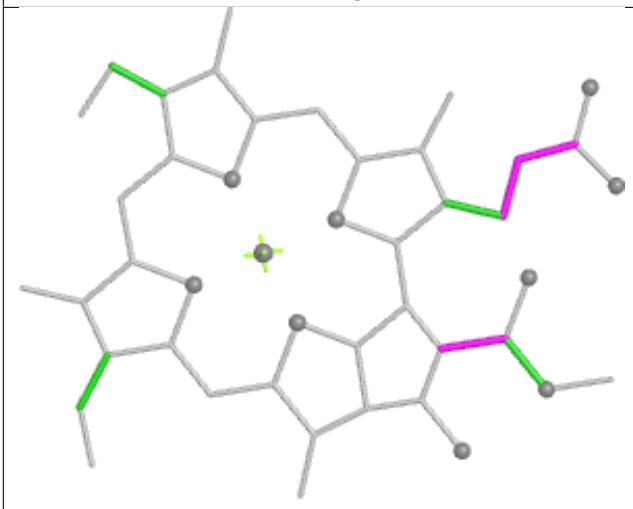
Ligand CLA cB 824



Bond lengths



Bond angles

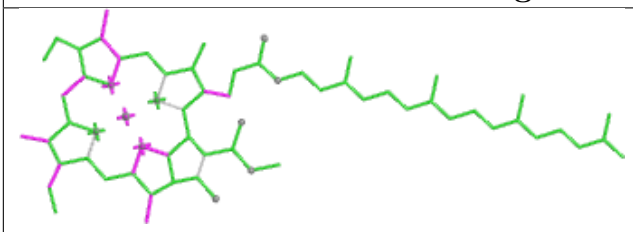


Torsions

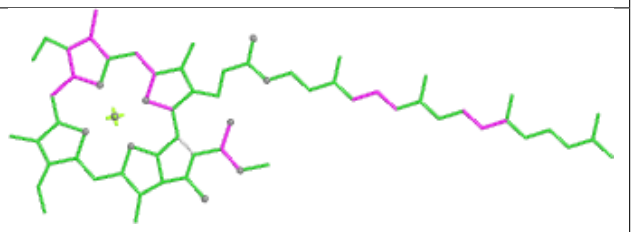


Rings

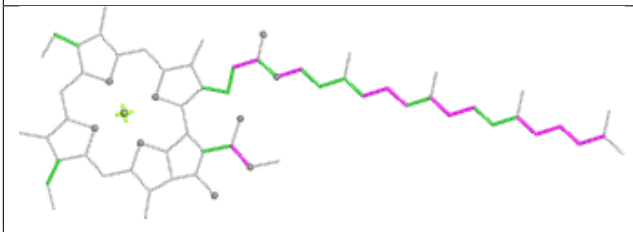
Ligand CLA bB 807



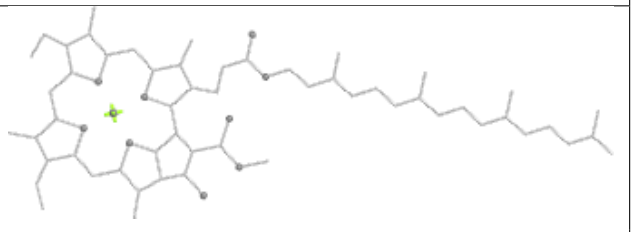
Bond lengths



Bond angles

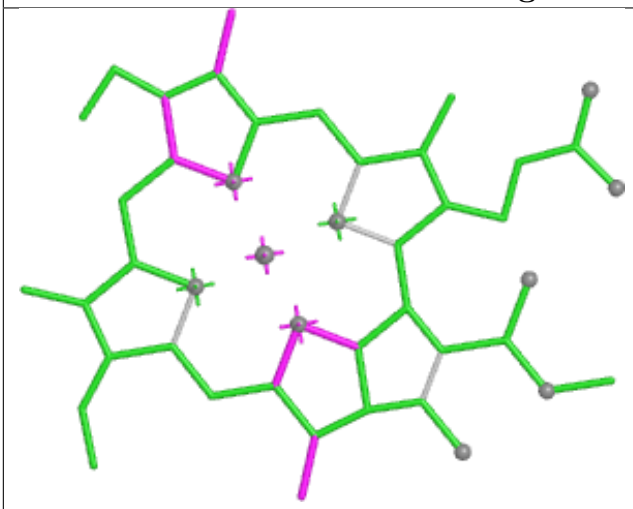


Torsions

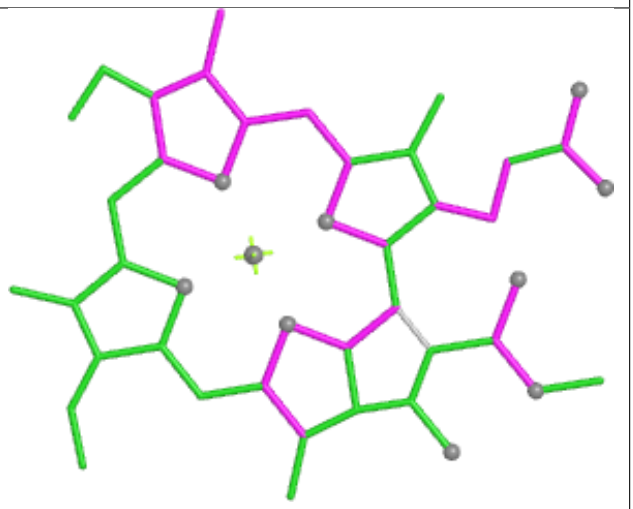


Rings

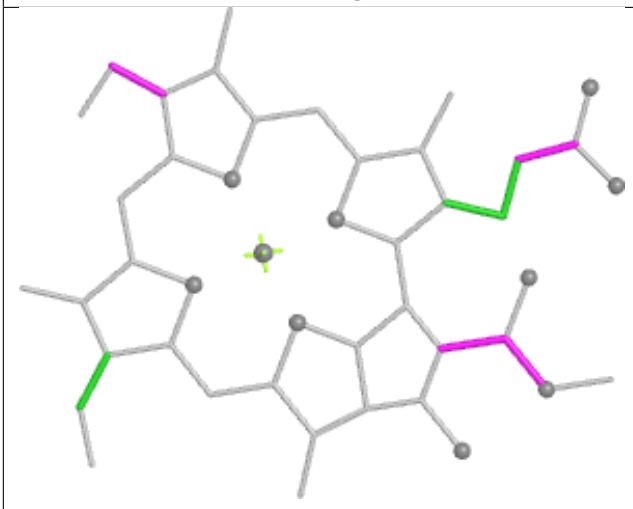
Ligand CLA b1 415



Bond lengths



Bond angles

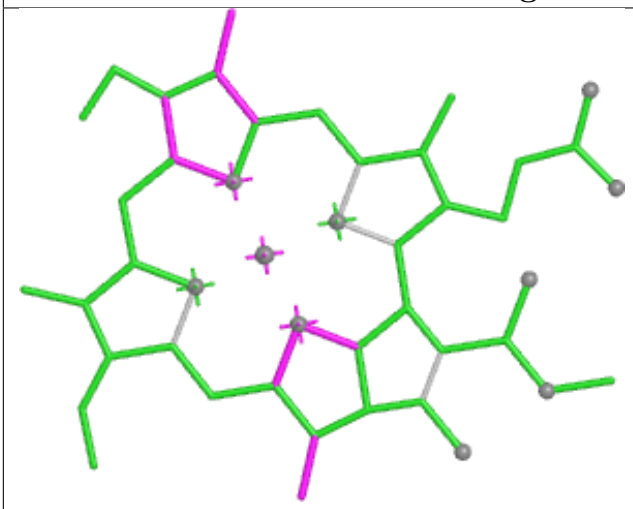


Torsions

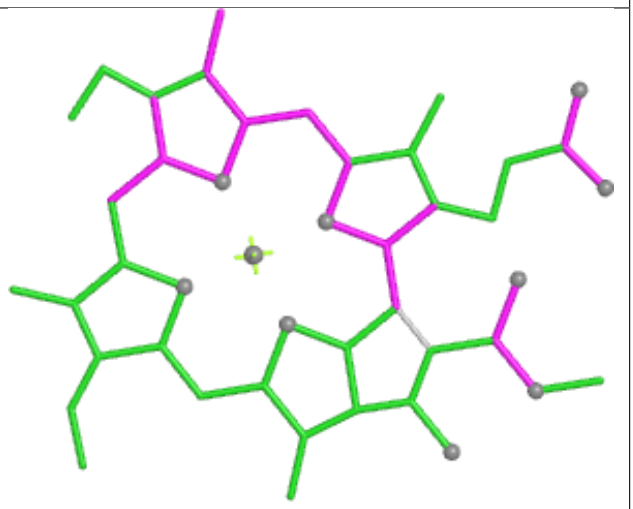


Rings

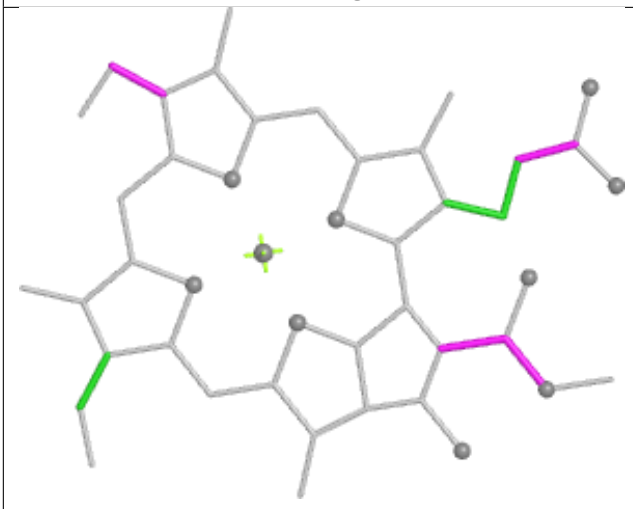
Ligand CLA a5 407



Bond lengths



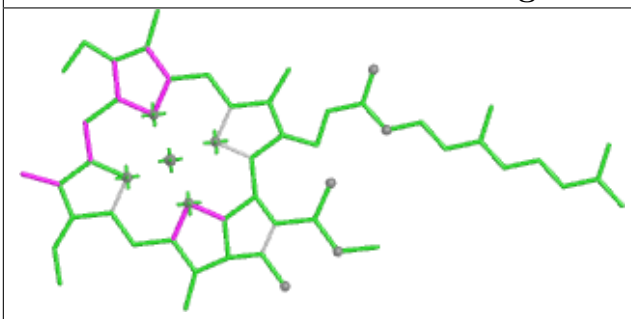
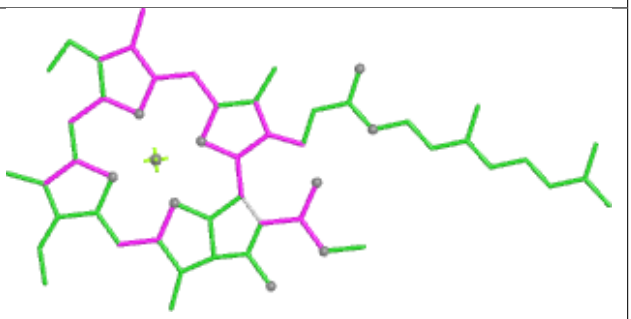
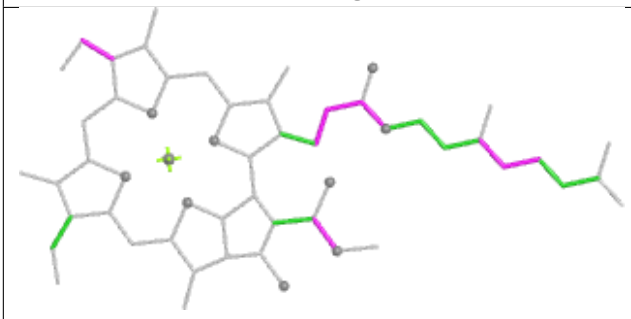
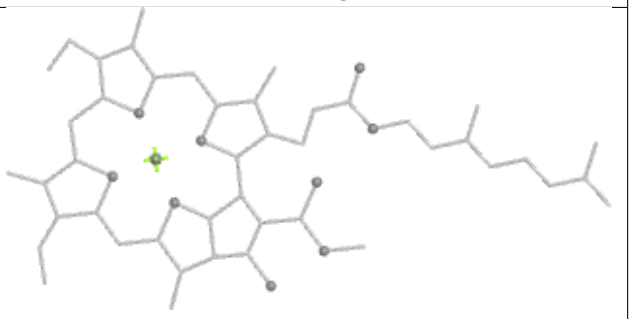
Bond angles

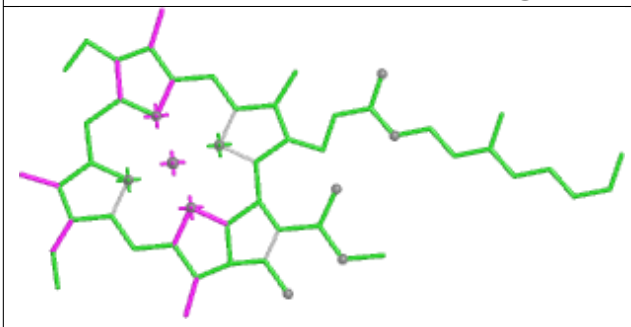
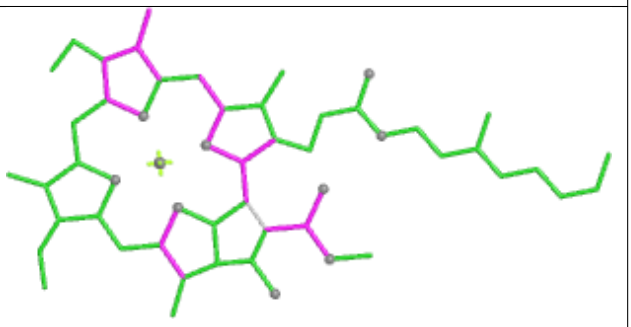
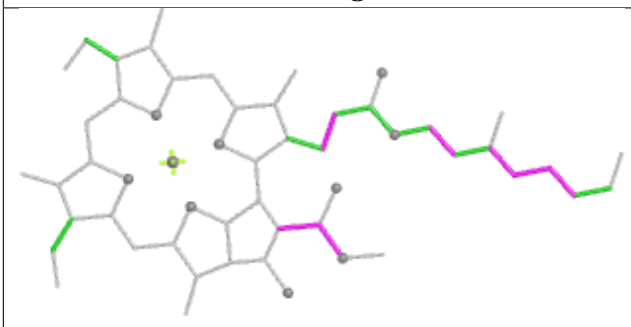
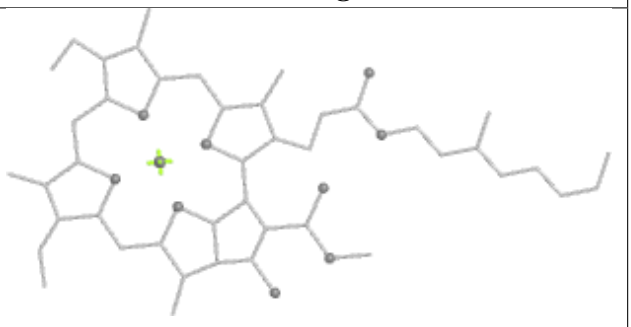


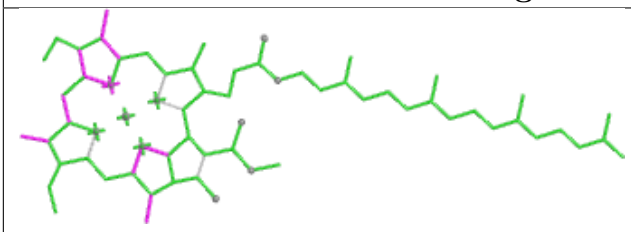
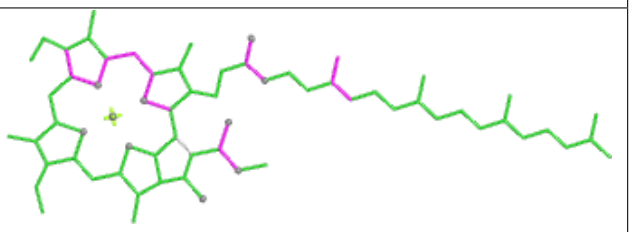
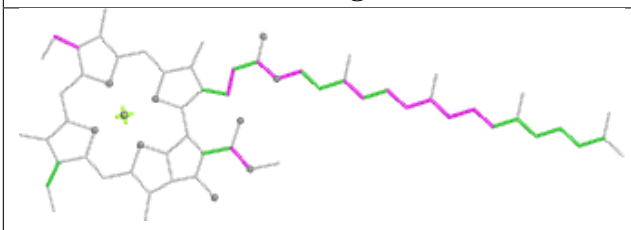
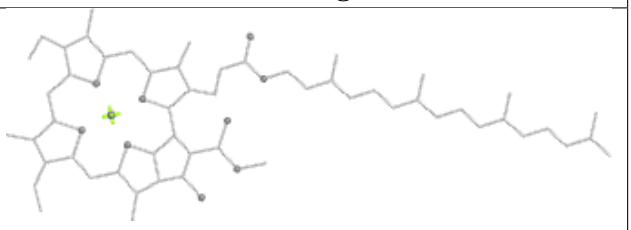
Torsions

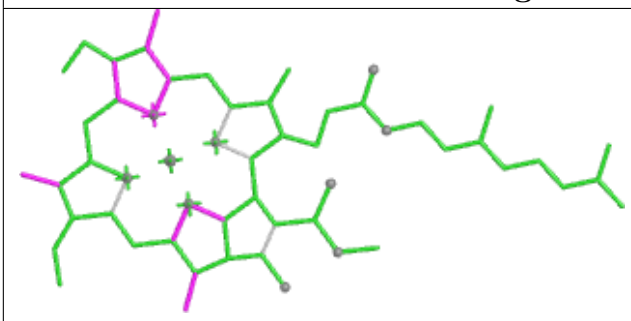
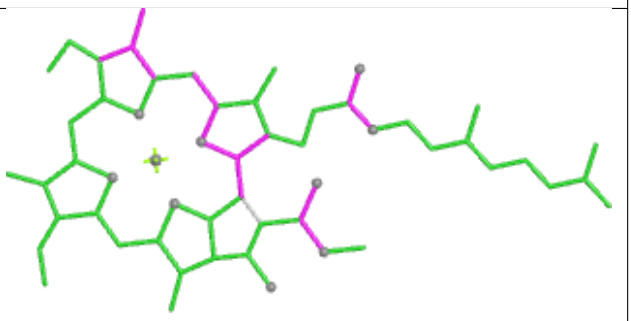
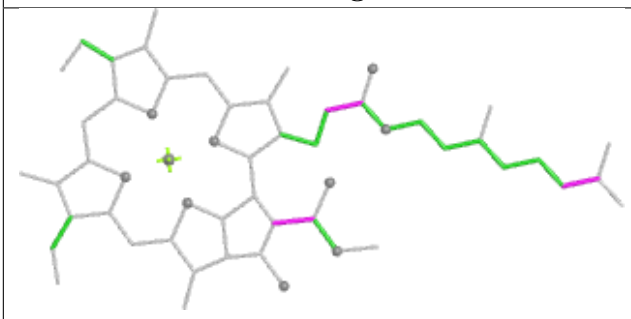
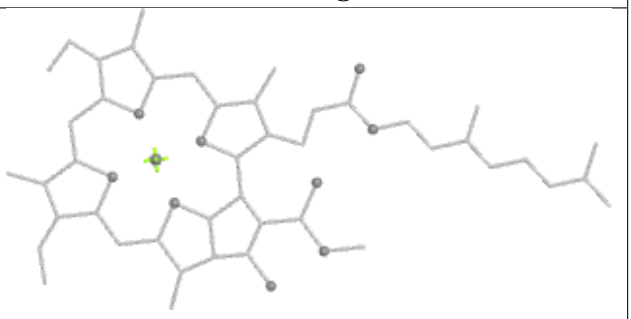


Rings

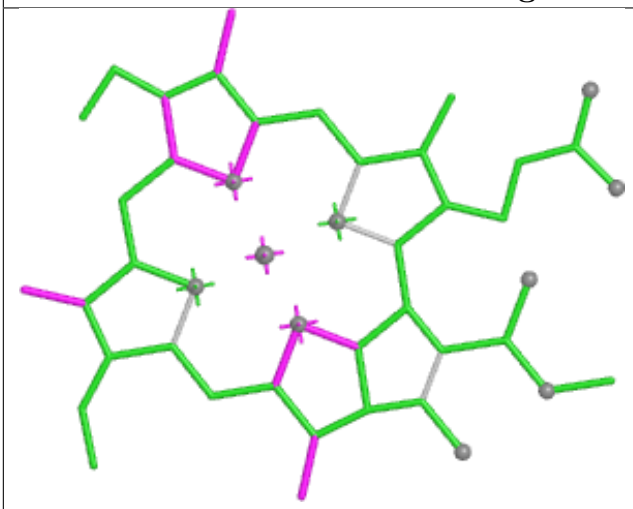
Ligand CLA b6 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

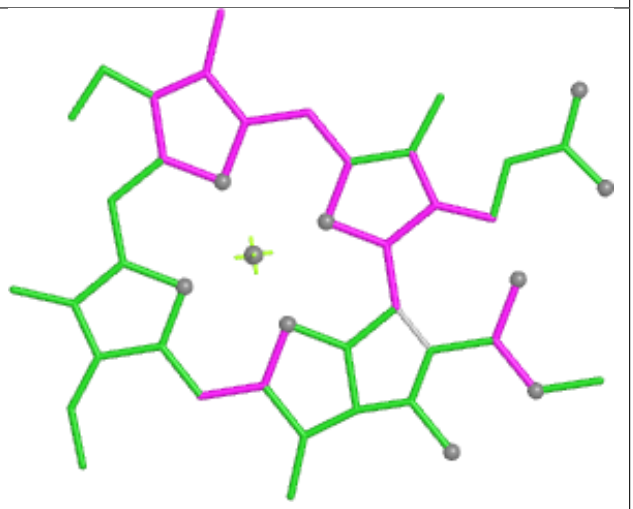
Ligand CLA aA 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

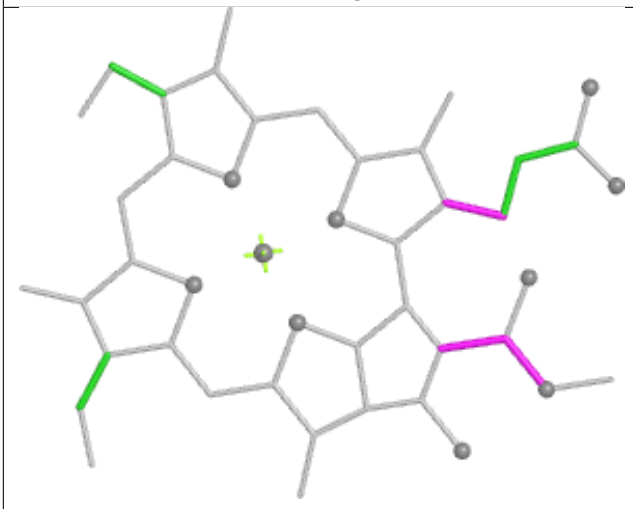
Ligand CLA b3 411



Bond lengths



Bond angles

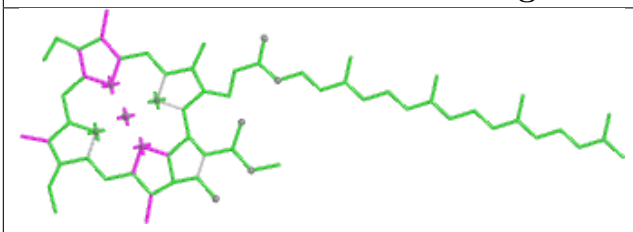


Torsions

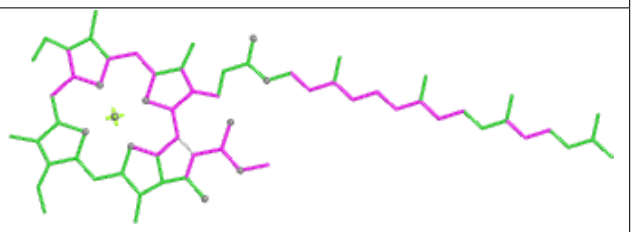


Rings

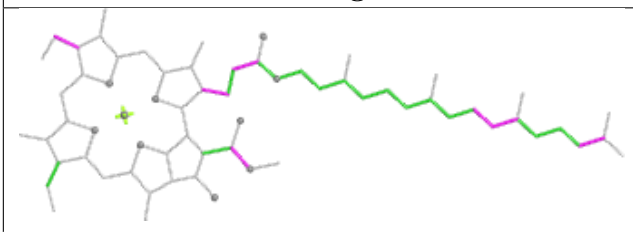
Ligand CLA b2 422



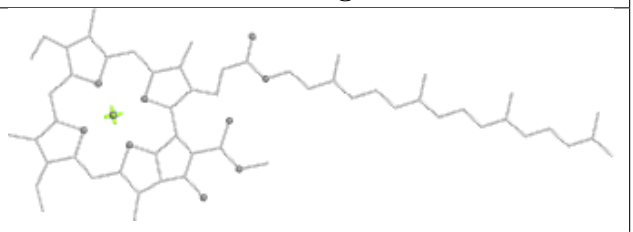
Bond lengths



Bond angles

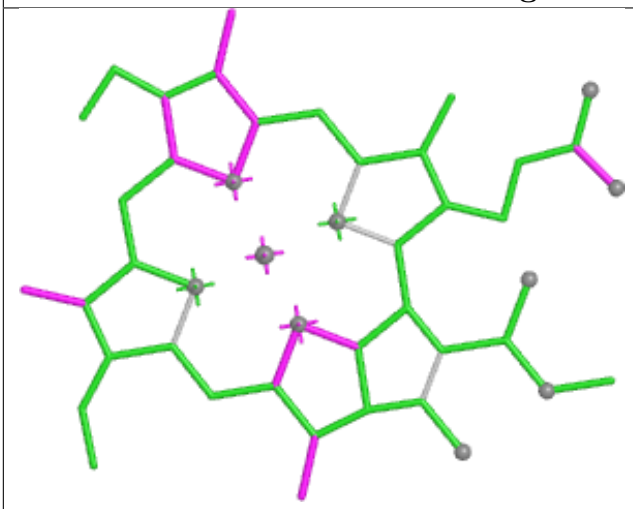


Torsions

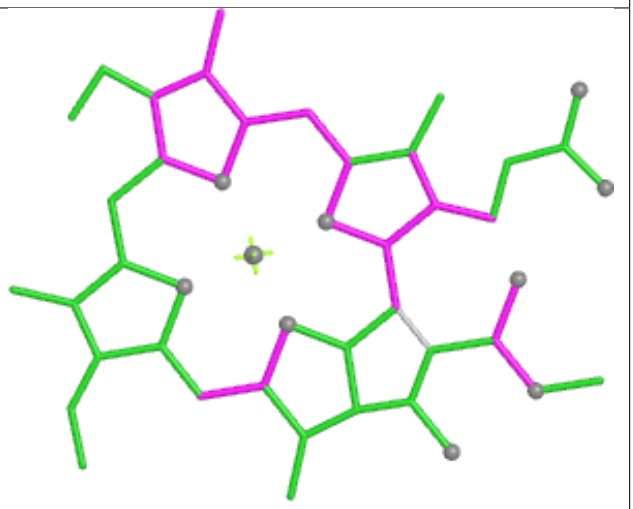


Rings

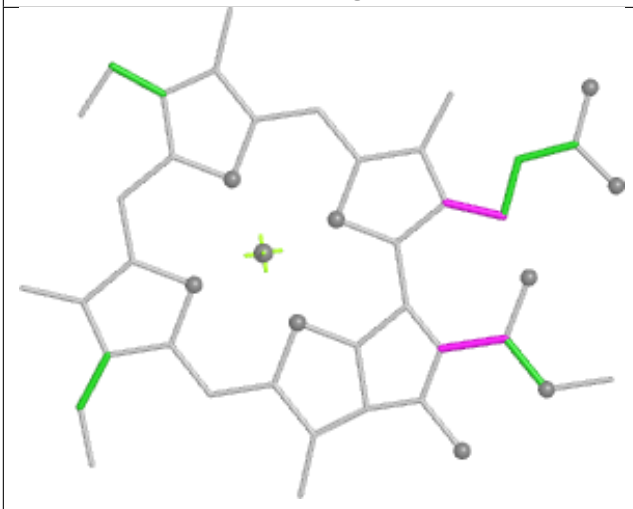
Ligand CLA a2 412



Bond lengths



Bond angles

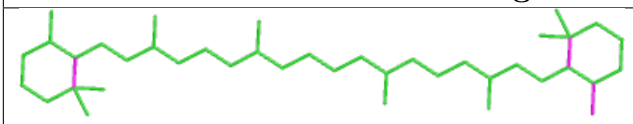


Torsions

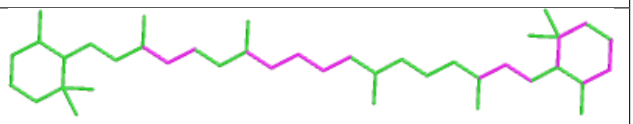


Rings

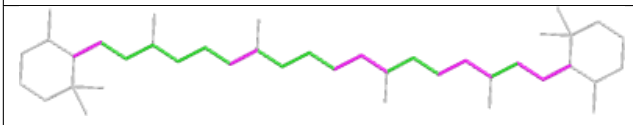
Ligand BCR aA 848



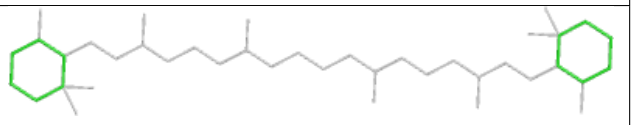
Bond lengths



Bond angles

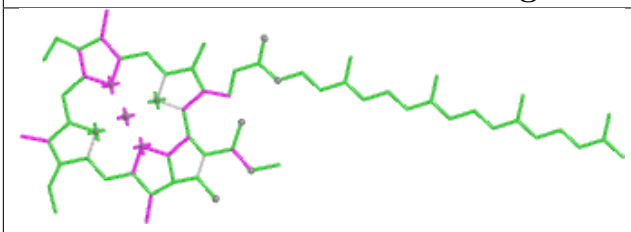


Torsions

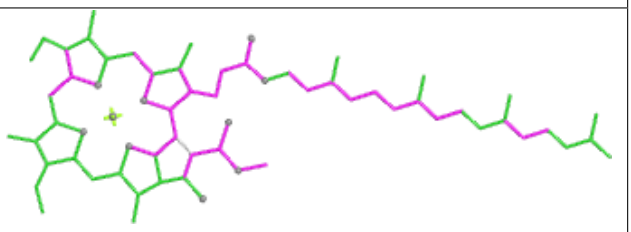


Rings

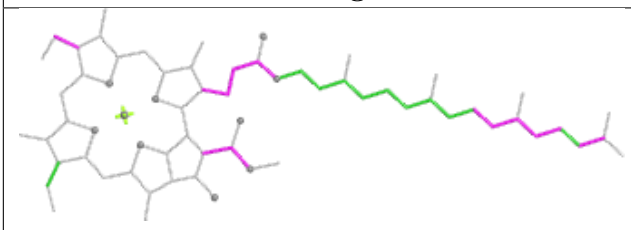
Ligand CLA a6 422



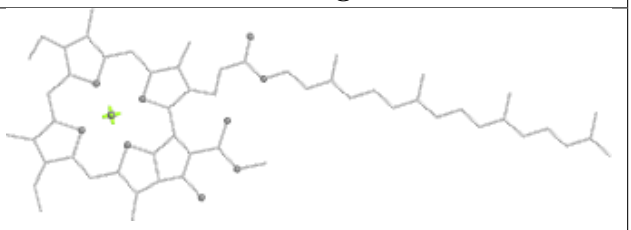
Bond lengths



Bond angles

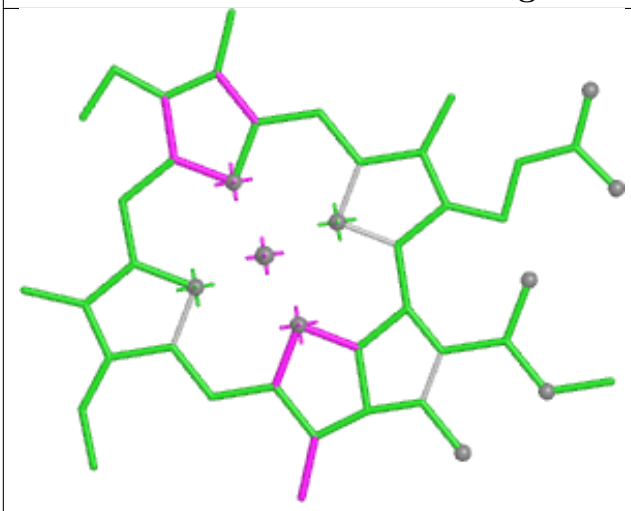


Torsions

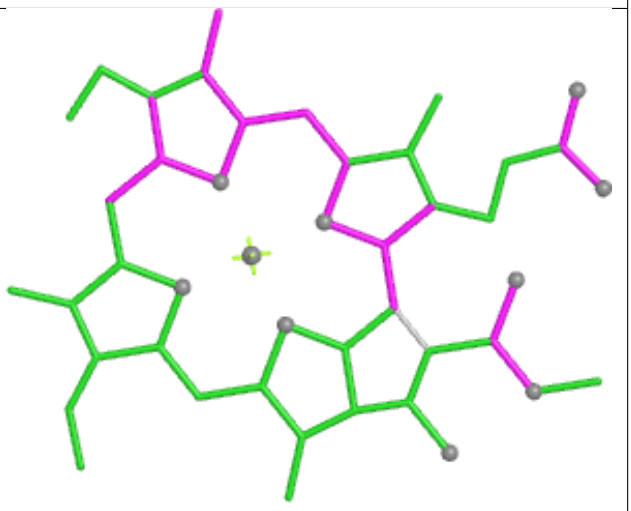


Rings

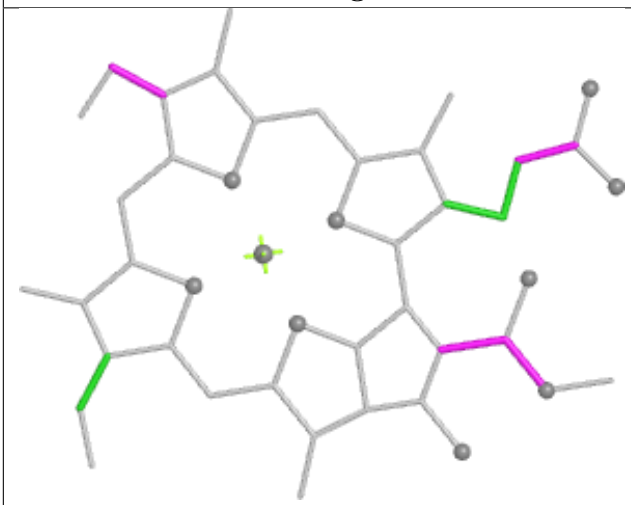
Ligand CLA b5 407



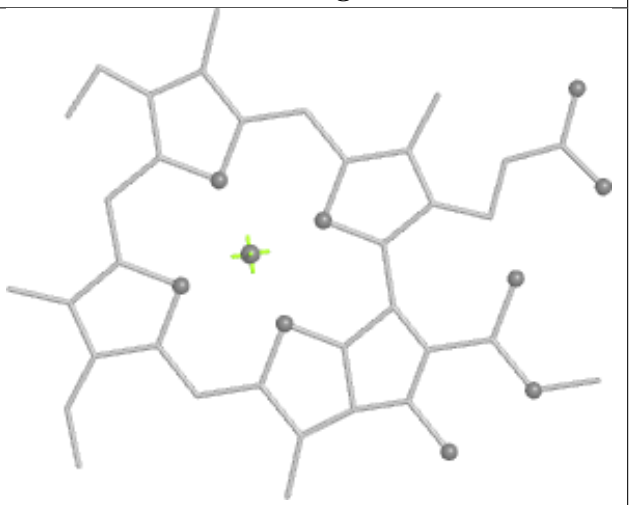
Bond lengths



Bond angles

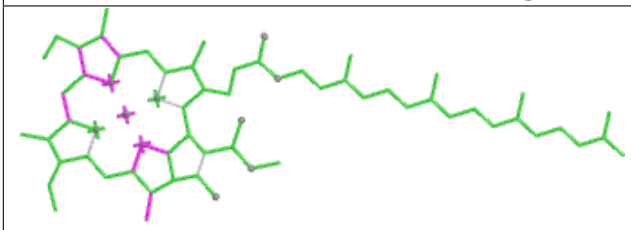


Torsions

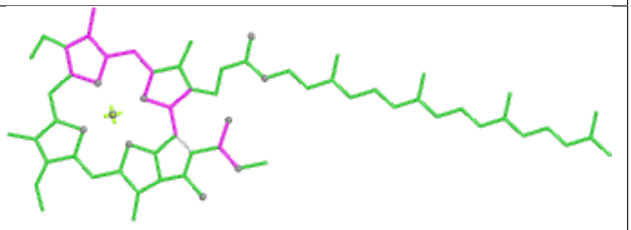


Rings

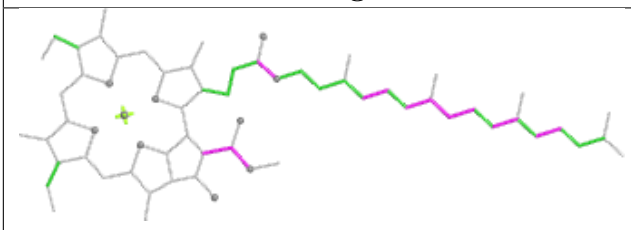
Ligand CLA a2 403



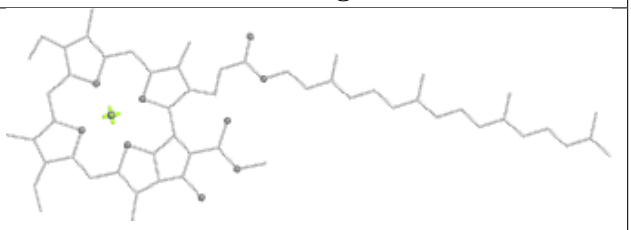
Bond lengths



Bond angles

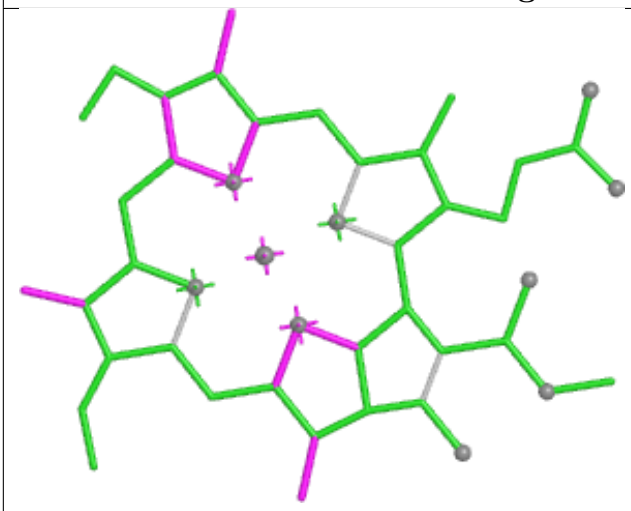


Torsions

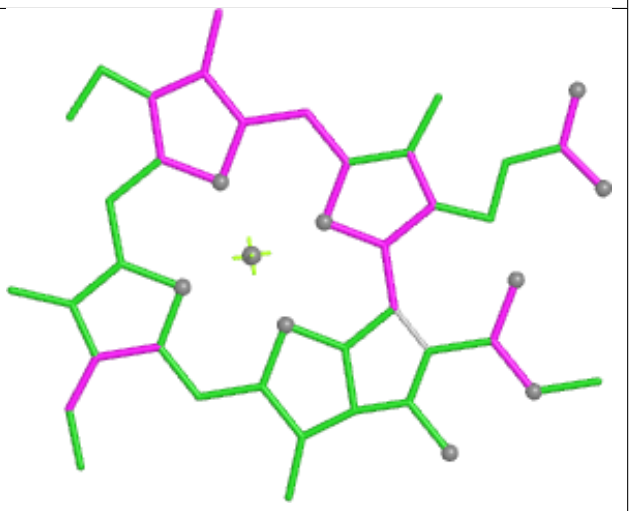


Rings

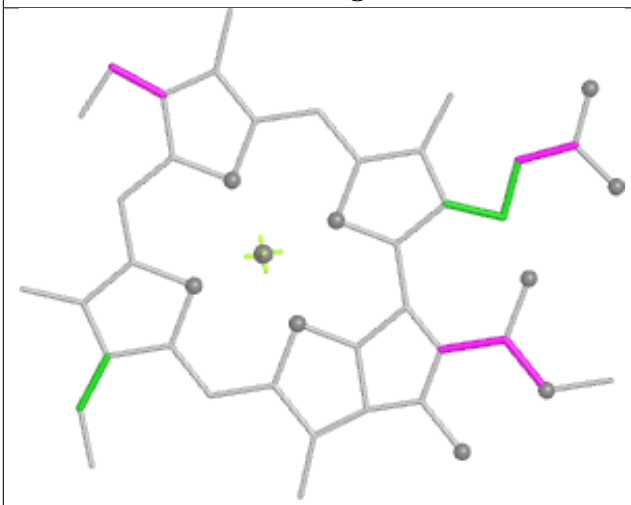
Ligand CLA cF 203



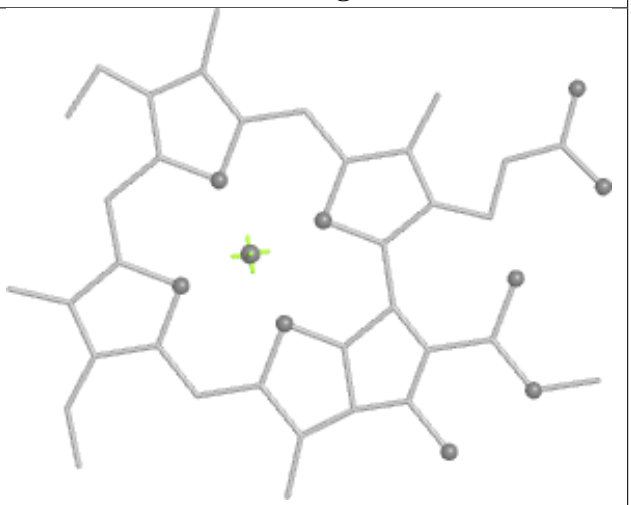
Bond lengths



Bond angles

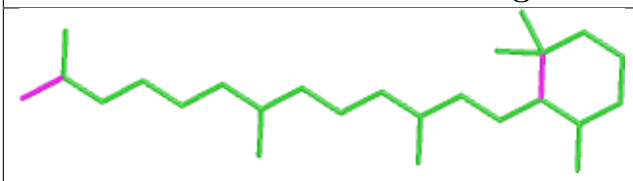


Torsions

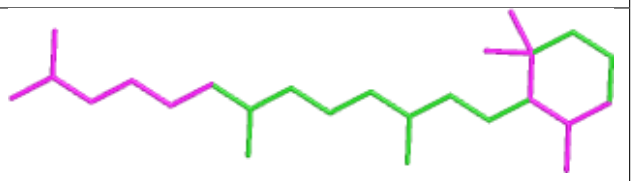


Rings

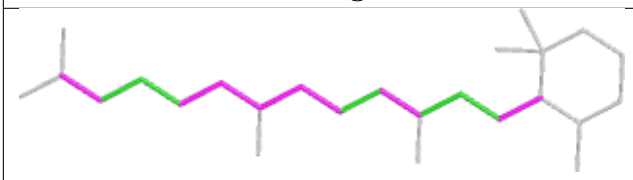
Ligand BCR bB 847



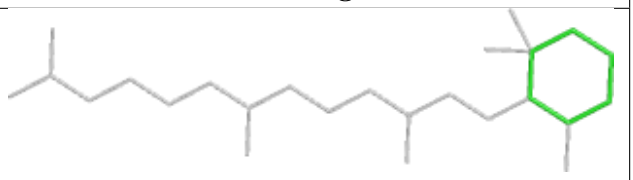
Bond lengths



Bond angles

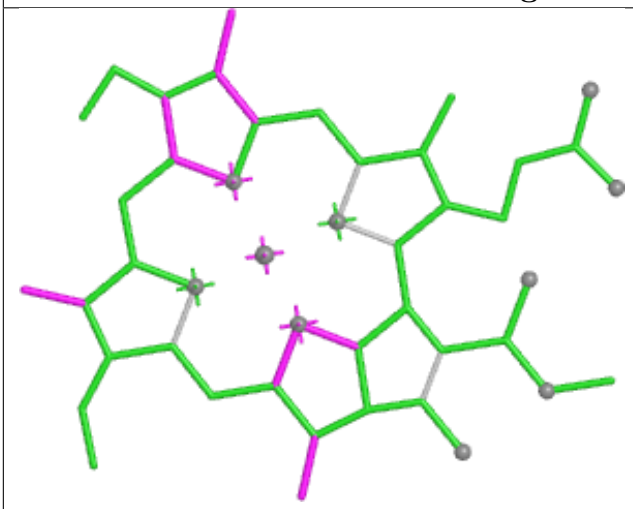


Torsions

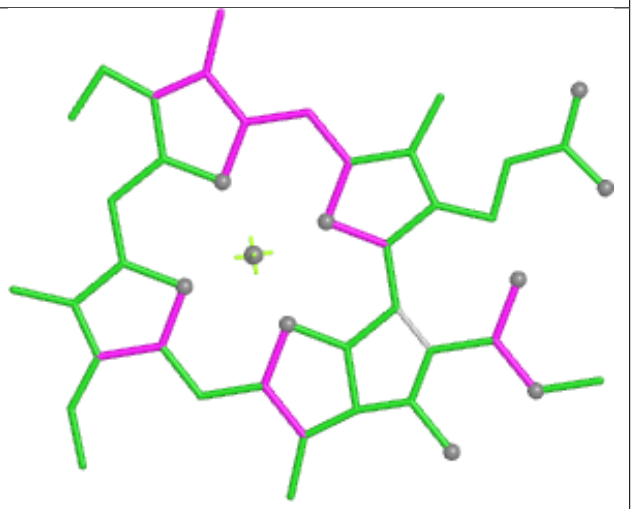


Rings

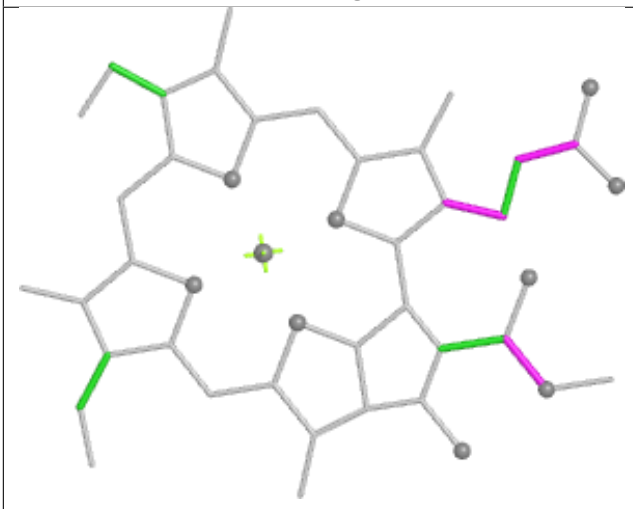
Ligand CLA c1 408



Bond lengths



Bond angles

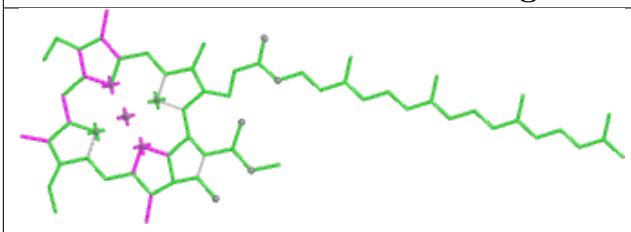


Torsions

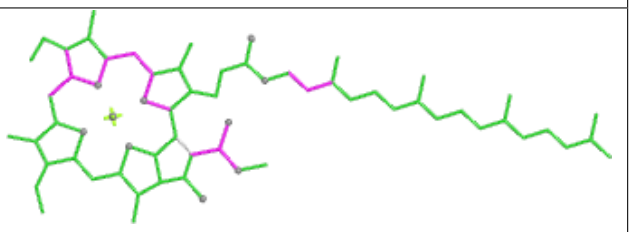


Rings

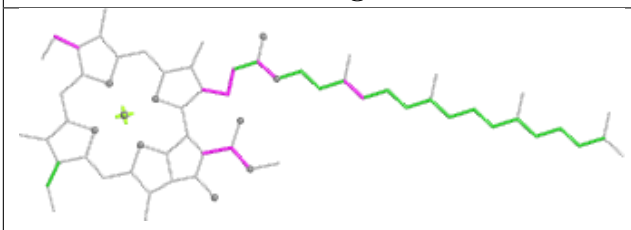
Ligand CLA a4 404



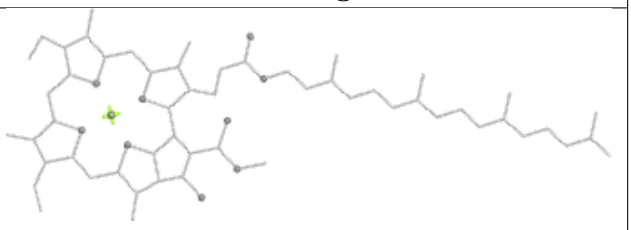
Bond lengths



Bond angles

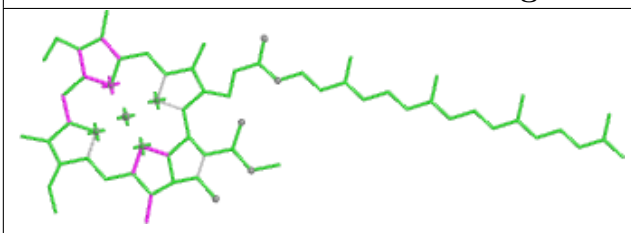


Torsions

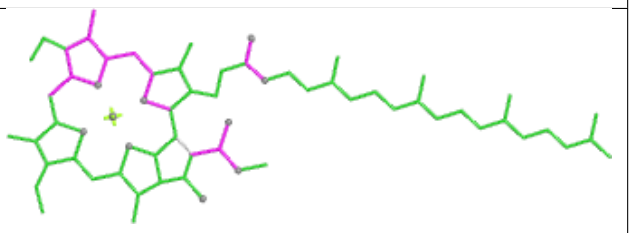


Rings

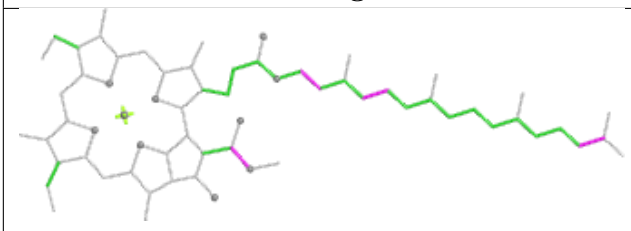
Ligand CLA c4 409



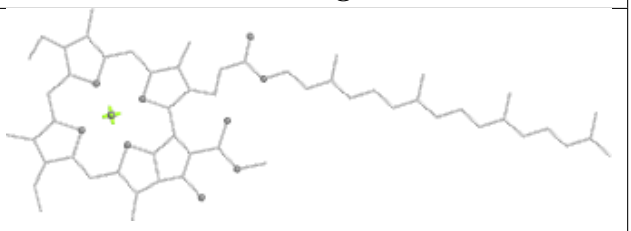
Bond lengths



Bond angles

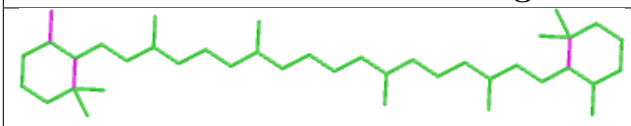


Torsions

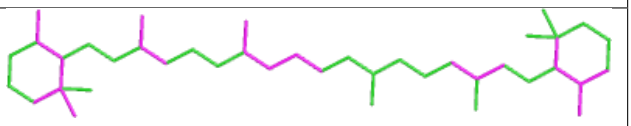


Rings

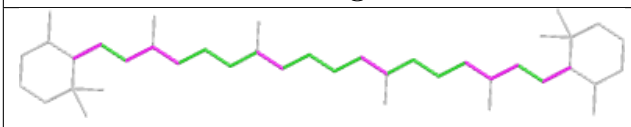
Ligand BCR bF 202



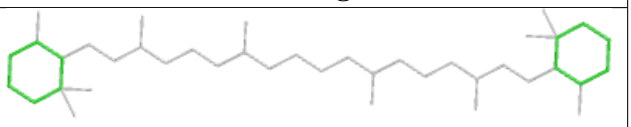
Bond lengths



Bond angles

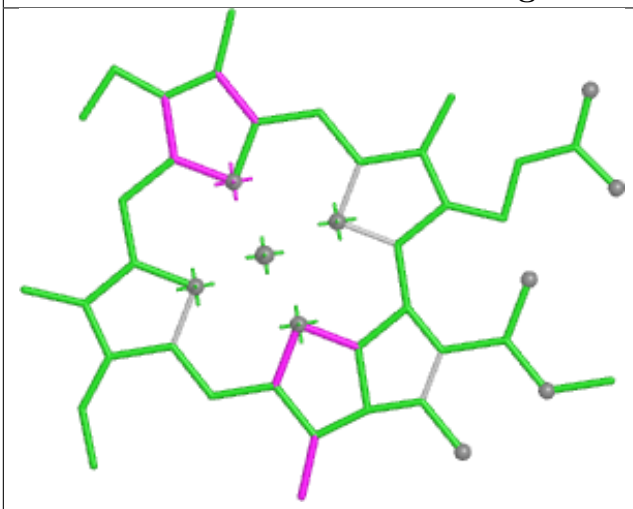


Torsions

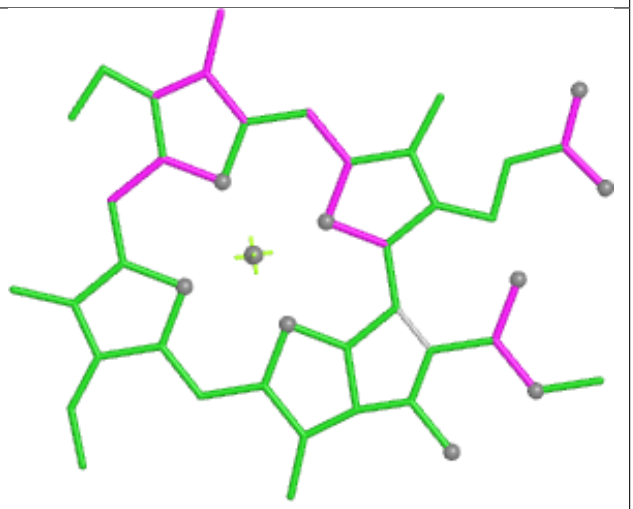


Rings

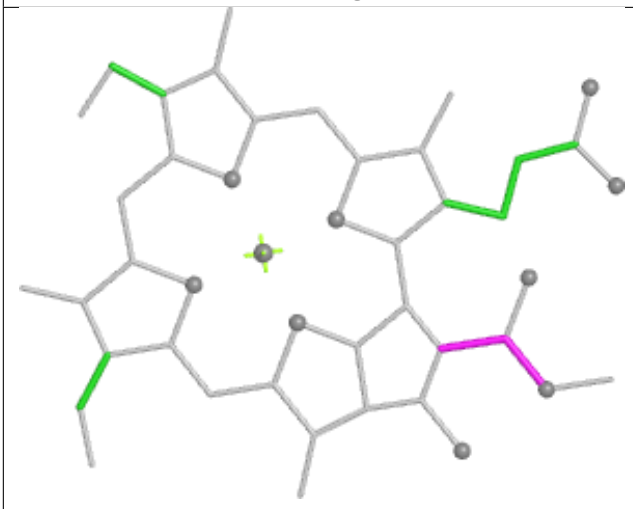
Ligand CLA b2 407



Bond lengths



Bond angles

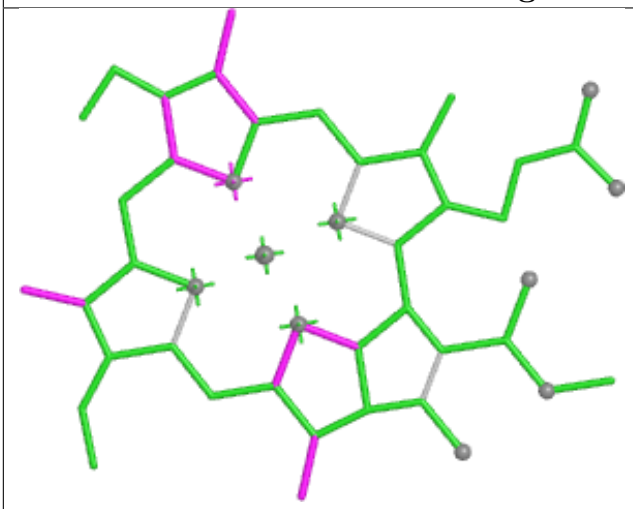


Torsions

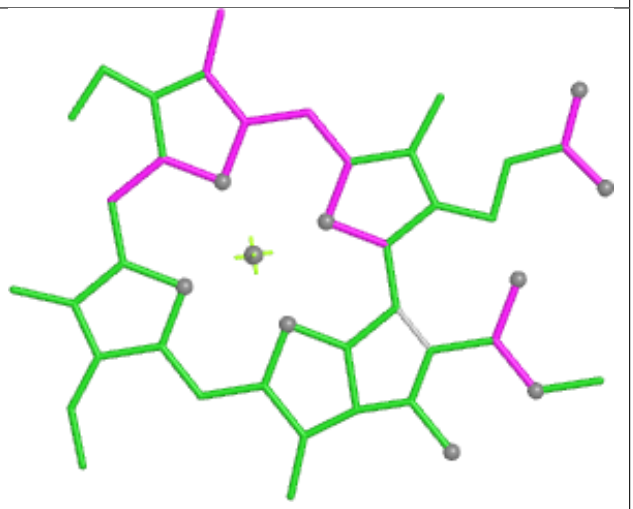


Rings

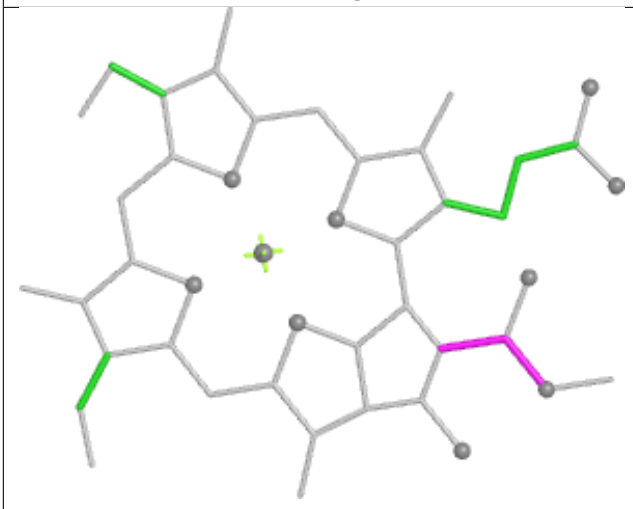
Ligand CLA b4 406



Bond lengths



Bond angles

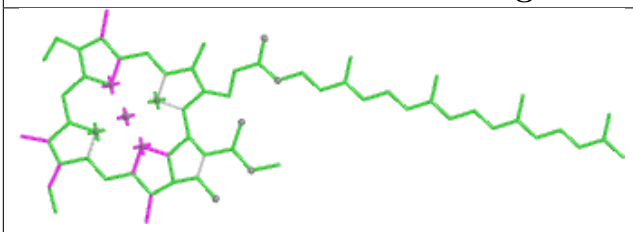


Torsions

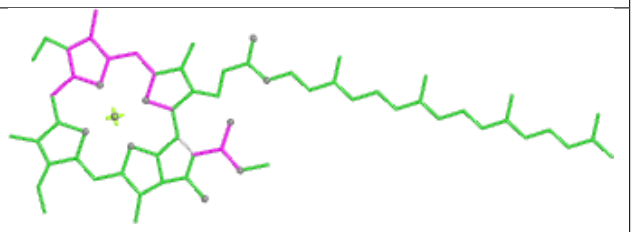


Rings

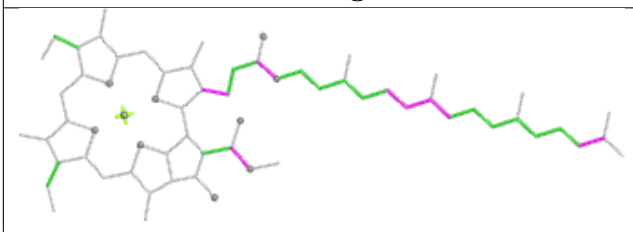
Ligand CLA cA 833



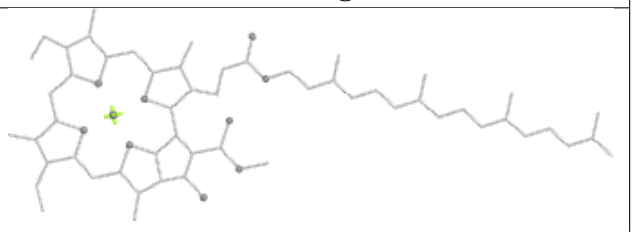
Bond lengths



Bond angles

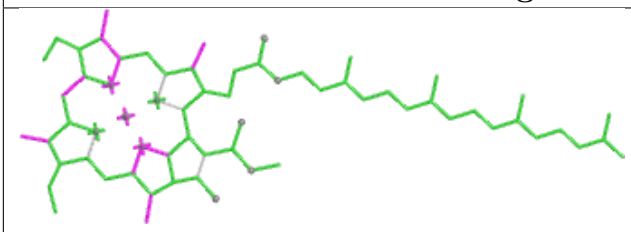


Torsions

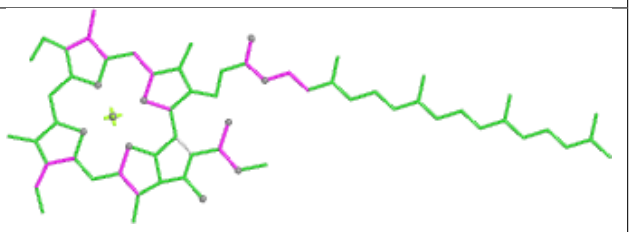


Rings

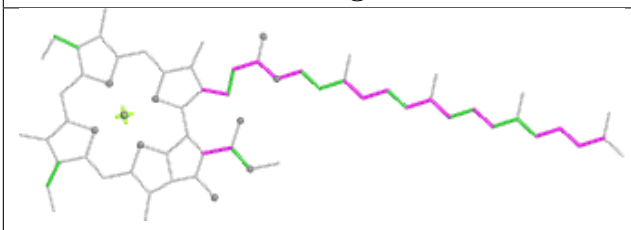
Ligand CLA cB 806



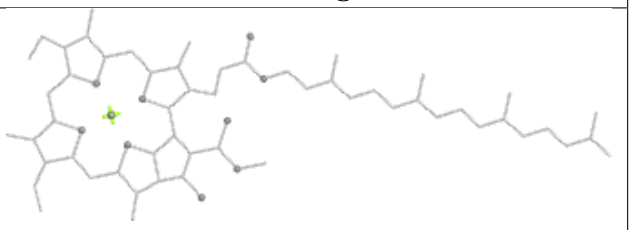
Bond lengths



Bond angles

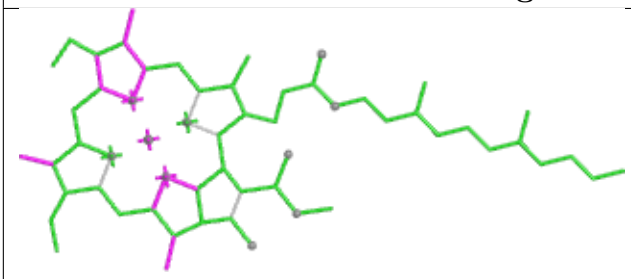


Torsions

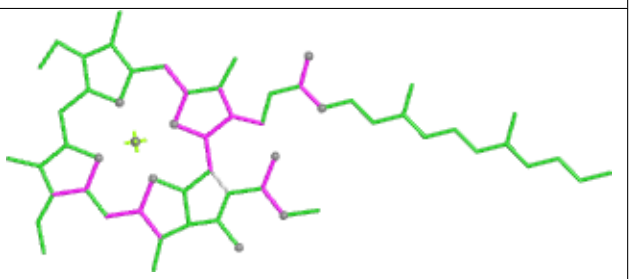


Rings

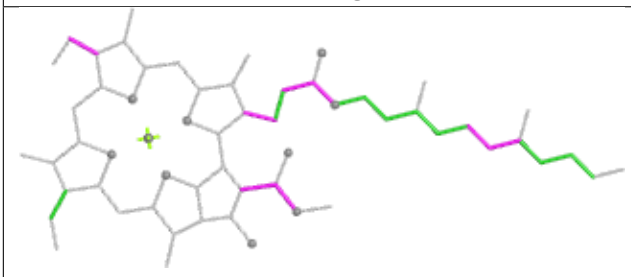
Ligand CLA cB 834



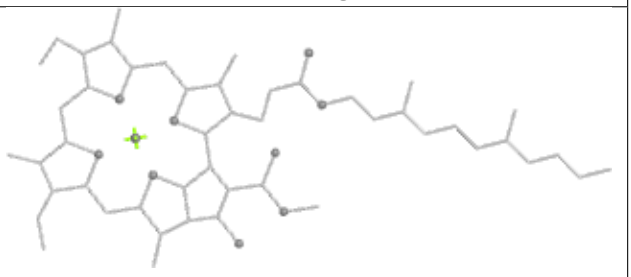
Bond lengths



Bond angles

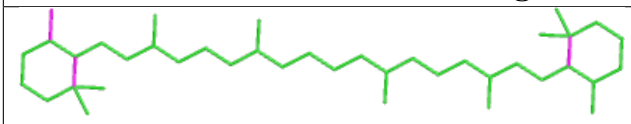


Torsions

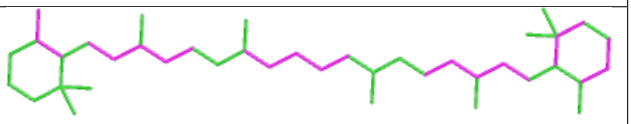


Rings

Ligand BCR cK 101



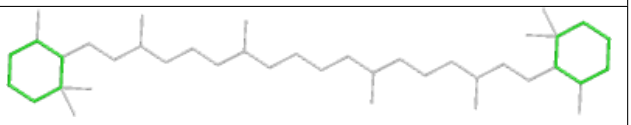
Bond lengths



Bond angles

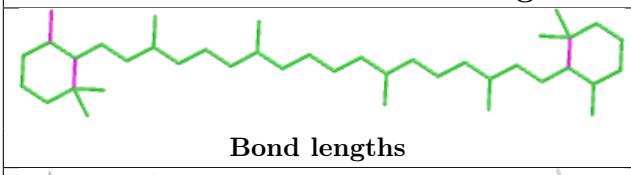


Torsions

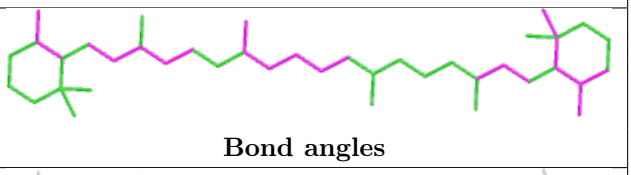


Rings

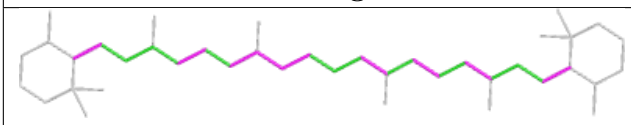
Ligand BCR bJ 103



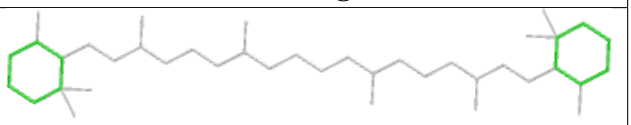
Bond lengths



Bond angles

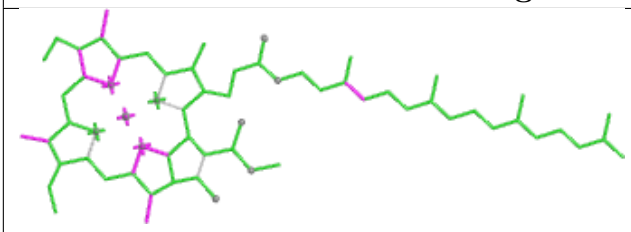


Torsions

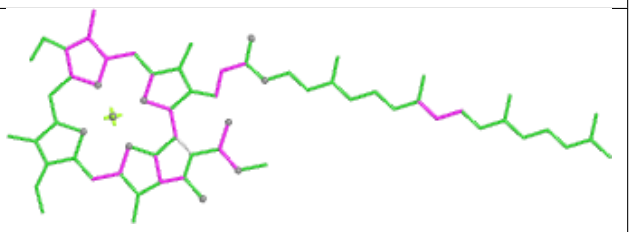


Rings

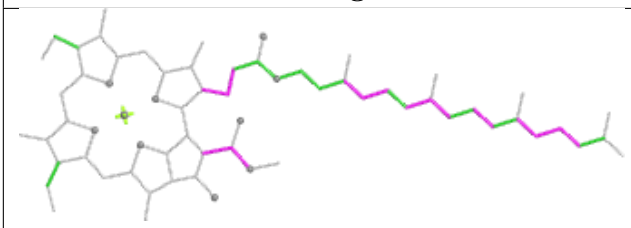
Ligand CLA aA 802



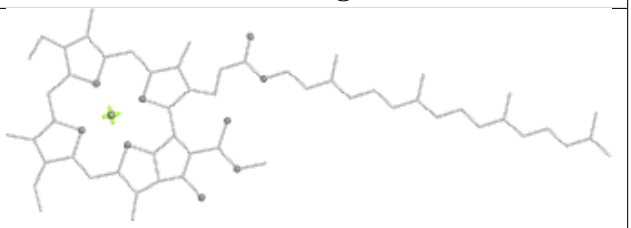
Bond lengths



Bond angles

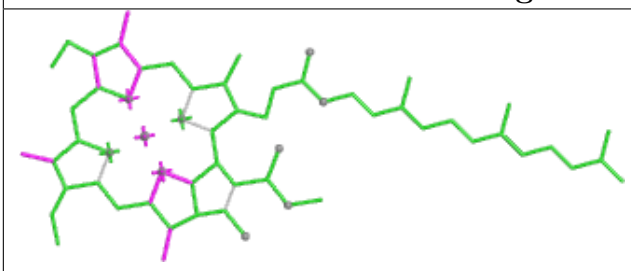


Torsions

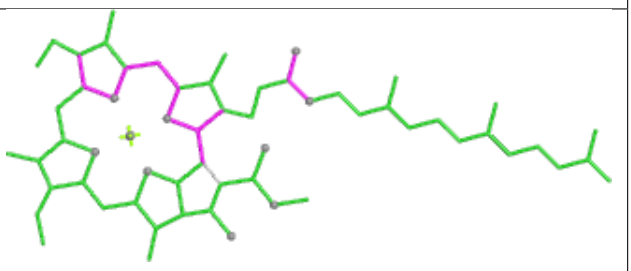


Rings

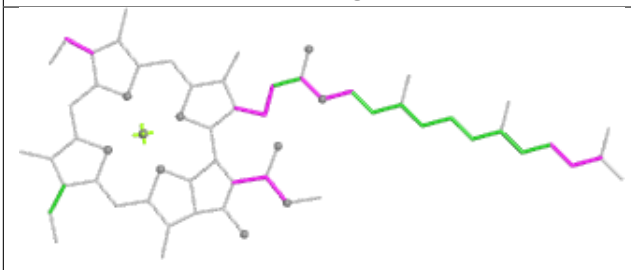
Ligand CLA cA 814



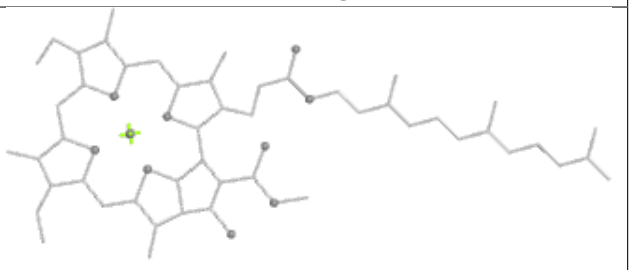
Bond lengths



Bond angles

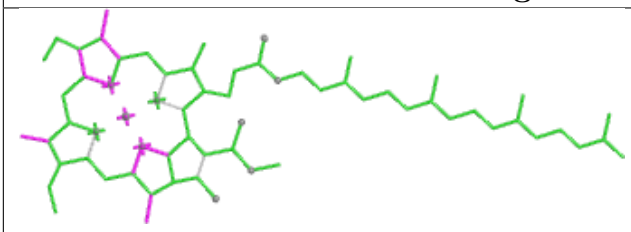


Torsions

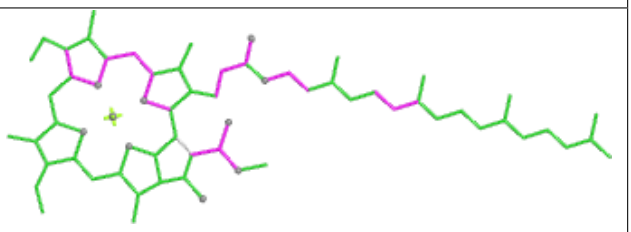


Rings

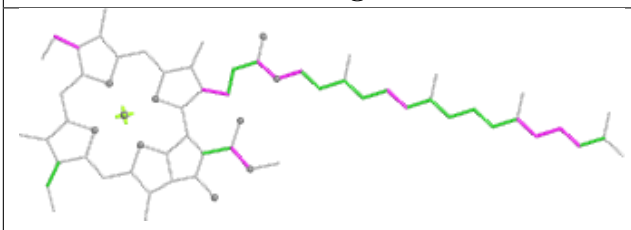
Ligand CLA bA 812



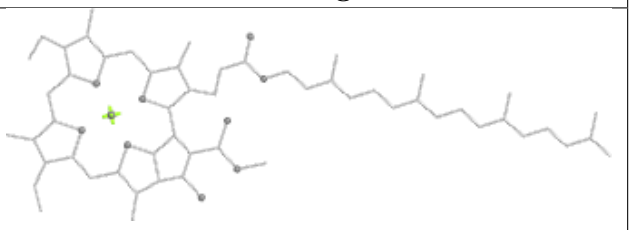
Bond lengths



Bond angles

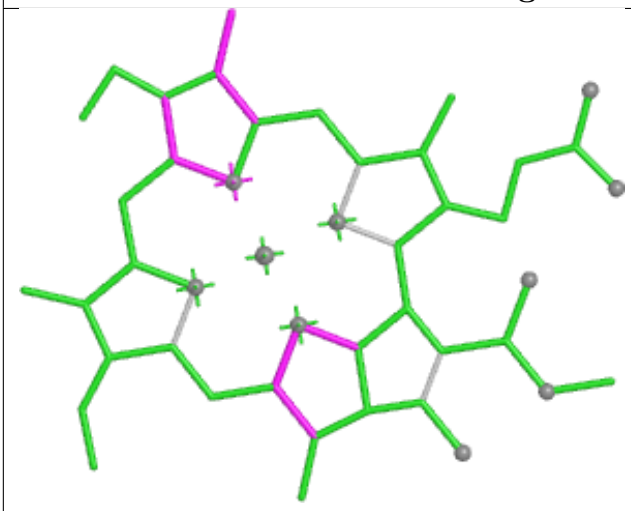


Torsions

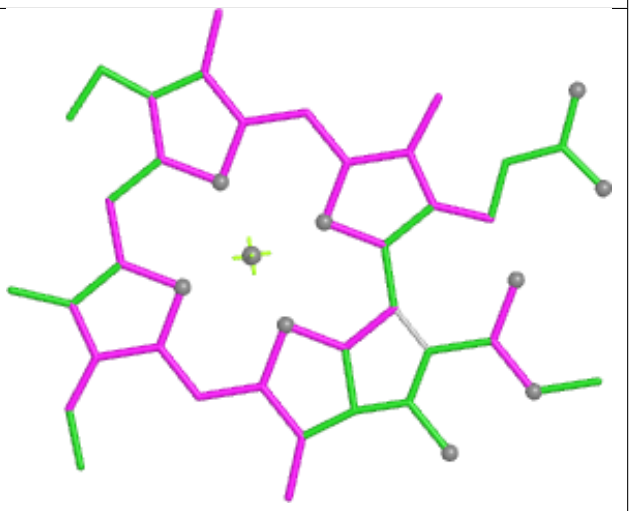


Rings

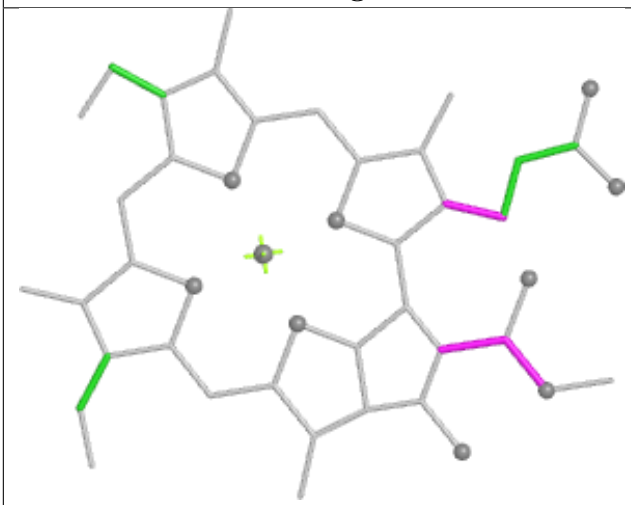
Ligand CLA b2 405



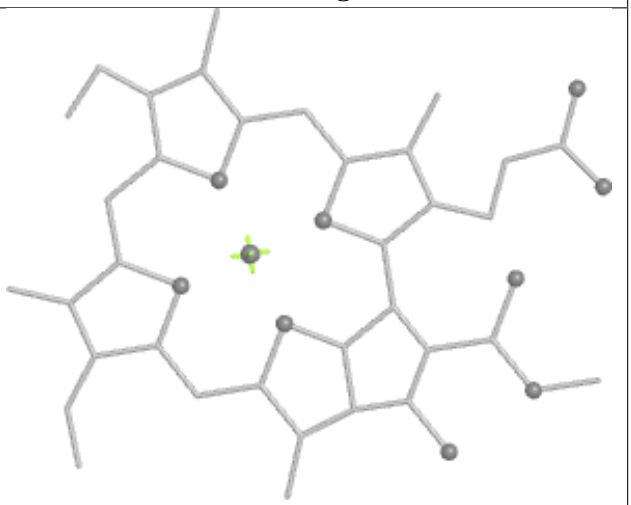
Bond lengths



Bond angles

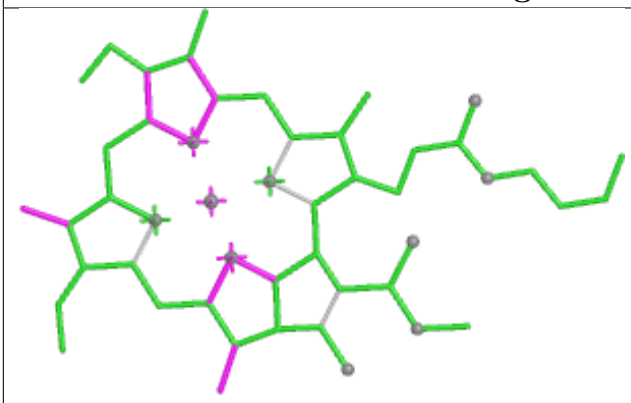


Torsions

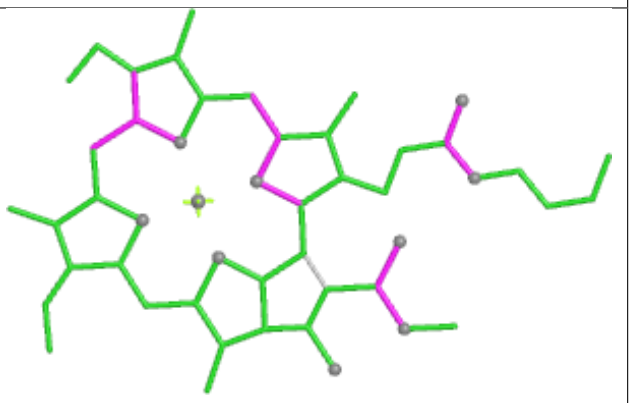


Rings

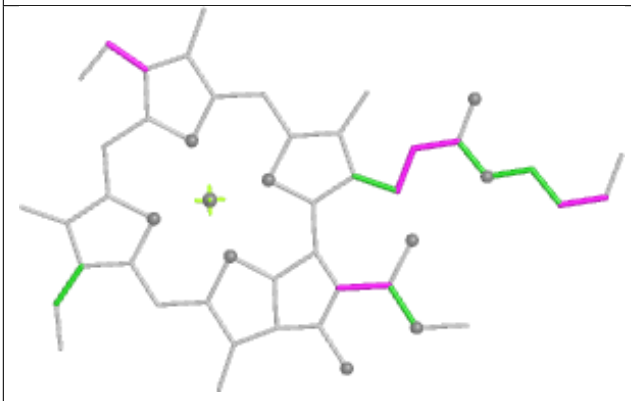
Ligand CLA bA 823



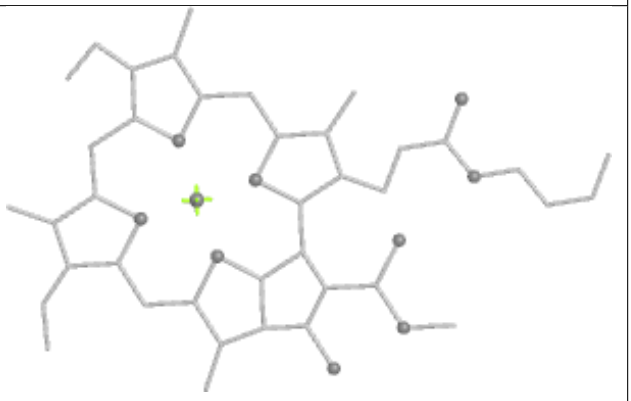
Bond lengths



Bond angles

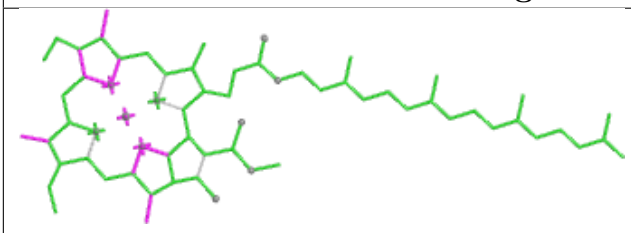


Torsions

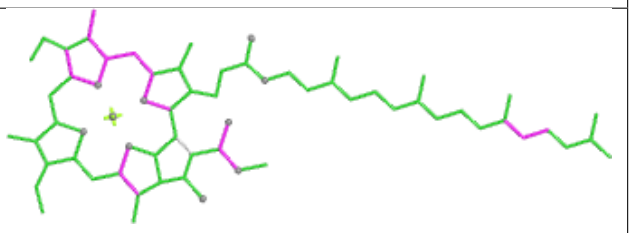


Rings

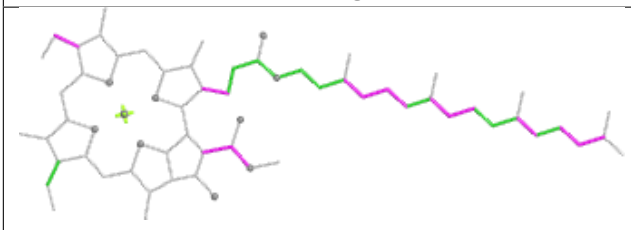
Ligand CLA aA 822



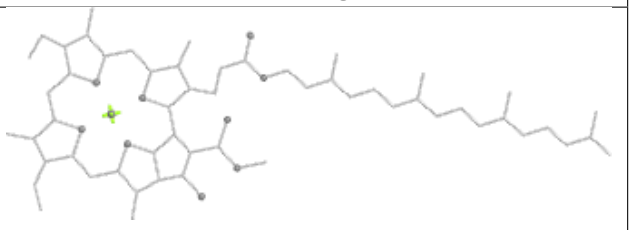
Bond lengths



Bond angles

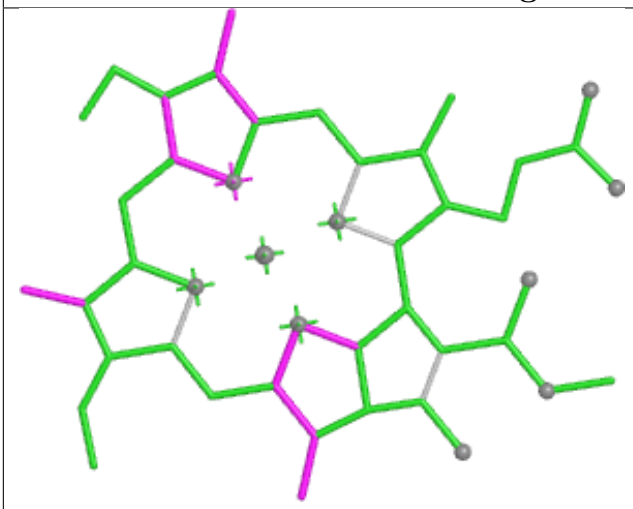


Torsions

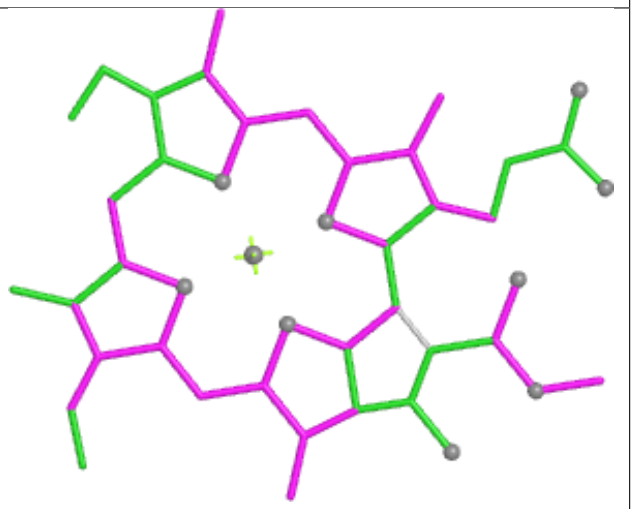


Rings

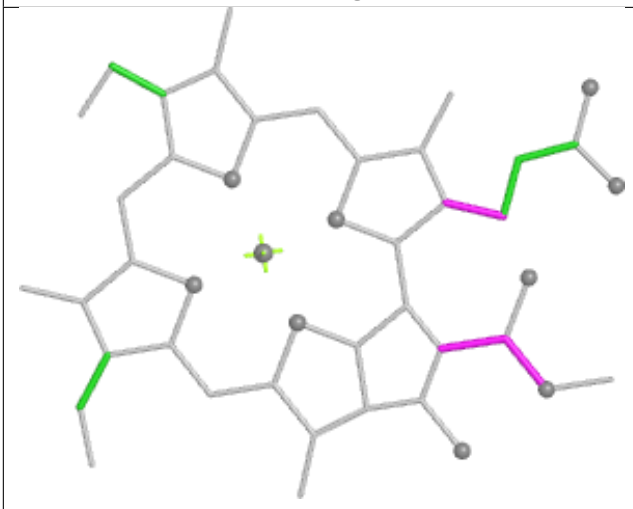
Ligand CLA a4 405



Bond lengths



Bond angles

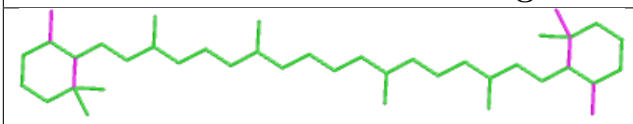


Torsions

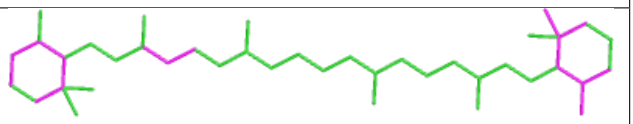


Rings

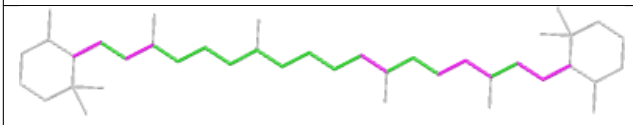
Ligand BCR b2 419



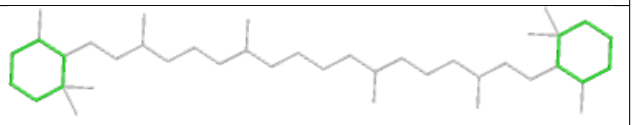
Bond lengths



Bond angles

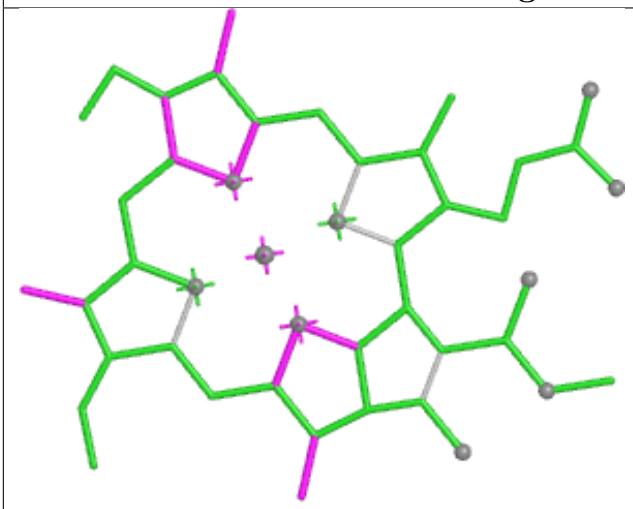


Torsions

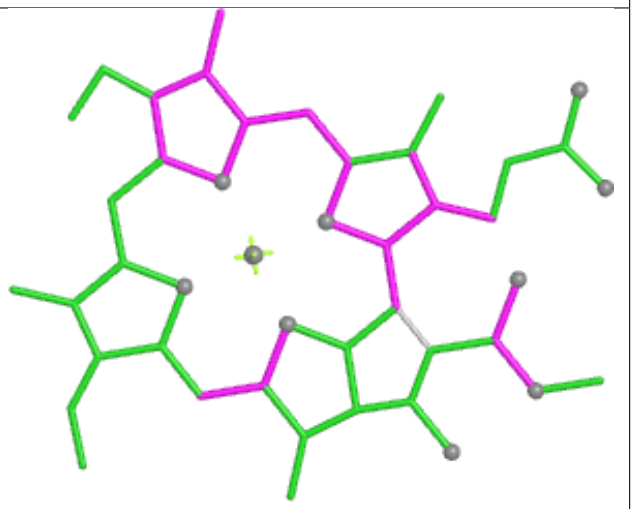


Rings

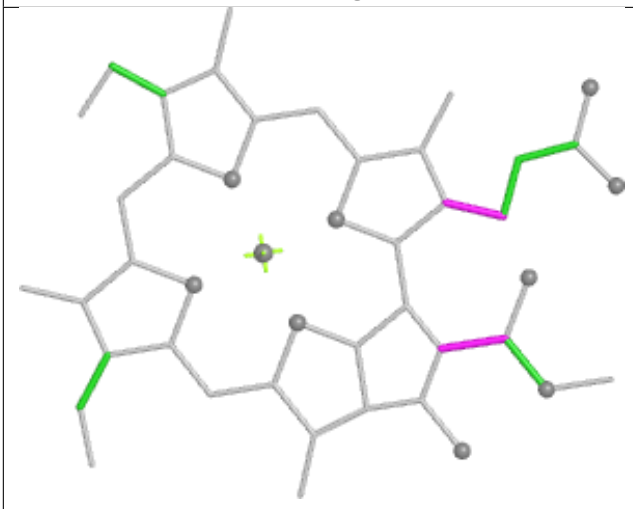
Ligand CLA b5 411



Bond lengths



Bond angles

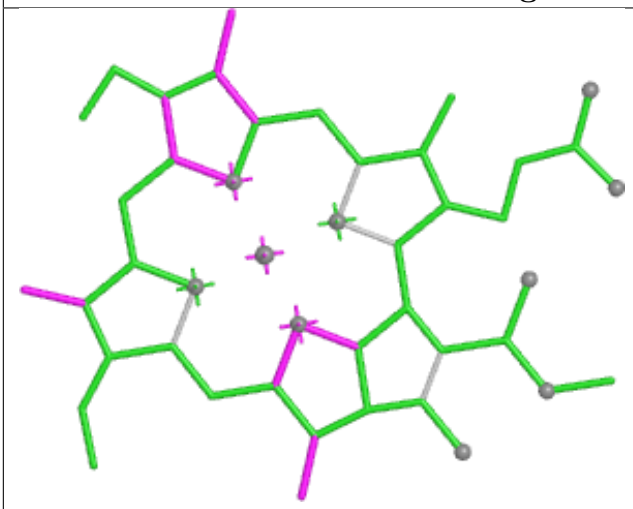


Torsions

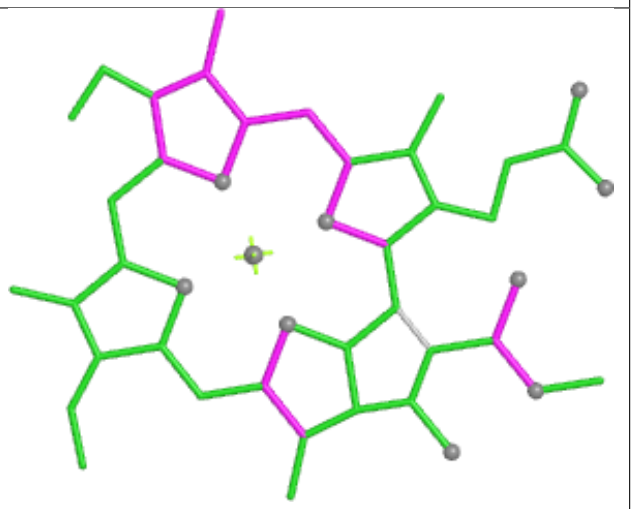


Rings

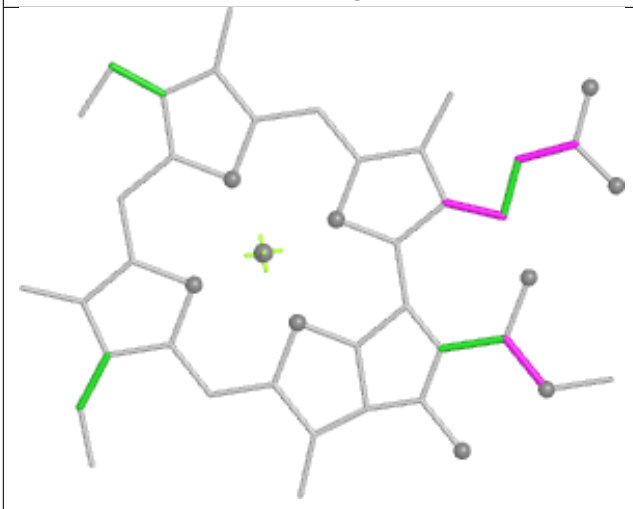
Ligand CLA a6 409



Bond lengths



Bond angles

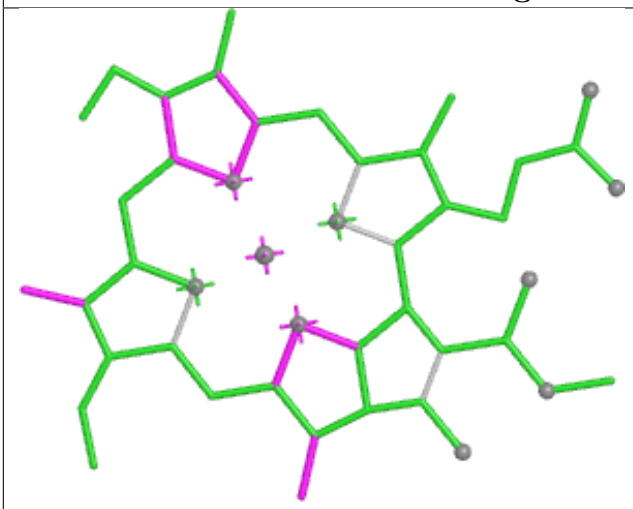


Torsions

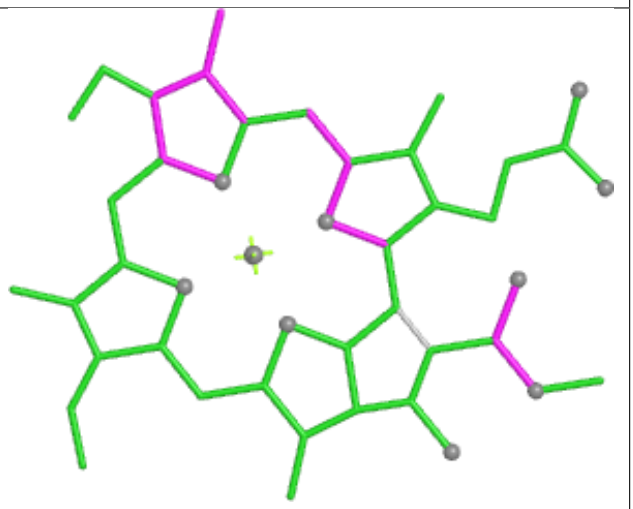


Rings

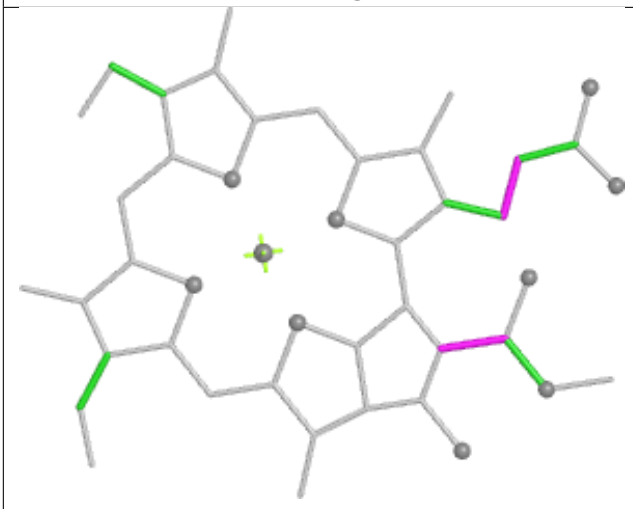
Ligand CLA bA 816



Bond lengths



Bond angles

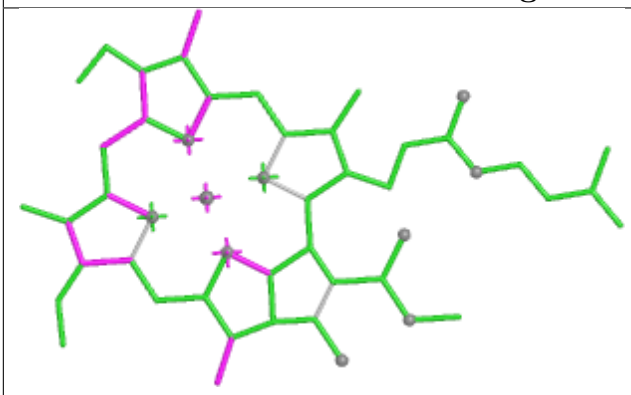


Torsions

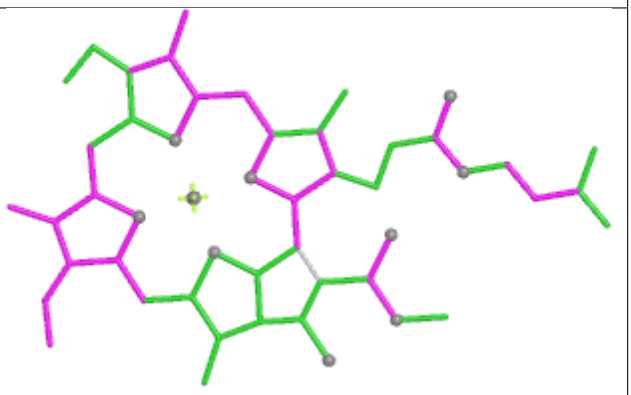


Rings

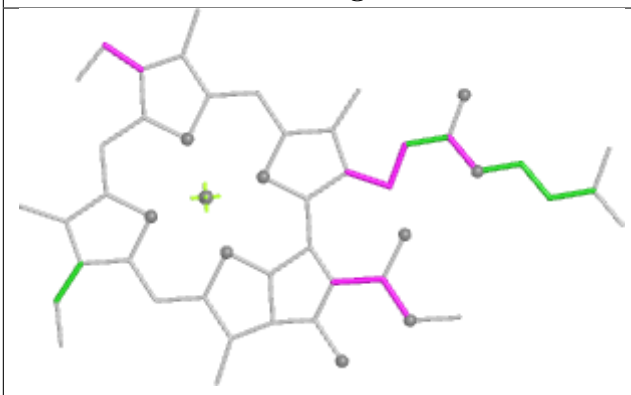
Ligand CLA a1 415



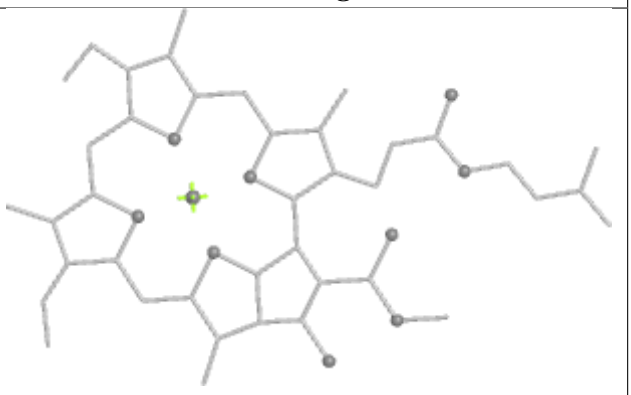
Bond lengths



Bond angles



Torsions

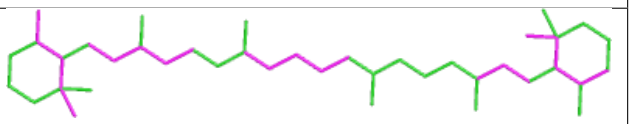


Rings

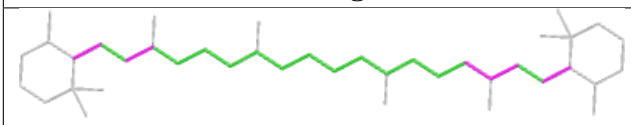
Ligand BCR bL 205



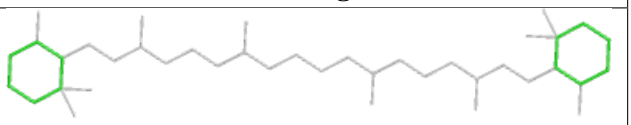
Bond lengths



Bond angles

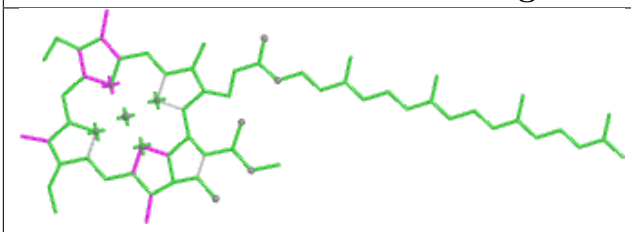


Torsions

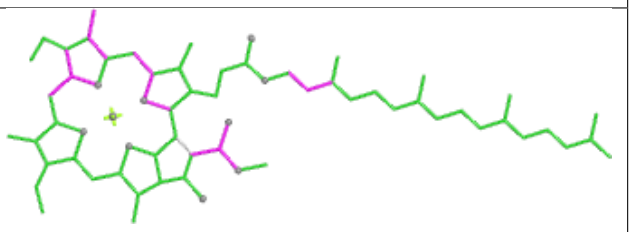


Rings

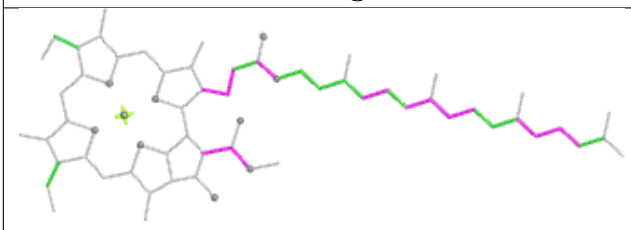
Ligand CLA b4 402



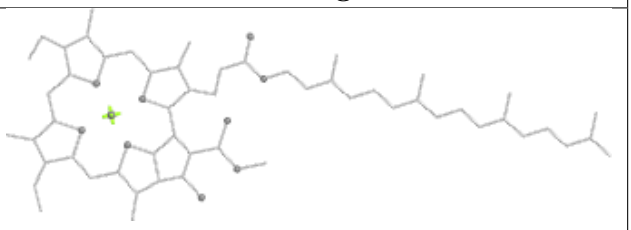
Bond lengths



Bond angles

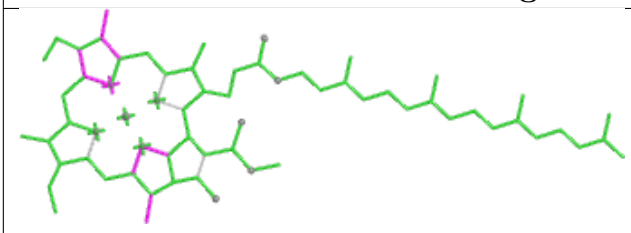


Torsions

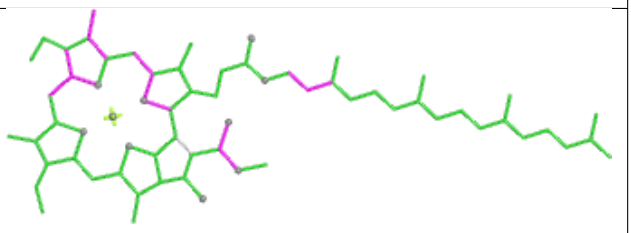


Rings

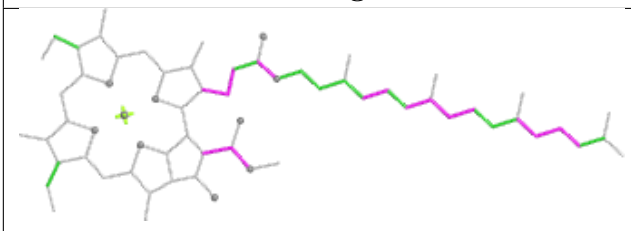
Ligand CLA a6 403



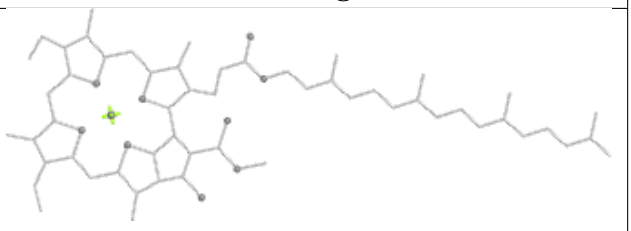
Bond lengths



Bond angles

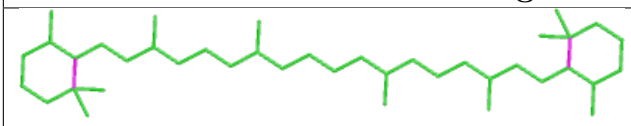


Torsions

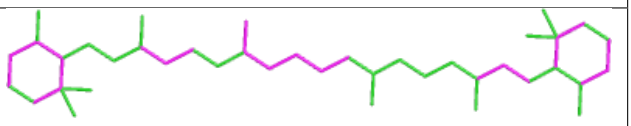


Rings

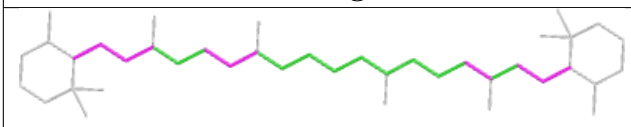
Ligand BCR b5 419



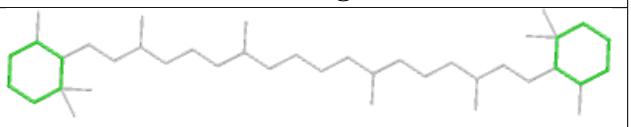
Bond lengths



Bond angles

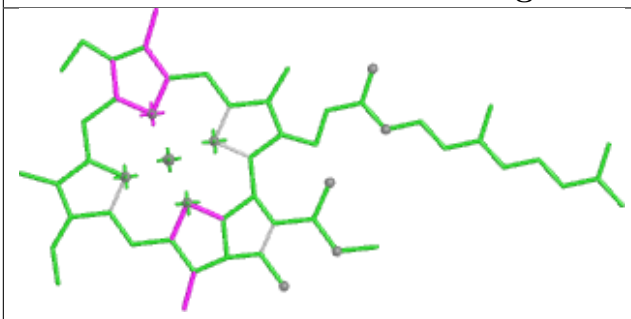


Torsions

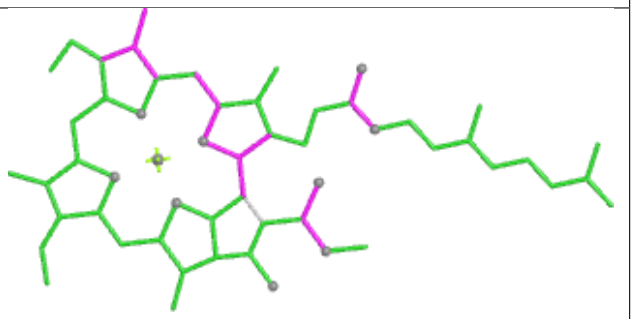


Rings

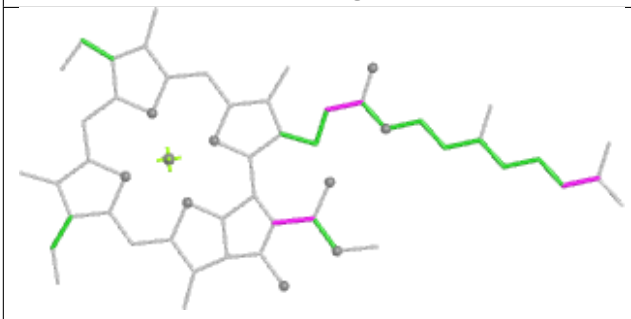
Ligand CLA aB 823



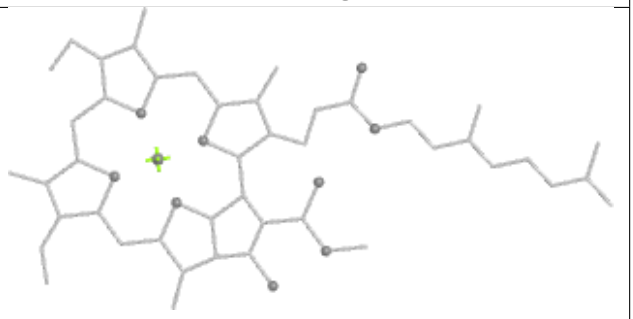
Bond lengths



Bond angles

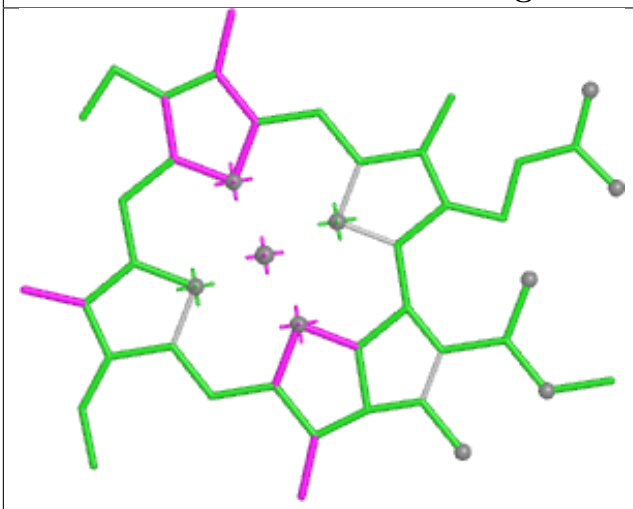


Torsions

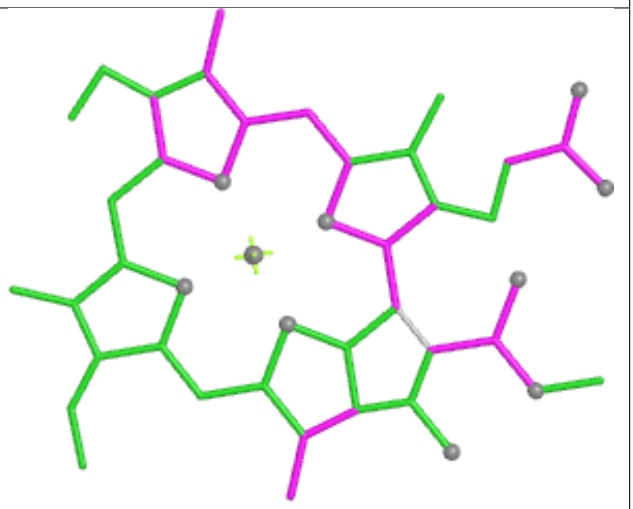


Rings

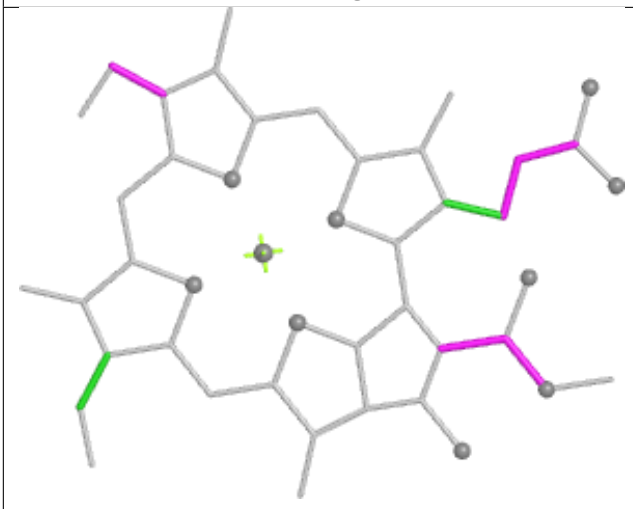
Ligand CLA aX 102



Bond lengths



Bond angles

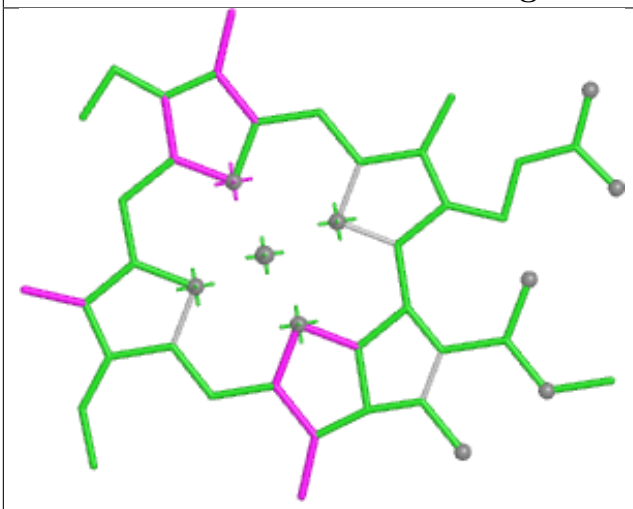


Torsions

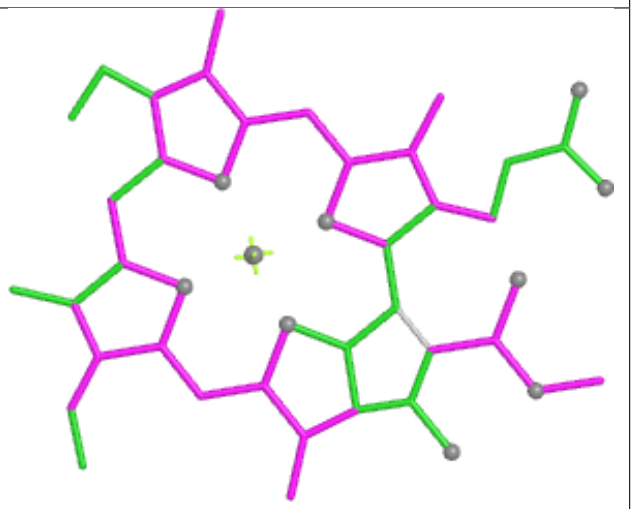


Rings

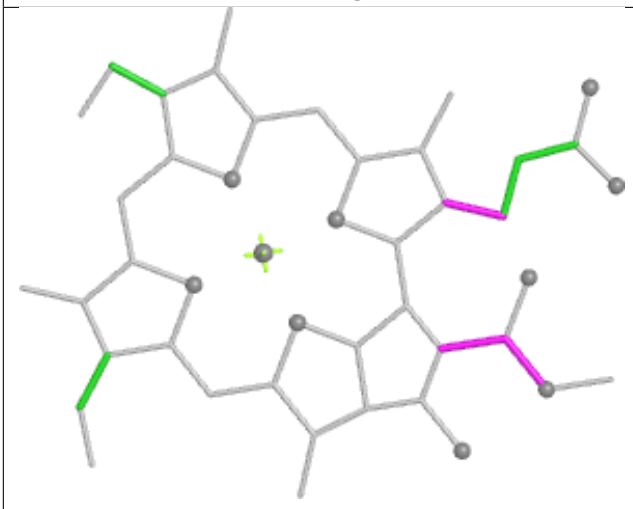
Ligand CLA a5 405



Bond lengths



Bond angles

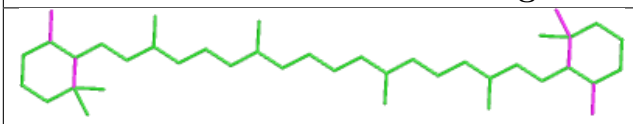


Torsions

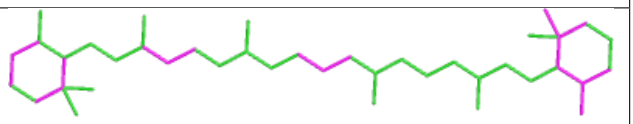


Rings

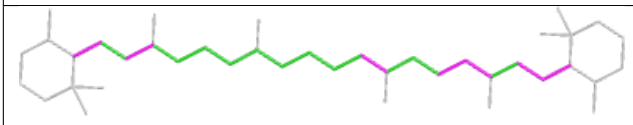
Ligand BCR c2 419



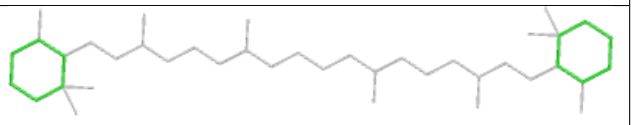
Bond lengths



Bond angles

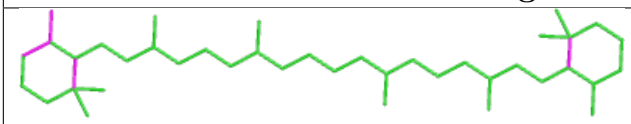


Torsions

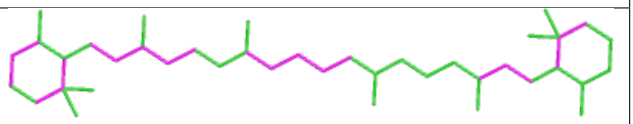


Rings

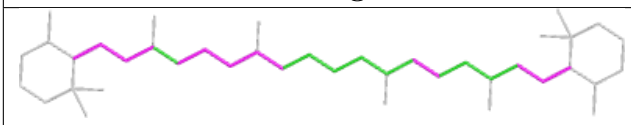
Ligand BCR c3 401



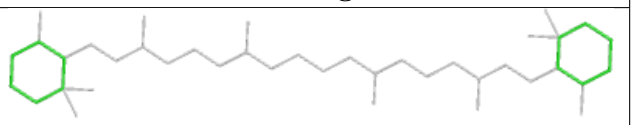
Bond lengths



Bond angles

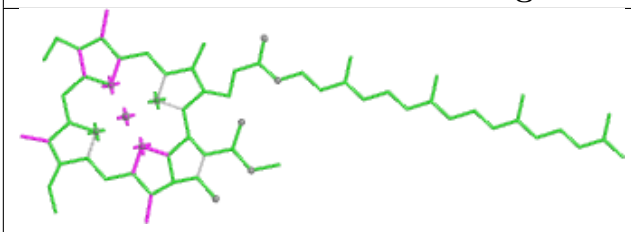


Torsions

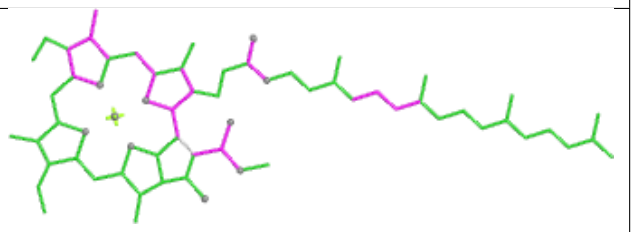


Rings

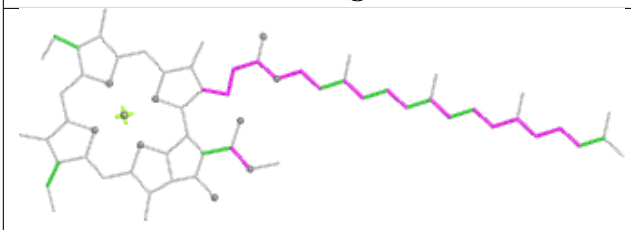
Ligand CLA cA 829



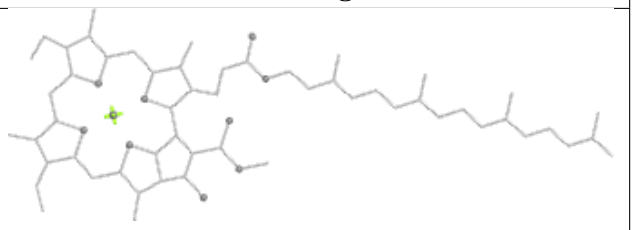
Bond lengths



Bond angles

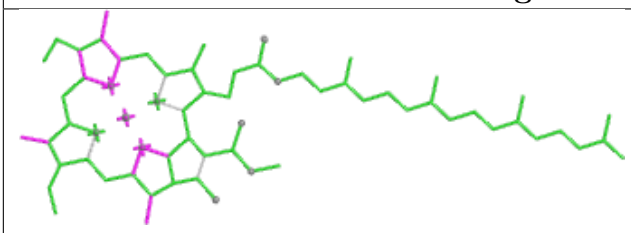


Torsions

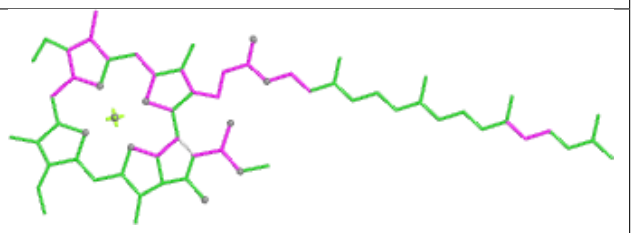


Rings

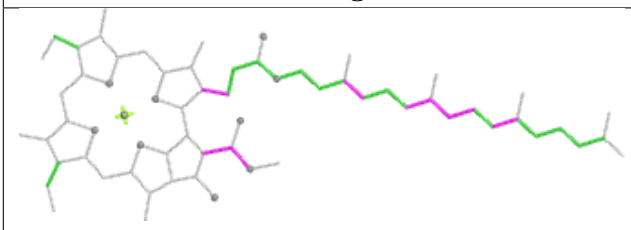
Ligand CLA bB 827



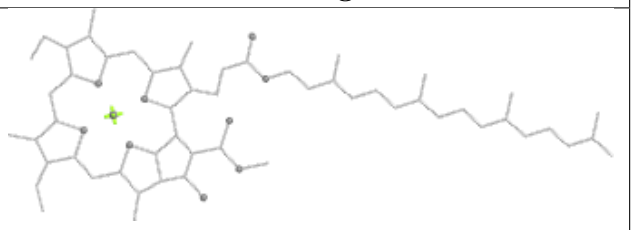
Bond lengths



Bond angles

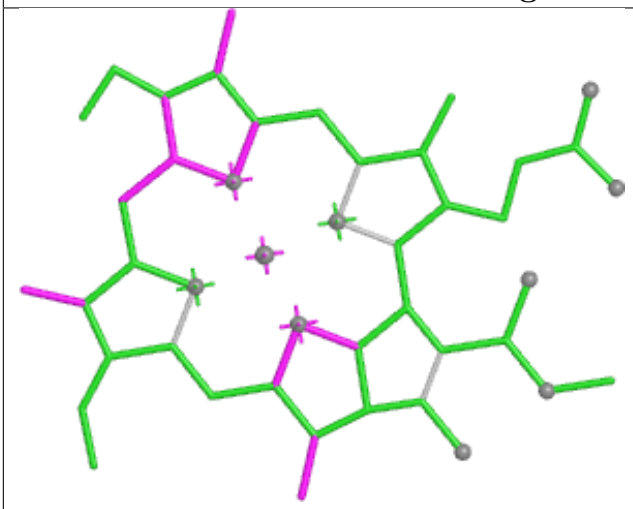


Torsions

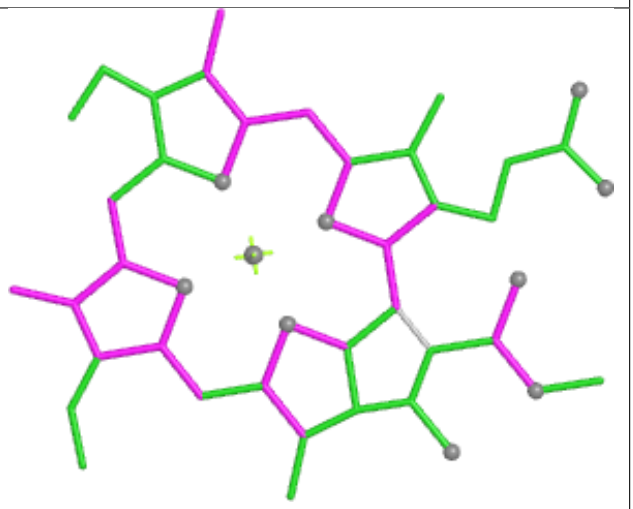


Rings

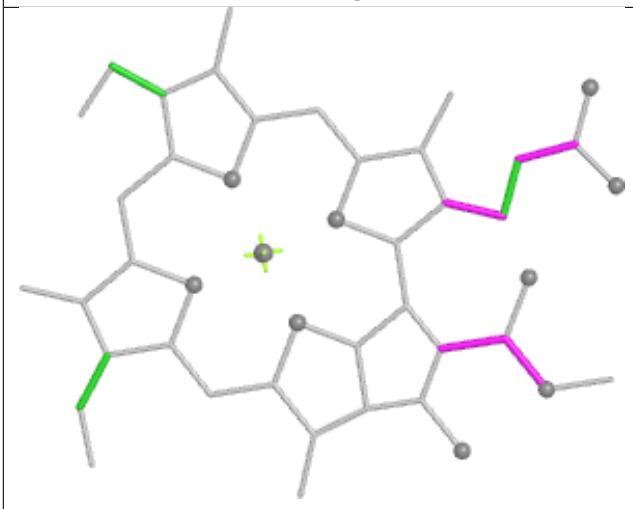
Ligand CLA a1 411



Bond lengths



Bond angles

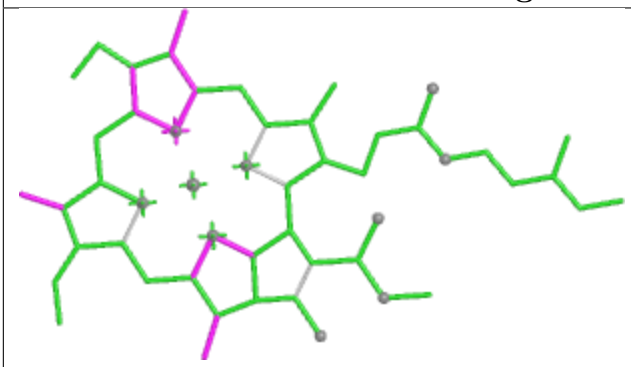


Torsions

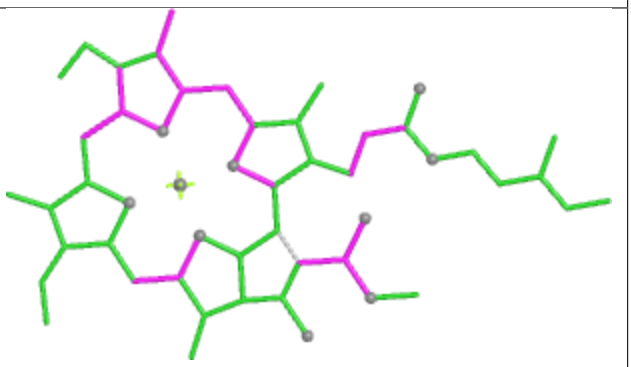


Rings

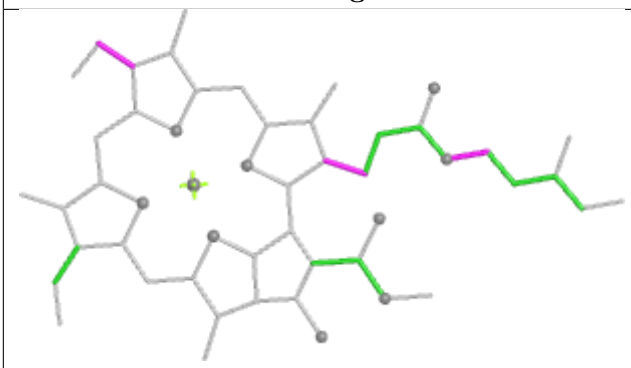
Ligand CLA cA 808



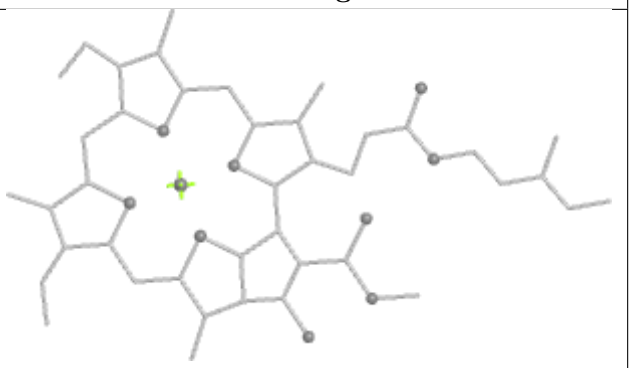
Bond lengths



Bond angles

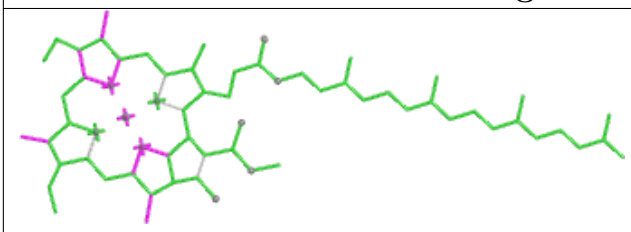


Torsions

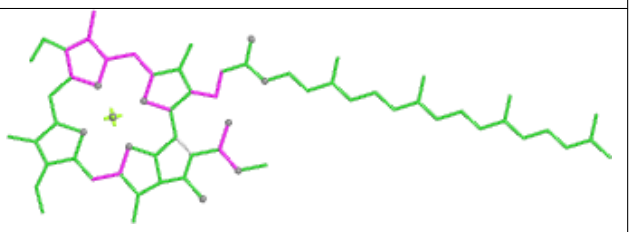


Rings

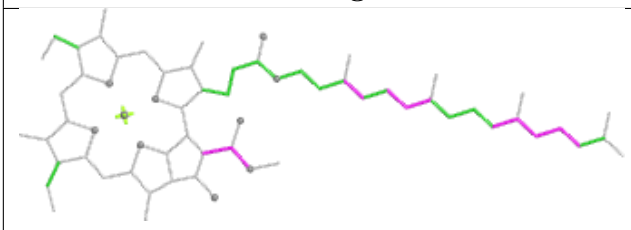
Ligand CLA cB 837



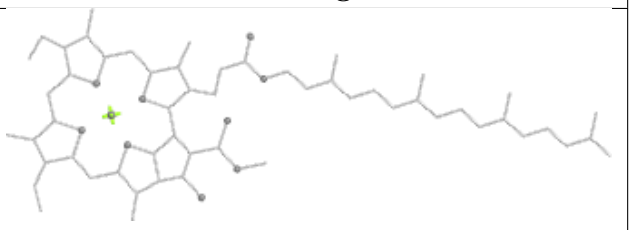
Bond lengths



Bond angles

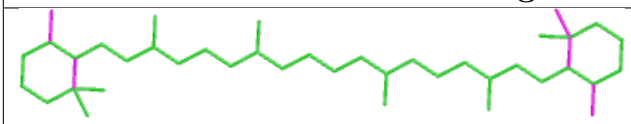


Torsions

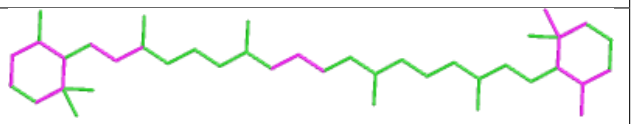


Rings

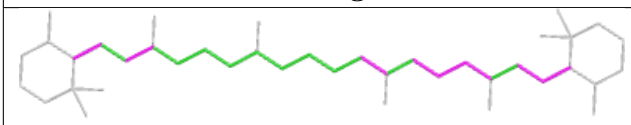
Ligand BCR a3 418



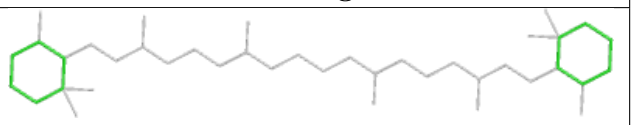
Bond lengths



Bond angles

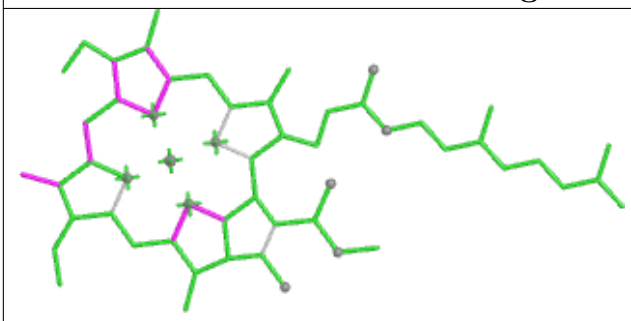


Torsions

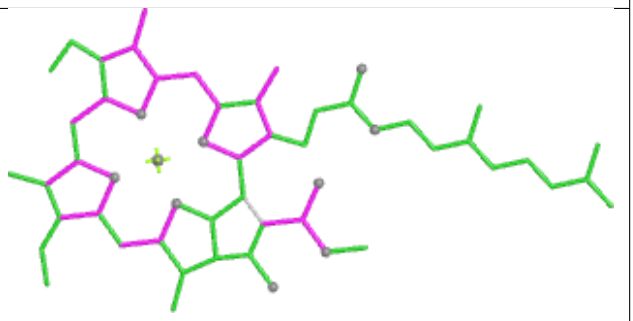


Rings

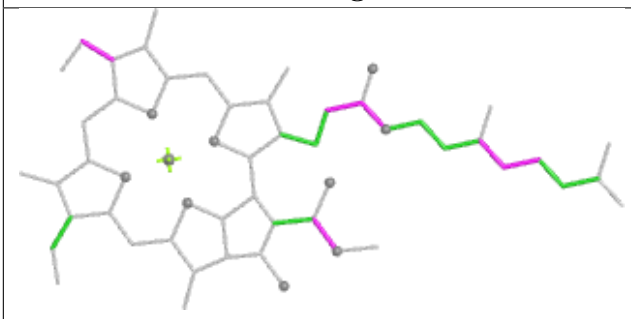
Ligand CLA c5 417



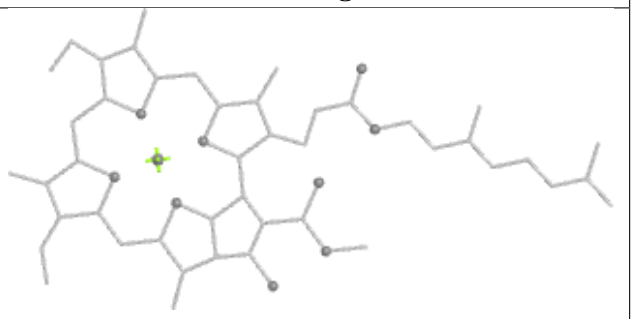
Bond lengths



Bond angles

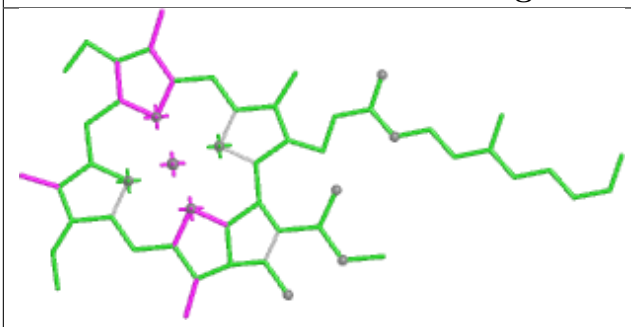


Torsions

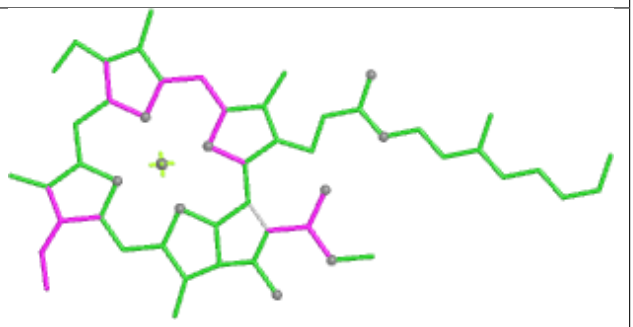


Rings

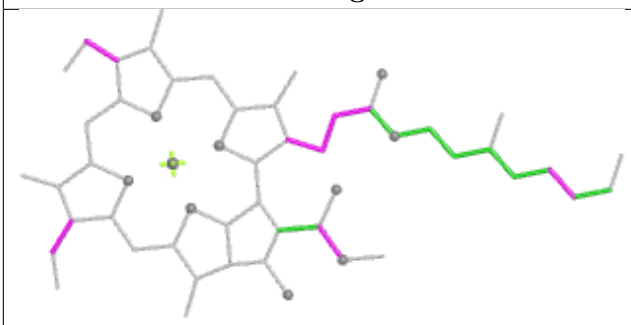
Ligand CLA aA 819



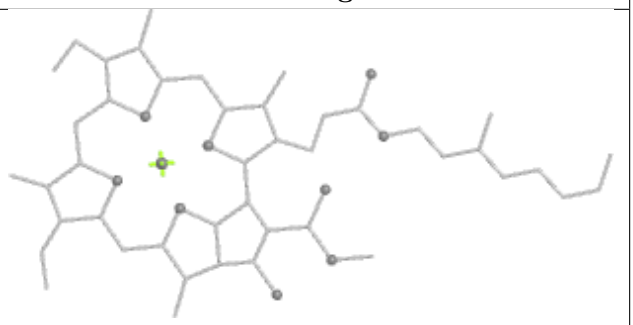
Bond lengths



Bond angles

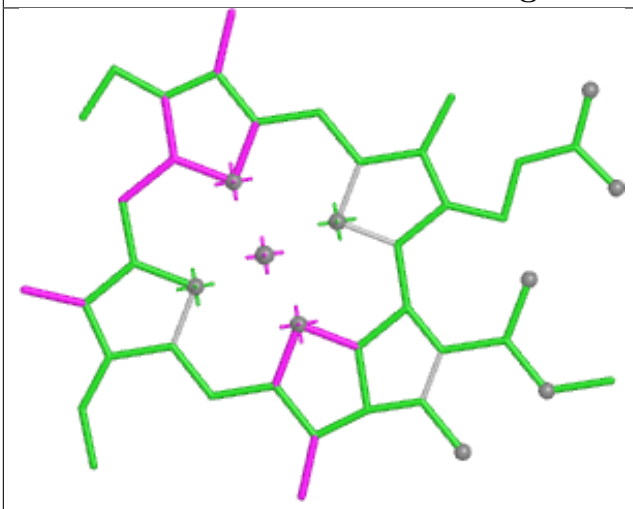


Torsions

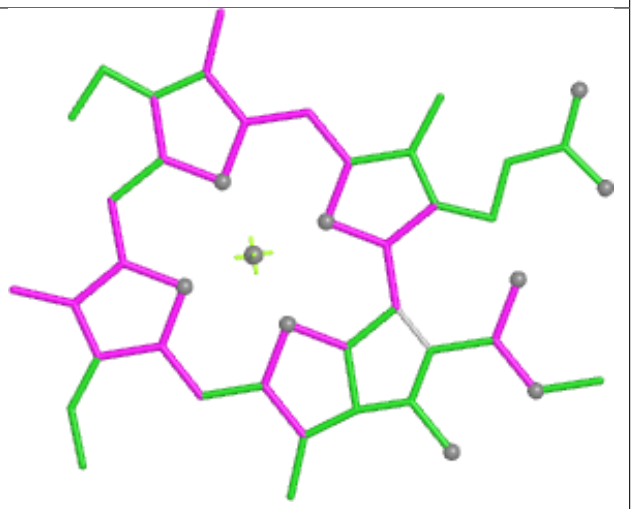


Rings

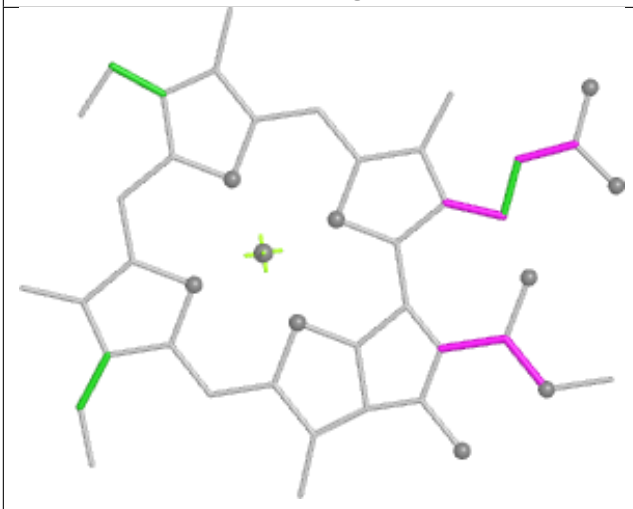
Ligand CLA a2 413



Bond lengths



Bond angles

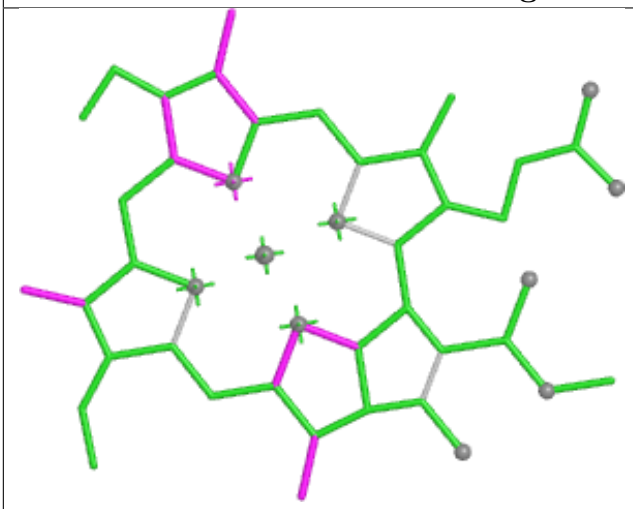


Torsions

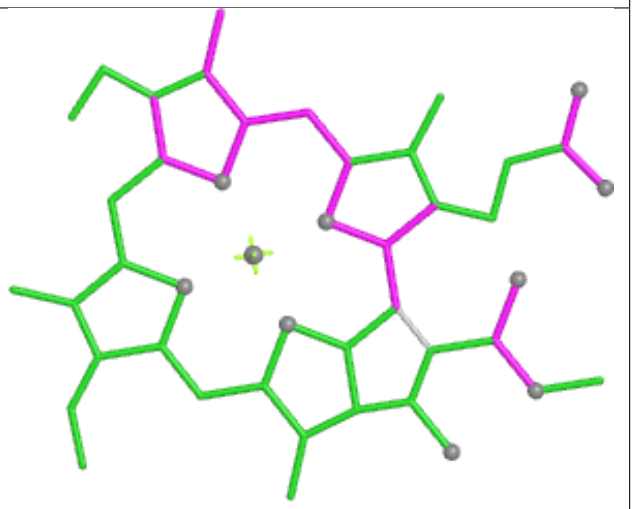


Rings

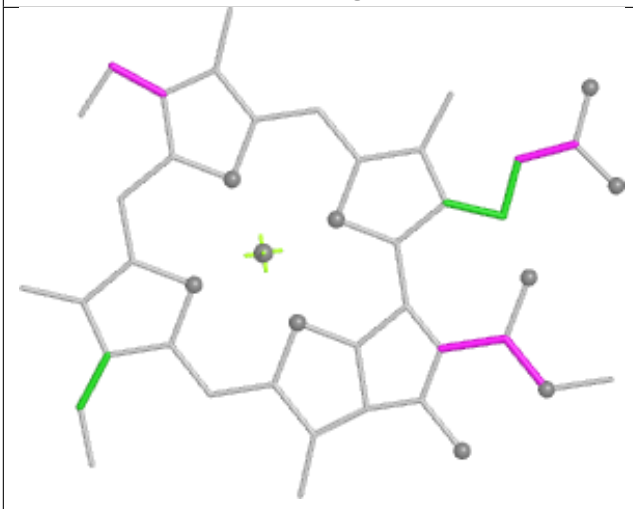
Ligand CLA a1 406



Bond lengths



Bond angles

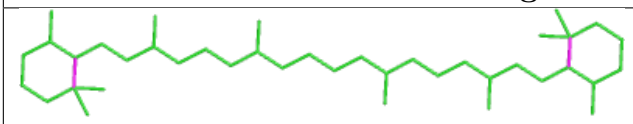


Torsions

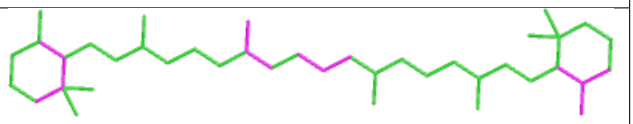


Rings

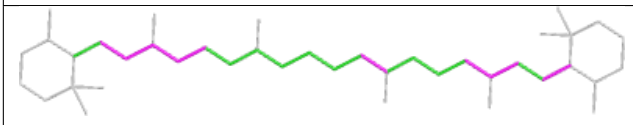
Ligand BCR aI 101



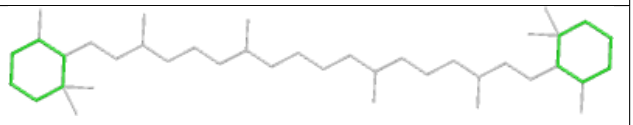
Bond lengths



Bond angles

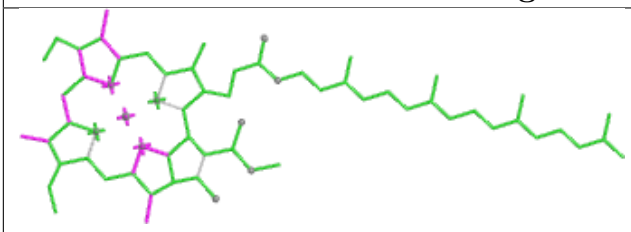


Torsions

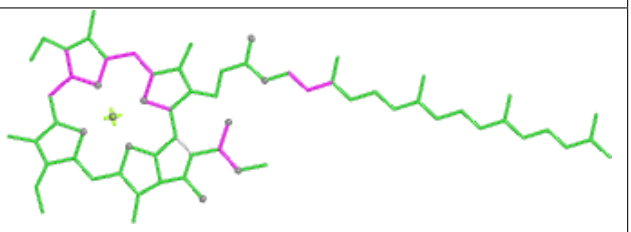


Rings

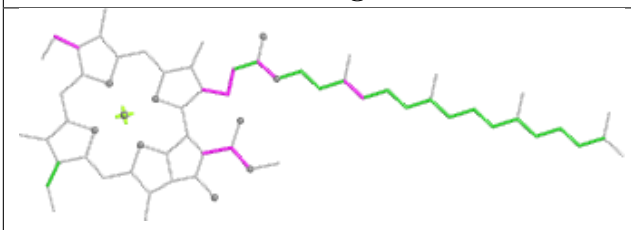
Ligand CLA b4 404



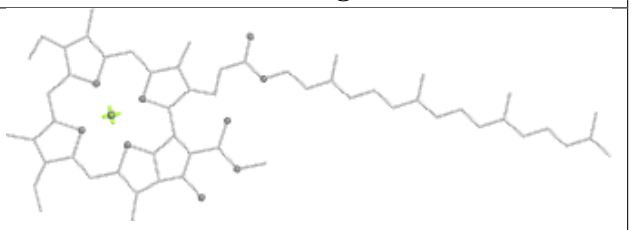
Bond lengths



Bond angles

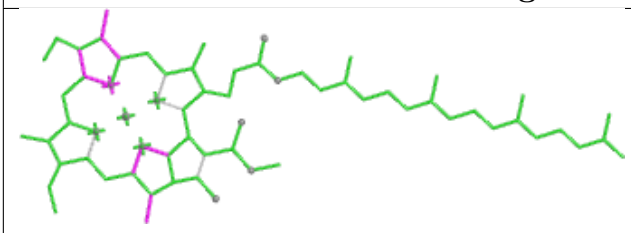


Torsions

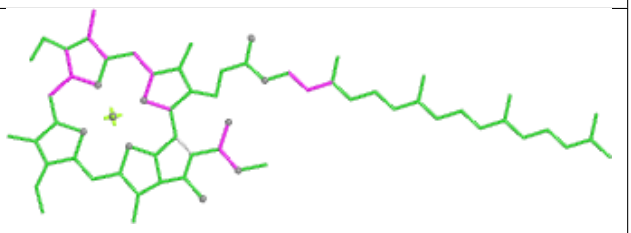


Rings

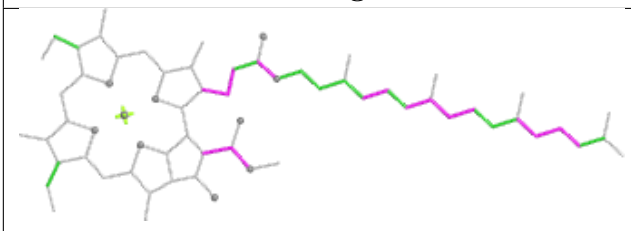
Ligand CLA b3 402



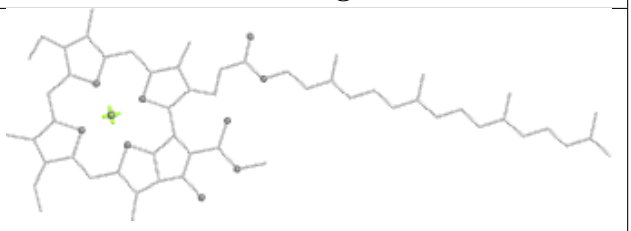
Bond lengths



Bond angles

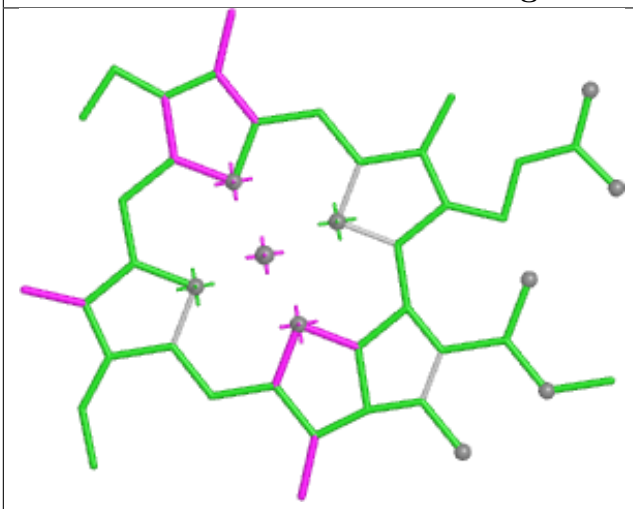


Torsions

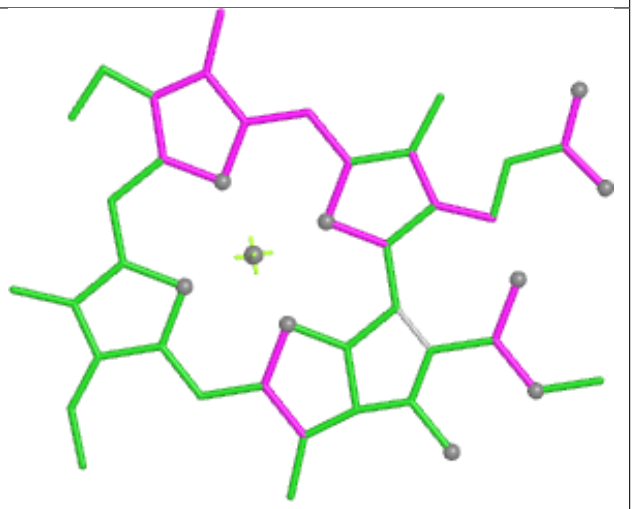


Rings

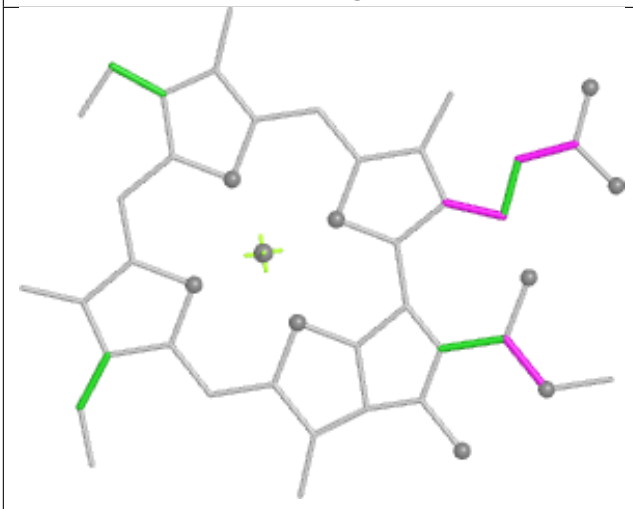
Ligand CLA c3 408



Bond lengths



Bond angles

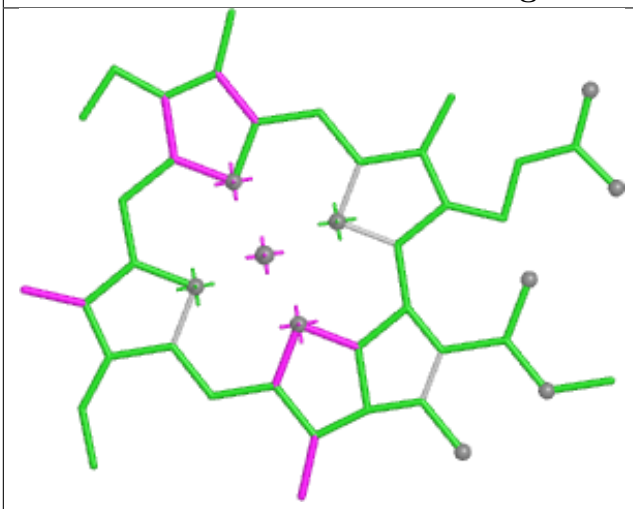


Torsions

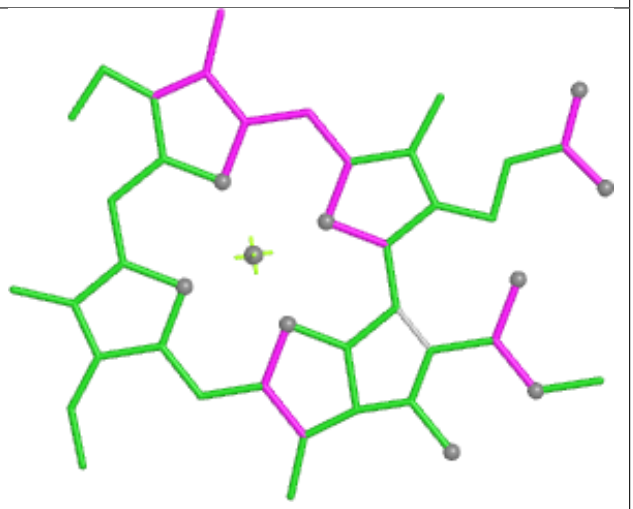


Rings

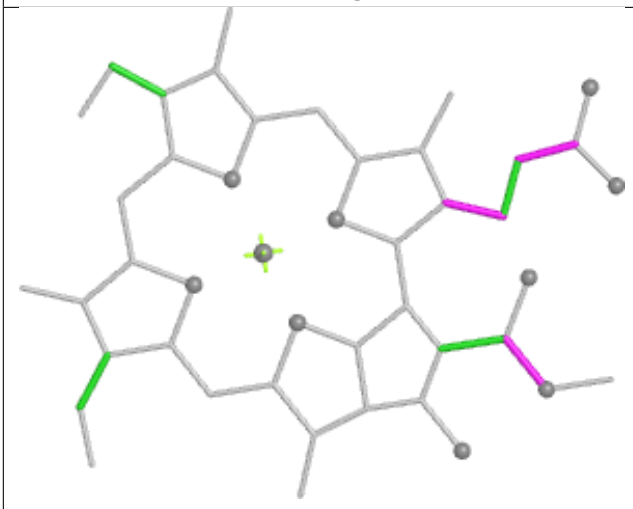
Ligand CLA a2 409



Bond lengths



Bond angles

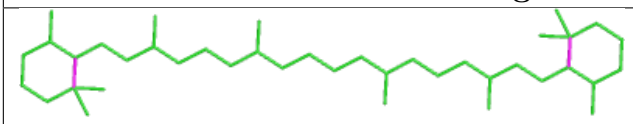


Torsions

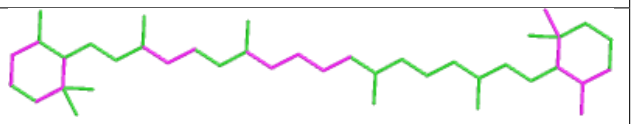


Rings

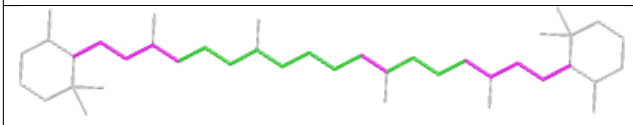
Ligand BCR aA 849



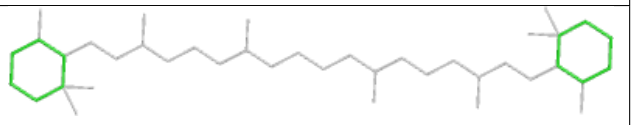
Bond lengths



Bond angles

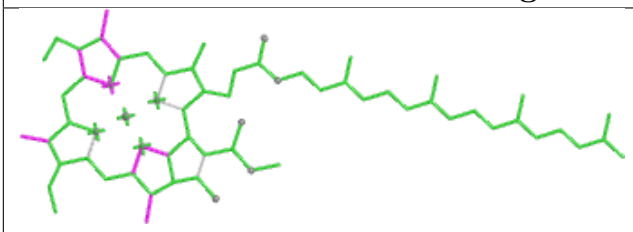


Torsions

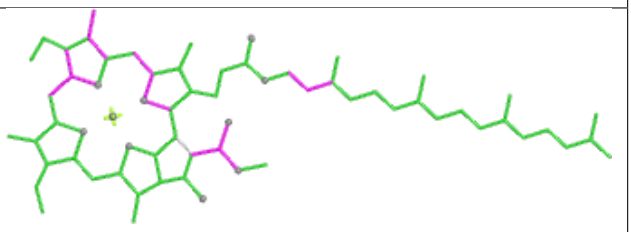


Rings

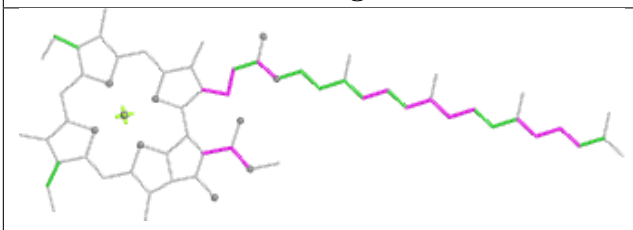
Ligand CLA a4 402



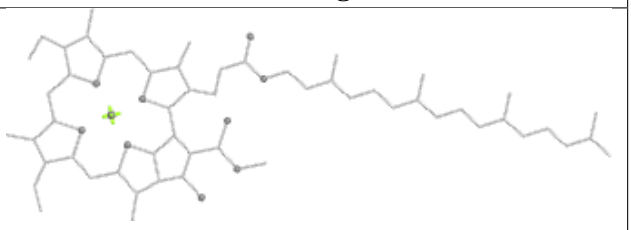
Bond lengths



Bond angles

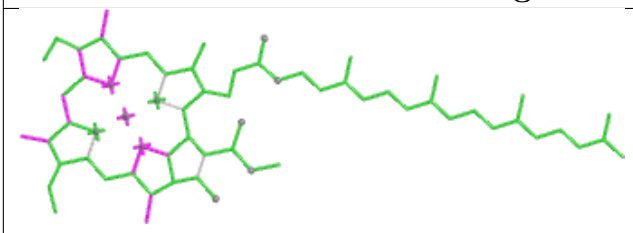


Torsions

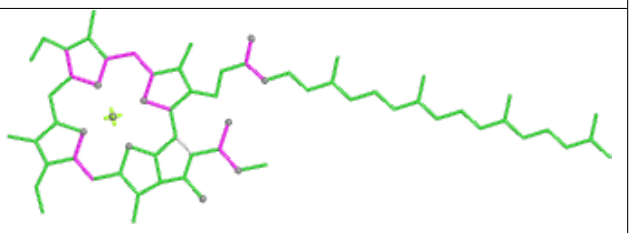


Rings

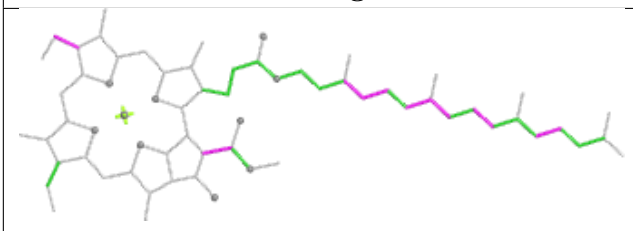
Ligand CLA bA 828



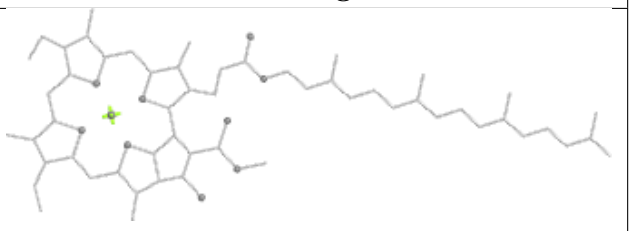
Bond lengths



Bond angles

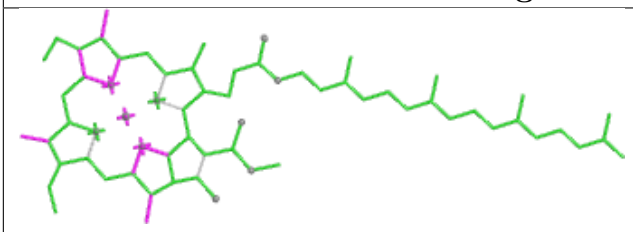


Torsions

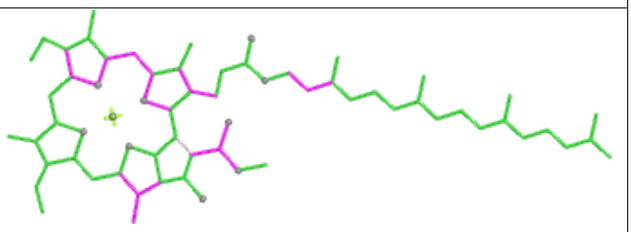


Rings

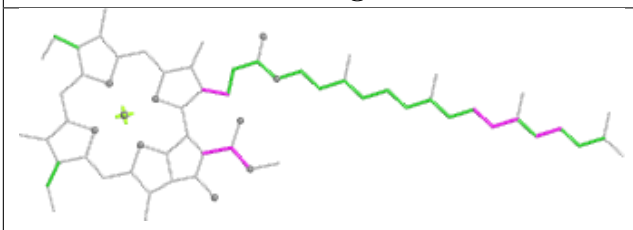
Ligand CLA cA 804



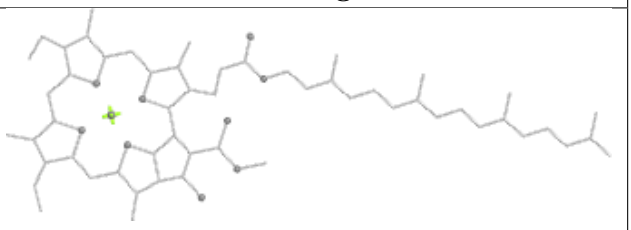
Bond lengths



Bond angles

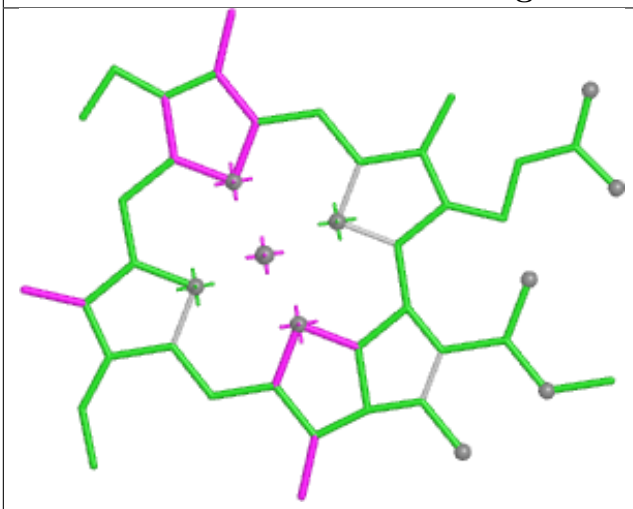


Torsions

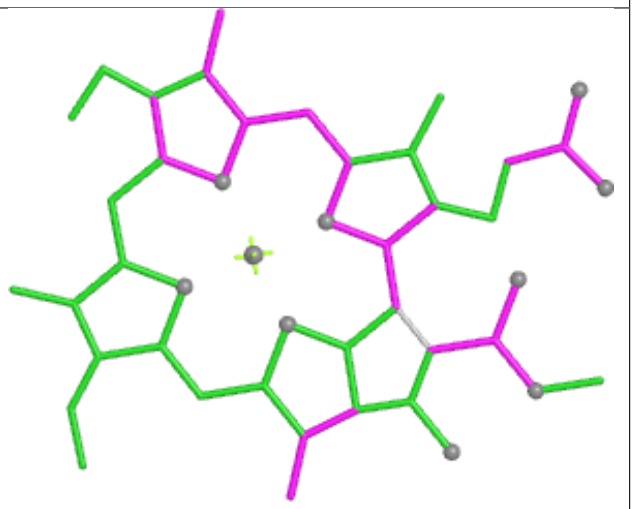


Rings

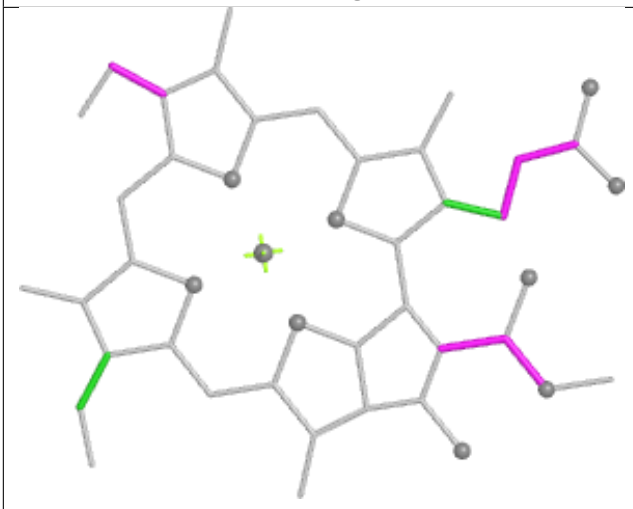
Ligand CLA cX 102



Bond lengths



Bond angles

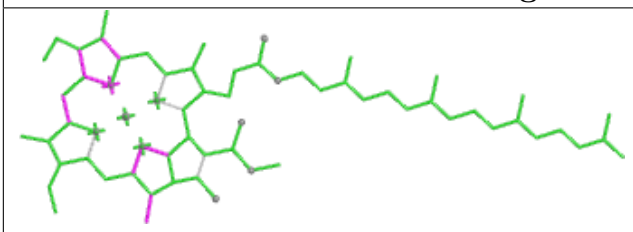


Torsions

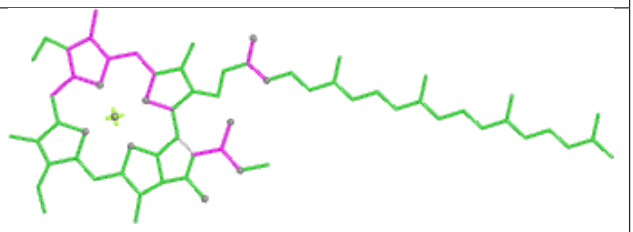


Rings

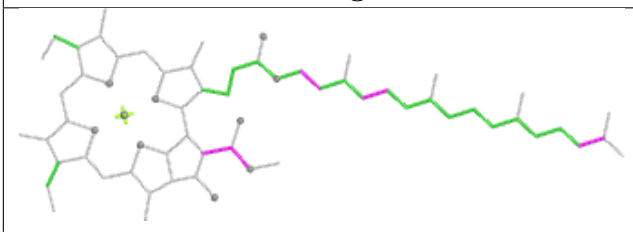
Ligand CLA a2 410



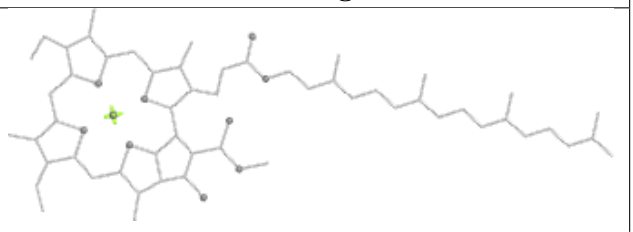
Bond lengths



Bond angles

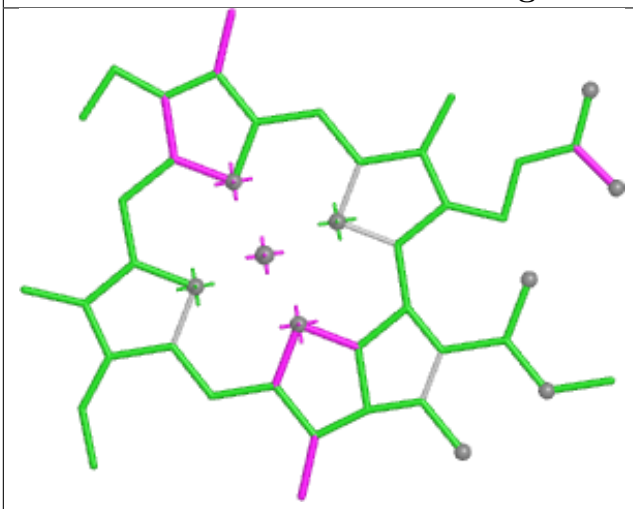


Torsions

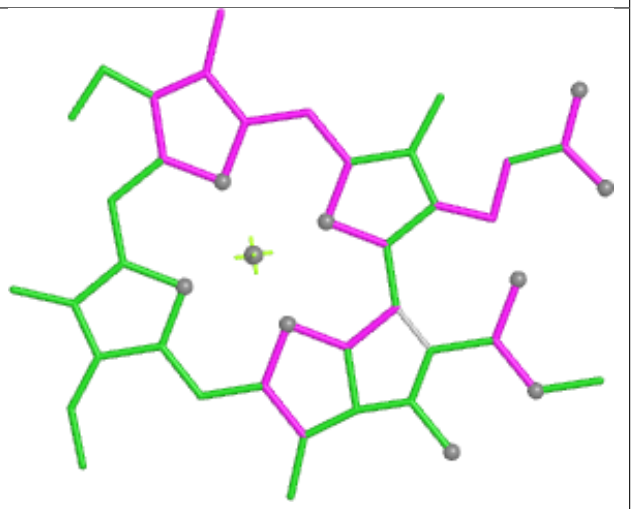


Rings

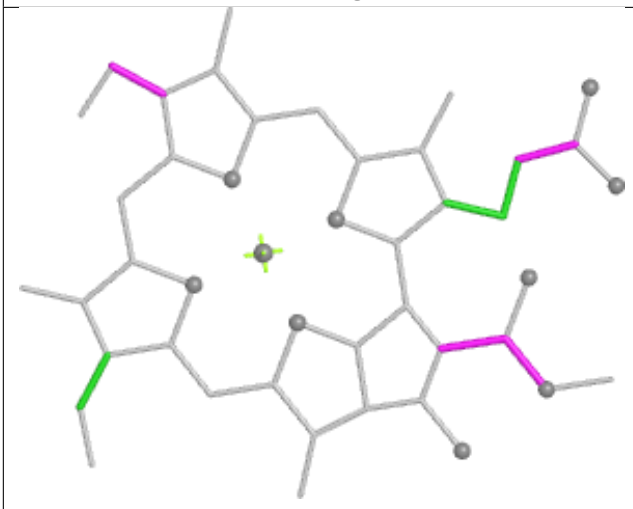
Ligand CLA b3 415



Bond lengths



Bond angles

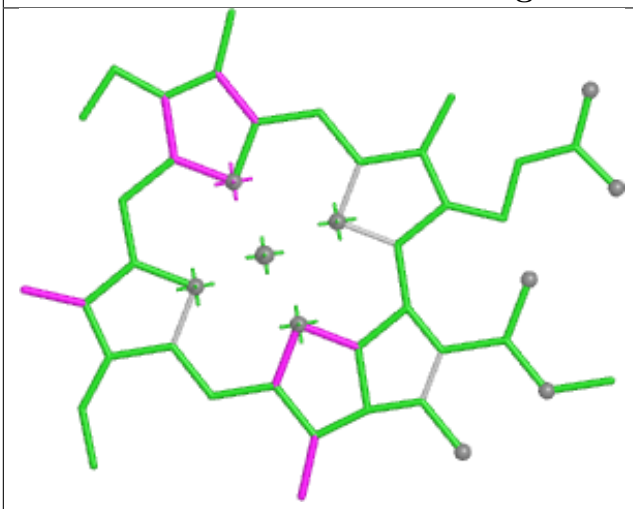


Torsions

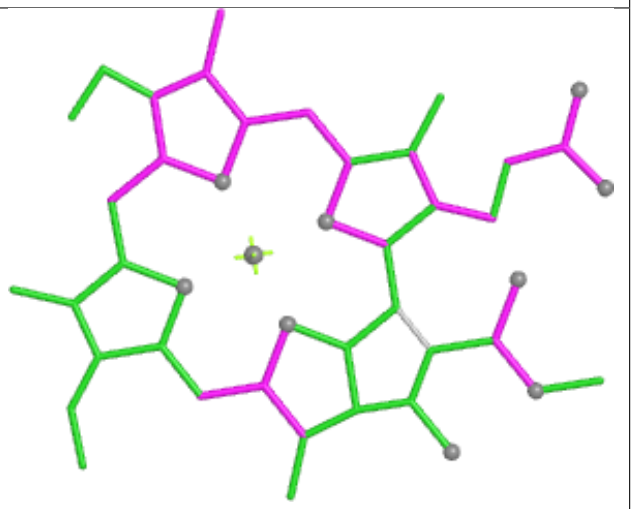


Rings

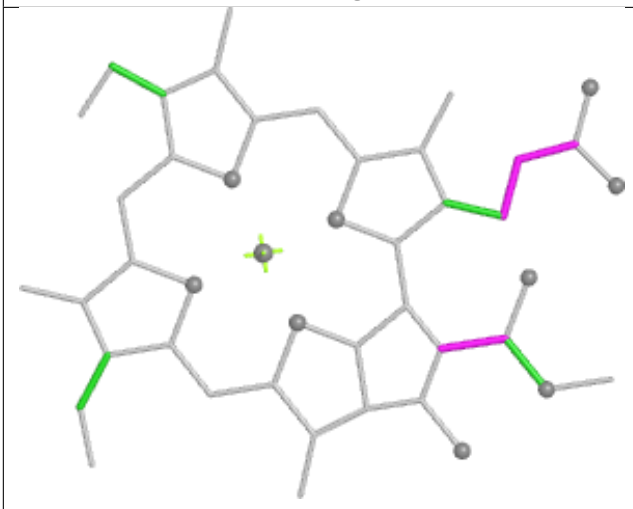
Ligand CLA aB 824



Bond lengths



Bond angles

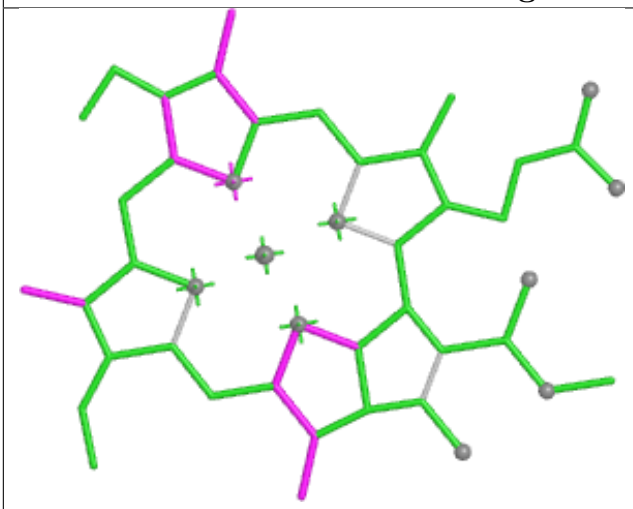


Torsions

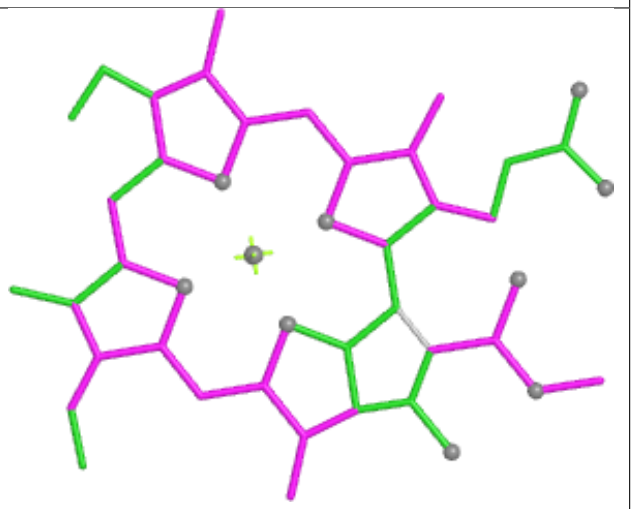


Rings

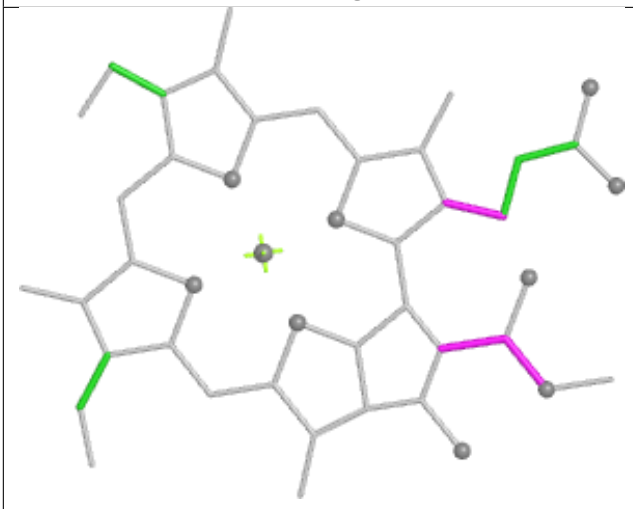
Ligand CLA b5 405



Bond lengths



Bond angles

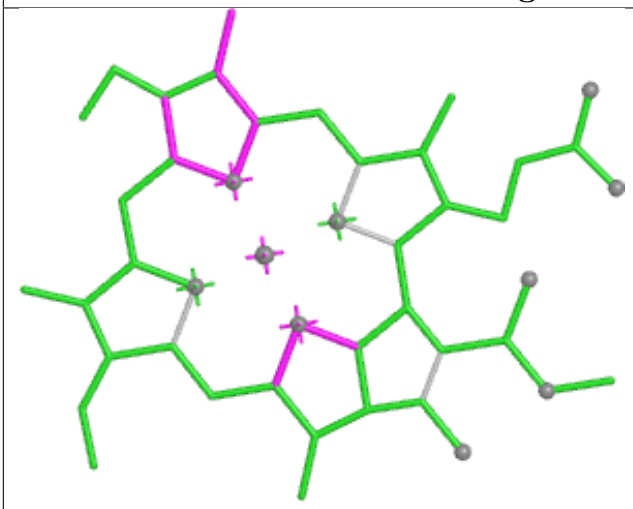


Torsions

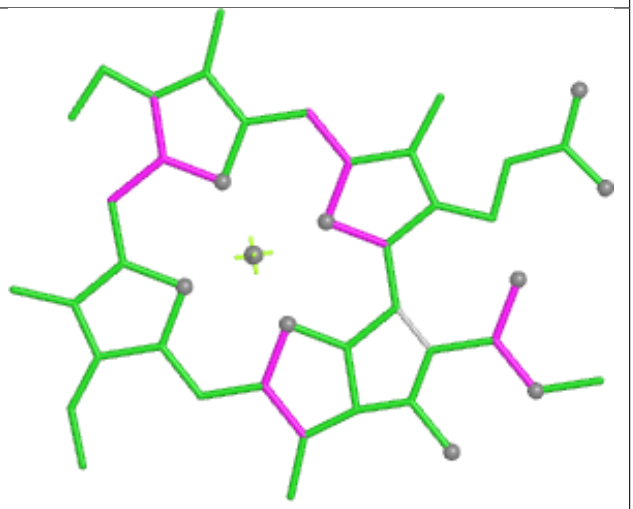


Rings

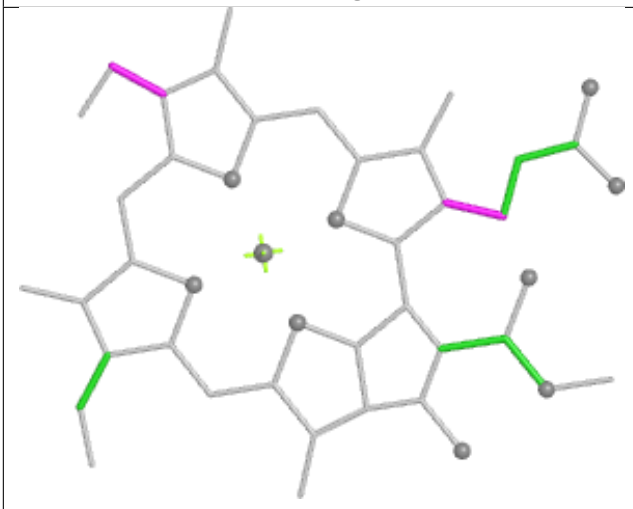
Ligand CLA b2 414



Bond lengths



Bond angles

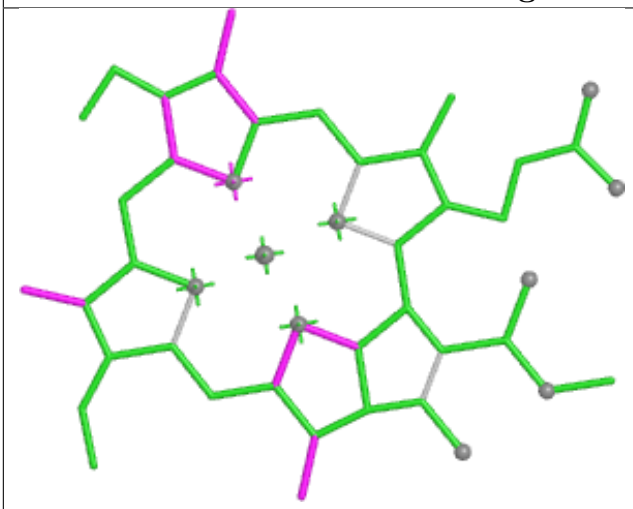


Torsions

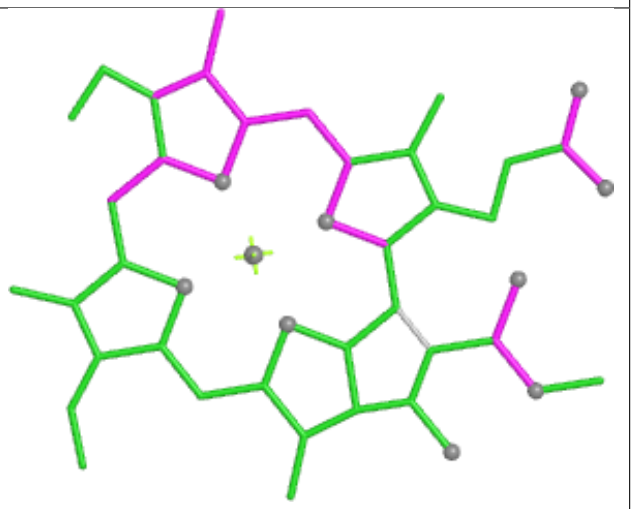


Rings

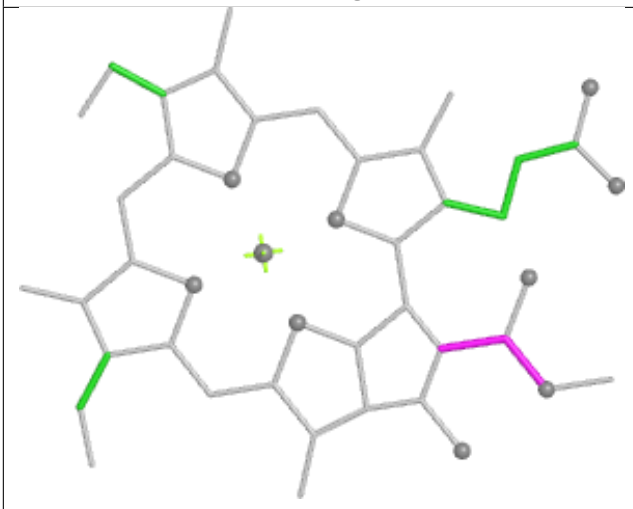
Ligand CLA b1 406



Bond lengths



Bond angles

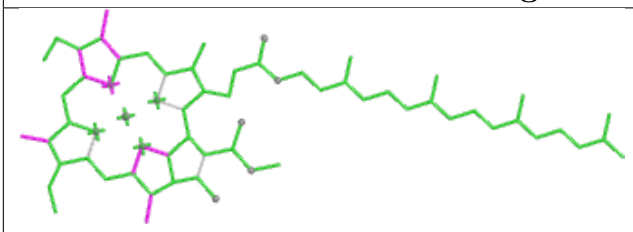


Torsions

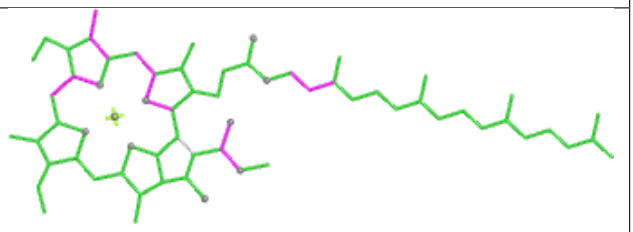


Rings

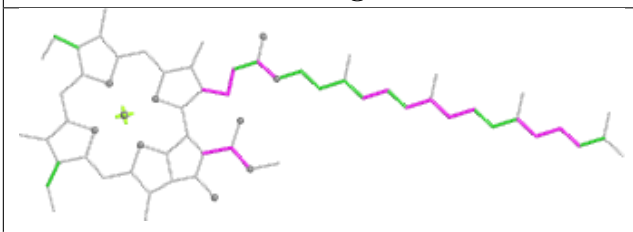
Ligand CLA c5 402



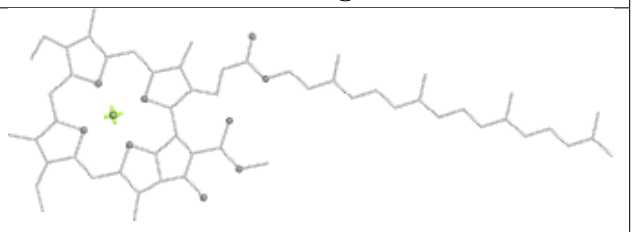
Bond lengths



Bond angles

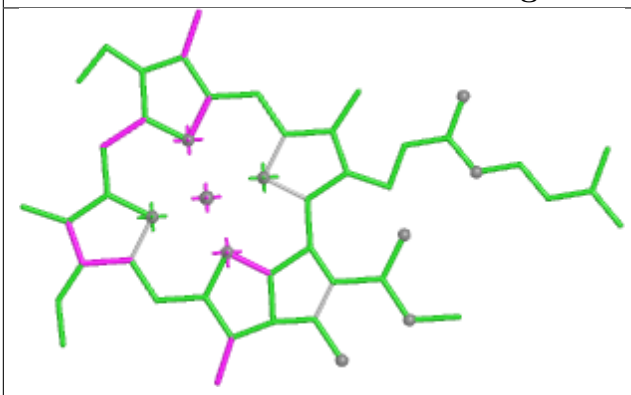


Torsions

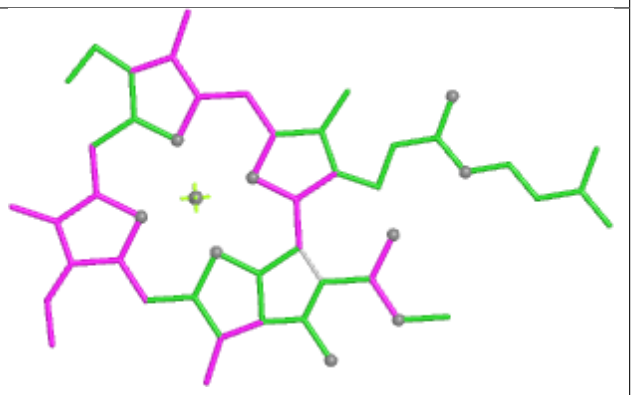


Rings

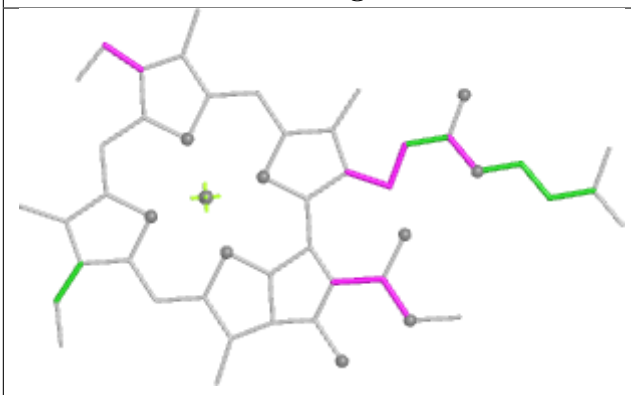
Ligand CLA c5 416



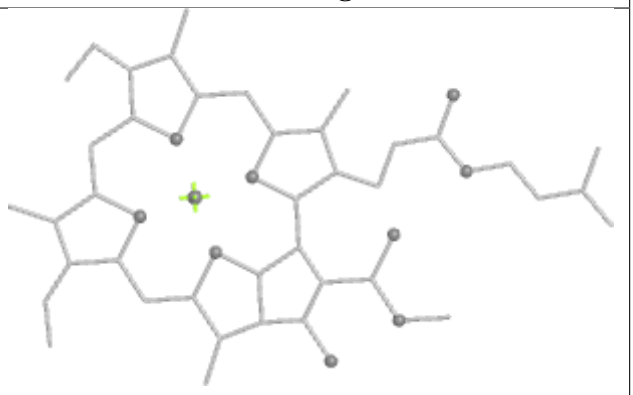
Bond lengths



Bond angles



Torsions

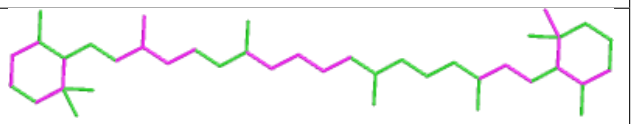


Rings

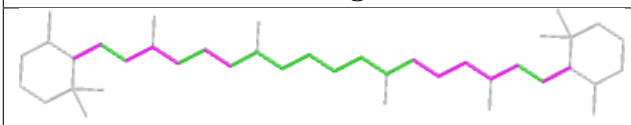
Ligand BCR a1 420



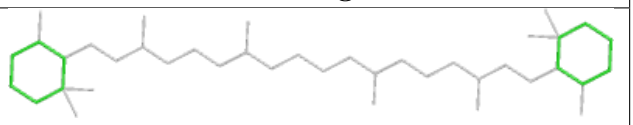
Bond lengths



Bond angles

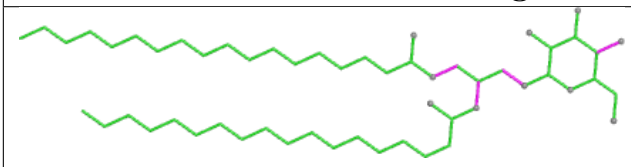


Torsions

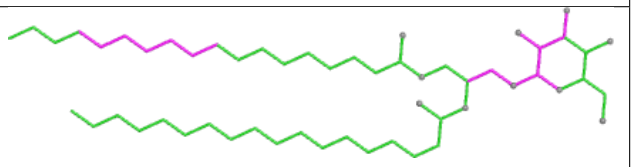


Rings

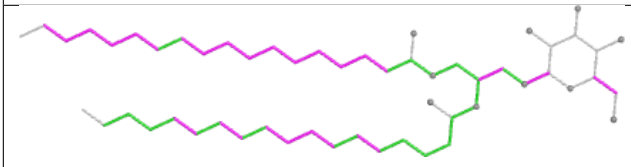
Ligand LMG aB 850



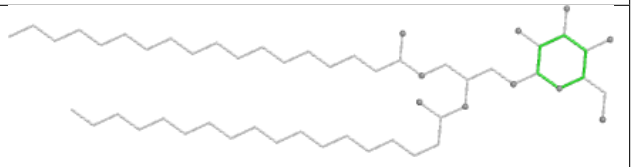
Bond lengths



Bond angles

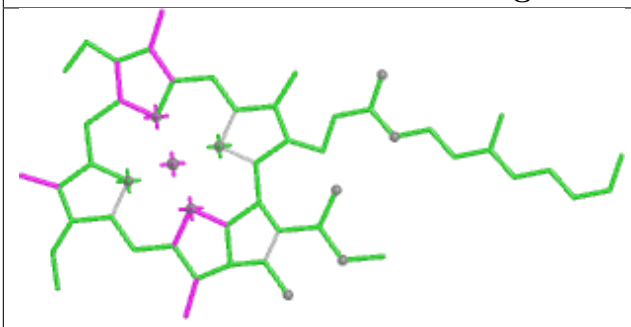


Torsions

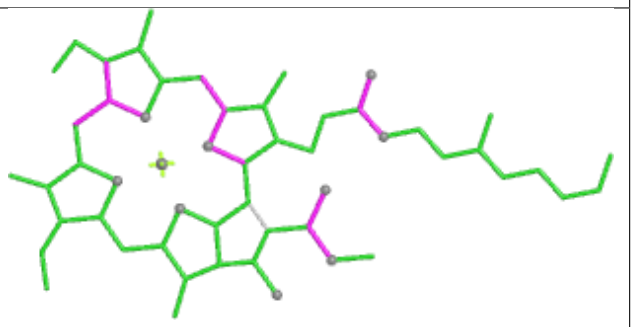


Rings

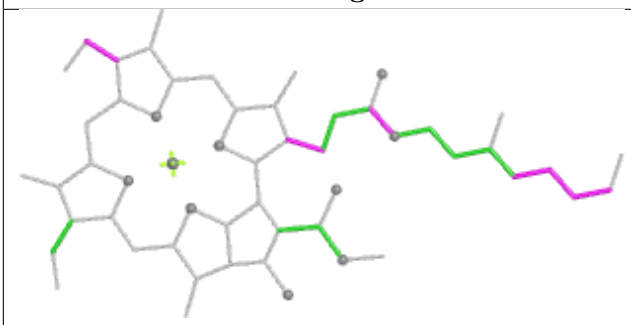
Ligand CLA bA 836



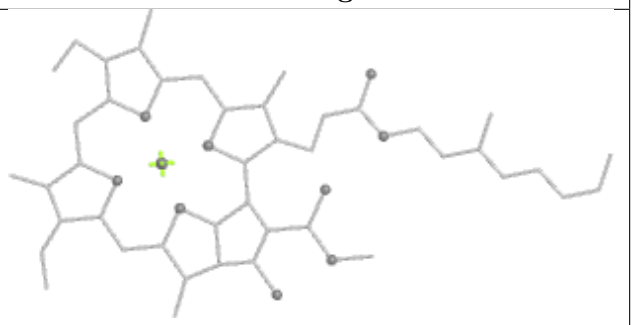
Bond lengths



Bond angles

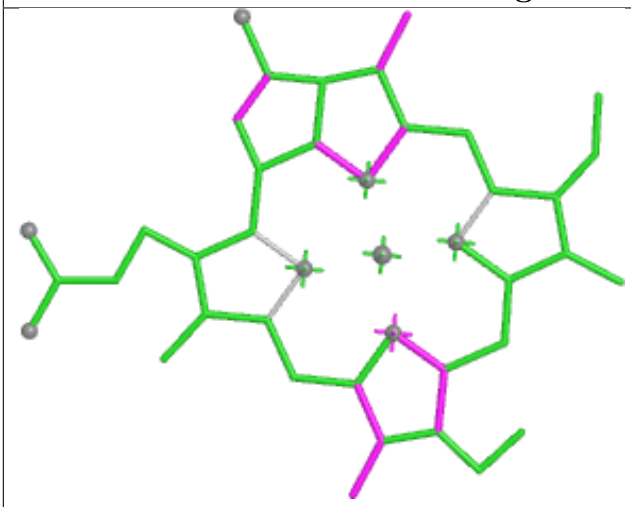


Torsions

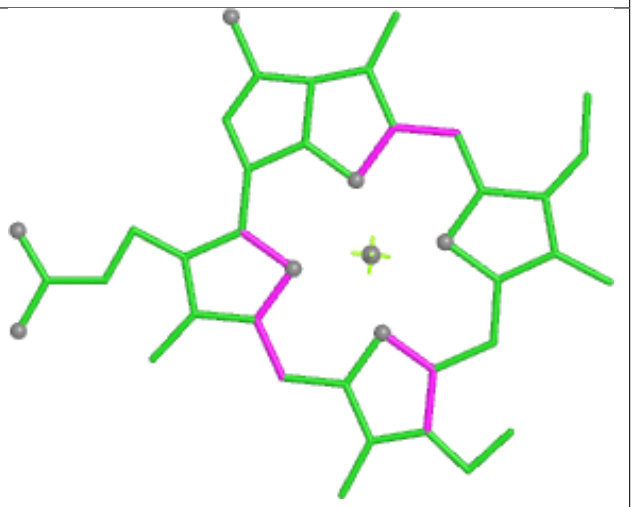


Rings

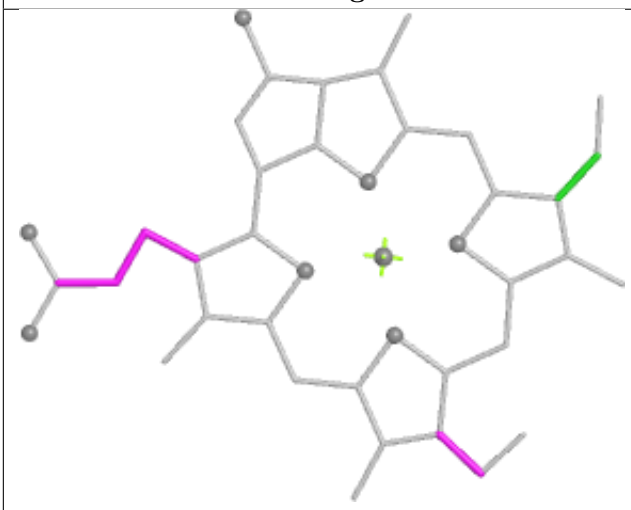
Ligand CLA aA 844



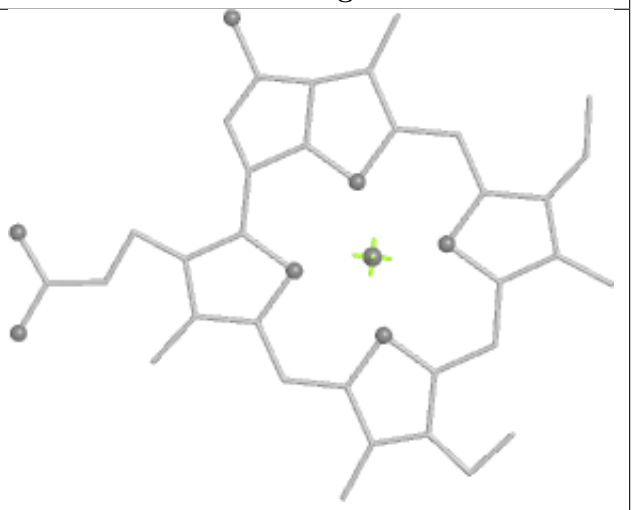
Bond lengths



Bond angles

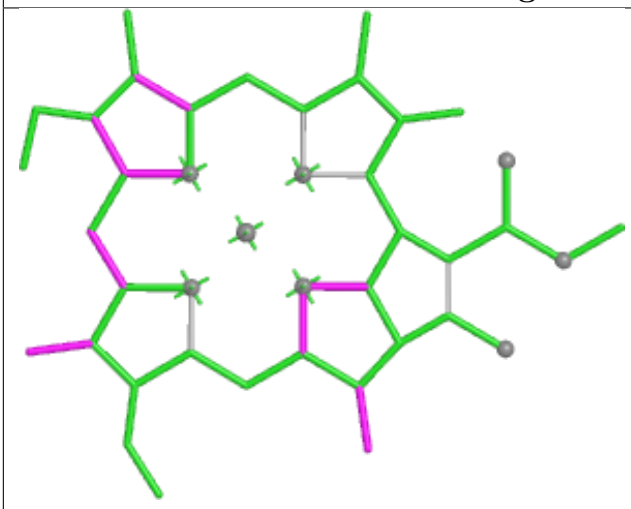


Torsions

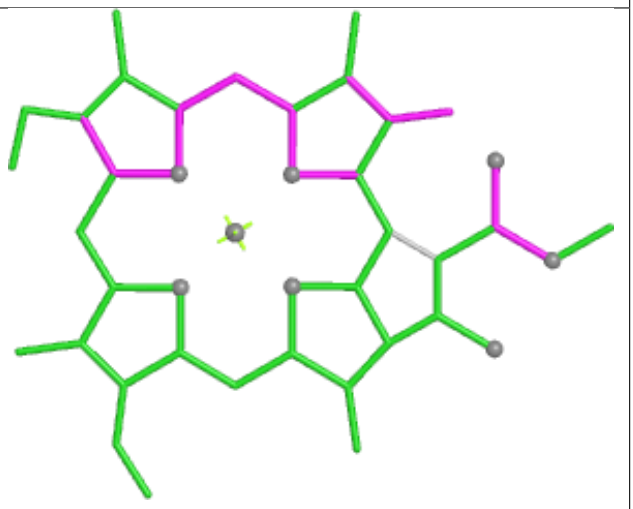


Rings

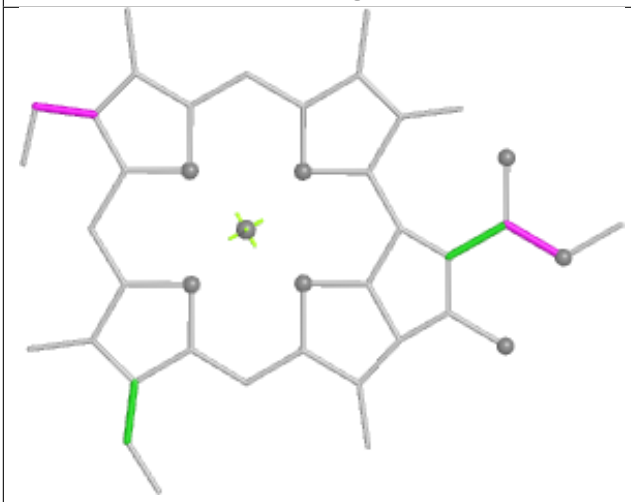
Ligand CLA b6 415



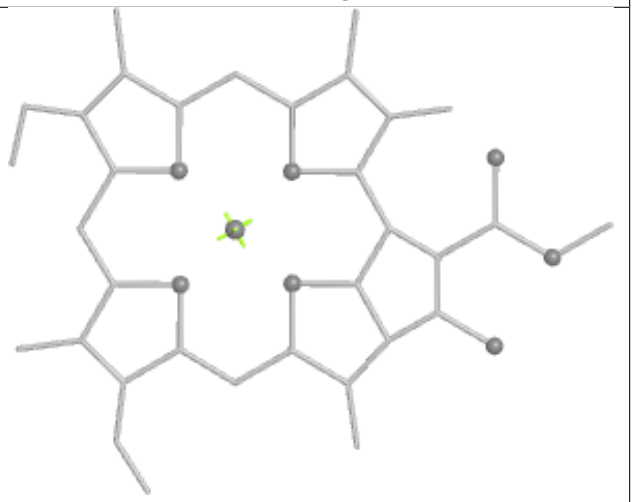
Bond lengths



Bond angles

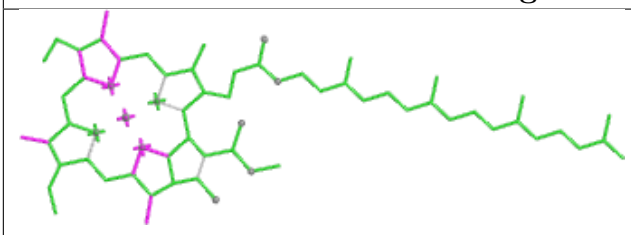


Torsions

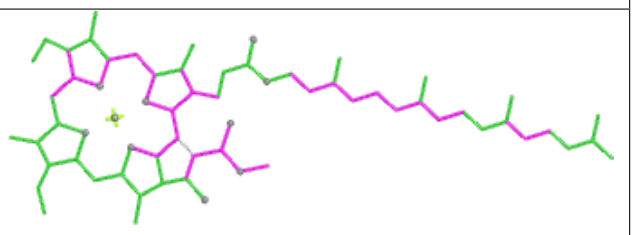


Rings

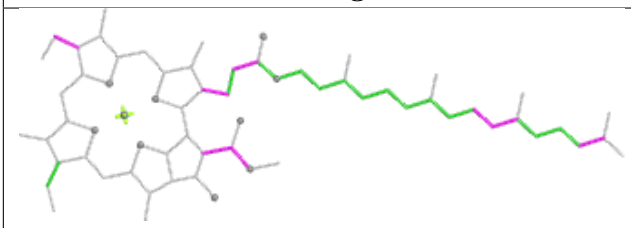
Ligand CLA a2 422



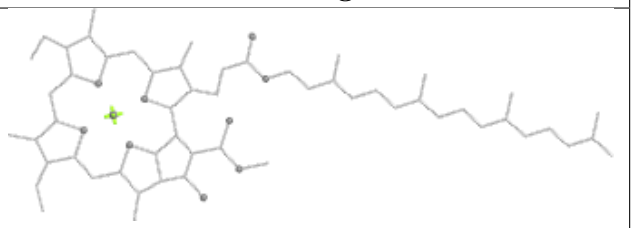
Bond lengths



Bond angles

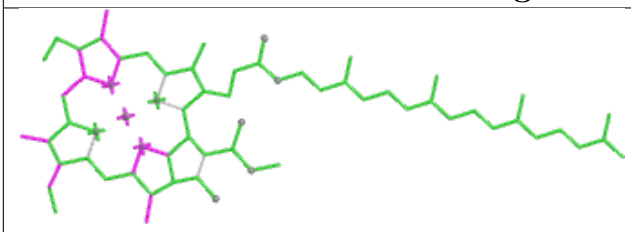


Torsions

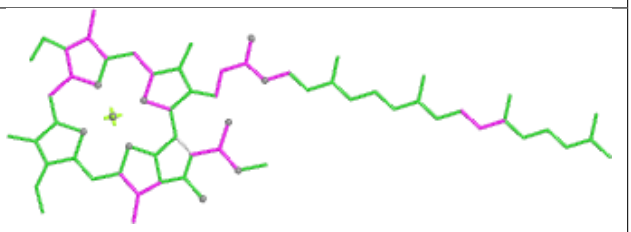


Rings

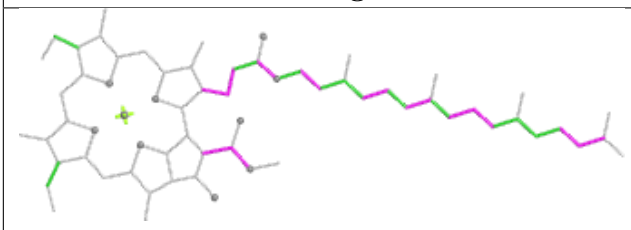
Ligand CLA bA 803



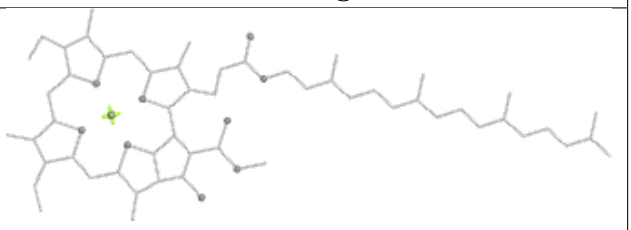
Bond lengths



Bond angles

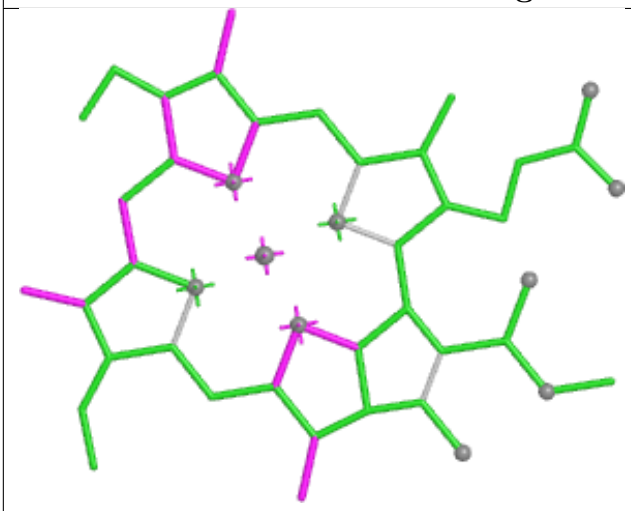


Torsions

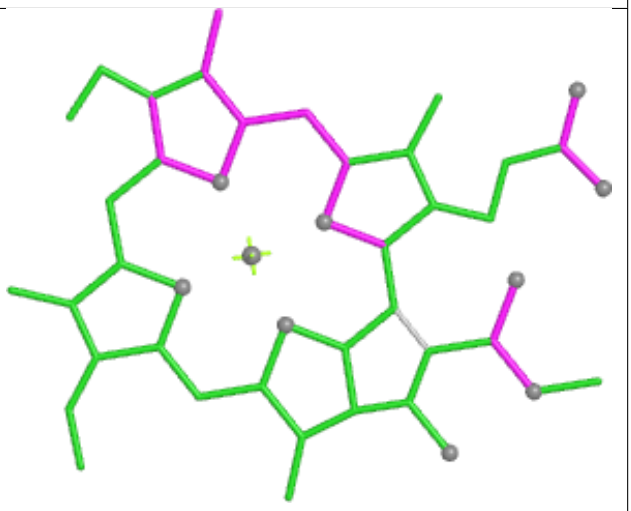


Rings

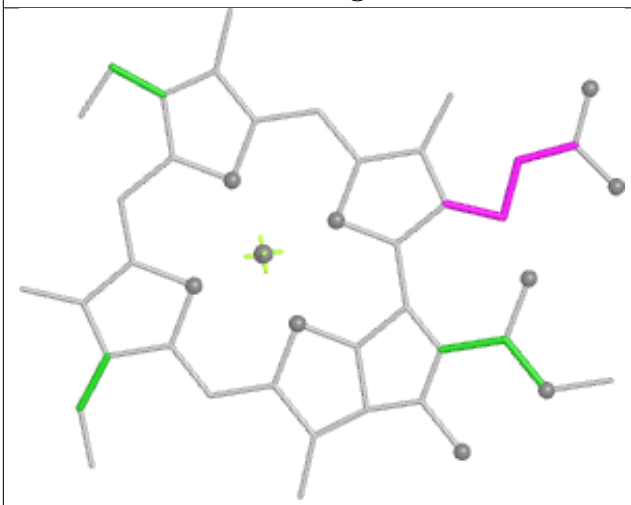
Ligand CLA aB 813



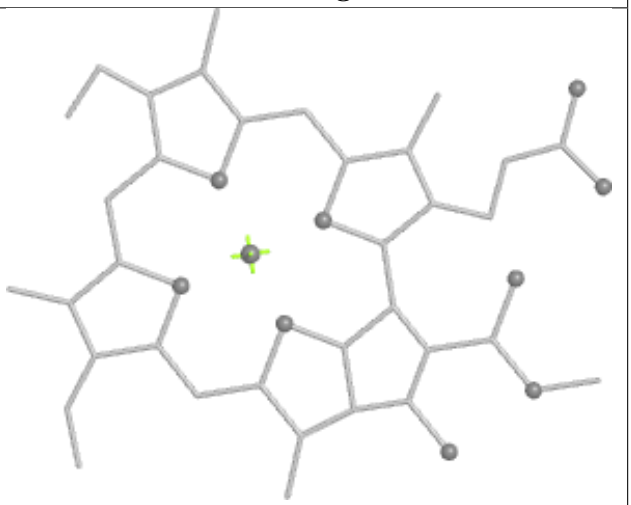
Bond lengths



Bond angles

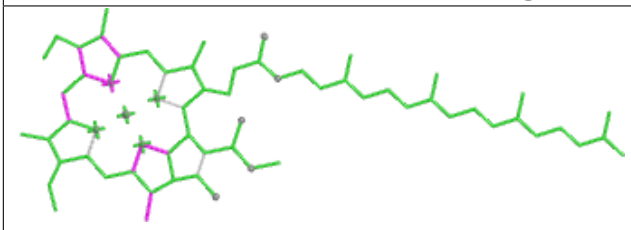


Torsions

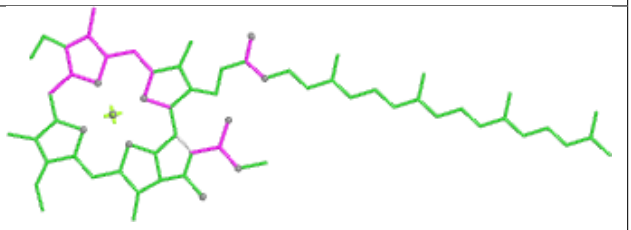


Rings

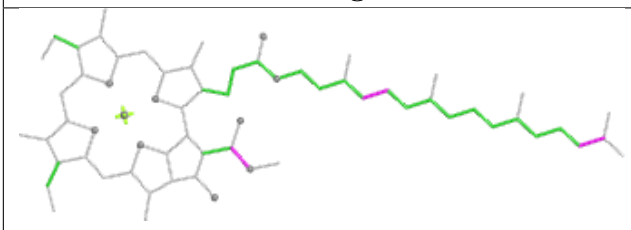
Ligand CLA a4 409



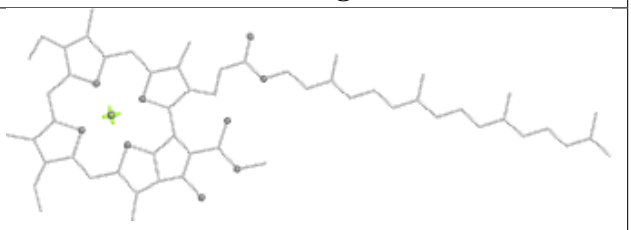
Bond lengths



Bond angles

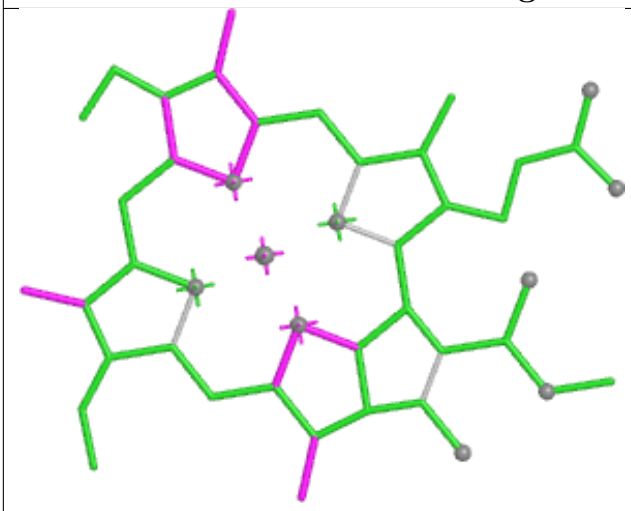


Torsions

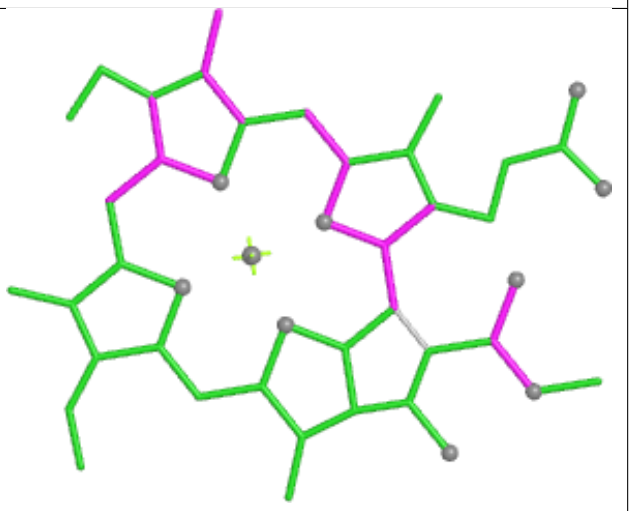


Rings

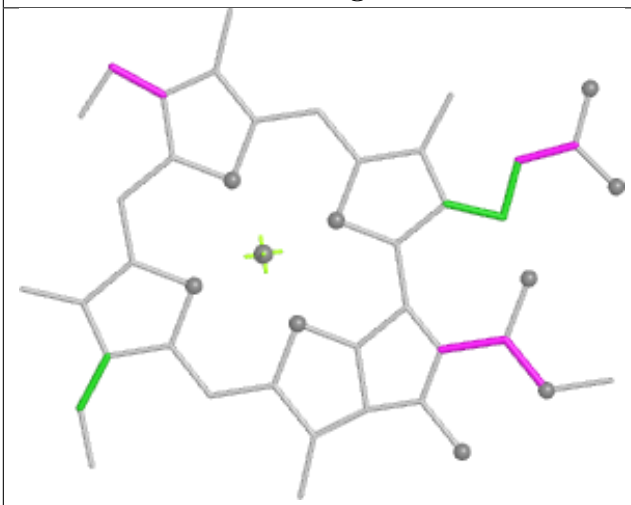
Ligand CLA b4 407



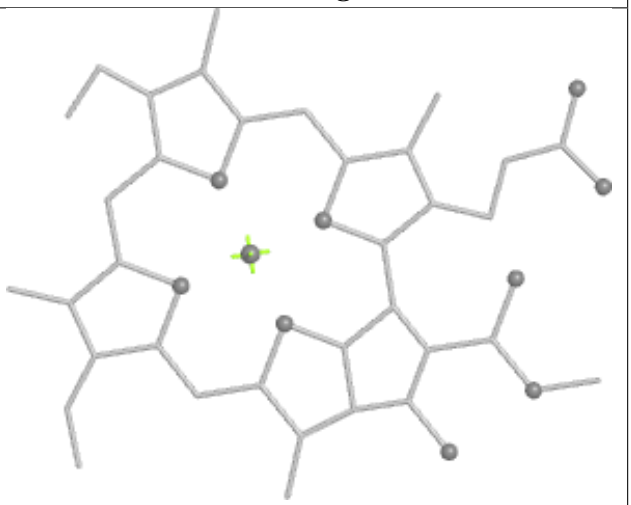
Bond lengths



Bond angles

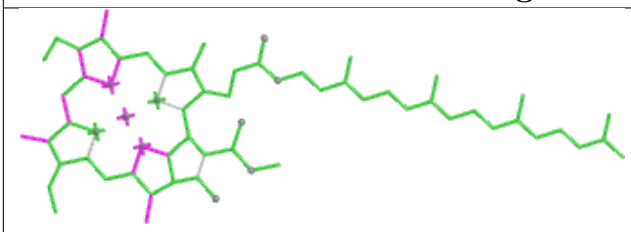


Torsions

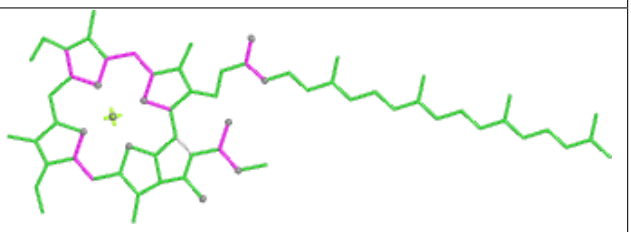


Rings

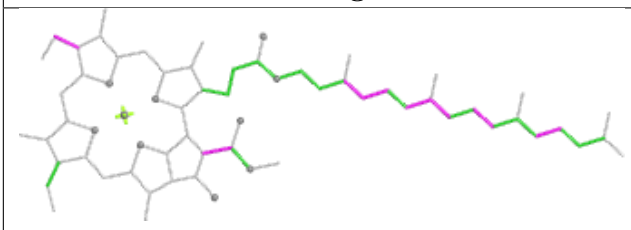
Ligand CLA cA 828



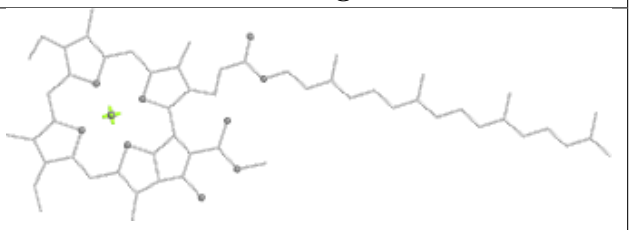
Bond lengths



Bond angles

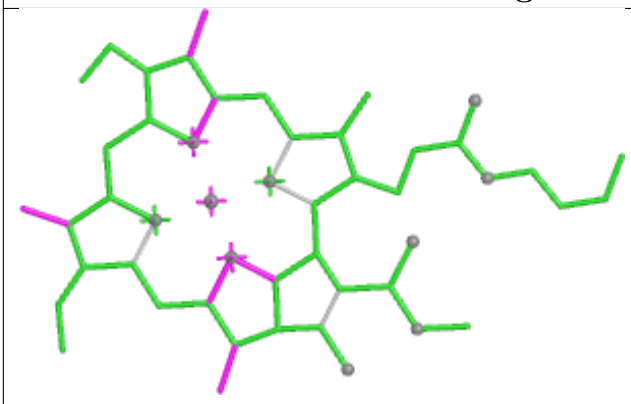


Torsions

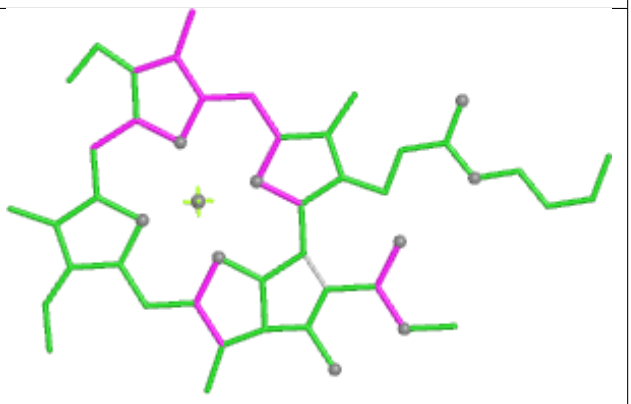


Rings

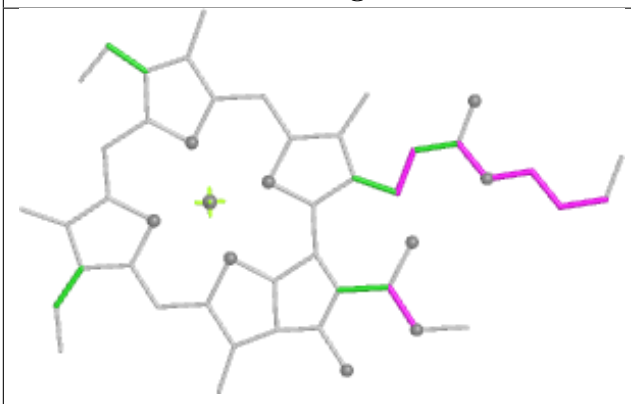
Ligand CLA aB 832



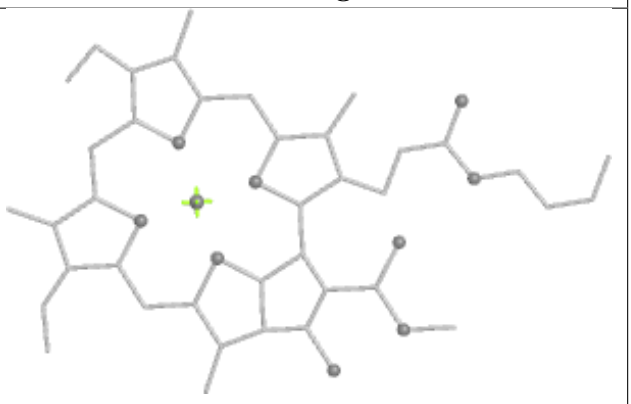
Bond lengths



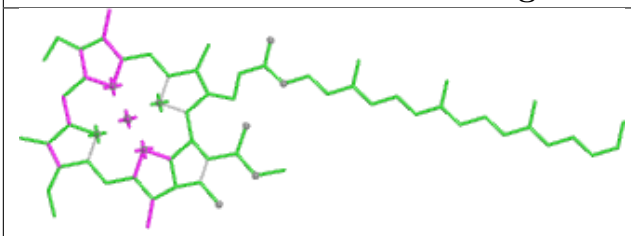
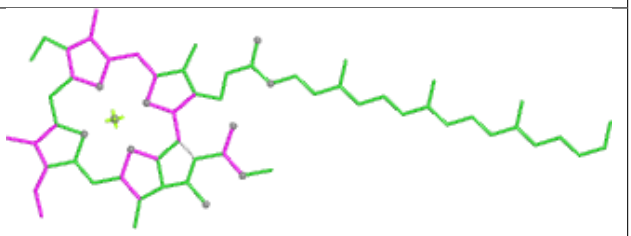
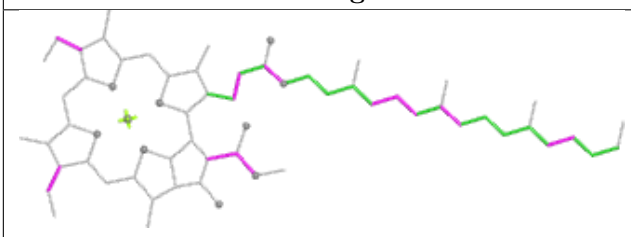
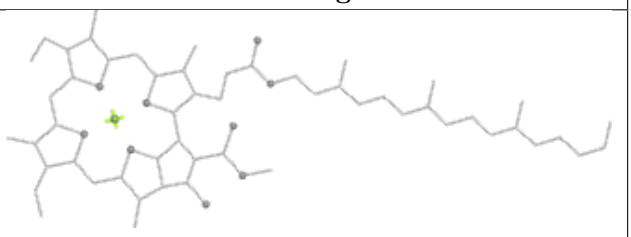
Bond angles

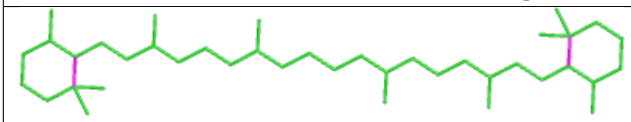
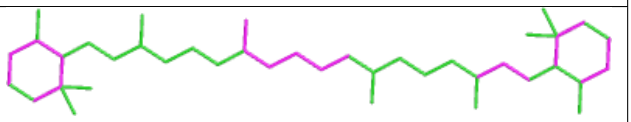
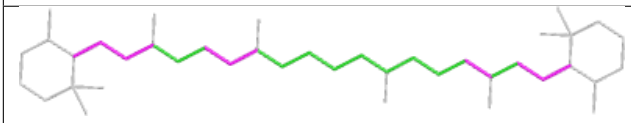
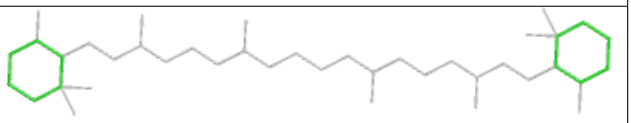


Torsions

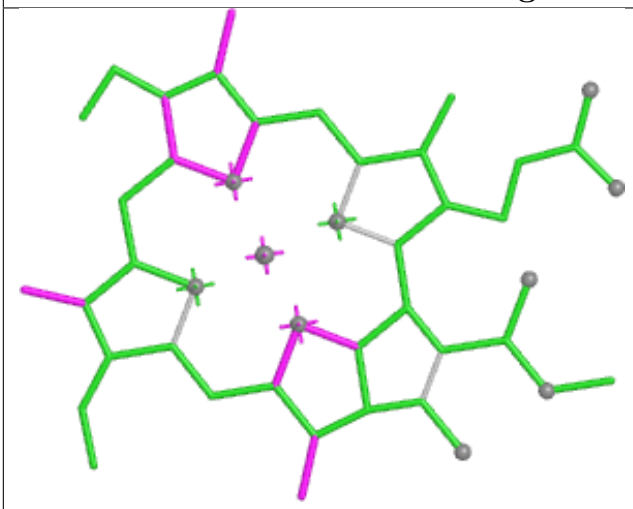


Rings

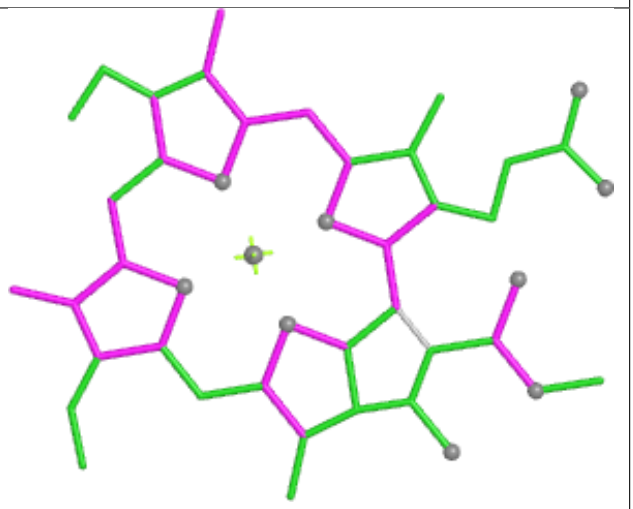
Ligand CLA b6 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a2 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

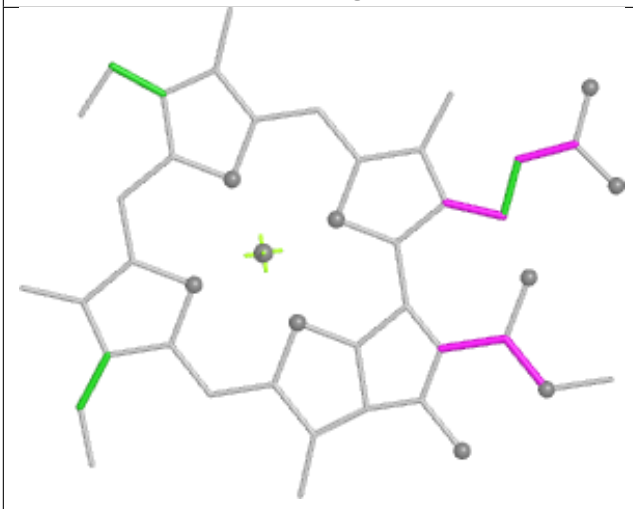
Ligand CLA b3 412



Bond lengths



Bond angles

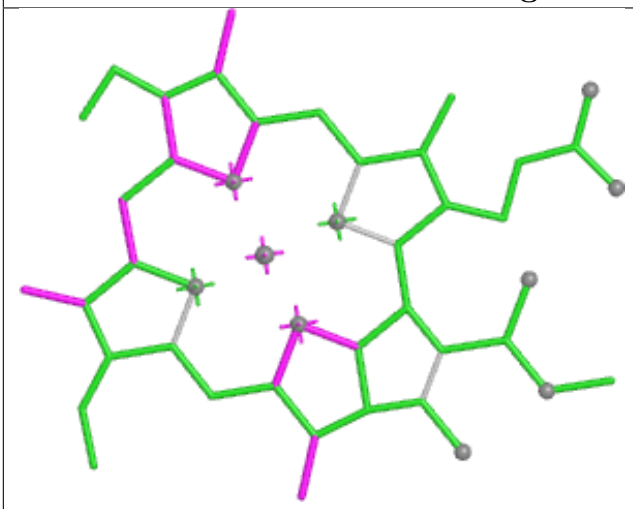


Torsions

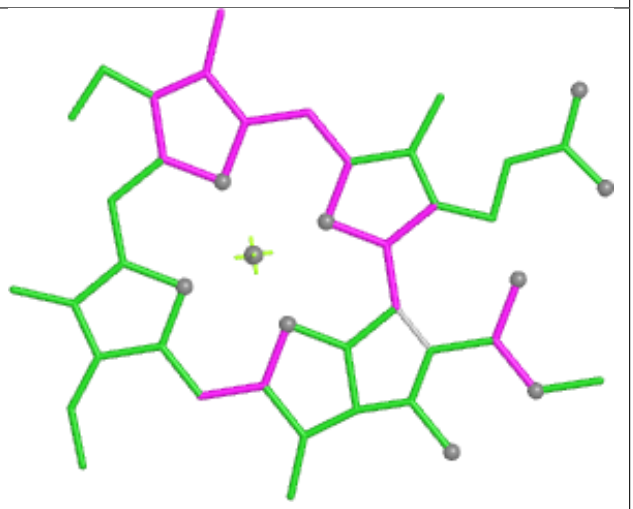


Rings

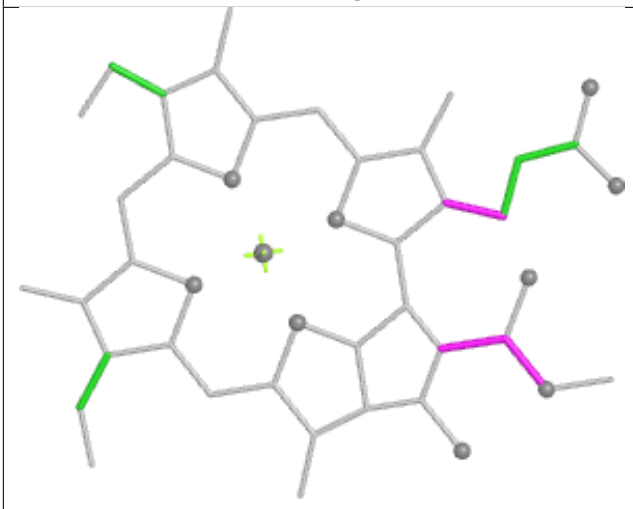
Ligand CLA c1 411



Bond lengths



Bond angles

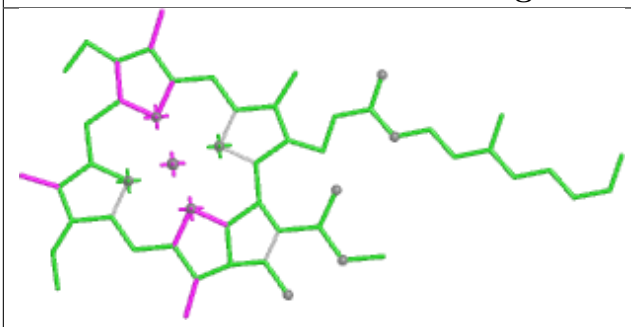


Torsions

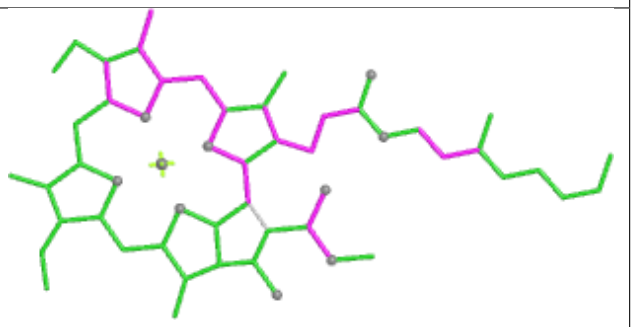


Rings

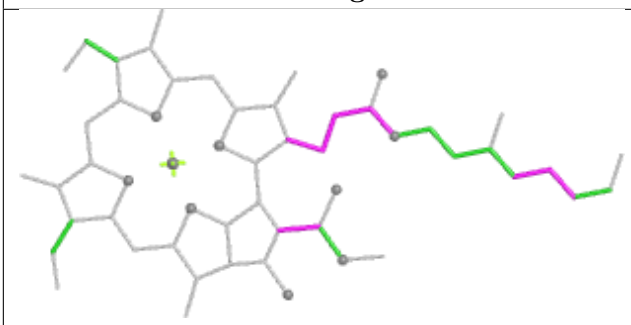
Ligand CLA aA 813



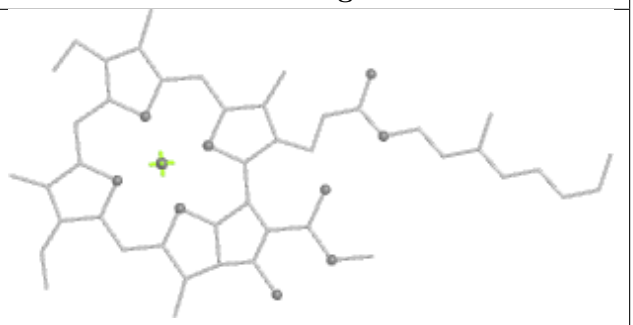
Bond lengths



Bond angles

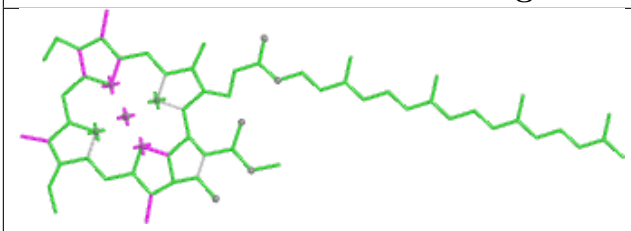


Torsions

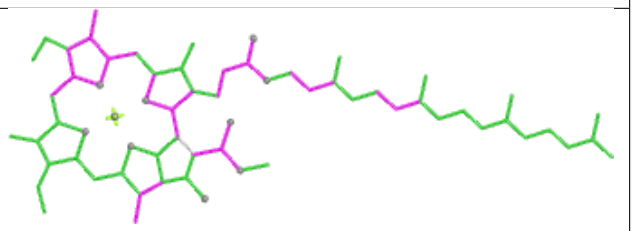


Rings

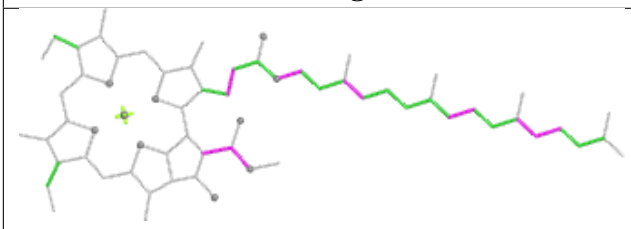
Ligand CLA aB 803



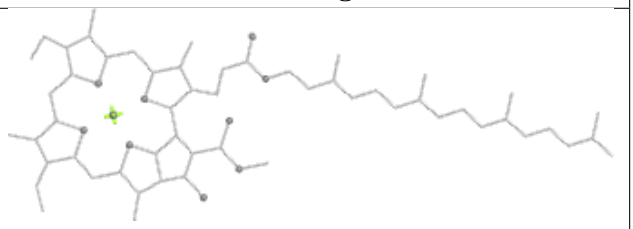
Bond lengths



Bond angles

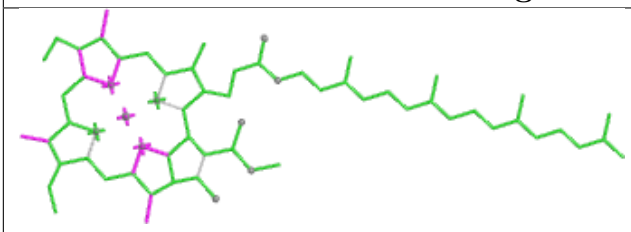


Torsions

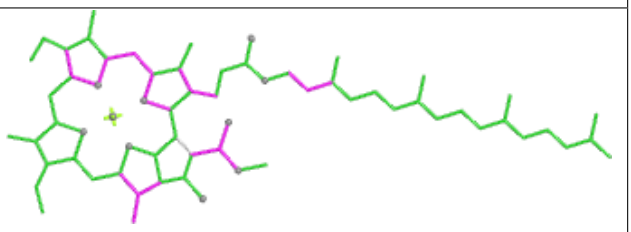


Rings

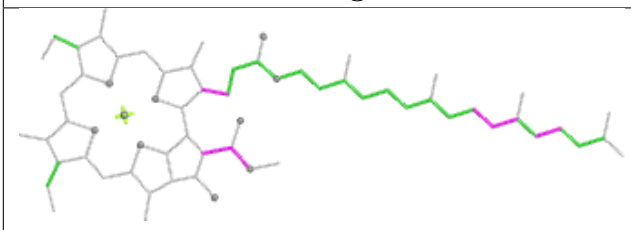
Ligand CLA aA 804



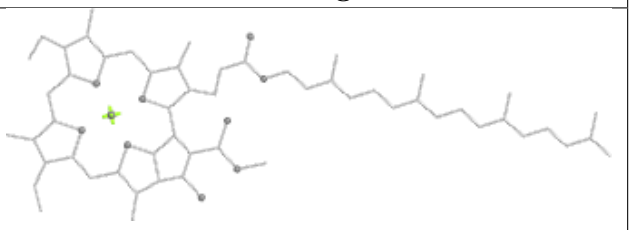
Bond lengths



Bond angles

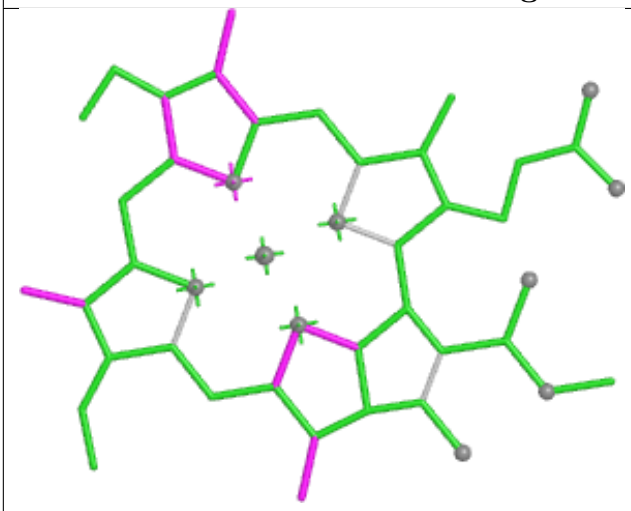


Torsions

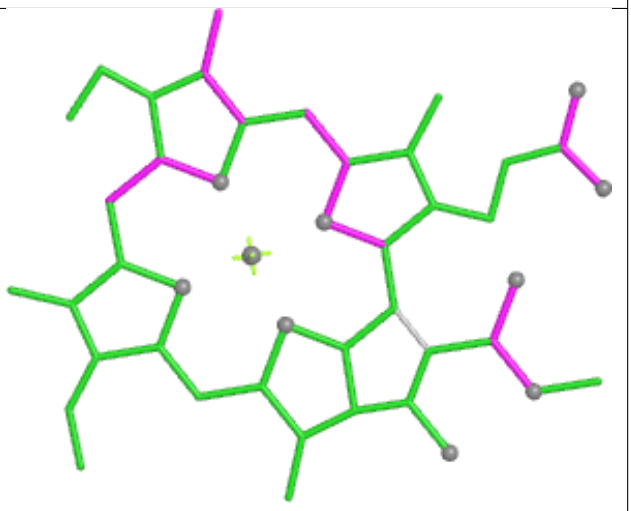


Rings

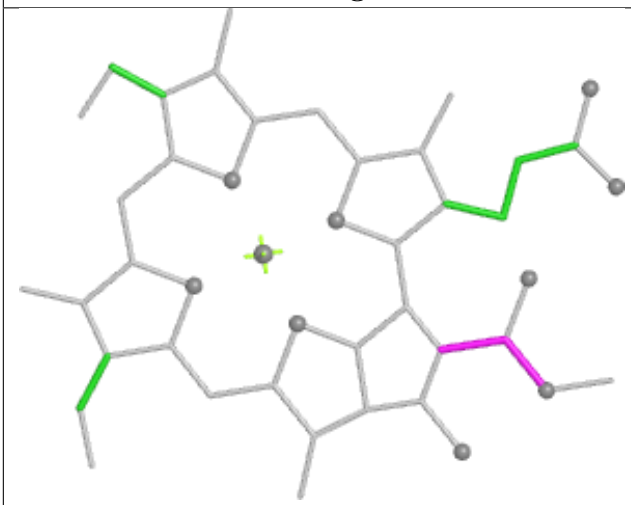
Ligand CLA c5 406



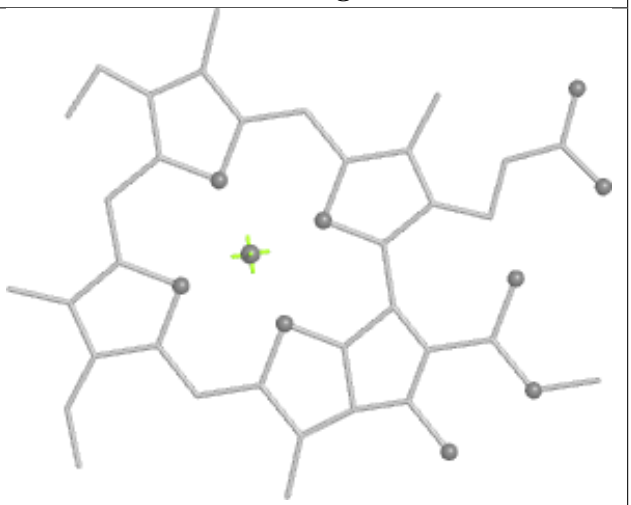
Bond lengths



Bond angles

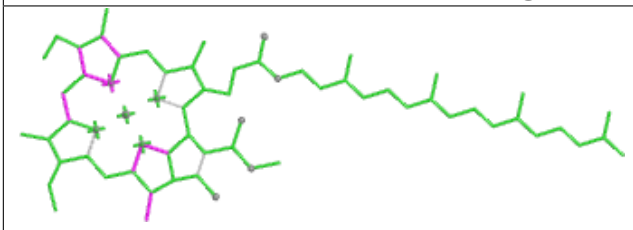


Torsions

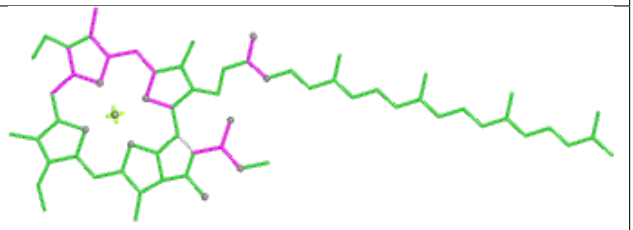


Rings

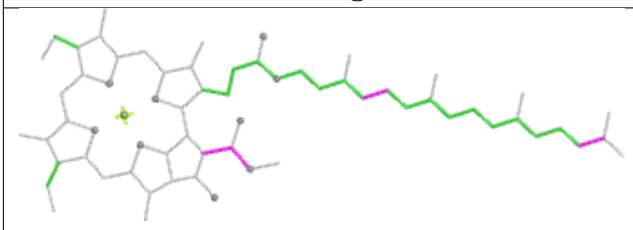
Ligand CLA a6 410



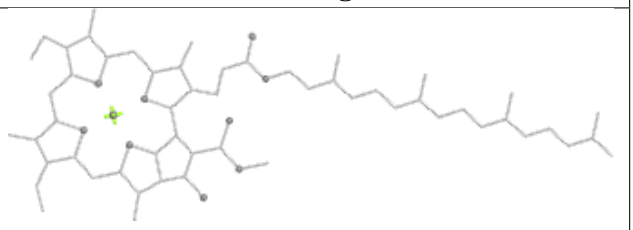
Bond lengths



Bond angles

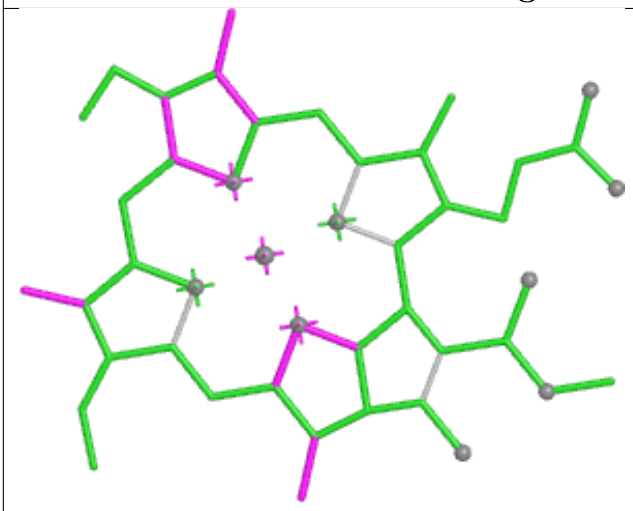


Torsions

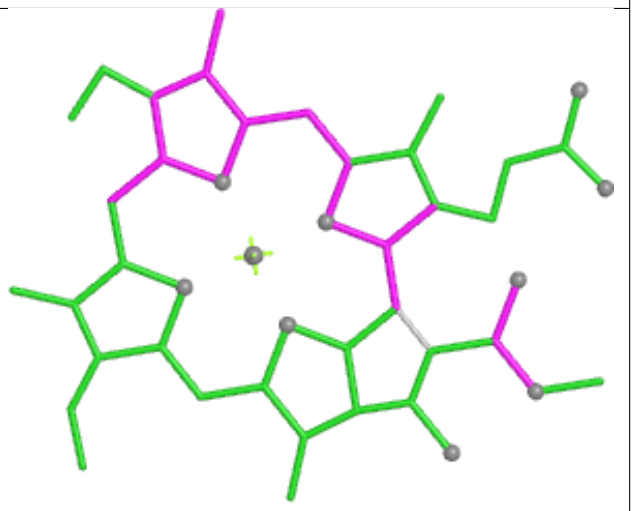


Rings

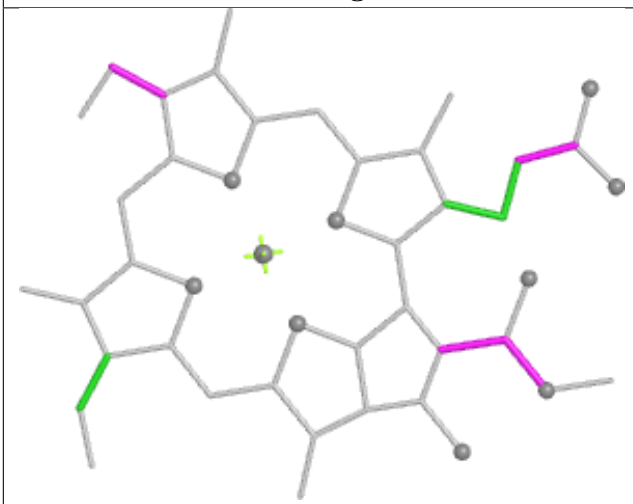
Ligand CLA b3 407



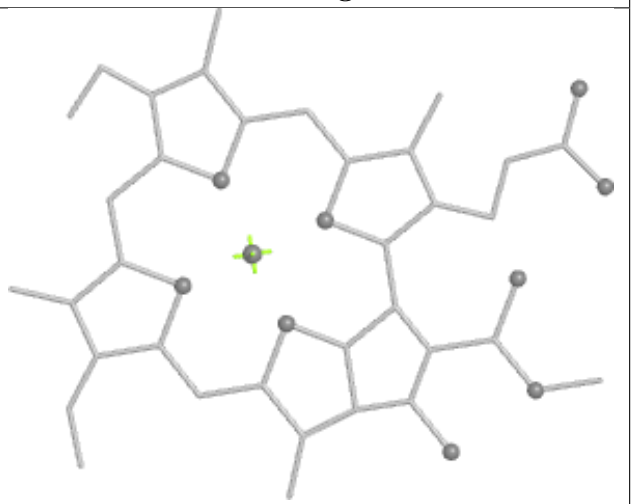
Bond lengths



Bond angles

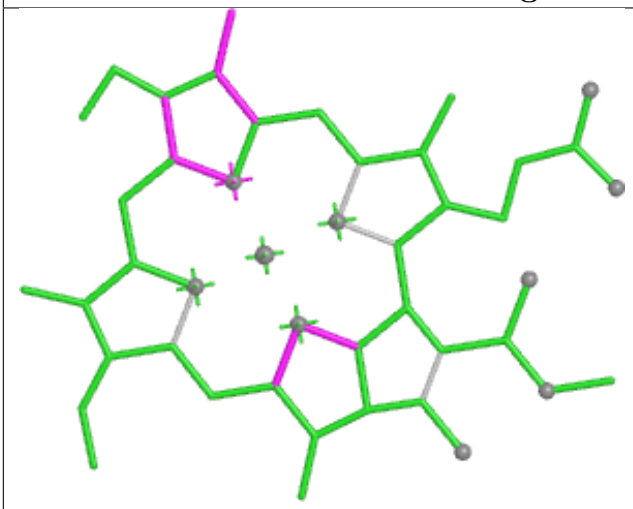


Torsions

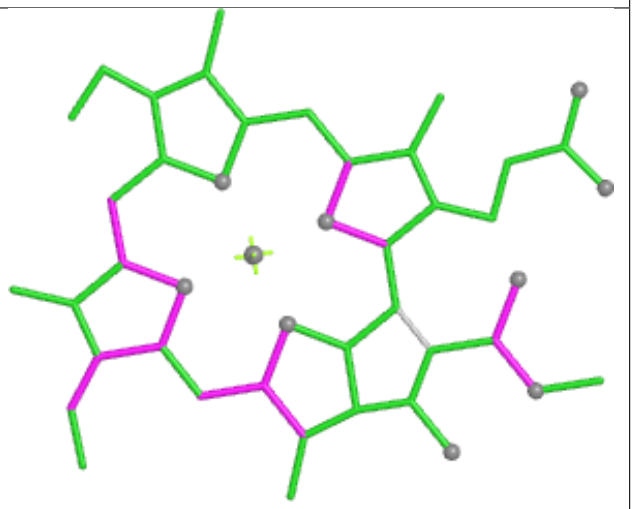


Rings

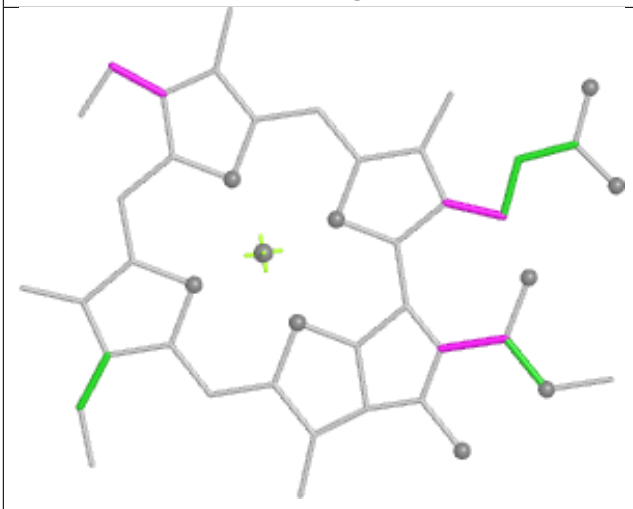
Ligand CLA c6 415



Bond lengths



Bond angles

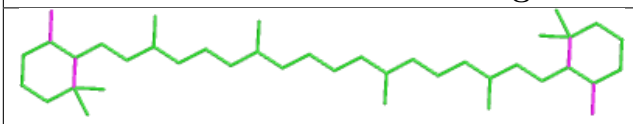


Torsions

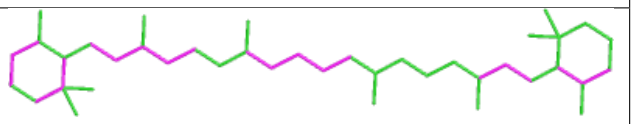


Rings

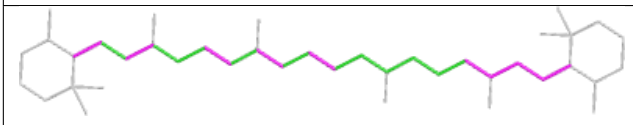
Ligand BCR bB 848



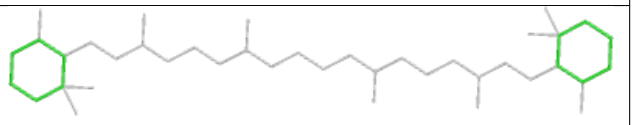
Bond lengths



Bond angles

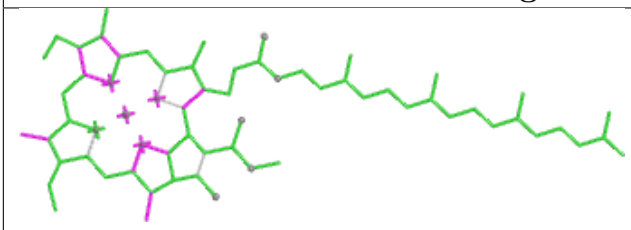


Torsions

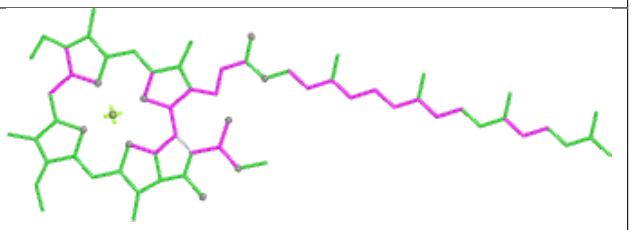


Rings

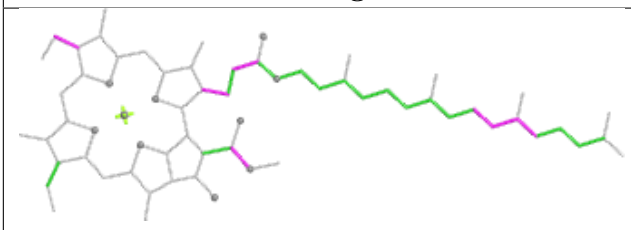
Ligand CLA a3 421



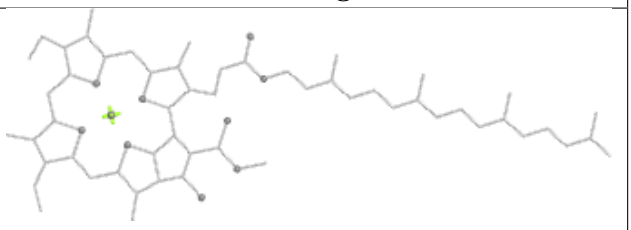
Bond lengths



Bond angles

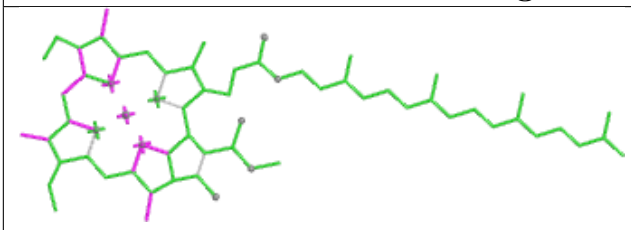


Torsions

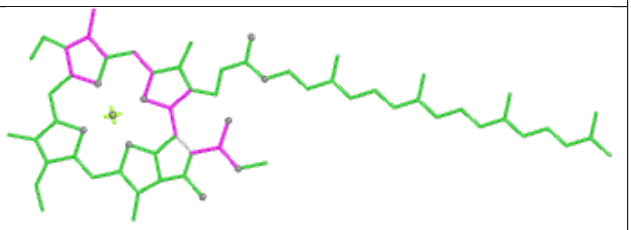


Rings

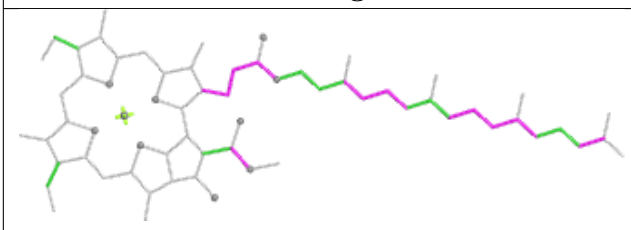
Ligand CLA cB 828



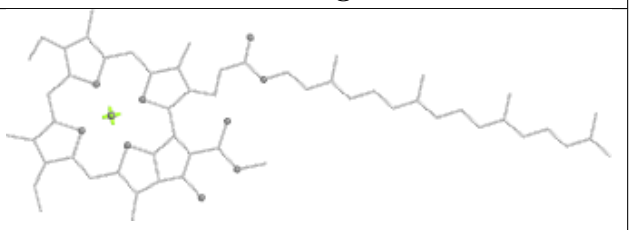
Bond lengths



Bond angles

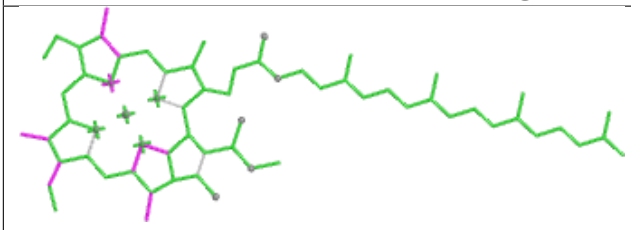


Torsions

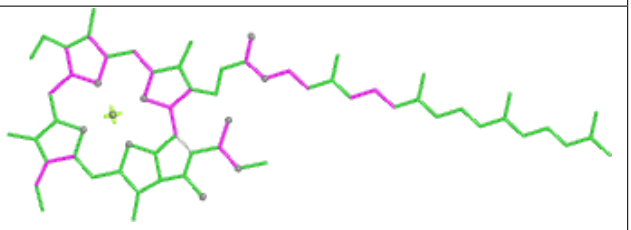


Rings

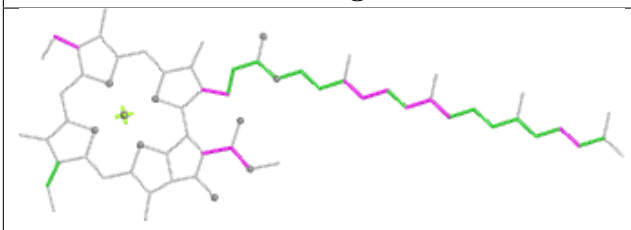
Ligand CLA cB 811



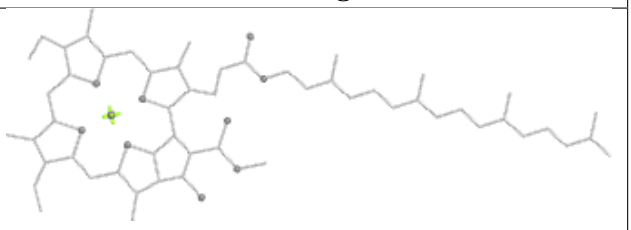
Bond lengths



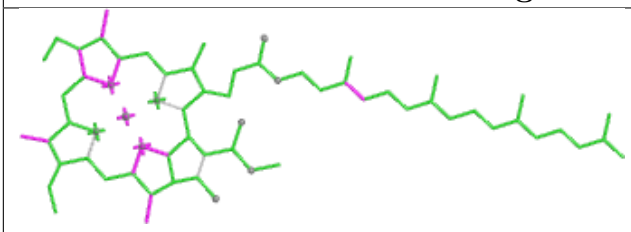
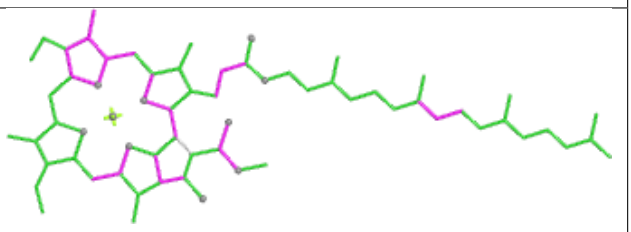
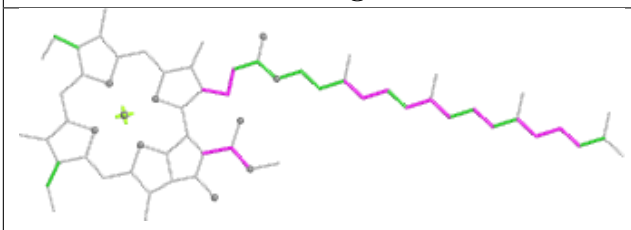
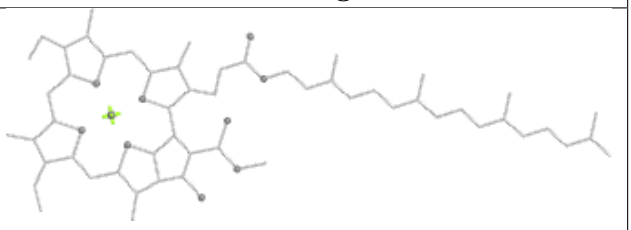
Bond angles

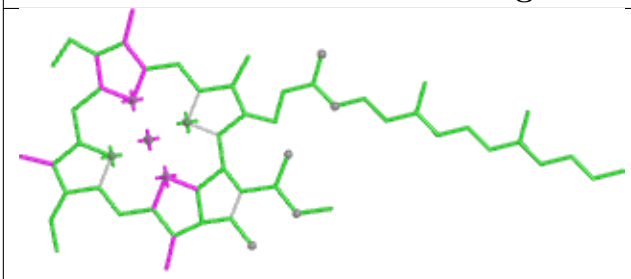
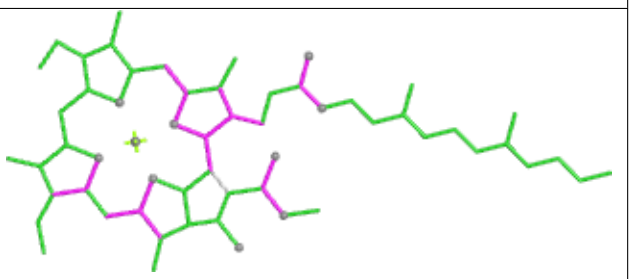
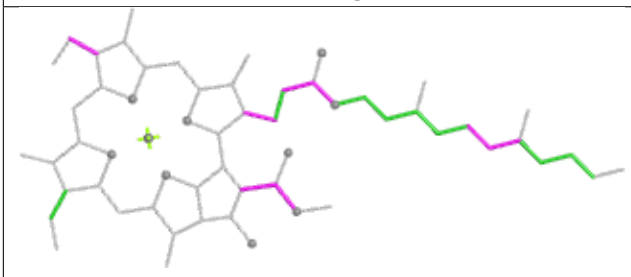
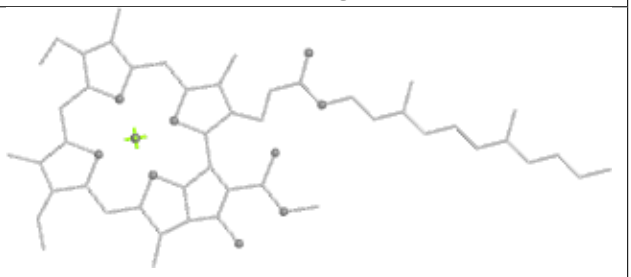


Torsions

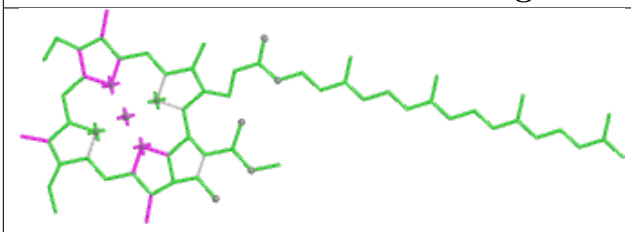


Rings

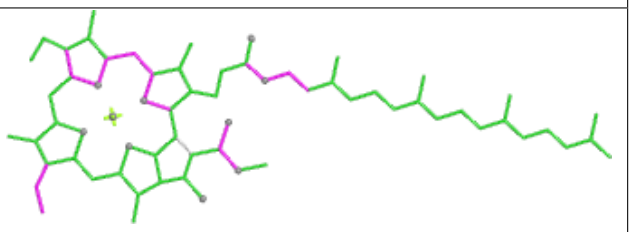
Ligand CLA cA 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aB 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

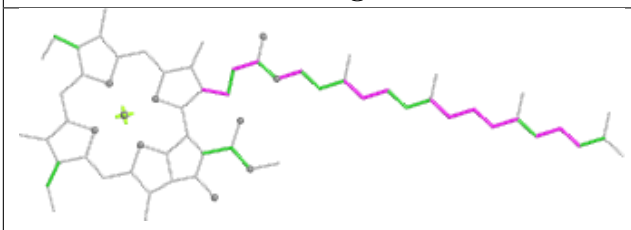
Ligand CLA aA 843



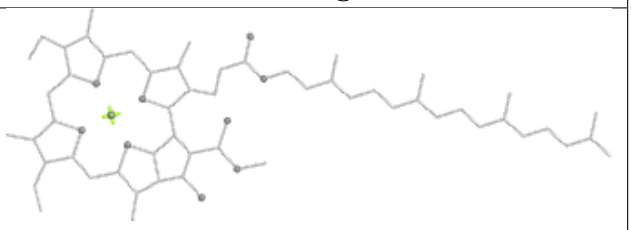
Bond lengths



Bond angles

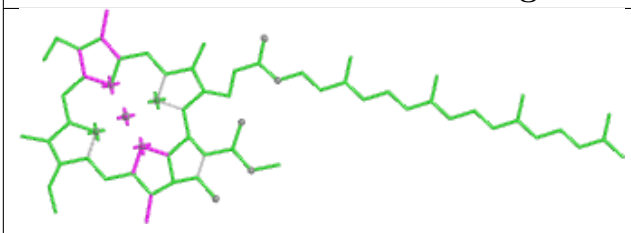


Torsions

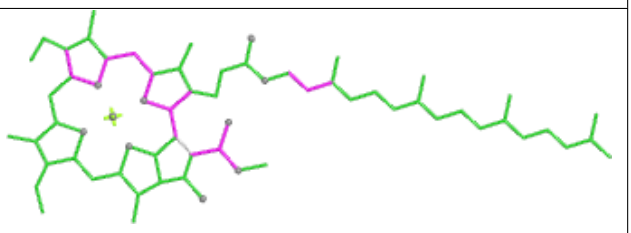


Rings

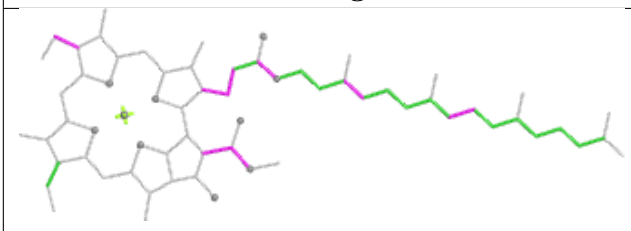
Ligand CLA a1 403



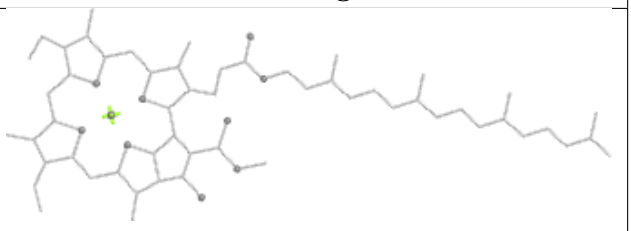
Bond lengths



Bond angles

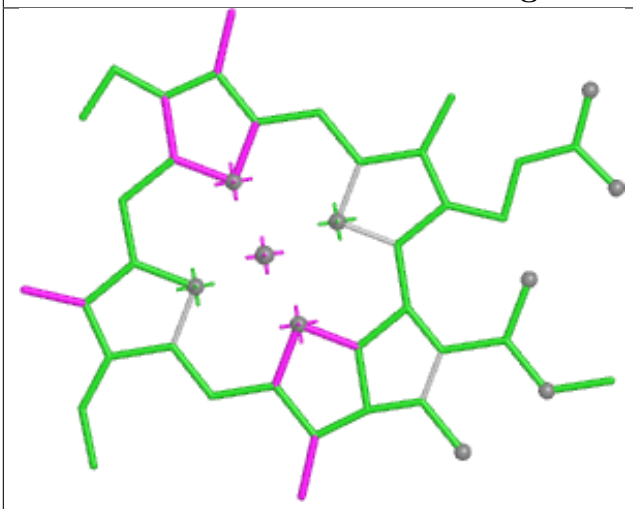


Torsions

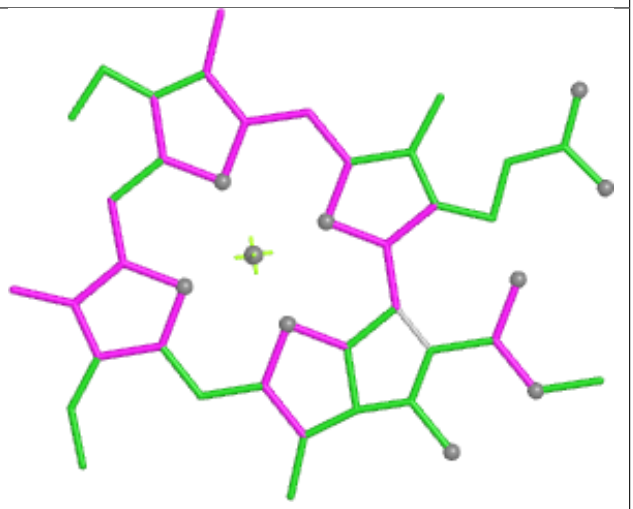


Rings

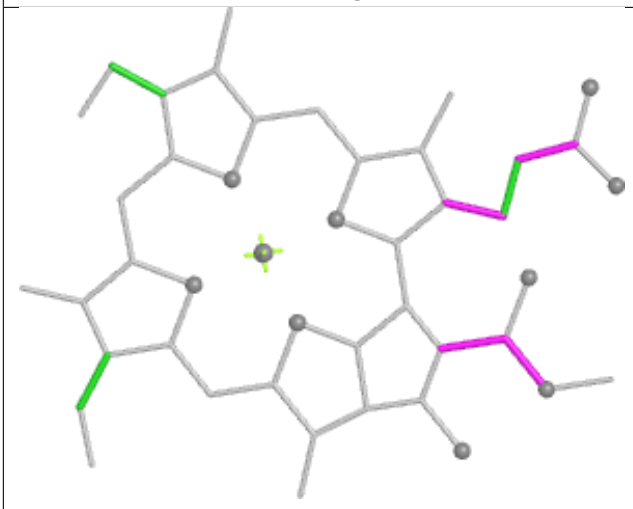
Ligand CLA c4 412



Bond lengths



Bond angles

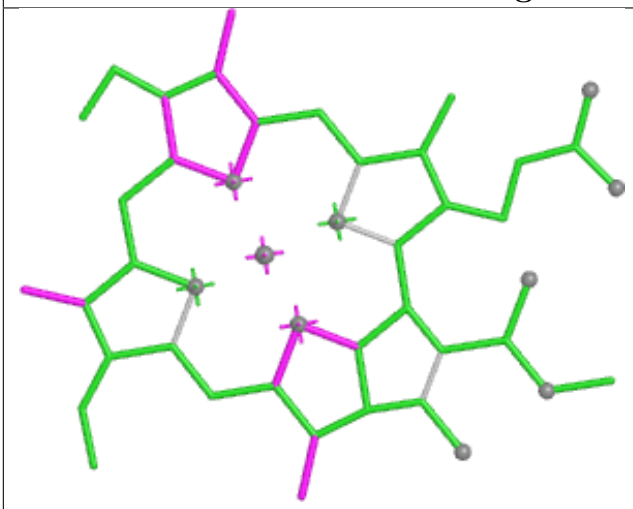


Torsions

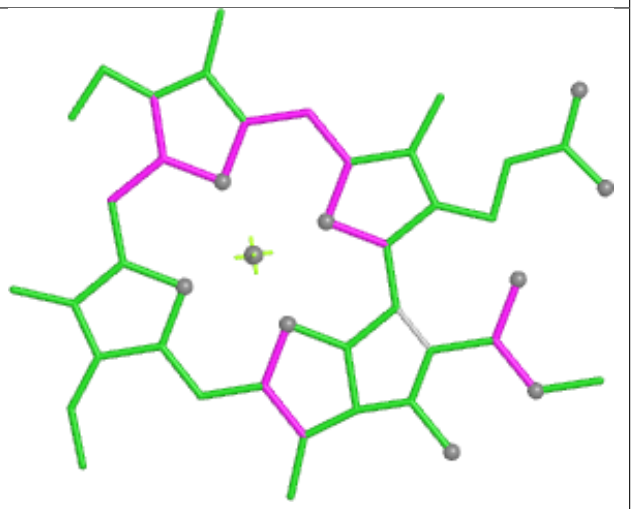


Rings

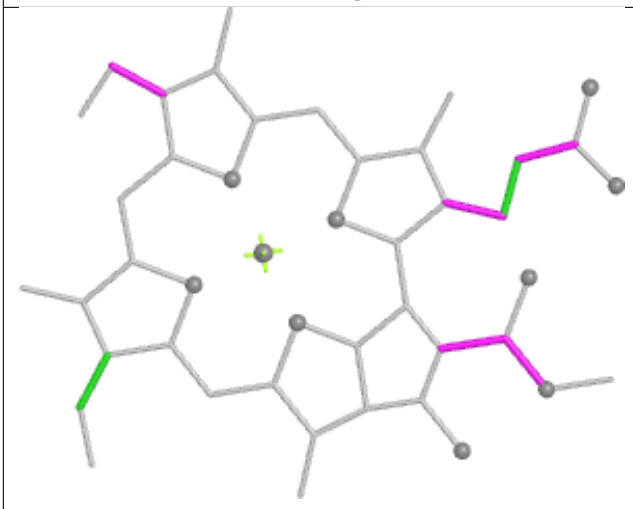
Ligand CLA aA 811



Bond lengths



Bond angles

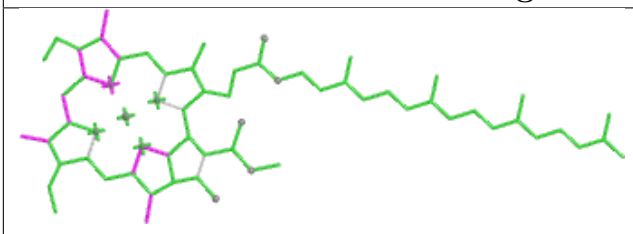


Torsions

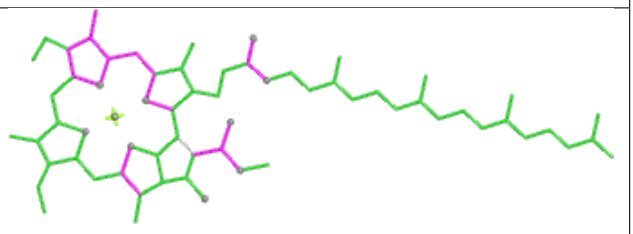


Rings

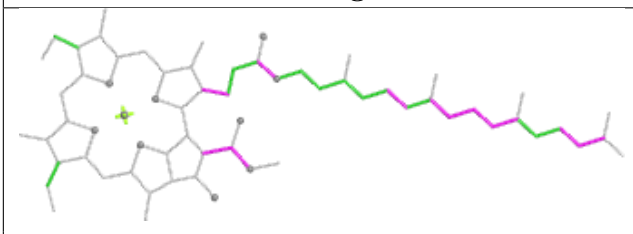
Ligand CLA cB 815



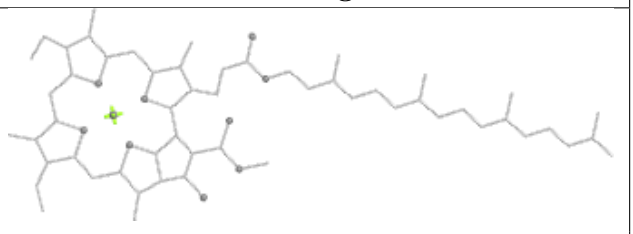
Bond lengths



Bond angles

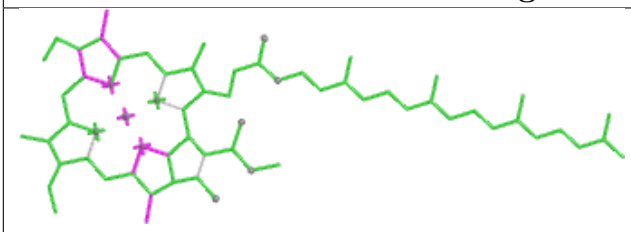


Torsions

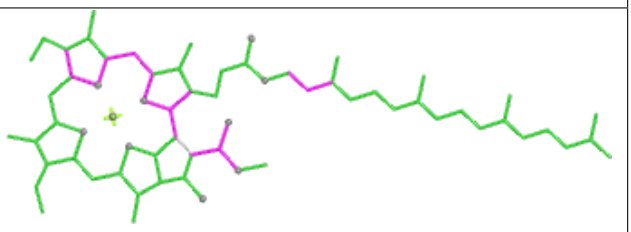


Rings

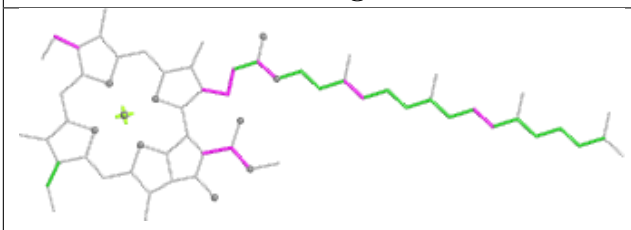
Ligand CLA b1 404



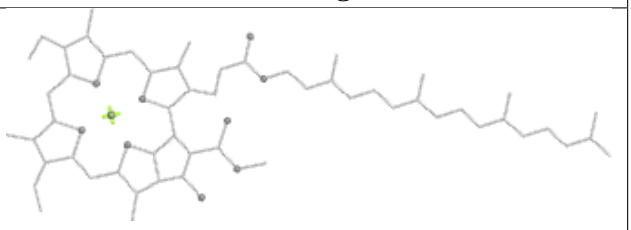
Bond lengths



Bond angles

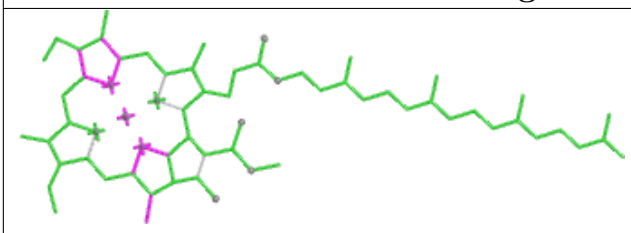


Torsions

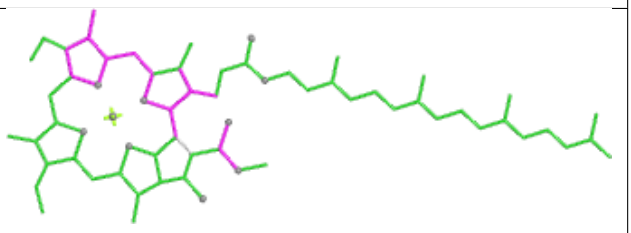


Rings

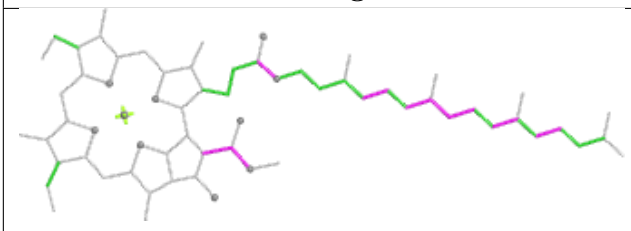
Ligand CLA b1 403



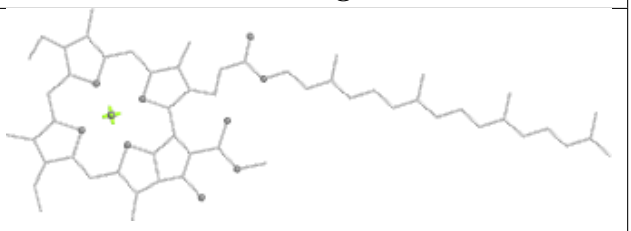
Bond lengths



Bond angles

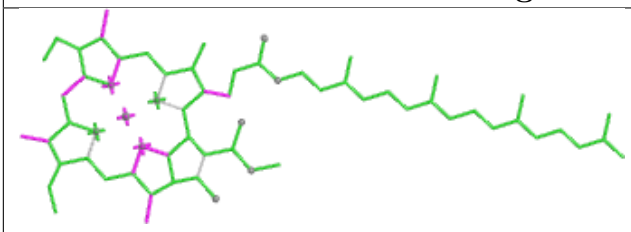


Torsions

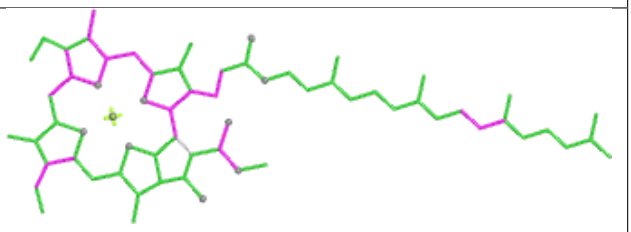


Rings

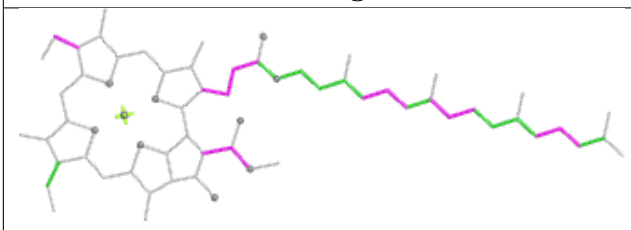
Ligand CLA aB 810



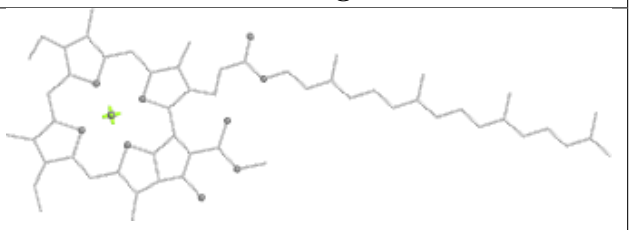
Bond lengths



Bond angles

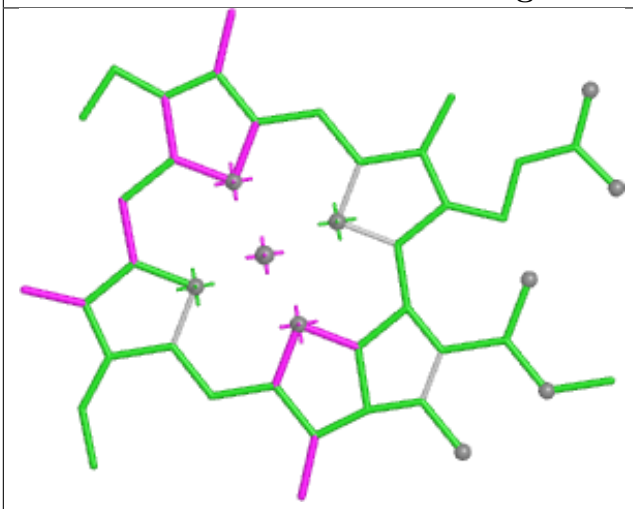


Torsions

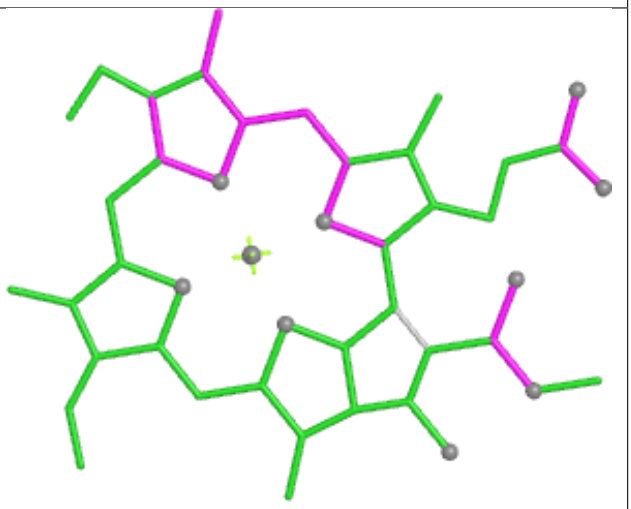


Rings

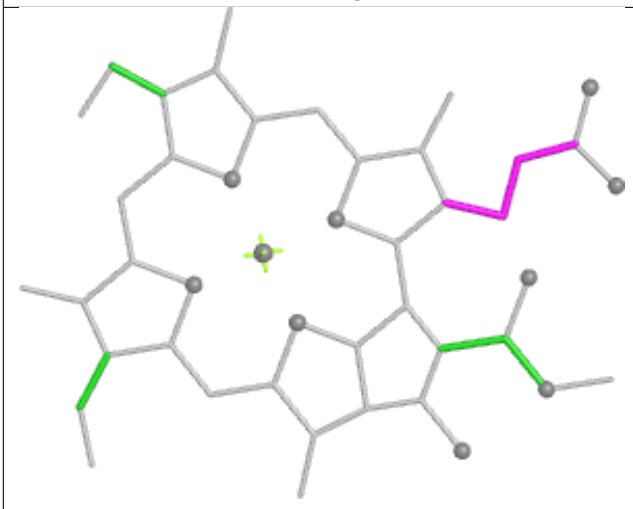
Ligand CLA cB 813



Bond lengths



Bond angles

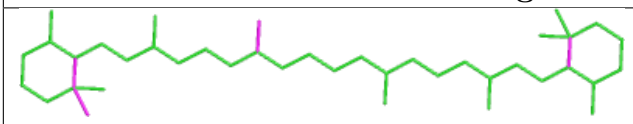


Torsions

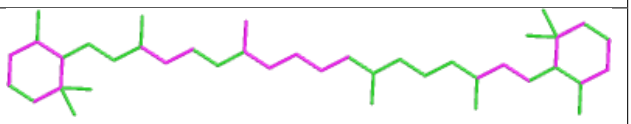


Rings

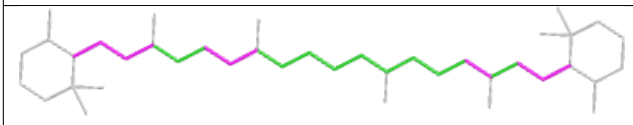
Ligand BCR b1 420



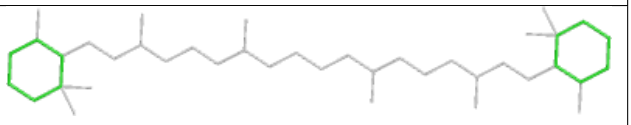
Bond lengths



Bond angles

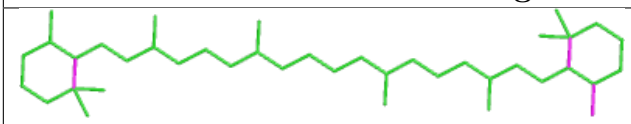


Torsions

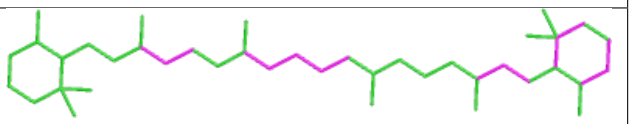


Rings

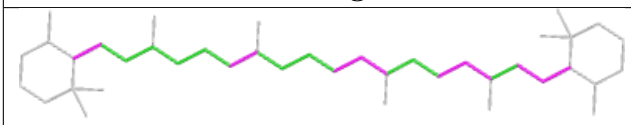
Ligand BCR cA 847



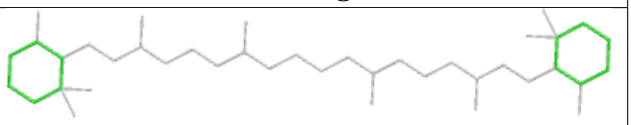
Bond lengths



Bond angles

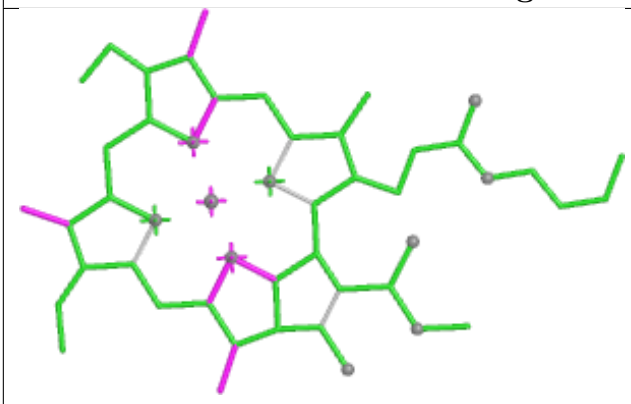


Torsions

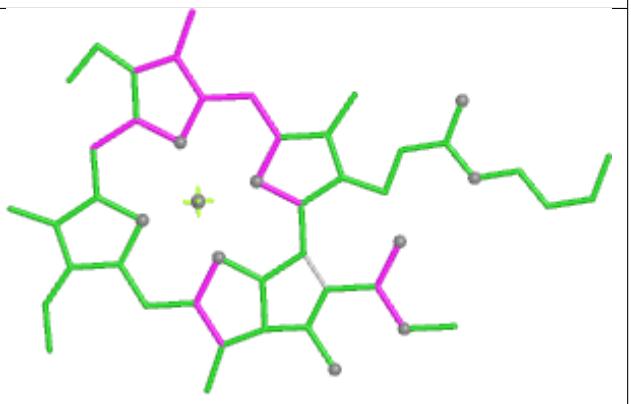


Rings

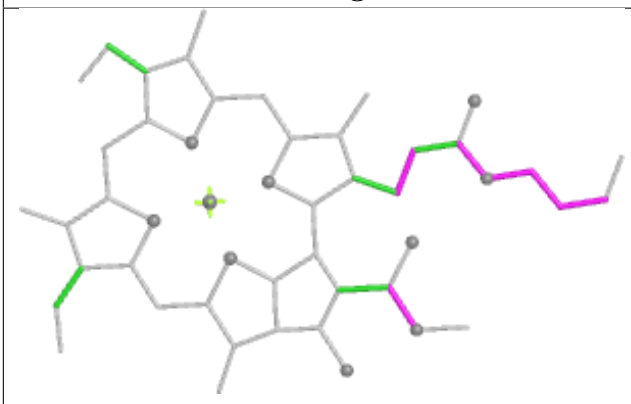
Ligand CLA cB 832



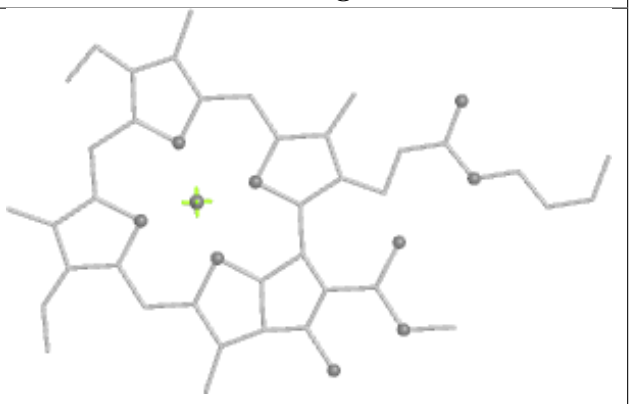
Bond lengths



Bond angles

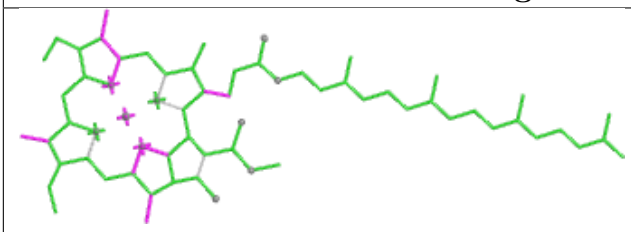


Torsions

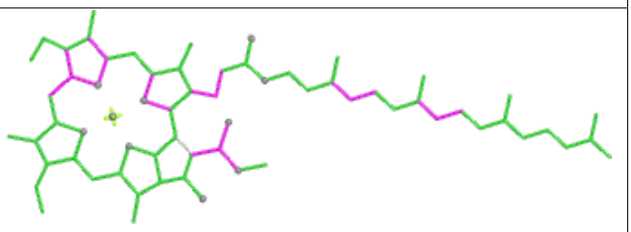


Rings

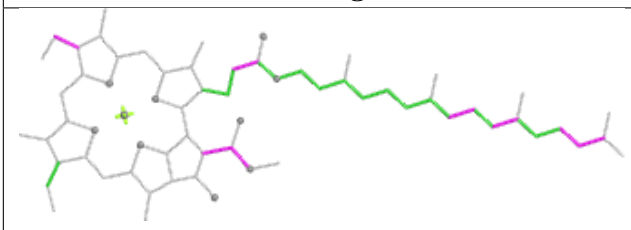
Ligand CLA bB 802



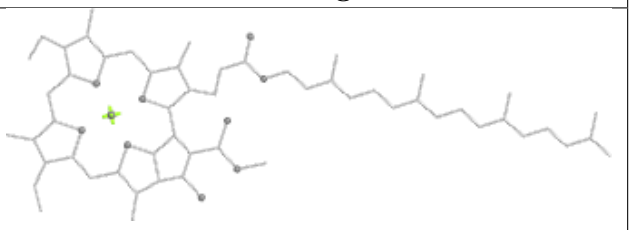
Bond lengths



Bond angles

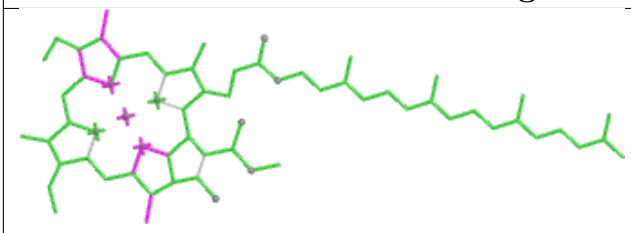


Torsions

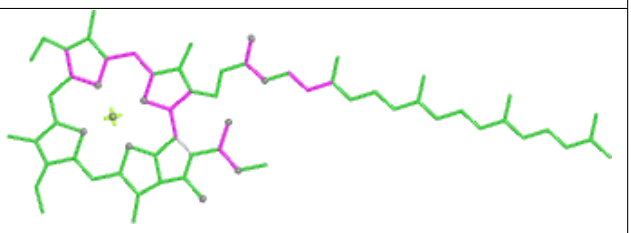


Rings

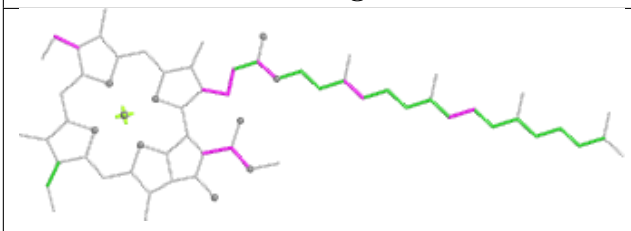
Ligand CLA b3 404



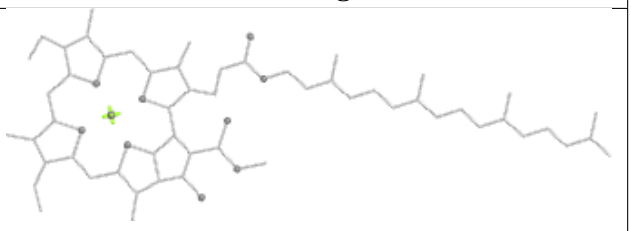
Bond lengths



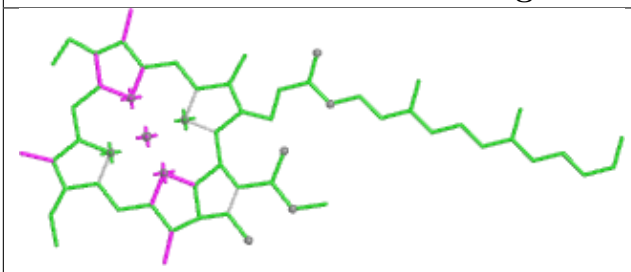
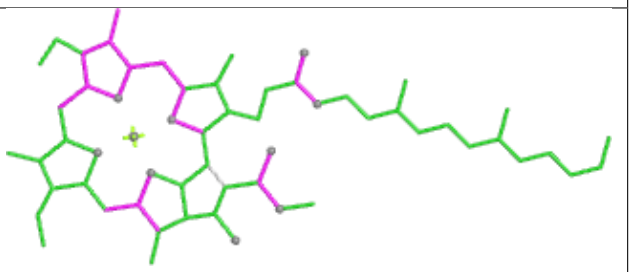
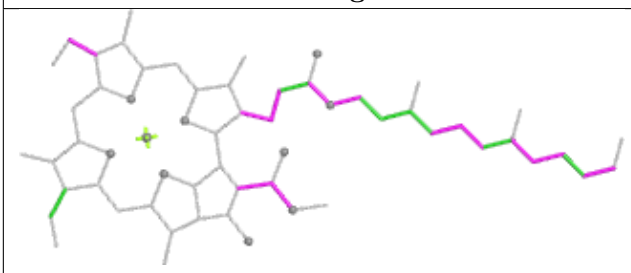
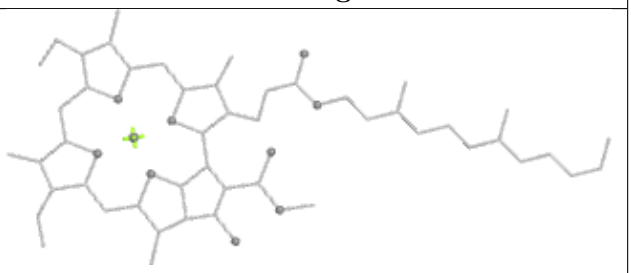
Bond angles

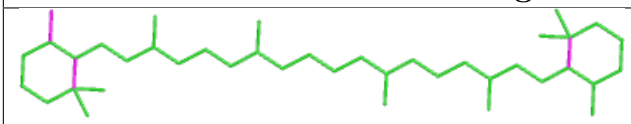
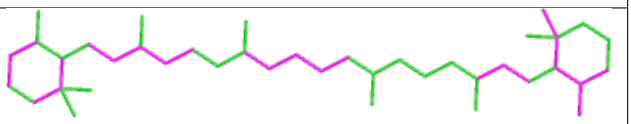
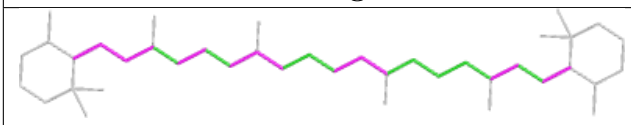
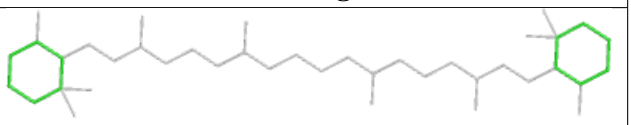


Torsions

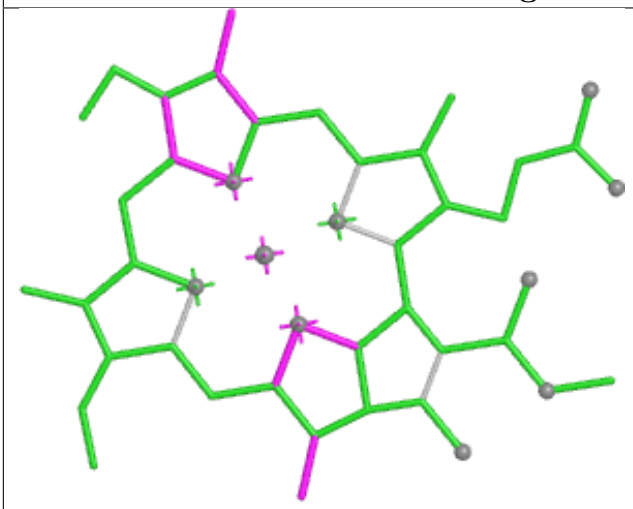


Rings

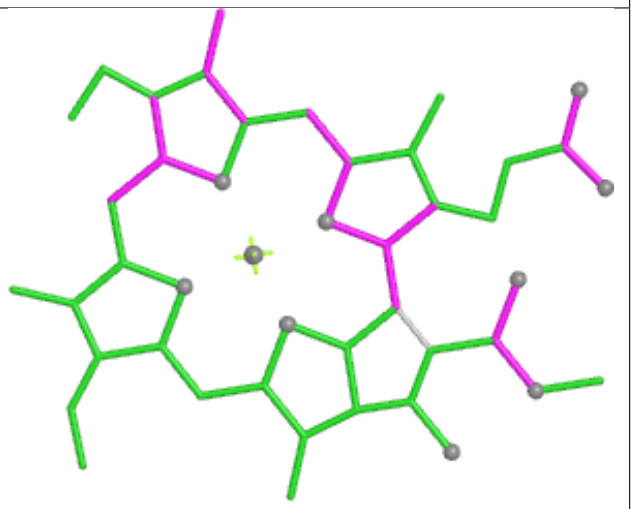
Ligand CLA cA 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR bL 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

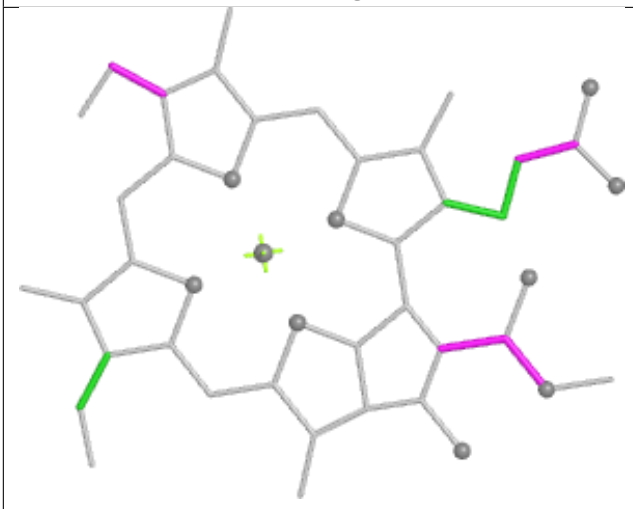
Ligand CLA a6 408



Bond lengths



Bond angles

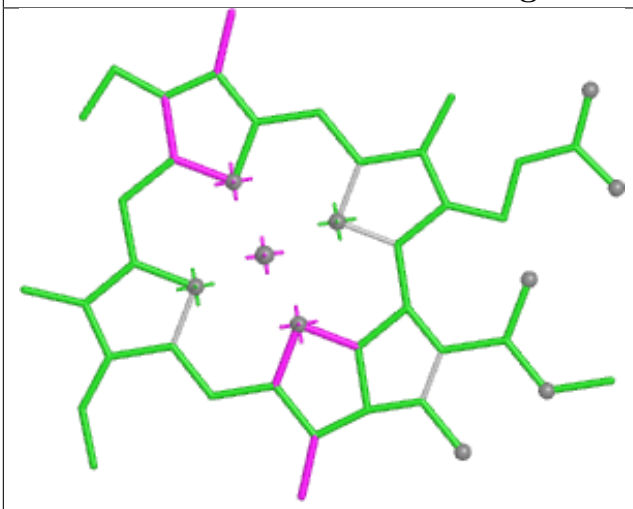


Torsions

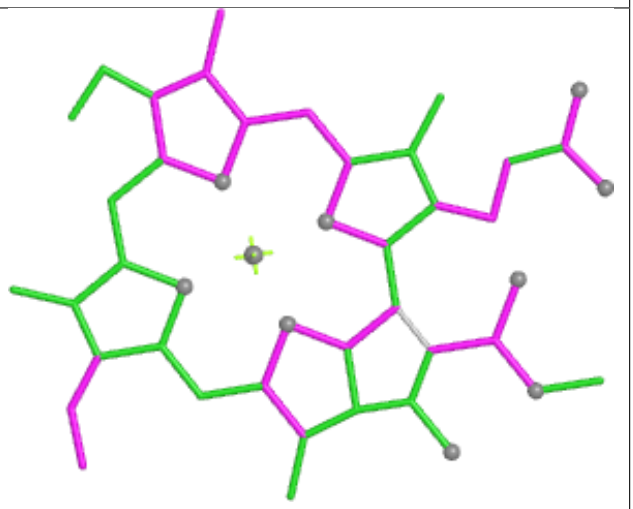


Rings

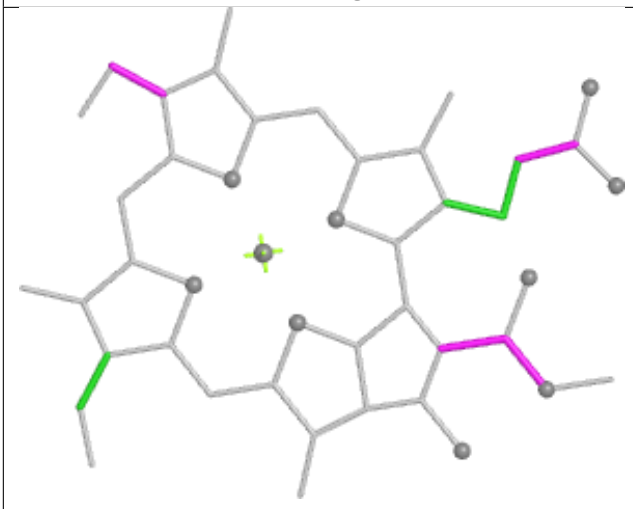
Ligand CLA a4 415



Bond lengths



Bond angles

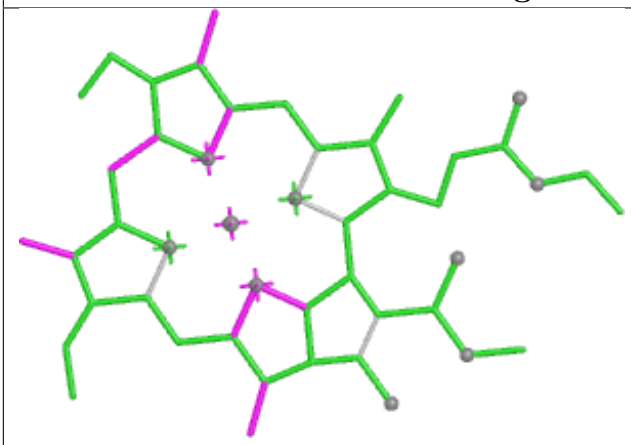


Torsions

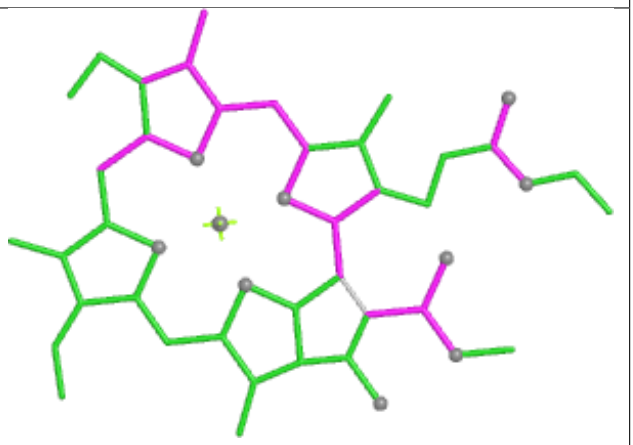


Rings

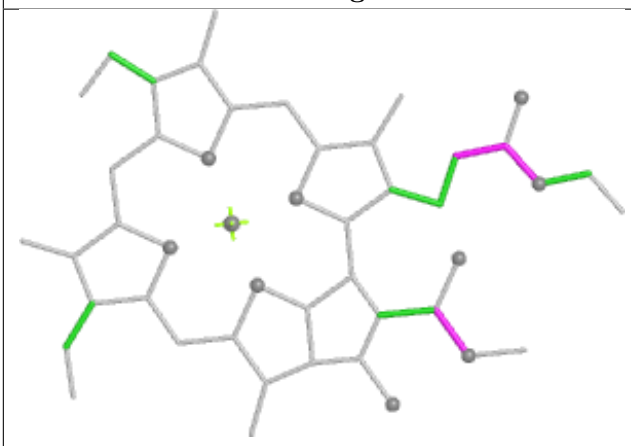
Ligand CLA bA 840



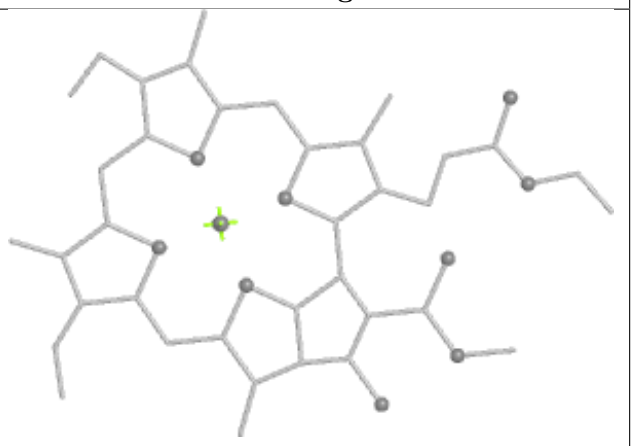
Bond lengths



Bond angles

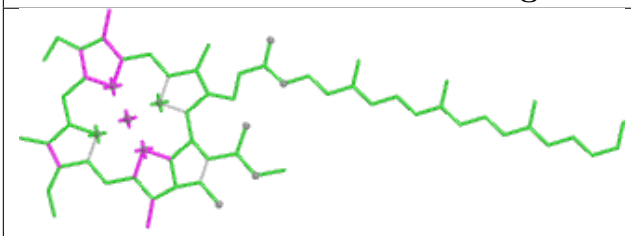


Torsions

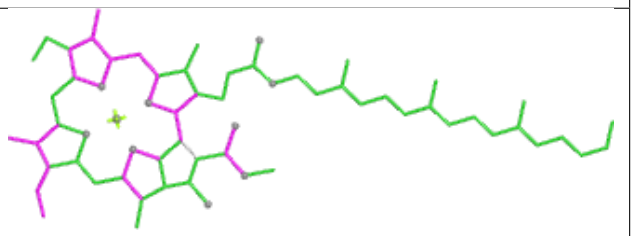


Rings

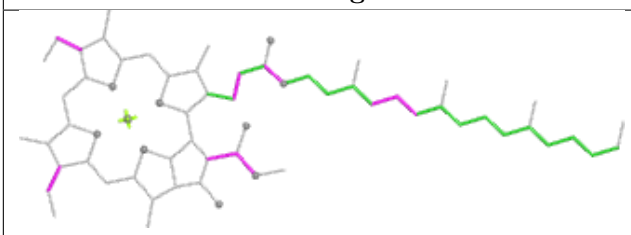
Ligand CLA c6 412



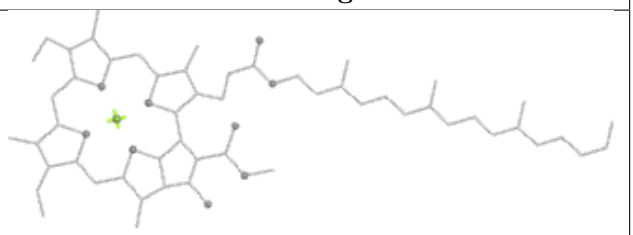
Bond lengths



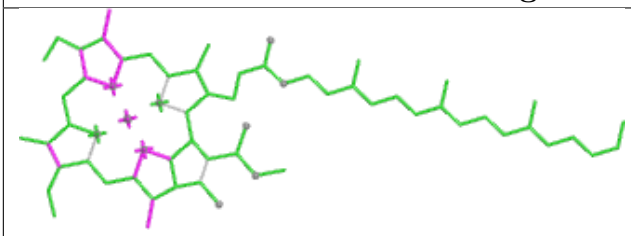
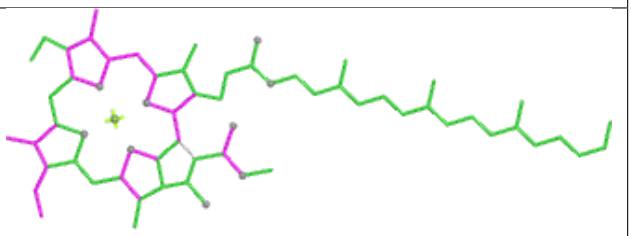
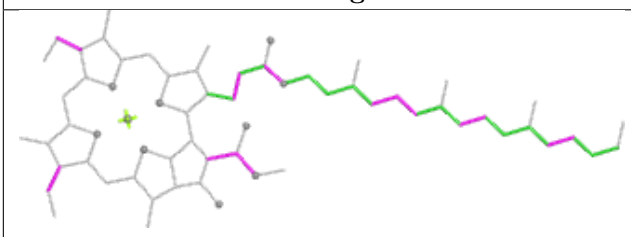
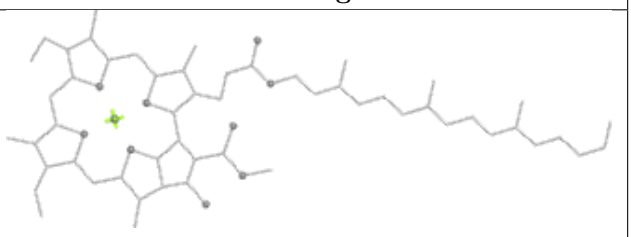
Bond angles

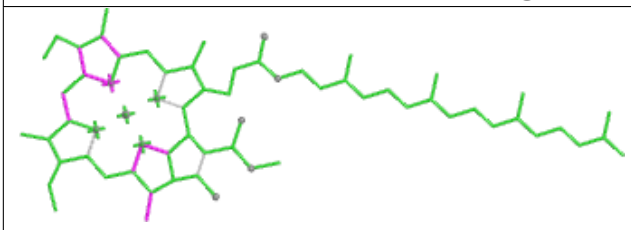
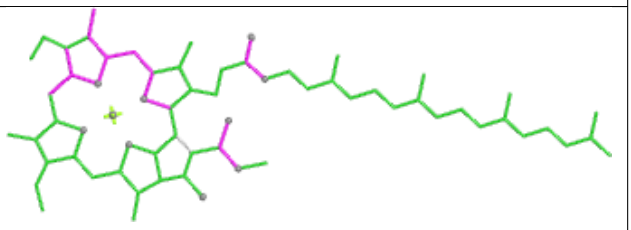
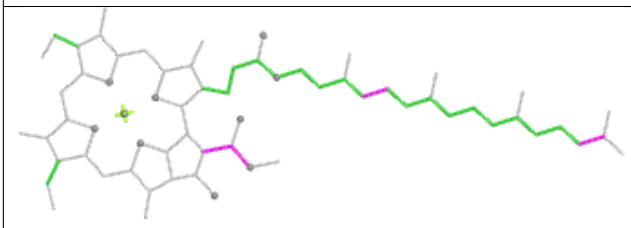
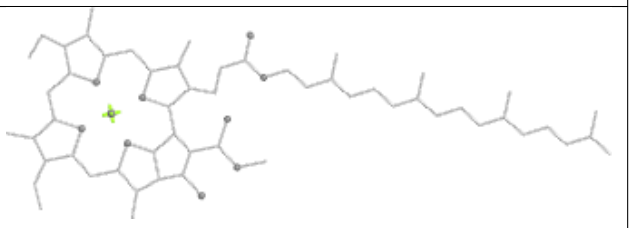


Torsions

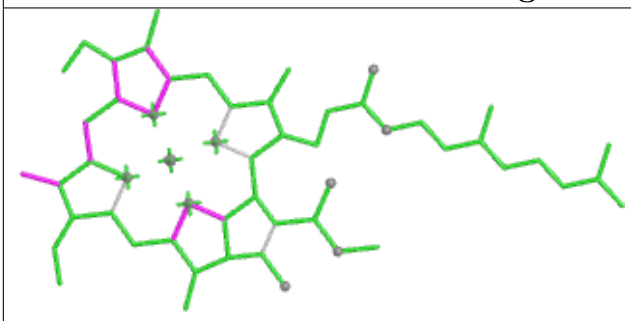


Rings

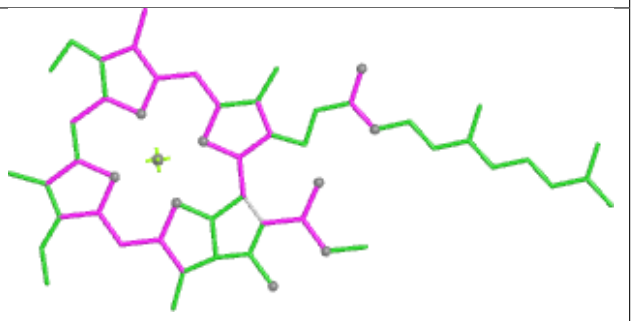
Ligand CLA a5 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b1 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

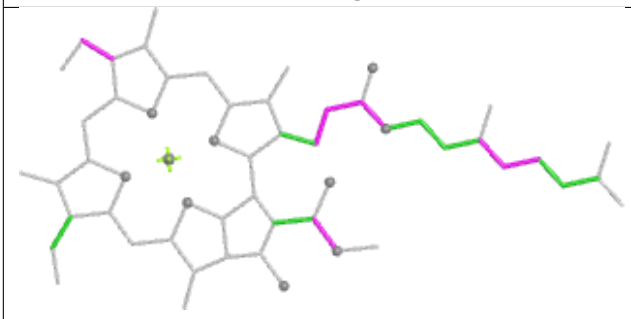
Ligand CLA b3 417



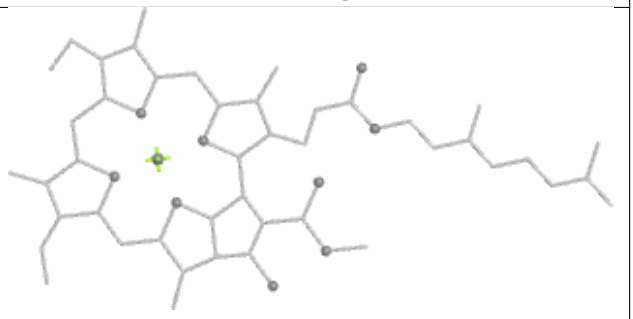
Bond lengths



Bond angles

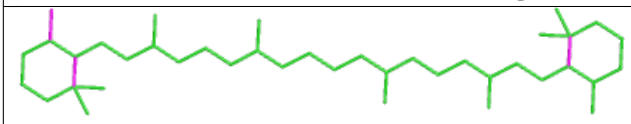


Torsions

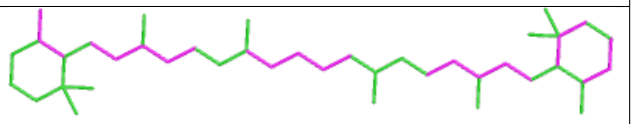


Rings

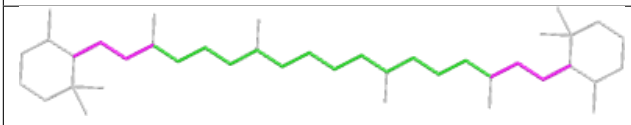
Ligand BCR bA 848



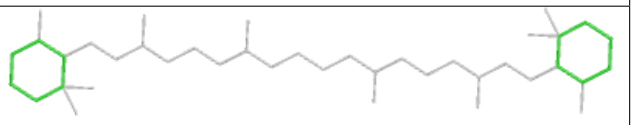
Bond lengths



Bond angles

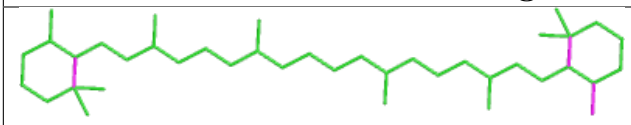


Torsions

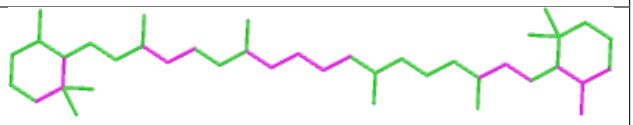


Rings

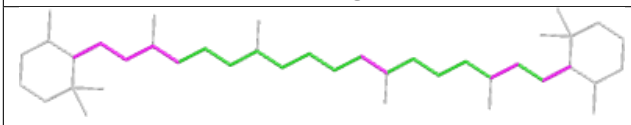
Ligand BCR cJ 104



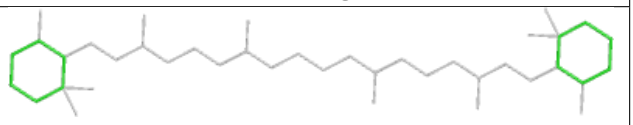
Bond lengths



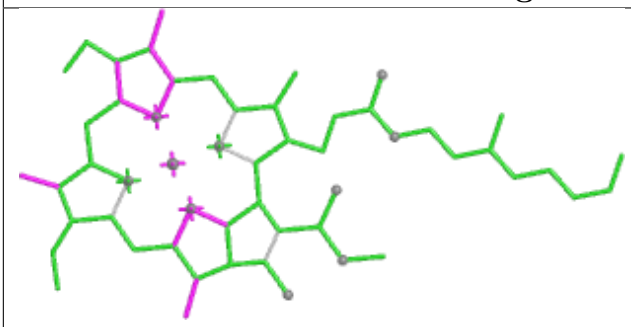
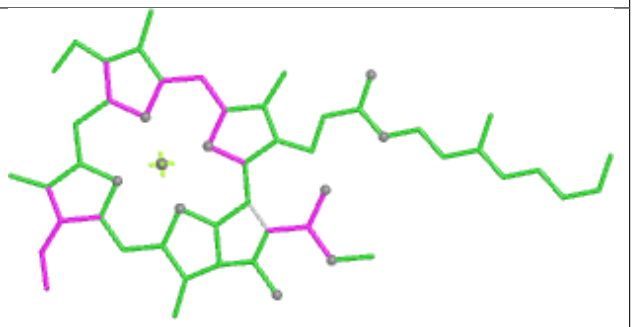
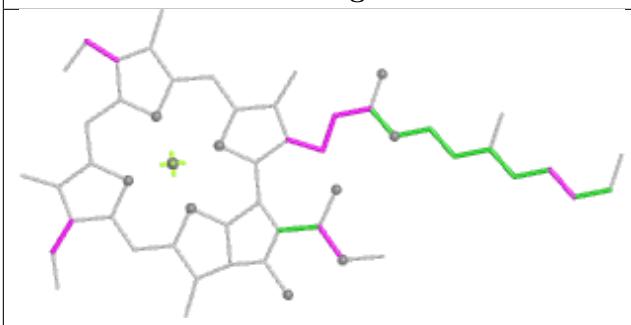
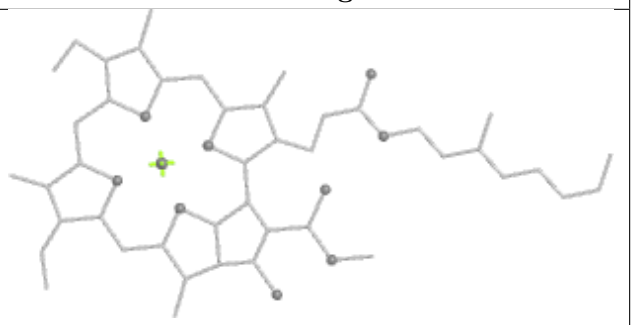
Bond angles



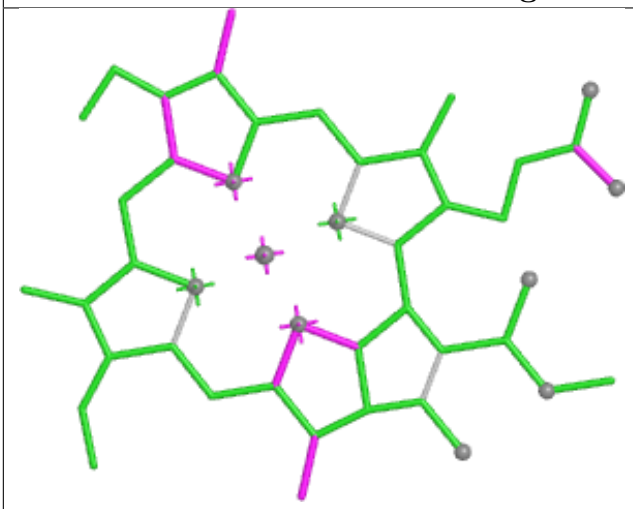
Torsions



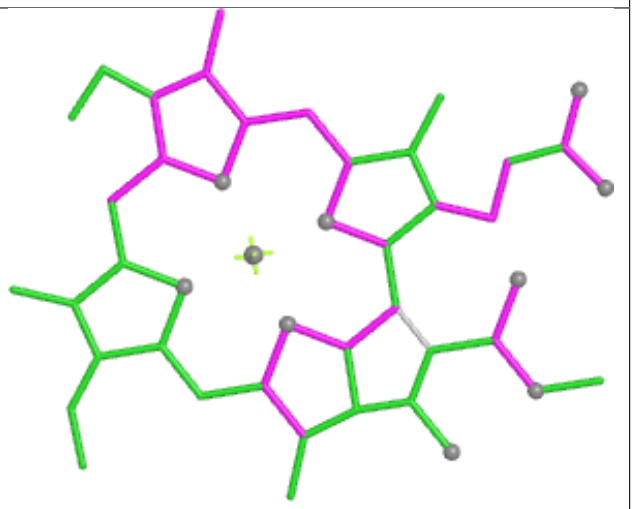
Rings

Ligand CLA cA 819	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

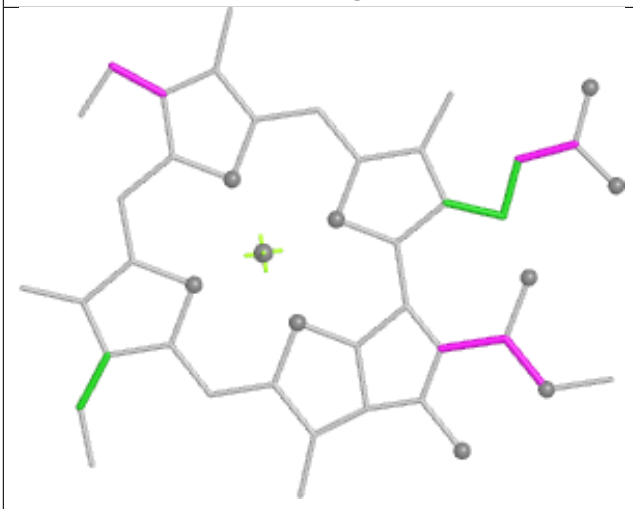
Ligand CLA a3 415



Bond lengths



Bond angles

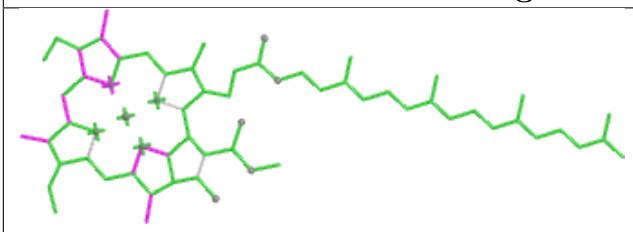


Torsions

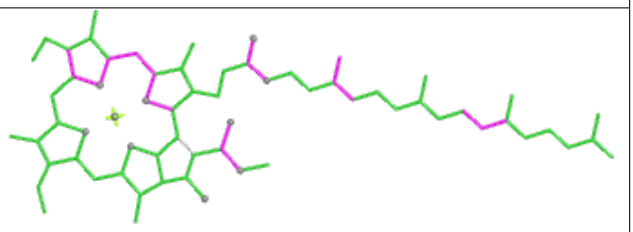


Rings

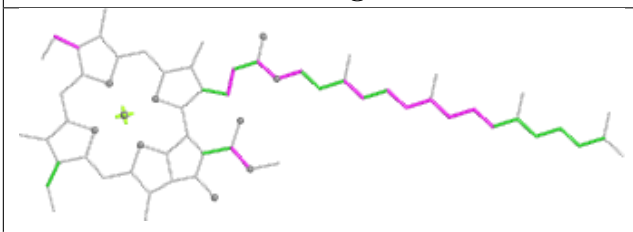
Ligand CLA cA 841



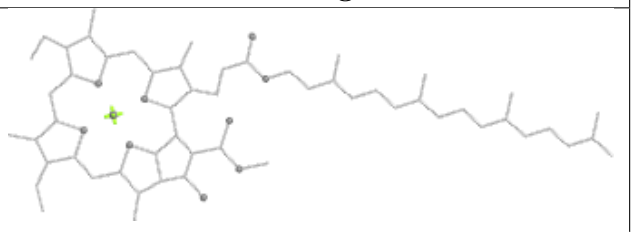
Bond lengths



Bond angles

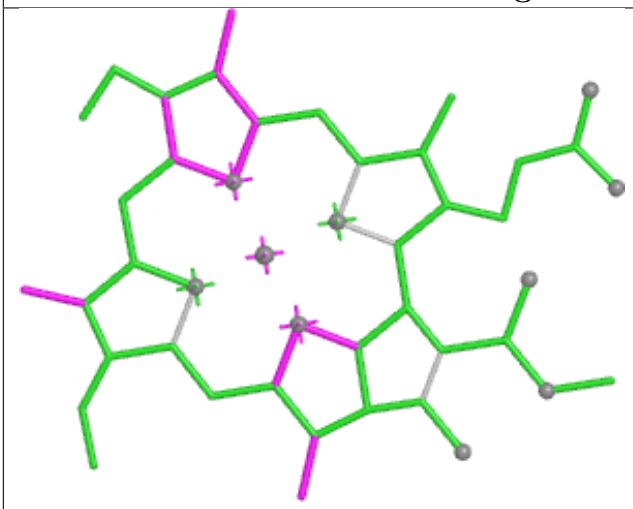


Torsions

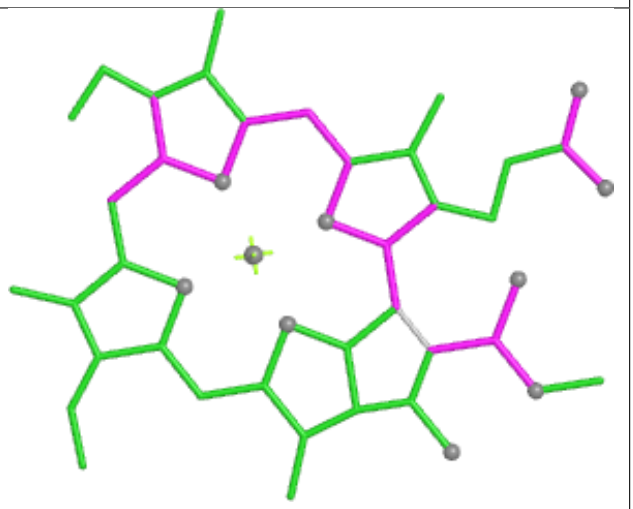


Rings

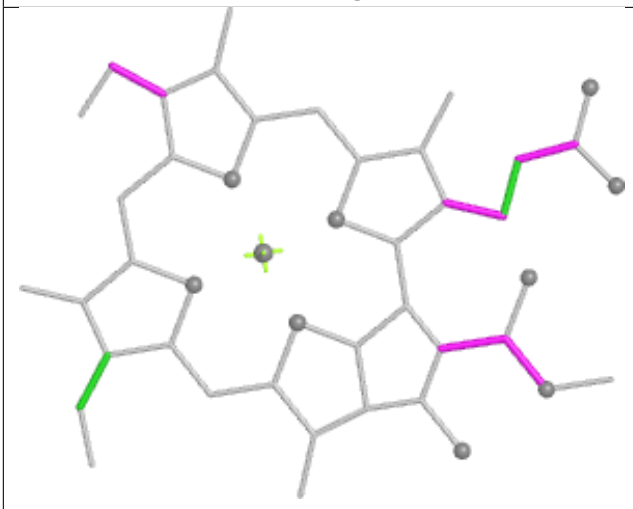
Ligand CLA aK 102



Bond lengths



Bond angles

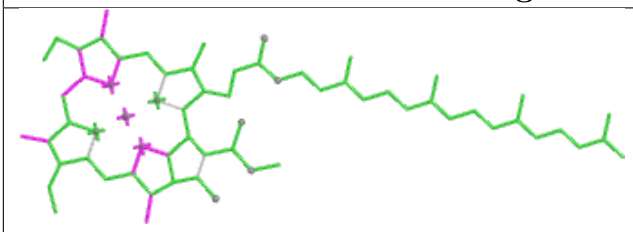


Torsions

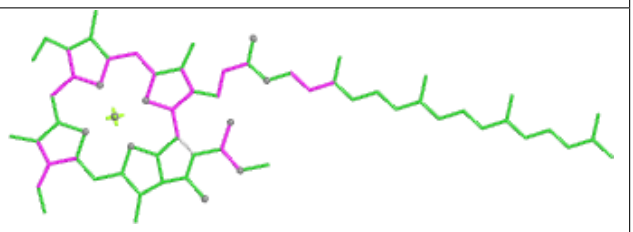


Rings

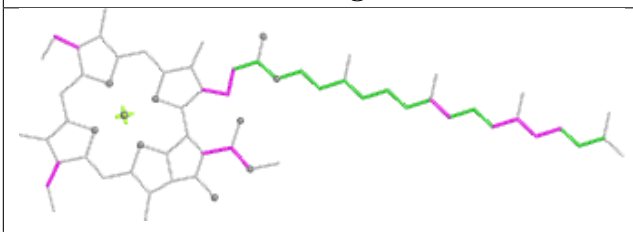
Ligand CLA aB 840



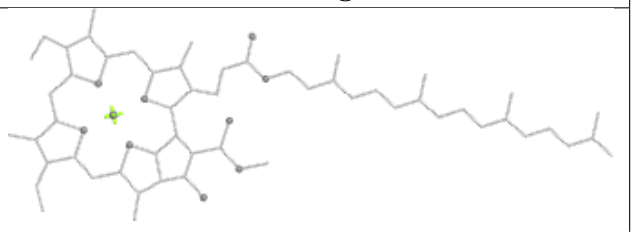
Bond lengths



Bond angles

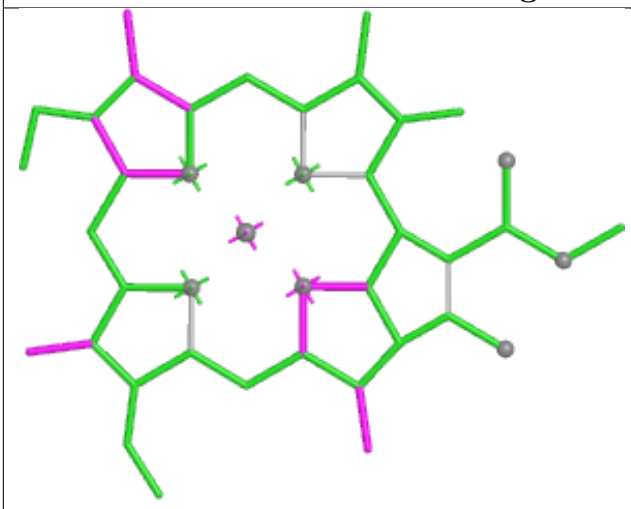


Torsions

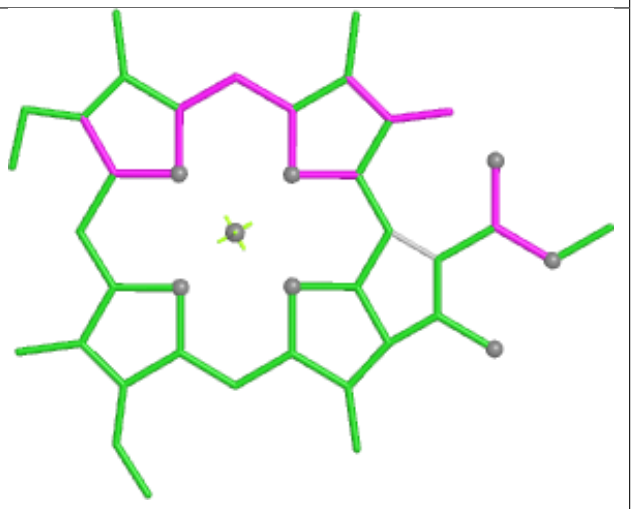


Rings

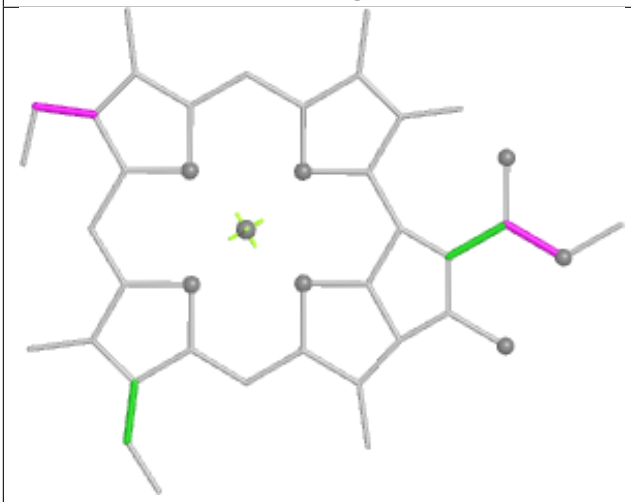
Ligand CLA a4 414



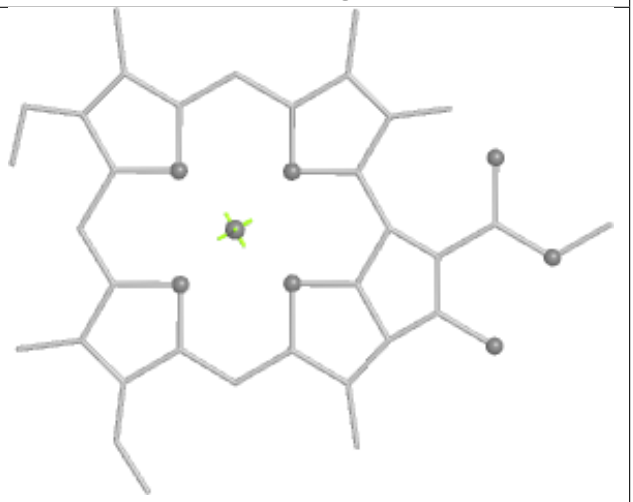
Bond lengths



Bond angles



Torsions

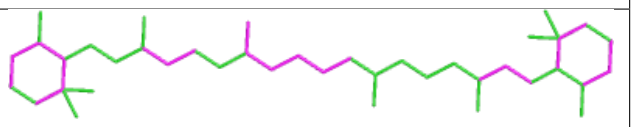


Rings

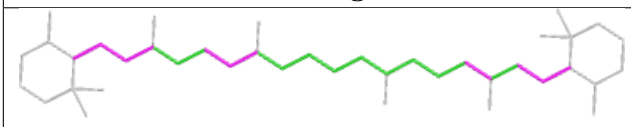
Ligand BCR c4 420



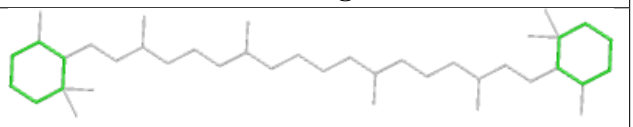
Bond lengths



Bond angles

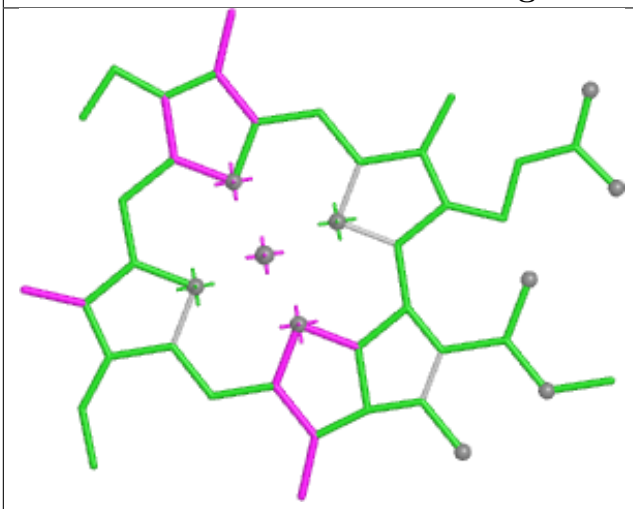


Torsions

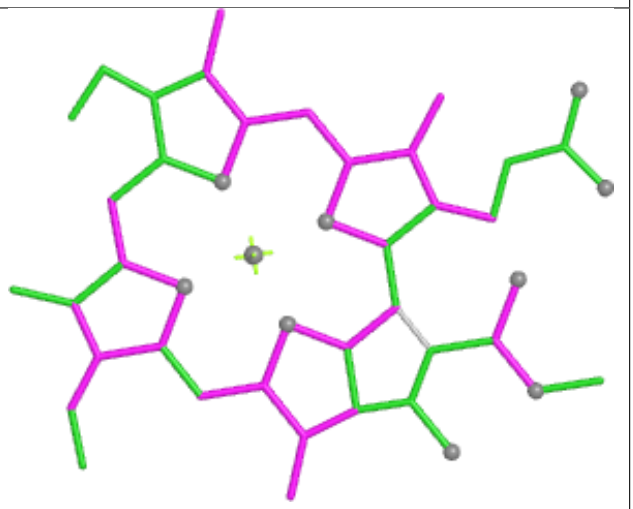


Rings

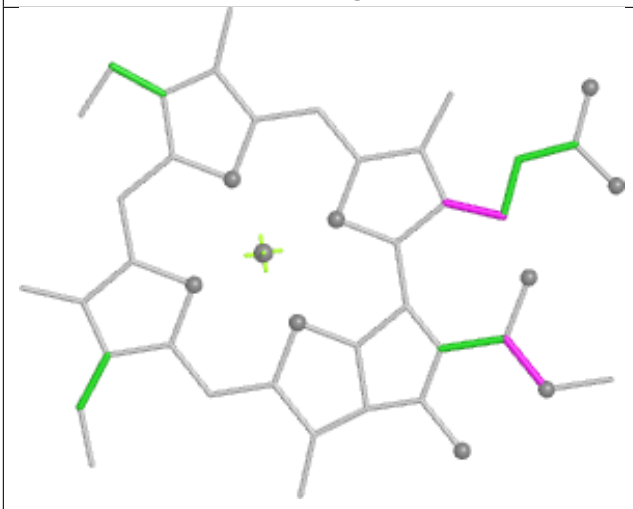
Ligand CLA b3 405



Bond lengths



Bond angles

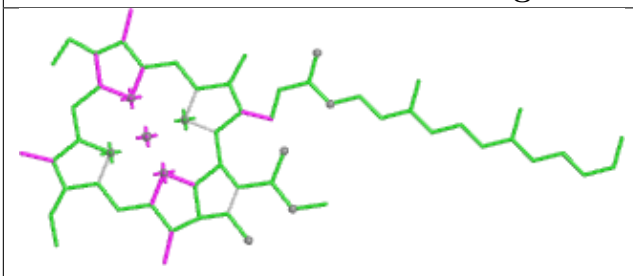


Torsions

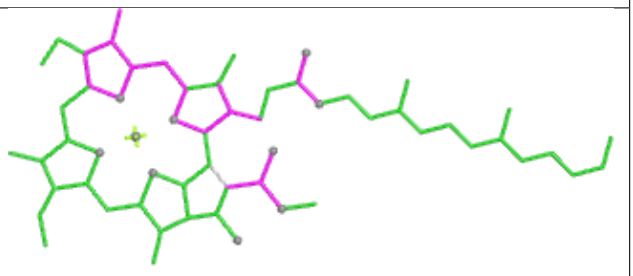


Rings

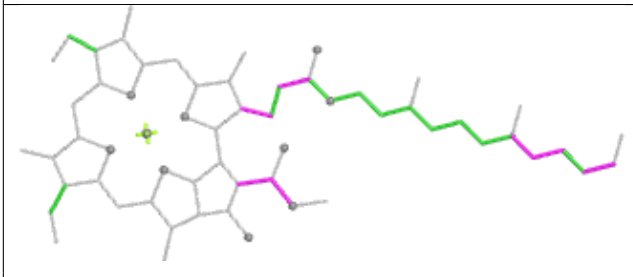
Ligand CLA bA 805



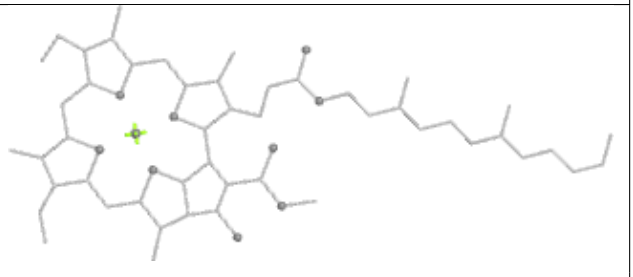
Bond lengths



Bond angles

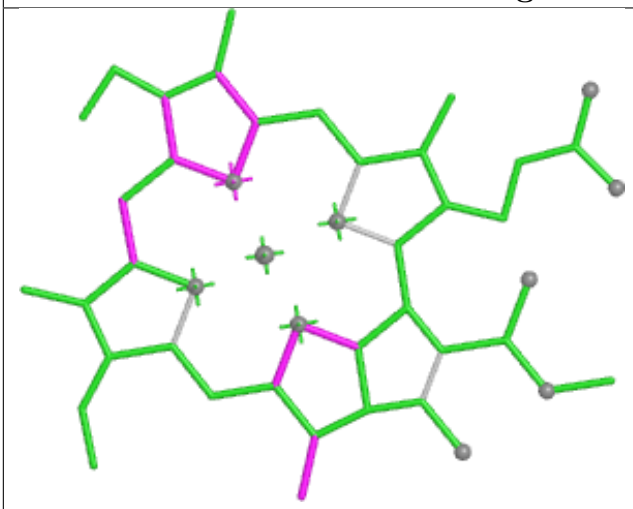


Torsions

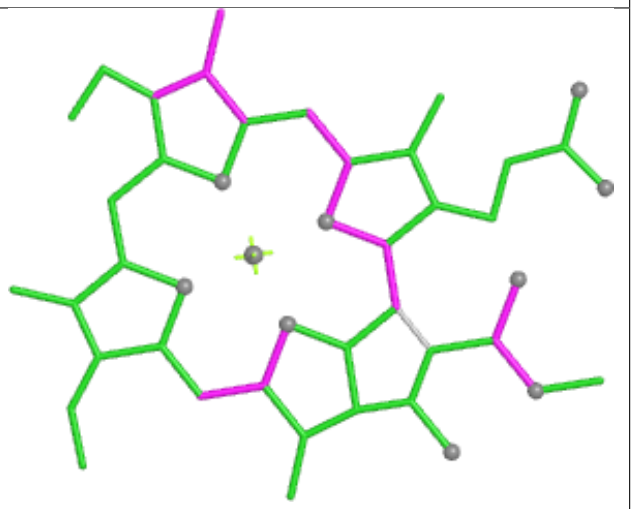


Rings

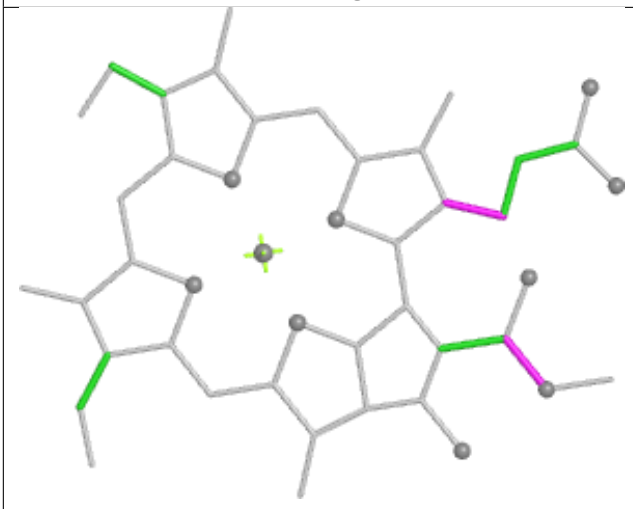
Ligand CLA cB 812



Bond lengths



Bond angles

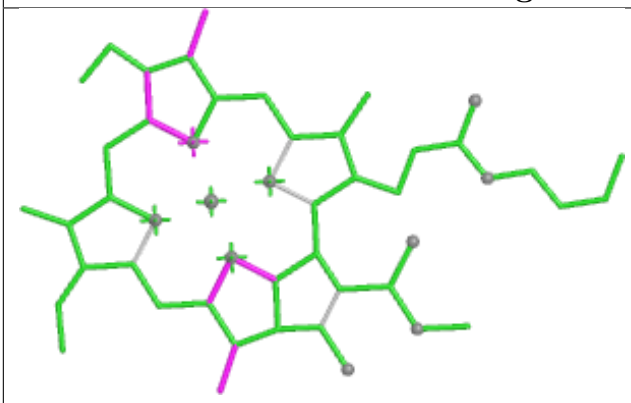


Torsions

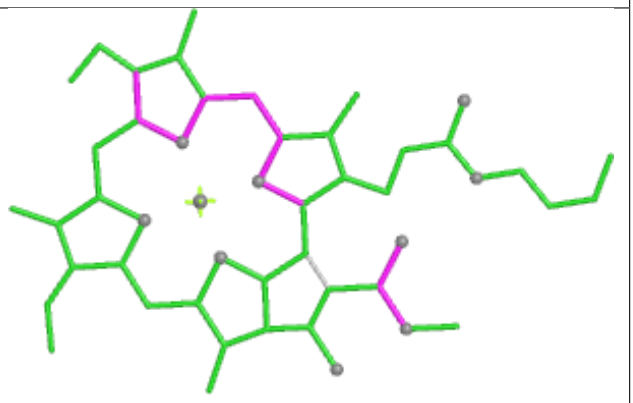


Rings

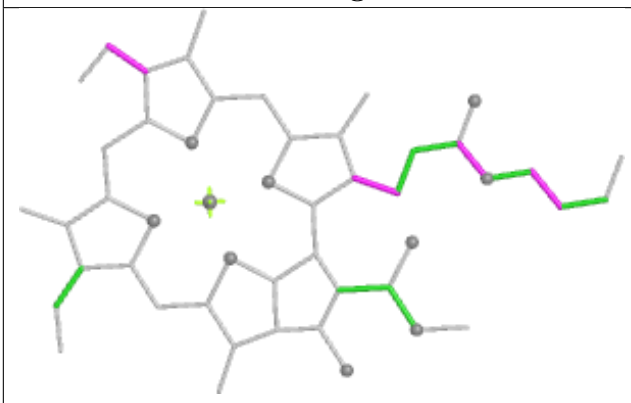
Ligand CLA cA 817



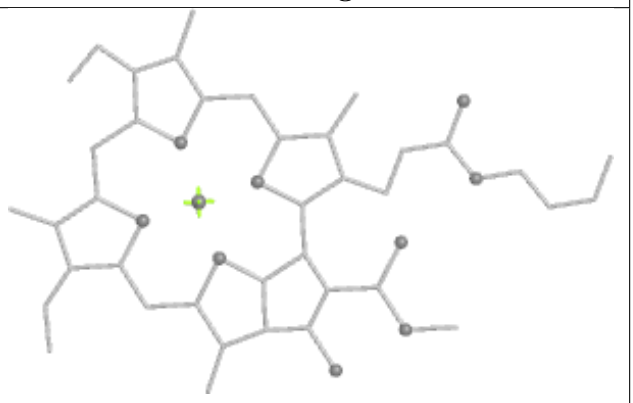
Bond lengths



Bond angles

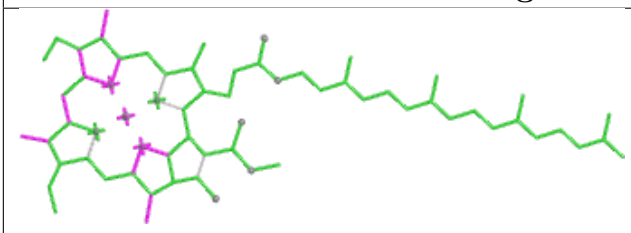


Torsions

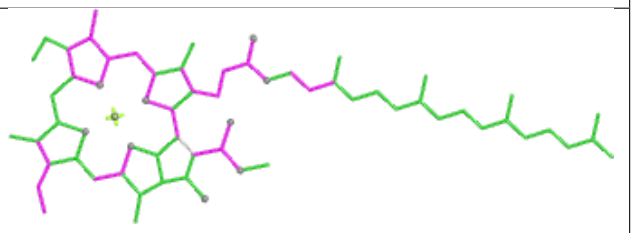


Rings

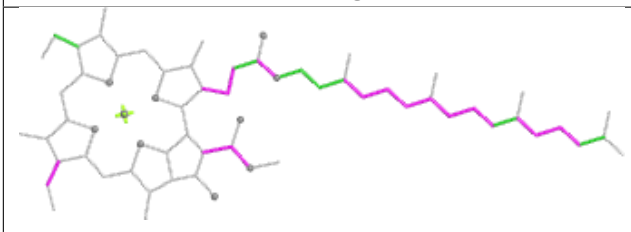
Ligand CLA cB 814



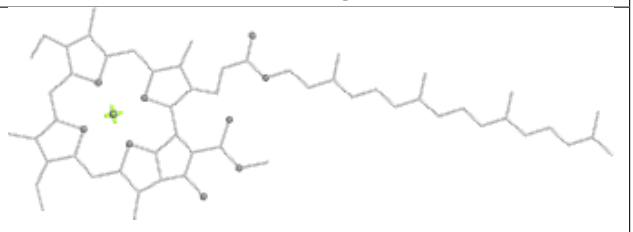
Bond lengths



Bond angles

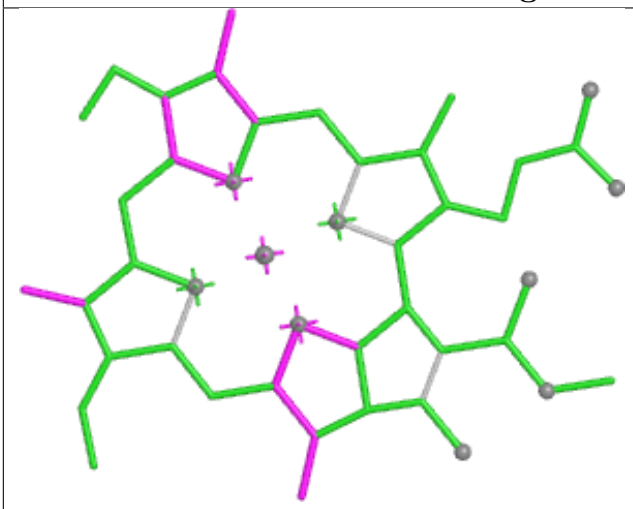


Torsions

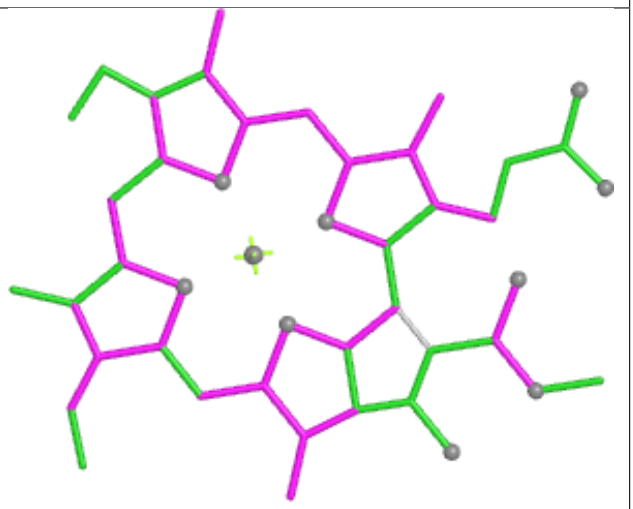


Rings

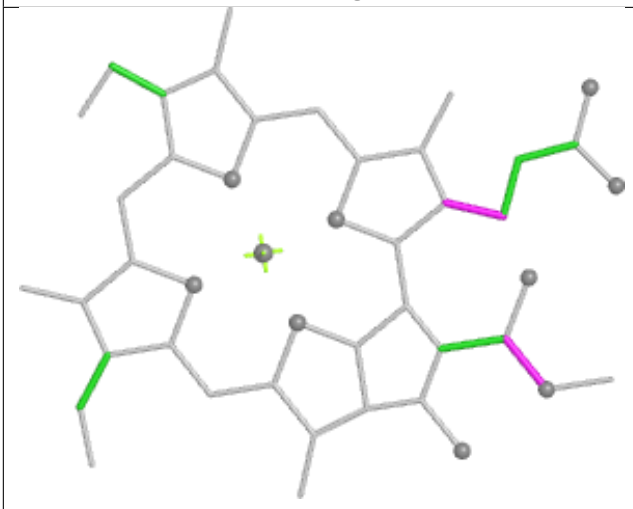
Ligand CLA a3 405



Bond lengths



Bond angles

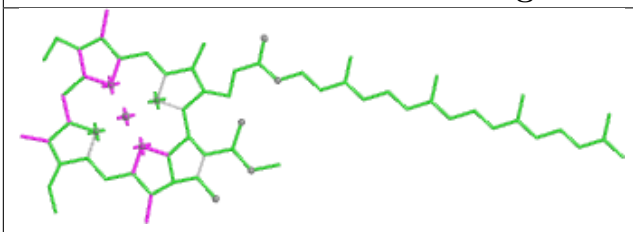


Torsions

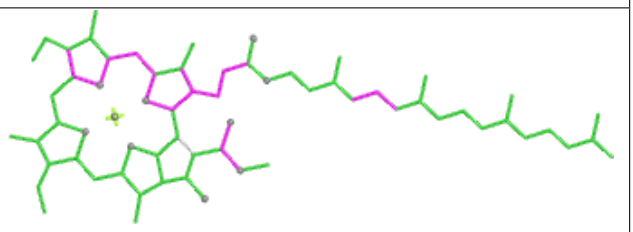


Rings

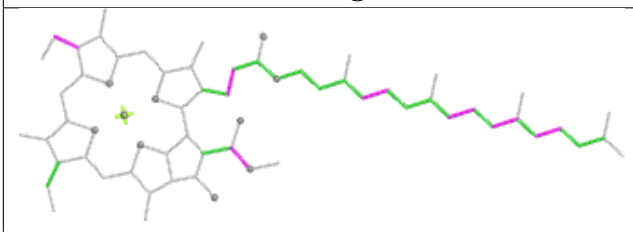
Ligand CLA cB 839



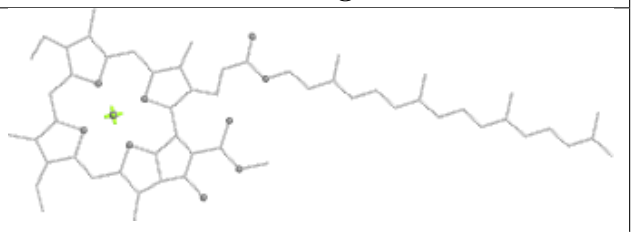
Bond lengths



Bond angles

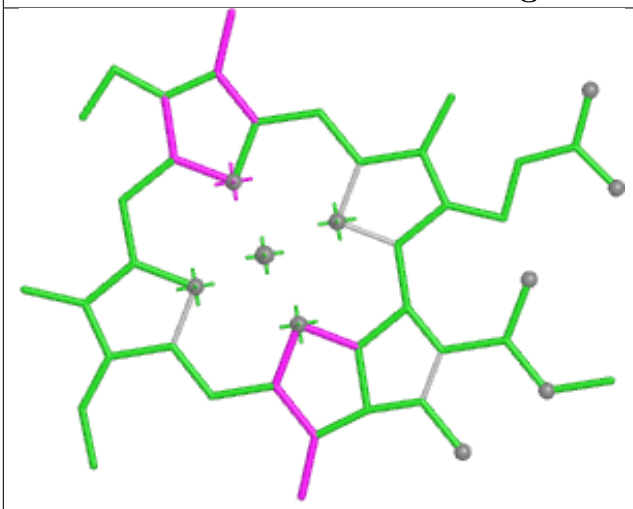


Torsions

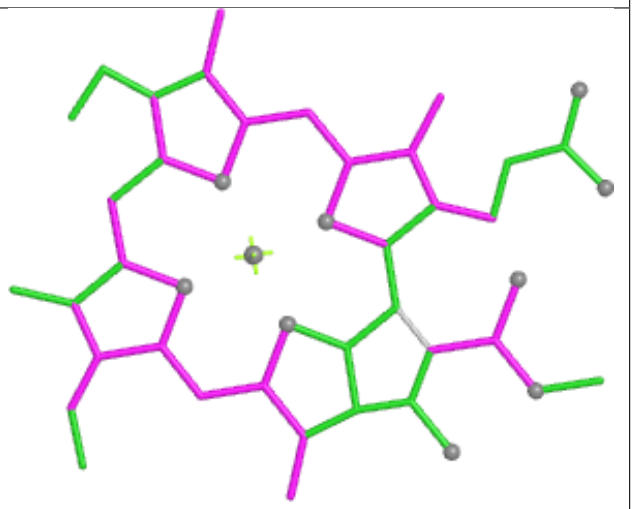


Rings

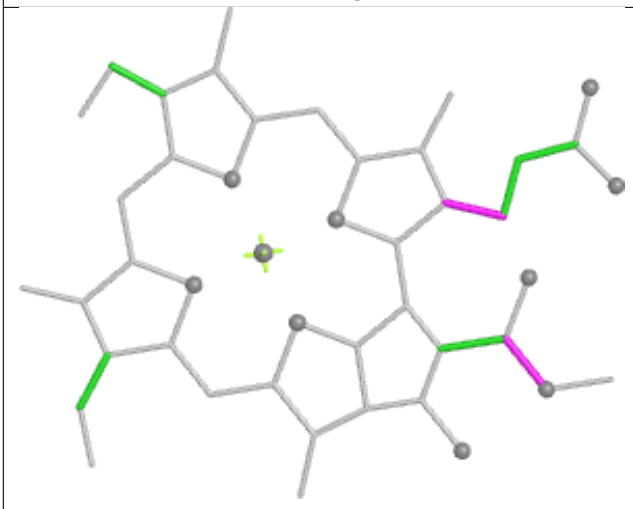
Ligand CLA c6 407



Bond lengths



Bond angles

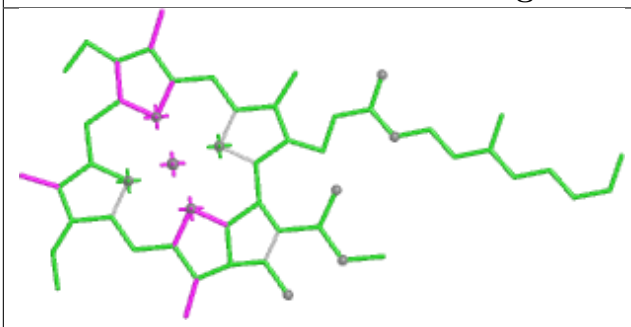


Torsions

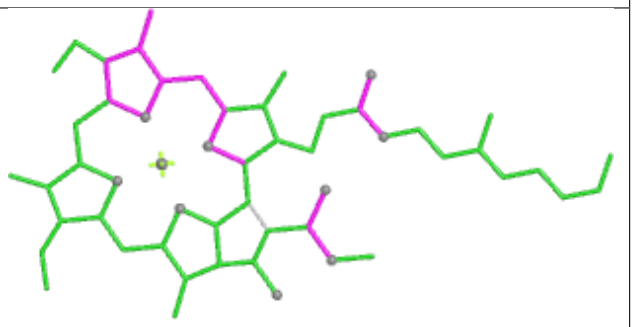


Rings

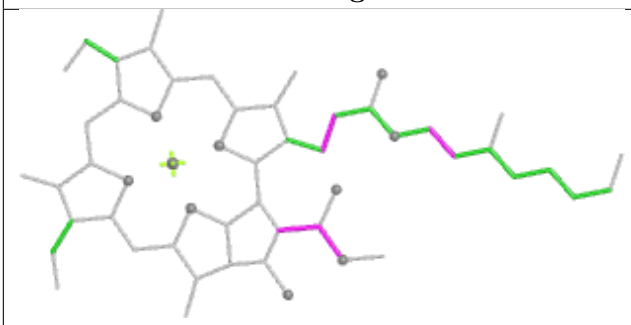
Ligand CLA cB 805



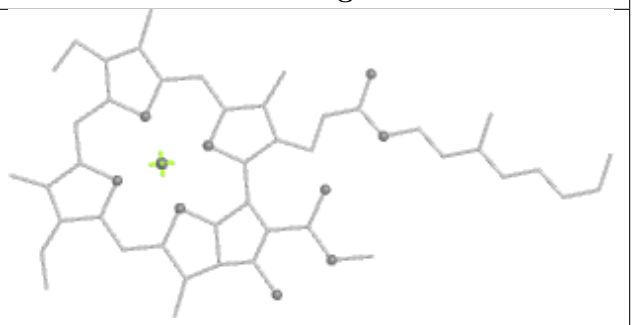
Bond lengths



Bond angles

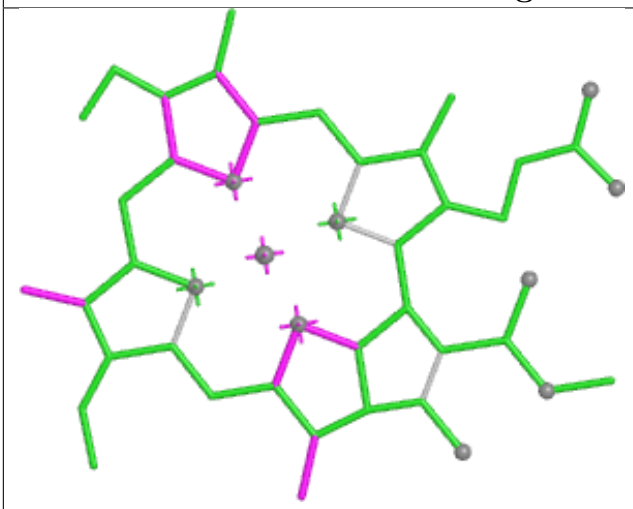


Torsions

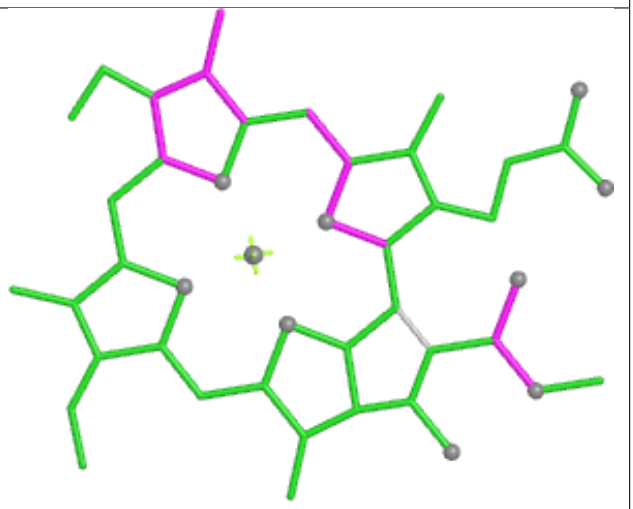


Rings

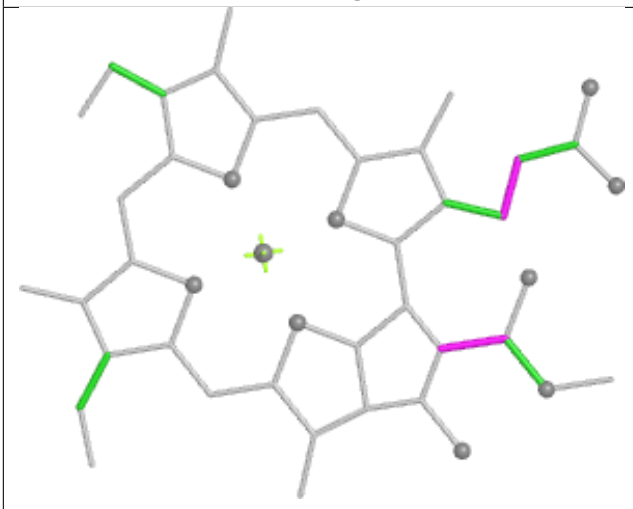
Ligand CLA cA 816



Bond lengths



Bond angles

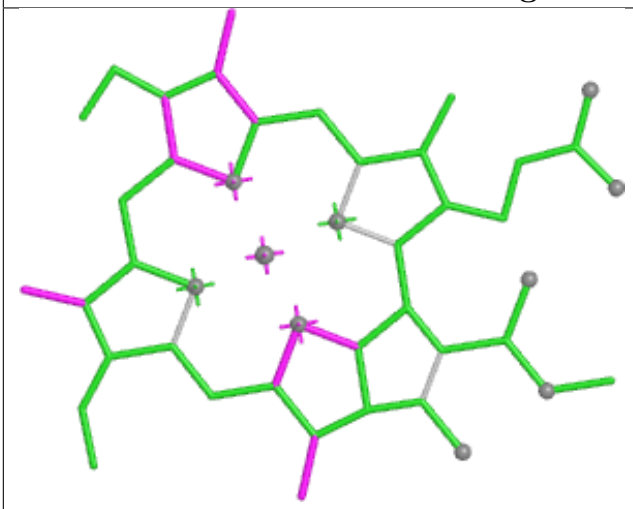


Torsions

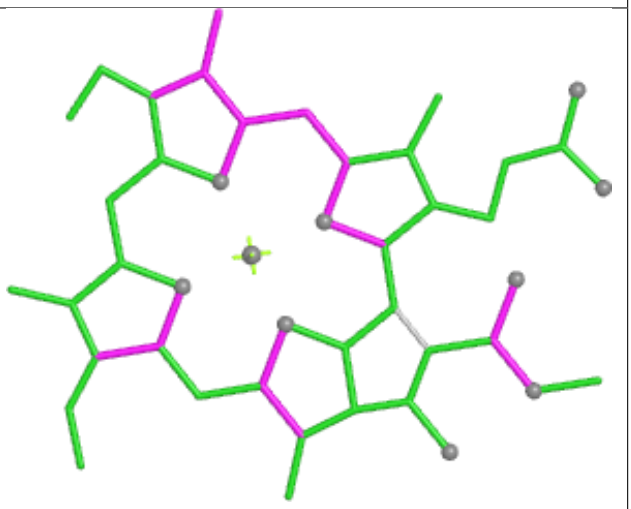


Rings

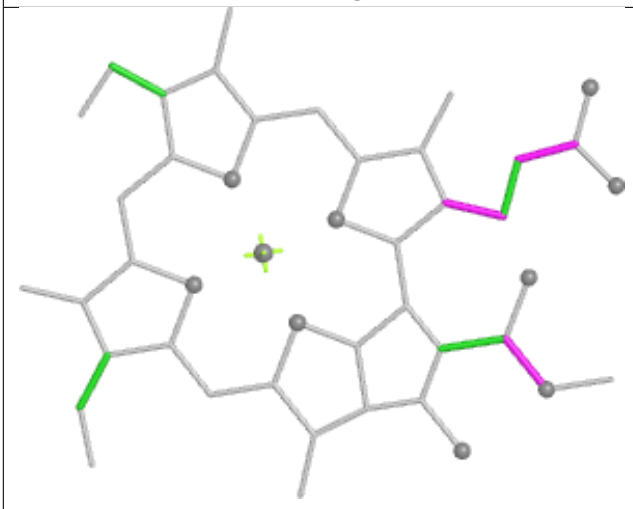
Ligand CLA a1 407



Bond lengths



Bond angles

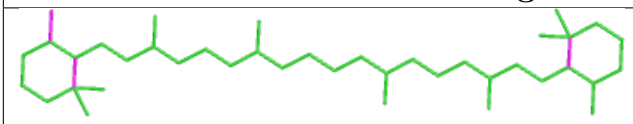


Torsions

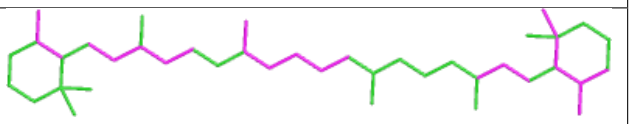


Rings

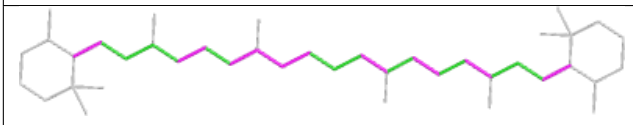
Ligand BCR aJ 204



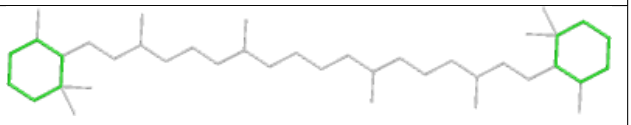
Bond lengths



Bond angles

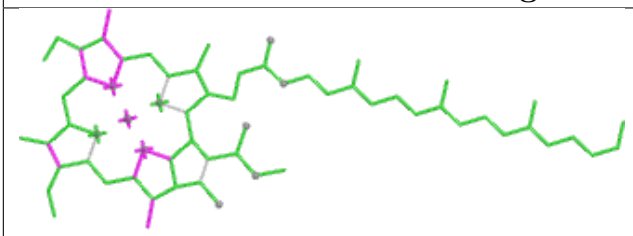


Torsions

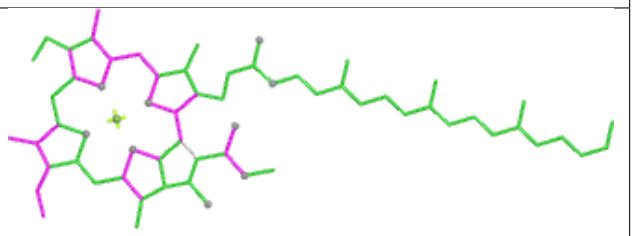


Rings

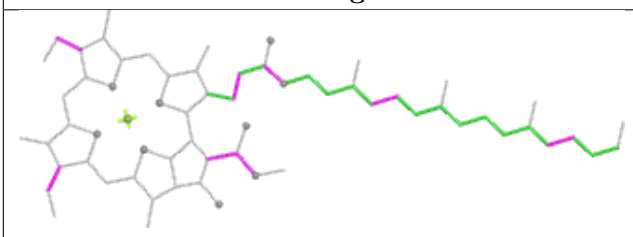
Ligand CLA a3 410



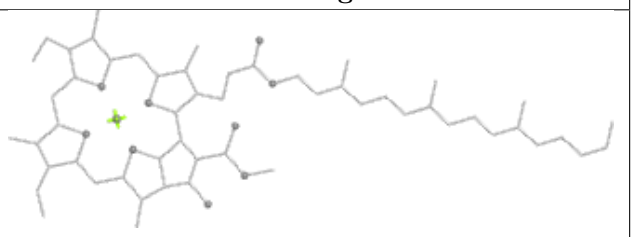
Bond lengths



Bond angles

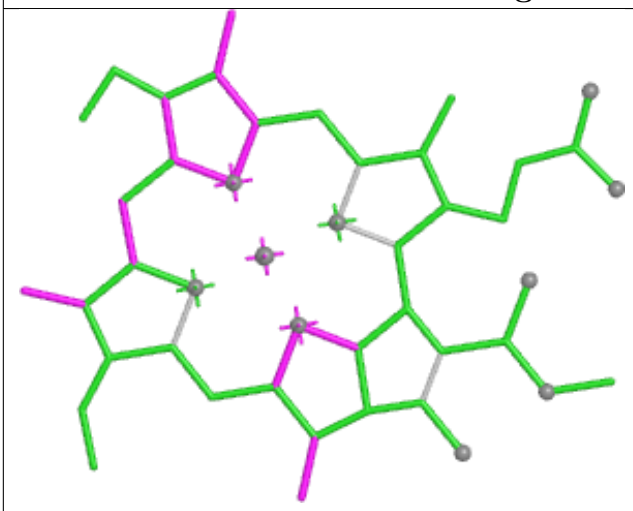


Torsions

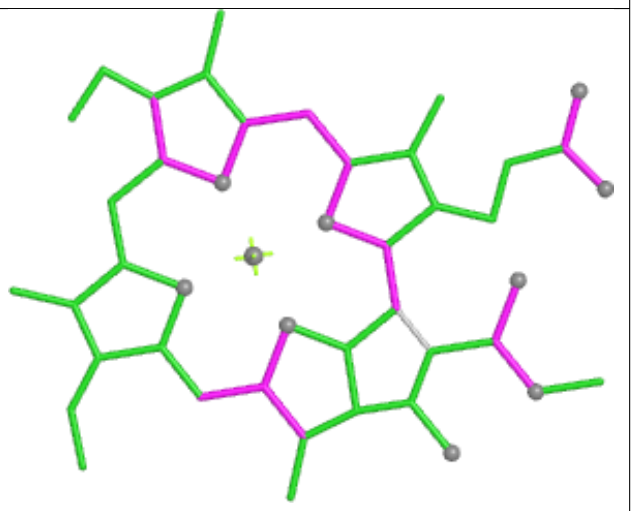


Rings

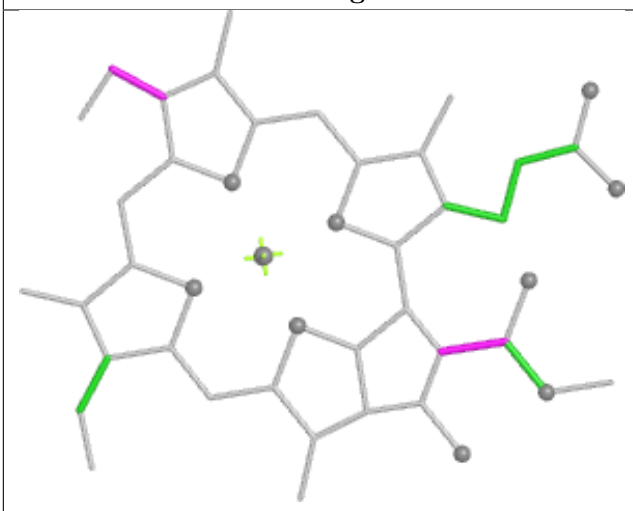
Ligand CLA aA 815



Bond lengths



Bond angles

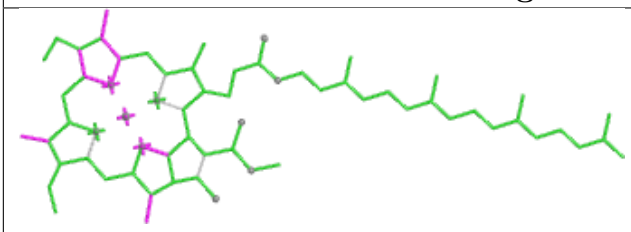


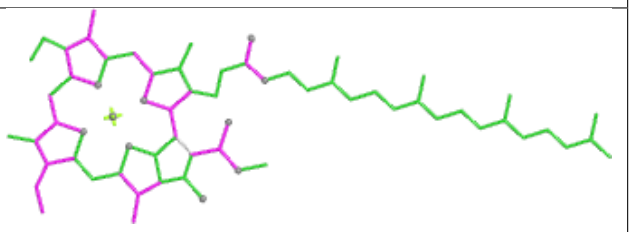
Torsions

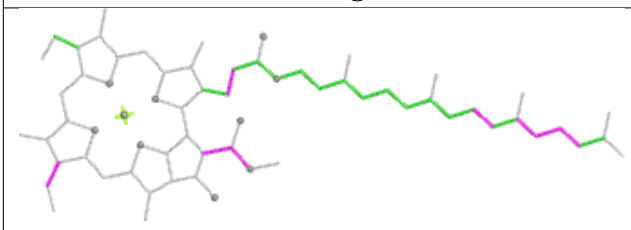


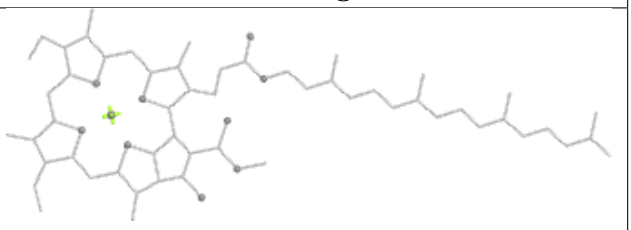
Rings

Ligand CLA cB 804

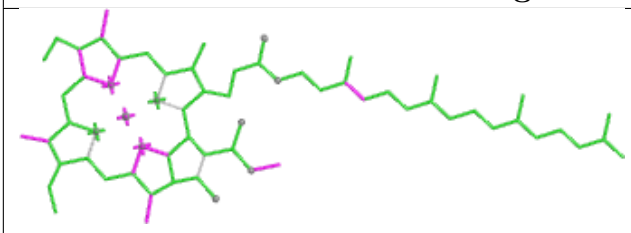

Bond lengths

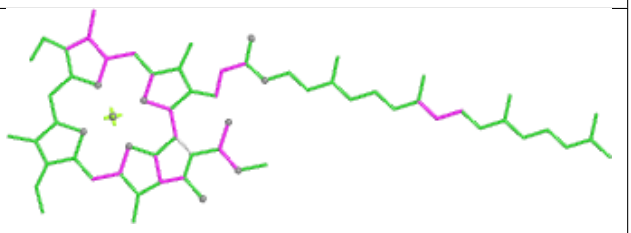

Bond angles

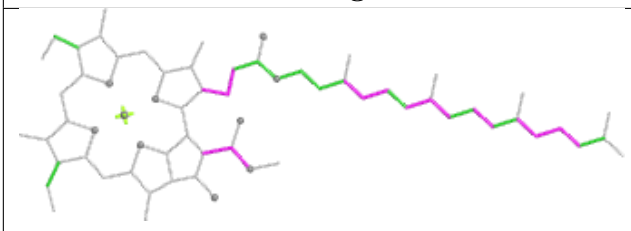

Torsions

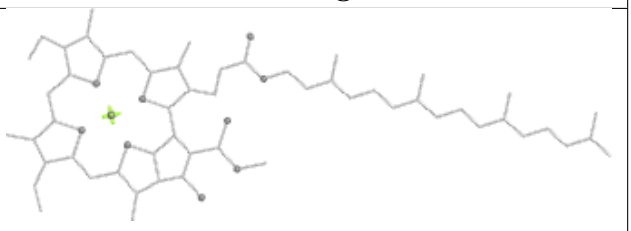

Rings

Ligand CLA bA 802

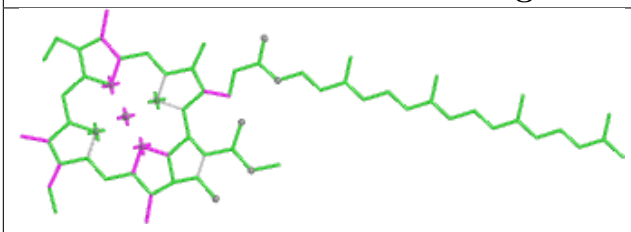

Bond lengths

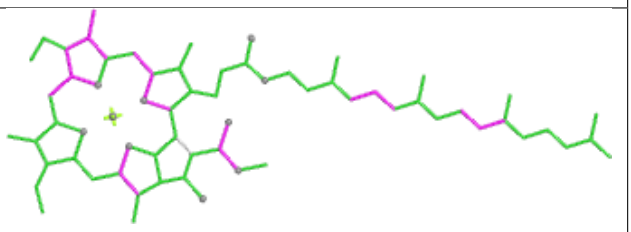

Bond angles

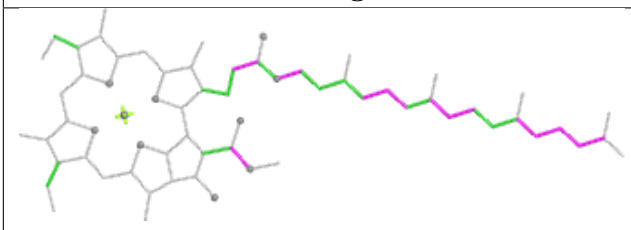

Torsions

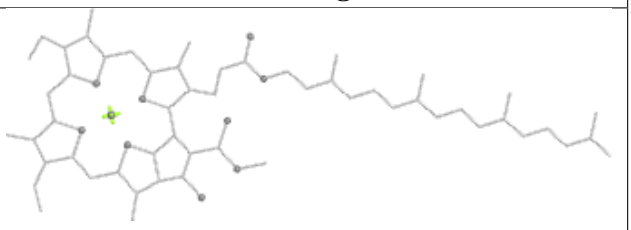

Rings

Ligand CLA aB 807

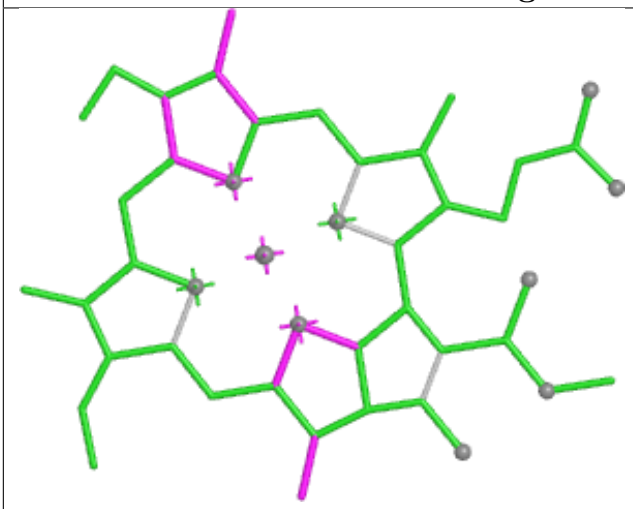

Bond lengths


Bond angles

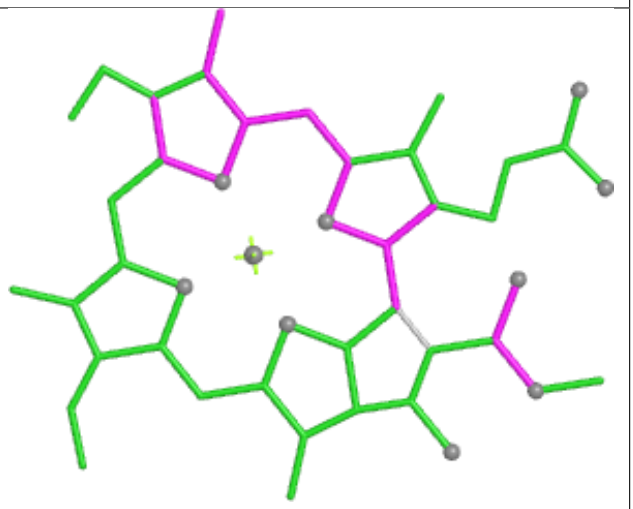

Torsions


Rings

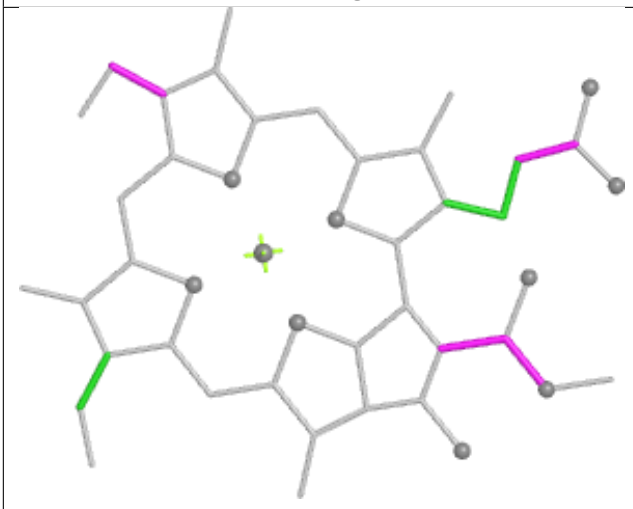
Ligand CLA b1 407



Bond lengths



Bond angles

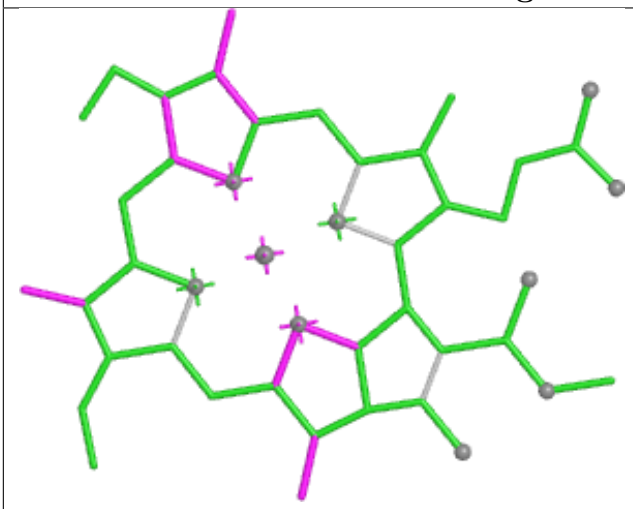


Torsions

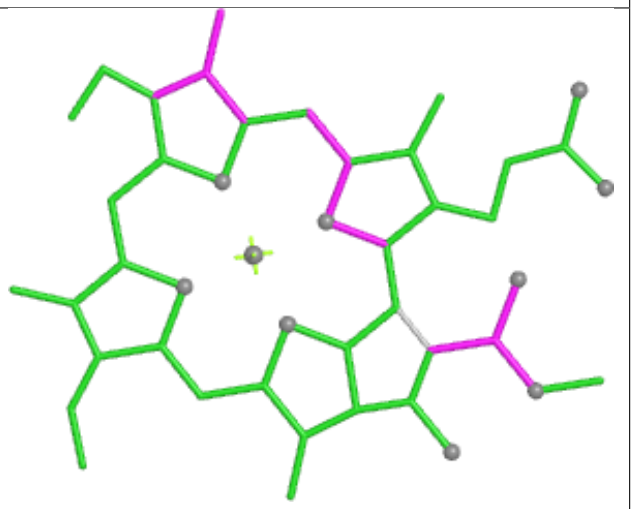


Rings

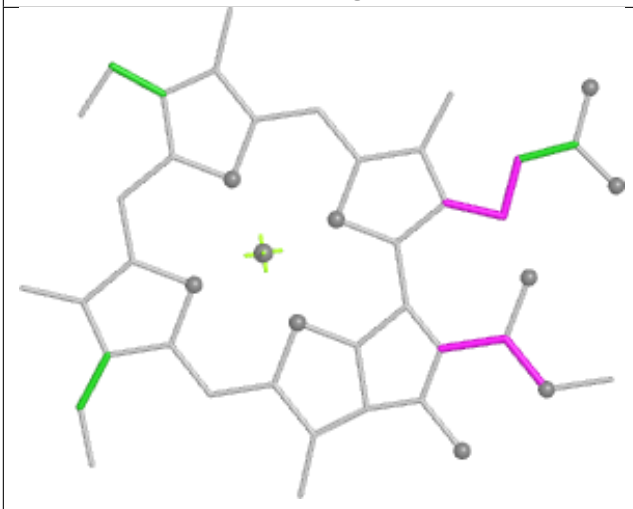
Ligand CLA cB 816



Bond lengths



Bond angles

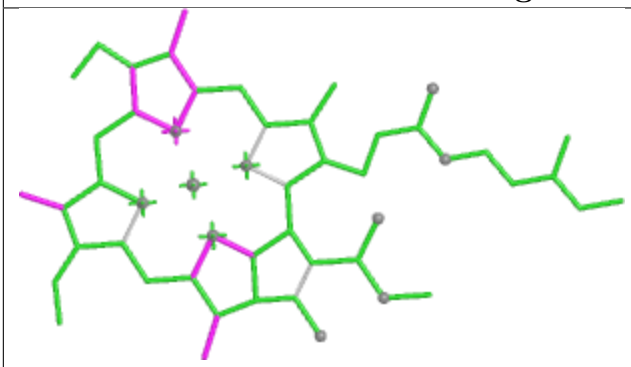


Torsions

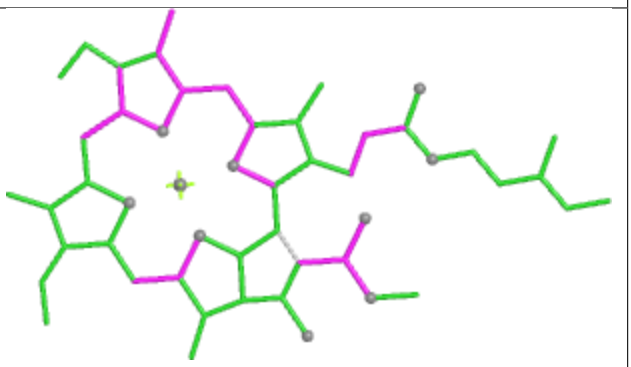


Rings

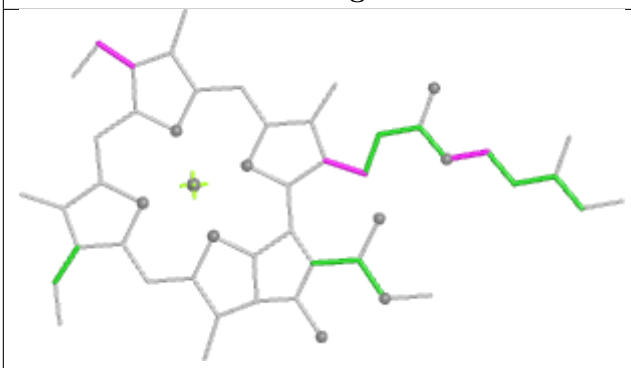
Ligand CLA aA 808



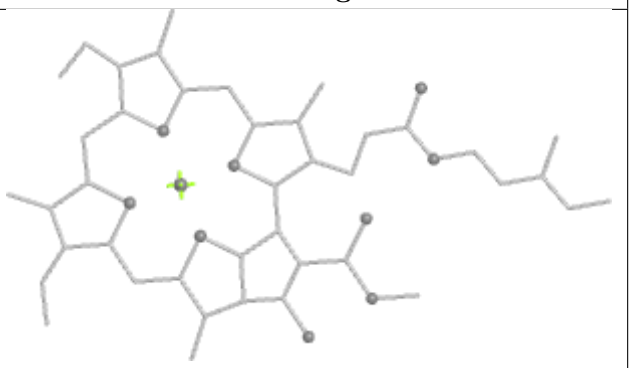
Bond lengths



Bond angles

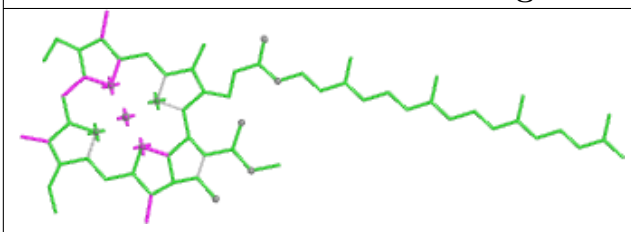


Torsions

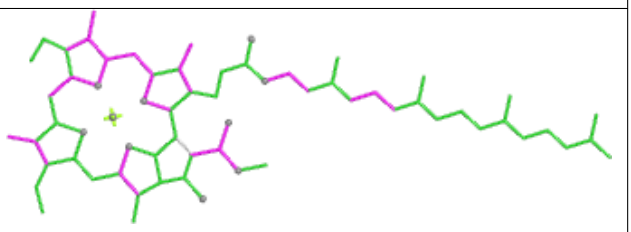


Rings

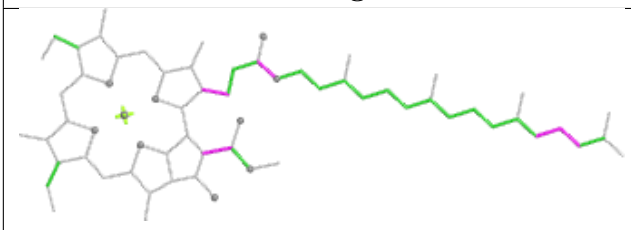
Ligand CLA cB 830



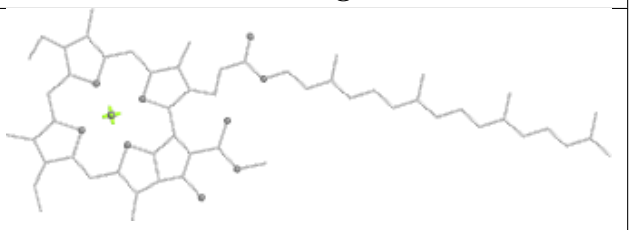
Bond lengths



Bond angles

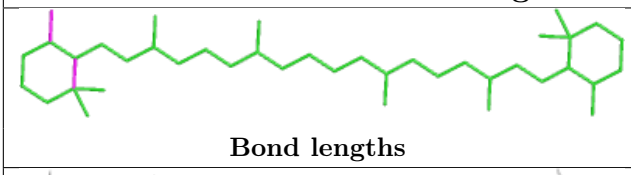


Torsions

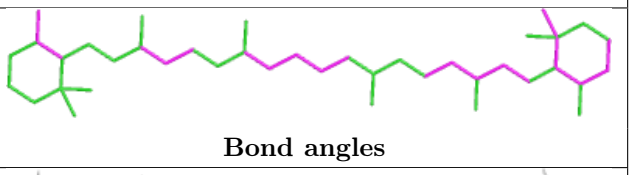


Rings

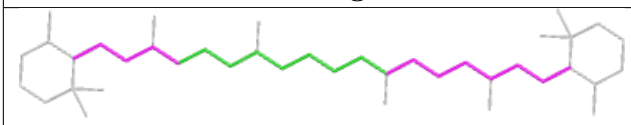
Ligand BCR bA 851



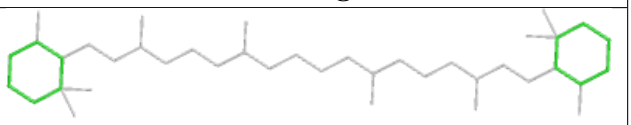
Bond lengths



Bond angles

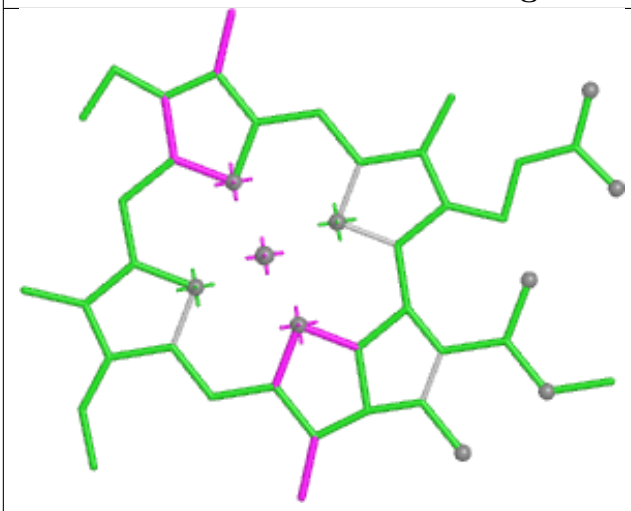


Torsions

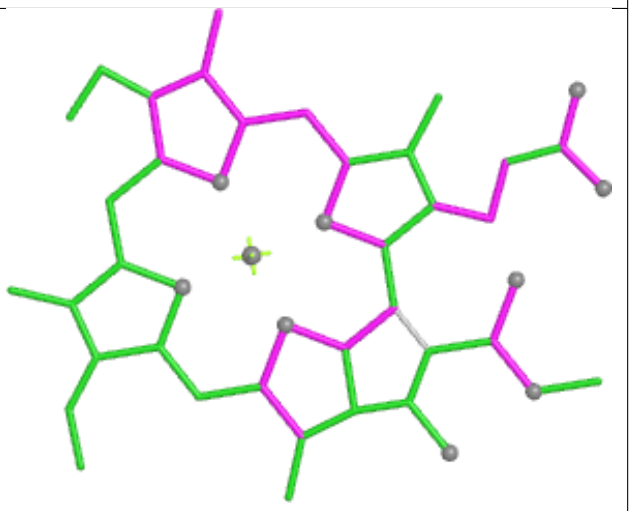


Rings

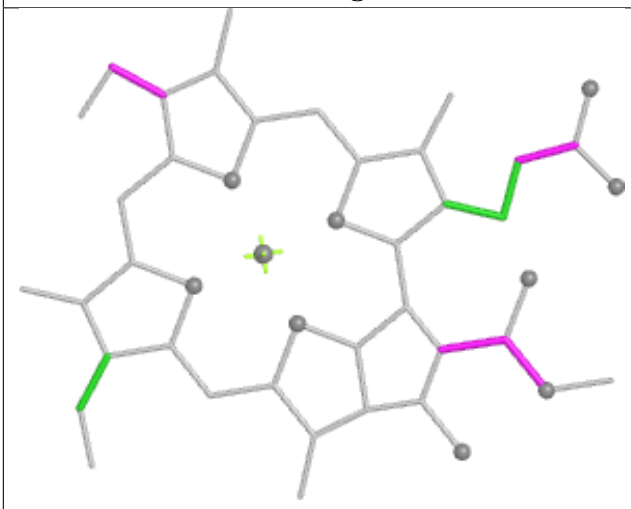
Ligand CLA c6 417



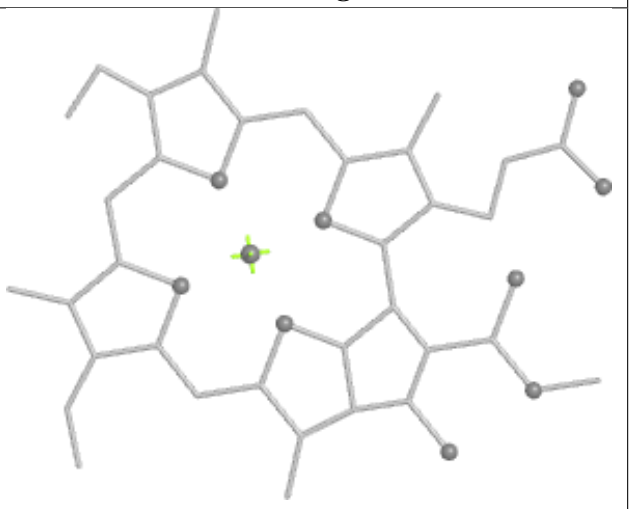
Bond lengths



Bond angles

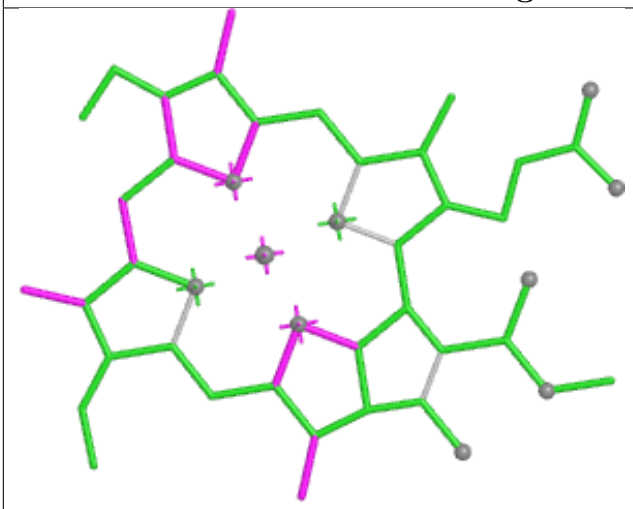


Torsions

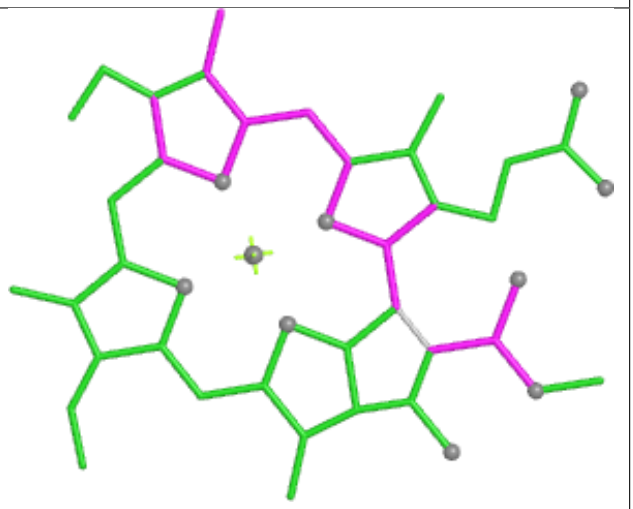


Rings

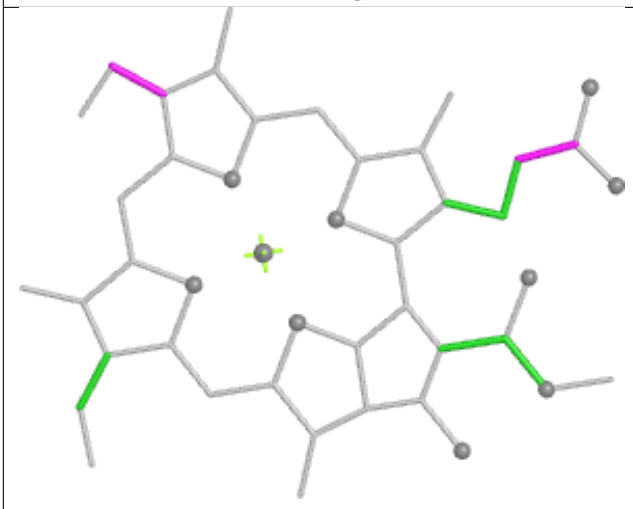
Ligand CLA cB 841



Bond lengths



Bond angles

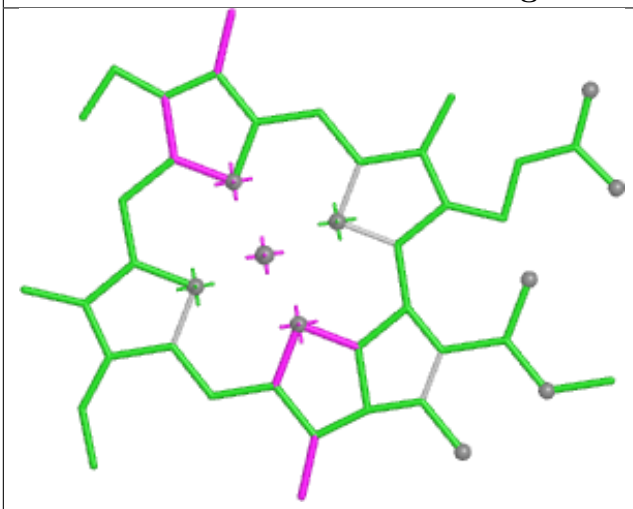


Torsions

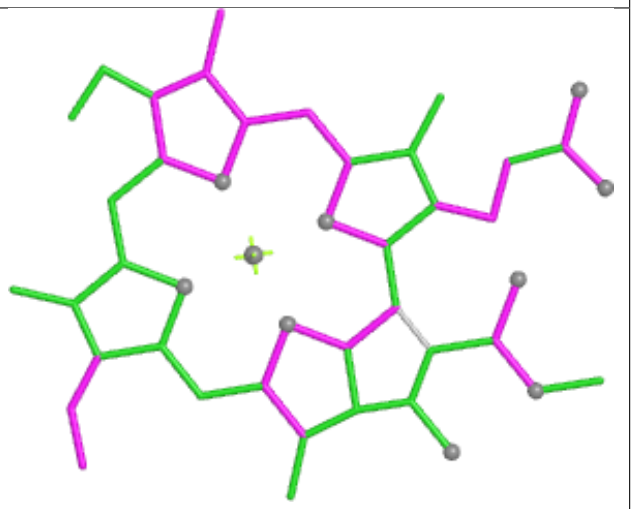


Rings

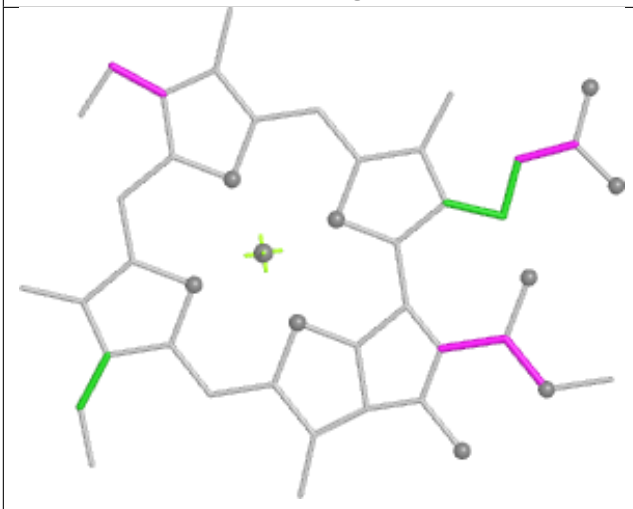
Ligand CLA c4 415



Bond lengths



Bond angles

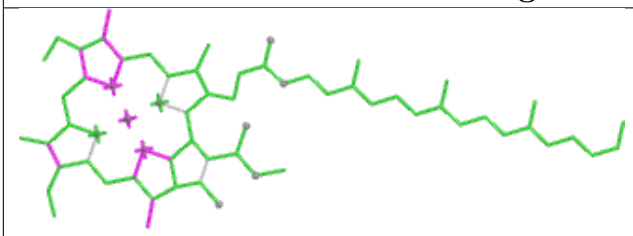


Torsions

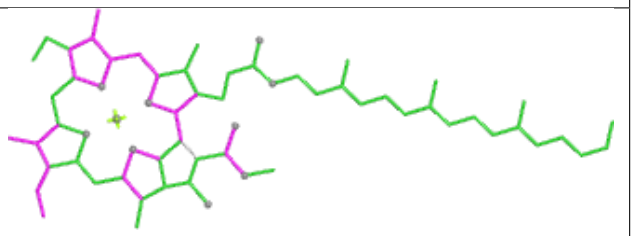


Rings

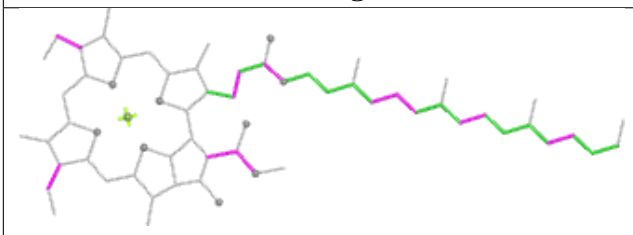
Ligand CLA b5 410



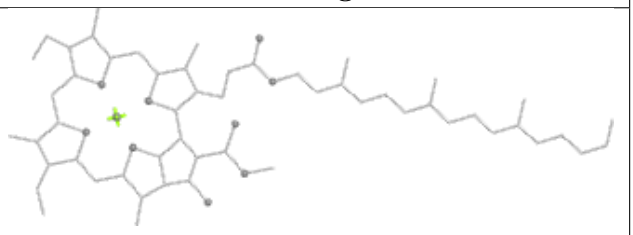
Bond lengths



Bond angles

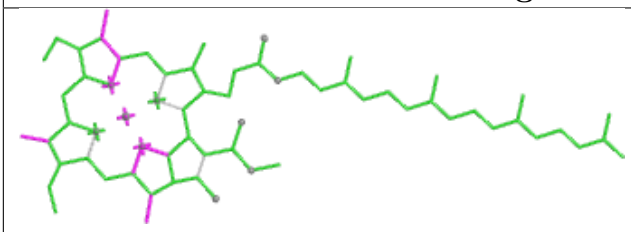


Torsions

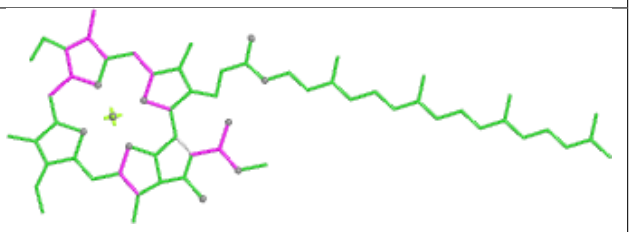


Rings

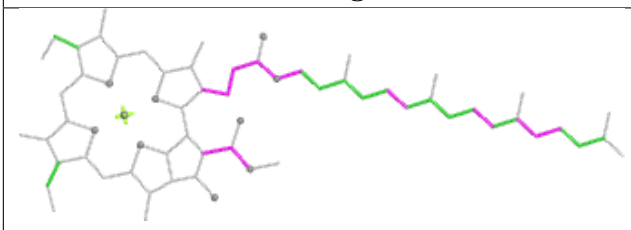
Ligand CLA aB 829



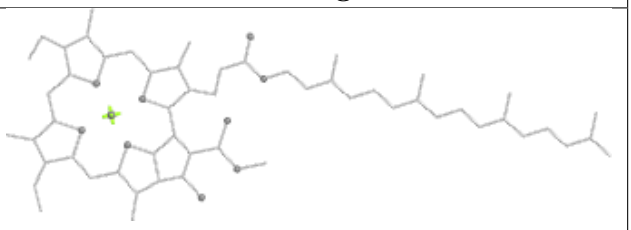
Bond lengths



Bond angles

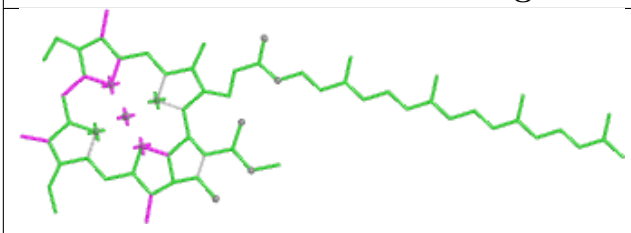


Torsions

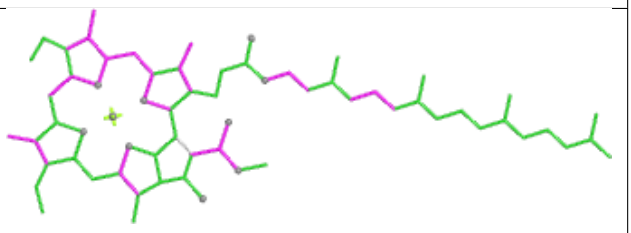


Rings

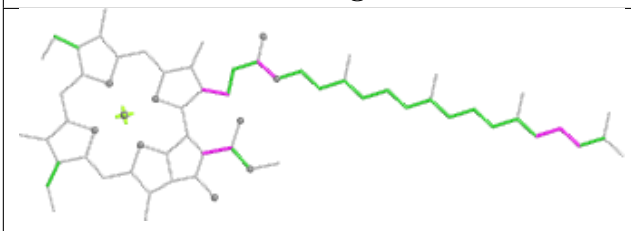
Ligand CLA bB 830



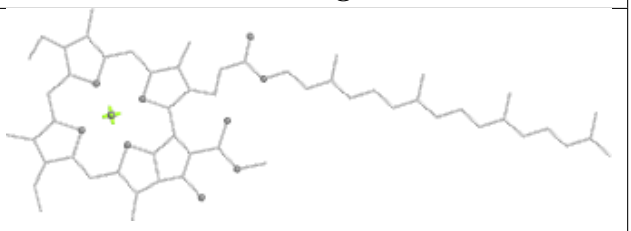
Bond lengths



Bond angles

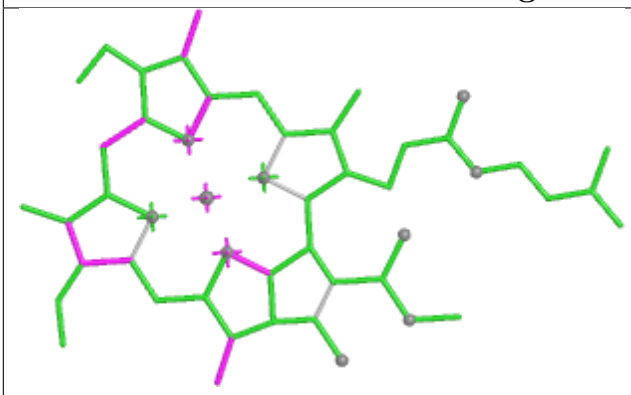


Torsions

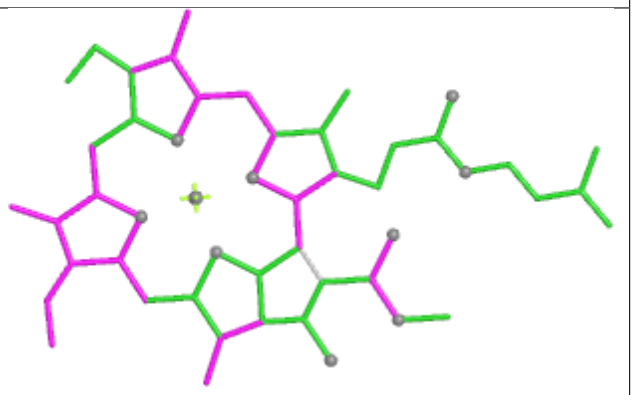


Rings

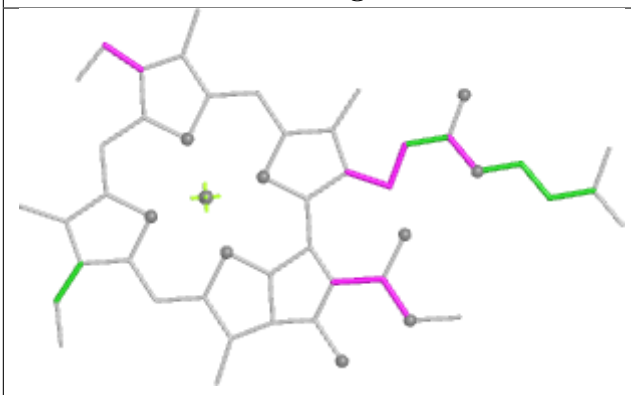
Ligand CLA b5 416



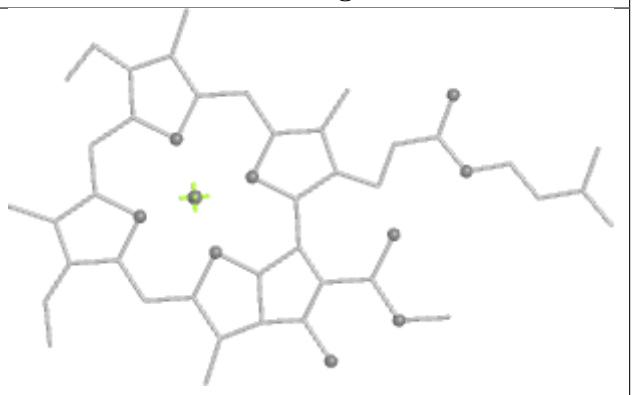
Bond lengths



Bond angles

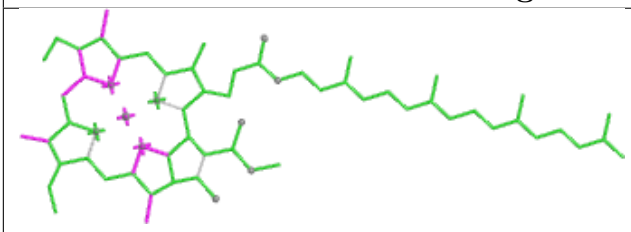


Torsions

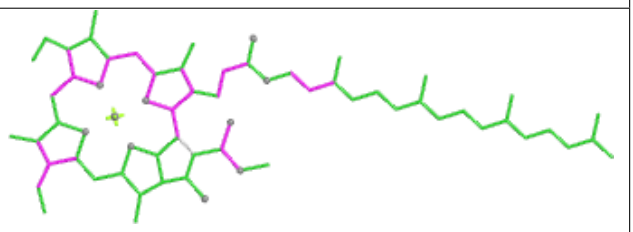


Rings

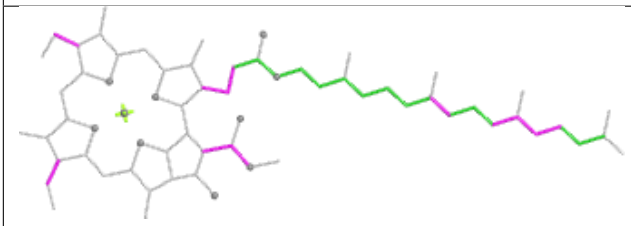
Ligand CLA cB 840



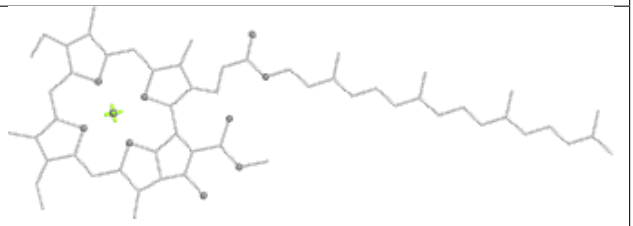
Bond lengths



Bond angles

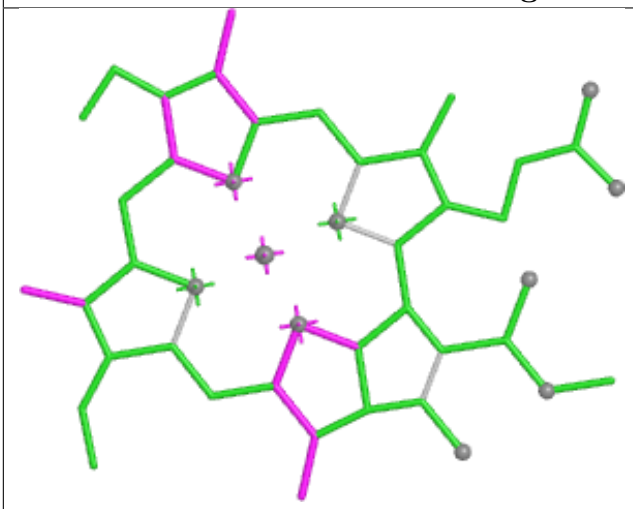


Torsions

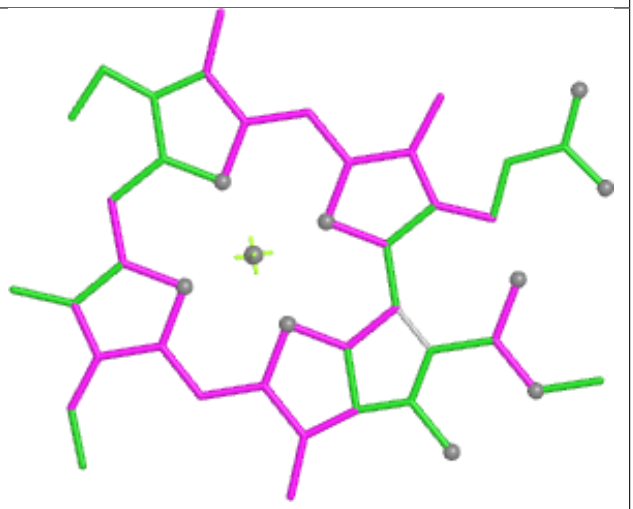


Rings

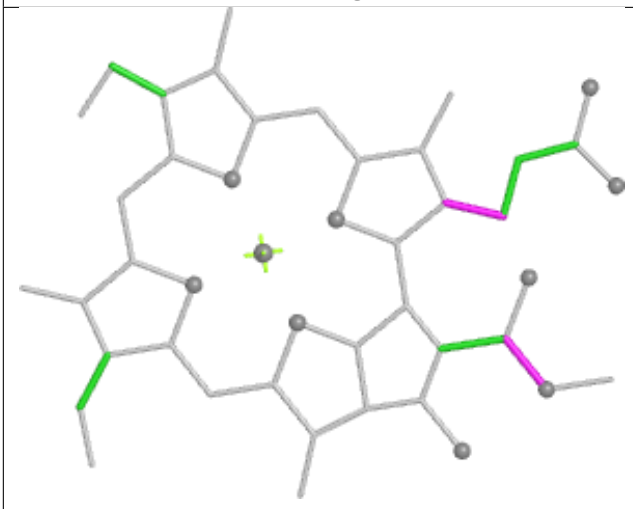
Ligand CLA c3 405



Bond lengths



Bond angles

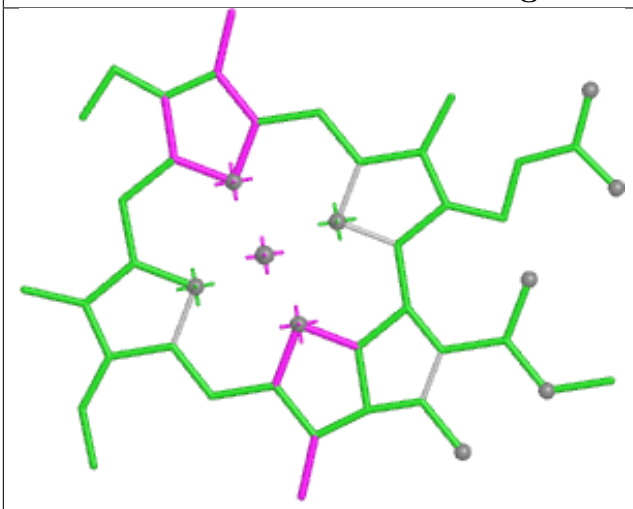


Torsions

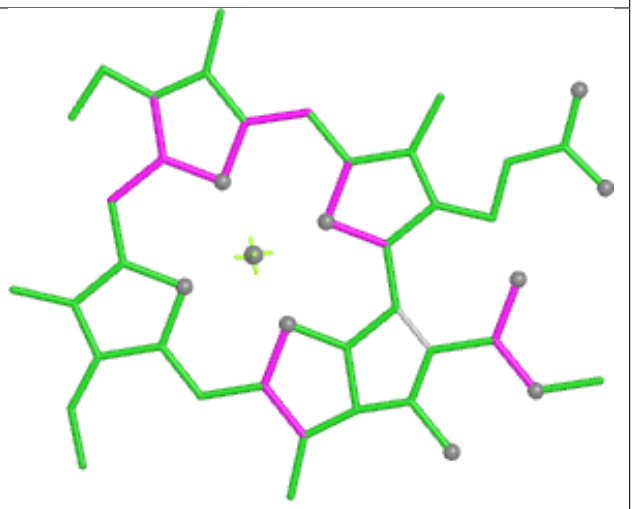


Rings

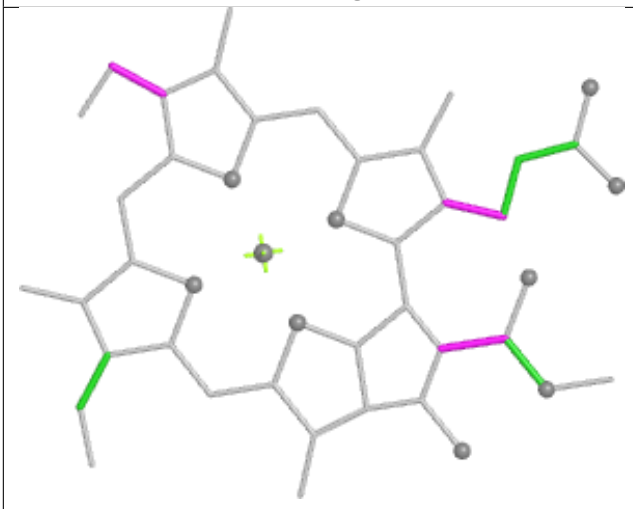
Ligand CLA c4 413



Bond lengths



Bond angles

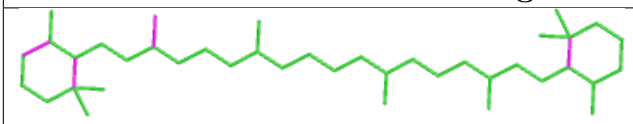


Torsions

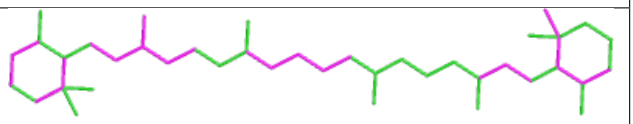


Rings

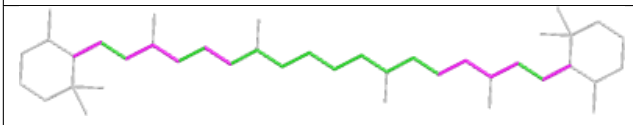
Ligand BCR b6 401



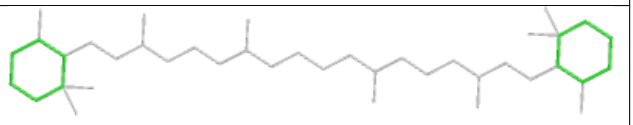
Bond lengths



Bond angles

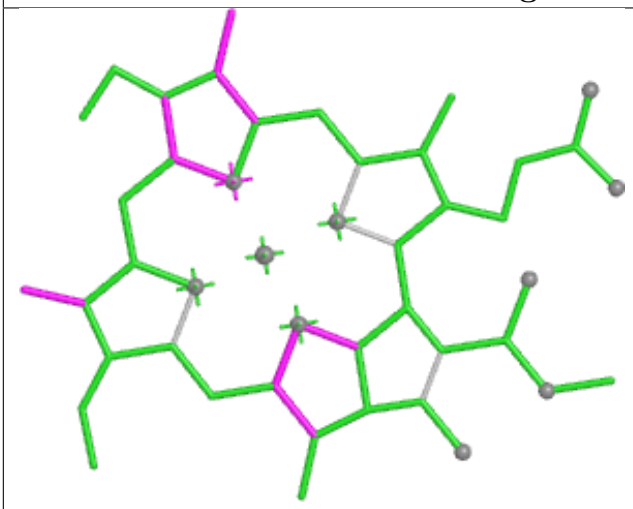


Torsions

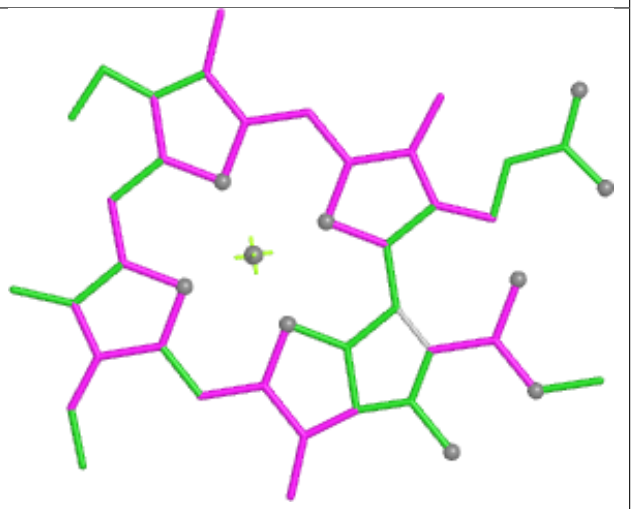


Rings

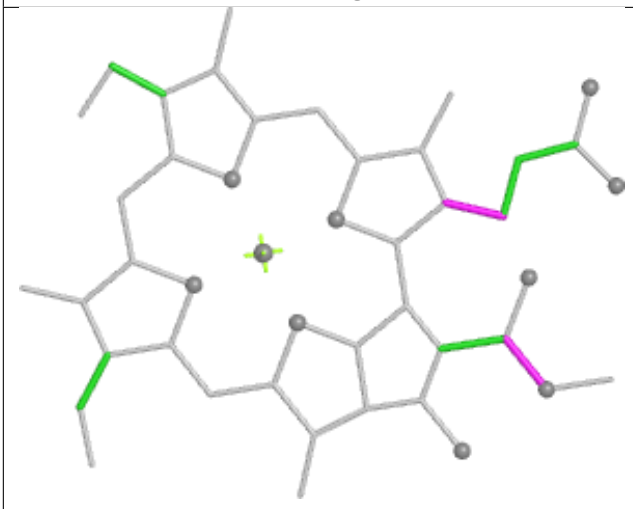
Ligand CLA a1 404



Bond lengths



Bond angles

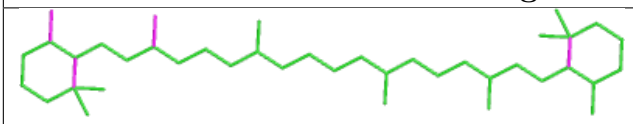


Torsions

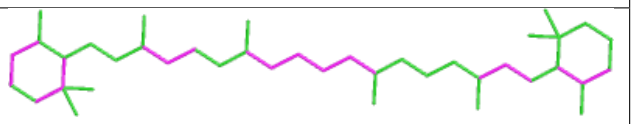


Rings

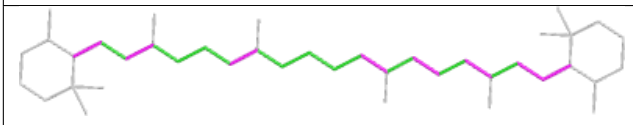
Ligand BCR aI 102



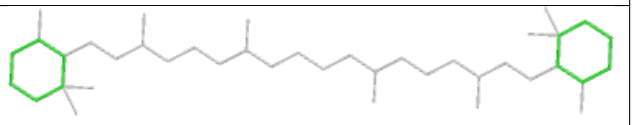
Bond lengths



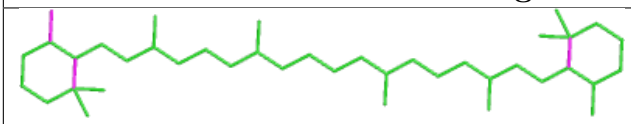
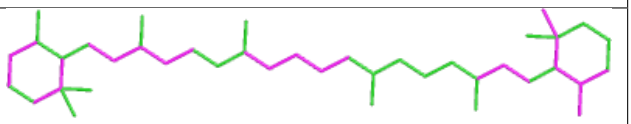
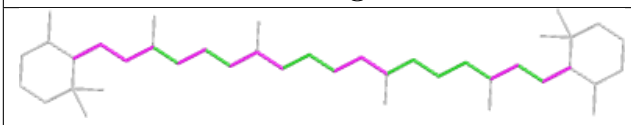
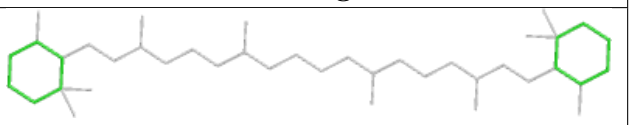
Bond angles

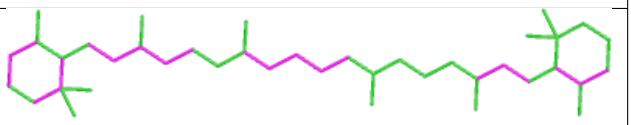
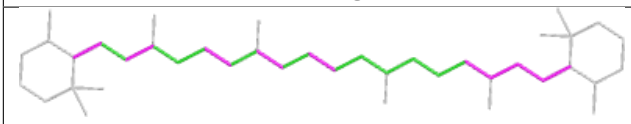
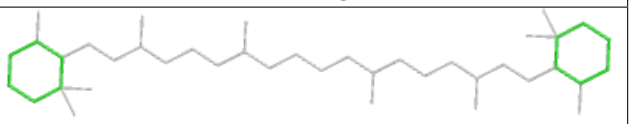


Torsions

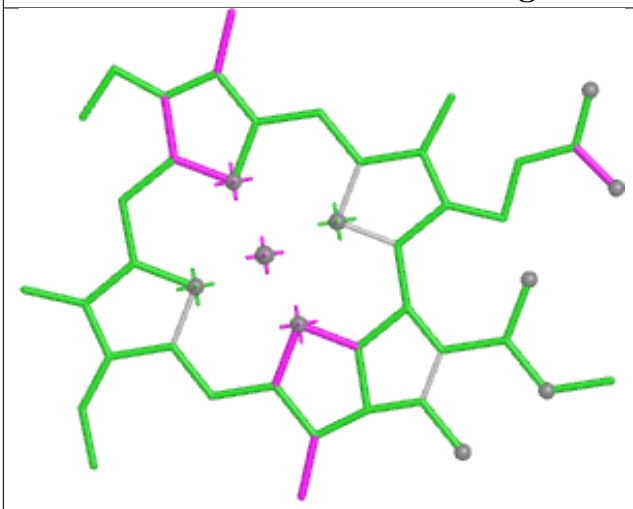


Rings

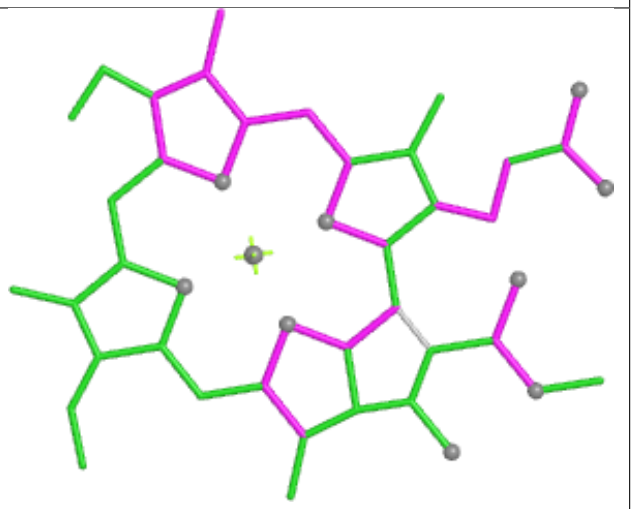
Ligand BCR bL 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cB 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

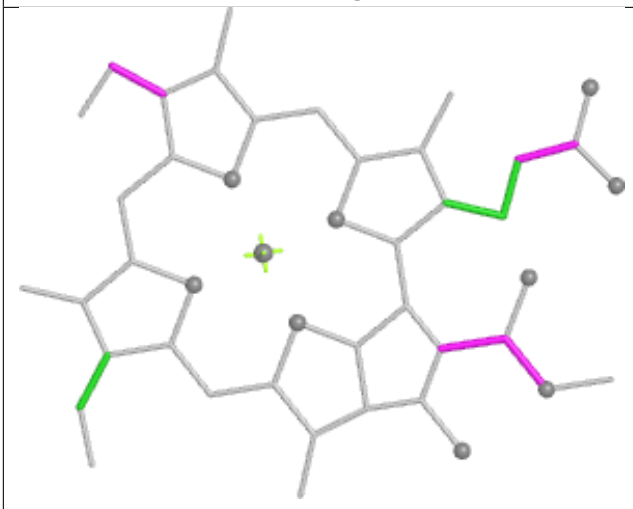
Ligand CLA b2 416



Bond lengths



Bond angles

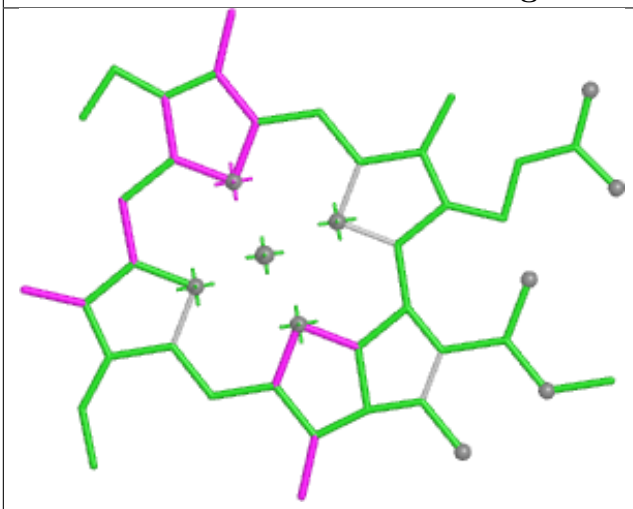


Torsions

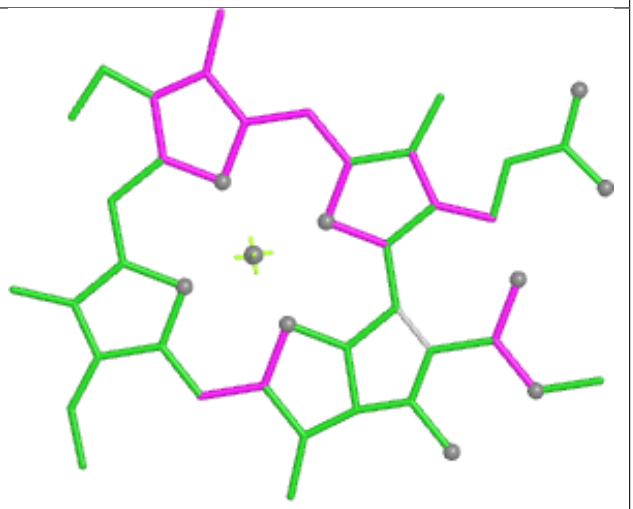


Rings

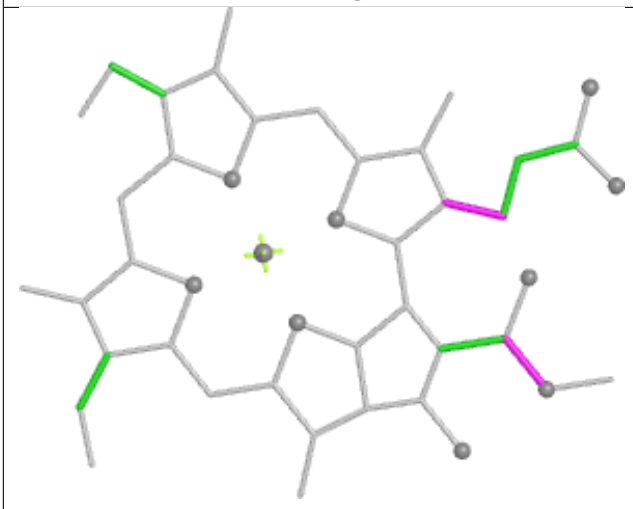
Ligand CLA c4 411



Bond lengths



Bond angles

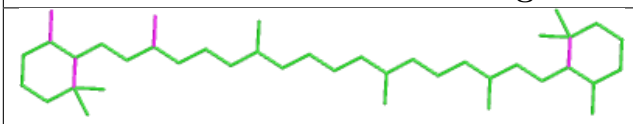


Torsions

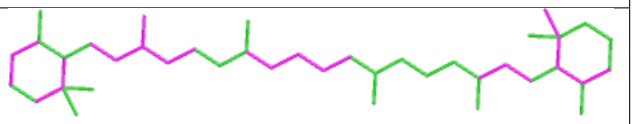


Rings

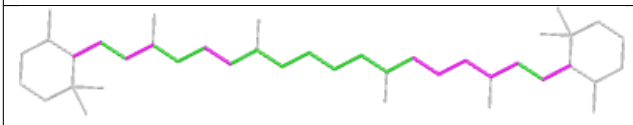
Ligand BCR b1 419



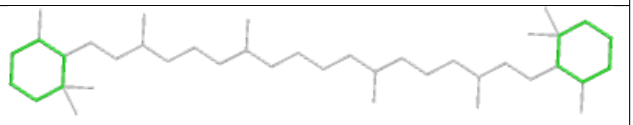
Bond lengths



Bond angles

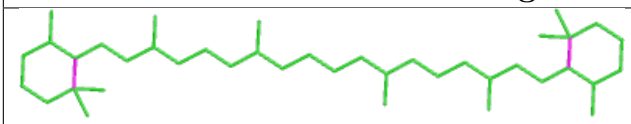


Torsions

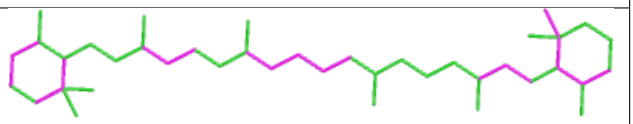


Rings

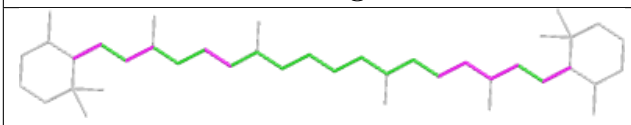
Ligand BCR c3 419



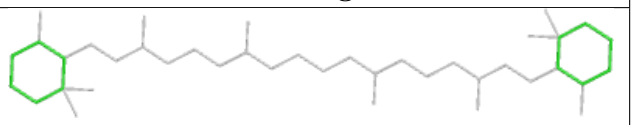
Bond lengths



Bond angles

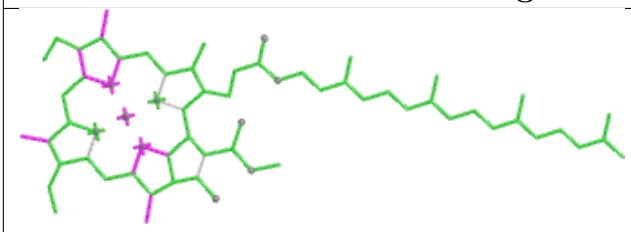


Torsions

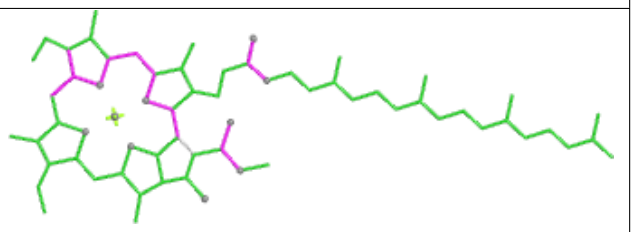


Rings

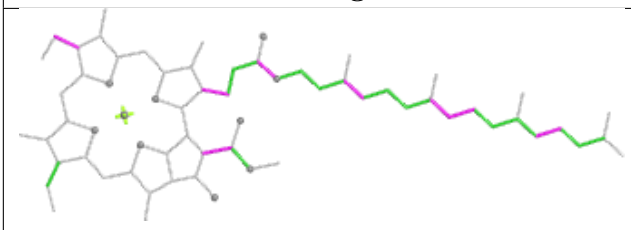
Ligand CLA bL 202



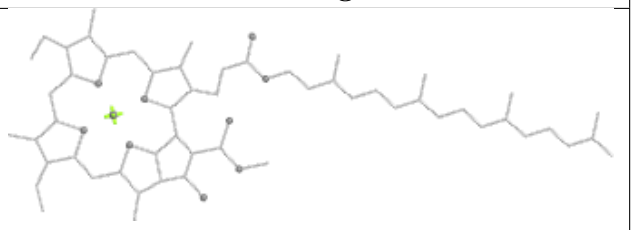
Bond lengths



Bond angles

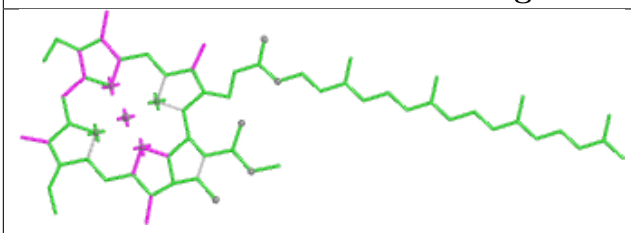


Torsions

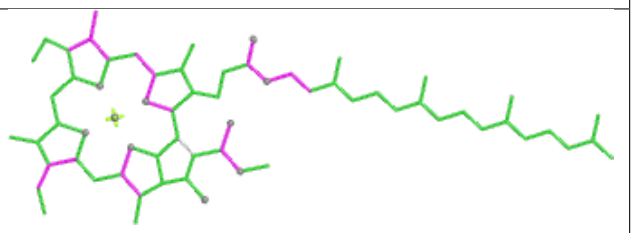


Rings

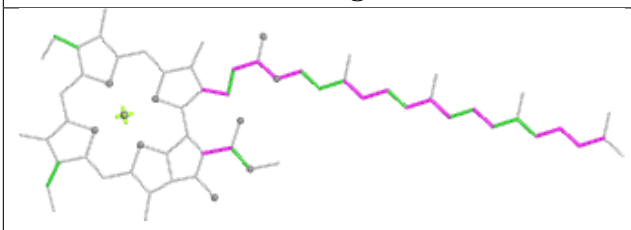
Ligand CLA bB 806



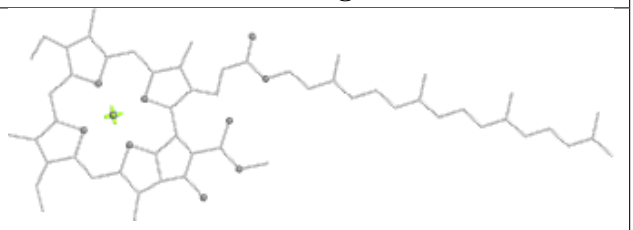
Bond lengths



Bond angles

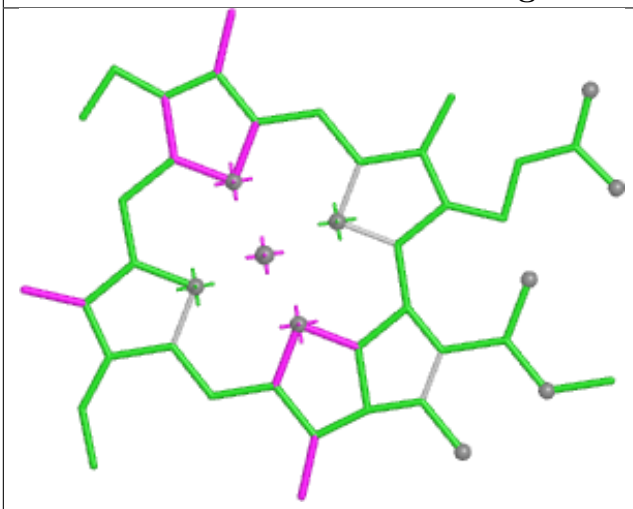


Torsions

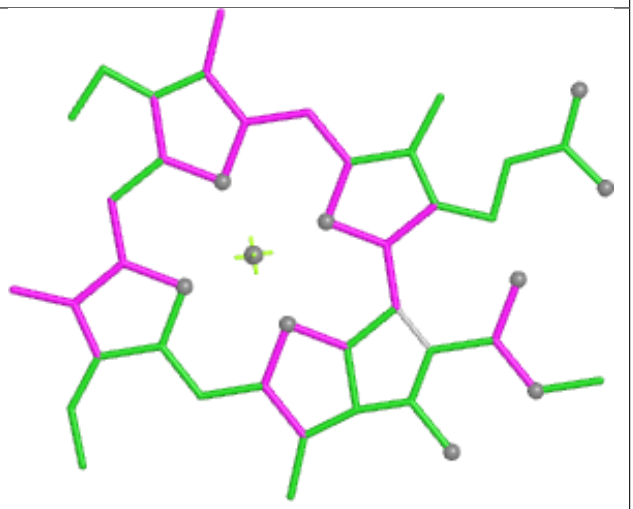


Rings

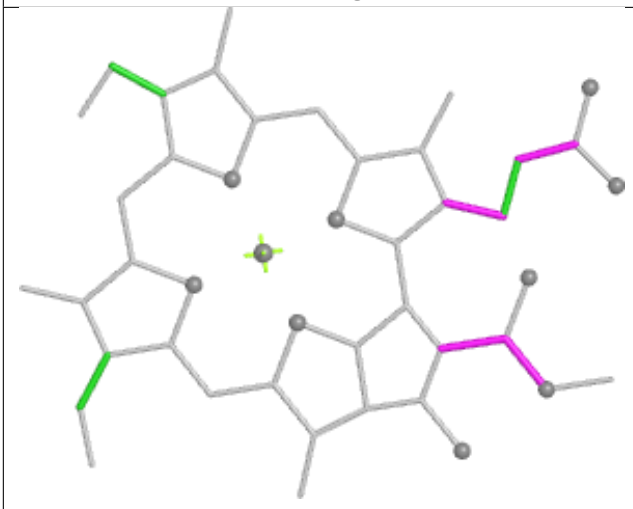
Ligand CLA b5 412



Bond lengths



Bond angles

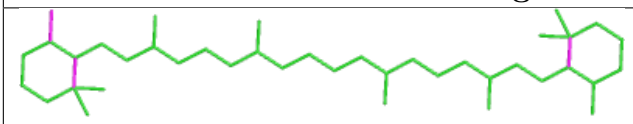


Torsions

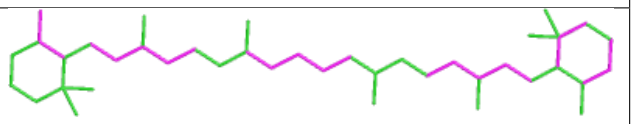


Rings

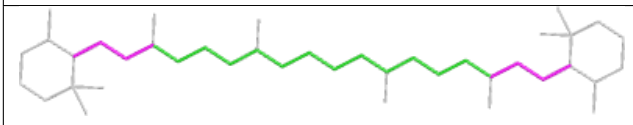
Ligand BCR aK 101



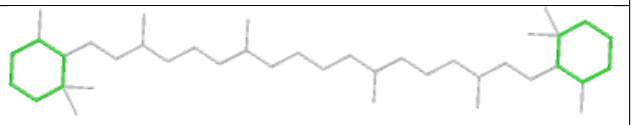
Bond lengths



Bond angles

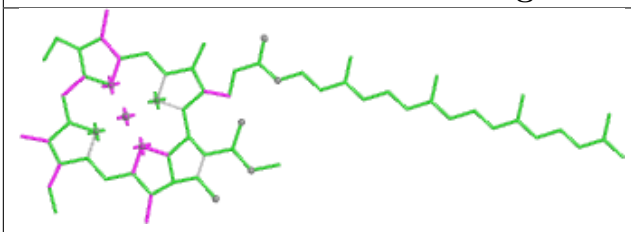


Torsions

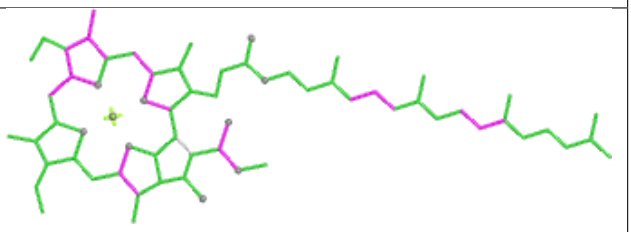


Rings

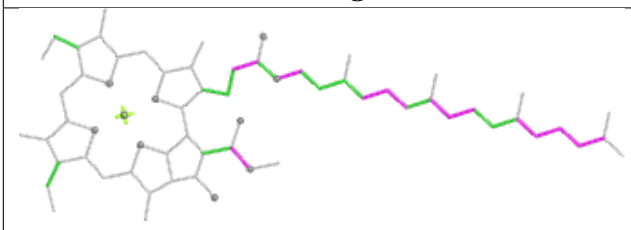
Ligand CLA cB 807



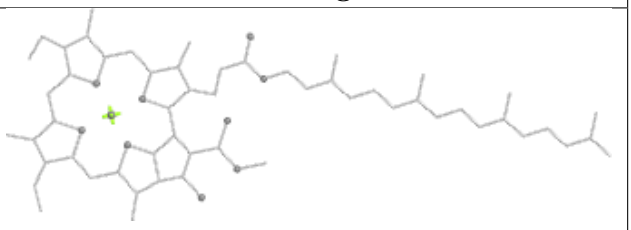
Bond lengths



Bond angles



Torsions

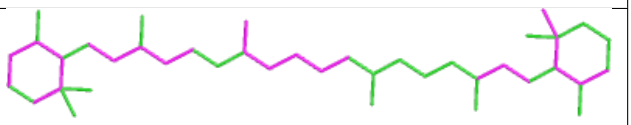


Rings

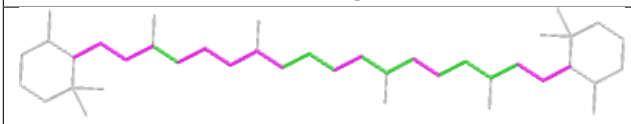
Ligand BCR b5 401



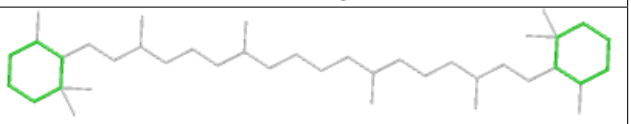
Bond lengths



Bond angles

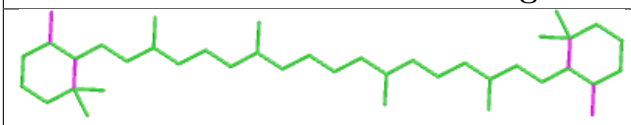


Torsions

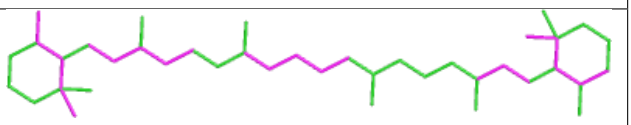


Rings

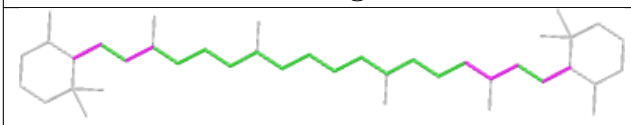
Ligand BCR aI 103



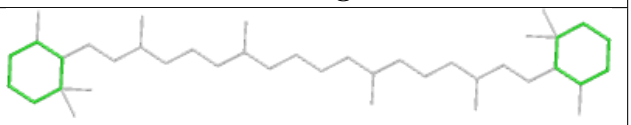
Bond lengths



Bond angles

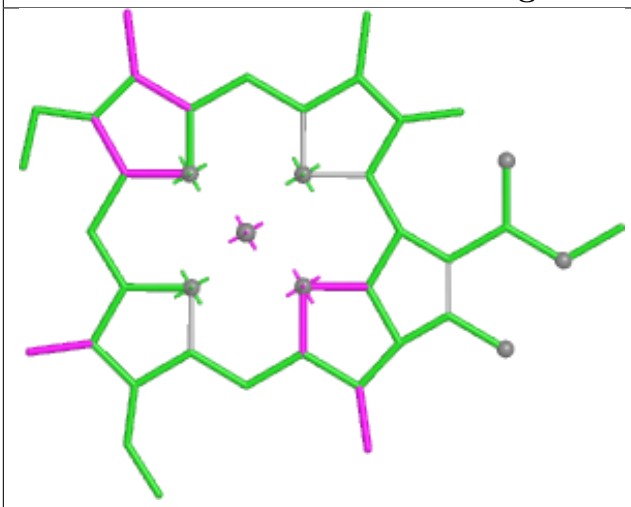


Torsions

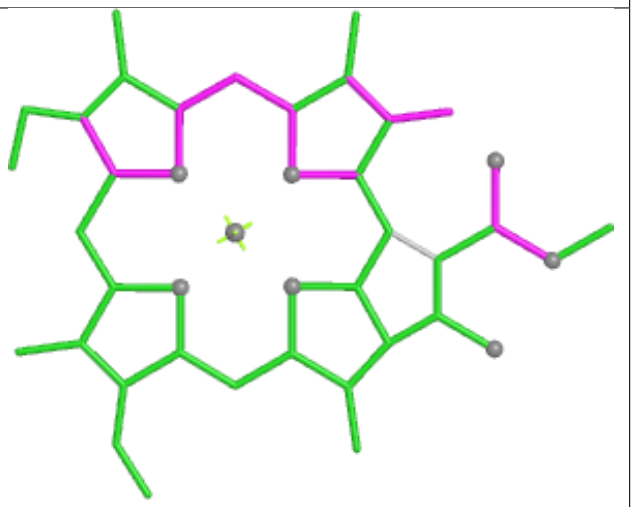


Rings

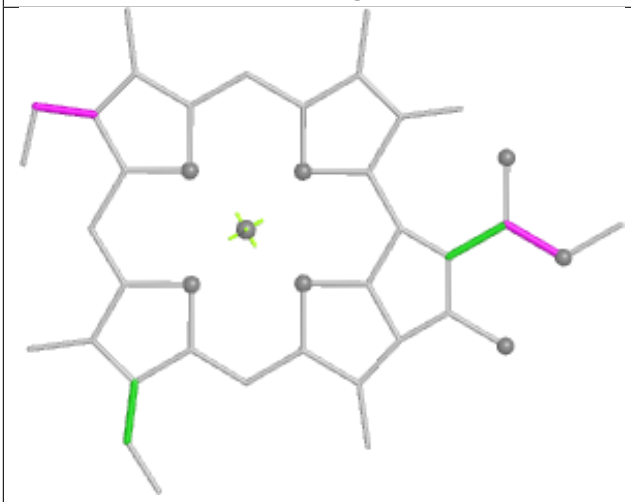
Ligand CLA b4 414



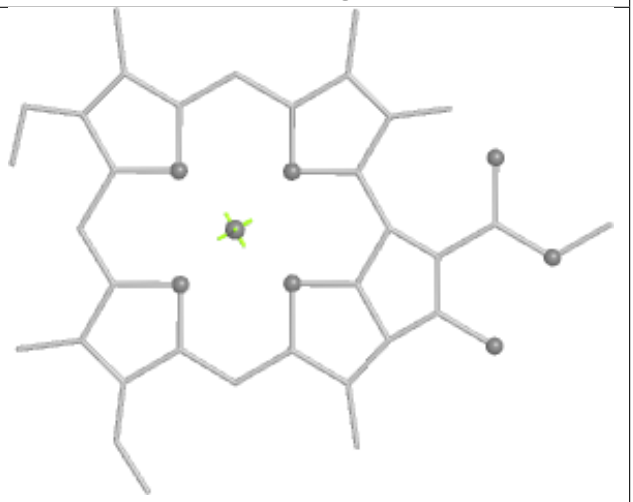
Bond lengths



Bond angles

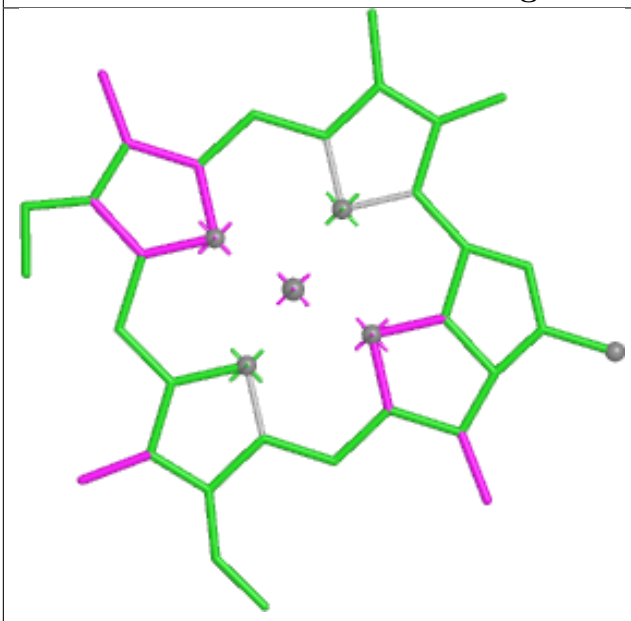


Torsions



Rings

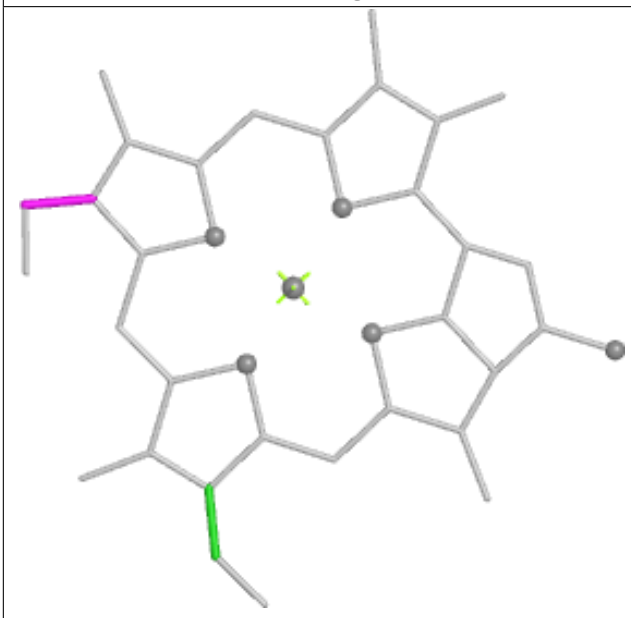
Ligand CLA cJ 102



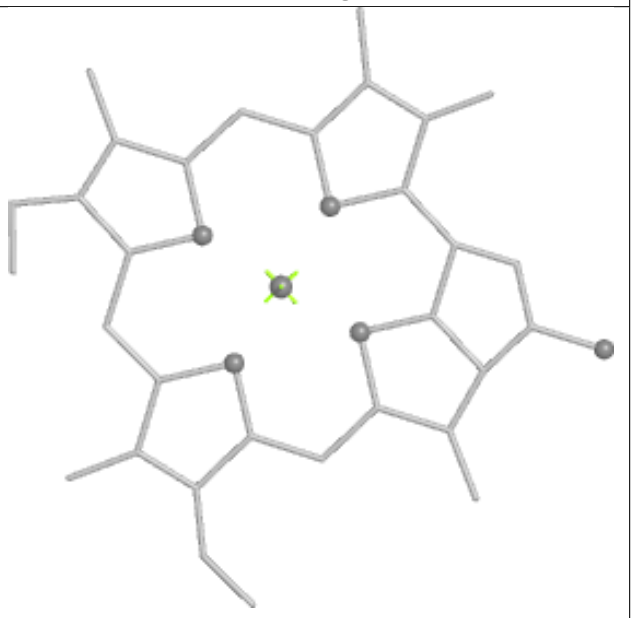
Bond lengths



Bond angles

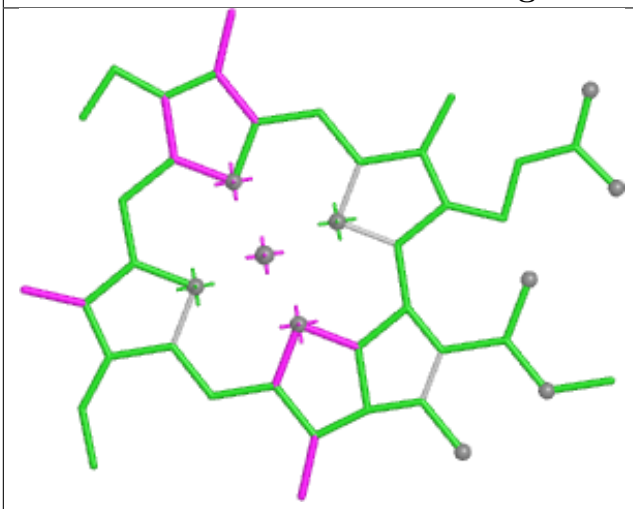


Torsions

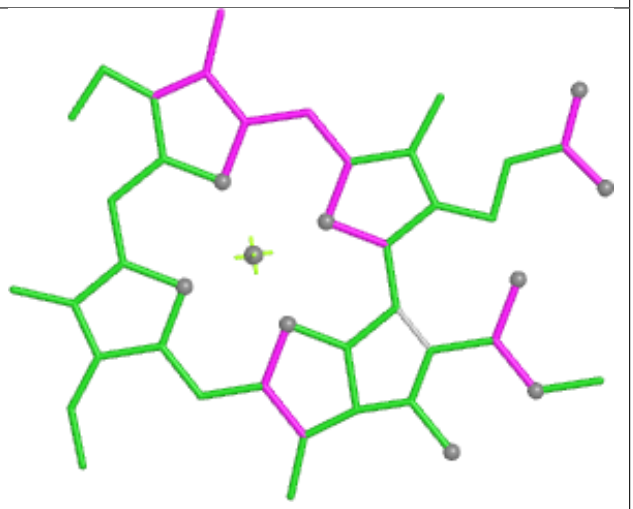


Rings

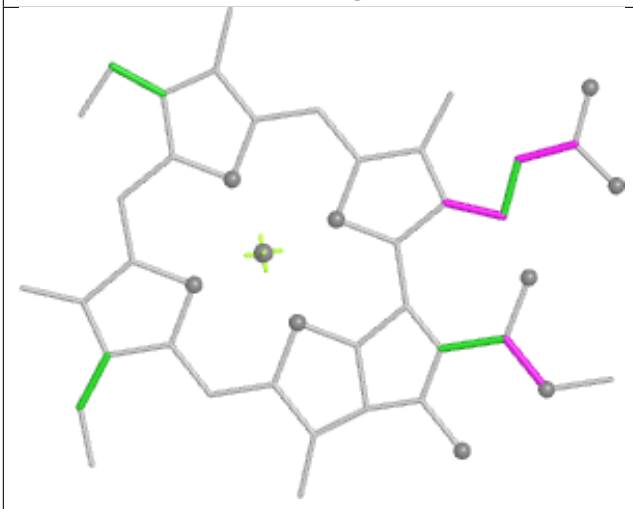
Ligand CLA b4 408



Bond lengths



Bond angles

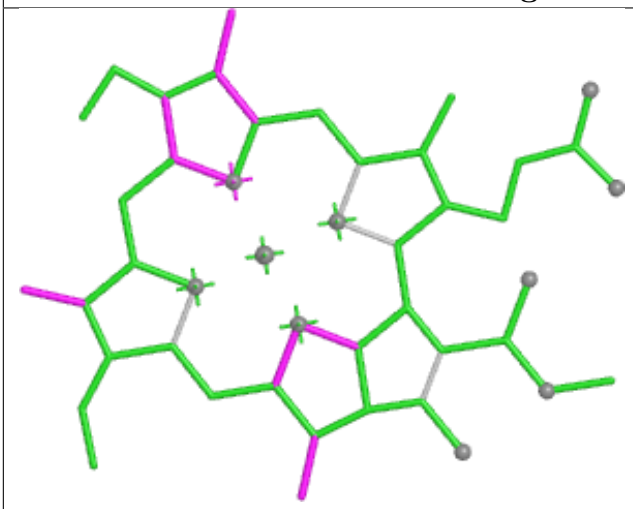


Torsions

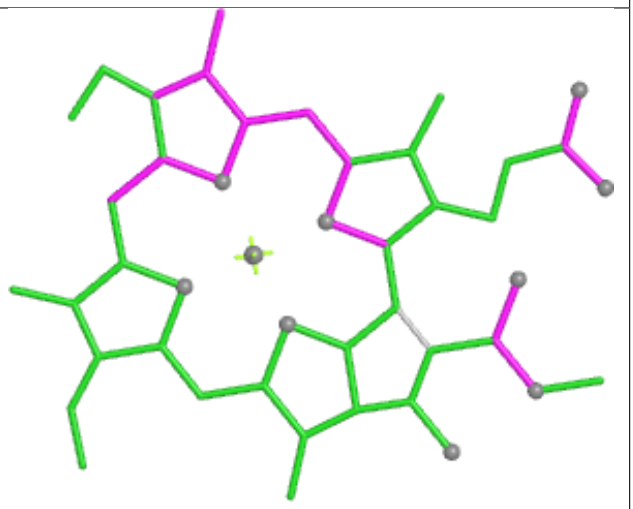


Rings

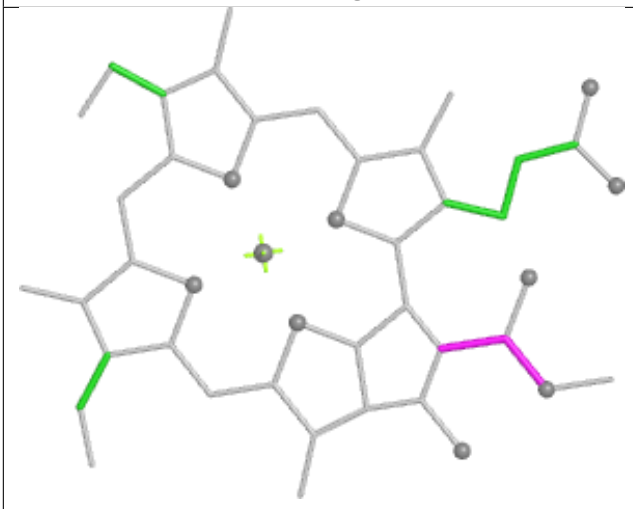
Ligand CLA c1 406



Bond lengths



Bond angles

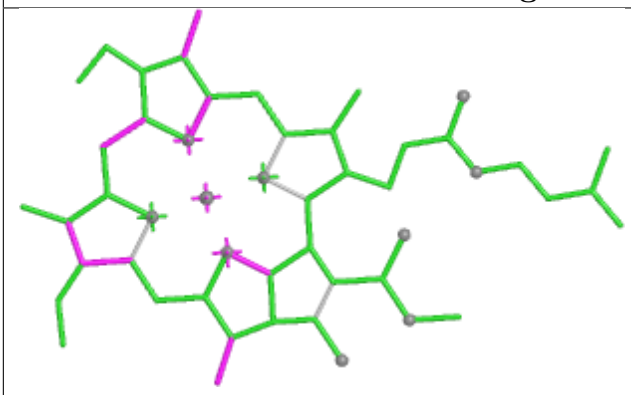


Torsions

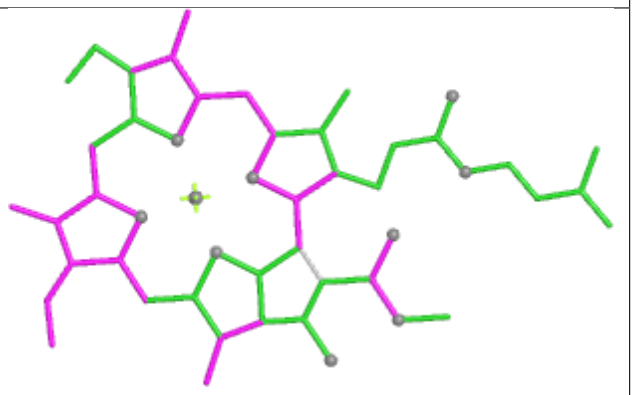


Rings

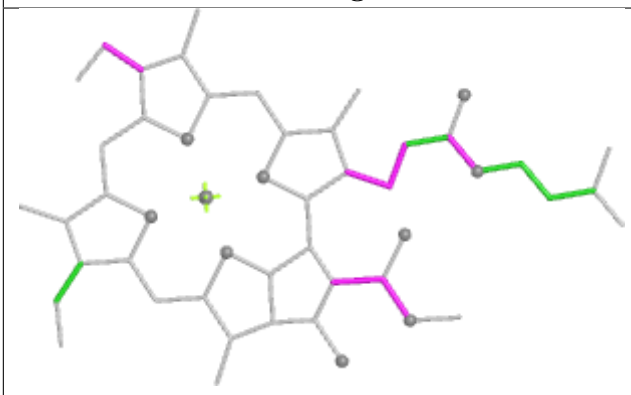
Ligand CLA a5 416



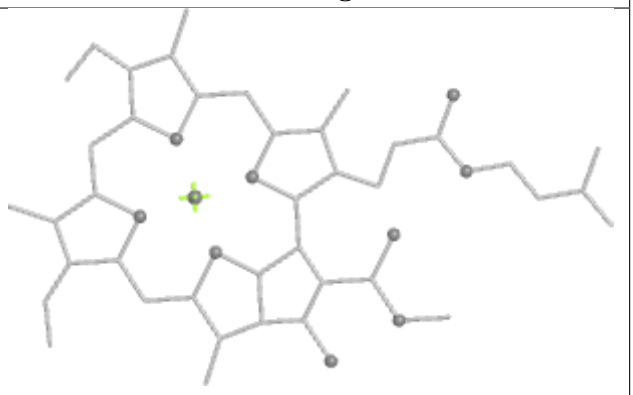
Bond lengths



Bond angles

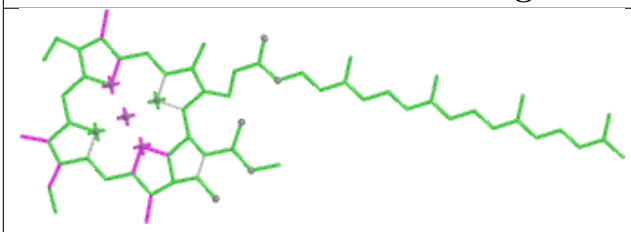


Torsions

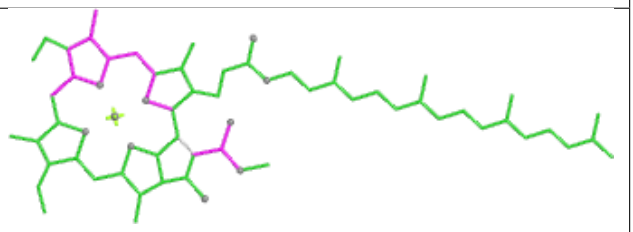


Rings

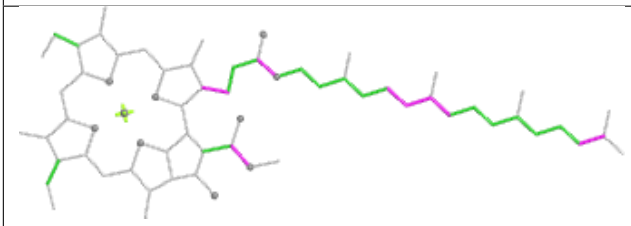
Ligand CLA aA 833



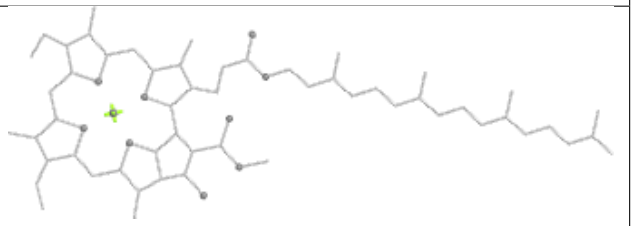
Bond lengths



Bond angles

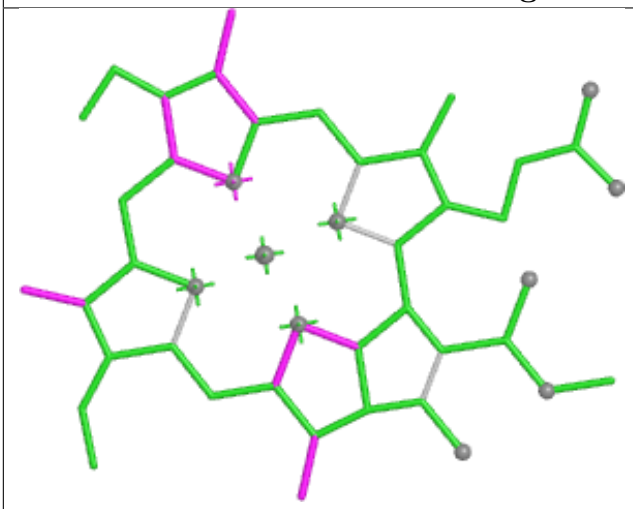


Torsions

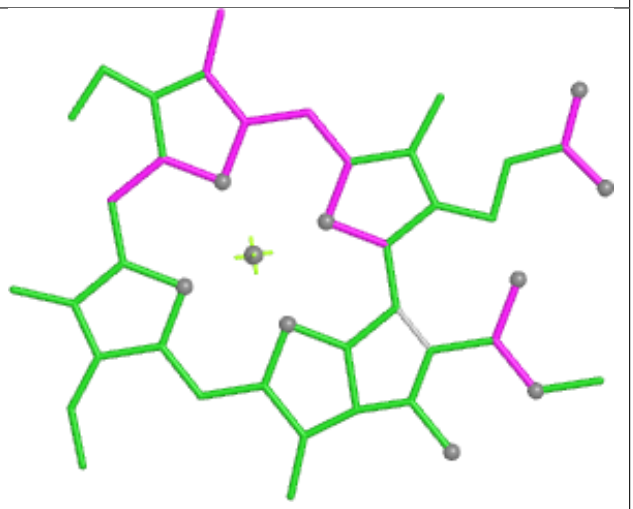


Rings

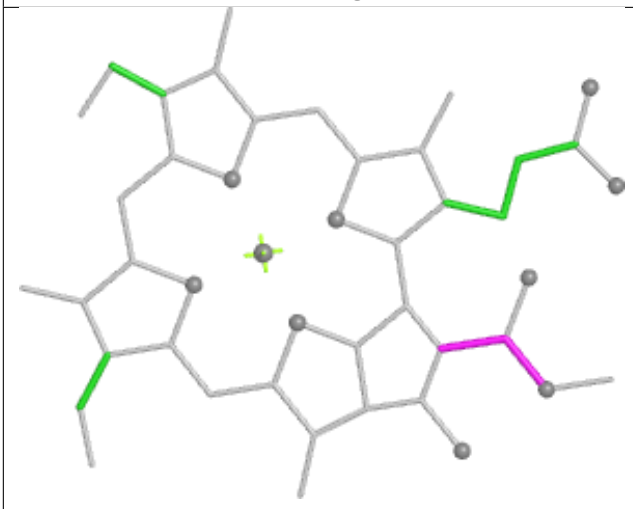
Ligand CLA a3 406



Bond lengths



Bond angles

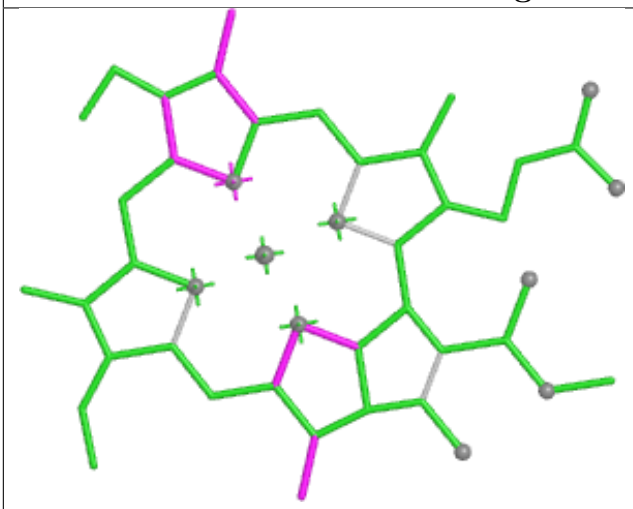


Torsions

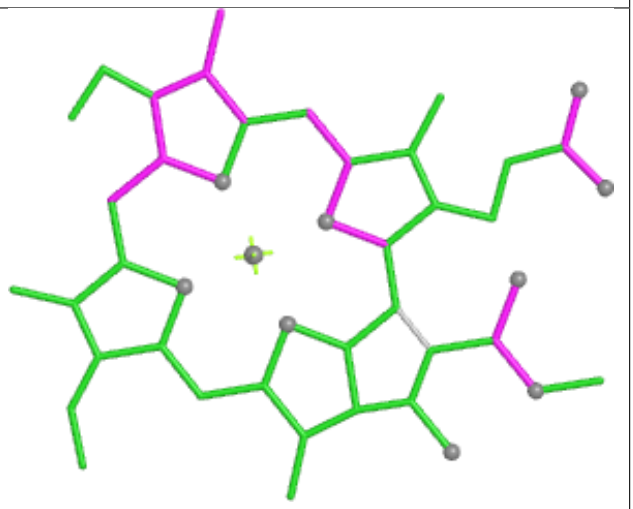


Rings

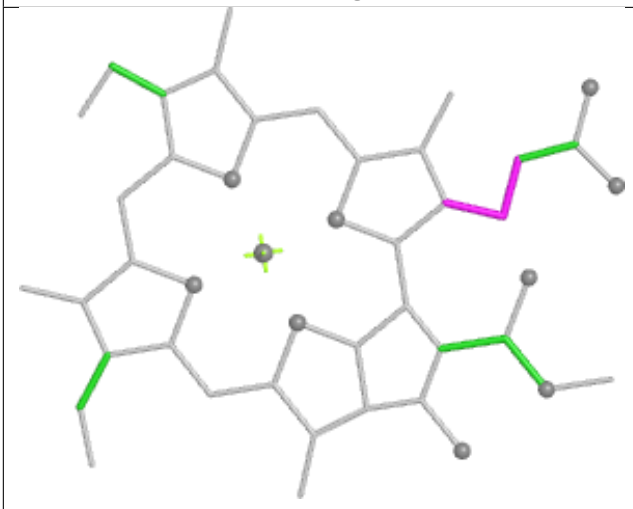
Ligand CLA bB 822



Bond lengths



Bond angles

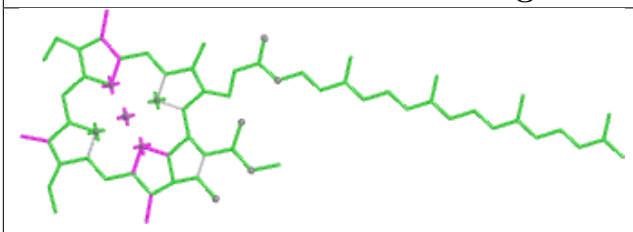


Torsions

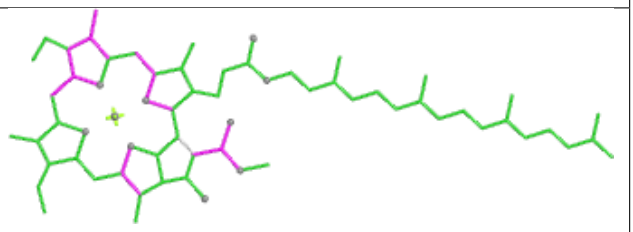


Rings

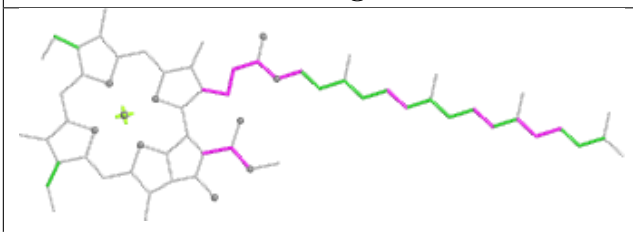
Ligand CLA cB 829



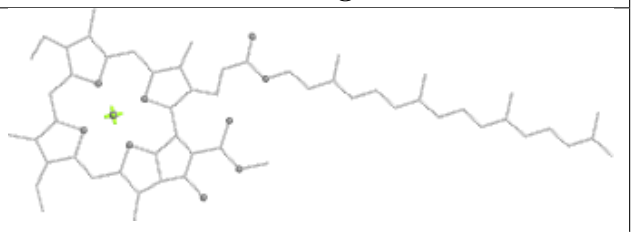
Bond lengths



Bond angles

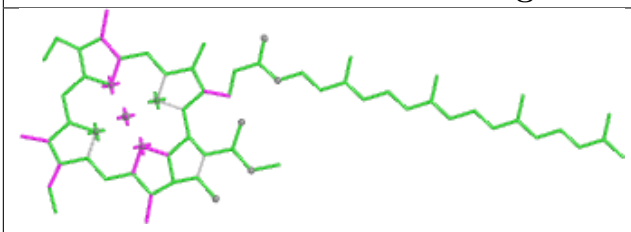


Torsions

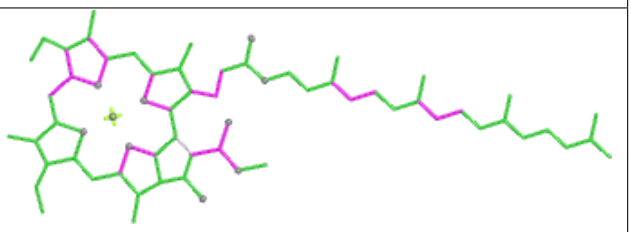


Rings

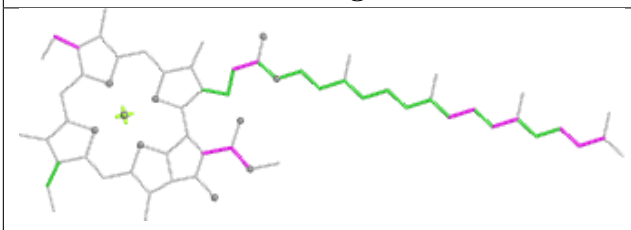
Ligand CLA cB 802



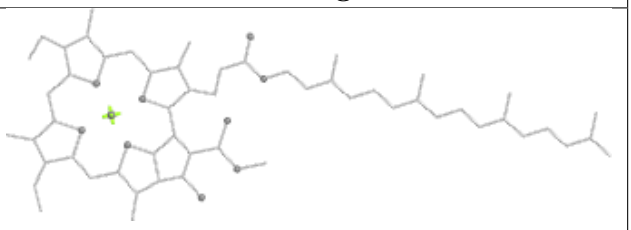
Bond lengths



Bond angles

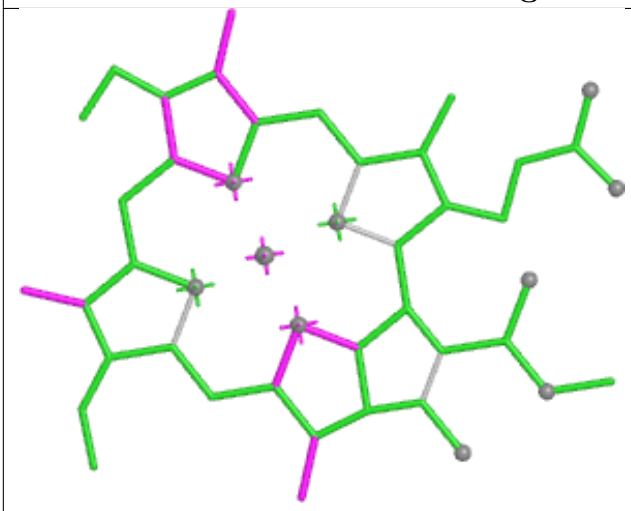


Torsions

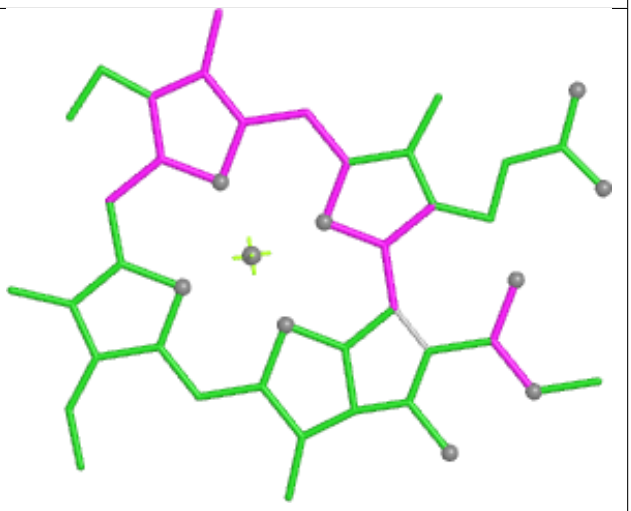


Rings

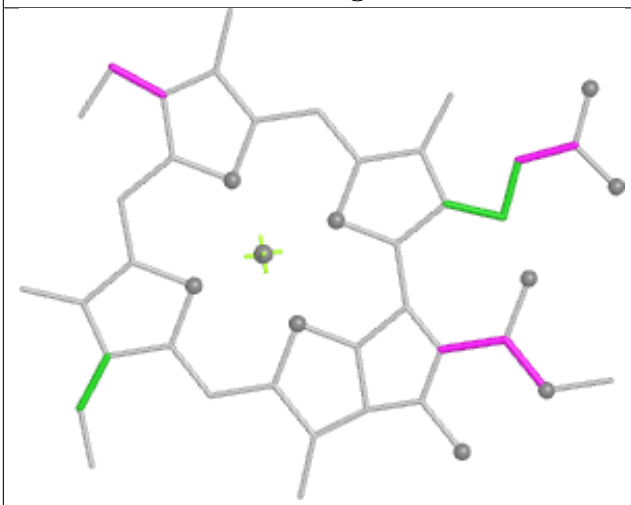
Ligand CLA c3 407



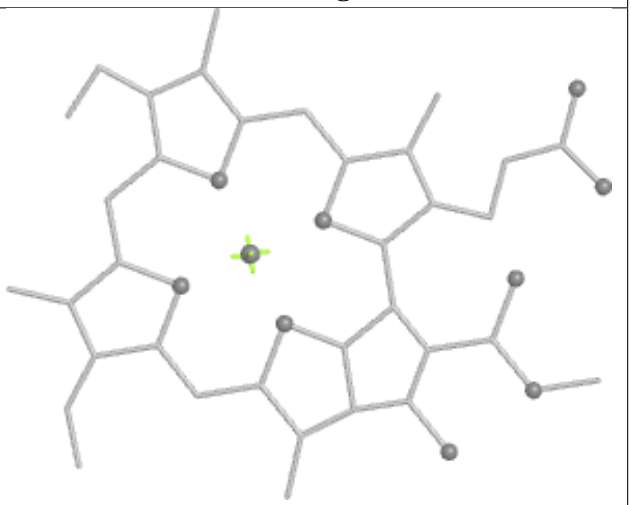
Bond lengths



Bond angles

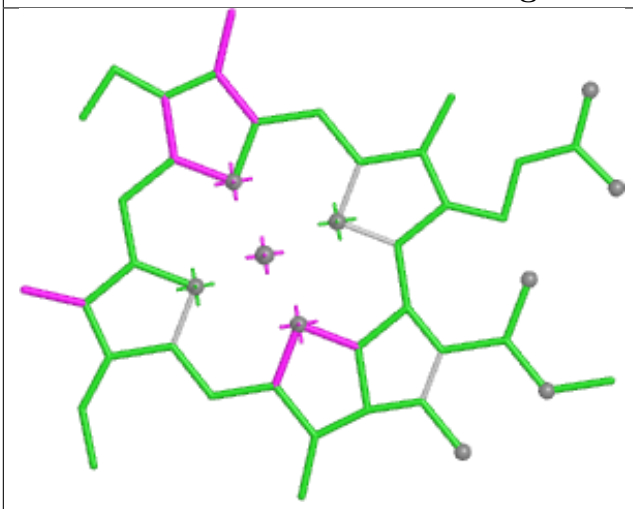


Torsions

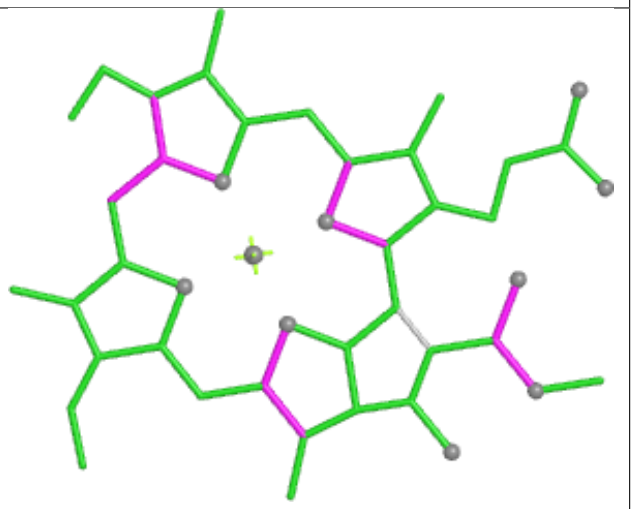


Rings

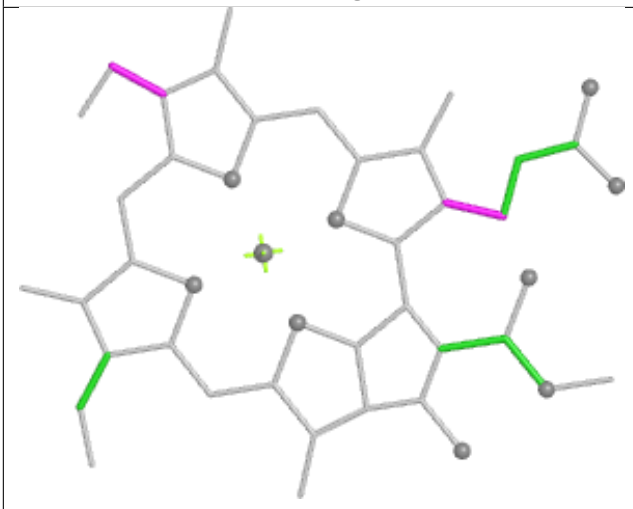
Ligand CLA a5 413



Bond lengths



Bond angles

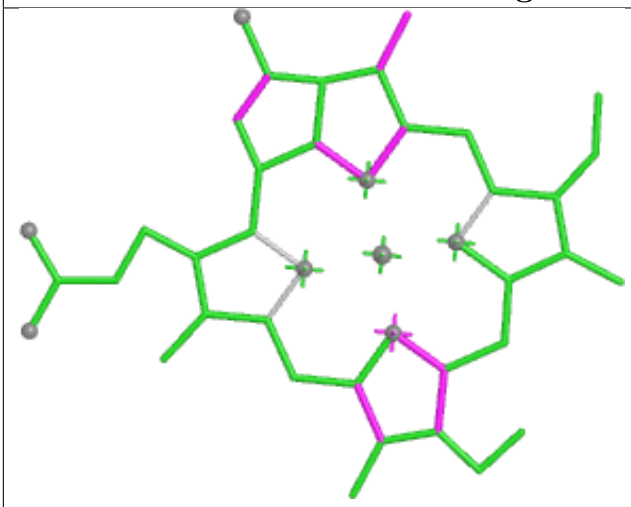


Torsions

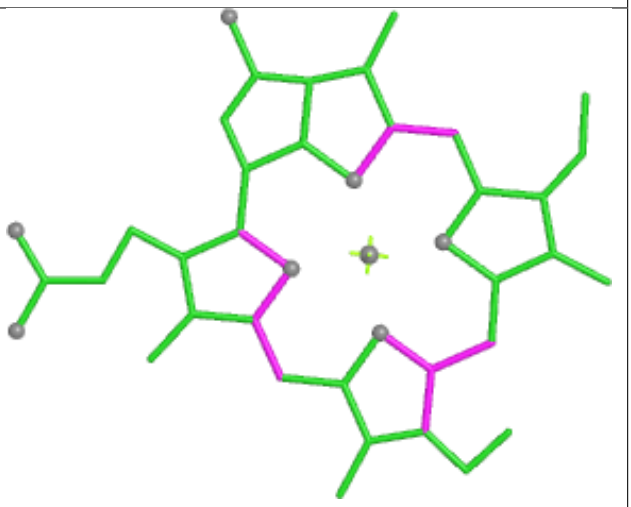


Rings

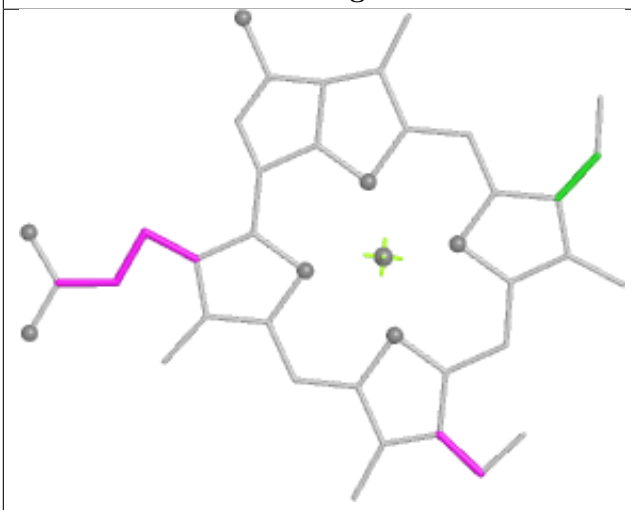
Ligand CLA cA 843



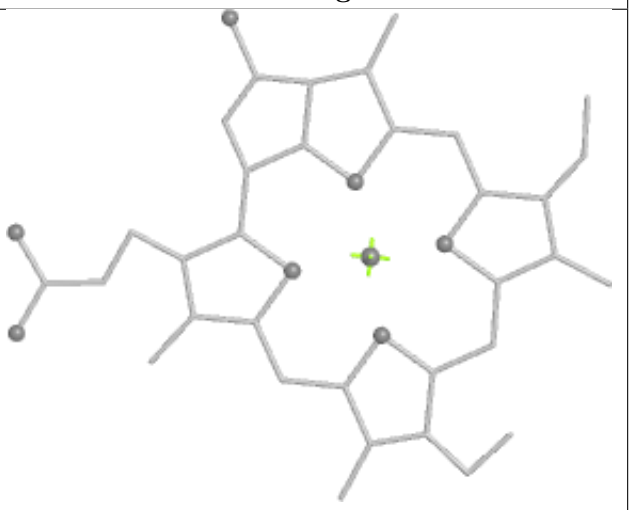
Bond lengths



Bond angles

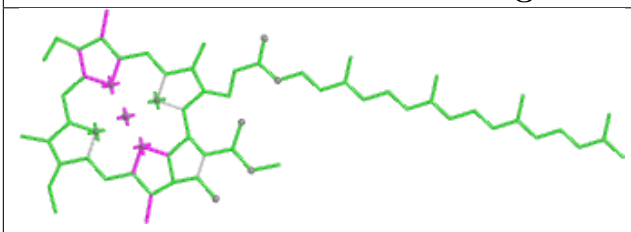


Torsions

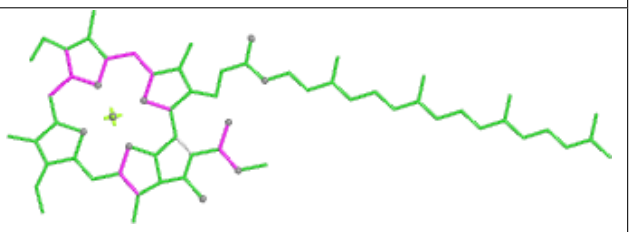


Rings

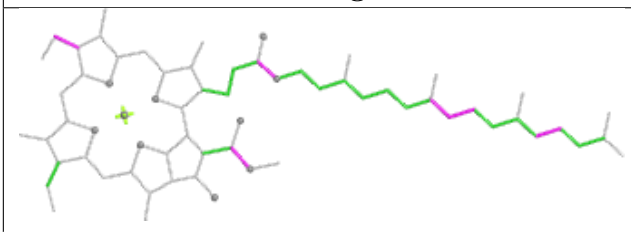
Ligand CLA aB 820



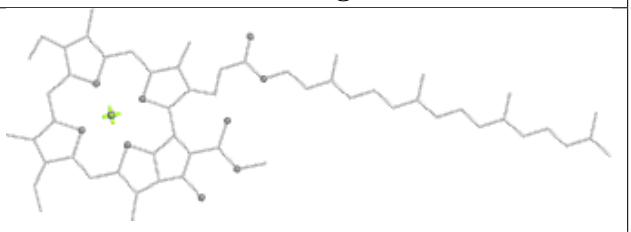
Bond lengths



Bond angles

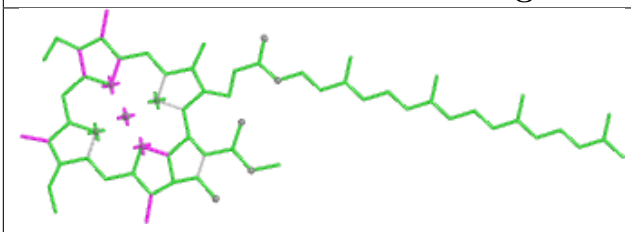


Torsions

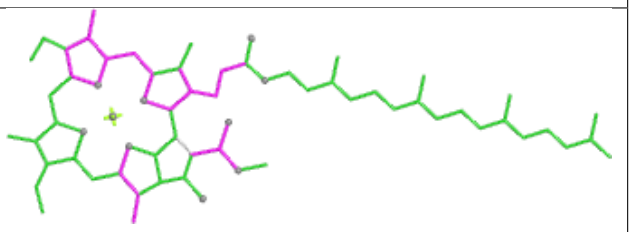


Rings

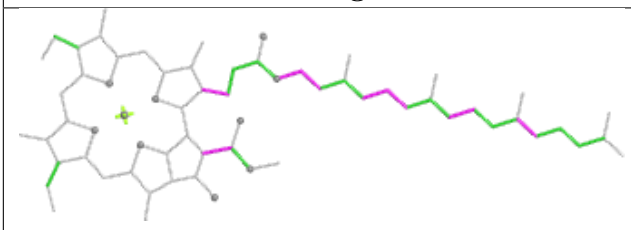
Ligand CLA cA 827



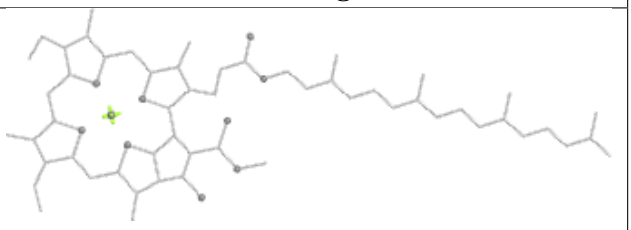
Bond lengths



Bond angles

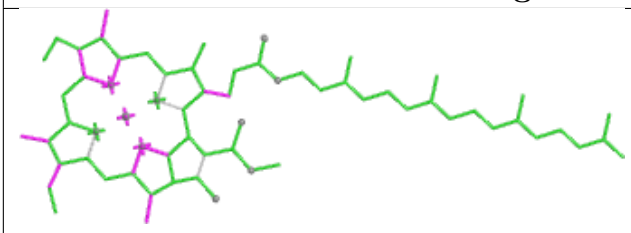


Torsions

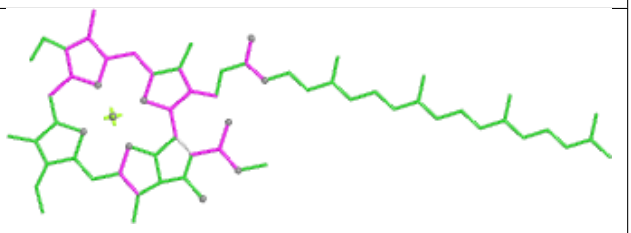


Rings

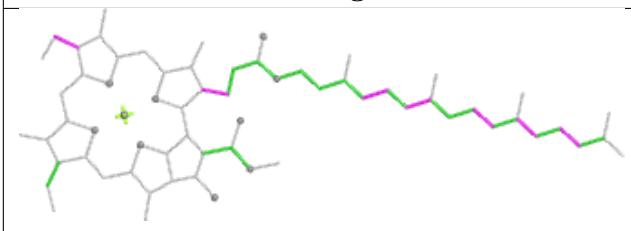
Ligand CLA bA 807



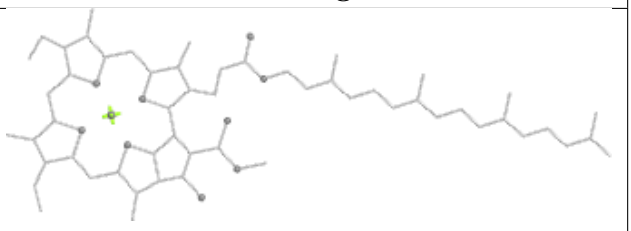
Bond lengths



Bond angles

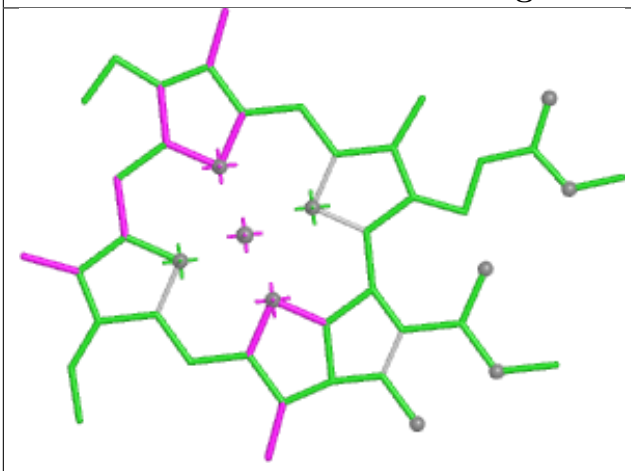


Torsions

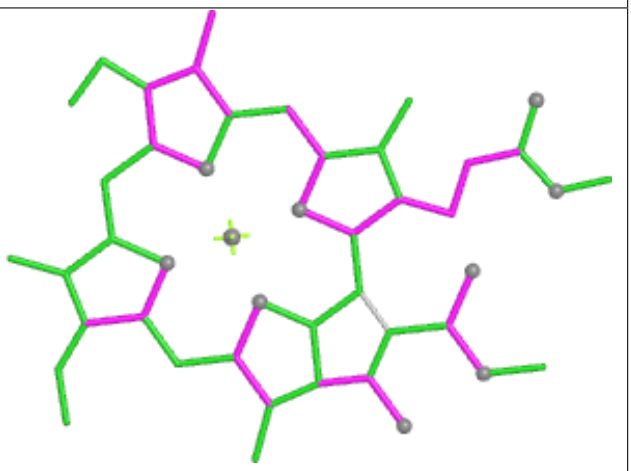


Rings

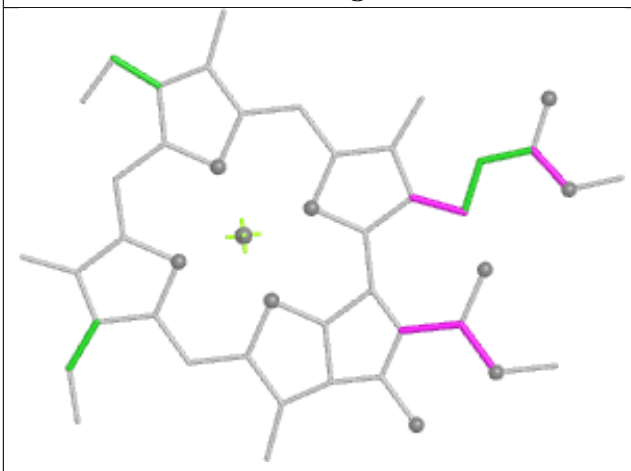
Ligand CLA aB 826



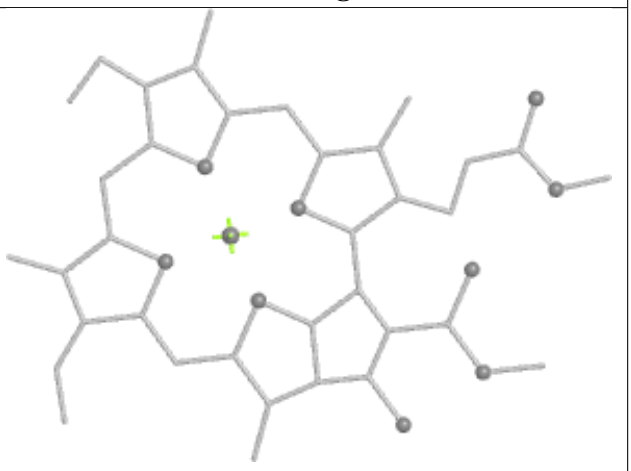
Bond lengths



Bond angles

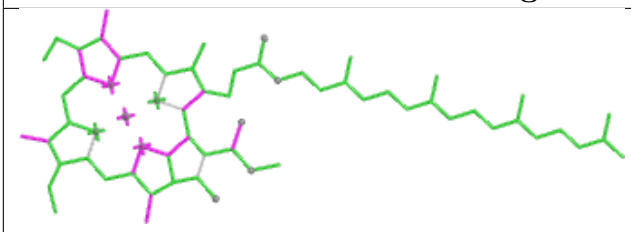


Torsions

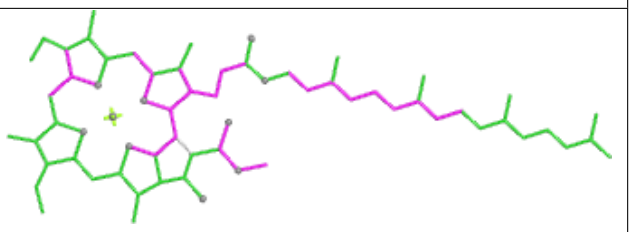


Rings

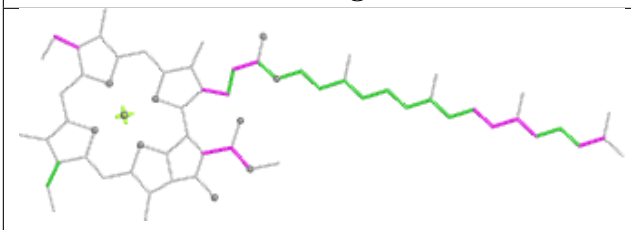
Ligand CLA c4 421



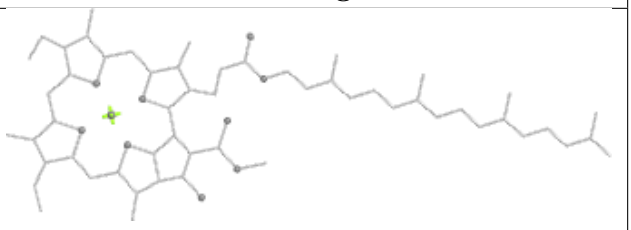
Bond lengths



Bond angles

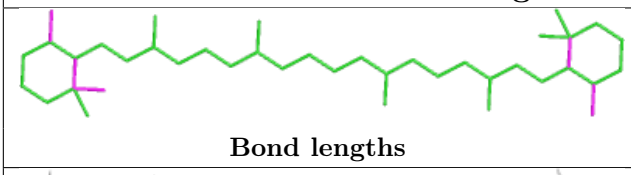


Torsions

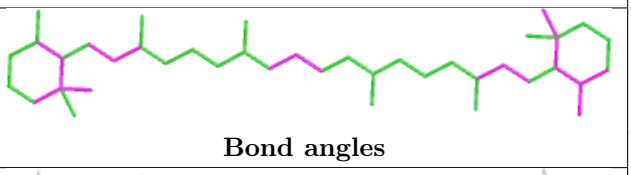


Rings

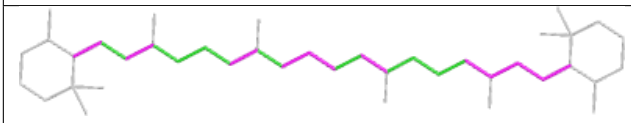
Ligand BCR bB 849



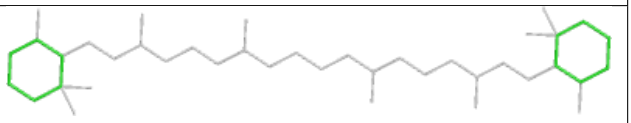
Bond lengths



Bond angles

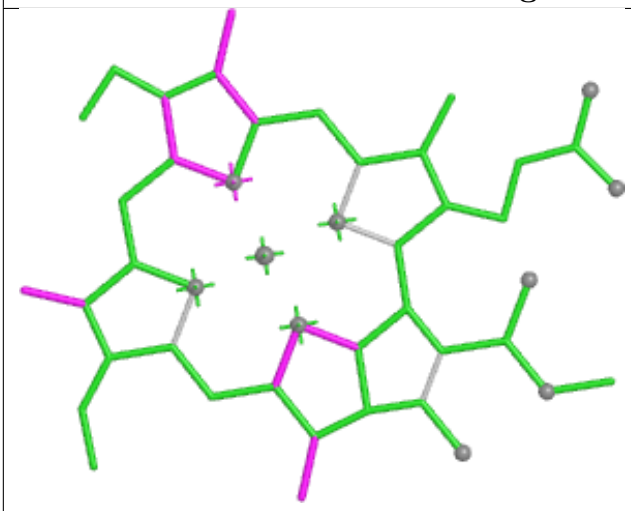


Torsions

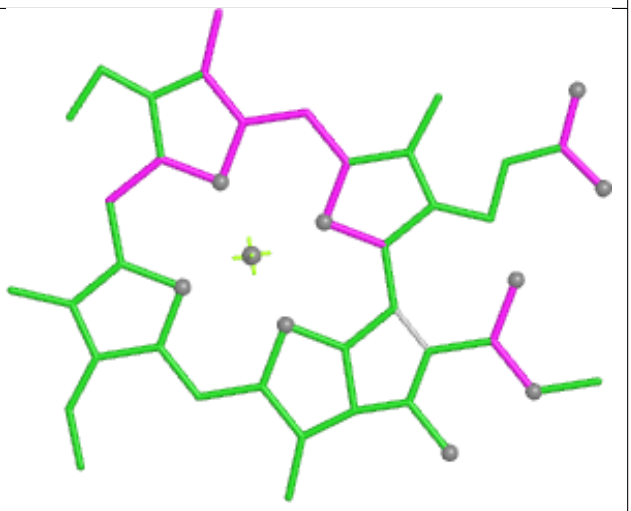


Rings

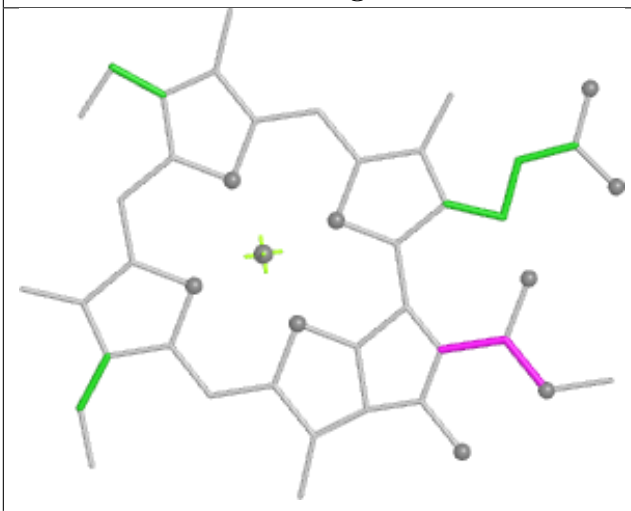
Ligand CLA a4 406



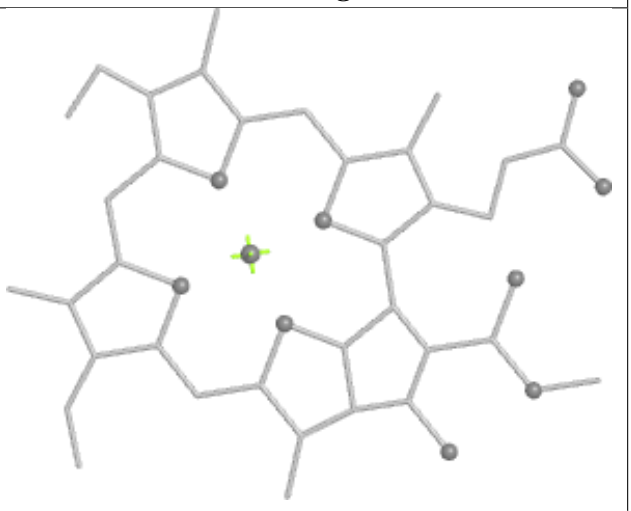
Bond lengths



Bond angles

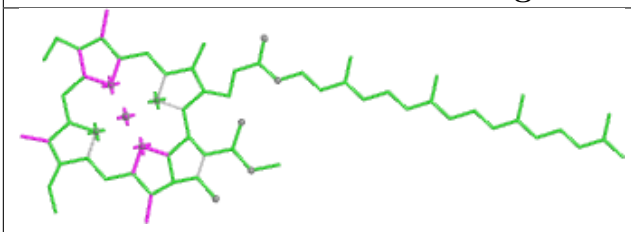


Torsions

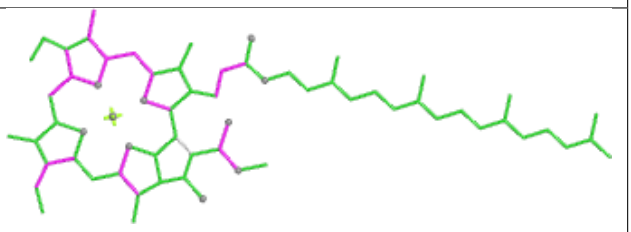


Rings

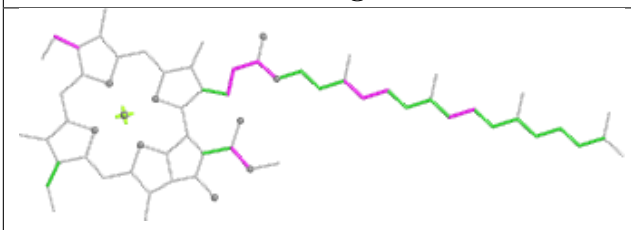
Ligand CLA bB 801



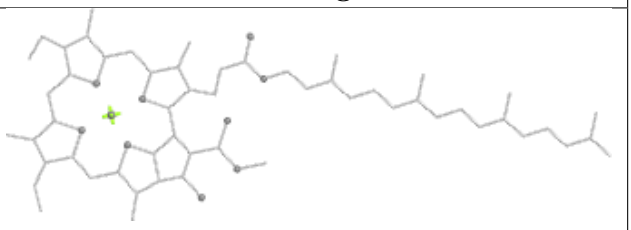
Bond lengths



Bond angles

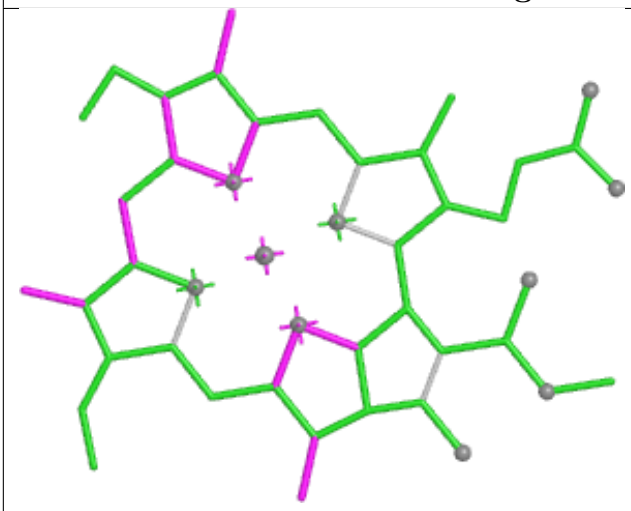


Torsions

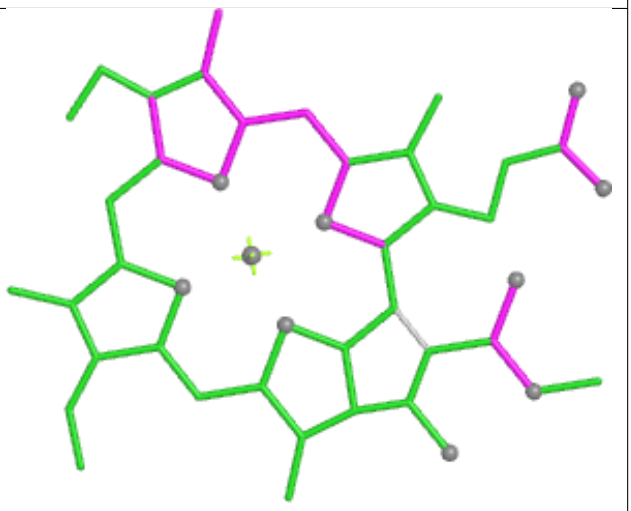


Rings

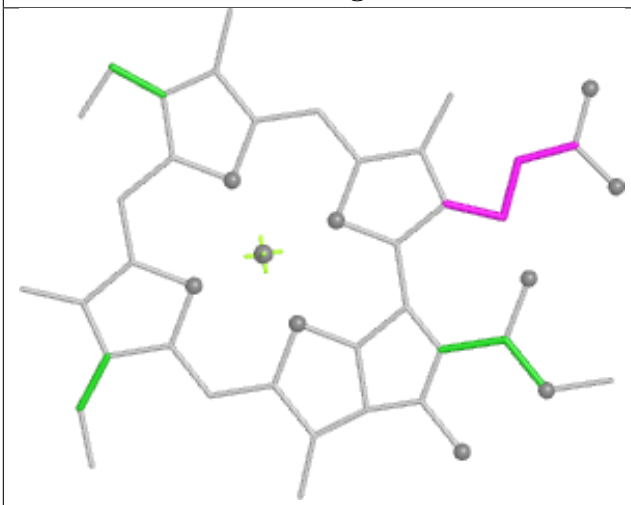
Ligand CLA bB 813



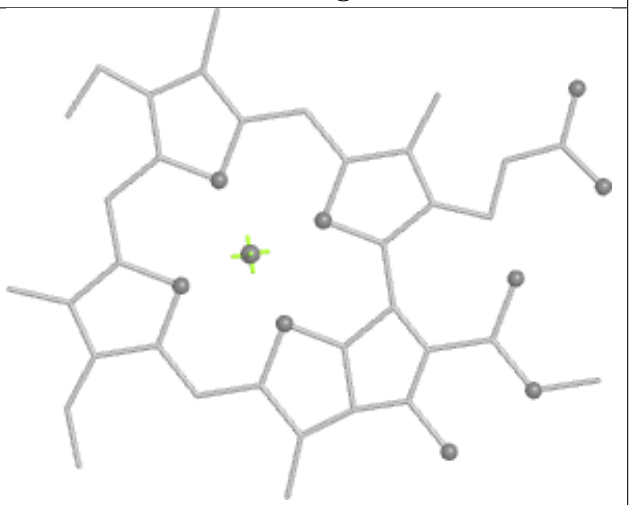
Bond lengths



Bond angles

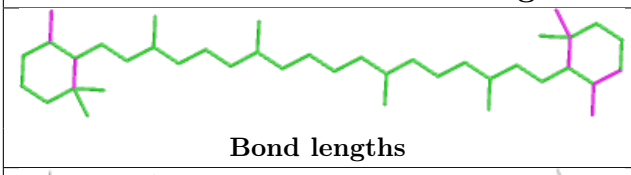


Torsions

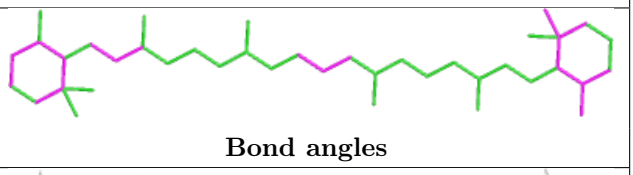


Rings

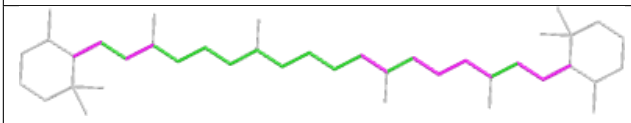
Ligand BCR a5 418



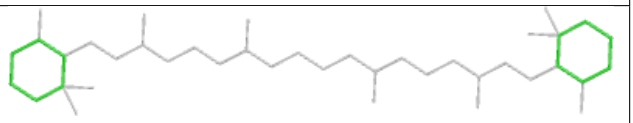
Bond lengths



Bond angles



Torsions

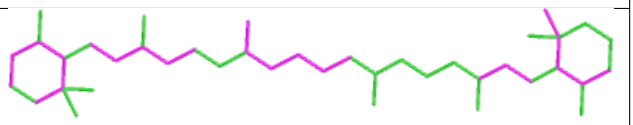


Rings

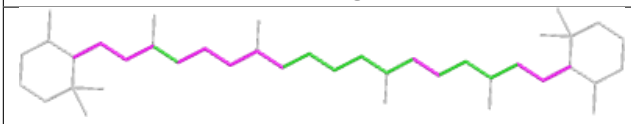
Ligand BCR a5 401



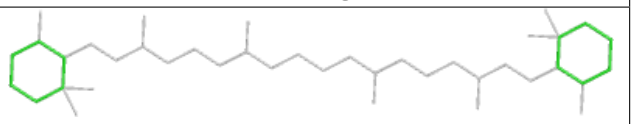
Bond lengths



Bond angles

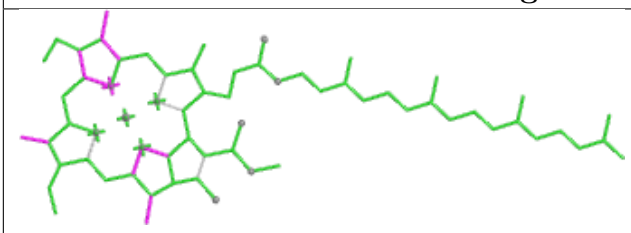


Torsions

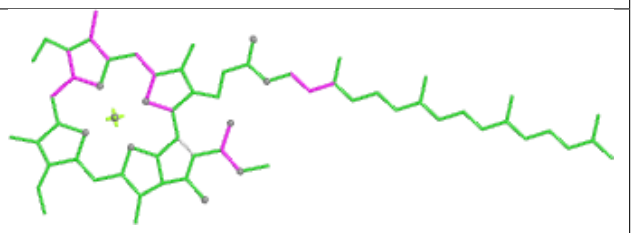


Rings

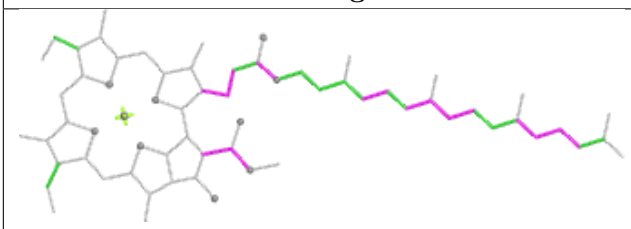
Ligand CLA c1 402



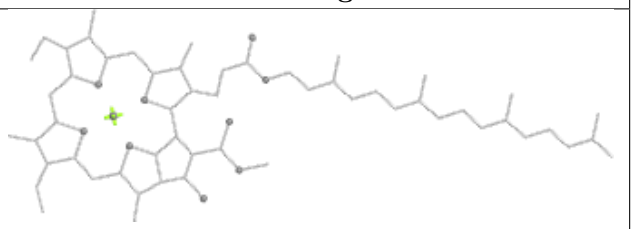
Bond lengths



Bond angles

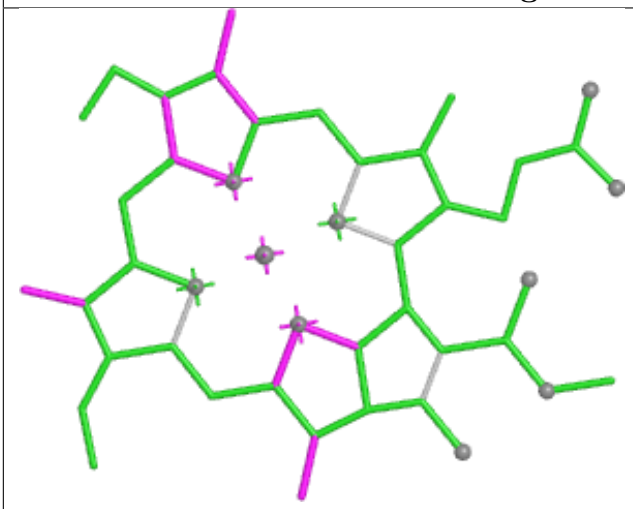


Torsions

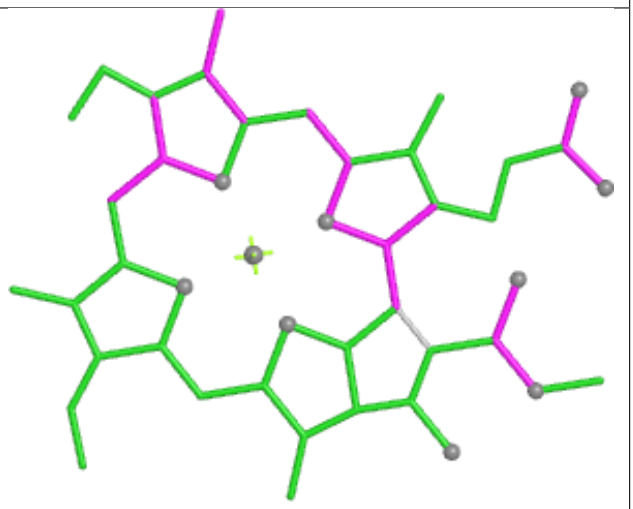


Rings

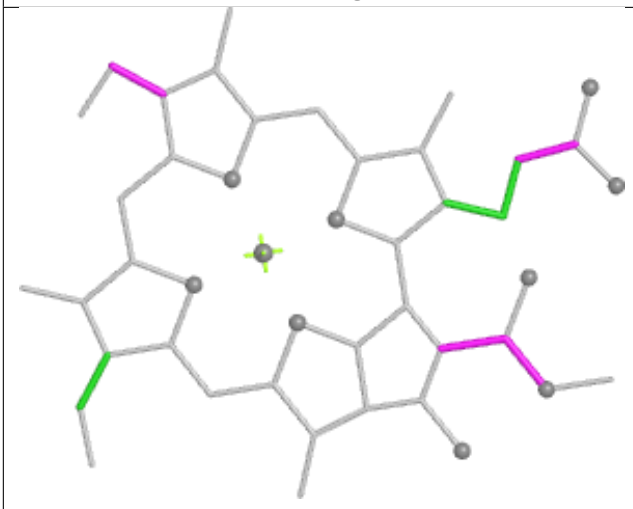
Ligand CLA c1 407



Bond lengths



Bond angles

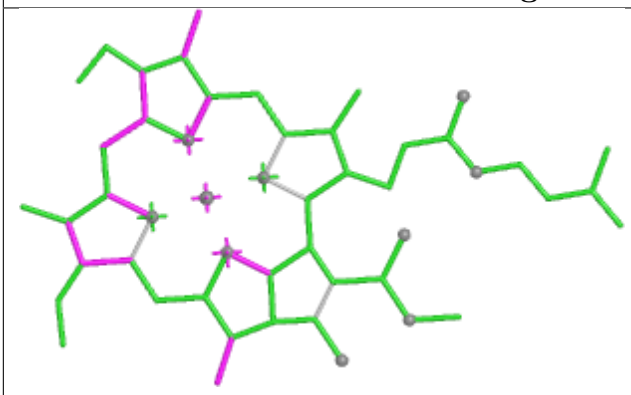


Torsions

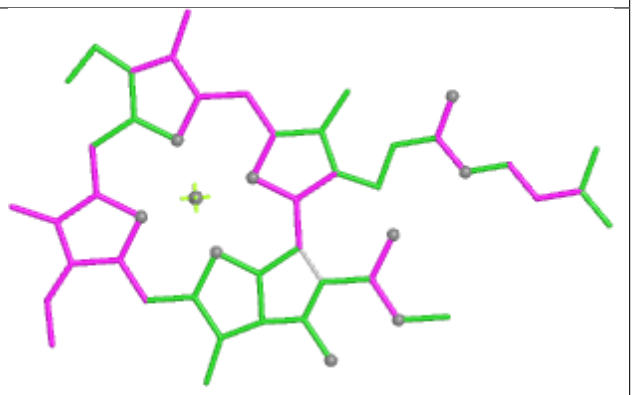


Rings

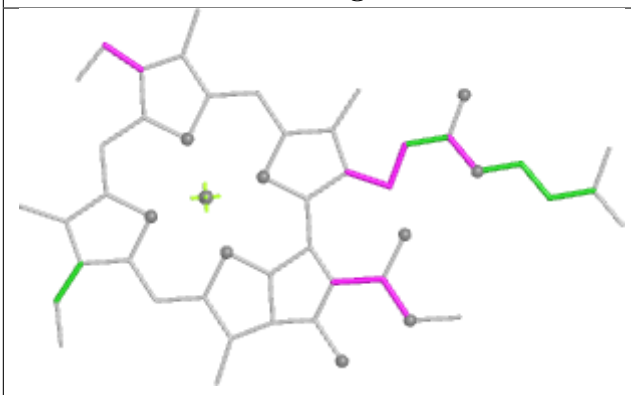
Ligand CLA c1 416



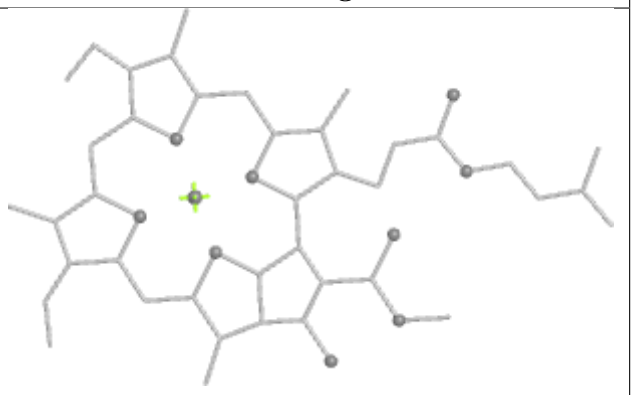
Bond lengths



Bond angles

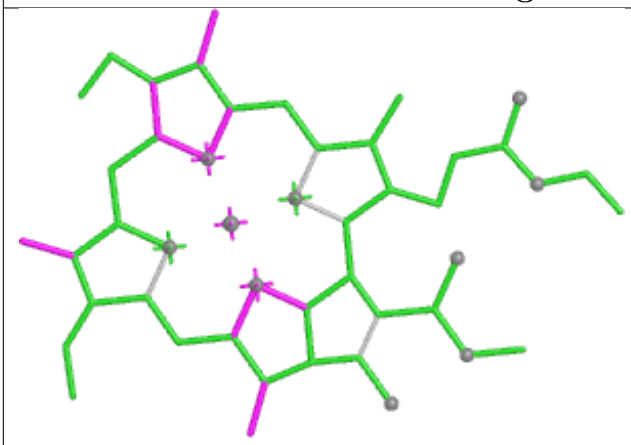


Torsions

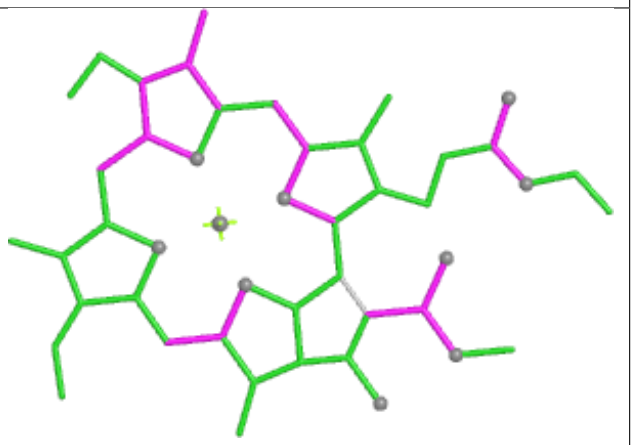


Rings

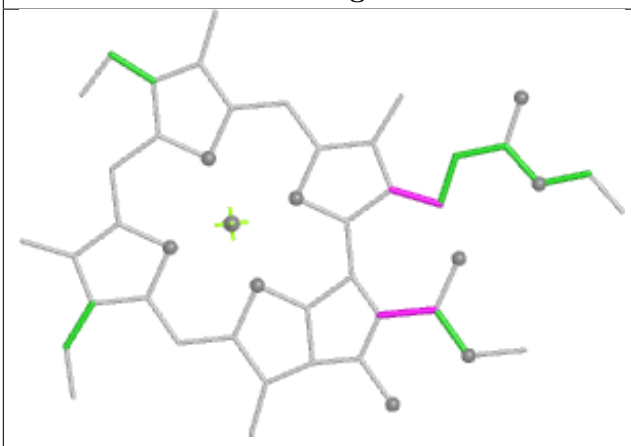
Ligand CLA cB 838



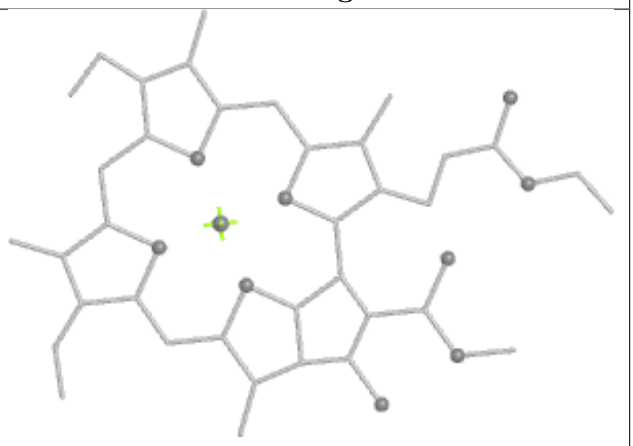
Bond lengths



Bond angles

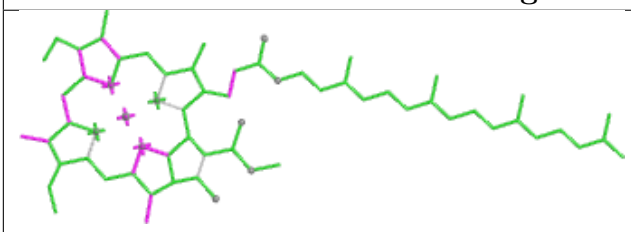


Torsions

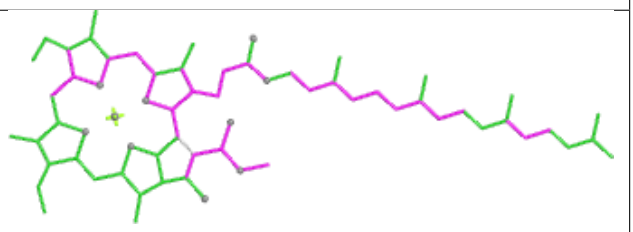


Rings

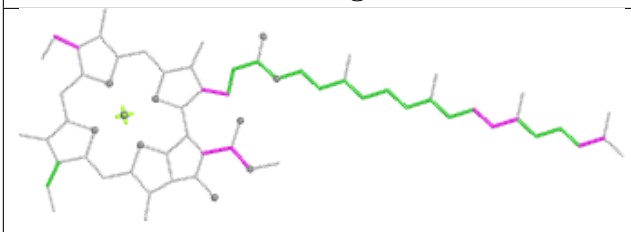
Ligand CLA c2 406



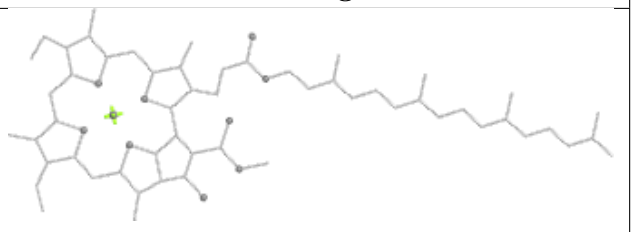
Bond lengths



Bond angles

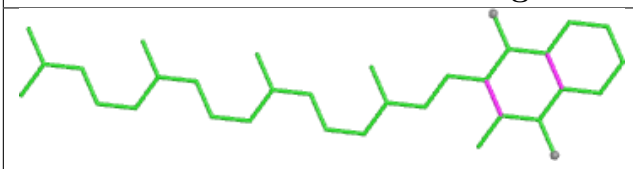


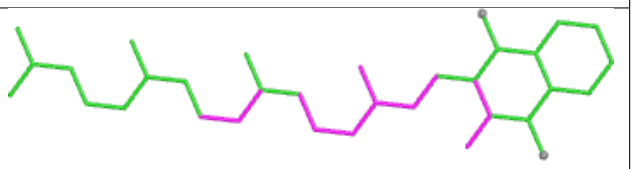
Torsions

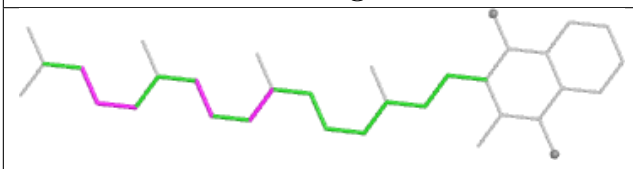


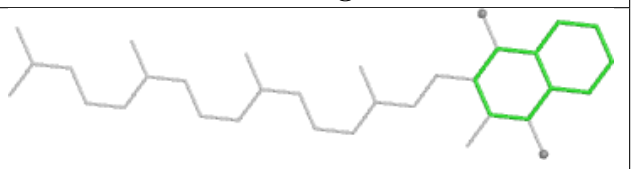
Rings

Ligand PQN bA 846

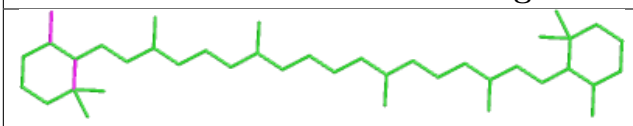

Bond lengths

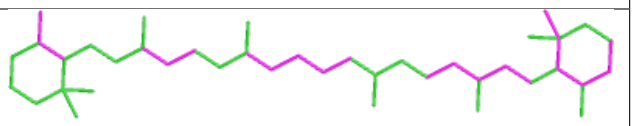

Bond angles

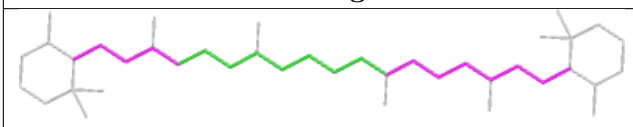

Torsions

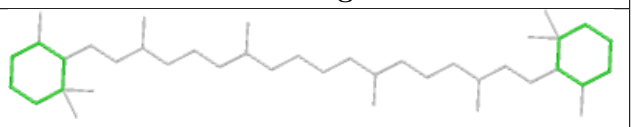

Rings

Ligand BCR cA 849

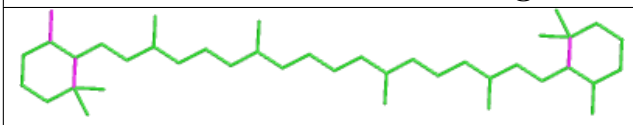

Bond lengths

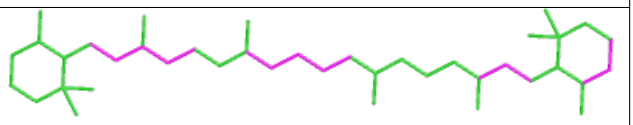

Bond angles

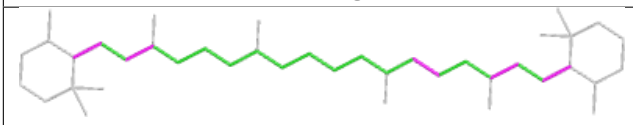

Torsions

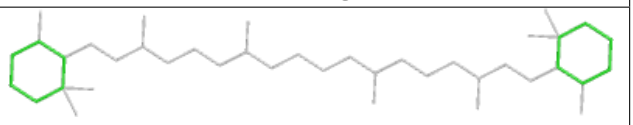

Rings

Ligand BCR cB 844

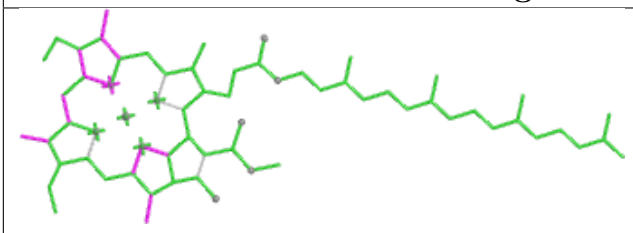

Bond lengths

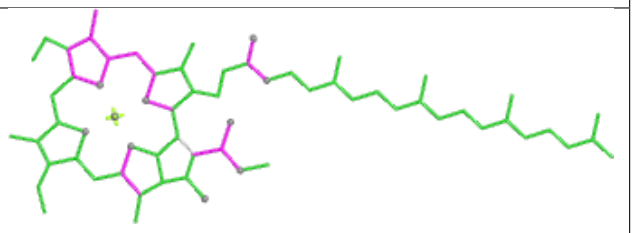

Bond angles

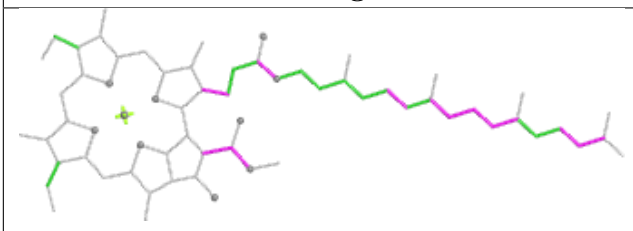

Torsions

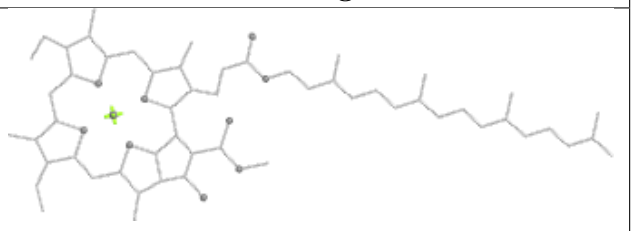

Rings

Ligand CLA bB 815

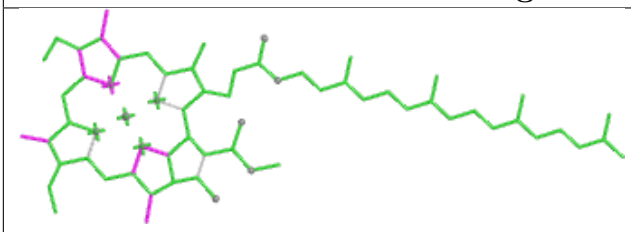

Bond lengths


Bond angles

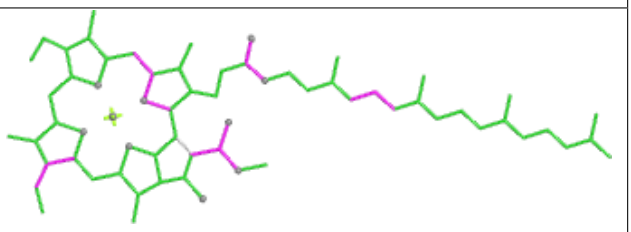

Torsions


Rings

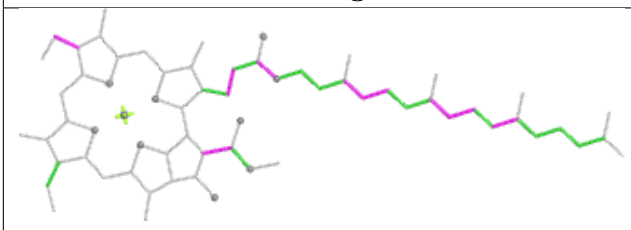
Ligand CLA cB 808



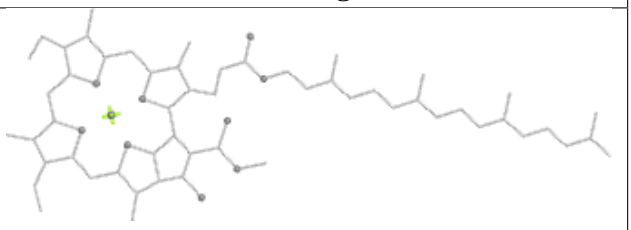
Bond lengths



Bond angles

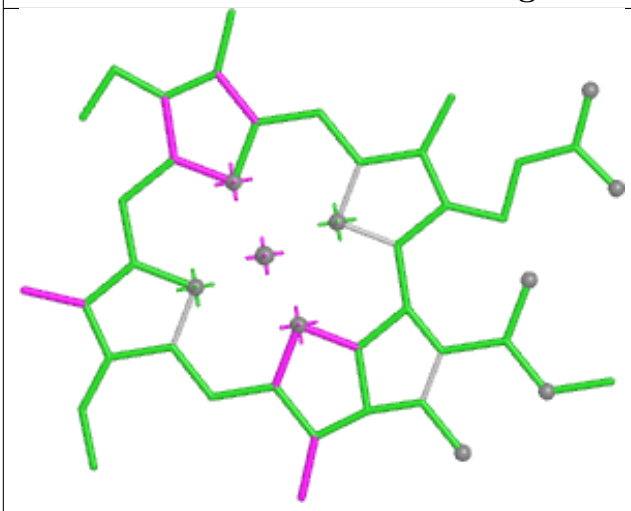


Torsions

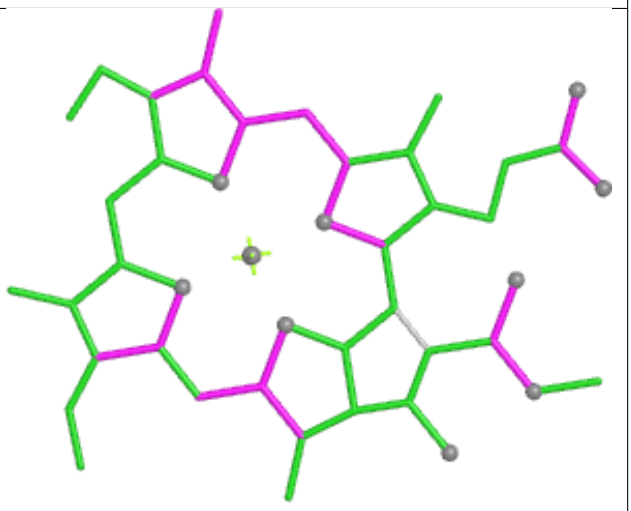


Rings

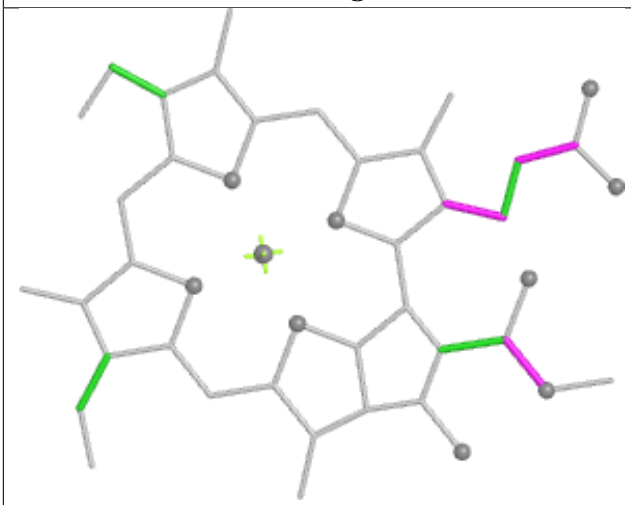
Ligand CLA b2 409



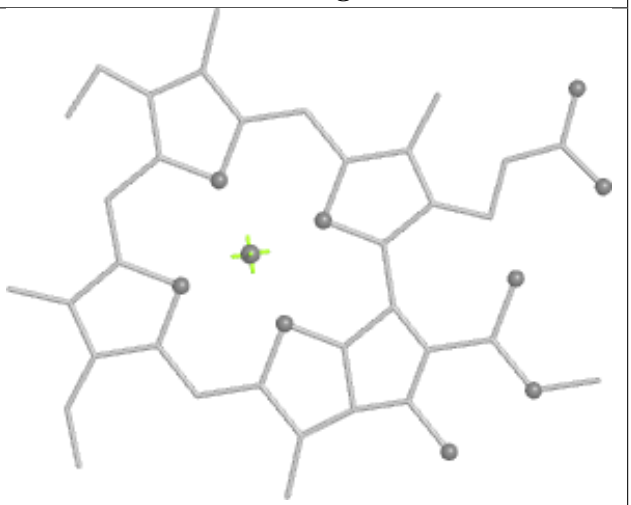
Bond lengths



Bond angles

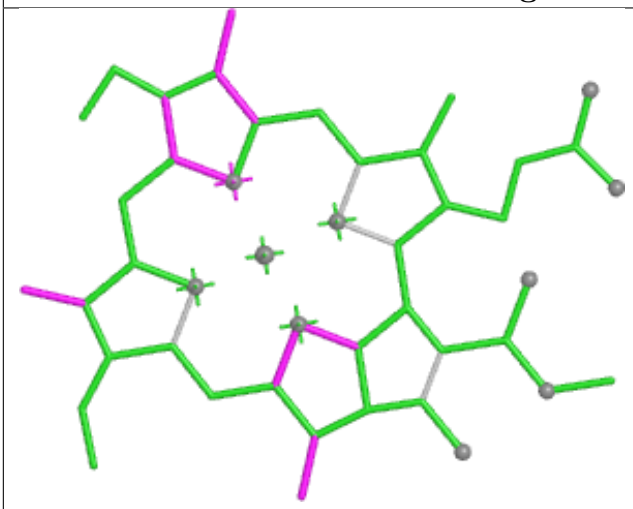


Torsions

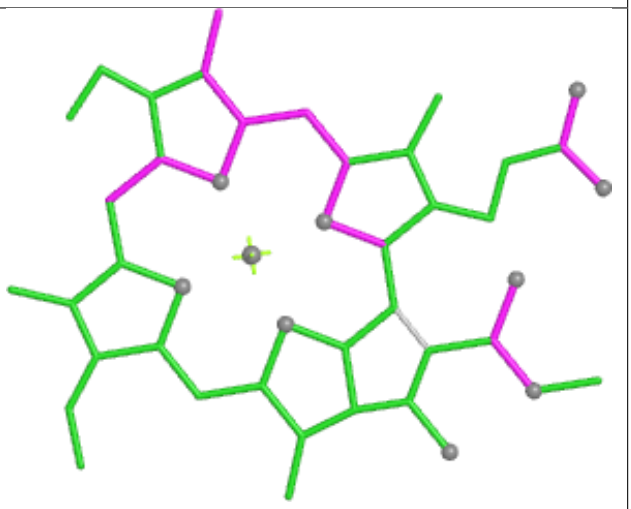


Rings

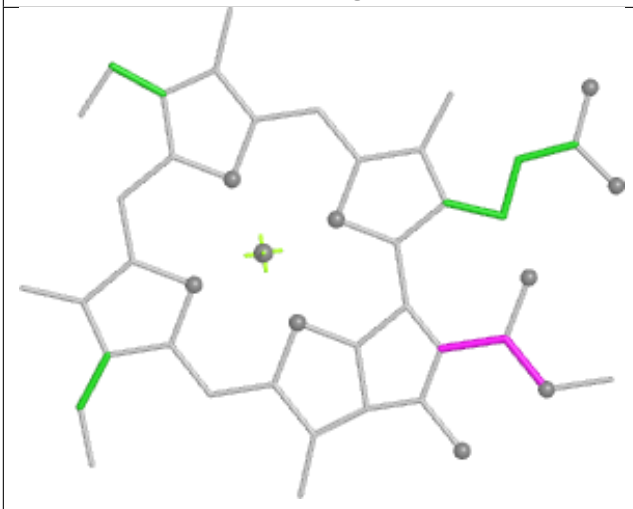
Ligand CLA a6 407



Bond lengths



Bond angles

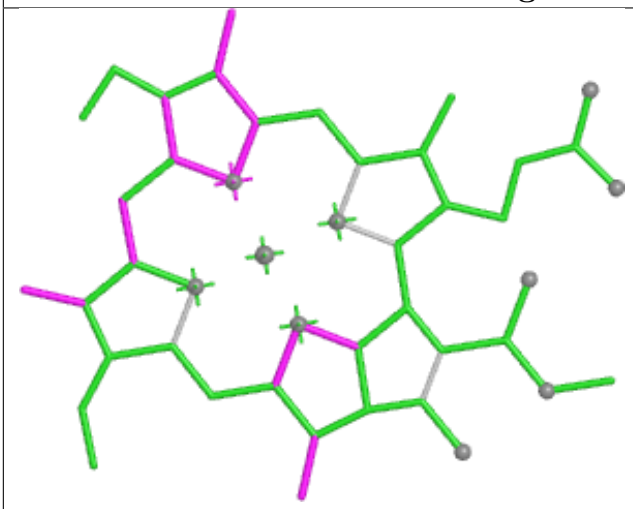


Torsions

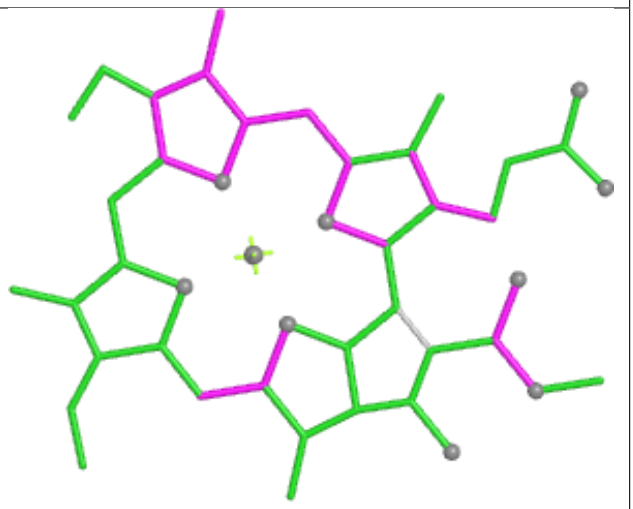


Rings

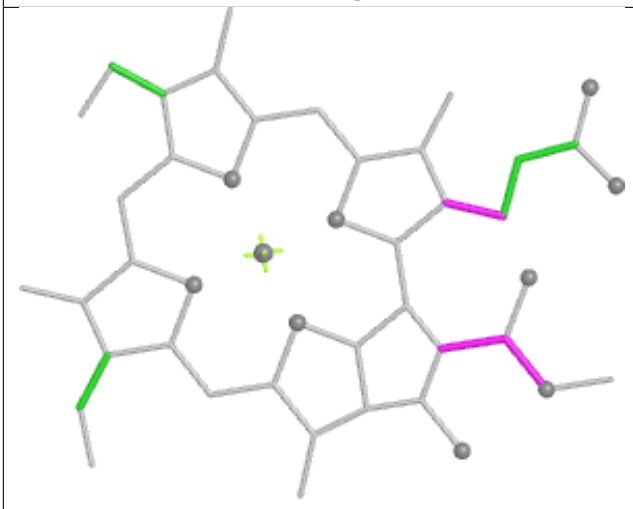
Ligand CLA b4 411



Bond lengths



Bond angles

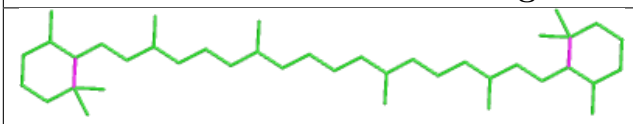


Torsions

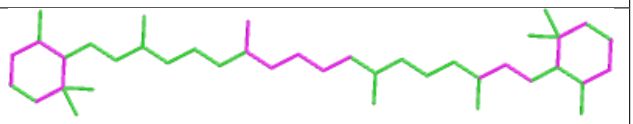


Rings

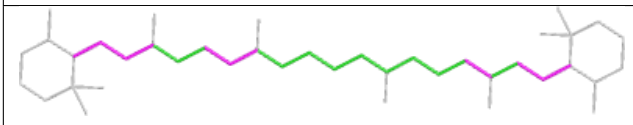
Ligand BCR c3 420



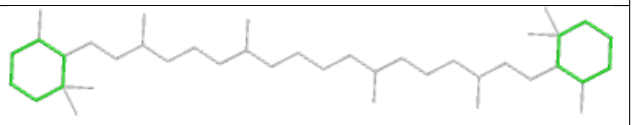
Bond lengths



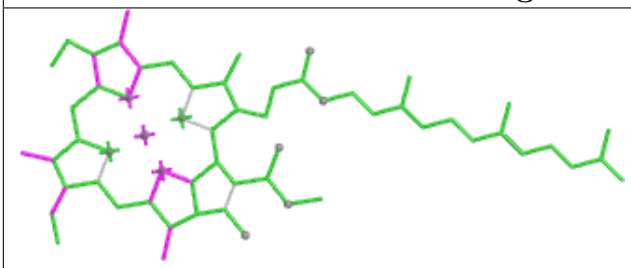
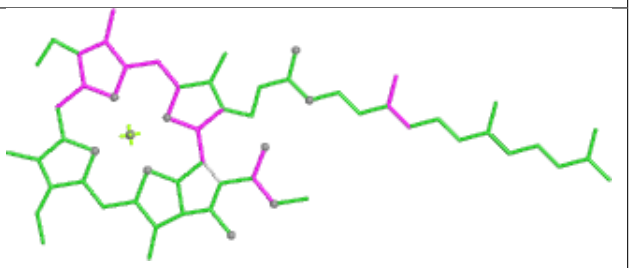
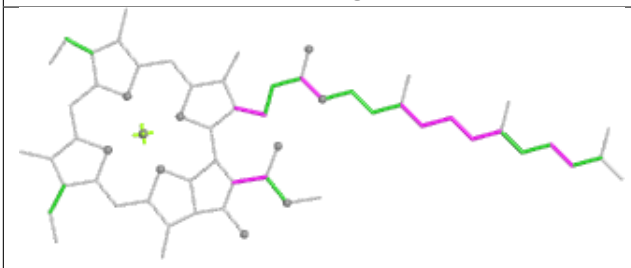
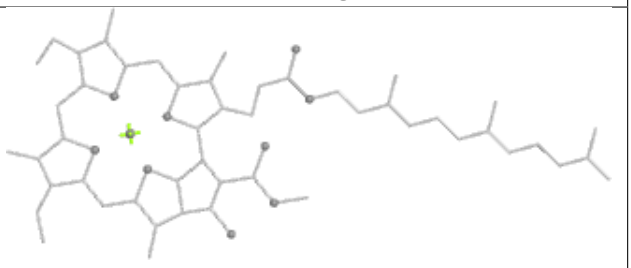
Bond angles

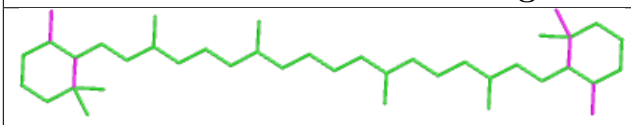
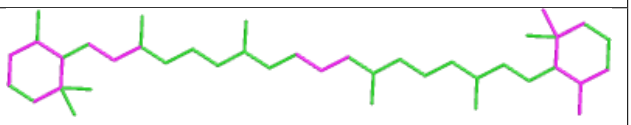
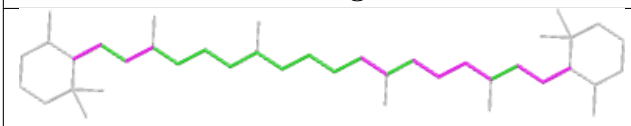
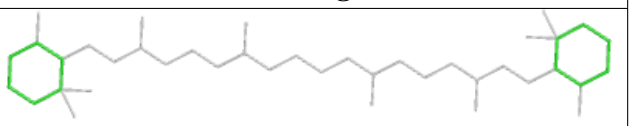


Torsions

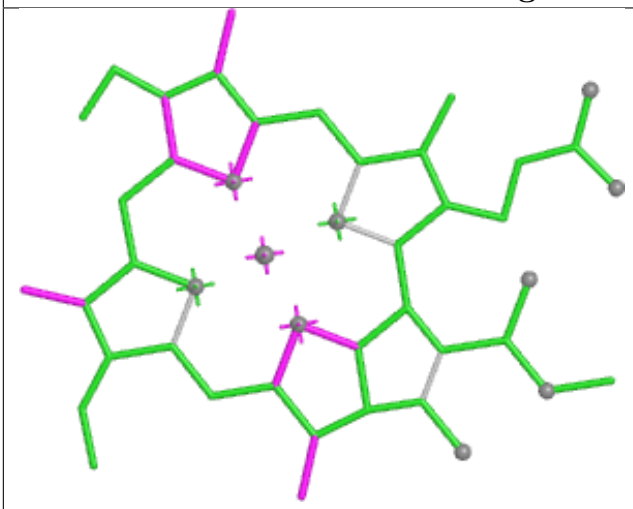


Rings

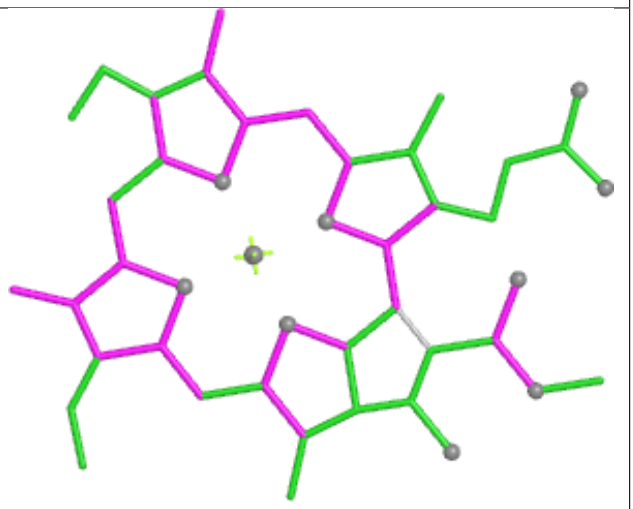
Ligand CLA cB 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR c5 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

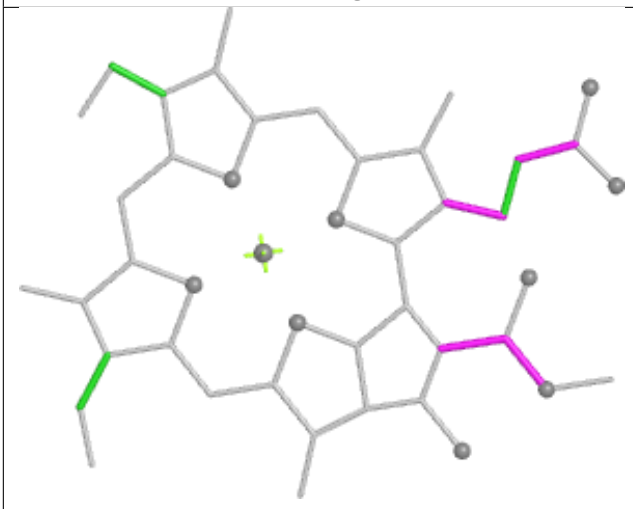
Ligand CLA b2 413



Bond lengths



Bond angles

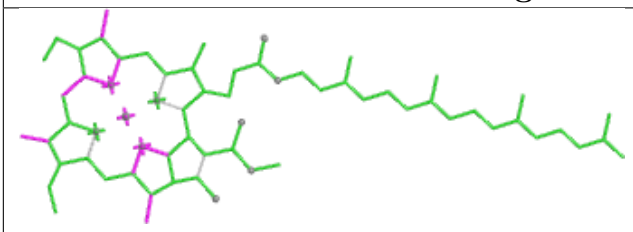


Torsions

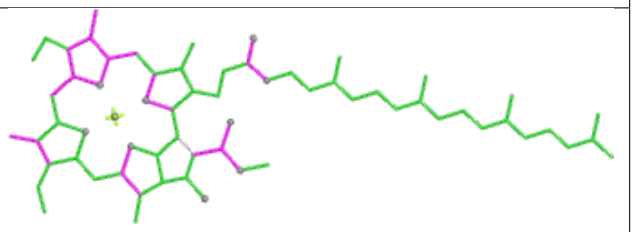


Rings

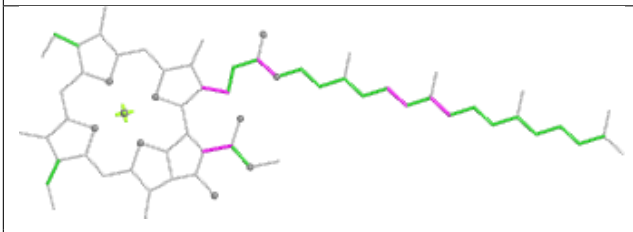
Ligand CLA aA 831



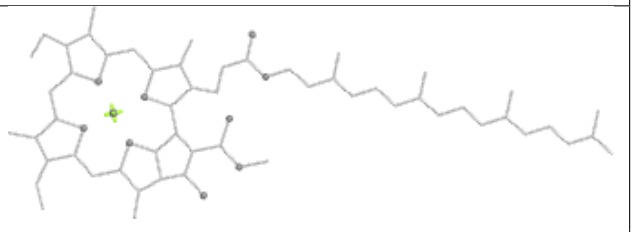
Bond lengths



Bond angles

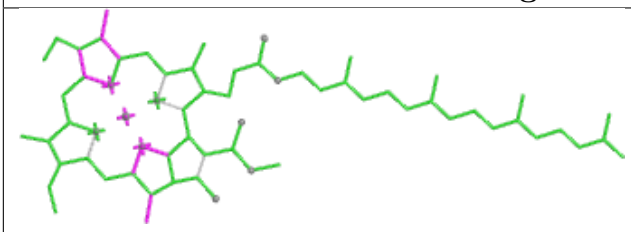


Torsions

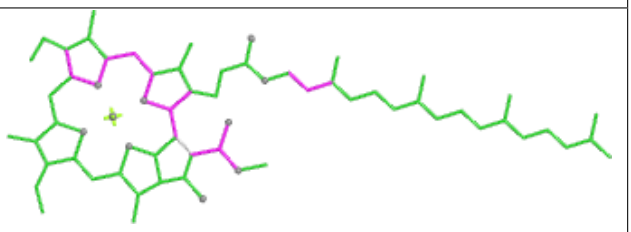


Rings

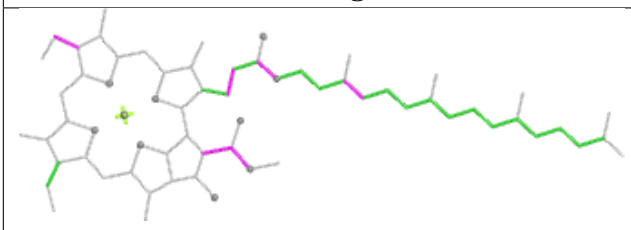
Ligand CLA a5 404



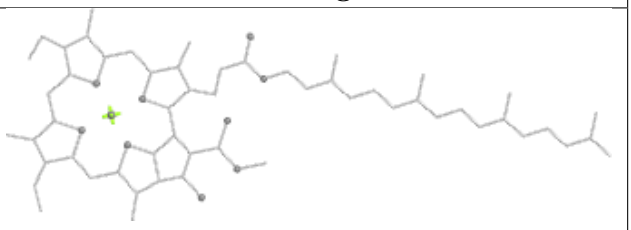
Bond lengths



Bond angles

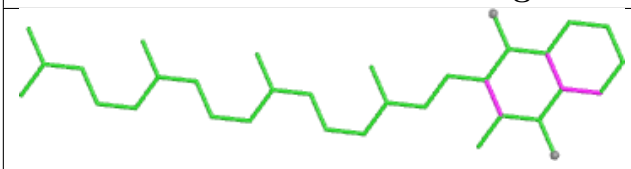


Torsions

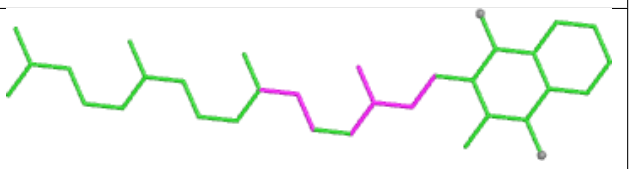


Rings

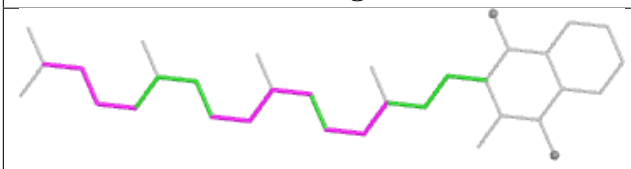
Ligand PQN aB 843



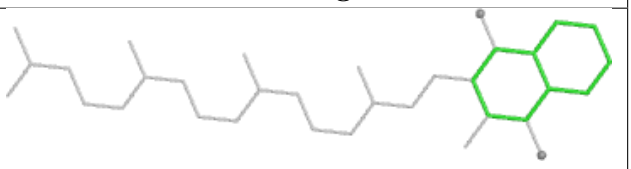
Bond lengths



Bond angles

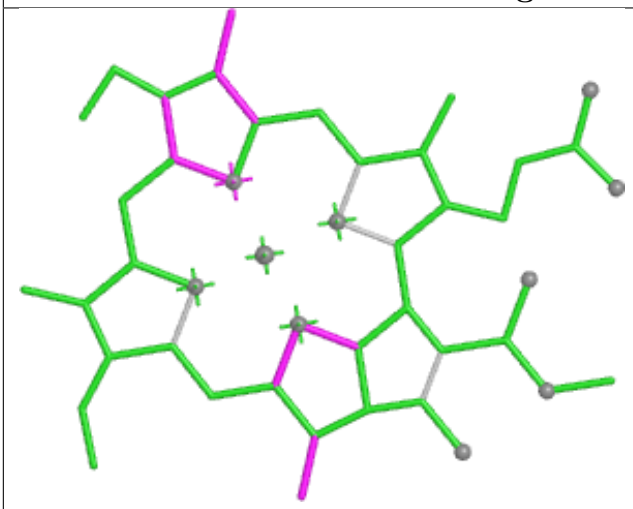


Torsions

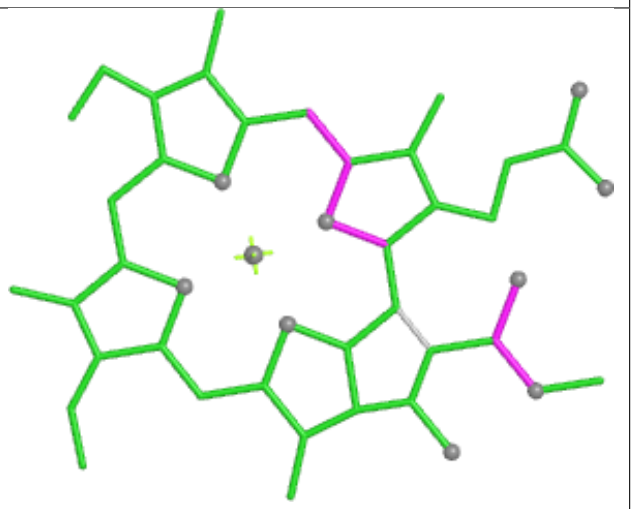


Rings

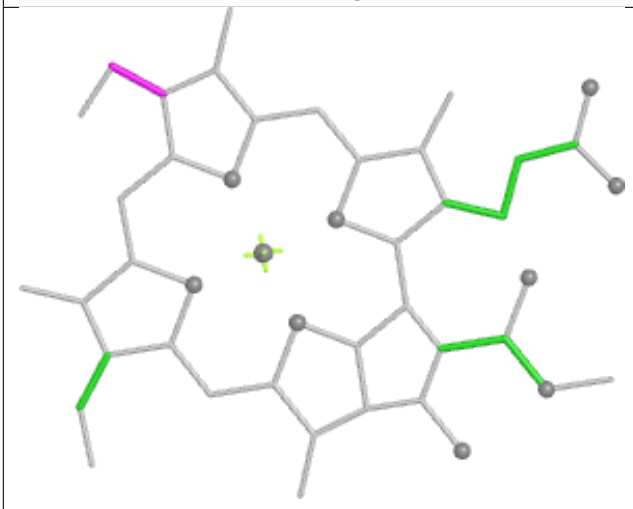
Ligand CLA cB 842



Bond lengths



Bond angles

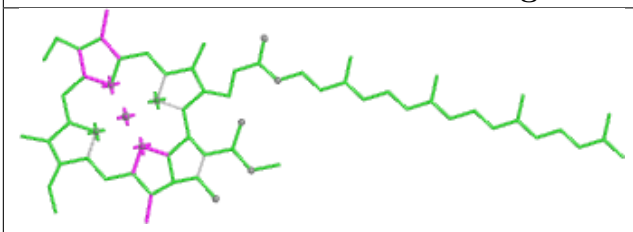


Torsions

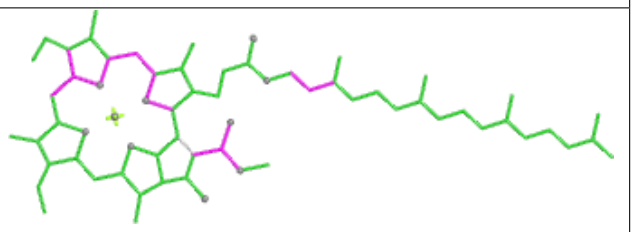


Rings

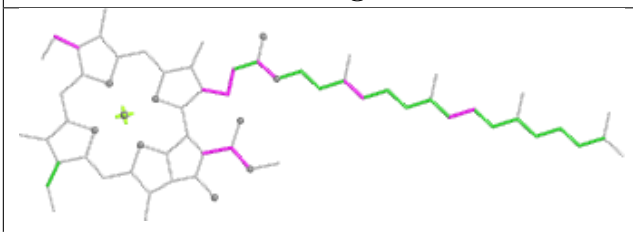
Ligand CLA c1 404



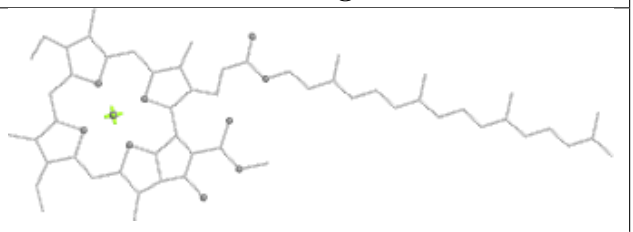
Bond lengths



Bond angles

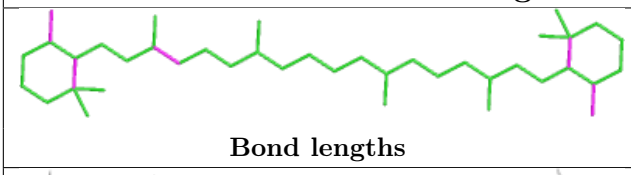


Torsions

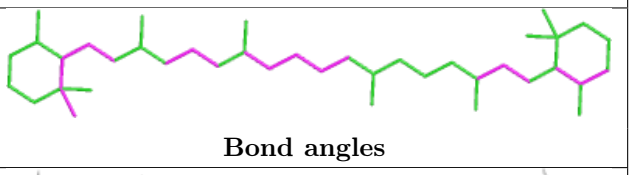


Rings

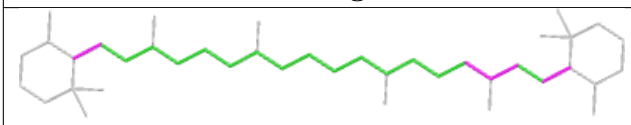
Ligand BCR cA 850



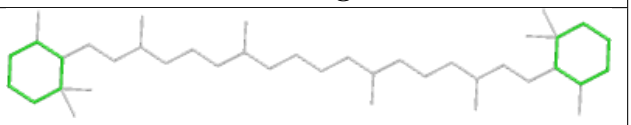
Bond lengths



Bond angles

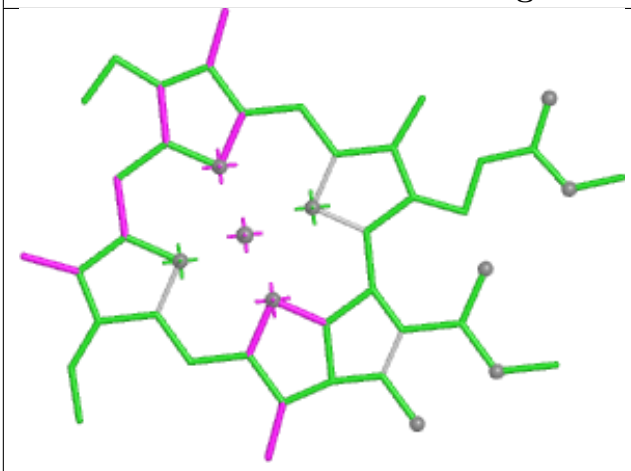


Torsions

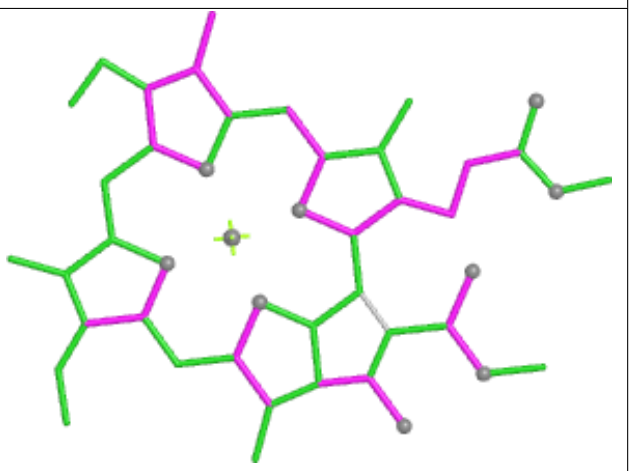


Rings

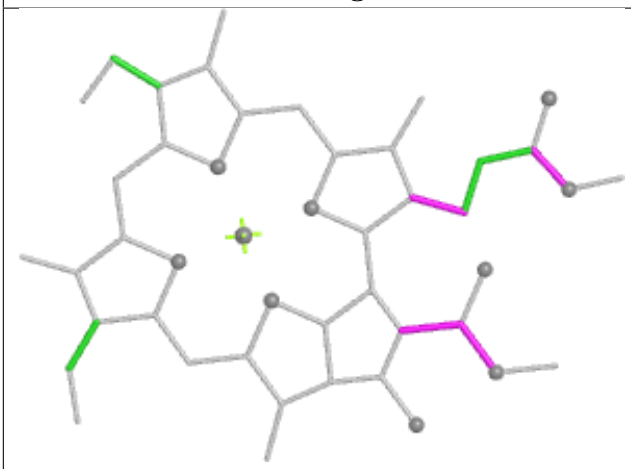
Ligand CLA cB 826



Bond lengths



Bond angles

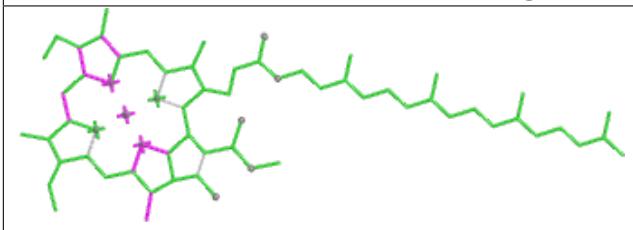


Torsions

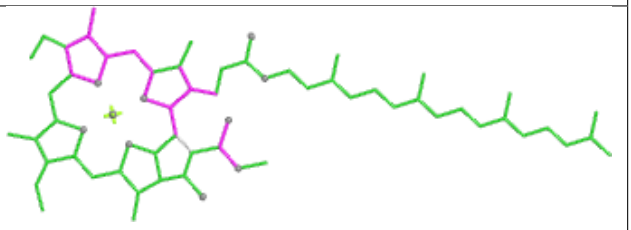


Rings

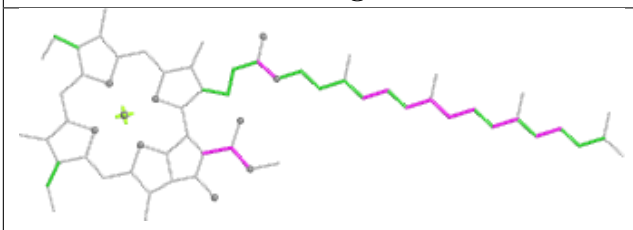
Ligand CLA c2 403



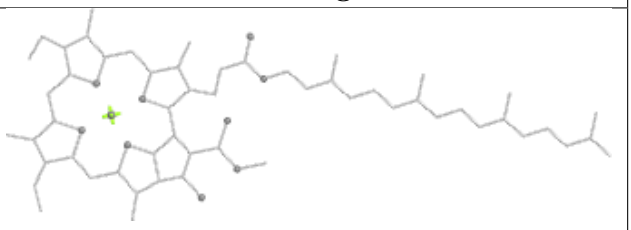
Bond lengths



Bond angles

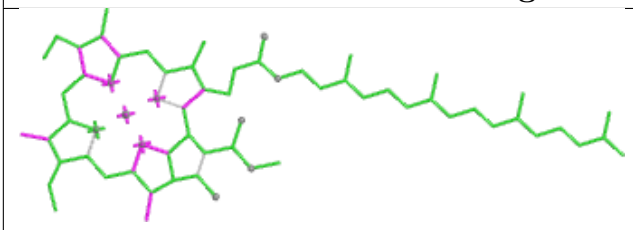


Torsions

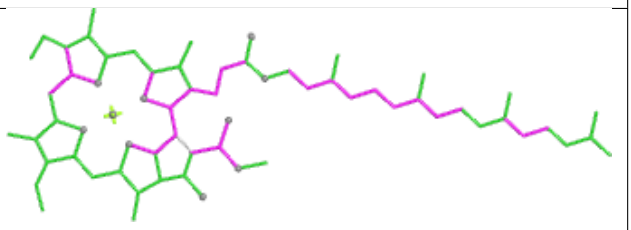


Rings

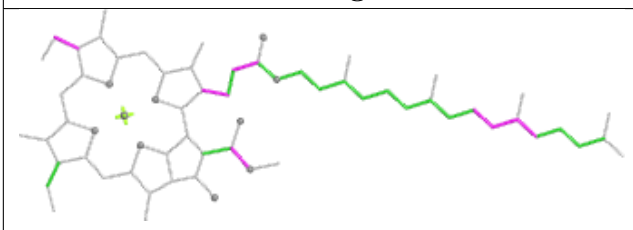
Ligand CLA b3 421



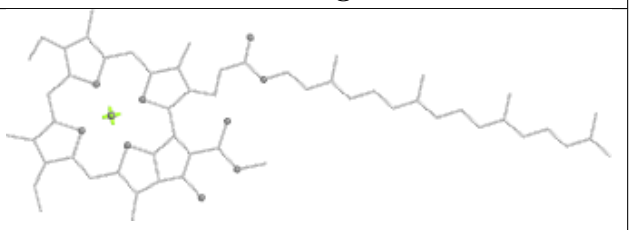
Bond lengths



Bond angles

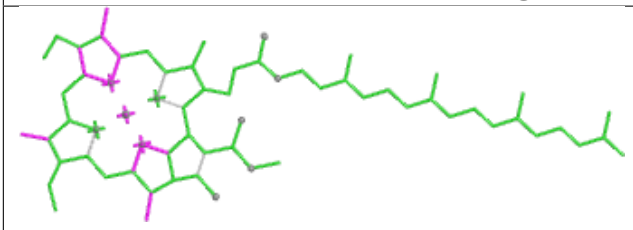


Torsions

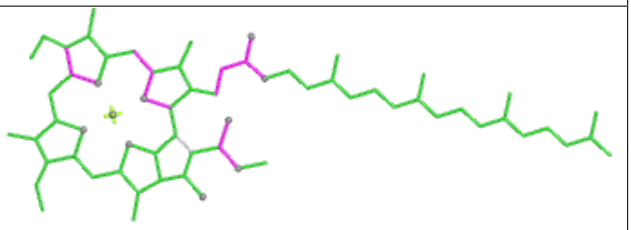


Rings

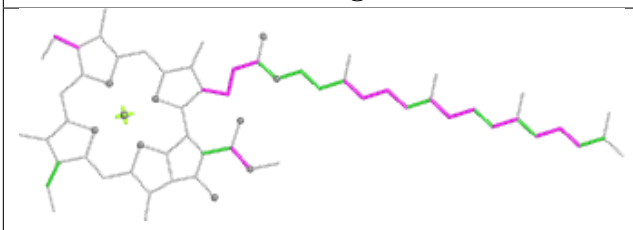
Ligand CLA aA 810



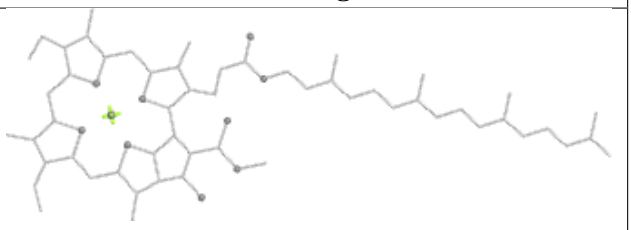
Bond lengths



Bond angles

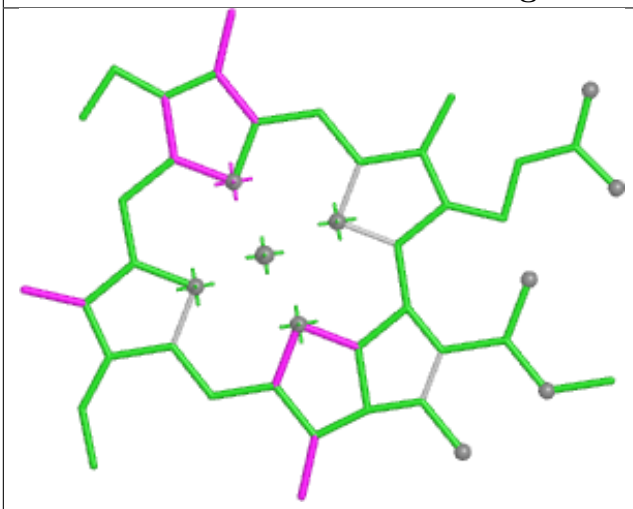


Torsions

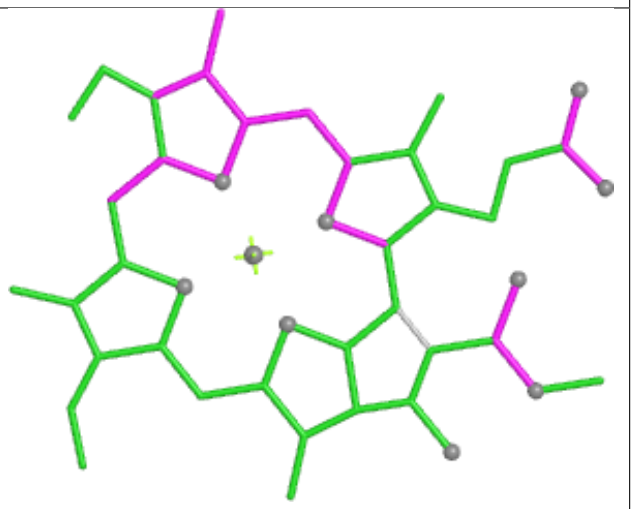


Rings

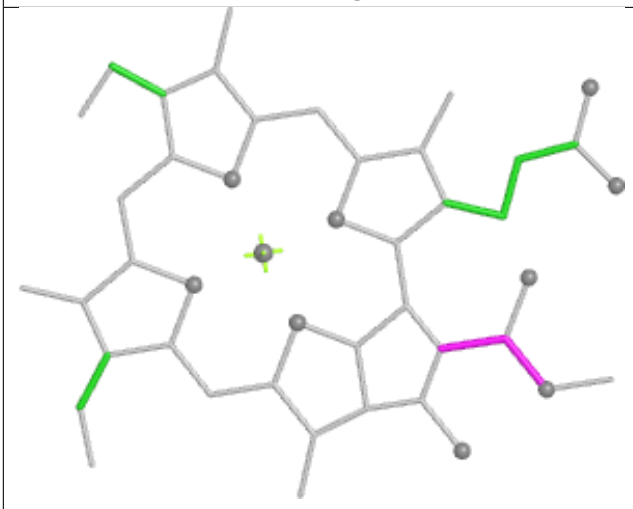
Ligand CLA a1 405



Bond lengths



Bond angles

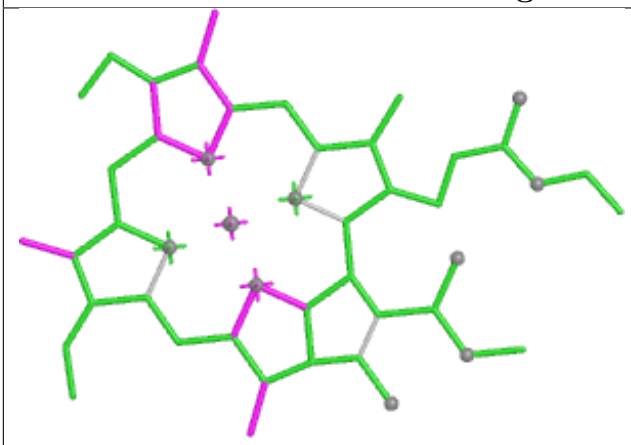


Torsions

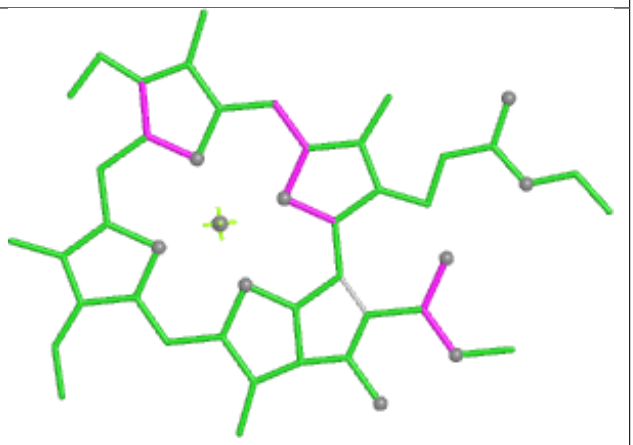


Rings

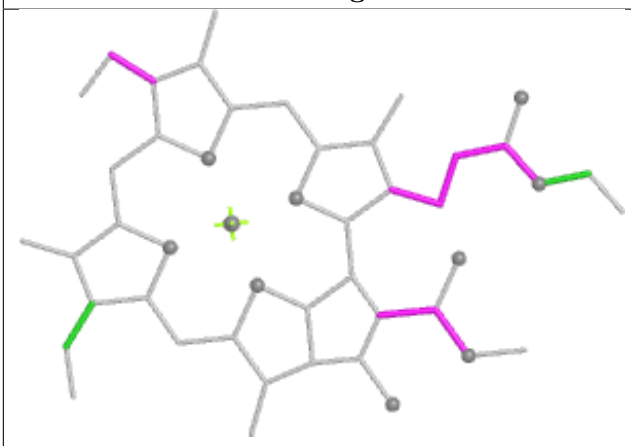
Ligand CLA cB 821



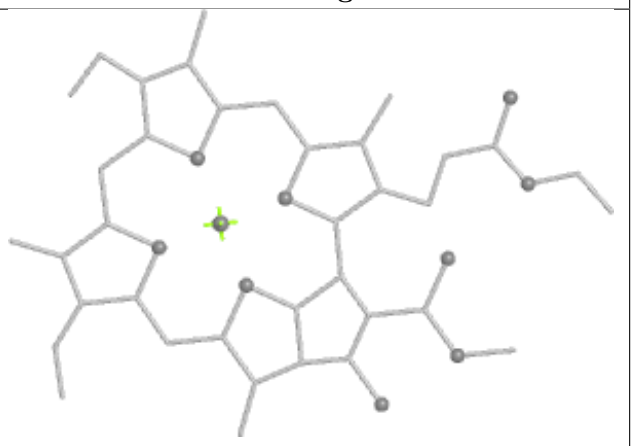
Bond lengths



Bond angles

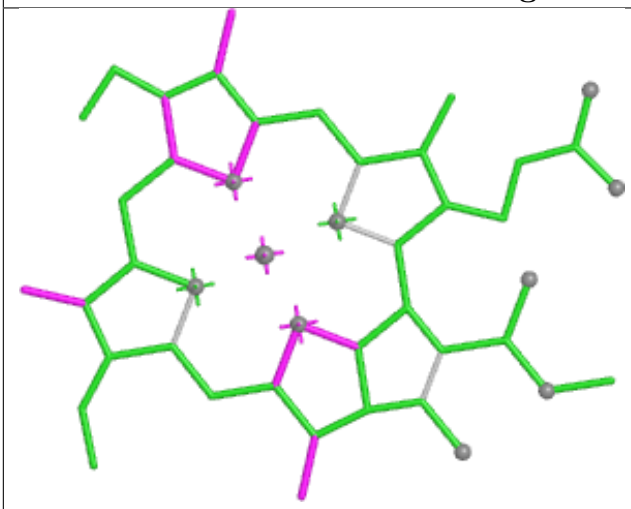


Torsions

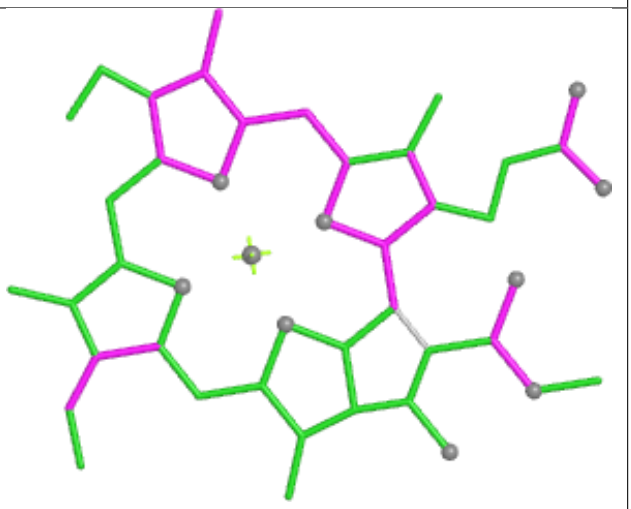


Rings

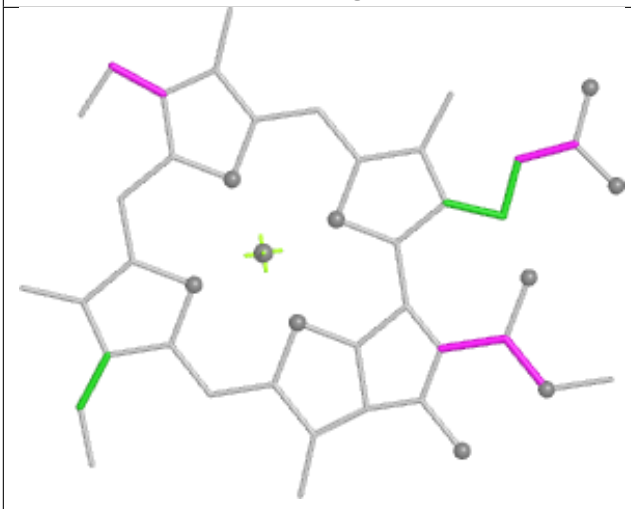
Ligand CLA aJ 201



Bond lengths



Bond angles

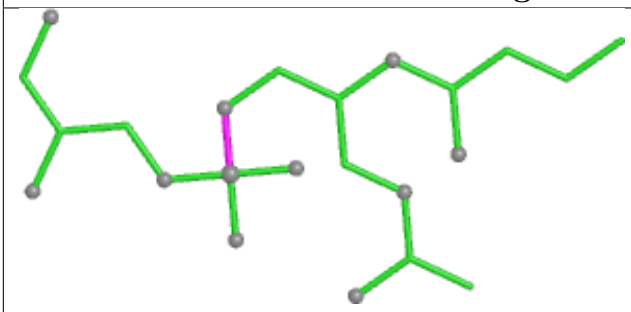


Torsions

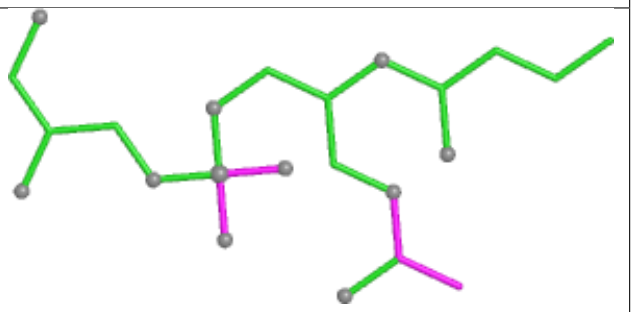


Rings

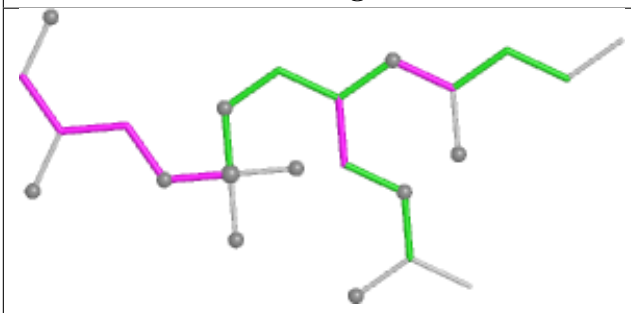
Ligand LHG aX 101



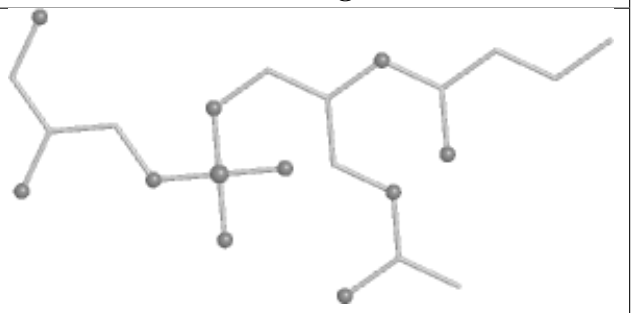
Bond lengths



Bond angles

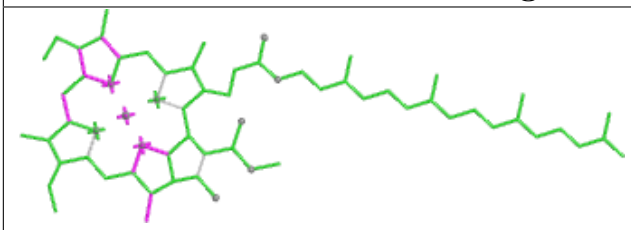


Torsions

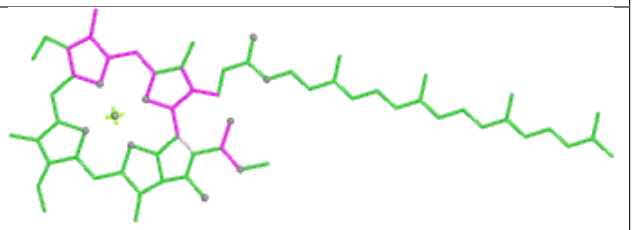


Rings

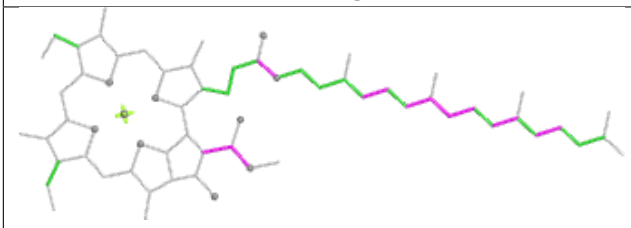
Ligand CLA a6 404



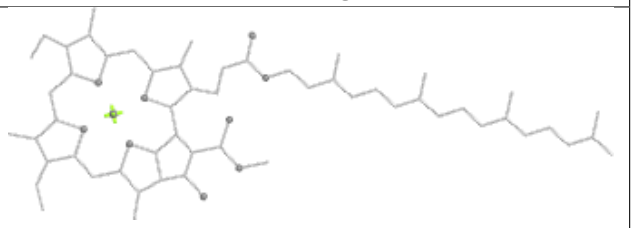
Bond lengths



Bond angles

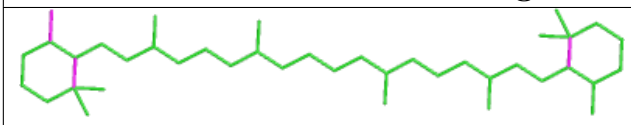


Torsions

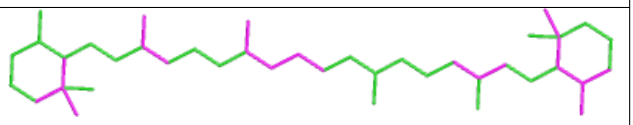


Rings

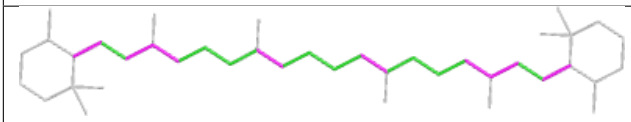
Ligand BCR aF 202



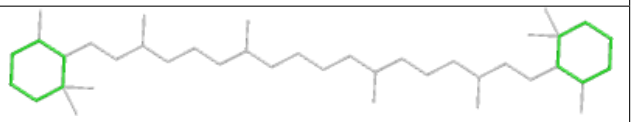
Bond lengths



Bond angles

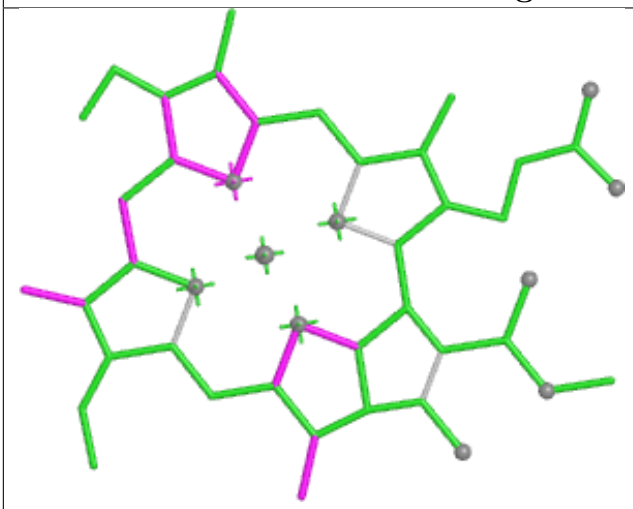


Torsions

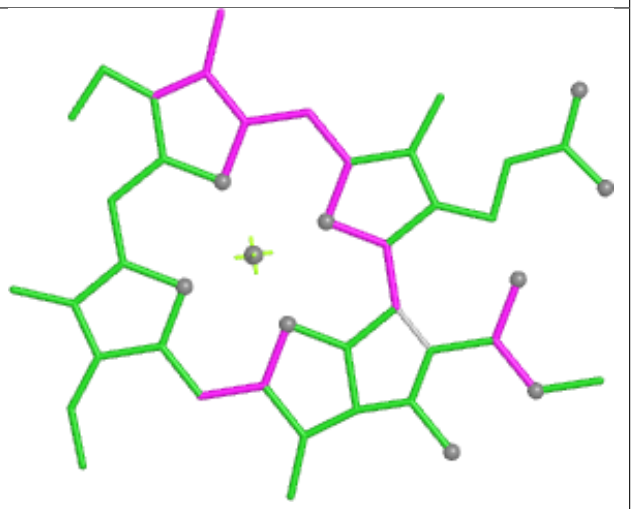


Rings

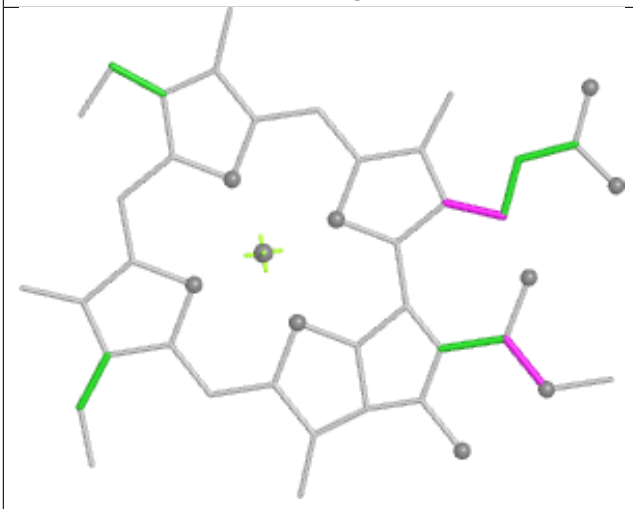
Ligand CLA aB 812



Bond lengths



Bond angles

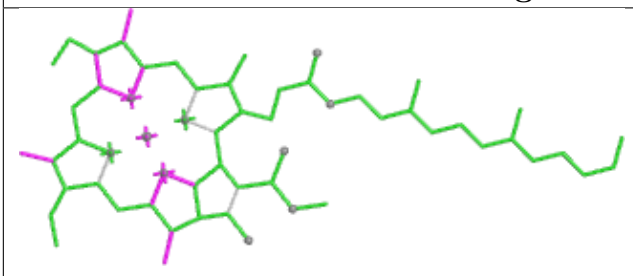


Torsions

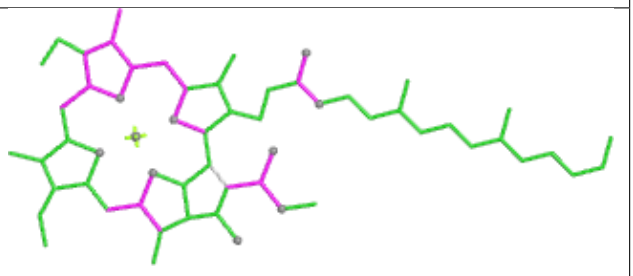


Rings

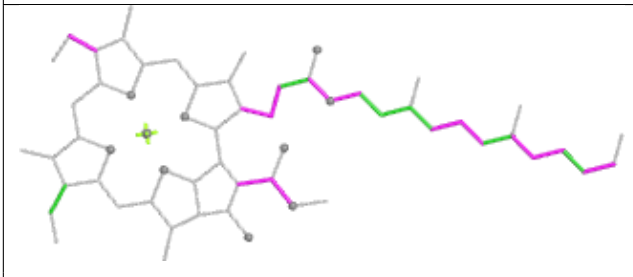
Ligand CLA aA 825



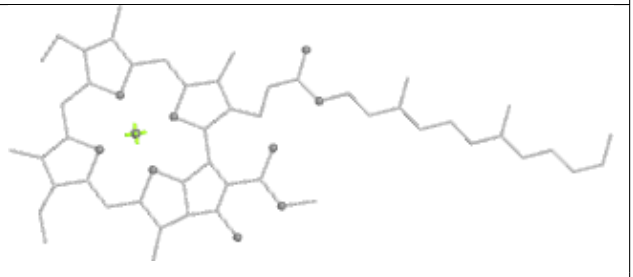
Bond lengths



Bond angles

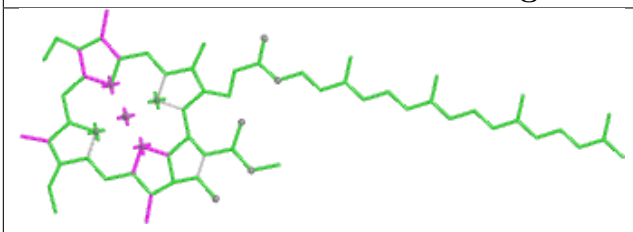


Torsions

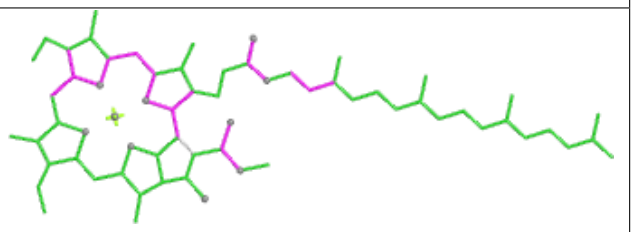


Rings

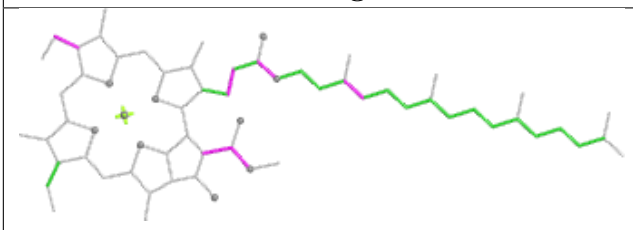
Ligand CLA c6 406



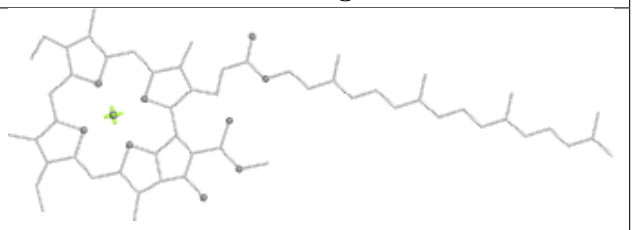
Bond lengths



Bond angles

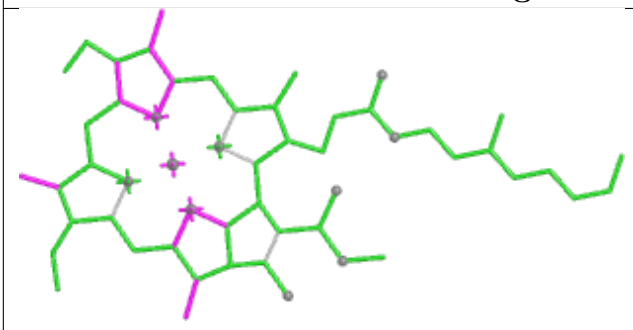


Torsions

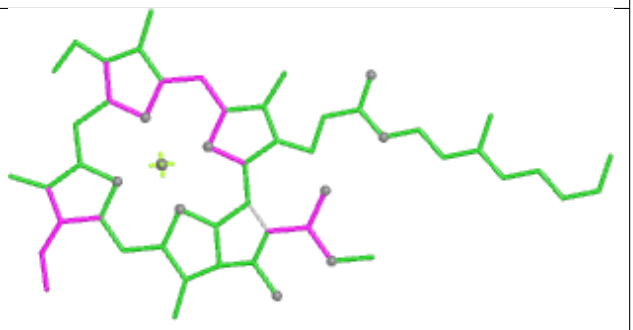


Rings

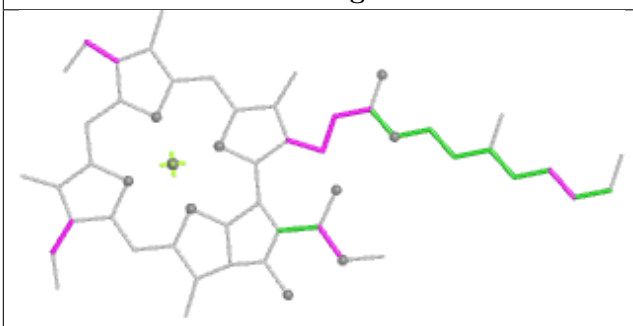
Ligand CLA bA 819



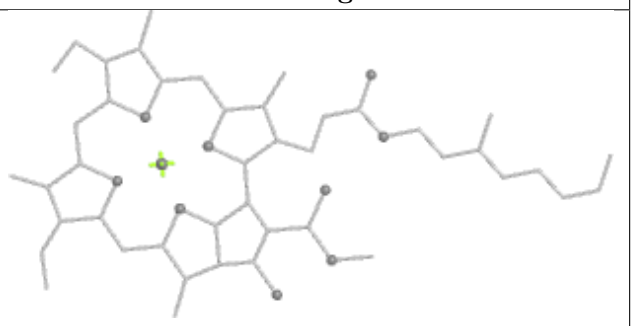
Bond lengths



Bond angles

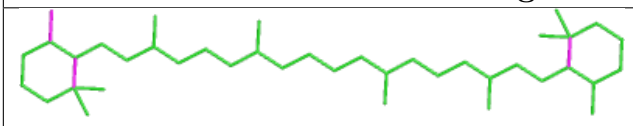


Torsions

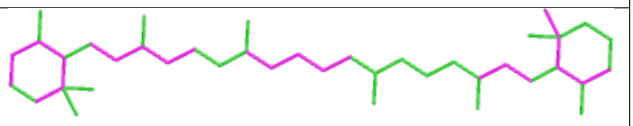


Rings

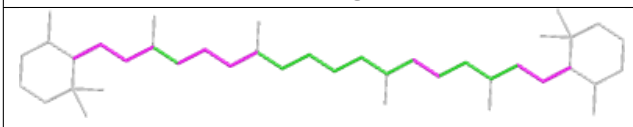
Ligand BCR a4 401



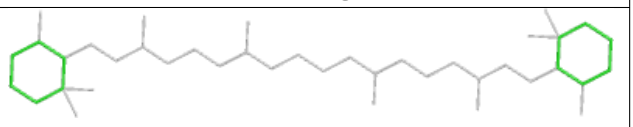
Bond lengths



Bond angles

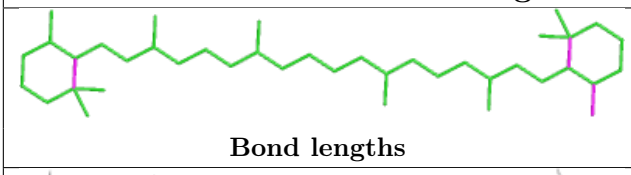


Torsions

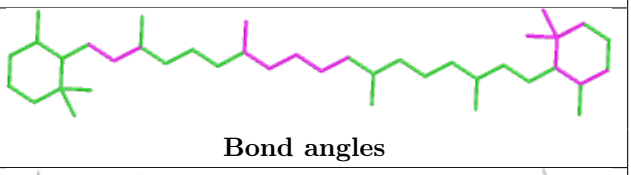


Rings

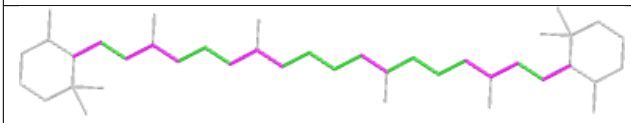
Ligand BCR aB 846



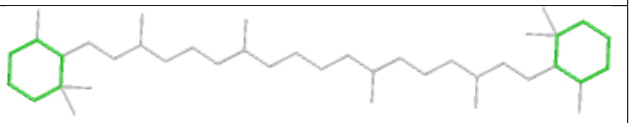
Bond lengths



Bond angles

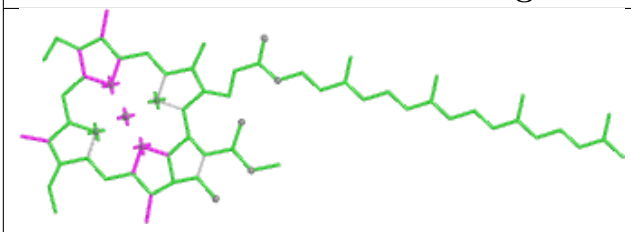


Torsions

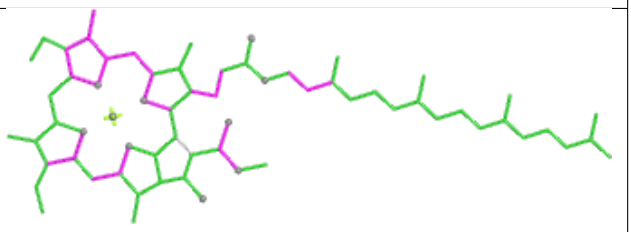


Rings

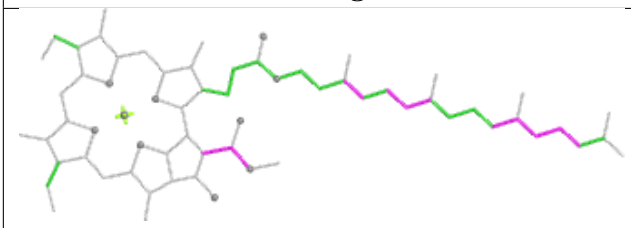
Ligand CLA aB 837



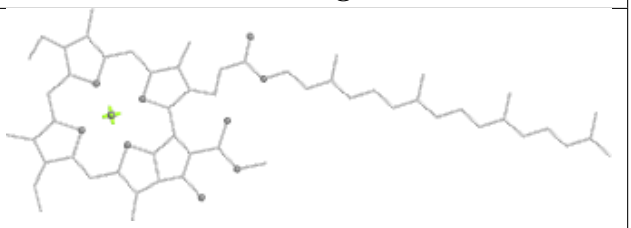
Bond lengths



Bond angles

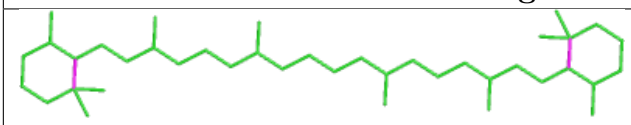


Torsions

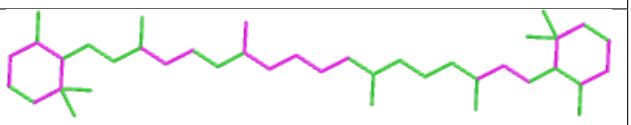


Rings

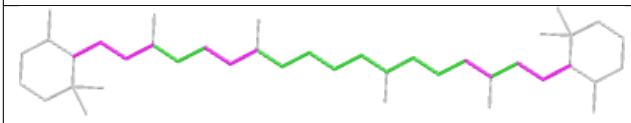
Ligand BCR c5 419



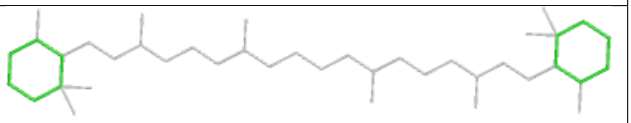
Bond lengths



Bond angles

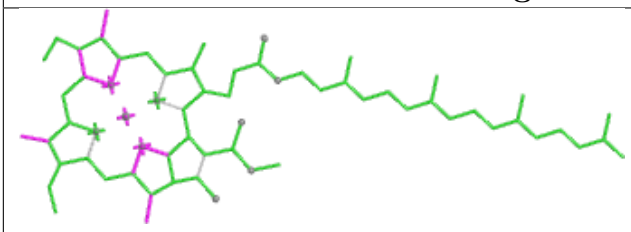


Torsions

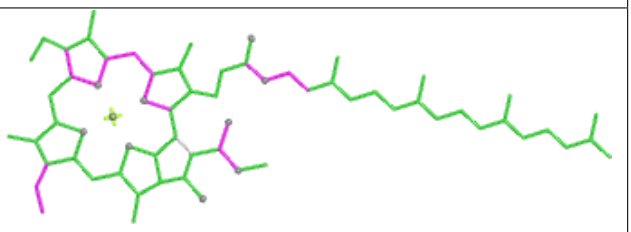


Rings

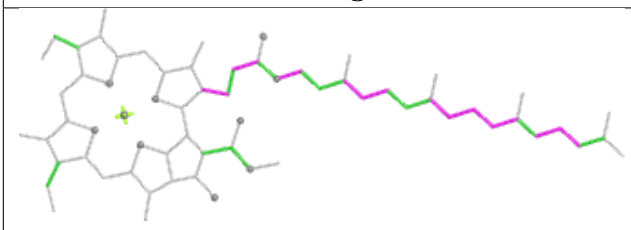
Ligand CLA bA 843



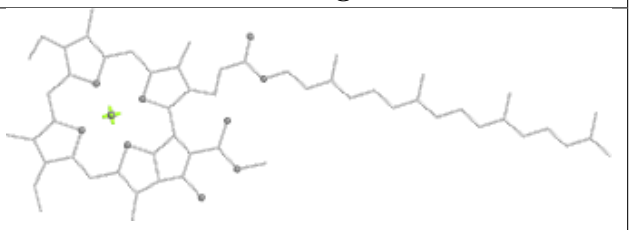
Bond lengths



Bond angles

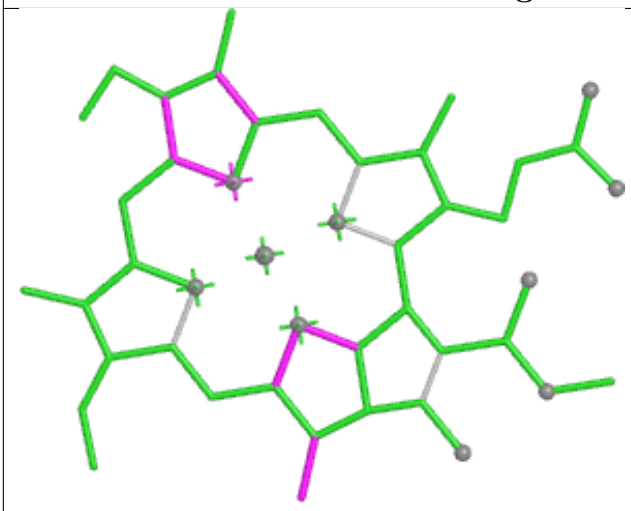


Torsions

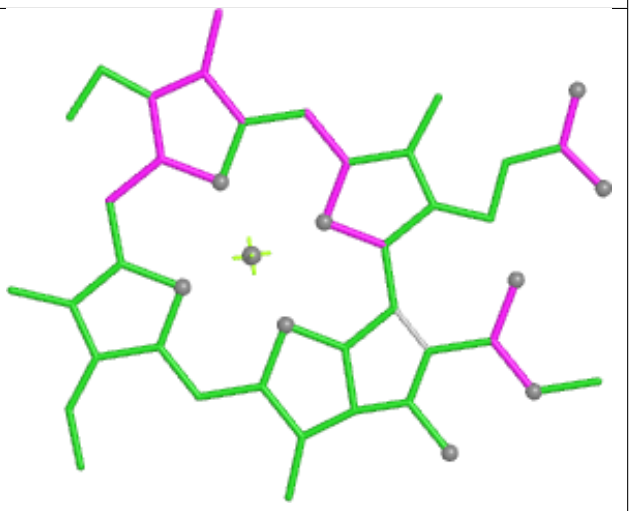


Rings

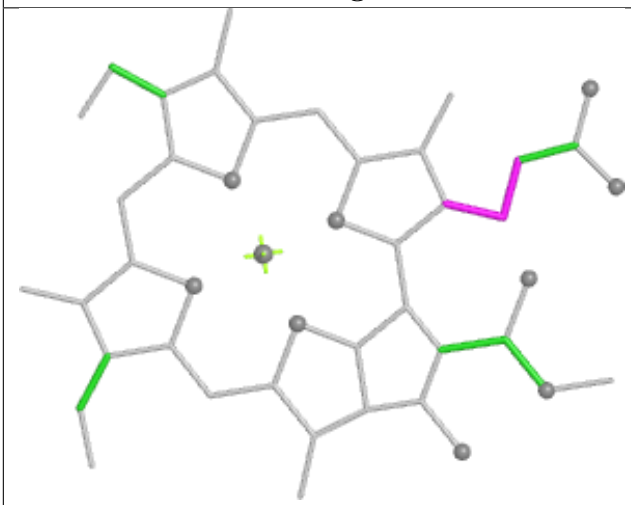
Ligand CLA aB 822



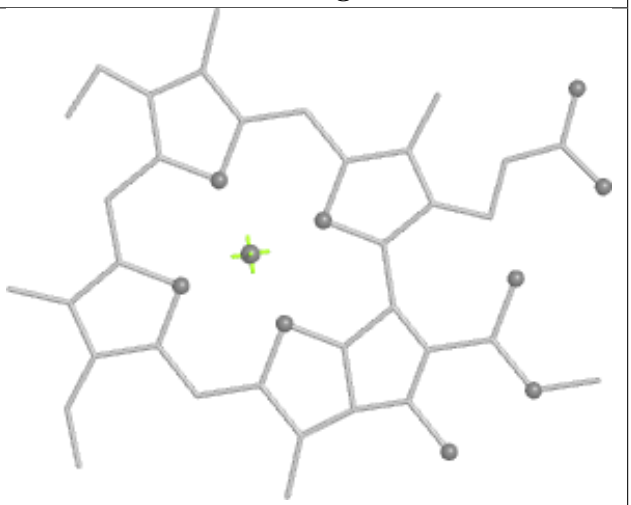
Bond lengths



Bond angles

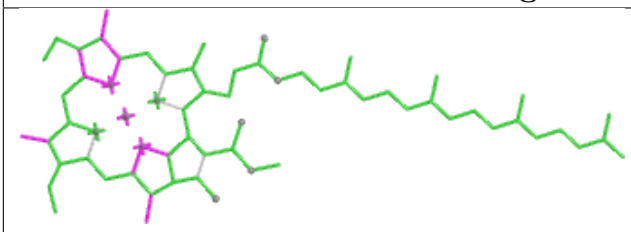


Torsions

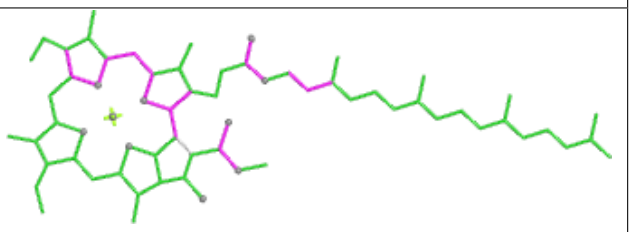


Rings

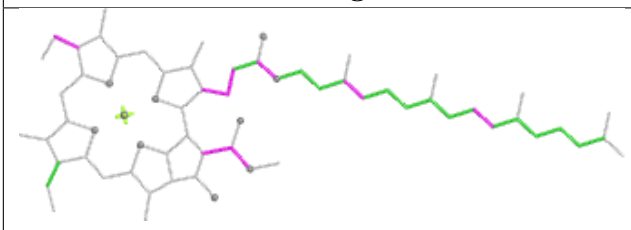
Ligand CLA a3 404



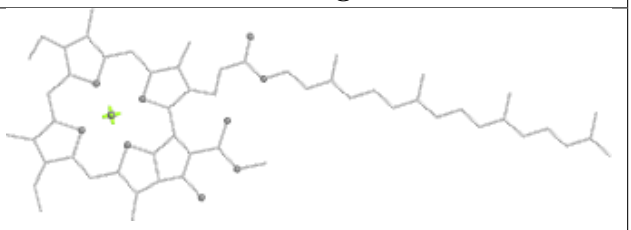
Bond lengths



Bond angles

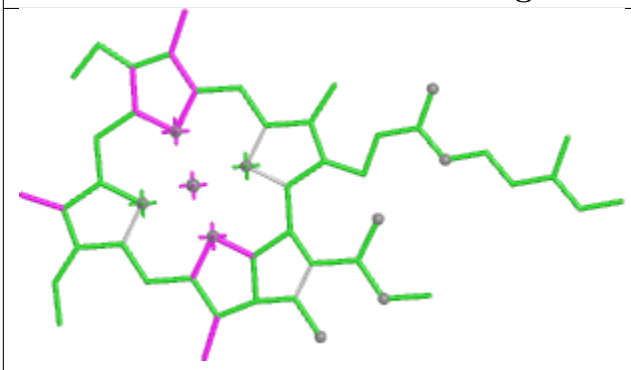


Torsions

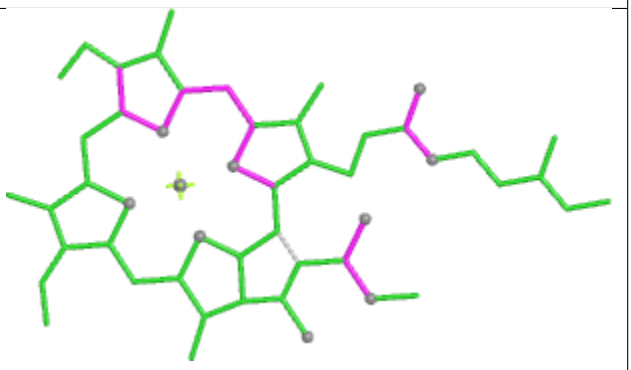


Rings

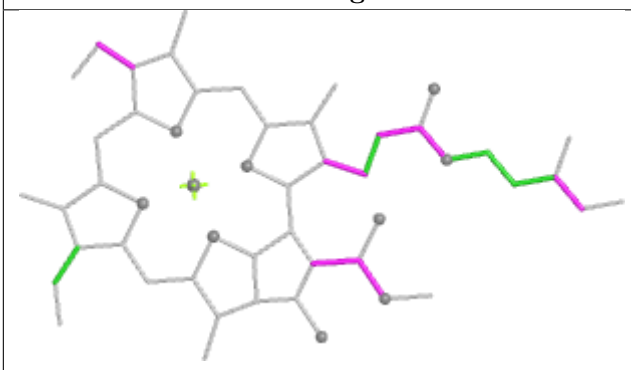
Ligand CLA aA 824



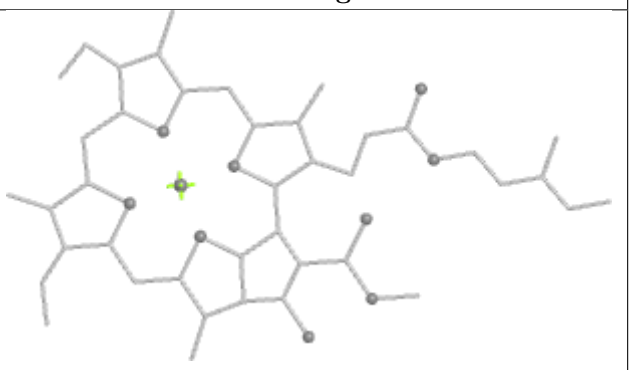
Bond lengths



Bond angles

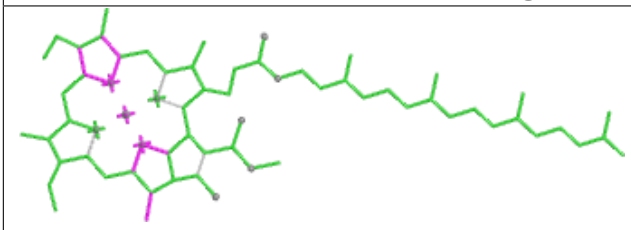


Torsions

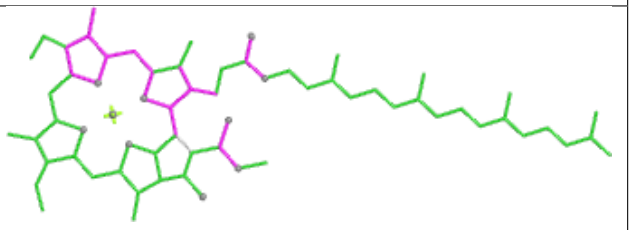


Rings

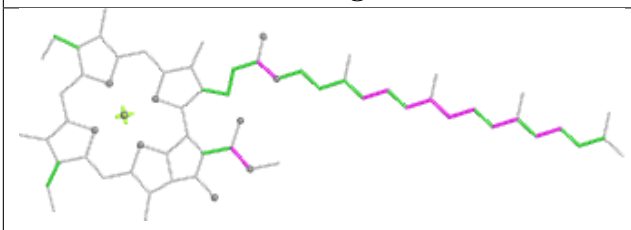
Ligand CLA a3 403



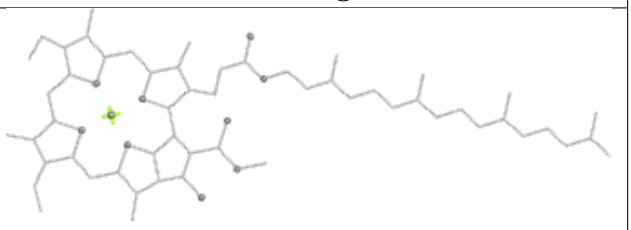
Bond lengths



Bond angles

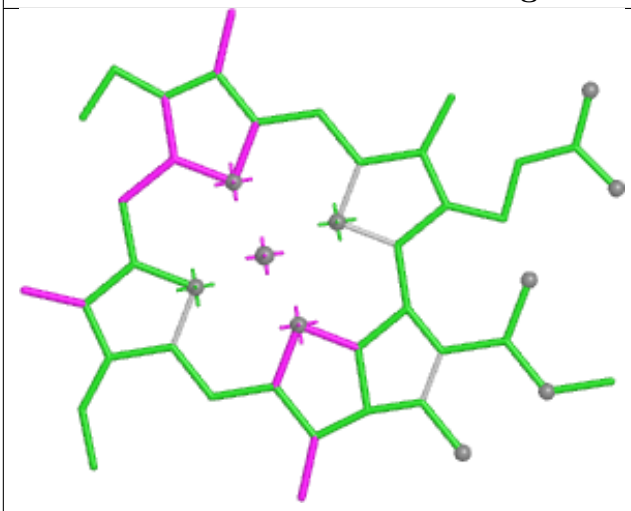


Torsions

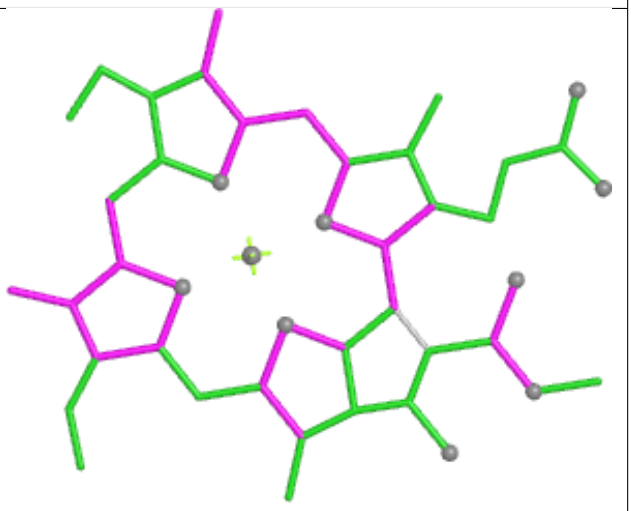


Rings

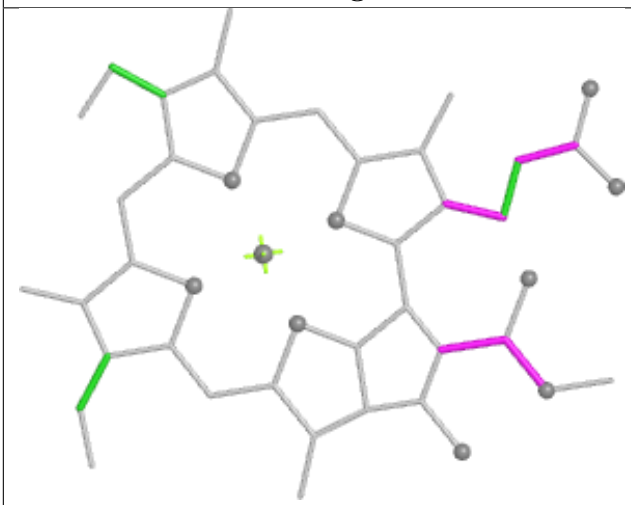
Ligand CLA c1 412



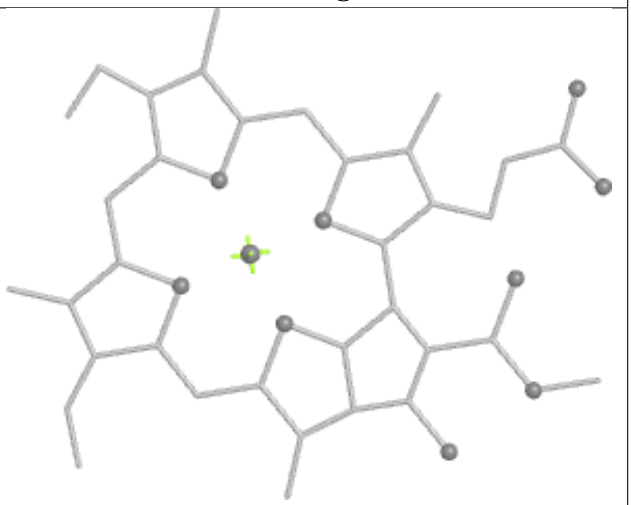
Bond lengths



Bond angles

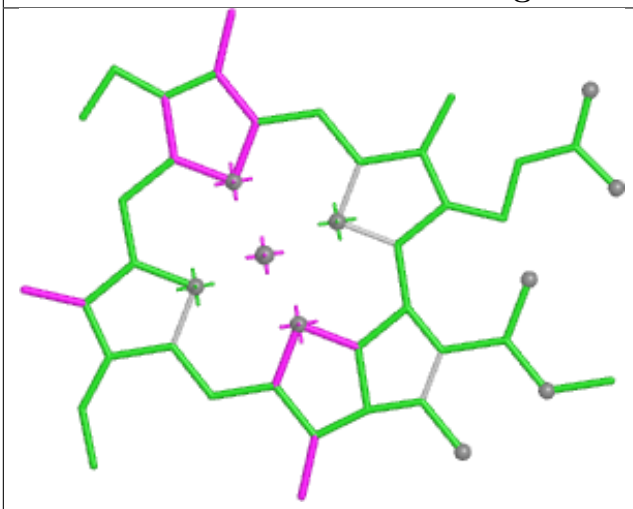


Torsions

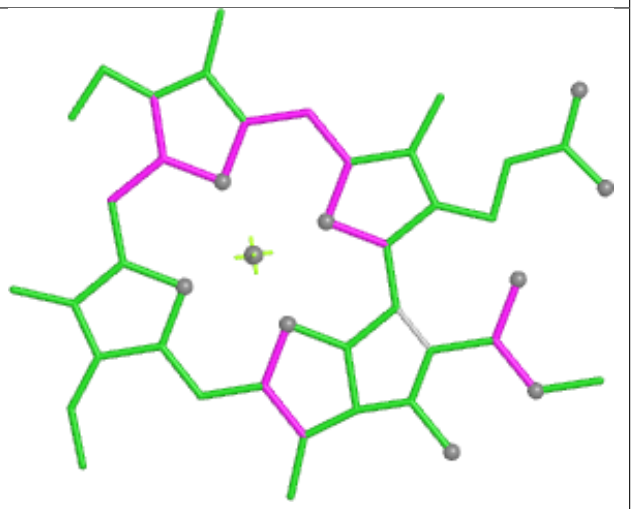


Rings

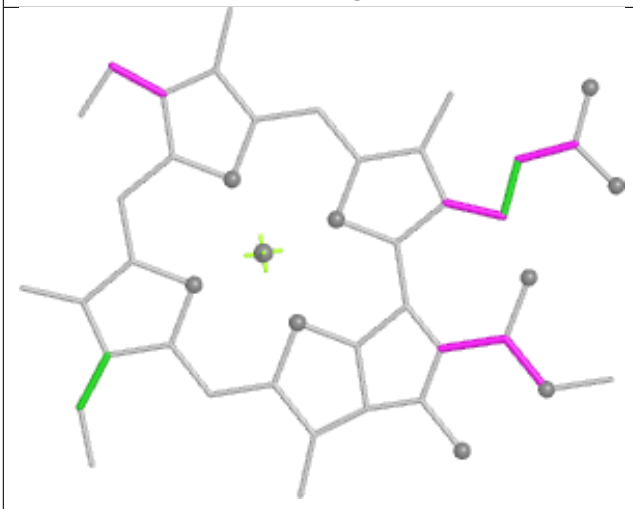
Ligand CLA bA 811



Bond lengths



Bond angles

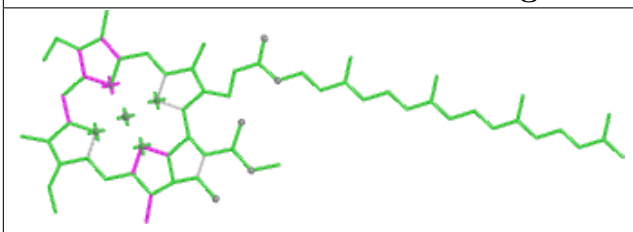


Torsions

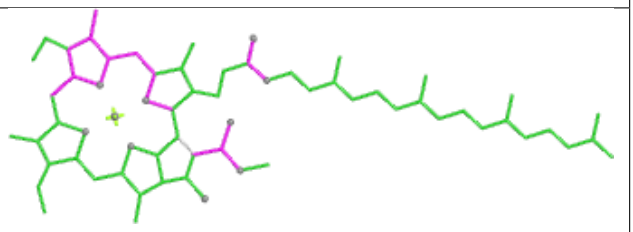


Rings

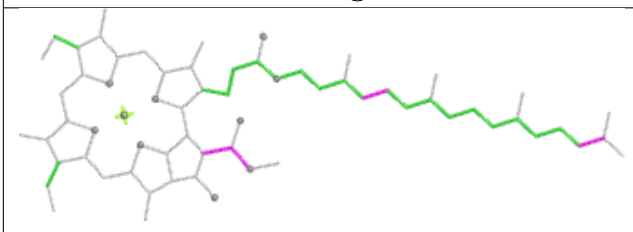
Ligand CLA c2 410



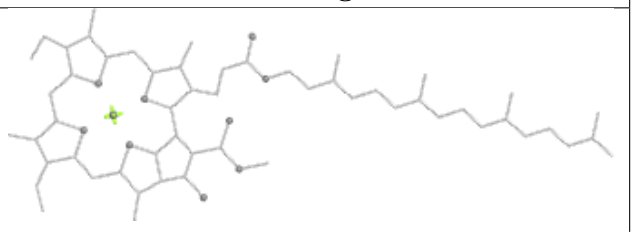
Bond lengths



Bond angles

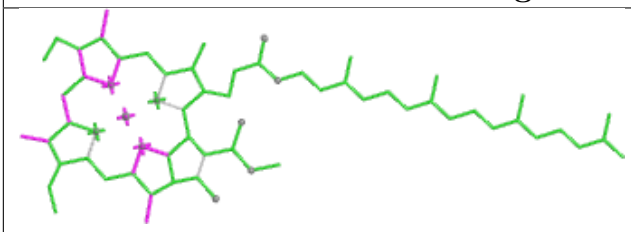


Torsions

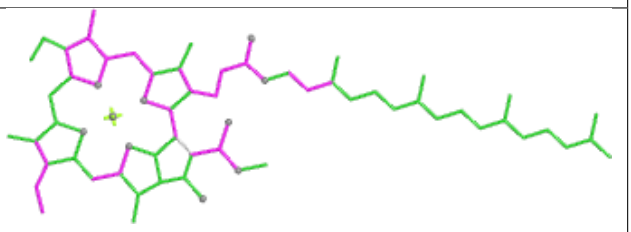


Rings

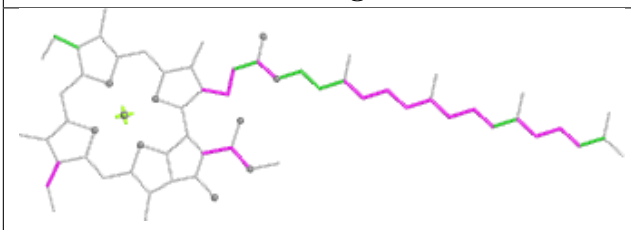
Ligand CLA bB 814



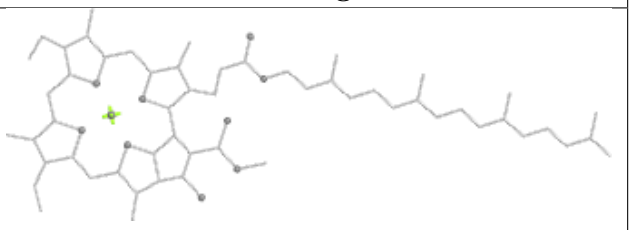
Bond lengths



Bond angles



Torsions

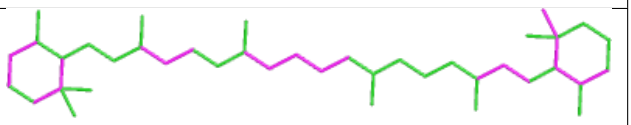


Rings

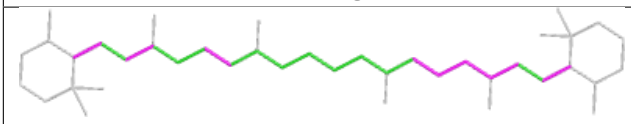
Ligand BCR b2 420



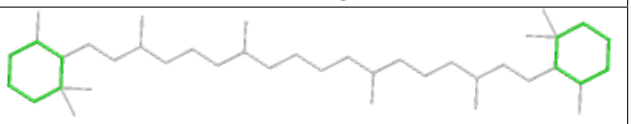
Bond lengths



Bond angles

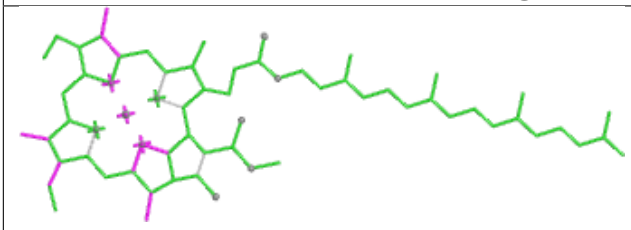


Torsions

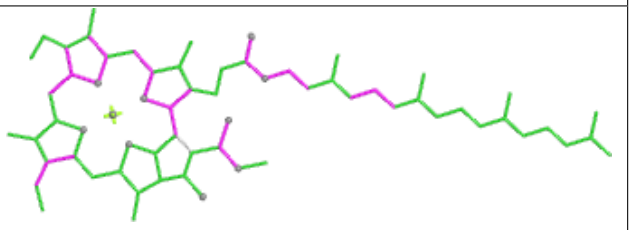


Rings

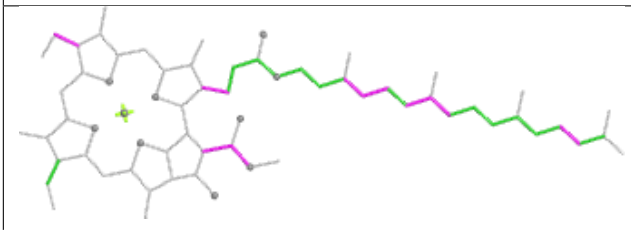
Ligand CLA aB 811



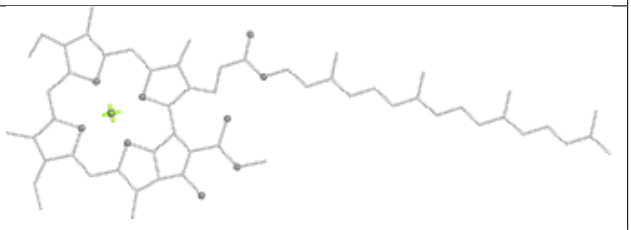
Bond lengths



Bond angles

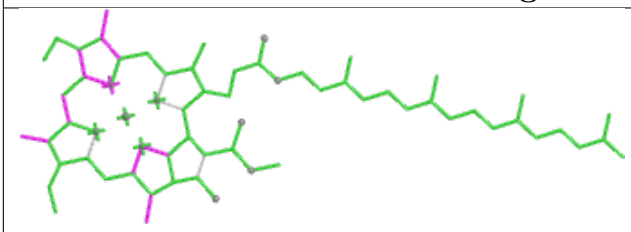


Torsions

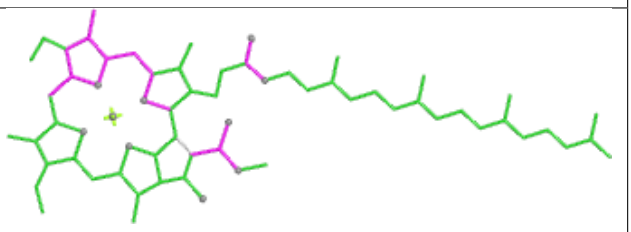


Rings

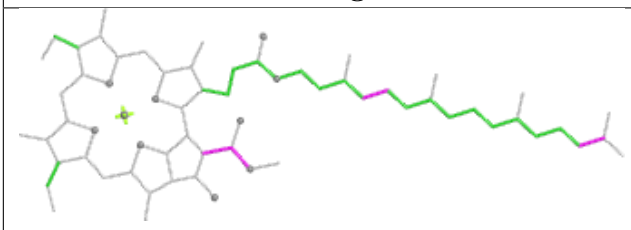
Ligand CLA a3 409



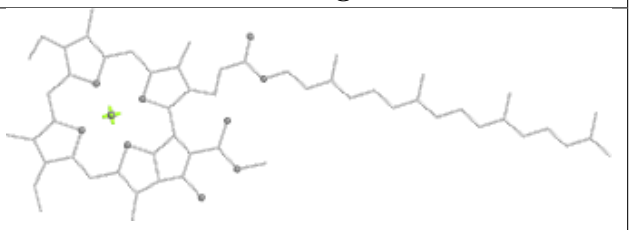
Bond lengths



Bond angles

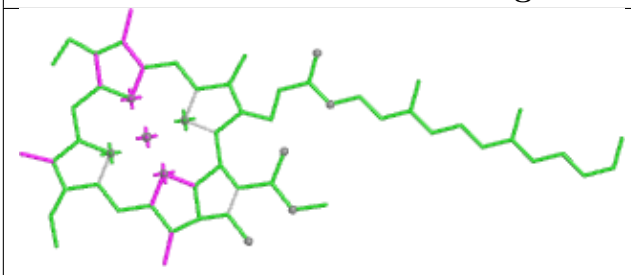


Torsions

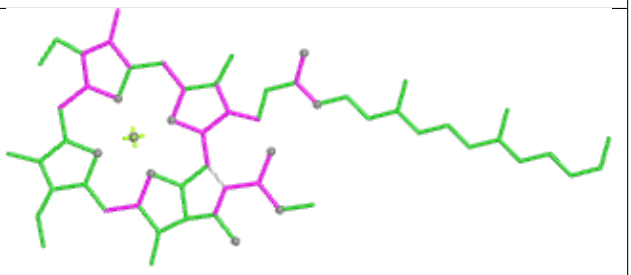


Rings

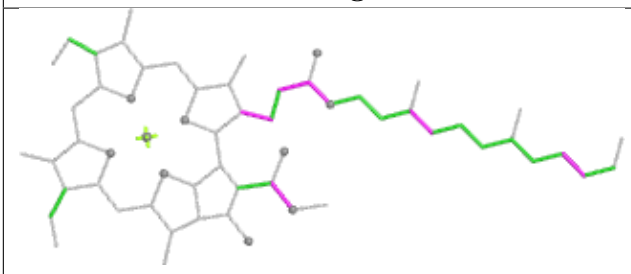
Ligand CLA bB 818



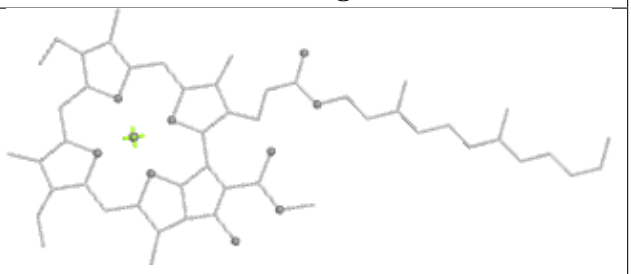
Bond lengths



Bond angles

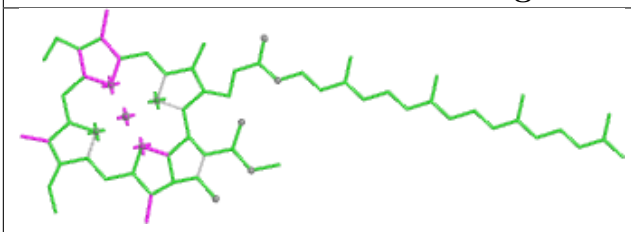


Torsions

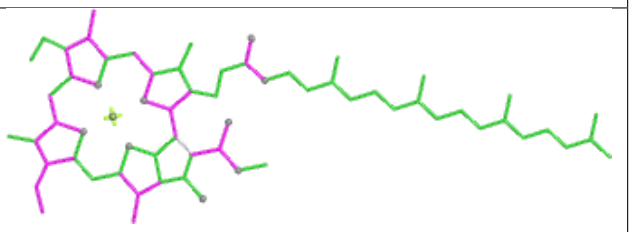


Rings

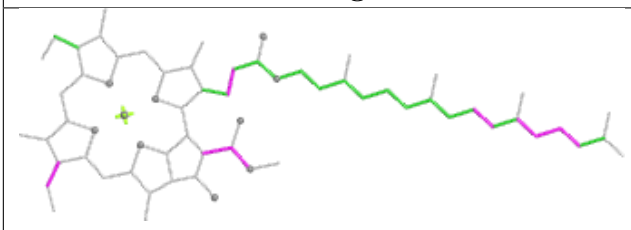
Ligand CLA bB 804



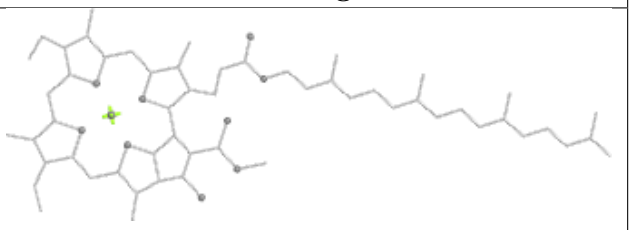
Bond lengths



Bond angles

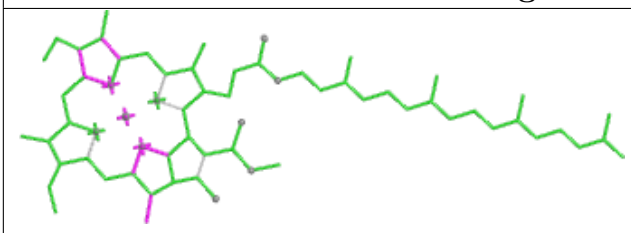


Torsions

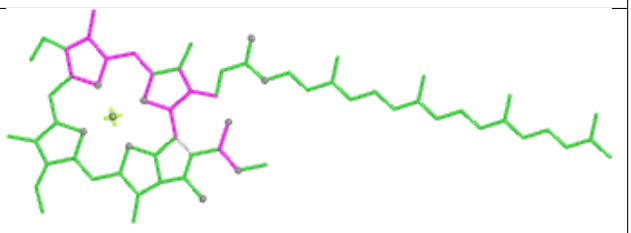


Rings

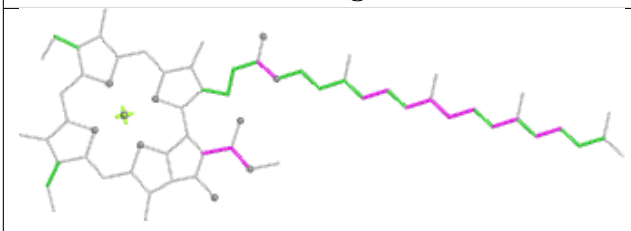
Ligand CLA b6 404



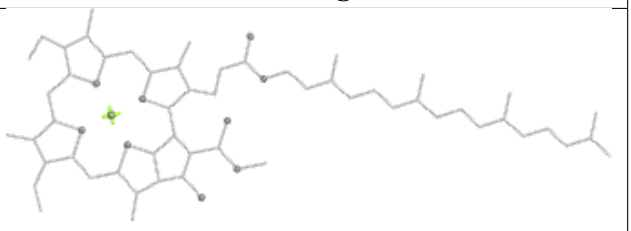
Bond lengths



Bond angles

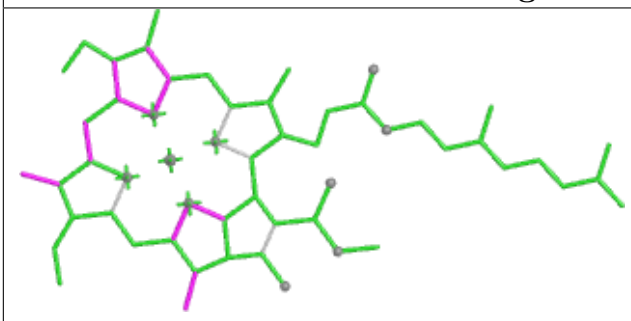


Torsions

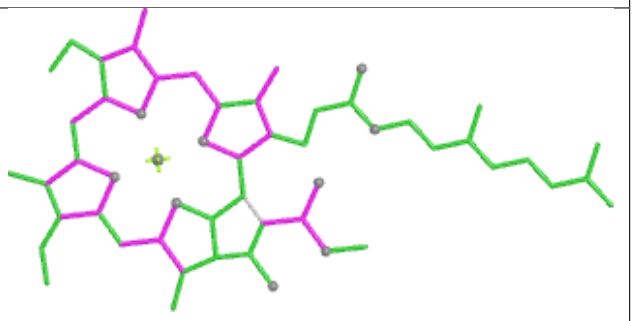


Rings

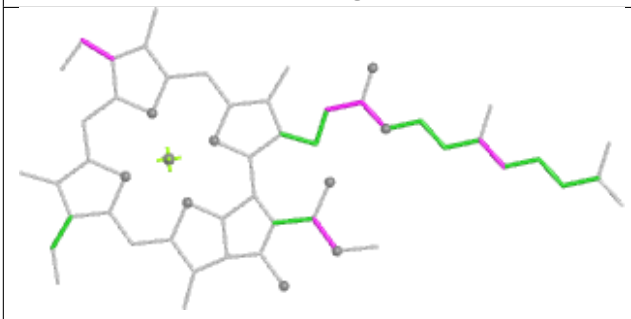
Ligand CLA b4 417



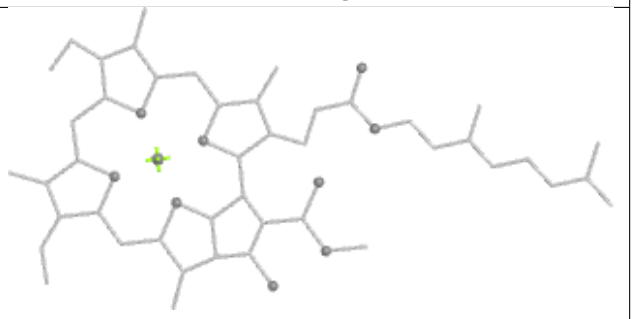
Bond lengths



Bond angles

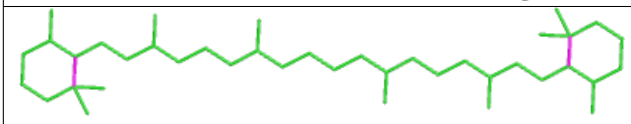


Torsions

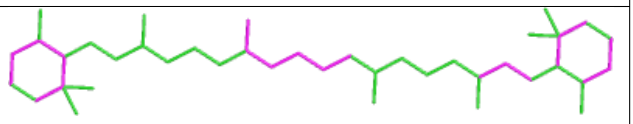


Rings

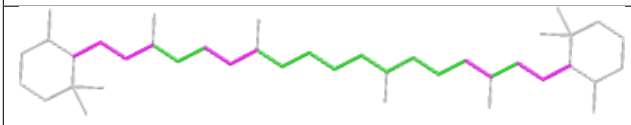
Ligand BCR b2 421



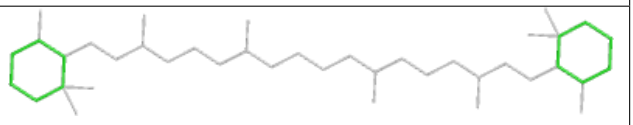
Bond lengths



Bond angles

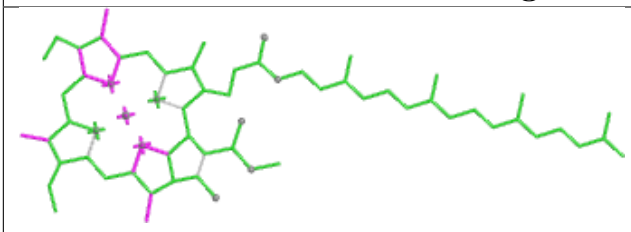


Torsions

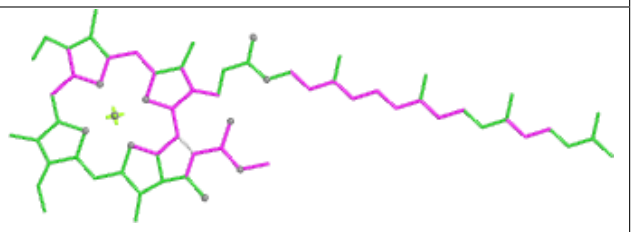


Rings

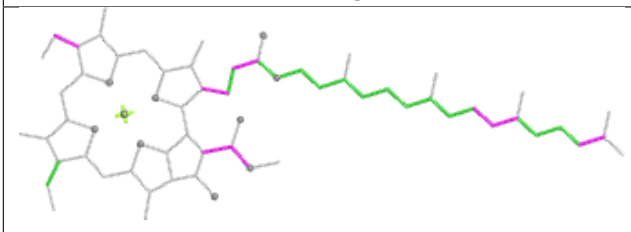
Ligand CLA c2 422



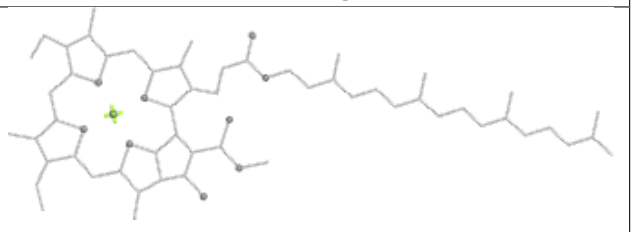
Bond lengths



Bond angles

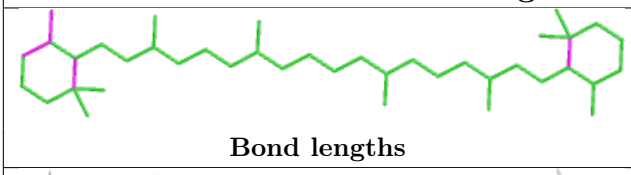


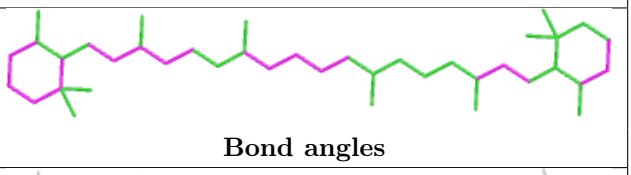
Torsions

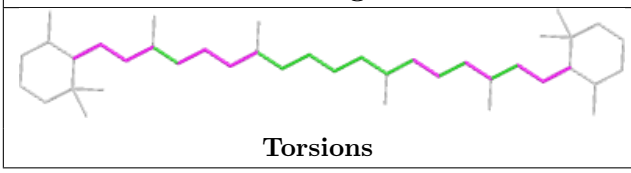


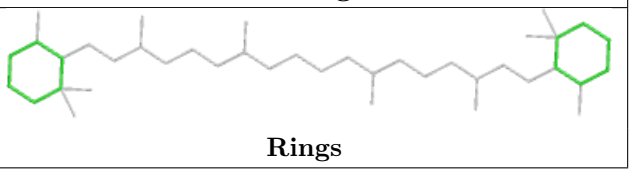
Rings

Ligand BCR a6 421

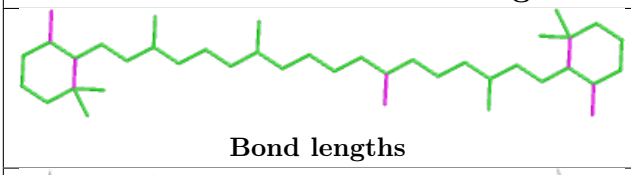

Bond lengths

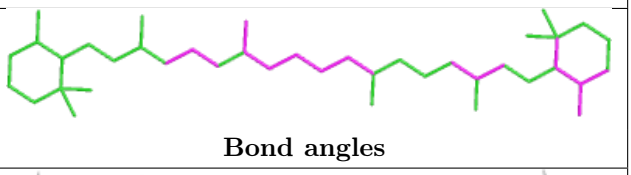

Bond angles

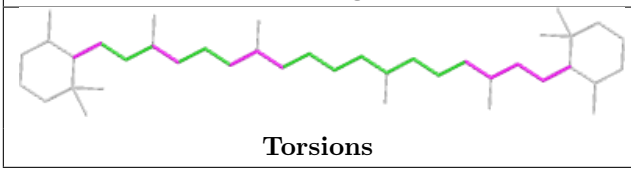

Torsions

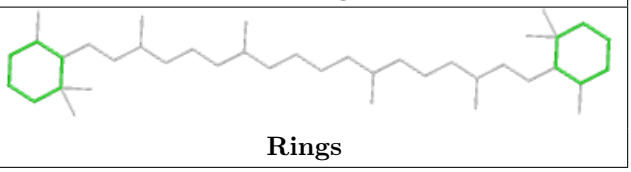

Rings

Ligand BCR bB 850

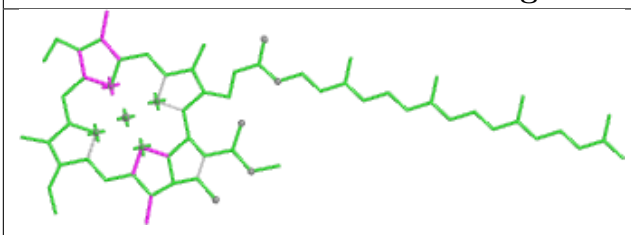

Bond lengths

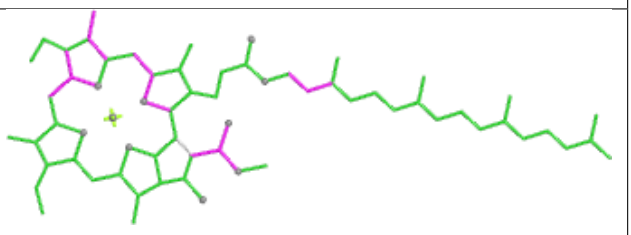

Bond angles

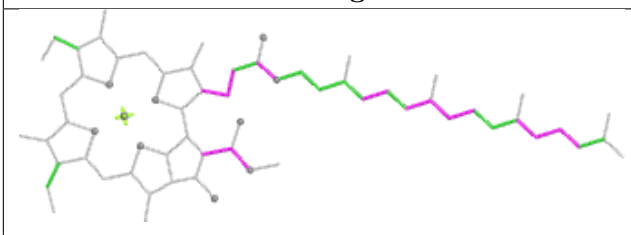

Torsions

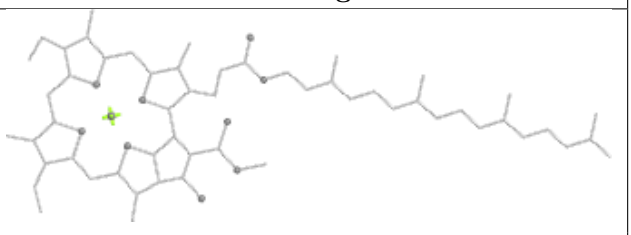

Rings

Ligand CLA c4 402


Bond lengths

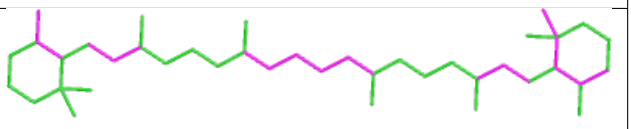

Bond angles

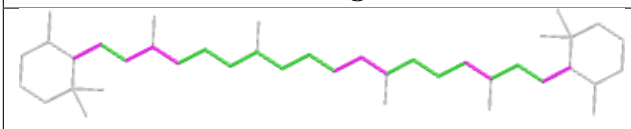

Torsions

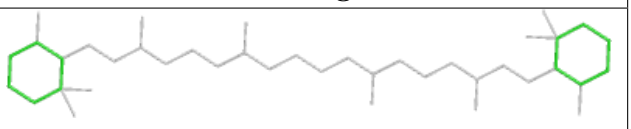

Rings

Ligand BCR bM 101

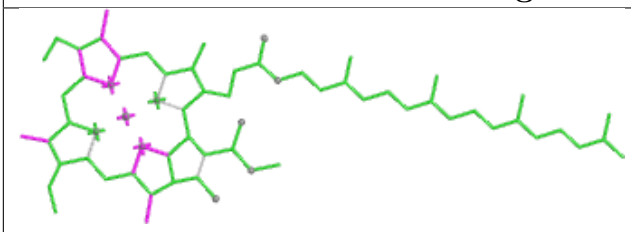

Bond lengths


Bond angles

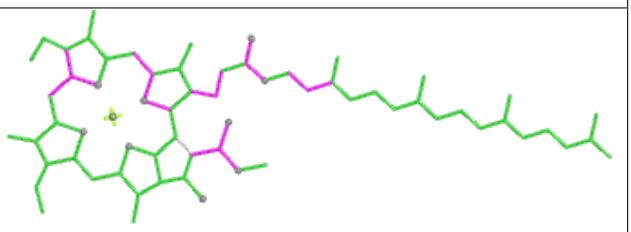

Torsions


Rings

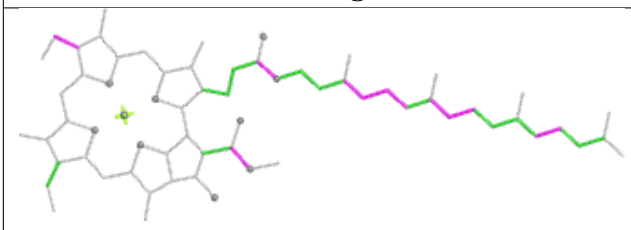
Ligand CLA aB 809



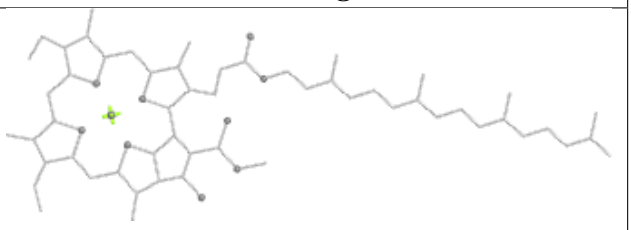
Bond lengths



Bond angles



Torsions

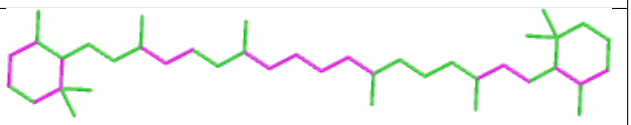


Rings

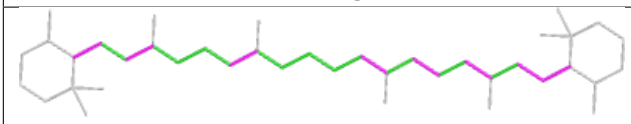
Ligand BCR cI 102



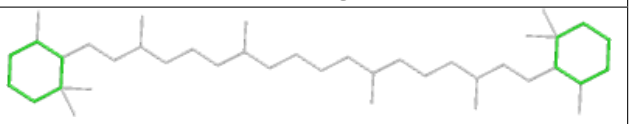
Bond lengths



Bond angles

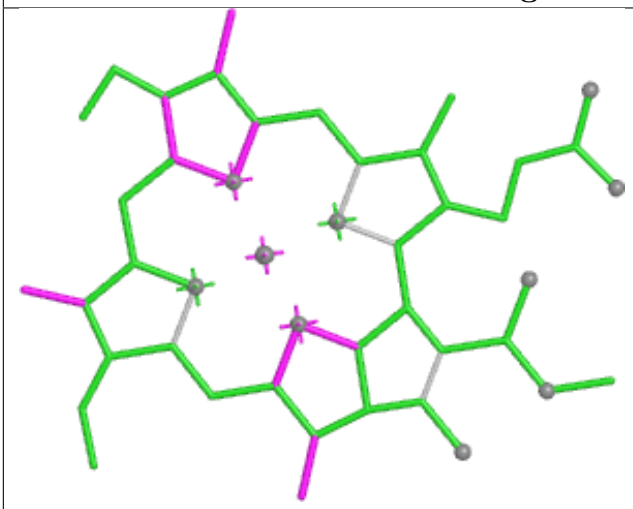


Torsions

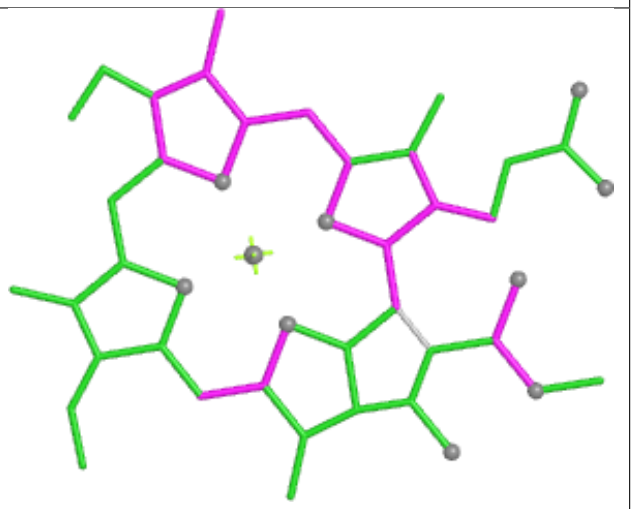


Rings

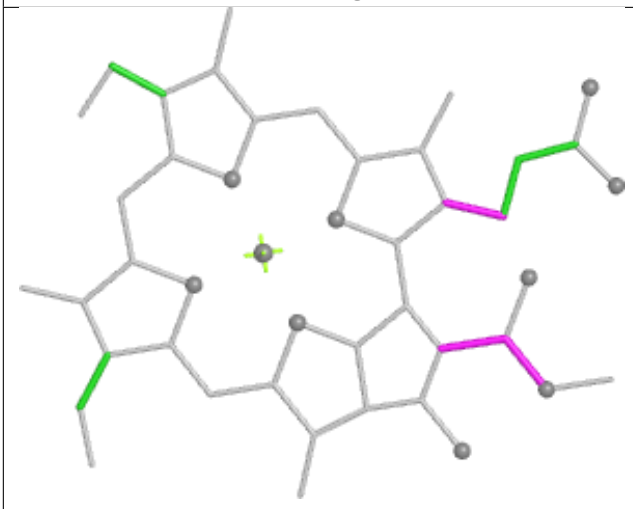
Ligand CLA c3 411



Bond lengths



Bond angles

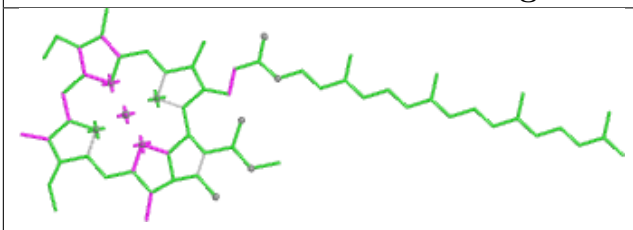


Torsions

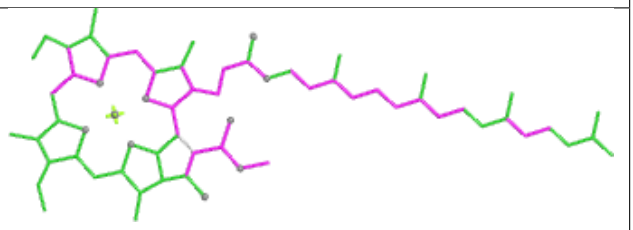


Rings

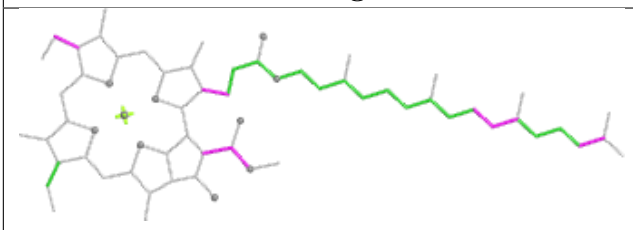
Ligand CLA a2 406



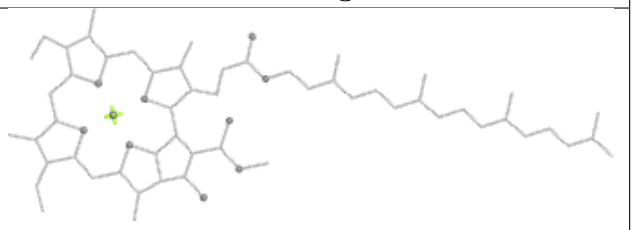
Bond lengths



Bond angles

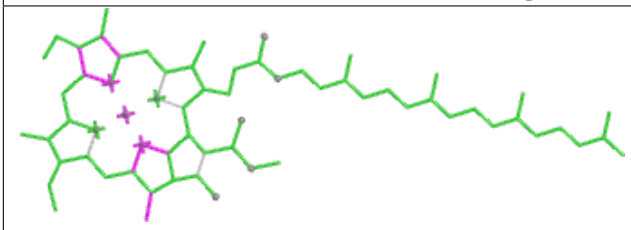


Torsions

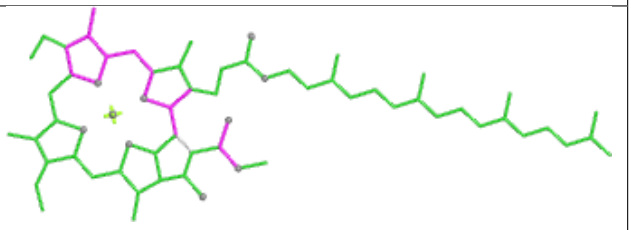


Rings

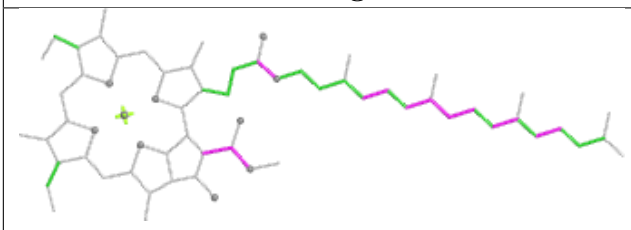
Ligand CLA c4 403



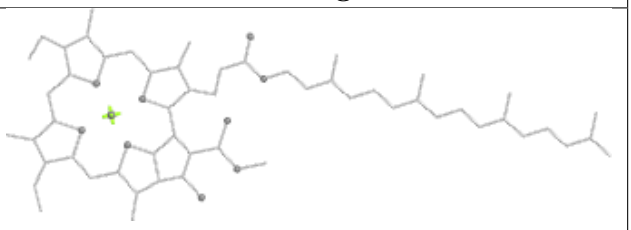
Bond lengths



Bond angles

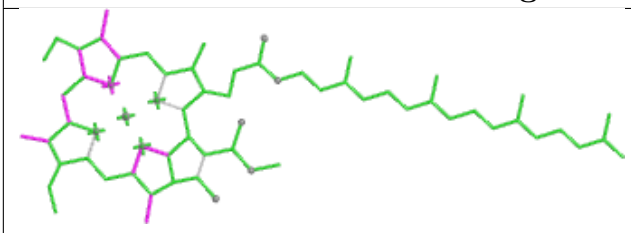


Torsions

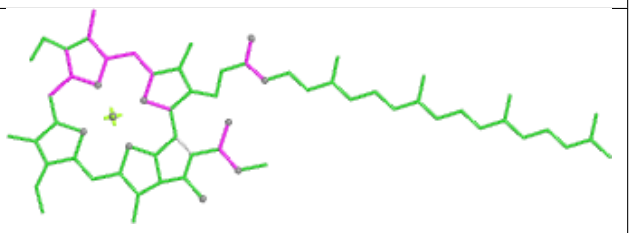


Rings

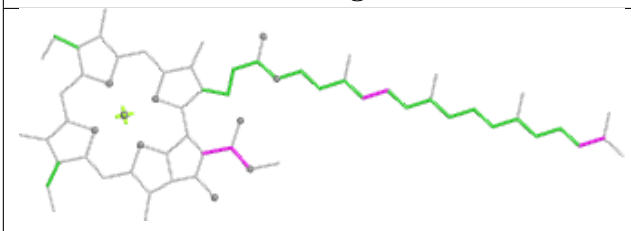
Ligand CLA a5 409



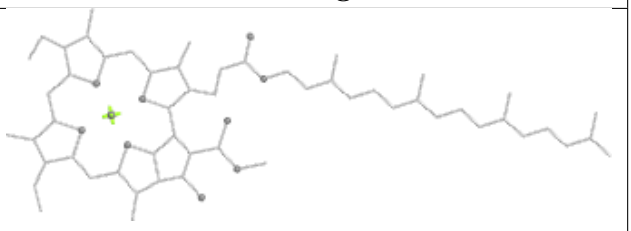
Bond lengths



Bond angles

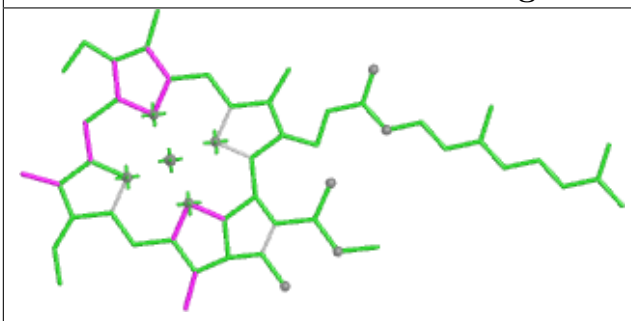


Torsions

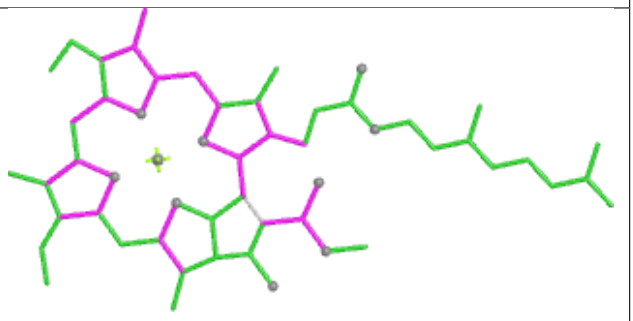


Rings

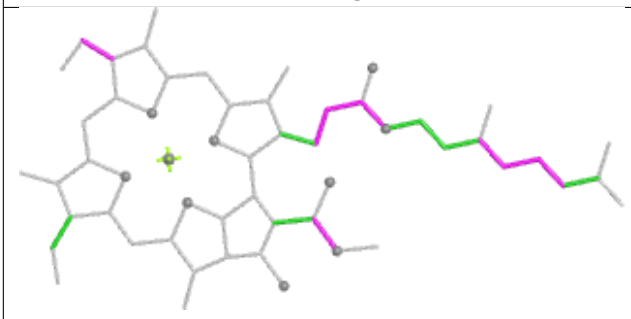
Ligand CLA b1 417



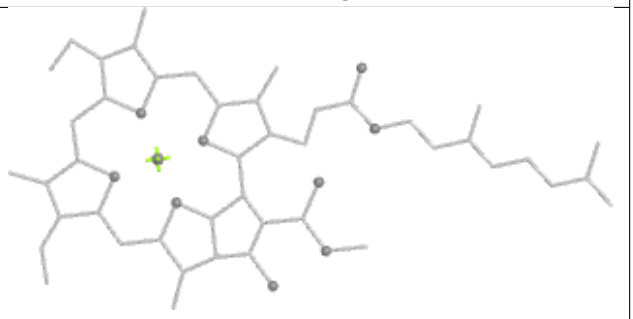
Bond lengths



Bond angles

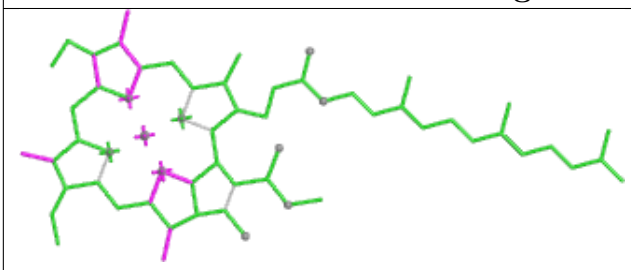


Torsions

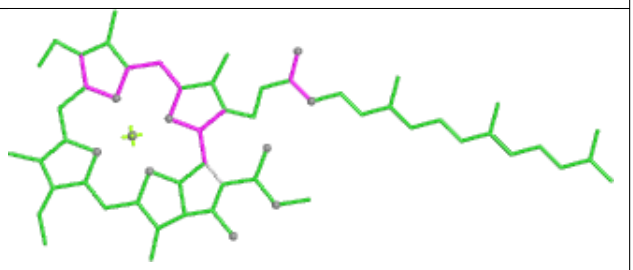


Rings

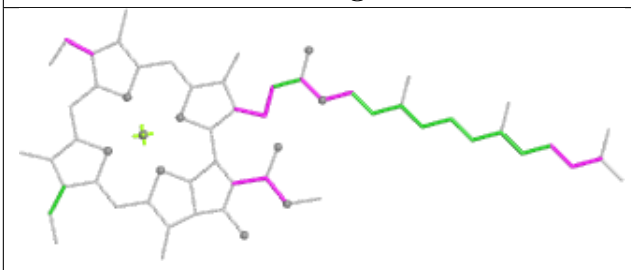
Ligand CLA bA 814



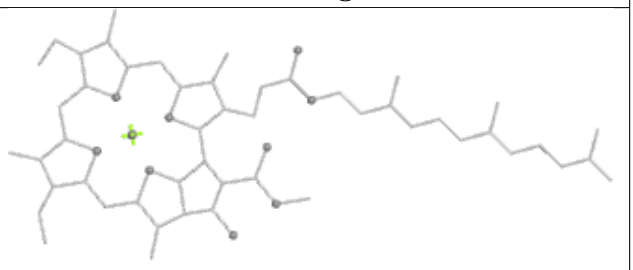
Bond lengths



Bond angles



Torsions

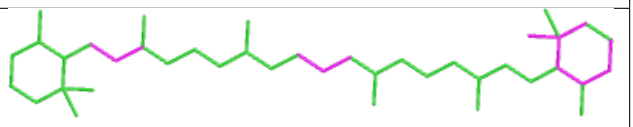


Rings

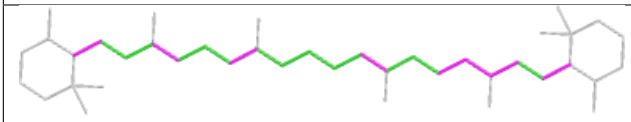
Ligand BCR aB 845



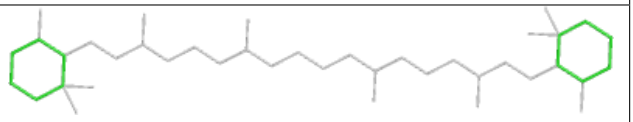
Bond lengths



Bond angles

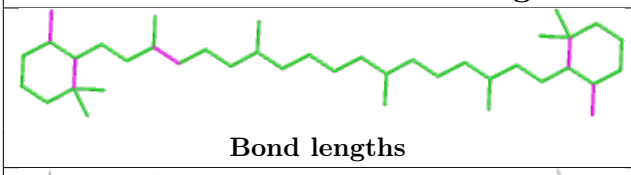


Torsions

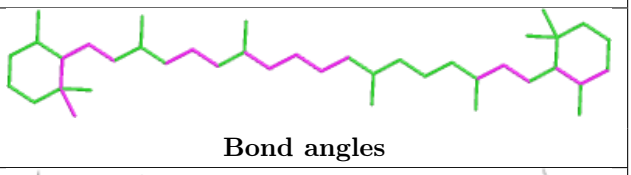


Rings

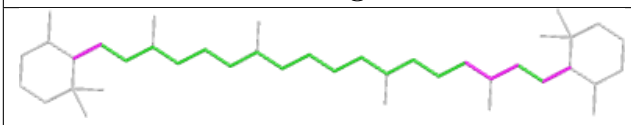
Ligand BCR aA 851



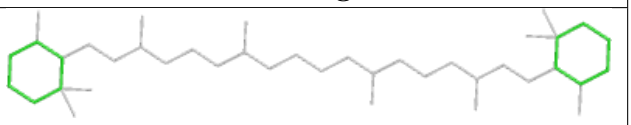
Bond lengths



Bond angles

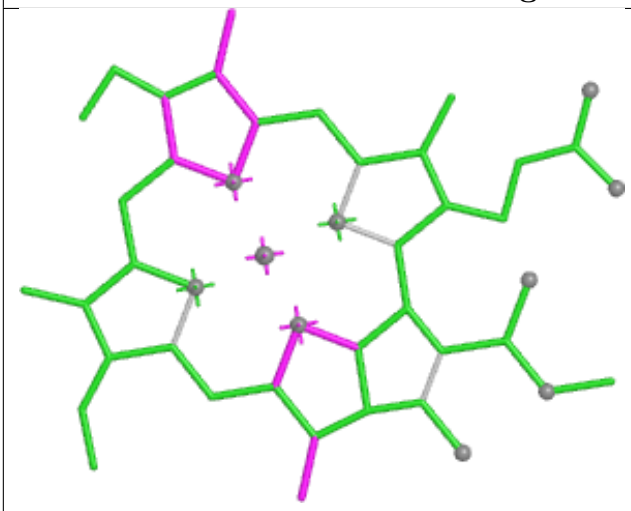


Torsions

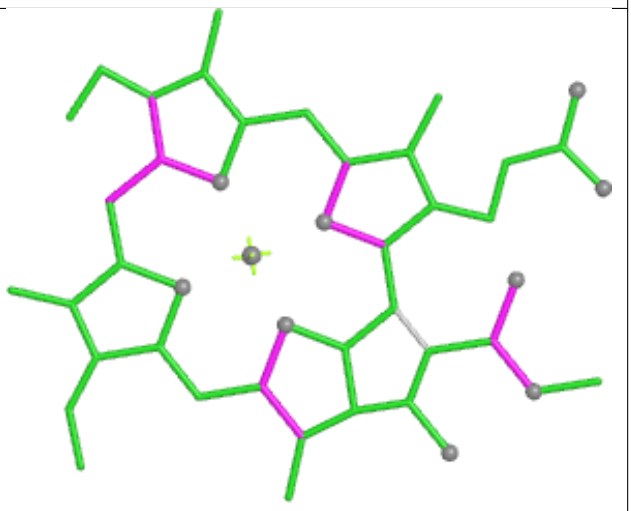


Rings

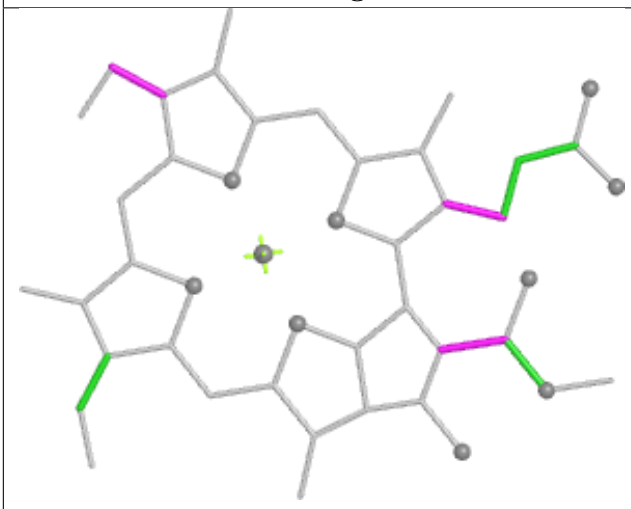
Ligand CLA a4 413



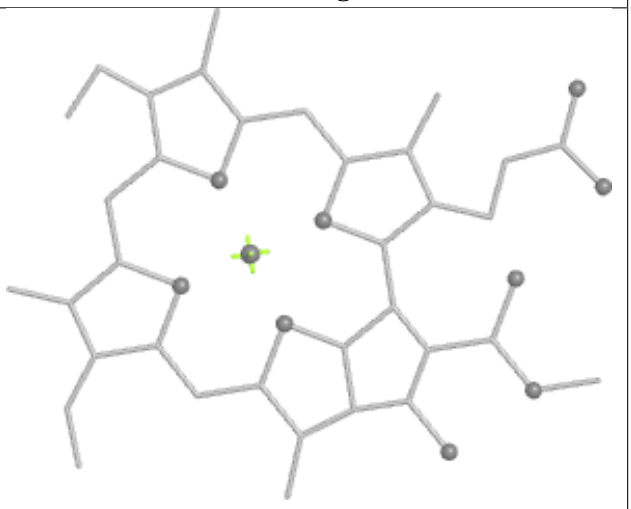
Bond lengths



Bond angles

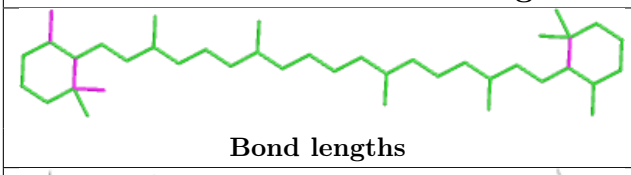


Torsions

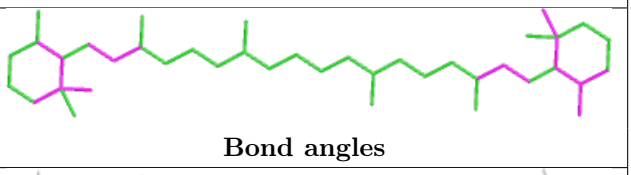


Rings

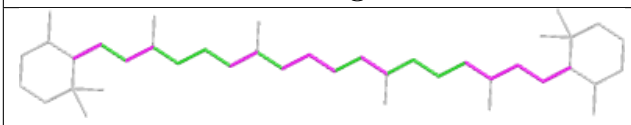
Ligand BCR aF 201



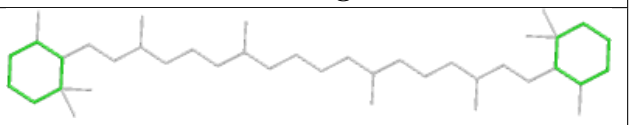
Bond lengths



Bond angles

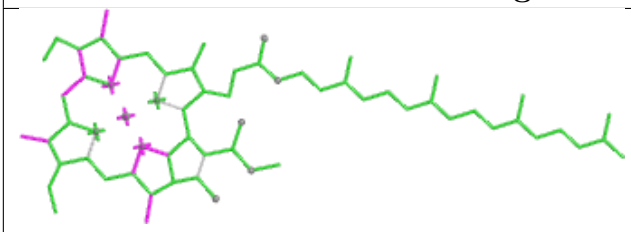


Torsions

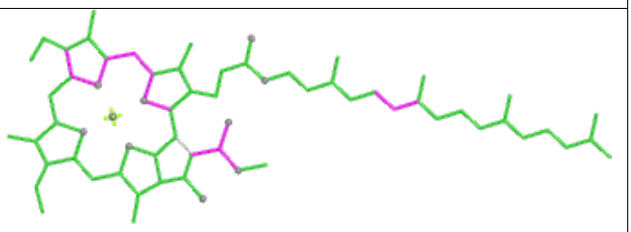


Rings

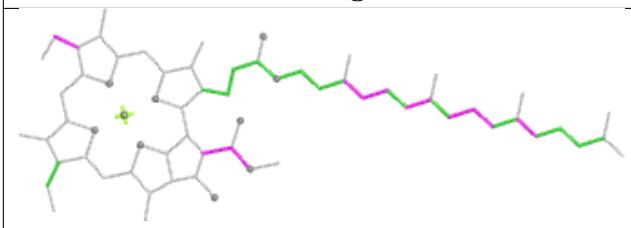
Ligand CLA bA 839



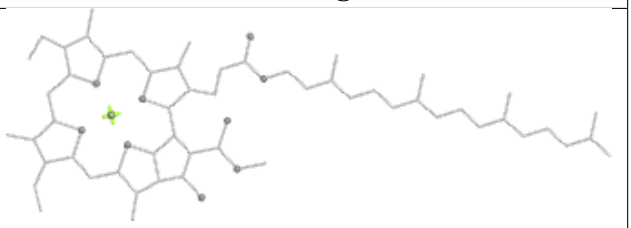
Bond lengths



Bond angles

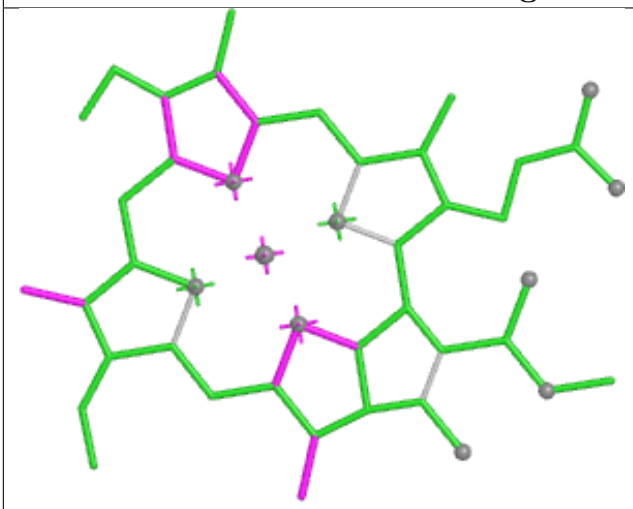


Torsions

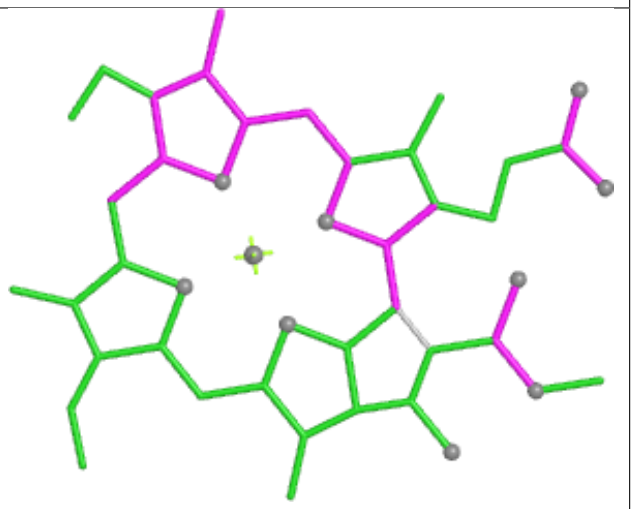


Rings

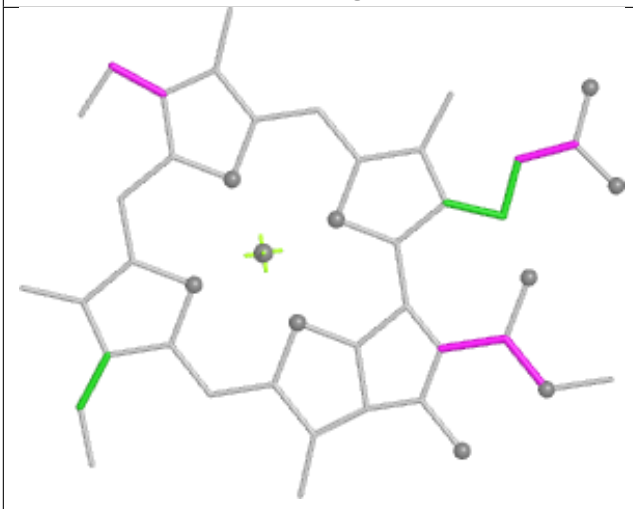
Ligand CLA a2 408



Bond lengths



Bond angles

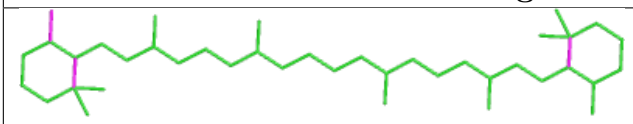


Torsions

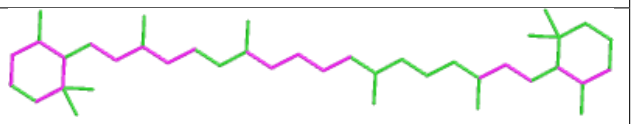


Rings

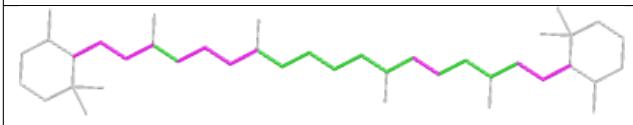
Ligand BCR b4 401



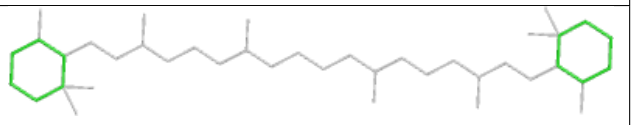
Bond lengths



Bond angles

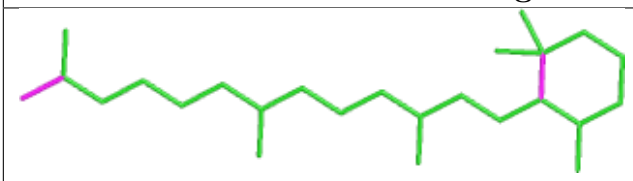


Torsions

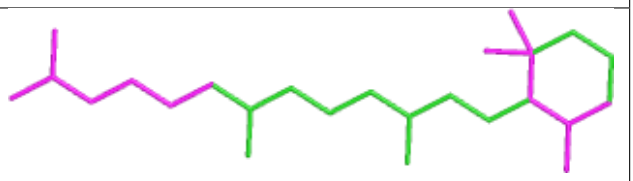


Rings

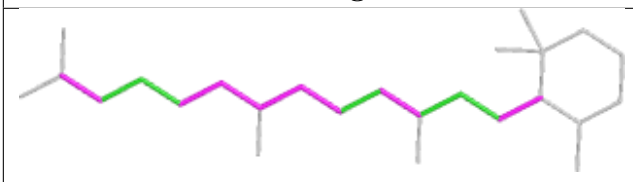
Ligand BCR cB 847



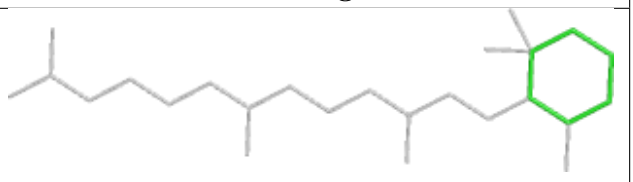
Bond lengths



Bond angles

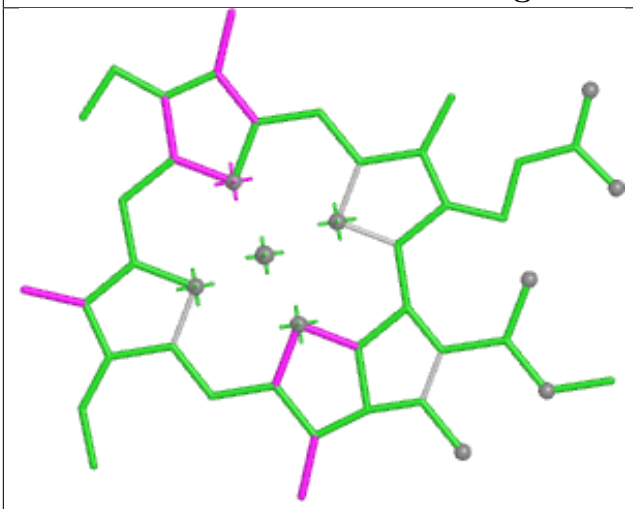


Torsions

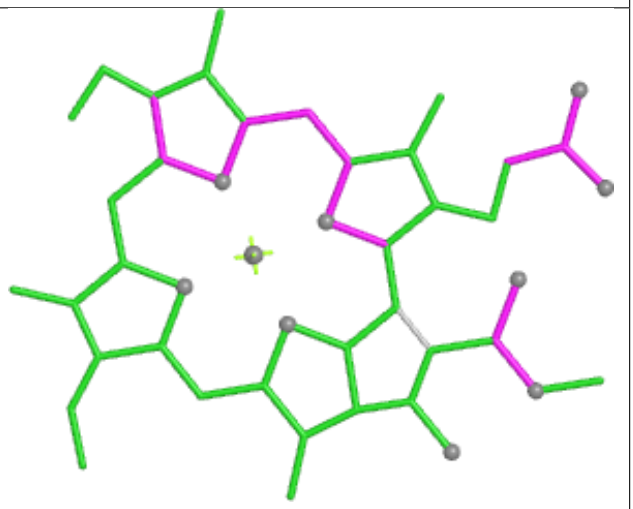


Rings

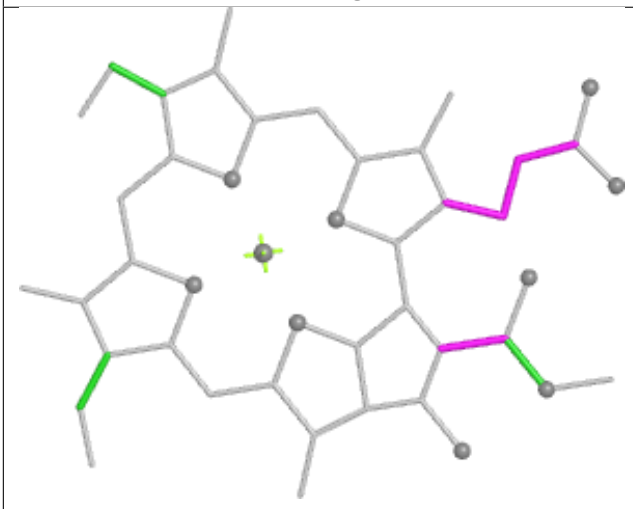
Ligand CLA bA 837



Bond lengths



Bond angles

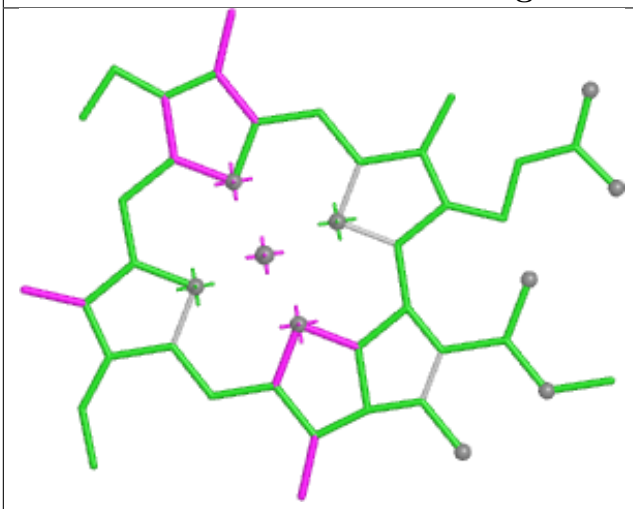


Torsions

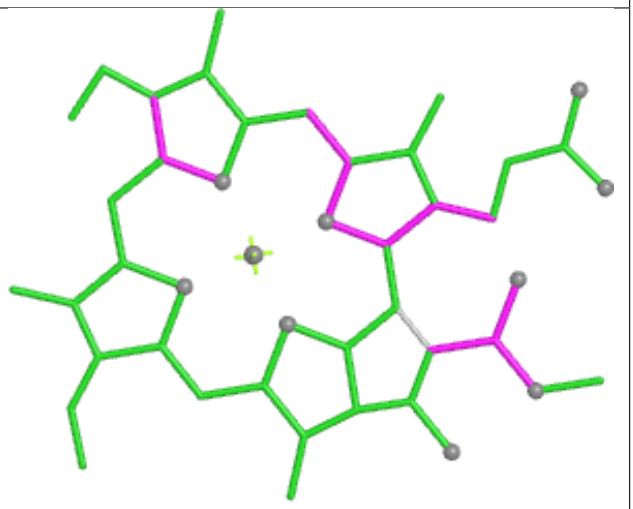


Rings

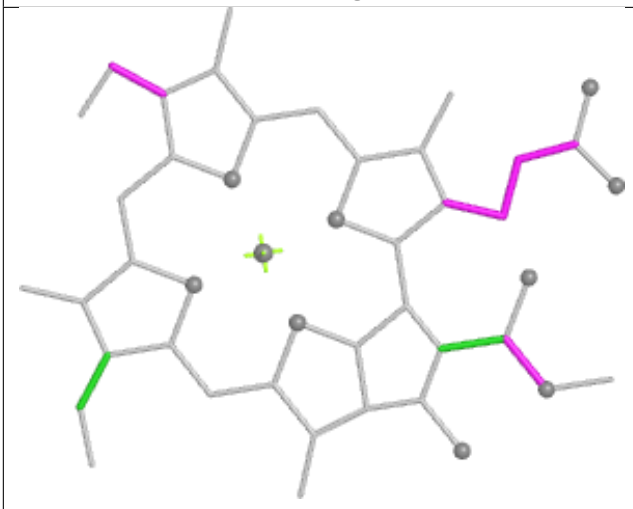
Ligand CLA aB 835



Bond lengths



Bond angles

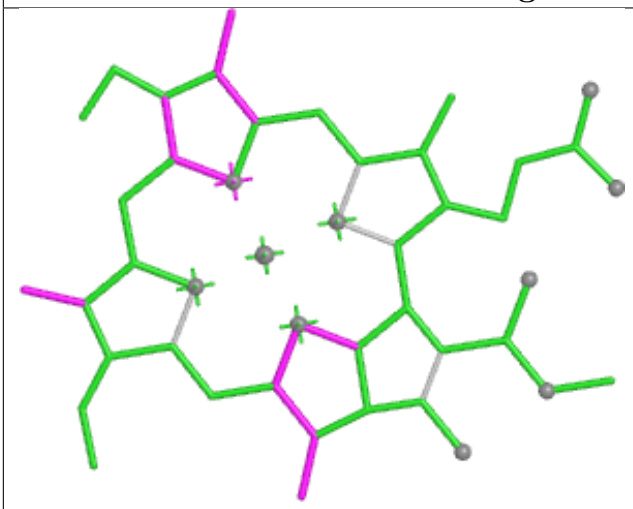


Torsions

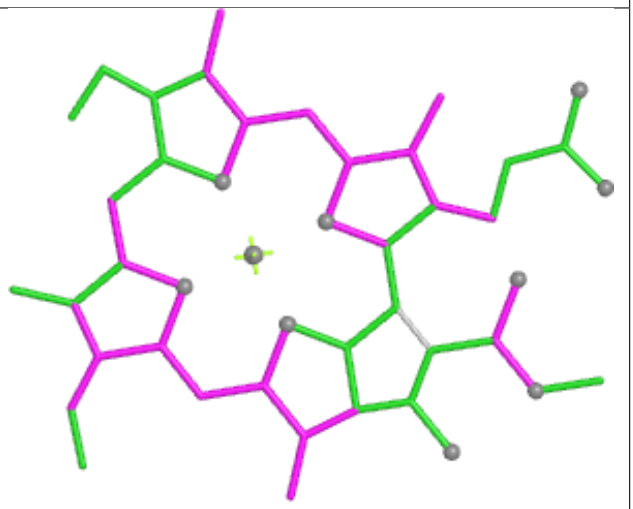


Rings

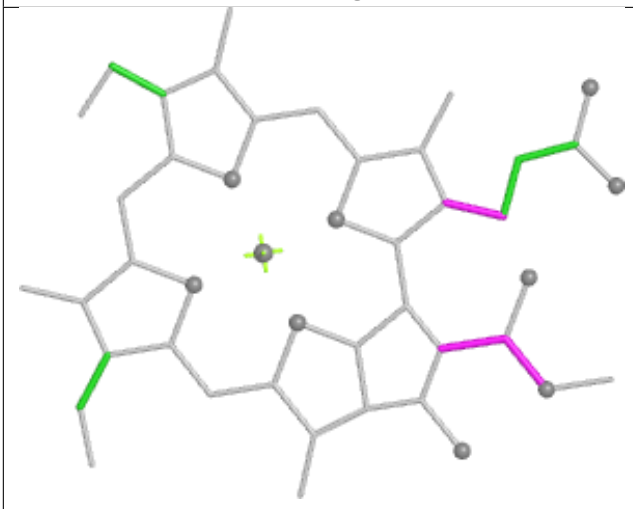
Ligand CLA b4 405



Bond lengths



Bond angles

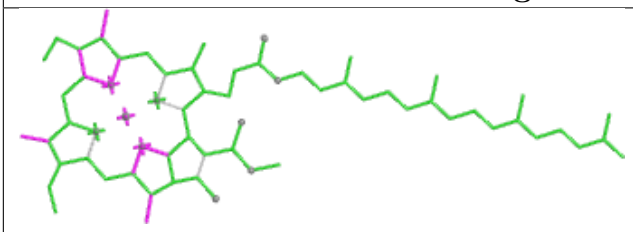


Torsions

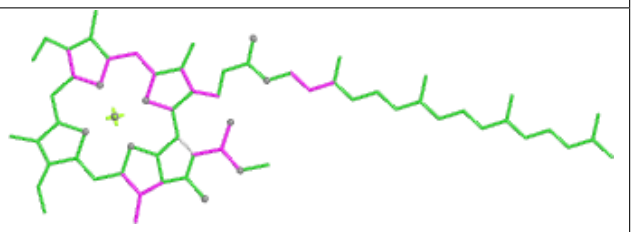


Rings

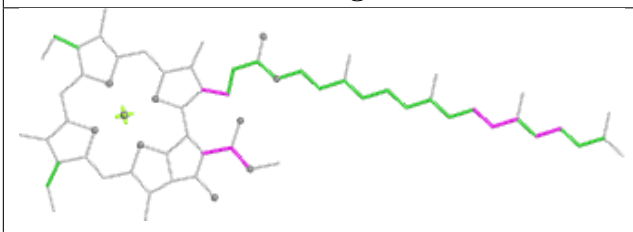
Ligand CLA bA 804



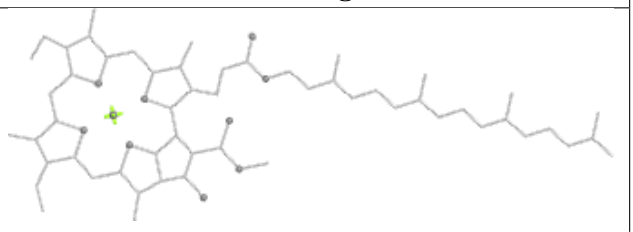
Bond lengths



Bond angles

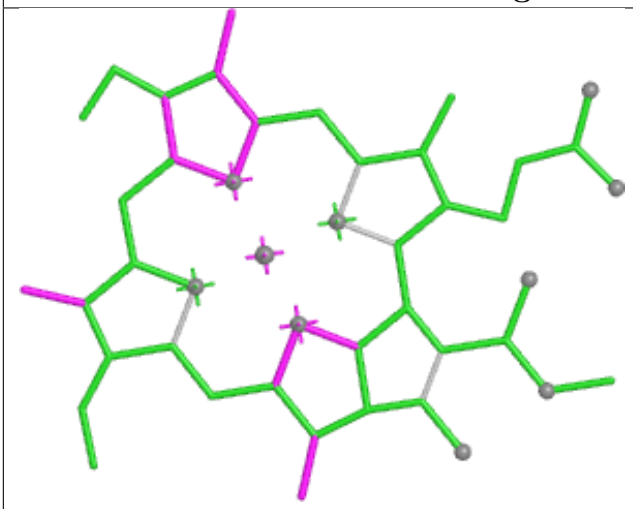


Torsions

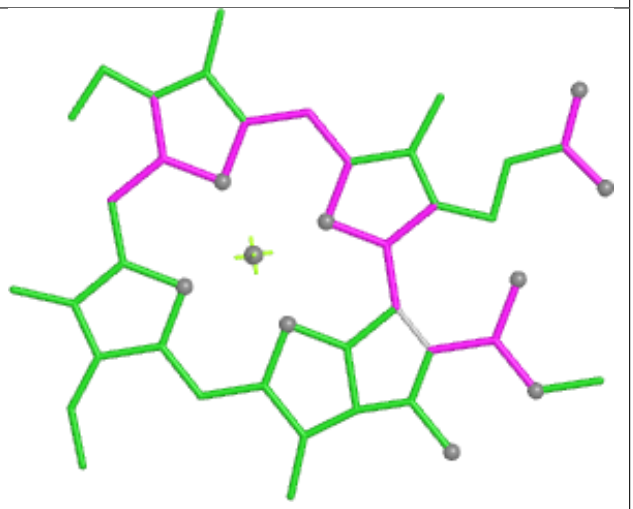


Rings

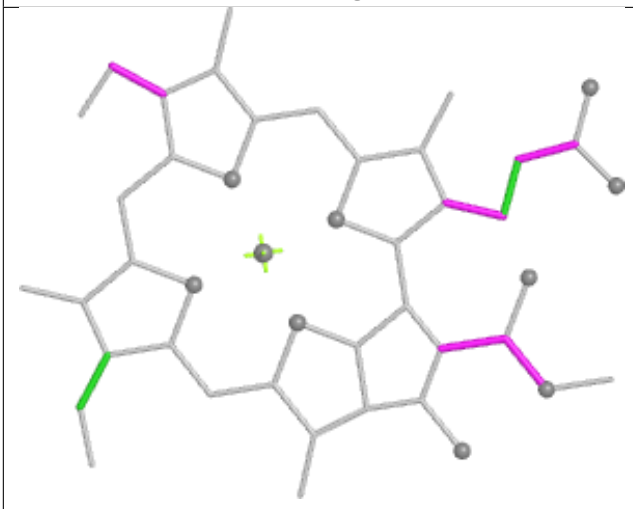
Ligand CLA bK 101



Bond lengths



Bond angles

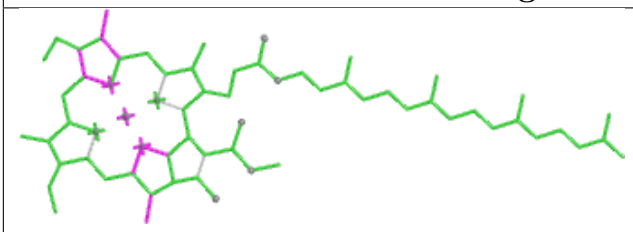


Torsions

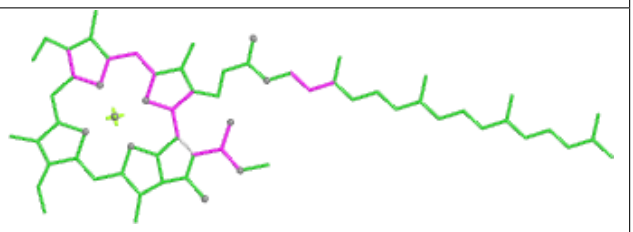


Rings

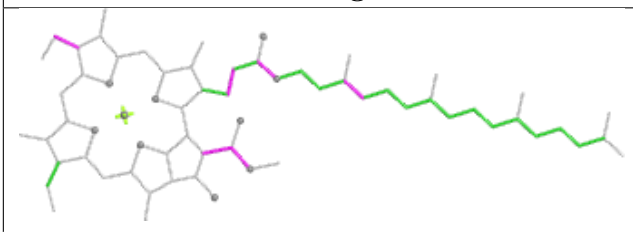
Ligand CLA b5 404



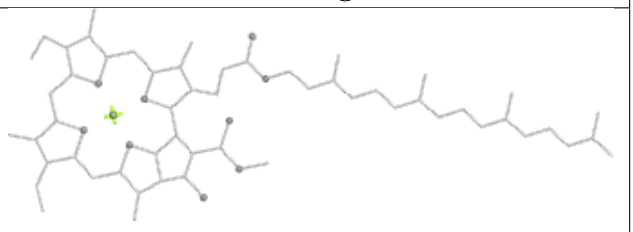
Bond lengths



Bond angles

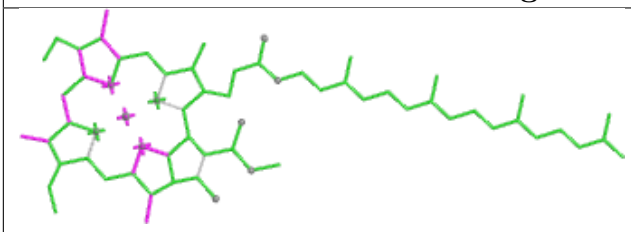


Torsions

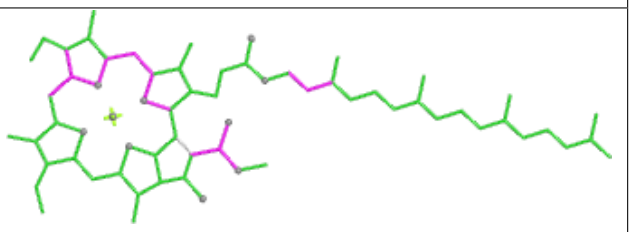


Rings

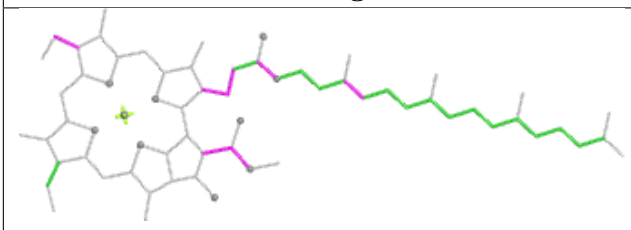
Ligand CLA c4 404



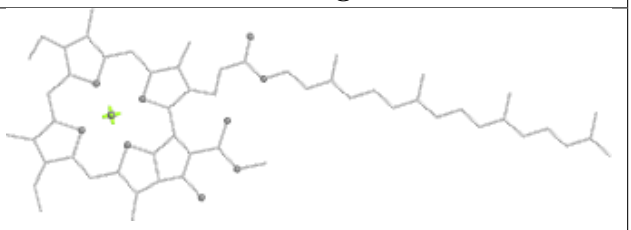
Bond lengths



Bond angles

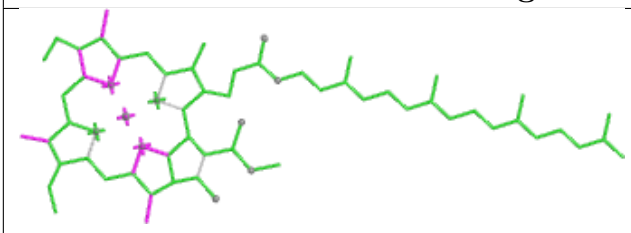


Torsions

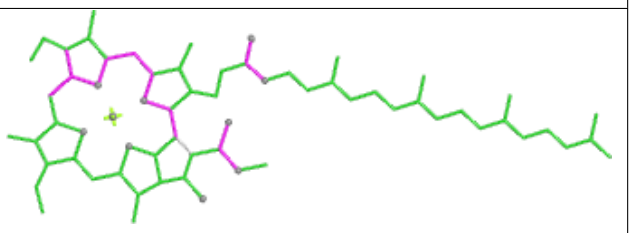


Rings

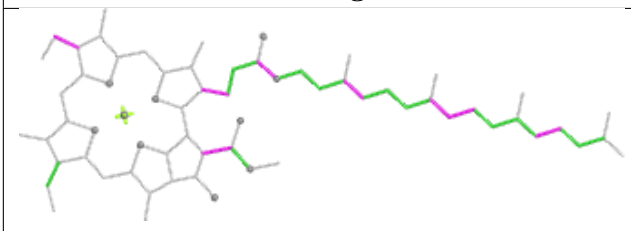
Ligand CLA aL 201



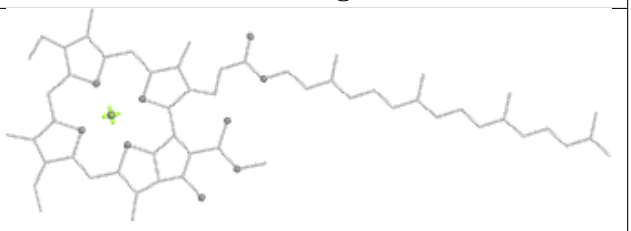
Bond lengths



Bond angles

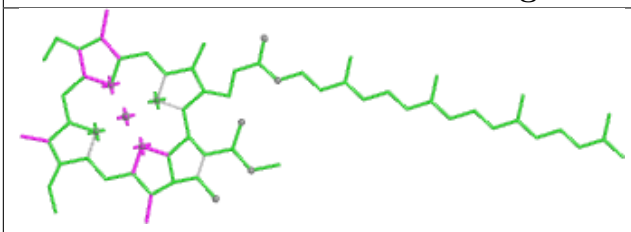


Torsions

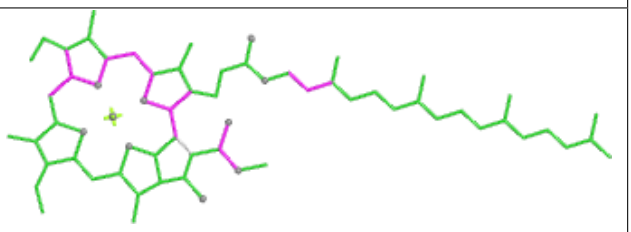


Rings

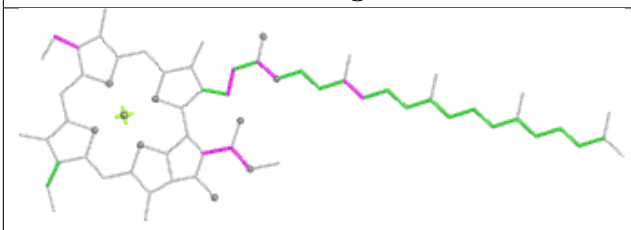
Ligand CLA a6 405



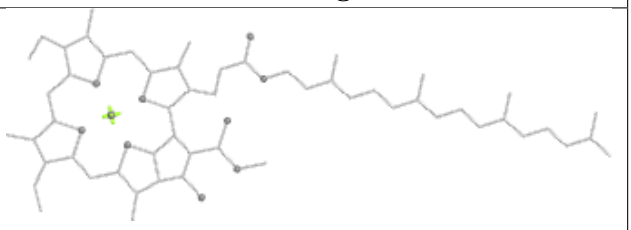
Bond lengths



Bond angles

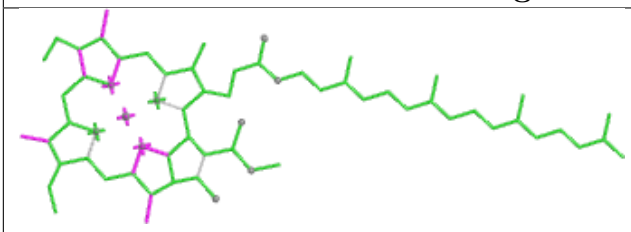


Torsions

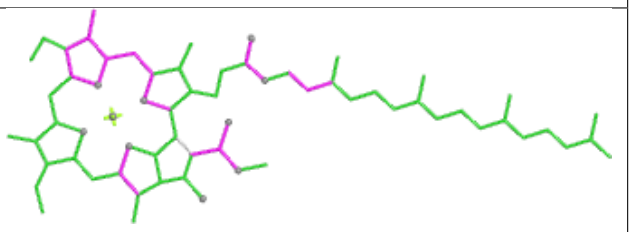


Rings

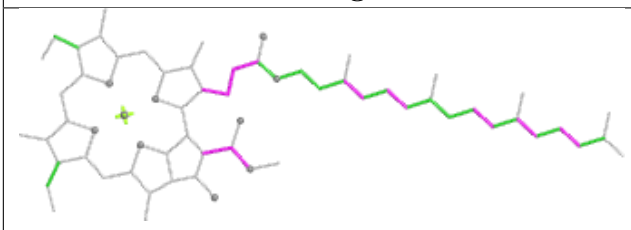
Ligand CLA bA 830



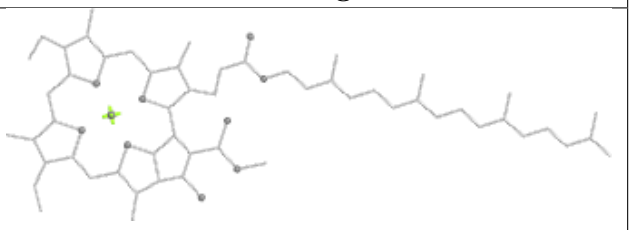
Bond lengths



Bond angles

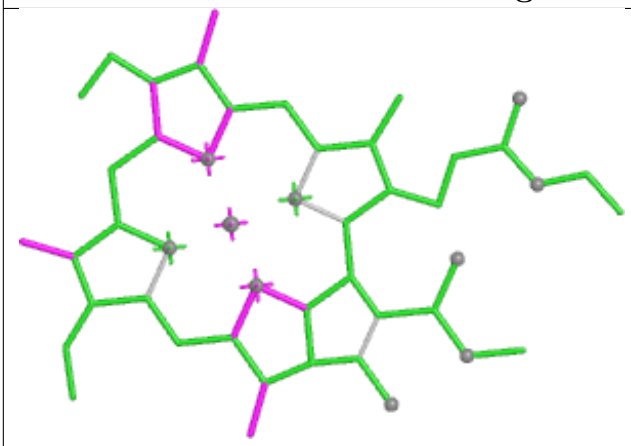


Torsions

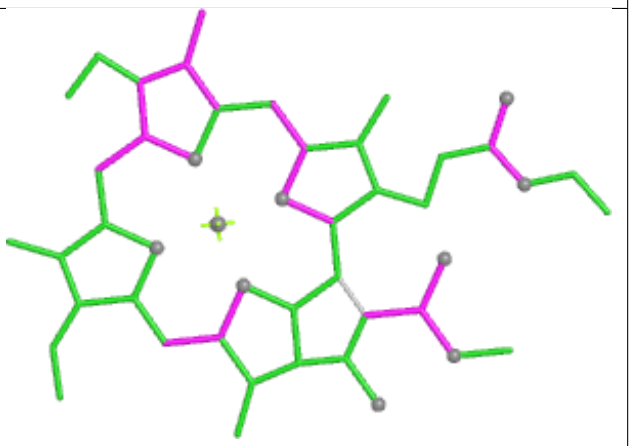


Rings

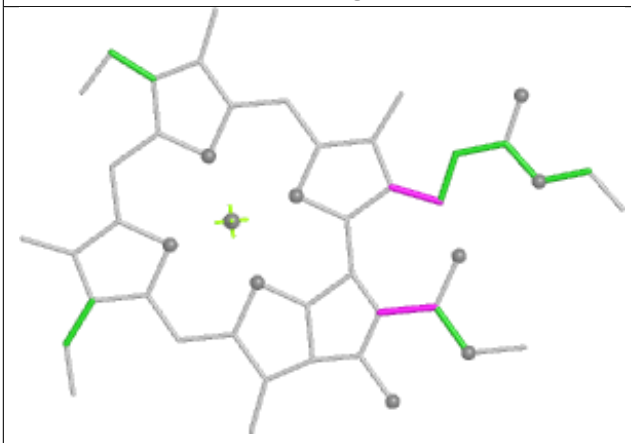
Ligand CLA aB 838



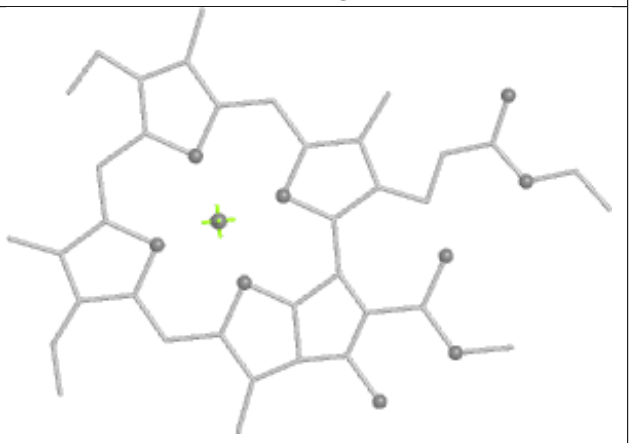
Bond lengths



Bond angles

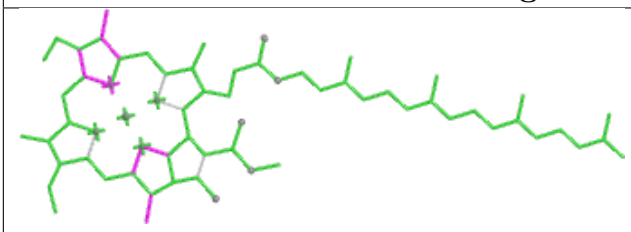


Torsions

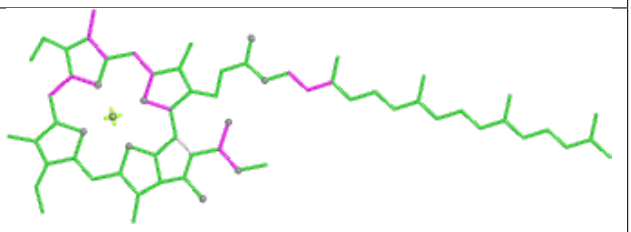


Rings

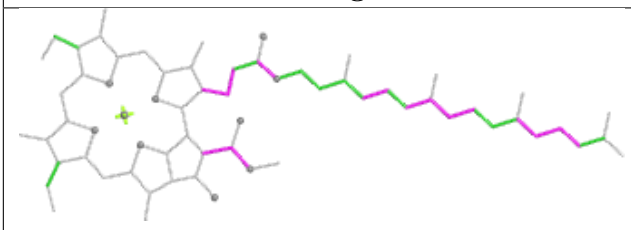
Ligand CLA a2 402



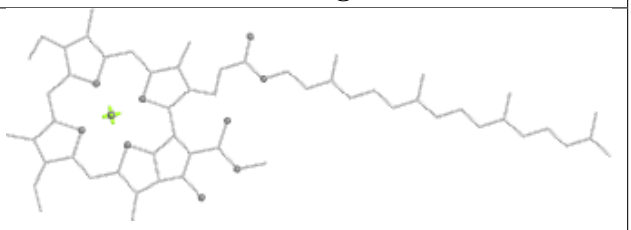
Bond lengths



Bond angles

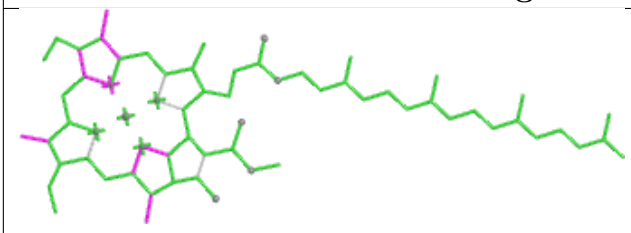


Torsions

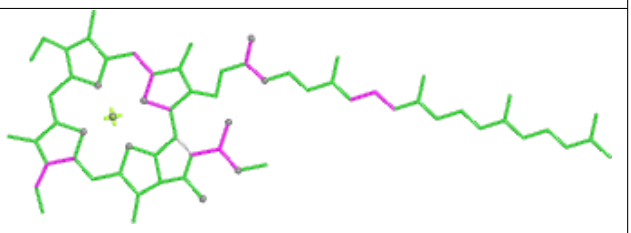


Rings

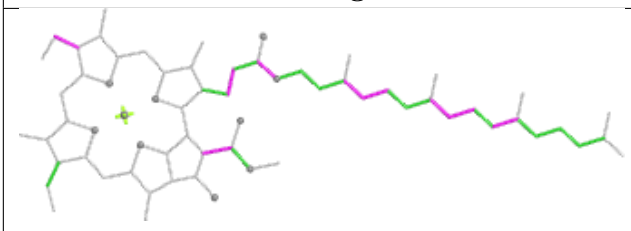
Ligand CLA aB 808



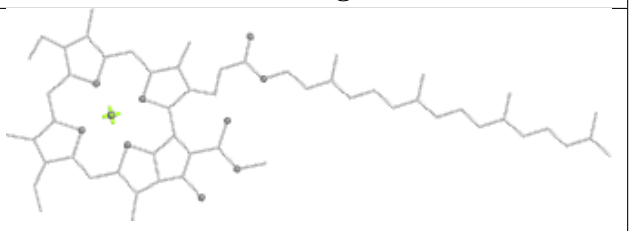
Bond lengths



Bond angles

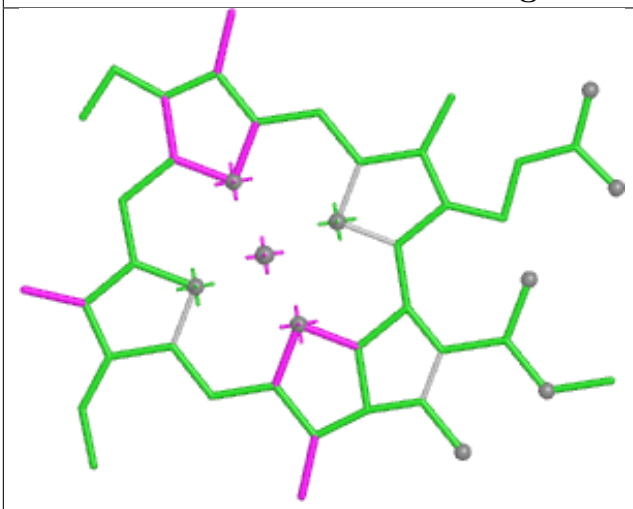


Torsions

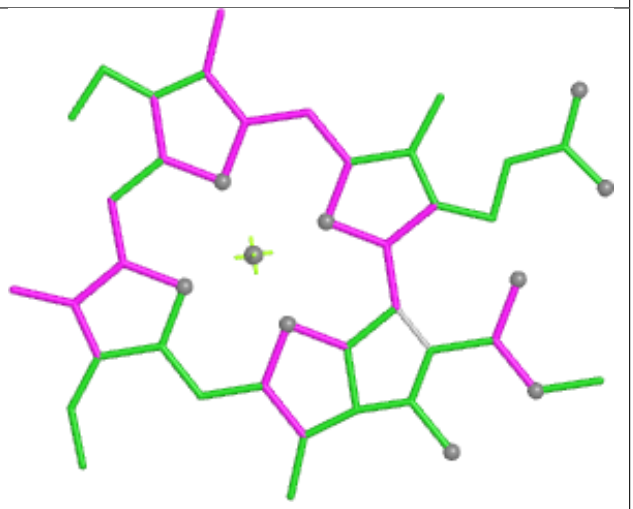


Rings

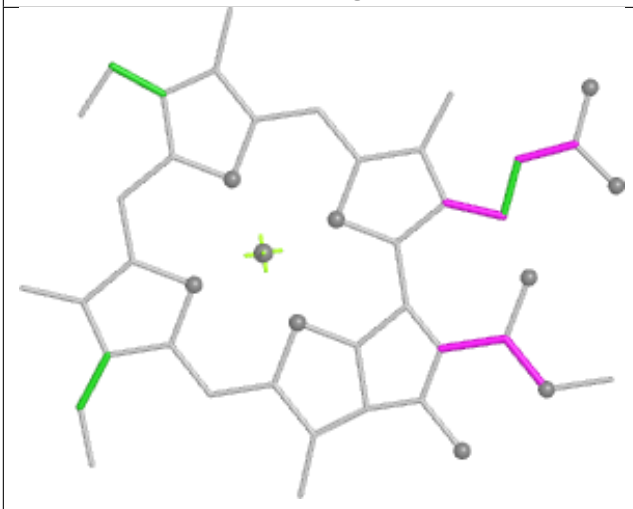
Ligand CLA a5 412



Bond lengths



Bond angles

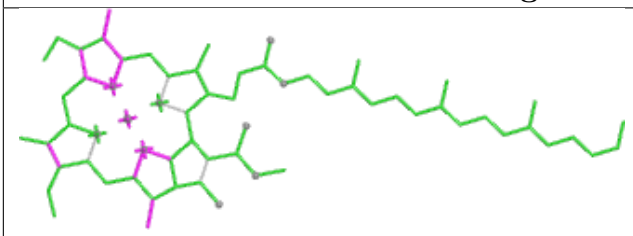


Torsions

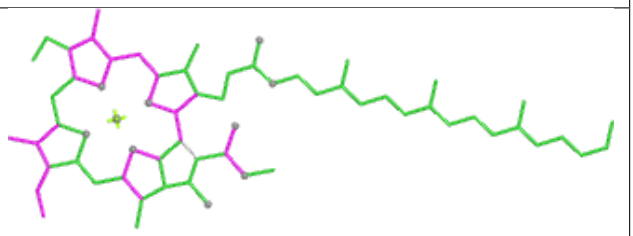


Rings

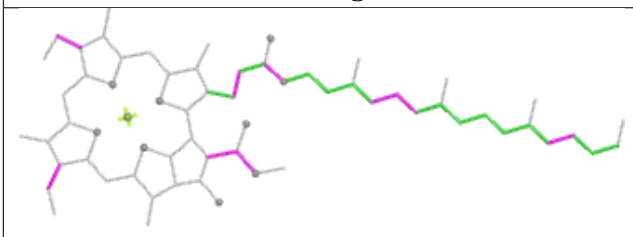
Ligand CLA c4 410



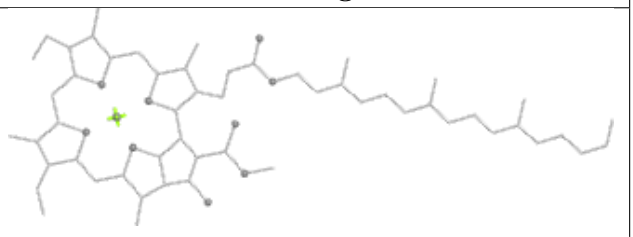
Bond lengths



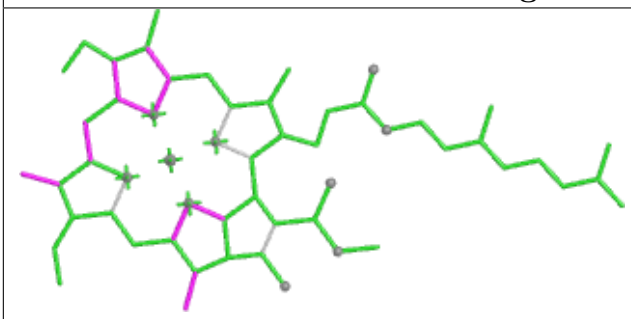
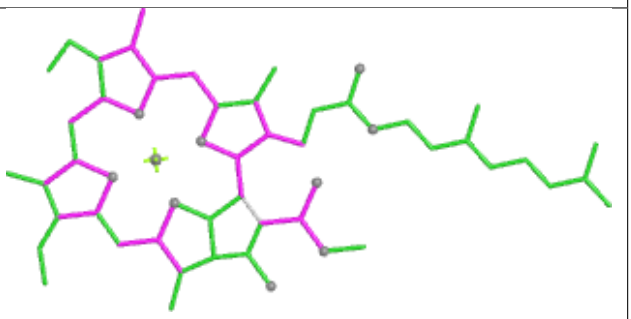
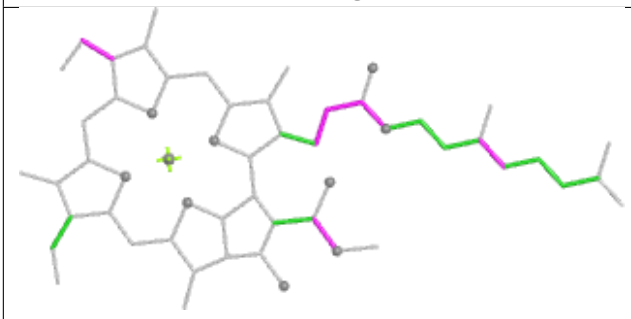
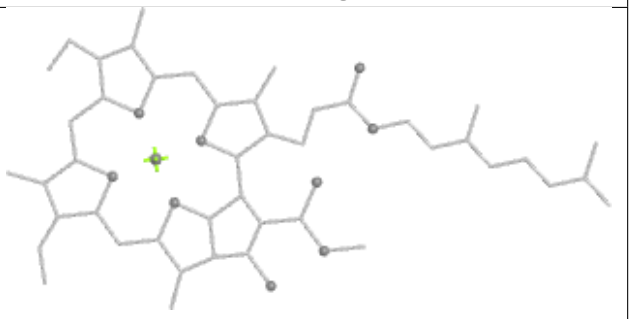
Bond angles

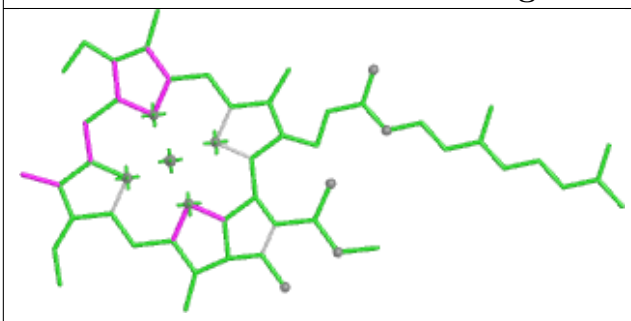
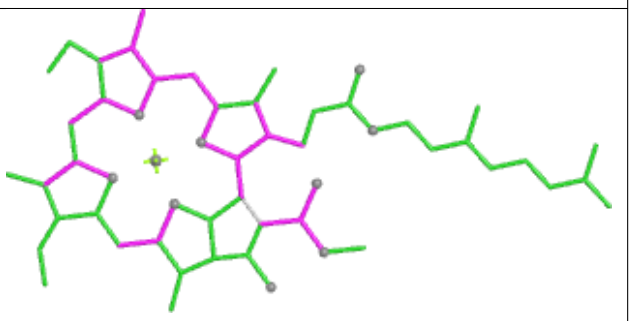
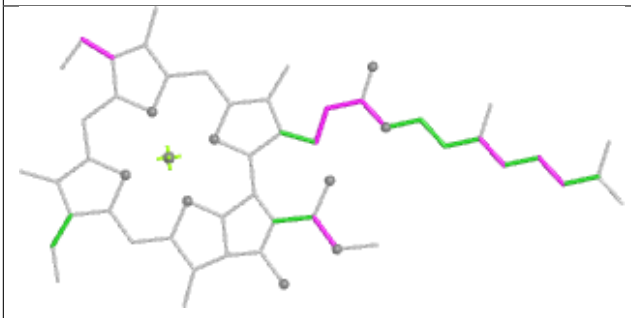
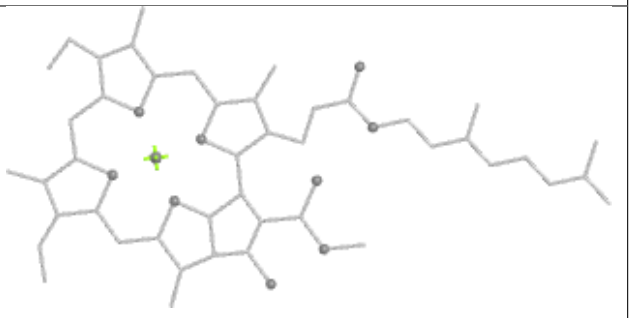


Torsions

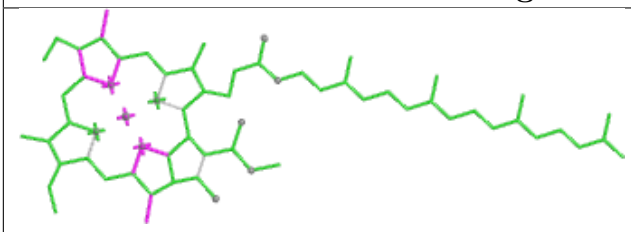


Rings

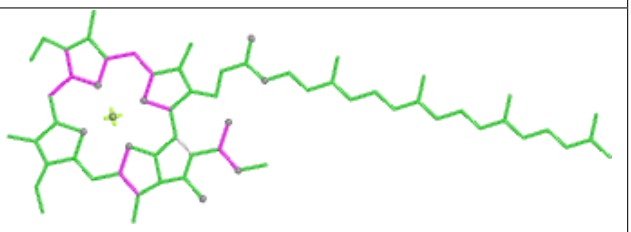
Ligand CLA a1 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b2 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

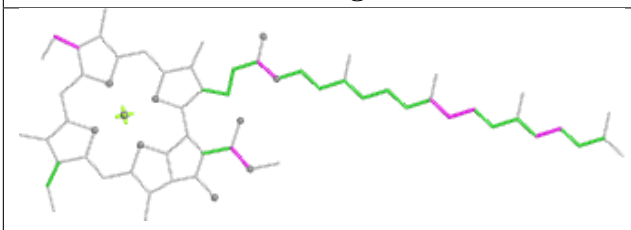
Ligand CLA cB 820



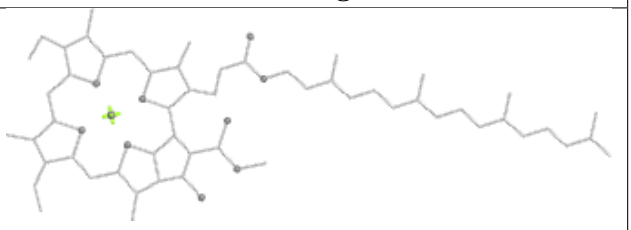
Bond lengths



Bond angles

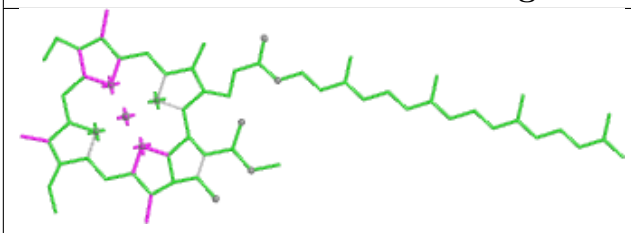


Torsions

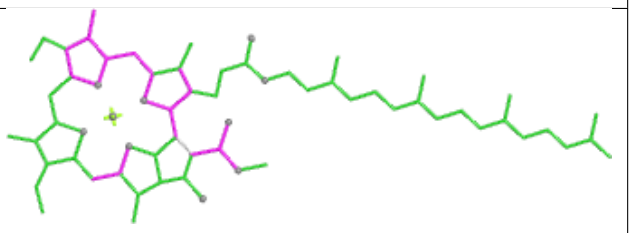


Rings

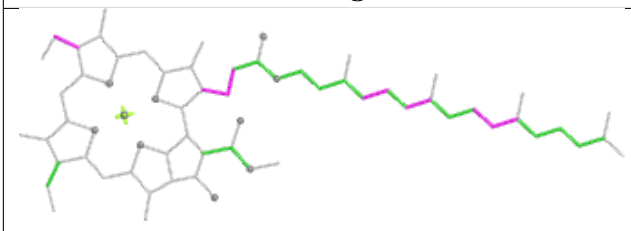
Ligand CLA cL 203



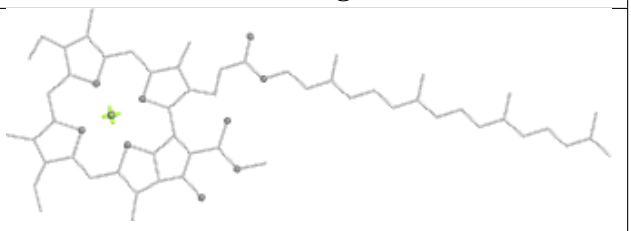
Bond lengths



Bond angles

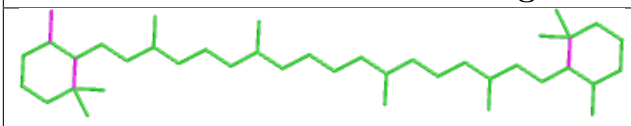


Torsions

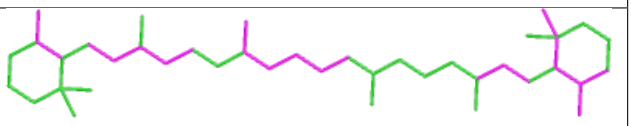


Rings

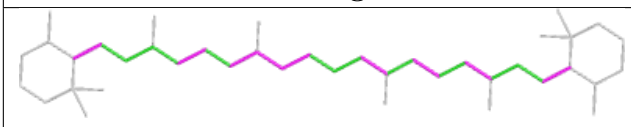
Ligand BCR cJ 103



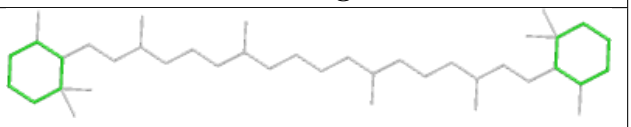
Bond lengths



Bond angles

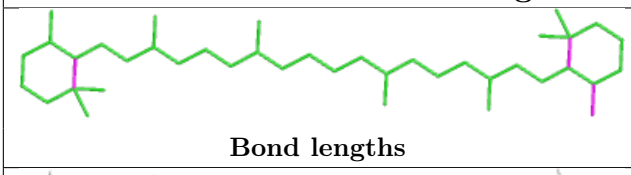


Torsions

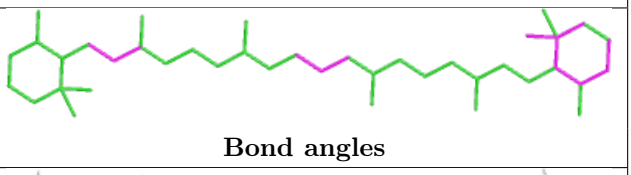


Rings

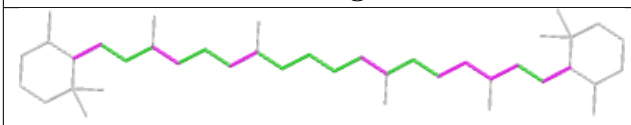
Ligand BCR cB 845



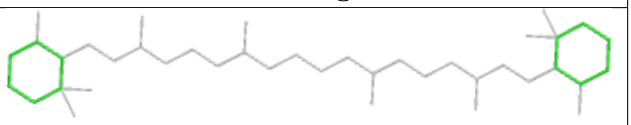
Bond lengths



Bond angles

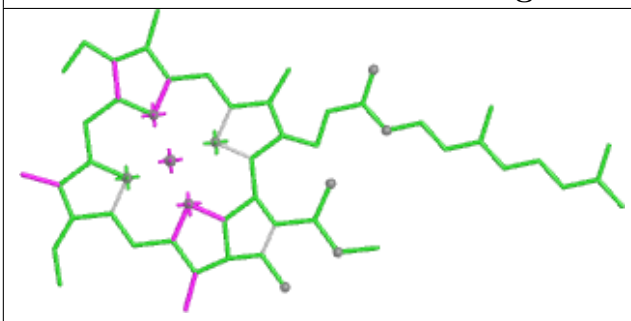


Torsions

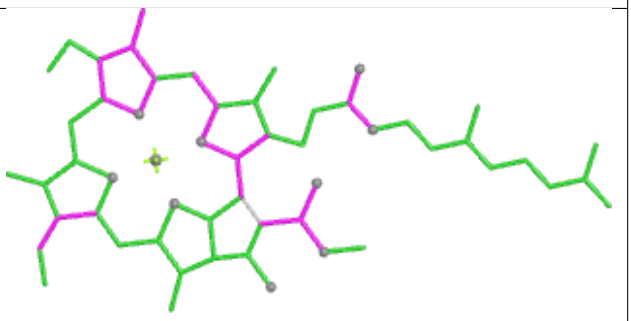


Rings

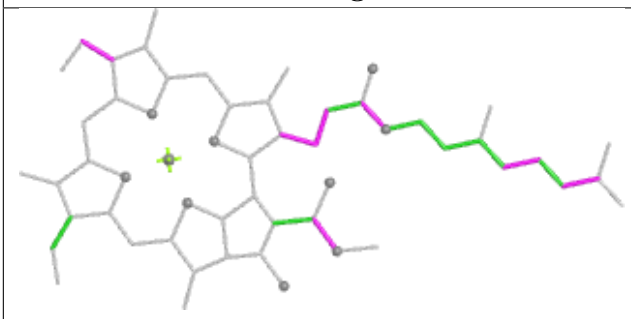
Ligand CLA aB 817



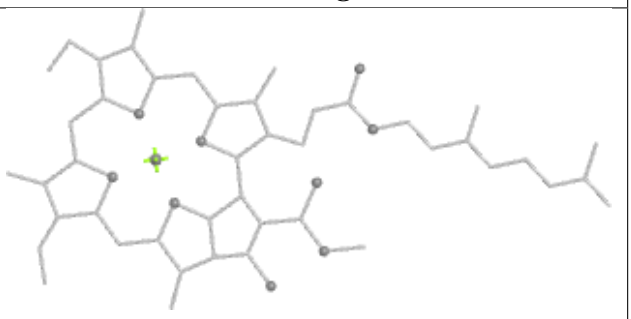
Bond lengths



Bond angles

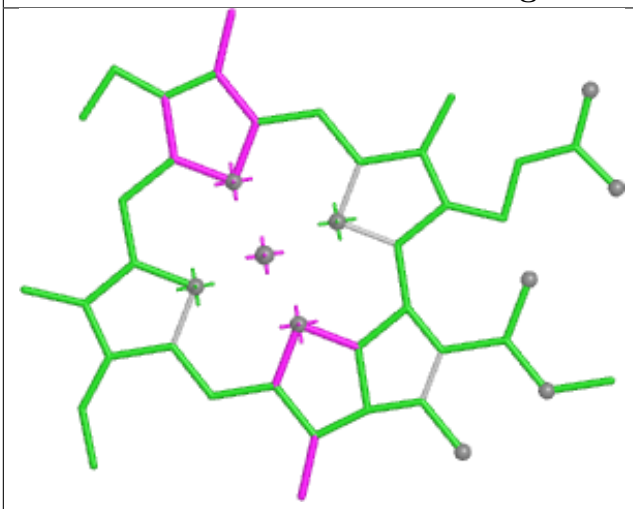


Torsions

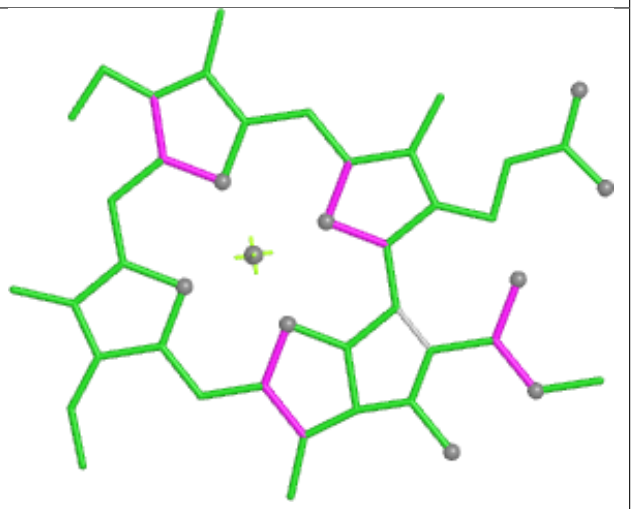


Rings

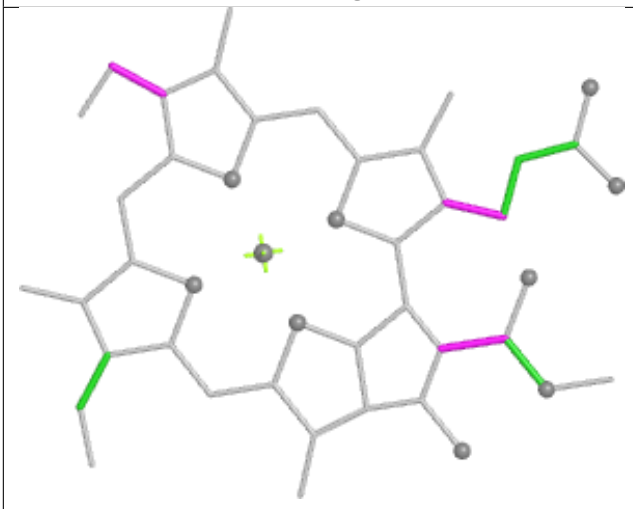
Ligand CLA a1 412



Bond lengths



Bond angles

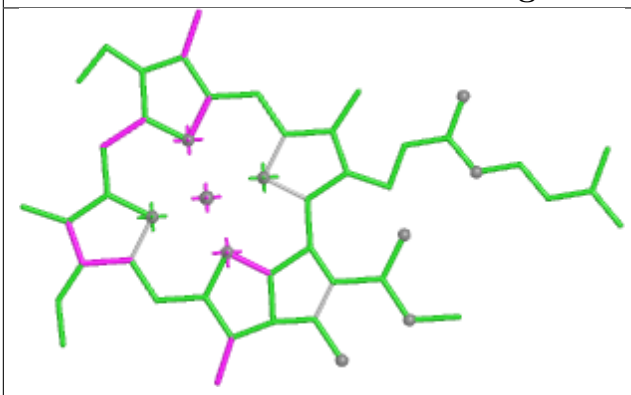


Torsions

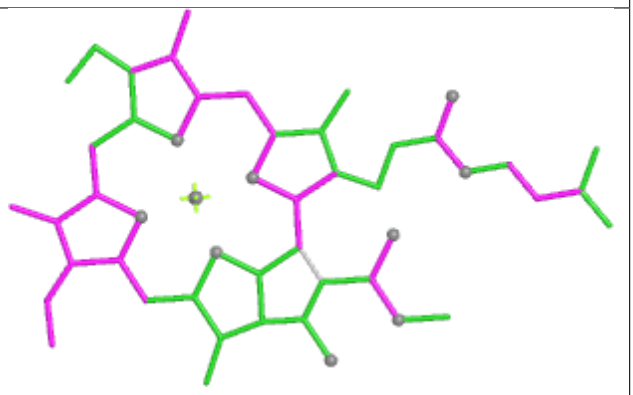


Rings

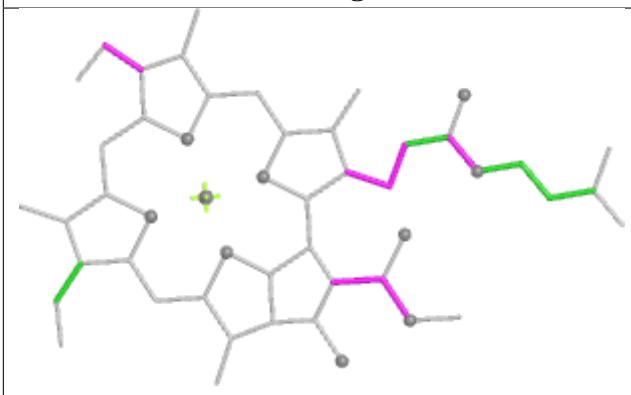
Ligand CLA b1 416



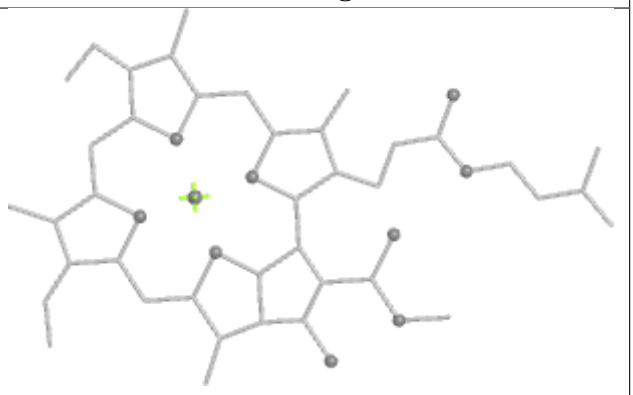
Bond lengths



Bond angles



Torsions

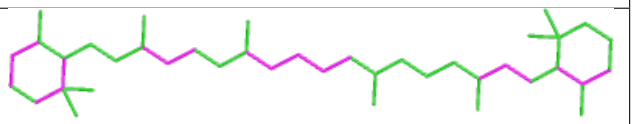


Rings

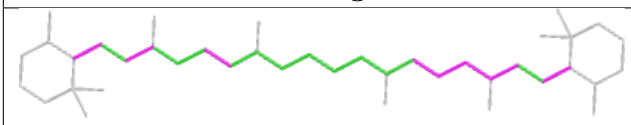
Ligand BCR a4 419



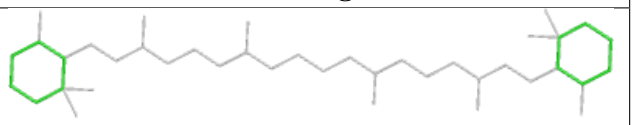
Bond lengths



Bond angles

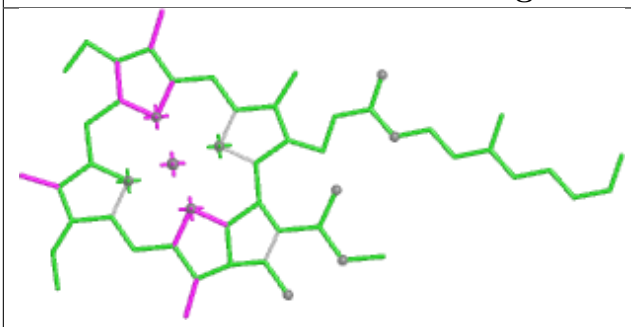


Torsions

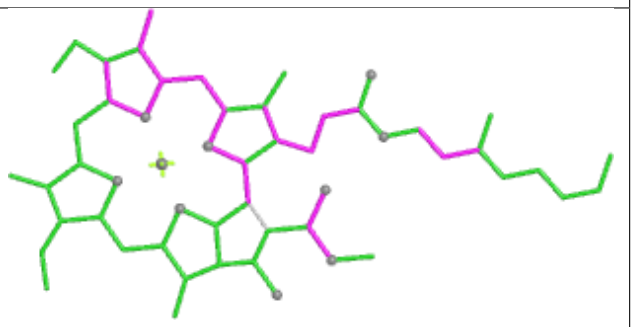


Rings

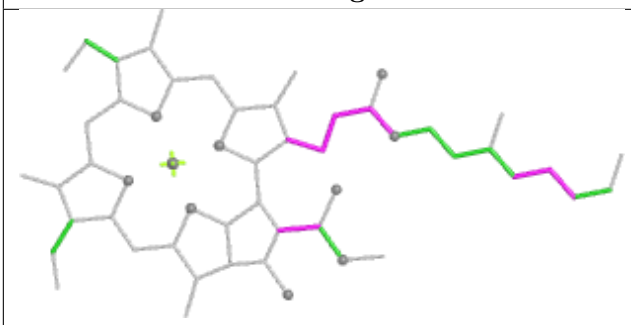
Ligand CLA cA 813



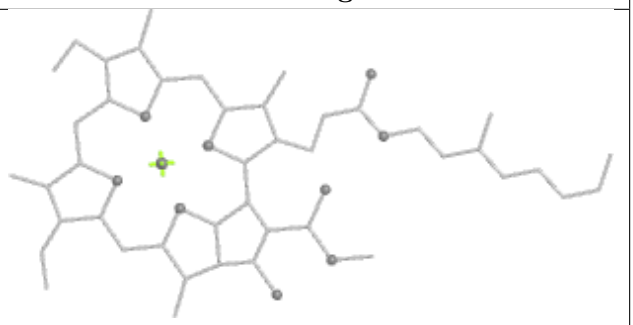
Bond lengths



Bond angles

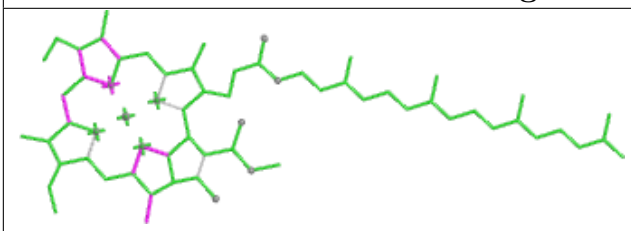


Torsions

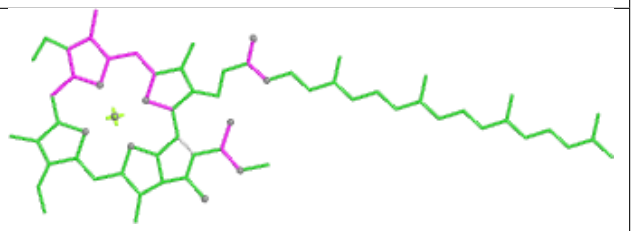


Rings

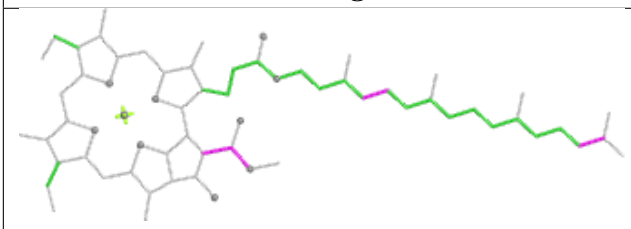
Ligand CLA a1 408



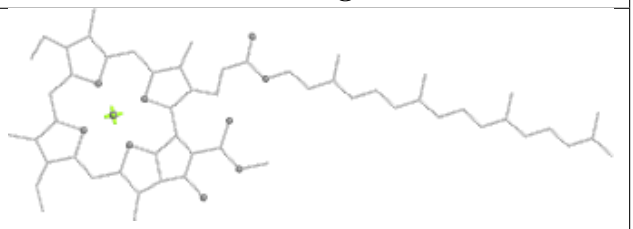
Bond lengths



Bond angles

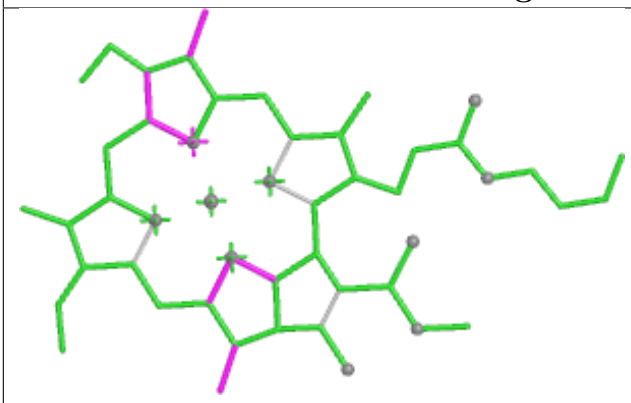


Torsions

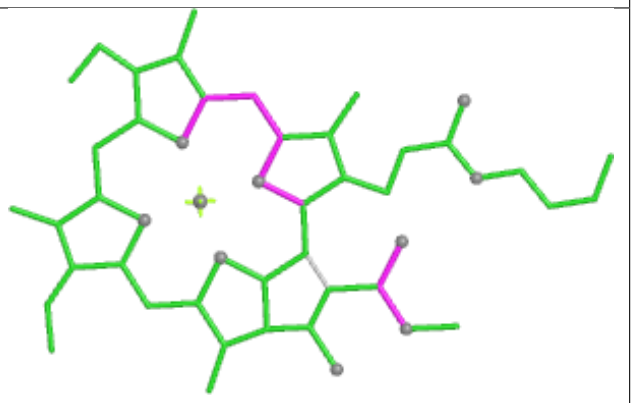


Rings

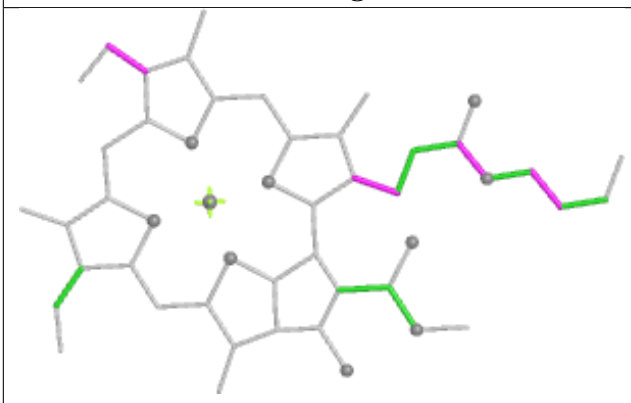
Ligand CLA aA 817



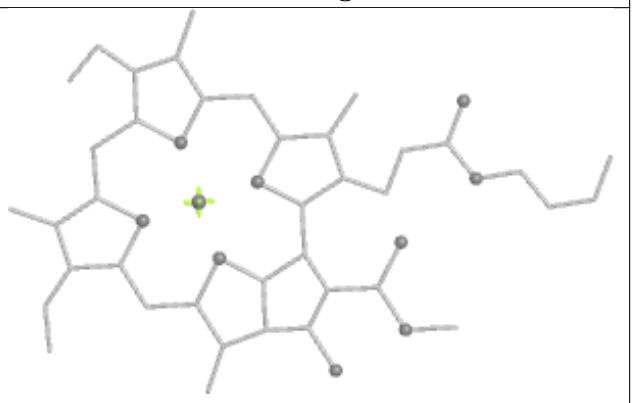
Bond lengths



Bond angles

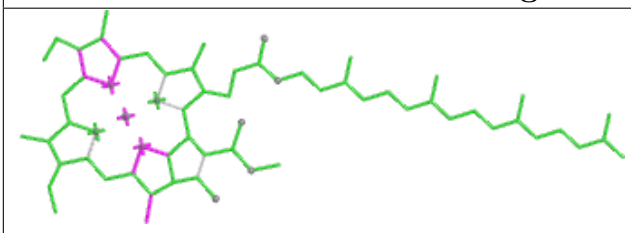


Torsions

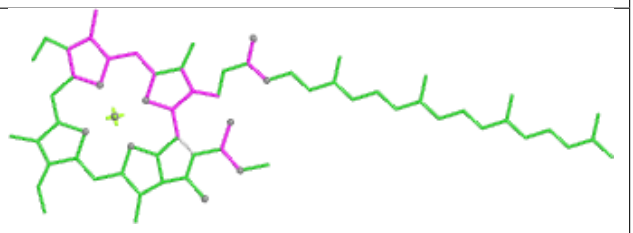


Rings

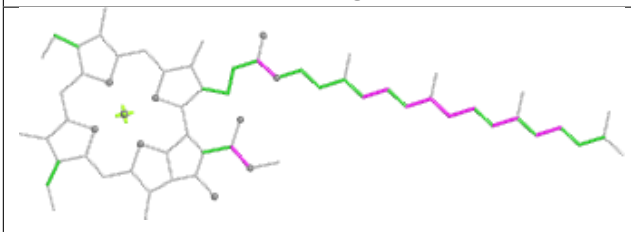
Ligand CLA c3 403



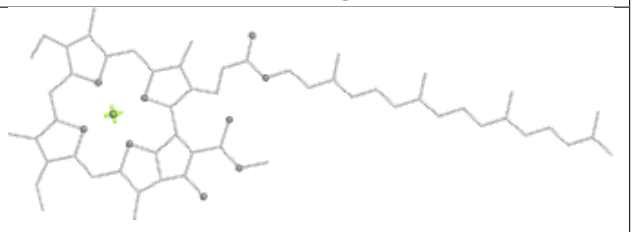
Bond lengths



Bond angles

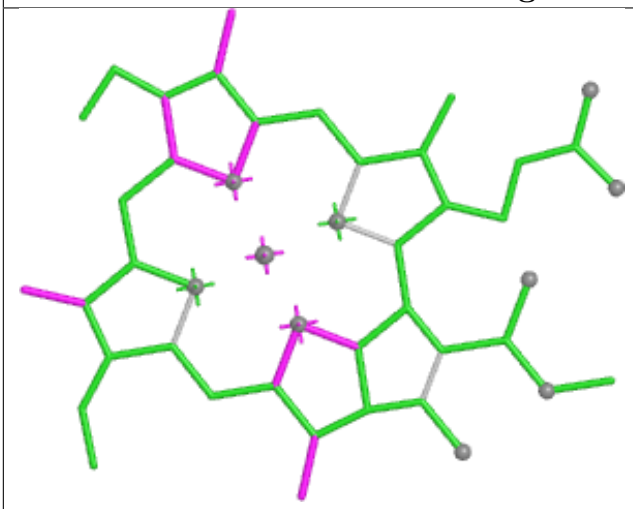


Torsions

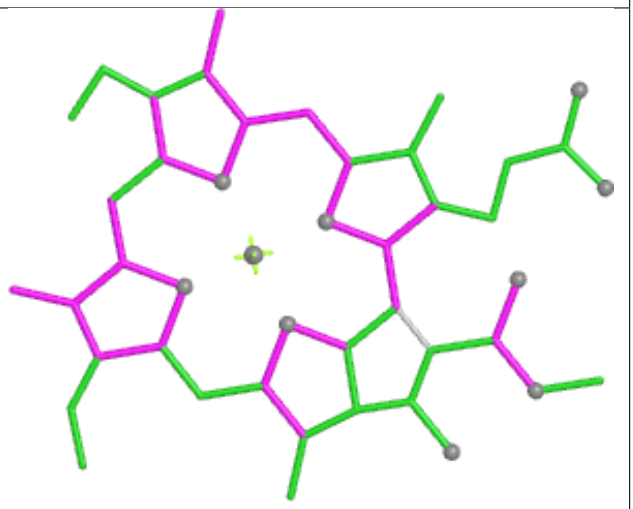


Rings

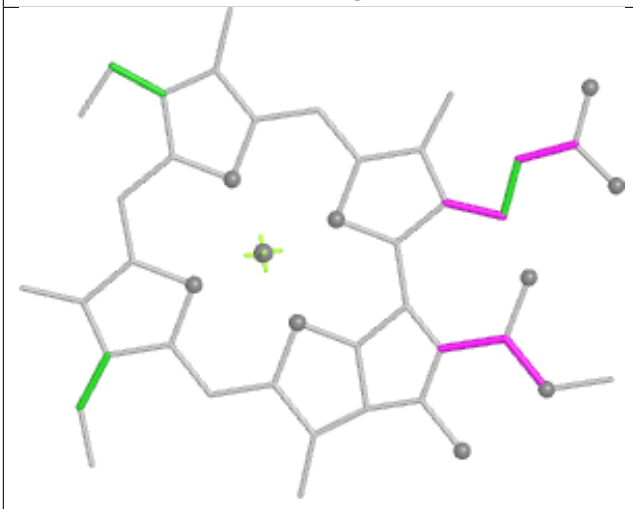
Ligand CLA b1 412



Bond lengths



Bond angles

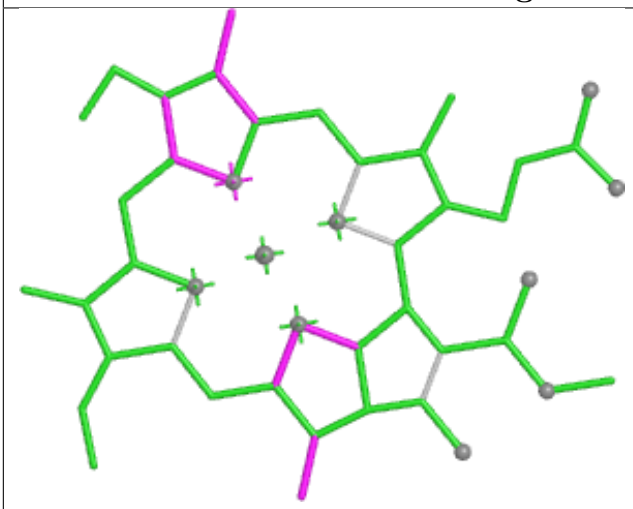


Torsions

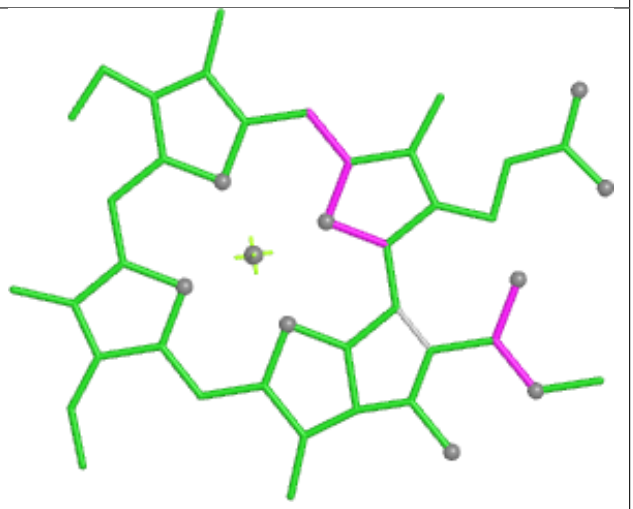


Rings

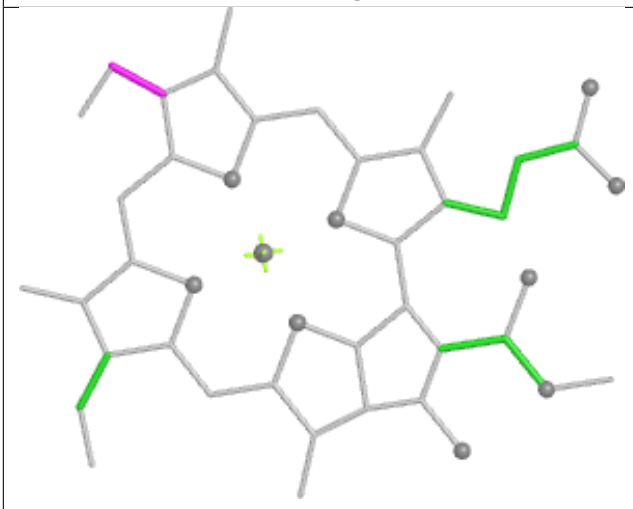
Ligand CLA aB 842



Bond lengths



Bond angles

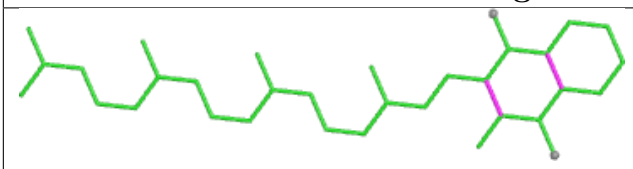


Torsions

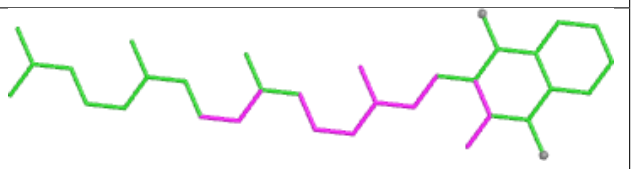


Rings

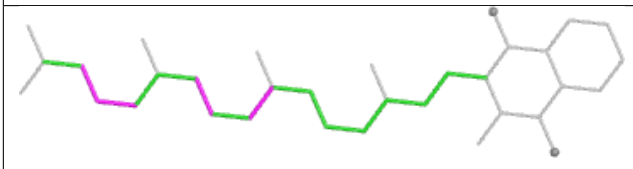
Ligand PQN cA 845



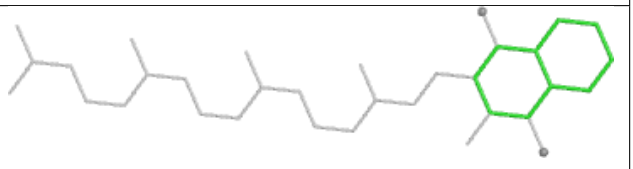
Bond lengths



Bond angles

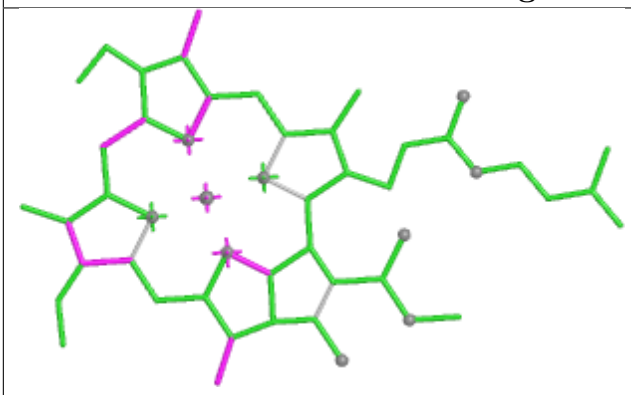


Torsions

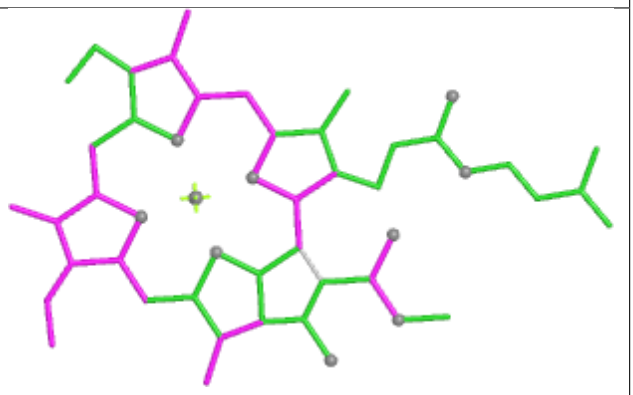


Rings

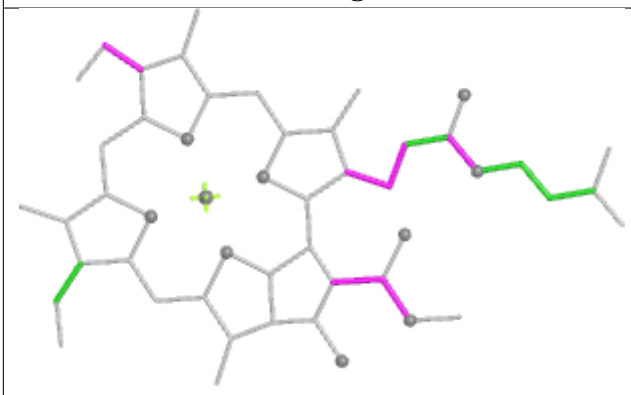
Ligand CLA b4 416



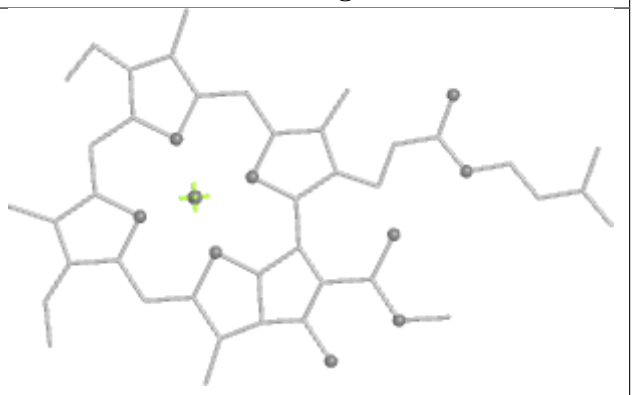
Bond lengths



Bond angles

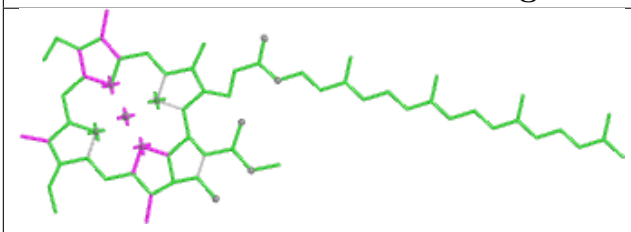


Torsions

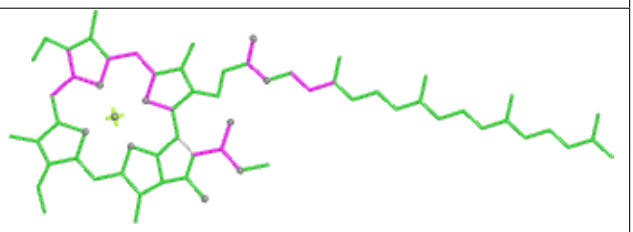


Rings

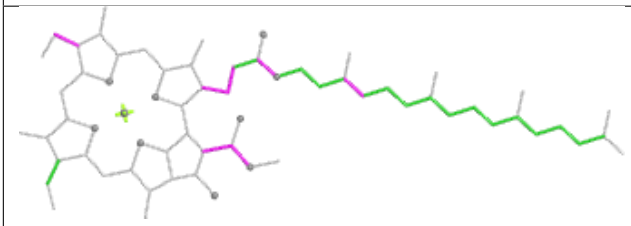
Ligand CLA a2 404



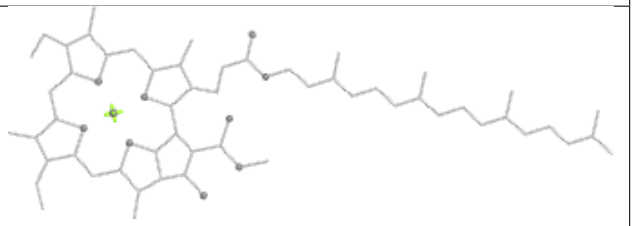
Bond lengths



Bond angles

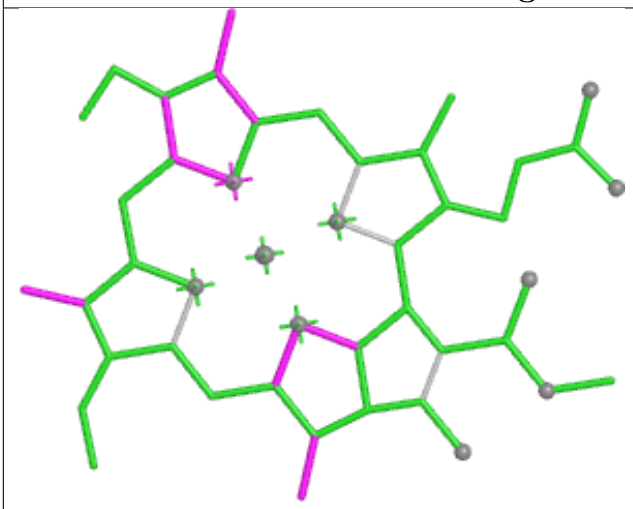


Torsions

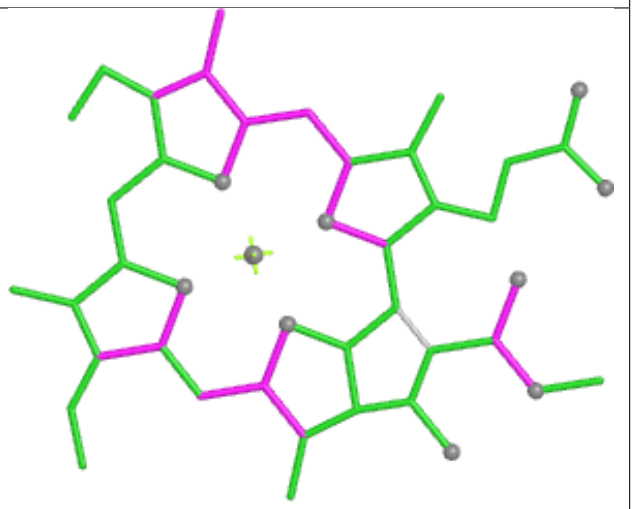


Rings

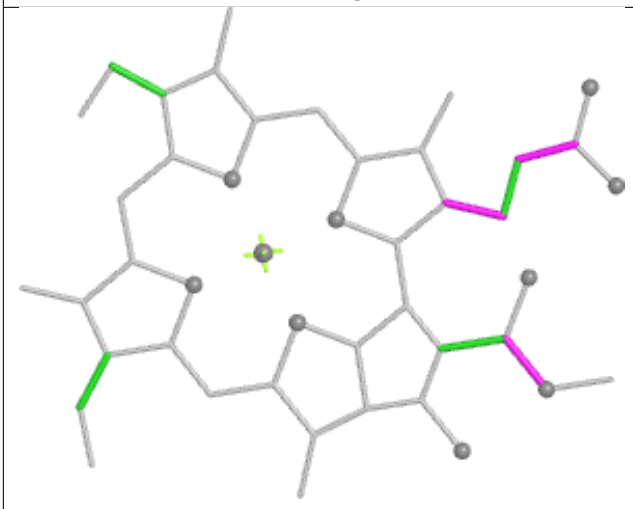
Ligand CLA b1 408



Bond lengths



Bond angles

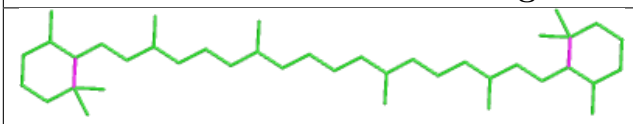


Torsions

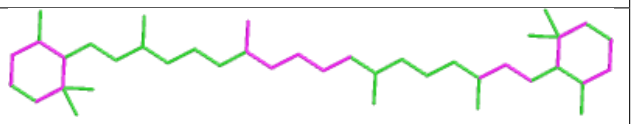


Rings

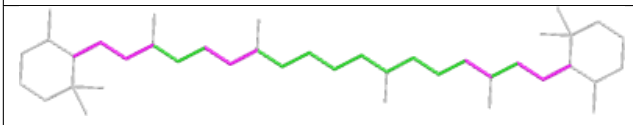
Ligand BCR c2 421



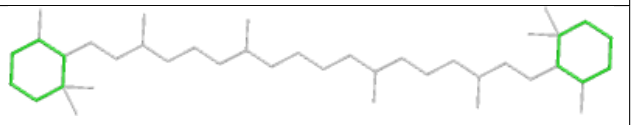
Bond lengths



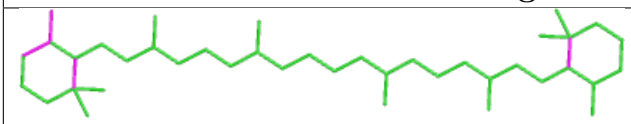
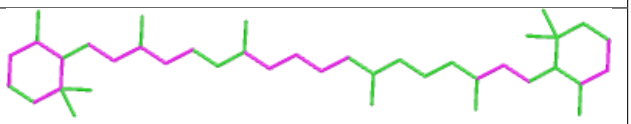
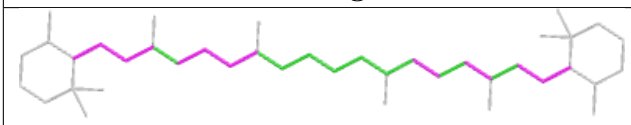
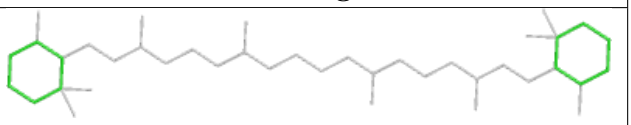
Bond angles

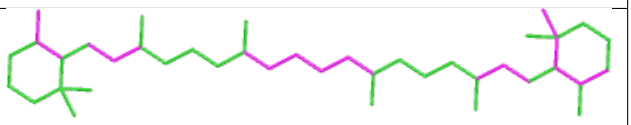
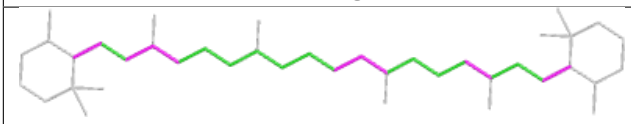
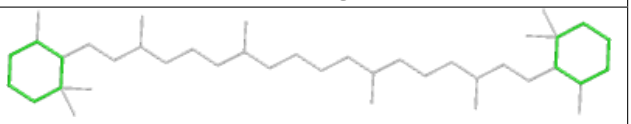


Torsions

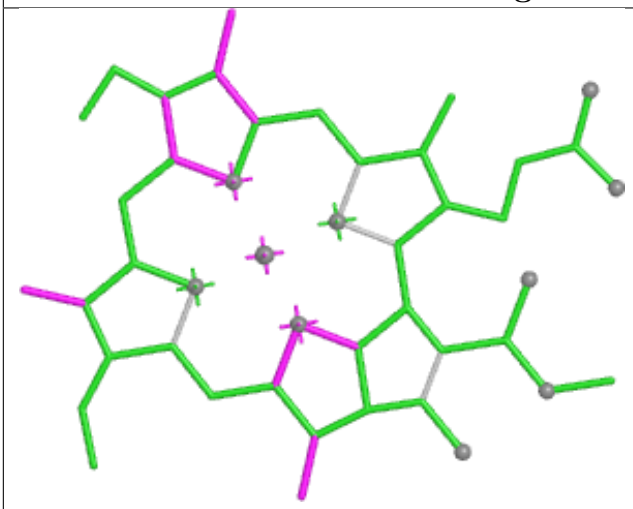


Rings

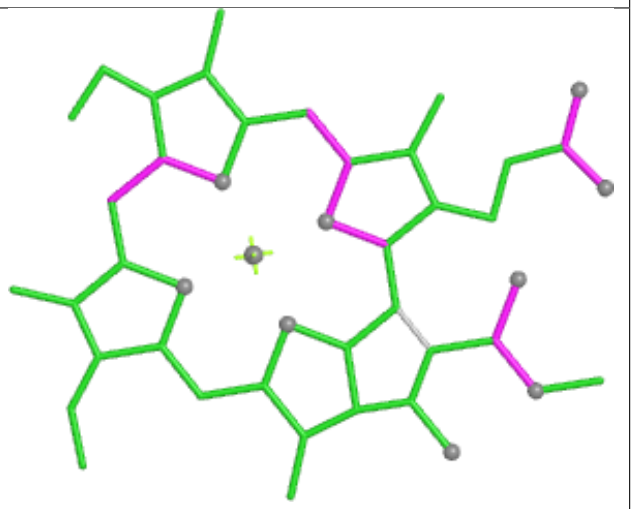
Ligand BCR c6 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR aM 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

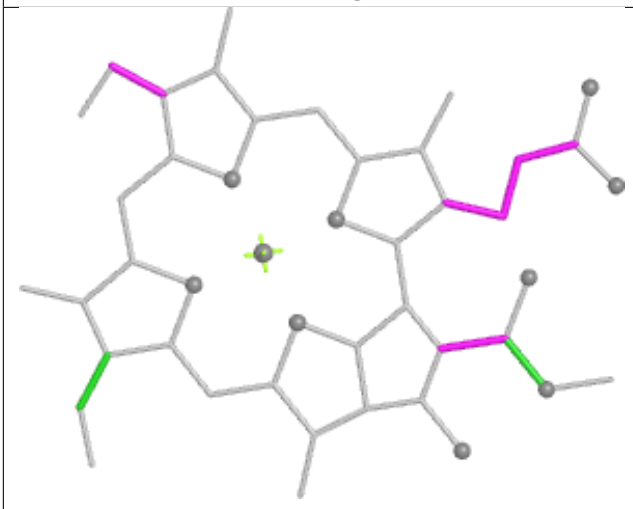
Ligand CLA bB 831



Bond lengths



Bond angles

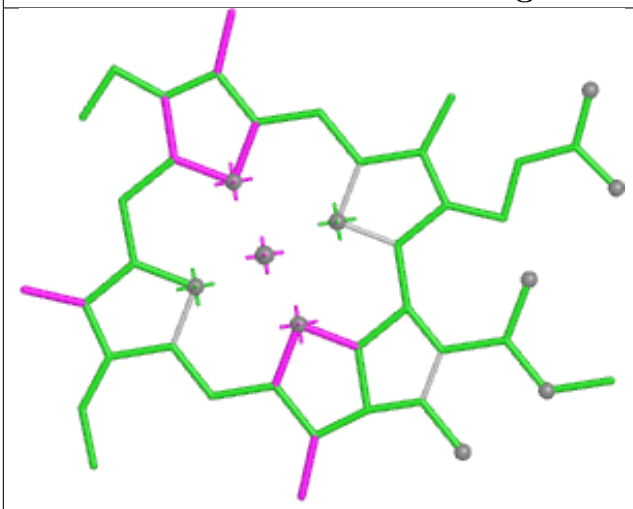


Torsions

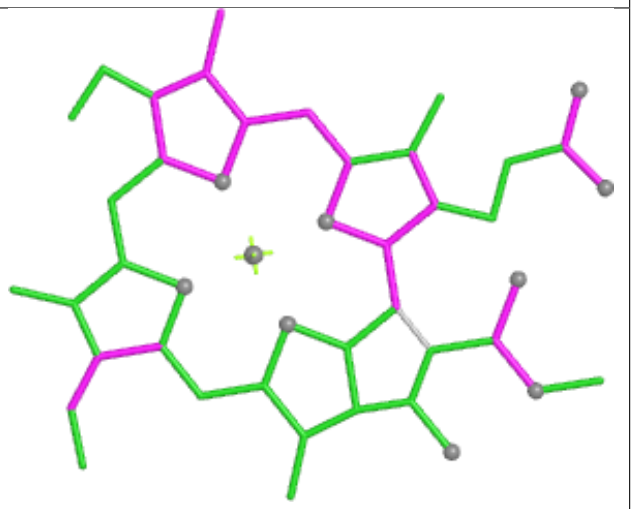


Rings

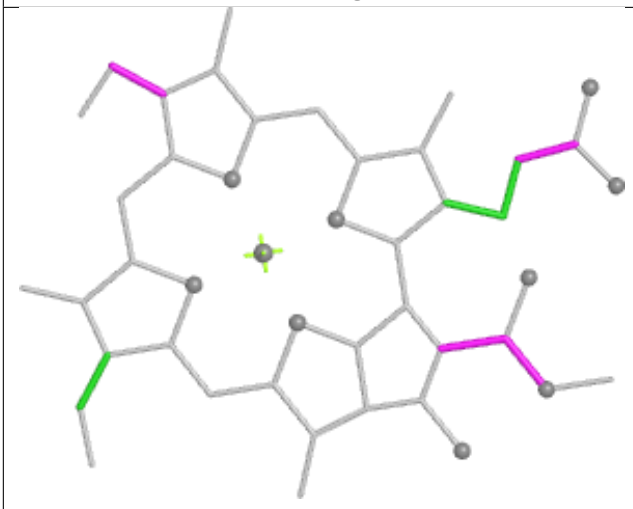
Ligand CLA bF 201



Bond lengths



Bond angles

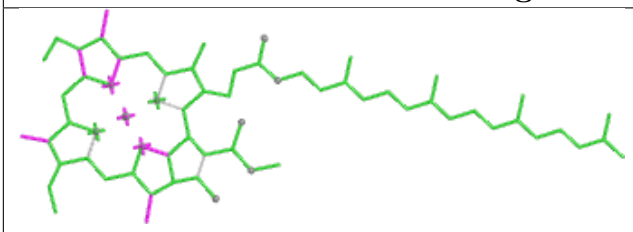


Torsions

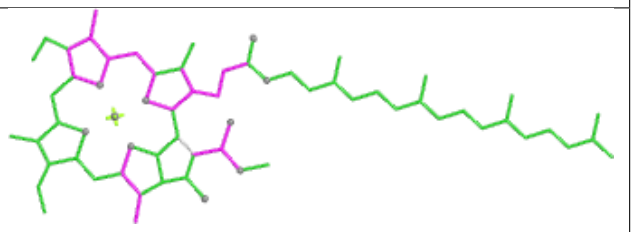


Rings

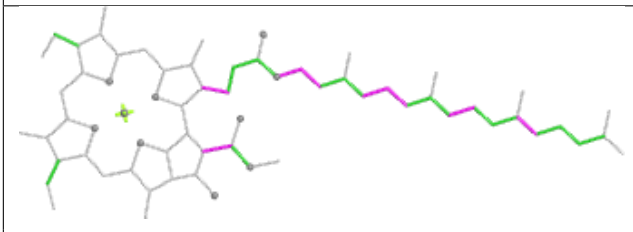
Ligand CLA aA 827



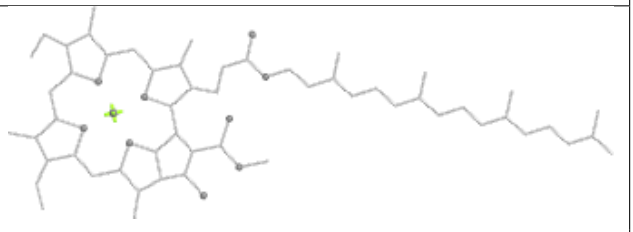
Bond lengths



Bond angles

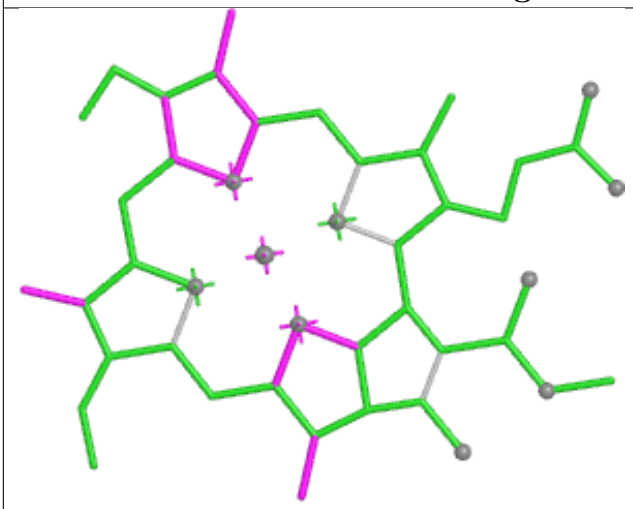


Torsions

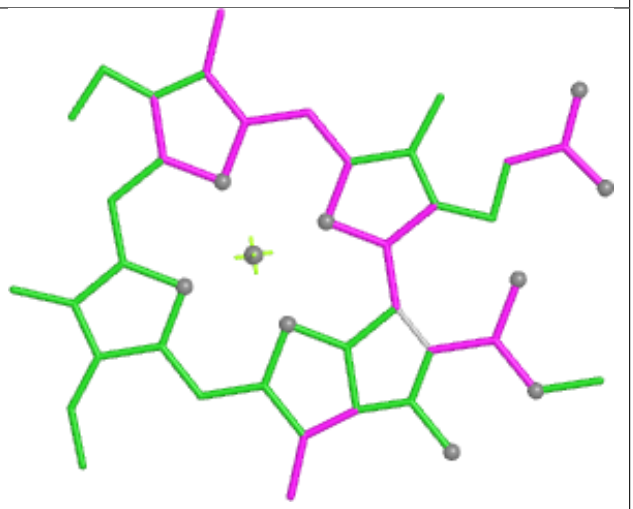


Rings

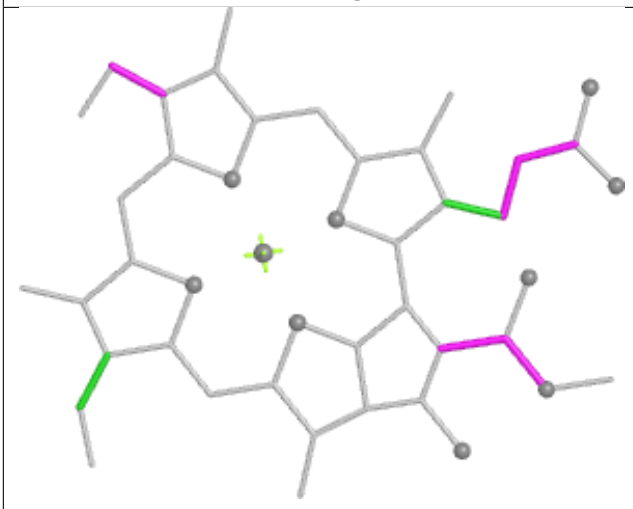
Ligand CLA bX 102



Bond lengths



Bond angles

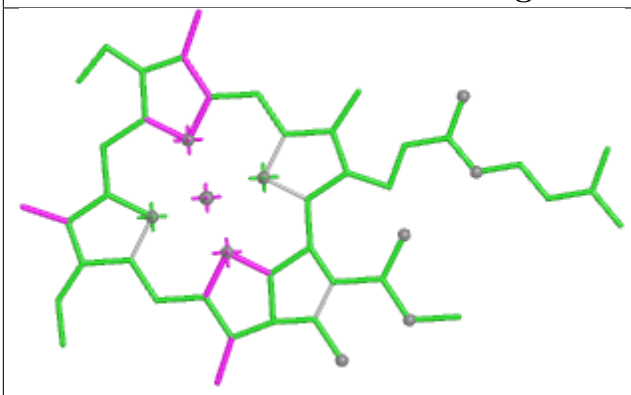


Torsions

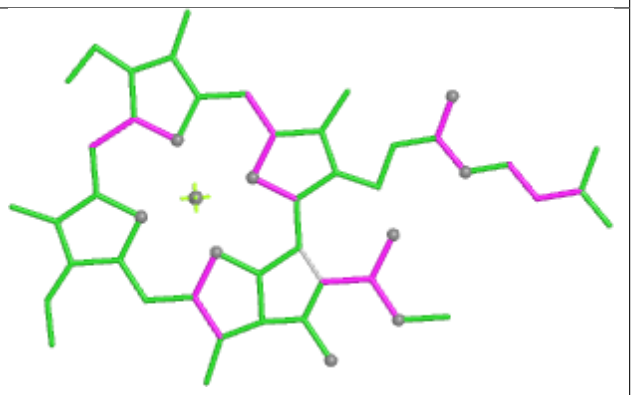


Rings

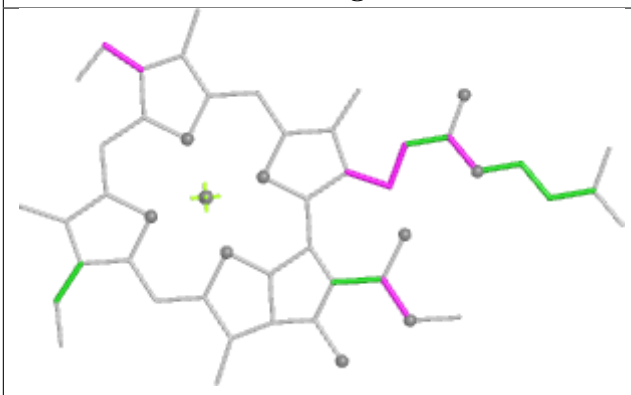
Ligand CLA aA 832



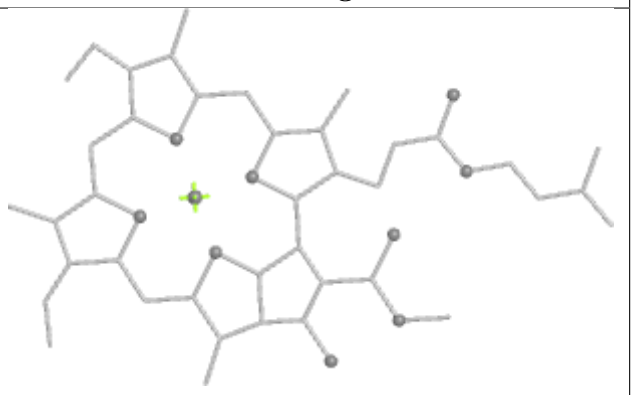
Bond lengths



Bond angles

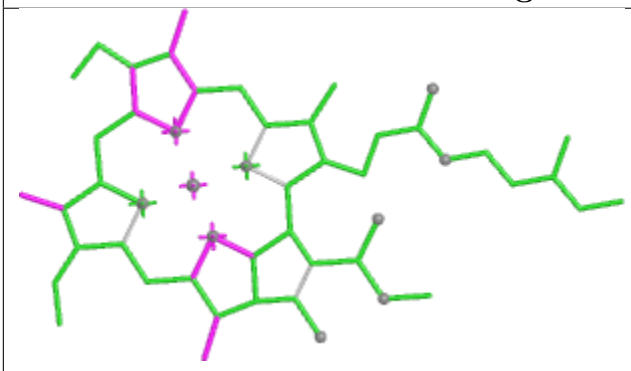


Torsions

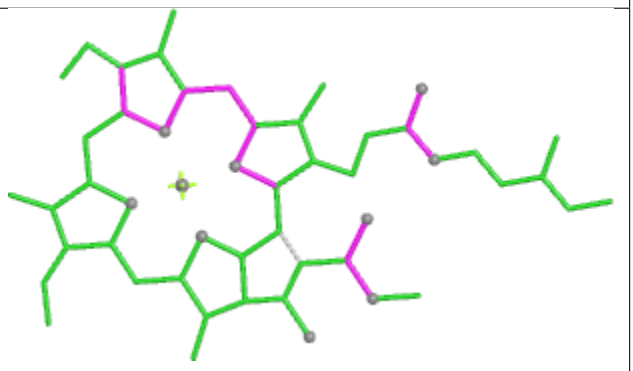


Rings

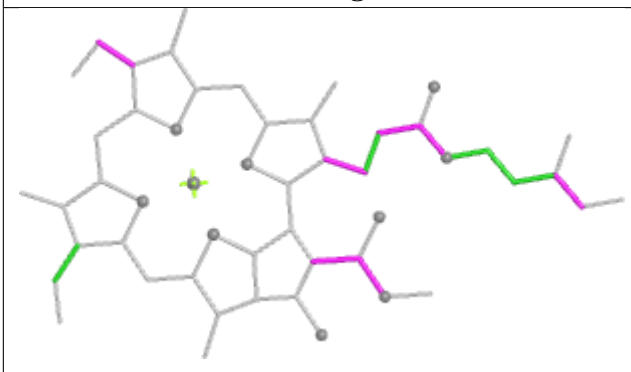
Ligand CLA cA 824



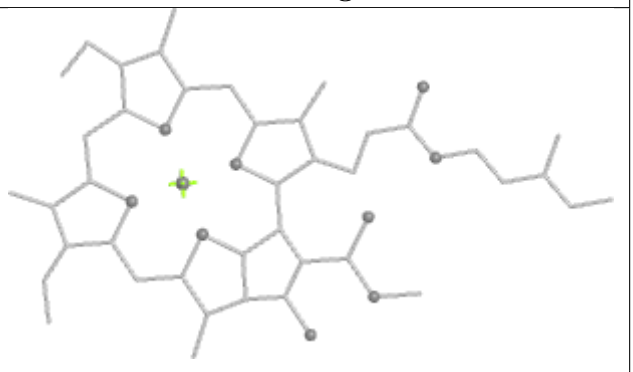
Bond lengths



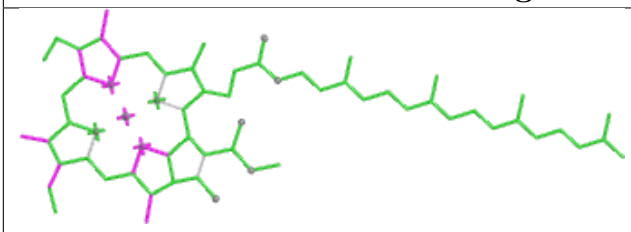
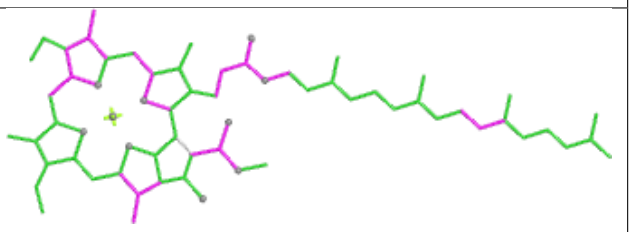
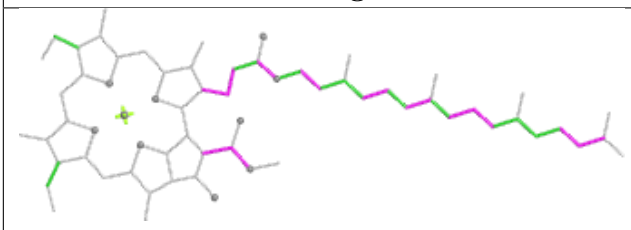
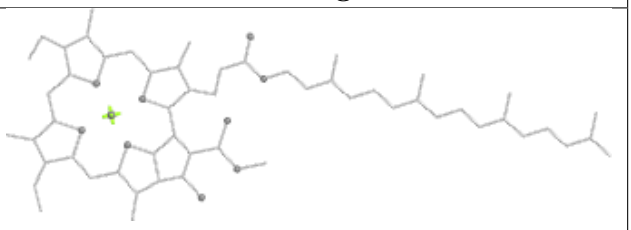
Bond angles



Torsions



Rings

Ligand CLA aA 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

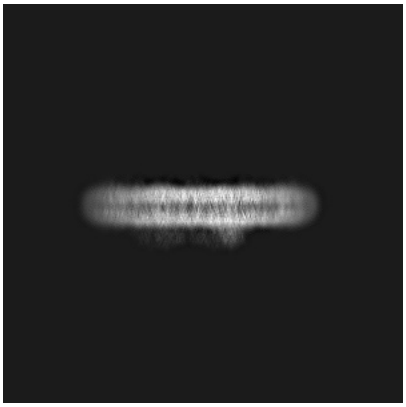
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9908. These allow visual inspection of the internal detail of the map and identification of artifacts.

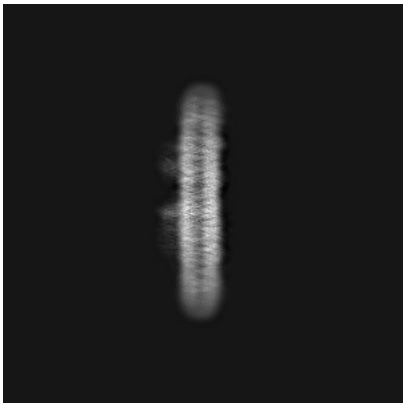
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

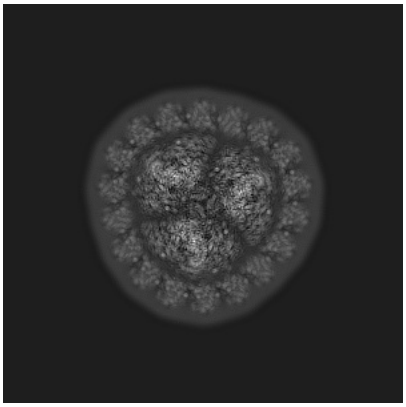
6.1.1 Primary map



X



Y

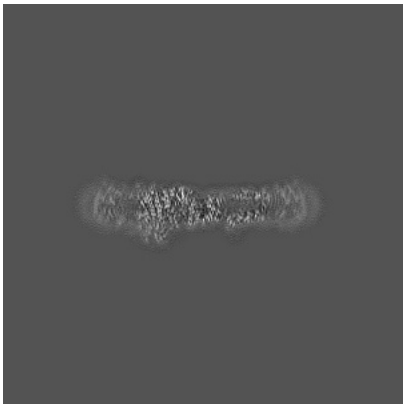


Z

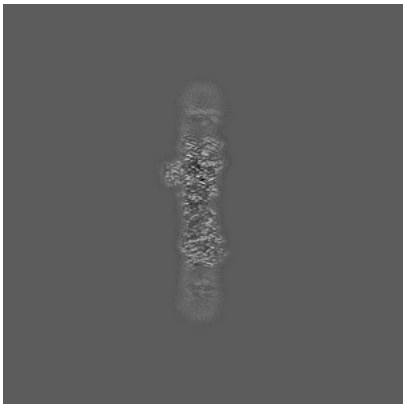
The images above show the map projected in three orthogonal directions.

6.2 Central slices

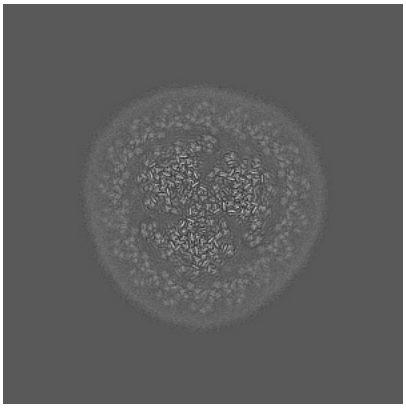
6.2.1 Primary map



X Index: 240



Y Index: 240

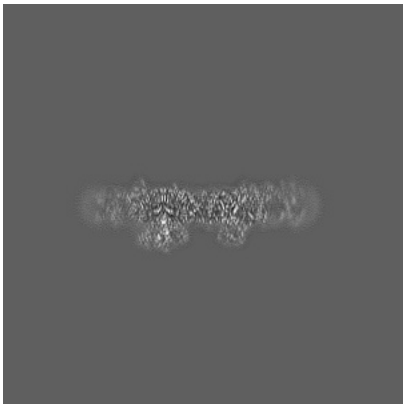


Z Index: 240

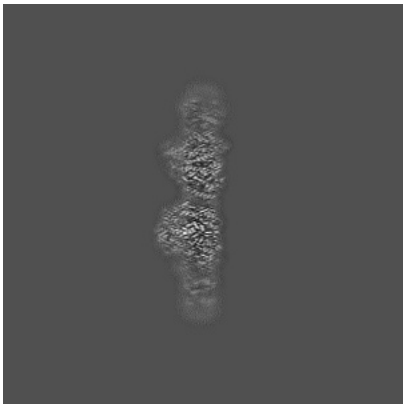
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

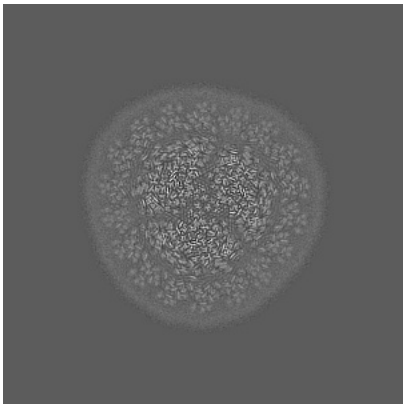
6.3.1 Primary map



X Index: 229



Y Index: 273

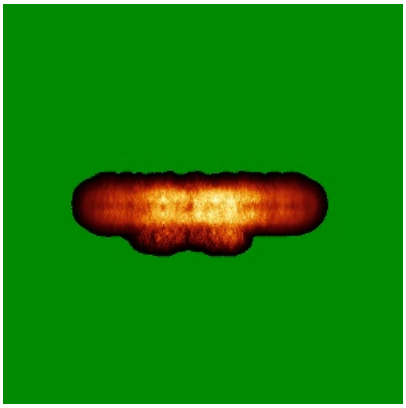


Z Index: 245

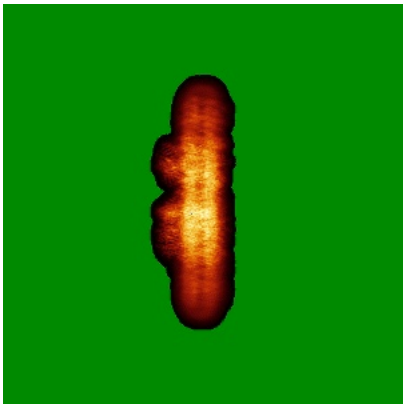
The images above show the largest variance slices of the map in three orthogonal directions.

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

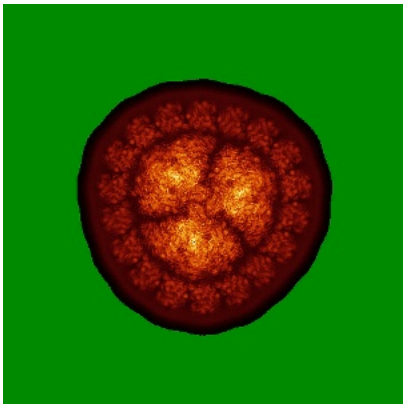
6.4.1 Primary map



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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

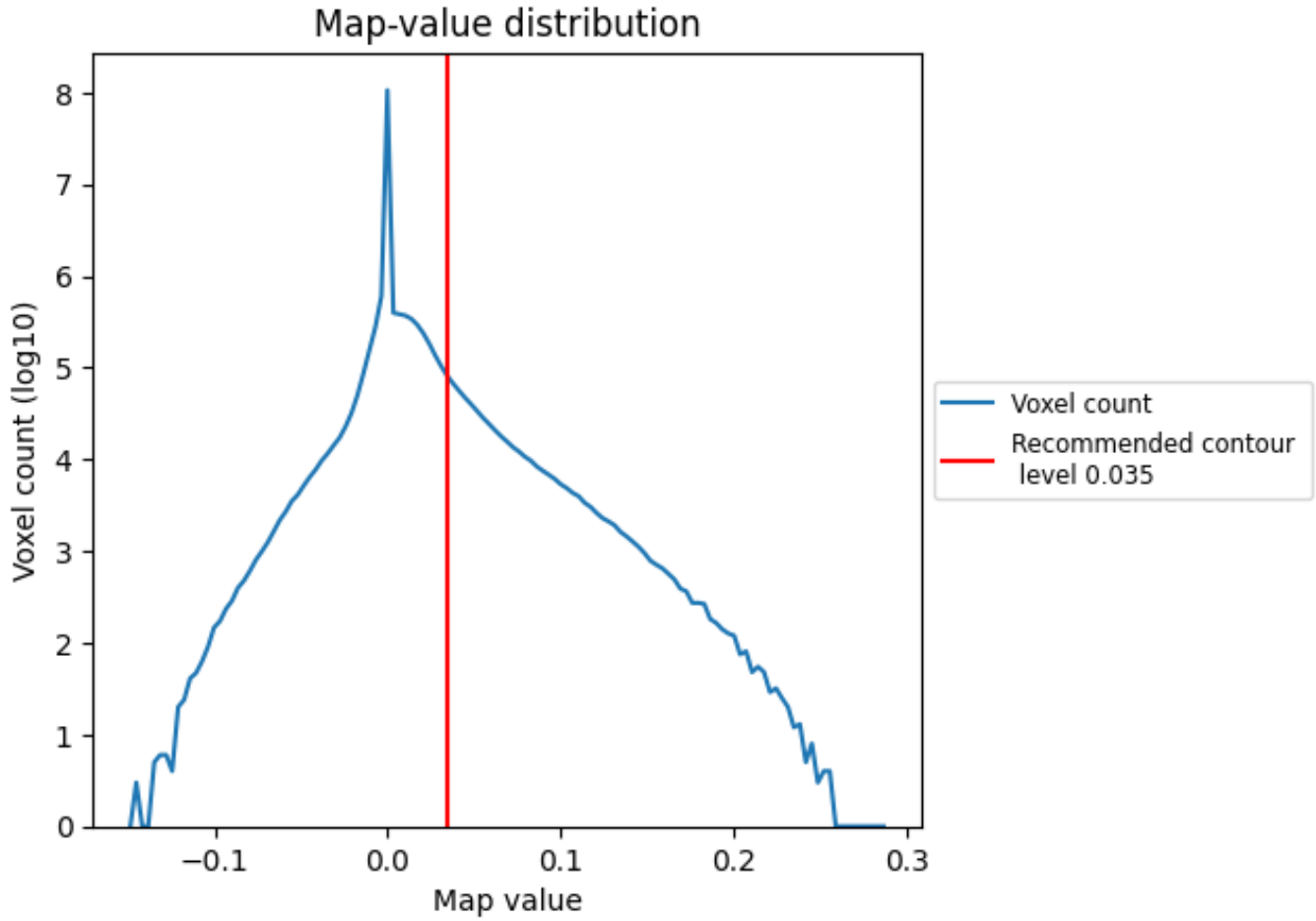
6.6 Mask visualisation (i)

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

7 Map analysis

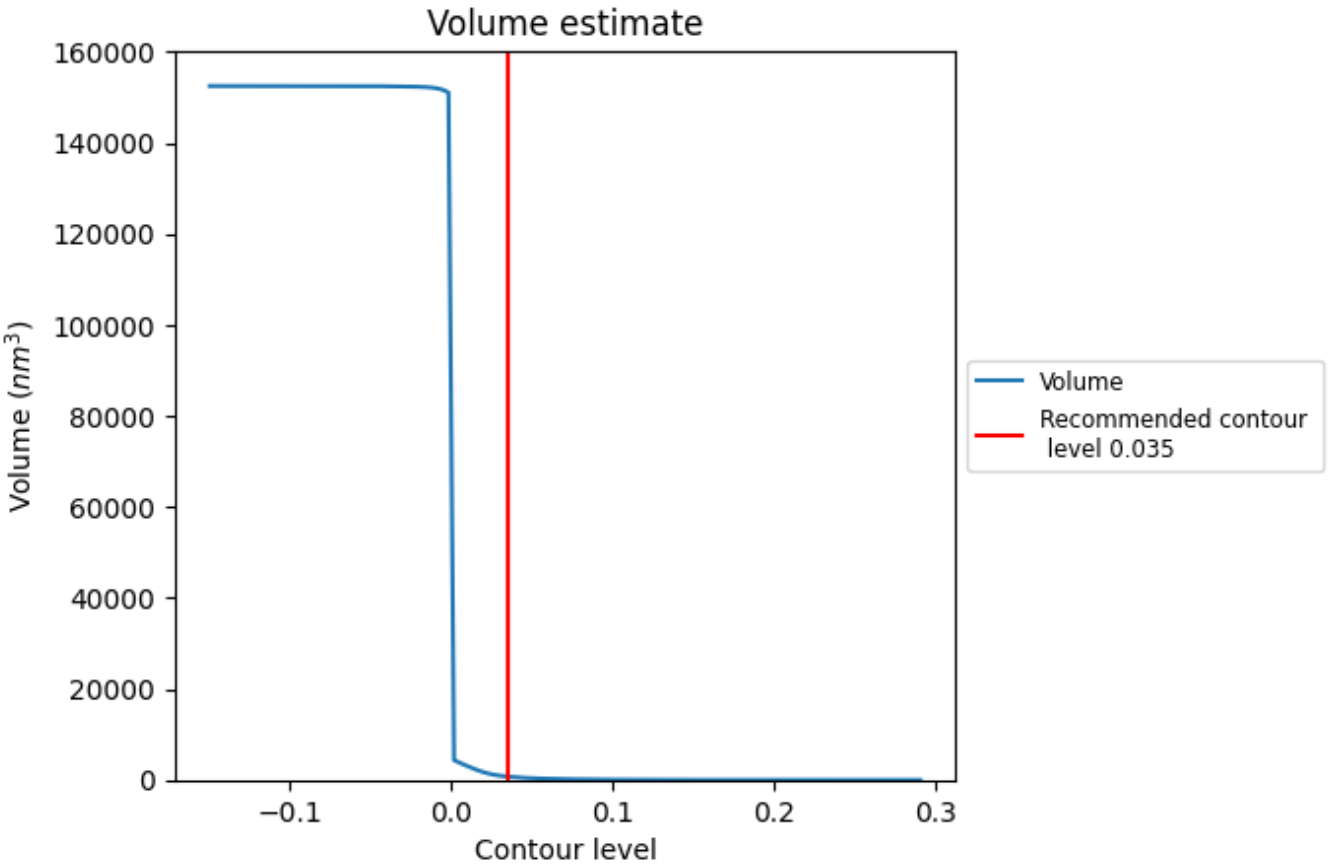
This section contains the results of statistical analysis of the map.

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.

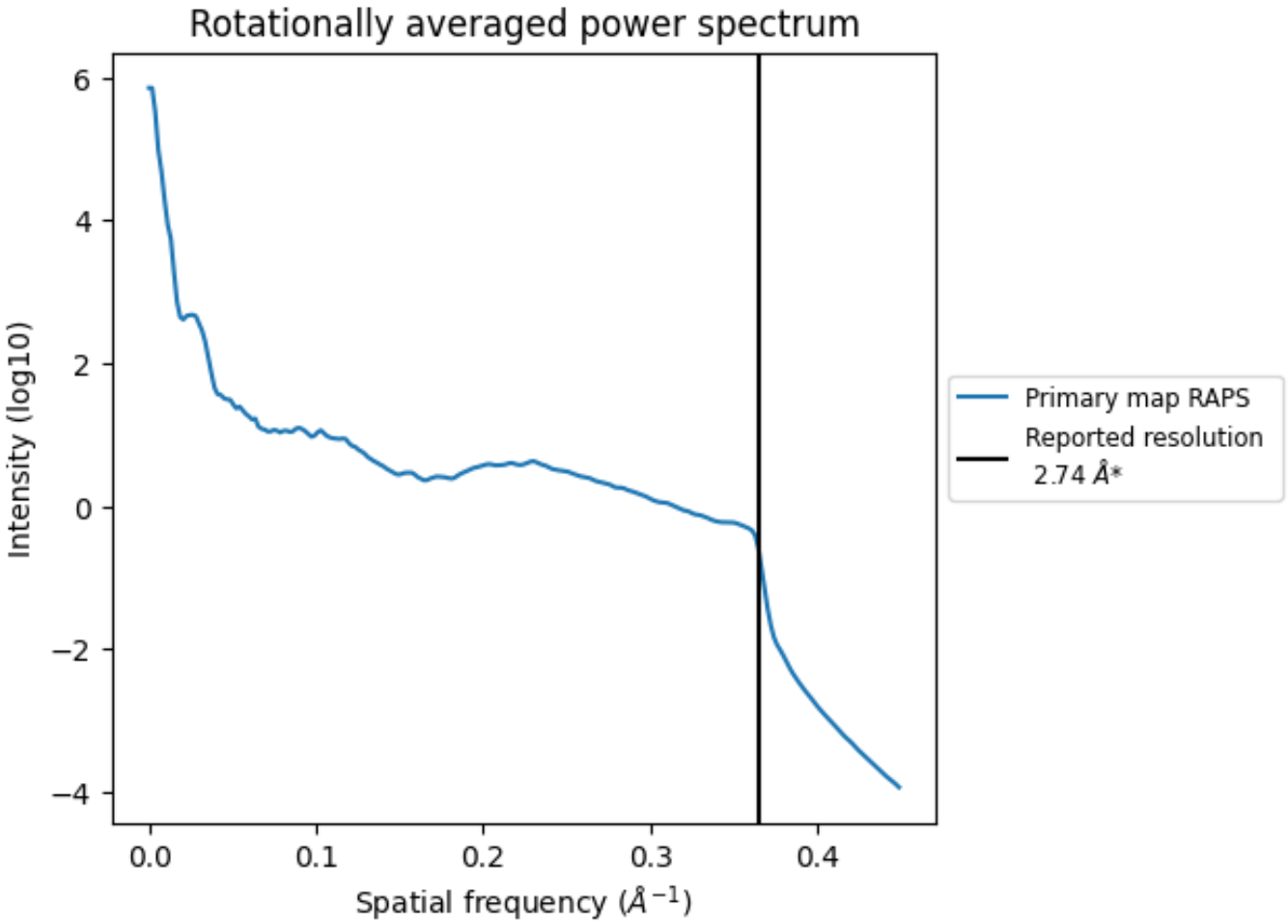
7.2 Volume estimate



The volume at the recommended contour level is 747 nm^3; this corresponds to an approximate mass of 675 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)

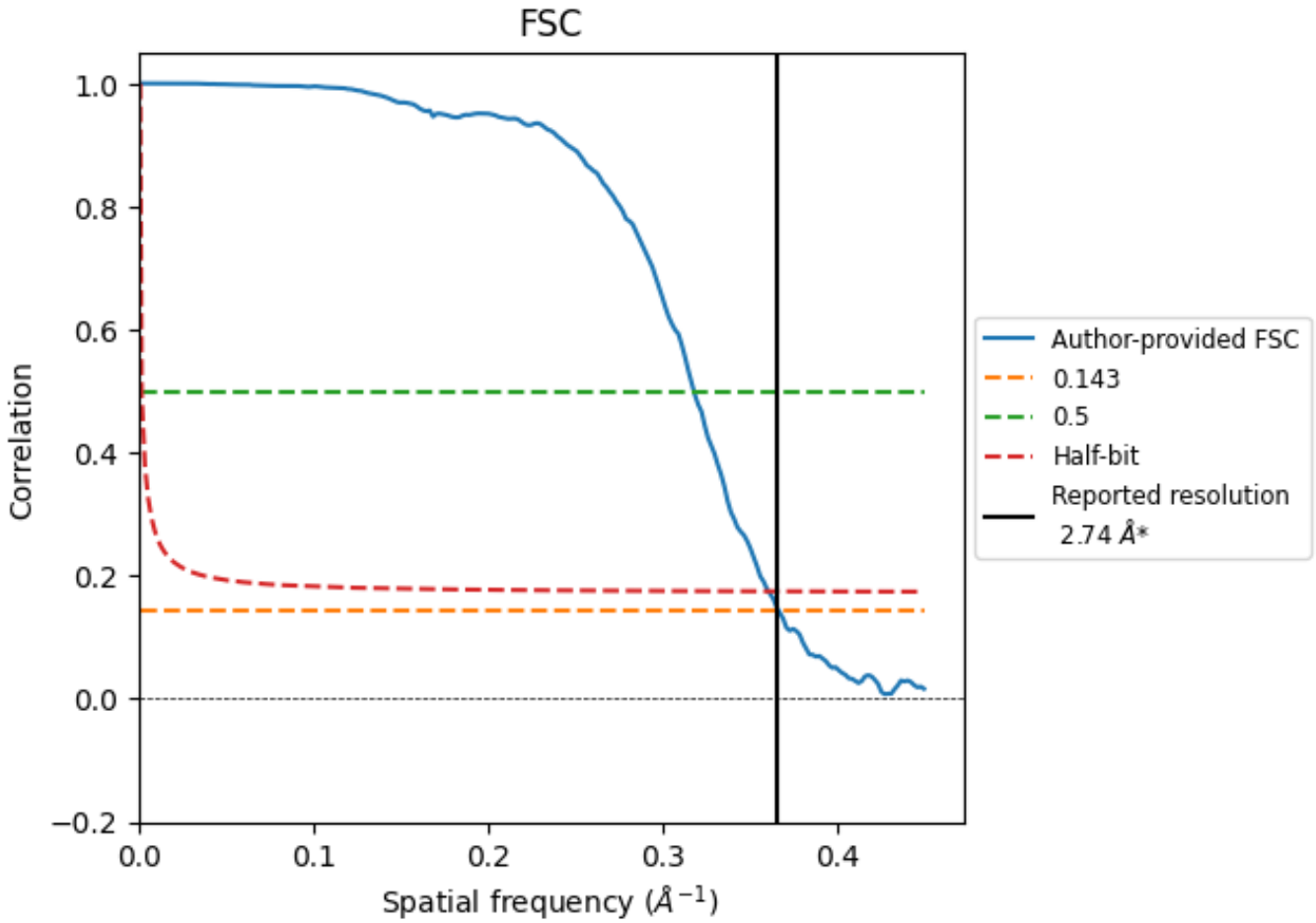


*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8.2 Resolution estimates (i)

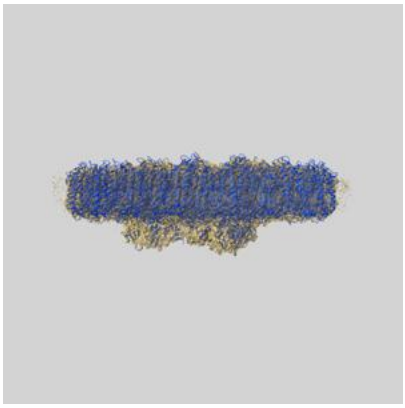
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.15	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

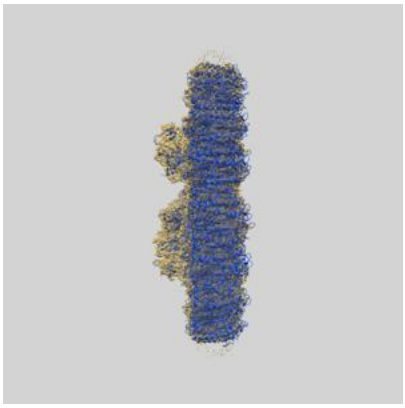
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9908 and PDB model 6K33. Per-residue inclusion information can be found in section 3 on page 50.

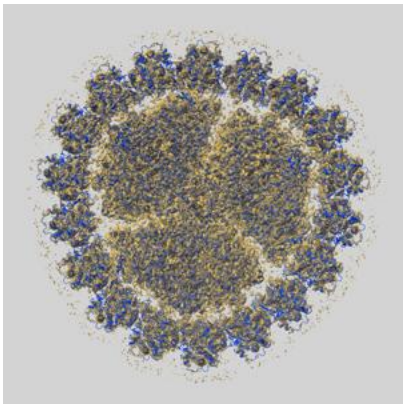
9.1 Map-model overlay



X



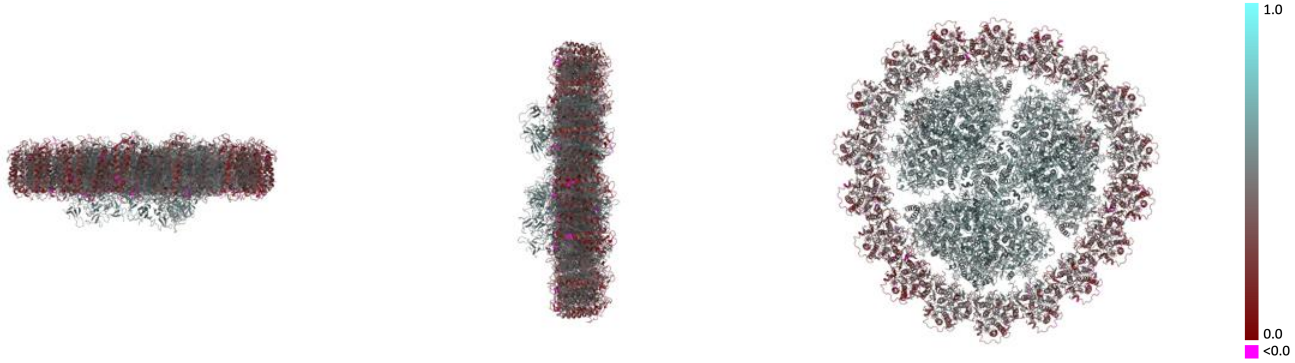
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

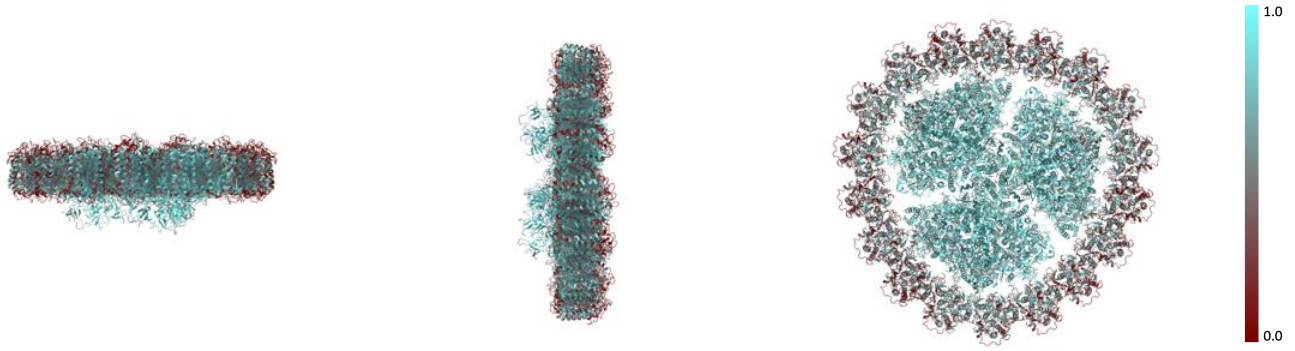
9.2 Q-score mapped to coordinate model



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.

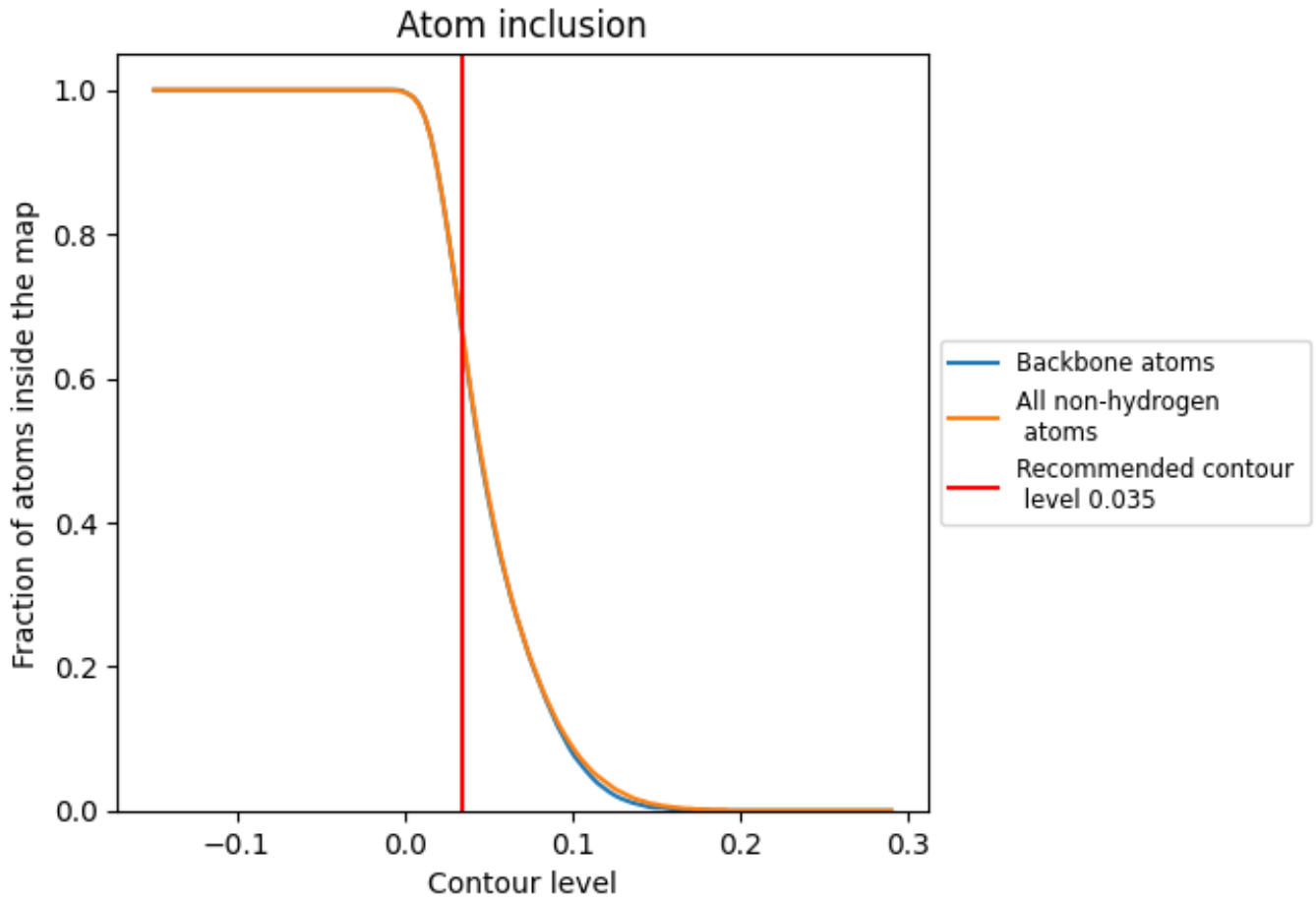
9.3 Atom inclusion mapped to coordinate model



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4450
a1	0.4050	0.2890
a2	0.3810	0.2690
a3	0.5040	0.3620
a4	0.4840	0.3610
a5	0.4290	0.3390
a6	0.3750	0.2970
aA	0.8720	0.5710
aB	0.8890	0.5690
aC	0.9200	0.5550
aD	0.8210	0.5560
aE	0.7720	0.5160
aF	0.7100	0.4700
aI	0.8900	0.5860
aJ	0.8030	0.5310
aK	0.8060	0.4710
aL	0.8830	0.5860
aM	0.8010	0.5490
aX	0.8250	0.5250
b1	0.4030	0.2870
b2	0.3720	0.2590
b3	0.4950	0.3600
b4	0.4810	0.3600
b5	0.4320	0.3380
b6	0.3710	0.2950
bA	0.8710	0.5680
bB	0.8900	0.5680
bC	0.9150	0.5500
bD	0.8220	0.5470
bE	0.7650	0.5100
bF	0.7370	0.5110
bI	0.9020	0.5940
bJ	0.8310	0.5420
bK	0.8190	0.4930
bL	0.8760	0.5850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
bM	0.7910	0.5420
bX	0.8250	0.5140
c1	0.4120	0.2890
c2	0.3680	0.2650
c3	0.4980	0.3590
c4	0.4880	0.3590
c5	0.4310	0.3390
c6	0.3710	0.2990
cA	0.8720	0.5700
cB	0.8870	0.5670
cC	0.9170	0.5510
cD	0.8250	0.5510
cE	0.7820	0.5150
cF	0.6930	0.4520
cI	0.8940	0.5930
cJ	0.8190	0.5400
cK	0.8300	0.4940
cL	0.8880	0.5900
cM	0.8090	0.5490
cX	0.8350	0.5280