Full wwPDB EM Validation Report ⓘ

Nov 9, 2026 – 06:25 PM JST

PDB ID	:	9XNV / pdb_00009xnv
EMDB ID	:	EMD-67061
Title	:	Cryo-EM structure of a PSI supercomplex in the leaves of Hevea brasiliensis
Authors	:	Wang, M.; Yang, Y.; Li, Z.H.; Wang, W.D.; Wang, X.C.
Deposited on	:	2025-11-13
Resolution	:	2.75 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

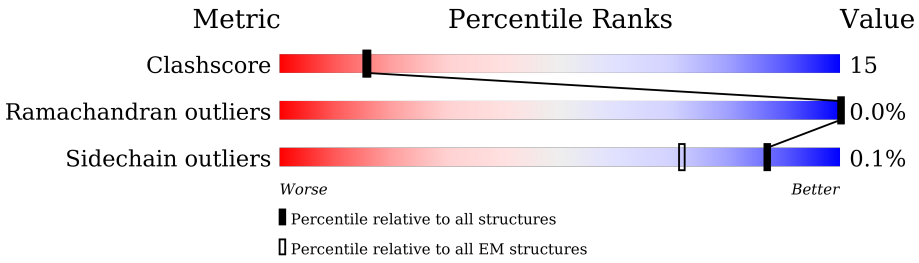
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

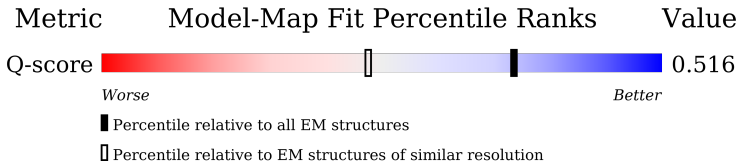
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	10570 (2.25 - 3.25)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	708	74% 26%
1	a	708	75% 25%
2	B	733	79% 21%
2	b	733	79% 21%

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Mol	Chain	Length	Quality of chain
3	C	80	88% 12%
3	c	80	86% 12%
4	D	142	89% 11%
4	d	142	89% 11%
5	E	65	88% 12%
5	e	65	88% 12%
6	H	95	79% 21%
6	h	95	80% 20%
7	I	35	71% 29%
7	i	35	69% 31%
8	L	159	62% 36%
8	l	159	65% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	A	819	-	-	X	-
9	CLA	a	820	-	-	X	-
9	CLA	h	201	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 42578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	708	Total	C	N	O	S	0	0
			5564	3650	944	952	18		
1	a	708	Total	C	N	O	S	0	0
			5564	3650	944	952	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5851	3841	998	999	13		
2	b	733	Total	C	N	O	S	0	0
			5851	3841	998	999	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			617	381	107	118	11		
3	c	80	Total	C	N	O	S	0	0
			617	381	107	118	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1129	726	196	204	3		
4	d	142	Total	C	N	O	S	0	0
			1129	726	196	204	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total 525	C 335	N 92	O 98	0	0
5	e	65	Total 525	C 335	N 92	O 98	0	0

- Molecule 6 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total 727	C 477	N 116	O 134	0	0
6	h	95	Total 727	C 477	N 116	O 134	0	0

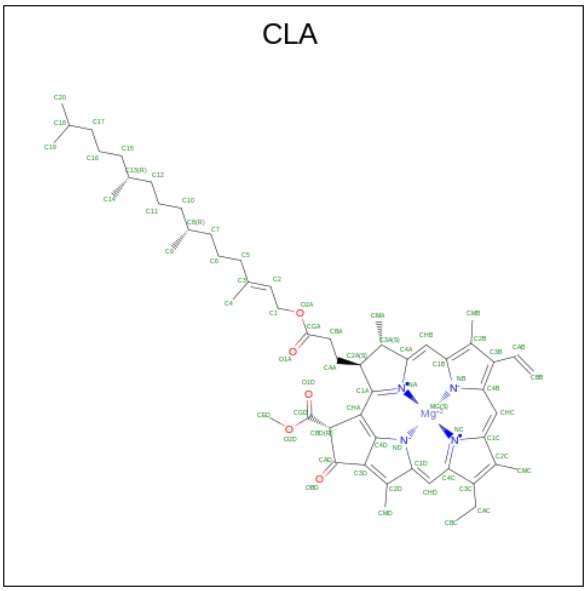
- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total 267	C 181	N 41	O 44	S 1	0	0
7	i	35	Total 267	C 181	N 41	O 44	S 1	0	0

- Molecule 8 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	159	Total 1185	C 782	N 187	O 214	S 2	0	0
8	l	159	Total 1185	C 782	N 187	O 214	S 2	0	0

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
9	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
9	B	1	Total 44	C 34	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
9	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
9	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
9	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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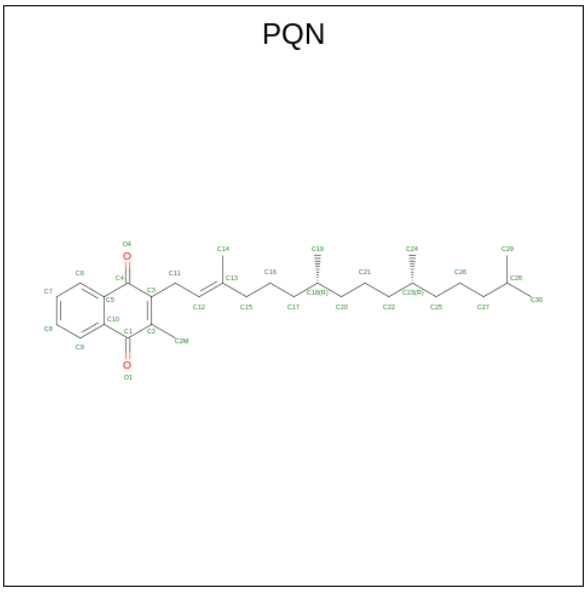
Mol	Chain	Residues	Atoms					AltConf
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			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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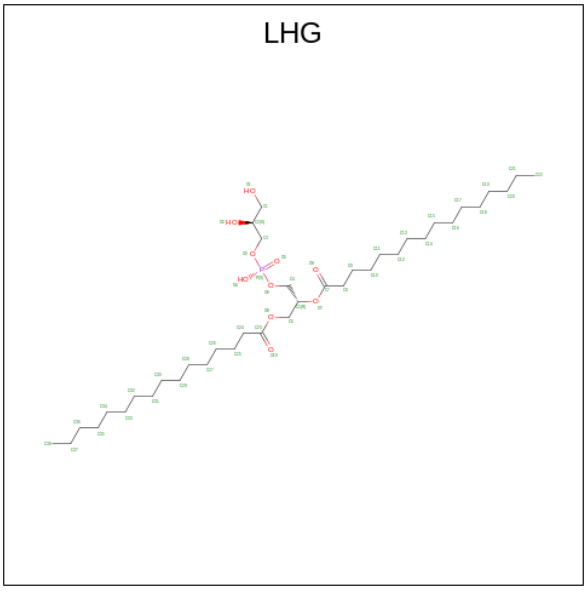
Mol	Chain	Residues	Atoms					AltConf
9	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



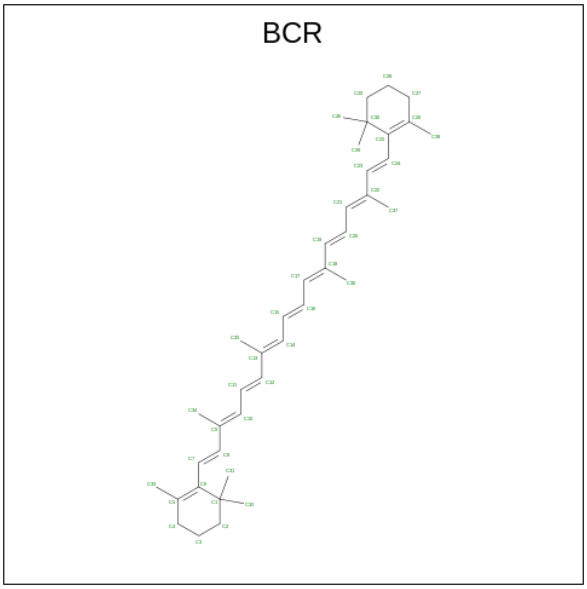
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 33 31 2	0
10	B	1	Total C O 33 31 2	0
10	a	1	Total C O 33 31 2	0
10	b	1	Total C O 33 31 2	0

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	A	1	Total	C	O	P	0
			27	16	10	1	
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	a	1	Total	C	O	P	0
			49	38	10	1	
11	a	1	Total	C	O	P	0
			27	16	10	1	
11	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



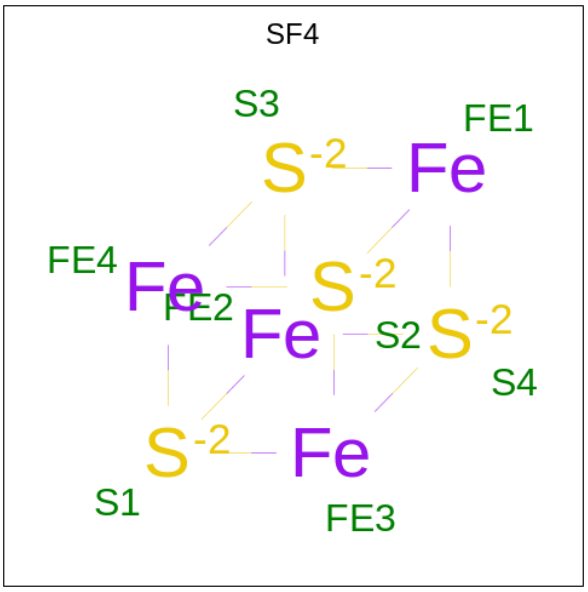
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	

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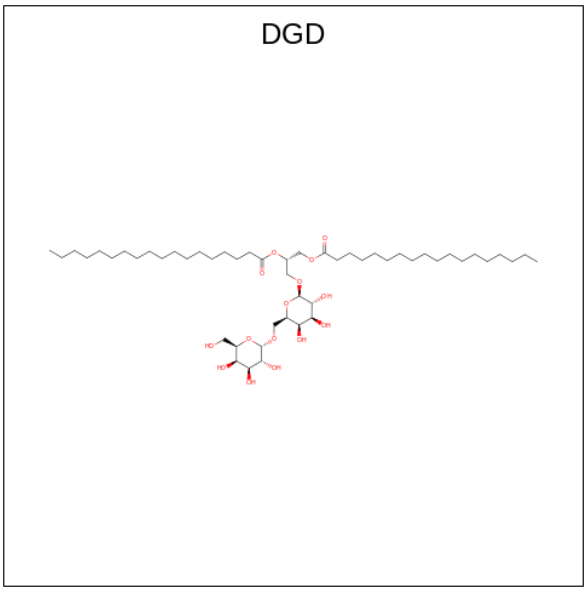
Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	H	1	Total C 40 40	0
12	I	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	h	1	Total C 40 40	0
12	i	1	Total C 40 40	0
12	l	1	Total C 40 40	0
12	l	1	Total C 40 40	0
12	l	1	Total C 40 40	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



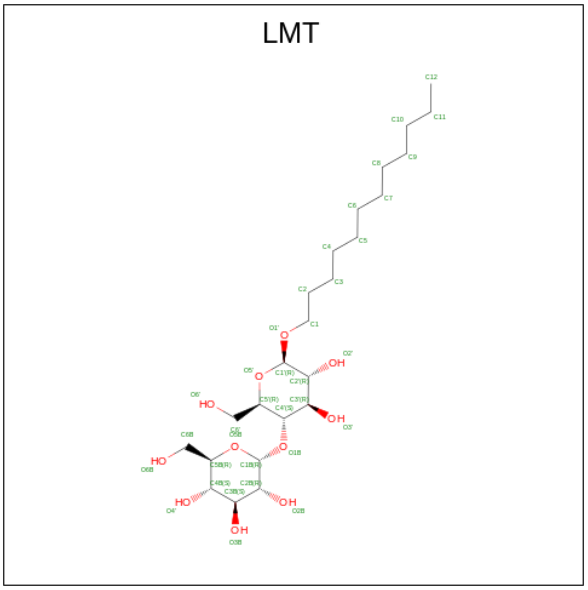
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0
13	a	1	Total Fe S 8 4 4	0
13	c	1	Total Fe S 8 4 4	0
13	c	1	Total Fe S 8 4 4	0

- Molecule 14 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	C	O	0
			66	51	15	
14	b	1	Total	C	O	0
			66	51	15	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			35	24	11	
15	b	1	Total	C	O	0
			35	24	11	

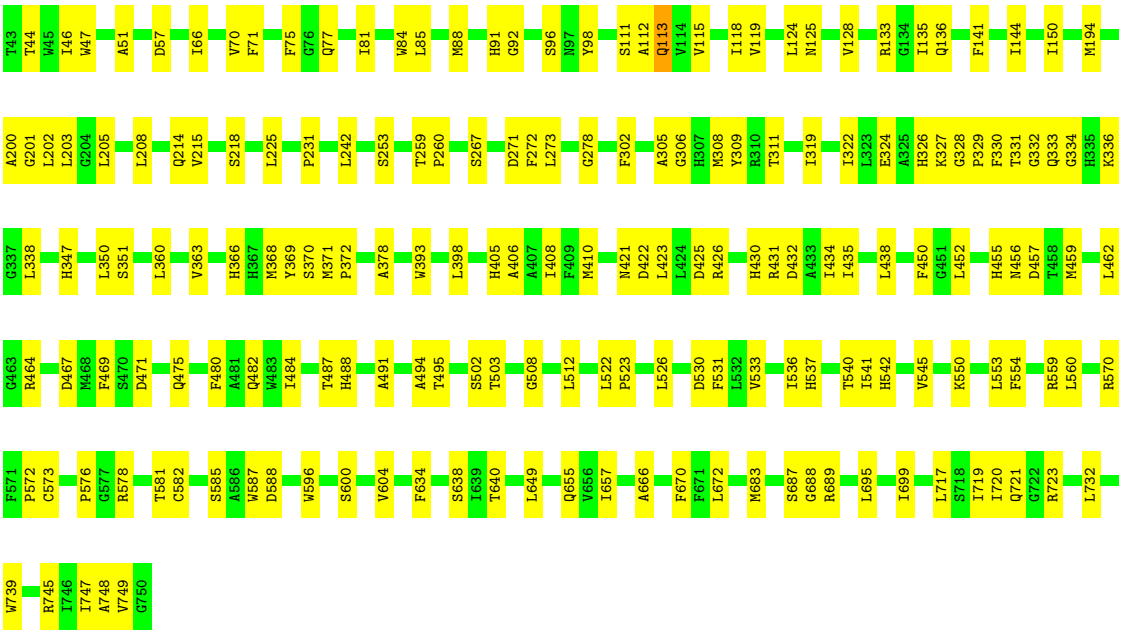
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

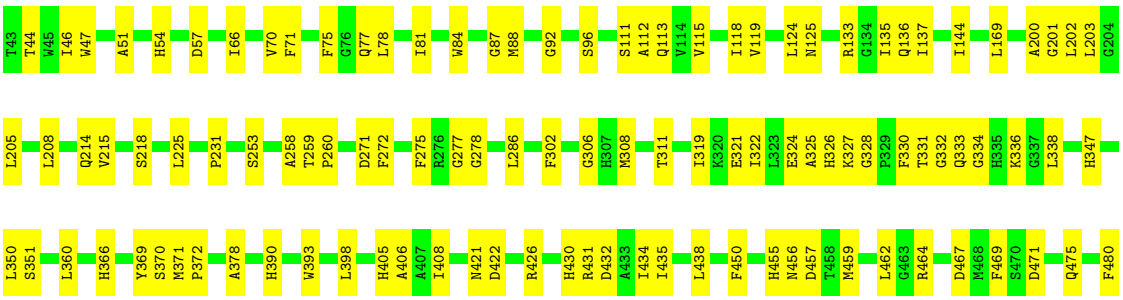


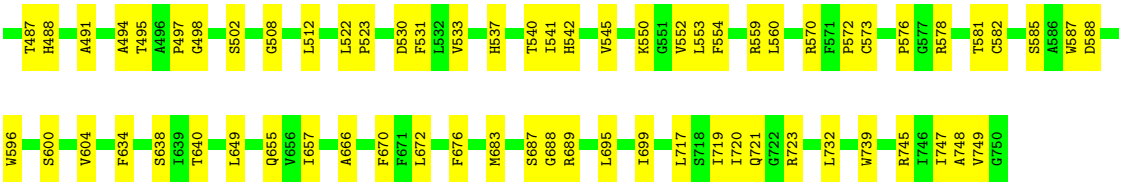


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



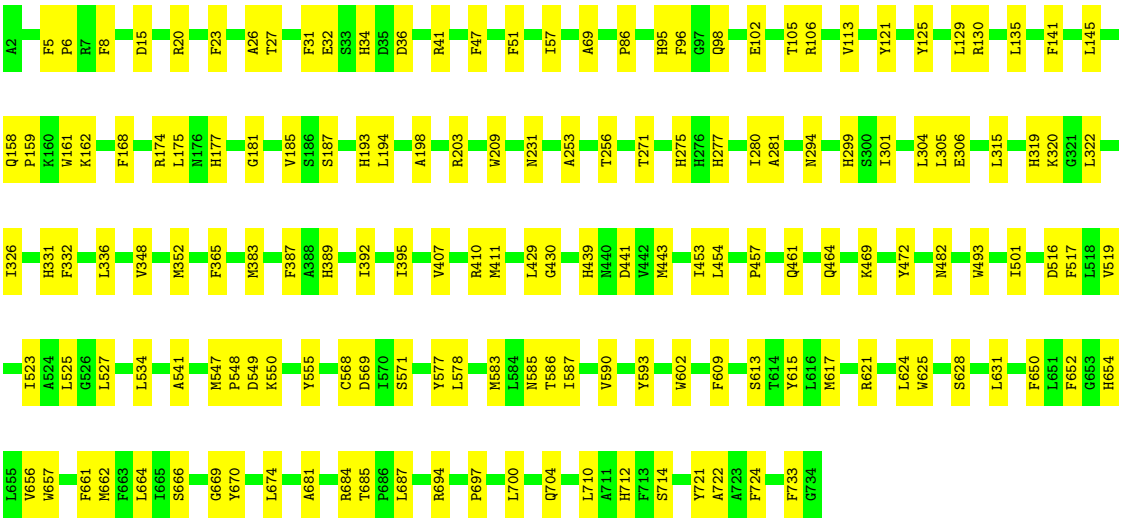




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

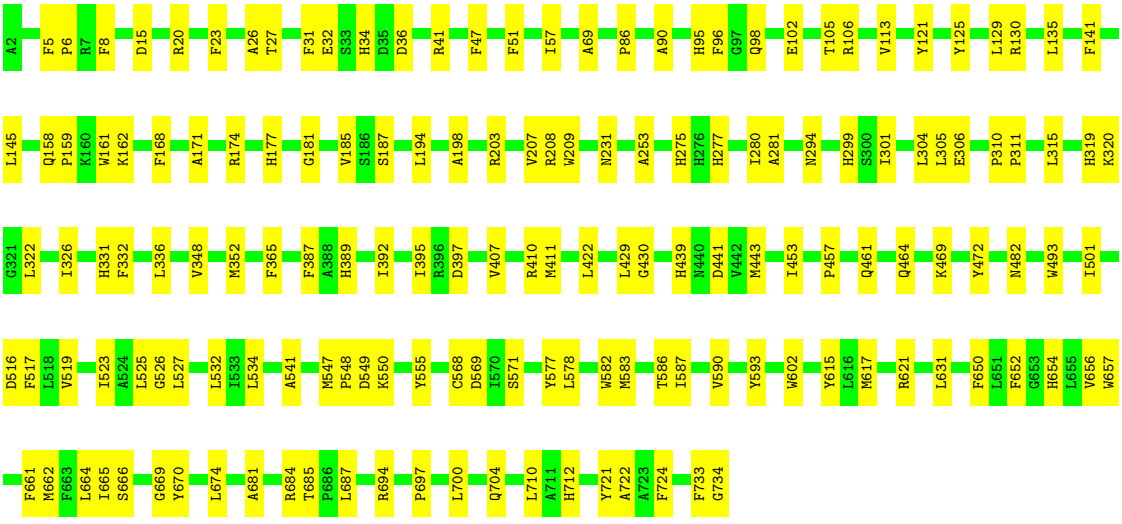




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:





• Molecule 3: Photosystem I iron-sulfur center

Chain C:

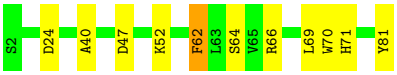




• Molecule 3: Photosystem I iron-sulfur center

Chain c:





• Molecule 4: PsaD

Chain D:

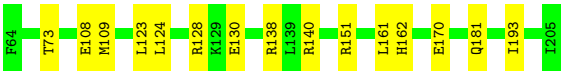




• Molecule 4: PsaD

Chain d:

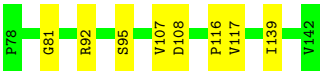




• Molecule 5: PsaE

Chain E:

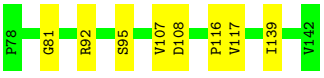




• Molecule 5: PsaE

Chain e:

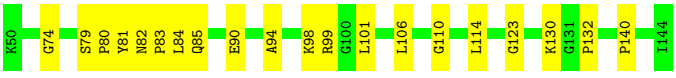




• Molecule 6: PsaH

Chain H:

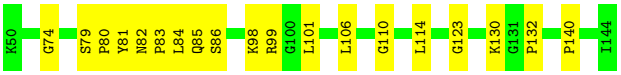




• Molecule 6: PsaH

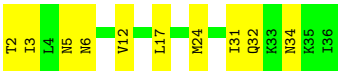
Chain h:





• Molecule 7: Photosystem I reaction center subunit VIII





• Molecule 7: Photosystem I reaction center subunit VIII

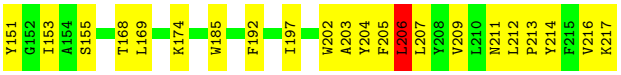




• Molecule 8: PsaL

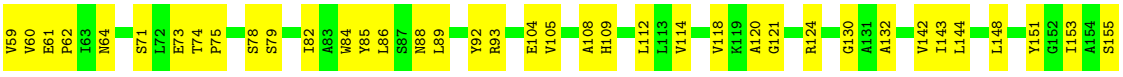






• Molecule 8: PsaL







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3309024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.526	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0614	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, BCR, LHG, SF4, PQN, LMT, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.16	0/5754	0.31	0/7852
1	a	0.13	0/5754	0.29	0/7852
2	B	0.13	0/6063	0.28	0/8280
2	b	0.13	0/6063	0.28	0/8280
3	C	0.11	0/630	0.30	0/853
3	c	0.23	0/630	0.59	3/853 (0.4%)
4	D	0.09	0/1159	0.24	0/1565
4	d	0.10	0/1159	0.25	0/1565
5	E	0.08	0/537	0.21	0/728
5	e	0.09	0/537	0.20	0/728
6	H	0.18	0/748	0.33	0/1014
6	h	0.18	0/748	0.34	0/1014
7	I	0.18	0/272	0.31	0/371
7	i	0.18	0/272	0.31	0/371
8	L	0.32	1/1218 (0.1%)	0.60	1/1664 (0.1%)
8	l	0.19	0/1218	0.54	3/1664 (0.2%)
All	All	0.15	1/32762 (0.0%)	0.33	7/44654 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	L	0	2
8	l	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	206	LEU	C-N	5.78	1.42	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	l	211	ASN	CA-C-N	-8.23	110.17	121.61
8	l	211	ASN	C-N-CA	-8.23	110.17	121.61
3	c	62	PHE	N-CA-CB	7.33	122.88	110.49
3	c	62	PHE	CA-CB-CG	-7.14	106.66	113.80
8	L	84	TRP	CA-CB-CG	7.05	127.00	113.60
3	c	64	SER	N-CA-C	-5.76	105.92	113.12
8	l	210	LEU	CA-CB-CG	5.49	135.52	116.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	L	206	LEU	Peptide,Mainchain
8	l	209	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5564	0	5418	174	0
1	a	5564	0	5417	182	0
2	B	5851	0	5636	123	0
2	b	5851	0	5636	121	0
3	C	617	0	592	9	0
3	c	617	0	592	9	0
4	D	1129	0	1134	11	0
4	d	1129	0	1134	10	0
5	E	525	0	526	4	0
5	e	525	0	526	4	0
6	H	727	0	734	42	0
6	h	727	0	734	31	0
7	I	267	0	296	10	0
7	i	267	0	296	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	1185	0	1199	69	0
8	l	1185	0	1199	69	0
9	A	2285	0	2317	225	0
9	B	1966	0	1928	86	0
9	H	65	0	72	3	0
9	L	261	0	210	40	0
9	a	2336	0	2387	238	0
9	b	1966	0	1928	90	0
9	h	116	0	109	42	0
9	l	261	0	226	35	0
10	A	33	0	46	6	0
10	B	33	0	46	2	0
10	a	33	0	46	5	0
10	b	33	0	46	2	0
11	A	125	0	172	9	0
11	a	76	0	98	5	0
11	l	49	0	74	4	0
12	A	160	0	224	12	0
12	B	120	0	168	11	0
12	H	40	0	56	3	0
12	I	40	0	56	1	0
12	L	120	0	168	11	0
12	a	160	0	224	22	0
12	b	120	0	168	12	0
12	h	40	0	56	2	0
12	i	40	0	56	1	0
12	l	120	0	168	12	0
13	A	8	0	0	0	0
13	C	16	0	0	0	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	B	66	0	96	8	0
14	b	66	0	96	6	0
15	B	35	0	46	5	0
15	b	35	0	46	5	0
All	All	42578	0	42402	1243	0

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

All (1243) 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)
9:L:307:CLA:HMD1	1:a:275:PHE:CD2	1.27	1.62
9:L:307:CLA:CMD	1:a:275:PHE:CD2	1.79	1.59
9:L:307:CLA:HMD3	1:a:275:PHE:CE2	1.39	1.57
9:A:819:CLA:CBB	9:A:821:CLA:CMA	1.84	1.52
1:A:322:ILE:HG21	9:A:819:CLA:CGA	1.45	1.44
9:A:819:CLA:CBB	9:A:821:CLA:HMA3	0.94	1.39
1:A:322:ILE:CG2	9:A:819:CLA:O1A	1.71	1.37
9:A:819:CLA:CAB	9:A:821:CLA:HMA3	1.61	1.30
9:L:307:CLA:CMD	1:a:275:PHE:CE2	2.03	1.30
9:A:819:CLA:H141	9:h:201:CLA:CBC	1.63	1.29
1:A:322:ILE:HD13	9:A:819:CLA:O2A	1.24	1.29
1:A:322:ILE:CD1	9:A:819:CLA:O2A	1.90	1.18
9:A:819:CLA:H143	9:A:820:CLA:HAA2	1.22	1.15
1:A:322:ILE:HG21	9:A:819:CLA:O1A	0.97	1.13
9:A:819:CLA:C14	9:A:820:CLA:HAA2	1.80	1.10
9:A:819:CLA:C14	9:h:201:CLA:CBC	2.30	1.10
9:A:819:CLA:H52	9:A:821:CLA:HMC2	1.23	1.09
9:A:819:CLA:HBB2	9:A:821:CLA:CMA	1.63	1.06
9:A:819:CLA:H143	9:A:820:CLA:CAA	1.87	1.04
1:A:319:ILE:HA	9:A:819:CLA:H12	1.36	1.02
9:A:819:CLA:HBB2	9:A:821:CLA:HMA3	1.04	1.01
9:L:307:CLA:HMD3	1:a:275:PHE:CD2	1.67	1.01
9:A:819:CLA:H141	9:h:201:CLA:CAC	1.94	0.96
9:A:819:CLA:C14	9:h:201:CLA:HBC1	1.95	0.95
1:A:319:ILE:HG23	9:A:819:CLA:C3	1.94	0.94
9:A:819:CLA:H141	9:h:201:CLA:HBC1	1.50	0.93
9:A:819:CLA:OBD	9:A:819:CLA:H171	1.67	0.93
6:H:83:PRO:HD3	9:a:820:CLA:HAA1	1.51	0.93
6:H:85:GLN:HB2	9:a:820:CLA:H52	1.52	0.92
9:A:819:CLA:HBB1	9:A:823:CLA:H72	1.51	0.92
9:L:307:CLA:HMD3	1:a:275:PHE:CZ	2.06	0.90
9:A:819:CLA:C14	9:A:820:CLA:CAA	2.48	0.90
9:A:819:CLA:C5	9:A:821:CLA:HMC2	2.00	0.90
9:A:819:CLA:HBB1	9:A:823:CLA:C7	2.04	0.89
1:a:326:HIS:HE1	9:a:820:CLA:C4D	1.85	0.89
2:b:517:PHE:HA	9:b:829:CLA:HED1	1.55	0.88
9:A:819:CLA:C14	9:h:201:CLA:HBC2	2.03	0.88
9:A:819:CLA:H52	9:A:821:CLA:CMC	2.06	0.84
1:A:322:ILE:HD13	9:A:819:CLA:CGA	2.07	0.83
9:A:819:CLA:H141	9:h:201:CLA:HAC2	1.58	0.83
9:A:808:CLA:HBB2	9:A:811:CLA:HMA3	1.59	0.83
1:A:322:ILE:CG2	9:A:819:CLA:CGA	2.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:PHE:HA	9:B:829:CLA:HED1	1.62	0.82
8:L:100:LEU:HD13	9:a:820:CLA:H2	1.61	0.82
9:A:819:CLA:HBB1	9:A:823:CLA:C8	2.10	0.81
6:h:82:ASN:HA	9:h:201:CLA:C4D	2.11	0.81
9:a:808:CLA:HBB2	9:a:811:CLA:HMA3	1.62	0.80
1:A:322:ILE:HD12	9:A:819:CLA:H12	1.64	0.79
1:a:322:ILE:HG12	9:a:820:CLA:CAD	2.11	0.79
2:b:453:ILE:HG23	15:b:838:LMT:H1B	1.63	0.79
6:H:79:SER:HB3	9:a:820:CLA:HBA1	1.65	0.78
9:L:307:CLA:C3C	1:a:497:PRO:CD	2.35	0.78
9:A:808:CLA:H51	9:A:810:CLA:H2	1.63	0.78
1:a:550:LYS:NZ	2:b:670:TYR:O	2.16	0.78
1:A:322:ILE:HD12	9:A:819:CLA:C1	2.12	0.78
9:A:819:CLA:HBB2	9:A:821:CLA:HMA2	1.63	0.78
2:B:453:ILE:HG23	15:B:838:LMT:H1B	1.66	0.78
9:a:834:CLA:H201	12:a:843:BCR:H10C	1.64	0.78
6:h:82:ASN:HA	9:h:201:CLA:CHA	2.14	0.78
9:A:830:CLA:CHD	8:l:212:LEU:HD22	2.14	0.77
1:a:325:ALA:HB1	9:a:820:CLA:H2A	1.67	0.77
6:H:83:PRO:CD	9:a:820:CLA:HBD	2.15	0.77
1:a:393:TRP:CD1	9:a:825:CLA:HAB	2.19	0.77
1:A:672:LEU:HD11	2:B:617:MET:HB2	1.65	0.77
1:a:326:HIS:CE1	9:a:820:CLA:C4D	2.68	0.77
9:A:830:CLA:HBC2	8:l:212:LEU:HD13	1.66	0.76
9:L:307:CLA:HMD1	1:a:275:PHE:HD2	0.96	0.76
1:a:672:LEU:HD11	2:b:617:MET:HB2	1.67	0.76
1:A:91:HIS:HE1	1:A:113:GLN:HG2	1.51	0.76
1:A:322:ILE:CD1	9:A:819:CLA:C1	2.64	0.75
1:A:96:SER:HA	1:A:112:ALA:HB3	1.67	0.75
6:h:82:ASN:H	9:h:201:CLA:H51	1.52	0.75
1:A:322:ILE:HG22	9:A:819:CLA:O1A	1.84	0.74
1:A:550:LYS:NZ	2:B:670:TYR:O	2.16	0.74
1:a:322:ILE:HG23	9:a:820:CLA:C2D	2.18	0.74
1:A:319:ILE:HA	9:A:819:CLA:C1	2.15	0.73
1:A:393:TRP:CD1	9:A:824:CLA:HAB	2.23	0.73
9:A:817:CLA:H142	9:A:819:CLA:HMC3	1.69	0.73
9:L:308:CLA:C3C	9:a:820:CLA:HMB3	2.18	0.73
9:a:820:CLA:HBC3	9:a:820:CLA:HHD	1.68	0.73
9:L:307:CLA:CMD	1:a:275:PHE:CG	2.67	0.73
1:a:739:TRP:HB2	9:a:825:CLA:HBB1	1.69	0.73
8:l:84:TRP:HB3	9:l:302:CLA:HAA2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:819:CLA:HBB1	9:A:823:CLA:H8	1.69	0.73
1:a:322:ILE:HG23	9:a:820:CLA:C3D	2.19	0.72
9:A:830:CLA:HHD	8:l:212:LEU:HD22	1.71	0.72
9:B:822:CLA:HAB	9:B:827:CLA:H3A	1.71	0.72
2:B:275:HIS:HD1	9:B:818:CLA:HAB	1.55	0.72
6:H:83:PRO:CD	9:a:820:CLA:HAA1	2.20	0.71
9:a:805:CLA:H11	9:a:827:CLA:HBA1	1.72	0.71
9:A:819:CLA:H41	9:A:821:CLA:HAC1	1.72	0.71
9:A:819:CLA:H142	9:h:201:CLA:HBC2	1.73	0.71
2:b:294:ASN:HB3	2:b:299:HIS:HA	1.72	0.71
2:B:294:ASN:HB3	2:B:299:HIS:HA	1.72	0.71
9:a:807:CLA:H11	9:a:825:CLA:H92	1.73	0.70
1:A:739:TRP:HB2	9:A:824:CLA:HBB1	1.72	0.70
4:D:106:ILE:HG12	4:D:116:ILE:HG12	1.74	0.70
1:a:96:SER:HA	1:a:112:ALA:HB3	1.72	0.70
9:A:805:CLA:H11	9:A:826:CLA:HBA1	1.72	0.70
1:A:531:PHE:HA	9:A:832:CLA:HED1	1.72	0.70
8:L:100:LEU:HD13	9:a:820:CLA:C2	2.21	0.70
1:A:330:PHE:O	1:A:426:ARG:NE	2.25	0.70
1:A:508:GLY:HA2	1:A:523:PRO:HB3	1.73	0.69
1:a:326:HIS:HE1	9:a:820:CLA:ND	1.84	0.69
1:a:326:HIS:CD2	9:a:820:CLA:NB	2.60	0.69
1:a:508:GLY:HA2	1:a:523:PRO:HB3	1.72	0.69
2:b:397:ASP:HA	4:d:193:ILE:HD13	1.74	0.69
8:l:209:VAL:HG23	9:l:301:CLA:HAC2	1.74	0.69
9:A:829:CLA:HMA2	8:L:120:ALA:HB1	1.73	0.69
8:L:100:LEU:HD22	9:a:820:CLA:H42	1.74	0.69
1:a:531:PHE:HA	9:a:833:CLA:HED1	1.75	0.69
1:A:302:PHE:HE1	9:A:819:CLA:HAC1	1.58	0.68
2:B:687:LEU:HD21	8:L:89:LEU:HD23	1.75	0.68
6:h:85:GLN:HB2	9:h:201:CLA:H52	1.76	0.68
1:A:689:ARG:H	2:B:568:CYS:HB2	1.58	0.68
9:L:307:CLA:C2D	1:a:275:PHE:CE2	2.76	0.68
1:a:371:MET:HE1	9:a:824:CLA:HAB	1.74	0.68
1:A:205:LEU:HB3	12:A:841:BCR:H20C	1.76	0.68
1:a:366:HIS:HA	1:a:369:TYR:CE2	2.29	0.68
6:H:80:PRO:O	9:a:820:CLA:C2B	2.41	0.68
9:b:822:CLA:HAB	9:b:827:CLA:H3A	1.76	0.68
1:a:689:ARG:H	2:b:568:CYS:HB2	1.58	0.67
2:B:305:LEU:HD13	2:B:322:LEU:HB3	1.77	0.67
2:b:733:PHE:HD2	6:h:140:PRO:HG2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:125:ASN:HB3	1:a:133:ARG:HB3	1.75	0.67
2:b:181:GLY:HA2	2:b:185:VAL:HB	1.77	0.67
1:A:309:TYR:HE1	9:A:819:CLA:H2	1.60	0.67
1:A:326:HIS:HA	9:l:302:CLA:HMC2	1.75	0.67
12:H:202:BCR:H24C	8:L:202:TRP:HE1	1.60	0.67
1:a:111:SER:HB2	1:a:137:ILE:H	1.58	0.67
1:A:208:LEU:HD21	12:A:840:BCR:HC42	1.77	0.66
1:A:366:HIS:HA	1:A:369:TYR:CE2	2.30	0.66
6:H:83:PRO:HD2	9:a:820:CLA:HBD	1.77	0.66
2:b:275:HIS:HD1	9:b:818:CLA:HAB	1.60	0.66
9:A:803:CLA:HBA2	9:A:809:CLA:H62	1.77	0.66
2:b:305:LEU:HD13	2:b:322:LEU:HB3	1.77	0.66
1:A:488:HIS:CD2	9:A:830:CLA:C1D	2.78	0.66
2:B:181:GLY:HA2	2:B:185:VAL:HB	1.78	0.66
2:B:733:PHE:HD2	6:H:140:PRO:HG2	1.59	0.66
8:L:203:ALA:O	8:L:207:LEU:HB2	1.95	0.65
1:a:325:ALA:O	9:a:820:CLA:HMA3	1.96	0.65
9:b:821:CLA:HHB	12:b:835:BCR:H12C	1.79	0.65
4:d:128:ARG:NH2	4:d:130:GLU:OE1	2.30	0.65
9:L:308:CLA:C2C	9:a:820:CLA:CMB	2.75	0.65
4:D:128:ARG:NH2	4:D:130:GLU:OE1	2.30	0.65
6:h:81:TYR:HB3	9:h:201:CLA:C3	2.27	0.65
6:H:80:PRO:O	9:a:820:CLA:C1B	2.45	0.65
6:H:84:LEU:HD22	1:a:308:MET:HE3	1.78	0.65
8:L:212:LEU:HD22	9:a:831:CLA:CHD	2.27	0.65
1:A:125:ASN:HB3	1:A:133:ARG:HB3	1.77	0.65
9:A:830:CLA:C1D	8:l:212:LEU:HD22	2.26	0.65
2:B:661:PHE:HA	2:B:664:LEU:HD12	1.79	0.65
9:a:811:CLA:HMA1	9:a:811:CLA:H72	1.78	0.65
9:a:830:CLA:HMA2	8:l:120:ALA:HB1	1.77	0.65
1:A:371:MET:HE1	9:A:823:CLA:HAB	1.79	0.65
2:B:168:PHE:O	2:B:174:ARG:NH2	2.30	0.65
8:L:204:TYR:O	9:L:307:CLA:HMB2	1.96	0.65
9:L:307:CLA:C3C	1:a:497:PRO:HD2	1.72	0.65
2:b:57:ILE:HD13	9:b:806:CLA:H43	1.78	0.65
9:A:819:CLA:C13	9:h:201:CLA:HBC1	2.27	0.64
2:B:57:ILE:HD13	9:B:806:CLA:H43	1.78	0.64
2:b:168:PHE:O	2:b:174:ARG:NH2	2.30	0.64
6:H:81:TYR:O	9:a:820:CLA:HBA2	1.97	0.64
1:A:332:GLY:N	1:A:422:ASP:OD2	2.31	0.64
9:A:820:CLA:NC	12:A:842:BCR:H19C	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:HA	1:A:47:TRP:HD1	1.63	0.64
1:a:44:THR:HA	1:a:47:TRP:HD1	1.63	0.63
1:a:322:ILE:HG12	9:a:820:CLA:C3D	2.28	0.63
9:a:823:CLA:H8	12:a:844:BCR:H383	1.80	0.63
9:a:803:CLA:HBA2	9:a:809:CLA:H62	1.80	0.63
2:B:26:ALA:HA	9:B:825:CLA:H42	1.80	0.63
1:a:202:LEU:HD22	1:a:203:LEU:HD12	1.81	0.63
1:A:328:GLY:H	11:A:839:LHG:HC2	1.63	0.63
1:A:503:THR:HG21	9:A:830:CLA:HMA2	1.81	0.63
8:l:89:LEU:HD11	9:l:306:CLA:HBD	1.79	0.63
1:A:202:LEU:HD22	1:A:203:LEU:HD12	1.81	0.63
2:b:661:PHE:HA	2:b:664:LEU:HD12	1.79	0.63
9:A:819:CLA:CBB	9:A:823:CLA:H72	2.27	0.62
1:a:350:LEU:HD11	9:a:827:CLA:HBB1	1.81	0.62
8:l:148:LEU:HD13	12:l:308:BCR:H24C	1.80	0.62
1:A:350:LEU:HD11	9:A:826:CLA:HBB1	1.82	0.62
1:a:480:PHE:HB3	9:a:832:CLA:H11	1.81	0.62
2:b:501:ILE:HD11	9:b:827:CLA:HMA3	1.79	0.62
8:L:211:ASN:HB2	1:a:491:ALA:HA	1.82	0.62
9:A:819:CLA:H171	9:A:819:CLA:CAD	2.30	0.62
9:a:847:CLA:H51	8:l:86:LEU:HD11	1.80	0.62
8:l:209:VAL:HG23	9:l:301:CLA:CAC	2.29	0.62
1:a:550:LYS:HZ2	2:b:674:LEU:HB2	1.65	0.62
2:B:174:ARG:HB3	9:B:814:CLA:HBC2	1.81	0.62
9:A:819:CLA:C16	9:A:819:CLA:HBD	2.30	0.62
2:b:26:ALA:HA	9:b:825:CLA:H42	1.82	0.61
8:L:205:PHE:HA	9:L:307:CLA:HMB2	1.81	0.61
9:a:807:CLA:H92	9:a:825:CLA:HBC2	1.82	0.61
6:H:82:ASN:OD1	9:a:820:CLA:C2D	2.48	0.61
9:L:308:CLA:C1C	9:a:820:CLA:HMB1	2.31	0.61
8:l:205:PHE:CD1	9:l:301:CLA:HBC3	2.35	0.61
2:B:332:PHE:CE2	12:B:835:BCR:H291	2.36	0.61
8:L:148:LEU:HD13	12:L:305:BCR:H24C	1.81	0.61
1:a:326:HIS:CD2	9:a:820:CLA:C1B	2.83	0.61
2:b:174:ARG:HB3	9:b:814:CLA:HBC2	1.82	0.61
9:A:819:CLA:H41	9:A:821:CLA:CAC	2.30	0.61
1:a:328:GLY:H	11:a:840:LHG:HC2	1.65	0.61
1:A:585:SER:OG	1:A:588:ASP:OD2	2.19	0.60
9:A:806:CLA:HMB3	9:A:807:CLA:HHB	1.82	0.60
2:b:209:TRP:HH2	12:b:834:BCR:H17C	1.66	0.60
6:h:81:TYR:HB2	9:h:201:CLA:O2A	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:HA	1:A:334:GLY:HA3	1.84	0.60
1:a:87:GLY:HA3	9:a:806:CLA:HHC	1.84	0.60
2:b:332:PHE:CE2	12:b:835:BCR:H291	2.36	0.60
2:B:501:ILE:HD11	9:B:827:CLA:HMA3	1.81	0.60
2:b:587:ILE:HA	2:b:590:VAL:HG22	1.84	0.60
8:L:100:LEU:CD1	9:a:820:CLA:H2	2.32	0.60
8:L:211:ASN:O	8:L:213:PRO:HD3	2.02	0.60
1:a:214:GLN:HA	1:a:218:SER:HB2	1.84	0.60
8:l:168:THR:HG22	8:l:174:LYS:HD2	1.84	0.60
1:A:214:GLN:HA	1:A:218:SER:HB2	1.84	0.59
9:A:822:CLA:H111	9:A:833:CLA:H72	1.84	0.59
1:A:319:ILE:HG21	9:A:821:CLA:HAC1	1.83	0.59
9:A:819:CLA:HBD	9:A:819:CLA:H161	1.85	0.59
1:a:326:HIS:CD2	9:a:820:CLA:CHB	2.85	0.59
2:b:407:VAL:HG12	2:b:411:MET:HE2	1.85	0.59
1:A:550:LYS:HZ2	2:B:674:LEU:HB2	1.67	0.59
9:A:819:CLA:H142	9:A:820:CLA:HBD	1.83	0.59
1:A:118:ILE:HG23	1:A:119:VAL:HG22	1.84	0.59
1:A:302:PHE:CE1	9:A:819:CLA:HAC1	2.37	0.59
9:b:802:CLA:HHB	9:b:803:CLA:H202	1.84	0.59
8:L:213:PRO:HD2	1:a:487:THR:HB	1.85	0.59
1:a:319:ILE:HG21	9:a:822:CLA:HAC1	1.83	0.59
9:a:819:CLA:H71	12:a:844:BCR:H12C	1.84	0.59
8:L:209:VAL:HA	1:a:495:THR:HB	1.85	0.59
1:A:322:ILE:HB	9:A:819:CLA:C1	2.33	0.59
1:A:495:THR:HB	8:l:209:VAL:HA	1.84	0.59
1:A:634:PHE:O	1:A:638:SER:OG	2.21	0.59
11:A:845:LHG:H322	8:L:216:VAL:HG11	1.83	0.59
8:L:168:THR:HG22	8:L:174:LYS:HD2	1.84	0.59
1:a:390:HIS:HE1	9:a:825:CLA:ND	2.00	0.59
8:l:88:ASN:OD1	9:l:302:CLA:HAA1	2.03	0.59
9:A:817:CLA:H203	9:A:823:CLA:H3A	1.85	0.59
1:a:327:LYS:HA	1:a:334:GLY:HA3	1.84	0.59
1:a:322:ILE:CG2	9:a:820:CLA:C2D	2.80	0.58
1:a:332:GLY:N	1:a:422:ASP:OD2	2.36	0.58
8:l:120:ALA:HB2	11:l:303:LHG:HC81	1.85	0.58
8:l:206:LEU:HD22	9:l:301:CLA:HBB1	1.85	0.58
2:B:587:ILE:HA	2:B:590:VAL:HG22	1.84	0.58
6:H:82:ASN:OD1	9:a:820:CLA:C3D	2.51	0.58
9:L:302:CLA:HBC2	9:a:820:CLA:HBB2	1.85	0.58
9:A:825:CLA:H12	12:A:841:BCR:HC7	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:VAL:HG12	2:B:411:MET:HE2	1.85	0.58
9:B:839:CLA:HHB	9:B:840:CLA:HAA1	1.85	0.58
4:D:140:ARG:NH2	4:D:170:GLU:OE2	2.36	0.58
6:H:82:ASN:OD1	9:a:820:CLA:C4D	2.51	0.58
1:a:488:HIS:CD2	9:a:831:CLA:C1D	2.87	0.58
9:A:813:CLA:HBB1	12:A:840:BCR:H333	1.85	0.58
9:A:836:CLA:HBC2	10:A:837:PQN:H251	1.85	0.58
1:a:585:SER:OG	1:a:588:ASP:OD2	2.18	0.58
1:A:201:GLY:O	1:A:205:LEU:HB2	2.03	0.58
1:A:329:PRO:HG3	9:l:302:CLA:C4D	2.34	0.58
9:a:801:CLA:HBB1	9:b:802:CLA:HED1	1.86	0.58
9:b:822:CLA:H12	12:b:835:BCR:HC8	1.84	0.58
9:A:819:CLA:H141	9:h:201:CLA:HBC2	1.61	0.58
1:a:634:PHE:O	1:a:638:SER:OG	2.21	0.58
9:a:817:CLA:H203	9:a:824:CLA:H3A	1.85	0.58
6:H:80:PRO:O	9:a:820:CLA:CMB	2.51	0.58
4:d:140:ARG:NH2	4:d:170:GLU:OE2	2.36	0.58
1:a:338:LEU:HD21	9:a:821:CLA:HBC3	1.85	0.58
8:L:79:SER:O	8:L:82:ILE:HG22	2.04	0.57
1:a:201:GLY:O	1:a:205:LEU:HB2	2.03	0.57
6:H:81:TYR:HB2	9:a:820:CLA:C1	2.34	0.57
5:e:108:ASP:HB2	5:e:116:PRO:HB3	1.87	0.57
9:b:822:CLA:CAB	9:b:827:CLA:H3A	2.34	0.57
1:A:194:MET:HB2	9:A:811:CLA:HBC2	1.86	0.57
8:L:203:ALA:HB1	8:L:207:LEU:HD12	1.86	0.57
6:h:114:LEU:HD21	7:i:17:LEU:HD12	1.86	0.57
8:l:73:GLU:HG3	8:l:78:SER:HB2	1.85	0.57
6:H:83:PRO:CG	9:a:820:CLA:HBD	2.35	0.57
10:a:838:PQN:H271	9:a:846:CLA:H161	1.86	0.57
1:A:309:TYR:CE1	9:A:819:CLA:H2	2.38	0.57
9:a:802:CLA:H172	12:b:836:BCR:H343	1.87	0.57
9:A:802:CLA:H172	12:B:836:BCR:H343	1.87	0.57
9:A:847:CLA:H52	9:L:303:CLA:H43	1.87	0.57
9:A:807:CLA:H143	9:A:824:CLA:H91	1.86	0.57
6:H:114:LEU:HD21	7:I:17:LEU:HD12	1.87	0.57
1:A:488:HIS:HD2	9:A:830:CLA:C2D	2.17	0.56
8:L:204:TYR:O	9:L:307:CLA:CMB	2.53	0.56
1:A:596:TRP:HE1	9:B:804:CLA:C1D	2.19	0.56
9:A:816:CLA:H121	9:A:816:CLA:HBC3	1.87	0.56
6:H:82:ASN:OD1	9:a:820:CLA:ND	2.38	0.56
6:H:83:PRO:HG3	9:a:820:CLA:HAA1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:74:THR:O	8:L:78:SER:N	2.38	0.56
1:a:588:ASP:OD1	1:a:723:ARG:NH1	2.38	0.56
2:b:315:LEU:HA	2:b:410:ARG:HG3	1.87	0.56
4:D:151:ARG:HB2	4:D:161:LEU:HD11	1.87	0.56
5:E:108:ASP:HB2	5:E:116:PRO:HB3	1.87	0.56
9:a:819:CLA:H72	9:a:821:CLA:H51	1.87	0.56
4:d:151:ARG:HB2	4:d:161:LEU:HD11	1.87	0.56
9:a:826:CLA:H12	12:a:842:BCR:HC7	1.86	0.56
9:B:822:CLA:CAB	9:B:827:CLA:H3A	2.35	0.56
6:H:82:ASN:OD1	9:a:820:CLA:C1D	2.53	0.56
1:a:322:ILE:HG12	9:a:820:CLA:OBD	2.05	0.56
12:i:101:BCR:H383	12:l:304:BCR:H362	1.88	0.56
9:l:302:CLA:H62	9:l:305:CLA:HHC	1.88	0.56
1:a:205:LEU:HB3	12:a:842:BCR:H20C	1.88	0.56
9:a:819:CLA:H172	12:a:844:BCR:HC42	1.86	0.56
8:L:212:LEU:HD22	9:a:831:CLA:HHD	1.88	0.56
9:a:847:CLA:H52	9:l:306:CLA:H43	1.86	0.56
2:b:203:ARG:NH2	2:b:253:ALA:O	2.35	0.56
1:A:405:HIS:HA	1:A:408:ILE:HD12	1.88	0.55
2:B:256:THR:OG1	2:B:271:THR:OG1	2.20	0.55
9:a:834:CLA:H43	12:a:844:BCR:H19C	1.89	0.55
1:A:491:ALA:HB2	9:A:830:CLA:HMD1	1.89	0.55
6:H:83:PRO:HD2	9:a:820:CLA:CBD	2.36	0.55
8:L:212:LEU:HD22	9:a:831:CLA:C1D	2.36	0.55
1:a:136:GLN:HG2	1:a:747:ILE:HG12	1.88	0.55
1:a:405:HIS:HA	1:a:408:ILE:HD12	1.88	0.55
1:a:450:PHE:HD2	9:b:804:CLA:H92	1.71	0.55
9:b:811:CLA:H42	8:l:132:ALA:HB1	1.88	0.55
9:b:821:CLA:H172	9:b:830:CLA:C1B	2.37	0.55
1:a:596:TRP:HE1	9:b:804:CLA:C1D	2.18	0.55
1:A:588:ASP:OD1	1:A:723:ARG:NH1	2.38	0.55
2:B:23:PHE:O	2:B:27:THR:OG1	2.22	0.55
2:B:141:PHE:HZ	9:B:815:CLA:H102	1.71	0.55
9:a:821:CLA:NC	12:a:843:BCR:H19C	2.21	0.55
2:b:161:TRP:HA	9:b:812:CLA:HED1	1.89	0.55
9:b:839:CLA:HHB	9:b:840:CLA:HAA1	1.88	0.55
6:h:82:ASN:N	9:h:201:CLA:H51	2.20	0.55
2:B:519:VAL:HG21	2:B:593:TYR:HB2	1.89	0.55
9:B:811:CLA:H42	8:L:132:ALA:HB1	1.89	0.55
9:a:807:CLA:H192	9:a:827:CLA:H203	1.89	0.55
9:A:810:CLA:HHC	9:A:810:CLA:HBB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:819:CLA:H142	9:h:201:CLA:CBC	2.28	0.55
9:A:819:CLA:H13	9:h:201:CLA:HBC1	1.88	0.55
8:L:104:GLU:HB2	9:L:302:CLA:HED1	1.89	0.55
9:a:801:CLA:HAB	9:b:803:CLA:NA	2.21	0.55
2:b:519:VAL:HG21	2:b:593:TYR:HB2	1.89	0.55
8:l:61:GLU:HG2	8:l:62:PRO:HD2	1.89	0.55
6:H:82:ASN:C	9:a:820:CLA:H11	2.32	0.55
1:a:491:ALA:HB2	9:a:831:CLA:HMD3	1.88	0.55
1:a:286:LEU:HD22	9:a:816:CLA:HBA1	1.89	0.55
1:a:118:ILE:HG23	1:a:119:VAL:HG22	1.89	0.54
2:b:129:LEU:HD23	2:b:135:LEU:HD23	1.89	0.54
2:B:315:LEU:HA	2:B:410:ARG:HG3	1.88	0.54
9:A:801:CLA:HBB1	9:B:802:CLA:HED1	1.89	0.54
9:a:816:CLA:H62	9:a:816:CLA:NC	2.23	0.54
9:B:821:CLA:H172	9:B:830:CLA:C1B	2.38	0.54
6:h:79:SER:OG	9:h:201:CLA:HBA1	2.07	0.54
1:A:200:ALA:HB2	1:A:306:GLY:HA3	1.89	0.54
9:L:308:CLA:C2C	9:a:820:CLA:HMB3	2.38	0.54
1:a:649:LEU:HD11	9:a:801:CLA:H71	1.90	0.54
8:L:211:ASN:HD21	1:a:495:THR:HG23	1.71	0.54
1:a:333:GLN:HB2	1:a:422:ASP:HB2	1.89	0.54
1:A:480:PHE:HB3	9:A:831:CLA:H11	1.88	0.54
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.89	0.54
1:a:512:LEU:HD12	1:a:522:LEU:HD21	1.90	0.54
6:h:83:PRO:HD3	9:h:201:CLA:HAA1	1.90	0.54
1:A:326:HIS:HE1	9:h:201:CLA:ND	2.01	0.54
1:A:649:LEU:HD11	9:A:801:CLA:H71	1.89	0.54
9:A:801:CLA:HAB	9:B:803:CLA:NA	2.22	0.54
12:h:203:BCR:H24C	8:l:202:TRP:HE1	1.73	0.54
1:A:372:PRO:HG2	1:A:378:ALA:HB2	1.90	0.54
1:A:464:ARG:NH1	2:B:95:HIS:O	2.41	0.54
1:A:512:LEU:HD12	1:A:522:LEU:HD21	1.90	0.54
9:A:817:CLA:HAB	9:A:817:CLA:H8	1.89	0.54
9:a:801:CLA:HBC3	9:b:803:CLA:HAC2	1.89	0.54
9:a:830:CLA:H93	12:l:304:BCR:H14C	1.89	0.54
2:B:203:ARG:NH2	2:B:253:ALA:O	2.35	0.53
1:a:111:SER:CB	1:a:137:ILE:H	2.21	0.53
1:a:464:ARG:NH1	2:b:95:HIS:O	2.41	0.53
9:a:819:CLA:H202	12:a:843:BCR:H402	1.89	0.53
9:b:815:CLA:CHC	12:b:834:BCR:H15C	2.38	0.53
1:A:253:SER:OG	1:A:271:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:837:CLA:HBC2	10:a:838:PQN:H251	1.90	0.53
9:A:819:CLA:H143	9:A:820:CLA:HAA1	1.82	0.53
2:b:687:LEU:HD21	8:l:89:LEU:HD23	1.90	0.53
8:l:206:LEU:HD22	9:l:301:CLA:CBB	2.39	0.53
2:B:129:LEU:HD23	2:B:135:LEU:HD23	1.89	0.53
9:B:809:CLA:O1A	9:B:823:CLA:HBD	2.09	0.53
9:L:308:CLA:CMC	9:a:820:CLA:C2B	2.87	0.53
2:B:577:TYR:CE1	2:B:710:LEU:HB2	2.44	0.53
6:H:83:PRO:CG	9:a:820:CLA:HAA1	2.39	0.53
2:b:32:GLU:OE1	2:b:331:HIS:NE2	2.40	0.53
9:h:201:CLA:HBB1	9:h:201:CLA:HMB1	1.89	0.53
8:l:104:GLU:HB2	9:l:305:CLA:HED1	1.89	0.53
9:A:817:CLA:HBC1	12:A:841:BCR:H15C	1.89	0.53
9:A:847:CLA:H51	8:L:86:LEU:HD11	1.91	0.53
1:a:325:ALA:C	9:a:820:CLA:HMA3	2.34	0.53
2:B:32:GLU:OE1	2:B:331:HIS:NE2	2.41	0.53
9:B:808:CLA:HHB	9:B:809:CLA:HMB3	1.91	0.53
8:L:61:GLU:HG2	8:L:62:PRO:HD2	1.90	0.53
1:A:456:ASN:HD21	1:A:469:PHE:HB2	1.73	0.53
6:h:82:ASN:H	9:h:201:CLA:C5	2.20	0.53
9:A:801:CLA:HBC3	9:B:803:CLA:HAC2	1.90	0.53
9:A:807:CLA:H51	9:A:824:CLA:H12	1.90	0.53
2:b:171:ALA:HB1	9:b:820:CLA:HAB	1.90	0.53
2:b:429:LEU:HB3	2:b:525:LEU:HB2	1.91	0.53
2:b:631:LEU:HD22	2:b:724:PHE:HA	1.90	0.53
9:B:801:CLA:HBC3	9:B:801:CLA:HHD	1.91	0.52
8:L:79:SER:HB3	8:L:82:ILE:HB	1.90	0.52
1:a:688:GLY:HA3	2:b:569:ASP:HB2	1.92	0.52
2:b:141:PHE:HZ	9:b:815:CLA:H102	1.74	0.52
2:b:322:LEU:O	2:b:326:ILE:HG12	2.10	0.52
1:A:398:LEU:HD21	9:A:805:CLA:H142	1.91	0.52
9:L:308:CLA:HMC2	11:a:840:LHG:HC11	1.92	0.52
6:h:81:TYR:C	9:h:201:CLA:HBA2	2.35	0.52
9:a:808:CLA:H41	9:a:810:CLA:H2	1.90	0.52
9:a:817:CLA:HBC1	12:a:842:BCR:H15C	1.90	0.52
1:A:136:GLN:HG2	1:A:747:ILE:HG12	1.92	0.52
12:I:101:BCR:H383	12:L:301:BCR:H362	1.91	0.52
1:A:331:THR:HG21	1:A:423:LEU:HD23	1.91	0.52
1:a:717:LEU:HD22	1:a:721:GLN:HB3	1.92	0.52
9:a:821:CLA:HBB2	11:a:840:LHG:HC82	1.92	0.52
9:b:801:CLA:HBC3	9:b:801:CLA:HHD	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:805:CLA:HHB	9:A:826:CLA:HAB	1.91	0.52
2:b:577:TYR:CE1	2:b:710:LEU:HB2	2.44	0.52
1:a:456:ASN:HD21	1:a:469:PHE:HB2	1.73	0.52
6:h:81:TYR:CA	9:h:201:CLA:HBA2	2.40	0.52
1:A:487:THR:HB	8:l:213:PRO:HD2	1.91	0.52
8:L:79:SER:O	8:L:82:ILE:N	2.42	0.52
1:a:488:HIS:HD2	9:a:831:CLA:C2D	2.22	0.52
1:a:683:MET:HB3	9:a:846:CLA:C1C	2.40	0.52
9:a:833:CLA:H101	9:a:834:CLA:HBC1	1.92	0.52
2:b:23:PHE:O	2:b:27:THR:OG1	2.23	0.52
2:b:158:GLN:HB2	2:b:161:TRP:HD1	1.75	0.52
2:b:662:MET:O	2:b:666:SER:OG	2.23	0.52
9:h:201:CLA:H42	9:l:305:CLA:HED3	1.92	0.52
1:A:717:LEU:HD22	1:A:721:GLN:HB3	1.92	0.51
9:B:815:CLA:CHC	12:B:834:BCR:H15C	2.40	0.51
6:H:80:PRO:HG3	8:L:93:ARG:CZ	2.40	0.51
9:b:811:CLA:H18	8:l:143:ILE:HD11	1.93	0.51
8:l:75:PRO:O	8:l:79:SER:OG	2.22	0.51
1:A:98:TYR:OH	1:A:150:ILE:O	2.27	0.51
1:A:324:GLU:HG2	1:A:336:LYS:HG3	1.92	0.51
2:B:277:HIS:HA	2:B:280:ILE:HG12	1.91	0.51
2:B:429:LEU:HB3	2:B:525:LEU:HB2	1.92	0.51
3:C:40:ALA:O	4:D:181:GLN:NE2	2.43	0.51
9:a:817:CLA:HAB	9:a:817:CLA:H8	1.91	0.51
2:b:493:TRP:HZ2	9:b:818:CLA:H12	1.74	0.51
9:b:810:CLA:H112	9:b:823:CLA:H193	1.92	0.51
1:A:91:HIS:CE1	1:A:113:GLN:HG2	2.40	0.51
9:A:832:CLA:H101	9:A:833:CLA:HBC1	1.91	0.51
6:H:81:TYR:O	9:a:820:CLA:C4A	2.58	0.51
8:l:211:ASN:O	8:l:213:PRO:HD3	2.10	0.51
8:L:64:ASN:HD21	8:L:169:LEU:HD12	1.76	0.51
12:L:301:BCR:H323	9:L:303:CLA:H51	1.91	0.51
6:h:123:GLY:HA3	6:h:130:LYS:HB3	1.93	0.51
1:A:683:MET:HB3	9:A:846:CLA:C1C	2.41	0.51
9:A:819:CLA:CAB	9:A:821:CLA:CMA	2.51	0.51
9:B:811:CLA:H18	8:L:143:ILE:HD11	1.93	0.51
9:B:815:CLA:H8	12:B:834:BCR:H14C	1.91	0.51
9:L:308:CLA:HMC3	9:a:820:CLA:C1B	2.41	0.51
2:b:125:TYR:O	2:b:130:ARG:NH1	2.41	0.51
2:b:277:HIS:HA	2:b:280:ILE:HG12	1.92	0.51
6:h:81:TYR:N	9:h:201:CLA:H3A	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:64:ASN:HD21	8:l:169:LEU:HD12	1.75	0.51
6:H:123:GLY:HA3	6:H:130:LYS:HB3	1.93	0.51
1:a:330:PHE:O	1:a:426:ARG:NE	2.44	0.51
2:b:105:THR:HG21	6:h:132:PRO:HG3	1.93	0.51
6:H:79:SER:O	9:a:820:CLA:H3A	2.11	0.51
2:b:31:PHE:HA	2:b:34:HIS:CD2	2.46	0.51
1:A:51:ALA:HB2	11:A:838:LHG:HC82	1.93	0.51
1:A:92:GLY:HA2	1:A:96:SER:HB3	1.93	0.51
1:A:111:SER:HB2	1:A:128:VAL:HG11	1.93	0.51
1:a:253:SER:OG	1:a:271:ASP:OD1	2.26	0.51
9:A:820:CLA:H2A	9:h:201:CLA:HBC2	1.92	0.50
2:B:125:TYR:O	2:B:130:ARG:NH1	2.41	0.50
1:a:92:GLY:HA2	1:a:96:SER:HB3	1.93	0.50
9:A:812:CLA:HBD	9:A:814:CLA:HMA1	1.93	0.50
9:A:819:CLA:H142	9:A:820:CLA:CAA	2.41	0.50
12:H:202:BCR:H382	12:L:306:BCR:H351	1.94	0.50
8:L:79:SER:O	8:L:80:PRO:C	2.54	0.50
1:a:203:LEU:HD23	1:a:302:PHE:CE2	2.46	0.50
2:b:661:PHE:HD1	2:b:664:LEU:HD12	1.76	0.50
2:b:697:PRO:O	3:c:81:TYR:OH	2.21	0.50
1:A:683:MET:HB3	9:A:846:CLA:C2C	2.42	0.50
2:B:275:HIS:HD1	9:B:818:CLA:CAB	2.22	0.50
9:b:808:CLA:HHB	9:b:809:CLA:HMB3	1.93	0.50
1:A:331:THR:HG22	1:A:426:ARG:HD3	1.94	0.50
12:A:842:BCR:H323	9:l:305:CLA:H42	1.93	0.50
9:B:822:CLA:HMA2	12:B:835:BCR:H323	1.93	0.50
6:H:83:PRO:HD3	9:a:820:CLA:CAA	2.33	0.50
7:I:2:THR:OG1	7:I:3:ILE:N	2.44	0.50
1:a:537:HIS:HB3	9:a:832:CLA:HAB	1.93	0.50
9:a:807:CLA:H171	9:a:827:CLA:H18	1.93	0.50
8:l:210:LEU:HD23	9:l:301:CLA:CHC	2.40	0.50
1:a:576:PRO:HB2	3:c:69:LEU:HD11	1.94	0.50
2:b:662:MET:HB3	9:b:804:CLA:C4C	2.42	0.50
2:B:158:GLN:HB2	2:B:161:TRP:HD1	1.77	0.50
2:B:516:ASP:HA	2:B:519:VAL:HG12	1.94	0.50
11:A:845:LHG:HC81	8:L:120:ALA:HB2	1.94	0.50
2:B:661:PHE:HD1	2:B:664:LEU:HD12	1.76	0.50
1:a:81:ILE:HG21	9:a:804:CLA:H8	1.94	0.50
9:a:805:CLA:HHB	9:a:827:CLA:HAB	1.93	0.50
4:d:108:GLU:O	4:d:138:ARG:NH1	2.44	0.50
1:A:435:ILE:HG13	1:A:554:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:LEU:O	2:B:326:ILE:HG12	2.11	0.50
2:B:684:ARG:HE	8:L:71:SER:HB3	1.76	0.50
9:L:307:CLA:OBD	9:a:816:CLA:C9	2.60	0.50
1:a:398:LEU:HD21	9:a:805:CLA:H142	1.92	0.50
3:c:40:ALA:O	4:d:181:GLN:NE2	2.44	0.50
9:A:819:CLA:HBC3	9:A:823:CLA:H162	1.93	0.50
9:B:811:CLA:H202	6:H:110:GLY:HA3	1.94	0.50
2:b:306:GLU:HG3	2:b:320:LYS:HD3	1.94	0.50
9:b:811:CLA:H202	6:h:110:GLY:HA3	1.94	0.50
6:h:80:PRO:HG3	8:l:93:ARG:CZ	2.41	0.50
1:A:81:ILE:HG21	9:A:804:CLA:H8	1.94	0.49
1:A:360:LEU:HD11	9:A:817:CLA:H72	1.94	0.49
1:A:494:ALA:HB3	8:l:211:ASN:ND2	2.27	0.49
2:B:306:GLU:HG3	2:B:320:LYS:HD3	1.94	0.49
2:b:275:HIS:HD1	9:b:818:CLA:CAB	2.23	0.49
4:d:109:MET:HE1	4:d:124:LEU:HD21	1.94	0.49
5:e:92:ARG:HD2	5:e:95:SER:HB2	1.94	0.49
1:A:688:GLY:HA3	2:B:569:ASP:HB2	1.93	0.49
8:L:88:ASN:ND2	9:L:308:CLA:OBD	2.42	0.49
1:a:676:PHE:HD1	9:b:802:CLA:HAA1	1.77	0.49
9:a:807:CLA:H143	9:a:825:CLA:H91	1.94	0.49
2:b:336:LEU:HD13	9:b:820:CLA:HAA1	1.94	0.49
1:A:66:ILE:O	1:A:70:VAL:HG13	2.13	0.49
1:A:203:LEU:HD23	1:A:302:PHE:CE2	2.48	0.49
9:A:810:CLA:HMD3	9:A:811:CLA:H141	1.94	0.49
2:B:31:PHE:HA	2:B:34:HIS:CD2	2.46	0.49
1:a:326:HIS:HD2	9:a:820:CLA:NB	2.11	0.49
2:b:516:ASP:HA	2:b:519:VAL:HG12	1.93	0.49
1:A:456:ASN:OD1	1:A:469:PHE:N	2.40	0.49
8:L:212:LEU:O	8:L:214:TYR:N	2.41	0.49
9:a:807:CLA:H121	9:a:807:CLA:H2	1.95	0.49
2:b:47:PHE:CE2	2:b:51:PHE:HE2	2.30	0.49
2:B:681:ALA:O	2:B:685:THR:OG1	2.23	0.49
2:b:36:ASP:O	2:b:41:ARG:NH2	2.33	0.49
2:b:684:ARG:HE	8:l:71:SER:HB3	1.78	0.49
1:A:88:MET:HE2	1:A:88:MET:HA	1.95	0.49
1:A:319:ILE:HG23	9:A:819:CLA:C5	2.42	0.49
9:A:806:CLA:H2	9:A:806:CLA:HBD	1.94	0.49
8:l:108:ALA:HB2	9:l:305:CLA:HMA1	1.95	0.49
1:A:450:PHE:HD2	9:B:804:CLA:H92	1.78	0.49
9:B:818:CLA:H92	9:B:818:CLA:H41	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:319:HIS:ND1	2:b:322:LEU:HD22	2.28	0.49
7:i:17:LEU:HD13	12:l:304:BCR:H291	1.95	0.49
2:B:98:GLN:NE2	2:B:102:GLU:OE2	2.46	0.49
2:B:319:HIS:ND1	2:B:322:LEU:HD22	2.28	0.49
2:B:697:PRO:O	3:C:81:TYR:OH	2.21	0.49
9:B:812:CLA:H2	9:B:813:CLA:C4D	2.43	0.49
5:E:81:GLY:HA3	5:E:107:VAL:HG11	1.95	0.49
1:a:326:HIS:HD2	9:a:820:CLA:C1B	2.26	0.49
9:A:807:CLA:H92	9:A:824:CLA:HBC2	1.95	0.49
2:B:523:ILE:HG12	2:B:590:VAL:HG12	1.95	0.49
1:a:200:ALA:HB2	1:a:306:GLY:HA3	1.94	0.49
1:a:324:GLU:HG2	1:a:336:LYS:HG3	1.95	0.49
1:a:455:HIS:O	1:a:459:MET:HG2	2.13	0.49
2:b:5:PHE:CG	7:i:31:ILE:HD13	2.47	0.49
1:A:455:HIS:O	1:A:459:MET:HG2	2.13	0.49
2:B:47:PHE:CE2	2:B:51:PHE:HE2	2.30	0.49
5:E:92:ARG:HD2	5:E:95:SER:HB2	1.95	0.49
2:b:523:ILE:HG12	2:b:590:VAL:HG12	1.95	0.49
1:A:530:ASP:HA	1:A:533:VAL:HG22	1.95	0.48
1:A:576:PRO:HB2	3:C:69:LEU:HD11	1.93	0.48
2:B:694:ARG:HD2	8:L:155:SER:HA	1.95	0.48
9:B:815:CLA:NA	12:B:834:BCR:H352	2.27	0.48
8:L:108:ALA:HB2	9:L:302:CLA:HMA1	1.95	0.48
9:a:802:CLA:HBB1	9:a:802:CLA:HMB3	1.95	0.48
9:a:804:CLA:H72	12:a:842:BCR:HC8	1.94	0.48
1:A:338:LEU:HD21	9:A:820:CLA:HBC3	1.94	0.48
9:A:820:CLA:H52	9:A:833:CLA:H12	1.94	0.48
9:A:830:CLA:NB	12:A:843:BCR:H292	2.28	0.48
2:B:105:THR:HG21	6:H:132:PRO:HG3	1.94	0.48
2:B:609:PHE:O	2:B:613:SER:OG	2.24	0.48
1:a:66:ILE:O	1:a:70:VAL:HG13	2.13	0.48
1:a:405:HIS:HE1	9:a:827:CLA:NA	2.11	0.48
1:a:695:LEU:O	1:a:699:ILE:HD12	2.14	0.48
8:L:59:VAL:HG23	8:L:60:VAL:HG23	1.94	0.48
1:a:530:ASP:HA	1:a:533:VAL:HG22	1.95	0.48
1:A:488:HIS:CD2	9:A:830:CLA:C2D	2.96	0.48
9:a:823:CLA:H111	9:a:834:CLA:H72	1.96	0.48
9:b:821:CLA:H8	9:b:830:CLA:HMD2	1.94	0.48
2:B:5:PHE:CG	7:I:31:ILE:HD13	2.48	0.48
1:a:57:ASP:OD2	1:a:347:HIS:NE2	2.47	0.48
9:a:819:CLA:H141	9:a:819:CLA:H161	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:838:LMT:H122	15:b:838:LMT:H91	1.72	0.48
7:i:2:THR:OG1	7:i:3:ILE:N	2.45	0.48
6:H:98:LYS:HB2	6:H:101:LEU:HB2	1.95	0.48
9:a:802:CLA:HBB2	9:b:804:CLA:HAA1	1.96	0.48
2:b:27:THR:HG21	14:b:837:DGD:HD5	1.95	0.48
2:b:549:ASP:OD1	3:c:66:ARG:NH2	2.42	0.48
5:e:81:GLY:HA3	5:e:107:VAL:HG11	1.95	0.48
6:h:81:TYR:HB2	9:h:201:CLA:HBA2	1.95	0.48
1:A:57:ASP:OD2	1:A:347:HIS:NE2	2.47	0.48
9:B:806:CLA:HBA2	9:B:806:CLA:H11	1.56	0.48
9:B:807:CLA:HAB	9:B:824:CLA:HMC1	1.96	0.48
8:l:74:THR:O	8:l:78:SER:N	2.29	0.48
2:b:86:PRO:HB3	2:b:121:TYR:CG	2.48	0.48
2:b:98:GLN:NE2	2:b:102:GLU:OE2	2.46	0.48
9:b:806:CLA:H11	9:b:806:CLA:HBA2	1.62	0.48
6:h:98:LYS:HB2	6:h:101:LEU:HB2	1.96	0.48
1:A:405:HIS:HE1	9:A:826:CLA:NA	2.12	0.48
2:B:493:TRP:HZ2	9:B:818:CLA:H12	1.78	0.48
9:B:825:CLA:H91	14:B:837:DGD:HBH1	1.95	0.48
6:H:80:PRO:O	9:a:820:CLA:HMB2	2.13	0.48
8:L:211:ASN:HD21	1:a:494:ALA:HB3	1.78	0.48
2:b:694:ARG:HD2	8:l:155:SER:HA	1.96	0.48
1:A:278:GLY:N	1:A:502:SER:O	2.44	0.47
1:a:88:MET:SD	9:a:807:CLA:HAA2	2.54	0.47
9:h:202:CLA:H101	12:l:309:BCR:H19C	1.96	0.47
9:A:810:CLA:H3A	9:A:810:CLA:HBA2	1.50	0.47
4:D:73:THR:HG23	4:D:123:LEU:HB2	1.97	0.47
6:H:82:ASN:H	9:a:820:CLA:H51	1.79	0.47
1:a:435:ILE:HG13	1:a:554:PHE:HE2	1.78	0.47
1:a:572:PRO:HB3	1:a:719:ILE:HB	1.96	0.47
9:h:202:CLA:H151	12:h:203:BCR:H272	1.97	0.47
9:h:202:CLA:HBB2	12:l:309:BCR:H311	1.96	0.47
8:l:212:LEU:O	8:l:214:TYR:N	2.43	0.47
1:A:657:ILE:HD12	2:B:621:ARG:HG3	1.96	0.47
9:A:817:CLA:H122	9:A:817:CLA:H162	1.41	0.47
9:b:807:CLA:HAB	9:b:824:CLA:HMC1	1.95	0.47
9:A:802:CLA:HBB1	9:A:802:CLA:HMB3	1.96	0.47
2:B:662:MET:HB3	9:B:804:CLA:C4C	2.43	0.47
1:a:278:GLY:N	1:a:502:SER:O	2.45	0.47
1:a:322:ILE:HD13	9:a:820:CLA:HMD1	1.95	0.47
1:A:333:GLN:HB2	1:A:422:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ARG:NE	1:A:467:ASP:OD2	2.43	0.47
1:A:695:LEU:O	1:A:699:ILE:HD12	2.14	0.47
9:A:802:CLA:HBB2	9:B:804:CLA:HAA1	1.97	0.47
4:D:108:GLU:O	4:D:138:ARG:NH1	2.46	0.47
1:a:488:HIS:CD2	9:a:831:CLA:C2D	2.98	0.47
6:h:80:PRO:C	9:h:201:CLA:H3A	2.39	0.47
9:l:302:CLA:H51	9:l:305:CLA:HMC1	1.96	0.47
1:A:111:SER:HB3	1:A:135:ILE:O	2.14	0.47
1:A:305:ALA:HB1	9:A:819:CLA:CHD	2.45	0.47
9:B:821:CLA:H102	9:B:821:CLA:H62	1.51	0.47
9:a:816:CLA:H92	9:a:816:CLA:H41	1.95	0.47
8:l:88:ASN:O	8:l:93:ARG:NH2	2.48	0.47
1:A:488:HIS:HD2	9:A:830:CLA:C1D	2.21	0.47
1:A:494:ALA:HB3	8:l:211:ASN:HD21	1.79	0.47
1:A:573:CYS:SG	1:A:582:CYS:HA	2.54	0.47
2:B:36:ASP:O	2:B:41:ARG:NH2	2.33	0.47
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.96	0.47
1:a:573:CYS:SG	1:a:582:CYS:HA	2.55	0.47
9:a:817:CLA:H142	9:a:819:CLA:HHC	1.96	0.47
8:l:202:TRP:O	8:l:206:LEU:HG	2.15	0.47
9:A:829:CLA:H91	9:A:829:CLA:H112	1.66	0.47
2:B:721:TYR:HB2	9:B:803:CLA:HED3	1.97	0.47
9:a:805:CLA:HAB	9:a:826:CLA:HMC1	1.96	0.47
12:a:841:BCR:H15C	12:a:842:BCR:H23C	1.97	0.47
1:A:739:TRP:HD1	9:A:824:CLA:HMB2	1.80	0.47
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.50	0.47
1:a:552:VAL:HG21	12:a:844:BCR:HC31	1.97	0.47
1:a:657:ILE:HD12	2:b:621:ARG:HG3	1.97	0.47
9:a:819:CLA:H2	9:a:819:CLA:H61	1.77	0.47
9:a:830:CLA:H202	9:a:830:CLA:H162	1.74	0.47
2:b:389:HIS:HA	2:b:392:ILE:HD12	1.97	0.47
1:A:438:LEU:HD22	9:A:833:CLA:HAB	1.97	0.47
9:A:806:CLA:H152	9:A:806:CLA:H112	1.50	0.47
11:A:845:LHG:H162	11:A:845:LHG:H132	1.51	0.47
9:B:814:CLA:H143	9:B:814:CLA:H112	1.80	0.47
1:a:432:ASP:OD2	1:a:559:ARG:NH1	2.47	0.47
8:l:210:LEU:HD23	9:l:301:CLA:C4B	2.44	0.47
9:A:807:CLA:H192	9:A:826:CLA:H203	1.97	0.46
2:B:275:HIS:ND1	9:B:818:CLA:HAB	2.28	0.46
9:B:812:CLA:H2	9:B:813:CLA:CHA	2.45	0.46
9:a:816:CLA:H3A	9:a:816:CLA:HBA2	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:803:CLA:H161	9:B:803:CLA:H122	1.56	0.46
1:a:745:ARG:O	1:a:749:VAL:HG22	2.15	0.46
2:b:194:LEU:HA	2:b:198:ALA:HB3	1.97	0.46
9:A:805:CLA:HAB	9:A:825:CLA:HMC1	1.98	0.46
9:a:820:CLA:HAC2	9:a:821:CLA:HAA2	1.97	0.46
9:a:847:CLA:H142	9:a:847:CLA:H111	1.71	0.46
9:b:809:CLA:H8	9:b:809:CLA:H51	1.77	0.46
14:b:837:DGD:HA52	14:b:837:DGD:HA21	1.69	0.46
8:l:205:PHE:O	8:l:206:LEU:HD23	2.15	0.46
9:B:824:CLA:H62	9:B:824:CLA:H41	1.41	0.46
9:L:307:CLA:OBD	9:a:816:CLA:H91	2.16	0.46
1:a:457:ASP:OD1	1:a:640:THR:HB	2.16	0.46
2:b:700:LEU:HD22	2:b:704:GLN:NE2	2.30	0.46
12:b:835:BCR:H342	12:b:835:BCR:H331	1.96	0.46
5:e:117:VAL:HG11	5:e:139:ILE:HD13	1.98	0.46
2:B:326:ILE:HD12	2:B:332:PHE:CE1	2.51	0.46
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.30	0.46
9:B:807:CLA:HHB	9:B:825:CLA:HAB	1.98	0.46
7:I:5:ASN:OD1	7:I:6:ASN:N	2.49	0.46
9:L:303:CLA:HMD3	12:L:305:BCR:H381	1.97	0.46
1:a:540:THR:HB	1:a:600:SER:OG	2.15	0.46
1:a:683:MET:HB3	9:a:846:CLA:C2C	2.45	0.46
9:a:816:CLA:H91	9:a:816:CLA:H111	1.71	0.46
9:a:833:CLA:H202	9:l:306:CLA:H91	1.97	0.46
9:b:818:CLA:H61	9:b:818:CLA:H41	1.57	0.46
1:A:572:PRO:HB3	1:A:719:ILE:HB	1.97	0.46
1:A:745:ARG:O	1:A:749:VAL:HG22	2.15	0.46
9:A:807:CLA:HAA1	9:A:824:CLA:HED2	1.97	0.46
9:a:801:CLA:H151	9:a:802:CLA:HMA1	1.97	0.46
2:b:348:VAL:HG12	2:b:352:MET:HE2	1.98	0.46
9:b:802:CLA:H112	9:b:802:CLA:H72	1.61	0.46
4:d:73:THR:HG23	4:d:123:LEU:HB2	1.97	0.46
1:A:540:THR:HB	1:A:600:SER:OG	2.15	0.46
9:A:826:CLA:H202	9:A:836:CLA:HHB	1.96	0.46
11:A:845:LHG:H362	9:L:304:CLA:H42	1.98	0.46
9:A:847:CLA:H142	9:A:847:CLA:H111	1.66	0.46
2:B:231:ASN:HA	9:B:817:CLA:HAA2	1.98	0.46
6:H:81:TYR:O	9:a:820:CLA:NA	2.48	0.46
1:a:88:MET:HA	1:a:88:MET:HE2	1.98	0.46
1:a:321:GLU:OE2	9:a:820:CLA:HED2	2.15	0.46
9:b:806:CLA:H162	9:b:806:CLA:H122	1.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:59:VAL:HG23	8:l:60:VAL:HG23	1.98	0.46
9:l:302:CLA:HBA1	9:l:302:CLA:H3A	1.55	0.46
9:A:835:CLA:H202	9:A:835:CLA:H161	1.78	0.46
9:B:802:CLA:H61	9:B:802:CLA:H41	1.63	0.46
6:H:83:PRO:HA	9:a:820:CLA:H12	1.97	0.46
1:a:225:LEU:HD21	1:a:231:PRO:HG3	1.98	0.46
1:a:322:ILE:HD13	9:a:820:CLA:CMD	2.45	0.46
9:a:811:CLA:H91	9:a:811:CLA:H111	1.60	0.46
9:a:825:CLA:H3A	9:a:825:CLA:HBA2	1.49	0.46
9:a:833:CLA:H102	9:l:306:CLA:H171	1.97	0.46
2:b:8:PHE:HB2	2:b:34:HIS:CG	2.51	0.46
9:b:829:CLA:HMC2	9:b:829:CLA:H112	1.97	0.46
9:b:839:CLA:HAA2	9:b:840:CLA:CHB	2.46	0.46
9:A:832:CLA:H142	9:A:832:CLA:H111	1.67	0.46
1:a:325:ALA:HB2	9:a:820:CLA:HED3	1.97	0.46
1:a:655:GLN:HG2	1:a:748:ALA:HB3	1.97	0.46
9:a:831:CLA:HAA2	12:a:844:BCR:H401	1.98	0.46
9:A:801:CLA:H151	9:A:802:CLA:HMA1	1.98	0.46
9:A:815:CLA:H122	9:A:815:CLA:H162	1.64	0.46
9:A:830:CLA:HMD2	8:l:212:LEU:HD23	1.97	0.46
9:A:832:CLA:H102	9:L:303:CLA:H171	1.98	0.46
9:A:846:CLA:O1A	2:B:430:GLY:HA3	2.16	0.46
2:B:383:MET:HE1	12:B:835:BCR:H17C	1.98	0.46
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.97	0.46
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.98	0.46
9:a:812:CLA:HBD	9:a:814:CLA:HMA1	1.98	0.46
1:A:462:LEU:HD22	2:B:96:PHE:HD1	1.82	0.45
9:A:811:CLA:H91	9:A:811:CLA:H111	1.63	0.45
2:B:159:PRO:HA	2:B:162:LYS:HE2	1.98	0.45
2:B:209:TRP:HH2	12:B:834:BCR:H17C	1.82	0.45
9:B:829:CLA:H112	9:B:829:CLA:HMC2	1.99	0.45
9:b:804:CLA:H92	9:b:804:CLA:H62	1.73	0.45
2:B:8:PHE:HB2	2:B:34:HIS:CG	2.51	0.45
9:a:810:CLA:H3A	9:a:810:CLA:HBA2	1.59	0.45
7:i:5:ASN:OD1	7:i:6:ASN:N	2.49	0.45
1:A:655:GLN:HG2	1:A:748:ALA:HB3	1.98	0.45
9:A:836:CLA:HHC	9:A:836:CLA:HBB1	1.97	0.45
9:B:818:CLA:H72	9:B:818:CLA:HBB1	1.99	0.45
1:a:325:ALA:HB1	9:a:820:CLA:HMA3	1.98	0.45
9:a:806:CLA:H101	9:a:806:CLA:H62	1.69	0.45
2:b:457:PRO:HG3	2:b:517:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:809:CLA:O1A	9:b:823:CLA:HBD	2.16	0.45
9:b:832:CLA:H172	7:i:24:MET:HE2	1.98	0.45
9:h:201:CLA:H2A	9:h:201:CLA:O2D	2.17	0.45
1:A:308:MET:SD	9:A:819:CLA:C4D	3.04	0.45
1:A:732:LEU:HD22	9:A:836:CLA:HMA1	1.98	0.45
2:B:662:MET:HB3	9:B:804:CLA:C3C	2.47	0.45
15:B:838:LMT:H122	15:B:838:LMT:H91	1.73	0.45
1:a:456:ASN:OD1	1:a:469:PHE:N	2.40	0.45
9:a:819:CLA:H121	12:a:844:BCR:H10C	1.98	0.45
9:a:836:CLA:HBA1	9:a:836:CLA:H3A	1.75	0.45
2:b:395:ILE:HD13	2:b:555:TYR:HA	1.98	0.45
9:b:807:CLA:HHB	9:b:825:CLA:HAB	1.99	0.45
9:b:819:CLA:HBA2	9:b:819:CLA:H3A	1.62	0.45
6:h:85:GLN:CB	9:h:201:CLA:H52	2.45	0.45
8:l:88:ASN:OD1	9:l:302:CLA:HBD	2.17	0.45
9:A:835:CLA:H13	9:A:835:CLA:H101	1.65	0.45
9:A:847:CLA:CBB	12:L:301:BCR:H342	2.47	0.45
2:B:5:PHE:HB3	2:B:6:PRO:HD3	1.98	0.45
2:B:657:TRP:CZ3	9:B:803:CLA:HHB	2.52	0.45
8:L:213:PRO:HG2	1:a:487:THR:HA	1.97	0.45
1:a:311:THR:HG21	9:a:818:CLA:OBD	2.17	0.45
1:a:360:LEU:HD11	9:a:817:CLA:H72	1.98	0.45
2:b:657:TRP:CZ3	9:b:803:CLA:HHB	2.51	0.45
1:A:326:HIS:HA	9:l:302:CLA:CMC	2.44	0.45
9:A:803:CLA:HAB	9:A:809:CLA:H161	1.99	0.45
9:B:815:CLA:HAA2	12:B:834:BCR:H332	1.99	0.45
1:a:325:ALA:HB1	9:a:820:CLA:C2A	2.40	0.45
9:a:819:CLA:H112	9:a:819:CLA:H91	1.74	0.45
9:a:830:CLA:H142	9:a:830:CLA:H111	1.71	0.45
2:b:662:MET:HB3	9:b:804:CLA:C3C	2.47	0.45
9:b:811:CLA:H91	9:b:811:CLA:H112	1.62	0.45
6:h:74:GLY:HA2	8:l:92:TYR:HB3	1.98	0.45
1:A:430:HIS:CE1	1:A:434:ILE:HD11	2.52	0.45
9:A:807:CLA:H112	9:A:807:CLA:H43	1.97	0.45
2:B:348:VAL:HG12	2:B:352:MET:HE2	1.98	0.45
2:B:441:ASP:OD1	2:B:615:TYR:HB2	2.17	0.45
2:B:464:GLN:HB3	2:B:469:LYS:HD3	1.98	0.45
14:B:837:DGD:HA71	14:B:837:DGD:HA42	1.66	0.45
7:I:17:LEU:HD13	12:L:301:BCR:H291	1.98	0.45
9:L:308:CLA:HBC2	1:a:327:LYS:C	2.42	0.45
9:a:805:CLA:H3A	9:a:827:CLA:HAB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:441:ASP:OD1	2:b:615:TYR:HB2	2.16	0.45
1:A:77:GLN:HG2	9:A:804:CLA:H3A	1.99	0.45
1:A:328:GLY:HA3	11:A:839:LHG:P	2.57	0.45
1:A:457:ASP:OD1	1:A:640:THR:HB	2.16	0.45
9:A:828:CLA:H71	9:A:828:CLA:H111	1.58	0.45
9:A:847:CLA:H141	9:A:847:CLA:H162	1.64	0.45
2:B:457:PRO:HG3	2:B:517:PHE:HB2	1.98	0.45
2:B:684:ARG:NE	8:L:71:SER:HB3	2.32	0.45
9:B:810:CLA:H112	9:B:823:CLA:H193	1.97	0.45
9:B:832:CLA:H172	7:I:24:MET:HE2	1.99	0.45
1:a:351:SER:OG	1:a:406:ALA:HB2	2.16	0.45
9:a:816:CLA:H41	9:a:816:CLA:H61	1.33	0.45
9:a:820:CLA:HBC3	9:a:820:CLA:CHD	2.43	0.45
9:b:806:CLA:H41	9:b:806:CLA:H61	1.62	0.45
9:A:807:CLA:H101	9:A:807:CLA:H61	1.35	0.45
5:E:117:VAL:HG11	5:E:139:ILE:HD13	1.98	0.45
2:b:231:ASN:HA	9:b:817:CLA:HAA2	1.99	0.45
2:b:661:PHE:O	2:b:665:ILE:N	2.45	0.45
2:b:684:ARG:NE	8:l:71:SER:HB3	2.32	0.45
15:b:838:LMT:H1B	15:b:838:LMT:H5'	1.67	0.45
7:i:11:LEU:HD23	7:i:11:LEU:HA	1.83	0.45
9:l:306:CLA:HMD3	12:l:308:BCR:H381	1.97	0.45
9:A:835:CLA:HED2	9:A:835:CLA:HBD	1.56	0.45
9:B:819:CLA:H91	9:B:819:CLA:H112	1.77	0.45
2:b:721:TYR:HB2	9:b:803:CLA:HED3	1.99	0.45
3:c:24:ASP:OD2	4:d:162:HIS:ND1	2.47	0.45
1:A:225:LEU:HD21	1:A:231:PRO:HG3	1.98	0.44
1:A:351:SER:OG	1:A:406:ALA:HB2	2.16	0.44
9:A:824:CLA:H3A	9:A:824:CLA:HBA2	1.51	0.44
10:A:837:PQN:H242	10:A:837:PQN:H212	1.85	0.44
2:B:549:ASP:OD1	3:C:66:ARG:NH2	2.42	0.44
9:L:307:CLA:HMA3	9:L:307:CLA:HED3	1.98	0.44
1:a:51:ALA:HB2	11:a:839:LHG:HC82	1.98	0.44
1:a:326:HIS:CE1	9:a:820:CLA:CHA	3.00	0.44
9:a:830:CLA:H41	9:a:830:CLA:H61	1.45	0.44
1:A:259:THR:OG1	1:A:260:PRO:HD3	2.17	0.44
9:B:832:CLA:H203	9:B:832:CLA:H162	1.80	0.44
9:a:816:CLA:H92	9:a:816:CLA:H61	1.69	0.44
9:a:833:CLA:H142	9:a:833:CLA:H111	1.68	0.44
9:b:803:CLA:H102	9:b:803:CLA:H62	1.81	0.44
9:b:825:CLA:H91	14:b:837:DGD:HBH1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:833:PQN:H172	10:b:833:PQN:H212	1.79	0.44
1:A:537:HIS:HB3	9:A:831:CLA:HAB	1.99	0.44
9:A:803:CLA:HED1	9:A:809:CLA:OBD	2.17	0.44
2:B:555:TYR:O	2:B:571:SER:OG	2.34	0.44
9:B:807:CLA:H8	14:B:837:DGD:HBH2	1.99	0.44
6:H:99:ARG:HB3	8:L:153:ILE:HG12	1.99	0.44
1:a:462:LEU:HD22	2:b:96:PHE:HD1	1.82	0.44
1:a:570:ARG:HG3	1:a:587:TRP:CG	2.52	0.44
1:a:670:PHE:HZ	9:a:825:CLA:H143	1.82	0.44
6:h:99:ARG:HB3	8:l:153:ILE:HG12	2.00	0.44
1:A:410:MET:HE3	1:A:410:MET:HB3	1.87	0.44
1:A:570:ARG:HG3	1:A:587:TRP:CG	2.53	0.44
9:A:804:CLA:H72	12:A:841:BCR:HC8	1.99	0.44
12:a:841:BCR:H20C	12:a:841:BCR:H361	1.89	0.44
10:b:833:PQN:H28	14:b:837:DGD:HA82	1.99	0.44
1:A:432:ASP:OD2	1:A:559:ARG:NH1	2.48	0.44
9:A:817:CLA:H142	9:A:819:CLA:CMC	2.45	0.44
9:A:819:CLA:H52	9:A:821:CLA:C2C	2.47	0.44
2:B:365:PHE:HB3	2:B:602:TRP:CZ3	2.53	0.44
2:B:585:ASN:HB2	9:B:802:CLA:HBC2	1.99	0.44
8:L:75:PRO:HB3	8:l:84:TRP:CZ3	2.53	0.44
1:a:372:PRO:HG2	1:a:378:ALA:HB2	1.99	0.44
9:a:817:CLA:H162	9:a:817:CLA:H122	1.50	0.44
9:b:802:CLA:H162	9:b:802:CLA:H122	1.76	0.44
8:l:85:TYR:HD1	9:l:302:CLA:H2	1.83	0.44
8:l:144:LEU:HD13	12:l:308:BCR:H401	2.00	0.44
1:A:482:GLN:NE2	1:A:526:LEU:O	2.48	0.44
1:A:541:ILE:O	1:A:545:VAL:HG13	2.18	0.44
9:A:806:CLA:H61	9:A:806:CLA:HBA2	2.00	0.44
2:B:187:SER:HB3	2:B:281:ALA:HB2	2.00	0.44
2:B:301:ILE:HA	2:B:304:LEU:HD12	2.00	0.44
2:B:527:LEU:HD23	2:B:586:THR:HG21	2.00	0.44
2:B:662:MET:O	2:B:666:SER:OG	2.24	0.44
2:B:722:ALA:HB2	9:B:823:CLA:HBB1	1.98	0.44
7:I:31:ILE:HG22	7:I:32:GLN:HE21	1.83	0.44
1:a:84:TRP:O	1:a:88:MET:HG2	2.17	0.44
1:a:541:ILE:O	1:a:545:VAL:HG13	2.18	0.44
10:a:838:PQN:H242	10:a:838:PQN:H212	1.84	0.44
1:A:582:CYS:O	2:B:669:GLY:N	2.50	0.44
9:A:829:CLA:H202	9:A:829:CLA:H162	1.73	0.44
2:B:583:MET:O	2:B:587:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:331:THR:HG22	1:a:426:ARG:HD3	2.00	0.44
1:a:604:VAL:HG21	9:a:832:CLA:HBB2	2.00	0.44
9:a:814:CLA:HHC	9:a:814:CLA:HBB1	1.99	0.44
9:a:846:CLA:H91	9:a:846:CLA:H111	1.60	0.44
2:b:650:PHE:CZ	2:b:654:HIS:HE1	2.36	0.44
6:h:81:TYR:N	9:h:201:CLA:HBA2	2.32	0.44
9:A:801:CLA:H203	9:A:801:CLA:H162	1.71	0.44
2:B:429:LEU:HD11	9:B:829:CLA:HMB2	2.00	0.44
2:B:548:PRO:HD2	3:C:62:PHE:CZ	2.53	0.44
9:B:825:CLA:H102	14:B:837:DGD:HBH1	2.00	0.44
1:a:471:ASP:HA	1:a:475:GLN:HG2	2.00	0.44
2:b:5:PHE:HB3	2:b:6:PRO:HD3	1.98	0.44
2:b:187:SER:HB3	2:b:281:ALA:HB2	1.99	0.44
2:b:365:PHE:HB3	2:b:602:TRP:CZ3	2.53	0.44
2:b:464:GLN:HB3	2:b:469:LYS:HD3	1.98	0.44
2:b:583:MET:O	2:b:587:ILE:HG12	2.17	0.44
9:b:828:CLA:HBB1	9:b:828:CLA:HMB1	2.00	0.44
9:b:829:CLA:HBC2	15:b:838:LMT:H82	1.99	0.44
9:A:847:CLA:H61	8:L:82:ILE:HD11	2.00	0.44
2:B:577:TYR:HE1	2:B:710:LEU:HB2	1.83	0.44
9:B:817:CLA:H41	9:B:817:CLA:H62	1.34	0.44
1:a:582:CYS:O	2:b:669:GLY:N	2.51	0.44
9:a:808:CLA:H92	9:a:808:CLA:H11	1.99	0.44
9:b:816:CLA:HHB	12:b:834:BCR:H24C	2.00	0.44
9:b:825:CLA:H102	14:b:837:DGD:HBH1	2.00	0.44
6:h:106:LEU:HD22	8:l:142:VAL:HG13	2.00	0.44
7:i:31:ILE:HG22	7:i:32:GLN:HE21	1.83	0.44
1:A:46:ILE:HG13	1:A:47:TRP:N	2.33	0.43
9:A:846:CLA:HMD1	2:B:578:LEU:HB3	2.00	0.43
9:a:817:CLA:H3A	9:a:817:CLA:HBA2	1.80	0.43
9:a:824:CLA:H161	9:a:824:CLA:H121	1.42	0.43
9:a:826:CLA:H91	9:a:826:CLA:H111	1.71	0.43
9:a:830:CLA:H112	9:a:830:CLA:H91	1.67	0.43
11:l:303:LHG:H132	11:l:303:LHG:H162	1.48	0.43
1:A:88:MET:HE1	9:A:807:CLA:HMA2	1.99	0.43
1:A:370:SER:OG	9:A:823:CLA:HAC2	2.18	0.43
9:A:847:CLA:H51	8:L:86:LEU:HD21	2.00	0.43
1:a:464:ARG:NE	1:a:467:ASP:OD2	2.43	0.43
9:a:825:CLA:H72	9:a:825:CLA:H111	1.29	0.43
2:b:159:PRO:HA	2:b:162:LYS:HE2	1.99	0.43
2:b:652:PHE:O	2:b:656:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:804:CLA:H142	9:b:804:CLA:H111	1.75	0.43
9:b:806:CLA:H62	9:b:806:CLA:H102	1.82	0.43
9:b:818:CLA:H41	9:b:818:CLA:H92	2.00	0.43
9:l:301:CLA:HBD	9:l:301:CLA:HBA1	2.00	0.43
11:l:303:LHG:H291	11:l:303:LHG:H322	1.68	0.43
1:A:687:SER:HA	2:B:578:LEU:HD21	2.00	0.43
9:A:833:CLA:H171	9:h:202:CLA:O1A	2.17	0.43
1:a:687:SER:HA	2:b:578:LEU:HD21	2.00	0.43
9:A:824:CLA:H141	9:A:824:CLA:H161	1.61	0.43
2:B:650:PHE:CZ	2:B:654:HIS:HE1	2.36	0.43
12:B:835:BCR:H342	12:B:835:BCR:H331	2.00	0.43
1:a:370:SER:OG	9:a:824:CLA:HAC2	2.17	0.43
1:a:455:HIS:CE1	1:a:459:MET:HE2	2.53	0.43
9:a:846:CLA:O1A	2:b:430:GLY:HA3	2.19	0.43
1:A:471:ASP:HA	1:A:475:GLN:HG2	2.00	0.43
9:A:829:CLA:H41	9:A:829:CLA:H61	1.43	0.43
2:B:336:LEU:HD13	9:B:820:CLA:HAA1	2.00	0.43
9:B:804:CLA:H142	9:B:804:CLA:H111	1.70	0.43
9:B:839:CLA:HAA2	9:B:840:CLA:CHB	2.48	0.43
1:a:328:GLY:HA3	11:a:840:LHG:P	2.59	0.43
9:a:808:CLA:H193	9:a:808:CLA:H162	1.78	0.43
9:a:809:CLA:H162	9:a:809:CLA:H121	1.28	0.43
9:a:836:CLA:HBD	9:a:836:CLA:HED2	1.56	0.43
9:a:847:CLA:CBB	12:l:304:BCR:H342	2.49	0.43
9:b:803:CLA:H161	9:b:803:CLA:H122	1.59	0.43
3:c:47:ASP:OD1	4:d:151:ARG:NH2	2.52	0.43
8:l:82:ILE:O	8:l:85:TYR:HB3	2.19	0.43
1:A:455:HIS:CE1	1:A:459:MET:HE2	2.54	0.43
9:A:816:CLA:CHC	9:A:816:CLA:H93	2.48	0.43
8:L:211:ASN:ND2	1:a:494:ALA:HB3	2.33	0.43
1:a:46:ILE:HG13	1:a:47:TRP:N	2.33	0.43
1:a:144:ILE:HD11	9:a:826:CLA:CED	2.49	0.43
1:a:215:VAL:HG22	1:a:272:PHE:CE2	2.54	0.43
1:a:259:THR:OG1	1:a:260:PRO:HD3	2.17	0.43
1:a:325:ALA:O	9:a:820:CLA:CMA	2.66	0.43
9:a:806:CLA:H93	9:a:806:CLA:H112	1.87	0.43
9:a:847:CLA:H112	9:l:306:CLA:H102	2.00	0.43
2:b:555:TYR:O	2:b:571:SER:OG	2.36	0.43
9:b:807:CLA:H92	9:b:807:CLA:H61	1.76	0.43
1:A:484:ILE:HD11	9:A:831:CLA:H12	2.01	0.43
9:A:824:CLA:H41	9:A:824:CLA:H62	1.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:829:CLA:H93	12:L:301:BCR:H14C	2.00	0.43
2:B:547:MET:HE2	2:B:550:LYS:HA	2.00	0.43
9:B:806:CLA:H41	9:B:806:CLA:H61	1.63	0.43
1:a:77:GLN:HG2	9:a:804:CLA:H3A	2.00	0.43
1:a:336:LYS:O	1:a:421:ASN:ND2	2.51	0.43
9:a:808:CLA:HED3	9:a:808:CLA:HBD	1.75	0.43
2:b:301:ILE:HA	2:b:304:LEU:HD12	2.00	0.43
2:b:422:LEU:HD13	2:b:532:LEU:HA	2.00	0.43
15:b:838:LMT:H102	15:b:838:LMT:H72	1.38	0.43
9:A:815:CLA:H202	9:A:815:CLA:H61	2.00	0.43
9:A:826:CLA:H142	9:A:826:CLA:H112	1.69	0.43
2:B:454:LEU:H	15:B:838:LMT:H2B	1.83	0.43
2:B:694:ARG:NH1	7:I:32:GLN:O	2.52	0.43
3:C:47:ASP:OD1	4:D:151:ARG:NH2	2.52	0.43
8:L:216:VAL:HG12	8:L:216:VAL:O	2.19	0.43
1:a:54:HIS:HB2	9:a:827:CLA:HAA2	2.01	0.43
9:a:823:CLA:H93	9:a:823:CLA:H62	1.68	0.43
9:a:829:CLA:H71	9:a:829:CLA:H111	1.54	0.43
9:a:847:CLA:H141	9:a:847:CLA:H162	1.59	0.43
2:b:694:ARG:NH1	7:i:32:GLN:O	2.52	0.43
9:b:825:CLA:H112	9:b:825:CLA:H72	1.85	0.43
8:l:114:VAL:HG21	8:l:203:ALA:HB3	2.01	0.43
8:l:206:LEU:HA	9:l:301:CLA:CHC	2.49	0.43
1:A:84:TRP:O	1:A:88:MET:HG2	2.19	0.43
1:A:363:VAL:HG11	9:A:817:CLA:H201	2.00	0.43
1:A:431:ARG:HB2	1:A:553:LEU:HD13	2.01	0.43
9:A:835:CLA:HBA1	9:A:835:CLA:H3A	1.73	0.43
9:B:801:CLA:H143	9:B:801:CLA:H112	1.73	0.43
9:B:819:CLA:H3A	9:B:819:CLA:HBA2	1.61	0.43
9:B:831:CLA:H111	9:B:831:CLA:H152	1.91	0.43
6:H:90:GLU:O	6:H:94:ALA:HB2	2.19	0.43
6:H:106:LEU:HD22	8:L:142:VAL:HG13	2.01	0.43
9:a:801:CLA:NA	9:b:803:CLA:HAB	2.33	0.43
2:b:577:TYR:HE1	2:b:710:LEU:HB2	1.83	0.43
2:b:681:ALA:O	2:b:685:THR:OG1	2.23	0.43
8:l:105:VAL:HG12	8:l:192:PHE:HE2	1.84	0.43
1:A:215:VAL:HG22	1:A:272:PHE:CE2	2.53	0.43
14:B:837:DGD:HA21	14:B:837:DGD:HA51	1.83	0.43
2:b:69:ALA:HB2	2:b:135:LEU:HB2	2.01	0.43
2:b:656:VAL:HG12	2:b:712:HIS:O	2.19	0.43
6:h:85:GLN:CD	9:h:201:CLA:H52	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:114:VAL:O	8:l:118:VAL:HG12	2.19	0.43
11:A:845:LHG:H181	11:A:845:LHG:H212	1.51	0.42
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.01	0.42
8:L:144:LEU:HD13	12:L:305:BCR:H401	2.00	0.42
9:a:805:CLA:H111	9:a:805:CLA:H71	1.75	0.42
2:b:527:LEU:HD23	2:b:586:THR:HG21	2.00	0.42
6:h:83:PRO:HA	6:h:86:SER:HB3	2.01	0.42
1:A:319:ILE:HG21	9:A:819:CLA:H41	1.76	0.42
9:A:806:CLA:H121	9:A:806:CLA:H8	1.47	0.42
9:B:808:CLA:HAA1	7:I:12:VAL:HG22	2.00	0.42
8:L:209:VAL:H	9:L:307:CLA:HMB1	1.85	0.42
9:b:818:CLA:H11	9:b:827:CLA:HBA1	2.01	0.42
9:b:818:CLA:H72	9:b:818:CLA:HBB1	2.01	0.42
9:A:801:CLA:H61	9:A:802:CLA:O1D	2.19	0.42
9:A:809:CLA:H162	9:A:809:CLA:H121	1.30	0.42
10:A:837:PQN:H141	10:A:837:PQN:H161	1.70	0.42
2:B:656:VAL:HG12	2:B:712:HIS:O	2.19	0.42
4:D:133:LEU:HD12	4:D:133:LEU:HA	1.85	0.42
9:L:308:CLA:C1C	9:a:820:CLA:CMB	2.96	0.42
9:a:813:CLA:HBB1	12:a:841:BCR:H333	2.00	0.42
9:a:846:CLA:HMD1	2:b:578:LEU:HB3	2.02	0.42
9:A:832:CLA:H202	9:L:303:CLA:H91	2.00	0.42
2:B:106:ARG:NH2	2:B:113:VAL:O	2.43	0.42
2:B:439:HIS:O	2:B:443:MET:HG2	2.20	0.42
9:B:806:CLA:H62	9:B:806:CLA:H102	1.75	0.42
9:B:810:CLA:H8	9:B:810:CLA:H122	1.78	0.42
9:B:832:CLA:H61	9:B:832:CLA:H41	1.83	0.42
9:H:201:CLA:H142	9:H:201:CLA:H112	1.83	0.42
9:a:801:CLA:H203	9:a:801:CLA:H162	1.71	0.42
9:a:815:CLA:H162	9:a:815:CLA:H122	1.58	0.42
2:b:548:PRO:HD2	3:c:62:PHE:CZ	2.54	0.42
1:A:328:GLY:HA3	11:A:839:LHG:O4	2.20	0.42
9:A:805:CLA:H3A	9:A:826:CLA:HAB	2.01	0.42
8:L:121:GLY:H	8:L:124:ARG:HD3	1.84	0.42
1:a:258:ALA:HB2	9:a:813:CLA:H11	2.00	0.42
1:a:322:ILE:HA	9:a:820:CLA:O1D	2.19	0.42
1:a:430:HIS:CE1	1:a:434:ILE:HD11	2.54	0.42
2:b:145:LEU:HD23	2:b:145:LEU:HA	1.88	0.42
8:l:216:VAL:HG12	8:l:216:VAL:O	2.20	0.42
1:A:308:MET:HE3	6:h:84:LEU:HD22	2.02	0.42
9:A:805:CLA:H71	9:A:805:CLA:H111	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:814:CLA:HHC	9:A:814:CLA:HBB1	2.00	0.42
9:A:830:CLA:HBA1	9:A:830:CLA:H12	1.66	0.42
2:B:177:HIS:HE1	9:B:813:CLA:HMA3	1.84	0.42
15:B:838:LMT:H1B	15:B:838:LMT:H5'	1.65	0.42
8:L:118:VAL:HG23	8:L:130:GLY:H	1.84	0.42
8:L:213:PRO:HA	8:L:217:LYS:HE3	2.02	0.42
9:a:836:CLA:H101	9:a:836:CLA:H13	1.63	0.42
9:b:821:CLA:H61	9:b:828:CLA:H2	2.01	0.42
8:l:121:GLY:H	8:l:124:ARG:HD3	1.84	0.42
2:B:624:LEU:O	2:B:628:SER:OG	2.21	0.42
12:L:301:BCR:H20C	12:L:301:BCR:H361	1.94	0.42
9:b:815:CLA:HAA2	12:b:834:BCR:H332	2.00	0.42
9:b:832:CLA:H92	9:b:832:CLA:H62	1.83	0.42
1:A:71:PHE:CE2	1:A:75:PHE:HE2	2.38	0.42
9:A:808:CLA:H151	9:A:808:CLA:H112	1.49	0.42
2:B:652:PHE:O	2:B:656:VAL:HG23	2.19	0.42
14:B:837:DGD:HAH2	14:B:837:DGD:HAT1	1.69	0.42
8:L:114:VAL:O	8:L:118:VAL:HG12	2.19	0.42
1:a:214:GLN:NE2	9:a:817:CLA:O1D	2.53	0.42
1:a:390:HIS:HE1	9:a:825:CLA:C1D	2.33	0.42
9:a:823:CLA:HBB1	9:a:834:CLA:HHB	2.01	0.42
2:b:722:ALA:HB2	9:b:823:CLA:HBB1	2.02	0.42
8:l:118:VAL:HG23	8:l:130:GLY:H	1.85	0.42
9:A:821:CLA:HHB	9:A:823:CLA:H92	2.02	0.42
9:B:803:CLA:H91	9:B:803:CLA:H111	1.89	0.42
6:H:81:TYR:HB2	9:a:820:CLA:C2	2.49	0.42
9:H:201:CLA:H61	12:a:843:BCR:HC21	2.01	0.42
8:L:89:LEU:O	8:L:93:ARG:HG3	2.19	0.42
1:a:732:LEU:HD22	9:a:837:CLA:HMA1	2.02	0.42
9:a:807:CLA:H101	9:a:807:CLA:H61	1.32	0.42
9:a:847:CLA:HBB2	12:l:304:BCR:H342	2.01	0.42
8:l:216:VAL:HB	9:l:307:CLA:HBA1	2.02	0.42
9:A:819:CLA:CBB	9:A:823:CLA:H8	2.46	0.42
1:a:431:ARG:HB2	1:a:553:LEU:HD13	2.01	0.42
9:b:824:CLA:H143	9:b:824:CLA:H112	1.73	0.42
1:A:194:MET:HE1	9:A:821:CLA:H121	2.01	0.41
1:A:542:HIS:HA	1:A:545:VAL:HG22	2.02	0.41
9:A:817:CLA:H2	9:A:817:CLA:H62	1.74	0.41
6:H:81:TYR:HE2	8:L:96:VAL:HG11	1.85	0.41
1:a:325:ALA:CB	9:a:820:CLA:H2A	2.43	0.41
9:a:807:CLA:H93	9:a:807:CLA:H112	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:829:CLA:H161	9:a:829:CLA:H141	1.80	0.41
9:a:837:CLA:HMC1	9:a:846:CLA:H151	2.02	0.41
2:b:106:ARG:NH2	2:b:113:VAL:O	2.42	0.41
2:b:326:ILE:HD12	2:b:332:PHE:CE1	2.55	0.41
8:l:151:TYR:O	8:l:185:TRP:NE1	2.53	0.41
1:A:144:ILE:HD11	9:A:825:CLA:CED	2.49	0.41
9:A:828:CLA:H93	9:A:828:CLA:H62	1.83	0.41
9:L:302:CLA:H42	12:a:843:BCR:H323	2.01	0.41
1:a:124:LEU:HD22	1:a:666:ALA:HB2	2.01	0.41
1:a:169:LEU:HD22	9:a:808:CLA:HBC1	2.02	0.41
1:a:438:LEU:HD22	9:a:834:CLA:HAB	2.03	0.41
9:a:803:CLA:H43	9:a:809:CLA:H92	2.02	0.41
9:a:833:CLA:H92	9:a:833:CLA:H61	1.86	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.95	0.41
9:B:803:CLA:H102	9:B:803:CLA:H62	1.85	0.41
9:B:804:CLA:H72	9:B:804:CLA:H112	1.70	0.41
12:B:836:BCR:H20C	12:B:836:BCR:H361	1.87	0.41
8:L:105:VAL:HG12	8:L:192:PHE:HE2	1.85	0.41
9:L:307:CLA:HHD	1:a:498:GLY:HA3	2.02	0.41
1:a:71:PHE:CE2	1:a:75:PHE:HE2	2.38	0.41
1:a:560:LEU:HD21	1:a:581:THR:HG22	2.01	0.41
9:a:811:CLA:H162	9:a:811:CLA:H141	1.74	0.41
9:a:819:CLA:H72	9:a:821:CLA:H2	2.02	0.41
9:a:819:CLA:H112	9:a:819:CLA:H151	1.70	0.41
9:a:835:CLA:HBA2	9:a:835:CLA:H3A	1.78	0.41
2:b:389:HIS:HE1	9:b:825:CLA:NA	2.18	0.41
2:b:501:ILE:HD11	9:b:827:CLA:CMA	2.48	0.41
1:A:670:PHE:HZ	9:A:824:CLA:H143	1.85	0.41
9:H:201:CLA:NB	12:H:202:BCR:H362	2.35	0.41
8:L:107:LEU:HD22	12:L:306:BCR:C11	2.50	0.41
8:L:151:TYR:O	8:L:185:TRP:NE1	2.53	0.41
1:a:87:GLY:CA	9:a:806:CLA:HHC	2.50	0.41
9:a:806:CLA:H13	9:a:806:CLA:H172	1.66	0.41
9:a:827:CLA:H122	9:a:827:CLA:H161	1.68	0.41
2:b:387:PHE:HB3	2:b:534:LEU:HB3	2.02	0.41
2:b:395:ILE:HD11	2:b:541:ALA:HB1	2.03	0.41
9:b:810:CLA:H8	9:b:810:CLA:H122	1.73	0.41
9:b:814:CLA:H143	9:b:814:CLA:H112	1.78	0.41
14:b:837:DGD:HAH2	14:b:837:DGD:HAT1	1.57	0.41
11:l:303:LHG:H282	9:l:307:CLA:HMB3	2.01	0.41
1:A:273:LEU:HB2	9:A:815:CLA:CMA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:803:CLA:H51	9:A:809:CLA:HBB1	2.01	0.41
10:A:837:PQN:H271	9:A:846:CLA:H18	2.02	0.41
2:B:27:THR:HG21	14:B:837:DGD:HD5	2.03	0.41
1:a:84:TRP:HZ3	12:a:842:BCR:H322	1.85	0.41
9:a:825:CLA:H62	9:a:825:CLA:H41	1.41	0.41
2:b:275:HIS:ND1	9:b:818:CLA:HAB	2.32	0.41
6:h:81:TYR:N	9:h:201:CLA:C4A	2.77	0.41
1:A:560:LEU:HD21	1:A:581:THR:HG22	2.01	0.41
1:A:604:VAL:HG21	9:A:831:CLA:HBB2	2.01	0.41
1:A:717:LEU:HB2	10:A:837:PQN:H6	2.02	0.41
2:B:714:SER:HB2	14:B:837:DGD:HBF1	2.02	0.41
1:a:438:LEU:HB2	9:a:834:CLA:HAB	2.03	0.41
9:a:810:CLA:HMD3	9:a:811:CLA:H141	2.02	0.41
9:b:810:CLA:H192	9:b:810:CLA:H161	1.82	0.41
9:b:822:CLA:HMA2	12:b:835:BCR:H322	2.01	0.41
1:A:311:THR:HG21	9:A:818:CLA:OBD	2.20	0.41
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.87	0.41
1:A:488:HIS:CD2	9:A:830:CLA:ND	2.88	0.41
9:A:817:CLA:H3A	9:A:817:CLA:HBA2	1.80	0.41
9:A:821:CLA:H102	9:A:821:CLA:H62	1.78	0.41
9:A:825:CLA:H91	9:A:825:CLA:H111	1.72	0.41
9:B:823:CLA:H192	9:B:823:CLA:H161	1.78	0.41
3:C:24:ASP:OD2	4:D:162:HIS:ND1	2.47	0.41
8:L:197:ILE:HD13	8:L:197:ILE:HA	1.96	0.41
8:L:211:ASN:CB	1:a:491:ALA:HA	2.48	0.41
1:a:542:HIS:HA	1:a:545:VAL:HG22	2.02	0.41
2:b:547:MET:HE2	2:b:550:LYS:HA	2.02	0.41
9:b:808:CLA:HAA1	7:i:12:VAL:HG22	2.03	0.41
1:A:124:LEU:HD22	1:A:666:ALA:HB2	2.01	0.41
1:A:336:LYS:O	1:A:421:ASN:ND2	2.54	0.41
9:A:830:CLA:H2A	9:A:830:CLA:CGD	2.51	0.41
9:B:802:CLA:H112	9:B:802:CLA:H72	1.29	0.41
9:B:811:CLA:H112	9:B:811:CLA:H91	1.62	0.41
9:L:308:CLA:C4B	9:a:820:CLA:CBB	2.99	0.41
1:a:570:ARG:HD2	1:a:720:ILE:HG21	2.03	0.41
1:a:576:PRO:HD2	3:c:52:LYS:HD2	2.03	0.41
9:a:819:CLA:HMB1	9:a:822:CLA:HMA3	2.02	0.41
8:l:105:VAL:HG12	8:l:192:PHE:CE2	2.55	0.41
8:l:207:LEU:HD21	9:l:307:CLA:H2A	2.03	0.41
1:A:322:ILE:HG21	9:A:819:CLA:O2A	2.05	0.41
1:A:576:PRO:HD2	3:C:52:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:822:CLA:HBB1	9:A:833:CLA:HHB	2.01	0.41
9:A:828:CLA:H112	9:A:828:CLA:H151	1.90	0.41
2:B:631:LEU:HD21	2:B:650:PHE:CG	2.56	0.41
9:B:821:CLA:H8	9:B:830:CLA:HMD2	2.03	0.41
9:B:831:CLA:H192	9:B:831:CLA:H161	1.76	0.41
10:B:833:PQN:H212	10:B:833:PQN:H172	1.79	0.41
15:B:838:LMT:H72	15:B:838:LMT:H102	1.38	0.41
9:B:839:CLA:CHB	9:B:840:CLA:HAA1	2.51	0.41
8:L:202:TRP:CZ2	8:L:206:LEU:HD21	2.56	0.41
1:a:277:GLY:HA2	9:a:816:CLA:O1A	2.21	0.41
1:a:717:LEU:HB2	10:a:838:PQN:H6	2.02	0.41
9:a:812:CLA:HMB1	12:a:841:BCR:H23C	2.03	0.41
9:a:829:CLA:H12	9:a:829:CLA:H51	1.84	0.41
9:a:847:CLA:H3A	9:a:847:CLA:HBA2	1.89	0.41
2:b:482:ASN:OD1	2:b:482:ASN:N	2.54	0.41
9:b:818:CLA:H91	9:b:818:CLA:H111	1.74	0.41
9:b:831:CLA:H91	9:b:831:CLA:H112	1.90	0.41
12:b:835:BCR:H11C	12:b:835:BCR:H341	1.86	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.92	0.41
1:A:267:SER:HA	9:A:815:CLA:HBA2	2.03	0.41
1:A:425:ASP:OD1	4:D:114:ALA:N	2.54	0.41
1:A:560:LEU:HD11	1:A:578:ARG:HB3	2.03	0.41
9:A:806:CLA:H2	9:A:806:CLA:CBD	2.51	0.41
9:A:816:CLA:H41	9:A:816:CLA:H61	1.53	0.41
9:A:819:CLA:CAB	9:A:821:CLA:C4A	2.98	0.41
10:A:837:PQN:H221	10:A:837:PQN:H18	1.70	0.41
8:L:109:HIS:HA	8:L:112:LEU:CD2	2.51	0.41
1:a:326:HIS:CE1	9:a:820:CLA:C1A	3.04	0.41
9:a:833:CLA:ND	9:a:833:CLA:H11	2.36	0.41
2:b:439:HIS:O	2:b:443:MET:HG2	2.20	0.41
12:b:836:BCR:H20C	12:b:836:BCR:H361	1.87	0.41
8:l:212:LEU:HG	9:l:301:CLA:HAB	2.03	0.41
1:A:487:THR:CB	8:l:213:PRO:HD2	2.50	0.40
9:A:811:CLA:H72	9:A:811:CLA:HMA1	2.03	0.40
2:B:389:HIS:HE1	9:B:825:CLA:NA	2.18	0.40
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.02	0.40
1:a:78:LEU:HD22	9:a:804:CLA:H92	2.02	0.40
9:a:833:CLA:H171	9:a:847:CLA:H122	2.02	0.40
10:a:838:PQN:H18	10:a:838:PQN:H221	1.72	0.40
9:b:807:CLA:H71	9:b:807:CLA:H111	1.67	0.40
9:h:202:CLA:H112	9:h:202:CLA:H142	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TYR:CE2	9:A:819:CLA:HMD2	2.56	0.40
1:A:368:MET:HE1	9:A:825:CLA:HED2	2.03	0.40
1:A:536:ILE:HD13	1:A:536:ILE:HA	1.92	0.40
2:B:15:ASP:HB3	2:B:20:ARG:HB2	2.03	0.40
2:b:15:ASP:HB3	2:b:20:ARG:HB2	2.03	0.40
2:b:310:PRO:HA	2:b:311:PRO:HD3	1.89	0.40
9:b:801:CLA:H91	9:b:801:CLA:H112	1.59	0.40
9:b:832:CLA:H203	9:b:832:CLA:H162	1.80	0.40
8:l:109:HIS:HE1	9:l:306:CLA:C4D	2.35	0.40
8:l:210:LEU:HD23	9:l:301:CLA:C1C	2.51	0.40
1:A:570:ARG:HD2	1:A:720:ILE:HG21	2.02	0.40
9:A:802:CLA:H142	9:A:802:CLA:H111	1.65	0.40
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.88	0.40
2:B:387:PHE:HB3	2:B:534:LEU:HB3	2.02	0.40
2:B:482:ASN:OD1	2:B:482:ASN:N	2.54	0.40
9:B:811:CLA:H141	9:B:811:CLA:H161	1.90	0.40
10:B:833:PQN:H211	10:B:833:PQN:H252	1.92	0.40
6:H:74:GLY:HA2	8:L:92:TYR:HB3	2.03	0.40
7:I:34:ASN:OD1	7:I:34:ASN:N	2.55	0.40
8:L:105:VAL:HG12	8:L:192:PHE:CE2	2.57	0.40
1:a:208:LEU:HD21	12:a:841:BCR:HC42	2.03	0.40
2:b:207:VAL:O	2:b:208:ARG:NH1	2.47	0.40
2:b:461:GLN:HG2	2:b:472:TYR:CZ	2.57	0.40
3:c:70:TRP:CG	3:c:71:HIS:H	2.39	0.40
8:l:109:HIS:HA	8:l:112:LEU:CD2	2.51	0.40
12:l:309:BCR:H20C	12:l:309:BCR:H361	1.95	0.40
9:A:801:CLA:NA	9:B:803:CLA:HAB	2.36	0.40
9:A:815:CLA:H101	9:A:815:CLA:H13	1.82	0.40
9:A:822:CLA:H52	9:A:831:CLA:H2	2.03	0.40
12:A:840:BCR:H15C	12:A:841:BCR:H23C	2.03	0.40
12:A:842:BCR:HC31	9:h:202:CLA:H112	2.03	0.40
3:C:70:TRP:CG	3:C:71:HIS:H	2.39	0.40
1:a:360:LEU:HD11	9:a:817:CLA:H102	2.02	0.40
1:a:560:LEU:HD11	1:a:578:ARG:HB3	2.03	0.40
9:a:819:CLA:O1A	9:a:820:CLA:HBC1	2.22	0.40
2:b:90:ALA:HA	2:b:113:VAL:HG12	2.03	0.40
2:b:177:HIS:HE1	9:b:813:CLA:HMA3	1.85	0.40
1:A:141:PHE:CZ	9:A:825:CLA:HBA1	2.57	0.40
9:A:801:CLA:HBC1	2:B:625:TRP:HD1	1.86	0.40
9:A:828:CLA:H141	9:A:828:CLA:H161	1.82	0.40
12:A:843:BCR:H341	12:A:843:BCR:H11C	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:846:CLA:H62	9:A:846:CLA:H41	1.82	0.40
2:B:175:LEU:HD12	2:B:175:LEU:HA	1.94	0.40
2:B:193:HIS:HB2	9:B:815:CLA:CHC	2.51	0.40
2:B:461:GLN:HG2	2:B:472:TYR:CZ	2.57	0.40
2:B:657:TRP:CZ2	2:B:661:PHE:HZ	2.40	0.40
9:B:806:CLA:H122	9:B:806:CLA:H162	1.42	0.40
1:a:113:GLN:HB3	1:a:135:ILE:HG12	2.02	0.40
2:b:365:PHE:CD2	2:b:734:GLY:HA2	2.57	0.40
2:b:526:GLY:HA2	2:b:582:TRP:CZ3	2.57	0.40
9:b:824:CLA:H61	9:b:824:CLA:H101	1.74	0.40
7:i:34:ASN:OD1	7:i:34:ASN:N	2.55	0.40
12:l:304:BCR:H20C	12:l:304:BCR:H361	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	706/708 (100%)	680 (96%)	25 (4%)	1 (0%)	48	71
1	a	706/708 (100%)	679 (96%)	26 (4%)	1 (0%)	48	71
2	B	731/733 (100%)	711 (97%)	20 (3%)	0	100	100
2	b	731/733 (100%)	710 (97%)	21 (3%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
4	d	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
5	E	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
5	e	63/65 (97%)	62 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
6	h	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
7	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
7	i	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
8	L	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
8	l	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
All	All	4002/4034 (99%)	3871 (97%)	129 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	115	VAL
1	A	115	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/571 (100%)	570 (100%)	1 (0%)	87	95
1	a	571/571 (100%)	571 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
2	b	596/596 (100%)	596 (100%)	0	100	100
3	C	71/71 (100%)	71 (100%)	0	100	100
3	c	71/71 (100%)	71 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
4	d	121/121 (100%)	121 (100%)	0	100	100
5	E	58/58 (100%)	58 (100%)	0	100	100
5	e	58/58 (100%)	58 (100%)	0	100	100
6	H	77/77 (100%)	77 (100%)	0	100	100
6	h	77/77 (100%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	I	31/31 (100%)	31 (100%)	0	100 100
7	i	31/31 (100%)	31 (100%)	0	100 100
8	L	123/123 (100%)	121 (98%)	2 (2%)	55 73
8	l	123/123 (100%)	123 (100%)	0	100 100
All	All	3296/3296 (100%)	3293 (100%)	3 (0%)	87 95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
8	L	80	PRO
8	L	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	312	ASN
1	A	384	GLN
1	A	439	ASN
1	A	475	GLN
2	B	114	ASN
2	B	158	GLN
2	B	294	ASN
2	B	333	GLN
2	B	350	GLN
2	B	502	ASN
8	L	211	ASN
1	a	214	GLN
1	a	312	ASN
1	a	384	GLN
1	a	439	ASN
2	b	114	ASN
2	b	158	GLN
2	b	294	ASN
2	b	328	ASN
2	b	350	GLN
2	b	502	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

202 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	CLA	B	816	2	50,54,73	1.34	6 (12%)	60,90,113	1.13	4 (6%)
9	CLA	B	817	2	59,63,73	1.26	6 (10%)	71,101,113	1.00	4 (5%)
9	CLA	b	840	-	52,56,73	1.35	7 (13%)	62,92,113	0.99	3 (4%)
9	CLA	A	823	1	69,73,73	1.19	7 (10%)	83,113,113	0.89	5 (6%)
9	CLA	a	802	-	69,73,73	1.15	7 (10%)	83,113,113	0.98	5 (6%)
13	SF4	a	845	1,2	0,12,12	-	-	-		
14	DGD	B	837	-	67,67,67	0.81	2 (2%)	81,81,81	1.01	3 (3%)
9	CLA	A	832	1	69,73,73	1.16	6 (8%)	83,113,113	0.98	4 (4%)
10	PQN	b	833	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
13	SF4	c	102	3	0,12,12	-	-	-		
9	CLA	B	806	2	69,73,73	1.18	7 (10%)	83,113,113	0.94	3 (3%)
9	CLA	a	807	-	69,73,73	1.10	6 (8%)	83,113,113	0.98	4 (4%)
9	CLA	B	810	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
12	BCR	B	834	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
9	CLA	A	809	-	69,73,73	1.16	6 (8%)	83,113,113	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SF4	c	101	3	0,12,12	-	-	-		
14	DGD	b	837	-	67,67,67	0.81	2 (2%)	81,81,81	1.02	4 (4%)
9	CLA	b	816	2	50,54,73	1.33	6 (12%)	60,90,113	1.15	4 (6%)
9	CLA	b	817	2	59,63,73	1.26	6 (10%)	71,101,113	1.00	4 (5%)
9	CLA	b	821	-	68,72,73	1.21	7 (10%)	85,112,113	0.96	4 (4%)
9	CLA	B	822	2	51,55,73	1.40	6 (11%)	61,91,113	1.06	4 (6%)
9	CLA	B	803	2	69,73,73	1.17	7 (10%)	83,113,113	0.89	4 (4%)
15	LMT	b	838	-	36,36,36	0.22	0	47,47,47	0.41	0
9	CLA	b	813	2	47,52,73	1.28	5 (10%)	55,87,113	1.07	3 (5%)
9	CLA	A	814	-	49,53,73	1.38	7 (14%)	59,89,113	1.18	6 (10%)
12	BCR	b	834	-	41,41,41	1.71	8 (19%)	56,56,56	1.68	13 (23%)
9	CLA	a	822	-	69,73,73	1.14	6 (8%)	83,113,113	0.94	4 (4%)
12	BCR	L	306	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
9	CLA	a	815	1	69,73,73	1.18	6 (8%)	83,113,113	0.92	3 (3%)
9	CLA	a	804	1	69,73,73	1.16	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	a	836	-	69,73,73	1.13	5 (7%)	83,113,113	1.06	5 (6%)
9	CLA	b	818	2	63,67,73	1.19	6 (9%)	75,105,113	1.07	5 (6%)
9	CLA	B	819	2	64,68,73	1.24	7 (10%)	77,107,113	0.98	4 (5%)
10	PQN	A	837	-	34,34,34	0.35	0	42,45,45	0.56	0
15	LMT	B	838	-	36,36,36	0.21	0	47,47,47	0.40	0
12	BCR	B	835	-	41,41,41	1.70	8 (19%)	56,56,56	1.70	12 (21%)
9	CLA	a	816	1	69,73,73	1.14	7 (10%)	83,113,113	1.07	8 (9%)
9	CLA	a	820	1	55,59,73	3.04	16 (29%)	66,96,113	3.57	30 (45%)
9	CLA	A	801	1	69,73,73	1.16	7 (10%)	83,113,113	1.00	5 (6%)
9	CLA	a	837	1	52,56,73	1.35	6 (11%)	62,92,113	1.08	5 (8%)
9	CLA	b	820	-	54,58,73	1.44	7 (12%)	65,95,113	1.12	5 (7%)
9	CLA	a	824	1	69,73,73	1.16	7 (10%)	83,113,113	0.91	5 (6%)
12	BCR	A	840	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	12 (21%)
9	CLA	A	846	-	69,73,73	1.17	7 (10%)	83,113,113	0.99	4 (4%)
9	CLA	A	805	1	69,73,73	1.17	6 (8%)	83,113,113	0.90	3 (3%)
13	SF4	A	844	1,2	0,12,12	-	-	-		
9	CLA	B	812	2	58,62,73	1.33	8 (13%)	73,100,113	1.10	4 (5%)
9	CLA	a	818	1	49,53,73	1.36	6 (12%)	59,89,113	0.96	3 (5%)
9	CLA	a	835	1	51,55,73	1.35	6 (11%)	61,91,113	1.01	4 (6%)
9	CLA	l	305	8	53,57,73	1.37	6 (11%)	62,93,113	1.20	5 (8%)
9	CLA	B	802	-	69,73,73	1.19	7 (10%)	83,113,113	0.91	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	SF4	C	102	3	0,12,12	-	-	-		
9	CLA	A	822	-	69,73,73	1.17	6 (8%)	83,113,113	0.89	3 (3%)
9	CLA	a	808	1	69,73,73	1.14	6 (8%)	83,113,113	1.02	5 (6%)
9	CLA	b	803	2	69,73,73	1.17	7 (10%)	83,113,113	0.90	4 (4%)
12	BCR	L	305	-	41,41,41	1.69	8 (19%)	56,56,56	1.59	10 (17%)
9	CLA	B	805	2	49,53,73	1.41	7 (14%)	59,89,113	1.11	4 (6%)
9	CLA	b	814	2	69,73,73	1.17	7 (10%)	83,113,113	0.93	3 (3%)
9	CLA	A	828	1	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	A	831	1	55,59,73	1.36	7 (12%)	66,96,113	1.05	4 (6%)
9	CLA	a	812	1	49,53,73	1.43	8 (16%)	59,89,113	1.24	5 (8%)
9	CLA	a	810	1	58,62,73	1.24	6 (10%)	69,99,113	1.03	4 (5%)
9	CLA	a	826	1	69,73,73	1.21	7 (10%)	83,113,113	0.92	4 (4%)
9	CLA	b	832	2	69,73,73	1.17	6 (8%)	83,113,113	0.98	3 (3%)
9	CLA	b	809	-	69,73,73	1.21	7 (10%)	83,113,113	0.91	4 (4%)
9	CLA	a	827	1	69,73,73	1.25	8 (11%)	83,113,113	0.95	4 (4%)
9	CLA	b	802	-	69,73,73	1.24	8 (11%)	83,113,113	0.98	5 (6%)
12	BCR	a	842	-	41,41,41	1.71	8 (19%)	56,56,56	1.58	11 (19%)
9	CLA	L	304	-	54,58,73	1.30	6 (11%)	65,95,113	1.18	5 (7%)
9	CLA	B	829	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
9	CLA	l	306	8	69,73,73	1.16	6 (8%)	83,113,113	0.95	4 (4%)
9	CLA	b	824	-	64,68,73	1.26	7 (10%)	77,107,113	0.94	3 (3%)
9	CLA	B	807	2	69,73,73	1.22	8 (11%)	83,113,113	0.88	3 (3%)
12	BCR	a	841	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	12 (21%)
9	CLA	b	810	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	L	308	11	56,60,73	1.40	7 (12%)	67,97,113	1.55	10 (14%)
9	CLA	b	830	2	51,55,73	1.36	7 (13%)	61,91,113	1.10	4 (6%)
9	CLA	A	833	1	69,73,73	1.17	6 (8%)	83,113,113	0.94	4 (4%)
9	CLA	b	807	2	69,73,73	1.21	8 (11%)	83,113,113	0.88	3 (3%)
9	CLA	b	806	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	3 (3%)
11	LHG	a	840	9	26,26,48	0.35	0	29,32,54	0.49	0
9	CLA	A	836	1	52,56,73	1.35	6 (11%)	62,92,113	1.10	5 (8%)
9	CLA	B	832	2	69,73,73	1.18	6 (8%)	83,113,113	0.98	3 (3%)
9	CLA	B	827	2	49,53,73	1.34	7 (14%)	59,89,113	1.25	5 (8%)
12	BCR	l	308	-	41,41,41	1.68	8 (19%)	56,56,56	1.59	10 (17%)
9	CLA	a	847	1	69,73,73	1.20	8 (11%)	83,113,113	0.98	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	LHG	A	838	-	48,48,48	0.28	0	51,54,54	0.32	0
9	CLA	b	826	2	52,56,73	1.34	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	b	839	2	52,56,73	1.33	6 (11%)	62,92,113	1.07	4 (6%)
9	CLA	A	808	1	69,73,73	1.13	6 (8%)	83,113,113	1.08	4 (4%)
9	CLA	b	805	2	49,53,73	1.41	7 (14%)	59,89,113	1.12	4 (6%)
9	CLA	A	825	1	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
9	CLA	B	804	-	69,73,73	1.17	7 (10%)	83,113,113	1.00	5 (6%)
12	BCR	h	203	-	41,41,41	1.70	8 (19%)	56,56,56	1.72	12 (21%)
12	BCR	a	844	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	11 (19%)
9	CLA	B	814	2	69,73,73	1.17	7 (10%)	83,113,113	0.92	3 (3%)
9	CLA	A	811	1	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
9	CLA	a	833	1	69,73,73	1.16	7 (10%)	83,113,113	0.97	4 (4%)
9	CLA	A	803	-	59,63,73	1.25	7 (11%)	71,101,113	1.04	5 (7%)
9	CLA	a	825	1	69,73,73	1.13	6 (8%)	83,113,113	1.05	5 (6%)
9	CLA	a	829	1	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	A	835	-	69,73,73	1.13	5 (7%)	83,113,113	1.06	5 (6%)
12	BCR	b	835	-	41,41,41	1.69	8 (19%)	56,56,56	1.68	13 (23%)
9	CLA	A	834	1	51,55,73	1.35	6 (11%)	61,91,113	1.01	4 (6%)
9	CLA	A	817	1	69,73,73	1.17	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	B	808	2	59,63,73	1.28	6 (10%)	71,101,113	1.01	3 (4%)
9	CLA	A	807	-	69,73,73	1.13	6 (8%)	83,113,113	0.94	4 (4%)
12	BCR	A	841	-	41,41,41	1.71	8 (19%)	56,56,56	1.56	11 (19%)
9	CLA	b	828	2	55,59,73	1.37	8 (14%)	66,96,113	1.05	4 (6%)
9	CLA	B	820	-	54,58,73	1.38	7 (12%)	65,95,113	1.01	4 (6%)
9	CLA	A	812	1	49,53,73	1.43	7 (14%)	59,89,113	1.29	7 (11%)
9	CLA	H	201	6	69,73,73	1.25	8 (11%)	83,113,113	0.98	4 (4%)
11	LHG	a	839	-	48,48,48	0.28	0	51,54,54	0.32	0
9	CLA	B	828	2	55,59,73	1.38	8 (14%)	66,96,113	1.06	4 (6%)
9	CLA	B	824	-	64,68,73	1.25	7 (10%)	77,107,113	0.94	3 (3%)
9	CLA	a	819	-	69,73,73	1.26	10 (14%)	83,113,113	1.17	7 (8%)
9	CLA	b	808	2	59,63,73	1.28	7 (11%)	71,101,113	1.02	4 (5%)
9	CLA	b	812	2	58,62,73	1.36	7 (12%)	73,100,113	1.09	5 (6%)
9	CLA	a	805	1	69,73,73	1.18	6 (8%)	83,113,113	0.90	4 (4%)
9	CLA	A	826	1	69,73,73	1.26	8 (11%)	83,113,113	0.95	4 (4%)
9	CLA	b	819	2	64,68,73	1.23	7 (10%)	77,107,113	1.01	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	b	827	2	49,53,73	1.34	7 (14%)	59,89,113	1.26	5 (8%)
9	CLA	A	813	1	54,58,73	1.28	6 (11%)	65,95,113	1.11	4 (6%)
9	CLA	B	831	-	69,73,73	1.21	8 (11%)	83,113,113	0.93	4 (4%)
9	CLA	h	202	6	69,73,73	1.23	8 (11%)	83,113,113	0.99	5 (6%)
9	CLA	h	201	1	55,59,73	1.58	11 (20%)	66,96,113	1.86	14 (21%)
9	CLA	a	801	1	69,73,73	1.16	7 (10%)	83,113,113	1.00	5 (6%)
9	CLA	A	802	-	69,73,73	1.15	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	B	826	2	52,56,73	1.34	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	a	806	-	69,73,73	1.14	6 (8%)	83,113,113	0.91	4 (4%)
9	CLA	A	821	-	69,73,73	1.16	7 (10%)	83,113,113	1.01	5 (6%)
9	CLA	a	814	-	49,53,73	1.37	7 (14%)	59,89,113	1.18	6 (10%)
9	CLA	a	828	1	54,58,73	1.31	6 (11%)	65,95,113	1.01	3 (4%)
9	CLA	b	801	-	69,73,73	1.20	7 (10%)	83,113,113	0.97	4 (4%)
9	CLA	B	813	2	47,52,73	1.29	5 (10%)	55,87,113	1.05	3 (5%)
9	CLA	l	302	-	56,60,73	1.35	8 (14%)	67,97,113	0.98	3 (4%)
9	CLA	a	830	1	69,73,73	1.21	8 (11%)	83,113,113	1.03	4 (4%)
12	BCR	L	301	-	41,41,41	1.68	8 (19%)	56,56,56	1.46	8 (14%)
11	LHG	l	303	-	48,48,48	0.28	0	51,54,54	0.34	0
13	SF4	C	101	3	0,12,12	-	-	-		
9	CLA	a	846	-	69,73,73	1.17	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	A	819	-	69,73,73	3.00	13 (18%)	83,113,113	10.30	14 (16%)
9	CLA	b	822	2	51,55,73	1.39	7 (13%)	61,91,113	1.09	5 (8%)
9	CLA	b	815	2	69,73,73	1.21	7 (10%)	83,113,113	0.98	5 (6%)
9	CLA	l	307	-	54,58,73	1.33	6 (11%)	65,95,113	1.09	5 (7%)
9	CLA	A	818	1	49,53,73	1.37	6 (12%)	59,89,113	0.97	3 (5%)
12	BCR	H	202	-	41,41,41	1.70	8 (19%)	56,56,56	1.78	13 (23%)
9	CLA	a	817	1	69,73,73	1.16	6 (8%)	83,113,113	0.99	4 (4%)
12	BCR	a	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	12 (21%)
9	CLA	A	829	1	69,73,73	1.20	7 (10%)	83,113,113	1.04	4 (4%)
9	CLA	b	811	2	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
9	CLA	L	303	8	69,73,73	1.15	6 (8%)	83,113,113	0.92	4 (4%)
9	CLA	B	823	2	69,73,73	1.19	7 (10%)	83,113,113	1.05	5 (6%)
9	CLA	A	816	1	69,73,73	1.14	6 (8%)	83,113,113	1.03	5 (6%)
9	CLA	B	839	2	52,56,73	1.33	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	b	804	-	69,73,73	1.16	7 (10%)	83,113,113	0.99	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	804	1	69,73,73	1.16	6 (8%)	83,113,113	0.97	4 (4%)
9	CLA	B	825	2	69,73,73	1.20	8 (11%)	83,113,113	0.96	4 (4%)
9	CLA	A	830	1	54,58,73	1.26	5 (9%)	65,95,113	1.05	5 (7%)
9	CLA	L	307	-	49,53,73	1.30	5 (10%)	59,89,113	1.53	11 (18%)
9	CLA	a	823	-	69,73,73	1.17	6 (8%)	83,113,113	0.91	3 (3%)
9	CLA	a	834	1	69,73,73	1.17	6 (8%)	83,113,113	0.94	4 (4%)
9	CLA	B	809	-	69,73,73	1.20	7 (10%)	83,113,113	0.89	4 (4%)
9	CLA	a	803	-	59,63,73	1.25	7 (11%)	71,101,113	1.03	5 (7%)
12	BCR	I	101	-	41,41,41	1.67	8 (19%)	56,56,56	1.53	11 (19%)
9	CLA	A	827	1	54,58,73	1.31	6 (11%)	65,95,113	1.04	3 (4%)
9	CLA	a	832	1	55,59,73	1.37	7 (12%)	66,96,113	1.04	4 (6%)
12	BCR	A	842	-	41,41,41	1.68	8 (19%)	56,56,56	1.52	11 (19%)
9	CLA	A	815	1	69,73,73	1.19	6 (8%)	83,113,113	0.91	3 (3%)
9	CLA	B	801	-	69,73,73	1.20	8 (11%)	83,113,113	0.98	5 (6%)
10	PQN	a	838	-	34,34,34	0.36	0	42,45,45	0.55	0
12	BCR	l	309	-	41,41,41	1.69	8 (19%)	56,56,56	1.69	13 (23%)
12	BCR	l	304	-	41,41,41	1.67	8 (19%)	56,56,56	1.47	9 (16%)
9	CLA	B	815	2	69,73,73	1.22	8 (11%)	83,113,113	0.96	6 (7%)
11	LHG	A	845	-	48,48,48	0.28	0	51,54,54	0.36	0
9	CLA	a	809	-	69,73,73	1.16	6 (8%)	83,113,113	0.91	3 (3%)
12	BCR	i	101	-	41,41,41	1.66	8 (19%)	56,56,56	1.53	11 (19%)
12	BCR	A	843	-	41,41,41	1.69	8 (19%)	56,56,56	1.57	10 (17%)
9	CLA	a	831	1	54,58,73	1.22	5 (9%)	65,95,113	1.09	7 (10%)
9	CLA	b	823	2	69,73,73	1.18	6 (8%)	83,113,113	1.06	5 (6%)
9	CLA	l	301	-	49,53,73	1.40	6 (12%)	59,89,113	1.83	12 (20%)
9	CLA	A	806	-	69,73,73	1.12	7 (10%)	83,113,113	1.13	9 (10%)
9	CLA	b	829	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	4 (4%)
9	CLA	A	847	1	69,73,73	1.20	8 (11%)	83,113,113	0.97	4 (4%)
9	CLA	B	830	2	51,55,73	1.35	7 (13%)	61,91,113	1.12	5 (8%)
9	CLA	a	813	1	54,58,73	1.28	6 (11%)	65,95,113	1.07	4 (6%)
9	CLA	A	820	1	59,63,73	1.20	6 (10%)	71,101,113	1.08	4 (5%)
12	BCR	B	836	-	41,41,41	1.66	8 (19%)	56,56,56	1.57	10 (17%)
9	CLA	B	818	2	63,67,73	1.19	6 (9%)	75,105,113	1.07	5 (6%)
9	CLA	b	825	2	69,73,73	1.20	8 (11%)	83,113,113	0.98	4 (4%)
11	LHG	A	839	-	26,26,48	0.36	0	29,32,54	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	B	821	-	68,72,73	1.21	7 (10%)	85,112,113	0.95	4 (4%)
9	CLA	B	840	-	52,56,73	1.34	7 (13%)	62,92,113	0.98	3 (4%)
9	CLA	a	811	1	69,73,73	1.16	6 (8%)	83,113,113	0.95	4 (4%)
9	CLA	b	831	-	69,73,73	1.21	8 (11%)	83,113,113	0.93	4 (4%)
10	PQN	B	833	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
9	CLA	A	810	1	58,62,73	1.25	6 (10%)	69,99,113	1.06	4 (5%)
9	CLA	A	824	1	69,73,73	1.14	6 (8%)	83,113,113	1.05	6 (7%)
9	CLA	L	302	8	53,57,73	1.37	6 (11%)	62,93,113	1.19	5 (8%)
9	CLA	a	821	1	59,63,73	1.22	6 (10%)	71,101,113	1.07	4 (5%)
9	CLA	B	811	2	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
12	BCR	b	836	-	41,41,41	1.66	8 (19%)	56,56,56	1.57	10 (17%)

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
9	CLA	B	816	2	-	11/17/93/115	-
9	CLA	B	817	2	-	12/27/103/115	-
9	CLA	b	840	-	-	8/19/95/115	-
9	CLA	A	823	1	-	13/39/115/115	-
9	CLA	a	802	-	-	17/39/115/115	-
14	DGD	B	837	-	-	32/55/95/95	0/2/2/2
13	SF4	a	845	1,2	-	-	0/6/5/5
9	CLA	A	832	1	-	14/39/115/115	-
10	PQN	b	833	-	-	2/23/43/43	0/2/2/2
13	SF4	c	102	3	-	-	0/6/5/5
9	CLA	B	806	2	-	17/39/115/115	-
9	CLA	a	807	-	-	23/39/115/115	-
9	CLA	B	810	2	-	16/39/115/115	-
12	BCR	B	834	-	-	22/29/63/63	0/2/2/2
9	CLA	A	809	-	-	20/39/115/115	-
14	DGD	b	837	-	-	29/55/95/95	0/2/2/2
13	SF4	c	101	3	-	-	0/6/5/5
9	CLA	b	816	2	-	11/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	b	817	2	-	12/27/103/115	-
9	CLA	b	821	-	-	15/37/113/115	-
9	CLA	B	822	2	-	10/18/94/115	-
9	CLA	B	803	2	-	15/39/115/115	-
15	LMT	b	838	-	-	17/21/61/61	0/2/2/2
9	CLA	b	813	2	-	4/14/91/115	-
9	CLA	A	814	-	-	4/15/91/115	-
12	BCR	b	834	-	-	20/29/63/63	0/2/2/2
9	CLA	a	822	-	-	14/39/115/115	-
12	BCR	L	306	-	-	18/29/63/63	0/2/2/2
9	CLA	a	815	1	-	27/39/115/115	-
9	CLA	a	804	1	-	11/39/115/115	-
9	CLA	a	836	-	-	21/39/115/115	-
9	CLA	b	818	2	-	17/32/108/115	-
9	CLA	B	819	2	-	18/33/109/115	-
10	PQN	A	837	-	-	12/23/43/43	0/2/2/2
15	LMT	B	838	-	-	16/21/61/61	0/2/2/2
12	BCR	B	835	-	-	26/29/63/63	0/2/2/2
9	CLA	a	816	1	-	19/39/115/115	-
9	CLA	a	820	1	-	12/23/99/115	-
9	CLA	A	801	1	-	18/39/115/115	-
9	CLA	a	837	1	-	6/19/95/115	-
9	CLA	b	820	-	-	9/21/97/115	-
9	CLA	a	824	1	-	23/39/115/115	-
12	BCR	A	840	-	-	18/29/63/63	0/2/2/2
9	CLA	A	846	-	-	17/39/115/115	-
9	CLA	A	805	1	-	17/39/115/115	-
13	SF4	A	844	1,2	-	-	0/6/5/5
9	CLA	B	812	2	-	11/25/101/115	-
9	CLA	a	818	1	-	7/15/91/115	-
9	CLA	a	835	1	-	10/18/94/115	-
9	CLA	l	305	8	-	8/20/96/115	-
9	CLA	B	802	-	-	22/39/115/115	-
13	SF4	C	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	822	-	-	14/39/115/115	-
9	CLA	a	808	1	-	23/39/115/115	-
9	CLA	b	803	2	-	15/39/115/115	-
12	BCR	L	305	-	-	16/29/63/63	0/2/2/2
9	CLA	B	805	2	-	5/15/91/115	-
9	CLA	b	814	2	-	19/39/115/115	-
9	CLA	A	828	1	-	13/39/115/115	-
9	CLA	A	831	1	-	12/23/99/115	-
9	CLA	a	812	1	-	3/15/91/115	-
9	CLA	a	810	1	-	10/26/102/115	-
9	CLA	a	826	1	-	16/39/115/115	-
9	CLA	b	832	2	-	13/39/115/115	-
9	CLA	b	809	-	-	10/39/115/115	-
9	CLA	a	827	1	-	14/39/115/115	-
9	CLA	b	802	-	-	20/39/115/115	-
12	BCR	a	842	-	-	20/29/63/63	0/2/2/2
9	CLA	L	304	-	-	9/21/97/115	-
9	CLA	B	829	2	-	13/39/115/115	-
9	CLA	l	306	8	-	20/39/115/115	-
9	CLA	b	824	-	-	19/33/109/115	-
9	CLA	B	807	2	-	19/39/115/115	-
12	BCR	a	841	-	-	20/29/63/63	0/2/2/2
9	CLA	b	810	2	-	16/39/115/115	-
9	CLA	L	308	11	-	11/24/100/115	-
9	CLA	b	830	2	-	3/18/94/115	-
9	CLA	A	833	1	-	22/39/115/115	-
9	CLA	b	807	2	-	19/39/115/115	-
9	CLA	b	806	2	-	14/39/115/115	-
11	LHG	a	840	9	-	16/31/31/53	-
9	CLA	A	836	1	-	6/19/95/115	-
9	CLA	B	832	2	-	11/39/115/115	-
9	CLA	B	827	2	-	7/15/91/115	-
12	BCR	l	308	-	-	17/29/63/63	0/2/2/2
9	CLA	a	847	1	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LHG	A	838	-	-	34/53/53/53	-
9	CLA	b	826	2	-	7/19/95/115	-
9	CLA	b	839	2	-	7/19/95/115	-
9	CLA	A	808	1	-	23/39/115/115	-
9	CLA	b	805	2	-	5/15/91/115	-
9	CLA	A	825	1	-	17/39/115/115	-
9	CLA	B	804	-	-	17/39/115/115	-
12	BCR	h	203	-	-	23/29/63/63	0/2/2/2
12	BCR	a	844	-	-	20/29/63/63	0/2/2/2
9	CLA	B	814	2	-	18/39/115/115	-
9	CLA	A	811	1	-	23/39/115/115	-
9	CLA	a	833	1	-	14/39/115/115	-
9	CLA	A	803	-	-	12/27/103/115	-
9	CLA	a	825	1	-	21/39/115/115	-
9	CLA	a	829	1	-	13/39/115/115	-
9	CLA	A	835	-	-	21/39/115/115	-
12	BCR	b	835	-	-	24/29/63/63	0/2/2/2
9	CLA	A	834	1	-	10/18/94/115	-
9	CLA	A	817	1	-	22/39/115/115	-
9	CLA	B	808	2	-	9/27/103/115	-
9	CLA	A	807	-	-	23/39/115/115	-
12	BCR	A	841	-	-	19/29/63/63	0/2/2/2
9	CLA	b	828	2	-	10/23/99/115	-
9	CLA	B	820	-	-	10/21/97/115	-
9	CLA	A	812	1	-	4/15/91/115	-
9	CLA	H	201	6	-	21/39/115/115	-
11	LHG	a	839	-	-	34/53/53/53	-
9	CLA	B	828	2	-	6/23/99/115	-
9	CLA	B	824	-	-	19/33/109/115	-
9	CLA	a	819	-	-	18/39/115/115	-
9	CLA	b	808	2	-	9/27/103/115	-
9	CLA	b	812	2	-	6/25/101/115	-
9	CLA	a	805	1	-	16/39/115/115	-
9	CLA	A	826	1	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	b	819	2	-	20/33/109/115	-
9	CLA	b	827	2	-	6/15/91/115	-
9	CLA	A	813	1	-	8/21/97/115	-
9	CLA	B	831	-	-	13/39/115/115	-
9	CLA	h	202	6	-	22/39/115/115	-
9	CLA	h	201	1	-	15/23/99/115	-
9	CLA	a	801	1	-	16/39/115/115	-
9	CLA	A	802	-	-	16/39/115/115	-
9	CLA	B	826	2	-	8/19/95/115	-
9	CLA	a	806	-	-	24/39/115/115	-
9	CLA	A	821	-	-	20/39/115/115	-
9	CLA	a	814	-	-	4/15/91/115	-
9	CLA	a	828	1	-	6/21/97/115	-
9	CLA	b	801	-	-	22/39/115/115	-
9	CLA	B	813	2	-	6/14/91/115	-
9	CLA	l	302	-	-	11/24/100/115	-
9	CLA	a	830	1	-	24/39/115/115	-
12	BCR	L	301	-	-	16/29/63/63	0/2/2/2
11	LHG	l	303	-	-	31/53/53/53	-
13	SF4	C	101	3	-	-	0/6/5/5
9	CLA	a	846	-	-	24/39/115/115	-
9	CLA	A	819	-	-	26/39/115/115	-
9	CLA	b	822	2	-	10/18/94/115	-
9	CLA	b	815	2	-	15/39/115/115	-
9	CLA	l	307	-	-	8/21/97/115	-
9	CLA	A	818	1	-	8/15/91/115	-
12	BCR	H	202	-	-	23/29/63/63	0/2/2/2
9	CLA	a	817	1	-	22/39/115/115	-
12	BCR	a	843	-	-	19/29/63/63	0/2/2/2
9	CLA	A	829	1	-	25/39/115/115	-
9	CLA	b	811	2	-	19/39/115/115	-
9	CLA	L	303	8	-	21/39/115/115	-
9	CLA	B	823	2	-	15/39/115/115	-
9	CLA	A	816	1	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	839	2	-	9/19/95/115	-
9	CLA	b	804	-	-	20/39/115/115	-
9	CLA	A	804	1	-	11/39/115/115	-
9	CLA	B	825	2	-	14/39/115/115	-
9	CLA	A	830	1	-	14/21/97/115	-
9	CLA	L	307	-	-	11/15/91/115	-
9	CLA	a	823	-	-	13/39/115/115	-
9	CLA	a	834	1	-	22/39/115/115	-
9	CLA	B	809	-	-	10/39/115/115	-
9	CLA	a	803	-	-	14/27/103/115	-
12	BCR	I	101	-	-	16/29/63/63	0/2/2/2
9	CLA	A	827	1	-	8/21/97/115	-
9	CLA	a	832	1	-	14/23/99/115	-
12	BCR	A	842	-	-	16/29/63/63	0/2/2/2
9	CLA	A	815	1	-	23/39/115/115	-
9	CLA	B	801	-	-	22/39/115/115	-
10	PQN	a	838	-	-	11/23/43/43	0/2/2/2
12	BCR	l	309	-	-	18/29/63/63	0/2/2/2
12	BCR	l	304	-	-	18/29/63/63	0/2/2/2
9	CLA	B	815	2	-	14/39/115/115	-
11	LHG	A	845	-	-	35/53/53/53	-
9	CLA	a	809	-	-	20/39/115/115	-
12	BCR	i	101	-	-	17/29/63/63	0/2/2/2
12	BCR	A	843	-	-	13/29/63/63	0/2/2/2
9	CLA	a	831	1	-	10/21/97/115	-
9	CLA	b	823	2	-	18/39/115/115	-
9	CLA	l	301	-	-	8/15/91/115	-
9	CLA	A	806	-	-	24/39/115/115	-
9	CLA	b	829	2	-	14/39/115/115	-
9	CLA	A	847	1	-	23/39/115/115	-
9	CLA	B	830	2	-	3/18/94/115	-
9	CLA	a	813	1	-	6/21/97/115	-
9	CLA	A	820	1	-	13/27/103/115	-
12	BCR	B	836	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	818	2	-	17/32/108/115	-
9	CLA	b	825	2	-	14/39/115/115	-
11	LHG	A	839	-	-	15/31/31/53	-
9	CLA	B	821	-	-	17/37/113/115	-
9	CLA	B	840	-	-	7/19/95/115	-
9	CLA	a	811	1	-	23/39/115/115	-
9	CLA	b	831	-	-	13/39/115/115	-
10	PQN	B	833	-	-	2/23/43/43	0/2/2/2
9	CLA	A	810	1	-	10/26/102/115	-
9	CLA	A	824	1	-	19/39/115/115	-
9	CLA	L	302	8	-	8/20/96/115	-
9	CLA	a	821	1	-	14/27/103/115	-
9	CLA	B	811	2	-	18/39/115/115	-
12	BCR	b	836	-	-	16/29/63/63	0/2/2/2

All (1268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	CLA	C1D-C2D	-16.73	1.12	1.45
9	a	820	CLA	MG-NB	12.48	2.30	2.05
9	A	819	CLA	C3D-C2D	11.31	1.70	1.39
9	a	820	CLA	MG-ND	11.03	2.27	2.05
9	A	819	CLA	C4D-ND	-7.44	1.27	1.37
9	a	820	CLA	CHB-C1B	6.49	1.54	1.39
9	a	820	CLA	C3D-C2D	4.85	1.52	1.39
9	B	801	CLA	C1C-C2C	-4.85	1.35	1.44
9	l	301	CLA	C1C-C2C	-4.84	1.35	1.44
9	A	819	CLA	C4C-C3C	-4.82	1.36	1.45
9	b	820	CLA	MG-NA	4.81	2.17	2.06
9	b	801	CLA	C1C-C2C	-4.79	1.35	1.44
9	l	302	CLA	C1C-C2C	-4.78	1.35	1.44
9	B	824	CLA	C4C-C3C	-4.77	1.36	1.45
9	A	819	CLA	C3D-CAD	4.76	1.61	1.45
9	b	824	CLA	C4C-C3C	-4.75	1.36	1.45
9	B	822	CLA	C4C-C3C	-4.69	1.37	1.45
9	l	306	CLA	C4C-C3C	-4.68	1.37	1.45
9	L	303	CLA	C4C-C3C	-4.67	1.37	1.45
9	A	825	CLA	C4C-C3C	-4.67	1.37	1.45
9	b	822	CLA	C4C-C3C	-4.66	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	818	CLA	C1C-C2C	-4.66	1.35	1.44
9	b	805	CLA	C4C-C3C	-4.65	1.37	1.45
9	a	824	CLA	C4C-C3C	-4.65	1.37	1.45
9	A	829	CLA	C1C-C2C	-4.64	1.35	1.44
9	b	803	CLA	C4C-C3C	-4.63	1.37	1.45
9	B	832	CLA	C4C-C3C	-4.63	1.37	1.45
9	b	819	CLA	C4C-C3C	-4.63	1.37	1.45
9	B	839	CLA	C1C-C2C	-4.62	1.35	1.44
9	B	818	CLA	C1C-C2C	-4.62	1.35	1.44
9	A	828	CLA	C1C-C2C	-4.62	1.35	1.44
9	B	803	CLA	C4C-C3C	-4.62	1.37	1.45
9	A	823	CLA	C4C-C3C	-4.62	1.37	1.45
9	b	808	CLA	C4C-C3C	-4.62	1.37	1.45
9	b	809	CLA	C4C-C3C	-4.62	1.37	1.45
9	B	805	CLA	C4C-C3C	-4.61	1.37	1.45
9	a	829	CLA	C1C-C2C	-4.61	1.35	1.44
9	h	201	CLA	C1B-C2B	4.61	1.54	1.43
9	B	809	CLA	C4C-C3C	-4.61	1.37	1.45
9	b	832	CLA	C4C-C3C	-4.60	1.37	1.45
9	l	305	CLA	C4C-C3C	-4.59	1.37	1.45
9	b	839	CLA	C1C-C2C	-4.59	1.35	1.44
9	B	807	CLA	C4C-C3C	-4.59	1.37	1.45
9	B	809	CLA	C1C-C2C	-4.59	1.35	1.44
9	a	826	CLA	C4C-C3C	-4.59	1.37	1.45
9	B	819	CLA	C4C-C3C	-4.59	1.37	1.45
9	b	809	CLA	C1C-C2C	-4.59	1.35	1.44
9	B	804	CLA	C1C-C2C	-4.59	1.35	1.44
9	B	808	CLA	C4C-C3C	-4.58	1.37	1.45
9	A	815	CLA	C4C-C3C	-4.58	1.37	1.45
9	B	822	CLA	C1C-C2C	-4.58	1.35	1.44
9	b	803	CLA	C1C-C2C	-4.58	1.35	1.44
9	a	821	CLA	C1C-C2C	-4.58	1.35	1.44
9	B	832	CLA	C1C-C2C	-4.58	1.35	1.44
9	a	815	CLA	C4C-C3C	-4.58	1.37	1.45
9	b	822	CLA	C1C-C2C	-4.57	1.35	1.44
9	a	802	CLA	C4C-C3C	-4.57	1.37	1.45
9	b	807	CLA	C4C-C3C	-4.57	1.37	1.45
9	b	812	CLA	MG-NA	4.57	2.17	2.06
9	A	819	CLA	C1C-C2C	-4.57	1.35	1.44
9	h	202	CLA	C1C-C2C	-4.56	1.35	1.44
9	A	832	CLA	C1C-C2C	-4.56	1.35	1.44
9	A	802	CLA	C4C-C3C	-4.56	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	802	CLA	C4C-C3C	-4.56	1.37	1.45
9	A	801	CLA	C4C-C3C	-4.55	1.37	1.45
9	A	808	CLA	C4C-C3C	-4.55	1.37	1.45
9	A	827	CLA	C4C-C3C	-4.55	1.37	1.45
9	A	836	CLA	C1C-C2C	-4.55	1.35	1.44
9	A	817	CLA	C4C-C3C	-4.55	1.37	1.45
9	b	815	CLA	C1C-C2C	-4.55	1.35	1.44
9	A	811	CLA	C1C-C2C	-4.55	1.35	1.44
9	b	804	CLA	C1C-C2C	-4.54	1.35	1.44
9	b	832	CLA	C1C-C2C	-4.54	1.35	1.44
9	A	822	CLA	C4C-C3C	-4.54	1.37	1.45
9	a	847	CLA	C4C-C3C	-4.54	1.37	1.45
9	B	803	CLA	C1C-C2C	-4.54	1.35	1.44
9	B	807	CLA	C1C-C2C	-4.54	1.35	1.44
9	b	828	CLA	C1C-C2C	-4.54	1.35	1.44
9	B	815	CLA	C4C-C3C	-4.54	1.37	1.45
9	A	826	CLA	C1C-C2C	-4.54	1.35	1.44
9	a	814	CLA	C4C-C3C	-4.54	1.37	1.45
9	a	831	CLA	C4C-C3C	-4.54	1.37	1.45
9	A	820	CLA	C1C-C2C	-4.54	1.35	1.44
9	a	819	CLA	C4C-C3C	-4.54	1.37	1.45
9	a	829	CLA	C4C-C3C	-4.53	1.37	1.45
9	a	820	CLA	C1C-C2C	-4.53	1.35	1.44
9	b	817	CLA	C4C-C3C	-4.53	1.37	1.45
9	a	830	CLA	C1C-C2C	-4.53	1.35	1.44
9	a	823	CLA	C4C-C3C	-4.53	1.37	1.45
9	A	814	CLA	C4C-C3C	-4.53	1.37	1.45
9	A	830	CLA	C4C-C3C	-4.53	1.37	1.45
9	a	828	CLA	C4C-C3C	-4.53	1.37	1.45
9	B	810	CLA	C1C-C2C	-4.53	1.35	1.44
9	b	810	CLA	C1C-C2C	-4.53	1.35	1.44
9	A	810	CLA	C4C-C3C	-4.53	1.37	1.45
9	b	808	CLA	C1C-C2C	-4.53	1.35	1.44
9	A	818	CLA	C4C-C3C	-4.52	1.37	1.45
9	B	839	CLA	C4C-C3C	-4.52	1.37	1.45
9	l	307	CLA	C4C-C3C	-4.52	1.37	1.45
9	A	847	CLA	C4C-C3C	-4.52	1.37	1.45
9	b	815	CLA	C4C-C3C	-4.52	1.37	1.45
9	A	823	CLA	C1C-C2C	-4.52	1.35	1.44
9	B	829	CLA	C4C-C3C	-4.52	1.37	1.45
9	B	814	CLA	C1C-C2C	-4.52	1.35	1.44
9	a	801	CLA	C4C-C3C	-4.51	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	831	CLA	C4C-C3C	-4.51	1.37	1.45
9	B	825	CLA	C1C-C2C	-4.51	1.35	1.44
9	b	810	CLA	C4C-C3C	-4.51	1.37	1.45
9	B	828	CLA	C1C-C2C	-4.51	1.35	1.44
9	B	817	CLA	C4C-C3C	-4.51	1.37	1.45
9	b	806	CLA	C4C-C3C	-4.51	1.37	1.45
9	a	817	CLA	C4C-C3C	-4.51	1.37	1.45
9	b	830	CLA	C4C-C3C	-4.51	1.37	1.45
9	b	816	CLA	C4C-C3C	-4.51	1.37	1.45
9	b	840	CLA	C4C-C3C	-4.50	1.37	1.45
9	b	829	CLA	C4C-C3C	-4.50	1.37	1.45
9	A	804	CLA	C4C-C3C	-4.50	1.37	1.45
9	B	815	CLA	C1C-C2C	-4.50	1.35	1.44
9	a	812	CLA	C1C-C2C	-4.50	1.35	1.44
9	B	802	CLA	C4C-C3C	-4.50	1.37	1.45
9	A	813	CLA	C4C-C3C	-4.50	1.37	1.45
9	B	821	CLA	C4C-C3C	-4.50	1.37	1.45
9	A	833	CLA	C4C-C3C	-4.50	1.37	1.45
9	a	813	CLA	C4C-C3C	-4.50	1.37	1.45
9	B	826	CLA	C4C-C3C	-4.50	1.37	1.45
9	A	832	CLA	C4C-C3C	-4.50	1.37	1.45
9	b	825	CLA	C1C-C2C	-4.50	1.35	1.44
9	a	810	CLA	C4C-C3C	-4.50	1.37	1.45
9	B	808	CLA	C1C-C2C	-4.49	1.35	1.44
9	B	819	CLA	C1C-C2C	-4.49	1.35	1.44
9	a	833	CLA	C1C-C2C	-4.49	1.35	1.44
9	a	837	CLA	C1C-C2C	-4.49	1.35	1.44
9	B	830	CLA	C4C-C3C	-4.49	1.37	1.45
9	a	827	CLA	C1C-C2C	-4.49	1.35	1.44
9	A	835	CLA	C1C-C2C	-4.49	1.35	1.44
9	b	811	CLA	C4C-C3C	-4.49	1.37	1.45
9	b	821	CLA	C4C-C3C	-4.49	1.37	1.45
9	B	811	CLA	C4C-C3C	-4.49	1.37	1.45
9	b	807	CLA	C1C-C2C	-4.49	1.35	1.44
9	b	814	CLA	C1C-C2C	-4.49	1.35	1.44
9	b	813	CLA	C4C-C3C	-4.49	1.37	1.45
9	A	828	CLA	C4C-C3C	-4.49	1.37	1.45
9	a	822	CLA	C4C-C3C	-4.49	1.37	1.45
9	A	824	CLA	C1C-C2C	-4.48	1.35	1.44
9	A	809	CLA	C4C-C3C	-4.48	1.37	1.45
9	A	813	CLA	C1C-C2C	-4.48	1.35	1.44
9	a	836	CLA	C1C-C2C	-4.48	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	805	CLA	C4C-C3C	-4.48	1.37	1.45
9	A	809	CLA	C1C-C2C	-4.48	1.35	1.44
9	a	811	CLA	C1C-C2C	-4.48	1.35	1.44
9	A	846	CLA	C4C-C3C	-4.48	1.37	1.45
9	a	825	CLA	C1C-C2C	-4.48	1.35	1.44
9	B	810	CLA	C4C-C3C	-4.47	1.37	1.45
9	A	807	CLA	C1C-C2C	-4.47	1.35	1.44
9	a	847	CLA	C1C-C2C	-4.47	1.35	1.44
9	B	813	CLA	C4C-C3C	-4.47	1.37	1.45
9	a	812	CLA	C4C-C3C	-4.47	1.37	1.45
9	a	835	CLA	C1C-C2C	-4.47	1.35	1.44
9	a	805	CLA	C4C-C3C	-4.47	1.37	1.45
9	a	846	CLA	C4C-C3C	-4.47	1.37	1.45
9	B	829	CLA	C1C-C2C	-4.47	1.35	1.44
9	A	812	CLA	C1C-C2C	-4.47	1.35	1.44
9	L	304	CLA	C4C-C3C	-4.47	1.37	1.45
9	B	823	CLA	C1C-C2C	-4.47	1.35	1.44
9	B	816	CLA	C4C-C3C	-4.47	1.37	1.45
9	b	820	CLA	C4C-C3C	-4.47	1.37	1.45
9	A	805	CLA	C1C-C2C	-4.47	1.35	1.44
9	A	817	CLA	C1C-C2C	-4.47	1.35	1.44
9	B	826	CLA	C1C-C2C	-4.46	1.35	1.44
9	A	803	CLA	C4C-C3C	-4.46	1.37	1.45
9	a	836	CLA	C4C-C3C	-4.46	1.37	1.45
9	b	839	CLA	C4C-C3C	-4.46	1.37	1.45
9	a	833	CLA	C4C-C3C	-4.46	1.37	1.45
9	b	819	CLA	C1C-C2C	-4.46	1.35	1.44
9	A	821	CLA	C4C-C3C	-4.46	1.37	1.45
9	a	804	CLA	C4C-C3C	-4.46	1.37	1.45
9	b	829	CLA	C1C-C2C	-4.46	1.35	1.44
9	B	820	CLA	C4C-C3C	-4.46	1.37	1.45
9	B	827	CLA	C4C-C3C	-4.46	1.37	1.45
9	a	817	CLA	C1C-C2C	-4.46	1.35	1.44
9	b	818	CLA	C4C-C3C	-4.46	1.37	1.45
9	B	831	CLA	C4C-C3C	-4.46	1.37	1.45
9	H	201	CLA	C1C-C2C	-4.45	1.35	1.44
9	a	818	CLA	C4C-C3C	-4.45	1.37	1.45
9	b	806	CLA	C1C-C2C	-4.45	1.35	1.44
9	B	806	CLA	C4C-C3C	-4.45	1.37	1.45
9	A	825	CLA	C1C-C2C	-4.45	1.35	1.44
9	L	303	CLA	C1C-C2C	-4.45	1.35	1.44
9	B	823	CLA	C4C-C3C	-4.45	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	826	CLA	C1C-C2C	-4.45	1.35	1.44
9	B	840	CLA	C4C-C3C	-4.45	1.37	1.45
9	a	834	CLA	C4C-C3C	-4.45	1.37	1.45
9	b	827	CLA	C4C-C3C	-4.45	1.37	1.45
9	a	809	CLA	C1C-C2C	-4.45	1.36	1.44
9	A	829	CLA	C4C-C3C	-4.44	1.37	1.45
9	a	809	CLA	C4C-C3C	-4.44	1.37	1.45
9	A	834	CLA	C1C-C2C	-4.44	1.36	1.44
9	a	814	CLA	C1C-C2C	-4.44	1.36	1.44
9	A	835	CLA	C4C-C3C	-4.44	1.37	1.45
9	a	830	CLA	C4C-C3C	-4.44	1.37	1.45
9	b	823	CLA	C1C-C2C	-4.44	1.36	1.44
9	A	826	CLA	C4C-C3C	-4.44	1.37	1.45
9	B	806	CLA	C1C-C2C	-4.44	1.36	1.44
9	a	846	CLA	C1C-C2C	-4.43	1.36	1.44
9	a	824	CLA	C1C-C2C	-4.43	1.36	1.44
9	B	813	CLA	C1C-C2C	-4.43	1.36	1.44
9	b	804	CLA	C4C-C3C	-4.43	1.37	1.45
9	a	808	CLA	C4C-C3C	-4.43	1.37	1.45
9	a	837	CLA	C4C-C3C	-4.42	1.37	1.45
9	B	831	CLA	C1C-C2C	-4.42	1.36	1.44
9	A	847	CLA	C1C-C2C	-4.42	1.36	1.44
9	a	803	CLA	C4C-C3C	-4.42	1.37	1.45
9	b	823	CLA	C4C-C3C	-4.42	1.37	1.45
9	A	804	CLA	C1C-C2C	-4.42	1.36	1.44
9	a	802	CLA	C1C-C2C	-4.42	1.36	1.44
9	B	804	CLA	C4C-C3C	-4.42	1.37	1.45
9	a	826	CLA	C1C-C2C	-4.42	1.36	1.44
9	a	813	CLA	C1C-C2C	-4.41	1.36	1.44
9	a	807	CLA	C4C-C3C	-4.41	1.37	1.45
9	b	826	CLA	C4C-C3C	-4.41	1.37	1.45
9	A	836	CLA	C4C-C3C	-4.41	1.37	1.45
9	a	816	CLA	C4C-C3C	-4.41	1.37	1.45
9	a	806	CLA	C1C-C2C	-4.41	1.36	1.44
9	L	304	CLA	C1C-C2C	-4.41	1.36	1.44
9	A	802	CLA	C1C-C2C	-4.41	1.36	1.44
9	a	815	CLA	C1C-C2C	-4.41	1.36	1.44
9	b	821	CLA	C1C-C2C	-4.41	1.36	1.44
9	A	812	CLA	C4C-C3C	-4.40	1.37	1.45
9	a	820	CLA	MG-NA	4.40	2.16	2.06
9	a	820	CLA	CHB-C4A	4.40	1.47	1.37
9	B	828	CLA	C4C-C3C	-4.40	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	805	CLA	C1C-C2C	-4.40	1.36	1.44
9	a	822	CLA	C1C-C2C	-4.40	1.36	1.44
9	A	801	CLA	C1C-C2C	-4.40	1.36	1.44
9	a	801	CLA	C1C-C2C	-4.40	1.36	1.44
9	b	813	CLA	C1C-C2C	-4.40	1.36	1.44
9	A	814	CLA	C1C-C2C	-4.40	1.36	1.44
9	a	827	CLA	C4C-C3C	-4.40	1.37	1.45
9	A	815	CLA	C1C-C2C	-4.40	1.36	1.44
9	L	307	CLA	C4C-C3C	-4.40	1.37	1.45
9	b	840	CLA	C1C-C2C	-4.40	1.36	1.44
9	l	306	CLA	C1C-C2C	-4.39	1.36	1.44
9	b	825	CLA	C4C-C3C	-4.39	1.37	1.45
9	B	812	CLA	C1C-C2C	-4.39	1.36	1.44
9	B	818	CLA	C4C-C3C	-4.39	1.37	1.45
9	A	807	CLA	C4C-C3C	-4.39	1.37	1.45
9	b	824	CLA	C1C-C2C	-4.39	1.36	1.44
9	b	831	CLA	C1C-C2C	-4.39	1.36	1.44
9	B	821	CLA	C1C-C2C	-4.39	1.36	1.44
9	A	834	CLA	C4C-C3C	-4.38	1.37	1.45
9	B	824	CLA	C1C-C2C	-4.38	1.36	1.44
9	L	302	CLA	C4C-C3C	-4.38	1.37	1.45
9	A	821	CLA	C1C-C2C	-4.38	1.36	1.44
9	B	816	CLA	C1C-C2C	-4.38	1.36	1.44
9	b	816	CLA	C1C-C2C	-4.38	1.36	1.44
9	a	832	CLA	C1C-C2C	-4.38	1.36	1.44
9	l	307	CLA	C1C-C2C	-4.38	1.36	1.44
9	B	830	CLA	C1C-C2C	-4.38	1.36	1.44
9	a	835	CLA	C4C-C3C	-4.38	1.37	1.45
9	B	814	CLA	C4C-C3C	-4.37	1.37	1.45
9	b	830	CLA	C1C-C2C	-4.37	1.36	1.44
9	B	802	CLA	C1C-C2C	-4.37	1.36	1.44
9	B	812	CLA	C4C-C3C	-4.37	1.37	1.45
9	a	816	CLA	C1C-C2C	-4.37	1.36	1.44
9	b	827	CLA	C1C-C2C	-4.37	1.36	1.44
9	B	825	CLA	C4C-C3C	-4.37	1.37	1.45
9	H	201	CLA	C4C-C3C	-4.37	1.37	1.45
9	A	846	CLA	C1C-C2C	-4.37	1.36	1.44
9	a	804	CLA	C1C-C2C	-4.36	1.36	1.44
9	A	831	CLA	C1C-C2C	-4.36	1.36	1.44
9	A	816	CLA	C1C-C2C	-4.36	1.36	1.44
9	a	819	CLA	C1C-C2C	-4.36	1.36	1.44
9	b	828	CLA	C4C-C3C	-4.35	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	820	CLA	C4C-C3C	-4.35	1.37	1.45
9	a	828	CLA	C1C-C2C	-4.35	1.36	1.44
9	B	817	CLA	C1C-C2C	-4.35	1.36	1.44
9	a	834	CLA	C1C-C2C	-4.35	1.36	1.44
9	h	202	CLA	C4C-C3C	-4.35	1.37	1.45
9	B	840	CLA	C1C-C2C	-4.35	1.36	1.44
9	a	825	CLA	C4C-C3C	-4.35	1.37	1.45
9	b	817	CLA	C1C-C2C	-4.35	1.36	1.44
9	B	820	CLA	C1C-C2C	-4.34	1.36	1.44
9	A	824	CLA	C4C-C3C	-4.34	1.37	1.45
9	A	833	CLA	C1C-C2C	-4.34	1.36	1.44
9	L	302	CLA	C1C-C2C	-4.33	1.36	1.44
9	A	806	CLA	C4C-C3C	-4.33	1.37	1.45
9	B	811	CLA	C1C-C2C	-4.33	1.36	1.44
9	b	811	CLA	C1C-C2C	-4.33	1.36	1.44
9	b	802	CLA	C1C-C2C	-4.33	1.36	1.44
9	b	820	CLA	C1C-C2C	-4.33	1.36	1.44
9	a	807	CLA	C1C-C2C	-4.33	1.36	1.44
9	B	827	CLA	C1C-C2C	-4.32	1.36	1.44
9	A	827	CLA	C1C-C2C	-4.32	1.36	1.44
9	A	816	CLA	C4C-C3C	-4.32	1.37	1.45
9	A	831	CLA	C4C-C3C	-4.32	1.37	1.45
9	a	806	CLA	C4C-C3C	-4.32	1.37	1.45
9	a	810	CLA	C1C-C2C	-4.32	1.36	1.44
9	A	818	CLA	C1C-C2C	-4.32	1.36	1.44
9	b	814	CLA	C4C-C3C	-4.32	1.37	1.45
9	a	820	CLA	C4D-ND	4.31	1.43	1.37
9	a	821	CLA	C4C-C3C	-4.31	1.37	1.45
9	A	811	CLA	C4C-C3C	-4.31	1.37	1.45
9	A	803	CLA	C1C-C2C	-4.30	1.36	1.44
9	a	832	CLA	C4C-C3C	-4.30	1.37	1.45
9	H	201	CLA	MG-NA	4.30	2.16	2.06
9	a	832	CLA	MG-NA	4.30	2.16	2.06
9	l	302	CLA	C4C-C3C	-4.30	1.37	1.45
9	a	818	CLA	C1C-C2C	-4.29	1.36	1.44
9	l	305	CLA	C1C-C2C	-4.28	1.36	1.44
9	A	822	CLA	C1C-C2C	-4.27	1.36	1.44
9	a	823	CLA	C1C-C2C	-4.27	1.36	1.44
9	a	811	CLA	C4C-C3C	-4.27	1.37	1.45
9	A	806	CLA	C1C-C2C	-4.26	1.36	1.44
9	a	803	CLA	C1C-C2C	-4.26	1.36	1.44
9	A	810	CLA	C1C-C2C	-4.26	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	820	CLA	C4C-C3C	-4.26	1.37	1.45
9	L	307	CLA	C1C-C2C	-4.25	1.36	1.44
9	A	831	CLA	MG-NA	4.24	2.16	2.06
9	A	830	CLA	C1C-C2C	-4.24	1.36	1.44
9	b	812	CLA	C1C-C2C	-4.24	1.36	1.44
9	a	808	CLA	C1C-C2C	-4.23	1.36	1.44
9	B	805	CLA	C1C-C2C	-4.20	1.36	1.44
9	a	831	CLA	C1C-C2C	-4.19	1.36	1.44
9	b	802	CLA	MG-NA	4.18	2.16	2.06
9	A	808	CLA	C1C-C2C	-4.18	1.36	1.44
9	b	805	CLA	C1C-C2C	-4.17	1.36	1.44
9	A	826	CLA	MG-NA	4.12	2.16	2.06
12	A	841	BCR	C21-C22	4.12	1.41	1.35
9	b	812	CLA	C4C-C3C	-4.11	1.38	1.45
12	a	842	BCR	C21-C22	4.11	1.41	1.35
9	a	827	CLA	MG-NA	4.11	2.16	2.06
9	B	820	CLA	MG-NA	4.08	2.16	2.06
12	B	834	BCR	C10-C9	4.06	1.41	1.35
9	h	201	CLA	C1D-ND	4.05	1.42	1.37
9	B	801	CLA	C4C-C3C	-4.04	1.38	1.45
9	B	831	CLA	MG-NA	4.03	2.15	2.06
12	a	843	BCR	C21-C22	4.03	1.41	1.35
9	B	828	CLA	MG-NA	4.01	2.15	2.06
12	h	203	BCR	C10-C9	4.00	1.41	1.35
12	a	844	BCR	C21-C22	4.00	1.41	1.35
14	b	837	DGD	O1G-C1A	4.00	1.45	1.33
9	h	202	CLA	MG-NA	4.00	2.15	2.06
9	b	831	CLA	MG-NA	3.99	2.15	2.06
9	b	801	CLA	C4C-C3C	-3.99	1.38	1.45
12	b	834	BCR	C21-C22	3.99	1.41	1.35
14	B	837	DGD	O1G-C1A	3.98	1.45	1.33
9	A	812	CLA	MG-NA	3.96	2.15	2.06
12	H	202	BCR	C10-C9	3.96	1.41	1.35
12	b	834	BCR	C10-C9	3.96	1.41	1.35
12	H	202	BCR	C14-C13	3.96	1.41	1.35
14	B	837	DGD	O2G-C1B	3.96	1.45	1.34
9	l	301	CLA	C4C-C3C	-3.96	1.38	1.45
9	B	815	CLA	MG-NA	3.96	2.15	2.06
12	B	835	BCR	C14-C13	3.95	1.41	1.35
12	a	841	BCR	C10-C9	3.94	1.41	1.35
12	h	203	BCR	C14-C13	3.94	1.41	1.35
12	A	843	BCR	C21-C22	3.93	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	837	DGD	O2G-C1B	3.93	1.45	1.34
12	B	834	BCR	C21-C22	3.92	1.41	1.35
9	b	828	CLA	MG-NA	3.92	2.15	2.06
12	A	840	BCR	C10-C9	3.91	1.41	1.35
9	A	819	CLA	MG-NC	3.91	2.15	2.06
12	A	843	BCR	C17-C18	3.89	1.40	1.35
12	B	834	BCR	C17-C18	3.89	1.40	1.35
12	a	842	BCR	C14-C13	3.88	1.40	1.35
9	a	812	CLA	MG-NA	3.87	2.15	2.06
9	A	819	CLA	MG-NA	3.85	2.15	2.06
12	h	203	BCR	C21-C22	3.85	1.40	1.35
9	l	302	CLA	MG-NA	3.85	2.15	2.06
9	L	308	CLA	C1D-ND	3.85	1.42	1.37
12	a	843	BCR	C14-C13	3.84	1.40	1.35
12	a	841	BCR	C14-C13	3.84	1.40	1.35
12	A	840	BCR	C14-C13	3.84	1.40	1.35
12	b	834	BCR	C17-C18	3.84	1.40	1.35
9	a	830	CLA	MG-NA	3.84	2.15	2.06
12	A	842	BCR	C10-C9	3.83	1.40	1.35
12	B	835	BCR	C17-C18	3.83	1.40	1.35
12	a	841	BCR	C17-C18	3.83	1.40	1.35
12	a	843	BCR	C10-C9	3.82	1.40	1.35
12	b	835	BCR	C10-C9	3.81	1.40	1.35
12	b	835	BCR	C21-C22	3.80	1.40	1.35
12	H	202	BCR	C21-C22	3.80	1.40	1.35
9	L	302	CLA	MG-NA	3.80	2.15	2.06
12	A	841	BCR	C14-C13	3.79	1.40	1.35
12	a	844	BCR	C14-C13	3.79	1.40	1.35
12	A	841	BCR	C17-C18	3.79	1.40	1.35
12	a	842	BCR	C17-C18	3.78	1.40	1.35
12	a	844	BCR	C17-C18	3.78	1.40	1.35
9	l	307	CLA	MG-NA	3.78	2.15	2.06
12	h	203	BCR	C17-C18	3.76	1.40	1.35
12	A	841	BCR	C10-C9	3.75	1.40	1.35
12	B	835	BCR	C21-C22	3.74	1.40	1.35
9	b	815	CLA	MG-NA	3.74	2.15	2.06
12	H	202	BCR	C17-C18	3.74	1.40	1.35
12	b	835	BCR	C14-C13	3.74	1.40	1.35
12	A	842	BCR	C21-C22	3.74	1.40	1.35
9	l	305	CLA	MG-NA	3.74	2.15	2.06
12	l	309	BCR	C17-C18	3.74	1.40	1.35
12	a	842	BCR	C10-C9	3.73	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	835	BCR	C10-C9	3.73	1.40	1.35
9	B	802	CLA	MG-NA	3.72	2.15	2.06
9	A	819	CLA	C1D-ND	-3.72	1.33	1.37
12	L	306	BCR	C17-C18	3.72	1.40	1.35
12	A	840	BCR	C17-C18	3.72	1.40	1.35
12	b	835	BCR	C17-C18	3.71	1.40	1.35
9	B	812	CLA	MG-NA	3.71	2.15	2.06
12	A	843	BCR	C14-C13	3.71	1.40	1.35
12	L	306	BCR	C14-C13	3.70	1.40	1.35
12	b	834	BCR	C14-C13	3.68	1.40	1.35
12	L	305	BCR	C17-C18	3.66	1.40	1.35
9	a	826	CLA	MG-NA	3.66	2.15	2.06
12	A	842	BCR	C14-C13	3.65	1.40	1.35
12	L	306	BCR	C21-C22	3.64	1.40	1.35
12	L	305	BCR	C10-C9	3.64	1.40	1.35
12	l	304	BCR	C21-C22	3.63	1.40	1.35
9	A	829	CLA	MG-NA	3.63	2.14	2.06
12	l	308	BCR	C14-C13	3.63	1.40	1.35
12	l	309	BCR	C21-C22	3.63	1.40	1.35
12	l	309	BCR	C10-C9	3.63	1.40	1.35
9	b	840	CLA	MG-NA	3.63	2.14	2.06
12	L	305	BCR	C21-C22	3.63	1.40	1.35
12	B	834	BCR	C14-C13	3.62	1.40	1.35
12	a	843	BCR	C17-C18	3.62	1.40	1.35
9	A	847	CLA	MG-NA	3.62	2.14	2.06
9	A	815	CLA	MG-NA	3.62	2.14	2.06
12	a	841	BCR	C21-C22	3.61	1.40	1.35
12	L	305	BCR	C14-C13	3.61	1.40	1.35
9	B	840	CLA	MG-NA	3.61	2.14	2.06
12	l	308	BCR	C17-C18	3.60	1.40	1.35
12	l	308	BCR	C21-C22	3.60	1.40	1.35
12	l	304	BCR	C17-C18	3.59	1.40	1.35
12	L	301	BCR	C17-C18	3.58	1.40	1.35
9	a	847	CLA	MG-NA	3.58	2.14	2.06
12	L	301	BCR	C21-C22	3.57	1.40	1.35
9	B	822	CLA	MG-NA	3.57	2.14	2.06
9	b	822	CLA	MG-NA	3.57	2.14	2.06
12	a	844	BCR	C10-C9	3.56	1.40	1.35
9	A	825	CLA	MG-NA	3.56	2.14	2.06
9	b	801	CLA	MG-NA	3.55	2.14	2.06
12	l	308	BCR	C10-C9	3.55	1.40	1.35
12	l	309	BCR	C14-C13	3.55	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	836	BCR	C21-C22	3.54	1.40	1.35
9	B	807	CLA	MG-NA	3.54	2.14	2.06
12	A	840	BCR	C21-C22	3.54	1.40	1.35
9	a	815	CLA	MG-NA	3.53	2.14	2.06
12	A	843	BCR	C10-C9	3.53	1.40	1.35
9	b	807	CLA	MG-NA	3.52	2.14	2.06
12	B	836	BCR	C21-C22	3.51	1.40	1.35
9	A	803	CLA	MG-NA	3.51	2.14	2.06
9	b	824	CLA	MG-NA	3.50	2.14	2.06
12	b	836	BCR	C14-C13	3.50	1.40	1.35
9	B	801	CLA	MG-NA	3.49	2.14	2.06
12	L	301	BCR	C14-C13	3.49	1.40	1.35
9	b	825	CLA	MG-NA	3.49	2.14	2.06
9	a	803	CLA	MG-NA	3.48	2.14	2.06
12	L	306	BCR	C10-C9	3.47	1.40	1.35
9	a	805	CLA	MG-NA	3.47	2.14	2.06
12	i	101	BCR	C14-C13	3.46	1.40	1.35
12	B	836	BCR	C10-C9	3.46	1.40	1.35
12	B	836	BCR	C14-C13	3.45	1.40	1.35
12	b	836	BCR	C17-C18	3.45	1.40	1.35
9	B	824	CLA	MG-NA	3.44	2.14	2.06
12	I	101	BCR	C10-C9	3.44	1.40	1.35
9	b	817	CLA	MG-NA	3.44	2.14	2.06
12	l	304	BCR	C14-C13	3.43	1.40	1.35
12	I	101	BCR	C14-C13	3.43	1.40	1.35
9	B	817	CLA	MG-NA	3.43	2.14	2.06
12	B	836	BCR	C17-C18	3.43	1.40	1.35
9	A	805	CLA	MG-NA	3.43	2.14	2.06
9	B	825	CLA	MG-NA	3.42	2.14	2.06
12	i	101	BCR	C10-C9	3.42	1.40	1.35
9	b	810	CLA	MG-NA	3.42	2.14	2.06
9	B	810	CLA	MG-NA	3.41	2.14	2.06
12	b	836	BCR	C10-C9	3.41	1.40	1.35
9	B	819	CLA	MG-NA	3.40	2.14	2.06
9	b	805	CLA	MG-NA	3.40	2.14	2.06
9	B	805	CLA	MG-NA	3.40	2.14	2.06
12	A	842	BCR	C17-C18	3.38	1.40	1.35
9	a	837	CLA	MG-NA	3.38	2.14	2.06
12	I	101	BCR	C17-C18	3.38	1.40	1.35
12	l	304	BCR	C10-C9	3.37	1.40	1.35
9	A	836	CLA	MG-NA	3.37	2.14	2.06
12	i	101	BCR	C17-C18	3.36	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	811	CLA	MG-NA	3.36	2.14	2.06
9	B	806	CLA	MG-NA	3.35	2.14	2.06
9	a	834	CLA	MG-NA	3.35	2.14	2.06
9	b	814	CLA	MG-NA	3.33	2.14	2.06
9	b	806	CLA	MG-NA	3.33	2.14	2.06
12	L	301	BCR	C10-C9	3.33	1.40	1.35
9	A	833	CLA	MG-NA	3.32	2.14	2.06
9	h	201	CLA	C4B-NB	3.32	1.41	1.37
12	L	306	BCR	C8-C9	-3.31	1.38	1.45
9	a	819	CLA	C1D-C2D	-3.31	1.38	1.45
9	a	833	CLA	MG-NA	3.31	2.14	2.06
9	a	835	CLA	MG-NA	3.31	2.14	2.06
9	A	832	CLA	MG-NA	3.29	2.14	2.06
9	a	820	CLA	C3B-C2B	-3.28	1.29	1.41
9	b	830	CLA	MG-NA	3.28	2.14	2.06
9	b	819	CLA	MG-NA	3.27	2.14	2.06
9	A	834	CLA	MG-NA	3.27	2.14	2.06
9	B	809	CLA	MG-NA	3.27	2.14	2.06
9	a	823	CLA	MG-NA	3.27	2.14	2.06
9	b	809	CLA	MG-NA	3.27	2.14	2.06
12	i	101	BCR	C23-C22	-3.26	1.38	1.45
12	I	101	BCR	C21-C22	3.25	1.40	1.35
12	l	309	BCR	C8-C9	-3.25	1.39	1.45
12	I	101	BCR	C23-C22	-3.24	1.39	1.45
9	A	823	CLA	MG-NA	3.23	2.13	2.06
9	a	804	CLA	MG-NA	3.23	2.13	2.06
9	A	822	CLA	MG-NA	3.23	2.13	2.06
9	A	811	CLA	MG-NA	3.23	2.13	2.06
9	a	809	CLA	MG-NA	3.22	2.13	2.06
9	b	820	CLA	MG-NC	3.21	2.13	2.06
9	B	814	CLA	MG-NA	3.21	2.13	2.06
9	A	828	CLA	MG-NA	3.21	2.13	2.06
9	B	830	CLA	MG-NA	3.20	2.13	2.06
9	L	308	CLA	C4B-NB	3.19	1.41	1.37
12	L	301	BCR	C23-C22	-3.18	1.39	1.45
12	i	101	BCR	C21-C22	3.17	1.40	1.35
9	A	817	CLA	MG-NA	3.17	2.13	2.06
9	b	826	CLA	MG-NA	3.17	2.13	2.06
9	A	810	CLA	MG-NA	3.16	2.13	2.06
9	H	201	CLA	MG-NC	3.15	2.13	2.06
9	a	829	CLA	MG-NA	3.15	2.13	2.06
9	B	826	CLA	MG-NA	3.14	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	304	BCR	C23-C22	-3.14	1.39	1.45
12	L	305	BCR	C23-C22	-3.13	1.39	1.45
9	A	821	CLA	MG-NA	3.11	2.13	2.06
12	I	101	BCR	C8-C9	-3.11	1.39	1.45
9	B	816	CLA	MG-NA	3.11	2.13	2.06
12	l	308	BCR	C23-C22	-3.11	1.39	1.45
12	i	101	BCR	C8-C9	-3.11	1.39	1.45
12	A	842	BCR	C23-C22	-3.11	1.39	1.45
9	A	809	CLA	MG-NA	3.10	2.13	2.06
9	a	817	CLA	MG-NA	3.09	2.13	2.06
9	A	814	CLA	MG-NA	3.08	2.13	2.06
9	b	829	CLA	MG-NA	3.08	2.13	2.06
9	L	304	CLA	MG-NA	3.07	2.13	2.06
12	L	306	BCR	C23-C22	-3.06	1.39	1.45
12	L	301	BCR	C8-C9	-3.06	1.39	1.45
9	a	810	CLA	MG-NA	3.06	2.13	2.06
12	B	836	BCR	C8-C9	-3.06	1.39	1.45
9	A	804	CLA	MG-NA	3.05	2.13	2.06
9	A	830	CLA	MG-NA	3.05	2.13	2.06
12	b	835	BCR	C23-C22	-3.05	1.39	1.45
12	B	835	BCR	C23-C22	-3.05	1.39	1.45
12	L	305	BCR	C8-C9	-3.05	1.39	1.45
9	a	806	CLA	MG-NA	3.04	2.13	2.06
12	A	840	BCR	C23-C22	-3.03	1.39	1.45
9	A	819	CLA	MG-ND	3.03	2.11	2.05
9	B	808	CLA	MG-NA	3.03	2.13	2.06
12	A	843	BCR	C8-C9	-3.02	1.39	1.45
12	l	308	BCR	C8-C9	-3.02	1.39	1.45
12	a	841	BCR	C23-C22	-3.02	1.39	1.45
12	l	304	BCR	C8-C9	-3.01	1.39	1.45
9	B	829	CLA	MG-NA	3.01	2.13	2.06
9	B	811	CLA	MG-NA	3.01	2.13	2.06
12	a	844	BCR	C8-C9	-3.00	1.39	1.45
9	a	822	CLA	MG-NA	3.00	2.13	2.06
9	a	836	CLA	MG-NA	3.00	2.13	2.06
9	b	811	CLA	MG-NA	2.99	2.13	2.06
12	b	836	BCR	C8-C9	-2.99	1.39	1.45
9	a	846	CLA	MG-NA	2.99	2.13	2.06
12	b	836	BCR	C23-C22	-2.99	1.39	1.45
9	A	846	CLA	MG-NA	2.98	2.13	2.06
12	B	836	BCR	C23-C22	-2.98	1.39	1.45
9	b	808	CLA	MG-NA	2.98	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	309	BCR	C23-C22	-2.98	1.39	1.45
9	a	824	CLA	MG-NA	2.97	2.13	2.06
9	a	814	CLA	MG-NA	2.95	2.13	2.06
12	H	202	BCR	C8-C9	-2.95	1.39	1.45
9	b	816	CLA	MG-NA	2.95	2.13	2.06
12	A	841	BCR	C23-C22	-2.95	1.39	1.45
9	a	808	CLA	MG-NA	2.95	2.13	2.06
12	a	842	BCR	C23-C22	-2.93	1.39	1.45
12	h	203	BCR	C8-C9	-2.93	1.39	1.45
12	a	843	BCR	C23-C22	-2.92	1.39	1.45
12	A	841	BCR	C8-C9	-2.92	1.39	1.45
9	A	835	CLA	MG-NA	2.91	2.13	2.06
12	A	840	BCR	C8-C9	-2.91	1.39	1.45
12	a	842	BCR	C8-C9	-2.89	1.39	1.45
12	B	834	BCR	C8-C9	-2.89	1.39	1.45
9	h	201	CLA	C4D-ND	-2.89	1.33	1.37
9	L	308	CLA	C3B-C4B	2.89	1.49	1.42
9	a	813	CLA	MG-NA	2.89	2.13	2.06
12	b	835	BCR	C8-C9	-2.89	1.39	1.45
9	h	202	CLA	MG-NC	2.88	2.13	2.06
9	A	813	CLA	MG-NA	2.87	2.13	2.06
12	H	202	BCR	C23-C22	-2.87	1.39	1.45
9	b	832	CLA	MG-NA	2.86	2.13	2.06
12	B	835	BCR	C8-C9	-2.85	1.39	1.45
12	b	834	BCR	C8-C9	-2.85	1.39	1.45
12	b	834	BCR	C23-C22	-2.84	1.39	1.45
12	a	841	BCR	C8-C9	-2.83	1.39	1.45
9	B	813	CLA	MG-NA	2.83	2.13	2.06
12	A	842	BCR	C19-C18	-2.83	1.39	1.45
9	B	823	CLA	MG-NA	2.83	2.13	2.06
9	A	807	CLA	MG-NA	2.83	2.13	2.06
9	L	302	CLA	C3D-C4D	-2.83	1.37	1.44
9	B	832	CLA	MG-NA	2.83	2.13	2.06
9	A	818	CLA	C1D-C2D	-2.83	1.39	1.45
9	b	821	CLA	MG-NA	2.83	2.13	2.06
12	a	844	BCR	C23-C22	-2.82	1.39	1.45
12	B	834	BCR	C23-C22	-2.82	1.39	1.45
9	b	823	CLA	MG-NA	2.82	2.13	2.06
12	h	203	BCR	C23-C22	-2.81	1.39	1.45
9	a	820	CLA	C4D-CHA	2.81	1.48	1.38
9	A	827	CLA	MG-NA	2.80	2.12	2.06
9	l	301	CLA	C3D-C4D	-2.80	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	816	CLA	MG-NA	2.80	2.12	2.06
9	a	818	CLA	MG-NA	2.79	2.12	2.06
9	l	305	CLA	C3D-C4D	-2.79	1.37	1.44
9	b	839	CLA	MG-NA	2.79	2.12	2.06
9	b	813	CLA	MG-NA	2.79	2.12	2.06
12	A	842	BCR	C8-C9	-2.78	1.40	1.45
9	a	828	CLA	MG-NA	2.78	2.12	2.06
9	A	818	CLA	MG-NA	2.77	2.12	2.06
12	a	843	BCR	C8-C9	-2.77	1.40	1.45
9	B	821	CLA	MG-NA	2.77	2.12	2.06
9	B	807	CLA	C3D-C4D	-2.77	1.37	1.44
12	A	843	BCR	C23-C22	-2.77	1.40	1.45
9	a	821	CLA	MG-NA	2.76	2.12	2.06
9	b	807	CLA	C3D-C4D	-2.76	1.38	1.44
9	B	823	CLA	C3D-C4D	-2.74	1.38	1.44
9	B	808	CLA	C3D-C4D	-2.74	1.38	1.44
9	B	824	CLA	C3D-C4D	-2.74	1.38	1.44
9	b	811	CLA	C3D-C4D	-2.74	1.38	1.44
9	b	825	CLA	C3D-C4D	-2.73	1.38	1.44
9	l	306	CLA	MG-NA	2.73	2.12	2.06
9	L	308	CLA	C1B-C2B	2.73	1.49	1.43
12	L	306	BCR	C12-C13	-2.72	1.40	1.45
9	A	818	CLA	C3D-C4D	-2.72	1.38	1.44
9	B	809	CLA	C3D-C4D	-2.72	1.38	1.44
9	B	825	CLA	C3D-C4D	-2.72	1.38	1.44
9	B	824	CLA	C1D-C2D	-2.71	1.40	1.45
9	B	832	CLA	C3D-C4D	-2.71	1.38	1.44
9	b	808	CLA	C3D-C4D	-2.71	1.38	1.44
9	b	809	CLA	C3D-C4D	-2.71	1.38	1.44
9	b	824	CLA	C1D-C2D	-2.71	1.40	1.45
9	a	816	CLA	C3D-C4D	-2.71	1.38	1.44
9	a	818	CLA	C1D-C2D	-2.70	1.40	1.45
9	A	833	CLA	C3D-C4D	-2.70	1.38	1.44
9	a	828	CLA	C3D-C4D	-2.70	1.38	1.44
9	b	803	CLA	C3D-C4D	-2.70	1.38	1.44
9	b	821	CLA	C3D-C4D	-2.70	1.38	1.44
9	a	826	CLA	C1D-C2D	-2.70	1.40	1.45
9	b	824	CLA	C3D-C4D	-2.69	1.38	1.44
9	A	827	CLA	C3D-C4D	-2.69	1.38	1.44
9	a	819	CLA	MG-NA	2.69	2.12	2.06
12	I	101	BCR	C19-C18	-2.69	1.40	1.45
12	i	101	BCR	C19-C18	-2.69	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	834	CLA	C3D-C4D	-2.68	1.38	1.44
9	A	820	CLA	C3D-C4D	-2.68	1.38	1.44
12	l	304	BCR	C12-C13	-2.68	1.40	1.45
9	B	803	CLA	C3D-C4D	-2.68	1.38	1.44
9	L	303	CLA	C3D-C4D	-2.68	1.38	1.44
9	A	802	CLA	C3D-C4D	-2.68	1.38	1.44
9	L	308	CLA	C4D-ND	-2.68	1.34	1.37
9	b	832	CLA	C1D-C2D	-2.68	1.40	1.45
9	b	808	CLA	C1D-C2D	-2.68	1.40	1.45
9	A	816	CLA	C3D-C4D	-2.68	1.38	1.44
9	B	839	CLA	MG-NA	2.67	2.12	2.06
9	a	818	CLA	C3D-C4D	-2.67	1.38	1.44
9	A	825	CLA	C1D-C2D	-2.67	1.40	1.45
9	b	832	CLA	C3D-C4D	-2.67	1.38	1.44
9	b	839	CLA	C3D-C4D	-2.67	1.38	1.44
9	A	829	CLA	C3D-C4D	-2.67	1.38	1.44
9	B	806	CLA	C3D-C4D	-2.67	1.38	1.44
9	B	811	CLA	C3D-C4D	-2.67	1.38	1.44
9	a	828	CLA	C1D-C2D	-2.66	1.40	1.45
9	A	824	CLA	C3D-C4D	-2.66	1.38	1.44
9	A	832	CLA	C3D-C4D	-2.66	1.38	1.44
9	b	831	CLA	C3D-C4D	-2.66	1.38	1.44
12	L	301	BCR	C12-C13	-2.66	1.40	1.45
9	B	832	CLA	C1D-C2D	-2.65	1.40	1.45
9	b	803	CLA	C1D-C2D	-2.65	1.40	1.45
12	I	101	BCR	C12-C13	-2.65	1.40	1.45
9	a	820	CLA	CHC-C1C	2.65	1.43	1.38
9	l	306	CLA	C3D-C4D	-2.65	1.38	1.44
9	B	821	CLA	C3D-C4D	-2.65	1.38	1.44
9	B	803	CLA	C1D-C2D	-2.64	1.40	1.45
9	b	823	CLA	C3D-C4D	-2.64	1.38	1.44
9	B	804	CLA	C3D-C4D	-2.64	1.38	1.44
9	b	804	CLA	C3D-C4D	-2.64	1.38	1.44
9	a	830	CLA	C3D-C4D	-2.64	1.38	1.44
9	b	815	CLA	C3D-C4D	-2.64	1.38	1.44
9	B	830	CLA	C3D-C4D	-2.63	1.38	1.44
9	B	831	CLA	C3D-C4D	-2.63	1.38	1.44
9	B	820	CLA	MG-NC	2.63	2.12	2.06
9	b	810	CLA	C1D-C2D	-2.63	1.40	1.45
9	a	846	CLA	C3D-C4D	-2.63	1.38	1.44
9	A	827	CLA	C1D-C2D	-2.63	1.40	1.45
9	A	804	CLA	C3D-C4D	-2.63	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	846	CLA	C3D-C4D	-2.63	1.38	1.44
9	B	804	CLA	MG-NA	2.63	2.12	2.06
9	B	839	CLA	C3D-C4D	-2.63	1.38	1.44
12	i	101	BCR	C12-C13	-2.63	1.40	1.45
9	a	802	CLA	C3D-C4D	-2.62	1.38	1.44
9	a	833	CLA	C3D-C4D	-2.62	1.38	1.44
9	a	804	CLA	C3D-C4D	-2.62	1.38	1.44
9	B	818	CLA	C3D-C4D	-2.62	1.38	1.44
9	b	830	CLA	C3D-C4D	-2.62	1.38	1.44
9	B	812	CLA	C3D-C4D	-2.62	1.38	1.44
9	B	815	CLA	C3D-C4D	-2.61	1.38	1.44
9	a	817	CLA	C3D-C4D	-2.61	1.38	1.44
9	B	810	CLA	C1D-C2D	-2.61	1.40	1.45
9	a	801	CLA	MG-NA	2.61	2.12	2.06
9	B	817	CLA	C3D-C4D	-2.61	1.38	1.44
9	B	819	CLA	C3D-C4D	-2.61	1.38	1.44
9	b	829	CLA	C3D-C4D	-2.61	1.38	1.44
9	b	826	CLA	C3D-C4D	-2.61	1.38	1.44
9	B	823	CLA	C1D-C2D	-2.61	1.40	1.45
9	B	808	CLA	C1D-C2D	-2.61	1.40	1.45
12	b	836	BCR	C12-C13	-2.61	1.40	1.45
9	b	827	CLA	C3D-C4D	-2.61	1.38	1.44
12	l	309	BCR	C12-C13	-2.60	1.40	1.45
9	B	829	CLA	C3D-C4D	-2.60	1.38	1.44
9	a	829	CLA	C3D-C4D	-2.60	1.38	1.44
9	a	808	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	806	CLA	C3D-C4D	-2.60	1.38	1.44
9	A	835	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	816	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	801	CLA	C3D-C4D	-2.60	1.38	1.44
9	A	812	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	810	CLA	C3D-C4D	-2.60	1.38	1.44
9	a	827	CLA	C3D-C4D	-2.60	1.38	1.44
9	a	821	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	823	CLA	C1D-C2D	-2.60	1.40	1.45
9	b	819	CLA	C3D-C4D	-2.60	1.38	1.44
9	b	804	CLA	MG-NA	2.60	2.12	2.06
12	B	836	BCR	C12-C13	-2.60	1.40	1.45
9	a	812	CLA	C3D-C4D	-2.59	1.38	1.44
9	L	302	CLA	C1B-C2B	-2.59	1.37	1.43
9	A	817	CLA	C3D-C4D	-2.59	1.38	1.44
9	b	818	CLA	C3D-C4D	-2.59	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	201	CLA	C3D-C4D	-2.59	1.38	1.44
9	B	820	CLA	C1D-C2D	-2.59	1.40	1.45
9	A	826	CLA	C1D-C2D	-2.59	1.40	1.45
9	A	828	CLA	C3D-C4D	-2.59	1.38	1.44
9	b	805	CLA	C3D-C4D	-2.59	1.38	1.44
9	l	305	CLA	C1D-C2D	-2.58	1.40	1.45
9	a	823	CLA	C3D-C4D	-2.58	1.38	1.44
9	b	828	CLA	C1D-C2D	-2.58	1.40	1.45
9	B	816	CLA	C3D-C4D	-2.58	1.38	1.44
9	a	836	CLA	C3D-C4D	-2.58	1.38	1.44
9	b	830	CLA	C1D-C2D	-2.58	1.40	1.45
9	a	835	CLA	C3D-C4D	-2.58	1.38	1.44
9	b	828	CLA	C3D-C4D	-2.58	1.38	1.44
9	a	846	CLA	C1B-C2B	-2.58	1.37	1.43
9	b	809	CLA	C1D-C2D	-2.58	1.40	1.45
12	b	836	BCR	C19-C18	-2.58	1.40	1.45
9	A	846	CLA	C1B-C2B	-2.58	1.37	1.43
9	B	819	CLA	C1B-C2B	-2.58	1.37	1.43
9	b	817	CLA	C3D-C4D	-2.57	1.38	1.44
9	l	306	CLA	C1D-C2D	-2.57	1.40	1.45
9	A	806	CLA	C3D-C4D	-2.57	1.38	1.44
12	a	843	BCR	C19-C18	-2.57	1.40	1.45
9	A	826	CLA	C3D-C4D	-2.57	1.38	1.44
9	B	810	CLA	C3D-C4D	-2.57	1.38	1.44
9	B	805	CLA	C3D-C4D	-2.57	1.38	1.44
9	A	822	CLA	C3D-C4D	-2.57	1.38	1.44
9	B	809	CLA	C1D-C2D	-2.57	1.40	1.45
9	B	801	CLA	C3D-C4D	-2.57	1.38	1.44
9	B	807	CLA	C1D-C2D	-2.57	1.40	1.45
9	l	305	CLA	C1B-C2B	-2.56	1.37	1.43
9	B	804	CLA	C1D-C2D	-2.56	1.40	1.45
9	a	827	CLA	C1D-C2D	-2.56	1.40	1.45
9	A	808	CLA	C3D-C4D	-2.56	1.38	1.44
9	B	822	CLA	C3D-C4D	-2.56	1.38	1.44
9	A	813	CLA	C3D-C4D	-2.56	1.38	1.44
9	B	827	CLA	C3D-C4D	-2.56	1.38	1.44
9	b	821	CLA	CAB-C3B	-2.56	1.45	1.50
9	A	808	CLA	MG-NA	2.56	2.12	2.06
9	a	832	CLA	C3D-C4D	-2.55	1.38	1.44
9	L	307	CLA	C3D-C4D	-2.55	1.38	1.44
9	B	828	CLA	C3D-C4D	-2.55	1.38	1.44
9	L	303	CLA	C1D-C2D	-2.55	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	831	CLA	C3D-C4D	-2.55	1.38	1.44
9	B	826	CLA	C3D-C4D	-2.55	1.38	1.44
9	a	813	CLA	C3D-C4D	-2.55	1.38	1.44
9	B	827	CLA	MG-NA	2.55	2.12	2.06
9	a	814	CLA	C3D-C4D	-2.54	1.38	1.44
9	B	813	CLA	C3D-C4D	-2.54	1.38	1.44
9	A	801	CLA	MG-NA	2.54	2.12	2.06
12	A	843	BCR	C12-C13	-2.54	1.40	1.45
9	b	807	CLA	C1D-C2D	-2.54	1.40	1.45
12	B	836	BCR	C19-C18	-2.54	1.40	1.45
9	B	828	CLA	C1D-C2D	-2.54	1.40	1.45
9	b	804	CLA	C1D-C2D	-2.54	1.40	1.45
9	a	811	CLA	C3D-C4D	-2.54	1.38	1.44
9	a	801	CLA	C1D-C2D	-2.54	1.40	1.45
9	l	302	CLA	C3D-C4D	-2.54	1.38	1.44
9	A	805	CLA	C3D-C4D	-2.54	1.38	1.44
9	A	847	CLA	C3D-C4D	-2.54	1.38	1.44
9	A	811	CLA	C3D-C4D	-2.54	1.38	1.44
9	A	834	CLA	C3D-C4D	-2.54	1.38	1.44
9	B	815	CLA	C1D-C2D	-2.53	1.40	1.45
9	A	825	CLA	C3D-C4D	-2.53	1.38	1.44
12	a	844	BCR	C12-C13	-2.53	1.40	1.45
9	a	825	CLA	C3D-C4D	-2.53	1.38	1.44
9	b	801	CLA	C1D-C2D	-2.53	1.40	1.45
9	A	809	CLA	C1D-C2D	-2.53	1.40	1.45
9	b	813	CLA	C3D-C4D	-2.53	1.38	1.44
9	l	302	CLA	C1D-C2D	-2.53	1.40	1.45
9	b	802	CLA	C3D-C4D	-2.53	1.38	1.44
9	A	809	CLA	C3D-C4D	-2.53	1.38	1.44
9	A	814	CLA	C3D-C4D	-2.53	1.38	1.44
9	B	821	CLA	CAB-C3B	-2.53	1.45	1.50
12	L	306	BCR	C19-C18	-2.53	1.40	1.45
9	a	826	CLA	C3D-C4D	-2.53	1.38	1.44
12	L	305	BCR	C19-C18	-2.53	1.40	1.45
9	a	837	CLA	C3D-C4D	-2.52	1.38	1.44
9	a	805	CLA	C3D-C4D	-2.52	1.38	1.44
9	a	809	CLA	C3D-C4D	-2.52	1.38	1.44
9	L	303	CLA	MG-NA	2.52	2.12	2.06
9	l	307	CLA	C3D-C4D	-2.52	1.38	1.44
9	b	820	CLA	C1D-C2D	-2.51	1.40	1.45
9	A	801	CLA	C3D-C4D	-2.51	1.38	1.44
9	B	828	CLA	MG-NC	2.51	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	802	CLA	C3D-C4D	-2.51	1.38	1.44
9	b	815	CLA	C1D-C2D	-2.51	1.40	1.45
9	a	806	CLA	C3D-C4D	-2.51	1.38	1.44
9	B	801	CLA	C1D-C2D	-2.51	1.40	1.45
9	b	822	CLA	C3D-C4D	-2.51	1.38	1.44
9	A	801	CLA	C1D-C2D	-2.51	1.40	1.45
9	a	807	CLA	C3D-C4D	-2.51	1.38	1.44
12	l	309	BCR	C19-C18	-2.51	1.40	1.45
9	a	820	CLA	CAB-C3B	2.51	1.54	1.47
12	l	304	BCR	C19-C18	-2.51	1.40	1.45
9	A	815	CLA	C1D-C2D	-2.51	1.40	1.45
9	L	302	CLA	C1D-C2D	-2.51	1.40	1.45
9	a	837	CLA	C1D-C2D	-2.50	1.40	1.45
9	A	815	CLA	C3D-C4D	-2.50	1.38	1.44
9	a	801	CLA	C3D-C4D	-2.50	1.38	1.44
9	b	802	CLA	C1B-C2B	-2.50	1.37	1.43
9	a	815	CLA	C3D-C4D	-2.50	1.38	1.44
12	L	301	BCR	C19-C18	-2.50	1.40	1.45
9	B	802	CLA	C1B-C2B	-2.50	1.37	1.43
9	b	828	CLA	MG-NC	2.50	2.12	2.06
9	b	827	CLA	MG-NA	2.50	2.12	2.06
12	A	840	BCR	C19-C18	-2.50	1.40	1.45
12	b	834	BCR	C12-C13	-2.50	1.40	1.45
9	a	847	CLA	C3D-C4D	-2.50	1.38	1.44
9	b	814	CLA	C3D-C4D	-2.49	1.38	1.44
9	A	823	CLA	C1D-C2D	-2.49	1.40	1.45
9	b	806	CLA	C1D-C2D	-2.49	1.40	1.45
12	B	834	BCR	C12-C13	-2.49	1.40	1.45
9	A	807	CLA	C3D-C4D	-2.49	1.38	1.44
9	h	202	CLA	C3D-C4D	-2.49	1.38	1.44
9	a	824	CLA	C1D-C2D	-2.49	1.40	1.45
9	A	836	CLA	C3D-C4D	-2.49	1.38	1.44
9	A	822	CLA	C1D-C2D	-2.49	1.40	1.45
9	B	814	CLA	C3D-C4D	-2.49	1.38	1.44
9	b	831	CLA	C1B-C2B	-2.48	1.37	1.43
12	L	305	BCR	C12-C13	-2.48	1.40	1.45
12	l	308	BCR	C12-C13	-2.48	1.40	1.45
9	a	803	CLA	C3D-C4D	-2.48	1.38	1.44
9	A	823	CLA	C3D-C4D	-2.48	1.38	1.44
9	a	823	CLA	C1D-C2D	-2.48	1.40	1.45
12	l	308	BCR	C19-C18	-2.48	1.40	1.45
9	B	804	CLA	C1B-C2B	-2.48	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	822	CLA	C3D-C4D	-2.48	1.38	1.44
9	a	834	CLA	C1D-C2D	-2.48	1.40	1.45
9	A	836	CLA	C1D-C2D	-2.48	1.40	1.45
9	B	802	CLA	C1D-C2D	-2.48	1.40	1.45
9	b	804	CLA	C1B-C2B	-2.47	1.37	1.43
9	L	304	CLA	C3D-C4D	-2.47	1.38	1.44
9	A	827	CLA	C1B-C2B	-2.47	1.37	1.43
9	a	824	CLA	C3D-C4D	-2.47	1.38	1.44
9	A	824	CLA	C1B-C2B	-2.47	1.37	1.43
9	b	805	CLA	C1B-C2B	-2.47	1.37	1.43
9	b	810	CLA	C1B-C2B	-2.47	1.37	1.43
9	B	805	CLA	C1B-C2B	-2.47	1.37	1.43
9	a	832	CLA	MG-NC	2.47	2.12	2.06
9	a	809	CLA	C1D-C2D	-2.47	1.40	1.45
9	b	840	CLA	C3D-C4D	-2.46	1.38	1.44
9	a	810	CLA	C3D-C4D	-2.46	1.38	1.44
9	A	821	CLA	C3D-C4D	-2.46	1.38	1.44
9	B	806	CLA	C1D-C2D	-2.46	1.40	1.45
9	A	831	CLA	C1B-C2B	-2.46	1.37	1.43
9	B	830	CLA	C1D-C2D	-2.46	1.40	1.45
9	A	803	CLA	C3D-C4D	-2.45	1.38	1.44
9	A	816	CLA	C1B-C2B	-2.45	1.37	1.43
9	b	805	CLA	C1D-C2D	-2.45	1.40	1.45
9	B	810	CLA	C1B-C2B	-2.45	1.37	1.43
12	a	841	BCR	C19-C18	-2.45	1.40	1.45
9	A	831	CLA	MG-NC	2.45	2.12	2.06
9	a	825	CLA	C1B-C2B	-2.44	1.37	1.43
9	B	807	CLA	C1B-C2B	-2.44	1.37	1.43
9	A	810	CLA	C3D-C4D	-2.44	1.38	1.44
9	b	840	CLA	C1D-C2D	-2.44	1.40	1.45
9	B	831	CLA	C1B-C2B	-2.44	1.37	1.43
9	a	825	CLA	C1D-C2D	-2.44	1.40	1.45
9	a	832	CLA	C1B-C2B	-2.44	1.37	1.43
9	a	831	CLA	C3D-C4D	-2.44	1.38	1.44
9	a	816	CLA	MG-NA	2.44	2.12	2.06
12	b	835	BCR	C19-C18	-2.43	1.40	1.45
9	A	820	CLA	MG-NA	2.43	2.12	2.06
9	A	833	CLA	C1D-C2D	-2.43	1.40	1.45
9	B	840	CLA	C3D-C4D	-2.43	1.38	1.44
9	A	802	CLA	C1B-C2B	-2.43	1.37	1.43
9	a	819	CLA	C3D-C4D	-2.43	1.38	1.44
9	h	201	CLA	O2A-CGA	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	820	CLA	C4B-NB	2.42	1.40	1.37
9	b	807	CLA	C1B-C2B	-2.42	1.37	1.43
9	A	828	CLA	C1D-C2D	-2.42	1.40	1.45
9	a	816	CLA	C1B-C2B	-2.42	1.37	1.43
9	A	847	CLA	C1D-C2D	-2.42	1.40	1.45
9	h	202	CLA	C1B-C2B	-2.42	1.37	1.43
9	a	847	CLA	C1D-C2D	-2.42	1.40	1.45
9	B	805	CLA	C1D-C2D	-2.42	1.40	1.45
9	a	827	CLA	C1B-NB	-2.41	1.34	1.37
9	A	814	CLA	C1B-C2B	-2.41	1.37	1.43
9	a	815	CLA	C1D-C2D	-2.41	1.40	1.45
9	A	824	CLA	C1D-C2D	-2.41	1.40	1.45
9	B	839	CLA	C1B-C2B	-2.41	1.37	1.43
9	A	817	CLA	C1B-C2B	-2.41	1.37	1.43
9	b	820	CLA	C3D-C4D	-2.40	1.38	1.44
9	B	820	CLA	C3D-C4D	-2.40	1.38	1.44
9	a	829	CLA	C1D-C2D	-2.40	1.40	1.45
9	a	802	CLA	C1B-C2B	-2.40	1.37	1.43
9	B	840	CLA	C1D-C2D	-2.40	1.40	1.45
9	b	821	CLA	C1D-C2D	-2.40	1.40	1.45
9	B	824	CLA	C1B-C2B	-2.40	1.37	1.43
9	b	824	CLA	C1B-C2B	-2.40	1.37	1.43
9	a	828	CLA	C1B-C2B	-2.40	1.37	1.43
9	A	847	CLA	C1B-C2B	-2.40	1.37	1.43
9	a	826	CLA	C1B-C2B	-2.39	1.37	1.43
9	B	828	CLA	C1B-C2B	-2.39	1.37	1.43
12	H	202	BCR	C12-C13	-2.39	1.40	1.45
9	A	826	CLA	C1B-NB	-2.39	1.34	1.37
9	A	834	CLA	C1D-C2D	-2.39	1.40	1.45
9	b	825	CLA	C1D-C2D	-2.39	1.40	1.45
9	a	847	CLA	C1B-C2B	-2.39	1.37	1.43
9	A	810	CLA	C1B-C2B	-2.39	1.37	1.43
9	b	819	CLA	C1B-C2B	-2.38	1.37	1.43
9	a	846	CLA	C1D-C2D	-2.38	1.40	1.45
9	A	826	CLA	C1B-C2B	-2.38	1.37	1.43
9	B	811	CLA	C1B-C2B	-2.38	1.37	1.43
9	B	821	CLA	C1D-C2D	-2.38	1.40	1.45
9	A	817	CLA	C1D-C2D	-2.38	1.40	1.45
9	a	835	CLA	C1D-C2D	-2.38	1.40	1.45
12	a	841	BCR	C12-C13	-2.38	1.40	1.45
9	b	839	CLA	C1D-C2D	-2.38	1.40	1.45
12	b	835	BCR	C12-C13	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	814	CLA	C1B-C2B	-2.37	1.37	1.43
9	A	846	CLA	C1D-C2D	-2.37	1.40	1.45
9	B	839	CLA	C1D-C2D	-2.37	1.40	1.45
12	A	840	BCR	C12-C13	-2.37	1.40	1.45
9	A	825	CLA	C1B-C2B	-2.37	1.37	1.43
9	b	806	CLA	C1B-C2B	-2.37	1.37	1.43
9	b	828	CLA	C1B-C2B	-2.37	1.37	1.43
9	B	812	CLA	C1D-C2D	-2.37	1.40	1.45
12	B	834	BCR	C19-C18	-2.37	1.40	1.45
9	b	831	CLA	C1D-C2D	-2.37	1.40	1.45
9	A	826	CLA	MG-NC	2.37	2.11	2.06
9	b	814	CLA	C1D-C2D	-2.37	1.40	1.45
9	a	802	CLA	C1B-NB	-2.36	1.34	1.37
12	A	841	BCR	C12-C13	-2.36	1.40	1.45
9	A	812	CLA	C1B-NB	-2.36	1.34	1.37
9	a	827	CLA	C1B-C2B	-2.36	1.37	1.43
12	B	835	BCR	C12-C13	-2.36	1.40	1.45
9	b	811	CLA	C1D-C2D	-2.36	1.40	1.45
9	b	839	CLA	C1B-C2B	-2.36	1.37	1.43
9	B	814	CLA	C1D-C2D	-2.36	1.40	1.45
12	a	843	BCR	C12-C13	-2.36	1.40	1.45
9	b	802	CLA	C1D-C2D	-2.35	1.40	1.45
9	b	802	CLA	MG-NC	2.35	2.11	2.06
12	a	842	BCR	C12-C13	-2.35	1.40	1.45
12	h	203	BCR	C12-C13	-2.35	1.40	1.45
9	A	831	CLA	C1D-C2D	-2.35	1.40	1.45
9	b	821	CLA	C1B-C2B	-2.35	1.37	1.43
9	b	826	CLA	C1B-C2B	-2.35	1.37	1.43
9	B	811	CLA	C1D-C2D	-2.35	1.40	1.45
9	B	826	CLA	C1B-C2B	-2.35	1.37	1.43
9	a	832	CLA	C1D-C2D	-2.35	1.40	1.45
9	B	825	CLA	C1B-C2B	-2.35	1.37	1.43
9	B	825	CLA	C1D-C2D	-2.35	1.40	1.45
9	A	824	CLA	MG-NA	2.34	2.11	2.06
9	b	801	CLA	C1B-C2B	-2.34	1.37	1.43
9	b	811	CLA	C1B-C2B	-2.34	1.37	1.43
9	B	822	CLA	C1D-C2D	-2.34	1.40	1.45
9	B	808	CLA	C1B-C2B	-2.34	1.37	1.43
9	B	819	CLA	C1D-C2D	-2.34	1.40	1.45
9	B	812	CLA	CAB-C3B	-2.34	1.45	1.50
9	b	829	CLA	C1D-C2D	-2.34	1.40	1.45
9	a	805	CLA	C1D-C2D	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	835	BCR	C19-C18	-2.34	1.40	1.45
9	b	823	CLA	C1B-C2B	-2.34	1.37	1.43
9	B	831	CLA	C1D-C2D	-2.34	1.40	1.45
9	B	801	CLA	C1B-C2B	-2.34	1.37	1.43
9	a	817	CLA	C1B-C2B	-2.34	1.37	1.43
9	l	307	CLA	C1B-C2B	-2.34	1.37	1.43
9	b	818	CLA	C1D-C2D	-2.34	1.40	1.45
9	b	825	CLA	C1B-C2B	-2.34	1.37	1.43
9	B	821	CLA	C1B-C2B	-2.34	1.37	1.43
9	B	829	CLA	C1B-C2B	-2.33	1.37	1.43
9	b	812	CLA	MG-NC	2.33	2.11	2.06
9	B	829	CLA	C1D-C2D	-2.33	1.40	1.45
9	B	816	CLA	C1B-C2B	-2.33	1.37	1.43
9	b	808	CLA	C1B-C2B	-2.33	1.37	1.43
12	b	834	BCR	C19-C18	-2.33	1.40	1.45
9	A	828	CLA	C1B-C2B	-2.32	1.37	1.43
12	A	842	BCR	C12-C13	-2.32	1.41	1.45
9	A	805	CLA	C1D-C2D	-2.32	1.40	1.45
9	B	806	CLA	C1B-C2B	-2.32	1.37	1.43
9	b	817	CLA	C1B-C2B	-2.32	1.37	1.43
9	a	803	CLA	C1B-C2B	-2.32	1.37	1.43
9	b	813	CLA	C1D-C2D	-2.32	1.40	1.45
9	l	307	CLA	C1D-C2D	-2.32	1.40	1.45
9	a	810	CLA	C1B-C2B	-2.32	1.37	1.43
9	a	819	CLA	MG-ND	-2.32	2.01	2.05
9	a	817	CLA	C1D-C2D	-2.32	1.40	1.45
9	B	809	CLA	C1B-C2B	-2.31	1.37	1.43
9	a	827	CLA	MG-NC	2.31	2.11	2.06
9	B	818	CLA	C1D-C2D	-2.31	1.40	1.45
9	B	803	CLA	MG-NA	2.31	2.11	2.06
9	B	823	CLA	C1B-C2B	-2.31	1.37	1.43
9	B	813	CLA	C1D-C2D	-2.31	1.40	1.45
9	A	819	CLA	MG-NB	2.31	2.10	2.05
9	B	817	CLA	C1B-C2B	-2.31	1.37	1.43
9	b	819	CLA	C1D-C2D	-2.31	1.40	1.45
9	a	815	CLA	C1B-C2B	-2.31	1.37	1.43
9	a	822	CLA	C1B-C2B	-2.31	1.37	1.43
9	a	829	CLA	C1B-C2B	-2.30	1.37	1.43
12	a	842	BCR	C19-C18	-2.30	1.41	1.45
9	a	802	CLA	MG-NA	2.30	2.11	2.06
9	A	803	CLA	C1B-C2B	-2.30	1.37	1.43
12	H	202	BCR	C19-C18	-2.30	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	823	CLA	C1B-C2B	-2.30	1.37	1.43
9	A	830	CLA	C3D-C4D	-2.30	1.39	1.44
9	A	829	CLA	C1D-C2D	-2.30	1.40	1.45
9	B	812	CLA	C1B-C2B	-2.30	1.37	1.43
9	l	306	CLA	C1B-C2B	-2.30	1.37	1.43
9	A	823	CLA	C1B-NB	-2.29	1.35	1.37
9	a	802	CLA	C1D-C2D	-2.29	1.40	1.45
9	A	808	CLA	C1B-C2B	-2.29	1.37	1.43
9	A	821	CLA	C1D-C2D	-2.29	1.40	1.45
9	A	802	CLA	C1B-NB	-2.29	1.35	1.37
9	A	834	CLA	C1B-C2B	-2.29	1.37	1.43
9	b	827	CLA	C1B-NB	-2.29	1.35	1.37
9	A	832	CLA	C1B-C2B	-2.29	1.37	1.43
9	a	812	CLA	C1B-NB	-2.29	1.35	1.37
9	A	814	CLA	C1D-C2D	-2.29	1.40	1.45
12	h	203	BCR	C19-C18	-2.29	1.41	1.45
9	b	809	CLA	C1B-C2B	-2.29	1.37	1.43
9	l	301	CLA	C1B-C2B	-2.29	1.37	1.43
9	b	803	CLA	MG-NA	2.29	2.11	2.06
9	b	829	CLA	C1B-C2B	-2.29	1.37	1.43
9	b	822	CLA	C1D-C2D	-2.29	1.40	1.45
9	A	822	CLA	C1B-C2B	-2.29	1.37	1.43
9	A	823	CLA	C1B-C2B	-2.29	1.37	1.43
9	B	817	CLA	C1D-C2D	-2.28	1.40	1.45
12	A	841	BCR	C19-C18	-2.28	1.41	1.45
9	a	808	CLA	C1B-C2B	-2.28	1.37	1.43
9	a	825	CLA	MG-NA	2.28	2.11	2.06
9	a	833	CLA	C1B-C2B	-2.28	1.37	1.43
9	b	816	CLA	C1B-C2B	-2.28	1.37	1.43
9	a	830	CLA	C1D-C2D	-2.28	1.40	1.45
9	A	812	CLA	C1B-C2B	-2.28	1.37	1.43
9	H	201	CLA	C1B-C2B	-2.28	1.37	1.43
9	B	805	CLA	C1B-NB	-2.28	1.35	1.37
9	b	817	CLA	C1D-C2D	-2.28	1.40	1.45
9	L	303	CLA	C1B-C2B	-2.28	1.37	1.43
9	A	806	CLA	C1D-C2D	-2.28	1.40	1.45
9	A	816	CLA	C1D-C2D	-2.28	1.40	1.45
9	A	815	CLA	C1B-C2B	-2.28	1.37	1.43
9	a	813	CLA	C1B-C2B	-2.28	1.37	1.43
9	A	813	CLA	C1B-C2B	-2.27	1.37	1.43
9	A	808	CLA	C1D-C2D	-2.27	1.40	1.45
9	b	802	CLA	C1B-NB	-2.27	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	816	CLA	C1D-C2D	-2.27	1.40	1.45
9	A	802	CLA	C1D-C2D	-2.27	1.40	1.45
9	B	820	CLA	C1B-C2B	-2.27	1.37	1.43
9	b	805	CLA	C1B-NB	-2.27	1.35	1.37
12	a	844	BCR	C19-C18	-2.27	1.41	1.45
9	b	815	CLA	C1B-C2B	-2.27	1.37	1.43
9	B	816	CLA	C1D-C2D	-2.27	1.40	1.45
9	B	832	CLA	C1B-C2B	-2.26	1.37	1.43
9	a	819	CLA	C1B-NB	-2.26	1.35	1.37
12	A	843	BCR	C19-C18	-2.26	1.41	1.45
9	a	814	CLA	C1D-C2D	-2.26	1.40	1.45
9	B	822	CLA	C1B-C2B	-2.26	1.37	1.43
9	a	807	CLA	C1B-C2B	-2.26	1.37	1.43
9	a	805	CLA	C1B-C2B	-2.26	1.37	1.43
9	l	302	CLA	C1B-NB	-2.26	1.35	1.37
9	B	815	CLA	C1B-C2B	-2.26	1.37	1.43
9	A	802	CLA	MG-NA	2.26	2.11	2.06
9	a	831	CLA	C1B-C2B	-2.26	1.37	1.43
9	h	202	CLA	C1B-NB	-2.26	1.35	1.37
9	a	834	CLA	C1B-C2B	-2.25	1.37	1.43
9	A	805	CLA	C1B-C2B	-2.25	1.37	1.43
9	a	812	CLA	C1B-C2B	-2.25	1.38	1.43
9	A	821	CLA	C1B-C2B	-2.25	1.38	1.43
9	b	831	CLA	MG-NC	2.24	2.11	2.06
9	b	818	CLA	C1B-C2B	-2.24	1.38	1.43
9	b	822	CLA	C1B-C2B	-2.24	1.38	1.43
9	a	811	CLA	C1B-C2B	-2.24	1.38	1.43
9	B	827	CLA	C1B-NB	-2.24	1.35	1.37
9	a	813	CLA	C1D-C2D	-2.24	1.40	1.45
9	L	304	CLA	C1D-C2D	-2.24	1.40	1.45
9	a	810	CLA	C1D-C2D	-2.24	1.40	1.45
9	b	832	CLA	C1B-C2B	-2.24	1.38	1.43
9	A	810	CLA	C1D-C2D	-2.24	1.40	1.45
9	b	810	CLA	C1B-NB	-2.24	1.35	1.37
9	A	846	CLA	C1B-NB	-2.24	1.35	1.37
9	A	811	CLA	C1D-C2D	-2.24	1.40	1.45
9	A	819	CLA	C1B-C2B	-2.24	1.38	1.43
9	a	829	CLA	C1B-NB	-2.24	1.35	1.37
9	B	818	CLA	MG-NA	2.24	2.11	2.06
9	a	830	CLA	C1B-C2B	-2.24	1.38	1.43
9	B	825	CLA	C1B-NB	-2.24	1.35	1.37
9	a	835	CLA	C1B-C2B	-2.23	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	827	CLA	C1B-C2B	-2.23	1.38	1.43
9	A	828	CLA	C1B-NB	-2.23	1.35	1.37
9	A	804	CLA	C1B-C2B	-2.23	1.38	1.43
9	b	814	CLA	C1B-C2B	-2.23	1.38	1.43
9	B	831	CLA	MG-NC	2.23	2.11	2.06
9	a	811	CLA	C1D-C2D	-2.23	1.40	1.45
9	A	803	CLA	C1D-C2D	-2.23	1.40	1.45
9	A	804	CLA	C1D-C2D	-2.23	1.40	1.45
9	b	827	CLA	C1B-C2B	-2.23	1.38	1.43
9	a	824	CLA	C1B-NB	-2.23	1.35	1.37
9	b	825	CLA	C1B-NB	-2.23	1.35	1.37
9	b	812	CLA	C3D-C4D	-2.23	1.39	1.44
9	a	804	CLA	C1B-C2B	-2.23	1.38	1.43
9	A	811	CLA	C1B-C2B	-2.23	1.38	1.43
9	a	819	CLA	C1B-C2B	-2.23	1.38	1.43
9	b	809	CLA	C1B-NB	-2.23	1.35	1.37
9	a	820	CLA	C1B-NB	-2.22	1.35	1.37
9	a	806	CLA	C1D-C2D	-2.22	1.40	1.45
9	a	808	CLA	C1D-C2D	-2.22	1.40	1.45
9	A	829	CLA	C1B-C2B	-2.22	1.38	1.43
9	b	818	CLA	MG-NA	2.22	2.11	2.06
9	a	824	CLA	C1B-C2B	-2.22	1.38	1.43
9	b	815	CLA	C1B-NB	-2.21	1.35	1.37
9	A	836	CLA	C1B-C2B	-2.21	1.38	1.43
9	a	809	CLA	C1B-C2B	-2.21	1.38	1.43
9	L	304	CLA	C1B-C2B	-2.21	1.38	1.43
9	B	818	CLA	C1B-C2B	-2.21	1.38	1.43
9	B	826	CLA	C1D-C2D	-2.21	1.41	1.45
9	b	826	CLA	C1D-C2D	-2.21	1.41	1.45
9	A	807	CLA	C1B-C2B	-2.21	1.38	1.43
9	a	821	CLA	C1B-C2B	-2.21	1.38	1.43
9	A	809	CLA	C1B-C2B	-2.21	1.38	1.43
9	B	810	CLA	C1B-NB	-2.21	1.35	1.37
9	A	820	CLA	C1B-C2B	-2.21	1.38	1.43
9	A	833	CLA	C1B-C2B	-2.21	1.38	1.43
9	B	825	CLA	MG-NC	2.20	2.11	2.06
9	A	818	CLA	C1B-C2B	-2.20	1.38	1.43
9	a	846	CLA	C1B-NB	-2.20	1.35	1.37
9	a	826	CLA	MG-NC	2.20	2.11	2.06
9	a	837	CLA	C1B-C2B	-2.20	1.38	1.43
9	B	814	CLA	C1B-C2B	-2.20	1.38	1.43
9	a	822	CLA	C1D-C2D	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	807	CLA	MG-NA	2.20	2.11	2.06
9	A	801	CLA	CHB-C1B	2.19	1.44	1.39
9	a	814	CLA	C1B-NB	-2.19	1.35	1.37
9	a	803	CLA	C1D-C2D	-2.19	1.41	1.45
9	a	818	CLA	C1B-C2B	-2.19	1.38	1.43
9	B	840	CLA	C1B-C2B	-2.19	1.38	1.43
9	b	812	CLA	C1B-C2B	-2.19	1.38	1.43
9	B	815	CLA	MG-NC	2.19	2.11	2.06
9	B	830	CLA	C1B-C2B	-2.18	1.38	1.43
9	b	830	CLA	C1B-C2B	-2.18	1.38	1.43
9	A	814	CLA	C1B-NB	-2.18	1.35	1.37
9	l	301	CLA	CHB-C1B	2.18	1.44	1.39
9	A	813	CLA	C1D-C2D	-2.18	1.41	1.45
9	b	824	CLA	C1B-NB	-2.18	1.35	1.37
9	b	804	CLA	C1B-NB	-2.18	1.35	1.37
9	b	840	CLA	C1B-C2B	-2.18	1.38	1.43
9	b	801	CLA	MG-NC	2.18	2.11	2.06
9	a	801	CLA	CHB-C1B	2.18	1.44	1.39
9	B	828	CLA	C1B-NB	-2.17	1.35	1.37
9	a	807	CLA	C1D-C2D	-2.17	1.41	1.45
9	A	829	CLA	C1B-NB	-2.17	1.35	1.37
9	a	830	CLA	C1B-NB	-2.16	1.35	1.37
9	a	816	CLA	C1D-C2D	-2.16	1.41	1.45
9	A	830	CLA	C1B-C2B	-2.16	1.38	1.43
9	B	802	CLA	C1B-NB	-2.16	1.35	1.37
9	B	807	CLA	C1B-NB	-2.16	1.35	1.37
9	h	201	CLA	CHB-C1B	2.16	1.44	1.39
9	B	824	CLA	C1B-NB	-2.16	1.35	1.37
9	A	835	CLA	C1B-C2B	-2.15	1.38	1.43
9	B	815	CLA	C1B-NB	-2.15	1.35	1.37
9	L	308	CLA	CHC-C1C	2.15	1.42	1.38
9	l	301	CLA	MG-NA	2.15	2.11	2.06
9	b	825	CLA	MG-NC	2.14	2.11	2.06
9	l	302	CLA	MG-NC	2.14	2.11	2.06
9	A	807	CLA	C1D-C2D	-2.14	1.41	1.45
9	B	809	CLA	C1B-NB	-2.14	1.35	1.37
9	A	806	CLA	CHB-C1B	2.14	1.44	1.39
9	a	804	CLA	C1D-C2D	-2.14	1.41	1.45
9	B	801	CLA	MG-NC	2.13	2.11	2.06
9	a	836	CLA	C1B-C2B	-2.13	1.38	1.43
9	L	307	CLA	C1B-C2B	-2.13	1.38	1.43
9	A	832	CLA	C1D-C2D	-2.13	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	833	CLA	C1D-C2D	-2.13	1.41	1.45
9	H	201	CLA	C1D-C2D	-2.12	1.41	1.45
9	a	801	CLA	C1B-C2B	-2.12	1.38	1.43
9	a	821	CLA	C1D-C2D	-2.12	1.41	1.45
9	B	804	CLA	C1B-NB	-2.12	1.35	1.37
9	b	807	CLA	C1B-NB	-2.12	1.35	1.37
9	b	812	CLA	CAB-C3B	-2.12	1.46	1.50
9	b	820	CLA	C1B-C2B	-2.12	1.38	1.43
9	A	820	CLA	C1D-C2D	-2.11	1.41	1.45
9	B	823	CLA	C1B-NB	-2.11	1.35	1.37
9	A	821	CLA	C1B-NB	-2.11	1.35	1.37
9	L	308	CLA	CMC-C2C	-2.11	1.46	1.50
9	L	307	CLA	C1B-NB	-2.11	1.35	1.37
9	b	840	CLA	C1B-NB	-2.11	1.35	1.37
9	h	202	CLA	C1D-C2D	-2.11	1.41	1.45
9	a	847	CLA	C1B-NB	-2.10	1.35	1.37
9	A	825	CLA	MG-NC	2.10	2.11	2.06
9	h	201	CLA	CAA-C2A	2.10	1.58	1.54
9	A	801	CLA	C1B-C2B	-2.10	1.38	1.43
9	h	201	CLA	C3B-C4B	2.10	1.47	1.42
9	a	820	CLA	CMA-C3A	-2.09	1.48	1.53
9	A	806	CLA	MG-NA	2.09	2.11	2.06
9	b	806	CLA	C1B-NB	-2.09	1.35	1.37
9	B	806	CLA	C1B-NB	-2.09	1.35	1.37
9	A	812	CLA	MG-NC	2.09	2.11	2.06
9	b	807	CLA	MG-NC	2.09	2.11	2.06
9	a	830	CLA	MG-NC	2.08	2.11	2.06
9	A	803	CLA	C1B-NB	-2.08	1.35	1.37
9	b	803	CLA	C1B-C2B	-2.08	1.38	1.43
9	b	814	CLA	MG-NC	2.08	2.11	2.06
9	b	828	CLA	C1B-NB	-2.08	1.35	1.37
9	h	201	CLA	C2-C3	2.08	1.38	1.33
9	B	827	CLA	C1D-C2D	-2.08	1.41	1.45
9	A	825	CLA	C1B-NB	-2.08	1.35	1.37
9	A	847	CLA	C1B-NB	-2.08	1.35	1.37
9	B	807	CLA	MG-NC	2.08	2.11	2.06
9	B	803	CLA	C1B-C2B	-2.07	1.38	1.43
9	b	830	CLA	C1B-NB	-2.07	1.35	1.37
9	A	847	CLA	MG-NC	2.07	2.11	2.06
9	b	822	CLA	C1B-NB	-2.07	1.35	1.37
9	B	812	CLA	MG-NC	2.07	2.11	2.06
9	a	812	CLA	C1D-C2D	-2.06	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	830	CLA	C1B-NB	-2.06	1.35	1.37
9	B	840	CLA	C1B-NB	-2.06	1.35	1.37
9	a	831	CLA	MG-NA	2.05	2.11	2.06
9	a	803	CLA	C1B-NB	-2.05	1.35	1.37
9	b	808	CLA	C1B-NB	-2.05	1.35	1.37
9	a	806	CLA	CHB-C1B	2.05	1.44	1.39
9	A	819	CLA	C3D-C4D	-2.05	1.39	1.44
9	a	847	CLA	MG-NC	2.04	2.11	2.06
9	a	819	CLA	CHB-C1B	2.04	1.44	1.39
9	b	819	CLA	C1B-NB	-2.04	1.35	1.37
9	a	819	CLA	MG-NC	2.04	2.11	2.06
9	H	201	CLA	C1B-NB	-2.04	1.35	1.37
9	a	812	CLA	MG-NC	2.04	2.11	2.06
9	a	816	CLA	C1B-NB	-2.03	1.35	1.37
9	B	814	CLA	MG-NC	2.03	2.11	2.06
9	A	806	CLA	C1B-C2B	-2.03	1.38	1.43
9	b	827	CLA	C1D-C2D	-2.03	1.41	1.45
9	B	831	CLA	C1B-NB	-2.02	1.35	1.37
9	B	819	CLA	C1B-NB	-2.02	1.35	1.37
9	h	201	CLA	CHB-C4A	2.02	1.42	1.37
9	a	804	CLA	C1B-NB	-2.02	1.35	1.37
9	l	302	CLA	C1B-C2B	-2.02	1.38	1.43
9	a	833	CLA	C1B-NB	-2.01	1.35	1.37
9	B	803	CLA	CHB-C1B	2.01	1.43	1.39
9	h	201	CLA	CMC-C2C	-2.01	1.46	1.50
9	A	817	CLA	C1B-NB	-2.00	1.35	1.37
9	B	801	CLA	C1B-NB	-2.00	1.35	1.37
9	b	803	CLA	CHB-C1B	2.00	1.43	1.39
9	b	831	CLA	C1B-NB	-2.00	1.35	1.37

All (1014) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	819	CLA	C3D-C4D-ND	-51.00	27.73	110.24
9	A	819	CLA	C3D-C2D-C1D	-47.75	40.67	105.83
9	A	819	CLA	C1D-ND-C4D	41.92	136.11	106.33
9	A	819	CLA	C2D-C1D-ND	-34.87	84.41	110.10
9	A	819	CLA	CHD-C1D-ND	22.23	144.88	124.45
9	A	819	CLA	CMD-C2D-C1D	14.98	151.11	124.71
9	a	820	CLA	CHC-C4B-NB	-12.98	110.52	124.26
9	a	820	CLA	CHD-C1D-ND	-9.30	115.91	124.45
9	a	820	CLA	C1D-ND-C4D	8.85	112.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	820	CLA	C4A-NA-C1A	8.43	110.50	106.71
9	h	201	CLA	C4A-NA-C1A	8.22	110.40	106.71
9	l	301	CLA	CHD-C1D-ND	-8.03	117.07	124.45
9	a	820	CLA	C2B-C1B-NB	-7.23	105.39	110.23
9	A	819	CLA	C1D-CHD-C4C	-7.11	110.71	126.06
9	A	819	CLA	C4D-C3D-CAD	-7.05	99.78	108.10
9	L	308	CLA	C4A-NA-C1A	7.01	109.86	106.71
9	A	819	CLA	CMD-C2D-C3D	-6.77	112.05	127.61
9	a	820	CLA	O2A-C1-C2	6.60	125.99	108.64
9	L	307	CLA	CHD-C1D-ND	-5.92	119.02	124.45
9	a	820	CLA	CMB-C2B-C3B	-5.76	112.62	126.59
9	A	819	CLA	CHA-C4D-ND	-5.64	120.70	132.50
9	A	808	CLA	CHD-C1D-ND	-5.36	119.53	124.45
9	a	820	CLA	CMB-C2B-C1B	5.34	133.50	125.37
9	b	827	CLA	CHD-C1D-ND	-5.07	119.79	124.45
9	a	820	CLA	C3B-C2B-C1B	5.06	113.27	107.16
9	B	827	CLA	CHD-C1D-ND	-5.03	119.83	124.45
9	a	820	CLA	CHD-C1D-C2D	4.93	135.82	125.48
9	a	836	CLA	CHD-C1D-ND	-4.91	119.94	124.45
9	A	835	CLA	CHD-C1D-ND	-4.88	119.97	124.45
9	a	820	CLA	C4D-CHA-C1A	4.86	127.16	121.25
9	l	301	CLA	CHD-C4C-C3C	4.74	131.81	124.84
9	A	812	CLA	CHD-C1D-ND	-4.74	120.10	124.45
9	b	820	CLA	CHD-C1D-ND	-4.73	120.11	124.45
14	B	837	DGD	O2G-C1B-C2B	4.59	121.38	111.50
9	h	201	CLA	CBA-CAA-C2A	4.58	127.37	113.86
14	b	837	DGD	O2G-C1B-C2B	4.54	121.29	111.50
9	b	816	CLA	CHD-C1D-ND	-4.54	120.28	124.45
9	A	813	CLA	CHD-C1D-ND	-4.53	120.29	124.45
12	b	834	BCR	C16-C15-C14	4.52	132.73	123.47
9	a	816	CLA	CHD-C1D-ND	-4.52	120.30	124.45
9	a	812	CLA	CHD-C1D-ND	-4.51	120.31	124.45
9	A	816	CLA	CHD-C1D-ND	-4.48	120.33	124.45
9	a	820	CLA	CBB-CAB-C3B	4.46	149.81	127.62
9	B	818	CLA	CHD-C1D-ND	-4.41	120.40	124.45
9	A	832	CLA	CHD-C1D-ND	-4.40	120.41	124.45
12	H	202	BCR	C30-C25-C26	-4.40	116.42	122.61
9	a	808	CLA	CHD-C1D-ND	-4.39	120.42	124.45
9	A	812	CLA	C4D-CHA-C1A	4.38	126.57	121.25
9	a	825	CLA	CHD-C1D-ND	-4.37	120.44	124.45
9	a	812	CLA	C4D-CHA-C1A	4.36	126.56	121.25
9	b	818	CLA	CHD-C1D-ND	-4.35	120.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	820	CLA	CHD-C1D-ND	-4.34	120.47	124.45
9	a	814	CLA	CHD-C1D-ND	-4.28	120.52	124.45
12	H	202	BCR	C37-C22-C21	-4.26	116.96	122.92
9	A	801	CLA	CHD-C1D-ND	-4.26	120.54	124.45
9	B	816	CLA	CHD-C1D-ND	-4.25	120.55	124.45
9	L	304	CLA	CHD-C1D-ND	-4.25	120.55	124.45
12	A	840	BCR	C37-C22-C21	-4.25	116.97	122.92
9	a	817	CLA	C4D-CHA-C1A	4.24	126.41	121.25
12	A	842	BCR	C34-C9-C10	-4.23	116.99	122.92
12	L	305	BCR	C37-C22-C21	-4.23	116.99	122.92
9	A	829	CLA	CHD-C1D-ND	-4.23	120.57	124.45
9	h	202	CLA	CHD-C1D-ND	-4.23	120.57	124.45
12	B	836	BCR	C37-C22-C21	-4.23	117.00	122.92
12	B	835	BCR	C34-C9-C10	-4.22	117.00	122.92
12	l	308	BCR	C37-C22-C21	-4.22	117.01	122.92
9	A	824	CLA	CHD-C1D-ND	-4.22	120.57	124.45
9	a	833	CLA	CHD-C1D-ND	-4.22	120.57	124.45
12	i	101	BCR	C37-C22-C21	-4.21	117.02	122.92
9	A	814	CLA	CHD-C1D-ND	-4.21	120.58	124.45
12	B	835	BCR	C37-C22-C21	-4.21	117.03	122.92
12	H	202	BCR	C34-C9-C10	-4.21	117.03	122.92
12	b	835	BCR	C34-C9-C10	-4.21	117.03	122.92
12	b	836	BCR	C34-C9-C10	-4.20	117.03	122.92
12	h	203	BCR	C37-C22-C21	-4.20	117.04	122.92
12	a	844	BCR	C34-C9-C10	-4.20	117.04	122.92
9	B	829	CLA	CHD-C1D-ND	-4.20	120.60	124.45
12	A	841	BCR	C34-C9-C10	-4.19	117.05	122.92
12	a	842	BCR	C34-C9-C10	-4.19	117.06	122.92
9	a	801	CLA	CHD-C1D-ND	-4.19	120.61	124.45
12	L	305	BCR	C34-C9-C10	-4.18	117.06	122.92
12	b	836	BCR	C37-C22-C21	-4.18	117.07	122.92
9	B	830	CLA	C4D-CHA-C1A	4.18	126.33	121.25
12	B	836	BCR	C34-C9-C10	-4.17	117.08	122.92
9	b	829	CLA	CHD-C1D-ND	-4.17	120.62	124.45
12	b	834	BCR	C34-C9-C10	-4.17	117.08	122.92
9	a	820	CLA	CHC-C1C-NC	4.16	130.52	124.20
9	A	802	CLA	CHD-C1D-ND	-4.16	120.63	124.45
12	I	101	BCR	C37-C22-C21	-4.16	117.10	122.92
9	A	846	CLA	CHD-C1D-ND	-4.15	120.64	124.45
12	B	834	BCR	C34-C9-C10	-4.15	117.11	122.92
12	a	841	BCR	C37-C22-C21	-4.15	117.12	122.92
12	h	203	BCR	C34-C9-C10	-4.14	117.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	843	BCR	C34-C9-C10	-4.14	117.12	122.92
12	I	101	BCR	C34-C9-C10	-4.14	117.13	122.92
12	i	101	BCR	C34-C9-C10	-4.13	117.13	122.92
9	a	819	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
12	A	843	BCR	C34-C9-C10	-4.13	117.14	122.92
9	b	802	CLA	CHD-C1D-ND	-4.13	120.66	124.45
9	b	819	CLA	CHD-C1D-ND	-4.13	120.66	124.45
9	B	823	CLA	CHD-C1D-ND	-4.13	120.66	124.45
9	H	201	CLA	CHD-C1D-ND	-4.12	120.66	124.45
9	b	825	CLA	CHD-C1D-ND	-4.12	120.66	124.45
12	l	309	BCR	C37-C22-C21	-4.12	117.15	122.92
9	a	846	CLA	CHD-C1D-ND	-4.12	120.67	124.45
12	b	835	BCR	C37-C22-C21	-4.12	117.15	122.92
12	l	304	BCR	C34-C9-C10	-4.12	117.15	122.92
12	a	844	BCR	C37-C22-C21	-4.12	117.16	122.92
12	l	308	BCR	C34-C9-C10	-4.12	117.16	122.92
12	A	843	BCR	C37-C22-C21	-4.11	117.16	122.92
9	b	823	CLA	CHD-C1D-ND	-4.10	120.68	124.45
9	b	830	CLA	C4D-CHA-C1A	4.10	126.24	121.25
9	a	802	CLA	CHD-C1D-ND	-4.09	120.69	124.45
9	A	804	CLA	CHD-C1D-ND	-4.09	120.70	124.45
12	b	834	BCR	C37-C22-C21	-4.09	117.19	122.92
9	l	301	CLA	CHD-C1D-C2D	4.08	134.05	125.48
9	l	307	CLA	CHD-C1D-ND	-4.08	120.71	124.45
12	L	306	BCR	C34-C9-C10	-4.07	117.22	122.92
12	B	834	BCR	C37-C22-C21	-4.06	117.24	122.92
12	L	306	BCR	C37-C22-C21	-4.06	117.24	122.92
9	a	813	CLA	CHD-C1D-ND	-4.05	120.73	124.45
9	a	830	CLA	CHD-C1D-ND	-4.05	120.73	124.45
12	l	309	BCR	C34-C9-C10	-4.05	117.25	122.92
9	b	819	CLA	C4D-CHA-C1A	4.04	126.17	121.25
9	l	305	CLA	C4D-CHA-C1A	4.04	126.17	121.25
9	B	825	CLA	CHD-C1D-ND	-4.04	120.74	124.45
12	B	835	BCR	C16-C15-C14	4.04	131.75	123.47
9	a	804	CLA	CHD-C1D-ND	-4.03	120.75	124.45
12	a	841	BCR	C34-C9-C10	-4.03	117.28	122.92
9	a	819	CLA	CHD-C1D-ND	-4.02	120.76	124.45
12	L	301	BCR	C34-C9-C10	-4.01	117.30	122.92
9	B	804	CLA	CHD-C1D-ND	-4.01	120.77	124.45
9	L	302	CLA	C4D-CHA-C1A	4.01	126.13	121.25
9	A	819	CLA	CHA-C1A-NA	-4.00	117.24	126.40
9	a	820	CLA	C2D-C1D-ND	-3.99	107.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	l	306	CLA	CHD-C1D-ND	-3.99	120.79	124.45
9	b	804	CLA	CHD-C1D-ND	-3.98	120.80	124.45
12	l	308	BCR	C15-C16-C17	3.98	131.62	123.47
12	L	305	BCR	C15-C16-C17	3.97	131.61	123.47
12	l	304	BCR	C37-C22-C21	-3.97	117.36	122.92
9	A	828	CLA	C4D-CHA-C1A	3.97	126.08	121.25
9	a	821	CLA	CHD-C1D-ND	-3.96	120.81	124.45
9	b	815	CLA	C4D-CHA-C1A	3.96	126.07	121.25
12	A	840	BCR	C34-C9-C10	-3.96	117.38	122.92
12	L	301	BCR	C37-C22-C21	-3.96	117.38	122.92
12	A	841	BCR	C37-C22-C21	-3.94	117.41	122.92
9	L	304	CLA	C4D-CHA-C1A	3.94	126.04	121.25
9	a	808	CLA	C4D-CHA-C1A	3.94	126.04	121.25
9	b	829	CLA	C4D-CHA-C1A	3.93	126.03	121.25
9	a	826	CLA	C4D-CHA-C1A	3.92	126.02	121.25
9	l	307	CLA	C4D-CHA-C1A	3.92	126.02	121.25
12	B	834	BCR	C16-C15-C14	3.92	131.50	123.47
9	A	829	CLA	C4D-CHA-C1A	3.92	126.02	121.25
9	a	830	CLA	C4D-CHA-C1A	3.92	126.02	121.25
9	B	829	CLA	C4D-CHA-C1A	3.91	126.01	121.25
12	a	842	BCR	C37-C22-C21	-3.91	117.45	122.92
9	B	812	CLA	CHD-C1D-ND	-3.90	120.87	124.45
9	B	812	CLA	C4D-CHA-C1A	3.90	125.99	121.25
9	B	820	CLA	CHD-C1D-ND	-3.89	120.88	124.45
9	B	819	CLA	C4D-CHA-C1A	3.89	125.98	121.25
9	L	303	CLA	CHD-C1D-ND	-3.87	120.90	124.45
9	B	819	CLA	CHD-C1D-ND	-3.87	120.90	124.45
9	A	806	CLA	CHD-C1D-ND	-3.87	120.90	124.45
9	A	825	CLA	C4D-CHA-C1A	3.86	125.95	121.25
9	B	821	CLA	CHD-C1D-ND	-3.86	120.91	124.45
9	a	817	CLA	CHD-C1D-ND	-3.85	120.91	124.45
9	A	830	CLA	CHD-C1D-ND	-3.85	120.91	124.45
9	a	829	CLA	C4D-CHA-C1A	3.85	125.94	121.25
9	B	815	CLA	C4D-CHA-C1A	3.85	125.94	121.25
9	b	821	CLA	CHD-C1D-ND	-3.84	120.92	124.45
9	B	808	CLA	C4D-CHA-C1A	3.84	125.92	121.25
12	l	309	BCR	C16-C15-C14	3.83	131.33	123.47
9	L	302	CLA	CHD-C1D-ND	-3.83	120.93	124.45
9	b	808	CLA	C4D-CHA-C1A	3.83	125.91	121.25
9	a	807	CLA	CHD-C1D-ND	-3.83	120.94	124.45
12	l	309	BCR	C12-C13-C14	3.82	124.81	118.94
9	b	823	CLA	C4D-CHA-C1A	3.82	125.90	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	817	CLA	C4D-CHA-C1A	3.82	125.90	121.25
12	A	842	BCR	C37-C22-C21	-3.82	117.57	122.92
12	A	843	BCR	C16-C15-C14	3.82	131.30	123.47
12	b	835	BCR	C1-C6-C5	-3.82	117.23	122.61
9	l	306	CLA	C4D-CHA-C1A	3.81	125.89	121.25
12	a	843	BCR	C37-C22-C21	-3.81	117.58	122.92
12	b	835	BCR	C16-C15-C14	3.81	131.28	123.47
9	A	803	CLA	CHD-C1D-ND	-3.80	120.96	124.45
12	l	309	BCR	C35-C13-C14	-3.79	117.61	122.92
12	H	202	BCR	C15-C16-C17	3.79	131.23	123.47
9	B	802	CLA	CHD-C1D-ND	-3.78	120.98	124.45
9	a	837	CLA	C4D-CHA-C1A	3.78	125.85	121.25
9	b	831	CLA	CHD-C1D-ND	-3.78	120.98	124.45
9	l	305	CLA	CHD-C1D-ND	-3.78	120.98	124.45
12	h	203	BCR	C30-C25-C26	-3.78	117.29	122.61
12	a	841	BCR	C15-C16-C17	3.78	131.21	123.47
9	B	830	CLA	CHD-C1D-ND	-3.77	120.99	124.45
9	B	832	CLA	C4D-CHA-C1A	3.77	125.84	121.25
9	b	832	CLA	C4D-CHA-C1A	3.77	125.84	121.25
9	a	803	CLA	CHD-C1D-ND	-3.76	121.00	124.45
9	b	812	CLA	C4D-CHA-C1A	3.76	125.83	121.25
9	b	811	CLA	CHD-C1D-ND	-3.76	121.00	124.45
9	B	828	CLA	C4D-CHA-C1A	3.76	125.82	121.25
9	a	829	CLA	CHD-C1D-ND	-3.76	121.00	124.45
12	a	844	BCR	C16-C15-C14	3.75	131.16	123.47
12	B	835	BCR	C15-C16-C17	3.75	131.16	123.47
9	b	822	CLA	CHD-C1D-ND	-3.75	121.01	124.45
9	b	817	CLA	CHD-C1D-ND	-3.75	121.01	124.45
9	b	828	CLA	C4D-CHA-C1A	3.74	125.81	121.25
9	a	810	CLA	CHD-C1D-ND	-3.74	121.02	124.45
9	b	809	CLA	CHD-C1D-ND	-3.73	121.02	124.45
9	a	815	CLA	CHD-C1D-ND	-3.73	121.02	124.45
9	B	811	CLA	CHD-C1D-ND	-3.73	121.03	124.45
9	B	809	CLA	CHD-C1D-ND	-3.72	121.03	124.45
9	b	830	CLA	CHD-C1D-ND	-3.71	121.04	124.45
9	B	817	CLA	CHD-C1D-ND	-3.71	121.04	124.45
9	A	824	CLA	C4D-CHA-C1A	3.71	125.76	121.25
9	a	825	CLA	C4D-CHA-C1A	3.71	125.76	121.25
9	A	817	CLA	CHD-C1D-ND	-3.70	121.05	124.45
9	b	806	CLA	CHD-C1D-ND	-3.70	121.05	124.45
9	A	808	CLA	C4D-CHA-C1A	3.70	125.75	121.25
9	a	813	CLA	C4D-CHA-C1A	3.70	125.75	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	806	CLA	CHD-C1D-ND	-3.70	121.06	124.45
9	B	831	CLA	CHD-C1D-ND	-3.70	121.06	124.45
9	b	805	CLA	CHD-C1D-ND	-3.69	121.06	124.45
9	A	836	CLA	C4D-CHA-C1A	3.69	125.74	121.25
9	b	815	CLA	CHD-C1D-ND	-3.68	121.07	124.45
9	b	826	CLA	CHD-C1D-ND	-3.68	121.07	124.45
9	B	826	CLA	CHD-C1D-ND	-3.68	121.07	124.45
12	a	843	BCR	C15-C16-C17	3.67	131.00	123.47
12	h	203	BCR	C15-C16-C17	3.67	130.99	123.47
9	a	822	CLA	CHD-C1D-ND	-3.67	121.08	124.45
9	a	831	CLA	CHD-C1D-ND	-3.66	121.09	124.45
9	B	823	CLA	C4D-CHA-C1A	3.66	125.71	121.25
12	L	306	BCR	C16-C15-C14	3.66	130.98	123.47
9	A	821	CLA	CHD-C1D-ND	-3.66	121.09	124.45
9	a	806	CLA	CHD-C1D-ND	-3.66	121.09	124.45
9	A	828	CLA	CHD-C1D-ND	-3.65	121.10	124.45
12	A	840	BCR	C15-C16-C17	3.65	130.95	123.47
9	A	807	CLA	CHD-C1D-ND	-3.64	121.11	124.45
9	a	820	CLA	CAA-C2A-C1A	3.64	123.90	111.97
12	L	306	BCR	C12-C13-C14	3.64	124.52	118.94
9	B	806	CLA	C4D-CHA-C1A	3.64	125.67	121.25
9	A	831	CLA	C4D-CHA-C1A	3.63	125.67	121.25
12	L	306	BCR	C15-C16-C17	3.63	130.91	123.47
12	A	840	BCR	C16-C15-C14	3.63	130.90	123.47
9	B	813	CLA	CHD-C1D-ND	-3.62	121.12	124.45
9	b	812	CLA	CHD-C1D-ND	-3.62	121.13	124.45
9	A	810	CLA	C4D-CHA-C1A	3.61	125.64	121.25
9	A	835	CLA	C4D-CHA-C1A	3.61	125.64	121.25
12	B	836	BCR	C36-C18-C17	-3.61	117.87	122.92
12	h	203	BCR	C16-C15-C14	3.60	130.85	123.47
9	b	839	CLA	CHD-C1D-ND	-3.60	121.14	124.45
9	b	806	CLA	C4D-CHA-C1A	3.60	125.63	121.25
9	A	810	CLA	CHD-C1D-ND	-3.60	121.15	124.45
9	b	811	CLA	C4D-CHA-C1A	3.59	125.62	121.25
9	B	817	CLA	C4D-CHA-C1A	3.59	125.62	121.25
9	b	817	CLA	C4D-CHA-C1A	3.59	125.62	121.25
9	A	815	CLA	C4D-CHA-C1A	3.59	125.62	121.25
9	B	810	CLA	C4D-CHA-C1A	3.59	125.61	121.25
9	b	810	CLA	C4D-CHA-C1A	3.59	125.61	121.25
9	B	839	CLA	CHD-C1D-ND	-3.59	121.16	124.45
12	b	836	BCR	C36-C18-C17	-3.58	117.90	122.92
9	A	813	CLA	C4D-CHA-C1A	3.58	125.61	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	805	CLA	CHD-C1D-ND	-3.58	121.17	124.45
9	b	813	CLA	CHD-C1D-ND	-3.58	121.17	124.45
9	a	832	CLA	C4D-CHA-C1A	3.58	125.60	121.25
9	A	815	CLA	CHD-C1D-ND	-3.58	121.17	124.45
9	B	816	CLA	C4D-CHA-C1A	3.57	125.60	121.25
9	a	836	CLA	C4D-CHA-C1A	3.56	125.59	121.25
9	a	823	CLA	C4D-CHA-C1A	3.56	125.58	121.25
9	b	831	CLA	C4D-CHA-C1A	3.55	125.58	121.25
12	a	842	BCR	C16-C15-C14	3.55	130.75	123.47
12	l	309	BCR	C15-C16-C17	3.55	130.75	123.47
12	a	841	BCR	C16-C15-C14	3.55	130.75	123.47
12	H	202	BCR	C16-C15-C14	3.55	130.74	123.47
9	B	831	CLA	C4D-CHA-C1A	3.55	125.57	121.25
9	A	814	CLA	C4D-CHA-C1A	3.55	125.56	121.25
9	B	811	CLA	C4D-CHA-C1A	3.55	125.56	121.25
9	L	303	CLA	C4D-CHA-C1A	3.54	125.56	121.25
9	B	814	CLA	C4D-CHA-C1A	3.54	125.56	121.25
12	A	841	BCR	C36-C18-C17	-3.54	117.96	122.92
12	b	836	BCR	C15-C16-C17	3.54	130.72	123.47
9	B	822	CLA	CHD-C1D-ND	-3.53	121.21	124.45
9	L	307	CLA	CHB-C1B-NB	-3.53	120.52	124.26
9	b	814	CLA	C4D-CHA-C1A	3.53	125.54	121.25
9	b	813	CLA	C4D-CHA-C1A	3.52	125.53	121.25
9	h	201	CLA	C1-O2A-CGA	3.52	125.68	116.44
9	A	832	CLA	C4D-CHA-C1A	3.52	125.53	121.25
9	a	821	CLA	C4D-CHA-C1A	3.52	125.53	121.25
12	L	306	BCR	C35-C13-C14	-3.51	118.00	122.92
9	a	804	CLA	C4D-CHA-C1A	3.51	125.52	121.25
12	a	842	BCR	C36-C18-C17	-3.51	118.00	122.92
9	a	814	CLA	C4D-CHA-C1A	3.51	125.52	121.25
12	B	836	BCR	C15-C16-C17	3.51	130.66	123.47
12	H	202	BCR	C35-C13-C14	-3.51	118.01	122.92
12	i	101	BCR	C36-C18-C17	-3.51	118.01	122.92
12	h	203	BCR	C35-C13-C14	-3.50	118.02	122.92
12	l	304	BCR	C16-C15-C14	3.50	130.64	123.47
9	A	804	CLA	C4D-CHA-C1A	3.50	125.50	121.25
9	b	827	CLA	C4D-CHA-C1A	3.49	125.50	121.25
12	I	101	BCR	C36-C18-C17	-3.49	118.04	122.92
12	B	834	BCR	C15-C16-C17	3.49	130.62	123.47
9	b	820	CLA	C4D-CHA-C1A	3.49	125.49	121.25
9	a	810	CLA	C4D-CHA-C1A	3.48	125.49	121.25
9	h	201	CLA	O2D-CGD-O1D	-3.48	117.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	202	BCR	C36-C18-C17	-3.47	118.06	122.92
12	L	301	BCR	C16-C15-C14	3.47	130.59	123.47
9	a	815	CLA	C4D-CHA-C1A	3.47	125.47	121.25
12	A	842	BCR	C35-C13-C14	-3.47	118.06	122.92
9	a	827	CLA	CHD-C1D-ND	-3.47	121.27	124.45
9	b	818	CLA	C4D-CHA-C1A	3.47	125.47	121.25
9	h	201	CLA	CAA-C2A-C3A	3.46	122.26	112.78
12	b	835	BCR	C15-C16-C17	3.46	130.55	123.47
12	B	836	BCR	C19-C18-C17	3.46	124.24	118.94
9	B	827	CLA	C4D-CHA-C1A	3.45	125.45	121.25
12	A	843	BCR	C36-C18-C17	-3.45	118.09	122.92
12	b	834	BCR	C8-C9-C10	3.45	124.23	118.94
9	b	808	CLA	CHD-C1D-ND	-3.45	121.29	124.45
12	B	835	BCR	C35-C13-C14	-3.45	118.10	122.92
9	a	833	CLA	C4D-CHA-C1A	3.44	125.44	121.25
9	b	821	CLA	C4D-CHA-C1A	3.44	125.44	121.25
12	h	203	BCR	C36-C18-C17	-3.44	118.10	122.92
12	a	843	BCR	C16-C15-C14	3.44	130.53	123.47
9	A	811	CLA	CHD-C1D-ND	-3.44	121.29	124.45
12	a	841	BCR	C36-C18-C17	-3.44	118.10	122.92
9	B	818	CLA	C4D-CHA-C1A	3.43	125.43	121.25
12	A	840	BCR	C36-C18-C17	-3.43	118.12	122.92
9	B	813	CLA	C4D-CHA-C1A	3.43	125.42	121.25
12	L	305	BCR	C36-C18-C17	-3.43	118.12	122.92
9	A	822	CLA	C4D-CHA-C1A	3.43	125.42	121.25
12	l	308	BCR	C36-C18-C17	-3.42	118.13	122.92
9	A	834	CLA	CHD-C1D-ND	-3.42	121.31	124.45
9	a	823	CLA	CHD-C1D-ND	-3.41	121.32	124.45
9	b	810	CLA	CHD-C1D-ND	-3.41	121.32	124.45
12	a	844	BCR	C36-C18-C17	-3.41	118.15	122.92
9	B	810	CLA	CHD-C1D-ND	-3.41	121.32	124.45
12	I	101	BCR	C15-C16-C17	3.40	130.45	123.47
9	b	824	CLA	CHD-C1D-ND	-3.40	121.33	124.45
9	b	839	CLA	C4D-CHA-C1A	3.39	125.38	121.25
12	a	842	BCR	C35-C13-C14	-3.39	118.17	122.92
12	a	844	BCR	C15-C16-C17	3.39	130.42	123.47
12	l	304	BCR	C36-C18-C17	-3.39	118.18	122.92
12	L	301	BCR	C36-C18-C17	-3.39	118.18	122.92
9	h	201	CLA	C2B-C1B-NB	-3.39	107.96	110.23
9	B	824	CLA	C4D-CHA-C1A	3.39	125.37	121.25
12	B	836	BCR	C16-C15-C14	3.38	130.41	123.47
12	a	843	BCR	C35-C13-C14	-3.38	118.18	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	824	CLA	C4D-CHA-C1A	3.38	125.37	121.25
9	l	301	CLA	CAC-C3C-C4C	3.38	129.20	124.81
9	A	822	CLA	CHD-C1D-ND	-3.38	121.34	124.45
9	b	840	CLA	C4D-CHA-C1A	3.38	125.36	121.25
9	A	826	CLA	CHD-C1D-ND	-3.38	121.35	124.45
9	B	821	CLA	C4D-CHA-C1A	3.38	125.36	121.25
12	B	834	BCR	C36-C18-C17	-3.38	118.19	122.92
9	a	805	CLA	CHD-C1D-ND	-3.38	121.35	124.45
12	i	101	BCR	C15-C16-C17	3.38	130.39	123.47
12	b	836	BCR	C16-C15-C14	3.38	130.39	123.47
12	A	841	BCR	C35-C13-C14	-3.38	118.19	122.92
12	i	101	BCR	C16-C15-C14	3.37	130.39	123.47
9	A	805	CLA	CHD-C1D-ND	-3.37	121.35	124.45
12	A	843	BCR	C15-C16-C17	3.37	130.39	123.47
9	B	839	CLA	C4D-CHA-C1A	3.37	125.35	121.25
9	B	808	CLA	CHD-C1D-ND	-3.37	121.36	124.45
12	l	309	BCR	C36-C18-C17	-3.37	118.20	122.92
12	b	836	BCR	C19-C18-C17	3.37	124.11	118.94
9	A	820	CLA	C4D-CHA-C1A	3.37	125.35	121.25
9	b	816	CLA	C4D-CHA-C1A	3.37	125.35	121.25
9	b	832	CLA	CHD-C1D-ND	-3.37	121.36	124.45
12	B	834	BCR	C8-C9-C10	3.37	124.11	118.94
12	B	836	BCR	C35-C13-C14	-3.36	118.21	122.92
9	A	809	CLA	C4D-CHA-C1A	3.36	125.34	121.25
12	a	841	BCR	C35-C13-C14	-3.36	118.21	122.92
9	B	801	CLA	C4D-CHA-C1A	3.36	125.34	121.25
9	B	815	CLA	CHD-C1D-ND	-3.36	121.37	124.45
12	b	835	BCR	C35-C13-C14	-3.35	118.22	122.92
12	b	836	BCR	C35-C13-C14	-3.35	118.22	122.92
12	b	834	BCR	C35-C13-C14	-3.35	118.23	122.92
12	I	101	BCR	C16-C15-C14	3.35	130.34	123.47
12	A	843	BCR	C35-C13-C14	-3.35	118.23	122.92
12	L	306	BCR	C36-C18-C17	-3.34	118.24	122.92
12	H	202	BCR	C12-C13-C14	3.34	124.07	118.94
9	B	832	CLA	CHD-C1D-ND	-3.34	121.39	124.45
12	h	203	BCR	C12-C13-C14	3.34	124.06	118.94
9	b	826	CLA	C4D-CHA-C1A	3.33	125.31	121.25
12	B	835	BCR	C36-C18-C17	-3.33	118.25	122.92
12	a	844	BCR	C35-C13-C14	-3.32	118.27	122.92
9	B	840	CLA	C4D-CHA-C1A	3.32	125.29	121.25
12	A	841	BCR	C16-C15-C14	3.32	130.27	123.47
12	b	834	BCR	C36-C18-C17	-3.32	118.28	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	101	BCR	C35-C13-C14	-3.32	118.28	122.92
12	A	840	BCR	C35-C13-C14	-3.32	118.28	122.92
9	a	835	CLA	CHD-C1D-ND	-3.32	121.41	124.45
9	A	827	CLA	CHD-C1D-ND	-3.31	121.41	124.45
9	b	801	CLA	C4D-CHA-C1A	3.31	125.28	121.25
9	a	827	CLA	C4D-CHA-C1A	3.31	125.28	121.25
12	B	834	BCR	C35-C13-C14	-3.31	118.29	122.92
9	a	811	CLA	CHD-C1D-ND	-3.31	121.42	124.45
9	l	301	CLA	CHA-C1A-NA	-3.31	118.83	126.40
9	A	833	CLA	CHD-C1D-ND	-3.31	121.42	124.45
9	A	807	CLA	C4D-CHA-C1A	3.31	125.27	121.25
9	B	824	CLA	CHD-C1D-ND	-3.30	121.42	124.45
9	A	826	CLA	C4D-CHA-C1A	3.30	125.27	121.25
9	A	846	CLA	C4D-CHA-C1A	3.30	125.27	121.25
12	i	101	BCR	C35-C13-C14	-3.29	118.31	122.92
9	a	809	CLA	C4D-CHA-C1A	3.29	125.25	121.25
9	B	826	CLA	C4D-CHA-C1A	3.29	125.25	121.25
9	h	201	CLA	CHC-C4B-NB	3.29	127.74	124.26
9	a	846	CLA	C4D-CHA-C1A	3.29	125.25	121.25
12	l	308	BCR	C35-C13-C14	-3.28	118.33	122.92
9	A	827	CLA	C4D-CHA-C1A	3.27	125.23	121.25
9	a	834	CLA	CHD-C1D-ND	-3.27	121.45	124.45
9	B	814	CLA	CHD-C1D-ND	-3.27	121.45	124.45
9	b	803	CLA	CHD-C1D-ND	-3.27	121.45	124.45
12	I	101	BCR	C19-C18-C17	3.27	123.96	118.94
12	L	305	BCR	C35-C13-C14	-3.27	118.35	122.92
9	A	847	CLA	C4D-CHA-C1A	3.26	125.22	121.25
12	a	842	BCR	C15-C16-C17	3.26	130.16	123.47
9	b	814	CLA	CHD-C1D-ND	-3.26	121.46	124.45
12	i	101	BCR	C19-C18-C17	3.26	123.94	118.94
12	B	835	BCR	C12-C13-C14	3.25	123.93	118.94
9	A	819	CLA	C2A-C1A-CHA	3.25	129.55	123.86
9	a	802	CLA	C4D-CHA-C1A	3.25	125.20	121.25
9	A	821	CLA	C4D-CHA-C1A	3.24	125.20	121.25
9	B	820	CLA	C4D-CHA-C1A	3.24	125.20	121.25
12	L	301	BCR	C35-C13-C14	-3.24	118.38	122.92
9	h	202	CLA	C4D-CHA-C1A	3.24	125.19	121.25
12	b	835	BCR	C36-C18-C17	-3.24	118.39	122.92
12	A	842	BCR	C15-C16-C17	3.24	130.10	123.47
9	B	801	CLA	CAC-C3C-C4C	3.23	129.00	124.81
9	L	307	CLA	CHD-C1D-C2D	3.22	132.24	125.48
12	l	304	BCR	C35-C13-C14	-3.22	118.42	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	847	CLA	C4D-CHA-C1A	3.22	125.16	121.25
9	A	811	CLA	C4D-CHA-C1A	3.21	125.16	121.25
9	b	805	CLA	C4D-CHA-C1A	3.21	125.16	121.25
9	a	803	CLA	C4D-CHA-C1A	3.20	125.15	121.25
9	a	847	CLA	CHD-C1D-ND	-3.20	121.51	124.45
9	A	802	CLA	C4D-CHA-C1A	3.20	125.14	121.25
9	A	806	CLA	CHA-C1A-NA	-3.20	119.07	126.40
9	A	847	CLA	CHD-C1D-ND	-3.20	121.52	124.45
9	B	805	CLA	C4D-CHA-C1A	3.20	125.14	121.25
12	a	841	BCR	C19-C18-C17	3.19	123.84	118.94
9	A	803	CLA	C4D-CHA-C1A	3.19	125.13	121.25
12	b	834	BCR	C15-C16-C17	3.19	130.00	123.47
9	A	816	CLA	C4D-CHA-C1A	3.18	125.12	121.25
9	a	807	CLA	C4D-CHA-C1A	3.18	125.12	121.25
9	a	811	CLA	C4D-CHA-C1A	3.18	125.11	121.25
9	A	833	CLA	C4D-CHA-C1A	3.17	125.11	121.25
12	l	308	BCR	C16-C15-C14	3.16	129.96	123.47
9	a	819	CLA	C4A-NA-C1A	3.16	108.13	106.71
9	A	809	CLA	CHD-C1D-ND	-3.16	121.55	124.45
12	A	843	BCR	C12-C13-C14	3.16	123.78	118.94
9	B	803	CLA	CHD-C1D-ND	-3.16	121.55	124.45
12	A	841	BCR	C19-C18-C17	3.15	123.78	118.94
9	H	201	CLA	C4D-CHA-C1A	3.15	125.08	121.25
9	a	828	CLA	CHD-C1D-ND	-3.15	121.56	124.45
9	b	807	CLA	C4D-CHA-C1A	3.15	125.08	121.25
12	a	842	BCR	C19-C18-C17	3.15	123.77	118.94
9	a	809	CLA	CHD-C1D-ND	-3.14	121.56	124.45
12	L	305	BCR	C23-C22-C21	3.14	123.75	118.94
9	b	807	CLA	CHD-C1D-ND	-3.13	121.57	124.45
9	a	828	CLA	C4D-CHA-C1A	3.13	125.06	121.25
12	L	305	BCR	C16-C15-C14	3.13	129.88	123.47
9	B	807	CLA	CHD-C1D-ND	-3.13	121.58	124.45
12	A	840	BCR	C19-C18-C17	3.13	123.74	118.94
9	B	807	CLA	C4D-CHA-C1A	3.12	125.05	121.25
12	L	301	BCR	C19-C18-C17	3.12	123.73	118.94
9	a	822	CLA	C4D-CHA-C1A	3.12	125.05	121.25
12	B	834	BCR	C19-C18-C17	3.12	123.72	118.94
9	a	806	CLA	C4D-CHA-C1A	3.12	125.04	121.25
9	b	801	CLA	CAC-C3C-C4C	3.11	128.85	124.81
12	B	834	BCR	C30-C25-C26	-3.11	118.23	122.61
12	L	301	BCR	C15-C16-C17	3.11	129.85	123.47
12	a	842	BCR	C12-C13-C14	3.11	123.71	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	822	CLA	C4D-CHA-C1A	3.10	125.02	121.25
12	l	309	BCR	C19-C18-C17	3.10	123.70	118.94
12	A	843	BCR	C19-C18-C17	3.10	123.69	118.94
9	A	823	CLA	C4D-CHA-C1A	3.09	125.01	121.25
12	l	308	BCR	C23-C22-C21	3.09	123.68	118.94
12	a	844	BCR	C12-C13-C14	3.09	123.68	118.94
9	B	804	CLA	C4D-CHA-C1A	3.09	125.00	121.25
12	L	306	BCR	C19-C18-C17	3.08	123.67	118.94
9	a	820	CLA	CHB-C1B-NB	-3.08	121.00	124.26
12	l	304	BCR	C15-C16-C17	3.08	129.78	123.47
9	a	834	CLA	C4D-CHA-C1A	3.08	124.99	121.25
12	l	304	BCR	C19-C18-C17	3.08	123.66	118.94
12	a	843	BCR	C36-C18-C17	-3.07	118.62	122.92
9	b	828	CLA	CHD-C1D-ND	-3.07	121.63	124.45
12	L	305	BCR	C19-C18-C17	3.07	123.65	118.94
12	H	202	BCR	C19-C18-C17	3.07	123.65	118.94
12	a	844	BCR	C30-C25-C26	-3.06	118.30	122.61
12	b	834	BCR	C19-C18-C17	3.06	123.63	118.94
9	h	201	CLA	O2D-CGD-CBD	3.05	116.69	111.27
9	b	840	CLA	CHD-C1D-ND	-3.05	121.65	124.45
12	A	841	BCR	C15-C16-C17	3.05	129.72	123.47
9	B	822	CLA	C4D-CHA-C1A	3.05	124.96	121.25
12	a	843	BCR	C12-C13-C14	3.04	123.61	118.94
12	h	203	BCR	C19-C18-C17	3.04	123.61	118.94
12	l	308	BCR	C19-C18-C17	3.04	123.60	118.94
9	A	831	CLA	CHD-C1D-ND	-3.04	121.66	124.45
9	B	828	CLA	CHD-C1D-ND	-3.03	121.67	124.45
12	B	836	BCR	C12-C13-C14	3.03	123.59	118.94
12	A	841	BCR	C12-C13-C14	3.03	123.59	118.94
12	a	844	BCR	C19-C18-C17	3.03	123.58	118.94
9	a	837	CLA	CHD-C1D-ND	-3.03	121.67	124.45
12	B	835	BCR	C19-C18-C17	3.02	123.58	118.94
12	a	841	BCR	C12-C13-C14	3.02	123.58	118.94
12	i	101	BCR	C12-C13-C14	3.02	123.58	118.94
9	b	804	CLA	C4D-CHA-C1A	3.02	124.92	121.25
12	I	101	BCR	C12-C13-C14	3.02	123.57	118.94
9	L	307	CLA	C4D-CHA-C1A	3.01	124.92	121.25
9	a	801	CLA	CHA-C1A-NA	-3.01	119.51	126.40
12	b	835	BCR	C12-C13-C14	3.01	123.56	118.94
12	b	836	BCR	C12-C13-C14	3.00	123.55	118.94
9	A	825	CLA	CHD-C1D-ND	-3.00	121.70	124.45
9	L	308	CLA	CHB-C4A-NA	3.00	128.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	825	CLA	C4D-CHA-C1A	2.99	124.89	121.25
12	A	841	BCR	C1-C6-C5	-2.99	118.41	122.61
9	A	801	CLA	CHA-C1A-NA	-2.99	119.56	126.40
9	B	823	CLA	C1D-ND-C4D	2.98	108.45	106.33
9	L	307	CLA	CHA-C1A-NA	-2.98	119.57	126.40
12	A	842	BCR	C12-C13-C14	2.98	123.51	118.94
9	B	825	CLA	C4D-CHA-C1A	2.97	124.87	121.25
12	b	834	BCR	C12-C13-C14	2.97	123.50	118.94
9	a	826	CLA	CHD-C1D-ND	-2.97	121.73	124.45
12	b	834	BCR	C30-C25-C26	-2.96	118.45	122.61
9	A	836	CLA	CHD-C1D-ND	-2.95	121.74	124.45
9	a	818	CLA	CHA-C1A-NA	-2.95	119.64	126.40
9	a	820	CLA	C4-C3-C5	-2.95	112.61	115.98
12	A	840	BCR	C12-C13-C14	2.94	123.46	118.94
12	L	305	BCR	C12-C13-C14	2.94	123.46	118.94
12	l	308	BCR	C12-C13-C14	2.94	123.46	118.94
9	B	840	CLA	CHD-C1D-ND	-2.94	121.75	124.45
9	A	806	CLA	C4A-NA-C1A	2.94	108.03	106.71
12	A	842	BCR	C8-C9-C10	2.93	123.44	118.94
9	a	824	CLA	CHD-C1D-ND	-2.93	121.76	124.45
9	a	835	CLA	CHA-C1A-NA	-2.93	119.69	126.40
9	b	823	CLA	C1D-ND-C4D	2.92	108.41	106.33
9	b	820	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
9	a	832	CLA	CHD-C1D-ND	-2.92	121.77	124.45
9	A	821	CLA	CHA-C1A-NA	-2.91	119.73	126.40
9	a	819	CLA	CHA-C1A-NA	-2.91	119.73	126.40
12	B	834	BCR	C12-C13-C14	2.91	123.41	118.94
9	A	809	CLA	CHA-C1A-NA	-2.91	119.74	126.40
12	B	835	BCR	C1-C6-C5	-2.90	118.53	122.61
9	A	823	CLA	CHA-C1A-NA	-2.90	119.75	126.40
9	A	818	CLA	CHA-C1A-NA	-2.90	119.76	126.40
9	a	820	CLA	C4D-C3D-CAD	-2.90	104.68	108.10
9	a	847	CLA	CHA-C1A-NA	-2.89	119.77	126.40
9	A	834	CLA	CHA-C1A-NA	-2.89	119.79	126.40
9	B	840	CLA	CHA-C1A-NA	-2.89	119.79	126.40
12	B	835	BCR	C23-C22-C21	2.88	123.37	118.94
9	l	302	CLA	CHA-C1A-NA	-2.88	119.79	126.40
12	b	835	BCR	C19-C18-C17	2.88	123.36	118.94
9	a	809	CLA	CHA-C1A-NA	-2.88	119.80	126.40
9	a	824	CLA	CHA-C1A-NA	-2.88	119.81	126.40
9	a	824	CLA	C4D-CHA-C1A	2.88	124.75	121.25
12	A	842	BCR	C36-C18-C17	-2.88	118.89	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	822	CLA	CHA-C1A-NA	-2.87	119.82	126.40
9	b	809	CLA	C4D-CHA-C1A	2.87	124.74	121.25
9	B	801	CLA	CHD-C1D-ND	-2.87	121.82	124.45
9	A	824	CLA	C1D-ND-C4D	2.87	108.37	106.33
9	B	802	CLA	CHA-C1A-NA	-2.86	119.84	126.40
9	A	806	CLA	CHB-C1B-NB	-2.86	121.23	124.26
9	b	802	CLA	CHA-C1A-NA	-2.85	119.86	126.40
9	A	805	CLA	C4D-CHA-C1A	2.85	124.72	121.25
9	B	809	CLA	C4D-CHA-C1A	2.85	124.72	121.25
9	a	816	CLA	C4D-CHA-C1A	2.85	124.72	121.25
9	A	847	CLA	CHA-C1A-NA	-2.85	119.88	126.40
9	l	301	CLA	C3B-C4B-NB	-2.84	107.88	110.52
12	l	309	BCR	C23-C22-C21	2.84	123.30	118.94
9	b	840	CLA	CHA-C1A-NA	-2.84	119.90	126.40
9	b	823	CLA	CHA-C1A-NA	-2.83	119.91	126.40
9	b	801	CLA	CHD-C1D-ND	-2.83	121.85	124.45
9	B	820	CLA	CHA-C1A-NA	-2.83	119.92	126.40
12	a	842	BCR	C1-C6-C5	-2.82	118.64	122.61
12	H	202	BCR	C8-C9-C10	2.82	123.27	118.94
9	a	816	CLA	CHA-C1A-NA	-2.82	119.95	126.40
12	L	301	BCR	C12-C13-C14	2.81	123.26	118.94
9	a	847	CLA	C4A-NA-C1A	2.81	107.97	106.71
9	A	812	CLA	CHD-C1D-C2D	2.81	131.38	125.48
9	a	803	CLA	CHA-C1A-NA	-2.81	119.96	126.40
9	A	847	CLA	C4A-NA-C1A	2.81	107.97	106.71
9	B	824	CLA	CHA-C1A-NA	-2.81	119.97	126.40
9	A	827	CLA	CHA-C1A-NA	-2.81	119.97	126.40
9	a	814	CLA	CHA-C1A-NA	-2.80	119.99	126.40
9	A	811	CLA	CHA-C1A-NA	-2.80	119.99	126.40
9	b	824	CLA	CHA-C1A-NA	-2.80	119.99	126.40
9	A	833	CLA	CHA-C1A-NA	-2.80	119.99	126.40
9	a	828	CLA	CHA-C1A-NA	-2.80	119.99	126.40
9	B	803	CLA	CHA-C1A-NA	-2.79	120.00	126.40
9	A	803	CLA	CHA-C1A-NA	-2.79	120.00	126.40
9	a	805	CLA	C4D-CHA-C1A	2.79	124.65	121.25
9	a	807	CLA	CHA-C1A-NA	-2.78	120.02	126.40
9	b	803	CLA	CHA-C1A-NA	-2.78	120.03	126.40
9	A	814	CLA	CHA-C1A-NA	-2.78	120.04	126.40
9	L	302	CLA	CHA-C1A-NA	-2.78	120.04	126.40
9	A	825	CLA	CHA-C1A-NA	-2.77	120.05	126.40
9	b	810	CLA	CHA-C1A-NA	-2.77	120.05	126.40
12	a	843	BCR	C8-C9-C10	2.77	123.19	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	823	CLA	CHA-C1A-NA	-2.77	120.05	126.40
9	B	828	CLA	CHA-C1A-NA	-2.77	120.06	126.40
9	L	308	CLA	CAC-C3C-C4C	2.77	128.40	124.81
9	a	815	CLA	CHA-C1A-NA	-2.77	120.06	126.40
9	B	831	CLA	CHA-C1A-NA	-2.76	120.07	126.40
9	l	305	CLA	CHA-C1A-NA	-2.76	120.07	126.40
9	A	836	CLA	CHA-C1A-NA	-2.76	120.08	126.40
9	a	837	CLA	CHA-C1A-NA	-2.76	120.08	126.40
9	B	810	CLA	CHA-C1A-NA	-2.76	120.08	126.40
9	A	818	CLA	C4D-CHA-C1A	2.76	124.61	121.25
9	A	830	CLA	CHA-C1A-NA	-2.76	120.08	126.40
9	b	828	CLA	CHA-C1A-NA	-2.76	120.08	126.40
9	b	827	CLA	CHD-C1D-C2D	2.76	131.26	125.48
9	a	826	CLA	CHA-C1A-NA	-2.76	120.09	126.40
9	a	820	CLA	C2C-C1C-NC	-2.75	107.39	109.97
9	A	808	CLA	CHD-C1D-C2D	2.75	131.25	125.48
9	B	832	CLA	CHA-C1A-NA	-2.75	120.10	126.40
9	a	834	CLA	CHA-C1A-NA	-2.75	120.10	126.40
9	b	822	CLA	CHA-C1A-NA	-2.75	120.10	126.40
9	B	839	CLA	CHA-C1A-NA	-2.75	120.11	126.40
12	b	835	BCR	C23-C22-C21	2.74	123.15	118.94
12	l	304	BCR	C12-C13-C14	2.74	123.15	118.94
9	b	832	CLA	CHA-C1A-NA	-2.74	120.12	126.40
9	a	811	CLA	CHA-C1A-NA	-2.74	120.12	126.40
9	a	818	CLA	CHD-C1D-ND	-2.74	121.93	124.45
9	b	839	CLA	CHA-C1A-NA	-2.74	120.12	126.40
9	B	827	CLA	CHD-C1D-C2D	2.73	131.22	125.48
9	B	822	CLA	CHA-C1A-NA	-2.73	120.15	126.40
9	B	826	CLA	CHA-C1A-NA	-2.73	120.15	126.40
9	A	815	CLA	CHA-C1A-NA	-2.73	120.15	126.40
9	a	820	CLA	C2A-C1A-CHA	2.73	128.62	123.86
9	a	816	CLA	CHD-C1D-C2D	2.72	131.19	125.48
9	a	802	CLA	CHA-C1A-NA	-2.72	120.16	126.40
9	L	304	CLA	CHA-C1A-NA	-2.72	120.16	126.40
9	a	827	CLA	CHA-C1A-NA	-2.72	120.17	126.40
9	b	826	CLA	CHA-C1A-NA	-2.72	120.17	126.40
9	a	818	CLA	C4D-CHA-C1A	2.72	124.56	121.25
12	H	202	BCR	C1-C6-C5	-2.72	118.79	122.61
9	b	831	CLA	CHA-C1A-NA	-2.72	120.18	126.40
9	b	827	CLA	CHA-C1A-NA	-2.71	120.19	126.40
9	B	801	CLA	CHA-C1A-NA	-2.71	120.19	126.40
9	A	826	CLA	CHA-C1A-NA	-2.71	120.20	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	802	CLA	CHA-C1A-NA	-2.71	120.20	126.40
9	a	820	CLA	CHD-C4C-NC	2.70	128.46	124.20
9	a	825	CLA	CHA-C1A-NA	-2.70	120.22	126.40
9	b	801	CLA	CHA-C1A-NA	-2.70	120.22	126.40
9	a	836	CLA	CHD-C1D-C2D	2.69	131.12	125.48
9	A	807	CLA	CHA-C1A-NA	-2.69	120.24	126.40
9	B	827	CLA	CHA-C1A-NA	-2.69	120.24	126.40
9	A	805	CLA	CHA-C1A-NA	-2.69	120.24	126.40
9	l	307	CLA	CHA-C1A-NA	-2.69	120.25	126.40
9	a	832	CLA	CHA-C1A-NA	-2.68	120.25	126.40
12	B	835	BCR	C30-C25-C26	-2.68	118.84	122.61
9	B	804	CLA	CHA-C1A-NA	-2.68	120.26	126.40
9	A	831	CLA	CHA-C1A-NA	-2.68	120.26	126.40
9	B	807	CLA	CHA-C1A-NA	-2.68	120.26	126.40
9	b	807	CLA	CHA-C1A-NA	-2.68	120.26	126.40
12	A	842	BCR	C16-C15-C14	2.68	128.96	123.47
9	a	820	CLA	CHA-C1A-NA	-2.67	120.28	126.40
9	b	830	CLA	CHA-C1A-NA	-2.67	120.29	126.40
9	a	805	CLA	CHA-C1A-NA	-2.67	120.29	126.40
9	A	816	CLA	CHA-C1A-NA	-2.67	120.29	126.40
9	b	805	CLA	CHA-C1A-NA	-2.67	120.29	126.40
12	h	203	BCR	C1-C6-C5	-2.66	118.86	122.61
12	h	203	BCR	C8-C9-C10	2.66	123.03	118.94
9	B	808	CLA	CHA-C1A-NA	-2.66	120.30	126.40
12	L	306	BCR	C23-C22-C21	2.66	123.03	118.94
9	B	805	CLA	CHA-C1A-NA	-2.66	120.30	126.40
9	L	303	CLA	CHA-C1A-NA	-2.66	120.31	126.40
9	b	804	CLA	CHA-C1A-NA	-2.66	120.31	126.40
9	a	831	CLA	CHA-C1A-NA	-2.66	120.31	126.40
9	A	817	CLA	CHA-C1A-NA	-2.66	120.32	126.40
9	B	817	CLA	CHA-C1A-NA	-2.66	120.32	126.40
9	L	304	CLA	C4A-NA-C1A	2.65	107.90	106.71
9	l	306	CLA	CHA-C1A-NA	-2.65	120.33	126.40
9	a	830	CLA	CHA-C1A-NA	-2.65	120.33	126.40
9	b	808	CLA	CHA-C1A-NA	-2.65	120.33	126.40
9	A	835	CLA	CHD-C1D-C2D	2.65	131.04	125.48
9	B	819	CLA	CHA-C1A-NA	-2.65	120.33	126.40
9	B	830	CLA	CHA-C1A-NA	-2.65	120.34	126.40
12	A	840	BCR	C29-C30-C25	2.65	114.55	110.48
9	a	806	CLA	CHA-C1A-NA	-2.64	120.34	126.40
9	b	819	CLA	CHA-C1A-NA	-2.64	120.34	126.40
9	B	812	CLA	CHA-C1A-NA	-2.64	120.34	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	812	CLA	CHD-C1D-C2D	2.64	131.02	125.48
9	b	817	CLA	CHA-C1A-NA	-2.64	120.35	126.40
9	B	815	CLA	CHA-C1A-NA	-2.64	120.36	126.40
12	a	843	BCR	C19-C18-C17	2.64	122.98	118.94
9	A	829	CLA	CHA-C1A-NA	-2.63	120.38	126.40
12	a	841	BCR	C1-C6-C5	-2.63	118.91	122.61
14	b	837	DGD	O1G-C1A-C2A	2.62	120.14	111.91
9	h	201	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
9	a	813	CLA	CHA-C1A-NA	-2.62	120.39	126.40
9	A	808	CLA	CHA-C1A-NA	-2.62	120.39	126.40
9	A	821	CLA	C4A-NA-C1A	2.62	107.89	106.71
9	a	817	CLA	CHA-C1A-NA	-2.62	120.39	126.40
9	b	818	CLA	CHA-C1A-NA	-2.62	120.40	126.40
9	L	308	CLA	CED-O2D-CGD	2.62	121.86	115.94
9	L	307	CLA	CHC-C4B-NB	-2.62	121.48	124.26
9	b	816	CLA	CHA-C1A-NA	-2.61	120.41	126.40
9	A	813	CLA	CHA-C1A-NA	-2.61	120.42	126.40
9	A	835	CLA	CHA-C1A-NA	-2.61	120.42	126.40
9	a	810	CLA	CHA-C1A-NA	-2.61	120.43	126.40
9	b	820	CLA	CHA-C1A-NA	-2.60	120.43	126.40
9	h	202	CLA	CHA-C1A-NA	-2.60	120.43	126.40
9	a	836	CLA	CHA-C1A-NA	-2.60	120.44	126.40
9	b	813	CLA	CHA-C1A-NA	-2.60	120.44	126.40
12	a	841	BCR	C29-C30-C25	2.60	114.48	110.48
9	A	824	CLA	CHD-C1D-C2D	2.60	130.93	125.48
9	H	201	CLA	CHA-C1A-NA	-2.60	120.45	126.40
9	A	836	CLA	C4A-NA-C1A	2.60	107.87	106.71
9	a	825	CLA	C1D-ND-C4D	2.60	108.18	106.33
9	b	815	CLA	CHA-C1A-NA	-2.59	120.46	126.40
9	B	814	CLA	CHA-C1A-NA	-2.59	120.46	126.40
9	l	301	CLA	C4A-NA-C1A	2.59	107.87	106.71
9	B	816	CLA	CHA-C1A-NA	-2.59	120.47	126.40
9	l	301	CLA	CHD-C4C-NC	-2.59	120.13	124.20
9	B	813	CLA	CHA-C1A-NA	-2.59	120.47	126.40
9	A	810	CLA	CHA-C1A-NA	-2.59	120.48	126.40
9	a	823	CLA	CHA-C1A-NA	-2.58	120.48	126.40
9	B	818	CLA	CHA-C1A-NA	-2.58	120.48	126.40
9	B	802	CLA	C4D-CHA-C1A	2.58	124.39	121.25
9	b	829	CLA	CHA-C1A-NA	-2.58	120.48	126.40
12	A	843	BCR	C23-C22-C21	2.58	122.90	118.94
9	b	814	CLA	CHA-C1A-NA	-2.58	120.49	126.40
9	A	828	CLA	CHA-C1A-NA	-2.58	120.50	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	846	CLA	CHA-C1A-NA	-2.57	120.50	126.40
9	A	816	CLA	CHD-C1D-C2D	2.57	130.88	125.48
12	a	842	BCR	C23-C22-C21	2.57	122.89	118.94
9	A	832	CLA	CHA-C1A-NA	-2.57	120.51	126.40
9	A	846	CLA	CHA-C1A-NA	-2.57	120.51	126.40
9	b	806	CLA	CHA-C1A-NA	-2.57	120.51	126.40
9	b	812	CLA	CHA-C1A-NA	-2.57	120.52	126.40
9	a	833	CLA	CHA-C1A-NA	-2.57	120.52	126.40
9	A	824	CLA	CHA-C1A-NA	-2.56	120.52	126.40
9	A	823	CLA	CHD-C1D-ND	-2.56	122.10	124.45
9	B	806	CLA	CHA-C1A-NA	-2.56	120.53	126.40
9	A	822	CLA	CHA-C1A-NA	-2.56	120.53	126.40
9	a	825	CLA	CHD-C1D-C2D	2.56	130.85	125.48
9	B	829	CLA	CHA-C1A-NA	-2.56	120.54	126.40
9	a	819	CLA	C4D-CHA-C1A	2.56	124.36	121.25
9	a	829	CLA	CHA-C1A-NA	-2.55	120.56	126.40
12	a	844	BCR	C23-C22-C21	2.55	122.85	118.94
9	a	808	CLA	CHA-C1A-NA	-2.55	120.56	126.40
9	B	821	CLA	CHA-C1A-NA	-2.55	120.56	126.40
9	L	307	CLA	C4A-NA-C1A	2.54	107.85	106.71
9	a	820	CLA	C3C-C4C-NC	-2.53	107.73	110.57
9	A	820	CLA	CHA-C1A-NA	-2.53	120.60	126.40
12	I	101	BCR	C23-C22-C21	2.53	122.82	118.94
9	a	804	CLA	CHA-C1A-NA	-2.53	120.61	126.40
9	h	201	CLA	C2A-C3A-C4A	2.52	105.94	101.87
9	b	825	CLA	CHA-C1A-NA	-2.52	120.62	126.40
12	l	309	BCR	C30-C25-C26	-2.52	119.06	122.61
9	a	821	CLA	CHA-C1A-NA	-2.52	120.63	126.40
14	B	837	DGD	O1G-C1A-C2A	2.52	119.80	111.91
9	h	201	CLA	C4-C3-C5	-2.51	113.11	115.98
9	a	834	CLA	C4A-NA-C1A	2.51	107.84	106.71
9	A	812	CLA	CHA-C1A-NA	-2.51	120.64	126.40
9	h	201	CLA	CAA-CBA-CGA	2.51	120.60	113.25
12	i	101	BCR	C23-C22-C21	2.51	122.80	118.94
9	b	811	CLA	CHA-C1A-NA	-2.51	120.65	126.40
9	A	834	CLA	C4D-CHA-C1A	2.51	124.31	121.25
9	a	812	CLA	CHA-C1A-NA	-2.51	120.66	126.40
9	B	818	CLA	CHD-C1D-C2D	2.51	130.74	125.48
12	L	305	BCR	C8-C9-C10	2.51	122.78	118.94
9	a	808	CLA	CHD-C1D-C2D	2.50	130.72	125.48
9	B	825	CLA	CHA-C1A-NA	-2.50	120.67	126.40
9	B	811	CLA	CHA-C1A-NA	-2.50	120.67	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	835	CLA	C4D-CHA-C1A	2.50	124.29	121.25
12	L	306	BCR	C30-C25-C26	-2.50	119.10	122.61
9	b	809	CLA	CHA-C1A-NA	-2.49	120.69	126.40
12	A	840	BCR	C1-C6-C5	-2.49	119.10	122.61
9	A	819	CLA	CAD-C3D-C2D	2.49	152.82	140.80
9	b	821	CLA	CHA-C1A-NA	-2.49	120.69	126.40
9	A	804	CLA	CHA-C1A-NA	-2.49	120.71	126.40
9	l	302	CLA	CHD-C1D-ND	-2.48	122.17	124.45
9	B	809	CLA	CHA-C1A-NA	-2.48	120.72	126.40
12	a	843	BCR	C23-C22-C21	2.48	122.74	118.94
12	H	202	BCR	C23-C22-C21	2.47	122.73	118.94
9	a	820	CLA	CHC-C4B-C3B	2.47	138.70	127.71
9	a	819	CLA	CHD-C4C-C3C	2.46	128.46	124.84
9	a	820	CLA	C3D-C4D-CHA	2.46	118.35	112.72
9	H	201	CLA	CHD-C1D-C2D	2.46	130.64	125.48
9	b	818	CLA	CHD-C1D-C2D	2.46	130.64	125.48
9	A	803	CLA	C4A-NA-C1A	2.46	107.81	106.71
12	B	836	BCR	C8-C9-C10	2.46	122.71	118.94
12	l	308	BCR	C8-C9-C10	2.46	122.71	118.94
9	b	816	CLA	CHD-C1D-C2D	2.46	130.63	125.48
9	b	802	CLA	C4D-CHA-C1A	2.45	124.23	121.25
9	a	820	CLA	C1C-C2C-C3C	2.45	109.53	106.96
12	A	841	BCR	C23-C22-C21	2.45	122.69	118.94
9	B	823	CLA	CHD-C1D-C2D	2.44	130.61	125.48
9	A	818	CLA	CHD-C1D-ND	-2.44	122.21	124.45
9	A	813	CLA	CHD-C1D-C2D	2.44	130.60	125.48
9	b	823	CLA	CHD-C1D-C2D	2.44	130.59	125.48
9	a	801	CLA	C2A-C1A-CHA	2.43	128.12	123.86
12	A	842	BCR	C19-C18-C17	2.43	122.67	118.94
9	L	308	CLA	C3B-C4B-NB	-2.43	108.26	110.52
12	b	836	BCR	C8-C9-C10	2.42	122.66	118.94
9	A	820	CLA	CHD-C1D-C2D	2.42	130.56	125.48
9	b	825	CLA	CHD-C1D-C2D	2.42	130.55	125.48
12	b	835	BCR	C8-C9-C10	2.42	122.65	118.94
14	B	837	DGD	O2G-C1B-O1B	-2.41	117.87	123.70
9	A	801	CLA	C2A-C1A-CHA	2.40	128.05	123.86
14	b	837	DGD	O2G-C1B-O1B	-2.39	117.92	123.70
12	h	203	BCR	C23-C22-C21	2.39	122.61	118.94
9	h	202	CLA	CHD-C1D-C2D	2.39	130.49	125.48
9	a	837	CLA	C4A-NA-C1A	2.39	107.78	106.71
9	A	814	CLA	CHC-C4B-NB	-2.39	121.73	124.26
9	l	302	CLA	C4A-NA-C1A	2.38	107.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	814	CLA	CHC-C4B-NB	-2.38	121.74	124.26
12	b	835	BCR	C30-C25-C26	-2.38	119.26	122.61
9	A	812	CLA	C1D-ND-C4D	2.38	108.02	106.33
9	B	825	CLA	CHD-C1D-C2D	2.38	130.46	125.48
9	A	801	CLA	C4D-CHA-C1A	2.38	124.14	121.25
9	A	806	CLA	C4D-CHA-C1A	2.38	124.14	121.25
12	l	309	BCR	C10-C11-C12	2.37	130.63	123.22
9	L	308	CLA	O2A-C1-C2	-2.37	102.40	108.64
9	a	820	CLA	C1D-CHD-C4C	2.36	131.16	126.06
9	a	831	CLA	C3A-C2A-C1A	-2.36	97.81	101.34
9	B	816	CLA	CHD-C1D-C2D	2.35	130.42	125.48
9	A	832	CLA	CHD-C1D-C2D	2.35	130.41	125.48
9	A	816	CLA	C3B-C4B-NB	-2.35	108.34	110.52
9	a	824	CLA	C4A-NA-C1A	2.34	107.76	106.71
9	B	829	CLA	CHD-C1D-C2D	2.34	130.39	125.48
9	a	801	CLA	C4D-CHA-C1A	2.34	124.10	121.25
9	A	829	CLA	CHD-C1D-C2D	2.34	130.38	125.48
9	b	829	CLA	CHD-C1D-C2D	2.34	130.38	125.48
12	A	841	BCR	C8-C9-C10	2.33	122.52	118.94
9	L	308	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
9	A	802	CLA	CHD-C1D-C2D	2.33	130.37	125.48
9	A	833	CLA	C4A-NA-C1A	2.33	107.75	106.71
9	a	833	CLA	CHD-C1D-C2D	2.33	130.37	125.48
9	a	820	CLA	C1-C2-C3	2.33	130.07	126.04
9	a	816	CLA	C1D-ND-C4D	2.33	107.99	106.33
9	a	821	CLA	CHD-C1D-C2D	2.32	130.35	125.48
12	b	834	BCR	C23-C22-C21	2.31	122.49	118.94
9	a	836	CLA	CMD-C2D-C1D	2.31	128.79	124.71
12	a	841	BCR	C8-C9-C10	2.31	122.49	118.94
9	a	830	CLA	CHD-C1D-C2D	2.31	130.32	125.48
12	a	842	BCR	C8-C9-C10	2.31	122.48	118.94
9	b	819	CLA	CHD-C1D-C2D	2.31	130.31	125.48
9	b	830	CLA	C4A-NA-C1A	2.30	107.74	106.71
9	a	831	CLA	C2A-C1A-CHA	2.30	127.88	123.86
12	B	835	BCR	C8-C9-C10	2.30	122.47	118.94
9	a	802	CLA	CHD-C1D-C2D	2.30	130.31	125.48
9	L	304	CLA	CHD-C1D-C2D	2.30	130.30	125.48
9	L	308	CLA	O2D-CGD-CBD	2.30	115.35	111.27
9	a	846	CLA	CHD-C1D-C2D	2.29	130.29	125.48
12	A	842	BCR	C2-C1-C6	2.29	114.01	110.48
9	A	846	CLA	CHD-C1D-C2D	2.29	130.29	125.48
9	a	820	CLA	C3D-C4D-ND	-2.29	106.53	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	806	CLA	CHD-C1D-C2D	2.29	130.28	125.48
9	a	804	CLA	CHD-C1D-C2D	2.29	130.28	125.48
9	a	814	CLA	CHD-C1D-C2D	2.29	130.27	125.48
9	B	830	CLA	C4A-NA-C1A	2.28	107.73	106.71
9	A	814	CLA	CHD-C1D-C2D	2.28	130.27	125.48
9	A	835	CLA	CMD-C2D-C1D	2.28	128.74	124.71
9	a	816	CLA	C3B-C4B-NB	-2.28	108.40	110.52
9	B	815	CLA	C4A-NA-C1A	2.28	107.73	106.71
9	A	804	CLA	CHD-C1D-C2D	2.27	130.25	125.48
9	b	820	CLA	CHD-C1D-C2D	2.27	130.24	125.48
9	A	801	CLA	CHD-C1D-C2D	2.27	130.23	125.48
9	a	807	CLA	CHD-C1D-C2D	2.26	130.23	125.48
9	A	806	CLA	C2A-C1A-CHA	2.26	127.81	123.86
12	H	202	BCR	C30-C25-C24	2.25	122.15	115.78
12	l	309	BCR	C8-C9-C10	2.25	122.39	118.94
9	L	302	CLA	CHD-C1D-C2D	2.25	130.19	125.48
9	a	813	CLA	CHD-C1D-C2D	2.25	130.19	125.48
9	A	823	CLA	C4A-NA-C1A	2.24	107.72	106.71
12	L	306	BCR	C10-C11-C12	2.24	130.22	123.22
9	b	827	CLA	C4A-NA-C1A	2.24	107.71	106.71
9	l	301	CLA	C3C-C4C-NC	-2.24	108.06	110.57
9	B	803	CLA	C4D-CHA-C1A	2.24	123.97	121.25
12	l	309	BCR	C1-C6-C5	-2.23	119.47	122.61
9	a	801	CLA	CHD-C1D-C2D	2.23	130.17	125.48
9	B	827	CLA	C4A-NA-C1A	2.23	107.71	106.71
9	A	806	CLA	CHC-C4B-NB	-2.23	121.90	124.26
12	B	834	BCR	C2-C1-C6	2.23	113.91	110.48
9	b	812	CLA	C1D-ND-C4D	2.22	107.92	106.33
9	L	307	CLA	C1D-ND-C4D	2.22	107.91	106.33
9	B	804	CLA	CHD-C1D-C2D	2.22	130.14	125.48
9	b	802	CLA	CHD-C1D-C2D	2.22	130.13	125.48
9	a	803	CLA	C4A-NA-C1A	2.22	107.70	106.71
12	A	840	BCR	C23-C22-C21	2.21	122.34	118.94
12	B	836	BCR	C23-C22-C21	2.21	122.33	118.94
12	I	101	BCR	C30-C25-C26	-2.21	119.50	122.61
9	A	830	CLA	CGD-CBD-CAD	-2.21	103.58	110.73
9	a	820	CLA	CHB-C1B-C2B	2.20	133.46	127.24
9	B	819	CLA	CHD-C1D-C2D	2.20	130.10	125.48
9	B	812	CLA	CHD-C1D-C2D	2.20	130.09	125.48
9	A	830	CLA	CHD-C1D-C2D	2.20	130.09	125.48
12	A	840	BCR	C8-C9-C10	2.20	122.31	118.94
12	B	834	BCR	C23-C22-C21	2.19	122.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	815	CLA	CHD-C1D-C2D	2.19	130.08	125.48
9	a	812	CLA	C1D-ND-C4D	2.19	107.89	106.33
12	b	836	BCR	C23-C22-C21	2.19	122.30	118.94
9	a	814	CLA	C4A-NA-C1A	2.19	107.69	106.71
9	A	824	CLA	C2D-C1D-ND	-2.19	108.49	110.10
9	b	804	CLA	CHD-C1D-C2D	2.19	130.06	125.48
12	L	306	BCR	C1-C6-C5	-2.18	119.54	122.61
9	A	819	CLA	CHD-C4C-C3C	2.18	128.04	124.84
12	a	841	BCR	C23-C22-C21	2.17	122.28	118.94
9	a	816	CLA	C2D-C1D-ND	-2.17	108.50	110.10
9	L	307	CLA	C3B-C4B-NB	-2.17	108.50	110.52
9	A	834	CLA	C4A-NA-C1A	2.17	107.68	106.71
9	l	301	CLA	C2A-C1A-CHA	2.17	127.64	123.86
9	h	201	CLA	C1-C2-C3	2.16	129.79	126.04
9	B	826	CLA	CHD-C1D-C2D	2.16	130.01	125.48
12	i	101	BCR	C30-C25-C26	-2.16	119.58	122.61
12	a	843	BCR	C29-C30-C25	2.16	113.80	110.48
9	a	817	CLA	CHD-C1D-C2D	2.16	130.00	125.48
9	A	814	CLA	C4A-NA-C1A	2.16	107.67	106.71
9	b	812	CLA	CHD-C1D-C2D	2.15	130.00	125.48
12	a	843	BCR	C2-C1-C6	2.15	113.80	110.48
9	b	821	CLA	CHD-C1D-C2D	2.15	130.00	125.48
9	b	803	CLA	C4D-CHA-C1A	2.15	123.87	121.25
9	L	302	CLA	CMD-C2D-C1D	2.15	128.51	124.71
9	l	307	CLA	CHD-C1D-C2D	2.15	129.99	125.48
10	B	833	PQN	C11-C3-C4	-2.15	116.20	118.50
9	B	815	CLA	C1D-ND-C4D	2.15	107.86	106.33
9	a	831	CLA	CHD-C1D-C2D	2.15	129.99	125.48
9	B	817	CLA	CHD-C1D-C2D	2.15	129.99	125.48
9	l	305	CLA	C3B-C4B-NB	-2.15	108.52	110.52
12	a	844	BCR	C8-C9-C10	2.15	122.23	118.94
9	L	307	CLA	C2A-C1A-CHA	2.14	127.61	123.86
9	a	829	CLA	CHD-C1D-C2D	2.14	129.97	125.48
9	B	821	CLA	CHD-C1D-C2D	2.14	129.97	125.48
9	A	812	CLA	C2D-C1D-ND	-2.14	108.53	110.10
9	b	826	CLA	CHD-C1D-C2D	2.14	129.97	125.48
9	A	836	CLA	C1D-ND-C4D	2.14	107.85	106.33
9	A	811	CLA	CHD-C1D-C2D	2.14	129.96	125.48
9	B	804	CLA	C3B-C4B-NB	-2.14	108.53	110.52
9	a	835	CLA	C4A-NA-C1A	2.14	107.67	106.71
9	A	807	CLA	CHD-C1D-C2D	2.13	129.95	125.48
9	L	308	CLA	C1-C2-C3	2.13	129.72	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	308	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
9	B	829	CLA	C4A-NA-C1A	2.12	107.66	106.71
9	h	202	CLA	C1D-ND-C4D	2.12	107.84	106.33
9	a	832	CLA	C3B-C4B-NB	-2.12	108.55	110.52
9	b	839	CLA	CHD-C1D-C2D	2.12	129.93	125.48
9	b	817	CLA	CHD-C1D-C2D	2.12	129.93	125.48
9	b	831	CLA	CHD-C1D-C2D	2.12	129.93	125.48
9	b	815	CLA	C1D-ND-C4D	2.12	107.84	106.33
9	b	818	CLA	C1D-ND-C4D	2.12	107.84	106.33
9	A	817	CLA	CHD-C1D-C2D	2.12	129.92	125.48
9	a	826	CLA	C4A-NA-C1A	2.12	107.66	106.71
10	b	833	PQN	C11-C3-C4	-2.11	116.24	118.50
9	b	804	CLA	C3B-C4B-NB	-2.11	108.56	110.52
9	B	839	CLA	CHD-C1D-C2D	2.11	129.91	125.48
9	b	811	CLA	CHD-C1D-C2D	2.11	129.91	125.48
9	b	810	CLA	C4A-NA-C1A	2.11	107.66	106.71
9	A	831	CLA	C3B-C4B-NB	-2.11	108.56	110.52
9	a	816	CLA	C3C-C4C-NC	-2.11	108.21	110.57
9	a	808	CLA	C1D-ND-C4D	2.10	107.83	106.33
12	i	101	BCR	C8-C9-C10	2.10	122.17	118.94
9	B	810	CLA	C4A-NA-C1A	2.10	107.65	106.71
9	B	803	CLA	C2A-C1A-CHA	2.10	127.53	123.86
9	B	801	CLA	CHD-C4C-C3C	2.10	127.92	124.84
12	I	101	BCR	C8-C9-C10	2.10	122.16	118.94
9	A	821	CLA	CHD-C1D-C2D	2.10	129.88	125.48
9	B	811	CLA	CHD-C1D-C2D	2.09	129.87	125.48
9	B	802	CLA	CHD-C1D-C2D	2.09	129.87	125.48
9	B	818	CLA	C1D-ND-C4D	2.09	107.82	106.33
9	a	810	CLA	CHD-C1D-C2D	2.09	129.86	125.48
9	l	306	CLA	CHD-C1D-C2D	2.09	129.86	125.48
9	B	831	CLA	CHD-C1D-C2D	2.09	129.86	125.48
9	l	305	CLA	CHD-C1D-C2D	2.09	129.86	125.48
9	A	828	CLA	CHD-C1D-C2D	2.08	129.85	125.48
9	a	822	CLA	CHD-C1D-C2D	2.08	129.85	125.48
12	b	834	BCR	C2-C1-C6	2.08	113.69	110.48
9	a	803	CLA	CHD-C1D-C2D	2.08	129.85	125.48
9	a	831	CLA	C3B-C4B-NB	-2.08	108.58	110.52
9	a	811	CLA	CHD-C1D-C2D	2.08	129.84	125.48
12	A	843	BCR	C8-C9-C10	2.08	122.13	118.94
9	A	825	CLA	C4A-NA-C1A	2.08	107.64	106.71
9	A	830	CLA	CMD-C2D-C1D	2.08	128.38	124.71
9	A	806	CLA	C1D-ND-C4D	2.08	107.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	803	CLA	C2A-C1A-CHA	2.08	127.49	123.86
9	A	803	CLA	CHD-C1D-C2D	2.08	129.83	125.48
9	b	822	CLA	C4A-NA-C1A	2.07	107.64	106.71
9	B	809	CLA	CHD-C1D-C2D	2.07	129.82	125.48
9	b	822	CLA	CHD-C1D-C2D	2.07	129.81	125.48
9	l	301	CLA	CAC-C3C-C2C	-2.07	124.00	127.53
9	B	828	CLA	C4A-NA-C1A	2.06	107.63	106.71
9	L	303	CLA	CHD-C1D-C2D	2.06	129.80	125.48
9	B	830	CLA	CHD-C1D-C2D	2.06	129.80	125.48
9	b	809	CLA	CHD-C1D-C2D	2.06	129.80	125.48
9	l	301	CLA	C1D-CHD-C4C	-2.05	121.63	126.06
9	l	307	CLA	C4A-NA-C1A	2.05	107.63	106.71
9	B	815	CLA	CHD-C1D-C2D	2.05	129.79	125.48
9	a	824	CLA	CHC-C4B-NB	-2.05	122.08	124.26
9	A	810	CLA	CHD-C1D-C2D	2.05	129.78	125.48
12	A	842	BCR	C23-C22-C21	2.05	122.09	118.94
9	h	201	CLA	CMB-C2B-C1B	2.04	128.47	125.37
9	A	826	CLA	C4A-NA-C1A	2.03	107.62	106.71
14	b	837	DGD	C2G-O2G-C1B	-2.03	112.79	117.79
9	B	820	CLA	CHC-C4B-NB	-2.03	122.11	124.26
9	a	837	CLA	C1D-ND-C4D	2.03	107.78	106.33
9	a	831	CLA	CGD-CBD-CAD	-2.03	104.17	110.73
9	b	805	CLA	CHD-C1D-C2D	2.03	129.73	125.48
9	a	802	CLA	C3B-C4B-NB	-2.03	108.64	110.52
9	b	802	CLA	C3B-C4B-NB	-2.02	108.64	110.52
9	L	307	CLA	C3C-C4C-NC	-2.02	108.31	110.57
9	A	812	CLA	C3C-C4C-NC	-2.02	108.31	110.57
9	a	806	CLA	CHD-C1D-C2D	2.02	129.71	125.48
9	b	808	CLA	CHD-C1D-C2D	2.01	129.70	125.48
12	l	304	BCR	C23-C22-C21	2.01	122.03	118.94
9	A	823	CLA	CHC-C4B-NB	-2.01	122.13	124.26
9	a	805	CLA	CHD-C1D-C2D	2.01	129.70	125.48
12	b	834	BCR	C7-C8-C9	-2.01	123.20	126.23
9	a	827	CLA	C4A-NA-C1A	2.01	107.61	106.71
9	B	822	CLA	CHD-C1D-C2D	2.01	129.69	125.48
12	b	835	BCR	C1-C6-C7	2.00	121.45	115.78
9	B	805	CLA	C3B-C4B-NB	-2.00	108.66	110.52
9	a	819	CLA	CHD-C1D-C2D	2.00	129.68	125.48
9	b	828	CLA	C4A-NA-C1A	2.00	107.61	106.71

There are no chirality outliers.

All (3012) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	801	CLA	C2B-C3B-CAB-CBB
9	A	801	CLA	C4B-C3B-CAB-CBB
9	A	801	CLA	CBD-CGD-O2D-CED
9	A	801	CLA	O1D-CGD-O2D-CED
9	A	801	CLA	C1-C2-C3-C4
9	A	803	CLA	C1-C2-C3-C4
9	A	804	CLA	CHA-CBD-CGD-O1D
9	A	804	CLA	CHA-CBD-CGD-O2D
9	A	804	CLA	C1-C2-C3-C4
9	A	804	CLA	C1-C2-C3-C5
9	A	805	CLA	C1A-C2A-CAA-CBA
9	A	805	CLA	C3A-C2A-CAA-CBA
9	A	806	CLA	CBD-CGD-O2D-CED
9	A	806	CLA	C1-C2-C3-C4
9	A	806	CLA	C1-C2-C3-C5
9	A	807	CLA	C2B-C3B-CAB-CBB
9	A	807	CLA	C4B-C3B-CAB-CBB
9	A	807	CLA	CBD-CGD-O2D-CED
9	A	807	CLA	O2A-C1-C2-C3
9	A	807	CLA	C1-C2-C3-C4
9	A	807	CLA	C11-C10-C8-C9
9	A	808	CLA	C1A-C2A-CAA-CBA
9	A	808	CLA	C3A-C2A-CAA-CBA
9	A	808	CLA	C2B-C3B-CAB-CBB
9	A	808	CLA	C4B-C3B-CAB-CBB
9	A	808	CLA	CBD-CGD-O2D-CED
9	A	808	CLA	C1-C2-C3-C4
9	A	808	CLA	C1-C2-C3-C5
9	A	809	CLA	C2B-C3B-CAB-CBB
9	A	809	CLA	C4B-C3B-CAB-CBB
9	A	809	CLA	CBD-CGD-O2D-CED
9	A	809	CLA	O1D-CGD-O2D-CED
9	A	810	CLA	C1A-C2A-CAA-CBA
9	A	810	CLA	C3A-C2A-CAA-CBA
9	A	812	CLA	C1A-C2A-CAA-CBA
9	A	812	CLA	C3A-C2A-CAA-CBA
9	A	813	CLA	C2B-C3B-CAB-CBB
9	A	813	CLA	C4B-C3B-CAB-CBB
9	A	813	CLA	C1-C2-C3-C4
9	A	813	CLA	C1-C2-C3-C5
9	A	815	CLA	C1A-C2A-CAA-CBA
9	A	815	CLA	C2B-C3B-CAB-CBB
9	A	815	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	A	815	CLA	CBD-CGD-O2D-CED
9	A	815	CLA	C1-C2-C3-C4
9	A	816	CLA	C4B-C3B-CAB-CBB
9	A	817	CLA	C1A-C2A-CAA-CBA
9	A	817	CLA	C3A-C2A-CAA-CBA
9	A	817	CLA	CHA-CBD-CGD-O1D
9	A	817	CLA	CHA-CBD-CGD-O2D
9	A	817	CLA	C1-C2-C3-C4
9	A	817	CLA	C12-C13-C15-C16
9	A	818	CLA	C4B-C3B-CAB-CBB
9	A	819	CLA	C1A-C2A-CAA-CBA
9	A	819	CLA	C2B-C3B-CAB-CBB
9	A	819	CLA	C4B-C3B-CAB-CBB
9	A	819	CLA	CAD-CBD-CGD-O2D
9	A	819	CLA	CBD-CGD-O2D-CED
9	A	819	CLA	C1-C2-C3-C4
9	A	819	CLA	C1-C2-C3-C5
9	A	819	CLA	C6-C7-C8-C10
9	A	820	CLA	C1A-C2A-CAA-CBA
9	A	820	CLA	C3A-C2A-CAA-CBA
9	A	820	CLA	C2B-C3B-CAB-CBB
9	A	820	CLA	C4B-C3B-CAB-CBB
9	A	821	CLA	C1A-C2A-CAA-CBA
9	A	821	CLA	C3A-C2A-CAA-CBA
9	A	821	CLA	O2A-C1-C2-C3
9	A	821	CLA	C1-C2-C3-C4
9	A	821	CLA	C1-C2-C3-C5
9	A	823	CLA	C1A-C2A-CAA-CBA
9	A	823	CLA	C3A-C2A-CAA-CBA
9	A	824	CLA	C1A-C2A-CAA-CBA
9	A	824	CLA	C3A-C2A-CAA-CBA
9	A	824	CLA	CHA-CBD-CGD-O1D
9	A	824	CLA	CHA-CBD-CGD-O2D
9	A	824	CLA	CBD-CGD-O2D-CED
9	A	824	CLA	C4-C3-C5-C6
9	A	825	CLA	C2A-CAA-CBA-CGA
9	A	826	CLA	C1A-C2A-CAA-CBA
9	A	826	CLA	C4-C3-C5-C6
9	A	827	CLA	C2B-C3B-CAB-CBB
9	A	827	CLA	C4B-C3B-CAB-CBB
9	A	828	CLA	C6-C7-C8-C9
9	A	829	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	A	829	CLA	C4B-C3B-CAB-CBB
9	A	829	CLA	C6-C7-C8-C9
9	A	830	CLA	C1A-C2A-CAA-CBA
9	A	830	CLA	C3A-C2A-CAA-CBA
9	A	830	CLA	C2B-C3B-CAB-CBB
9	A	830	CLA	C4B-C3B-CAB-CBB
9	A	830	CLA	CBD-CGD-O2D-CED
9	A	830	CLA	O2A-C1-C2-C3
9	A	830	CLA	C1-C2-C3-C4
9	A	830	CLA	C1-C2-C3-C5
9	A	833	CLA	C2B-C3B-CAB-CBB
9	A	833	CLA	C4B-C3B-CAB-CBB
9	A	833	CLA	CHA-CBD-CGD-O1D
9	A	833	CLA	CHA-CBD-CGD-O2D
9	A	833	CLA	C1-C2-C3-C4
9	A	834	CLA	CHA-CBD-CGD-O1D
9	A	834	CLA	CHA-CBD-CGD-O2D
9	A	835	CLA	C2B-C3B-CAB-CBB
9	A	835	CLA	C4B-C3B-CAB-CBB
9	A	835	CLA	CHA-CBD-CGD-O1D
9	A	835	CLA	CHA-CBD-CGD-O2D
9	A	835	CLA	CBD-CGD-O2D-CED
9	A	847	CLA	C1-C2-C3-C4
9	A	847	CLA	C6-C7-C8-C9
9	B	801	CLA	C2-C1-O2A-CGA
9	B	801	CLA	C1-C2-C3-C4
9	B	801	CLA	C1-C2-C3-C5
9	B	801	CLA	C2-C3-C5-C6
9	B	801	CLA	C4-C3-C5-C6
9	B	802	CLA	C11-C10-C8-C7
9	B	803	CLA	C2B-C3B-CAB-CBB
9	B	803	CLA	C4B-C3B-CAB-CBB
9	B	803	CLA	CHA-CBD-CGD-O1D
9	B	803	CLA	C1-C2-C3-C4
9	B	804	CLA	CBD-CGD-O2D-CED
9	B	806	CLA	C2-C3-C5-C6
9	B	806	CLA	C4-C3-C5-C6
9	B	807	CLA	C2B-C3B-CAB-CBB
9	B	807	CLA	C4B-C3B-CAB-CBB
9	B	807	CLA	C6-C7-C8-C9
9	B	808	CLA	C2B-C3B-CAB-CBB
9	B	808	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	B	808	CLA	C1-C2-C3-C4
9	B	808	CLA	C1-C2-C3-C5
9	B	808	CLA	C4-C3-C5-C6
9	B	809	CLA	CHA-CBD-CGD-O1D
9	B	809	CLA	CHA-CBD-CGD-O2D
9	B	811	CLA	C1-C2-C3-C4
9	B	811	CLA	C1-C2-C3-C5
9	B	812	CLA	C1-C2-C3-C4
9	B	812	CLA	C1-C2-C3-C5
9	B	814	CLA	C1A-C2A-CAA-CBA
9	B	814	CLA	C11-C12-C13-C14
9	B	816	CLA	C2B-C3B-CAB-CBB
9	B	817	CLA	C2B-C3B-CAB-CBB
9	B	817	CLA	C4B-C3B-CAB-CBB
9	B	818	CLA	C1A-C2A-CAA-CBA
9	B	818	CLA	C3A-C2A-CAA-CBA
9	B	818	CLA	C2B-C3B-CAB-CBB
9	B	818	CLA	C4B-C3B-CAB-CBB
9	B	818	CLA	C1-C2-C3-C4
9	B	818	CLA	C2-C3-C5-C6
9	B	818	CLA	C4-C3-C5-C6
9	B	818	CLA	C6-C7-C8-C9
9	B	819	CLA	C1A-C2A-CAA-CBA
9	B	819	CLA	C3A-C2A-CAA-CBA
9	B	819	CLA	C2B-C3B-CAB-CBB
9	B	819	CLA	C4B-C3B-CAB-CBB
9	B	820	CLA	CBD-CGD-O2D-CED
9	B	821	CLA	C1-C2-C3-C4
9	B	822	CLA	C1A-C2A-CAA-CBA
9	B	823	CLA	C1-C2-C3-C4
9	B	824	CLA	C1A-C2A-CAA-CBA
9	B	824	CLA	C1-C2-C3-C4
9	B	824	CLA	C1-C2-C3-C5
9	B	824	CLA	C4-C3-C5-C6
9	B	825	CLA	C1A-C2A-CAA-CBA
9	B	825	CLA	CHA-CBD-CGD-O1D
9	B	825	CLA	CHA-CBD-CGD-O2D
9	B	825	CLA	CAD-CBD-CGD-O1D
9	B	825	CLA	CAD-CBD-CGD-O2D
9	B	826	CLA	C1A-C2A-CAA-CBA
9	B	826	CLA	C3A-C2A-CAA-CBA
9	B	826	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	B	826	CLA	C4B-C3B-CAB-CBB
9	B	826	CLA	CBD-CGD-O2D-CED
9	B	829	CLA	C2B-C3B-CAB-CBB
9	B	829	CLA	C4B-C3B-CAB-CBB
9	B	831	CLA	C2B-C3B-CAB-CBB
9	B	831	CLA	C4B-C3B-CAB-CBB
9	B	832	CLA	C1A-C2A-CAA-CBA
9	B	840	CLA	C4B-C3B-CAB-CBB
9	H	201	CLA	C2B-C3B-CAB-CBB
9	H	201	CLA	C4B-C3B-CAB-CBB
9	H	201	CLA	CBD-CGD-O2D-CED
9	H	201	CLA	C1-C2-C3-C4
9	H	201	CLA	C1-C2-C3-C5
9	L	303	CLA	C1A-C2A-CAA-CBA
9	L	303	CLA	C2B-C3B-CAB-CBB
9	L	303	CLA	C4B-C3B-CAB-CBB
9	L	303	CLA	C1-C2-C3-C4
9	L	303	CLA	C1-C2-C3-C5
9	L	303	CLA	C6-C7-C8-C9
9	L	304	CLA	C2B-C3B-CAB-CBB
9	L	304	CLA	C4B-C3B-CAB-CBB
9	L	304	CLA	O2A-C1-C2-C3
9	L	304	CLA	C1-C2-C3-C4
9	L	304	CLA	C1-C2-C3-C5
9	L	307	CLA	C1A-C2A-CAA-CBA
9	L	307	CLA	C2B-C3B-CAB-CBB
9	L	307	CLA	C4B-C3B-CAB-CBB
9	L	307	CLA	CHA-CBD-CGD-O1D
9	L	307	CLA	CHA-CBD-CGD-O2D
9	L	308	CLA	C2-C3-C5-C6
9	L	308	CLA	C4-C3-C5-C6
9	a	801	CLA	C2B-C3B-CAB-CBB
9	a	801	CLA	C4B-C3B-CAB-CBB
9	a	801	CLA	CBD-CGD-O2D-CED
9	a	801	CLA	O1D-CGD-O2D-CED
9	a	801	CLA	C1-C2-C3-C4
9	a	803	CLA	C1-C2-C3-C4
9	a	803	CLA	C1-C2-C3-C5
9	a	804	CLA	CHA-CBD-CGD-O1D
9	a	804	CLA	CHA-CBD-CGD-O2D
9	a	804	CLA	CAD-CBD-CGD-O1D
9	a	804	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
9	a	804	CLA	C1-C2-C3-C5
9	a	805	CLA	C3A-C2A-CAA-CBA
9	a	805	CLA	C1-C2-C3-C4
9	a	806	CLA	C2A-CAA-CBA-CGA
9	a	806	CLA	C4B-C3B-CAB-CBB
9	a	806	CLA	C1-C2-C3-C4
9	a	806	CLA	C1-C2-C3-C5
9	a	807	CLA	C1A-C2A-CAA-CBA
9	a	807	CLA	C3A-C2A-CAA-CBA
9	a	807	CLA	C2B-C3B-CAB-CBB
9	a	807	CLA	C4B-C3B-CAB-CBB
9	a	807	CLA	CBD-CGD-O2D-CED
9	a	807	CLA	O2A-C1-C2-C3
9	a	807	CLA	C1-C2-C3-C4
9	a	807	CLA	C1-C2-C3-C5
9	a	807	CLA	C6-C7-C8-C10
9	a	807	CLA	C11-C10-C8-C9
9	a	808	CLA	C1A-C2A-CAA-CBA
9	a	808	CLA	C3A-C2A-CAA-CBA
9	a	808	CLA	CBD-CGD-O2D-CED
9	a	808	CLA	C1-C2-C3-C4
9	a	808	CLA	C1-C2-C3-C5
9	a	809	CLA	C2B-C3B-CAB-CBB
9	a	809	CLA	C4B-C3B-CAB-CBB
9	a	809	CLA	CBD-CGD-O2D-CED
9	a	810	CLA	C1A-C2A-CAA-CBA
9	a	810	CLA	C3A-C2A-CAA-CBA
9	a	810	CLA	C1-C2-C3-C4
9	a	811	CLA	C2B-C3B-CAB-CBB
9	a	811	CLA	C4B-C3B-CAB-CBB
9	a	812	CLA	C1A-C2A-CAA-CBA
9	a	812	CLA	C3A-C2A-CAA-CBA
9	a	813	CLA	C2B-C3B-CAB-CBB
9	a	813	CLA	C4B-C3B-CAB-CBB
9	a	813	CLA	C1-C2-C3-C4
9	a	813	CLA	C1-C2-C3-C5
9	a	815	CLA	C1A-C2A-CAA-CBA
9	a	815	CLA	C2B-C3B-CAB-CBB
9	a	815	CLA	C4B-C3B-CAB-CBB
9	a	815	CLA	C1-C2-C3-C4
9	a	815	CLA	C1-C2-C3-C5
9	a	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	a	816	CLA	C3A-C2A-CAA-CBA
9	a	816	CLA	C1-C2-C3-C4
9	a	816	CLA	C1-C2-C3-C5
9	a	817	CLA	C1A-C2A-CAA-CBA
9	a	817	CLA	C3A-C2A-CAA-CBA
9	a	817	CLA	CBD-CGD-O2D-CED
9	a	817	CLA	C1-C2-C3-C4
9	a	817	CLA	C12-C13-C15-C16
9	a	818	CLA	C4B-C3B-CAB-CBB
9	a	819	CLA	C1-C2-C3-C4
9	a	819	CLA	C1-C2-C3-C5
9	a	820	CLA	C1A-C2A-CAA-CBA
9	a	820	CLA	C3A-C2A-CAA-CBA
9	a	820	CLA	C1-C2-C3-C4
9	a	820	CLA	C1-C2-C3-C5
9	a	820	CLA	C2-C3-C5-C6
9	a	820	CLA	C4-C3-C5-C6
9	a	821	CLA	C1A-C2A-CAA-CBA
9	a	821	CLA	C3A-C2A-CAA-CBA
9	a	822	CLA	C1A-C2A-CAA-CBA
9	a	822	CLA	O2A-C1-C2-C3
9	a	822	CLA	C1-C2-C3-C4
9	a	822	CLA	C1-C2-C3-C5
9	a	824	CLA	C1A-C2A-CAA-CBA
9	a	824	CLA	C3A-C2A-CAA-CBA
9	a	825	CLA	C1A-C2A-CAA-CBA
9	a	825	CLA	C3A-C2A-CAA-CBA
9	a	825	CLA	C2-C3-C5-C6
9	a	825	CLA	C4-C3-C5-C6
9	a	826	CLA	C2A-CAA-CBA-CGA
9	a	827	CLA	C1A-C2A-CAA-CBA
9	a	827	CLA	C2-C3-C5-C6
9	a	827	CLA	C4-C3-C5-C6
9	a	828	CLA	C2B-C3B-CAB-CBB
9	a	828	CLA	C4B-C3B-CAB-CBB
9	a	829	CLA	C6-C7-C8-C9
9	a	830	CLA	C2B-C3B-CAB-CBB
9	a	830	CLA	C4B-C3B-CAB-CBB
9	a	831	CLA	C2B-C3B-CAB-CBB
9	a	831	CLA	C4B-C3B-CAB-CBB
9	a	832	CLA	C2-C3-C5-C6
9	a	832	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	a	834	CLA	C2B-C3B-CAB-CBB
9	a	834	CLA	C4B-C3B-CAB-CBB
9	a	834	CLA	CHA-CBD-CGD-O1D
9	a	834	CLA	CHA-CBD-CGD-O2D
9	a	834	CLA	C1-C2-C3-C4
9	a	835	CLA	CHA-CBD-CGD-O1D
9	a	835	CLA	CHA-CBD-CGD-O2D
9	a	836	CLA	C2B-C3B-CAB-CBB
9	a	836	CLA	C4B-C3B-CAB-CBB
9	a	836	CLA	CHA-CBD-CGD-O1D
9	a	836	CLA	CHA-CBD-CGD-O2D
9	a	836	CLA	CBD-CGD-O2D-CED
9	a	846	CLA	C1-C2-C3-C4
9	a	846	CLA	C1-C2-C3-C5
9	a	846	CLA	C11-C12-C13-C15
9	a	847	CLA	C2B-C3B-CAB-CBB
9	b	801	CLA	C2-C1-O2A-CGA
9	b	801	CLA	C1-C2-C3-C4
9	b	801	CLA	C1-C2-C3-C5
9	b	801	CLA	C2-C3-C5-C6
9	b	801	CLA	C4-C3-C5-C6
9	b	802	CLA	C1-C2-C3-C4
9	b	802	CLA	C2-C3-C5-C6
9	b	802	CLA	C4-C3-C5-C6
9	b	803	CLA	C2B-C3B-CAB-CBB
9	b	803	CLA	C4B-C3B-CAB-CBB
9	b	803	CLA	CHA-CBD-CGD-O1D
9	b	803	CLA	C1-C2-C3-C4
9	b	804	CLA	CBD-CGD-O2D-CED
9	b	804	CLA	C11-C12-C13-C14
9	b	806	CLA	O1A-CGA-O2A-C1
9	b	806	CLA	C2-C3-C5-C6
9	b	806	CLA	C4-C3-C5-C6
9	b	807	CLA	C2B-C3B-CAB-CBB
9	b	807	CLA	C4B-C3B-CAB-CBB
9	b	807	CLA	C6-C7-C8-C9
9	b	808	CLA	C2B-C3B-CAB-CBB
9	b	808	CLA	C4B-C3B-CAB-CBB
9	b	808	CLA	C1-C2-C3-C4
9	b	808	CLA	C1-C2-C3-C5
9	b	808	CLA	C2-C3-C5-C6
9	b	808	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	b	809	CLA	CHA-CBD-CGD-O1D
9	b	809	CLA	CHA-CBD-CGD-O2D
9	b	811	CLA	C1-C2-C3-C4
9	b	811	CLA	C1-C2-C3-C5
9	b	814	CLA	C1A-C2A-CAA-CBA
9	b	814	CLA	C3A-C2A-CAA-CBA
9	b	814	CLA	C11-C12-C13-C14
9	b	817	CLA	C2B-C3B-CAB-CBB
9	b	817	CLA	C4B-C3B-CAB-CBB
9	b	818	CLA	C1A-C2A-CAA-CBA
9	b	818	CLA	C3A-C2A-CAA-CBA
9	b	818	CLA	C2B-C3B-CAB-CBB
9	b	818	CLA	C4B-C3B-CAB-CBB
9	b	818	CLA	C1-C2-C3-C4
9	b	818	CLA	C2-C3-C5-C6
9	b	818	CLA	C4-C3-C5-C6
9	b	819	CLA	C1A-C2A-CAA-CBA
9	b	819	CLA	C3A-C2A-CAA-CBA
9	b	819	CLA	C2B-C3B-CAB-CBB
9	b	819	CLA	C4B-C3B-CAB-CBB
9	b	820	CLA	CBD-CGD-O2D-CED
9	b	821	CLA	C1-C2-C3-C4
9	b	822	CLA	C1A-C2A-CAA-CBA
9	b	822	CLA	C3A-C2A-CAA-CBA
9	b	823	CLA	C1-C2-C3-C4
9	b	823	CLA	C1-C2-C3-C5
9	b	824	CLA	C1A-C2A-CAA-CBA
9	b	824	CLA	C1-C2-C3-C4
9	b	824	CLA	C1-C2-C3-C5
9	b	824	CLA	C4-C3-C5-C6
9	b	825	CLA	C1A-C2A-CAA-CBA
9	b	825	CLA	CHA-CBD-CGD-O1D
9	b	825	CLA	CAD-CBD-CGD-O1D
9	b	825	CLA	CAD-CBD-CGD-O2D
9	b	826	CLA	C1A-C2A-CAA-CBA
9	b	826	CLA	C3A-C2A-CAA-CBA
9	b	826	CLA	C2B-C3B-CAB-CBB
9	b	826	CLA	C4B-C3B-CAB-CBB
9	b	828	CLA	C1A-C2A-CAA-CBA
9	b	828	CLA	C1-C2-C3-C4
9	b	828	CLA	C4-C3-C5-C6
9	b	829	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	b	829	CLA	C4B-C3B-CAB-CBB
9	b	831	CLA	C2B-C3B-CAB-CBB
9	b	831	CLA	C4B-C3B-CAB-CBB
9	b	832	CLA	C1A-C2A-CAA-CBA
9	b	840	CLA	C4B-C3B-CAB-CBB
9	h	201	CLA	C1A-C2A-CAA-CBA
9	h	201	CLA	C2-C3-C5-C6
9	h	201	CLA	C4-C3-C5-C6
9	l	301	CLA	C4C-C3C-CAC-CBC
9	l	301	CLA	CBD-CGD-O2D-CED
9	l	302	CLA	C1A-C2A-CAA-CBA
9	l	302	CLA	C3A-C2A-CAA-CBA
9	l	302	CLA	CBD-CGD-O2D-CED
9	l	302	CLA	O2A-C1-C2-C3
9	l	302	CLA	C1-C2-C3-C4
9	l	306	CLA	C2B-C3B-CAB-CBB
9	l	306	CLA	C4B-C3B-CAB-CBB
9	l	306	CLA	C6-C7-C8-C9
9	l	307	CLA	C2B-C3B-CAB-CBB
11	A	838	LHG	C1-C2-C3-O3
11	A	839	LHG	C3-O3-P-O5
11	A	839	LHG	C4-O6-P-O3
11	A	839	LHG	C4-O6-P-O4
11	A	845	LHG	O1-C1-C2-C3
11	A	845	LHG	C4-O6-P-O4
11	a	839	LHG	C1-C2-C3-O3
11	a	840	LHG	C3-O3-P-O5
11	l	303	LHG	C4-O6-P-O4
11	l	303	LHG	C5-C4-O6-P
12	A	840	BCR	C6-C7-C8-C9
12	A	840	BCR	C7-C8-C9-C10
12	A	840	BCR	C7-C8-C9-C34
12	A	840	BCR	C11-C10-C9-C8
12	A	840	BCR	C11-C10-C9-C34
12	A	840	BCR	C10-C11-C12-C13
12	A	840	BCR	C11-C12-C13-C14
12	A	840	BCR	C11-C12-C13-C35
12	A	840	BCR	C12-C13-C14-C15
12	A	840	BCR	C35-C13-C14-C15
12	A	840	BCR	C14-C15-C16-C17
12	A	840	BCR	C22-C23-C24-C25
12	A	840	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
12	A	841	BCR	C7-C8-C9-C10
12	A	841	BCR	C7-C8-C9-C34
12	A	841	BCR	C11-C12-C13-C14
12	A	841	BCR	C11-C12-C13-C35
12	A	841	BCR	C12-C13-C14-C15
12	A	841	BCR	C35-C13-C14-C15
12	A	841	BCR	C14-C15-C16-C17
12	A	841	BCR	C16-C17-C18-C19
12	A	841	BCR	C16-C17-C18-C36
12	A	841	BCR	C18-C19-C20-C21
12	A	841	BCR	C22-C23-C24-C25
12	A	842	BCR	C6-C7-C8-C9
12	A	842	BCR	C10-C11-C12-C13
12	A	842	BCR	C12-C13-C14-C15
12	A	842	BCR	C35-C13-C14-C15
12	A	842	BCR	C14-C15-C16-C17
12	A	842	BCR	C17-C18-C19-C20
12	A	842	BCR	C36-C18-C19-C20
12	A	843	BCR	C10-C11-C12-C13
12	A	843	BCR	C11-C12-C13-C14
12	A	843	BCR	C11-C12-C13-C35
12	A	843	BCR	C15-C16-C17-C18
12	A	843	BCR	C18-C19-C20-C21
12	A	843	BCR	C23-C24-C25-C30
12	B	834	BCR	C9-C10-C11-C12
12	B	834	BCR	C15-C16-C17-C18
12	B	834	BCR	C19-C20-C21-C22
12	B	834	BCR	C20-C21-C22-C23
12	B	834	BCR	C20-C21-C22-C37
12	B	834	BCR	C21-C22-C23-C24
12	B	834	BCR	C37-C22-C23-C24
12	B	834	BCR	C22-C23-C24-C25
12	B	835	BCR	C1-C6-C7-C8
12	B	835	BCR	C5-C6-C7-C8
12	B	835	BCR	C6-C7-C8-C9
12	B	835	BCR	C10-C11-C12-C13
12	B	835	BCR	C11-C12-C13-C14
12	B	835	BCR	C11-C12-C13-C35
12	B	835	BCR	C12-C13-C14-C15
12	B	835	BCR	C35-C13-C14-C15
12	B	835	BCR	C14-C15-C16-C17
12	B	835	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	B	835	BCR	C16-C17-C18-C36
12	B	835	BCR	C17-C18-C19-C20
12	B	835	BCR	C18-C19-C20-C21
12	B	835	BCR	C21-C22-C23-C24
12	B	835	BCR	C37-C22-C23-C24
12	B	835	BCR	C22-C23-C24-C25
12	B	835	BCR	C23-C24-C25-C26
12	B	836	BCR	C11-C10-C9-C8
12	B	836	BCR	C11-C10-C9-C34
12	B	836	BCR	C21-C22-C23-C24
12	B	836	BCR	C37-C22-C23-C24
12	B	836	BCR	C22-C23-C24-C25
12	H	202	BCR	C6-C7-C8-C9
12	H	202	BCR	C11-C10-C9-C8
12	H	202	BCR	C11-C10-C9-C34
12	H	202	BCR	C11-C12-C13-C14
12	H	202	BCR	C11-C12-C13-C35
12	H	202	BCR	C18-C19-C20-C21
12	H	202	BCR	C20-C21-C22-C23
12	H	202	BCR	C20-C21-C22-C37
12	H	202	BCR	C22-C23-C24-C25
12	H	202	BCR	C23-C24-C25-C26
12	H	202	BCR	C23-C24-C25-C30
12	I	101	BCR	C7-C8-C9-C10
12	I	101	BCR	C7-C8-C9-C34
12	I	101	BCR	C9-C10-C11-C12
12	I	101	BCR	C10-C11-C12-C13
12	I	101	BCR	C11-C12-C13-C14
12	I	101	BCR	C11-C12-C13-C35
12	I	101	BCR	C14-C15-C16-C17
12	I	101	BCR	C21-C22-C23-C24
12	I	101	BCR	C37-C22-C23-C24
12	I	101	BCR	C22-C23-C24-C25
12	L	301	BCR	C6-C7-C8-C9
12	L	301	BCR	C14-C15-C16-C17
12	L	301	BCR	C20-C21-C22-C23
12	L	301	BCR	C20-C21-C22-C37
12	L	301	BCR	C21-C22-C23-C24
12	L	301	BCR	C37-C22-C23-C24
12	L	301	BCR	C22-C23-C24-C25
12	L	305	BCR	C7-C8-C9-C10
12	L	305	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
12	L	305	BCR	C11-C12-C13-C14
12	L	305	BCR	C11-C12-C13-C35
12	L	305	BCR	C19-C20-C21-C22
12	L	305	BCR	C22-C23-C24-C25
12	L	305	BCR	C23-C24-C25-C26
12	L	305	BCR	C23-C24-C25-C30
12	L	306	BCR	C1-C6-C7-C8
12	L	306	BCR	C10-C11-C12-C13
12	L	306	BCR	C11-C12-C13-C14
12	L	306	BCR	C11-C12-C13-C35
12	L	306	BCR	C14-C15-C16-C17
12	L	306	BCR	C16-C17-C18-C19
12	L	306	BCR	C16-C17-C18-C36
12	L	306	BCR	C18-C19-C20-C21
12	L	306	BCR	C20-C21-C22-C23
12	L	306	BCR	C20-C21-C22-C37
12	L	306	BCR	C22-C23-C24-C25
12	a	841	BCR	C1-C6-C7-C8
12	a	841	BCR	C7-C8-C9-C10
12	a	841	BCR	C7-C8-C9-C34
12	a	841	BCR	C11-C10-C9-C8
12	a	841	BCR	C11-C10-C9-C34
12	a	841	BCR	C10-C11-C12-C13
12	a	841	BCR	C11-C12-C13-C14
12	a	841	BCR	C12-C13-C14-C15
12	a	841	BCR	C35-C13-C14-C15
12	a	841	BCR	C14-C15-C16-C17
12	a	841	BCR	C22-C23-C24-C25
12	a	842	BCR	C7-C8-C9-C10
12	a	842	BCR	C7-C8-C9-C34
12	a	842	BCR	C11-C12-C13-C14
12	a	842	BCR	C11-C12-C13-C35
12	a	842	BCR	C12-C13-C14-C15
12	a	842	BCR	C35-C13-C14-C15
12	a	842	BCR	C13-C14-C15-C16
12	a	842	BCR	C14-C15-C16-C17
12	a	842	BCR	C16-C17-C18-C19
12	a	842	BCR	C16-C17-C18-C36
12	a	842	BCR	C18-C19-C20-C21
12	a	842	BCR	C22-C23-C24-C25
12	a	843	BCR	C6-C7-C8-C9
12	a	843	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
12	a	843	BCR	C7-C8-C9-C34
12	a	843	BCR	C11-C10-C9-C8
12	a	843	BCR	C11-C10-C9-C34
12	a	843	BCR	C9-C10-C11-C12
12	a	843	BCR	C11-C12-C13-C14
12	a	843	BCR	C11-C12-C13-C35
12	a	843	BCR	C16-C17-C18-C19
12	a	843	BCR	C16-C17-C18-C36
12	a	843	BCR	C17-C18-C19-C20
12	a	843	BCR	C36-C18-C19-C20
12	a	843	BCR	C19-C20-C21-C22
12	a	843	BCR	C22-C23-C24-C25
12	a	844	BCR	C10-C11-C12-C13
12	a	844	BCR	C11-C12-C13-C35
12	a	844	BCR	C16-C17-C18-C19
12	a	844	BCR	C16-C17-C18-C36
12	a	844	BCR	C17-C18-C19-C20
12	a	844	BCR	C36-C18-C19-C20
12	a	844	BCR	C18-C19-C20-C21
12	a	844	BCR	C20-C21-C22-C23
12	a	844	BCR	C20-C21-C22-C37
12	a	844	BCR	C21-C22-C23-C24
12	a	844	BCR	C37-C22-C23-C24
12	a	844	BCR	C22-C23-C24-C25
12	b	834	BCR	C15-C16-C17-C18
12	b	834	BCR	C19-C20-C21-C22
12	b	834	BCR	C20-C21-C22-C23
12	b	834	BCR	C20-C21-C22-C37
12	b	834	BCR	C22-C23-C24-C25
12	b	835	BCR	C1-C6-C7-C8
12	b	835	BCR	C5-C6-C7-C8
12	b	835	BCR	C6-C7-C8-C9
12	b	835	BCR	C7-C8-C9-C10
12	b	835	BCR	C7-C8-C9-C34
12	b	835	BCR	C10-C11-C12-C13
12	b	835	BCR	C12-C13-C14-C15
12	b	835	BCR	C35-C13-C14-C15
12	b	835	BCR	C14-C15-C16-C17
12	b	835	BCR	C15-C16-C17-C18
12	b	835	BCR	C17-C18-C19-C20
12	b	835	BCR	C36-C18-C19-C20
12	b	835	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
12	b	835	BCR	C21-C22-C23-C24
12	b	835	BCR	C37-C22-C23-C24
12	b	835	BCR	C22-C23-C24-C25
12	b	836	BCR	C11-C10-C9-C8
12	b	836	BCR	C11-C10-C9-C34
12	b	836	BCR	C21-C22-C23-C24
12	b	836	BCR	C37-C22-C23-C24
12	b	836	BCR	C22-C23-C24-C25
12	h	203	BCR	C6-C7-C8-C9
12	h	203	BCR	C11-C10-C9-C8
12	h	203	BCR	C11-C10-C9-C34
12	h	203	BCR	C11-C12-C13-C14
12	h	203	BCR	C11-C12-C13-C35
12	h	203	BCR	C35-C13-C14-C15
12	h	203	BCR	C20-C21-C22-C23
12	h	203	BCR	C20-C21-C22-C37
12	h	203	BCR	C22-C23-C24-C25
12	h	203	BCR	C23-C24-C25-C26
12	h	203	BCR	C23-C24-C25-C30
12	i	101	BCR	C7-C8-C9-C34
12	i	101	BCR	C9-C10-C11-C12
12	i	101	BCR	C10-C11-C12-C13
12	i	101	BCR	C11-C12-C13-C14
12	i	101	BCR	C11-C12-C13-C35
12	i	101	BCR	C21-C22-C23-C24
12	i	101	BCR	C37-C22-C23-C24
12	i	101	BCR	C22-C23-C24-C25
12	l	304	BCR	C6-C7-C8-C9
12	l	304	BCR	C7-C8-C9-C10
12	l	304	BCR	C7-C8-C9-C34
12	l	304	BCR	C14-C15-C16-C17
12	l	304	BCR	C16-C17-C18-C36
12	l	304	BCR	C20-C21-C22-C23
12	l	304	BCR	C20-C21-C22-C37
12	l	304	BCR	C21-C22-C23-C24
12	l	304	BCR	C37-C22-C23-C24
12	l	304	BCR	C22-C23-C24-C25
12	l	308	BCR	C7-C8-C9-C10
12	l	308	BCR	C7-C8-C9-C34
12	l	308	BCR	C11-C12-C13-C35
12	l	308	BCR	C22-C23-C24-C25
12	l	308	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
12	l	308	BCR	C23-C24-C25-C30
12	l	309	BCR	C1-C6-C7-C8
12	l	309	BCR	C14-C15-C16-C17
12	l	309	BCR	C22-C23-C24-C25
14	B	837	DGD	C2B-C1B-O2G-C2G
14	b	837	DGD	C2B-C1B-O2G-C2G
15	B	838	LMT	C2'-C1'-O1'-C1
15	B	838	LMT	O5'-C1'-O1'-C1
15	B	838	LMT	C2-C1-O1'-C1'
15	b	838	LMT	C2'-C1'-O1'-C1
15	b	838	LMT	O5'-C1'-O1'-C1
15	b	838	LMT	C2-C1-O1'-C1'
9	l	301	CLA	C2C-C3C-CAC-CBC
9	A	808	CLA	O1D-CGD-O2D-CED
9	A	814	CLA	O1D-CGD-O2D-CED
9	A	824	CLA	O1D-CGD-O2D-CED
9	A	834	CLA	O1D-CGD-O2D-CED
9	a	806	CLA	O1D-CGD-O2D-CED
9	a	808	CLA	O1D-CGD-O2D-CED
9	a	809	CLA	O1D-CGD-O2D-CED
9	a	814	CLA	O1D-CGD-O2D-CED
9	a	835	CLA	O1D-CGD-O2D-CED
9	a	846	CLA	C13-C15-C16-C17
9	A	819	CLA	O1D-CGD-O2D-CED
9	B	831	CLA	O1D-CGD-O2D-CED
9	A	813	CLA	CBD-CGD-O2D-CED
9	A	814	CLA	CBD-CGD-O2D-CED
9	A	821	CLA	CBD-CGD-O2D-CED
9	A	831	CLA	CBD-CGD-O2D-CED
9	A	834	CLA	CBD-CGD-O2D-CED
9	B	803	CLA	CBD-CGD-O2D-CED
9	B	807	CLA	CBD-CGD-O2D-CED
9	B	812	CLA	CBD-CGD-O2D-CED
9	B	831	CLA	CBD-CGD-O2D-CED
9	B	832	CLA	CBD-CGD-O2D-CED
9	L	304	CLA	CBD-CGD-O2D-CED
9	L	307	CLA	CBD-CGD-O2D-CED
9	L	308	CLA	CBD-CGD-O2D-CED
9	a	806	CLA	CBD-CGD-O2D-CED
9	a	813	CLA	CBD-CGD-O2D-CED
9	a	814	CLA	CBD-CGD-O2D-CED
9	a	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	a	831	CLA	CBD-CGD-O2D-CED
9	a	832	CLA	CBD-CGD-O2D-CED
9	a	835	CLA	CBD-CGD-O2D-CED
9	a	846	CLA	CBD-CGD-O2D-CED
9	b	803	CLA	CBD-CGD-O2D-CED
9	b	807	CLA	CBD-CGD-O2D-CED
9	b	826	CLA	CBD-CGD-O2D-CED
9	b	831	CLA	CBD-CGD-O2D-CED
9	b	832	CLA	CBD-CGD-O2D-CED
9	h	202	CLA	CBD-CGD-O2D-CED
9	l	307	CLA	CBD-CGD-O2D-CED
9	A	817	CLA	O1A-CGA-O2A-C1
9	A	830	CLA	O1A-CGA-O2A-C1
9	B	806	CLA	O1A-CGA-O2A-C1
9	a	817	CLA	O1A-CGA-O2A-C1
9	B	804	CLA	O1D-CGD-O2D-CED
9	L	307	CLA	O1D-CGD-O2D-CED
9	a	831	CLA	O1D-CGD-O2D-CED
9	b	804	CLA	O1D-CGD-O2D-CED
9	b	831	CLA	O1D-CGD-O2D-CED
9	l	307	CLA	O1D-CGD-O2D-CED
9	A	819	CLA	C15-C16-C17-C18
9	A	806	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	O1D-CGD-O2D-CED
9	A	815	CLA	O1D-CGD-O2D-CED
9	A	830	CLA	O1D-CGD-O2D-CED
9	A	835	CLA	O1D-CGD-O2D-CED
9	B	803	CLA	O1D-CGD-O2D-CED
9	B	820	CLA	O1D-CGD-O2D-CED
9	H	201	CLA	O1D-CGD-O2D-CED
9	a	815	CLA	O1D-CGD-O2D-CED
9	a	836	CLA	O1D-CGD-O2D-CED
9	b	803	CLA	O1D-CGD-O2D-CED
9	b	820	CLA	O1D-CGD-O2D-CED
9	l	301	CLA	O1D-CGD-O2D-CED
9	A	830	CLA	CBA-CGA-O2A-C1
9	B	806	CLA	CBA-CGA-O2A-C1
9	B	814	CLA	CBA-CGA-O2A-C1
9	a	817	CLA	CBA-CGA-O2A-C1
9	b	814	CLA	CBA-CGA-O2A-C1
9	A	825	CLA	CBD-CGD-O2D-CED
9	A	828	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	A	833	CLA	CBD-CGD-O2D-CED
9	A	846	CLA	CBD-CGD-O2D-CED
9	B	811	CLA	CBD-CGD-O2D-CED
9	B	816	CLA	CBD-CGD-O2D-CED
9	B	840	CLA	CBD-CGD-O2D-CED
9	a	822	CLA	CBD-CGD-O2D-CED
9	a	825	CLA	CBD-CGD-O2D-CED
9	a	826	CLA	CBD-CGD-O2D-CED
9	a	829	CLA	CBD-CGD-O2D-CED
9	a	834	CLA	CBD-CGD-O2D-CED
9	b	811	CLA	CBD-CGD-O2D-CED
9	b	822	CLA	CBD-CGD-O2D-CED
9	b	828	CLA	CBD-CGD-O2D-CED
9	b	840	CLA	CBD-CGD-O2D-CED
9	l	306	CLA	CBD-CGD-O2D-CED
9	A	809	CLA	O1A-CGA-O2A-C1
9	A	833	CLA	O1A-CGA-O2A-C1
9	B	811	CLA	O1A-CGA-O2A-C1
9	B	814	CLA	O1A-CGA-O2A-C1
9	H	201	CLA	O1A-CGA-O2A-C1
9	a	809	CLA	O1A-CGA-O2A-C1
9	a	821	CLA	O1A-CGA-O2A-C1
9	a	834	CLA	O1A-CGA-O2A-C1
9	b	811	CLA	O1A-CGA-O2A-C1
9	b	814	CLA	O1A-CGA-O2A-C1
9	a	807	CLA	O1D-CGD-O2D-CED
9	a	817	CLA	O1D-CGD-O2D-CED
9	l	302	CLA	O1D-CGD-O2D-CED
9	A	806	CLA	C8-C10-C11-C12
9	a	815	CLA	C10-C11-C12-C13
9	B	826	CLA	O1D-CGD-O2D-CED
9	B	822	CLA	CBD-CGD-O2D-CED
9	B	823	CLA	CBD-CGD-O2D-CED
9	b	826	CLA	O1D-CGD-O2D-CED
14	B	837	DGD	O1B-C1B-O2G-C2G
14	b	837	DGD	O1B-C1B-O2G-C2G
9	A	807	CLA	O1A-CGA-O2A-C1
9	A	801	CLA	C3-C5-C6-C7
9	A	806	CLA	C3-C5-C6-C7
9	A	821	CLA	C3-C5-C6-C7
9	A	828	CLA	C3-C5-C6-C7
9	B	801	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	B	806	CLA	C3-C5-C6-C7
9	B	810	CLA	C3-C5-C6-C7
9	B	817	CLA	C3-C5-C6-C7
9	a	801	CLA	C3-C5-C6-C7
9	a	816	CLA	C3-C5-C6-C7
9	a	825	CLA	C3-C5-C6-C7
9	a	829	CLA	C3-C5-C6-C7
9	a	846	CLA	C3-C5-C6-C7
9	b	801	CLA	C3-C5-C6-C7
9	b	806	CLA	C3-C5-C6-C7
9	b	810	CLA	C3-C5-C6-C7
9	A	809	CLA	CBA-CGA-O2A-C1
9	A	815	CLA	CBA-CGA-O2A-C1
9	A	817	CLA	CBA-CGA-O2A-C1
9	A	833	CLA	CBA-CGA-O2A-C1
9	H	201	CLA	CBA-CGA-O2A-C1
9	a	809	CLA	CBA-CGA-O2A-C1
9	a	834	CLA	CBA-CGA-O2A-C1
9	b	806	CLA	CBA-CGA-O2A-C1
9	a	806	CLA	C13-C15-C16-C17
9	B	832	CLA	O1D-CGD-O2D-CED
9	L	308	CLA	O1D-CGD-O2D-CED
9	b	832	CLA	O1D-CGD-O2D-CED
9	A	836	CLA	CBD-CGD-O2D-CED
9	B	809	CLA	CBD-CGD-O2D-CED
9	B	825	CLA	CBD-CGD-O2D-CED
9	B	828	CLA	CBD-CGD-O2D-CED
9	a	837	CLA	CBD-CGD-O2D-CED
9	b	814	CLA	CBD-CGD-O2D-CED
9	b	823	CLA	CBD-CGD-O2D-CED
9	b	825	CLA	CBD-CGD-O2D-CED
9	a	830	CLA	O1A-CGA-O2A-C1
9	a	820	CLA	C2C-C3C-CAC-CBC
14	b	837	DGD	O6E-C5E-C6E-O5E
9	B	811	CLA	C4-C3-C5-C6
9	b	811	CLA	C4-C3-C5-C6
9	A	824	CLA	C2-C3-C5-C6
9	B	808	CLA	C2-C3-C5-C6
9	B	824	CLA	C2-C3-C5-C6
9	b	824	CLA	C2-C3-C5-C6
9	b	809	CLA	CBD-CGD-O2D-CED
9	A	806	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	A	809	CLA	C2A-CAA-CBA-CGA
9	A	810	CLA	C2A-CAA-CBA-CGA
9	A	815	CLA	C2A-CAA-CBA-CGA
9	A	829	CLA	C2A-CAA-CBA-CGA
9	A	833	CLA	C2A-CAA-CBA-CGA
9	B	801	CLA	C2A-CAA-CBA-CGA
9	B	815	CLA	C2A-CAA-CBA-CGA
9	B	822	CLA	C2A-CAA-CBA-CGA
9	B	831	CLA	C2A-CAA-CBA-CGA
9	B	840	CLA	C2A-CAA-CBA-CGA
9	a	809	CLA	C2A-CAA-CBA-CGA
9	a	816	CLA	C2A-CAA-CBA-CGA
9	a	818	CLA	C2A-CAA-CBA-CGA
9	a	830	CLA	C2A-CAA-CBA-CGA
9	a	834	CLA	C2A-CAA-CBA-CGA
9	b	801	CLA	C2A-CAA-CBA-CGA
9	b	815	CLA	C2A-CAA-CBA-CGA
9	b	820	CLA	C2A-CAA-CBA-CGA
9	b	822	CLA	C2A-CAA-CBA-CGA
9	b	831	CLA	C2A-CAA-CBA-CGA
9	b	840	CLA	C2A-CAA-CBA-CGA
9	b	807	CLA	O1D-CGD-O2D-CED
9	A	805	CLA	C3-C5-C6-C7
9	A	815	CLA	C3-C5-C6-C7
9	A	824	CLA	C3-C5-C6-C7
9	b	817	CLA	C3-C5-C6-C7
9	A	805	CLA	CBA-CGA-O2A-C1
9	A	807	CLA	CBA-CGA-O2A-C1
9	B	811	CLA	CBA-CGA-O2A-C1
9	a	805	CLA	CBA-CGA-O2A-C1
9	a	819	CLA	CBA-CGA-O2A-C1
9	a	821	CLA	CBA-CGA-O2A-C1
9	b	811	CLA	CBA-CGA-O2A-C1
9	B	807	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	C1-C2-C3-C5
9	A	815	CLA	C1-C2-C3-C5
9	A	833	CLA	C1-C2-C3-C5
9	a	834	CLA	C1-C2-C3-C5
9	b	821	CLA	C1-C2-C3-C5
9	b	828	CLA	C1-C2-C3-C5
9	l	302	CLA	C1-C2-C3-C5
9	B	812	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	A	805	CLA	O1A-CGA-O2A-C1
9	A	815	CLA	O1A-CGA-O2A-C1
9	A	820	CLA	O1A-CGA-O2A-C1
9	A	829	CLA	O1A-CGA-O2A-C1
9	A	834	CLA	O1A-CGA-O2A-C1
9	B	817	CLA	O1A-CGA-O2A-C1
9	a	805	CLA	O1A-CGA-O2A-C1
9	a	835	CLA	O1A-CGA-O2A-C1
9	b	817	CLA	O1A-CGA-O2A-C1
9	L	304	CLA	O1D-CGD-O2D-CED
9	h	202	CLA	O1D-CGD-O2D-CED
12	A	841	BCR	C9-C10-C11-C12
12	A	841	BCR	C19-C20-C21-C22
12	a	842	BCR	C9-C10-C11-C12
12	a	844	BCR	C13-C14-C15-C16
12	a	844	BCR	C15-C16-C17-C18
12	b	834	BCR	C9-C10-C11-C12
12	b	835	BCR	C13-C14-C15-C16
12	l	308	BCR	C19-C20-C21-C22
15	B	838	LMT	O5'-C5'-C6'-O6'
9	B	819	CLA	CBD-CGD-O2D-CED
9	L	303	CLA	CBD-CGD-O2D-CED
9	a	802	CLA	CBD-CGD-O2D-CED
9	a	819	CLA	CBD-CGD-O2D-CED
9	b	816	CLA	CBD-CGD-O2D-CED
9	b	819	CLA	CBD-CGD-O2D-CED
9	a	813	CLA	O1D-CGD-O2D-CED
9	a	846	CLA	O1D-CGD-O2D-CED
11	A	838	LHG	O2-C2-C3-O3
11	a	839	LHG	O2-C2-C3-O3
9	a	805	CLA	C3-C5-C6-C7
9	a	817	CLA	C3-C5-C6-C7
9	B	817	CLA	CBA-CGA-O2A-C1
9	a	830	CLA	CBA-CGA-O2A-C1
9	a	835	CLA	CBA-CGA-O2A-C1
9	b	817	CLA	CBA-CGA-O2A-C1
9	b	822	CLA	CBA-CGA-O2A-C1
15	b	838	LMT	O5'-C5'-C6'-O6'
9	A	821	CLA	O1D-CGD-O2D-CED
9	B	814	CLA	CBD-CGD-O2D-CED
11	A	845	LHG	C13-C14-C15-C16
11	A	845	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	l	303	LHG	C29-C30-C31-C32
15	b	838	LMT	C7-C8-C9-C10
11	a	840	LHG	C9-C10-C11-C12
11	l	303	LHG	C13-C14-C15-C16
15	B	838	LMT	C7-C8-C9-C10
12	a	843	BCR	C14-C15-C16-C17
12	i	101	BCR	C14-C15-C16-C17
9	a	832	CLA	O1D-CGD-O2D-CED
9	b	804	CLA	C3-C5-C6-C7
9	b	818	CLA	C3-C5-C6-C7
9	A	820	CLA	CBA-CGA-O2A-C1
9	A	829	CLA	CBA-CGA-O2A-C1
9	A	834	CLA	CBA-CGA-O2A-C1
14	b	837	DGD	C4A-C5A-C6A-C7A
9	a	819	CLA	O1A-CGA-O2A-C1
9	A	833	CLA	C15-C16-C17-C18
9	A	810	CLA	C4-C3-C5-C6
9	A	816	CLA	C4-C3-C5-C6
9	A	829	CLA	C4-C3-C5-C6
9	B	802	CLA	C4-C3-C5-C6
9	B	817	CLA	C4-C3-C5-C6
9	a	816	CLA	C4-C3-C5-C6
9	a	830	CLA	C4-C3-C5-C6
9	b	817	CLA	C4-C3-C5-C6
15	B	838	LMT	C4'-C5'-C6'-O6'
15	b	838	LMT	C4'-C5'-C6'-O6'
9	A	810	CLA	C2-C3-C5-C6
9	A	816	CLA	C2-C3-C5-C6
9	A	826	CLA	C2-C3-C5-C6
9	A	829	CLA	C2-C3-C5-C6
9	B	802	CLA	C2-C3-C5-C6
9	B	817	CLA	C2-C3-C5-C6
9	a	816	CLA	C2-C3-C5-C6
9	a	830	CLA	C2-C3-C5-C6
9	b	817	CLA	C2-C3-C5-C6
9	A	836	CLA	C2A-CAA-CBA-CGA
9	B	819	CLA	C2A-CAA-CBA-CGA
9	B	820	CLA	C2A-CAA-CBA-CGA
9	L	308	CLA	C2A-CAA-CBA-CGA
9	a	810	CLA	C2A-CAA-CBA-CGA
9	a	837	CLA	C2A-CAA-CBA-CGA
9	l	302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	B	837	DGD	O6E-C5E-C6E-O5E
9	b	822	CLA	O1A-CGA-O2A-C1
14	b	837	DGD	C4E-C5E-C6E-O5E
9	A	831	CLA	O1D-CGD-O2D-CED
11	A	845	LHG	C9-C10-C11-C12
9	A	835	CLA	CBA-CGA-O2A-C1
9	a	806	CLA	CBA-CGA-O2A-C1
9	A	802	CLA	CBD-CGD-O2D-CED
11	l	303	LHG	C18-C19-C20-C21
9	A	813	CLA	O1D-CGD-O2D-CED
9	A	833	CLA	O1D-CGD-O2D-CED
9	a	834	CLA	O1D-CGD-O2D-CED
9	B	821	CLA	C1-C2-C3-C5
9	A	828	CLA	O1D-CGD-O2D-CED
9	a	829	CLA	O1D-CGD-O2D-CED
9	b	828	CLA	O1D-CGD-O2D-CED
9	l	306	CLA	O1D-CGD-O2D-CED
9	b	805	CLA	CBD-CGD-O2D-CED
9	b	818	CLA	CBD-CGD-O2D-CED
9	a	826	CLA	O1D-CGD-O2D-CED
11	l	303	LHG	C1-C2-C3-O3
9	B	818	CLA	C3-C5-C6-C7
9	a	819	CLA	C3-C5-C6-C7
9	A	825	CLA	O1D-CGD-O2D-CED
9	b	840	CLA	O1D-CGD-O2D-CED
9	A	806	CLA	CBA-CGA-O2A-C1
9	A	831	CLA	CBA-CGA-O2A-C1
9	B	801	CLA	CBA-CGA-O2A-C1
9	B	840	CLA	CBA-CGA-O2A-C1
9	L	308	CLA	CBA-CGA-O2A-C1
9	a	815	CLA	CBA-CGA-O2A-C1
9	a	820	CLA	CBA-CGA-O2A-C1
9	a	832	CLA	CBA-CGA-O2A-C1
9	a	836	CLA	CBA-CGA-O2A-C1
9	b	801	CLA	CBA-CGA-O2A-C1
9	b	840	CLA	CBA-CGA-O2A-C1
11	A	845	LHG	C24-C23-O8-C6
9	a	821	CLA	CBD-CGD-O2D-CED
14	B	837	DGD	C4E-C5E-C6E-O5E
9	B	840	CLA	O1D-CGD-O2D-CED
12	A	840	BCR	C9-C10-C11-C12
12	B	834	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	a	841	BCR	C9-C10-C11-C12
12	a	842	BCR	C15-C16-C17-C18
12	a	842	BCR	C19-C20-C21-C22
12	a	844	BCR	C19-C20-C21-C22
14	B	837	DGD	CDA-CEA-CFA-CGA
9	A	815	CLA	C8-C10-C11-C12
11	l	303	LHG	C9-C10-C11-C12
9	A	802	CLA	C10-C11-C12-C13
9	A	822	CLA	C5-C6-C7-C8
9	B	801	CLA	C13-C15-C16-C17
9	a	802	CLA	C10-C11-C12-C13
9	a	836	CLA	C10-C11-C12-C13
9	b	821	CLA	C8-C10-C11-C12
9	h	202	CLA	C15-C16-C17-C18
11	a	840	LHG	C7-C8-C9-C10
9	B	839	CLA	O2A-C1-C2-C3
9	B	820	CLA	CBA-CGA-O2A-C1
9	a	806	CLA	O1A-CGA-O2A-C1
9	B	811	CLA	C2-C3-C5-C6
9	b	811	CLA	C2-C3-C5-C6
9	A	802	CLA	C11-C12-C13-C14
9	A	808	CLA	C14-C13-C15-C16
9	A	809	CLA	C11-C12-C13-C14
9	A	811	CLA	C11-C10-C8-C9
9	A	816	CLA	C6-C7-C8-C9
9	A	816	CLA	C11-C10-C8-C9
9	A	822	CLA	C6-C7-C8-C9
9	A	822	CLA	C14-C13-C15-C16
9	A	823	CLA	C11-C10-C8-C9
9	A	824	CLA	C14-C13-C15-C16
9	A	829	CLA	C11-C10-C8-C9
9	A	829	CLA	C11-C12-C13-C14
9	A	832	CLA	C11-C12-C13-C14
9	B	801	CLA	C11-C10-C8-C9
9	B	804	CLA	C11-C12-C13-C14
9	B	810	CLA	C14-C13-C15-C16
9	B	814	CLA	C6-C7-C8-C9
9	B	815	CLA	C11-C12-C13-C14
9	B	819	CLA	C11-C10-C8-C9
9	B	824	CLA	C11-C10-C8-C9
9	L	303	CLA	C14-C13-C15-C16
9	a	802	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	a	808	CLA	C11-C12-C13-C14
9	a	809	CLA	C11-C12-C13-C14
9	a	811	CLA	C11-C10-C8-C9
9	a	816	CLA	C6-C7-C8-C9
9	a	819	CLA	C14-C13-C15-C16
9	a	823	CLA	C6-C7-C8-C9
9	a	823	CLA	C14-C13-C15-C16
9	a	824	CLA	C11-C12-C13-C14
9	a	825	CLA	C11-C12-C13-C14
9	a	830	CLA	C6-C7-C8-C9
9	a	830	CLA	C11-C12-C13-C14
9	a	833	CLA	C11-C12-C13-C14
9	a	846	CLA	C11-C10-C8-C9
9	a	847	CLA	C6-C7-C8-C9
9	a	847	CLA	C14-C13-C15-C16
9	b	801	CLA	C11-C10-C8-C9
9	b	810	CLA	C14-C13-C15-C16
9	b	814	CLA	C6-C7-C8-C9
9	b	815	CLA	C11-C12-C13-C14
9	b	818	CLA	C6-C7-C8-C9
9	b	819	CLA	C11-C10-C8-C9
9	b	824	CLA	C11-C10-C8-C9
9	l	306	CLA	C14-C13-C15-C16
10	A	837	PQN	C21-C22-C23-C24
10	a	838	PQN	C21-C22-C23-C24
9	A	846	CLA	O1D-CGD-O2D-CED
9	A	811	CLA	CBD-CGD-O2D-CED
9	B	805	CLA	CBD-CGD-O2D-CED
9	A	832	CLA	C10-C11-C12-C13
9	A	847	CLA	C5-C6-C7-C8
9	B	806	CLA	C10-C11-C12-C13
9	a	833	CLA	C10-C11-C12-C13
9	b	801	CLA	C13-C15-C16-C17
9	b	810	CLA	C10-C11-C12-C13
9	A	821	CLA	C2A-CAA-CBA-CGA
9	A	824	CLA	C2A-CAA-CBA-CGA
9	b	819	CLA	C2A-CAA-CBA-CGA
9	h	201	CLA	C2A-CAA-CBA-CGA
12	A	843	BCR	C36-C18-C19-C20
12	A	843	BCR	C37-C22-C23-C24
12	B	834	BCR	C11-C12-C13-C35
12	B	835	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
12	B	835	BCR	C36-C18-C19-C20
12	B	836	BCR	C11-C12-C13-C35
12	H	202	BCR	C7-C8-C9-C34
12	H	202	BCR	C36-C18-C19-C20
12	H	202	BCR	C37-C22-C23-C24
12	L	306	BCR	C7-C8-C9-C34
12	a	841	BCR	C11-C12-C13-C35
12	b	834	BCR	C37-C22-C23-C24
12	b	835	BCR	C11-C12-C13-C35
12	b	836	BCR	C11-C12-C13-C35
12	h	203	BCR	C7-C8-C9-C34
12	h	203	BCR	C36-C18-C19-C20
12	h	203	BCR	C37-C22-C23-C24
12	l	309	BCR	C7-C8-C9-C34
12	l	309	BCR	C11-C12-C13-C35
12	A	843	BCR	C17-C18-C19-C20
12	A	843	BCR	C21-C22-C23-C24
12	B	834	BCR	C11-C12-C13-C14
12	B	835	BCR	C7-C8-C9-C10
12	H	202	BCR	C7-C8-C9-C10
12	H	202	BCR	C17-C18-C19-C20
12	H	202	BCR	C21-C22-C23-C24
12	L	306	BCR	C7-C8-C9-C10
12	a	844	BCR	C11-C12-C13-C14
12	b	834	BCR	C11-C12-C13-C14
12	b	834	BCR	C21-C22-C23-C24
12	h	203	BCR	C7-C8-C9-C10
12	h	203	BCR	C17-C18-C19-C20
12	h	203	BCR	C21-C22-C23-C24
12	l	308	BCR	C21-C22-C23-C24
12	l	309	BCR	C7-C8-C9-C10
9	A	806	CLA	O1A-CGA-O2A-C1
9	B	801	CLA	O1A-CGA-O2A-C1
9	B	840	CLA	O1A-CGA-O2A-C1
9	a	815	CLA	O1A-CGA-O2A-C1
9	b	801	CLA	O1A-CGA-O2A-C1
9	b	840	CLA	O1A-CGA-O2A-C1
9	A	846	CLA	C10-C11-C12-C13
9	B	810	CLA	C10-C11-C12-C13
9	b	821	CLA	C13-C15-C16-C17
9	a	822	CLA	O1D-CGD-O2D-CED
9	b	822	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	838	LMT	C5'-C4'-O1B-C1B
9	A	811	CLA	C3-C5-C6-C7
9	A	829	CLA	C3-C5-C6-C7
9	b	814	CLA	C3-C5-C6-C7
9	A	819	CLA	CBA-CGA-O2A-C1
9	l	306	CLA	CBA-CGA-O2A-C1
9	A	805	CLA	C10-C11-C12-C13
9	A	817	CLA	C15-C16-C17-C18
9	A	828	CLA	C5-C6-C7-C8
9	A	832	CLA	C15-C16-C17-C18
9	A	835	CLA	C15-C16-C17-C18
9	B	804	CLA	C8-C10-C11-C12
9	B	811	CLA	C5-C6-C7-C8
9	a	805	CLA	C10-C11-C12-C13
9	a	817	CLA	C15-C16-C17-C18
9	a	836	CLA	C15-C16-C17-C18
9	a	847	CLA	C5-C6-C7-C8
9	a	847	CLA	C8-C10-C11-C12
9	b	802	CLA	C15-C16-C17-C18
9	b	807	CLA	C10-C11-C12-C13
10	a	838	PQN	C20-C21-C22-C23
9	a	820	CLA	C4C-C3C-CAC-CBC
15	b	838	LMT	C5'-C4'-O1B-C1B
9	A	801	CLA	C15-C16-C17-C18
9	A	806	CLA	C10-C11-C12-C13
9	A	808	CLA	C8-C10-C11-C12
9	A	809	CLA	C13-C15-C16-C17
9	A	823	CLA	C10-C11-C12-C13
9	A	847	CLA	C8-C10-C11-C12
9	B	801	CLA	C5-C6-C7-C8
9	B	807	CLA	C10-C11-C12-C13
9	B	818	CLA	C8-C10-C11-C12
9	B	821	CLA	C8-C10-C11-C12
9	B	821	CLA	C13-C15-C16-C17
9	B	829	CLA	C13-C15-C16-C17
9	a	801	CLA	C15-C16-C17-C18
9	a	808	CLA	C15-C16-C17-C18
9	a	809	CLA	C10-C11-C12-C13
9	a	811	CLA	C10-C11-C12-C13
9	a	819	CLA	C13-C15-C16-C17
9	a	829	CLA	C5-C6-C7-C8
9	b	801	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	b	804	CLA	C8-C10-C11-C12
9	b	806	CLA	C10-C11-C12-C13
9	b	814	CLA	C8-C10-C11-C12
9	b	823	CLA	C10-C11-C12-C13
9	b	829	CLA	C13-C15-C16-C17
9	A	803	CLA	C1-C2-C3-C5
9	B	803	CLA	C1-C2-C3-C5
9	b	803	CLA	C1-C2-C3-C5
11	l	303	LHG	C23-C24-C25-C26
9	a	811	CLA	CBD-CGD-O2D-CED
9	A	801	CLA	C13-C15-C16-C17
9	A	817	CLA	C5-C6-C7-C8
9	B	804	CLA	C10-C11-C12-C13
9	B	815	CLA	C10-C11-C12-C13
9	B	824	CLA	C8-C10-C11-C12
9	a	801	CLA	C13-C15-C16-C17
9	a	811	CLA	C15-C16-C17-C18
9	a	823	CLA	C5-C6-C7-C8
9	a	827	CLA	C10-C11-C12-C13
9	b	815	CLA	C10-C11-C12-C13
9	b	821	CLA	C10-C11-C12-C13
9	b	824	CLA	C8-C10-C11-C12
9	l	306	CLA	C10-C11-C12-C13
9	a	807	CLA	C3-C5-C6-C7
9	A	816	CLA	CBA-CGA-O2A-C1
9	B	830	CLA	CBA-CGA-O2A-C1
9	a	825	CLA	O1D-CGD-O2D-CED
9	A	806	CLA	C2-C1-O2A-CGA
9	L	308	CLA	C2-C1-O2A-CGA
9	B	802	CLA	C15-C16-C17-C18
9	B	814	CLA	C8-C10-C11-C12
9	B	821	CLA	C10-C11-C12-C13
9	B	823	CLA	C10-C11-C12-C13
9	a	809	CLA	C13-C15-C16-C17
9	a	811	CLA	C8-C10-C11-C12
9	b	811	CLA	C5-C6-C7-C8
9	a	818	CLA	CBD-CGD-O2D-CED
9	B	801	CLA	C2C-C3C-CAC-CBC
9	A	809	CLA	C5-C6-C7-C8
9	A	823	CLA	C13-C15-C16-C17
9	A	835	CLA	C10-C11-C12-C13
9	b	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	A	805	CLA	C11-C10-C8-C7
9	A	806	CLA	C11-C12-C13-C15
9	A	807	CLA	C6-C7-C8-C10
9	A	809	CLA	C12-C13-C15-C16
9	A	815	CLA	C11-C10-C8-C7
9	A	821	CLA	C6-C7-C8-C10
9	A	824	CLA	C11-C10-C8-C7
9	A	826	CLA	C12-C13-C15-C16
9	A	846	CLA	C12-C13-C15-C16
9	B	804	CLA	C11-C10-C8-C7
9	B	807	CLA	C11-C10-C8-C7
9	B	810	CLA	C11-C10-C8-C7
9	B	824	CLA	C6-C7-C8-C10
9	a	805	CLA	C11-C10-C8-C7
9	a	809	CLA	C12-C13-C15-C16
9	a	819	CLA	C11-C12-C13-C15
9	a	824	CLA	C12-C13-C15-C16
9	a	825	CLA	C11-C10-C8-C7
9	b	804	CLA	C11-C10-C8-C7
9	b	807	CLA	C11-C10-C8-C7
9	b	824	CLA	C6-C7-C8-C10
9	a	836	CLA	O1A-CGA-O2A-C1
11	A	845	LHG	O10-C23-O8-C6
12	A	842	BCR	C9-C10-C11-C12
12	A	842	BCR	C19-C20-C21-C22
12	A	843	BCR	C13-C14-C15-C16
12	A	843	BCR	C19-C20-C21-C22
12	B	835	BCR	C9-C10-C11-C12
12	H	202	BCR	C19-C20-C21-C22
9	B	811	CLA	O1D-CGD-O2D-CED
9	B	816	CLA	O1D-CGD-O2D-CED
9	b	811	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	C15-C16-C17-C18
9	A	808	CLA	C5-C6-C7-C8
9	A	811	CLA	C10-C11-C12-C13
9	A	824	CLA	C13-C15-C16-C17
9	A	826	CLA	C10-C11-C12-C13
9	B	801	CLA	C8-C10-C11-C12
9	B	802	CLA	C8-C10-C11-C12
9	B	803	CLA	C15-C16-C17-C18
9	B	809	CLA	C15-C16-C17-C18
9	H	201	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	a	806	CLA	C8-C10-C11-C12
9	a	809	CLA	C5-C6-C7-C8
9	b	803	CLA	C15-C16-C17-C18
9	b	814	CLA	C13-C15-C16-C17
12	a	841	BCR	C6-C7-C8-C9
12	A	842	BCR	C18-C19-C20-C21
12	B	834	BCR	C18-C19-C20-C21
12	L	301	BCR	C18-C19-C20-C21
12	a	843	BCR	C10-C11-C12-C13
12	a	843	BCR	C18-C19-C20-C21
12	b	834	BCR	C18-C19-C20-C21
12	h	203	BCR	C18-C19-C20-C21
12	l	309	BCR	C10-C11-C12-C13
12	l	309	BCR	C18-C19-C20-C21
9	B	814	CLA	C3-C5-C6-C7
9	a	847	CLA	C3-C5-C6-C7
9	b	824	CLA	C3-C5-C6-C7
9	A	824	CLA	C8-C10-C11-C12
9	A	829	CLA	C15-C16-C17-C18
9	A	846	CLA	C5-C6-C7-C8
9	B	801	CLA	C10-C11-C12-C13
9	B	832	CLA	C15-C16-C17-C18
9	H	201	CLA	C13-C15-C16-C17
9	L	303	CLA	C10-C11-C12-C13
9	a	830	CLA	C15-C16-C17-C18
9	a	846	CLA	C8-C10-C11-C12
9	b	801	CLA	C10-C11-C12-C13
9	b	804	CLA	C5-C6-C7-C8
9	b	832	CLA	C15-C16-C17-C18
10	A	837	PQN	C20-C21-C22-C23
9	A	818	CLA	CBD-CGD-O2D-CED
9	A	819	CLA	O1A-CGA-O2A-C1
9	A	831	CLA	O1A-CGA-O2A-C1
9	A	835	CLA	O1A-CGA-O2A-C1
9	L	308	CLA	O1A-CGA-O2A-C1
9	a	820	CLA	O1A-CGA-O2A-C1
9	a	832	CLA	O1A-CGA-O2A-C1
9	l	306	CLA	O1A-CGA-O2A-C1
11	A	839	LHG	C7-C8-C9-C10
9	b	801	CLA	C2C-C3C-CAC-CBC
14	b	837	DGD	CAA-CBA-CCA-CDA
9	A	809	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	B	810	CLA	C13-C15-C16-C17
9	B	823	CLA	C15-C16-C17-C18
9	H	201	CLA	C8-C10-C11-C12
9	a	825	CLA	C10-C11-C12-C13
9	a	826	CLA	C15-C16-C17-C18
9	a	830	CLA	C10-C11-C12-C13
9	a	833	CLA	C15-C16-C17-C18
9	b	824	CLA	C10-C11-C12-C13
9	h	202	CLA	C13-C15-C16-C17
9	B	822	CLA	O1D-CGD-O2D-CED
9	B	823	CLA	O1D-CGD-O2D-CED
9	a	837	CLA	O1D-CGD-O2D-CED
9	b	802	CLA	CBD-CGD-O2D-CED
9	B	820	CLA	O1A-CGA-O2A-C1
9	A	823	CLA	C8-C10-C11-C12
9	A	847	CLA	C10-C11-C12-C13
9	a	807	CLA	C5-C6-C7-C8
9	a	808	CLA	C13-C15-C16-C17
9	a	829	CLA	C10-C11-C12-C13
9	a	846	CLA	C10-C11-C12-C13
9	b	801	CLA	C8-C10-C11-C12
9	b	810	CLA	C13-C15-C16-C17
9	b	823	CLA	C15-C16-C17-C18
9	h	202	CLA	C8-C10-C11-C12
11	A	839	LHG	C3-O3-P-O6
11	A	845	LHG	C4-O6-P-O3
11	a	840	LHG	C3-O3-P-O6
11	l	303	LHG	C4-O6-P-O3
9	A	817	CLA	C3-C5-C6-C7
9	B	807	CLA	C3-C5-C6-C7
9	A	803	CLA	CBA-CGA-O2A-C1
9	b	828	CLA	CBA-CGA-O2A-C1
9	A	836	CLA	O1D-CGD-O2D-CED
9	B	828	CLA	O1D-CGD-O2D-CED
9	A	803	CLA	CBD-CGD-O2D-CED
9	A	846	CLA	C8-C10-C11-C12
9	B	809	CLA	O1D-CGD-O2D-CED
9	b	814	CLA	O1D-CGD-O2D-CED
9	B	815	CLA	C4-C3-C5-C6
9	b	819	CLA	C4-C3-C5-C6
9	a	817	CLA	C5-C6-C7-C8
9	a	847	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	b	807	CLA	C5-C6-C7-C8
9	b	823	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	C2A-CAA-CBA-CGA
9	A	818	CLA	C2A-CAA-CBA-CGA
9	A	830	CLA	C2A-CAA-CBA-CGA
9	B	802	CLA	C2A-CAA-CBA-CGA
9	a	825	CLA	C2A-CAA-CBA-CGA
9	b	802	CLA	C2A-CAA-CBA-CGA
9	A	803	CLA	C6-C7-C8-C9
9	A	808	CLA	C16-C17-C18-C20
9	a	833	CLA	C16-C17-C18-C19
9	B	824	CLA	C3-C5-C6-C7
9	a	830	CLA	C3-C5-C6-C7
9	a	816	CLA	CBA-CGA-O2A-C1
12	b	834	BCR	C14-C15-C16-C17
9	A	815	CLA	C15-C16-C17-C18
9	B	824	CLA	C10-C11-C12-C13
9	a	802	CLA	C15-C16-C17-C18
9	b	814	CLA	C10-C11-C12-C13
12	A	841	BCR	C13-C14-C15-C16
12	A	841	BCR	C15-C16-C17-C18
12	B	835	BCR	C19-C20-C21-C22
12	b	834	BCR	C13-C14-C15-C16
12	b	835	BCR	C19-C20-C21-C22
12	h	203	BCR	C19-C20-C21-C22
11	A	845	LHG	C32-C33-C34-C35
14	b	837	DGD	CDA-CEA-CFA-CGA
9	B	827	CLA	CBD-CGD-O2D-CED
11	A	838	LHG	C8-C7-O7-C5
11	A	839	LHG	C8-C7-O7-C5
11	a	840	LHG	C8-C7-O7-C5
9	A	807	CLA	C5-C6-C7-C8
9	B	810	CLA	C15-C16-C17-C18
9	a	806	CLA	C10-C11-C12-C13
12	A	840	BCR	C20-C21-C22-C37
12	A	841	BCR	C20-C21-C22-C37
12	B	834	BCR	C11-C10-C9-C34
12	B	834	BCR	C35-C13-C14-C15
12	B	834	BCR	C16-C17-C18-C36
12	B	835	BCR	C11-C10-C9-C34
12	B	836	BCR	C35-C13-C14-C15
12	H	202	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
12	H	202	BCR	C16-C17-C18-C36
12	I	101	BCR	C11-C10-C9-C34
12	I	101	BCR	C20-C21-C22-C37
12	L	301	BCR	C16-C17-C18-C36
12	L	305	BCR	C16-C17-C18-C36
12	a	841	BCR	C20-C21-C22-C37
12	a	842	BCR	C20-C21-C22-C37
12	b	834	BCR	C11-C10-C9-C34
12	b	835	BCR	C16-C17-C18-C36
12	b	836	BCR	C35-C13-C14-C15
12	h	203	BCR	C16-C17-C18-C36
12	i	101	BCR	C11-C10-C9-C34
12	i	101	BCR	C20-C21-C22-C37
12	l	304	BCR	C11-C10-C9-C34
12	l	308	BCR	C16-C17-C18-C36
12	l	309	BCR	C16-C17-C18-C36
12	l	309	BCR	C20-C21-C22-C37
9	A	807	CLA	C3-C5-C6-C7
11	A	838	LHG	C27-C28-C29-C30
11	A	845	LHG	C31-C32-C33-C34
11	l	303	LHG	C14-C15-C16-C17
15	b	838	LMT	C11-C10-C9-C8
9	b	809	CLA	O1D-CGD-O2D-CED
9	A	816	CLA	C16-C17-C18-C19
9	A	825	CLA	C16-C17-C18-C20
9	A	832	CLA	C16-C17-C18-C19
9	B	819	CLA	C11-C12-C13-C14
9	a	803	CLA	C6-C7-C8-C9
9	b	819	CLA	C11-C12-C13-C14
9	b	830	CLA	CBA-CGA-O2A-C1
11	A	845	LHG	C14-C15-C16-C17
14	b	837	DGD	CCB-CDB-CEB-CFB
15	b	838	LMT	C4-C5-C6-C7
9	B	825	CLA	O1D-CGD-O2D-CED
9	b	825	CLA	O1D-CGD-O2D-CED
11	A	838	LHG	O9-C7-O7-C5
11	A	839	LHG	O9-C7-O7-C5
9	A	802	CLA	C15-C16-C17-C18
9	a	831	CLA	C1-C2-C3-C4
9	a	831	CLA	C1-C2-C3-C5
9	b	820	CLA	C1-C2-C3-C4
9	b	820	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
9	l	307	CLA	C1-C2-C3-C4
9	l	307	CLA	C1-C2-C3-C5
11	a	839	LHG	C7-C8-C9-C10
9	B	802	CLA	CBD-CGD-O2D-CED
9	b	827	CLA	CBD-CGD-O2D-CED
14	B	837	DGD	CAB-CBB-CCB-CDB
15	B	838	LMT	C11-C10-C9-C8
9	A	816	CLA	O1A-CGA-O2A-C1
11	a	839	LHG	C24-C25-C26-C27
14	B	837	DGD	C9B-CAB-CBB-CCB
15	B	838	LMT	C4-C5-C6-C7
15	b	838	LMT	C6-C7-C8-C9
9	b	816	CLA	O1D-CGD-O2D-CED
9	b	819	CLA	O1D-CGD-O2D-CED
9	B	829	CLA	C10-C11-C12-C13
9	b	826	CLA	O2A-C1-C2-C3
12	A	840	BCR	C20-C21-C22-C23
12	A	841	BCR	C20-C21-C22-C23
12	B	834	BCR	C11-C10-C9-C8
12	B	834	BCR	C12-C13-C14-C15
12	B	834	BCR	C16-C17-C18-C19
12	B	835	BCR	C11-C10-C9-C8
12	B	836	BCR	C12-C13-C14-C15
12	H	202	BCR	C12-C13-C14-C15
12	H	202	BCR	C16-C17-C18-C19
12	I	101	BCR	C11-C10-C9-C8
12	I	101	BCR	C20-C21-C22-C23
12	L	301	BCR	C16-C17-C18-C19
12	L	305	BCR	C16-C17-C18-C19
12	a	841	BCR	C20-C21-C22-C23
12	a	842	BCR	C20-C21-C22-C23
12	b	834	BCR	C11-C10-C9-C8
12	b	835	BCR	C16-C17-C18-C19
12	b	836	BCR	C12-C13-C14-C15
12	h	203	BCR	C12-C13-C14-C15
12	h	203	BCR	C16-C17-C18-C19
12	i	101	BCR	C11-C10-C9-C8
12	i	101	BCR	C20-C21-C22-C23
12	l	304	BCR	C11-C10-C9-C8
12	l	304	BCR	C16-C17-C18-C19
12	l	308	BCR	C16-C17-C18-C19
12	l	309	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	l	309	BCR	C20-C21-C22-C23
9	B	832	CLA	CBA-CGA-O2A-C1
9	L	303	CLA	CBA-CGA-O2A-C1
9	a	803	CLA	CBA-CGA-O2A-C1
9	b	832	CLA	CBA-CGA-O2A-C1
11	A	838	LHG	C17-C18-C19-C20
11	a	839	LHG	C17-C18-C19-C20
14	B	837	DGD	C6B-C7B-C8B-C9B
14	B	837	DGD	CCB-CDB-CEB-CFB
9	a	836	CLA	C5-C6-C7-C8
9	b	815	CLA	C15-C16-C17-C18
9	B	830	CLA	O1A-CGA-O2A-C1
9	B	802	CLA	C16-C17-C18-C19
9	B	815	CLA	C16-C17-C18-C20
9	a	826	CLA	C16-C17-C18-C20
9	b	815	CLA	C16-C17-C18-C20
9	a	819	CLA	O1D-CGD-O2D-CED
9	a	824	CLA	C4-C3-C5-C6
9	b	815	CLA	C4-C3-C5-C6
11	A	838	LHG	C25-C26-C27-C28
11	a	839	LHG	C16-C17-C18-C19
14	B	837	DGD	CBA-CCA-CDA-CEA
15	B	838	LMT	C5-C6-C7-C8
15	B	838	LMT	C6-C7-C8-C9
9	B	815	CLA	C2-C3-C5-C6
9	A	811	CLA	C11-C12-C13-C14
9	A	821	CLA	C6-C7-C8-C9
9	A	826	CLA	C11-C12-C13-C14
9	B	807	CLA	C11-C12-C13-C14
9	B	809	CLA	C14-C13-C15-C16
9	a	811	CLA	C11-C12-C13-C14
9	b	824	CLA	C6-C7-C8-C9
10	a	838	PQN	C24-C23-C25-C26
9	L	308	CLA	C2C-C3C-CAC-CBC
11	A	838	LHG	C24-C25-C26-C27
11	A	845	LHG	C29-C30-C31-C32
14	b	837	DGD	C4B-C5B-C6B-C7B
14	b	837	DGD	C9B-CAB-CBB-CCB
9	A	828	CLA	C10-C11-C12-C13
9	A	833	CLA	C13-C15-C16-C17
9	B	814	CLA	C13-C15-C16-C17
9	b	831	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	A	805	CLA	C2A-CAA-CBA-CGA
9	A	827	CLA	C2A-CAA-CBA-CGA
9	a	805	CLA	C2A-CAA-CBA-CGA
9	a	815	CLA	C2A-CAA-CBA-CGA
9	l	301	CLA	C2A-CAA-CBA-CGA
9	b	828	CLA	O1A-CGA-O2A-C1
12	L	305	BCR	C36-C18-C19-C20
12	L	305	BCR	C37-C22-C23-C24
12	l	308	BCR	C36-C18-C19-C20
12	l	308	BCR	C37-C22-C23-C24
14	b	837	DGD	C9A-CAA-CBA-CCA
11	A	838	LHG	O1-C1-C2-C3
11	a	839	LHG	O1-C1-C2-C3
11	a	840	LHG	O1-C1-C2-C3
12	L	305	BCR	C17-C18-C19-C20
12	L	305	BCR	C21-C22-C23-C24
12	b	835	BCR	C11-C12-C13-C14
12	i	101	BCR	C7-C8-C9-C10
12	l	308	BCR	C11-C12-C13-C14
12	l	308	BCR	C17-C18-C19-C20
9	b	807	CLA	C3-C5-C6-C7
10	A	837	PQN	C13-C15-C16-C17
10	a	838	PQN	C13-C15-C16-C17
11	a	840	LHG	O9-C7-O7-C5
9	A	811	CLA	C8-C10-C11-C12
9	B	831	CLA	C15-C16-C17-C18
9	a	822	CLA	C8-C10-C11-C12
11	l	303	LHG	C24-C25-C26-C27
15	b	838	LMT	C5-C6-C7-C8
9	B	813	CLA	C4B-C3B-CAB-CBB
11	A	838	LHG	C16-C17-C18-C19
14	b	837	DGD	CBA-CCA-CDA-CEA
9	A	806	CLA	C4B-C3B-CAB-CBB
9	A	811	CLA	C4B-C3B-CAB-CBB
9	A	822	CLA	C4B-C3B-CAB-CBB
9	A	823	CLA	C4B-C3B-CAB-CBB
9	A	847	CLA	C4B-C3B-CAB-CBB
9	B	804	CLA	C4B-C3B-CAB-CBB
9	B	816	CLA	C4B-C3B-CAB-CBB
9	B	822	CLA	C4B-C3B-CAB-CBB
9	a	808	CLA	C4B-C3B-CAB-CBB
9	a	816	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	a	821	CLA	C4B-C3B-CAB-CBB
9	a	823	CLA	C4B-C3B-CAB-CBB
9	a	824	CLA	C4B-C3B-CAB-CBB
9	a	847	CLA	C4B-C3B-CAB-CBB
9	b	804	CLA	C4B-C3B-CAB-CBB
9	b	816	CLA	C4B-C3B-CAB-CBB
9	b	822	CLA	C4B-C3B-CAB-CBB
9	h	202	CLA	C4B-C3B-CAB-CBB
9	l	305	CLA	C4B-C3B-CAB-CBB
9	l	307	CLA	C4B-C3B-CAB-CBB
9	A	833	CLA	C16-C17-C18-C19
9	A	833	CLA	C16-C17-C18-C20
9	B	819	CLA	C11-C12-C13-C15
9	a	821	CLA	C6-C7-C8-C10
9	a	825	CLA	C16-C17-C18-C19
9	a	833	CLA	C16-C17-C18-C20
9	a	834	CLA	C16-C17-C18-C19
9	a	834	CLA	C16-C17-C18-C20
9	a	836	CLA	C16-C17-C18-C19
9	b	802	CLA	C16-C17-C18-C20
9	A	835	CLA	C5-C6-C7-C8
9	a	827	CLA	C15-C16-C17-C18
11	l	303	LHG	C25-C26-C27-C28
14	B	837	DGD	C4B-C5B-C6B-C7B
14	B	837	DGD	C8B-C9B-CAB-CBB
9	b	810	CLA	C8-C10-C11-C12
9	b	810	CLA	C15-C16-C17-C18
9	b	815	CLA	C5-C6-C7-C8
9	b	821	CLA	C5-C6-C7-C8
9	B	828	CLA	CBA-CGA-O2A-C1
11	A	845	LHG	C33-C34-C35-C36
9	L	303	CLA	O1D-CGD-O2D-CED
9	A	811	CLA	C3A-C2A-CAA-CBA
9	A	815	CLA	C3A-C2A-CAA-CBA
9	A	826	CLA	C3A-C2A-CAA-CBA
9	A	828	CLA	C3A-C2A-CAA-CBA
9	A	831	CLA	C3A-C2A-CAA-CBA
9	B	813	CLA	C3A-C2A-CAA-CBA
9	B	814	CLA	C3A-C2A-CAA-CBA
9	B	822	CLA	C3A-C2A-CAA-CBA
9	B	824	CLA	C3A-C2A-CAA-CBA
9	B	828	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	B	839	CLA	C3A-C2A-CAA-CBA
9	L	307	CLA	C3A-C2A-CAA-CBA
9	a	811	CLA	C3A-C2A-CAA-CBA
9	a	822	CLA	C3A-C2A-CAA-CBA
9	a	827	CLA	C3A-C2A-CAA-CBA
9	a	829	CLA	C3A-C2A-CAA-CBA
9	a	832	CLA	C3A-C2A-CAA-CBA
9	b	813	CLA	C3A-C2A-CAA-CBA
9	b	824	CLA	C3A-C2A-CAA-CBA
9	b	828	CLA	C3A-C2A-CAA-CBA
9	b	839	CLA	C3A-C2A-CAA-CBA
9	h	202	CLA	C3A-C2A-CAA-CBA
9	A	829	CLA	C10-C11-C12-C13
9	B	807	CLA	C5-C6-C7-C8
9	B	815	CLA	C15-C16-C17-C18
11	A	839	LHG	C9-C10-C11-C12
9	B	819	CLA	O1D-CGD-O2D-CED
9	A	803	CLA	C6-C7-C8-C10
9	A	816	CLA	C16-C17-C18-C20
9	A	832	CLA	C16-C17-C18-C20
9	A	835	CLA	C16-C17-C18-C19
9	H	201	CLA	C16-C17-C18-C19
9	a	821	CLA	C6-C7-C8-C9
9	b	819	CLA	C11-C12-C13-C15
11	a	839	LHG	C10-C11-C12-C13
14	B	837	DGD	C5A-C6A-C7A-C8A
9	b	829	CLA	C10-C11-C12-C13
14	b	837	DGD	O1G-C1G-C2G-C3G
9	A	817	CLA	CBD-CGD-O2D-CED
11	A	838	LHG	C10-C11-C12-C13
9	B	821	CLA	O2A-C1-C2-C3
9	b	802	CLA	O2A-C1-C2-C3
12	B	834	BCR	C14-C15-C16-C17
9	B	812	CLA	C3-C5-C6-C7
11	A	838	LHG	C7-C8-C9-C10
11	a	839	LHG	C9-C10-C11-C12
9	a	801	CLA	C5-C6-C7-C8
9	A	808	CLA	C4-C3-C5-C6
9	A	823	CLA	C4-C3-C5-C6
9	A	825	CLA	C4-C3-C5-C6
9	B	822	CLA	CBA-CGA-O2A-C1
11	a	839	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
9	b	816	CLA	C2A-CAA-CBA-CGA
11	A	845	LHG	O1-C1-C2-O2
11	a	839	LHG	O1-C1-C2-O2
11	a	840	LHG	O1-C1-C2-O2
11	A	838	LHG	C26-C27-C28-C29
11	A	845	LHG	C24-C25-C26-C27
14	b	837	DGD	CAB-CBB-CCB-CDB
9	a	816	CLA	O1A-CGA-O2A-C1
9	A	815	CLA	C16-C17-C18-C20
9	A	825	CLA	C16-C17-C18-C19
9	B	802	CLA	C16-C17-C18-C20
9	a	803	CLA	C6-C7-C8-C10
9	a	825	CLA	C16-C17-C18-C20
9	A	806	CLA	C2B-C3B-CAB-CBB
9	A	811	CLA	C2B-C3B-CAB-CBB
9	A	816	CLA	C2B-C3B-CAB-CBB
9	A	818	CLA	C2B-C3B-CAB-CBB
9	A	822	CLA	C2B-C3B-CAB-CBB
9	A	823	CLA	C2B-C3B-CAB-CBB
9	A	847	CLA	C2B-C3B-CAB-CBB
9	B	804	CLA	C2B-C3B-CAB-CBB
9	B	822	CLA	C2B-C3B-CAB-CBB
9	B	840	CLA	C2B-C3B-CAB-CBB
9	a	806	CLA	C2B-C3B-CAB-CBB
9	a	808	CLA	C2B-C3B-CAB-CBB
9	a	816	CLA	C2B-C3B-CAB-CBB
9	a	818	CLA	C2B-C3B-CAB-CBB
9	a	821	CLA	C2B-C3B-CAB-CBB
9	a	823	CLA	C2B-C3B-CAB-CBB
9	a	824	CLA	C2B-C3B-CAB-CBB
9	b	804	CLA	C2B-C3B-CAB-CBB
9	b	816	CLA	C2B-C3B-CAB-CBB
9	b	822	CLA	C2B-C3B-CAB-CBB
9	b	840	CLA	C2B-C3B-CAB-CBB
9	h	202	CLA	C2B-C3B-CAB-CBB
9	l	305	CLA	C2B-C3B-CAB-CBB
9	A	802	CLA	C13-C15-C16-C17
9	A	811	CLA	C15-C16-C17-C18
9	A	815	CLA	C5-C6-C7-C8
9	a	802	CLA	C13-C15-C16-C17
9	b	809	CLA	C15-C16-C17-C18
9	A	803	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	b	830	CLA	O1A-CGA-O2A-C1
9	b	832	CLA	O1A-CGA-O2A-C1
9	B	819	CLA	C8-C10-C11-C12
9	b	818	CLA	C8-C10-C11-C12
9	b	839	CLA	CBD-CGD-O2D-CED
11	a	839	LHG	O9-C7-O7-C5
14	B	837	DGD	C9A-CAA-CBA-CCA
9	A	821	CLA	C5-C6-C7-C8
9	A	825	CLA	C10-C11-C12-C13
9	B	804	CLA	C5-C6-C7-C8
9	B	821	CLA	C5-C6-C7-C8
9	a	826	CLA	C10-C11-C12-C13
9	B	832	CLA	O1A-CGA-O2A-C1
9	a	803	CLA	O1A-CGA-O2A-C1
11	a	839	LHG	C30-C31-C32-C33
9	A	819	CLA	C16-C17-C18-C19
12	A	842	BCR	C1-C6-C7-C8
12	A	842	BCR	C5-C6-C7-C8
12	A	843	BCR	C23-C24-C25-C26
12	B	835	BCR	C23-C24-C25-C30
12	B	836	BCR	C23-C24-C25-C26
12	B	836	BCR	C23-C24-C25-C30
12	I	101	BCR	C1-C6-C7-C8
12	I	101	BCR	C5-C6-C7-C8
12	L	301	BCR	C1-C6-C7-C8
12	L	301	BCR	C5-C6-C7-C8
12	L	306	BCR	C5-C6-C7-C8
12	L	306	BCR	C23-C24-C25-C26
12	L	306	BCR	C23-C24-C25-C30
12	a	841	BCR	C5-C6-C7-C8
12	a	843	BCR	C1-C6-C7-C8
12	a	843	BCR	C5-C6-C7-C8
12	a	844	BCR	C23-C24-C25-C26
12	a	844	BCR	C23-C24-C25-C30
12	b	835	BCR	C23-C24-C25-C26
12	b	835	BCR	C23-C24-C25-C30
12	b	836	BCR	C23-C24-C25-C26
12	b	836	BCR	C23-C24-C25-C30
12	i	101	BCR	C1-C6-C7-C8
12	i	101	BCR	C5-C6-C7-C8
12	l	304	BCR	C1-C6-C7-C8
12	l	304	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	l	309	BCR	C5-C6-C7-C8
12	l	309	BCR	C23-C24-C25-C26
12	l	309	BCR	C23-C24-C25-C30
15	b	838	LMT	C3'-C4'-O1B-C1B
15	b	838	LMT	C9-C10-C11-C12
11	A	838	LHG	C24-C23-O8-C6
11	A	839	LHG	C24-C23-O8-C6
9	B	815	CLA	C5-C6-C7-C8
9	B	818	CLA	C5-C6-C7-C8
9	a	806	CLA	C15-C16-C17-C18
9	a	808	CLA	C5-C6-C7-C8
9	h	202	CLA	C10-C11-C12-C13
15	B	838	LMT	C1-C2-C3-C4
15	b	838	LMT	C1-C2-C3-C4
11	A	845	LHG	C16-C17-C18-C19
11	l	303	LHG	C16-C17-C18-C19
14	B	837	DGD	CDB-CEB-CFB-CGB
14	b	837	DGD	CFA-CGA-CHA-CIA
15	B	838	LMT	C9-C10-C11-C12
9	l	302	CLA	C3-C5-C6-C7
9	B	826	CLA	O2A-C1-C2-C3
9	L	303	CLA	O1A-CGA-O2A-C1
11	A	845	LHG	C28-C29-C30-C31
14	b	837	DGD	C3B-C4B-C5B-C6B
9	b	804	CLA	C15-C16-C17-C18
15	B	838	LMT	C3'-C4'-O1B-C1B
9	a	826	CLA	C4-C3-C5-C6
9	A	806	CLA	C12-C13-C15-C16
9	A	807	CLA	C11-C12-C13-C15
9	A	808	CLA	C2-C3-C5-C6
9	A	808	CLA	C11-C12-C13-C15
9	A	816	CLA	C12-C13-C15-C16
9	A	822	CLA	C12-C13-C15-C16
9	A	823	CLA	C2-C3-C5-C6
9	A	825	CLA	C2-C3-C5-C6
9	A	828	CLA	C11-C10-C8-C7
9	A	846	CLA	C11-C12-C13-C15
9	B	802	CLA	C6-C7-C8-C10
9	B	807	CLA	C11-C12-C13-C15
9	B	810	CLA	C12-C13-C15-C16
9	B	821	CLA	C11-C10-C8-C7
9	B	821	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	B	823	CLA	C6-C7-C8-C10
9	a	808	CLA	C6-C7-C8-C10
9	a	811	CLA	C11-C12-C13-C15
9	a	823	CLA	C6-C7-C8-C10
9	a	823	CLA	C12-C13-C15-C16
9	a	824	CLA	C11-C12-C13-C15
9	a	829	CLA	C11-C10-C8-C7
9	a	846	CLA	C6-C7-C8-C10
9	a	847	CLA	C11-C10-C8-C7
9	b	807	CLA	C11-C12-C13-C15
9	b	810	CLA	C11-C10-C8-C7
9	b	814	CLA	C6-C7-C8-C10
9	b	815	CLA	C2-C3-C5-C6
9	b	821	CLA	C11-C10-C8-C7
9	b	821	CLA	C11-C12-C13-C15
9	b	832	CLA	C12-C13-C15-C16
9	B	822	CLA	O1A-CGA-O2A-C1
9	B	828	CLA	O1A-CGA-O2A-C1
14	B	837	DGD	CFA-CGA-CHA-CIA
9	a	834	CLA	C13-C15-C16-C17
9	a	846	CLA	C5-C6-C7-C8
9	A	816	CLA	CBD-CGD-O2D-CED
9	B	815	CLA	C16-C17-C18-C19
9	a	846	CLA	C16-C17-C18-C20
9	a	808	CLA	CBA-CGA-O2A-C1
9	b	803	CLA	CBA-CGA-O2A-C1
11	a	840	LHG	C24-C23-O8-C6
14	b	837	DGD	C8B-C9B-CAB-CBB
9	A	802	CLA	C2A-CAA-CBA-CGA
9	A	811	CLA	C2A-CAA-CBA-CGA
9	B	827	CLA	C2A-CAA-CBA-CGA
9	a	802	CLA	C2A-CAA-CBA-CGA
9	a	811	CLA	C2A-CAA-CBA-CGA
9	b	827	CLA	C2A-CAA-CBA-CGA
9	a	802	CLA	O1D-CGD-O2D-CED
9	a	824	CLA	C13-C15-C16-C17
9	b	802	CLA	C8-C10-C11-C12
11	a	839	LHG	C12-C13-C14-C15
9	B	814	CLA	O1D-CGD-O2D-CED
11	l	303	LHG	C33-C34-C35-C36
9	a	807	CLA	C15-C16-C17-C18
14	B	837	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
14	b	837	DGD	C7A-C8A-C9A-CAA
14	b	837	DGD	CDB-CEB-CFB-CGB
12	A	842	BCR	C22-C23-C24-C25
9	a	826	CLA	C8-C10-C11-C12
9	b	802	CLA	C13-C15-C16-C17
11	A	845	LHG	C12-C13-C14-C15
12	B	834	BCR	C10-C11-C12-C13
9	A	815	CLA	C10-C11-C12-C13
9	B	814	CLA	C10-C11-C12-C13
9	B	815	CLA	C13-C15-C16-C17
9	a	847	CLA	C10-C11-C12-C13
9	b	818	CLA	C5-C6-C7-C8
9	b	819	CLA	C8-C10-C11-C12
9	a	827	CLA	CBD-CGD-O2D-CED
14	b	837	DGD	C6B-C7B-C8B-C9B
9	B	802	CLA	C3-C5-C6-C7
11	l	303	LHG	C12-C13-C14-C15
11	a	839	LHG	C28-C29-C30-C31
9	a	803	CLA	CBD-CGD-O2D-CED
9	b	815	CLA	C16-C17-C18-C19
11	a	839	LHG	C26-C27-C28-C29
9	b	808	CLA	C5-C6-C7-C8
9	b	821	CLA	C15-C16-C17-C18
10	A	837	PQN	C14-C13-C15-C16
10	a	838	PQN	C14-C13-C15-C16
11	A	845	LHG	C23-C24-C25-C26
9	a	824	CLA	C2-C3-C5-C6
9	a	826	CLA	C2-C3-C5-C6
9	b	819	CLA	C2-C3-C5-C6
9	A	805	CLA	C11-C10-C8-C9
9	A	826	CLA	C14-C13-C15-C16
9	A	846	CLA	C11-C12-C13-C14
9	B	801	CLA	C11-C12-C13-C14
9	B	802	CLA	C6-C7-C8-C9
9	B	810	CLA	C11-C10-C8-C9
9	B	821	CLA	C11-C10-C8-C9
9	a	805	CLA	C11-C10-C8-C9
9	a	816	CLA	C11-C10-C8-C9
9	a	824	CLA	C14-C13-C15-C16
9	a	825	CLA	C11-C10-C8-C9
9	a	847	CLA	C11-C10-C8-C9
9	b	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	b	810	CLA	C11-C10-C8-C9
9	b	821	CLA	C11-C10-C8-C9
9	b	821	CLA	C11-C12-C13-C14
10	B	833	PQN	C16-C17-C18-C19
10	b	833	PQN	C16-C17-C18-C19
9	a	821	CLA	O1D-CGD-O2D-CED
9	A	816	CLA	C2A-CAA-CBA-CGA
9	B	824	CLA	C2A-CAA-CBA-CGA
9	L	302	CLA	C2A-CAA-CBA-CGA
9	b	824	CLA	C2A-CAA-CBA-CGA
12	b	834	BCR	C11-C12-C13-C35
9	b	805	CLA	O1D-CGD-O2D-CED
11	l	303	LHG	C34-C35-C36-C37
14	b	837	DGD	C2A-C3A-C4A-C5A
9	a	808	CLA	O1A-CGA-O2A-C1
11	A	838	LHG	O10-C23-O8-C6
11	A	839	LHG	O10-C23-O8-C6
9	A	818	CLA	C1A-C2A-CAA-CBA
9	A	828	CLA	C1A-C2A-CAA-CBA
9	A	831	CLA	C1A-C2A-CAA-CBA
9	B	805	CLA	C1A-C2A-CAA-CBA
9	B	812	CLA	C1A-C2A-CAA-CBA
9	B	813	CLA	C1A-C2A-CAA-CBA
9	B	817	CLA	C1A-C2A-CAA-CBA
9	B	823	CLA	C1A-C2A-CAA-CBA
9	B	828	CLA	C1A-C2A-CAA-CBA
9	B	839	CLA	C1A-C2A-CAA-CBA
9	a	805	CLA	C1A-C2A-CAA-CBA
9	a	818	CLA	C1A-C2A-CAA-CBA
9	a	819	CLA	C1A-C2A-CAA-CBA
9	a	829	CLA	C1A-C2A-CAA-CBA
9	a	832	CLA	C1A-C2A-CAA-CBA
9	b	805	CLA	C1A-C2A-CAA-CBA
9	b	812	CLA	C1A-C2A-CAA-CBA
9	b	813	CLA	C1A-C2A-CAA-CBA
9	b	817	CLA	C1A-C2A-CAA-CBA
9	b	823	CLA	C1A-C2A-CAA-CBA
9	b	839	CLA	C1A-C2A-CAA-CBA
9	h	202	CLA	C1A-C2A-CAA-CBA
9	A	819	CLA	C16-C17-C18-C20
9	H	201	CLA	C16-C17-C18-C20
9	a	826	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	b	802	CLA	C16-C17-C18-C19
9	h	202	CLA	C16-C17-C18-C19
12	A	842	BCR	C13-C14-C15-C16
11	A	838	LHG	C3-O3-P-O6
9	b	817	CLA	CBD-CGD-O2D-CED
9	B	831	CLA	C13-C15-C16-C17
10	A	837	PQN	C18-C20-C21-C22
11	A	838	LHG	O6-C4-C5-C6
9	a	824	CLA	C16-C17-C18-C20
9	l	306	CLA	C16-C17-C18-C19
9	l	306	CLA	C3-C5-C6-C7
9	A	825	CLA	C8-C10-C11-C12
9	B	821	CLA	C15-C16-C17-C18
9	B	803	CLA	CBA-CGA-O2A-C1
9	a	834	CLA	C15-C16-C17-C18
9	b	831	CLA	C13-C15-C16-C17
9	B	810	CLA	C8-C10-C11-C12
9	B	811	CLA	C13-C15-C16-C17
9	B	805	CLA	O1D-CGD-O2D-CED
9	a	806	CLA	C3-C5-C6-C7
11	A	845	LHG	C4-C5-C6-O8
9	a	816	CLA	C5-C6-C7-C8
9	b	815	CLA	C13-C15-C16-C17
11	A	838	LHG	C34-C35-C36-C37
9	b	818	CLA	O1D-CGD-O2D-CED
9	a	823	CLA	C15-C16-C17-C18
11	A	845	LHG	C19-C20-C21-C22
9	b	803	CLA	O1A-CGA-O2A-C1
11	a	840	LHG	O10-C23-O8-C6
9	A	846	CLA	C16-C17-C18-C20
9	B	818	CLA	C1-C2-C3-C5
9	A	826	CLA	C8-C10-C11-C12
9	A	802	CLA	O1D-CGD-O2D-CED
9	b	812	CLA	CBA-CGA-O2A-C1
11	l	303	LHG	C19-C20-C21-C22
10	a	838	PQN	C18-C20-C21-C22
9	B	806	CLA	C13-C15-C16-C17
9	A	821	CLA	C4-C3-C5-C6
9	A	811	CLA	O1D-CGD-O2D-CED
9	B	815	CLA	CBA-CGA-O2A-C1
9	a	804	CLA	CBA-CGA-O2A-C1
9	b	815	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	h	202	CLA	CBA-CGA-O2A-C1
9	A	803	CLA	C5-C6-C7-C8
9	A	811	CLA	C13-C15-C16-C17
9	b	806	CLA	C13-C15-C16-C17
9	b	811	CLA	C13-C15-C16-C17
11	l	303	LHG	C35-C36-C37-C38
9	l	305	CLA	C2A-CAA-CBA-CGA
9	B	811	CLA	C8-C10-C11-C12
9	a	819	CLA	C8-C10-C11-C12
9	a	811	CLA	O1D-CGD-O2D-CED
9	A	829	CLA	C8-C10-C11-C12
9	B	829	CLA	C15-C16-C17-C18
9	b	811	CLA	C8-C10-C11-C12
9	A	804	CLA	CBA-CGA-O2A-C1
9	A	811	CLA	CBA-CGA-O2A-C1
11	a	839	LHG	C24-C23-O8-C6
9	A	820	CLA	C6-C7-C8-C10
9	a	815	CLA	CAA-CBA-CGA-O2A
9	A	808	CLA	C6-C7-C8-C10
9	A	817	CLA	C11-C12-C13-C15
9	A	822	CLA	C6-C7-C8-C10
9	A	825	CLA	C11-C12-C13-C15
9	A	828	CLA	C6-C7-C8-C10
9	A	829	CLA	C6-C7-C8-C10
9	A	835	CLA	C6-C7-C8-C10
9	B	801	CLA	C11-C12-C13-C15
9	B	803	CLA	C12-C13-C15-C16
9	B	804	CLA	C11-C12-C13-C15
9	B	806	CLA	C12-C13-C15-C16
9	B	811	CLA	C11-C12-C13-C15
9	B	814	CLA	C6-C7-C8-C10
9	B	819	CLA	C6-C7-C8-C10
9	B	821	CLA	C6-C7-C8-C10
9	B	823	CLA	C11-C10-C8-C7
9	B	823	CLA	C12-C13-C15-C16
9	B	824	CLA	C11-C10-C8-C7
9	B	832	CLA	C12-C13-C15-C16
9	a	807	CLA	C11-C12-C13-C15
9	a	807	CLA	C12-C13-C15-C16
9	a	808	CLA	C11-C12-C13-C15
9	a	815	CLA	C6-C7-C8-C10
9	a	817	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	a	819	CLA	C12-C13-C15-C16
9	a	824	CLA	C6-C7-C8-C10
9	a	826	CLA	C11-C12-C13-C15
9	a	830	CLA	C6-C7-C8-C10
9	a	836	CLA	C6-C7-C8-C10
9	a	846	CLA	C12-C13-C15-C16
9	a	847	CLA	C6-C7-C8-C10
9	b	803	CLA	C12-C13-C15-C16
9	b	806	CLA	C12-C13-C15-C16
9	b	810	CLA	C6-C7-C8-C10
9	b	810	CLA	C12-C13-C15-C16
9	b	811	CLA	C11-C12-C13-C15
9	b	819	CLA	C6-C7-C8-C10
9	b	819	CLA	C11-C10-C8-C7
9	b	824	CLA	C11-C10-C8-C7
9	h	202	CLA	C11-C10-C8-C7
10	A	837	PQN	C16-C17-C18-C20
10	B	833	PQN	C16-C17-C18-C20
10	a	838	PQN	C16-C17-C18-C20
10	b	833	PQN	C16-C17-C18-C20
9	a	822	CLA	C3-C5-C6-C7
14	B	837	DGD	C3A-C4A-C5A-C6A
9	A	802	CLA	C11-C10-C8-C9
9	A	804	CLA	C14-C13-C15-C16
9	A	806	CLA	C11-C10-C8-C9
9	A	806	CLA	C14-C13-C15-C16
9	A	807	CLA	C11-C12-C13-C14
9	A	809	CLA	C14-C13-C15-C16
9	A	817	CLA	C11-C12-C13-C14
9	A	819	CLA	C14-C13-C15-C16
9	A	824	CLA	C6-C7-C8-C9
9	A	824	CLA	C11-C10-C8-C9
9	A	833	CLA	C11-C12-C13-C14
9	A	835	CLA	C6-C7-C8-C9
9	A	847	CLA	C11-C12-C13-C14
9	B	811	CLA	C11-C10-C8-C9
9	B	819	CLA	C6-C7-C8-C9
9	B	821	CLA	C11-C12-C13-C14
9	B	832	CLA	C14-C13-C15-C16
9	a	802	CLA	C11-C10-C8-C9
9	a	807	CLA	C6-C7-C8-C9
9	a	807	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	a	808	CLA	C6-C7-C8-C9
9	a	809	CLA	C14-C13-C15-C16
9	a	815	CLA	C6-C7-C8-C9
9	a	817	CLA	C11-C12-C13-C14
9	a	825	CLA	C6-C7-C8-C9
9	a	836	CLA	C6-C7-C8-C9
9	a	846	CLA	C6-C7-C8-C9
9	a	846	CLA	C11-C12-C13-C14
9	b	801	CLA	C11-C12-C13-C14
9	b	811	CLA	C11-C10-C8-C9
9	b	832	CLA	C14-C13-C15-C16
12	B	835	BCR	C15-C16-C17-C18
9	A	826	CLA	CBA-CGA-O2A-C1
9	a	827	CLA	CBA-CGA-O2A-C1
9	A	803	CLA	O1D-CGD-O2D-CED
9	b	812	CLA	O1A-CGA-O2A-C1
9	b	815	CLA	O1A-CGA-O2A-C1
9	A	822	CLA	C8-C10-C11-C12
9	A	847	CLA	C3-C5-C6-C7
9	B	804	CLA	C3-C5-C6-C7
9	b	802	CLA	C10-C11-C12-C13
9	b	829	CLA	C15-C16-C17-C18
9	A	801	CLA	C5-C6-C7-C8
9	A	825	CLA	C15-C16-C17-C18
9	B	804	CLA	C15-C16-C17-C18
9	H	201	CLA	C10-C11-C12-C13
9	a	803	CLA	C5-C6-C7-C8
9	B	817	CLA	CBD-CGD-O2D-CED
9	A	805	CLA	C4B-C3B-CAB-CBB
9	A	825	CLA	C4B-C3B-CAB-CBB
9	A	826	CLA	C4B-C3B-CAB-CBB
9	B	823	CLA	C4B-C3B-CAB-CBB
9	L	302	CLA	C4B-C3B-CAB-CBB
9	a	805	CLA	C4B-C3B-CAB-CBB
9	a	826	CLA	C4B-C3B-CAB-CBB
9	a	827	CLA	C4B-C3B-CAB-CBB
9	a	833	CLA	C4B-C3B-CAB-CBB
9	a	846	CLA	C4B-C3B-CAB-CBB
9	b	814	CLA	C4B-C3B-CAB-CBB
9	b	823	CLA	C4B-C3B-CAB-CBB
9	a	806	CLA	C5-C6-C7-C8
11	a	839	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
11	l	303	LHG	O6-C4-C5-C6
11	l	303	LHG	C7-C8-C9-C10
9	a	804	CLA	O1A-CGA-O2A-C1
9	a	815	CLA	C5-C6-C7-C8
9	A	817	CLA	O1D-CGD-O2D-CED
9	B	803	CLA	O1A-CGA-O2A-C1
9	B	815	CLA	O1A-CGA-O2A-C1
14	B	837	DGD	CEB-CFB-CGB-CHB
9	L	303	CLA	C16-C17-C18-C19
9	a	815	CLA	C16-C17-C18-C20
9	a	815	CLA	C13-C15-C16-C17
11	a	839	LHG	C2-C3-O3-P
11	l	303	LHG	C2-C3-O3-P
9	A	834	CLA	C3A-C2A-CAA-CBA
9	L	302	CLA	C3A-C2A-CAA-CBA
9	L	303	CLA	C3A-C2A-CAA-CBA
9	a	835	CLA	C3A-C2A-CAA-CBA
9	l	305	CLA	C3A-C2A-CAA-CBA
11	A	838	LHG	C35-C36-C37-C38
14	B	837	DGD	CAA-CBA-CCA-CDA
11	a	839	LHG	C23-C24-C25-C26
9	h	202	CLA	C16-C17-C18-C20
9	a	811	CLA	CBA-CGA-O2A-C1
14	b	837	DGD	CEB-CFB-CGB-CHB
11	A	839	LHG	C4-C5-C6-O8
11	a	840	LHG	C4-C5-C6-O8
14	B	837	DGD	O1G-C1G-C2G-C3G
9	A	826	CLA	CBD-CGD-O2D-CED
9	A	816	CLA	O1D-CGD-O2D-CED
9	B	827	CLA	O1D-CGD-O2D-CED
11	A	845	LHG	C15-C16-C17-C18
9	a	823	CLA	C3-C5-C6-C7
9	A	804	CLA	O1A-CGA-O2A-C1
9	a	846	CLA	C4-C3-C5-C6
11	a	839	LHG	C3-O3-P-O6
9	h	202	CLA	O1A-CGA-O2A-C1
11	a	839	LHG	O10-C23-O8-C6
11	A	838	LHG	C29-C30-C31-C32
9	a	827	CLA	O1D-CGD-O2D-CED
9	b	827	CLA	O1D-CGD-O2D-CED
9	H	201	CLA	C2A-CAA-CBA-CGA
9	a	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	a	839	LHG	O6-C4-C5-O7
9	b	824	CLA	CBA-CGA-O2A-C1
9	A	808	CLA	C16-C17-C18-C19
9	A	815	CLA	C16-C17-C18-C19
9	a	815	CLA	C16-C17-C18-C19
9	a	824	CLA	C16-C17-C18-C19
9	A	818	CLA	O1D-CGD-O2D-CED
9	b	839	CLA	O1D-CGD-O2D-CED
9	A	826	CLA	C2B-C3B-CAB-CBB
9	B	823	CLA	C2B-C3B-CAB-CBB
9	L	302	CLA	C2B-C3B-CAB-CBB
9	a	805	CLA	C2B-C3B-CAB-CBB
9	a	826	CLA	C2B-C3B-CAB-CBB
9	a	827	CLA	C2B-C3B-CAB-CBB
9	a	833	CLA	C2B-C3B-CAB-CBB
9	a	846	CLA	C2B-C3B-CAB-CBB
9	b	823	CLA	C2B-C3B-CAB-CBB
9	A	811	CLA	O1A-CGA-O2A-C1
9	a	827	CLA	O1A-CGA-O2A-C1
9	A	816	CLA	C3-C5-C6-C7
11	l	303	LHG	C15-C16-C17-C18
11	A	838	LHG	O7-C5-C6-O8
11	A	839	LHG	O7-C5-C6-O8
11	a	839	LHG	O7-C5-C6-O8
11	a	840	LHG	O7-C5-C6-O8
9	a	816	CLA	C8-C10-C11-C12
11	a	839	LHG	C35-C36-C37-C38
9	A	846	CLA	C16-C17-C18-C19
9	B	831	CLA	C16-C17-C18-C19
9	a	830	CLA	C16-C17-C18-C20
9	a	846	CLA	C16-C17-C18-C19
9	b	831	CLA	C16-C17-C18-C19
9	B	808	CLA	C5-C6-C7-C8
15	b	838	LMT	O5B-C5B-C6B-O6B
14	b	837	DGD	C7B-C8B-C9B-CAB
9	a	815	CLA	C4-C3-C5-C6
9	B	802	CLA	C2-C1-O2A-CGA
9	B	821	CLA	C2-C1-O2A-CGA
9	H	201	CLA	C2-C1-O2A-CGA
9	a	803	CLA	C2-C1-O2A-CGA
9	b	823	CLA	C2-C1-O2A-CGA
9	h	201	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
9	A	807	CLA	C6-C7-C8-C9
9	A	815	CLA	C11-C10-C8-C9
9	A	819	CLA	C6-C7-C8-C9
9	A	847	CLA	C14-C13-C15-C16
9	B	804	CLA	C11-C10-C8-C9
9	B	823	CLA	C11-C10-C8-C9
9	a	804	CLA	C14-C13-C15-C16
9	a	817	CLA	C11-C10-C8-C9
9	a	830	CLA	C11-C10-C8-C9
9	a	834	CLA	C11-C12-C13-C14
9	a	846	CLA	C14-C13-C15-C16
9	a	847	CLA	C11-C12-C13-C14
9	b	809	CLA	C14-C13-C15-C16
9	b	819	CLA	C6-C7-C8-C9
9	b	823	CLA	C11-C10-C8-C9
10	A	837	PQN	C24-C23-C25-C26
11	a	839	LHG	C25-C26-C27-C28
9	b	825	CLA	C13-C15-C16-C17
11	A	838	LHG	C2-C3-O3-P
11	A	838	LHG	C5-C4-O6-P
9	A	826	CLA	O1A-CGA-O2A-C1
9	A	802	CLA	C16-C17-C18-C19
9	A	835	CLA	C16-C17-C18-C20
9	a	836	CLA	C16-C17-C18-C20
9	l	306	CLA	C16-C17-C18-C20
12	A	840	BCR	C23-C24-C25-C26
12	A	841	BCR	C23-C24-C25-C26
12	A	841	BCR	C23-C24-C25-C30
12	B	836	BCR	C1-C6-C7-C8
12	B	836	BCR	C5-C6-C7-C8
12	a	841	BCR	C23-C24-C25-C30
12	a	842	BCR	C23-C24-C25-C26
12	a	842	BCR	C23-C24-C25-C30
12	b	836	BCR	C1-C6-C7-C8
12	b	836	BCR	C5-C6-C7-C8
9	h	202	CLA	C5-C6-C7-C8
12	B	836	BCR	C11-C12-C13-C14
12	b	836	BCR	C11-C12-C13-C14
12	l	309	BCR	C11-C12-C13-C14
9	A	822	CLA	C15-C16-C17-C18
9	A	847	CLA	C13-C15-C16-C17
9	a	825	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	b	818	CLA	C11-C12-C13-C14
9	A	846	CLA	C13-C15-C16-C17
9	A	829	CLA	C16-C17-C18-C20
9	A	847	CLA	C16-C17-C18-C20
9	L	303	CLA	C16-C17-C18-C20
9	a	817	CLA	C16-C17-C18-C19
9	a	819	CLA	C16-C17-C18-C19
9	a	803	CLA	O1D-CGD-O2D-CED
14	B	837	DGD	C7A-C8A-C9A-CAA
9	B	825	CLA	C13-C15-C16-C17
9	a	824	CLA	C10-C11-C12-C13
11	A	845	LHG	O8-C23-C24-C25
11	l	303	LHG	O2-C2-C3-O3
9	A	802	CLA	C11-C10-C8-C7
9	A	806	CLA	C11-C10-C8-C7
9	A	807	CLA	C11-C10-C8-C7
9	A	808	CLA	C12-C13-C15-C16
9	A	811	CLA	C6-C7-C8-C10
9	A	816	CLA	C11-C12-C13-C15
9	A	817	CLA	C6-C7-C8-C10
9	A	817	CLA	C11-C10-C8-C7
9	A	819	CLA	C12-C13-C15-C16
9	A	821	CLA	C2-C3-C5-C6
9	A	824	CLA	C6-C7-C8-C10
9	A	832	CLA	C12-C13-C15-C16
9	A	833	CLA	C11-C12-C13-C15
9	A	847	CLA	C6-C7-C8-C10
9	B	807	CLA	C6-C7-C8-C10
9	B	810	CLA	C6-C7-C8-C10
9	B	814	CLA	C11-C12-C13-C15
9	B	818	CLA	C6-C7-C8-C10
9	B	819	CLA	C11-C10-C8-C7
9	B	825	CLA	C6-C7-C8-C10
9	B	829	CLA	C11-C10-C8-C7
9	B	831	CLA	C12-C13-C15-C16
9	L	303	CLA	C6-C7-C8-C10
9	a	801	CLA	C6-C7-C8-C10
9	a	802	CLA	C11-C10-C8-C7
9	a	807	CLA	C11-C10-C8-C7
9	a	809	CLA	C11-C12-C13-C15
9	a	815	CLA	C2-C3-C5-C6
9	a	815	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	a	816	CLA	C6-C7-C8-C10
9	a	817	CLA	C6-C7-C8-C10
9	a	817	CLA	C11-C10-C8-C7
9	a	825	CLA	C6-C7-C8-C10
9	a	829	CLA	C6-C7-C8-C10
9	a	833	CLA	C11-C12-C13-C15
9	a	834	CLA	C11-C12-C13-C15
9	b	801	CLA	C11-C12-C13-C15
9	b	806	CLA	C11-C12-C13-C15
9	b	807	CLA	C6-C7-C8-C10
9	b	814	CLA	C11-C12-C13-C15
9	b	818	CLA	C6-C7-C8-C10
9	b	823	CLA	C11-C10-C8-C7
9	b	823	CLA	C12-C13-C15-C16
9	b	825	CLA	C6-C7-C8-C10
9	b	829	CLA	C11-C10-C8-C7
9	b	831	CLA	C12-C13-C15-C16
9	L	303	CLA	C3-C5-C6-C7
9	a	803	CLA	C3-C5-C6-C7
9	B	801	CLA	C4C-C3C-CAC-CBC
9	A	829	CLA	C1-C2-C3-C4
12	L	306	BCR	C9-C10-C11-C12
9	A	801	CLA	C16-C17-C18-C20
9	B	812	CLA	CBA-CGA-O2A-C1
9	B	824	CLA	CBA-CGA-O2A-C1
9	a	801	CLA	CBA-CGA-O2A-C1
9	h	201	CLA	CBA-CGA-O2A-C1
9	a	822	CLA	C5-C6-C7-C8
9	L	307	CLA	C2A-CAA-CBA-CGA
9	a	822	CLA	C2A-CAA-CBA-CGA
9	l	306	CLA	C2A-CAA-CBA-CGA
12	L	305	BCR	C35-C13-C14-C15
12	b	834	BCR	C16-C17-C18-C36
9	A	847	CLA	CBD-CGD-O2D-CED
9	A	827	CLA	CBA-CGA-O2A-C1
9	B	829	CLA	CBA-CGA-O2A-C1
11	a	839	LHG	C18-C19-C20-C21
9	A	802	CLA	CAD-CBD-CGD-O2D
9	A	807	CLA	CAD-CBD-CGD-O2D
9	A	822	CLA	CAD-CBD-CGD-O2D
9	B	813	CLA	CAD-CBD-CGD-O2D
9	B	815	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	B	817	CLA	CAD-CBD-CGD-O2D
9	B	821	CLA	CAD-CBD-CGD-O2D
9	B	822	CLA	CAD-CBD-CGD-O2D
9	B	826	CLA	CAD-CBD-CGD-O2D
9	B	827	CLA	CAD-CBD-CGD-O2D
9	B	831	CLA	CAD-CBD-CGD-O2D
9	L	302	CLA	CAD-CBD-CGD-O2D
9	a	802	CLA	CAD-CBD-CGD-O2D
9	a	807	CLA	CAD-CBD-CGD-O2D
9	a	815	CLA	CAD-CBD-CGD-O2D
9	a	823	CLA	CAD-CBD-CGD-O2D
9	a	832	CLA	CAD-CBD-CGD-O2D
9	b	815	CLA	CAD-CBD-CGD-O2D
9	b	817	CLA	CAD-CBD-CGD-O2D
9	b	831	CLA	CAD-CBD-CGD-O2D
9	l	302	CLA	CAD-CBD-CGD-O2D
9	l	305	CLA	CAD-CBD-CGD-O2D
9	B	825	CLA	C5-C6-C7-C8
9	A	801	CLA	CBA-CGA-O2A-C1
9	A	810	CLA	CBA-CGA-O2A-C1
9	a	801	CLA	C16-C17-C18-C20
9	B	812	CLA	O1A-CGA-O2A-C1
9	b	824	CLA	O1A-CGA-O2A-C1
11	l	303	LHG	O6-C4-C5-O7
9	L	302	CLA	O2A-C1-C2-C3
9	a	809	CLA	C16-C17-C18-C19
9	a	847	CLA	C16-C17-C18-C20
9	A	819	CLA	CHA-CBD-CGD-O1D
9	A	820	CLA	CHA-CBD-CGD-O1D
9	A	820	CLA	CHA-CBD-CGD-O2D
9	A	830	CLA	CHA-CBD-CGD-O1D
9	A	832	CLA	CHA-CBD-CGD-O1D
9	B	802	CLA	CHA-CBD-CGD-O1D
9	B	802	CLA	CHA-CBD-CGD-O2D
9	B	805	CLA	CHA-CBD-CGD-O1D
9	a	820	CLA	CHA-CBD-CGD-O1D
9	a	820	CLA	CHA-CBD-CGD-O2D
9	a	821	CLA	CHA-CBD-CGD-O1D
9	a	821	CLA	CHA-CBD-CGD-O2D
9	a	831	CLA	CHA-CBD-CGD-O1D
9	a	833	CLA	CHA-CBD-CGD-O1D
9	b	802	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	b	802	CLA	CHA-CBD-CGD-O2D
9	b	805	CLA	CHA-CBD-CGD-O1D
9	b	812	CLA	CHA-CBD-CGD-O1D
9	b	812	CLA	CHA-CBD-CGD-O2D
9	b	825	CLA	CHA-CBD-CGD-O2D
9	a	811	CLA	O1A-CGA-O2A-C1
12	b	834	BCR	C16-C17-C18-C19
15	b	838	LMT	C3-C4-C5-C6
9	B	824	CLA	O1A-CGA-O2A-C1
9	A	826	CLA	O1D-CGD-O2D-CED
9	b	817	CLA	O1D-CGD-O2D-CED
9	A	811	CLA	C6-C7-C8-C9
9	A	817	CLA	C6-C7-C8-C9
9	A	817	CLA	C11-C10-C8-C9
9	A	817	CLA	C14-C13-C15-C16
9	A	819	CLA	C11-C12-C13-C14
9	A	832	CLA	C14-C13-C15-C16
9	A	847	CLA	C11-C10-C8-C9
9	B	802	CLA	C11-C10-C8-C9
9	B	824	CLA	C6-C7-C8-C9
9	B	825	CLA	C6-C7-C8-C9
9	a	801	CLA	C6-C7-C8-C9
9	a	805	CLA	C6-C7-C8-C9
9	a	817	CLA	C6-C7-C8-C9
9	a	817	CLA	C14-C13-C15-C16
9	b	807	CLA	C11-C10-C8-C9
9	b	825	CLA	C6-C7-C8-C9
9	b	802	CLA	O1D-CGD-O2D-CED
9	a	801	CLA	O1A-CGA-O2A-C1
9	a	825	CLA	C15-C16-C17-C18
9	B	816	CLA	C2A-CAA-CBA-CGA
9	h	201	CLA	CBD-CGD-O2D-CED
12	B	836	BCR	C7-C8-C9-C34
9	b	825	CLA	C5-C6-C7-C8
9	A	811	CLA	C1A-C2A-CAA-CBA
9	A	827	CLA	C1A-C2A-CAA-CBA
9	B	810	CLA	C1A-C2A-CAA-CBA
9	a	811	CLA	C1A-C2A-CAA-CBA
9	b	810	CLA	C1A-C2A-CAA-CBA
9	A	809	CLA	C16-C17-C18-C19
9	A	817	CLA	C16-C17-C18-C19
9	B	832	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	b	832	CLA	C16-C17-C18-C20
9	B	802	CLA	O1D-CGD-O2D-CED
9	a	824	CLA	CBA-CGA-O2A-C1
9	a	837	CLA	CBA-CGA-O2A-C1
12	h	203	BCR	C9-C10-C11-C12
11	A	838	LHG	C15-C16-C17-C18
9	A	819	CLA	C4-C3-C5-C6
11	A	839	LHG	C2-C3-O3-P
11	A	845	LHG	C2-C3-O3-P
11	a	839	LHG	C5-C4-O6-P
10	A	837	PQN	C12-C13-C15-C16
10	a	838	PQN	C12-C13-C15-C16
9	A	827	CLA	O1A-CGA-O2A-C1
9	A	828	CLA	C4B-C3B-CAB-CBB
9	A	832	CLA	C4B-C3B-CAB-CBB
9	A	834	CLA	C4B-C3B-CAB-CBB
9	B	801	CLA	C4B-C3B-CAB-CBB
9	B	809	CLA	C4B-C3B-CAB-CBB
9	B	811	CLA	C4B-C3B-CAB-CBB
9	B	839	CLA	C4B-C3B-CAB-CBB
9	a	810	CLA	C4B-C3B-CAB-CBB
9	a	829	CLA	C4B-C3B-CAB-CBB
9	a	832	CLA	C4B-C3B-CAB-CBB
9	a	835	CLA	C4B-C3B-CAB-CBB
9	b	801	CLA	C4B-C3B-CAB-CBB
9	b	809	CLA	C4B-C3B-CAB-CBB
9	b	811	CLA	C4B-C3B-CAB-CBB
9	b	820	CLA	C4B-C3B-CAB-CBB
9	b	839	CLA	C4B-C3B-CAB-CBB
11	A	839	LHG	C3-O3-P-O4
11	A	839	LHG	C4-O6-P-O5
11	a	840	LHG	C3-O3-P-O4
9	A	806	CLA	C16-C17-C18-C20
9	a	802	CLA	C16-C17-C18-C19
9	A	819	CLA	C13-C15-C16-C17
9	A	836	CLA	CBA-CGA-O2A-C1
9	a	806	CLA	C16-C17-C18-C20
9	A	804	CLA	CAD-CBD-CGD-O1D
9	A	819	CLA	CAD-CBD-CGD-O1D
9	A	832	CLA	CAD-CBD-CGD-O1D
9	B	802	CLA	CAD-CBD-CGD-O1D
9	B	811	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	a	811	CLA	CAD-CBD-CGD-O1D
9	a	824	CLA	CAD-CBD-CGD-O1D
9	a	833	CLA	CAD-CBD-CGD-O1D
9	b	802	CLA	CAD-CBD-CGD-O1D
9	b	811	CLA	CAD-CBD-CGD-O1D
9	b	812	CLA	CAD-CBD-CGD-O1D
9	b	814	CLA	CAD-CBD-CGD-O1D
9	b	828	CLA	C2-C3-C5-C6
11	A	838	LHG	C9-C10-C11-C12
9	B	808	CLA	CBA-CGA-O2A-C1
9	B	817	CLA	O1D-CGD-O2D-CED
9	A	801	CLA	C6-C7-C8-C10
9	A	804	CLA	C6-C7-C8-C10
9	A	809	CLA	C6-C7-C8-C10
9	A	809	CLA	C11-C12-C13-C15
9	A	816	CLA	C6-C7-C8-C10
9	A	846	CLA	C6-C7-C8-C10
9	B	806	CLA	C11-C12-C13-C15
9	a	804	CLA	C6-C7-C8-C10
9	a	809	CLA	C6-C7-C8-C10
9	a	833	CLA	C12-C13-C15-C16
9	a	834	CLA	C3A-C2A-CAA-CBA
9	b	804	CLA	C3A-C2A-CAA-CBA
9	b	804	CLA	C11-C12-C13-C15
9	l	306	CLA	C6-C7-C8-C10
11	A	838	LHG	O6-C4-C5-O7
11	A	845	LHG	O6-C4-C5-O7
9	A	803	CLA	C3-C5-C6-C7
9	A	801	CLA	O1A-CGA-O2A-C1
9	a	824	CLA	O1A-CGA-O2A-C1
9	h	201	CLA	O1A-CGA-O2A-C1
14	B	837	DGD	O6D-C5D-C6D-O5D
11	l	303	LHG	C8-C7-O7-C5
9	L	308	CLA	C4C-C3C-CAC-CBC
9	A	810	CLA	O1A-CGA-O2A-C1
9	A	847	CLA	C16-C17-C18-C19
9	a	808	CLA	C16-C17-C18-C19
9	a	823	CLA	C16-C17-C18-C19
9	b	823	CLA	C16-C17-C18-C19
15	b	838	LMT	C4B-C5B-C6B-O6B
9	a	830	CLA	C8-C10-C11-C12
11	l	303	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	B	837	DGD	O1G-C1G-C2G-O2G
14	b	837	DGD	O1G-C1G-C2G-O2G
9	A	802	CLA	C16-C17-C18-C20
9	A	820	CLA	C6-C7-C8-C9
9	b	801	CLA	C4C-C3C-CAC-CBC
9	a	837	CLA	O1A-CGA-O2A-C1
9	b	802	CLA	CBA-CGA-O2A-C1
9	A	801	CLA	C6-C7-C8-C9
9	A	805	CLA	C6-C7-C8-C9
9	A	806	CLA	C11-C12-C13-C14
9	A	816	CLA	C11-C12-C13-C14
9	A	846	CLA	C14-C13-C15-C16
9	B	807	CLA	C11-C10-C8-C9
9	B	825	CLA	C11-C12-C13-C14
9	B	829	CLA	C11-C10-C8-C9
9	B	831	CLA	C14-C13-C15-C16
9	a	806	CLA	C14-C13-C15-C16
9	a	819	CLA	C11-C12-C13-C14
9	a	833	CLA	C14-C13-C15-C16
9	b	810	CLA	C6-C7-C8-C9
9	b	829	CLA	C11-C10-C8-C9
9	b	831	CLA	C14-C13-C15-C16
9	A	836	CLA	O1A-CGA-O2A-C1
9	B	818	CLA	CBD-CGD-O2D-CED
9	b	802	CLA	C1-C2-C3-C5
11	a	839	LHG	C11-C12-C13-C14
11	A	838	LHG	O1-C1-C2-O2
12	A	840	BCR	C15-C16-C17-C18
12	b	836	BCR	C7-C8-C9-C34
9	a	829	CLA	C13-C15-C16-C17
9	B	829	CLA	O1A-CGA-O2A-C1
9	A	805	CLA	C2B-C3B-CAB-CBB
9	A	825	CLA	C2B-C3B-CAB-CBB
9	A	828	CLA	C2B-C3B-CAB-CBB
9	A	832	CLA	C2B-C3B-CAB-CBB
9	B	801	CLA	C2B-C3B-CAB-CBB
9	B	810	CLA	C2B-C3B-CAB-CBB
9	B	814	CLA	C2B-C3B-CAB-CBB
9	a	810	CLA	C2B-C3B-CAB-CBB
9	a	829	CLA	C2B-C3B-CAB-CBB
9	b	801	CLA	C2B-C3B-CAB-CBB
9	b	810	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	b	814	CLA	C2B-C3B-CAB-CBB
11	l	303	LHG	O9-C7-O7-C5
11	l	303	LHG	C28-C29-C30-C31
9	L	302	CLA	C1-C2-C3-C4
9	l	305	CLA	C1-C2-C3-C4
9	A	835	CLA	C3-C5-C6-C7
9	h	202	CLA	C3-C5-C6-C7
9	A	847	CLA	O1D-CGD-O2D-CED
9	B	806	CLA	C2A-CAA-CBA-CGA
9	b	806	CLA	C2A-CAA-CBA-CGA
9	A	804	CLA	C2-C1-O2A-CGA
9	A	824	CLA	C2-C1-O2A-CGA
9	B	824	CLA	C2-C1-O2A-CGA
9	L	303	CLA	C2-C1-O2A-CGA
9	a	804	CLA	C2-C1-O2A-CGA
9	a	808	CLA	C2-C1-O2A-CGA
9	b	824	CLA	C2-C1-O2A-CGA
9	a	817	CLA	C16-C17-C18-C20
9	A	832	CLA	C5-C6-C7-C8
9	A	846	CLA	C15-C16-C17-C18
9	b	829	CLA	CBA-CGA-O2A-C1
9	A	808	CLA	O1A-CGA-O2A-C1
9	a	808	CLA	CAA-CBA-CGA-O2A
9	a	816	CLA	CAA-CBA-CGA-O2A
12	a	841	BCR	C23-C24-C25-C26
9	A	819	CLA	C2-C3-C5-C6
9	a	811	CLA	C16-C17-C18-C19
9	a	819	CLA	C16-C17-C18-C20
9	A	806	CLA	C5-C6-C7-C8
9	a	832	CLA	C2A-CAA-CBA-CGA
9	b	802	CLA	O1A-CGA-O2A-C1
11	A	845	LHG	O7-C5-C6-O8
11	l	303	LHG	C11-C12-C13-C14
9	A	808	CLA	CBA-CGA-O2A-C1
9	A	847	CLA	C1-C2-C3-C5
9	a	810	CLA	C1-C2-C3-C5
9	b	818	CLA	C1-C2-C3-C5
11	A	845	LHG	C3-O3-P-O6
11	a	840	LHG	C4-O6-P-O3
9	a	807	CLA	C13-C15-C16-C17
9	B	823	CLA	C16-C17-C18-C19
9	a	802	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
11	l	303	LHG	C4-C5-C6-O8
9	a	833	CLA	C5-C6-C7-C8
9	A	811	CLA	C11-C12-C13-C15
9	H	201	CLA	C11-C10-C8-C7
9	a	846	CLA	C2-C3-C5-C6
9	b	823	CLA	C6-C7-C8-C10
9	B	829	CLA	C3-C5-C6-C7
9	A	816	CLA	C14-C13-C15-C16
9	A	825	CLA	C11-C12-C13-C14
9	B	810	CLA	C6-C7-C8-C9
9	B	823	CLA	C14-C13-C15-C16
9	a	807	CLA	C14-C13-C15-C16
9	a	815	CLA	C11-C12-C13-C14
9	a	826	CLA	C11-C12-C13-C14
9	h	202	CLA	C11-C10-C8-C9
9	A	823	CLA	C15-C16-C17-C18
11	A	845	LHG	C10-C11-C12-C13
9	A	820	CLA	C3-C5-C6-C7
9	a	806	CLA	C16-C17-C18-C19
9	a	824	CLA	C15-C16-C17-C18
11	A	838	LHG	C11-C12-C13-C14
9	a	811	CLA	C3-C5-C6-C7
9	B	831	CLA	C16-C17-C18-C20
9	b	831	CLA	C16-C17-C18-C20
9	b	808	CLA	CBA-CGA-O2A-C1
9	B	808	CLA	O1A-CGA-O2A-C1
11	a	839	LHG	C32-C33-C34-C35
9	B	810	CLA	C4B-C3B-CAB-CBB
9	B	814	CLA	C4B-C3B-CAB-CBB
9	b	810	CLA	C4B-C3B-CAB-CBB
9	a	808	CLA	C16-C17-C18-C20
12	B	836	BCR	C9-C10-C11-C12
12	H	202	BCR	C9-C10-C11-C12
12	b	836	BCR	C9-C10-C11-C12
14	b	837	DGD	O6D-C5D-C6D-O5D
12	b	834	BCR	C10-C11-C12-C13
12	l	304	BCR	C10-C11-C12-C13
9	A	847	CLA	O1A-CGA-O2A-C1
9	A	822	CLA	C3-C5-C6-C7
9	a	808	CLA	C4-C3-C5-C6
9	B	802	CLA	C10-C11-C12-C13
15	B	838	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
9	a	808	CLA	C2-C3-C5-C6
9	b	829	CLA	O1A-CGA-O2A-C1
9	B	814	CLA	C2-C1-O2A-CGA
9	b	802	CLA	C2-C1-O2A-CGA
9	b	814	CLA	C2-C1-O2A-CGA
9	b	821	CLA	C2-C1-O2A-CGA
11	l	303	LHG	C11-C10-C9-C8
9	B	804	CLA	C2C-C3C-CAC-CBC
9	A	813	CLA	C2A-CAA-CBA-CGA
9	A	831	CLA	C2A-CAA-CBA-CGA
9	A	835	CLA	C2A-CAA-CBA-CGA
9	B	823	CLA	C2A-CAA-CBA-CGA
11	A	845	LHG	C5-C4-O6-P
9	A	819	CLA	C3A-C2A-CAA-CBA
9	A	829	CLA	C3A-C2A-CAA-CBA
9	A	833	CLA	C3A-C2A-CAA-CBA
9	A	835	CLA	C3A-C2A-CAA-CBA
9	B	804	CLA	C3A-C2A-CAA-CBA
9	B	810	CLA	C3A-C2A-CAA-CBA
9	B	820	CLA	C3A-C2A-CAA-CBA
9	B	832	CLA	C3A-C2A-CAA-CBA
9	a	815	CLA	C3A-C2A-CAA-CBA
9	a	830	CLA	C3A-C2A-CAA-CBA
9	a	831	CLA	C3A-C2A-CAA-CBA
9	b	810	CLA	C3A-C2A-CAA-CBA
9	h	201	CLA	C3A-C2A-CAA-CBA
12	l	304	BCR	C13-C14-C15-C16
12	l	309	BCR	C15-C16-C17-C18
9	a	814	CLA	CAA-CBA-CGA-O1A
14	b	837	DGD	C6A-C7A-C8A-C9A
9	A	809	CLA	C6-C7-C8-C9
9	A	809	CLA	C11-C10-C8-C9
9	a	806	CLA	C11-C10-C8-C9
9	a	809	CLA	C11-C10-C8-C9
9	a	836	CLA	C11-C12-C13-C14
9	b	804	CLA	C6-C7-C8-C9
9	b	825	CLA	C11-C12-C13-C14
9	b	832	CLA	C6-C7-C8-C9
9	A	814	CLA	CAA-CBA-CGA-O1A
9	A	816	CLA	C15-C16-C17-C18
12	A	842	BCR	C16-C17-C18-C36
12	L	301	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
9	a	823	CLA	C16-C17-C18-C20
9	A	827	CLA	O2A-C1-C2-C3
9	a	828	CLA	O2A-C1-C2-C3
9	l	306	CLA	O2A-C1-C2-C3
9	b	803	CLA	C5-C6-C7-C8
12	B	836	BCR	C7-C8-C9-C10
9	A	818	CLA	CAA-CBA-CGA-O2A
9	a	806	CLA	C4-C3-C5-C6
9	A	802	CLA	C1A-C2A-CAA-CBA
9	A	809	CLA	C1A-C2A-CAA-CBA
9	A	829	CLA	C1A-C2A-CAA-CBA
9	A	833	CLA	C1A-C2A-CAA-CBA
9	A	834	CLA	C1A-C2A-CAA-CBA
9	A	835	CLA	C1A-C2A-CAA-CBA
9	B	804	CLA	C1A-C2A-CAA-CBA
9	B	816	CLA	C1A-C2A-CAA-CBA
9	L	302	CLA	C1A-C2A-CAA-CBA
9	a	802	CLA	C1A-C2A-CAA-CBA
9	a	830	CLA	C1A-C2A-CAA-CBA
9	a	834	CLA	C1A-C2A-CAA-CBA
9	a	835	CLA	C1A-C2A-CAA-CBA
9	b	804	CLA	C1A-C2A-CAA-CBA
9	b	815	CLA	C1A-C2A-CAA-CBA
9	b	816	CLA	C1A-C2A-CAA-CBA
9	l	305	CLA	C1A-C2A-CAA-CBA
9	A	829	CLA	C11-C10-C8-C7
9	A	829	CLA	C11-C12-C13-C15
9	A	832	CLA	C11-C12-C13-C15
9	B	815	CLA	C11-C12-C13-C15
9	a	815	CLA	C12-C13-C15-C16
9	b	801	CLA	C11-C10-C8-C7
9	b	815	CLA	C11-C12-C13-C15
9	A	828	CLA	C13-C15-C16-C17
9	a	814	CLA	CAA-CBA-CGA-O2A
11	a	839	LHG	C34-C35-C36-C37
9	b	829	CLA	C3-C5-C6-C7
9	h	201	CLA	O1D-CGD-O2D-CED
9	B	811	CLA	C2A-CAA-CBA-CGA
9	b	811	CLA	C2A-CAA-CBA-CGA
9	B	829	CLA	C5-C6-C7-C8
9	A	818	CLA	CAA-CBA-CGA-O1A
9	a	830	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	A	814	CLA	CAA-CBA-CGA-O2A
9	b	813	CLA	CAA-CBA-CGA-O1A
9	b	827	CLA	CAA-CBA-CGA-O2A
9	A	833	CLA	C4-C3-C5-C6
9	a	834	CLA	C4-C3-C5-C6
9	b	804	CLA	C2C-C3C-CAC-CBC
11	A	845	LHG	C26-C27-C28-C29
9	A	834	CLA	C2B-C3B-CAB-CBB
9	B	809	CLA	C2B-C3B-CAB-CBB
9	B	811	CLA	C2B-C3B-CAB-CBB
9	B	839	CLA	C2B-C3B-CAB-CBB
9	a	832	CLA	C2B-C3B-CAB-CBB
9	a	835	CLA	C2B-C3B-CAB-CBB
9	b	809	CLA	C2B-C3B-CAB-CBB
9	b	811	CLA	C2B-C3B-CAB-CBB
9	b	820	CLA	C2B-C3B-CAB-CBB
9	b	839	CLA	C2B-C3B-CAB-CBB
9	B	803	CLA	C8-C10-C11-C12
9	a	822	CLA	C15-C16-C17-C18
10	a	838	PQN	C23-C25-C26-C27
15	B	838	LMT	O5B-C5B-C6B-O6B
12	A	842	BCR	C16-C17-C18-C19
12	L	301	BCR	C11-C10-C9-C8
9	A	821	CLA	CBA-CGA-O2A-C1
14	B	837	DGD	C2A-C1A-O1G-C1G
11	A	838	LHG	C30-C31-C32-C33
9	B	803	CLA	C5-C6-C7-C8
12	l	309	BCR	C9-C10-C11-C12
9	B	813	CLA	CAA-CBA-CGA-O1A
9	B	824	CLA	C11-C12-C13-C14
9	b	813	CLA	CAA-CBA-CGA-O2A
9	a	836	CLA	C3-C5-C6-C7
9	A	807	CLA	C4-C3-C5-C6
9	a	807	CLA	C4-C3-C5-C6
9	l	306	CLA	C4-C3-C5-C6
9	B	818	CLA	C2-C1-O2A-CGA
9	a	831	CLA	C2-C1-O2A-CGA
9	b	818	CLA	C2-C1-O2A-CGA
9	A	821	CLA	O1A-CGA-O2A-C1
14	B	837	DGD	O1A-C1A-O1G-C1G
12	a	842	BCR	C10-C11-C12-C13
9	B	827	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	b	827	CLA	CAA-CBA-CGA-O1A
9	A	815	CLA	C11-C12-C13-C14
9	B	832	CLA	C11-C12-C13-C14
9	a	805	CLA	C11-C12-C13-C14
9	b	832	CLA	C11-C12-C13-C14
9	b	819	CLA	C5-C6-C7-C8
9	B	827	CLA	CAA-CBA-CGA-O1A
11	A	845	LHG	C11-C10-C9-C8
9	A	831	CLA	C4-C3-C5-C6
9	A	815	CLA	CAA-CBA-CGA-O2A
9	a	810	CLA	CAA-CBA-CGA-O2A
9	b	808	CLA	O1A-CGA-O2A-C1
9	a	828	CLA	C2A-CAA-CBA-CGA
9	B	810	CLA	C16-C17-C18-C19
12	B	834	BCR	C1-C6-C7-C8
12	B	834	BCR	C5-C6-C7-C8
12	L	301	BCR	C23-C24-C25-C30
12	b	834	BCR	C1-C6-C7-C8
12	l	308	BCR	C1-C6-C7-C8
9	L	308	CLA	CAA-CBA-CGA-O2A
9	a	815	CLA	CAA-CBA-CGA-O1A
9	A	847	CLA	CBA-CGA-O2A-C1
12	b	836	BCR	C7-C8-C9-C10
9	a	811	CLA	C13-C15-C16-C17
9	a	825	CLA	CAA-CBA-CGA-O2A
9	B	821	CLA	C3-C5-C6-C7
9	B	813	CLA	CAA-CBA-CGA-O2A
9	b	824	CLA	C11-C12-C13-C14
9	A	821	CLA	C15-C16-C17-C18
9	b	809	CLA	C8-C10-C11-C12
9	A	801	CLA	CAA-CBA-CGA-O2A
9	A	808	CLA	CAA-CBA-CGA-O2A
9	a	801	CLA	CAA-CBA-CGA-O2A
9	A	810	CLA	C6-C7-C8-C9
9	B	827	CLA	C4B-C3B-CAB-CBB
9	B	818	CLA	O1D-CGD-O2D-CED
11	A	845	LHG	O6-C4-C5-C6
9	A	822	CLA	C4-C3-C5-C6
9	B	819	CLA	C4-C3-C5-C6
9	A	807	CLA	C12-C13-C15-C16
9	A	815	CLA	C12-C13-C15-C16
9	A	825	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
9	L	303	CLA	C12-C13-C15-C16
9	a	805	CLA	C12-C13-C15-C16
9	a	806	CLA	C2-C3-C5-C6
9	A	805	CLA	C1-C2-C3-C4
9	A	809	CLA	C1-C2-C3-C4
9	A	816	CLA	C1-C2-C3-C4
9	A	825	CLA	C1-C2-C3-C4
9	A	835	CLA	C1-C2-C3-C4
9	A	846	CLA	C1-C2-C3-C4
9	B	802	CLA	C1-C2-C3-C4
9	B	806	CLA	C1-C2-C3-C4
9	B	807	CLA	C1-C2-C3-C4
9	B	817	CLA	C1-C2-C3-C4
9	B	819	CLA	C1-C2-C3-C4
9	B	831	CLA	C1-C2-C3-C4
9	a	809	CLA	C1-C2-C3-C4
9	a	826	CLA	C1-C2-C3-C4
9	a	830	CLA	C1-C2-C3-C4
9	a	832	CLA	C1-C2-C3-C4
9	a	836	CLA	C1-C2-C3-C4
9	a	847	CLA	C1-C2-C3-C4
9	b	807	CLA	C1-C2-C3-C4
9	b	810	CLA	C1-C2-C3-C4
9	b	817	CLA	C1-C2-C3-C4
9	b	819	CLA	C1-C2-C3-C4
9	b	831	CLA	C1-C2-C3-C4
9	l	306	CLA	C1-C2-C3-C4
9	a	837	CLA	O2A-C1-C2-C3
12	L	301	BCR	C13-C14-C15-C16
12	L	306	BCR	C15-C16-C17-C18
9	A	816	CLA	C5-C6-C7-C8
14	B	837	DGD	O2G-C2G-C3G-O3G
9	B	824	CLA	C11-C12-C13-C15
9	A	808	CLA	C13-C15-C16-C17
12	a	844	BCR	C35-C13-C14-C15
12	i	101	BCR	C16-C17-C18-C36
12	l	308	BCR	C35-C13-C14-C15
9	L	303	CLA	C4-C3-C5-C6
9	a	802	CLA	C4-C3-C5-C6
9	a	817	CLA	C2-C3-C5-C6
9	a	834	CLA	C2-C3-C5-C6
9	b	824	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	b	820	CLA	CAA-CBA-CGA-O2A
9	A	808	CLA	C11-C12-C13-C14
9	A	846	CLA	C6-C7-C8-C9
9	B	806	CLA	C11-C12-C13-C14
9	B	811	CLA	C11-C12-C13-C14
9	B	821	CLA	C6-C7-C8-C9
9	a	809	CLA	C6-C7-C8-C9
9	b	804	CLA	C11-C10-C8-C9
9	b	806	CLA	C11-C12-C13-C14
9	b	823	CLA	C14-C13-C15-C16
10	A	837	PQN	C16-C17-C18-C19
9	A	802	CLA	C3A-C2A-CAA-CBA
9	B	816	CLA	C3A-C2A-CAA-CBA
9	a	802	CLA	C3A-C2A-CAA-CBA
9	a	836	CLA	C3A-C2A-CAA-CBA
9	b	816	CLA	C3A-C2A-CAA-CBA
9	b	832	CLA	C3A-C2A-CAA-CBA
9	l	306	CLA	C3A-C2A-CAA-CBA
9	A	805	CLA	CAD-CBD-CGD-O2D
9	A	806	CLA	CAD-CBD-CGD-O2D
9	A	810	CLA	CAD-CBD-CGD-O2D
9	A	812	CLA	CAD-CBD-CGD-O2D
9	A	821	CLA	CAD-CBD-CGD-O2D
9	A	831	CLA	CAD-CBD-CGD-O2D
9	B	806	CLA	CAD-CBD-CGD-O2D
9	B	812	CLA	CAD-CBD-CGD-O2D
9	B	829	CLA	CAD-CBD-CGD-O2D
9	B	839	CLA	CAD-CBD-CGD-O2D
9	a	805	CLA	CAD-CBD-CGD-O2D
9	a	810	CLA	CAD-CBD-CGD-O2D
9	a	812	CLA	CAD-CBD-CGD-O2D
9	a	822	CLA	CAD-CBD-CGD-O2D
9	b	806	CLA	CAD-CBD-CGD-O2D
9	b	821	CLA	CAD-CBD-CGD-O2D
9	b	822	CLA	CAD-CBD-CGD-O2D
9	b	827	CLA	CAD-CBD-CGD-O2D
9	b	829	CLA	CAD-CBD-CGD-O2D
9	b	839	CLA	CAD-CBD-CGD-O2D
9	h	201	CLA	CAD-CBD-CGD-O2D
9	h	202	CLA	CAD-CBD-CGD-O2D
9	a	815	CLA	C15-C16-C17-C18
9	a	836	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	B	803	CLA	C2-C1-O2A-CGA
9	A	802	CLA	C4-C3-C5-C6
9	B	812	CLA	C4-C3-C5-C6
9	a	819	CLA	C5-C6-C7-C8
9	A	802	CLA	C2-C3-C5-C6
9	A	833	CLA	C2-C3-C5-C6
9	a	802	CLA	C2-C3-C5-C6
9	a	811	CLA	CAA-CBA-CGA-O2A
9	h	202	CLA	CAA-CBA-CGA-O2A
11	a	839	LHG	C11-C10-C9-C8
11	A	838	LHG	C4-C5-C6-O8
11	a	839	LHG	C4-C5-C6-O8
9	L	304	CLA	CAA-CBA-CGA-O2A
9	a	810	CLA	C6-C7-C8-C9
9	A	822	CLA	O2A-C1-C2-C3
9	A	826	CLA	O2A-C1-C2-C3
9	A	833	CLA	O2A-C1-C2-C3
9	B	802	CLA	O2A-C1-C2-C3
9	B	804	CLA	O2A-C1-C2-C3
9	a	827	CLA	O2A-C1-C2-C3
9	a	834	CLA	O2A-C1-C2-C3
9	b	804	CLA	O2A-C1-C2-C3
9	b	821	CLA	O2A-C1-C2-C3
9	h	201	CLA	O2A-C1-C2-C3
9	B	839	CLA	CBA-CGA-O2A-C1
9	B	839	CLA	C2A-CAA-CBA-CGA
9	b	825	CLA	CAA-CBA-CGA-O2A
9	l	307	CLA	CAA-CBA-CGA-O2A
9	A	823	CLA	C3-C5-C6-C7
9	A	821	CLA	C16-C17-C18-C20
9	A	803	CLA	CHA-CBD-CGD-O1D
9	A	803	CLA	CHA-CBD-CGD-O2D
9	A	819	CLA	CHA-CBD-CGD-O2D
9	A	826	CLA	CHA-CBD-CGD-O1D
9	A	826	CLA	CHA-CBD-CGD-O2D
9	A	827	CLA	CHA-CBD-CGD-O1D
9	A	830	CLA	CHA-CBD-CGD-O2D
9	A	832	CLA	CHA-CBD-CGD-O2D
9	B	803	CLA	CHA-CBD-CGD-O2D
9	B	805	CLA	CHA-CBD-CGD-O2D
9	B	816	CLA	CHA-CBD-CGD-O1D
9	B	816	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	B	820	CLA	CHA-CBD-CGD-O2D
9	H	201	CLA	CHA-CBD-CGD-O1D
9	a	803	CLA	CHA-CBD-CGD-O1D
9	a	803	CLA	CHA-CBD-CGD-O2D
9	a	819	CLA	CHA-CBD-CGD-O2D
9	a	824	CLA	CHA-CBD-CGD-O1D
9	a	825	CLA	CHA-CBD-CGD-O2D
9	a	827	CLA	CHA-CBD-CGD-O2D
9	a	828	CLA	CHA-CBD-CGD-O1D
9	a	828	CLA	CHA-CBD-CGD-O2D
9	a	831	CLA	CHA-CBD-CGD-O2D
9	a	833	CLA	CHA-CBD-CGD-O2D
9	b	803	CLA	CHA-CBD-CGD-O2D
9	b	805	CLA	CHA-CBD-CGD-O2D
9	b	814	CLA	CHA-CBD-CGD-O1D
9	b	816	CLA	CHA-CBD-CGD-O1D
9	b	816	CLA	CHA-CBD-CGD-O2D
9	h	201	CLA	CHA-CBD-CGD-O1D
9	l	301	CLA	CHA-CBD-CGD-O2D
9	B	825	CLA	CAA-CBA-CGA-O2A
9	A	806	CLA	C2-C3-C5-C6
9	B	812	CLA	C2-C3-C5-C6
9	B	809	CLA	C5-C6-C7-C8
9	b	804	CLA	C13-C15-C16-C17
9	B	819	CLA	CAA-CBA-CGA-O2A
14	b	837	DGD	O2G-C2G-C3G-O3G
9	B	809	CLA	C13-C15-C16-C17
9	b	803	CLA	C8-C10-C11-C12
9	L	307	CLA	CAA-CBA-CGA-O1A
9	l	301	CLA	CAA-CBA-CGA-O1A
9	A	807	CLA	C13-C15-C16-C17
9	b	819	CLA	CAA-CBA-CGA-O2A
14	B	837	DGD	O2G-C1B-C2B-C3B
14	b	837	DGD	O2G-C1B-C2B-C3B
9	A	822	CLA	C2A-CAA-CBA-CGA
9	A	811	CLA	CAA-CBA-CGA-O2A
9	B	807	CLA	CAA-CBA-CGA-O2A
9	A	801	CLA	C8-C10-C11-C12
9	A	806	CLA	C6-C7-C8-C10
9	A	811	CLA	C11-C10-C8-C7
9	A	819	CLA	C11-C12-C13-C15
9	A	847	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	B	801	CLA	C11-C10-C8-C7
9	H	201	CLA	C6-C7-C8-C10
9	a	802	CLA	C11-C12-C13-C15
10	A	837	PQN	C21-C22-C23-C25
9	A	829	CLA	C16-C17-C18-C19
9	A	824	CLA	CAA-CBA-CGA-O2A
9	b	807	CLA	CAA-CBA-CGA-O2A
9	A	804	CLA	C6-C7-C8-C9
9	A	805	CLA	C11-C12-C13-C14
9	A	835	CLA	C11-C12-C13-C14
9	H	201	CLA	C11-C10-C8-C9
9	a	804	CLA	C6-C7-C8-C9
9	a	824	CLA	C6-C7-C8-C9
9	b	811	CLA	C11-C12-C13-C14
10	a	838	PQN	C16-C17-C18-C19
12	a	841	BCR	C15-C16-C17-C18
12	l	308	BCR	C15-C16-C17-C18
9	l	305	CLA	O2A-C1-C2-C3
9	B	830	CLA	CAA-CBA-CGA-O2A
11	A	838	LHG	C11-C10-C9-C8
11	A	838	LHG	C19-C20-C21-C22
9	a	824	CLA	C2A-CAA-CBA-CGA
9	b	830	CLA	CAA-CBA-CGA-O2A
9	b	809	CLA	C5-C6-C7-C8
9	a	811	CLA	C16-C17-C18-C20
9	b	829	CLA	C4-C3-C5-C6
9	B	806	CLA	C2C-C3C-CAC-CBC
14	B	837	DGD	C4A-C5A-C6A-C7A
9	B	806	CLA	C1A-C2A-CAA-CBA
9	B	820	CLA	C1A-C2A-CAA-CBA
9	H	201	CLA	C1A-C2A-CAA-CBA
9	a	803	CLA	C1A-C2A-CAA-CBA
9	a	836	CLA	C1A-C2A-CAA-CBA
9	b	806	CLA	C1A-C2A-CAA-CBA
9	l	306	CLA	C1A-C2A-CAA-CBA
9	b	820	CLA	CAA-CBA-CGA-O1A
9	B	816	CLA	CAA-CBA-CGA-O2A
9	a	821	CLA	CAA-CBA-CGA-O2A
9	a	830	CLA	CAA-CBA-CGA-O2A
10	A	837	PQN	C23-C25-C26-C27
9	b	823	CLA	C2A-CAA-CBA-CGA
9	A	817	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
9	a	816	CLA	C16-C17-C18-C20
9	a	822	CLA	C16-C17-C18-C20
9	L	304	CLA	CAA-CBA-CGA-O1A
11	A	838	LHG	C18-C19-C20-C21
9	A	829	CLA	CAA-CBA-CGA-O2A
9	b	829	CLA	C5-C6-C7-C8
9	b	829	CLA	C8-C10-C11-C12
10	a	838	PQN	C15-C16-C17-C18
11	a	840	LHG	C2-C3-O3-P
9	b	825	CLA	CAA-CBA-CGA-O1A
9	h	202	CLA	CAA-CBA-CGA-O1A
14	b	837	DGD	O1B-C1B-C2B-C3B
9	A	831	CLA	C4B-C3B-CAB-CBB
11	A	838	LHG	C3-O3-P-O5
11	a	839	LHG	C3-O3-P-O5
11	a	840	LHG	C4-O6-P-O5
11	A	845	LHG	O10-C23-C24-C25
14	B	837	DGD	O1B-C1B-C2B-C3B
14	B	837	DGD	C2A-C3A-C4A-C5A
12	L	305	BCR	C1-C6-C7-C8
12	a	844	BCR	C1-C6-C7-C8
12	b	834	BCR	C5-C6-C7-C8
9	A	811	CLA	CAA-CBA-CGA-O1A
9	B	819	CLA	CAA-CBA-CGA-O1A
9	B	825	CLA	CAA-CBA-CGA-O1A
9	a	811	CLA	CAA-CBA-CGA-O1A
9	b	819	CLA	CAA-CBA-CGA-O1A
9	l	307	CLA	CAA-CBA-CGA-O1A
9	B	839	CLA	O1A-CGA-O2A-C1
9	B	820	CLA	CAA-CBA-CGA-O2A
9	A	801	CLA	C16-C17-C18-C19
12	l	304	BCR	C18-C19-C20-C21
14	B	837	DGD	C7B-C8B-C9B-CAB
9	B	829	CLA	C8-C10-C11-C12
9	a	823	CLA	C4-C3-C5-C6
11	A	845	LHG	C17-C18-C19-C20
9	L	307	CLA	CAA-CBA-CGA-O2A
9	l	301	CLA	CAA-CBA-CGA-O2A
9	A	811	CLA	CAD-CBD-CGD-O1D
9	A	812	CLA	CAD-CBD-CGD-O1D
9	A	823	CLA	CAD-CBD-CGD-O1D
9	A	829	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	B	801	CLA	CAD-CBD-CGD-O1D
9	B	814	CLA	CAD-CBD-CGD-O1D
9	a	825	CLA	CAD-CBD-CGD-O1D
9	a	830	CLA	CAD-CBD-CGD-O1D
9	b	801	CLA	CAD-CBD-CGD-O1D
9	b	823	CLA	CAD-CBD-CGD-O1D
9	b	832	CLA	CAD-CBD-CGD-O1D
9	b	840	CLA	CAD-CBD-CGD-O1D
11	A	845	LHG	C7-C8-C9-C10
9	B	818	CLA	O1A-CGA-O2A-C1
9	B	807	CLA	CAA-CBA-CGA-O1A
9	b	807	CLA	CAA-CBA-CGA-O1A
9	A	820	CLA	CAA-CBA-CGA-O2A
9	b	807	CLA	C8-C10-C11-C12
10	A	837	PQN	C15-C16-C17-C18
9	A	805	CLA	C14-C13-C15-C16
9	A	825	CLA	C11-C10-C8-C9
9	B	806	CLA	C11-C10-C8-C9
9	B	807	CLA	C14-C13-C15-C16
9	a	826	CLA	C11-C10-C8-C9
9	b	807	CLA	C14-C13-C15-C16
9	b	821	CLA	C3-C5-C6-C7
9	A	847	CLA	CAA-CBA-CGA-O2A
9	a	806	CLA	CAA-CBA-CGA-O2A
9	a	847	CLA	CAA-CBA-CGA-O2A
9	b	816	CLA	CAA-CBA-CGA-O2A
9	B	807	CLA	C8-C10-C11-C12
9	a	832	CLA	CAA-CBA-CGA-O2A
9	B	816	CLA	CAA-CBA-CGA-O1A
9	a	847	CLA	C4-C3-C5-C6
9	a	801	CLA	C8-C10-C11-C12
9	A	805	CLA	C12-C13-C15-C16
9	A	821	CLA	C11-C12-C13-C15
9	B	806	CLA	C6-C7-C8-C10
9	B	807	CLA	C12-C13-C15-C16
9	a	806	CLA	C11-C10-C8-C7
9	a	806	CLA	C12-C13-C15-C16
9	a	809	CLA	C11-C10-C8-C7
9	a	811	CLA	C11-C10-C8-C7
9	a	846	CLA	C11-C10-C8-C7
9	b	807	CLA	C12-C13-C15-C16
9	b	811	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	h	202	CLA	C12-C13-C15-C16
9	l	306	CLA	C11-C10-C8-C7
9	A	829	CLA	CAA-CBA-CGA-O1A
9	A	810	CLA	CAA-CBA-CGA-O2A
9	A	831	CLA	CAA-CBA-CGA-O2A
9	b	804	CLA	CAA-CBA-CGA-O2A
9	h	201	CLA	CAA-CBA-CGA-O2A
9	A	820	CLA	CAA-CBA-CGA-O1A
9	A	847	CLA	CAA-CBA-CGA-O1A
9	a	821	CLA	CAA-CBA-CGA-O1A
9	a	830	CLA	CAA-CBA-CGA-O1A
9	h	201	CLA	CAA-CBA-CGA-O1A
9	A	813	CLA	CAA-CBA-CGA-O2A
9	A	846	CLA	CAA-CBA-CGA-O2A
9	b	806	CLA	C2C-C3C-CAC-CBC
9	B	820	CLA	CAA-CBA-CGA-O1A
9	A	801	CLA	C10-C11-C12-C13
9	B	802	CLA	C13-C15-C16-C17
9	a	824	CLA	C8-C10-C11-C12
9	a	830	CLA	C13-C15-C16-C17
9	A	831	CLA	CAA-CBA-CGA-O1A
9	L	303	CLA	C2A-CAA-CBA-CGA
9	a	846	CLA	C2A-CAA-CBA-CGA
9	b	816	CLA	CAA-CBA-CGA-O1A
9	a	817	CLA	C4-C3-C5-C6
9	l	302	CLA	C4-C3-C5-C6
9	b	803	CLA	CAA-CBA-CGA-O2A
9	A	836	CLA	O2A-C1-C2-C3
9	a	818	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

187 monomers are involved in 793 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	817	CLA	2	0
9	b	840	CLA	2	0
9	A	823	CLA	11	0
9	a	802	CLA	4	0
14	B	837	DGD	8	0
9	A	832	CLA	5	0
10	b	833	PQN	2	0
9	B	806	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	807	CLA	9	0
9	B	810	CLA	2	0
12	B	834	BCR	5	0
9	A	809	CLA	5	0
14	b	837	DGD	6	0
9	b	816	CLA	1	0
9	b	817	CLA	1	0
9	b	821	CLA	4	0
9	B	822	CLA	3	0
9	B	803	CLA	8	0
15	b	838	LMT	5	0
9	b	813	CLA	1	0
9	A	814	CLA	2	0
12	b	834	BCR	4	0
9	a	822	CLA	2	0
12	L	306	BCR	2	0
9	a	815	CLA	1	0
9	a	804	CLA	4	0
9	a	836	CLA	3	0
9	b	818	CLA	9	0
9	B	819	CLA	2	0
10	A	837	PQN	6	0
15	B	838	LMT	5	0
12	B	835	BCR	4	0
9	a	816	CLA	10	0
9	a	820	CLA	74	0
9	A	801	CLA	9	0
9	a	837	CLA	3	0
9	b	820	CLA	2	0
9	a	824	CLA	4	0
12	A	840	BCR	3	0
9	A	846	CLA	6	0
9	A	805	CLA	6	0
9	B	812	CLA	2	0
9	a	818	CLA	1	0
9	a	835	CLA	1	0
9	l	305	CLA	6	0
9	B	802	CLA	4	0
9	A	822	CLA	3	0
9	a	808	CLA	6	0
9	b	803	CLA	8	0
12	L	305	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	b	814	CLA	2	0
9	A	828	CLA	4	0
9	A	831	CLA	5	0
9	a	812	CLA	2	0
9	a	810	CLA	3	0
9	a	826	CLA	4	0
9	b	832	CLA	3	0
9	b	809	CLA	3	0
9	a	827	CLA	9	0
9	b	802	CLA	5	0
12	a	842	BCR	6	0
9	L	304	CLA	1	0
9	B	829	CLA	3	0
9	l	306	CLA	7	0
9	b	824	CLA	3	0
9	B	807	CLA	3	0
12	a	841	BCR	5	0
9	b	810	CLA	3	0
9	L	308	CLA	11	0
9	b	830	CLA	2	0
9	A	833	CLA	6	0
9	b	807	CLA	4	0
9	b	806	CLA	5	0
11	a	840	LHG	4	0
9	A	836	CLA	4	0
9	B	832	CLA	3	0
9	B	827	CLA	3	0
12	l	308	BCR	3	0
9	a	847	CLA	9	0
11	A	838	LHG	1	0
9	b	839	CLA	2	0
9	A	808	CLA	3	0
9	A	825	CLA	6	0
9	B	804	CLA	7	0
12	h	203	BCR	2	0
12	a	844	BCR	7	0
9	B	814	CLA	2	0
9	A	811	CLA	5	0
9	a	833	CLA	8	0
9	A	803	CLA	4	0
9	a	825	CLA	11	0
9	a	829	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	835	CLA	4	0
12	b	835	BCR	6	0
9	A	817	CLA	10	0
9	B	808	CLA	2	0
9	A	807	CLA	9	0
12	A	841	BCR	5	0
9	b	828	CLA	2	0
9	B	820	CLA	1	0
9	A	812	CLA	1	0
9	H	201	CLA	3	0
11	a	839	LHG	1	0
9	B	824	CLA	2	0
9	a	819	CLA	13	0
9	b	808	CLA	2	0
9	b	812	CLA	1	0
9	a	805	CLA	6	0
9	A	826	CLA	8	0
9	b	819	CLA	1	0
9	b	827	CLA	5	0
9	A	813	CLA	1	0
9	B	831	CLA	2	0
9	h	202	CLA	6	0
9	h	201	CLA	36	0
9	a	801	CLA	7	0
9	A	802	CLA	6	0
9	a	806	CLA	5	0
9	A	821	CLA	18	0
9	a	814	CLA	2	0
9	b	801	CLA	2	0
9	B	813	CLA	3	0
9	l	302	CLA	10	0
9	a	830	CLA	6	0
12	L	301	BCR	6	0
11	l	303	LHG	4	0
9	a	846	CLA	7	0
9	A	819	CLA	71	0
9	b	822	CLA	4	0
9	b	815	CLA	3	0
9	l	307	CLA	3	0
9	A	818	CLA	1	0
12	H	202	BCR	3	0
9	a	817	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	843	BCR	5	0
9	A	829	CLA	5	0
9	b	811	CLA	4	0
9	L	303	CLA	5	0
9	B	823	CLA	4	0
9	A	816	CLA	3	0
9	B	839	CLA	3	0
9	b	804	CLA	7	0
9	A	804	CLA	3	0
9	B	825	CLA	5	0
9	A	830	CLA	15	0
9	L	307	CLA	19	0
9	a	823	CLA	4	0
9	a	834	CLA	7	0
9	B	809	CLA	2	0
9	a	803	CLA	2	0
12	I	101	BCR	1	0
9	a	832	CLA	3	0
12	A	842	BCR	3	0
9	A	815	CLA	5	0
9	B	801	CLA	2	0
10	a	838	PQN	5	0
12	l	309	BCR	3	0
12	l	304	BCR	6	0
9	B	815	CLA	6	0
11	A	845	LHG	5	0
9	a	809	CLA	3	0
12	i	101	BCR	1	0
12	A	843	BCR	2	0
9	a	831	CLA	8	0
9	b	823	CLA	3	0
9	l	301	CLA	11	0
9	A	806	CLA	6	0
9	b	829	CLA	3	0
9	A	847	CLA	7	0
9	B	830	CLA	2	0
9	a	813	CLA	2	0
9	A	820	CLA	11	0
12	B	836	BCR	2	0
9	B	818	CLA	6	0
9	b	825	CLA	6	0
11	A	839	LHG	3	0

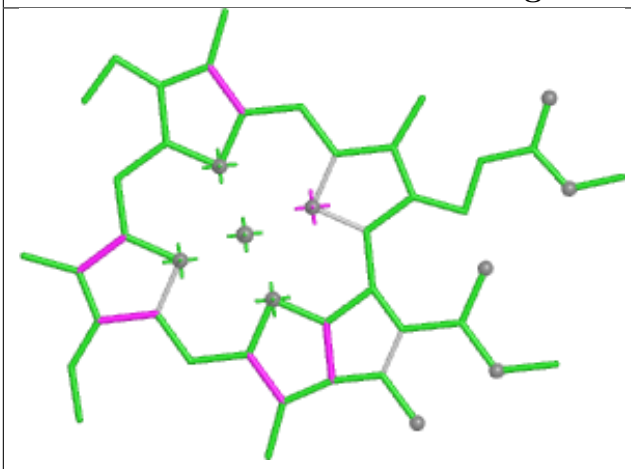
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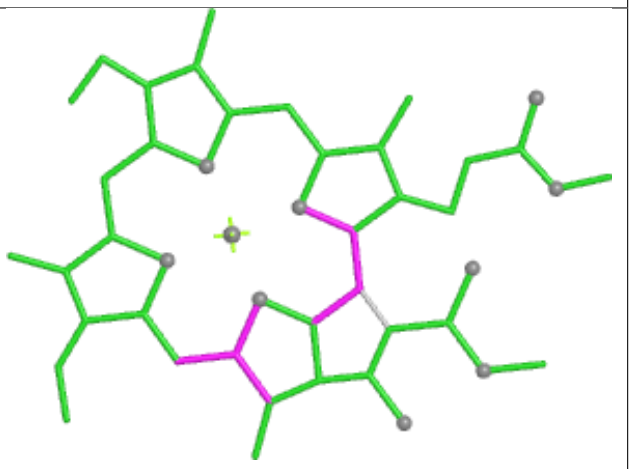
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	821	CLA	3	0
9	B	840	CLA	3	0
9	a	811	CLA	5	0
9	b	831	CLA	1	0
10	B	833	PQN	2	0
9	A	810	CLA	4	0
9	A	824	CLA	11	0
9	L	302	CLA	4	0
9	a	821	CLA	6	0
9	B	811	CLA	5	0
12	b	836	BCR	2	0

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

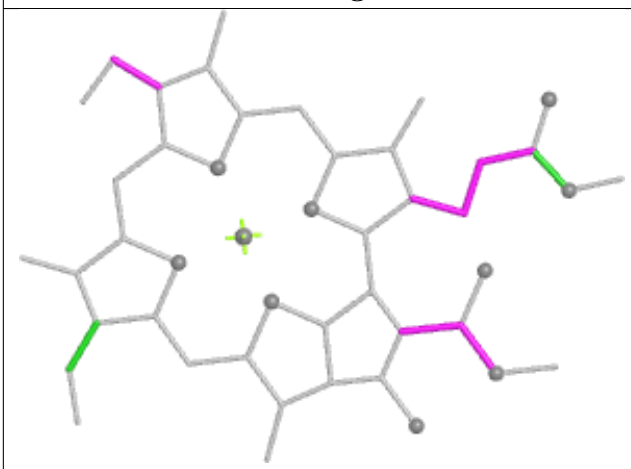
Ligand CLA B 816



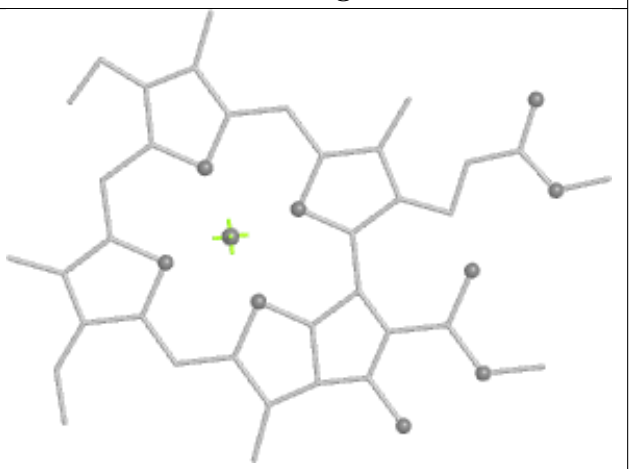
Bond lengths



Bond angles

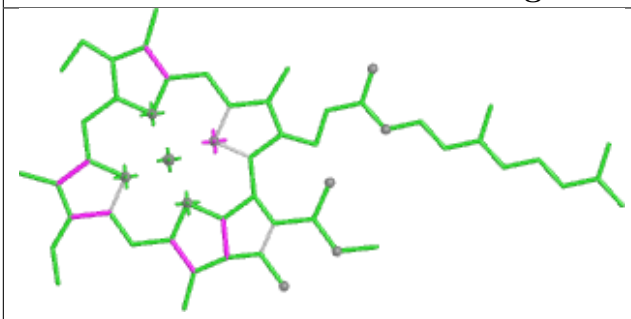


Torsions

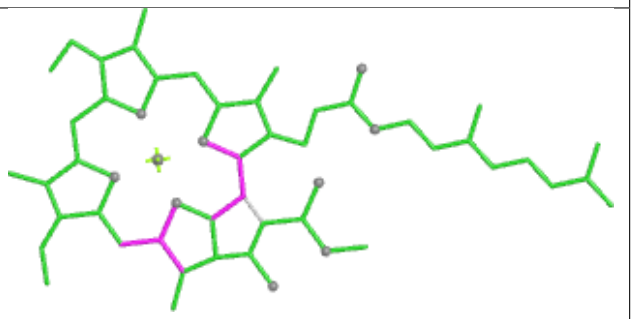


Rings

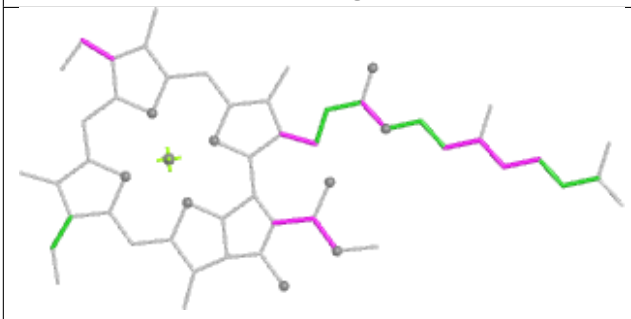
Ligand CLA B 817



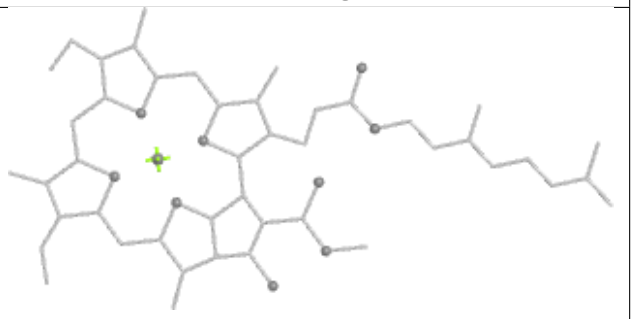
Bond lengths



Bond angles

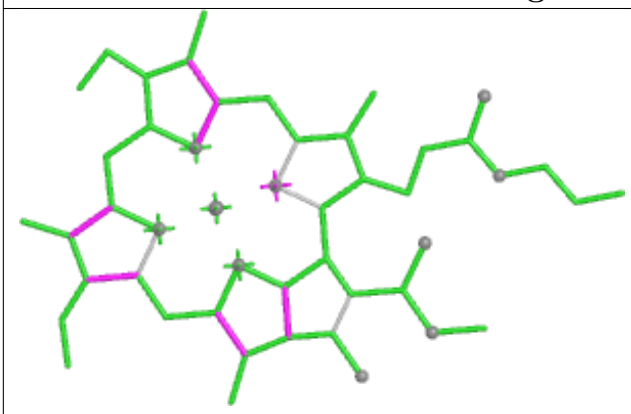


Torsions

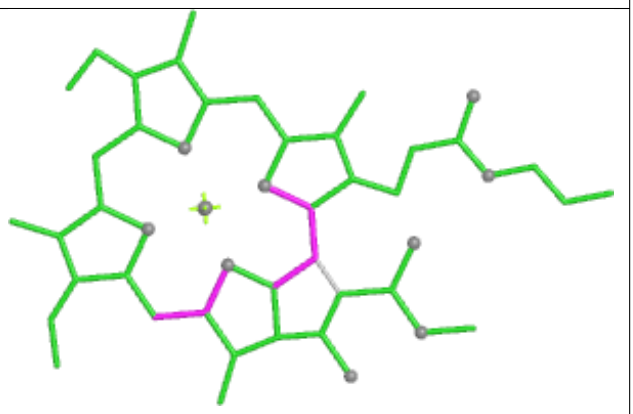


Rings

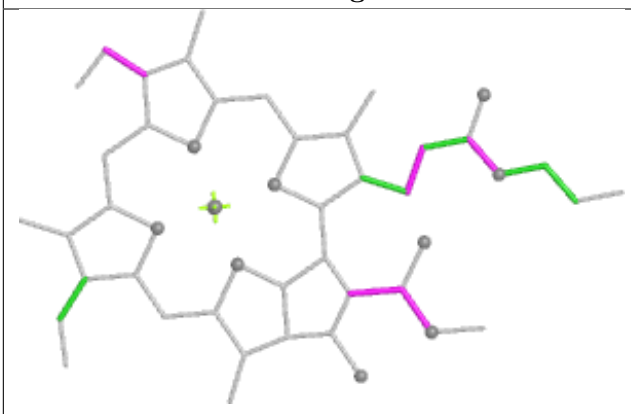
Ligand CLA b 840



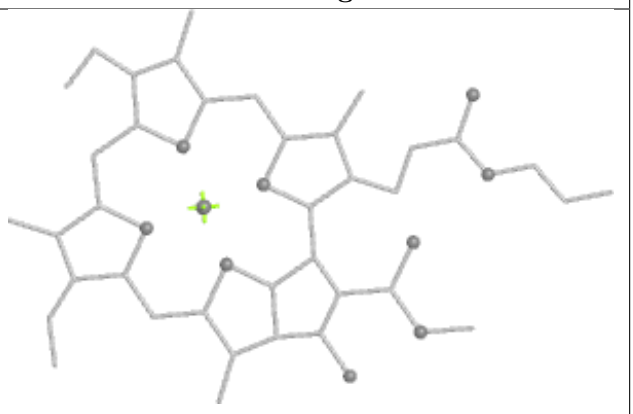
Bond lengths



Bond angles

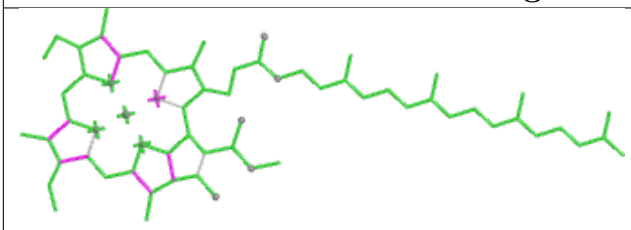


Torsions

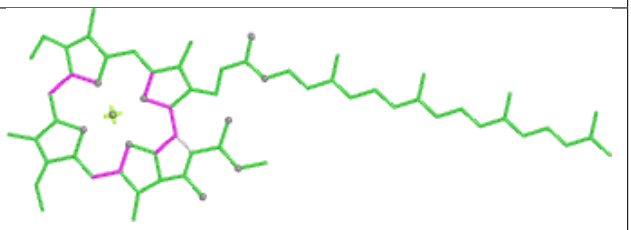


Rings

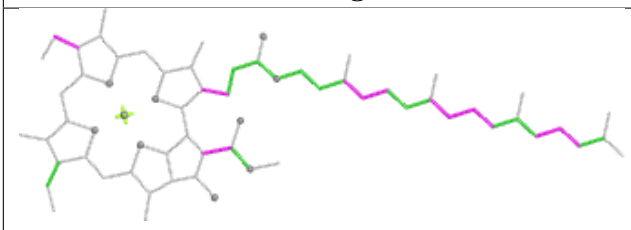
Ligand CLA A 823



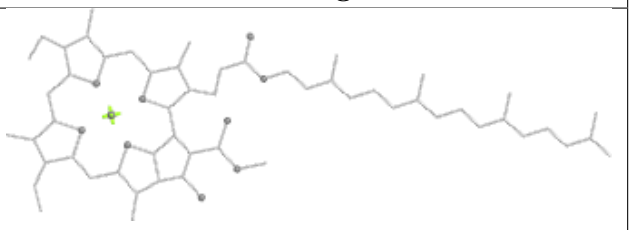
Bond lengths



Bond angles

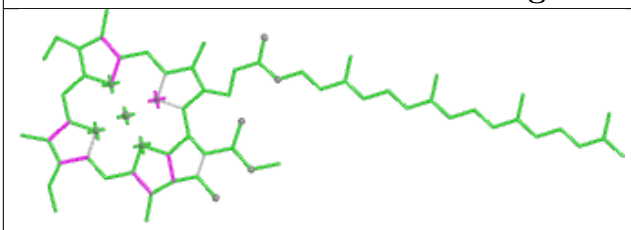


Torsions

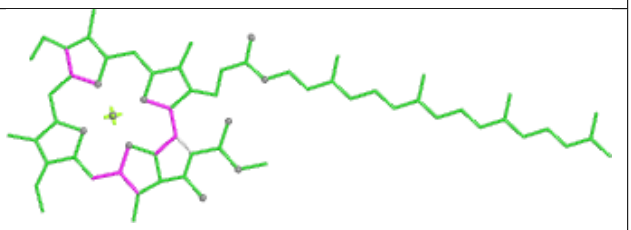


Rings

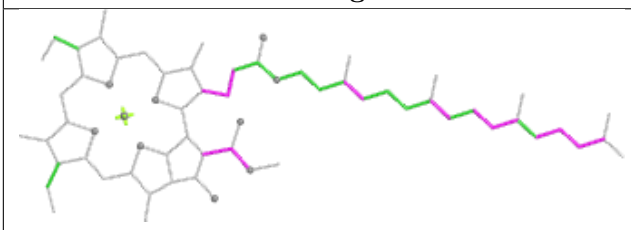
Ligand CLA a 802



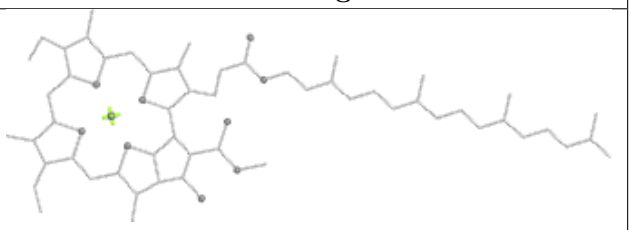
Bond lengths



Bond angles

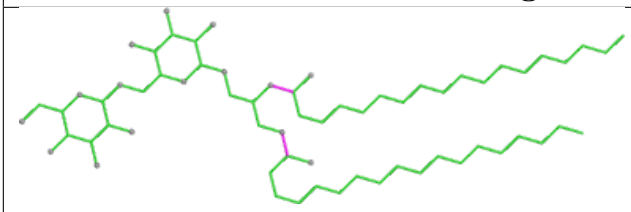


Torsions

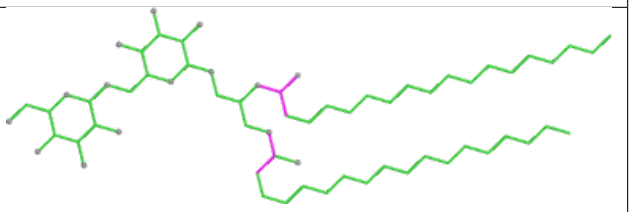


Rings

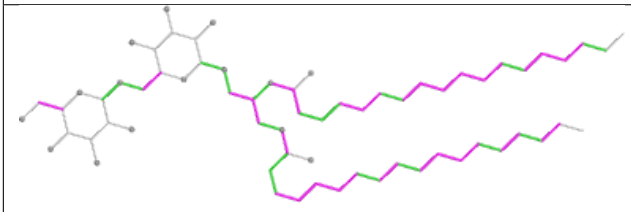
Ligand DGD B 837



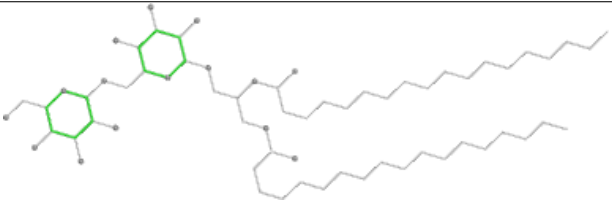
Bond lengths



Bond angles

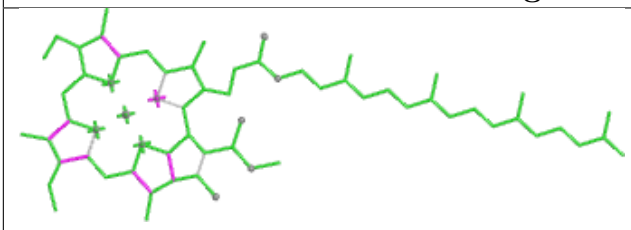


Torsions

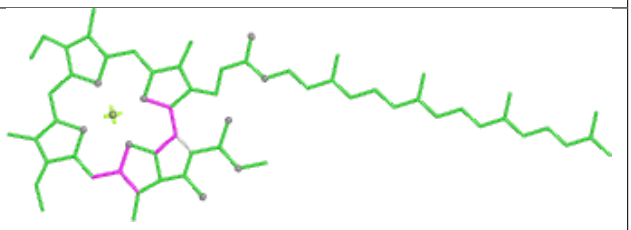


Rings

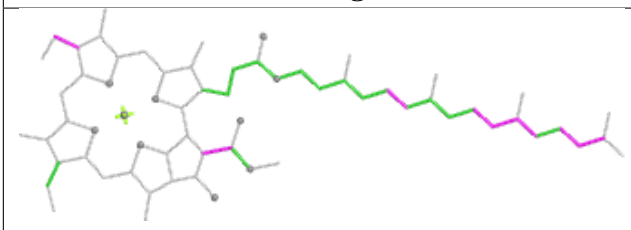
Ligand CLA A 832



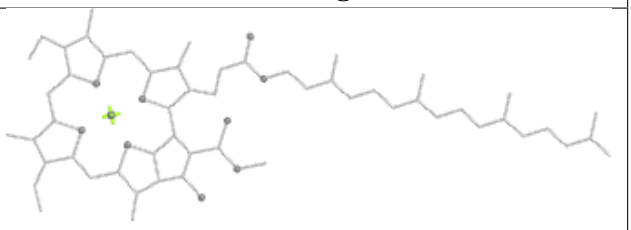
Bond lengths



Bond angles

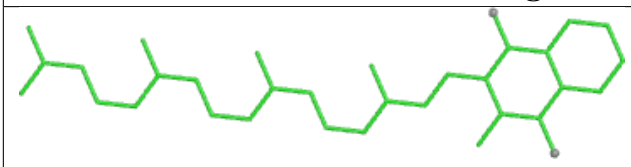


Torsions

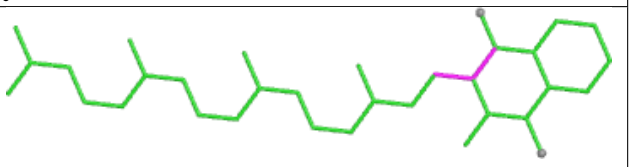


Rings

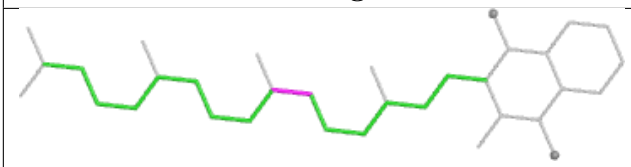
Ligand PQN b 833



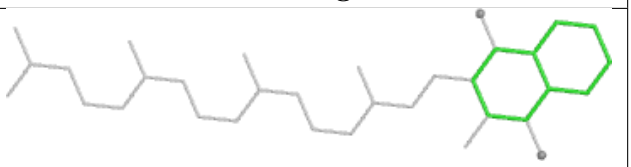
Bond lengths



Bond angles

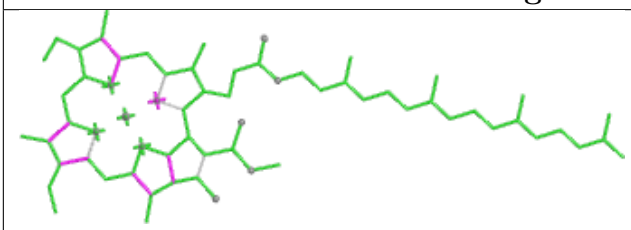


Torsions

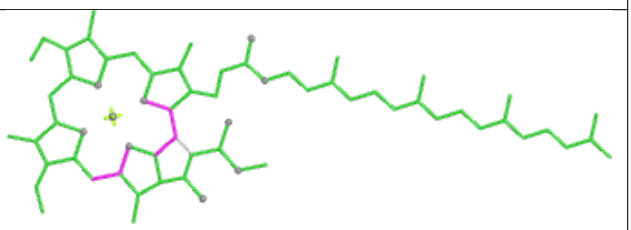


Rings

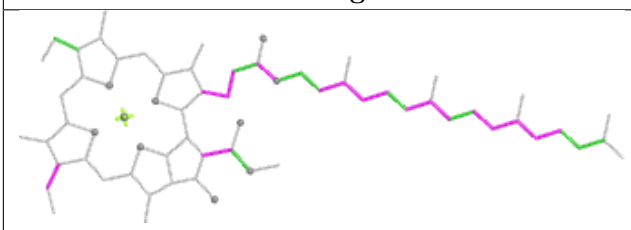
Ligand CLA B 806



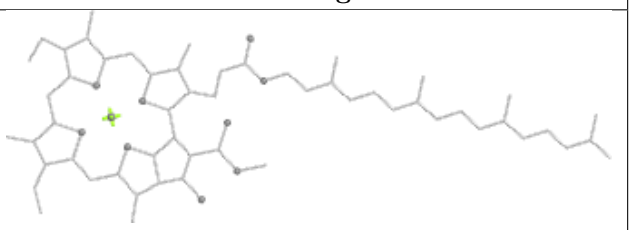
Bond lengths



Bond angles

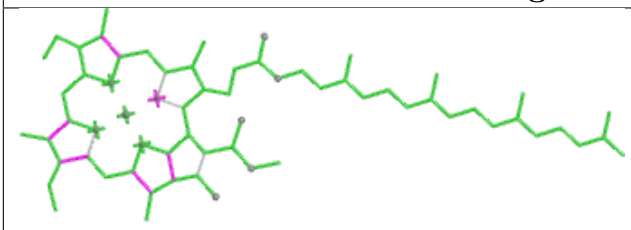


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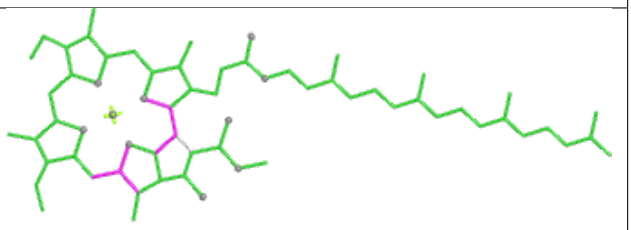


Rings

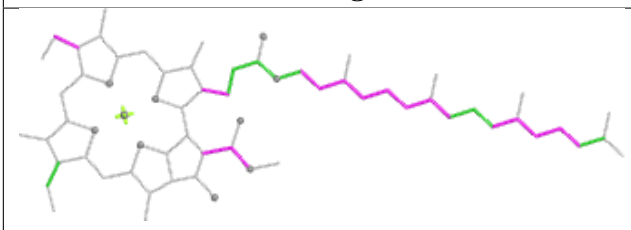
Ligand CLA a 807



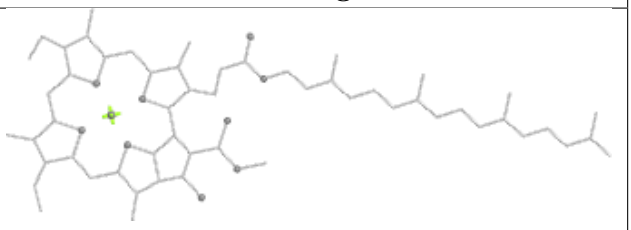
Bond lengths



Bond angles

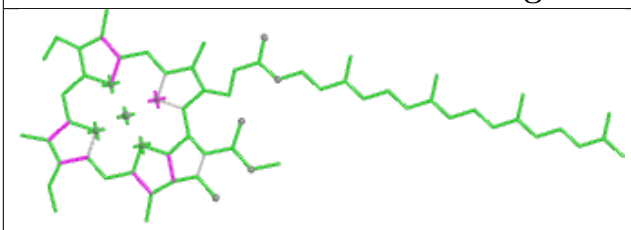


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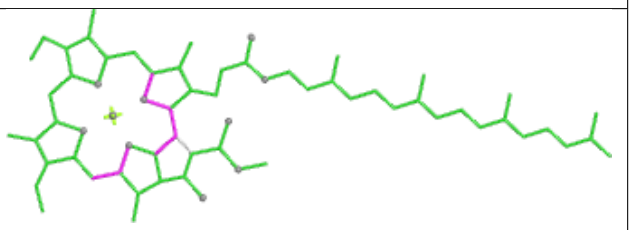


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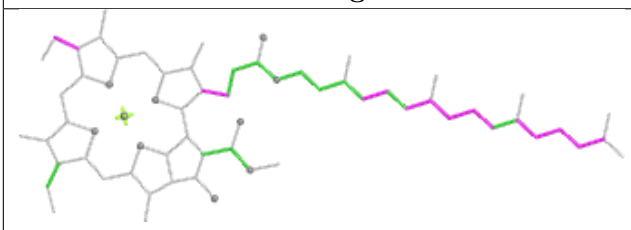
Ligand CLA B 810



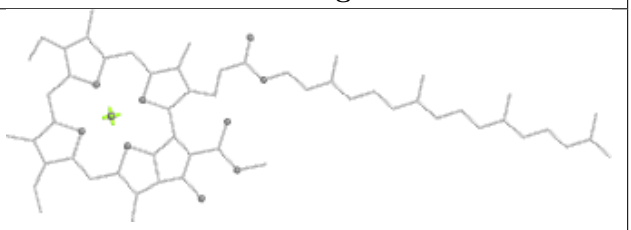
Bond lengths



Bond angles

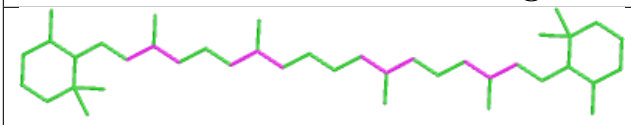


Torsions



Rings

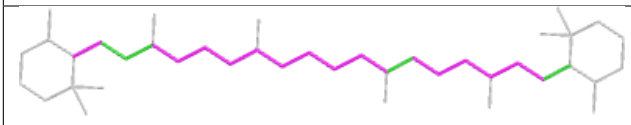
Ligand BCR B 834



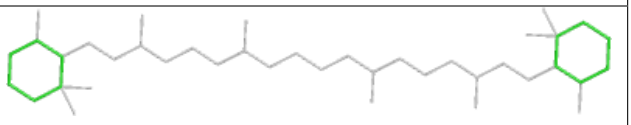
Bond lengths



Bond angles

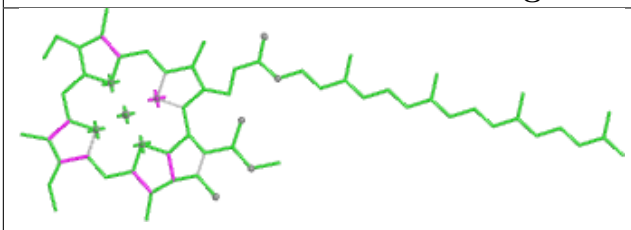


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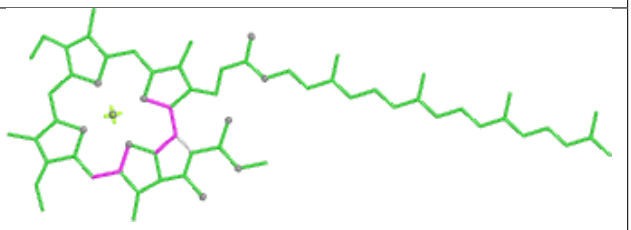


Rings

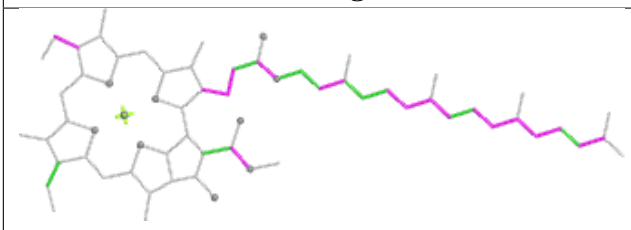
Ligand CLA A 809



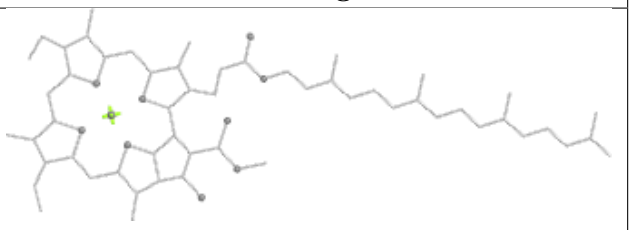
Bond lengths



Bond angles

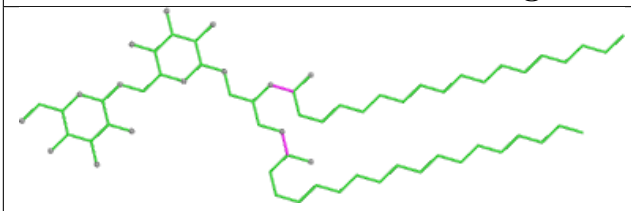


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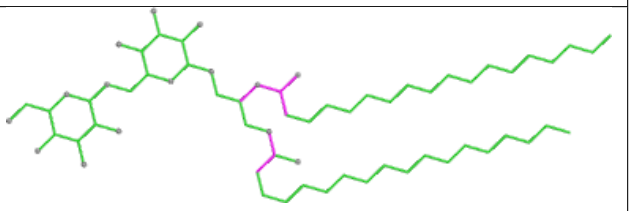


Rings

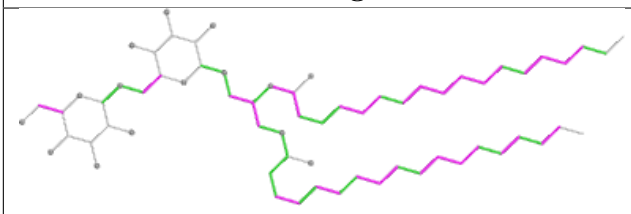
Ligand DGD b 837



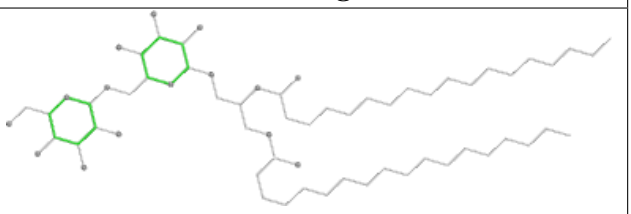
Bond lengths



Bond angles

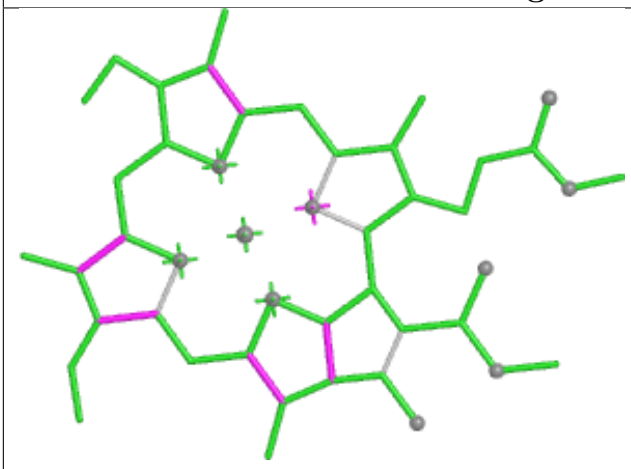


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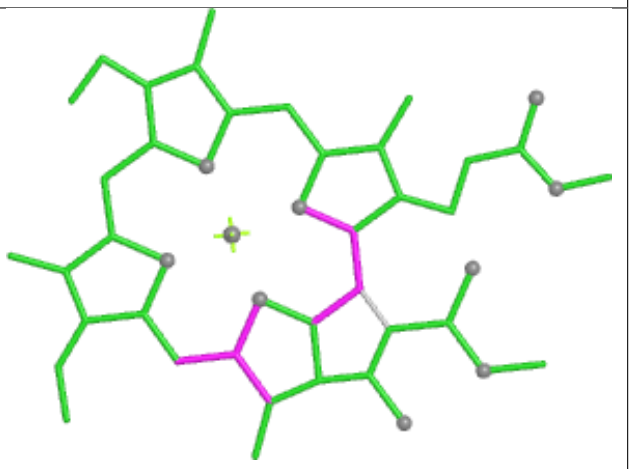


Rings

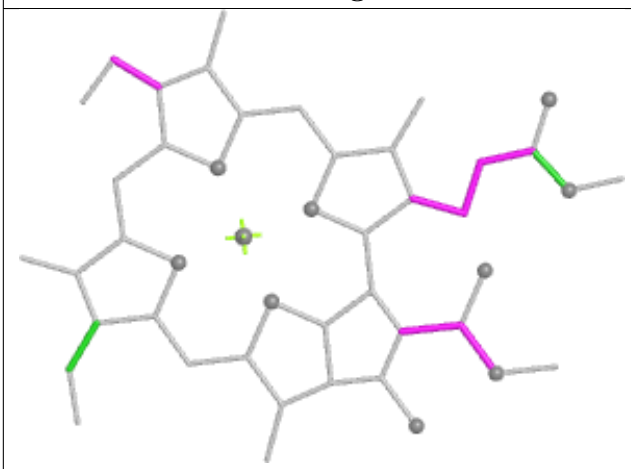
Ligand CLA b 816



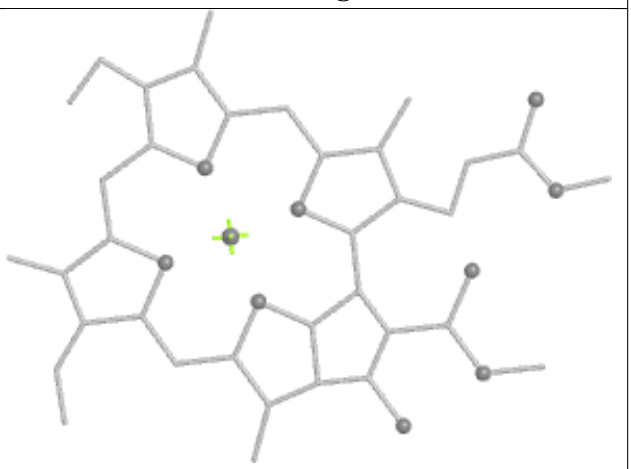
Bond lengths



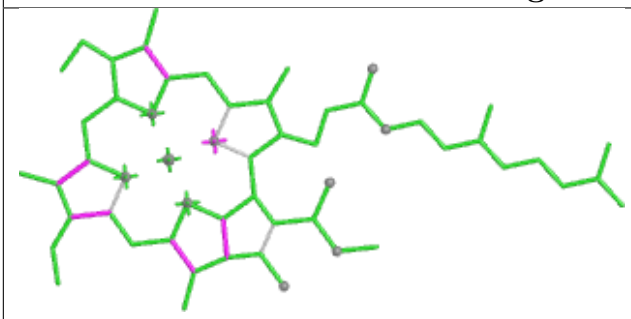
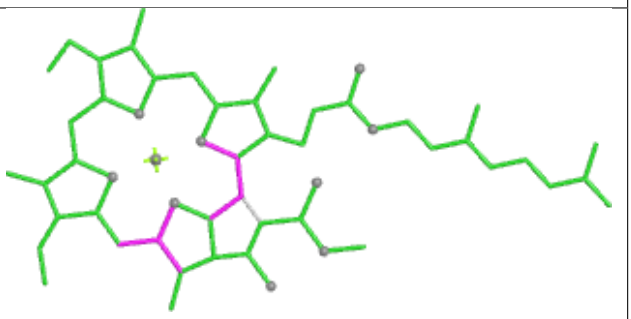
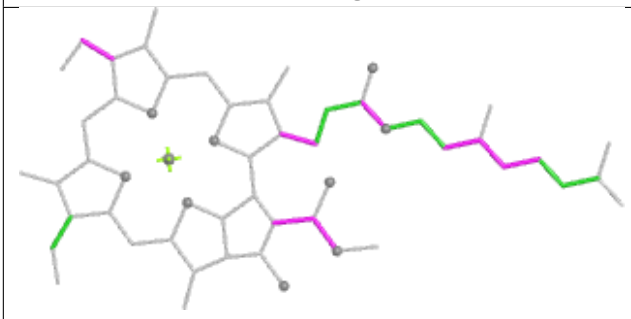
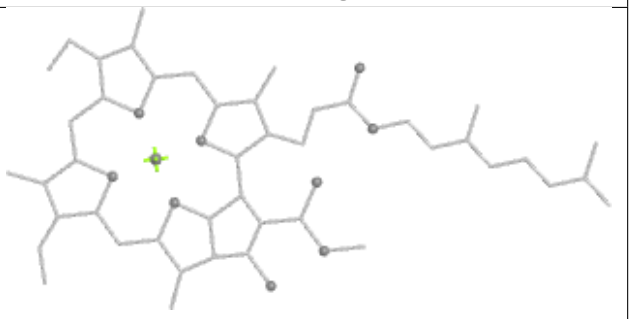
Bond angles

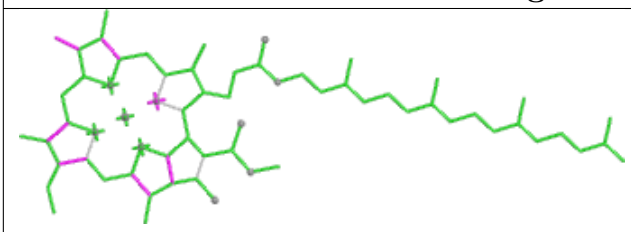
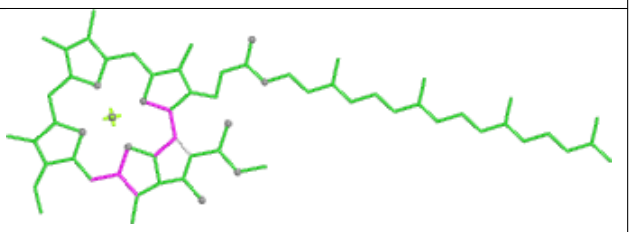
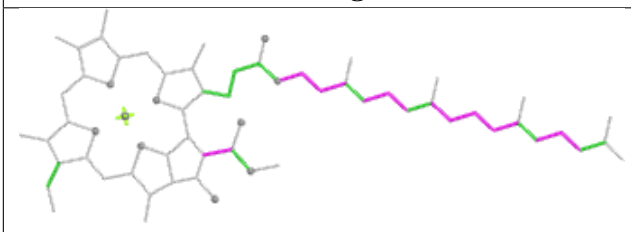
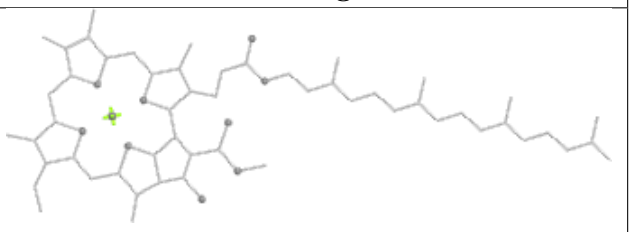


Torsions

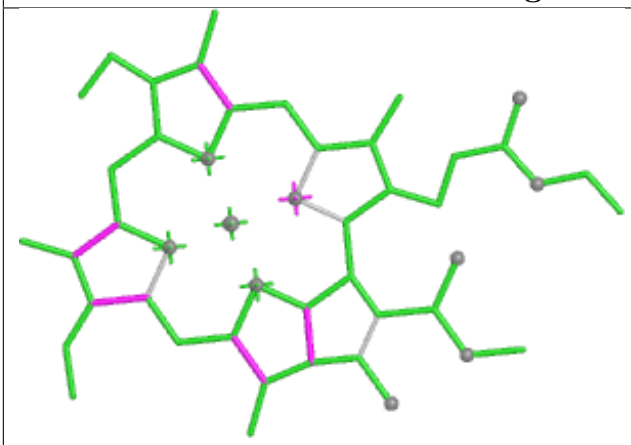


Rings

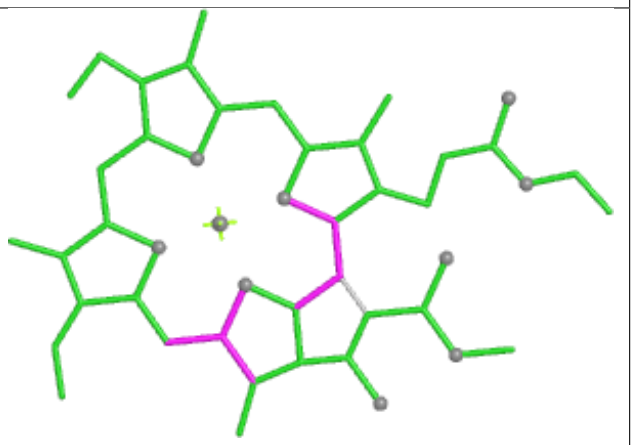
Ligand CLA b 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

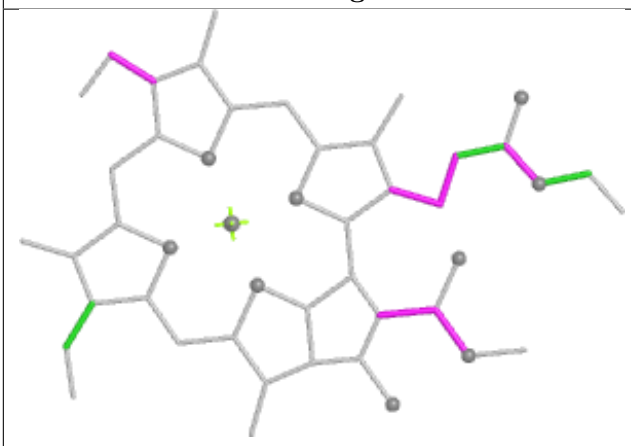
Ligand CLA B 822



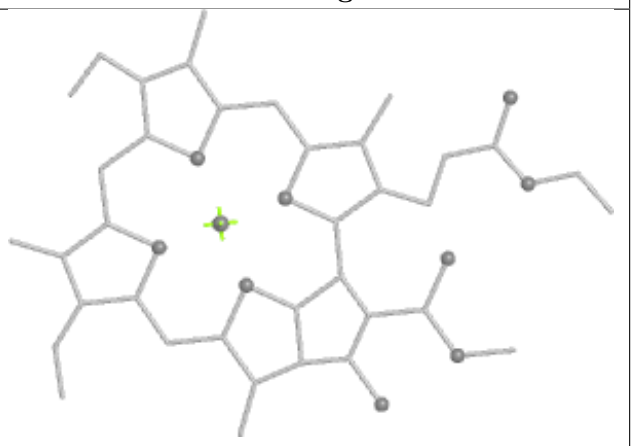
Bond lengths



Bond angles

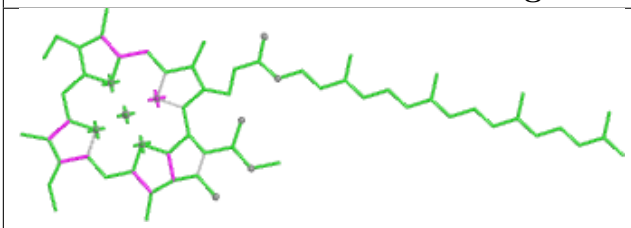


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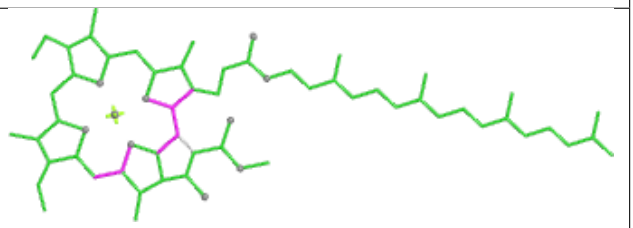


Rings

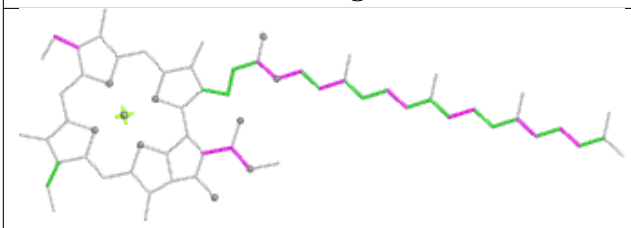
Ligand CLA B 803



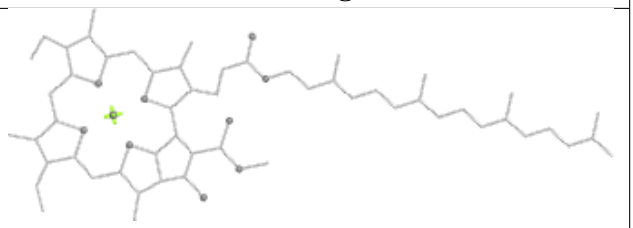
Bond lengths



Bond angles

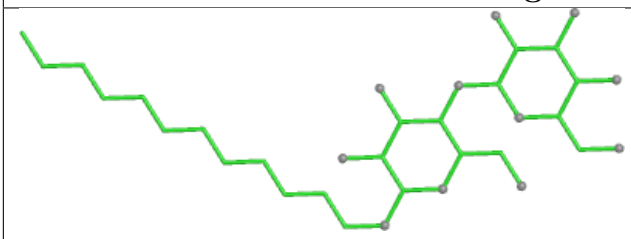


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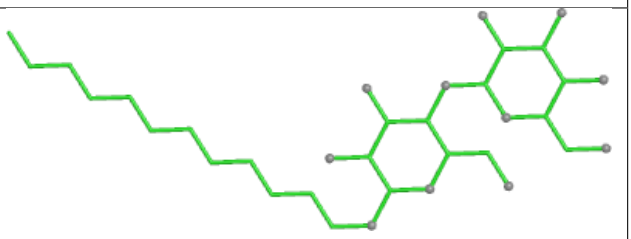


Rings

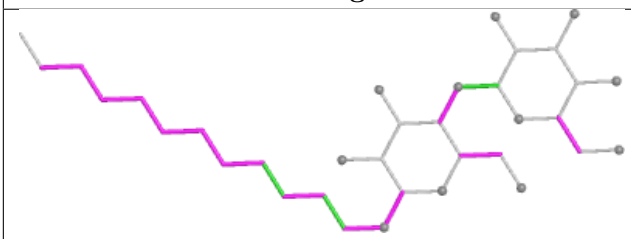
Ligand LMT b 838



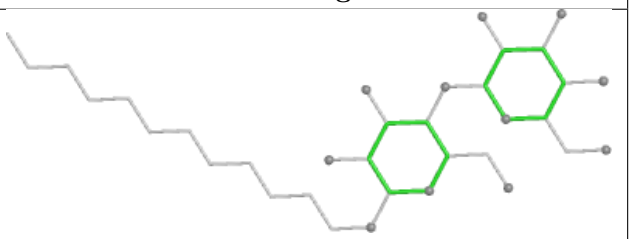
Bond lengths



Bond angles

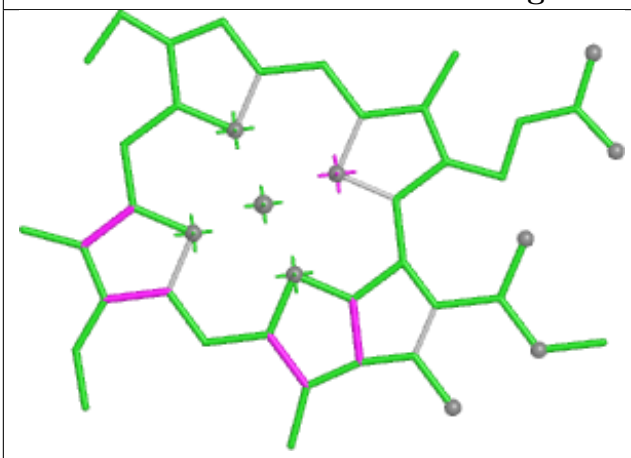


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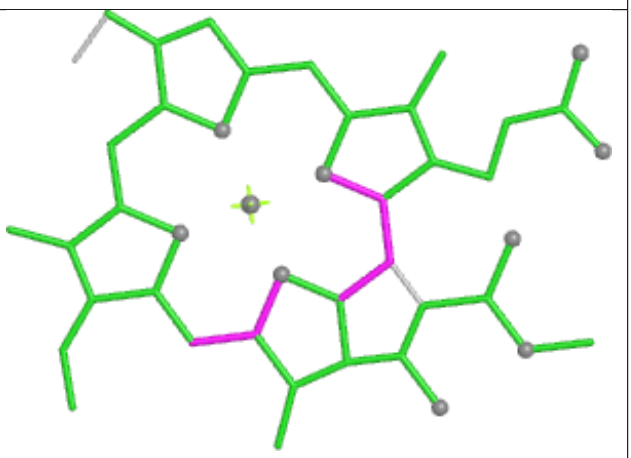


Rings

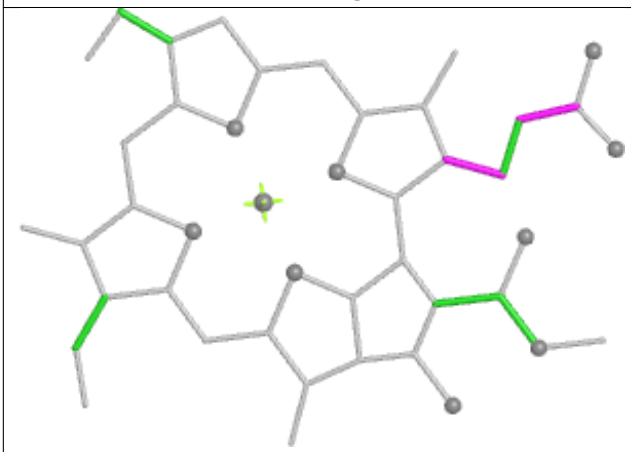
Ligand CLA b 813



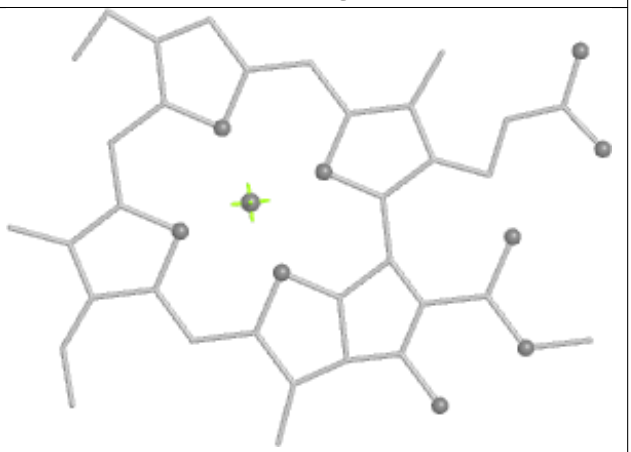
Bond lengths



Bond angles

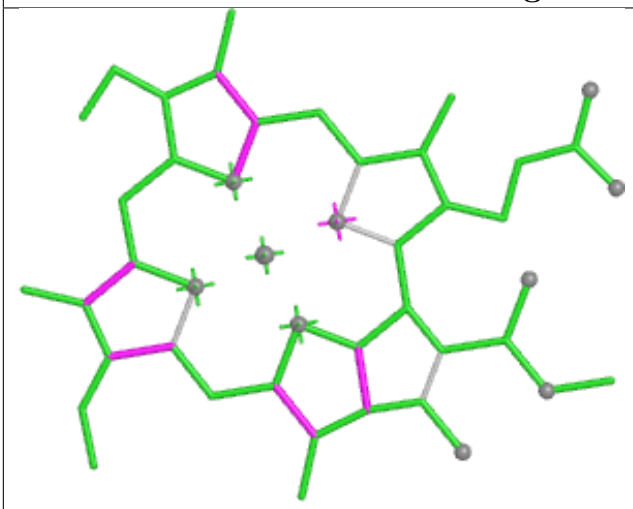


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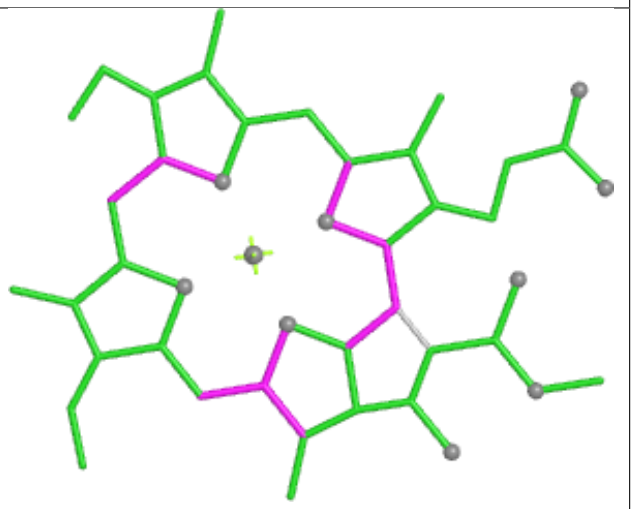


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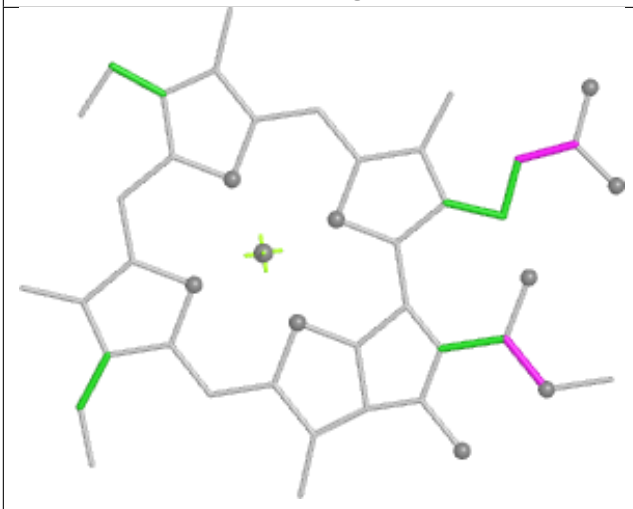
Ligand CLA A 814



Bond lengths



Bond angles

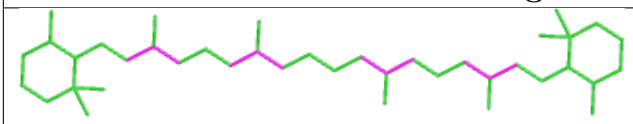


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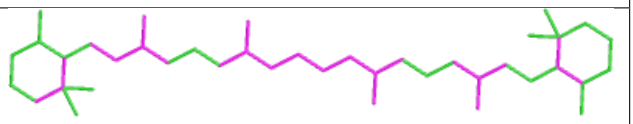


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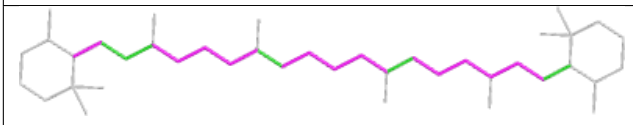
Ligand BCR b 834



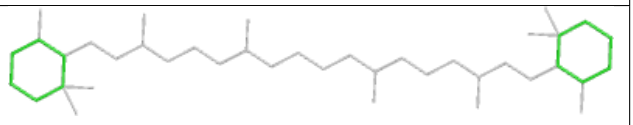
Bond lengths



Bond angles

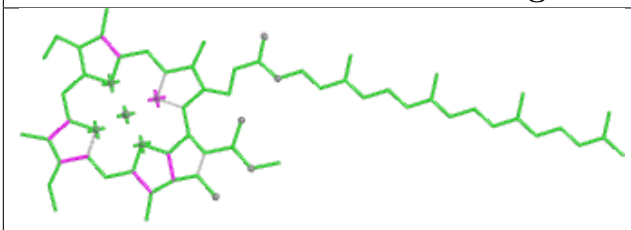


Torsions

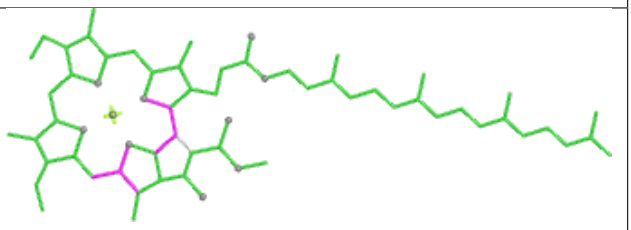


Rings

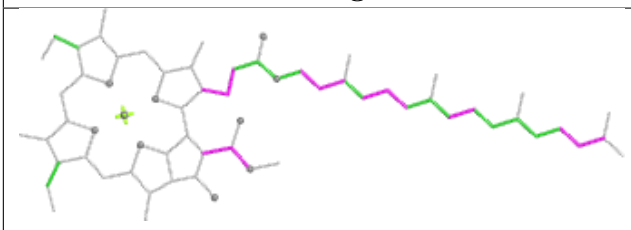
Ligand CLA a 822



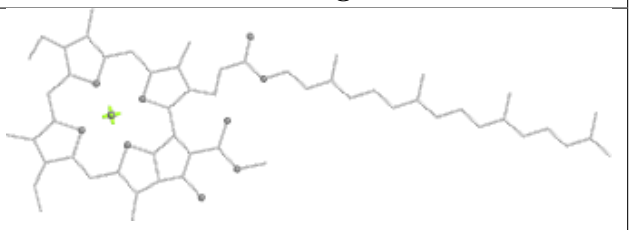
Bond lengths



Bond angles

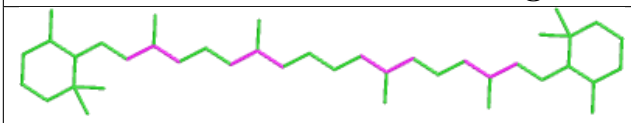


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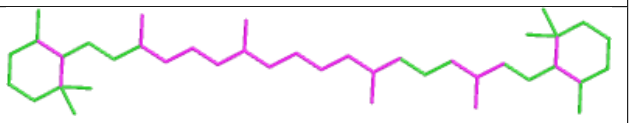


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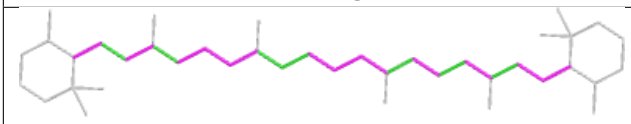
Ligand BCR L 306



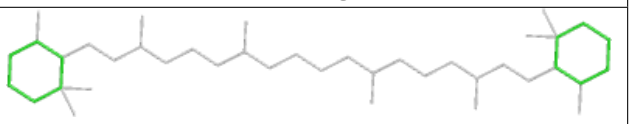
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Bond angles

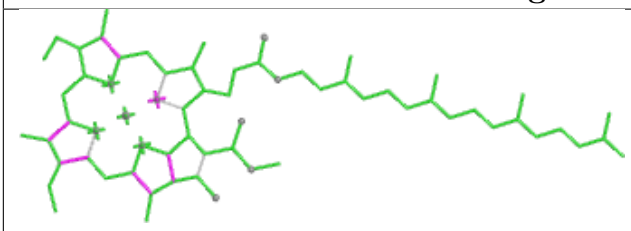


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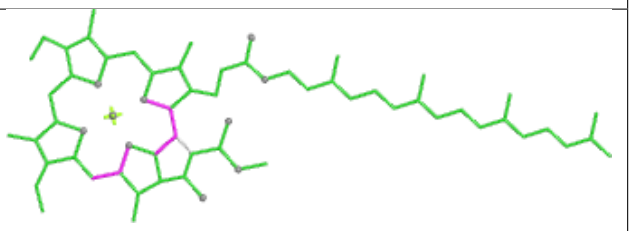


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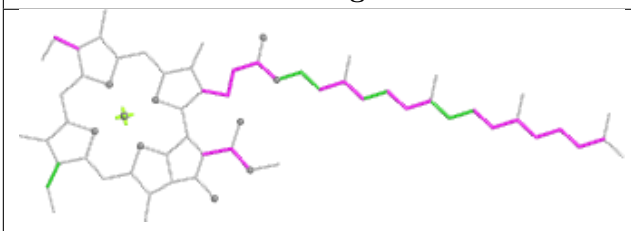
Ligand CLA a 815



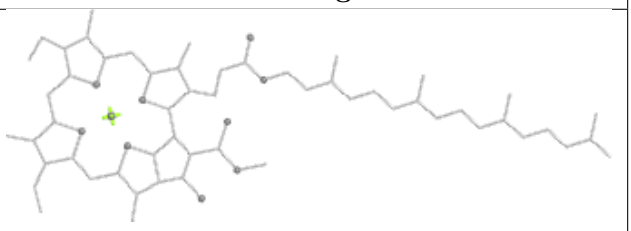
Bond lengths



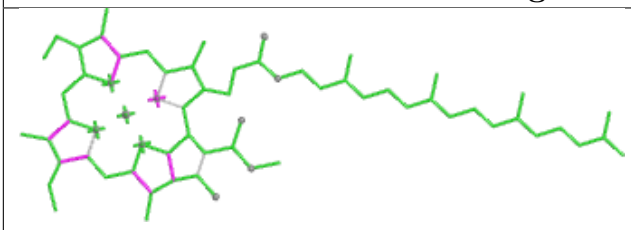
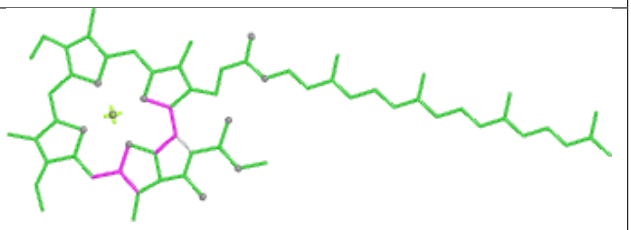
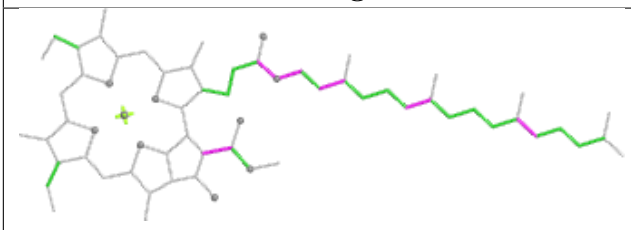
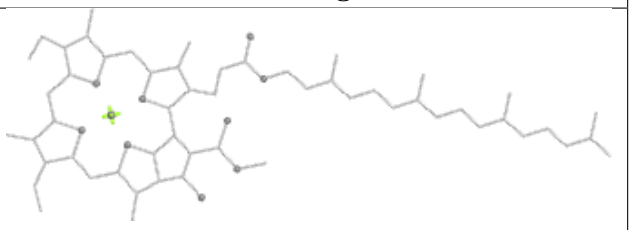
Bond angles

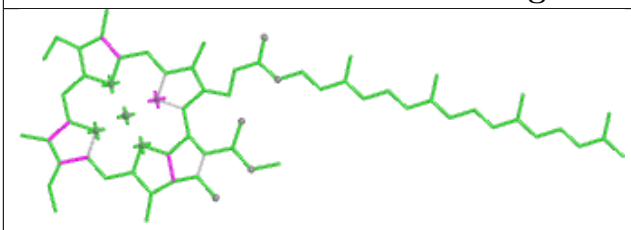
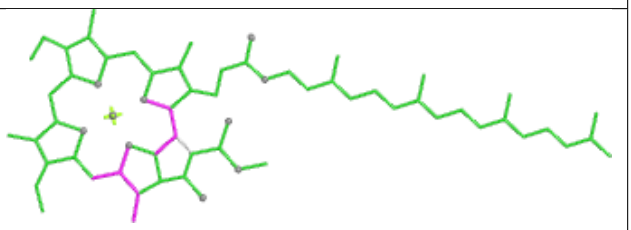
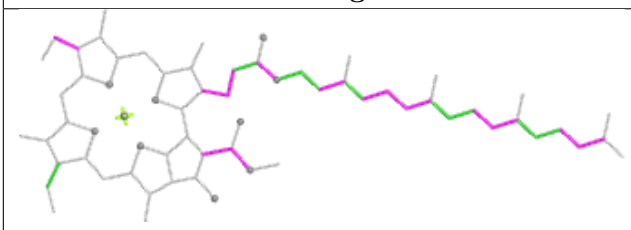
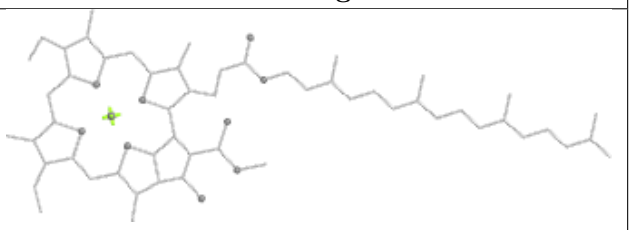


Torsions

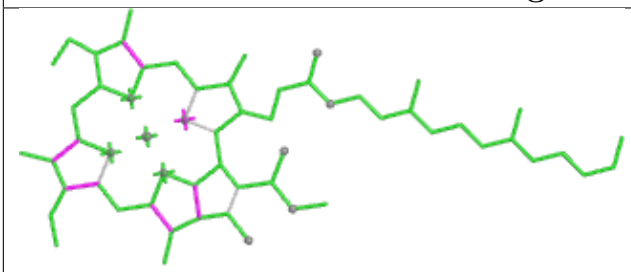


Rings

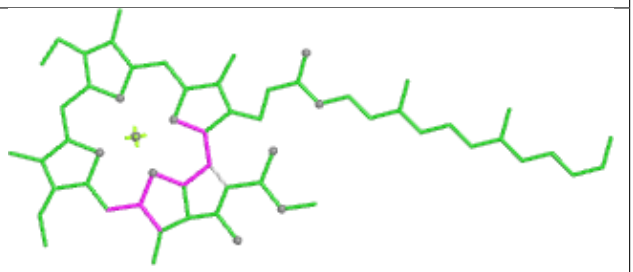
Ligand CLA a 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

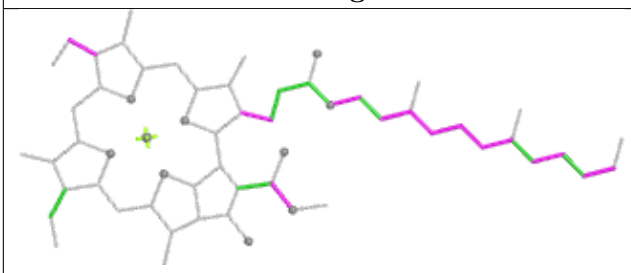
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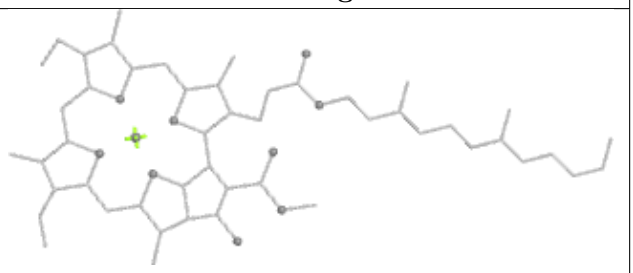
Bond lengths



Bond angles

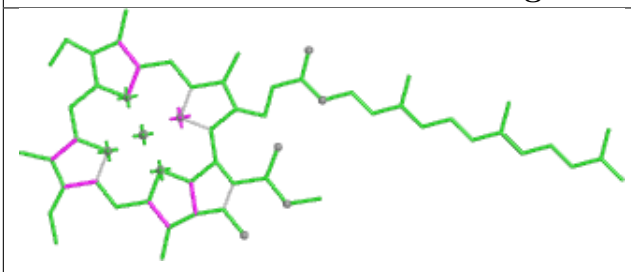


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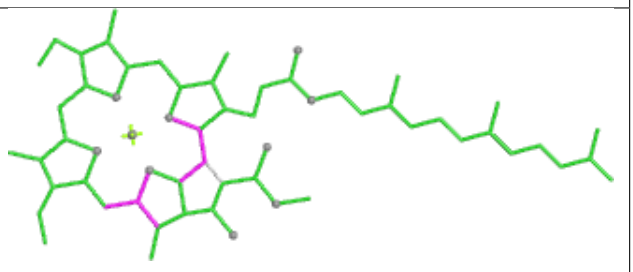


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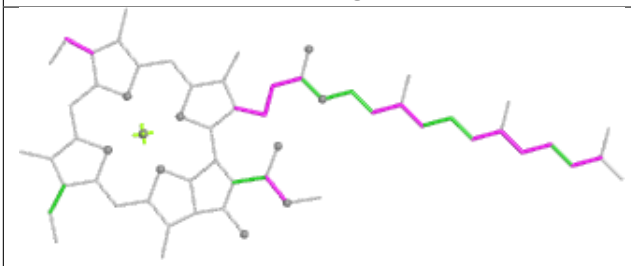
Ligand CLA B 819



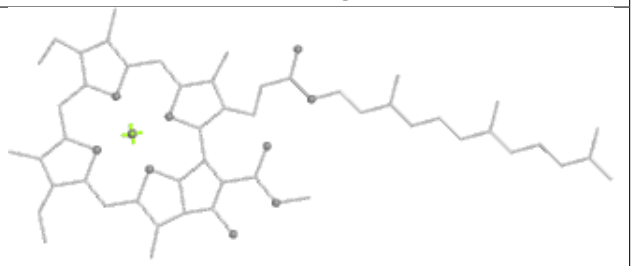
Bond lengths



Bond angles

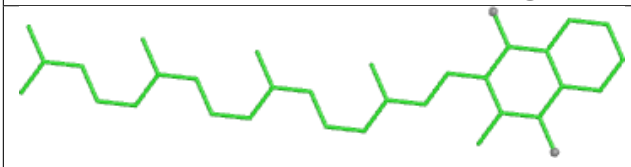


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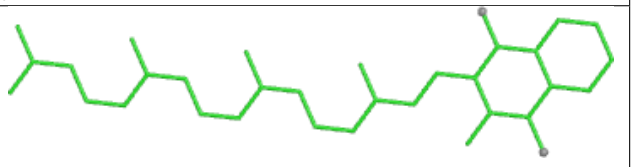


Rings

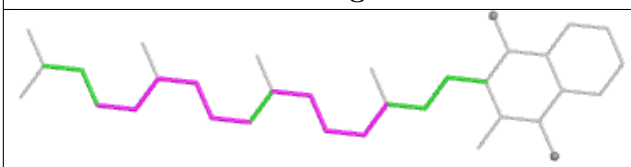
Ligand PQN A 837



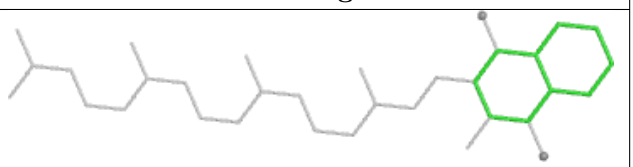
Bond lengths



Bond angles

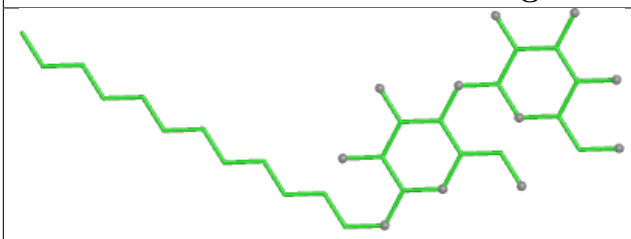


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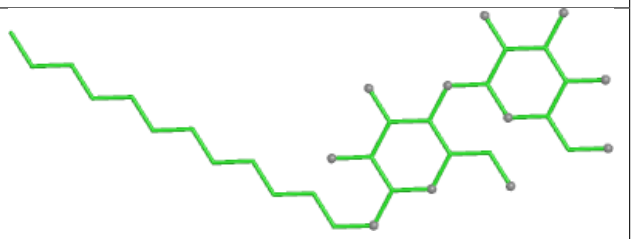


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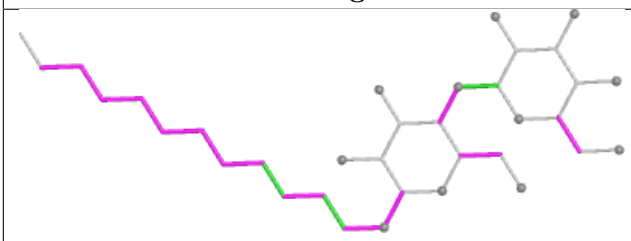
Ligand LMT B 838



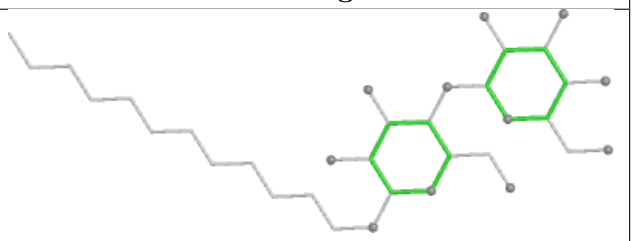
Bond lengths



Bond angles

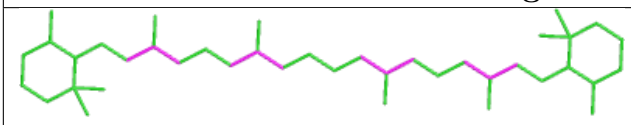


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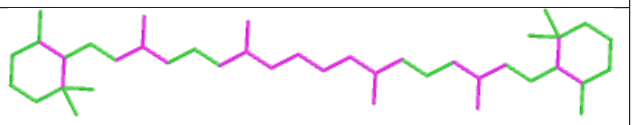


Rings

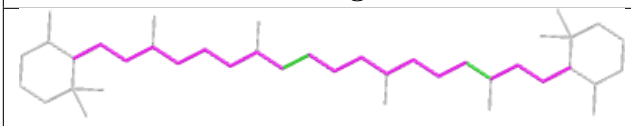
Ligand BCR B 835



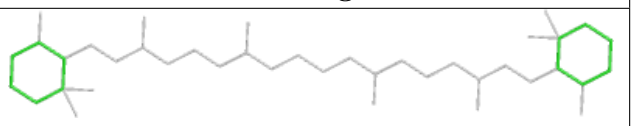
Bond lengths



Bond angles

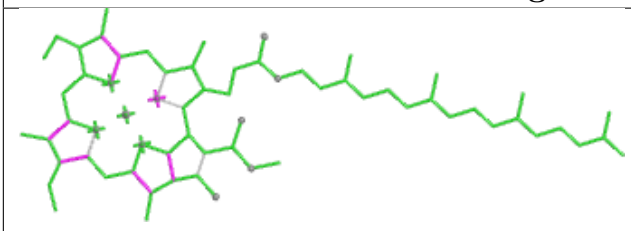


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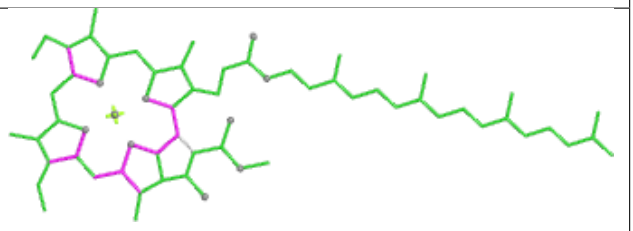


Rings

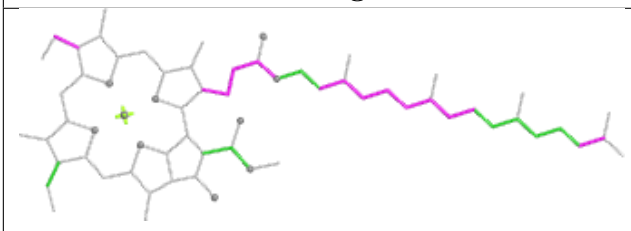
Ligand CLA a 816



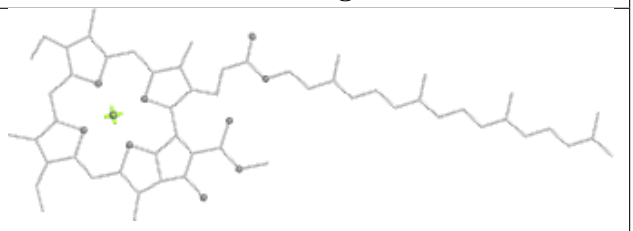
Bond lengths



Bond angles

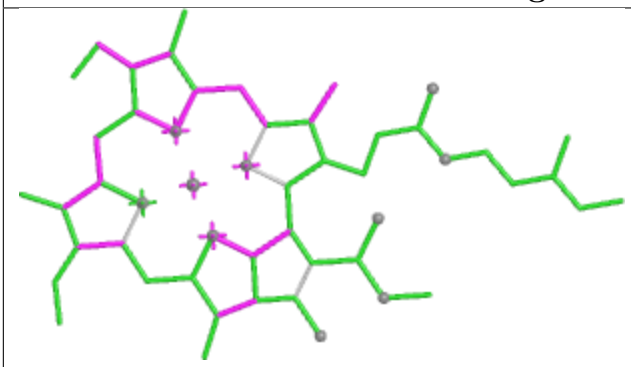


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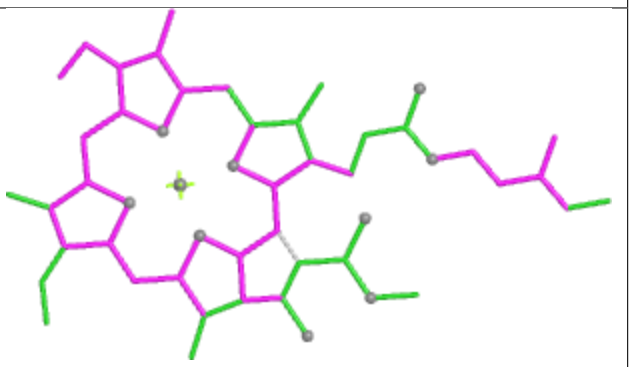


Rings

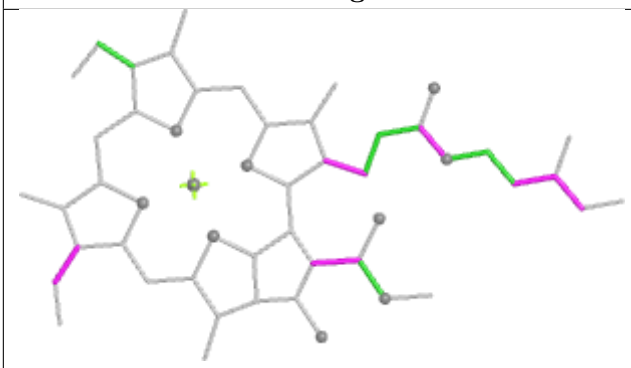
Ligand CLA a 820



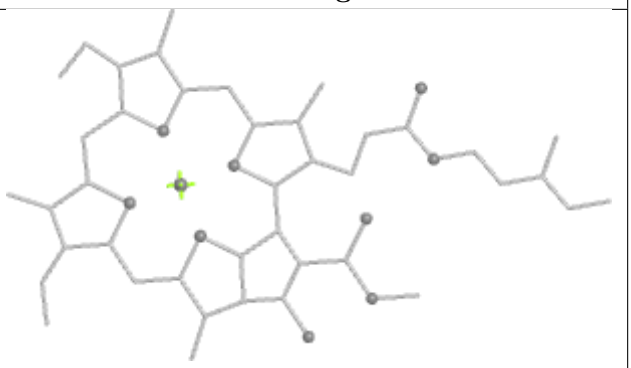
Bond lengths



Bond angles

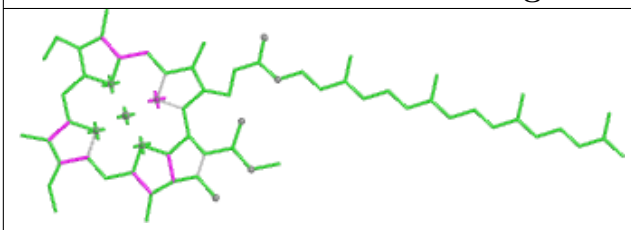


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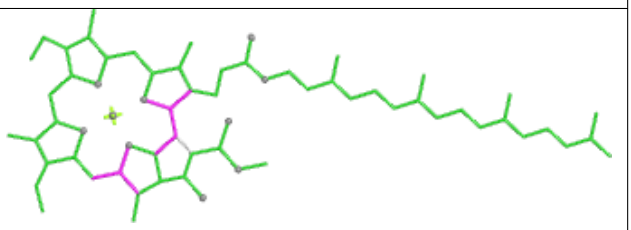


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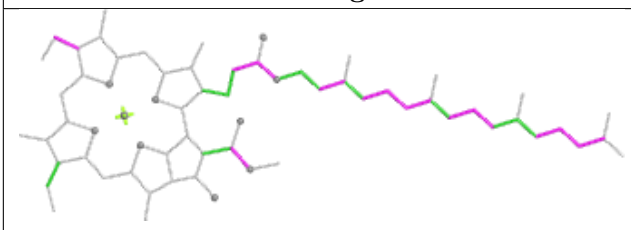
Ligand CLA A 801



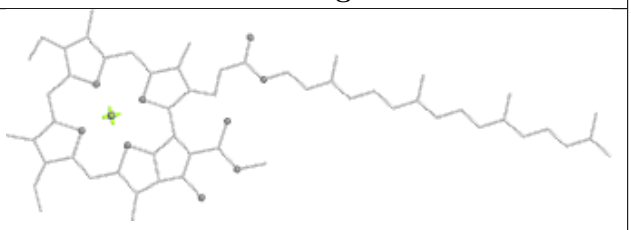
Bond lengths



Bond angles

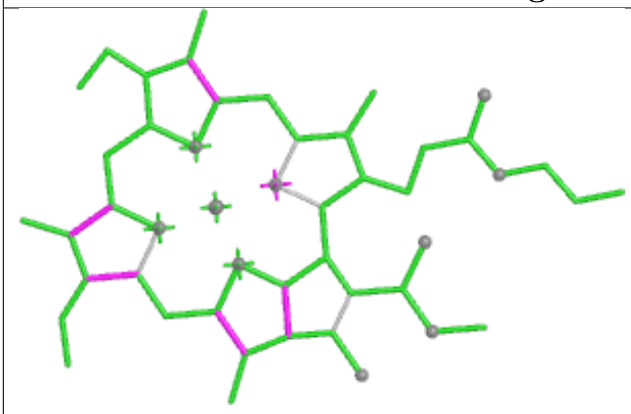


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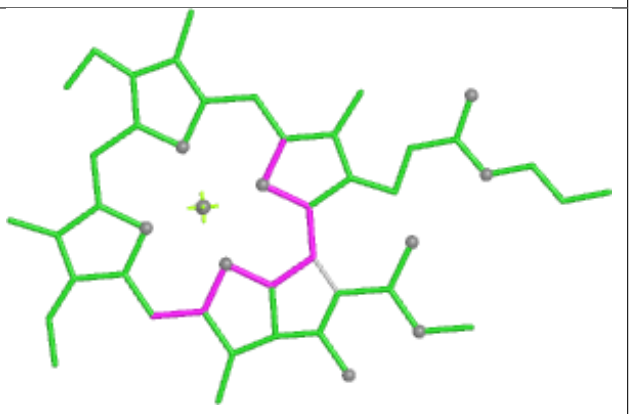


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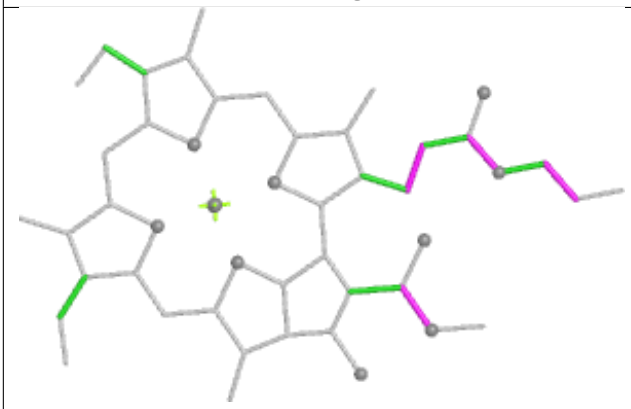
Ligand CLA a 837



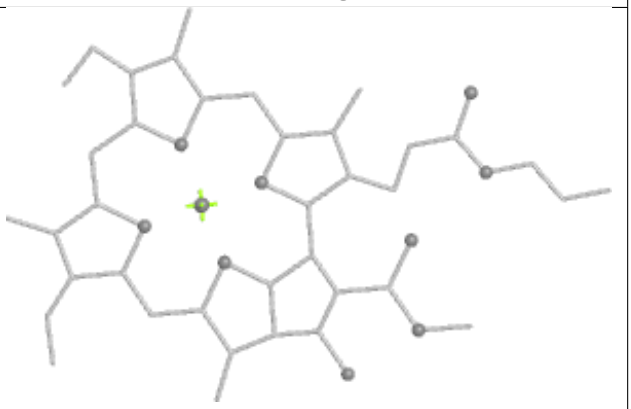
Bond lengths



Bond angles

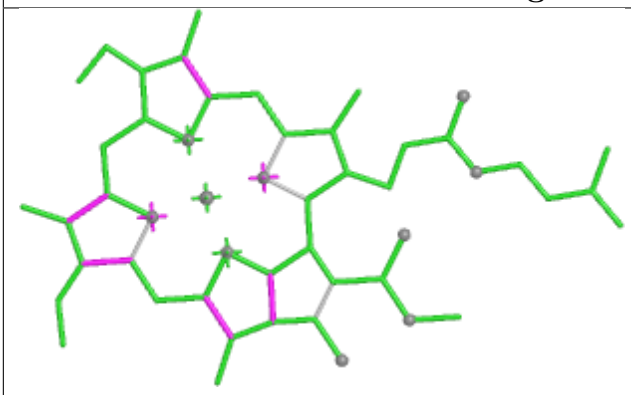


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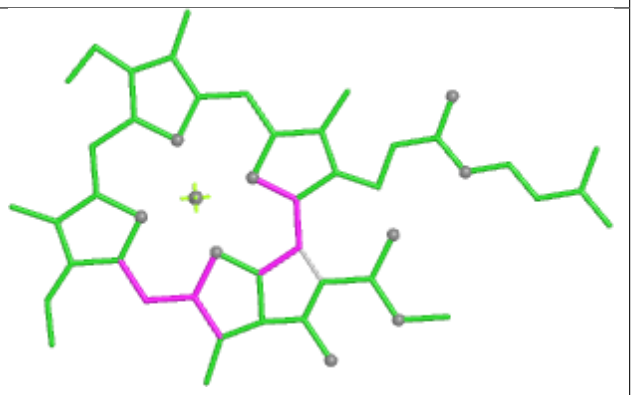


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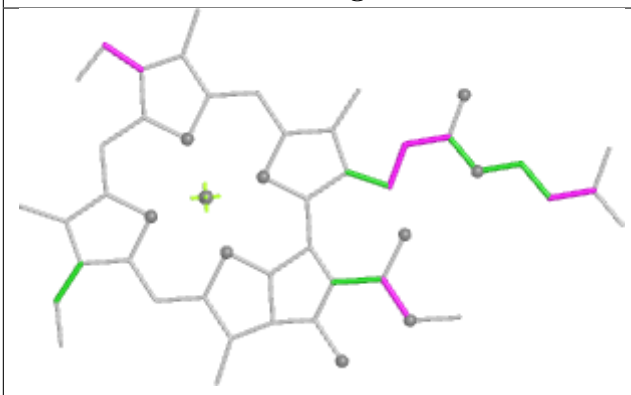
Ligand CLA b 820



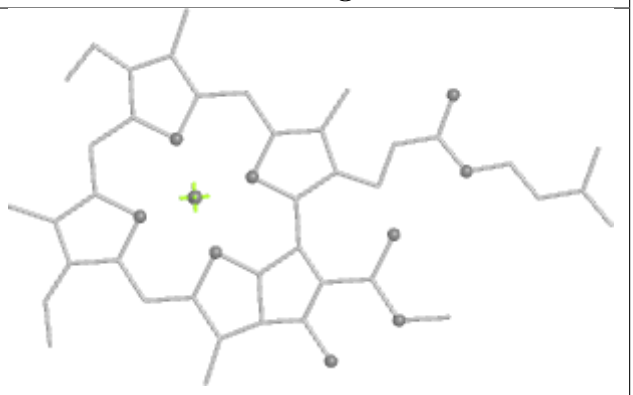
Bond lengths



Bond angles

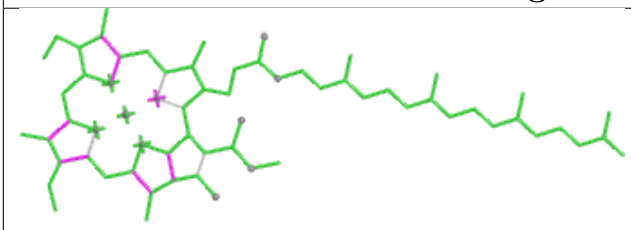


Torsions

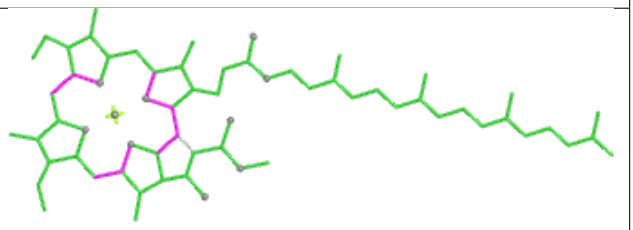


Rings

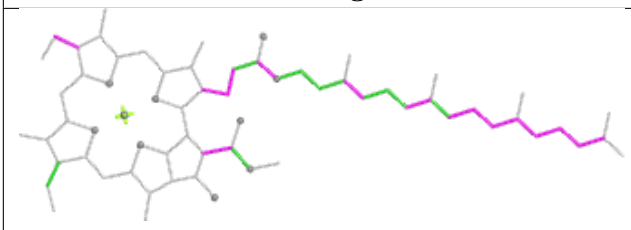
Ligand CLA a 824



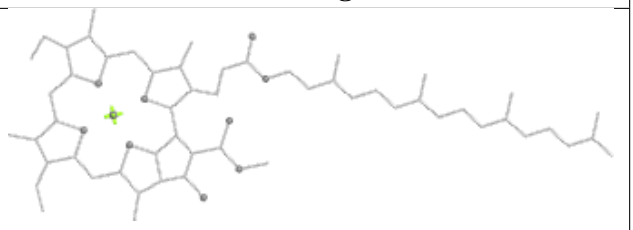
Bond lengths



Bond angles



Torsions

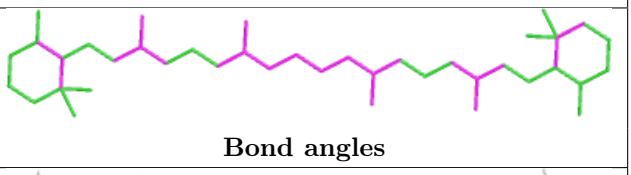


Rings

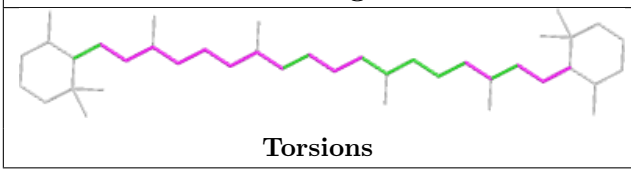
Ligand BCR A 840



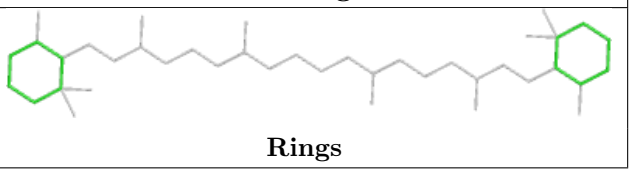
Bond lengths



Bond angles

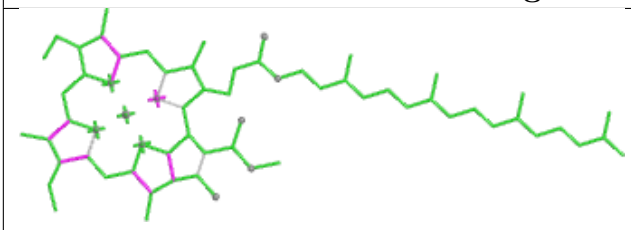


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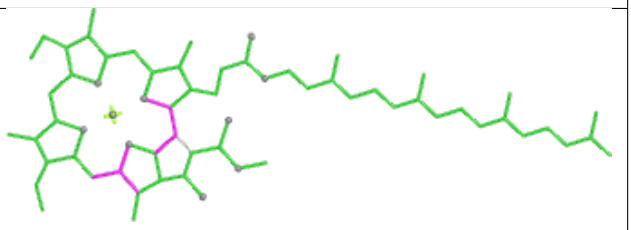


Rings

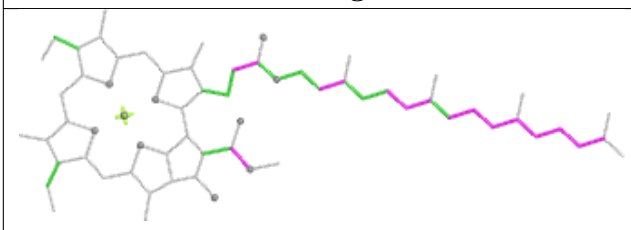
Ligand CLA A 846



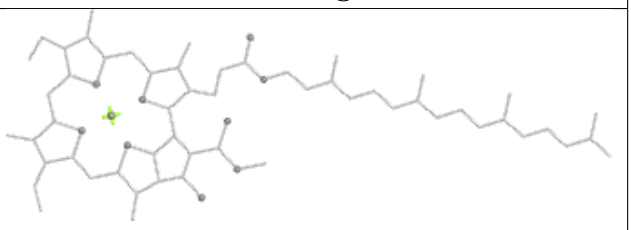
Bond lengths



Bond angles

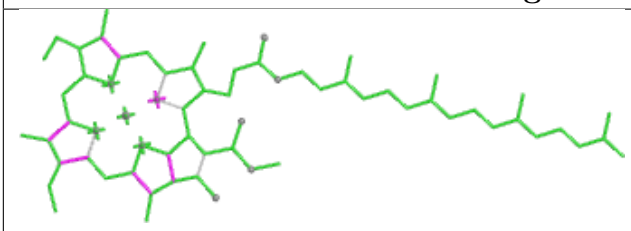


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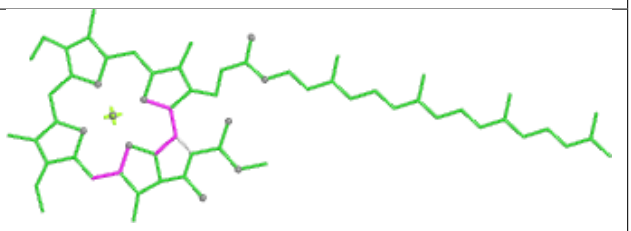


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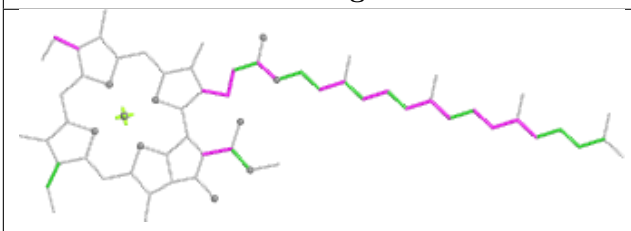
Ligand CLA A 805



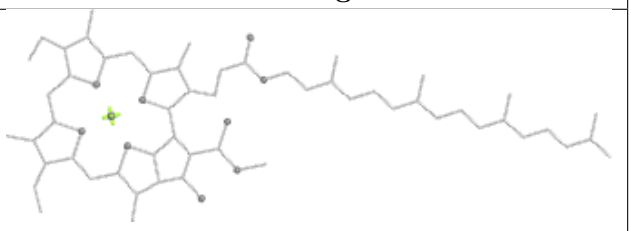
Bond lengths



Bond angles

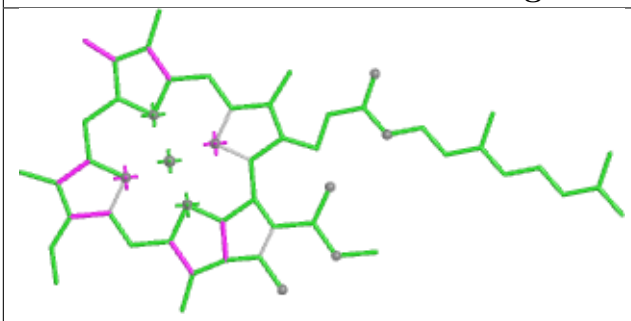


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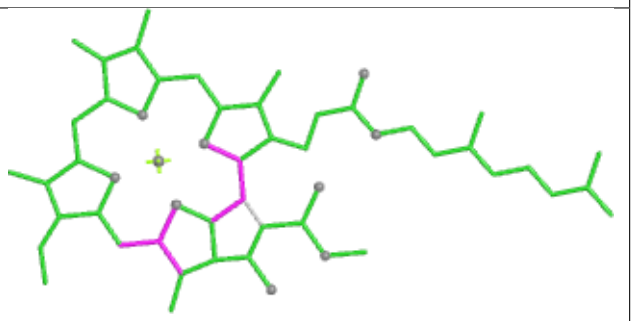


Rings

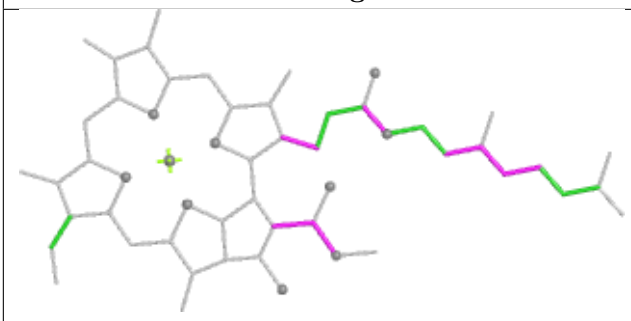
Ligand CLA B 812



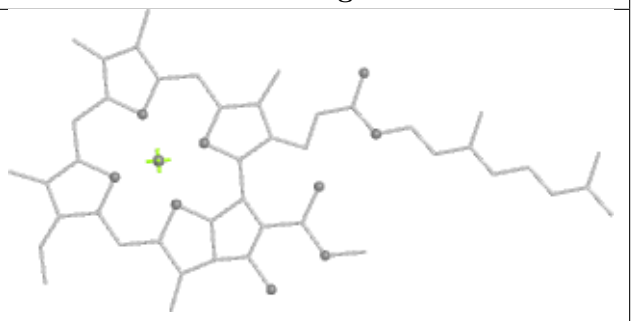
Bond lengths



Bond angles

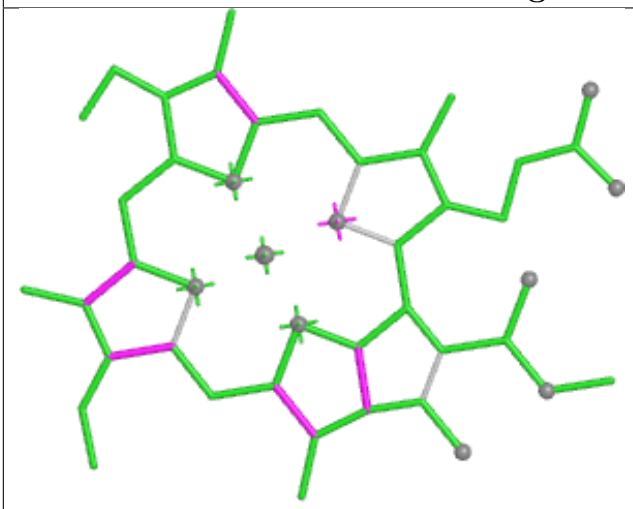


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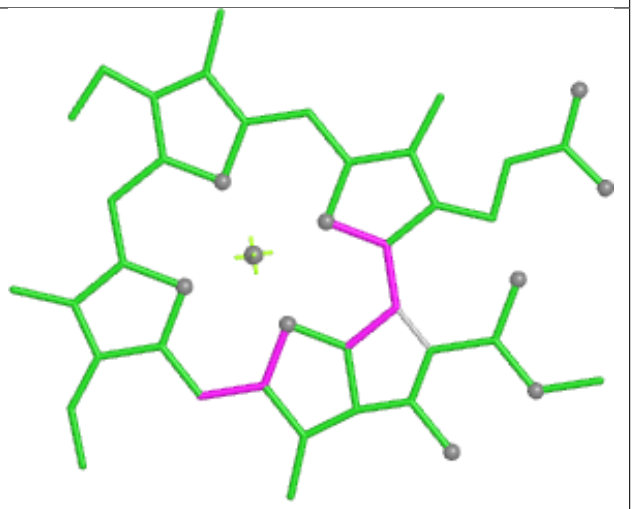


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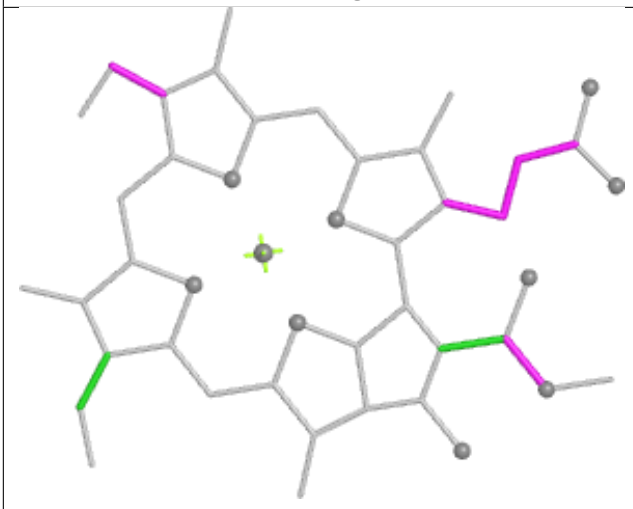
Ligand CLA a 818



Bond lengths



Bond angles

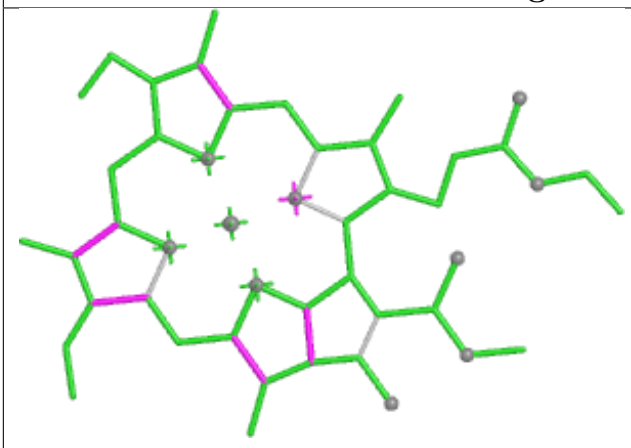


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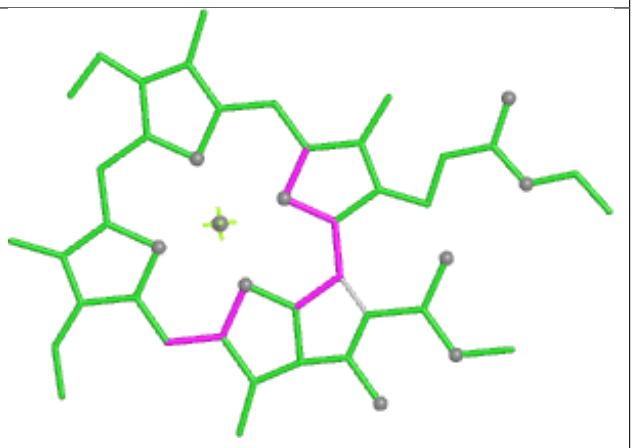


Rings

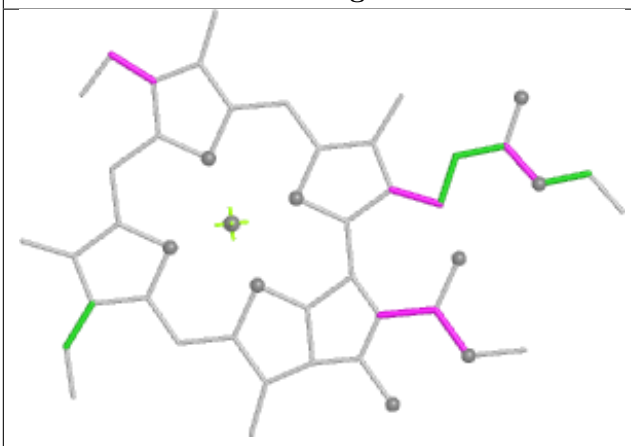
Ligand CLA a 835



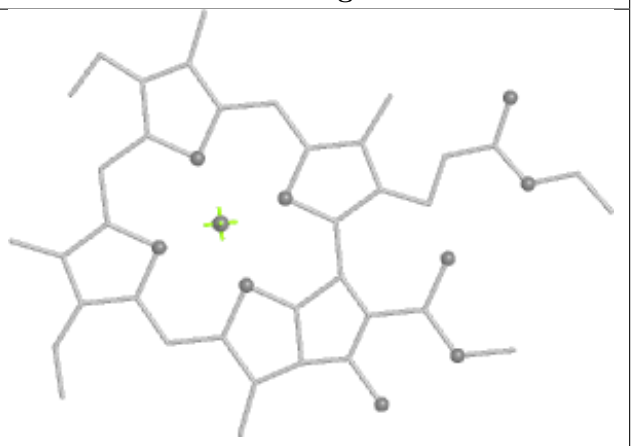
Bond lengths



Bond angles

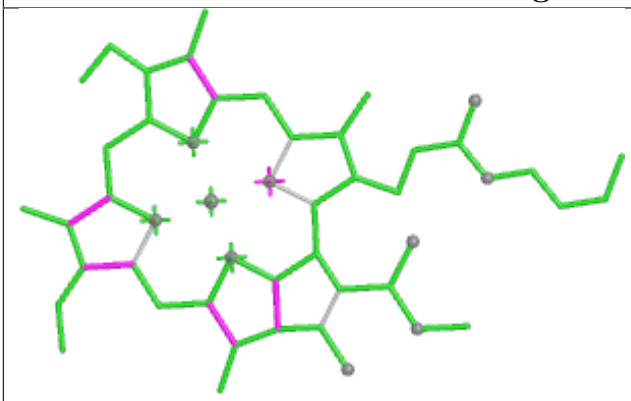


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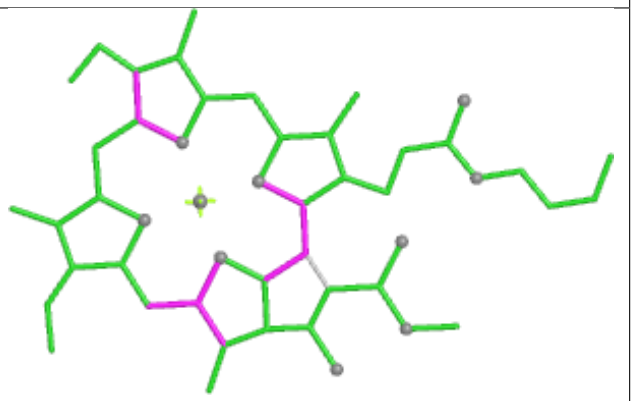


Rings

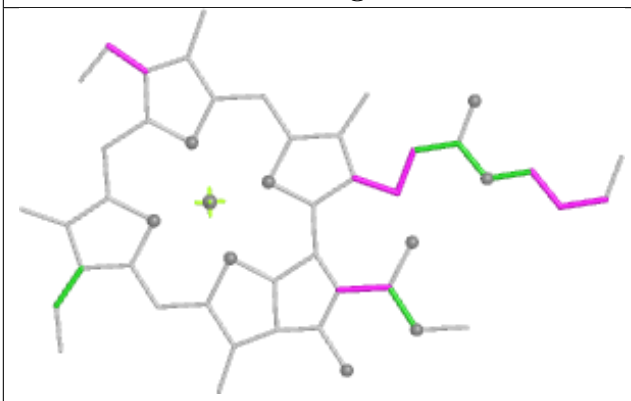
Ligand CLA l 305



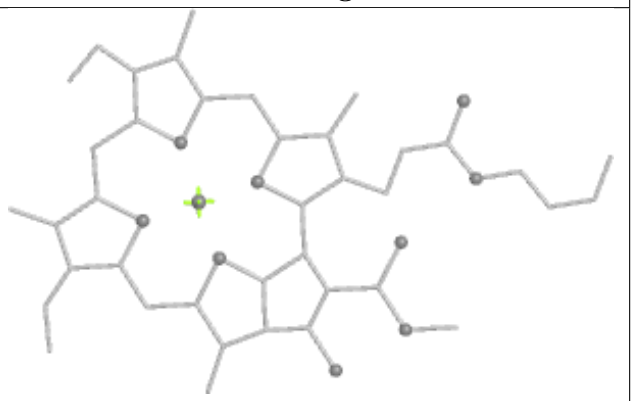
Bond lengths



Bond angles

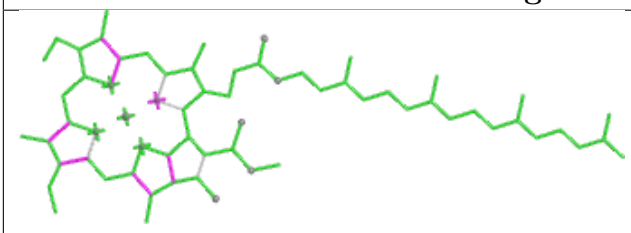


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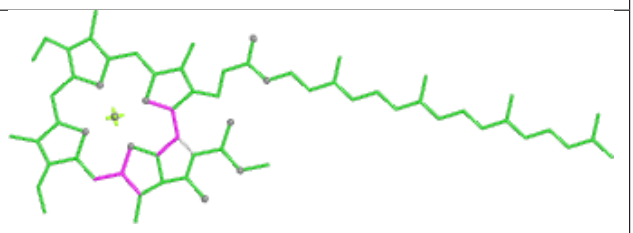


Rings

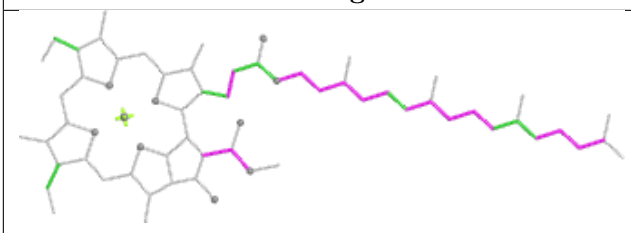
Ligand CLA B 802



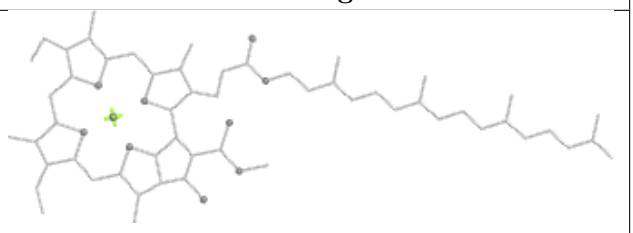
Bond lengths



Bond angles

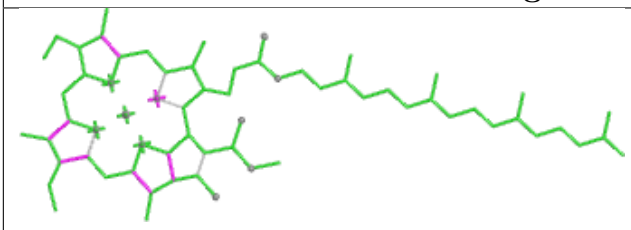


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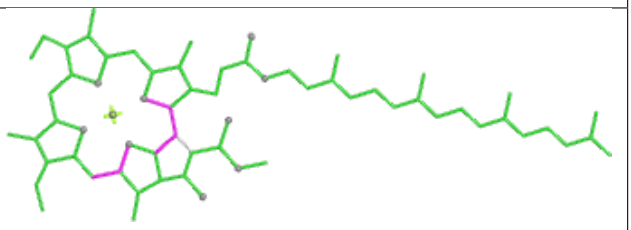


Rings

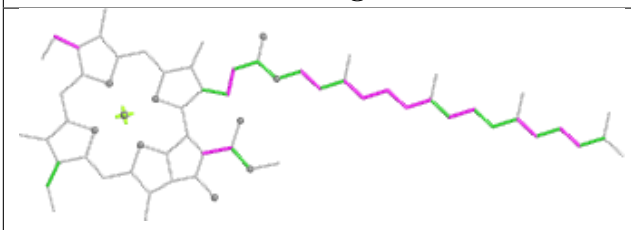
Ligand CLA A 822



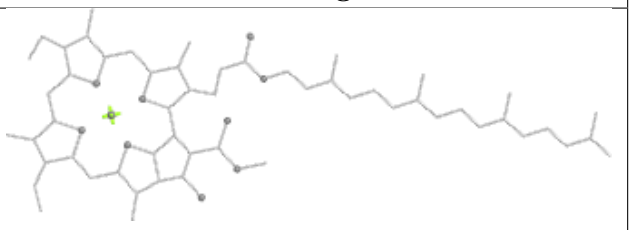
Bond lengths



Bond angles

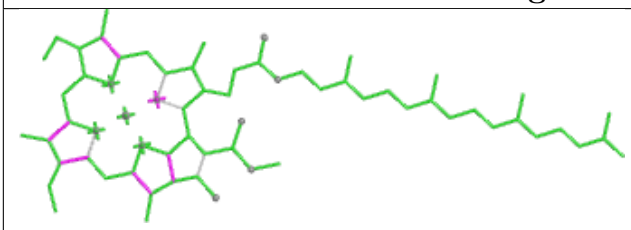


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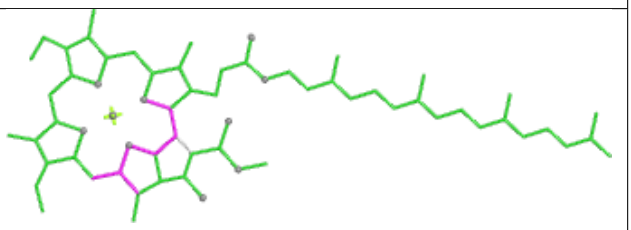


Rings

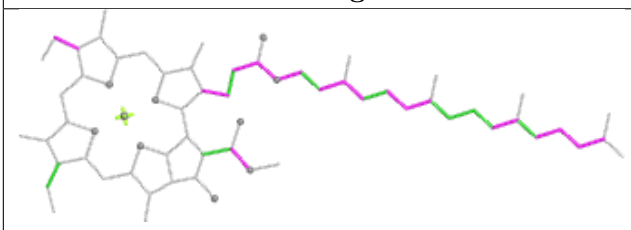
Ligand CLA a 808



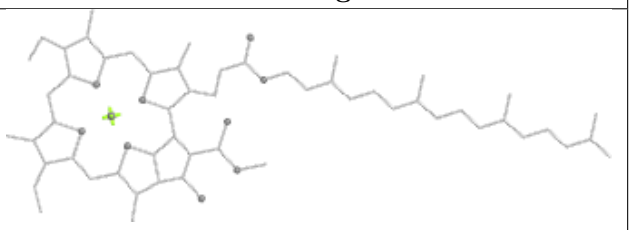
Bond lengths



Bond angles

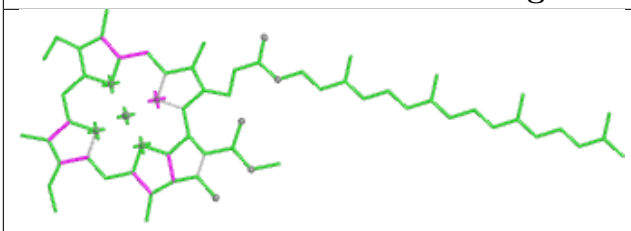


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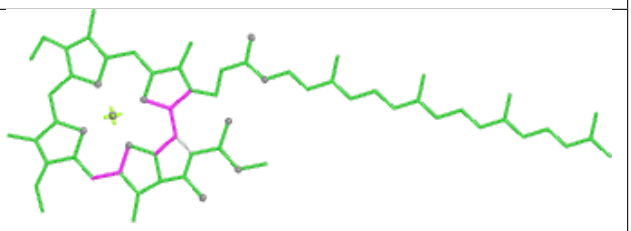


Rings

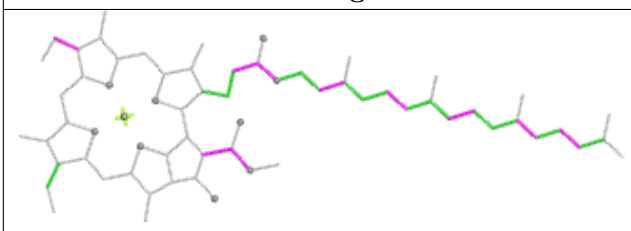
Ligand CLA b 803



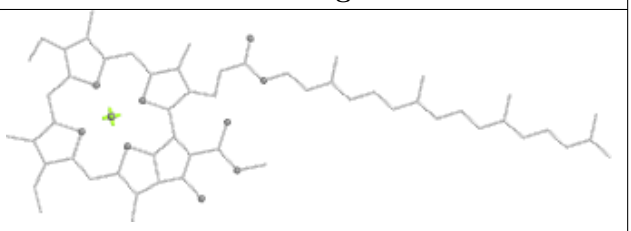
Bond lengths



Bond angles



Torsions

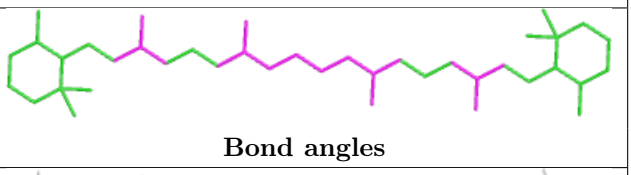


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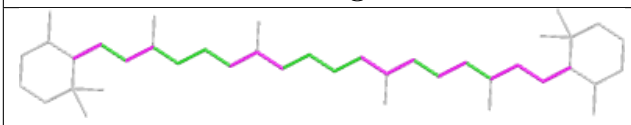
Ligand BCR L 305



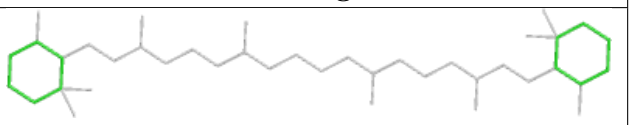
Bond lengths



Bond angles

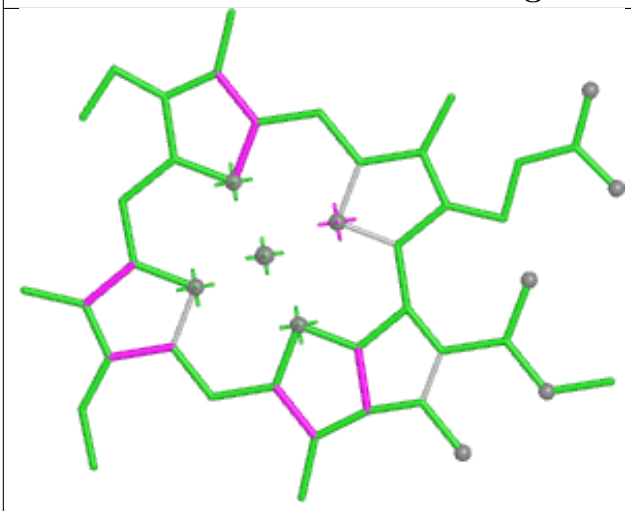


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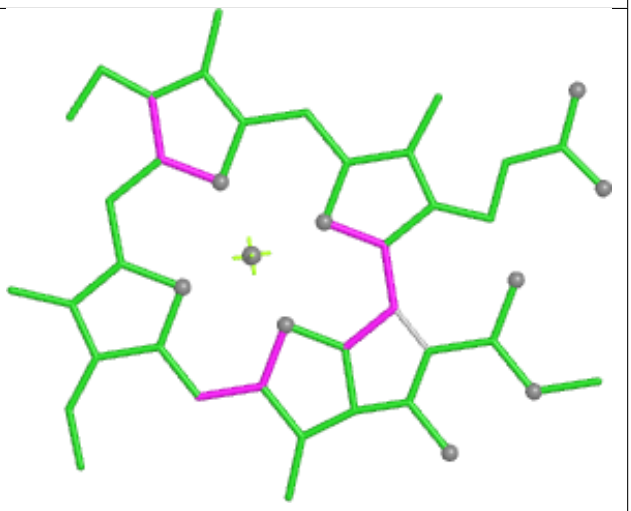


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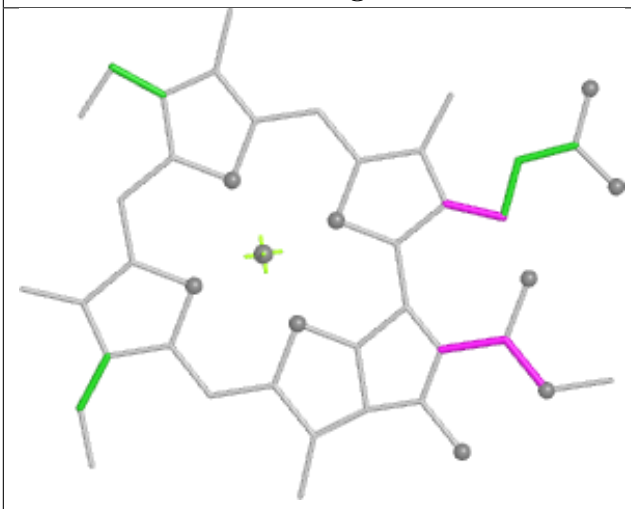
Ligand CLA B 805



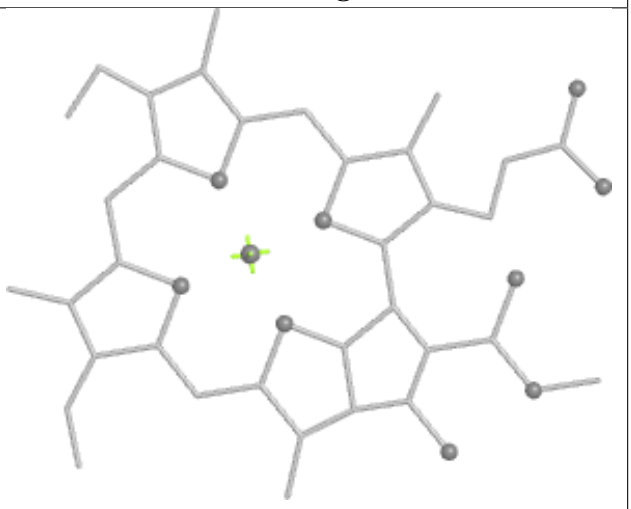
Bond lengths



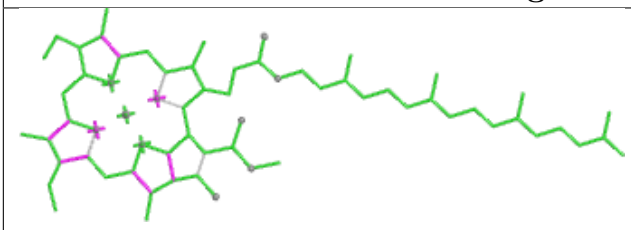
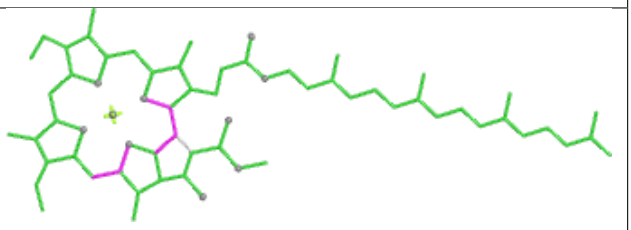
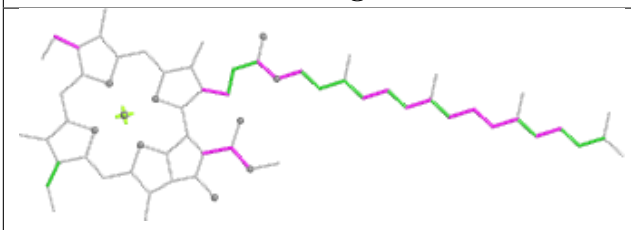
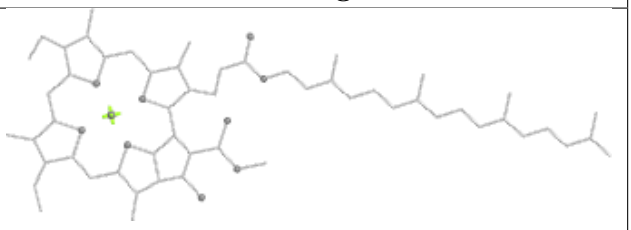
Bond angles

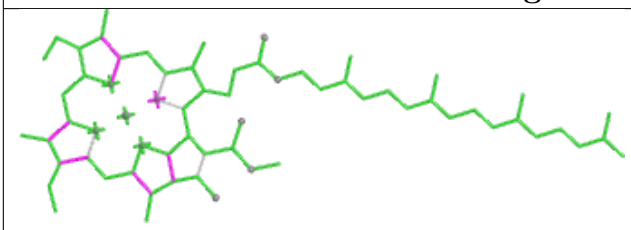
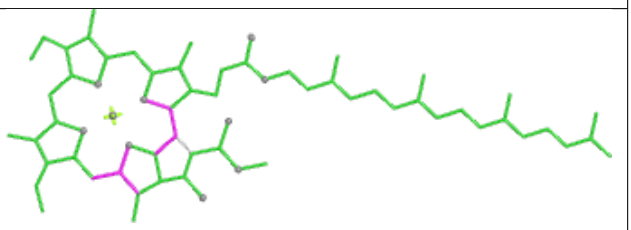
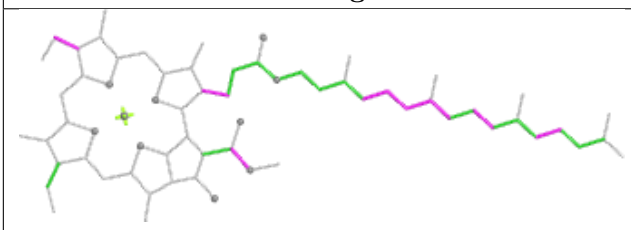
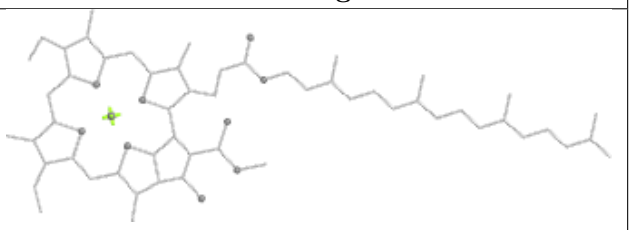


Torsions

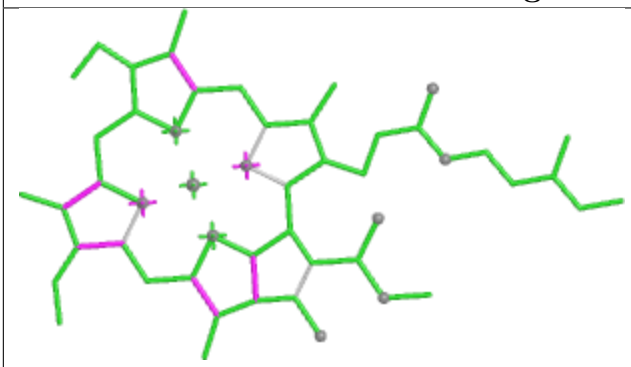


Rings

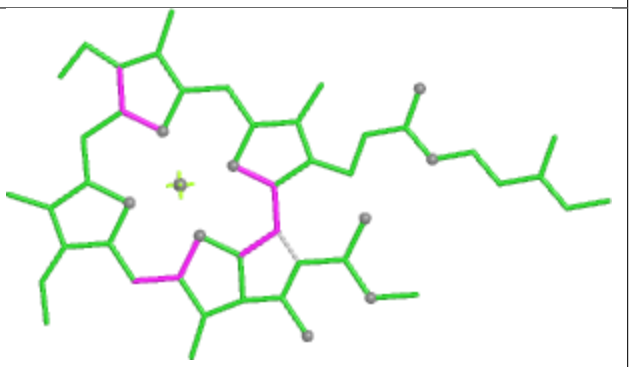
Ligand CLA b 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

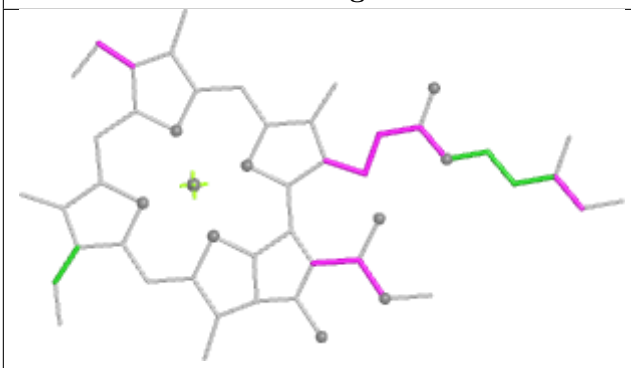
Ligand CLA A 831



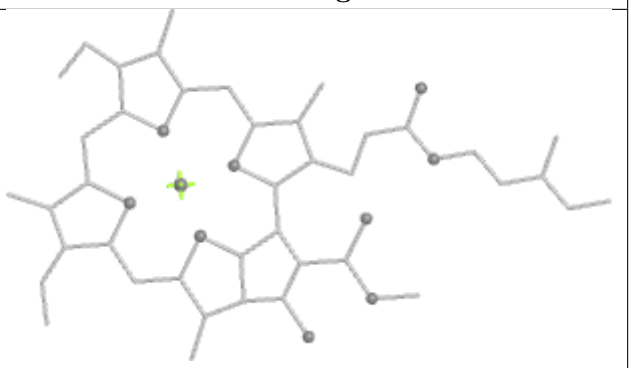
Bond lengths



Bond angles

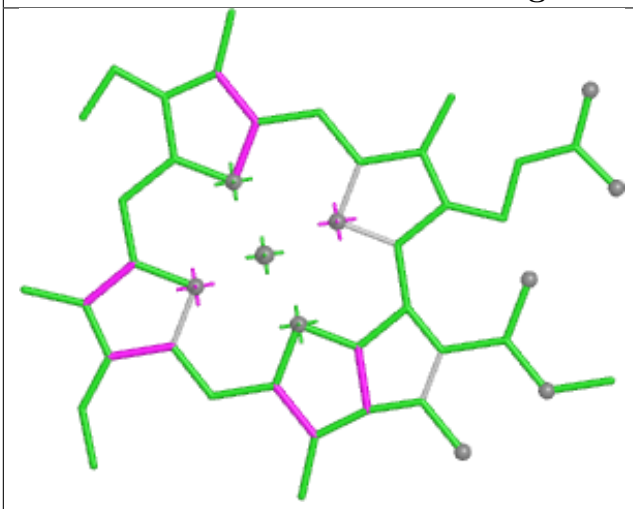


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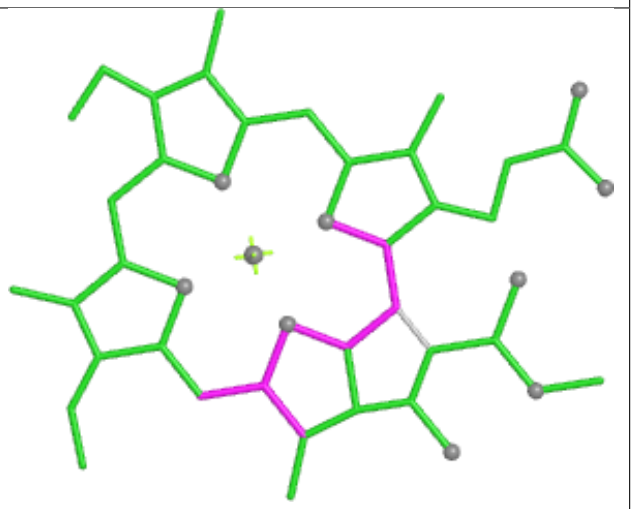


Rings

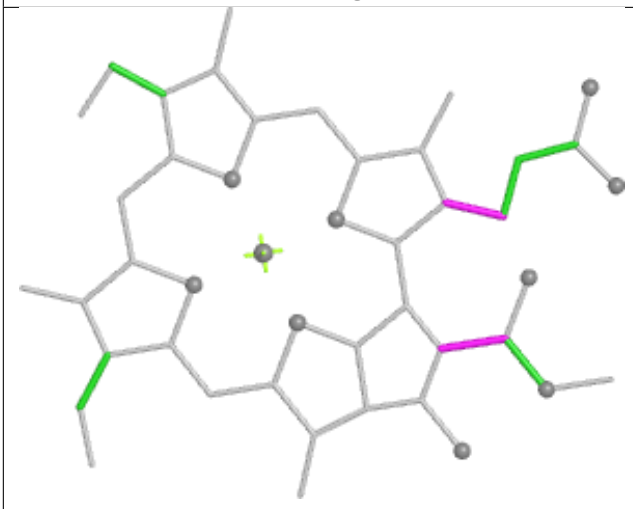
Ligand CLA a 812



Bond lengths



Bond angles

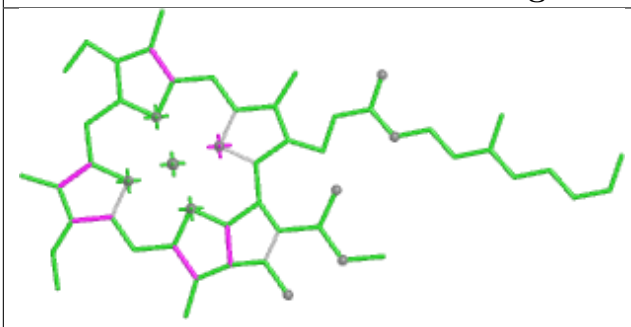


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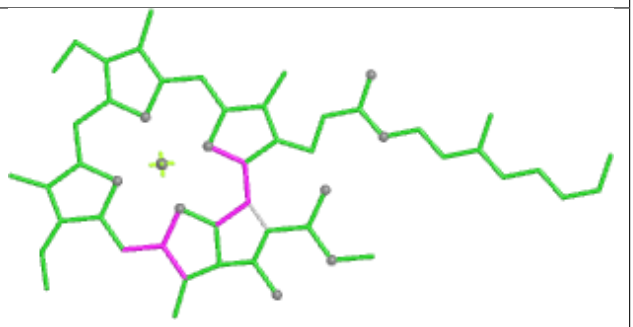


Rings

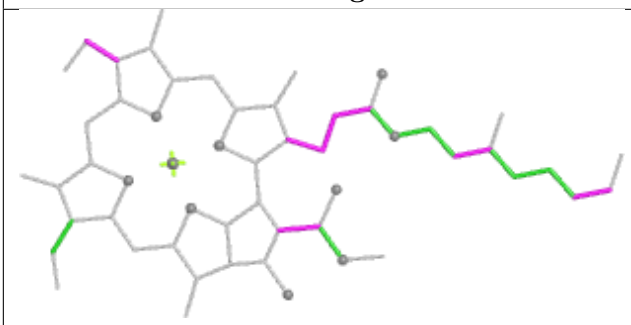
Ligand CLA a 810



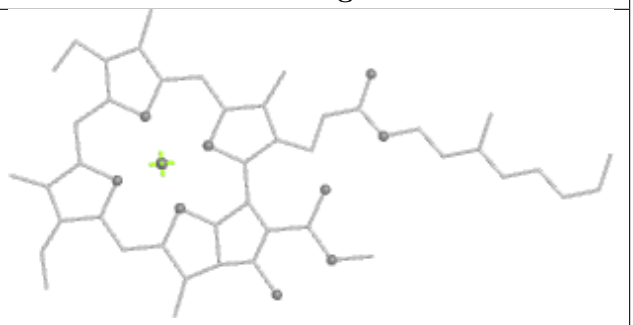
Bond lengths



Bond angles

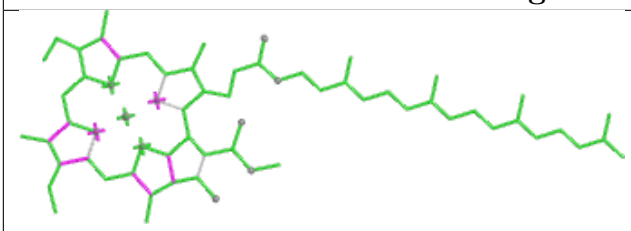


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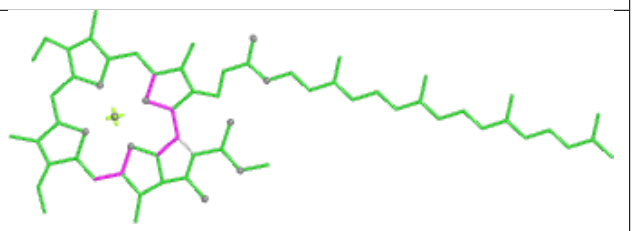


Rings

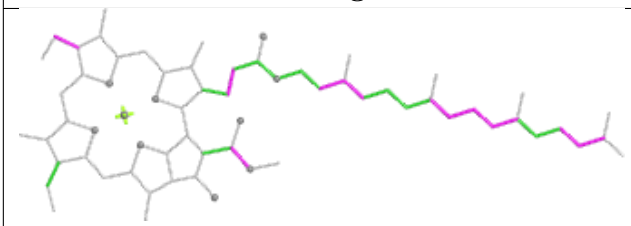
Ligand CLA a 826



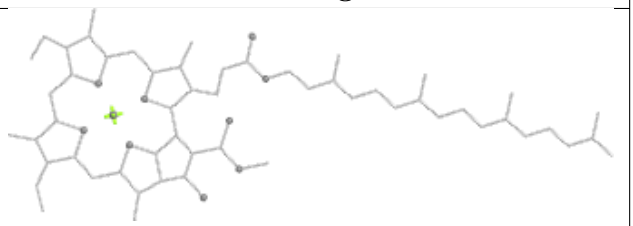
Bond lengths



Bond angles

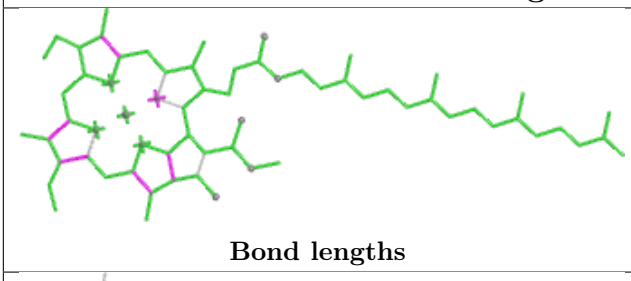


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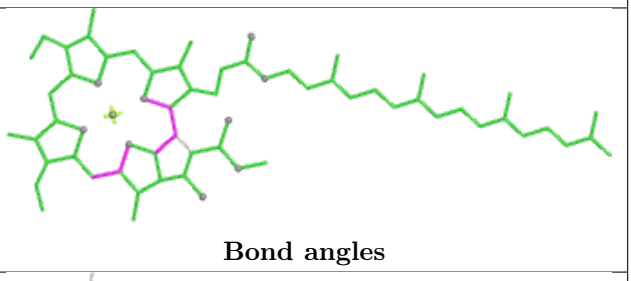


Rings

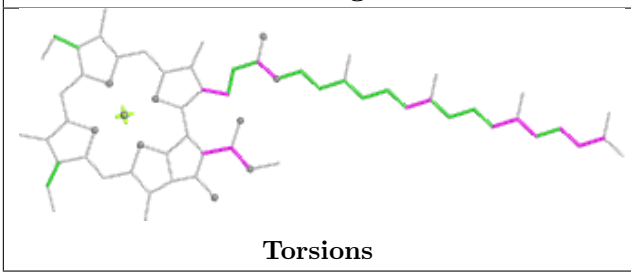
Ligand CLA b 832



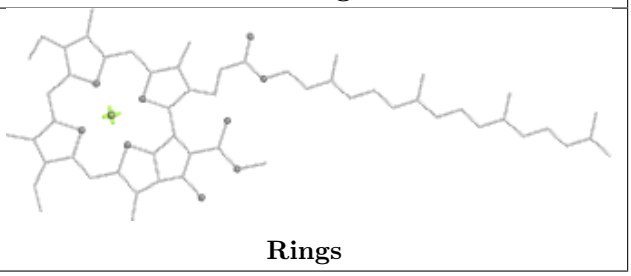
Bond lengths



Bond angles

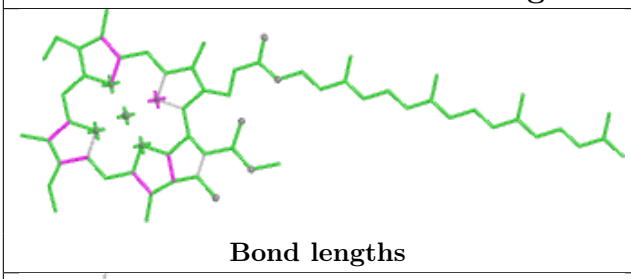


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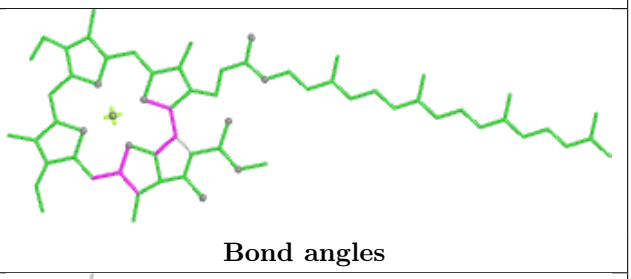


Rings

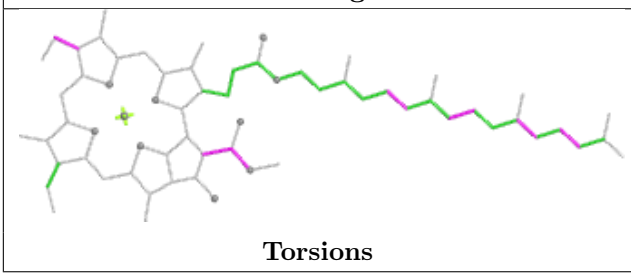
Ligand CLA b 809



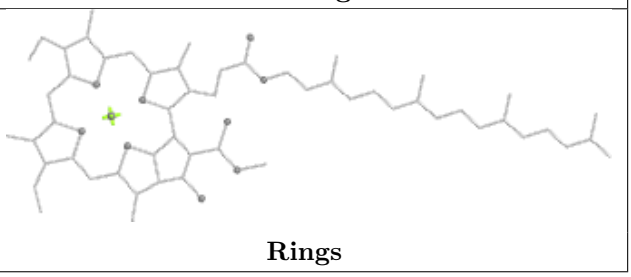
Bond lengths



Bond angles

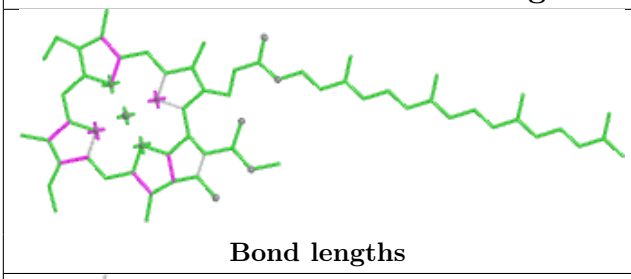


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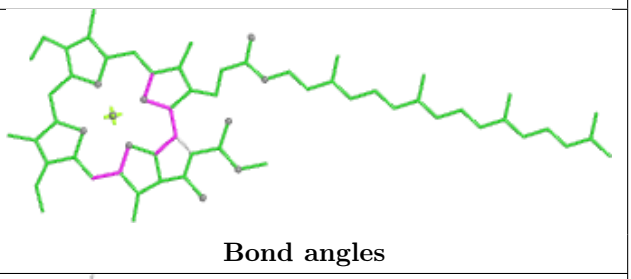


Rings

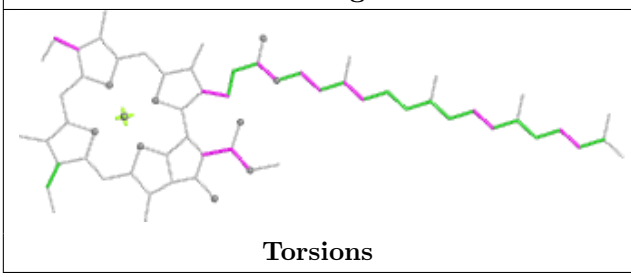
Ligand CLA a 827



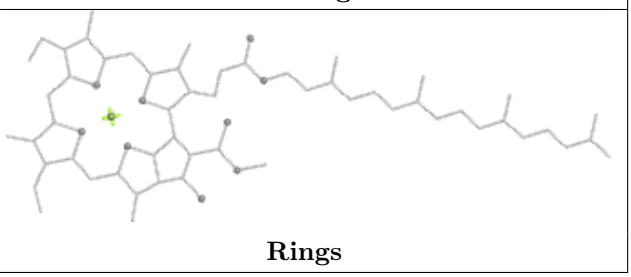
Bond lengths



Bond angles

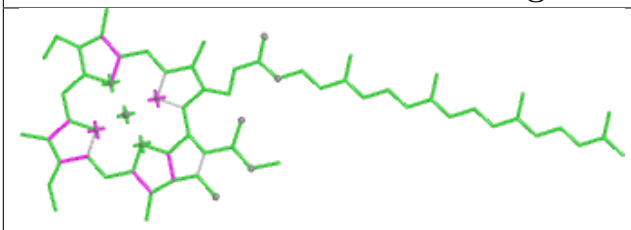


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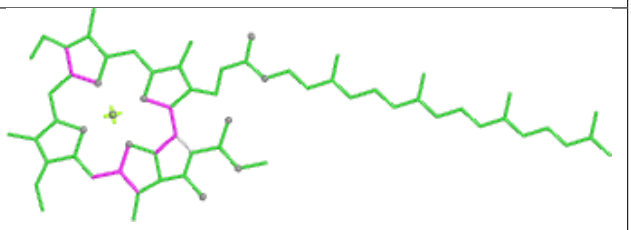


Rings

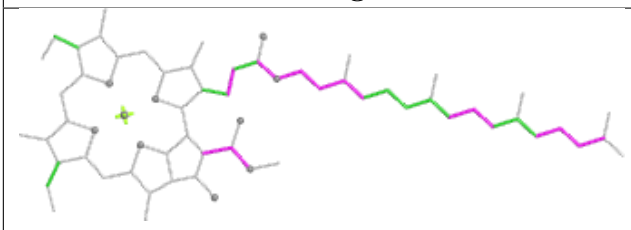
Ligand CLA b 802



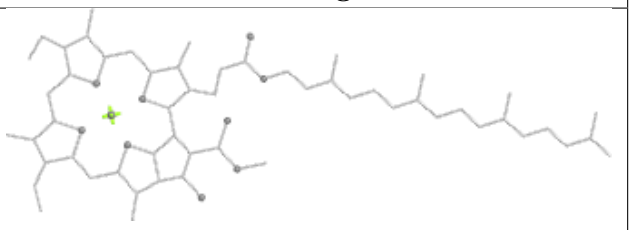
Bond lengths



Bond angles

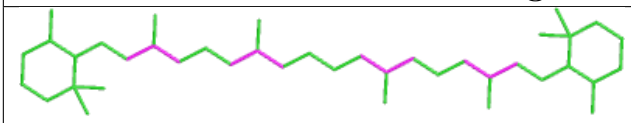


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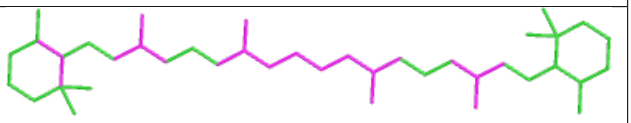


Rings

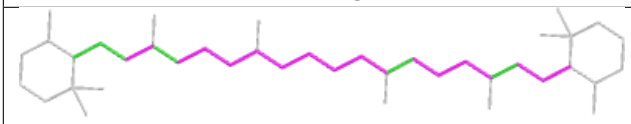
Ligand BCR a 842



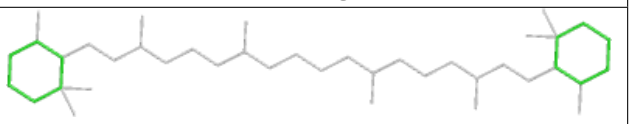
Bond lengths



Bond angles

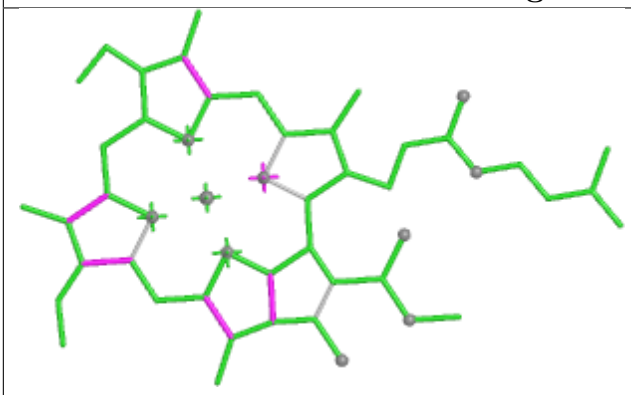


Torsions

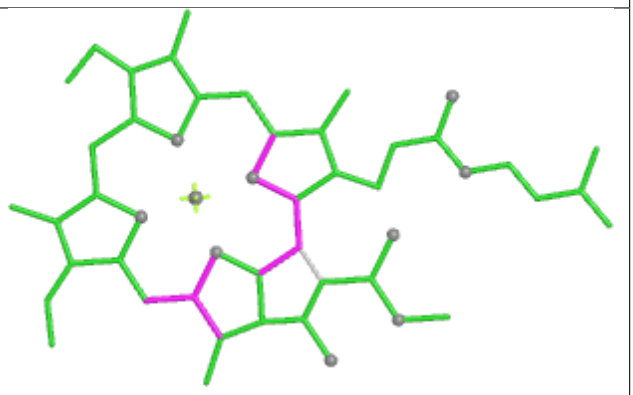


Rings

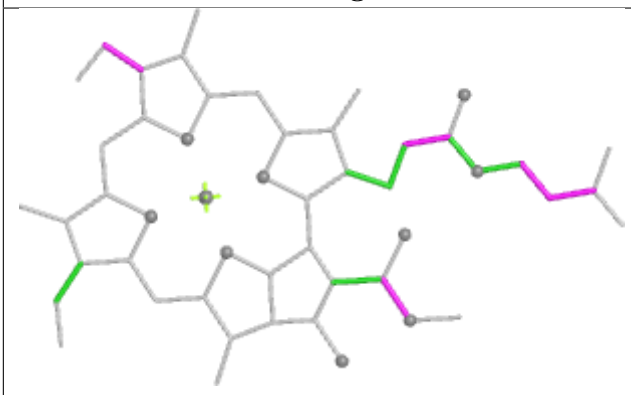
Ligand CLA L 304



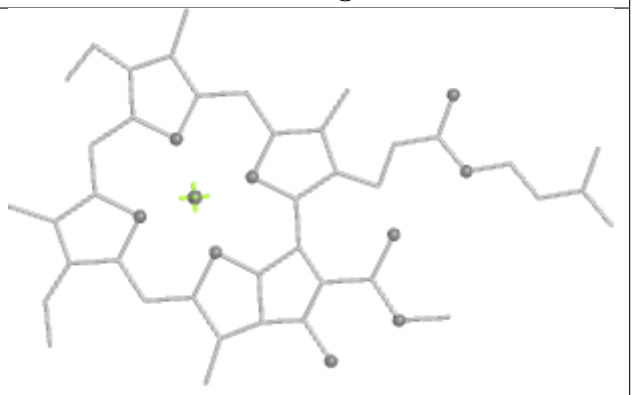
Bond lengths



Bond angles

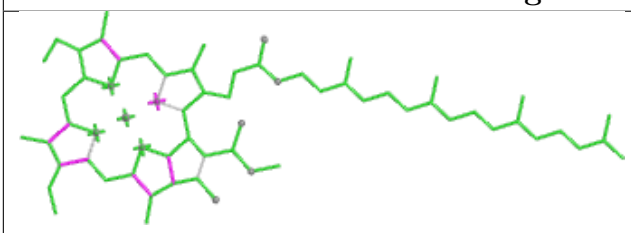


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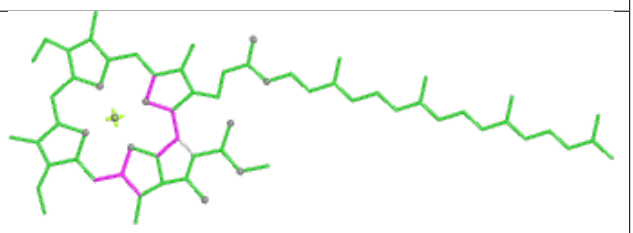


Rings

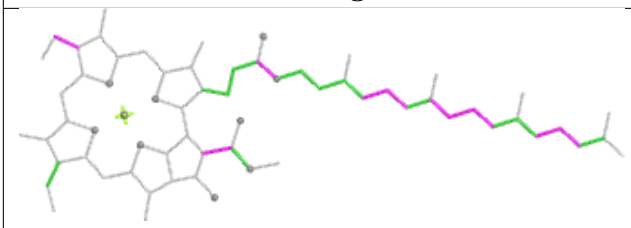
Ligand CLA B 829



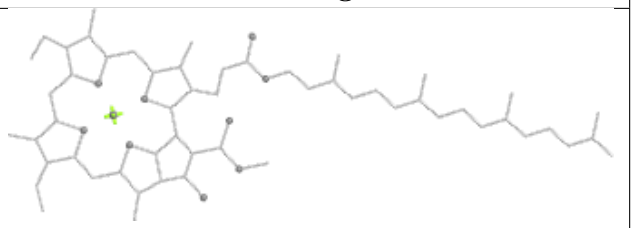
Bond lengths



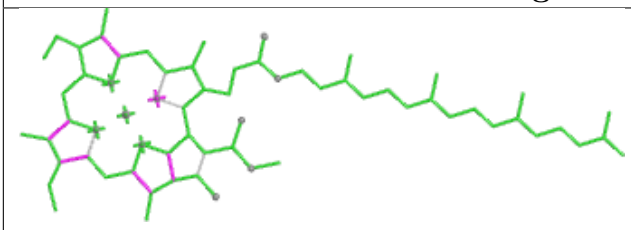
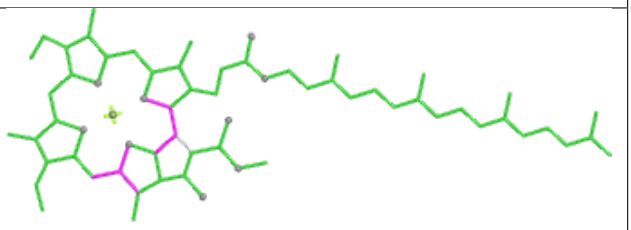
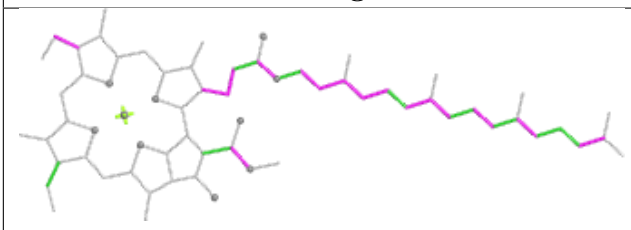
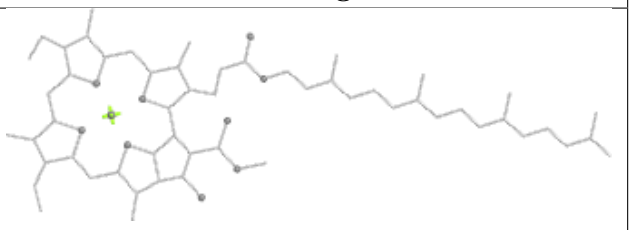
Bond angles

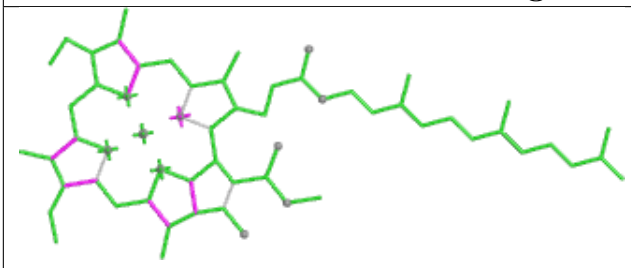
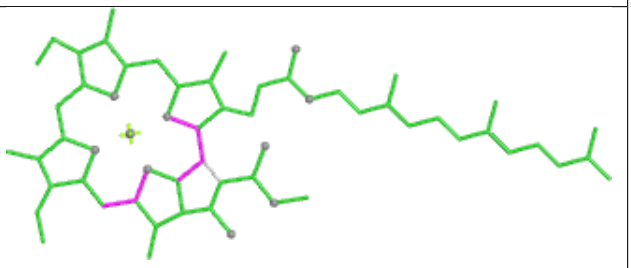
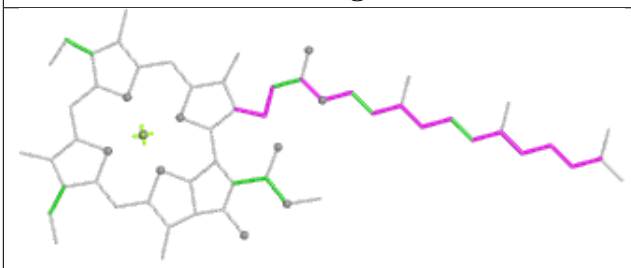
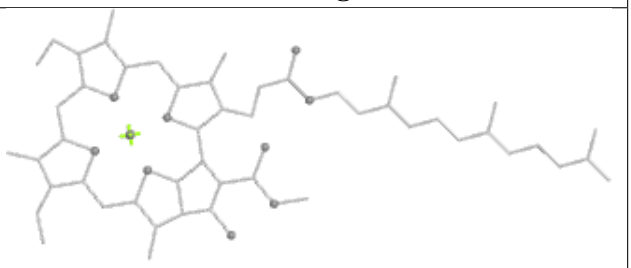


Torsions

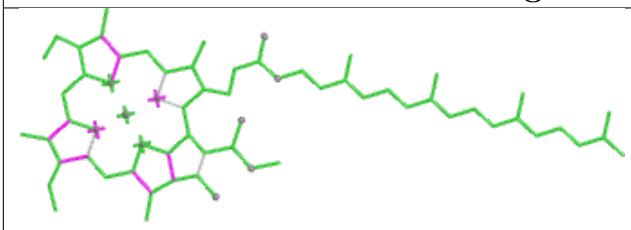


Rings

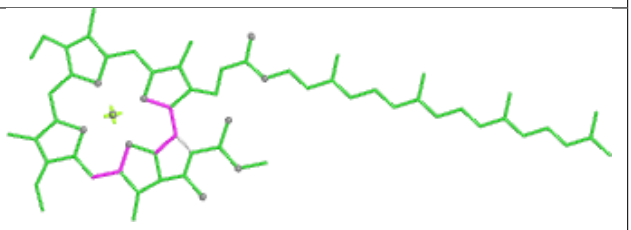
Ligand CLA l 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

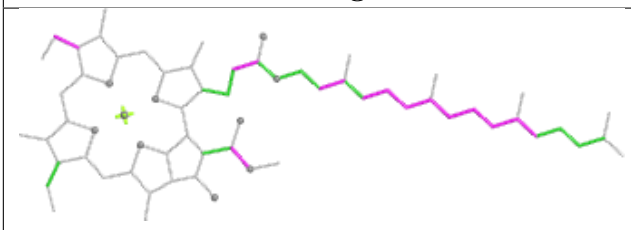
Ligand CLA B 807



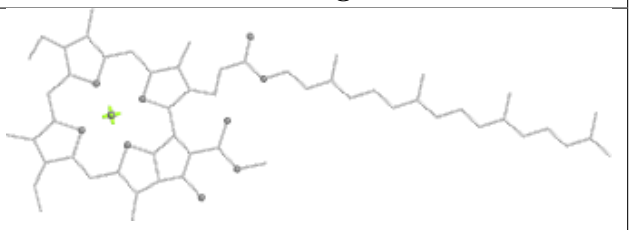
Bond lengths



Bond angles

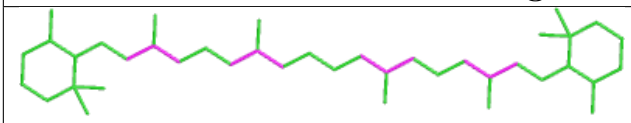


Torsions

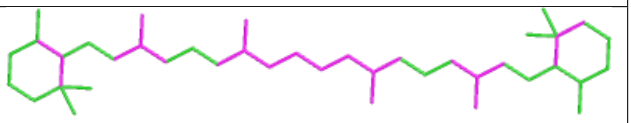


Rings

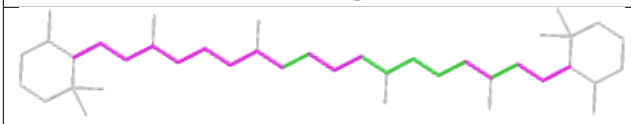
Ligand BCR a 841



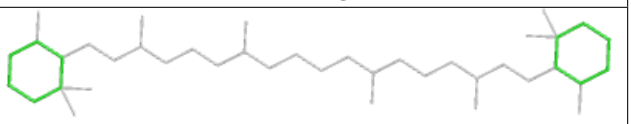
Bond lengths



Bond angles

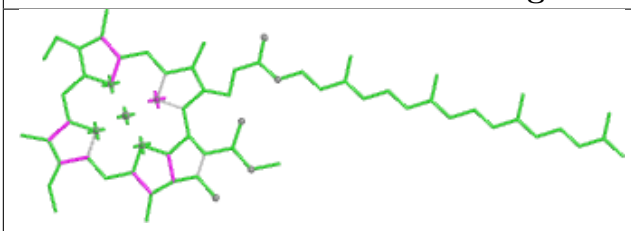


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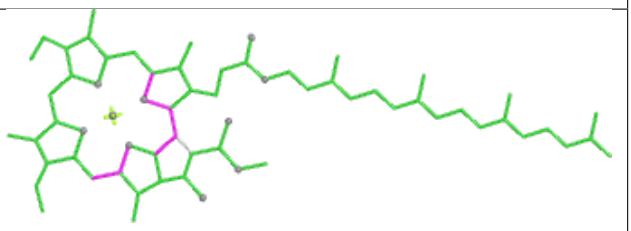


Rings

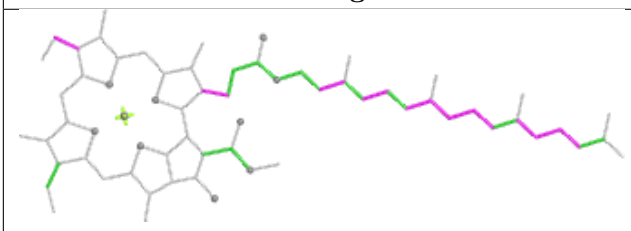
Ligand CLA b 810



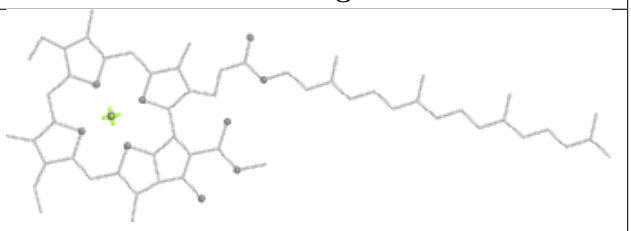
Bond lengths



Bond angles

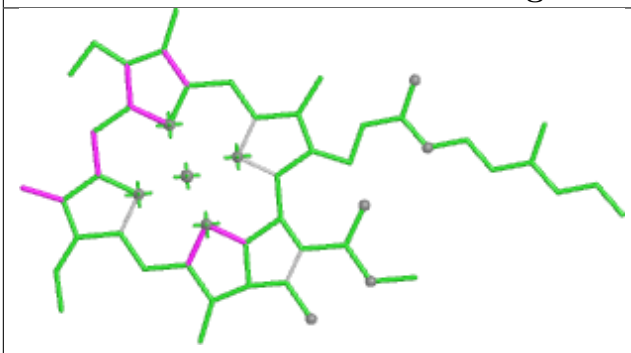


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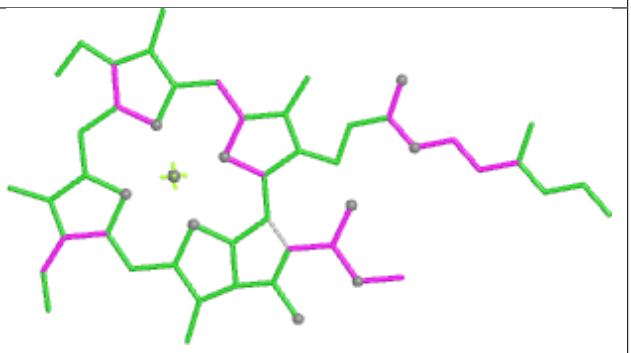


Rings

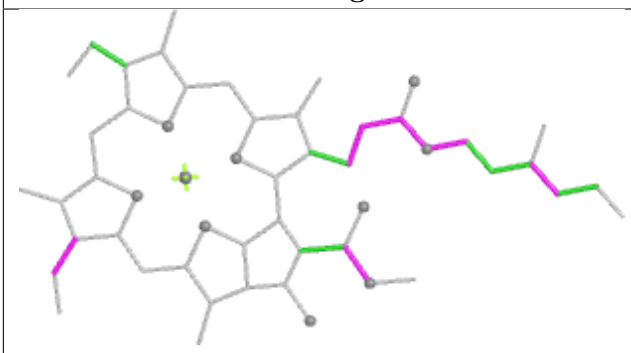
Ligand CLA L 308



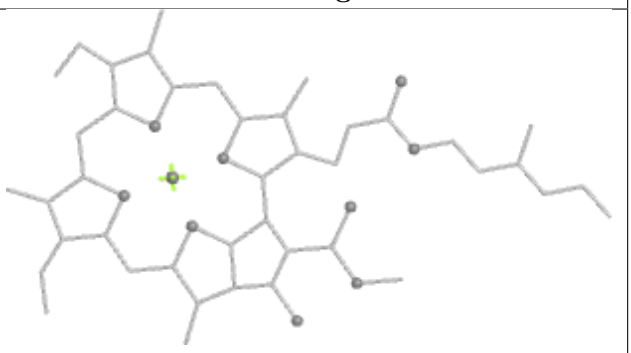
Bond lengths



Bond angles

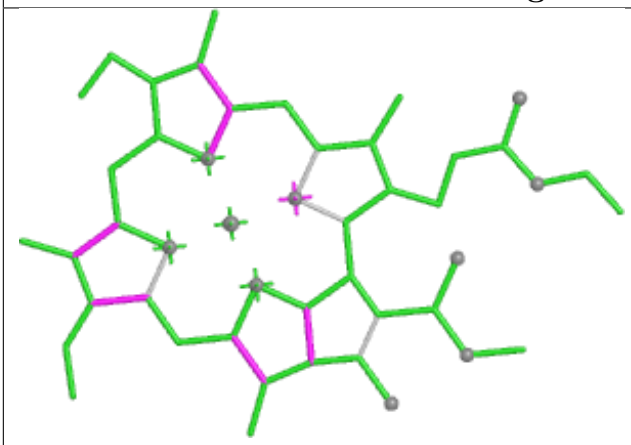


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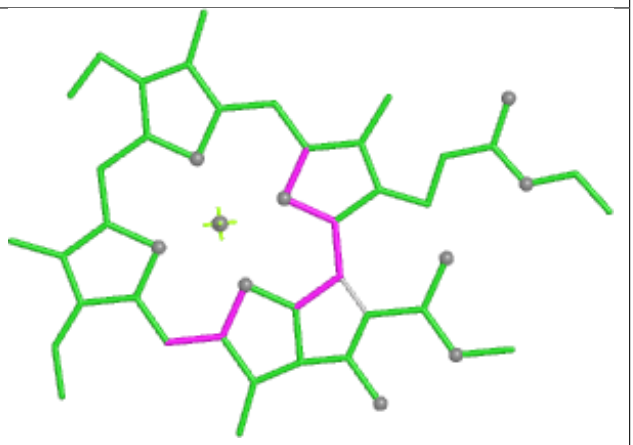


Rings

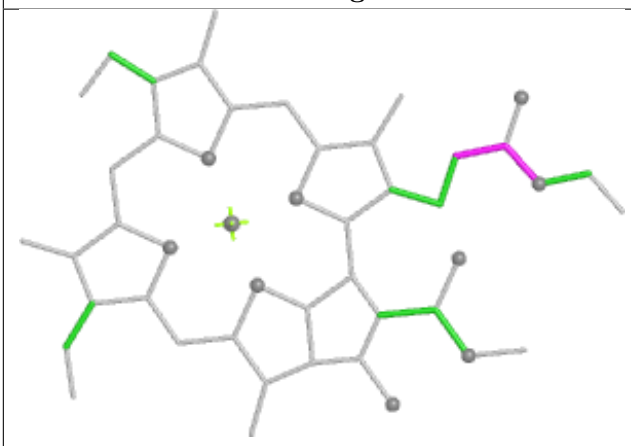
Ligand CLA b 830



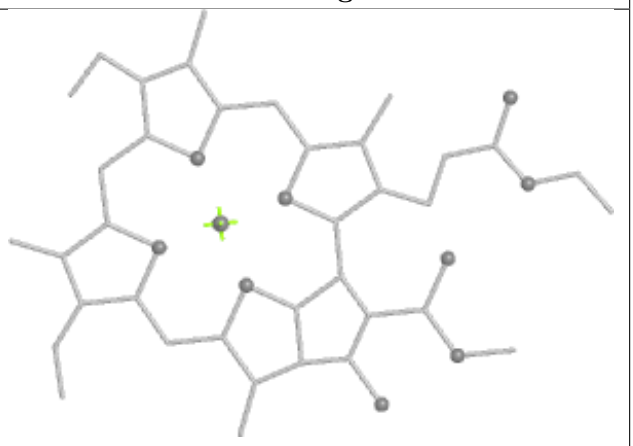
Bond lengths



Bond angles

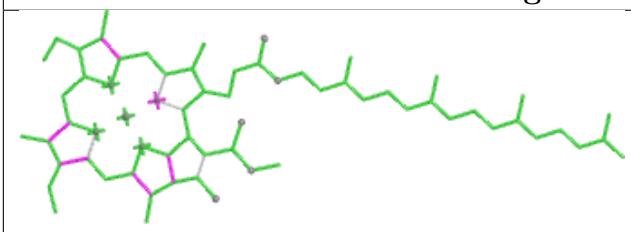


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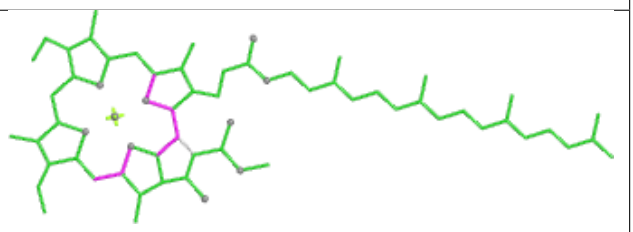


Rings

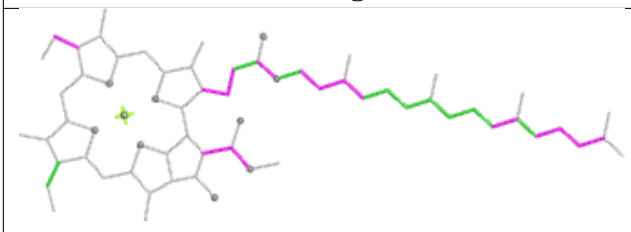
Ligand CLA A 833



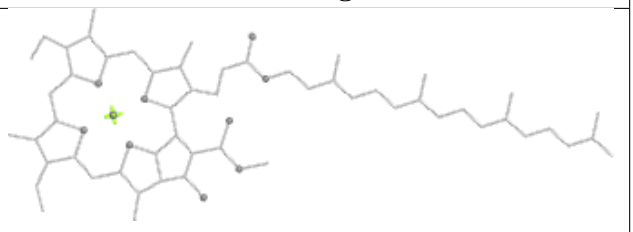
Bond lengths



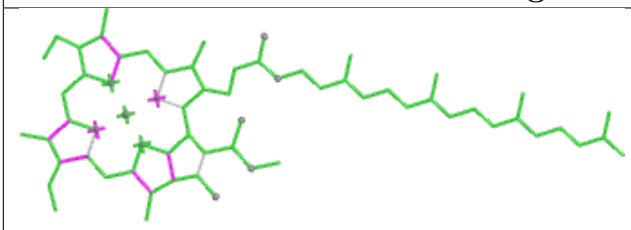
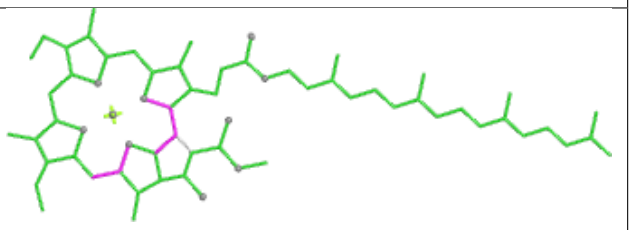
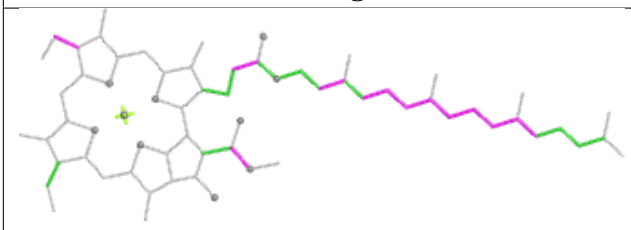
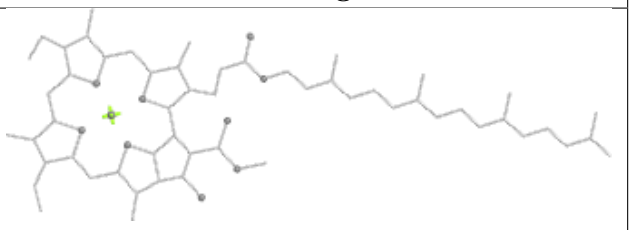
Bond angles

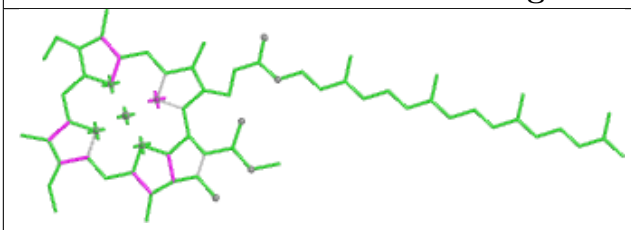
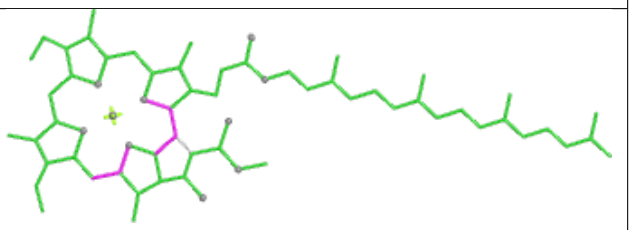
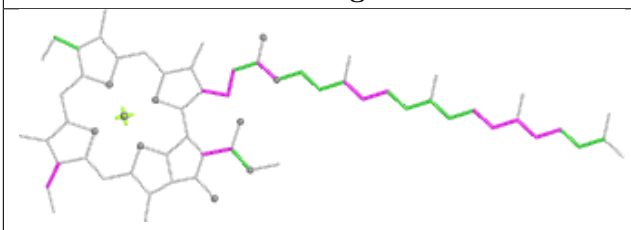
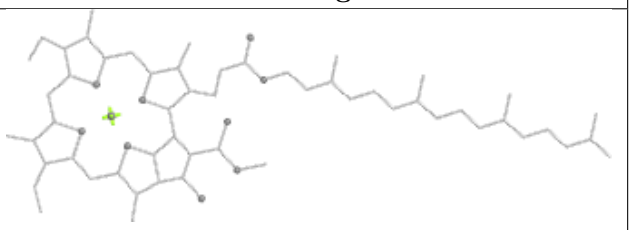


Torsions

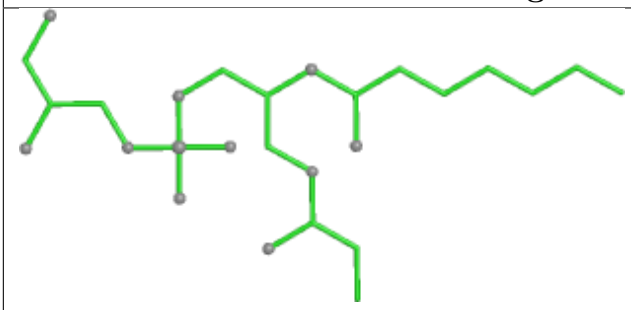


Rings

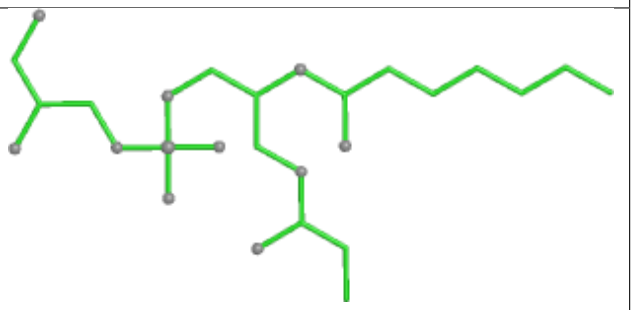
Ligand CLA b 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

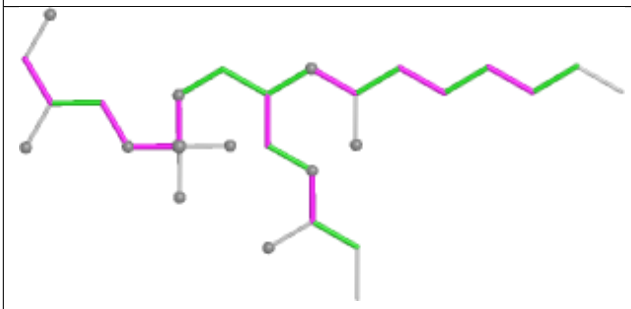
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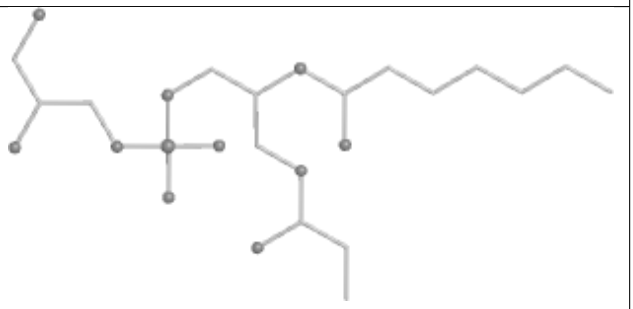
Bond lengths



Bond angles

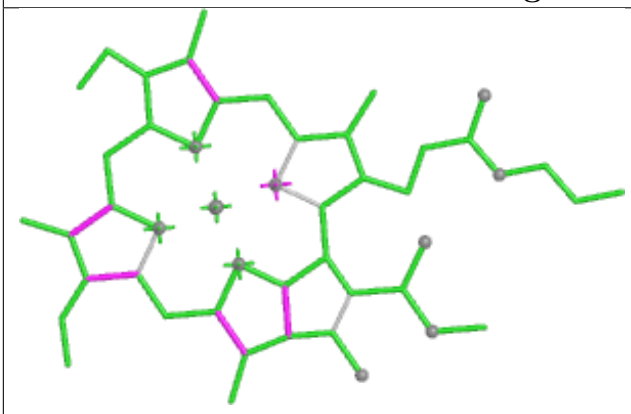


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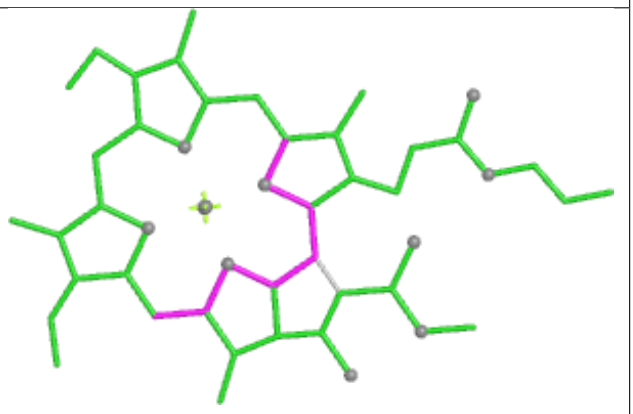


Rings

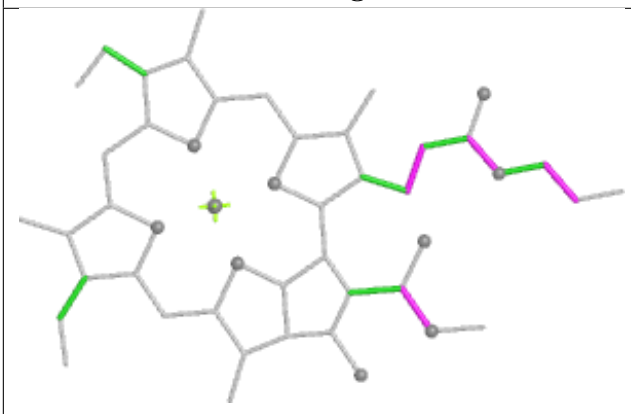
Ligand CLA A 836



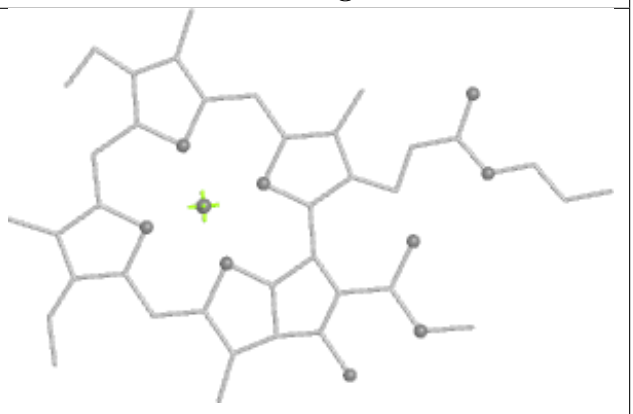
Bond lengths



Bond angles

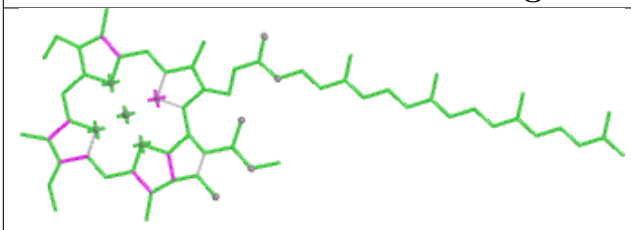


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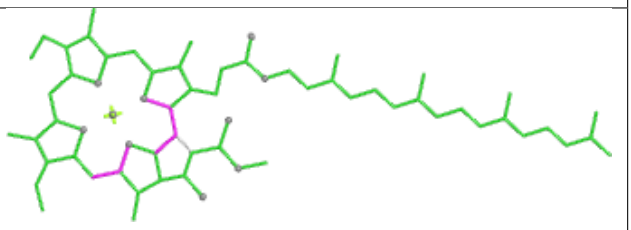


Rings

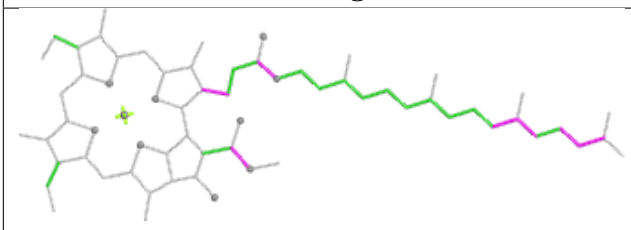
Ligand CLA B 832



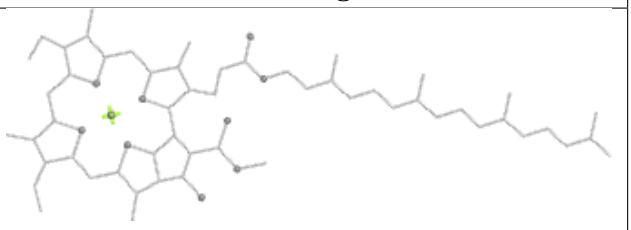
Bond lengths



Bond angles

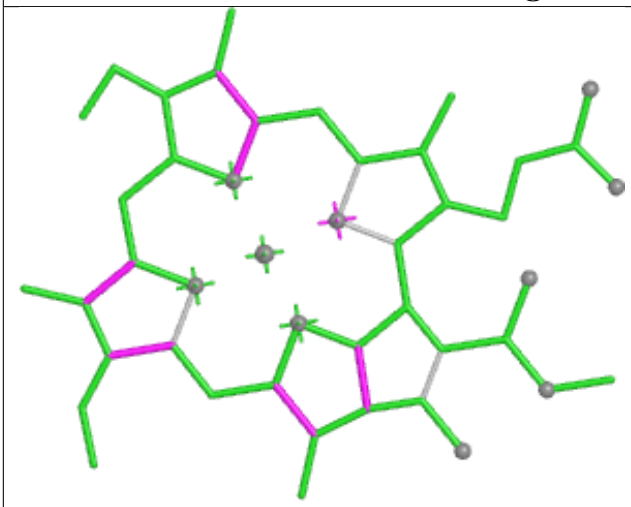


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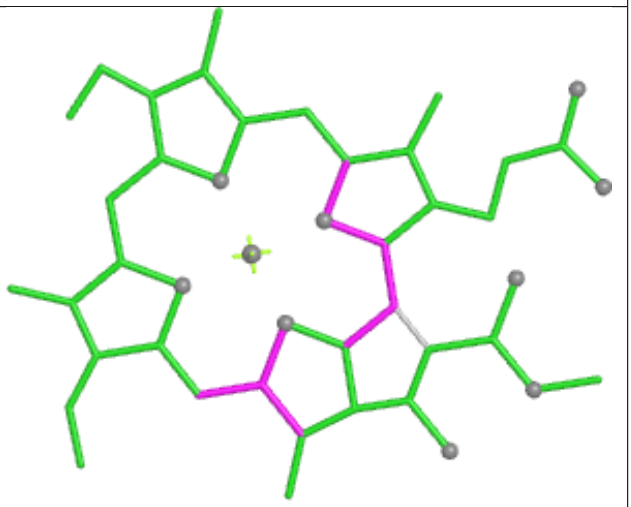


Rings

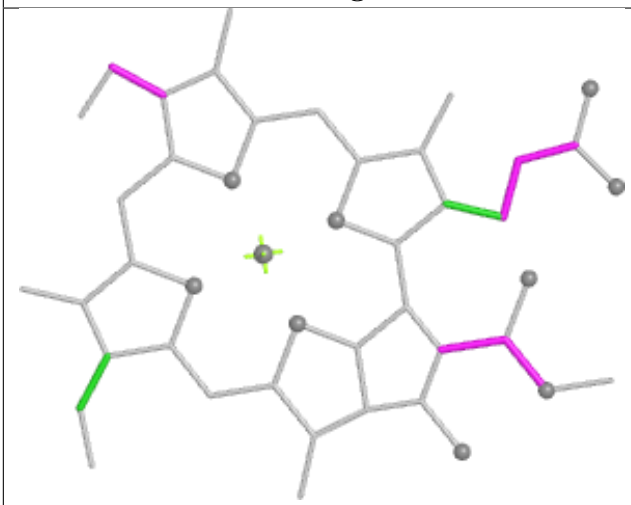
Ligand CLA B 827



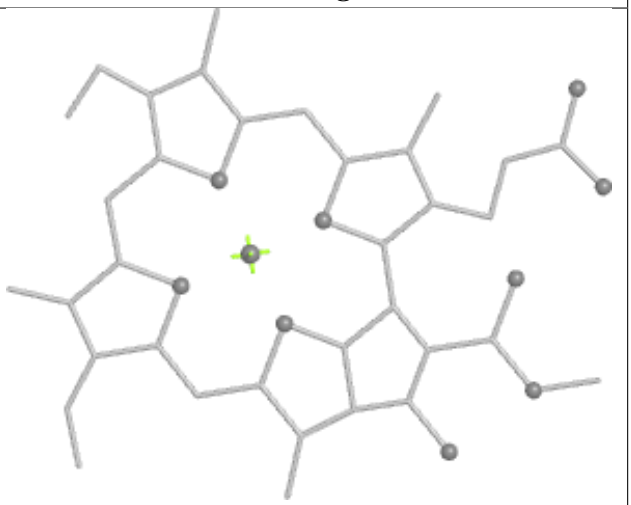
Bond lengths



Bond angles

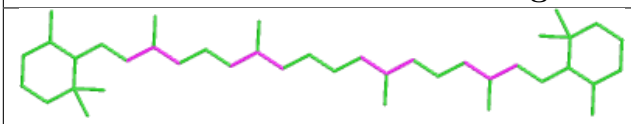


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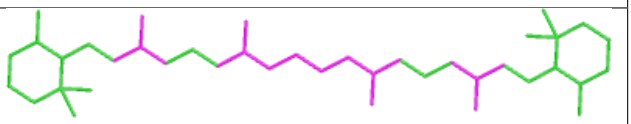


Rings

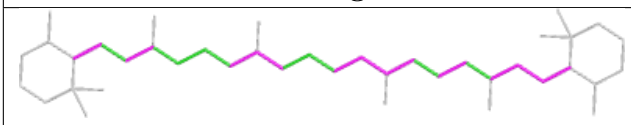
Ligand BCR l 308



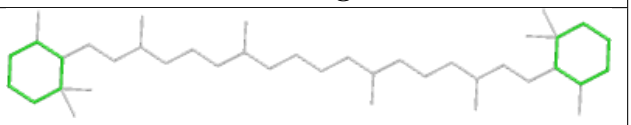
Bond lengths



Bond angles

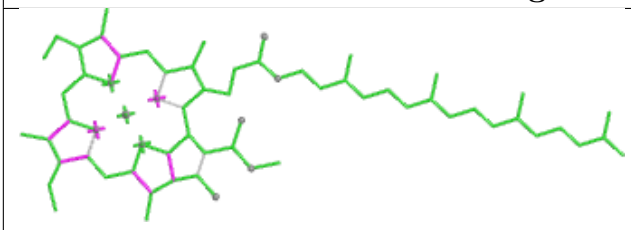


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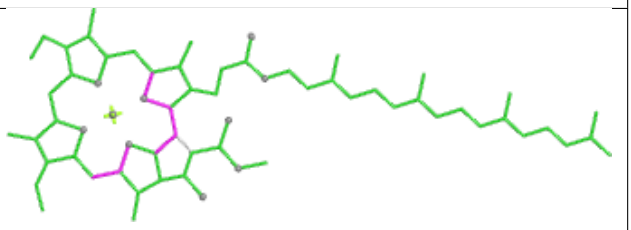


Rings

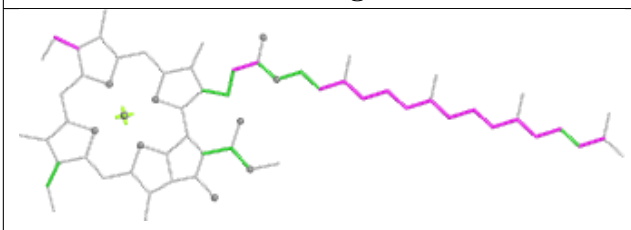
Ligand CLA a 847



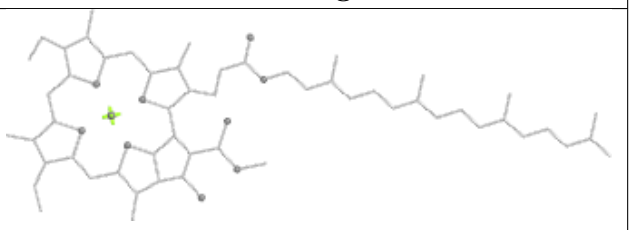
Bond lengths



Bond angles

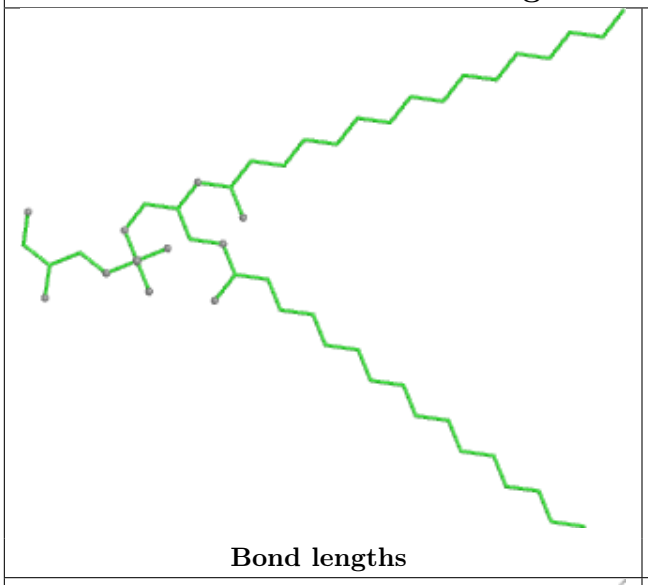


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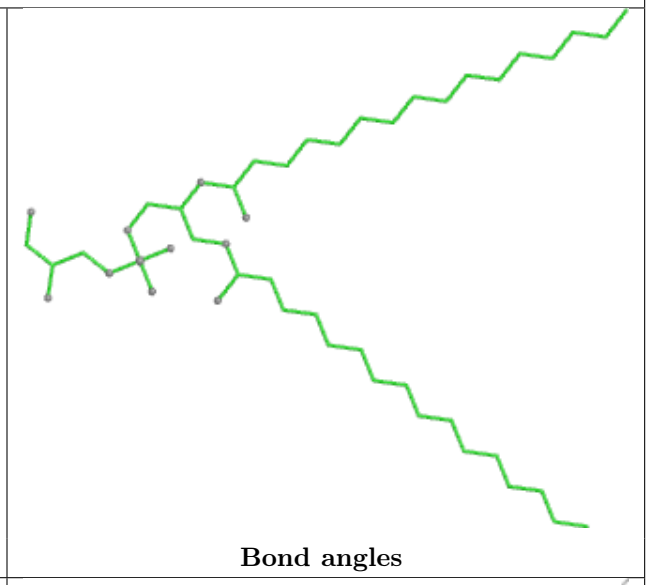


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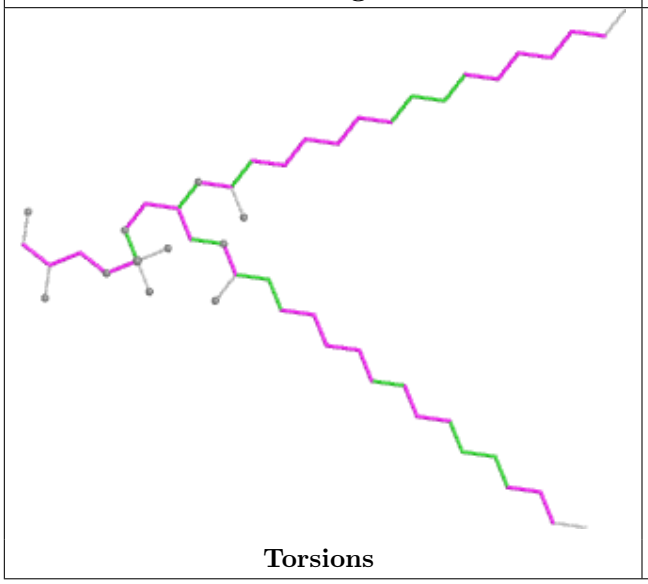
Ligand LHG A 838



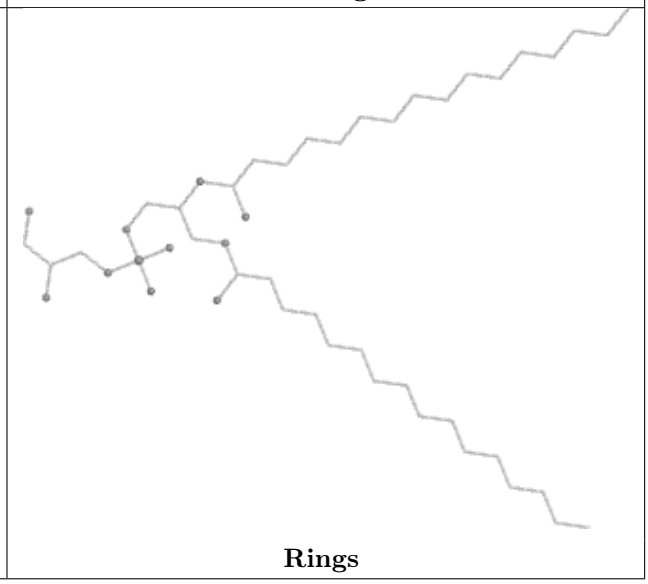
Bond lengths



Bond angles

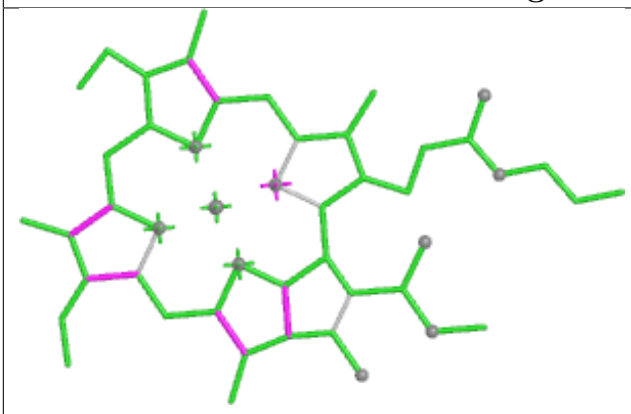


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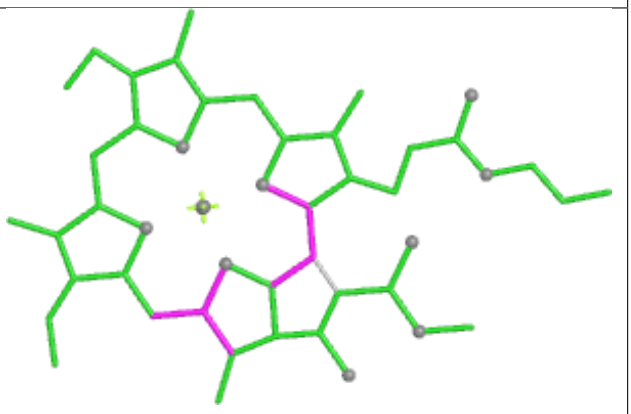


Rings

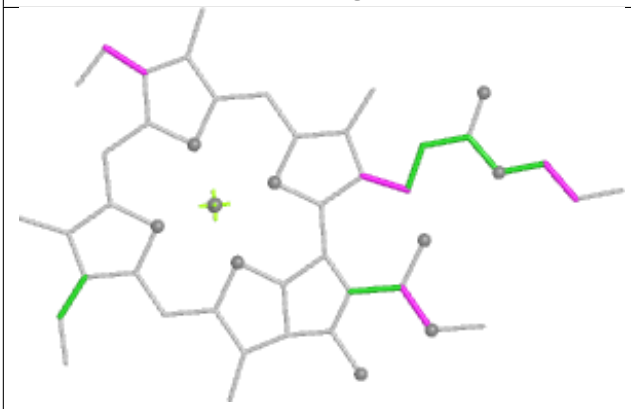
Ligand CLA b 826



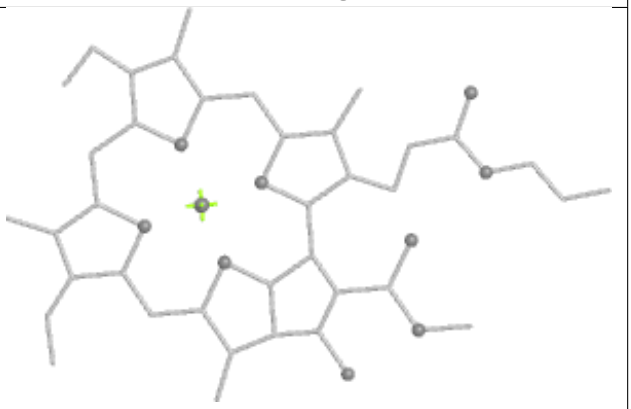
Bond lengths



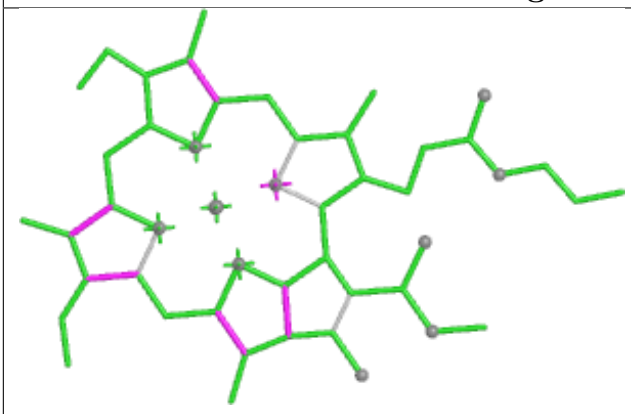
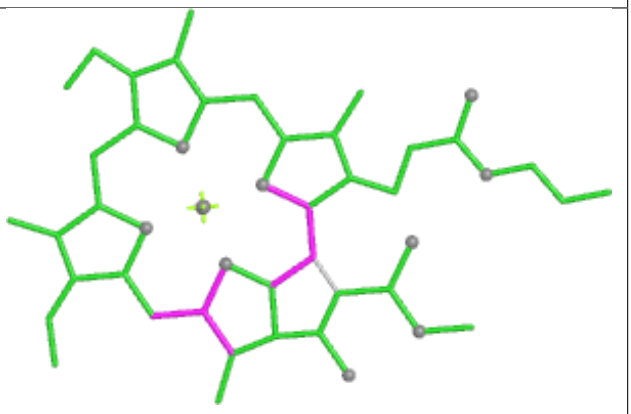
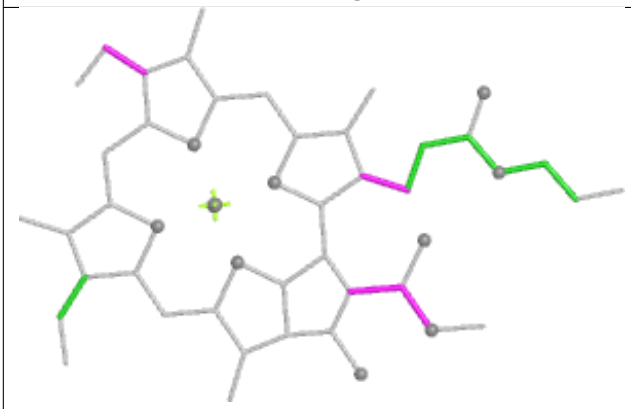
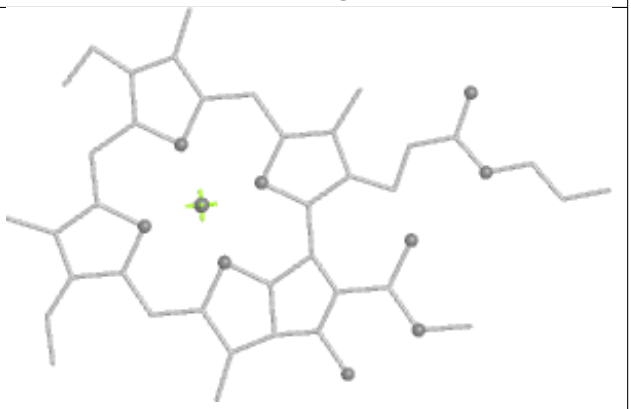
Bond angles

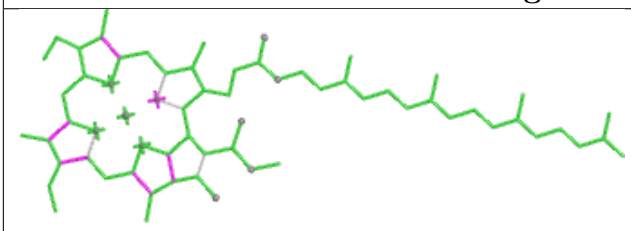
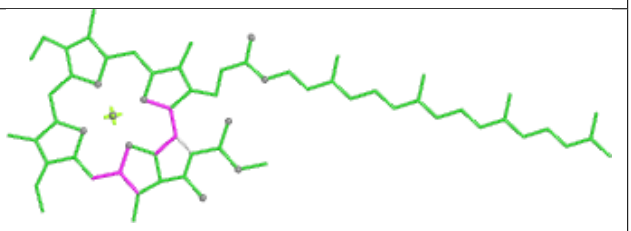
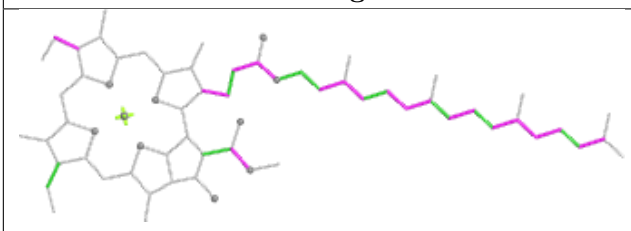
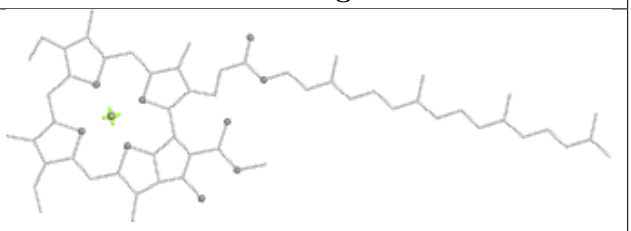


Torsions

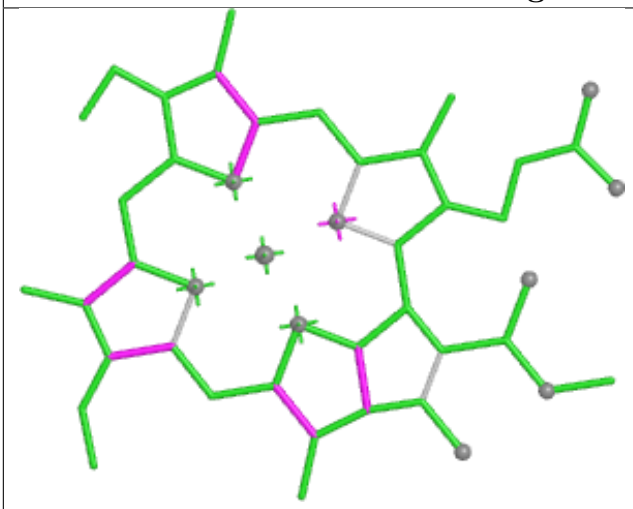


Rings

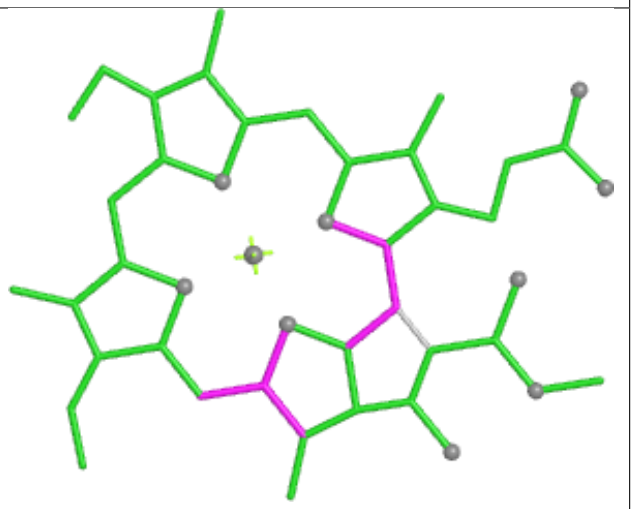
Ligand CLA b 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

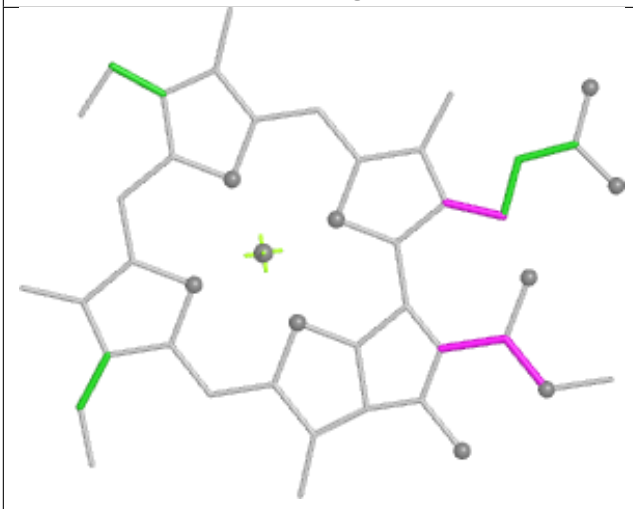
Ligand CLA b 805



Bond lengths



Bond angles

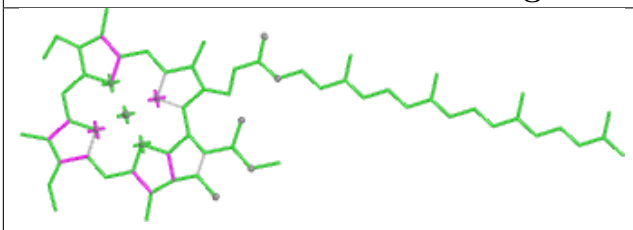


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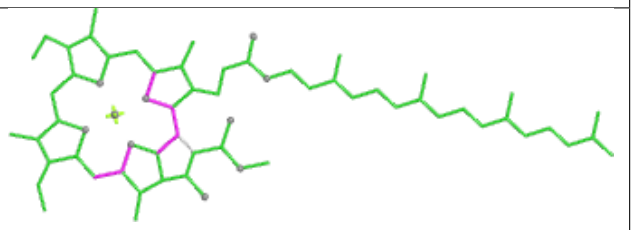


Rings

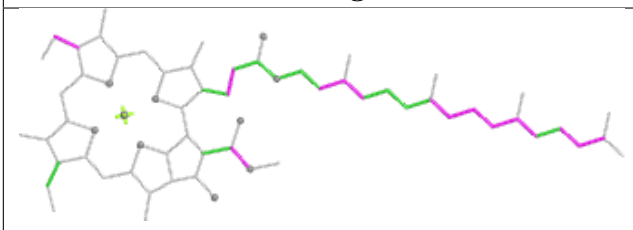
Ligand CLA A 825



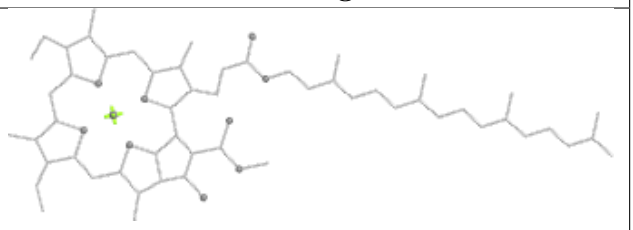
Bond lengths



Bond angles

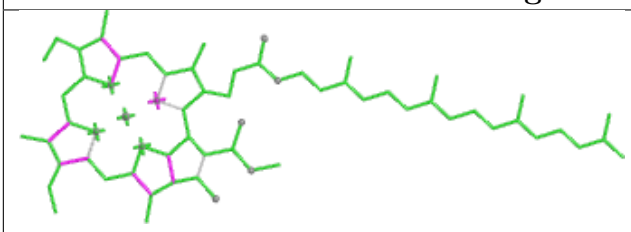


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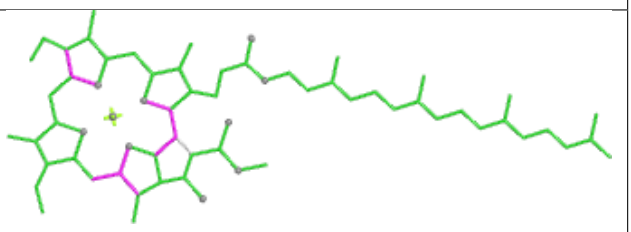


Rings

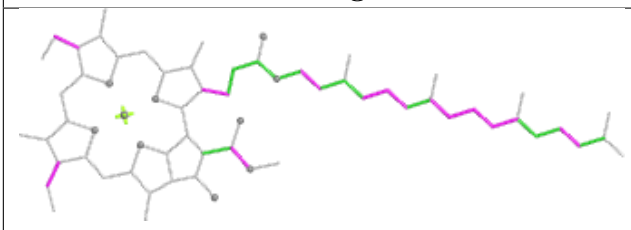
Ligand CLA B 804



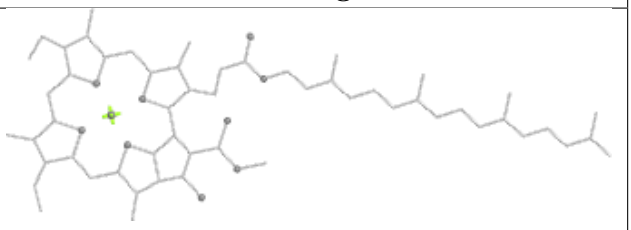
Bond lengths



Bond angles

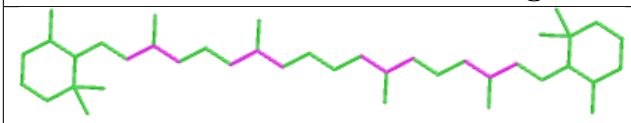


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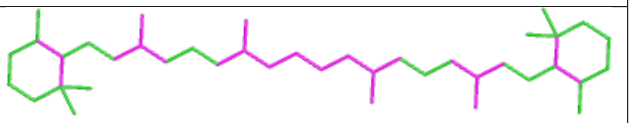


Rings

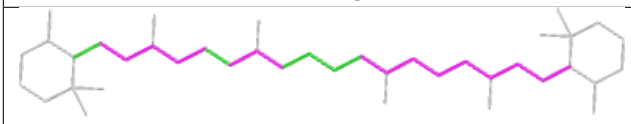
Ligand BCR h 203



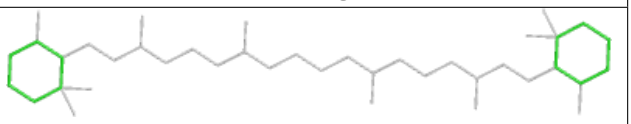
Bond lengths



Bond angles

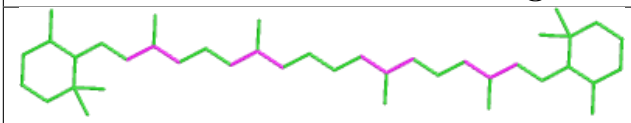


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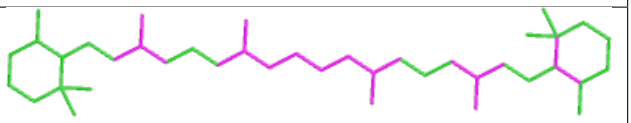


Rings

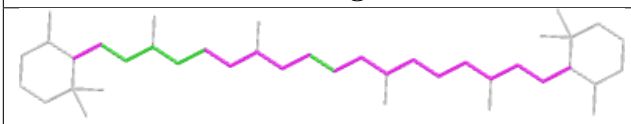
Ligand BCR a 844



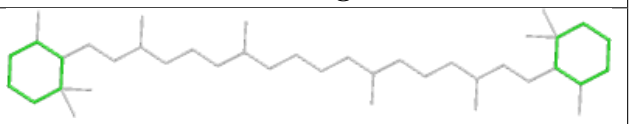
Bond lengths



Bond angles

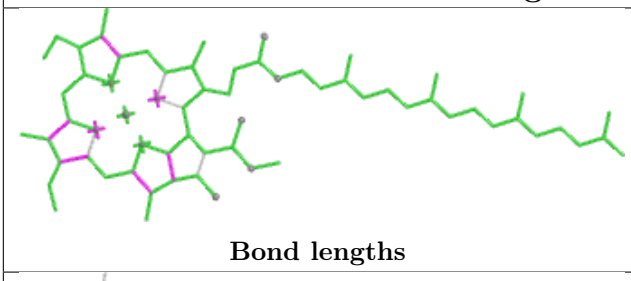


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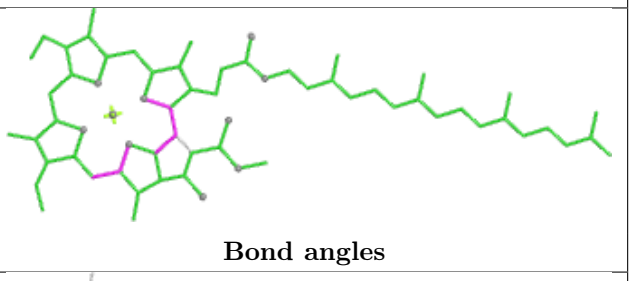


Rings

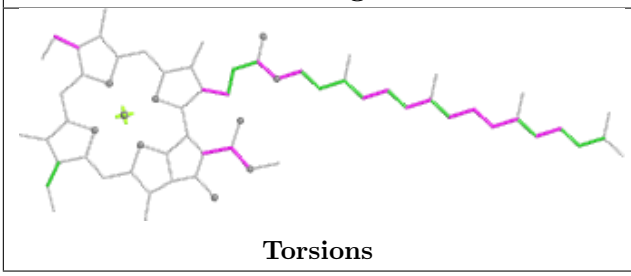
Ligand CLA B 814



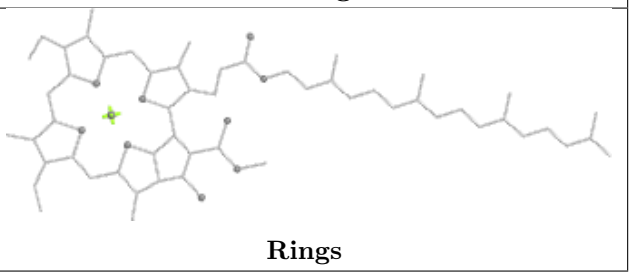
Bond lengths



Bond angles

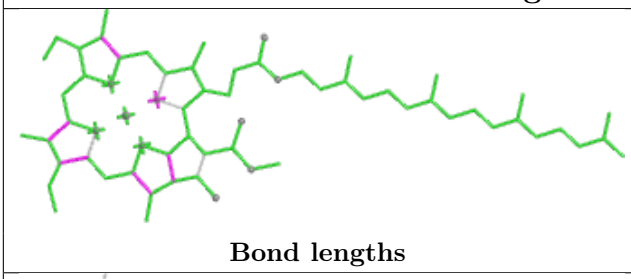


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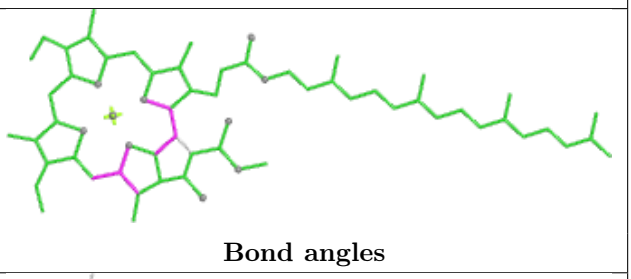


Rings

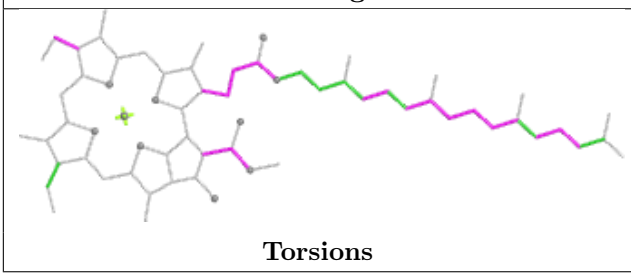
Ligand CLA A 811



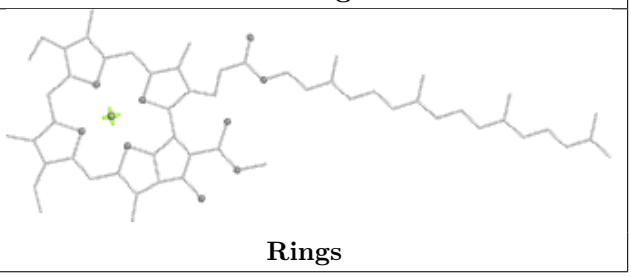
Bond lengths



Bond angles

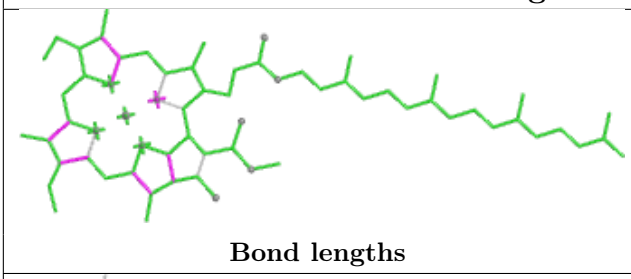


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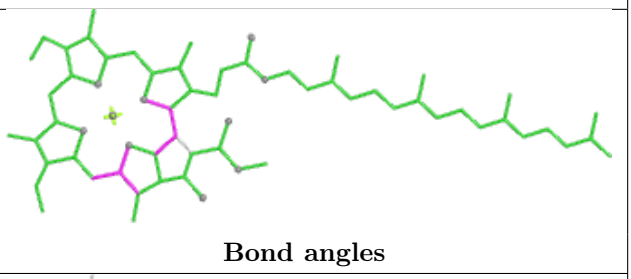


Rings

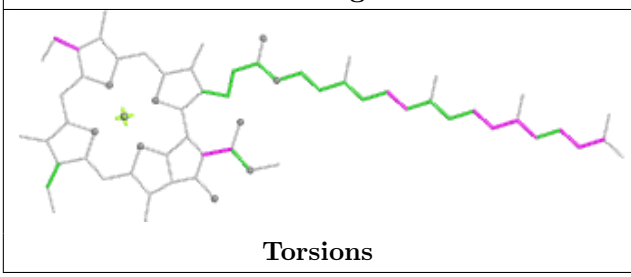
Ligand CLA a 833



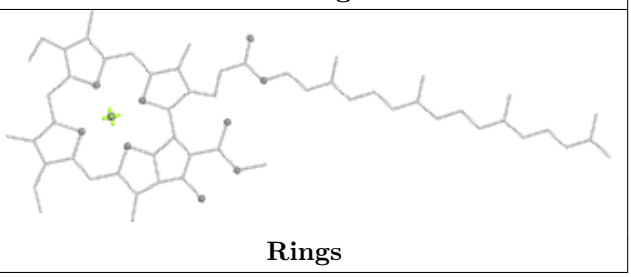
Bond lengths



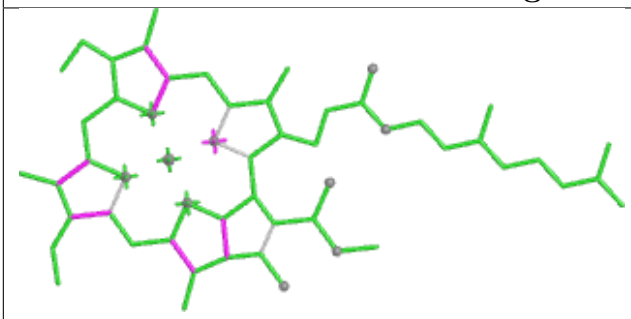
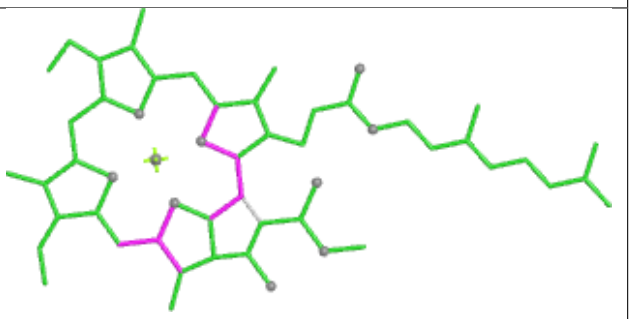
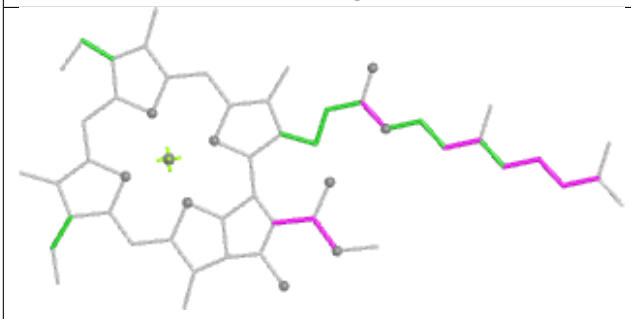
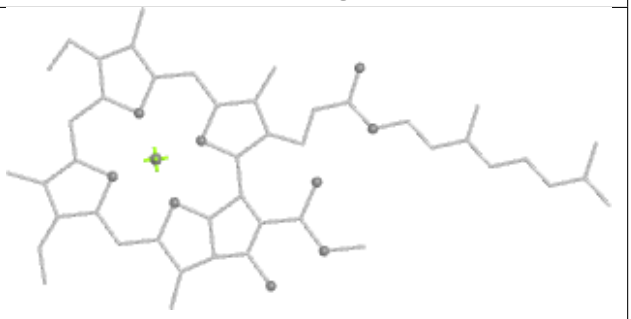
Bond angles

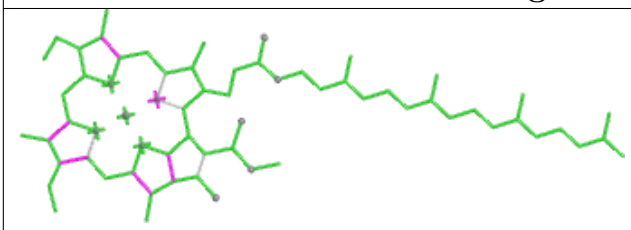
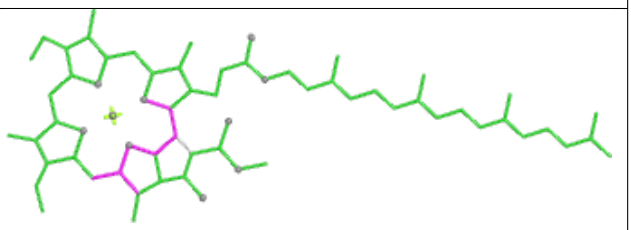
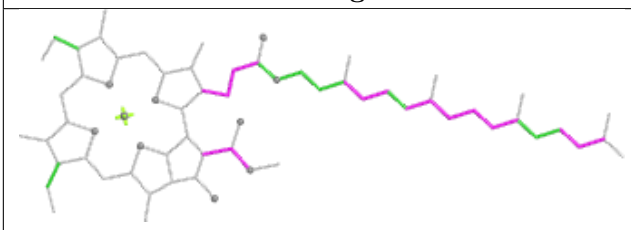
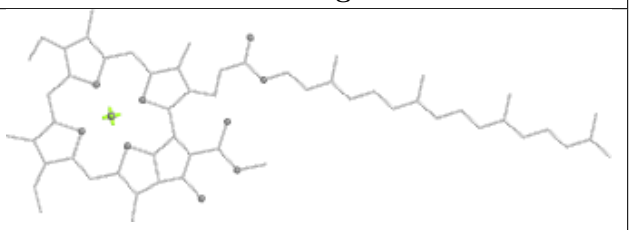


Torsions

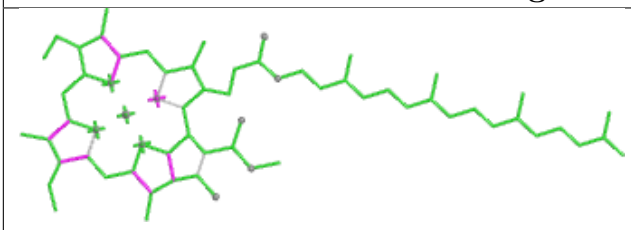


Rings

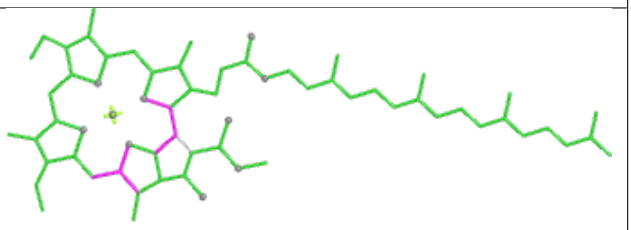
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

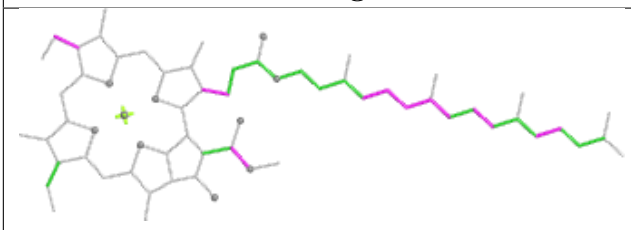
Ligand CLA a 829



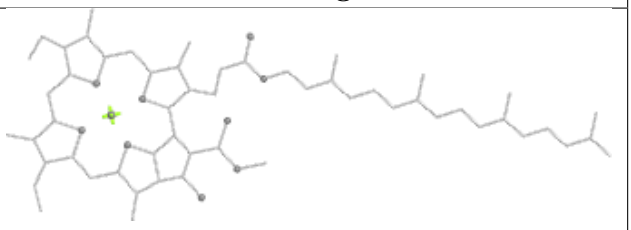
Bond lengths



Bond angles

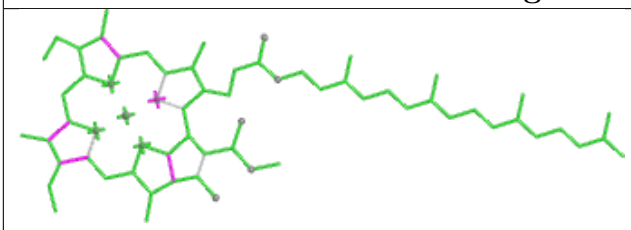


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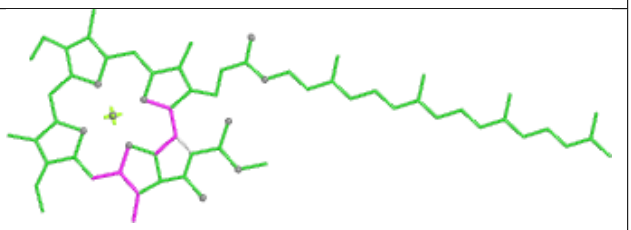


Rings

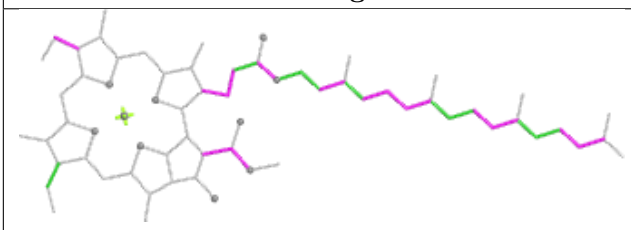
Ligand CLA A 835



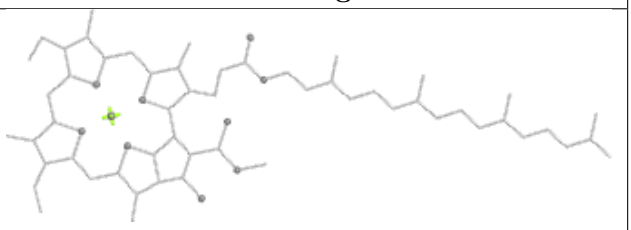
Bond lengths



Bond angles

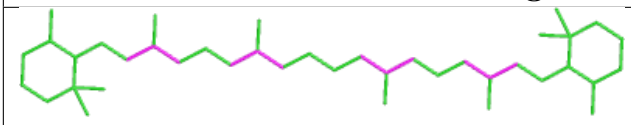


Torsions



Rings

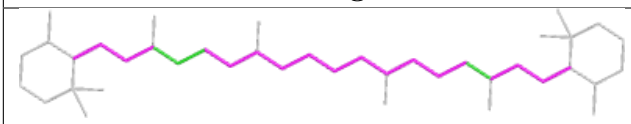
Ligand BCR b 835



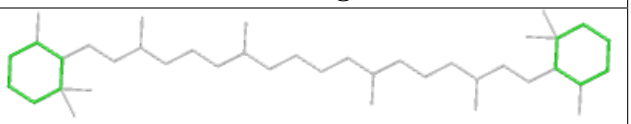
Bond lengths



Bond angles

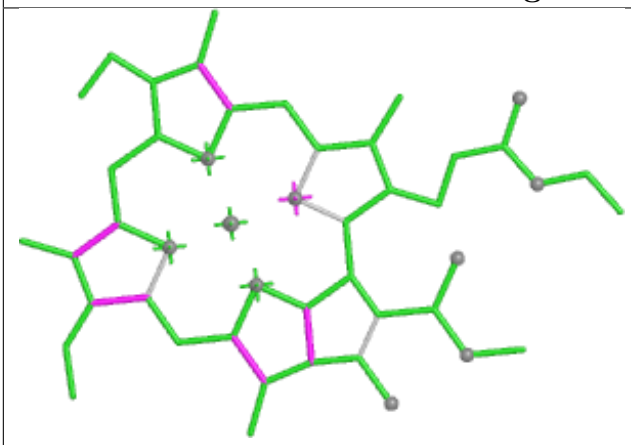


Torsions

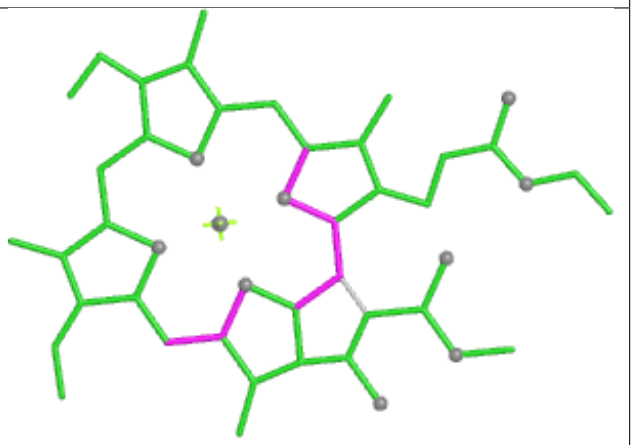


Rings

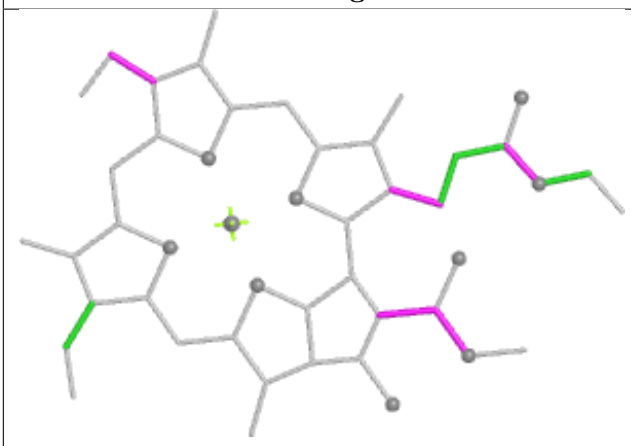
Ligand CLA A 834



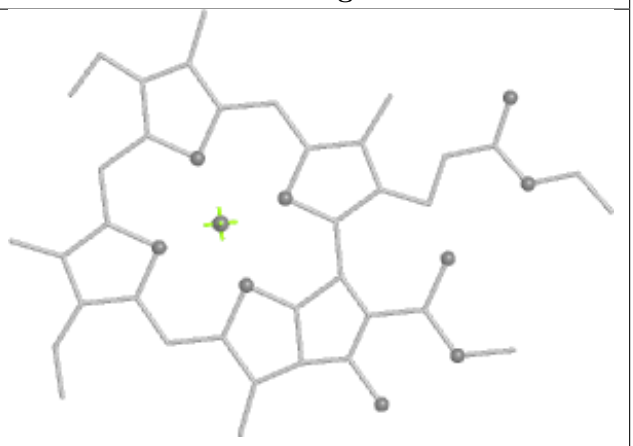
Bond lengths



Bond angles

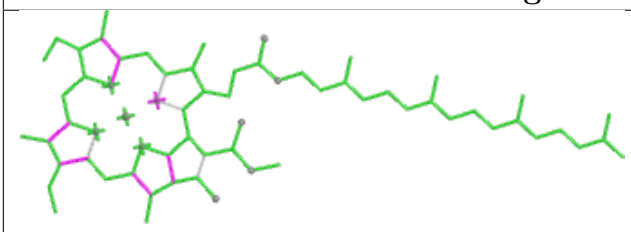


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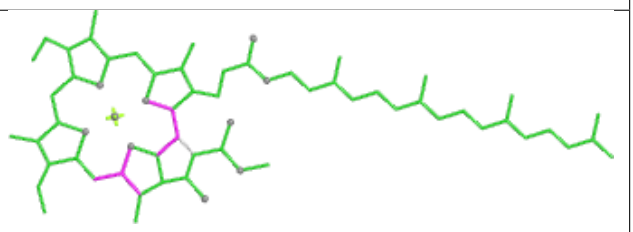


Rings

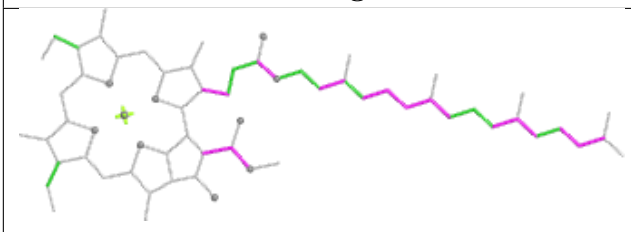
Ligand CLA A 817



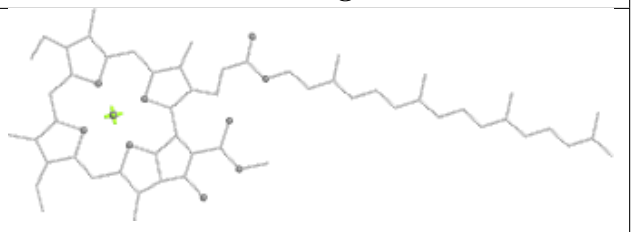
Bond lengths



Bond angles

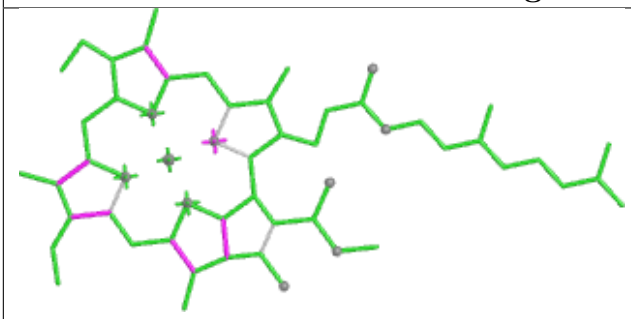


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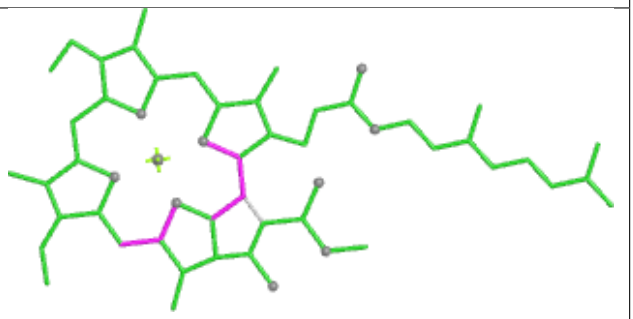


Rings

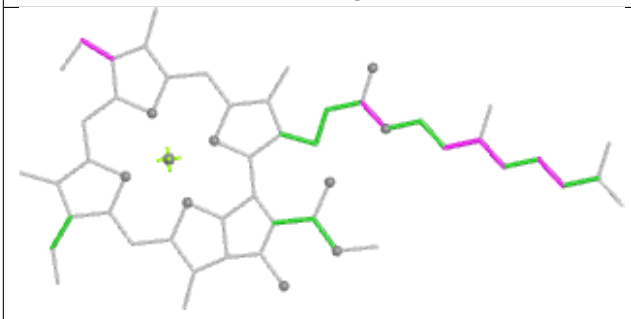
Ligand CLA B 808



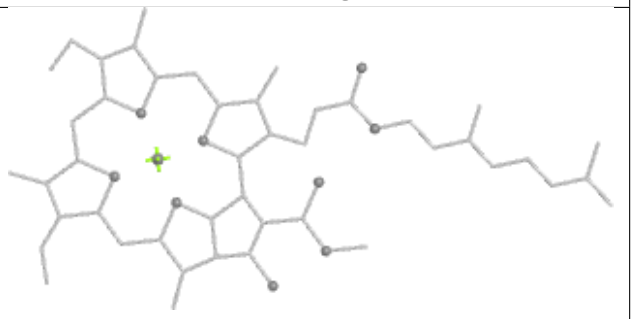
Bond lengths



Bond angles

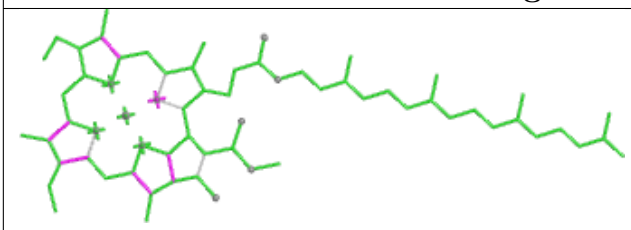


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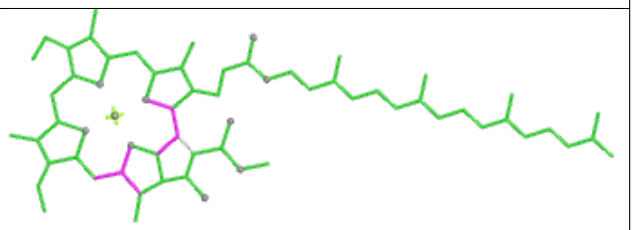


Rings

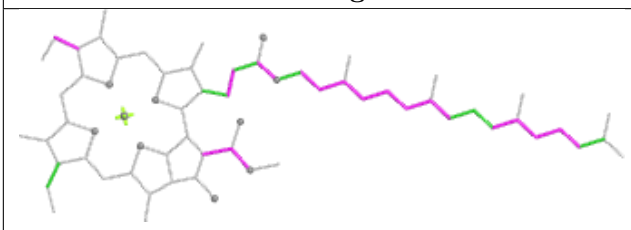
Ligand CLA A 807



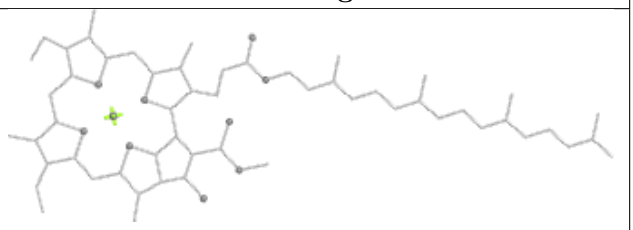
Bond lengths



Bond angles

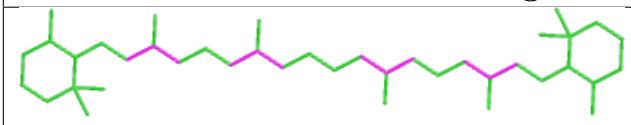


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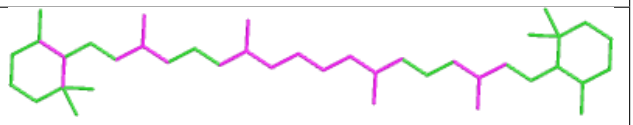


Rings

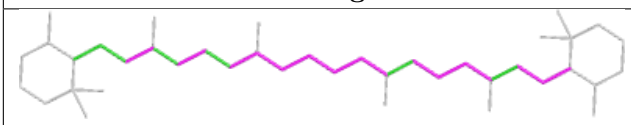
Ligand BCR A 841



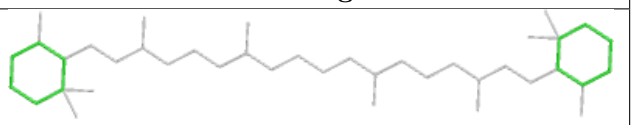
Bond lengths



Bond angles

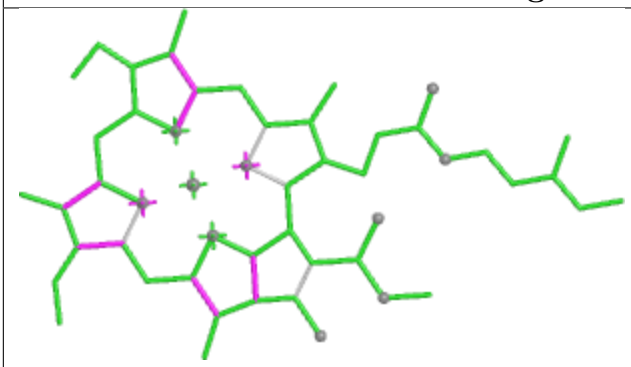


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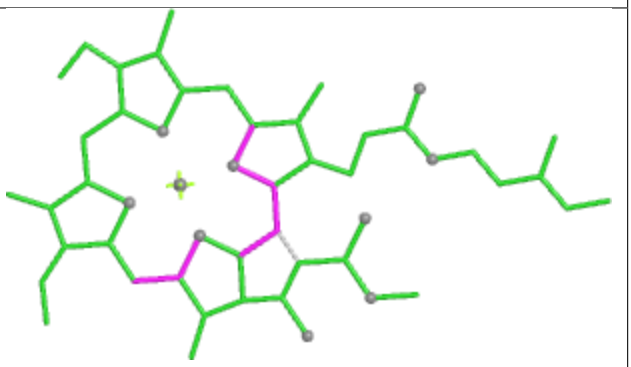


Rings

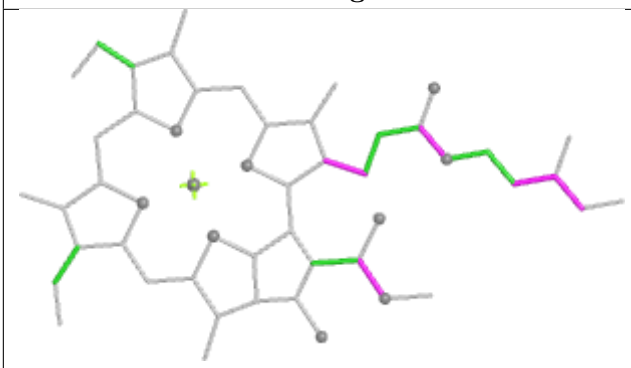
Ligand CLA b 828



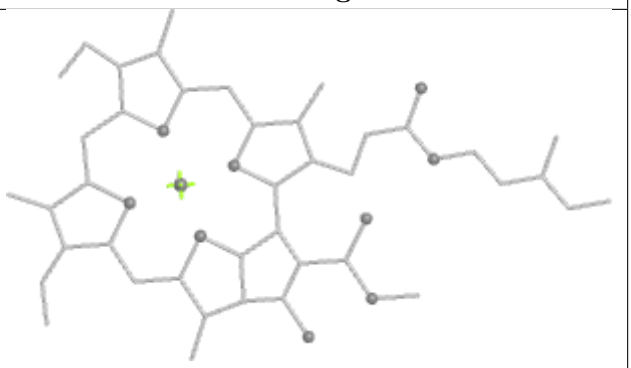
Bond lengths



Bond angles

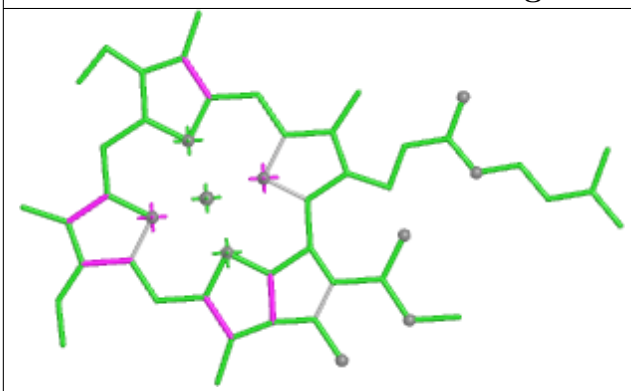


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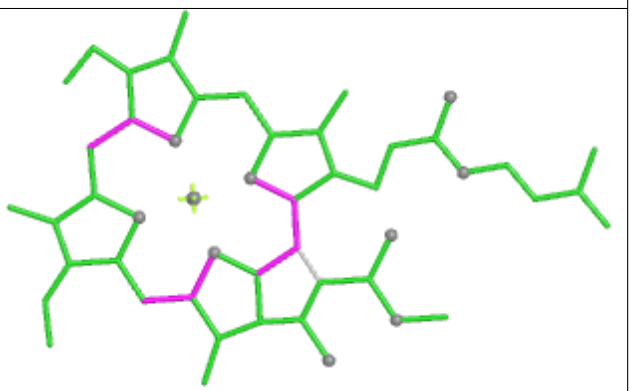


Rings

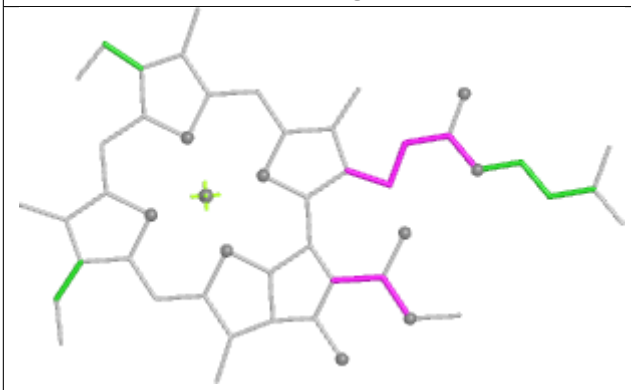
Ligand CLA B 820



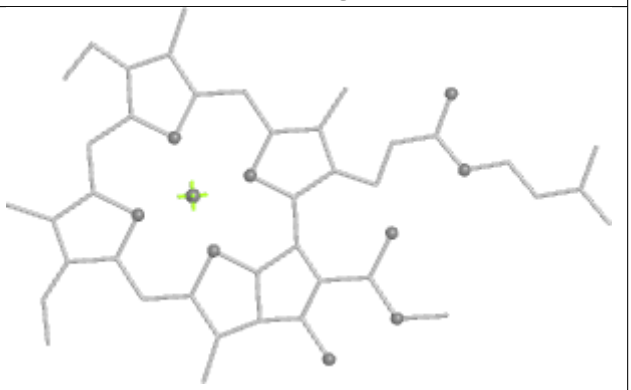
Bond lengths



Bond angles

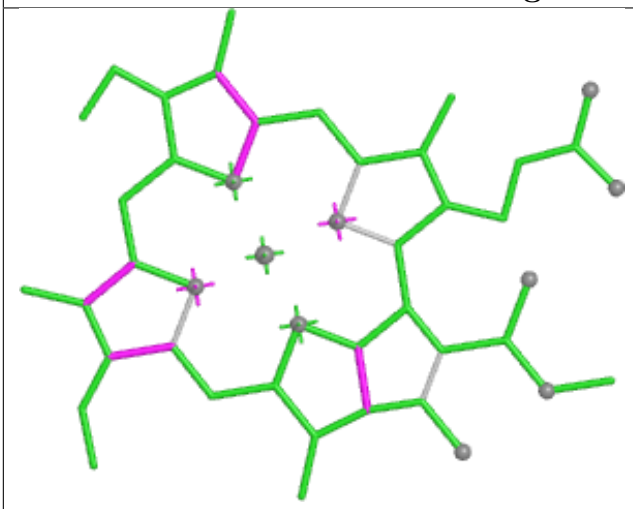


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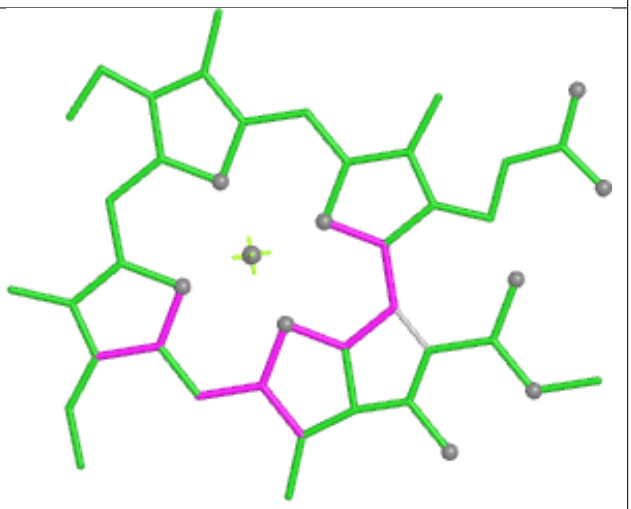


Rings

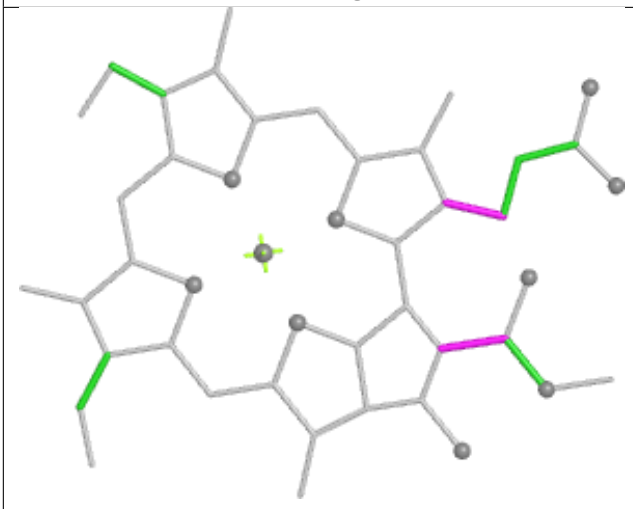
Ligand CLA A 812



Bond lengths



Bond angles

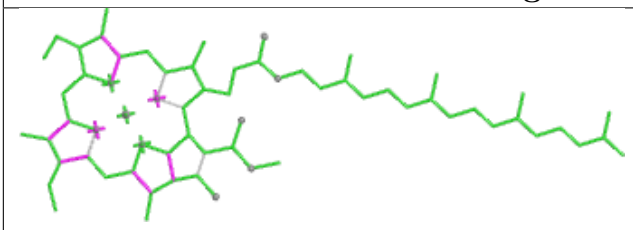


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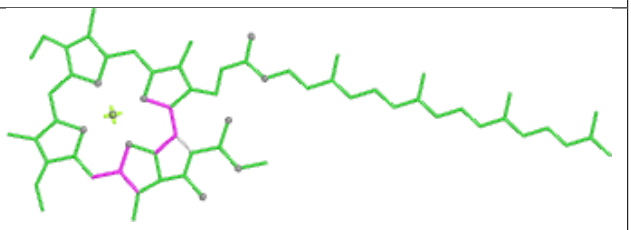


Rings

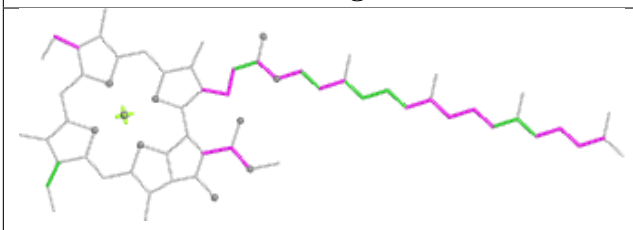
Ligand CLA H 201



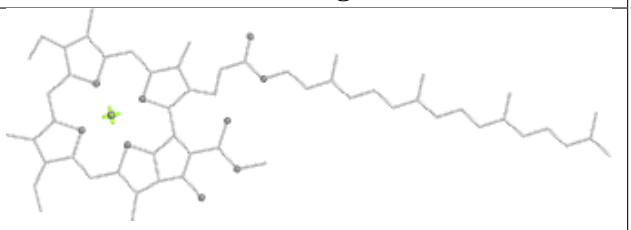
Bond lengths



Bond angles

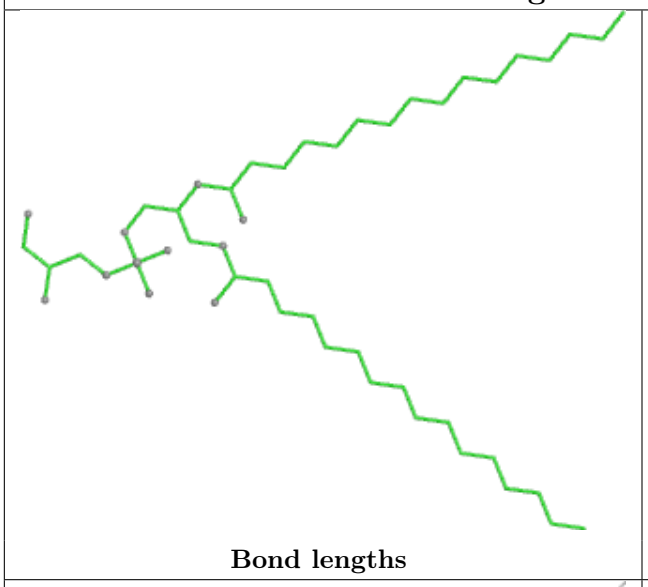


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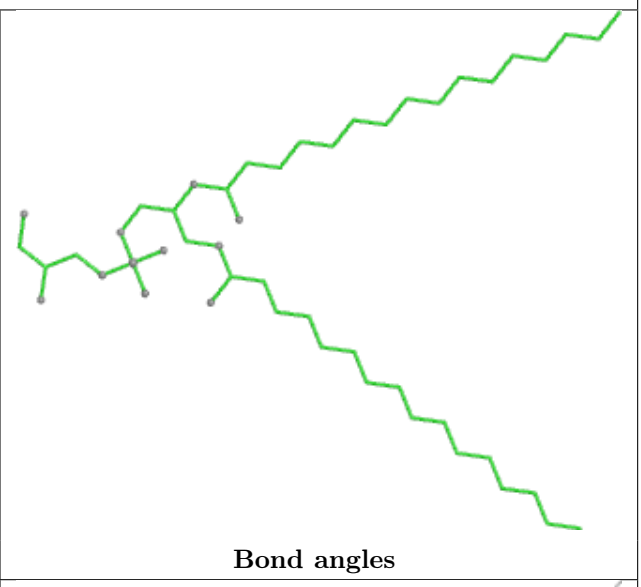


Rings

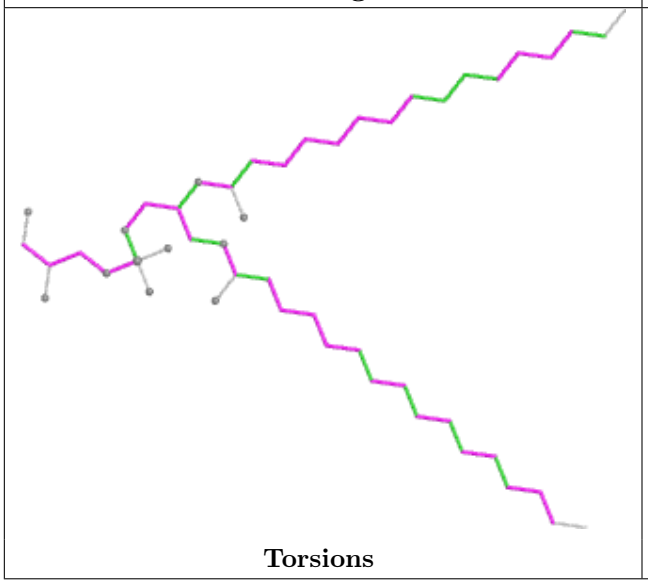
Ligand LHG a 839



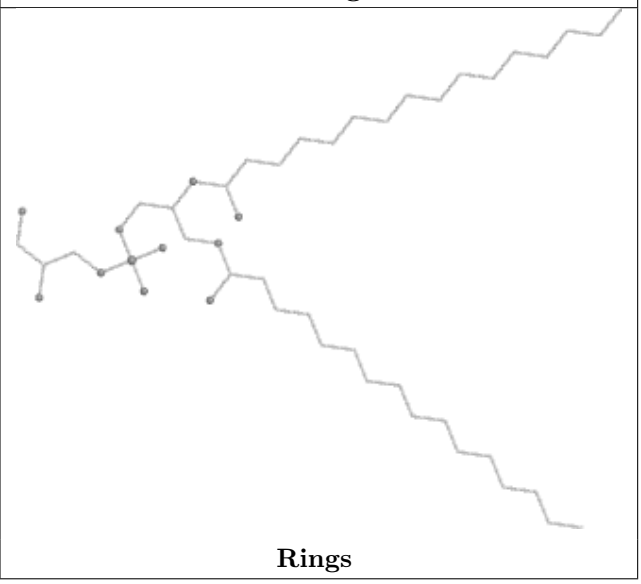
Bond lengths



Bond angles

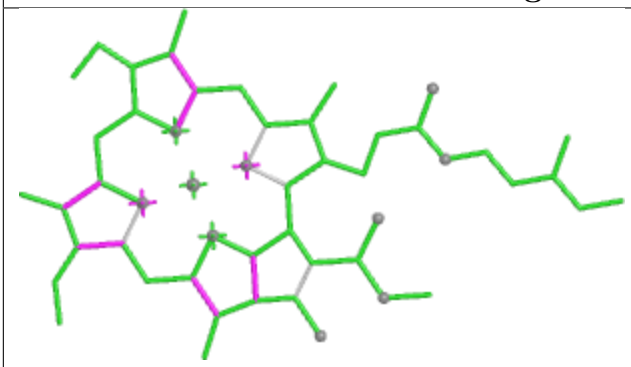


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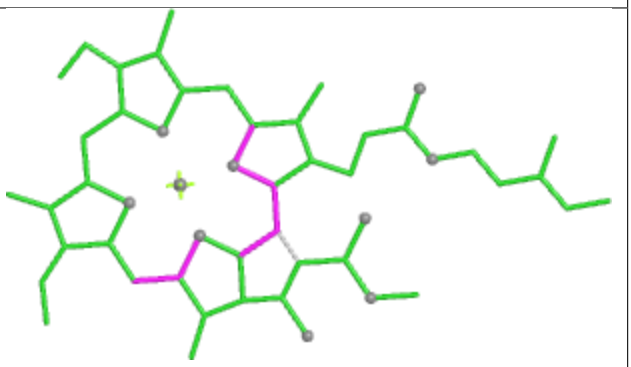


Rings

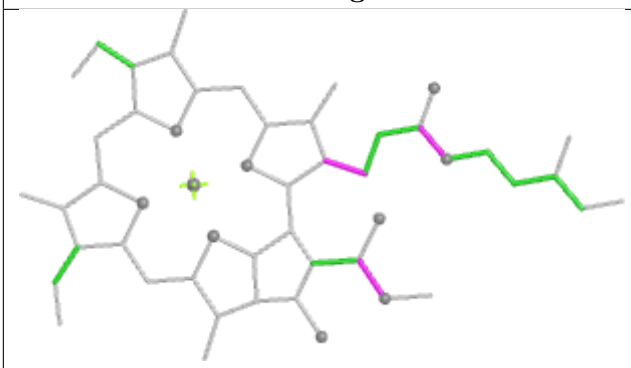
Ligand CLA B 828



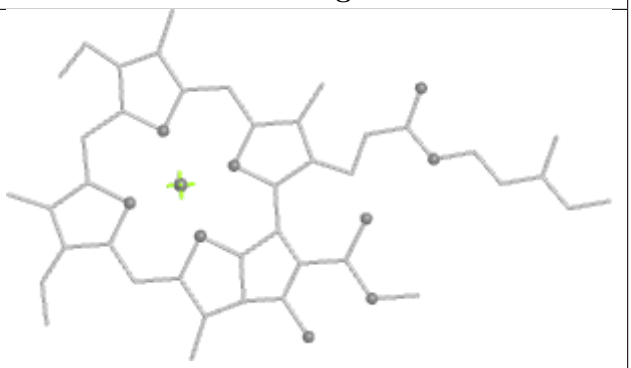
Bond lengths



Bond angles

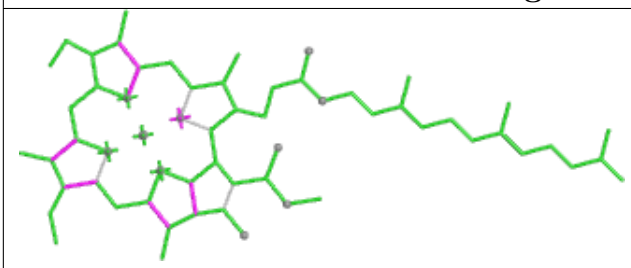


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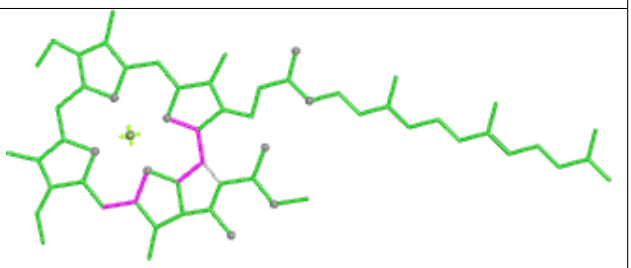


Rings

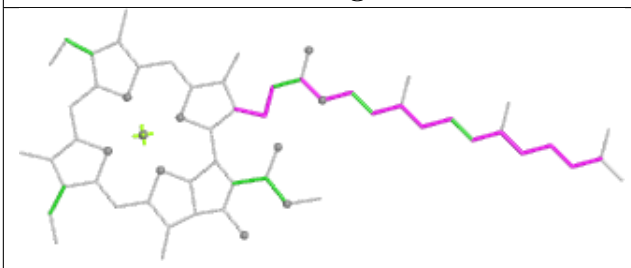
Ligand CLA B 824



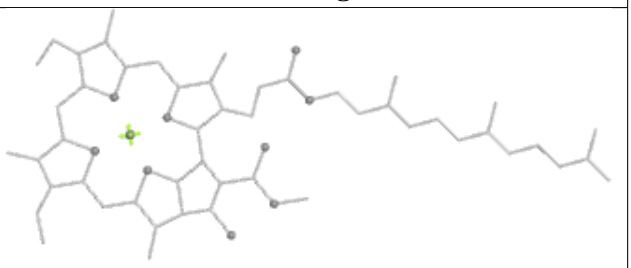
Bond lengths



Bond angles

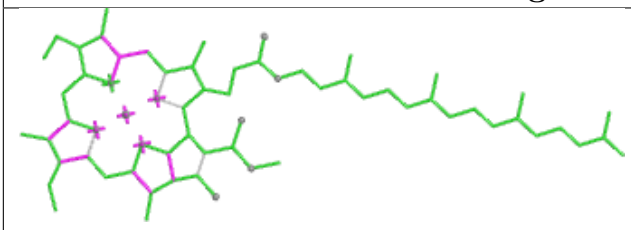


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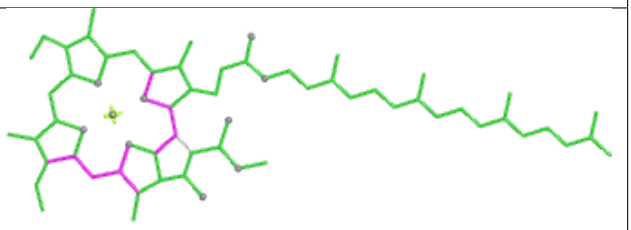


Rings

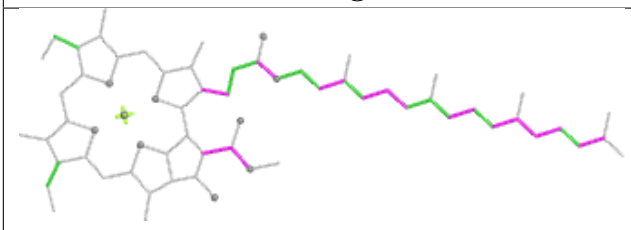
Ligand CLA a 819



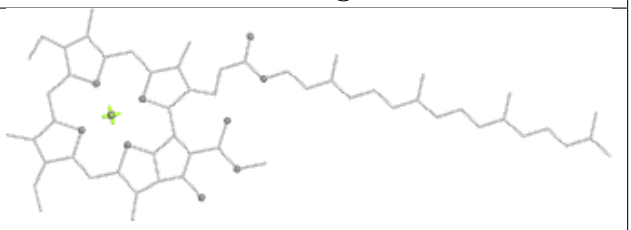
Bond lengths



Bond angles

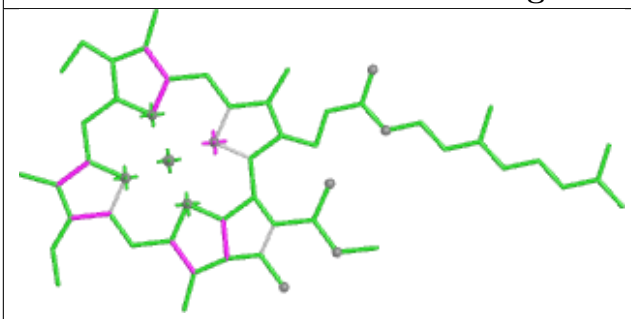


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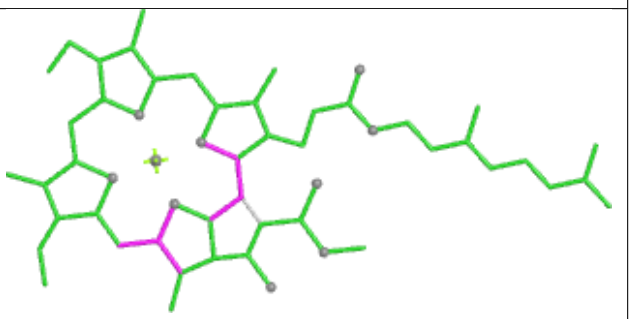


Rings

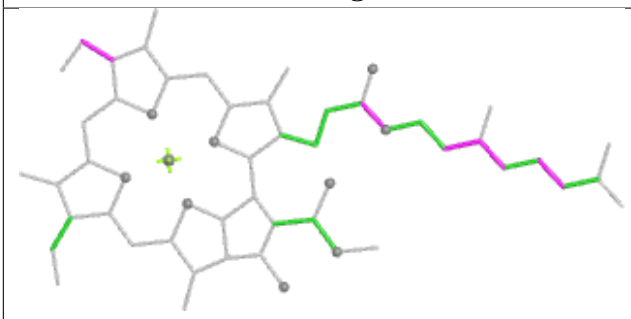
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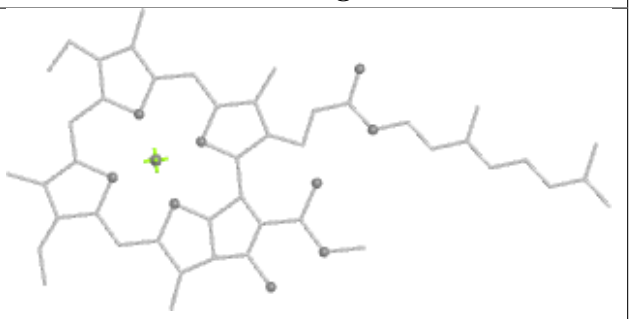
Bond lengths



Bond angles

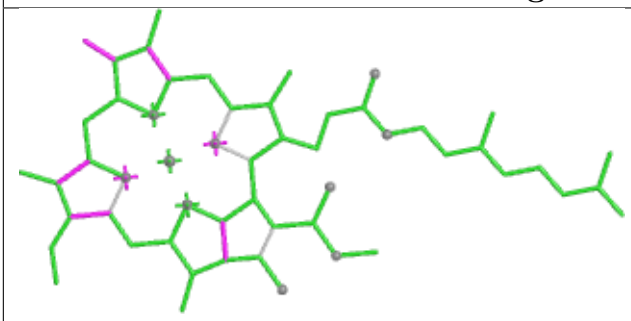


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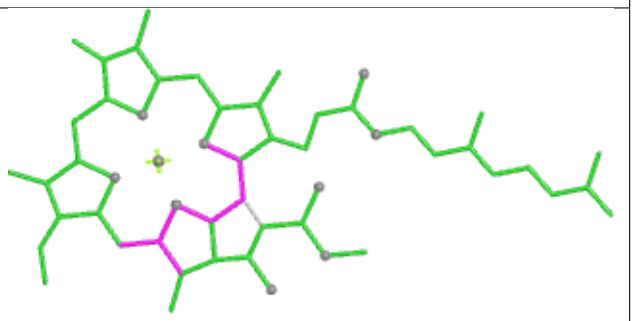


Rings

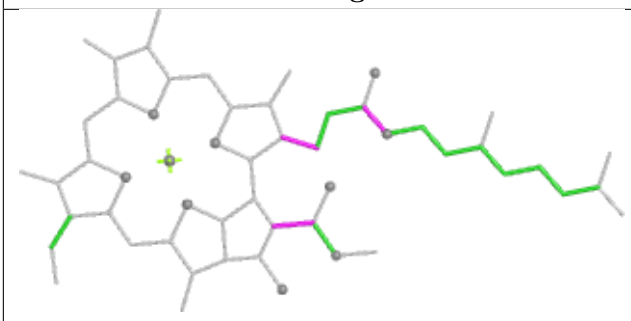
Ligand CLA b 812



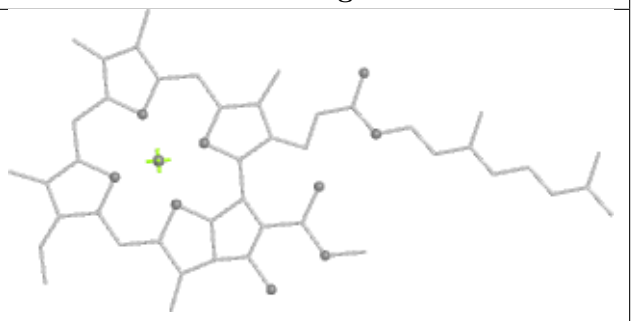
Bond lengths



Bond angles

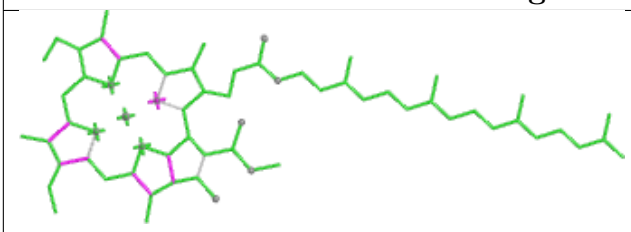


Torsions

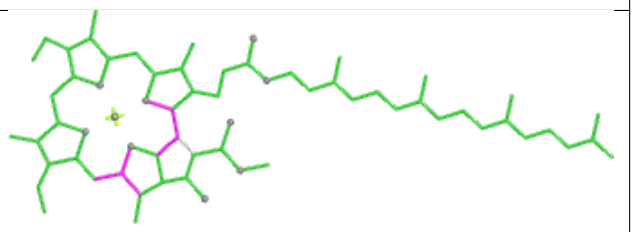


Rings

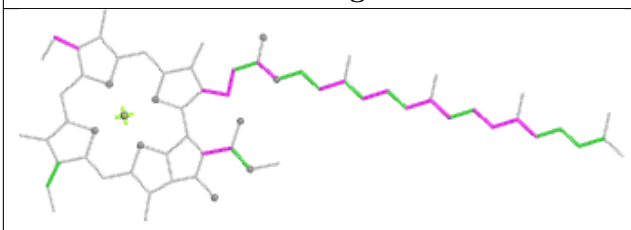
Ligand CLA a 805



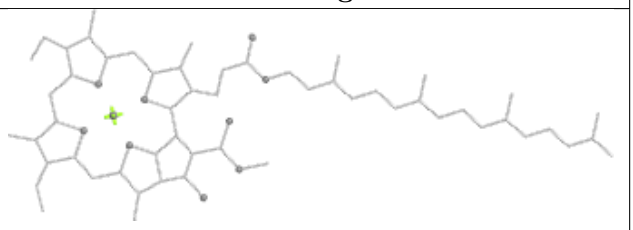
Bond lengths



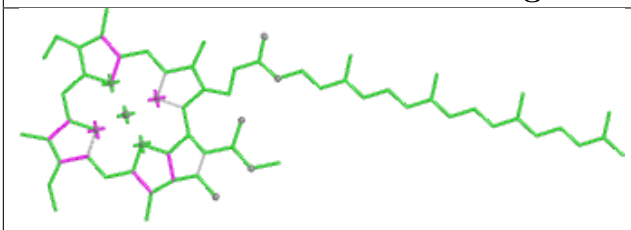
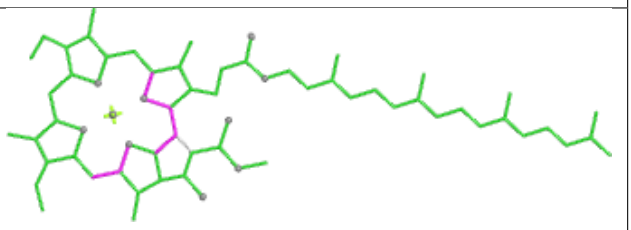
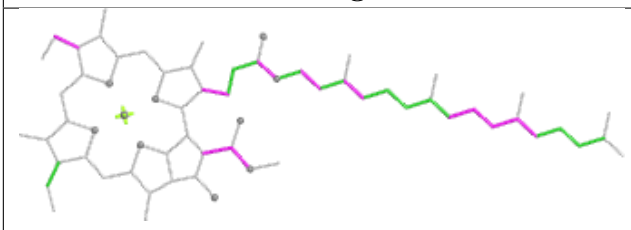
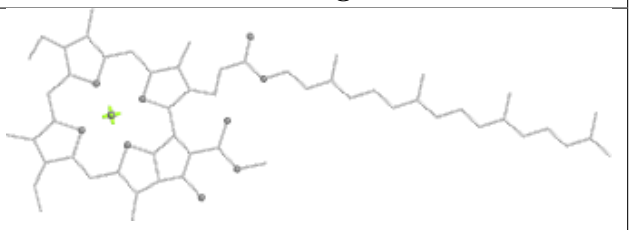
Bond angles

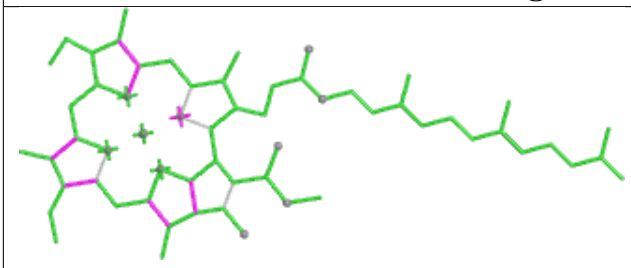
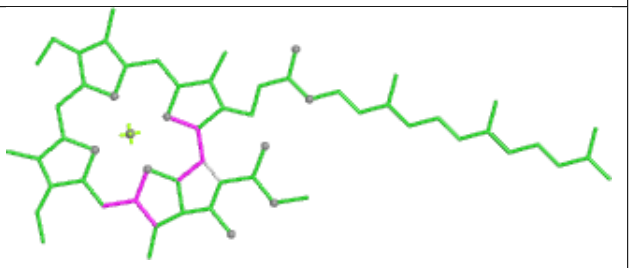
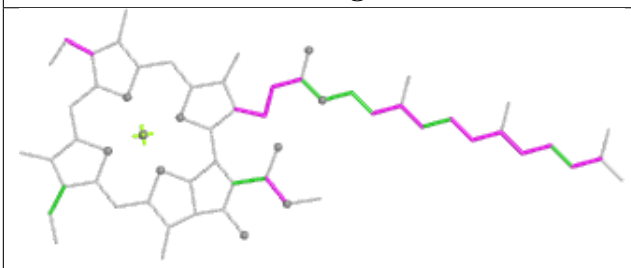
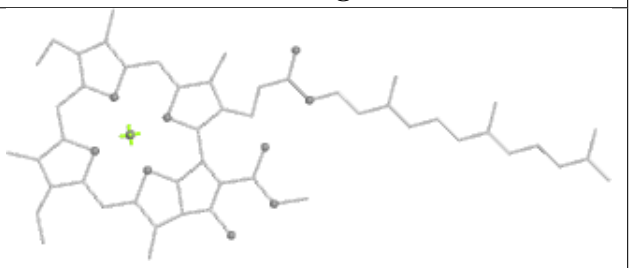


Torsions

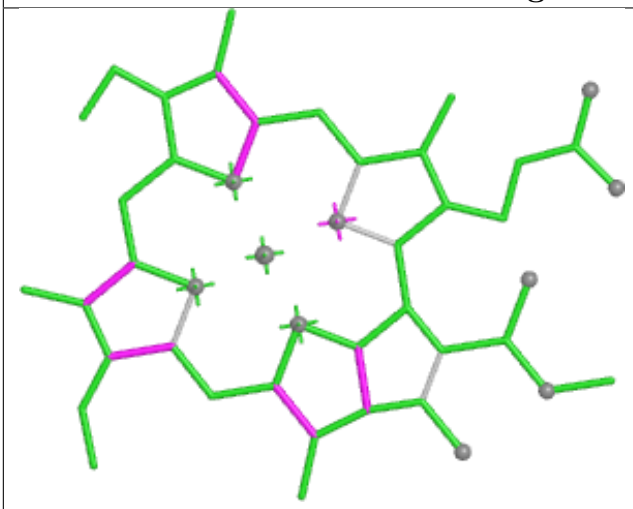


Rings

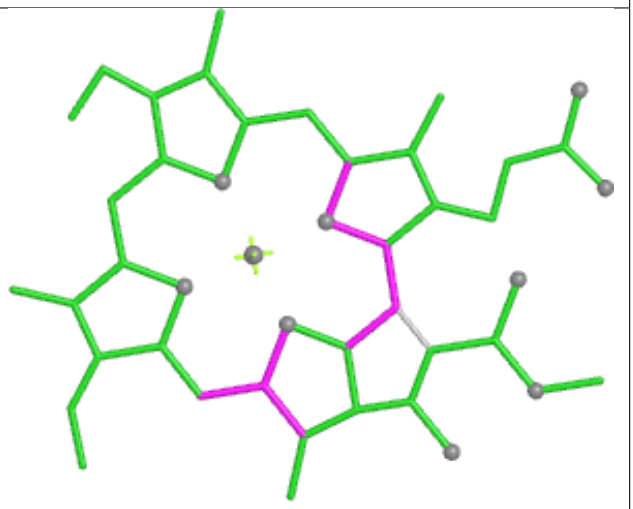
Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

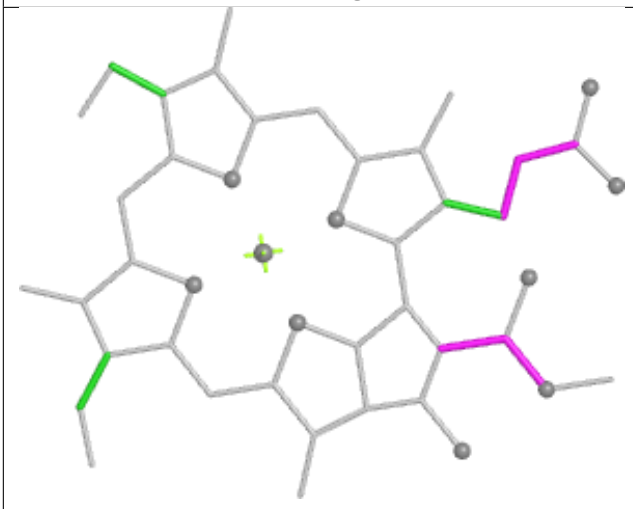
Ligand CLA b 827



Bond lengths



Bond angles

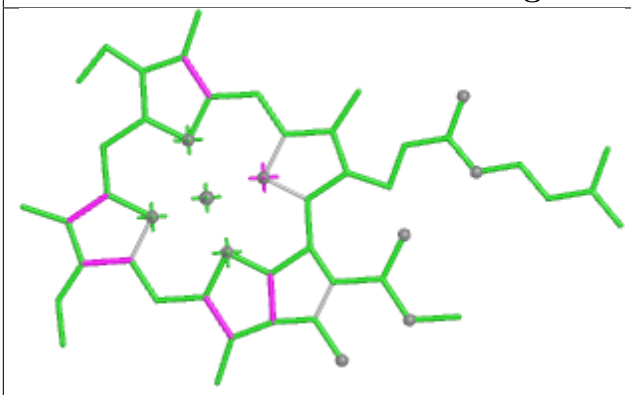


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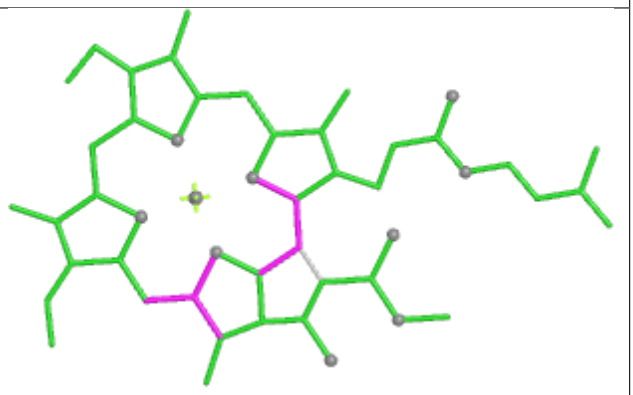


Rings

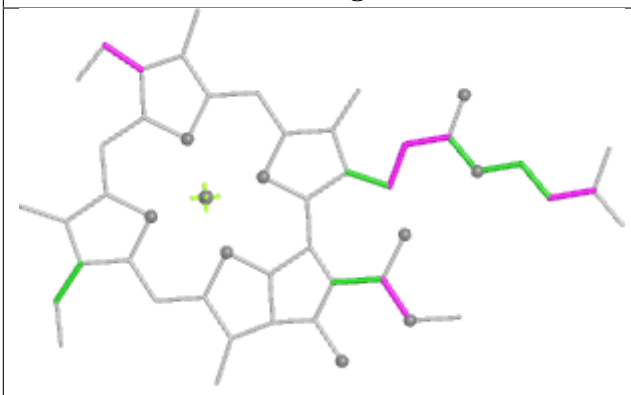
Ligand CLA A 813



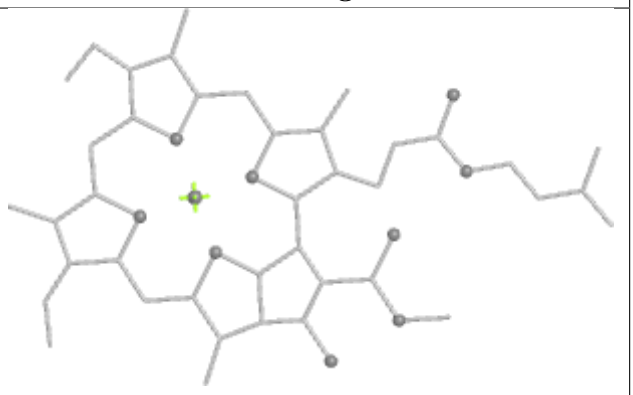
Bond lengths



Bond angles

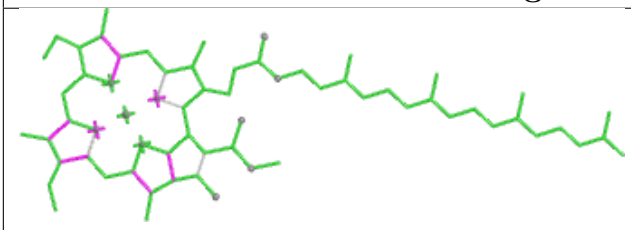


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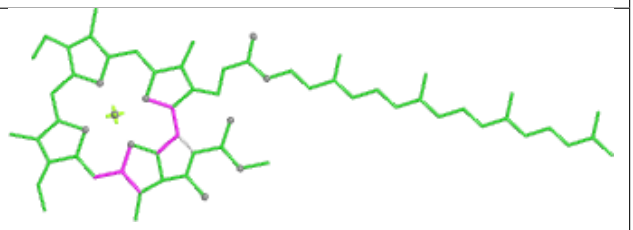


Rings

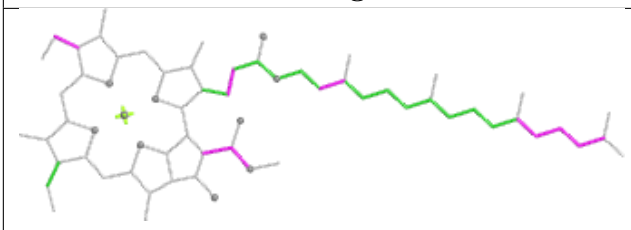
Ligand CLA B 831



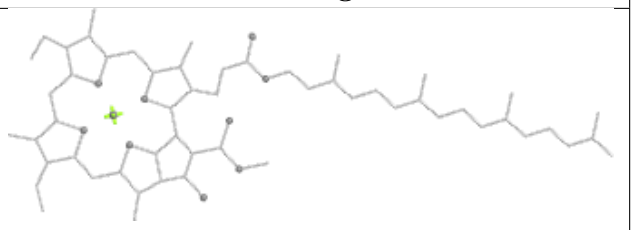
Bond lengths



Bond angles

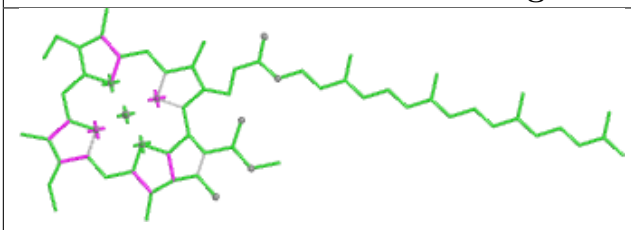


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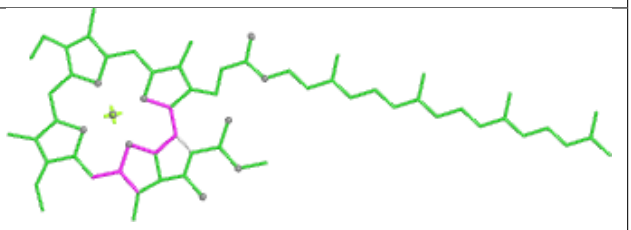


Rings

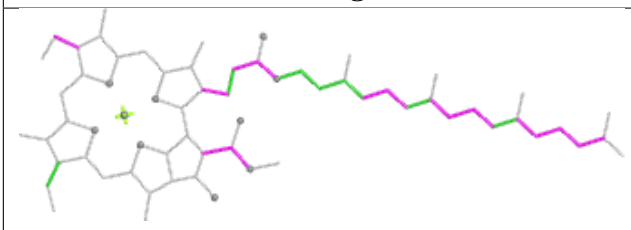
Ligand CLA h 202



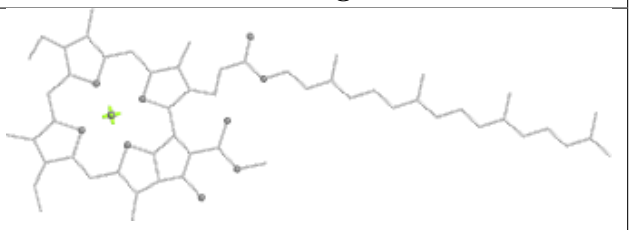
Bond lengths



Bond angles

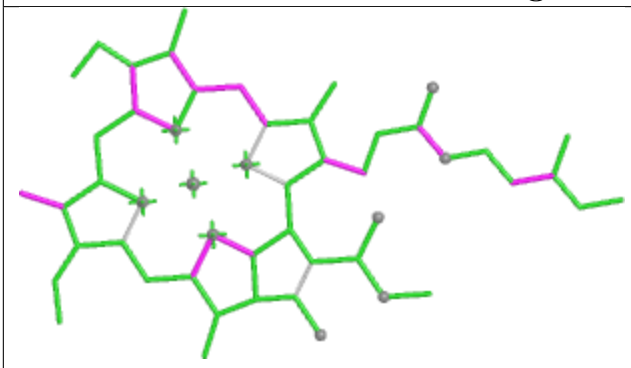


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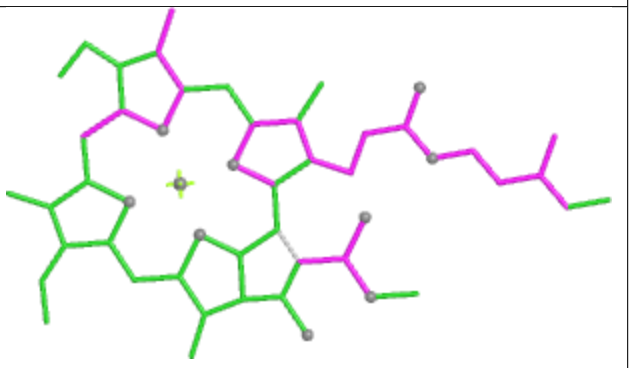


Rings

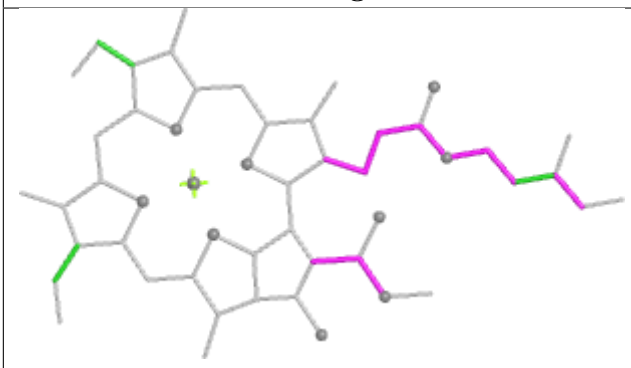
Ligand CLA h 201



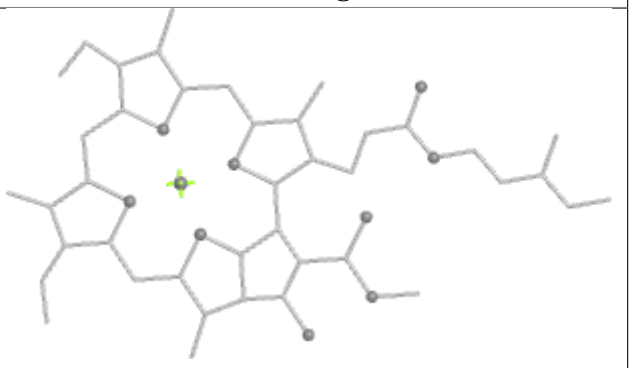
Bond lengths



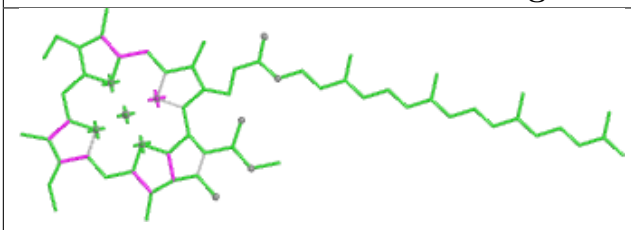
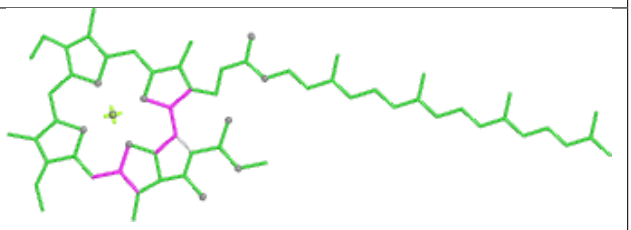
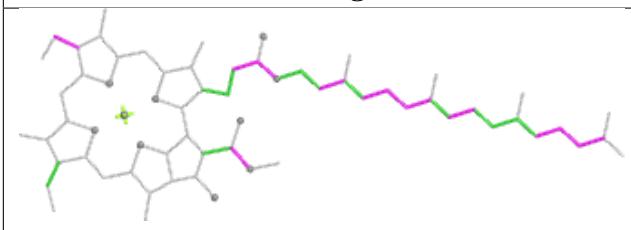
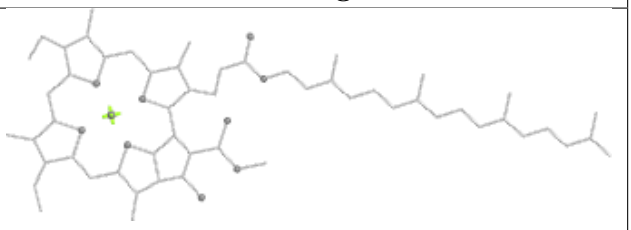
Bond angles

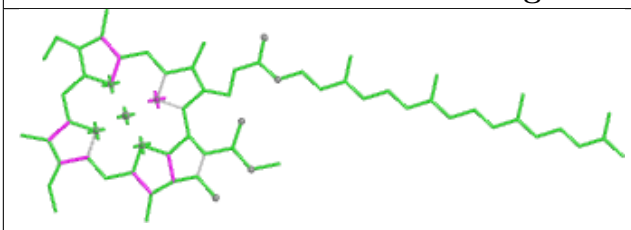
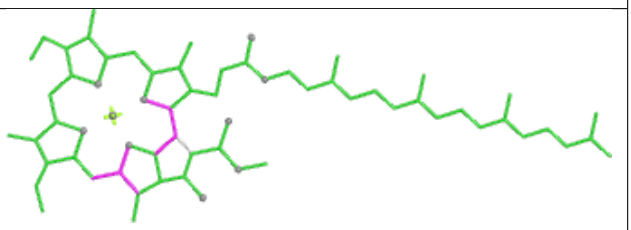
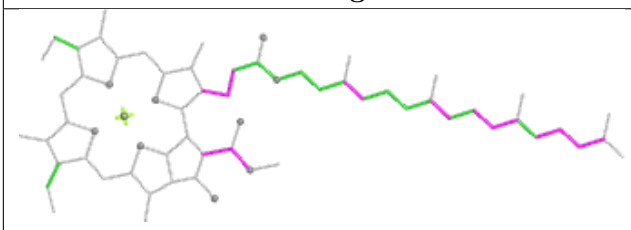
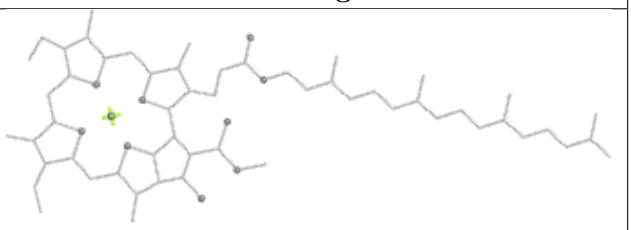


Torsions

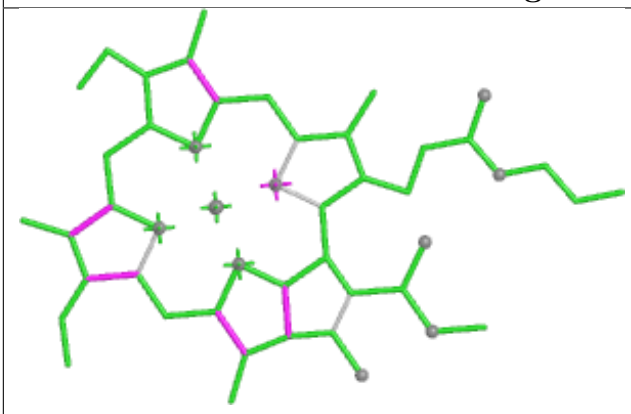


Rings

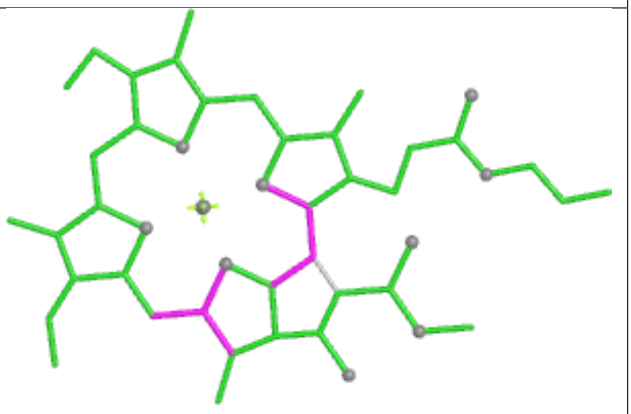
Ligand CLA a 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

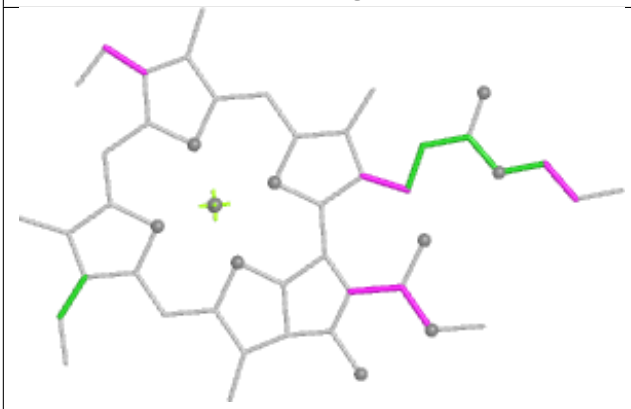
Ligand CLA B 826



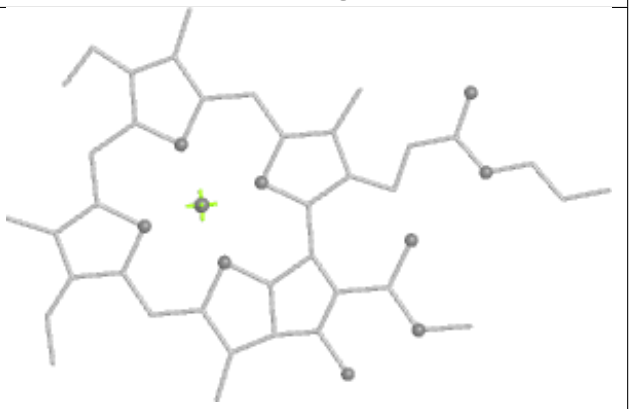
Bond lengths



Bond angles

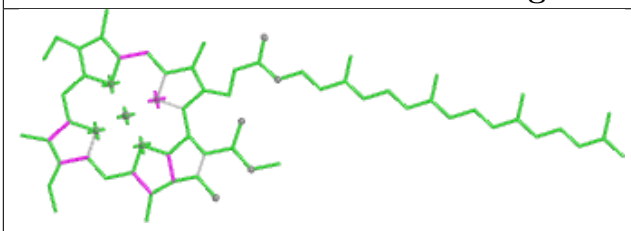


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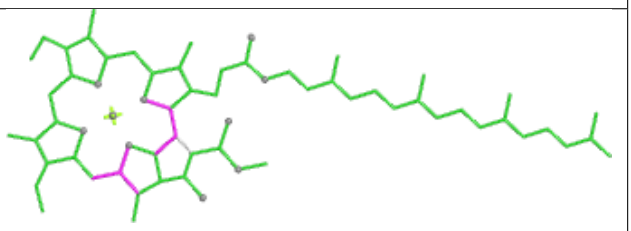


Rings

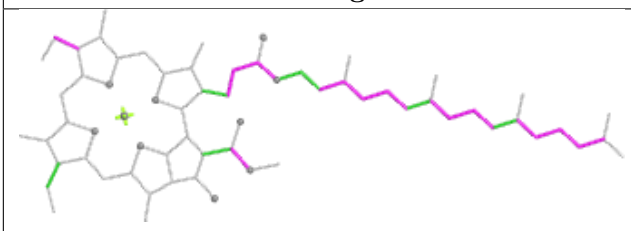
Ligand CLA a 806



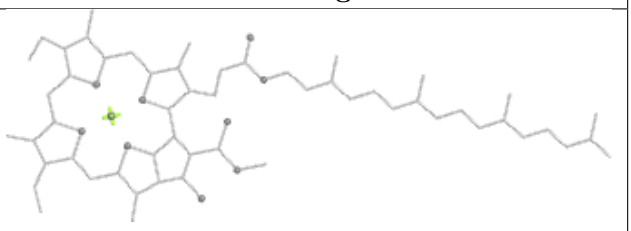
Bond lengths



Bond angles

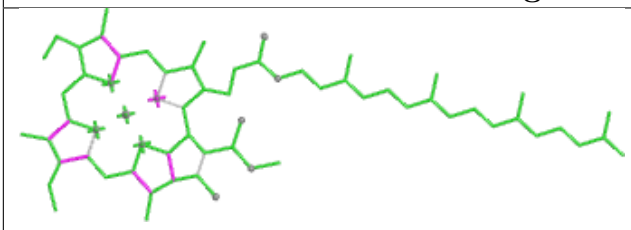


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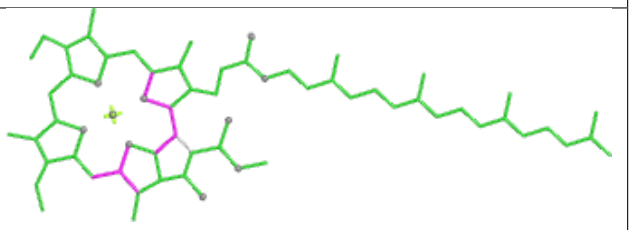


Rings

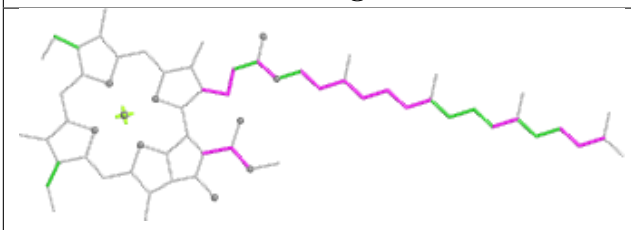
Ligand CLA A 821



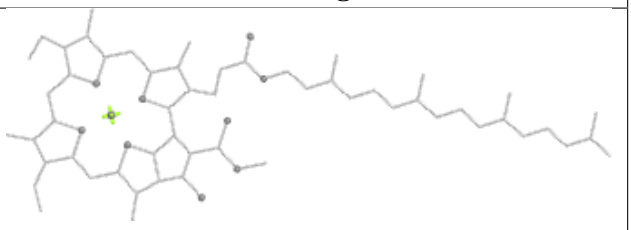
Bond lengths



Bond angles

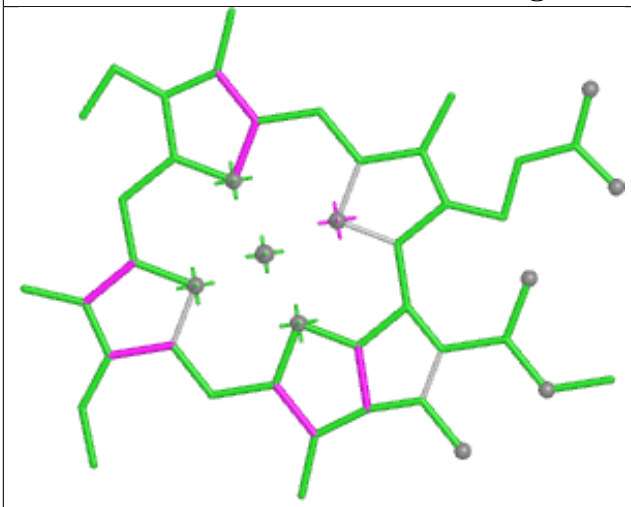


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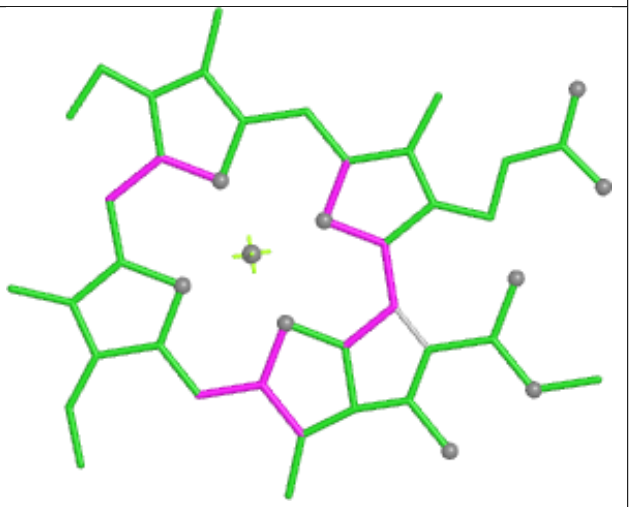


Rings

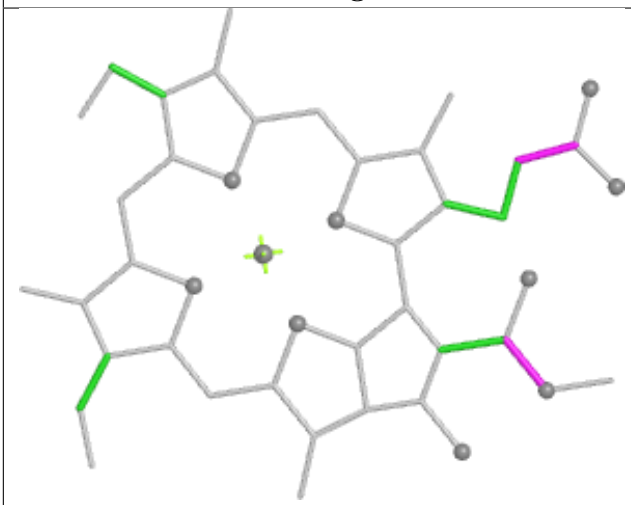
Ligand CLA a 814



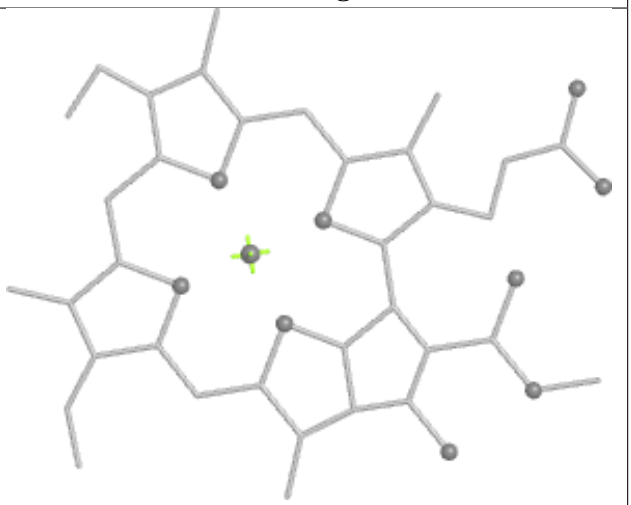
Bond lengths



Bond angles

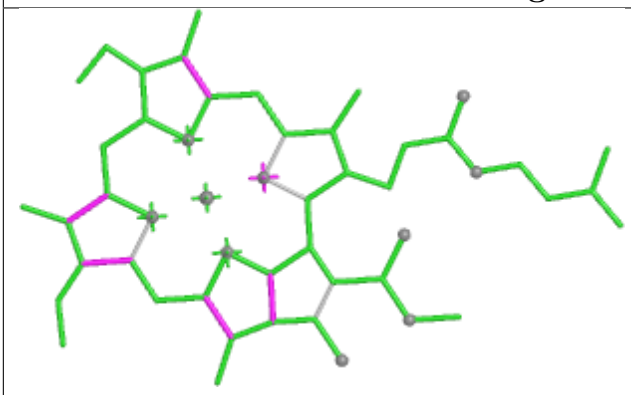


Torsions

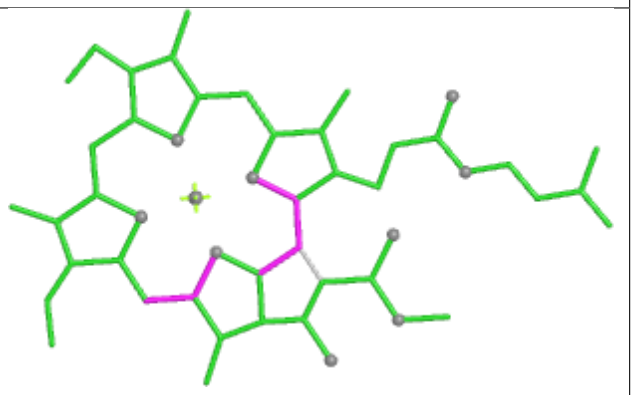


Rings

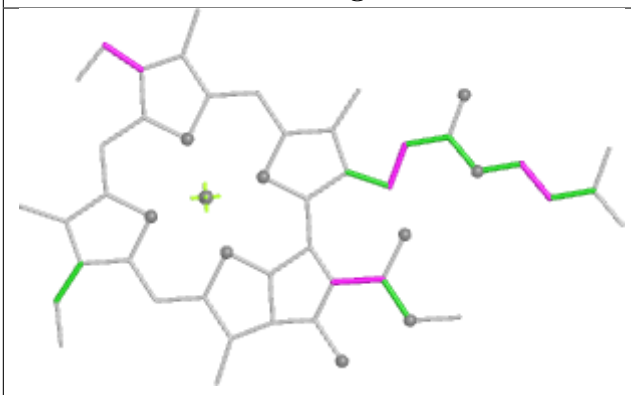
Ligand CLA a 828



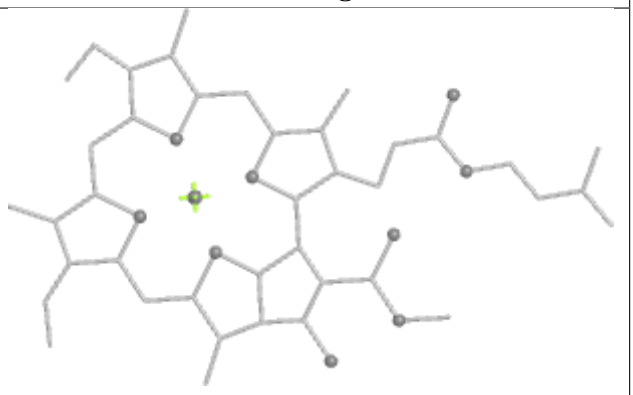
Bond lengths



Bond angles

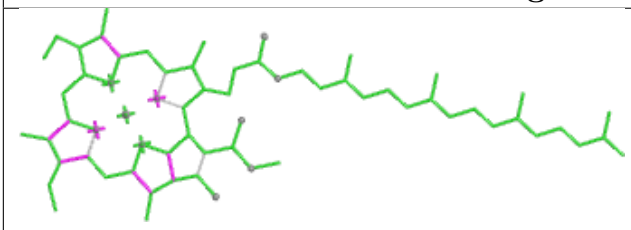


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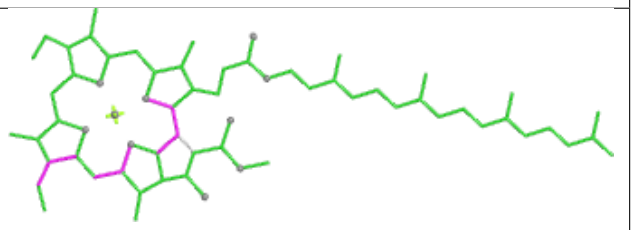


Rings

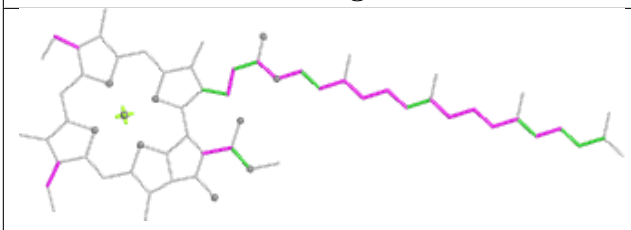
Ligand CLA b 801



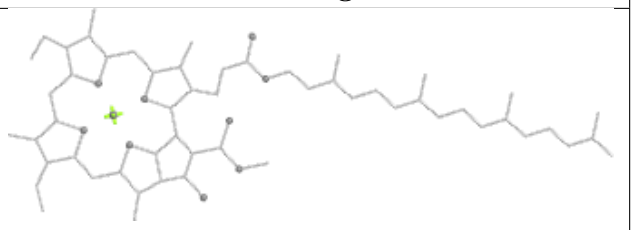
Bond lengths



Bond angles

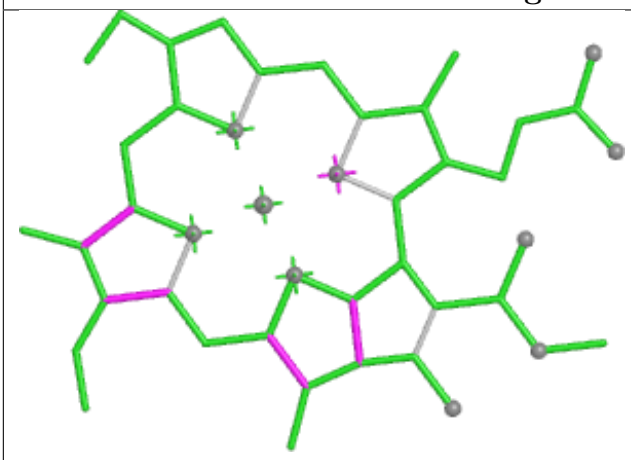


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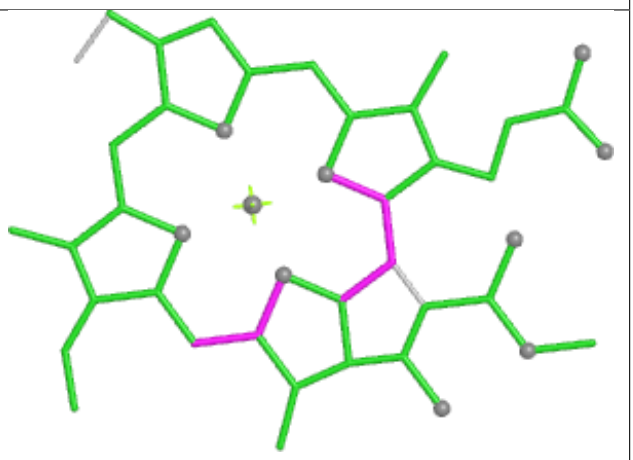


Rings

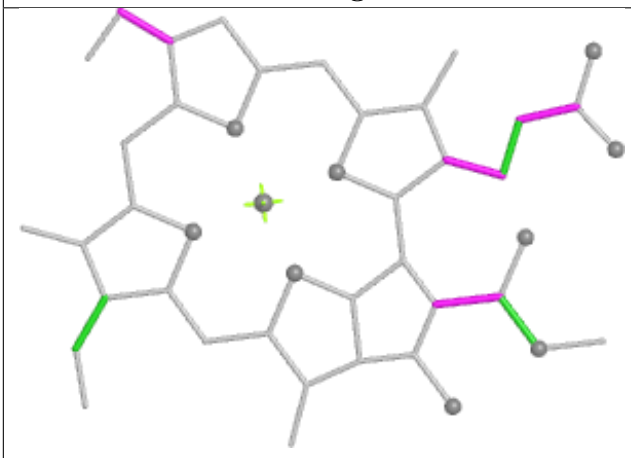
Ligand CLA B 813



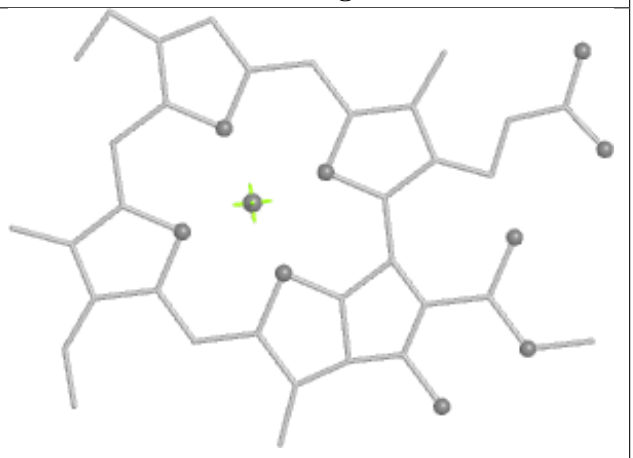
Bond lengths



Bond angles

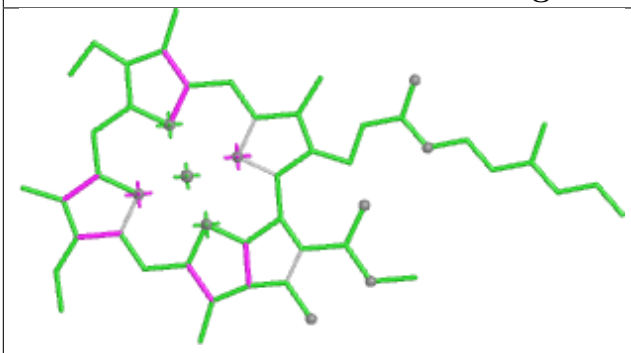


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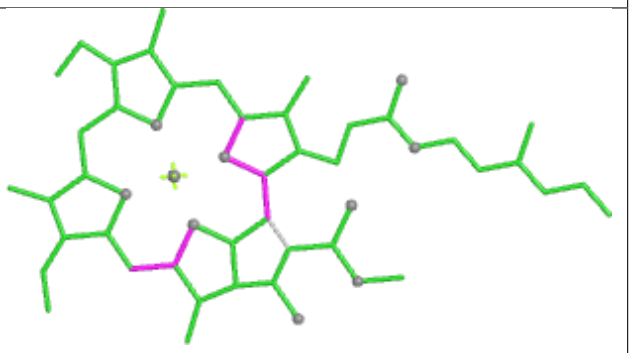


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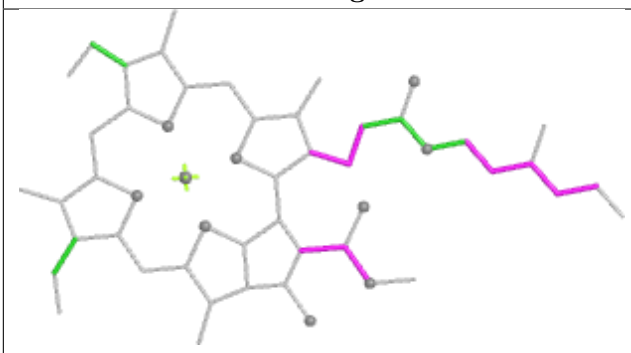
Ligand CLA l 302



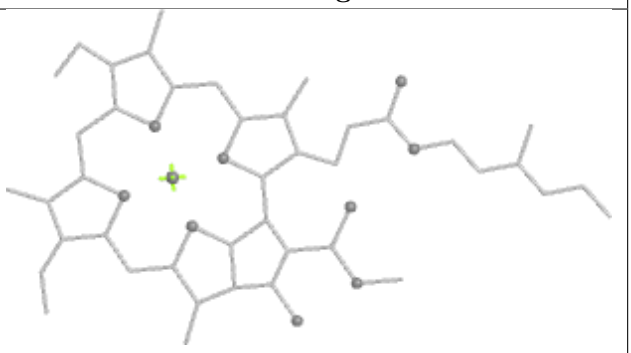
Bond lengths



Bond angles

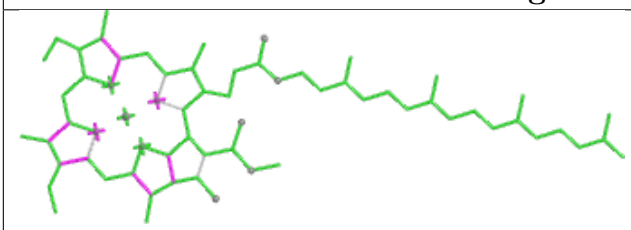


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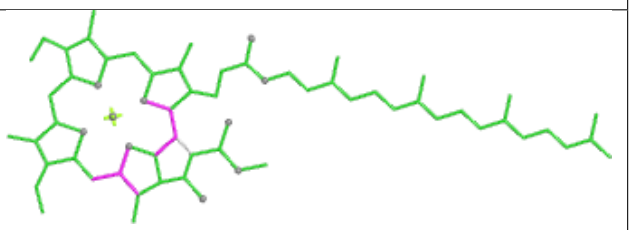


Rings

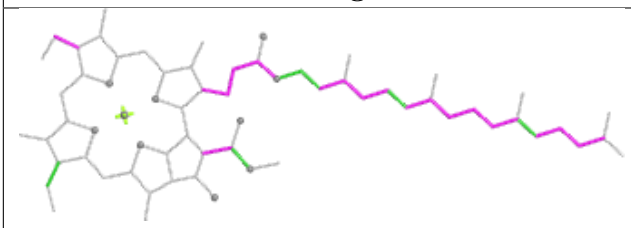
Ligand CLA a 830



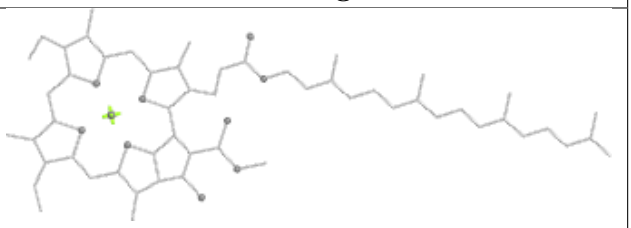
Bond lengths



Bond angles

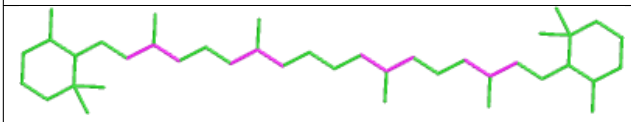


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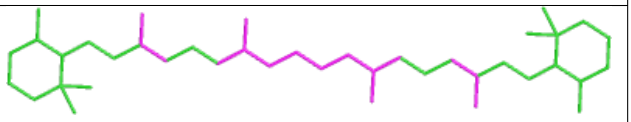


Rings

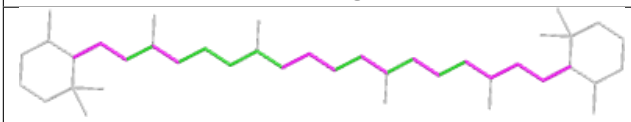
Ligand BCR L 301



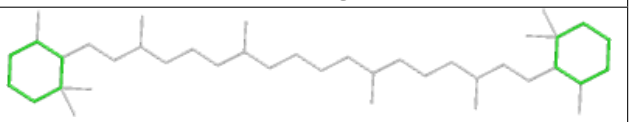
Bond lengths



Bond angles

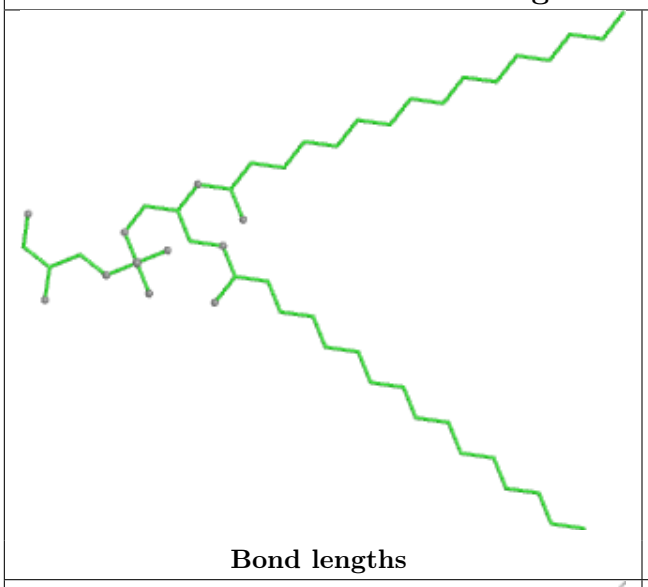


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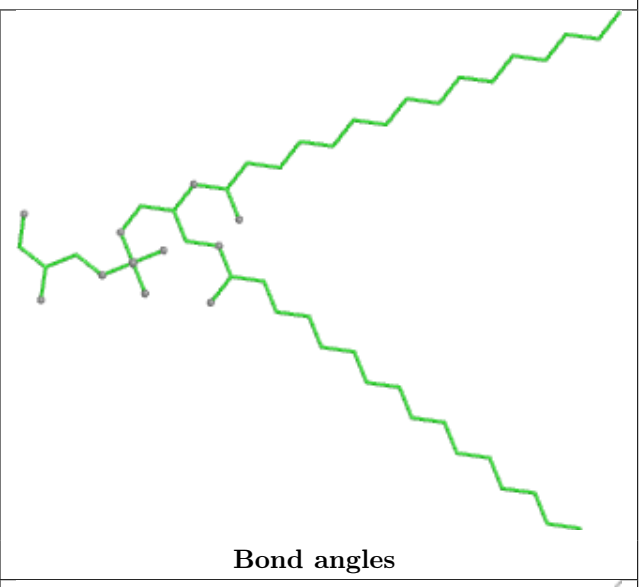


Rings

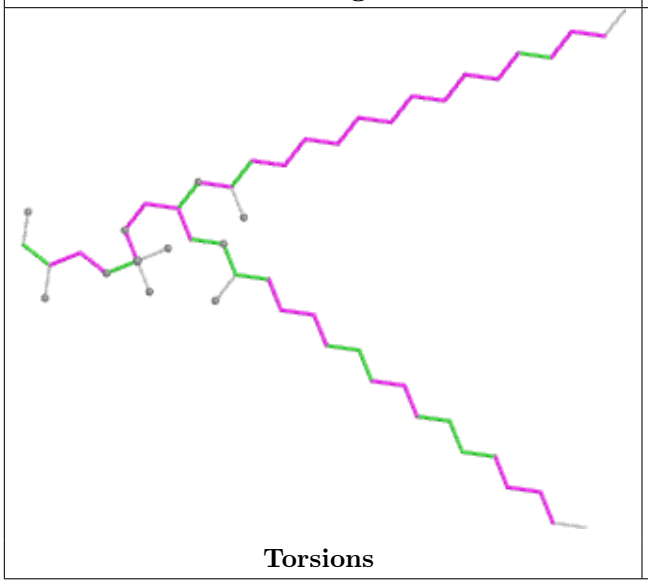
Ligand LHG l 303



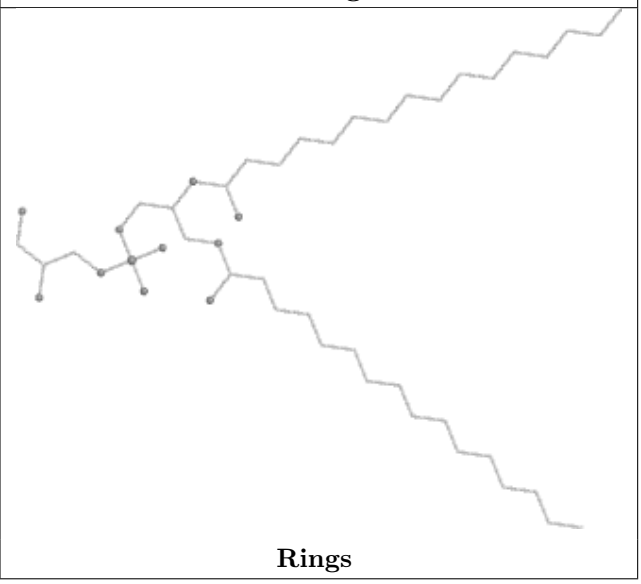
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Bond angles

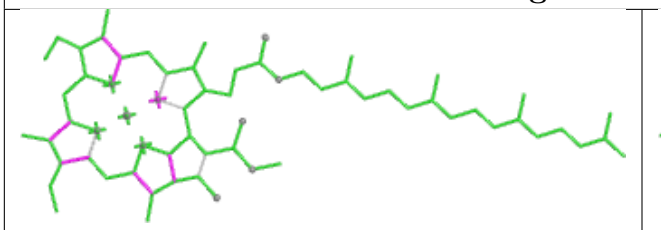


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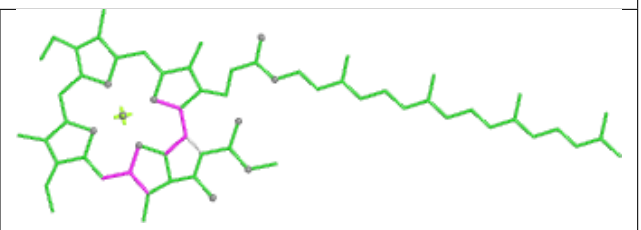


Rings

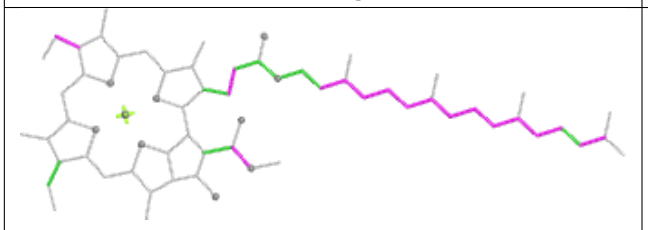
Ligand CLA a 846



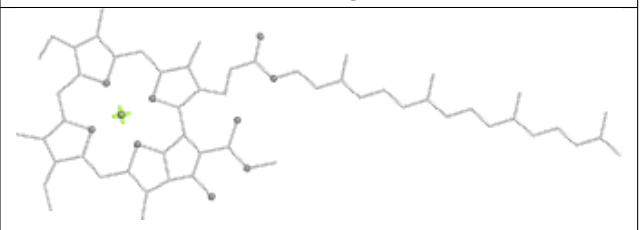
Bond lengths



Bond angles

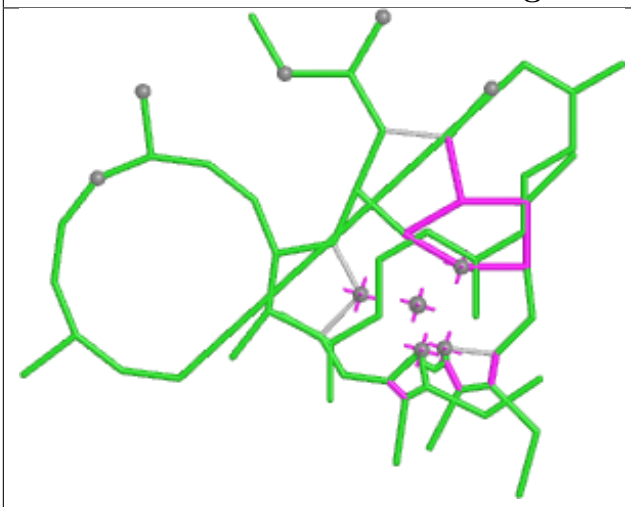


Torsions



Rings

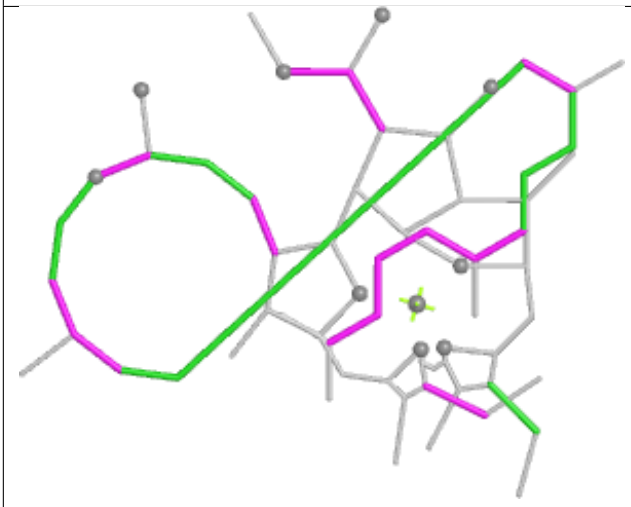
Ligand CLA A 819



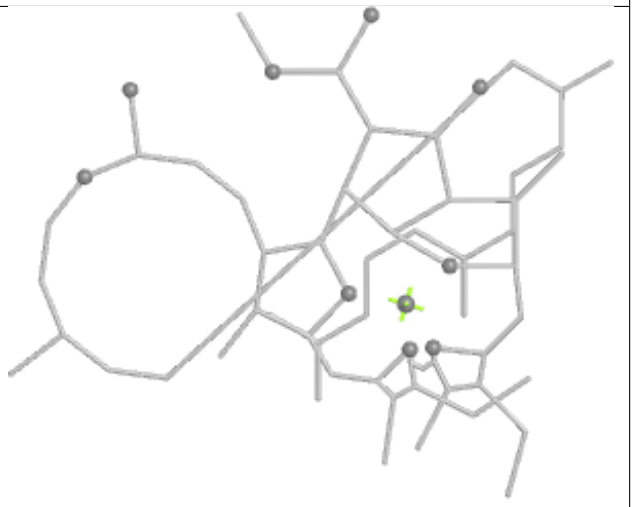
Bond lengths



Bond angles

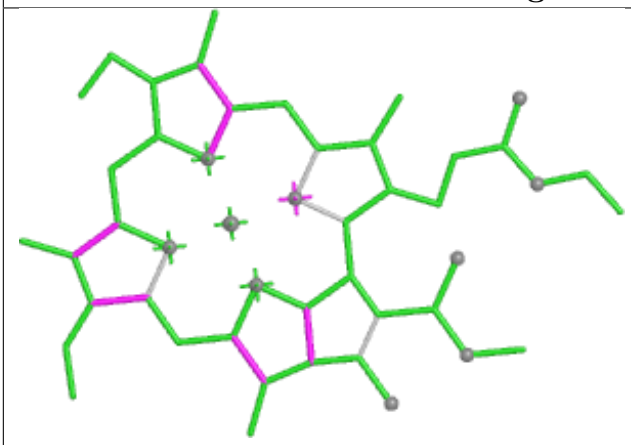


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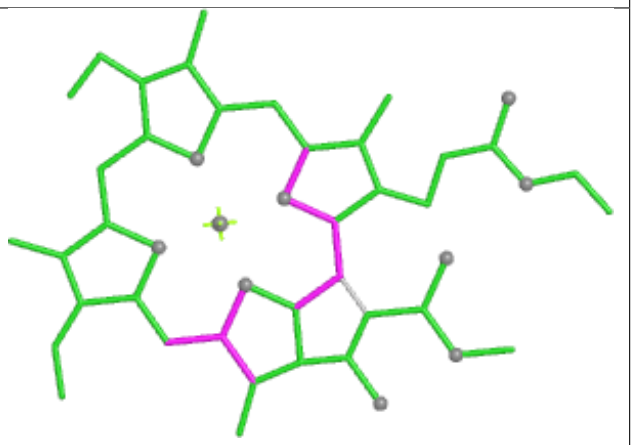


Rings

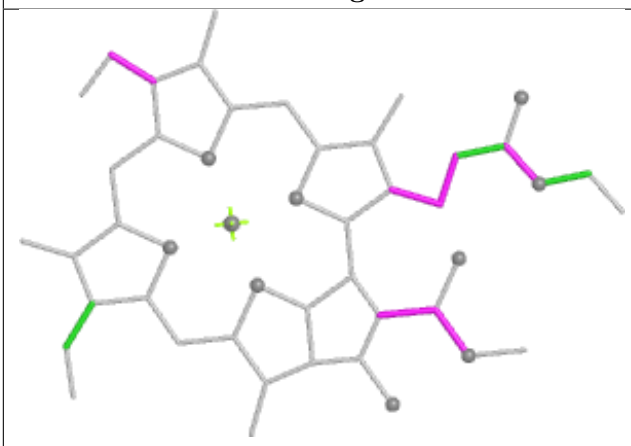
Ligand CLA b 822



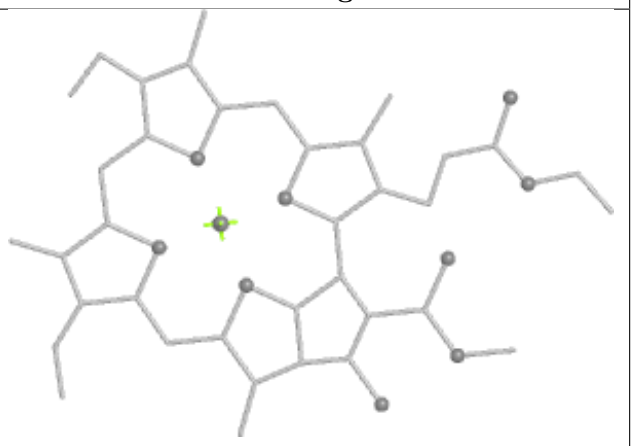
Bond lengths



Bond angles

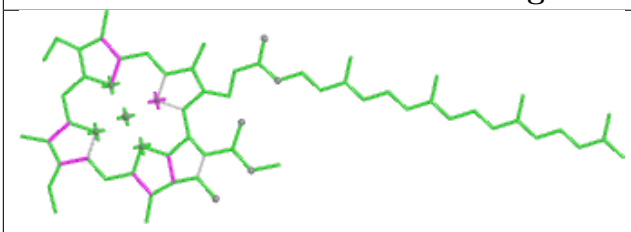


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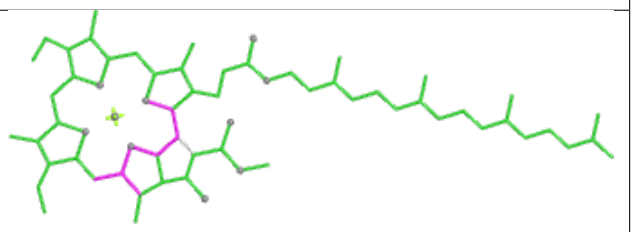


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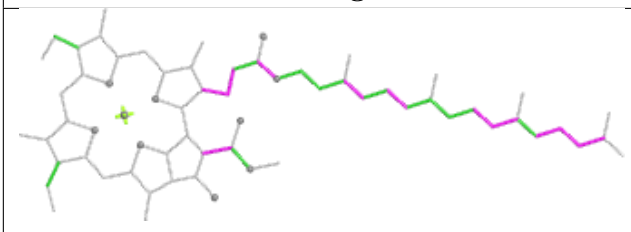
Ligand CLA b 815



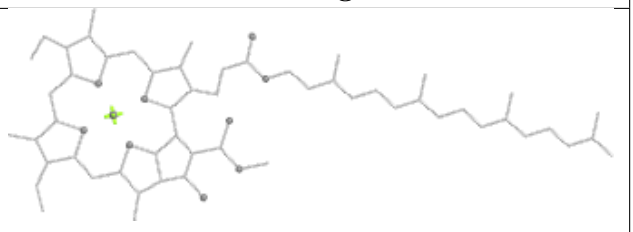
Bond lengths



Bond angles

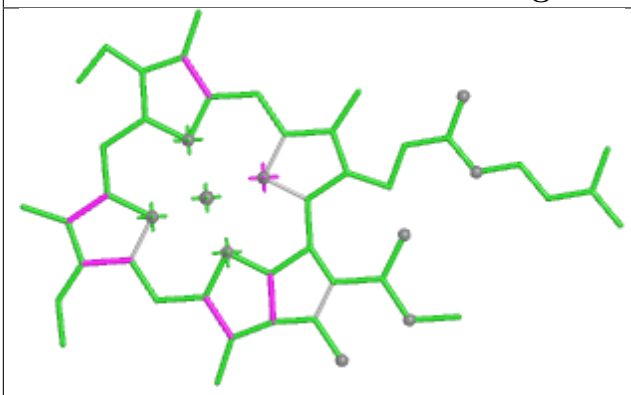


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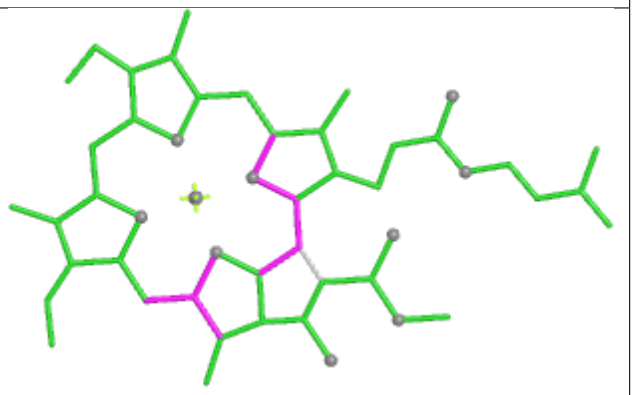


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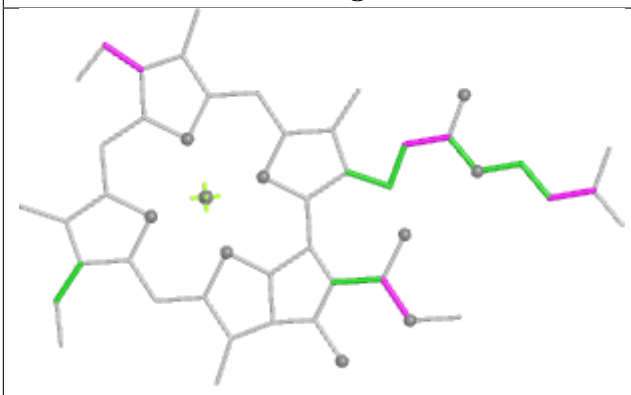
Ligand CLA l 307



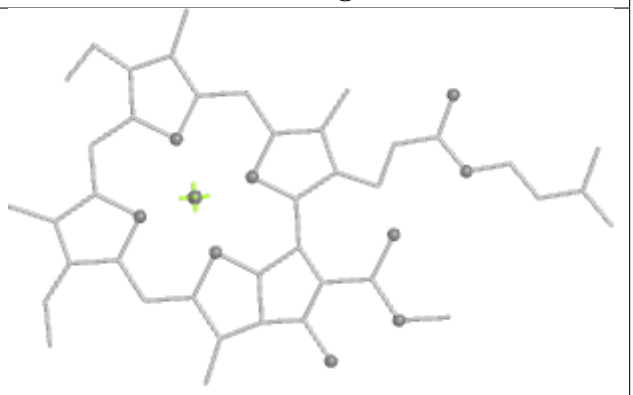
Bond lengths



Bond angles

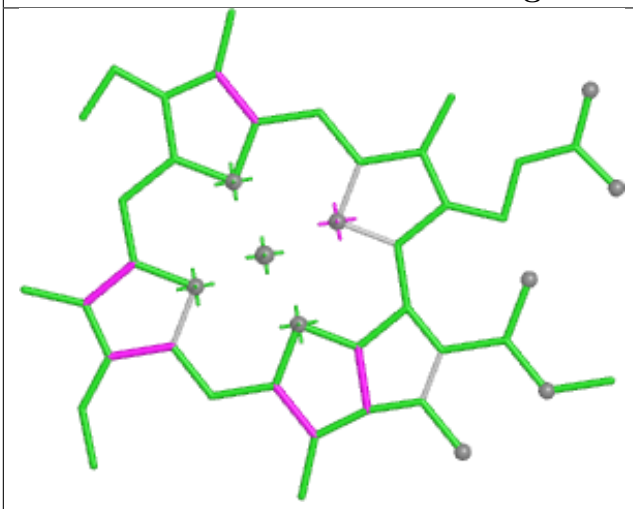


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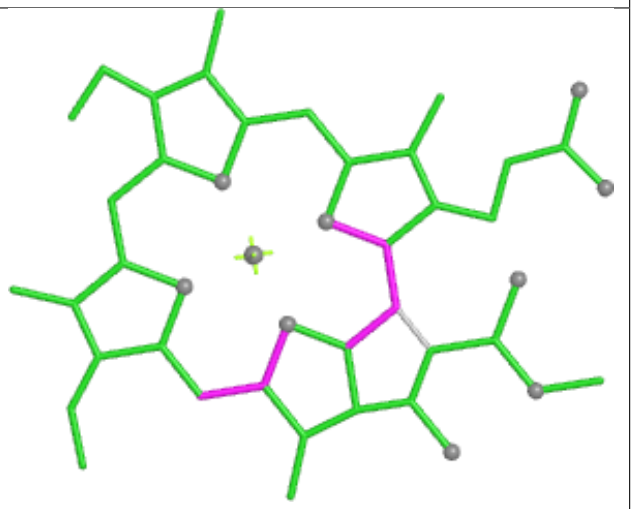


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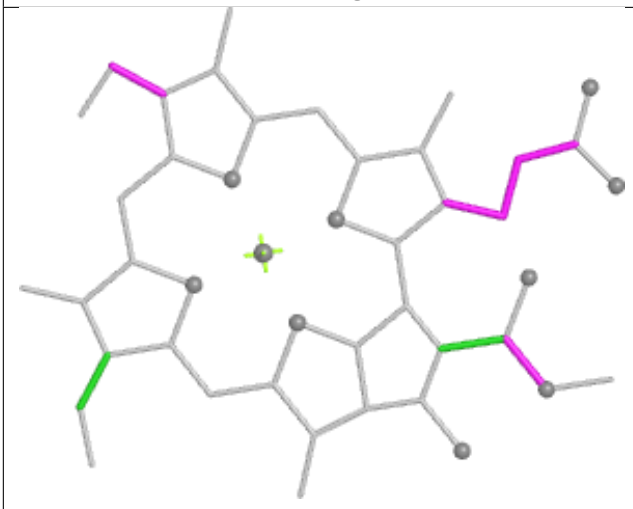
Ligand CLA A 818



Bond lengths



Bond angles

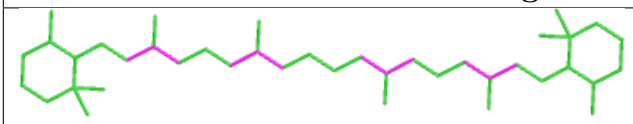


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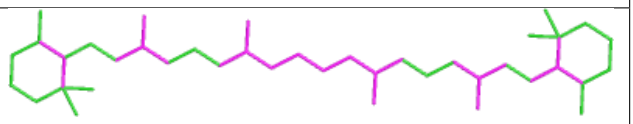


Rings

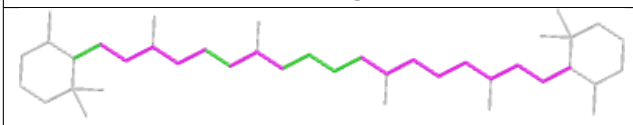
Ligand BCR H 202



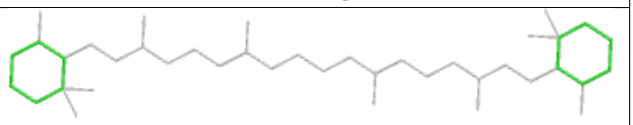
Bond lengths



Bond angles

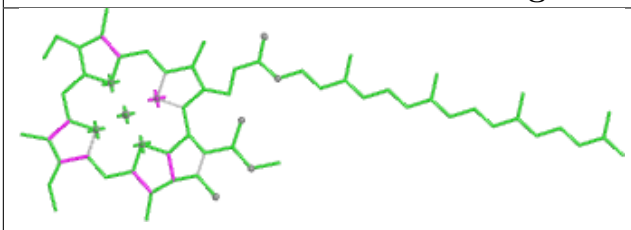


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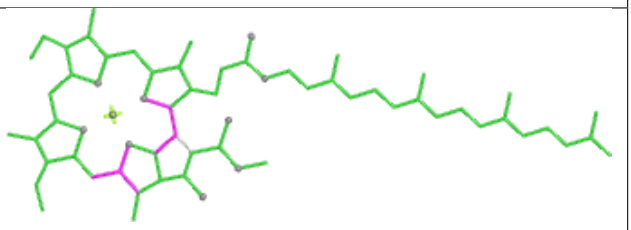


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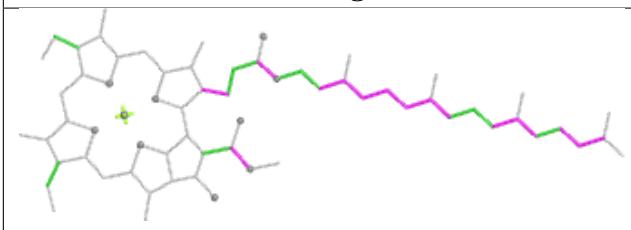
Ligand CLA a 817



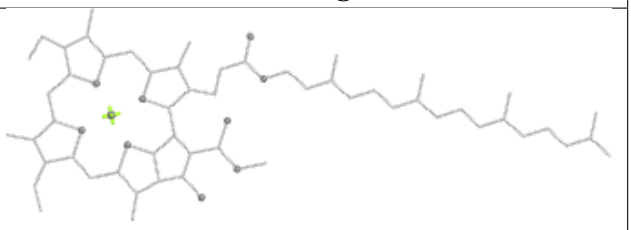
Bond lengths



Bond angles

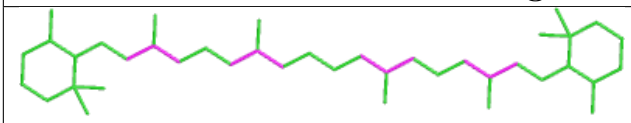


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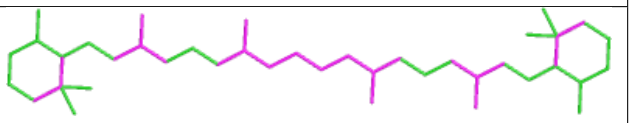


Rings

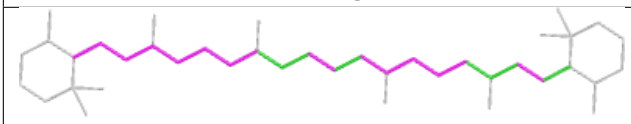
Ligand BCR a 843



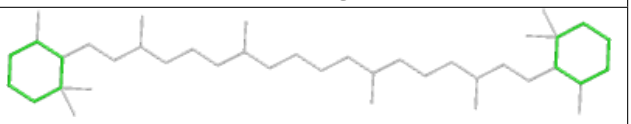
Bond lengths



Bond angles

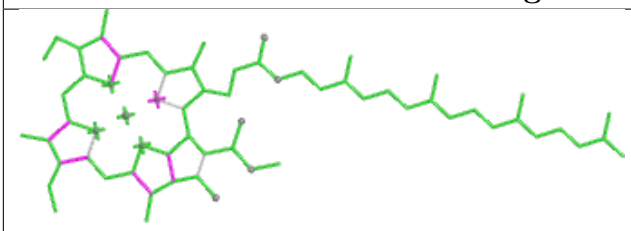


Torsions

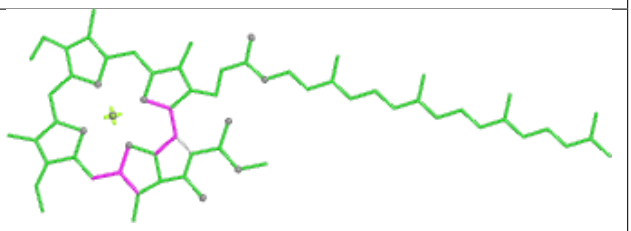


Rings

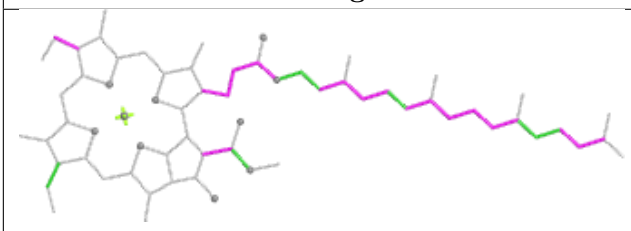
Ligand CLA A 829



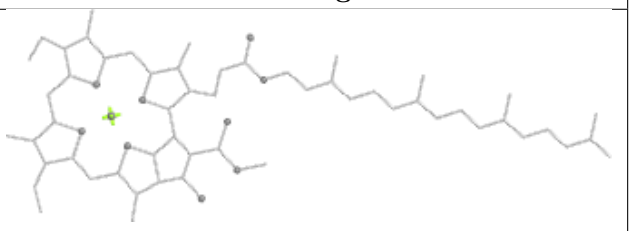
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Bond angles

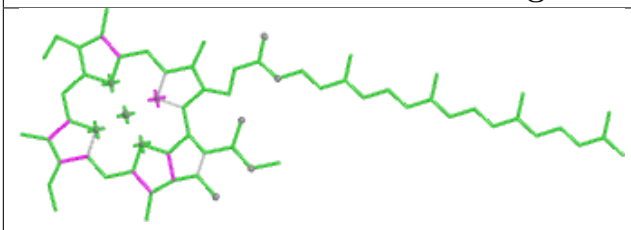


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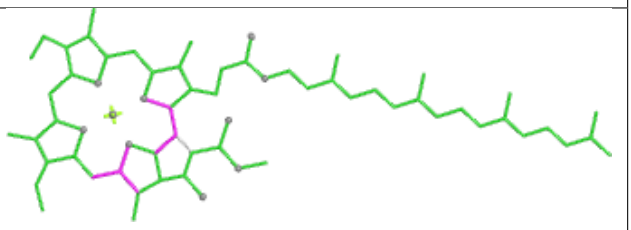


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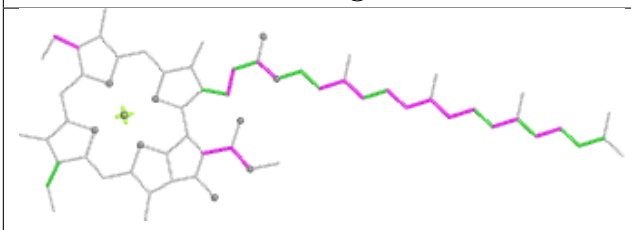
Ligand CLA b 811



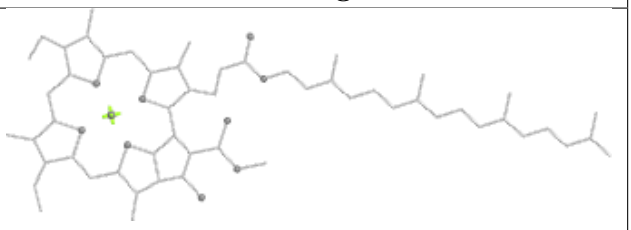
Bond lengths



Bond angles

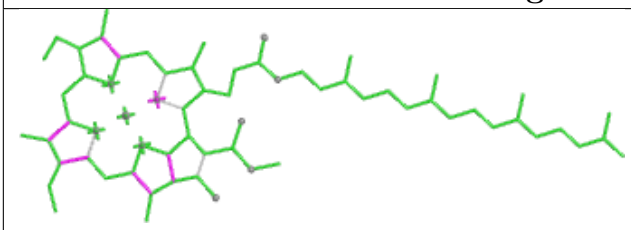


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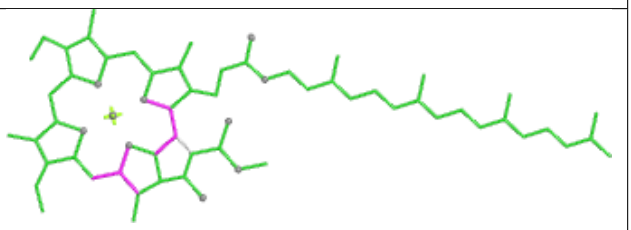


Rings

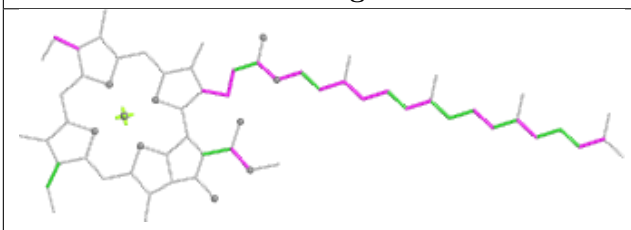
Ligand CLA L 303



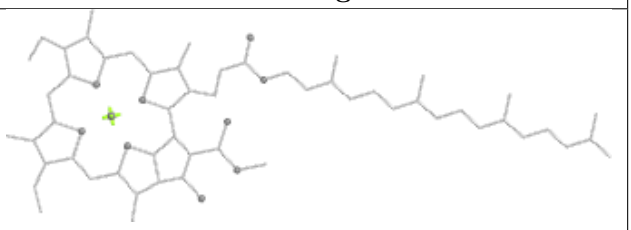
Bond lengths



Bond angles

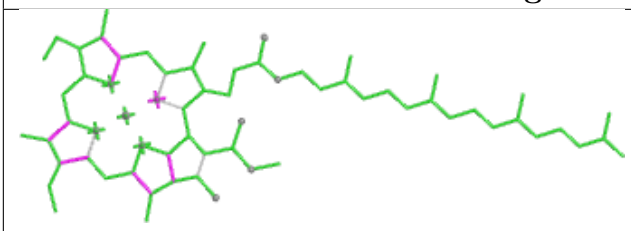


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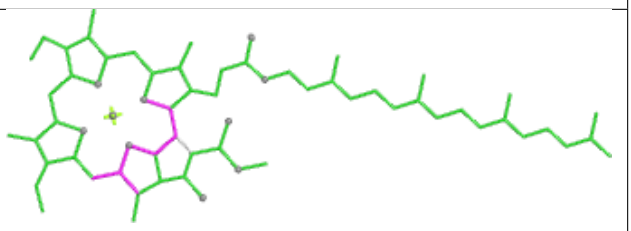


Rings

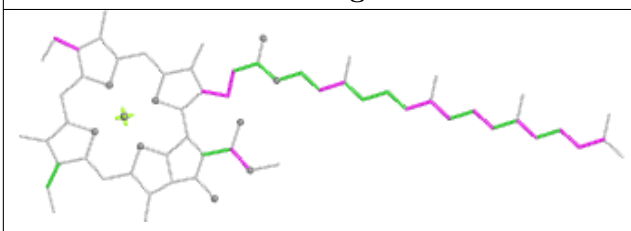
Ligand CLA B 823



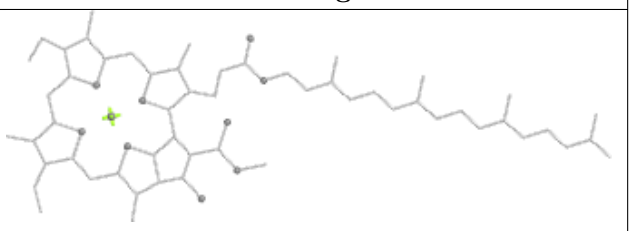
Bond lengths



Bond angles

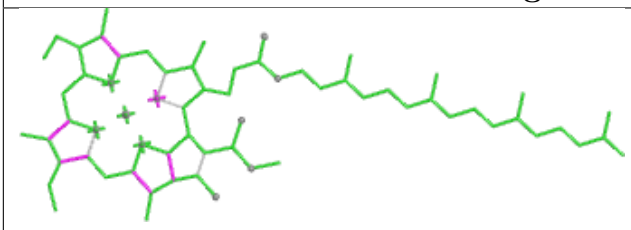


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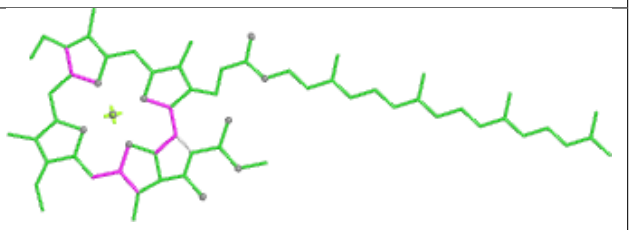


Rings

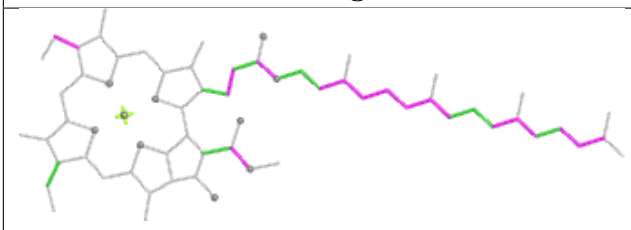
Ligand CLA A 816



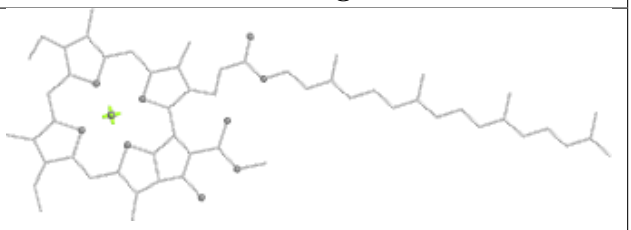
Bond lengths



Bond angles

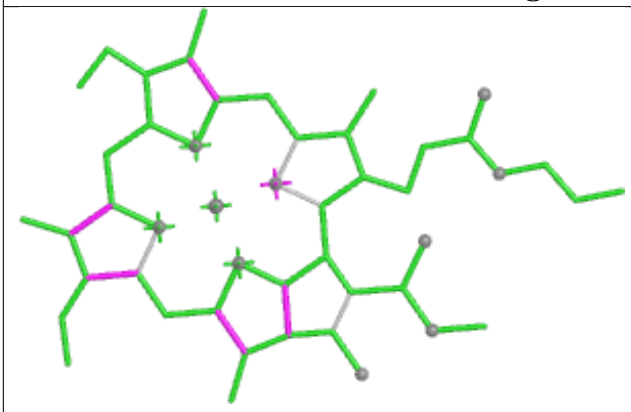


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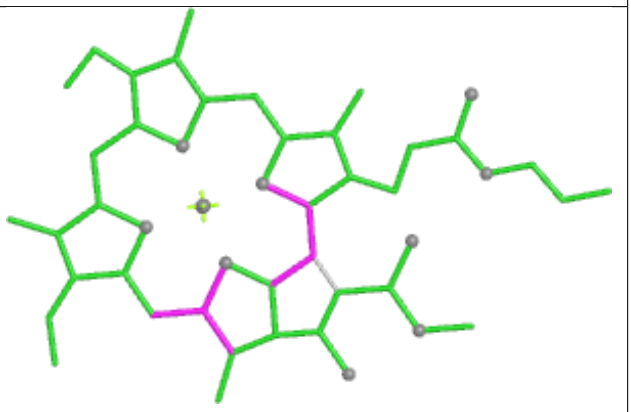


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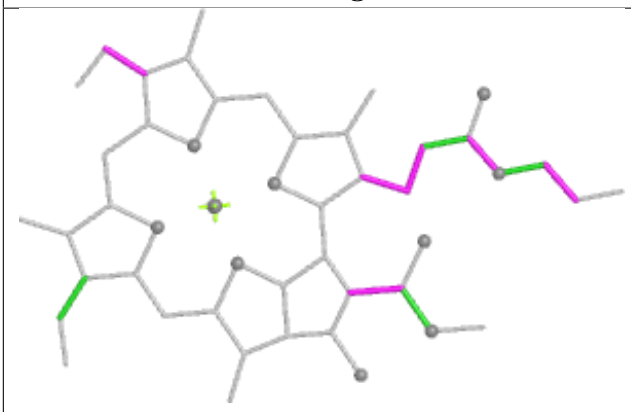
Ligand CLA B 839



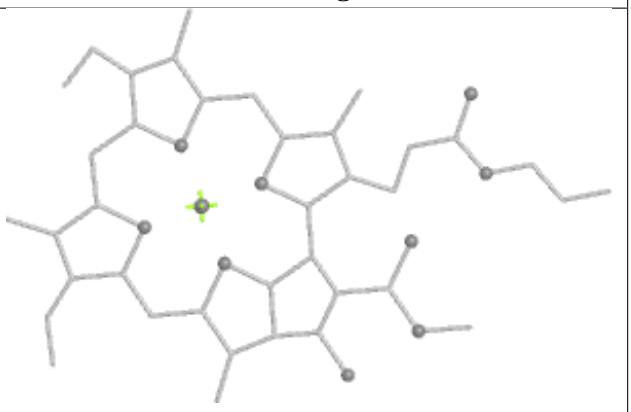
Bond lengths



Bond angles

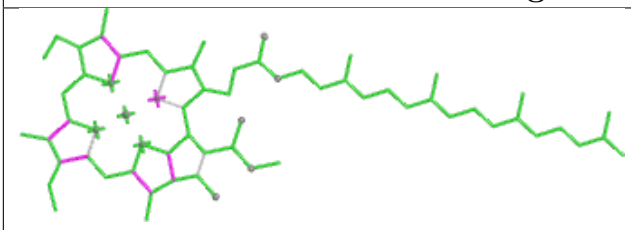


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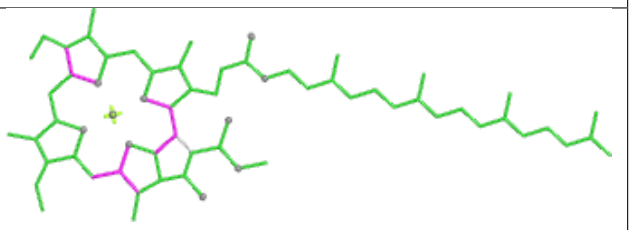


Rings

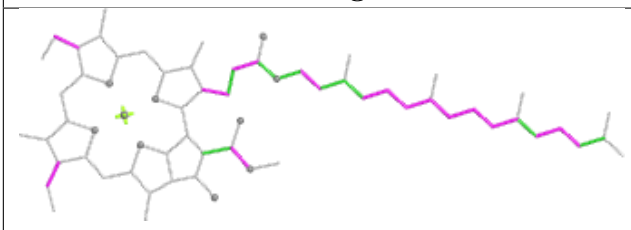
Ligand CLA b 804



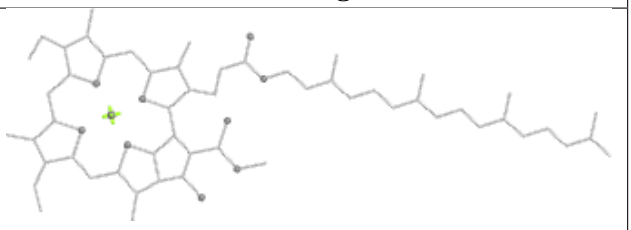
Bond lengths



Bond angles

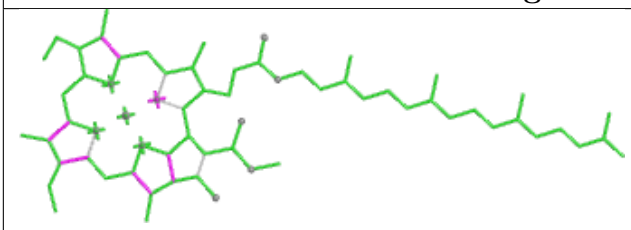


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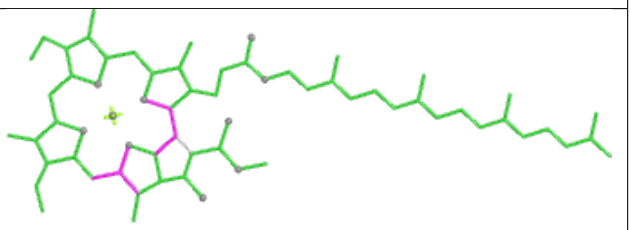


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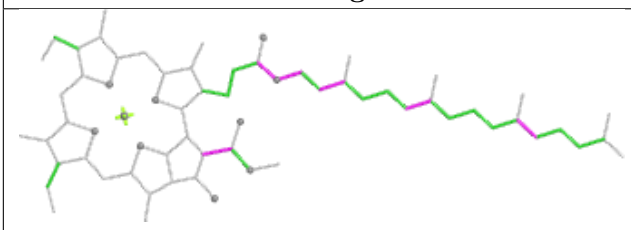
Ligand CLA A 804



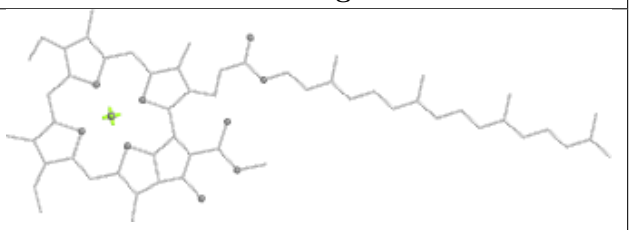
Bond lengths



Bond angles

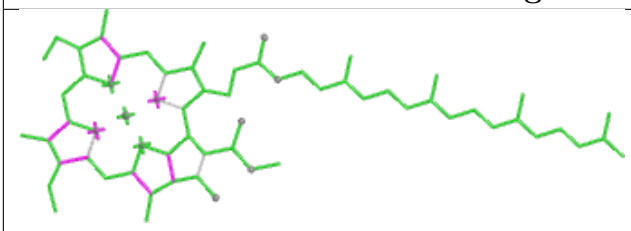


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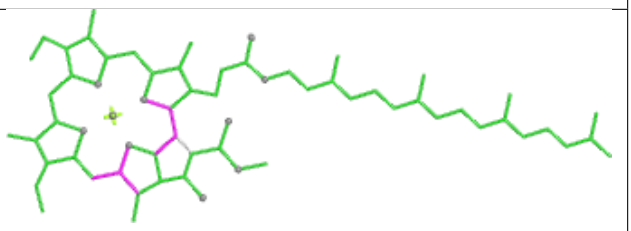


Rings

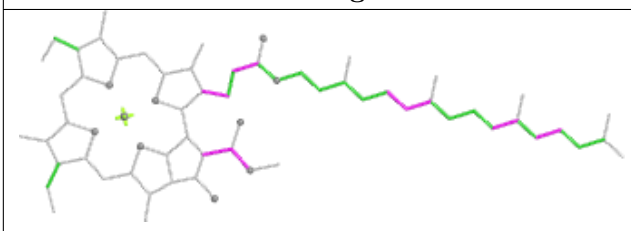
Ligand CLA B 825



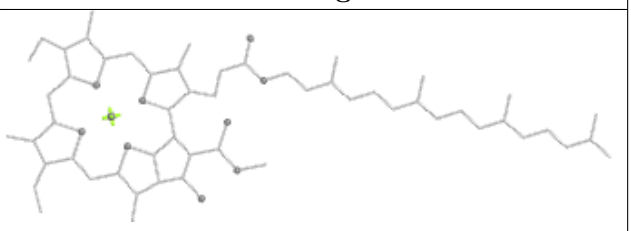
Bond lengths



Bond angles

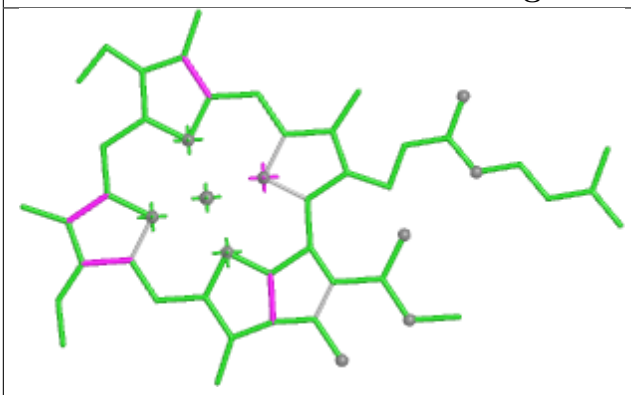


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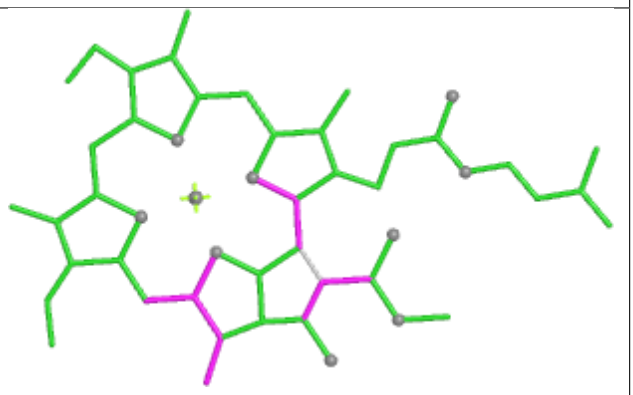


Rings

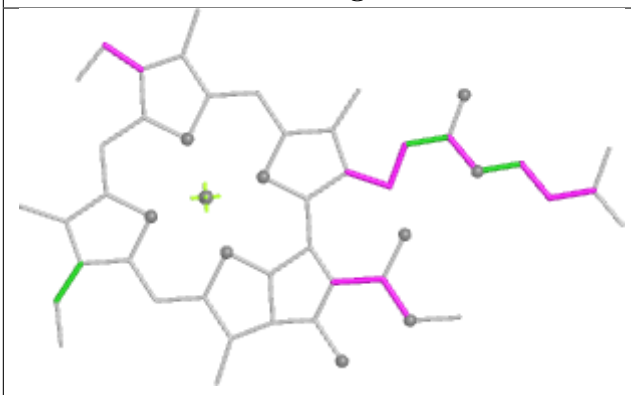
Ligand CLA A 830



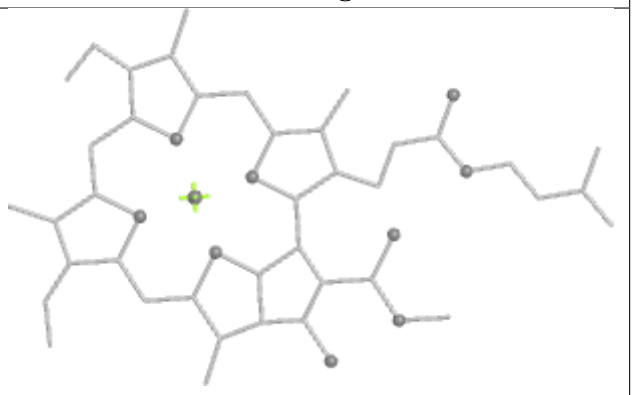
Bond lengths



Bond angles

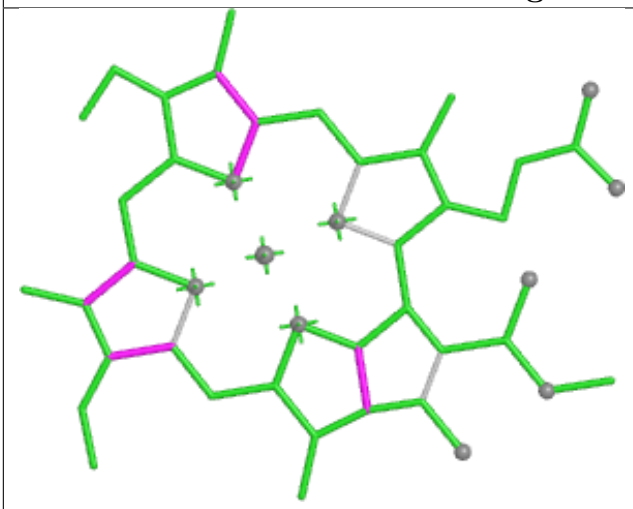


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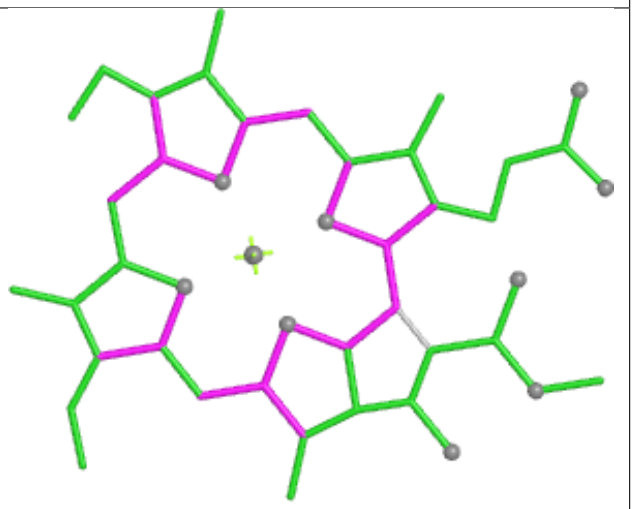


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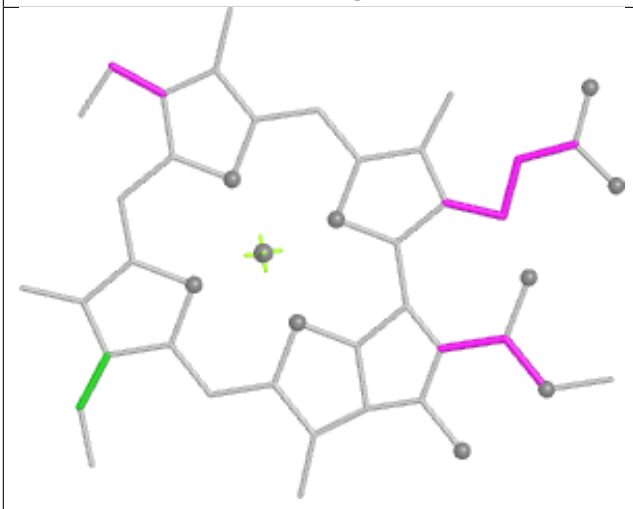
Ligand CLA L 307



Bond lengths



Bond angles

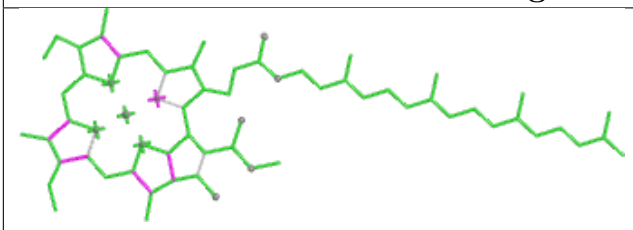


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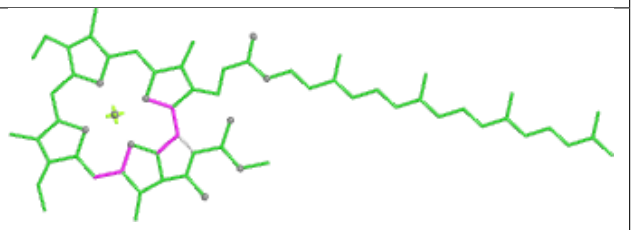


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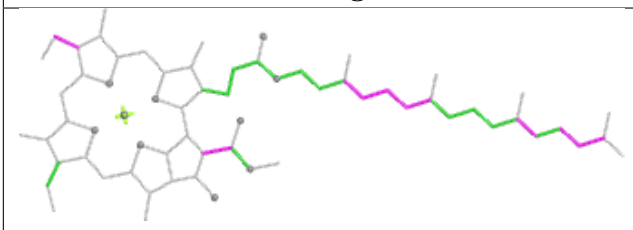
Ligand CLA a 823



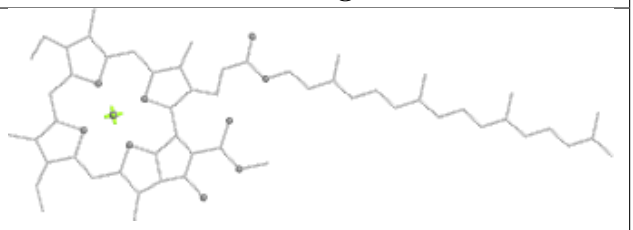
Bond lengths



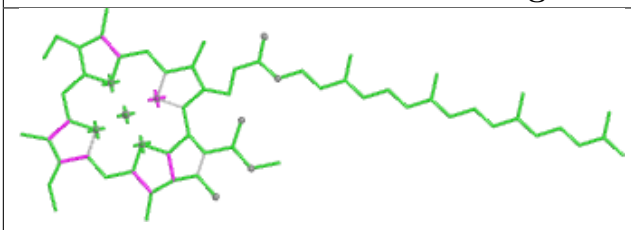
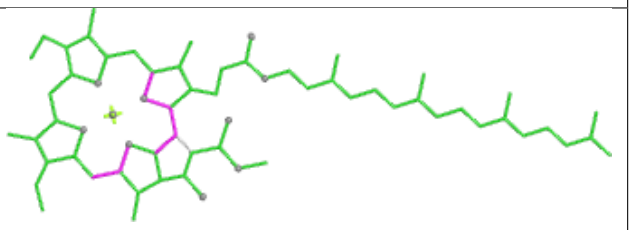
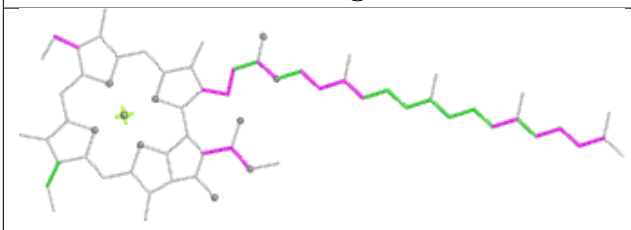
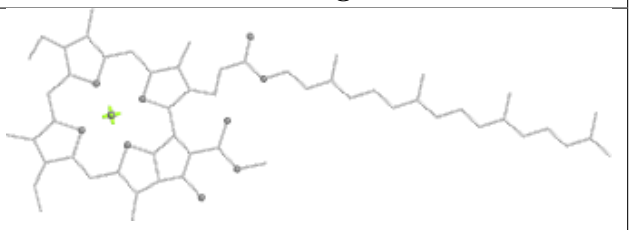
Bond angles

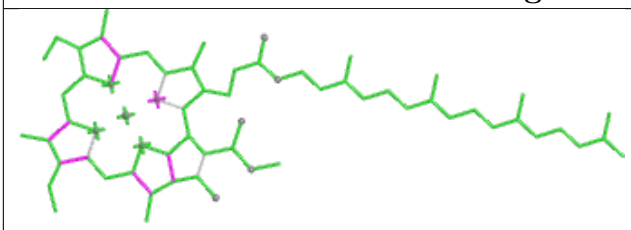
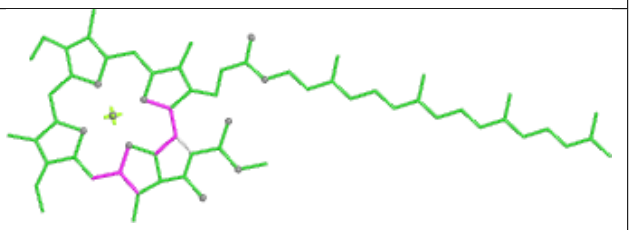
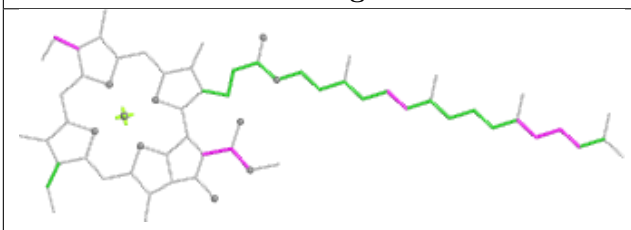
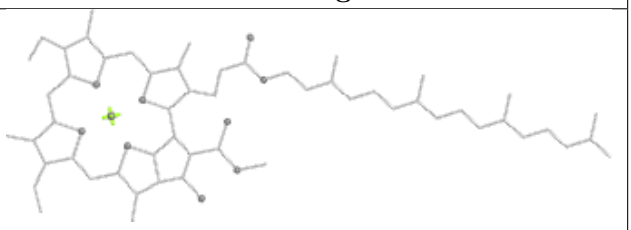


Torsions

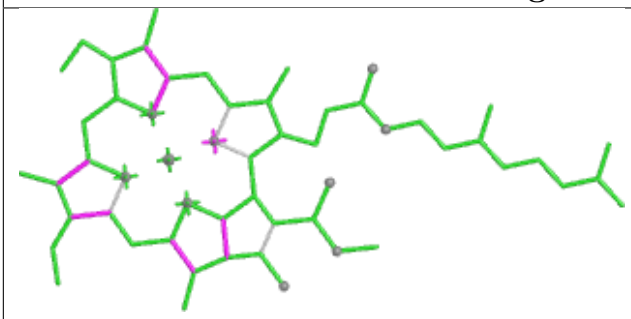


Rings

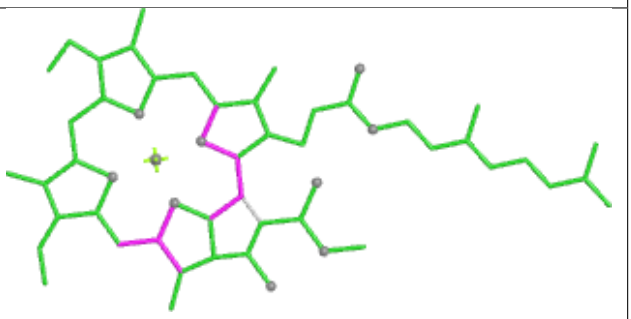
Ligand CLA a 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

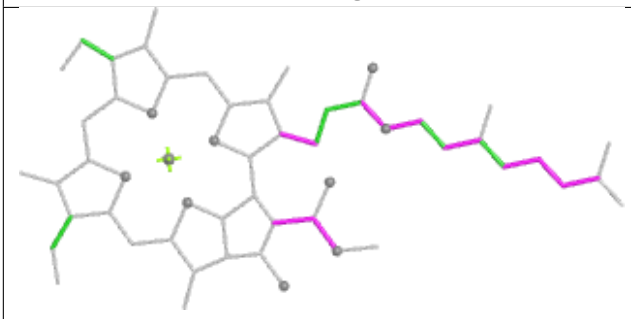
Ligand CLA a 803



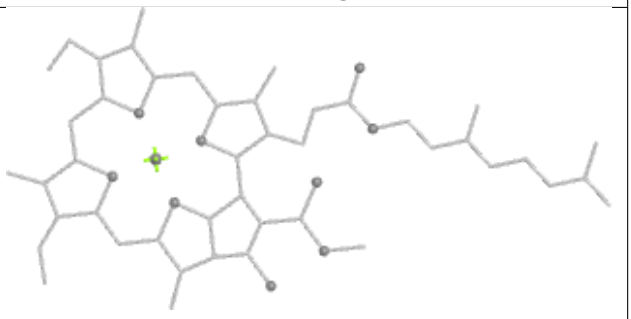
Bond lengths



Bond angles

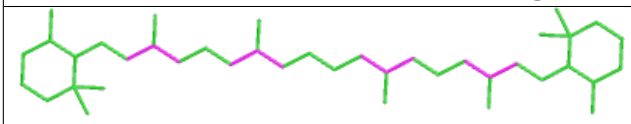


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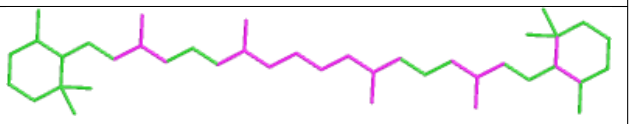


Rings

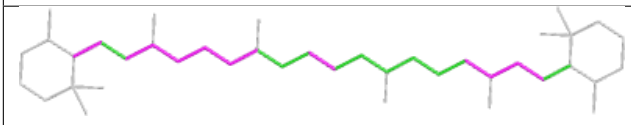
Ligand BCR I 101



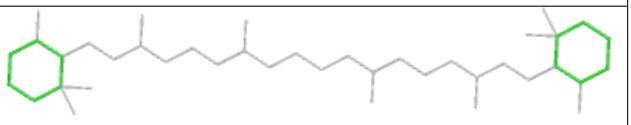
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Bond angles

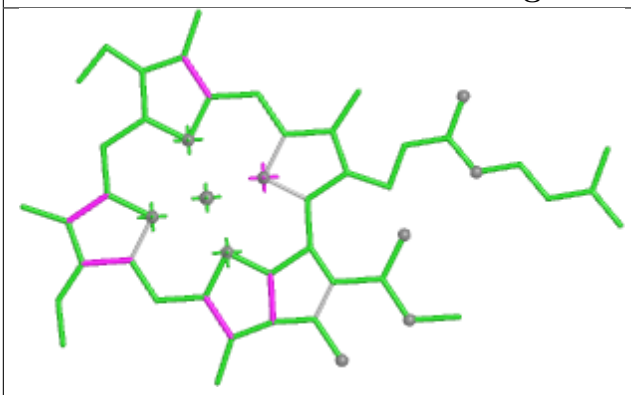


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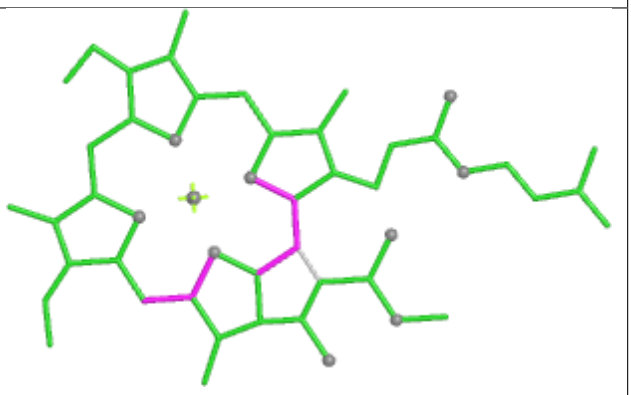


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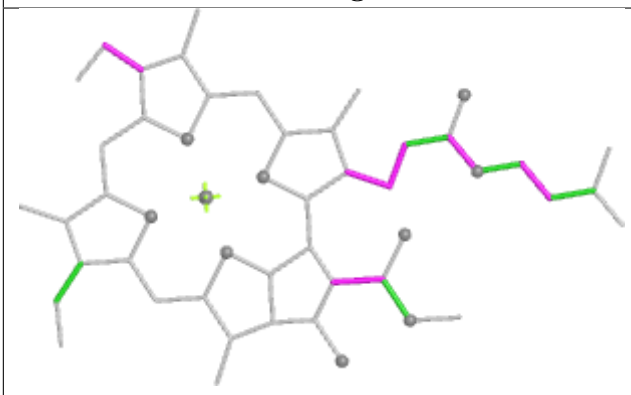
Ligand CLA A 827



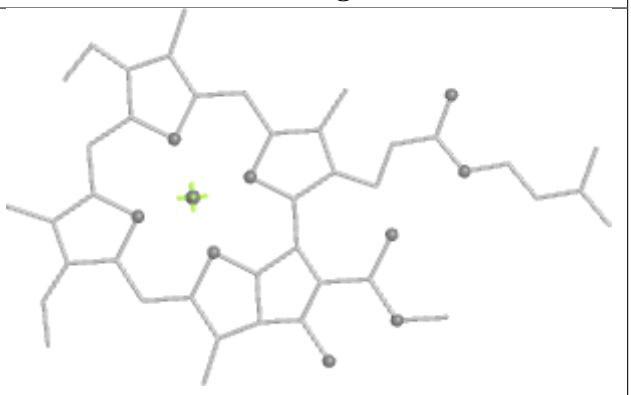
Bond lengths



Bond angles

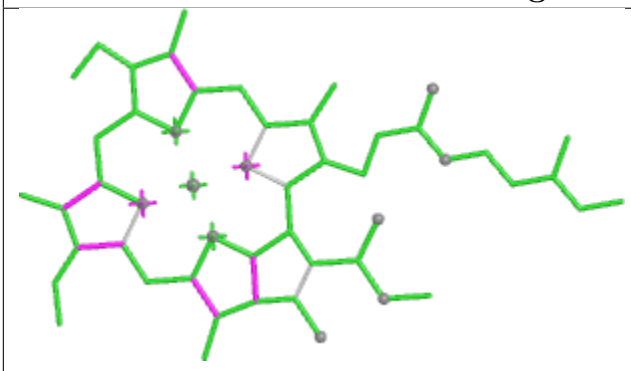


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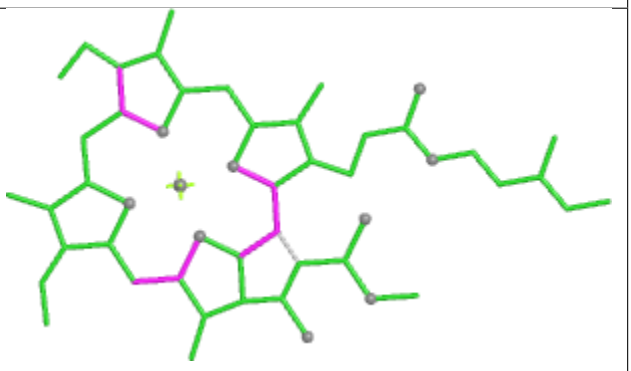


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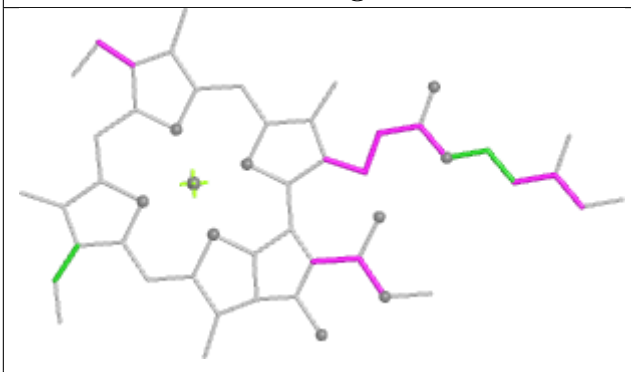
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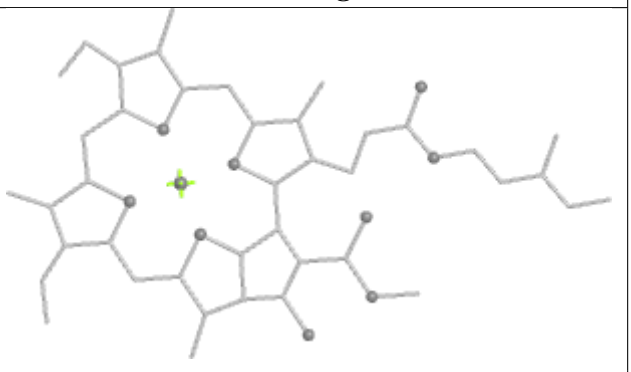
Bond lengths



Bond angles



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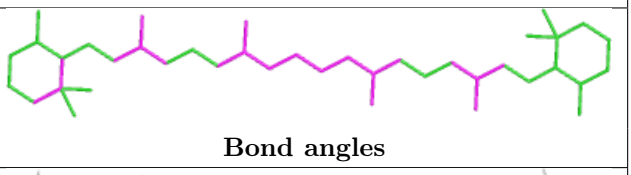


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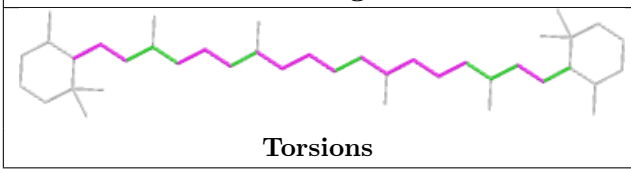
Ligand BCR A 842



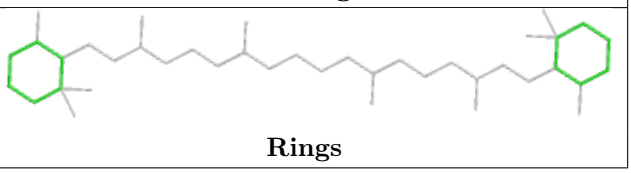
Bond lengths



Bond angles

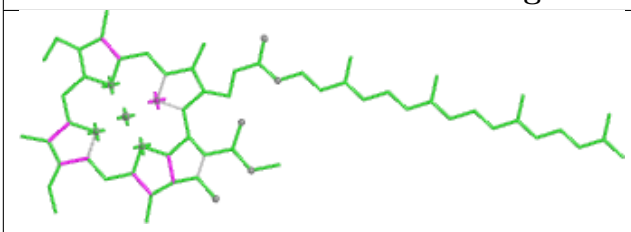


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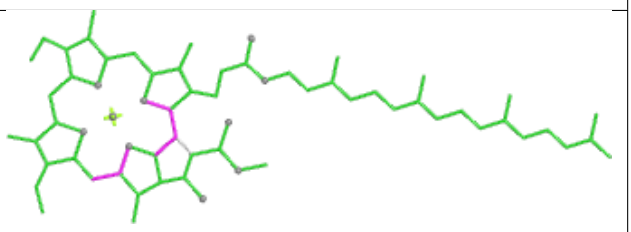


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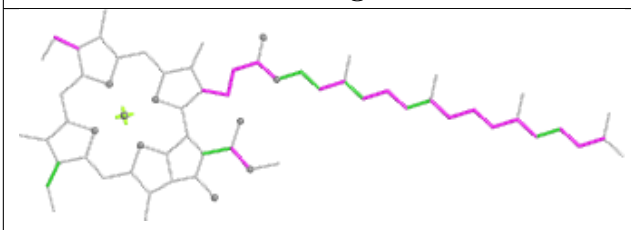
Ligand CLA A 815



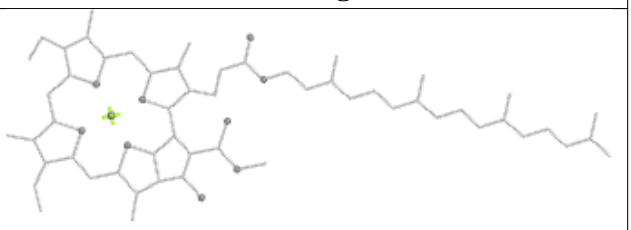
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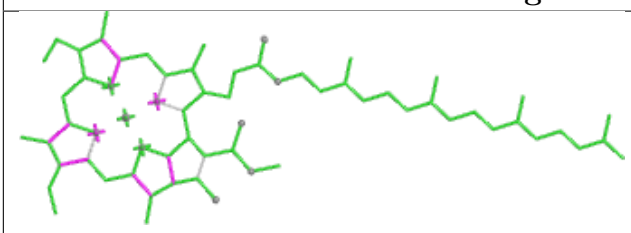


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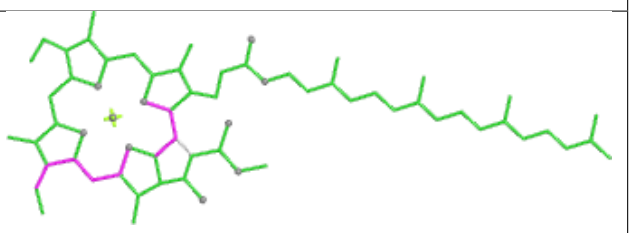


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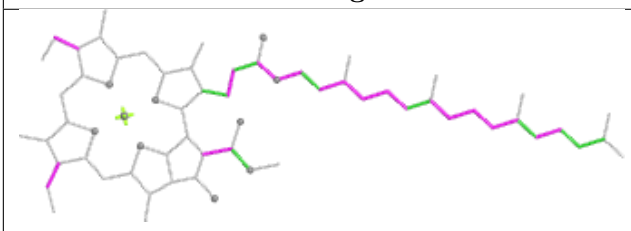
Ligand CLA B 801



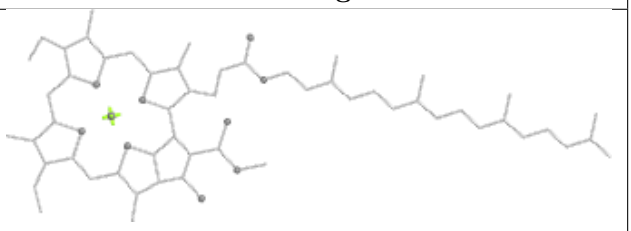
Bond lengths



Bond angles

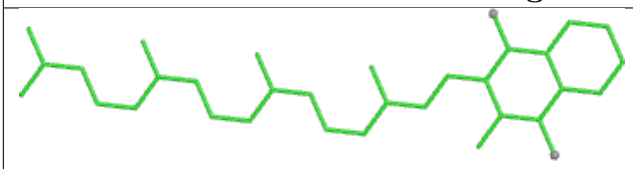


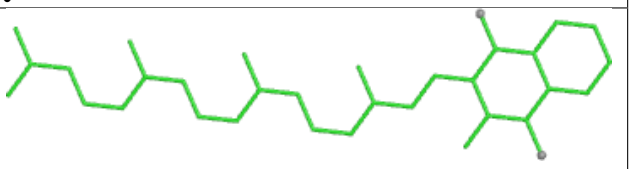
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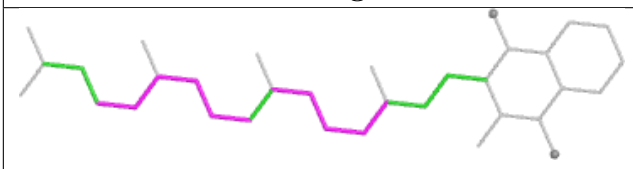


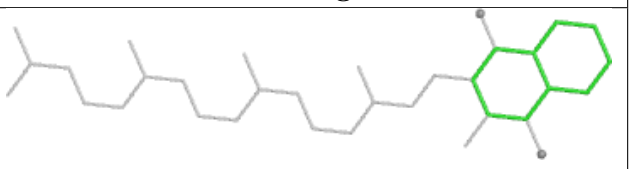
Rings

Ligand PQN a 838

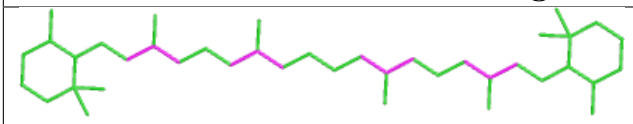

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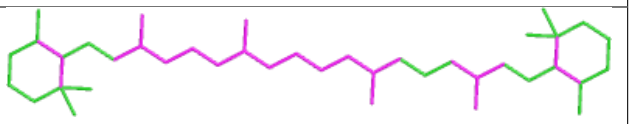

Bond angles

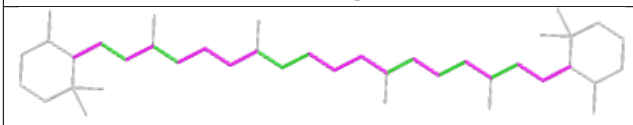

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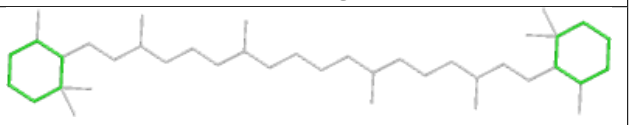

Rings

Ligand BCR l 309

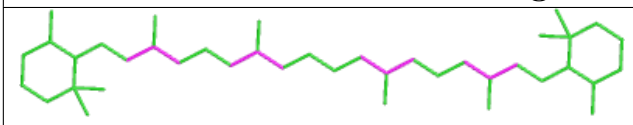

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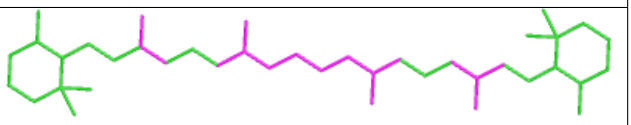

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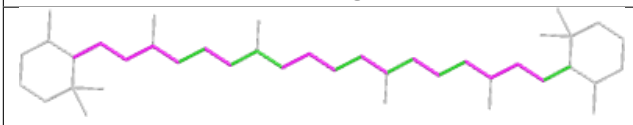

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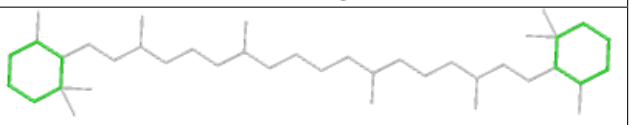

Rings

Ligand BCR l 304

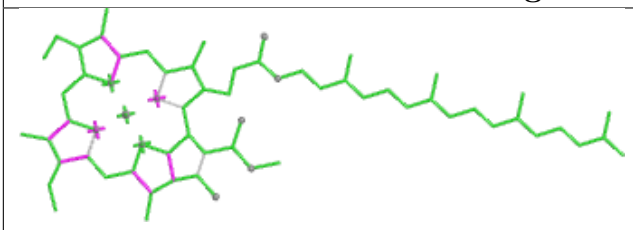

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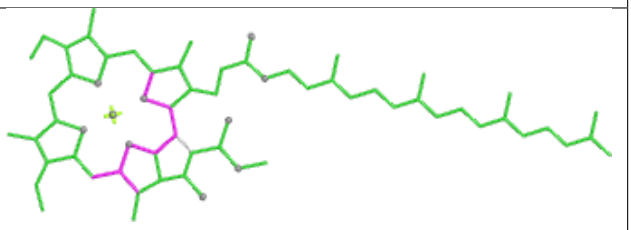

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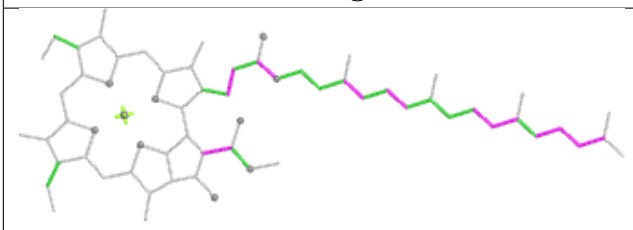

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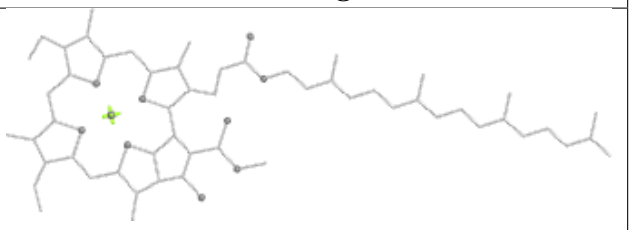

Rings

Ligand CLA B 815

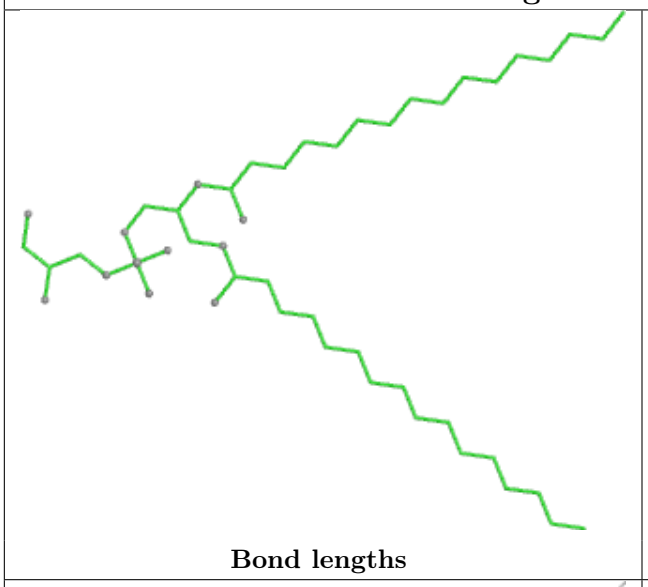

Bond lengths


Bond angles

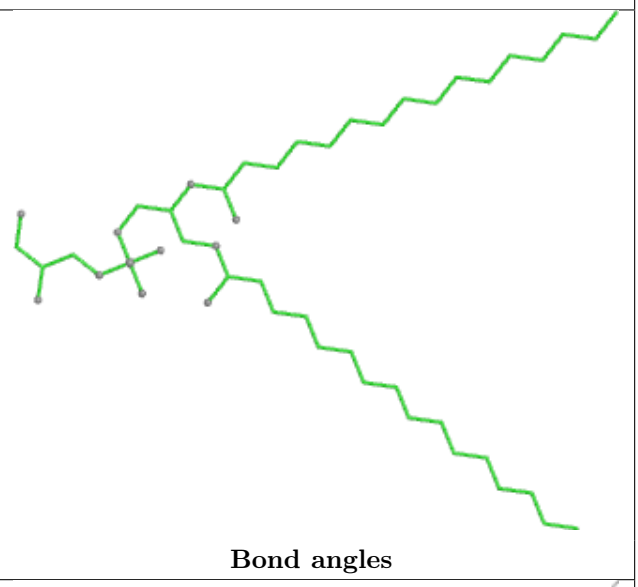

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Rings

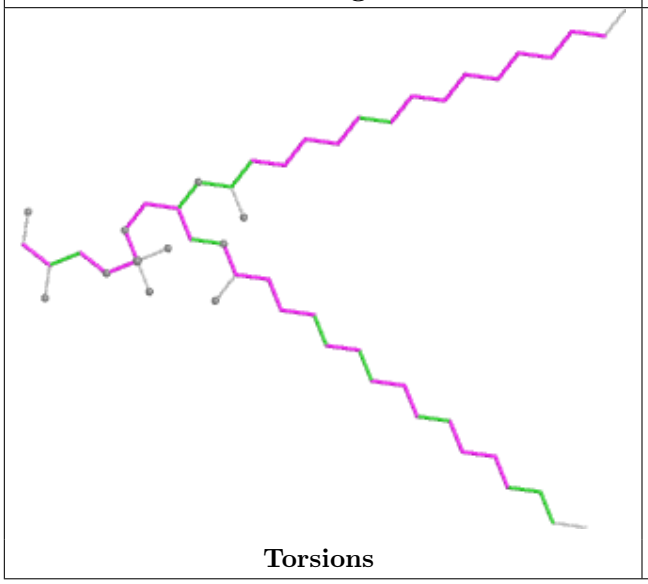
Ligand LHG A 845



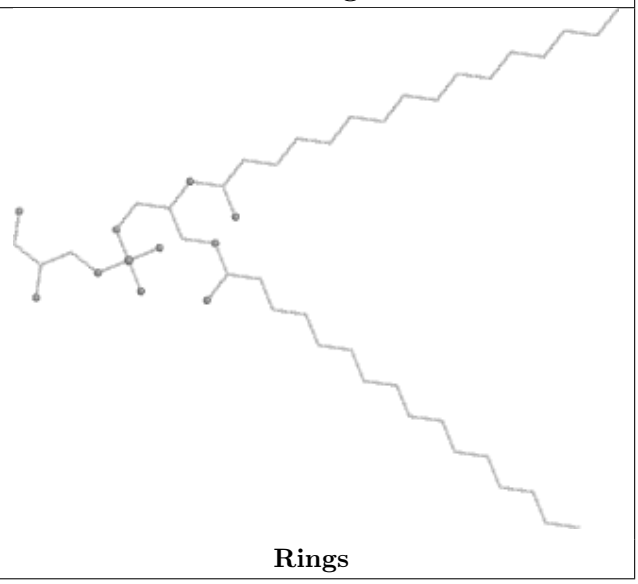
Bond lengths



Bond angles

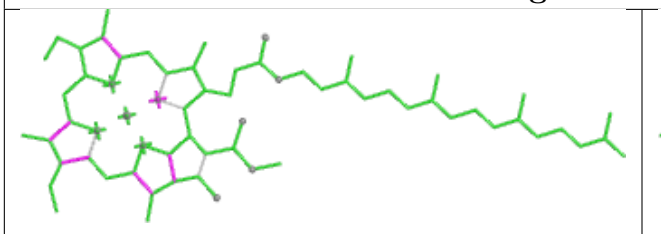


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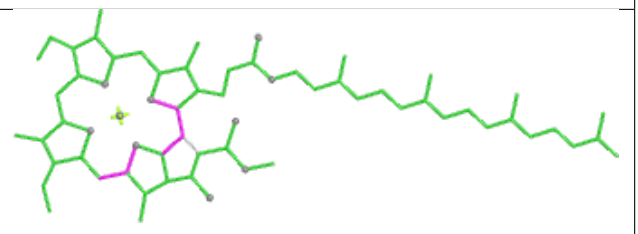


Rings

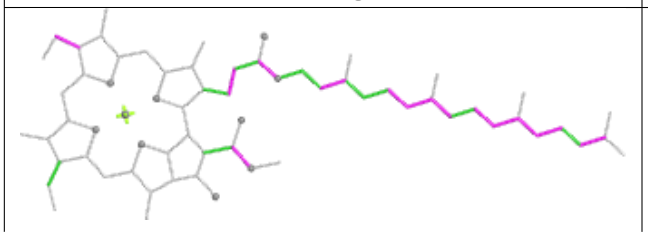
Ligand CLA a 809



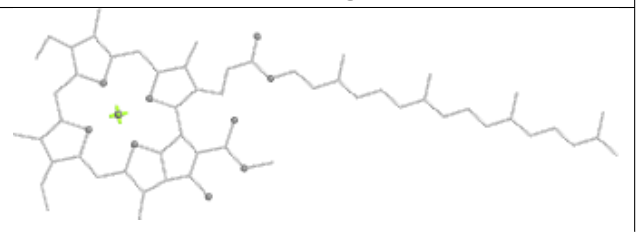
Bond lengths



Bond angles



Torsions

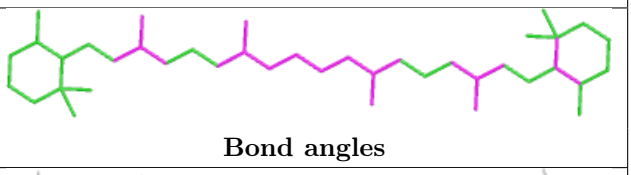


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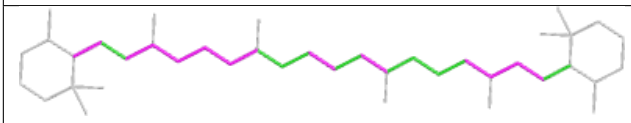
Ligand BCR i 101



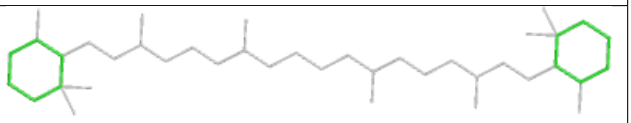
Bond lengths



Bond angles

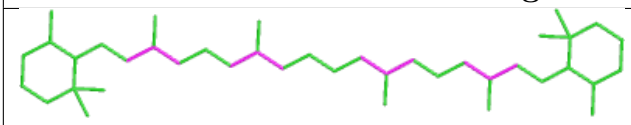


Torsions



Rings

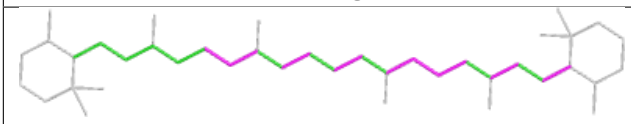
Ligand BCR A 843



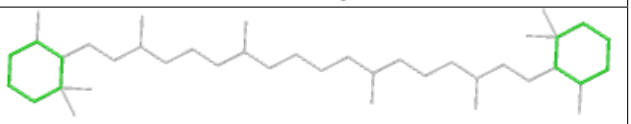
Bond lengths



Bond angles

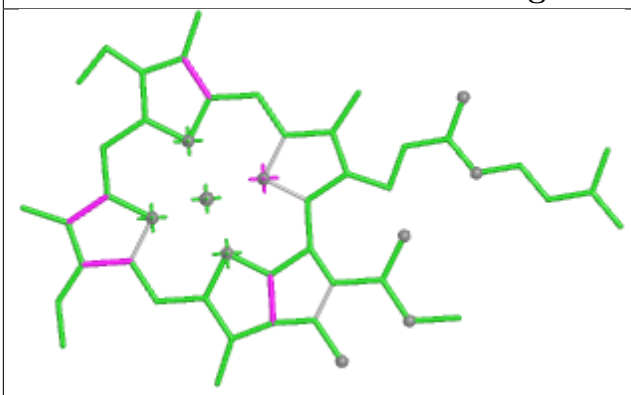


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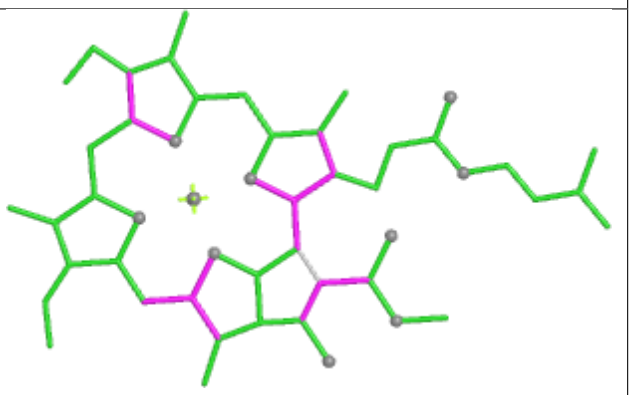


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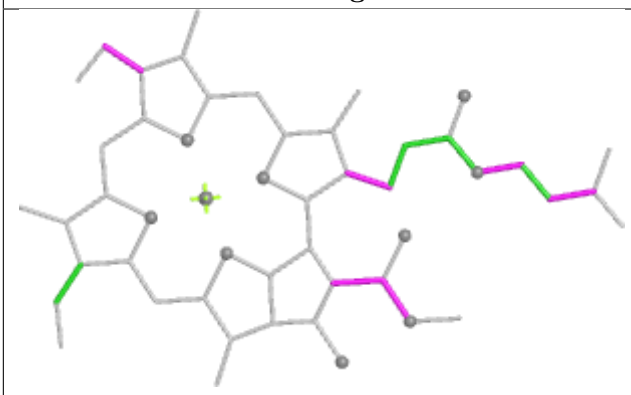
Ligand CLA a 831



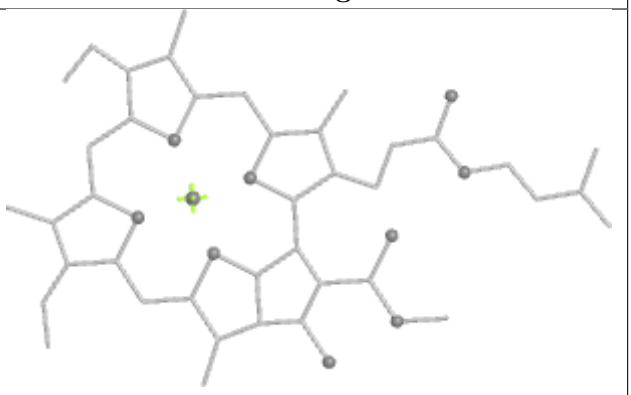
Bond lengths



Bond angles

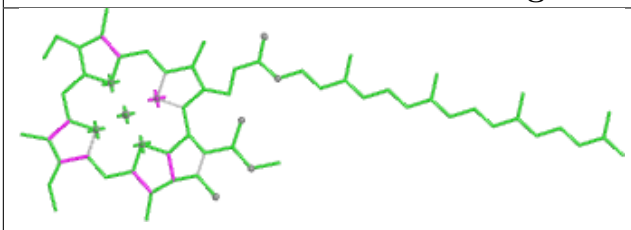


Torsions

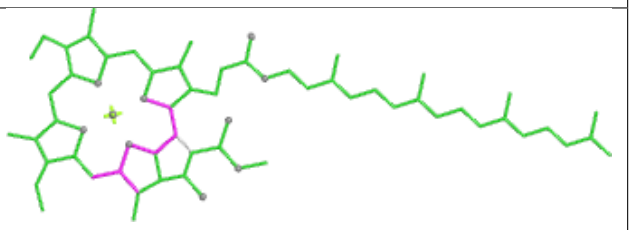


Rings

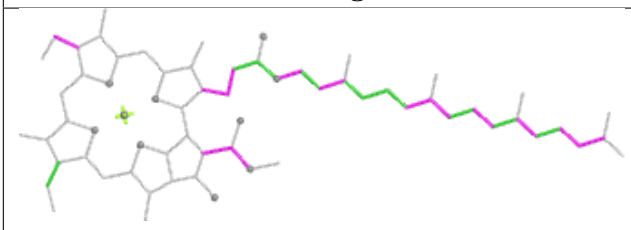
Ligand CLA b 823



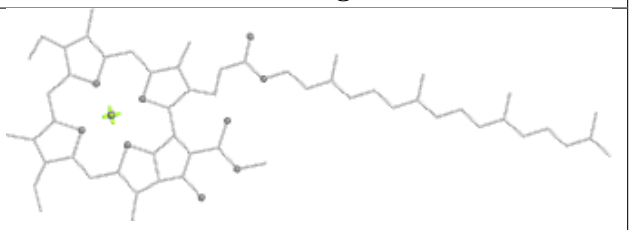
Bond lengths



Bond angles

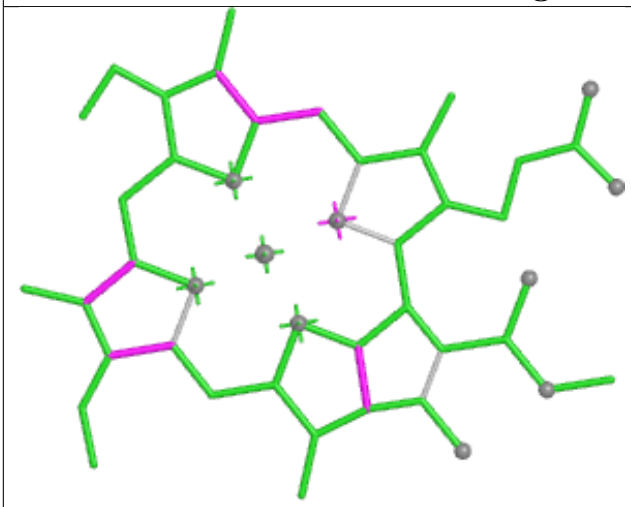


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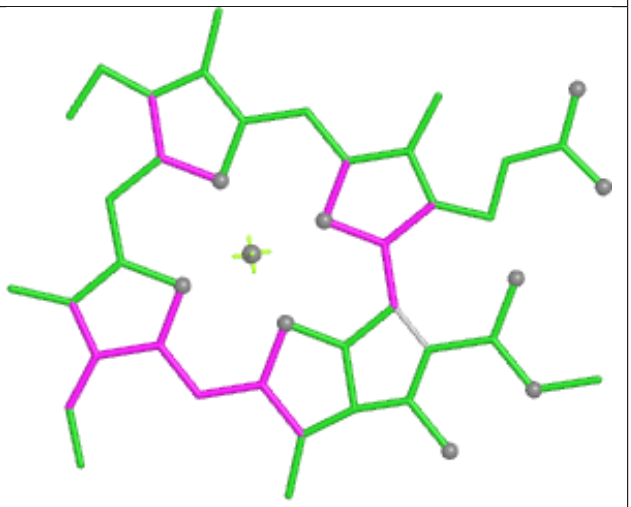


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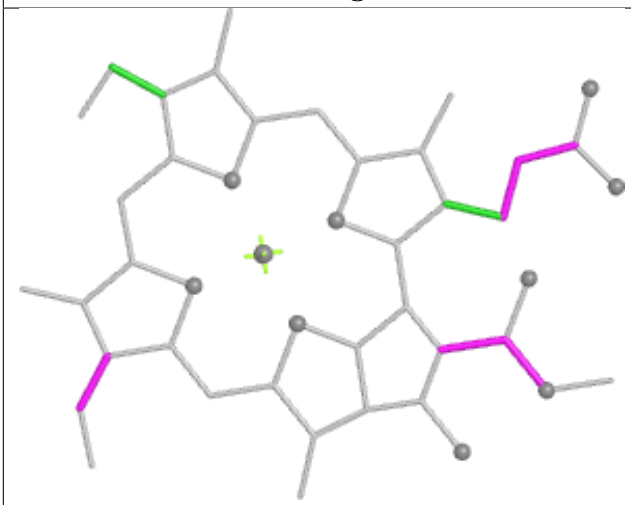
Ligand CLA l 301



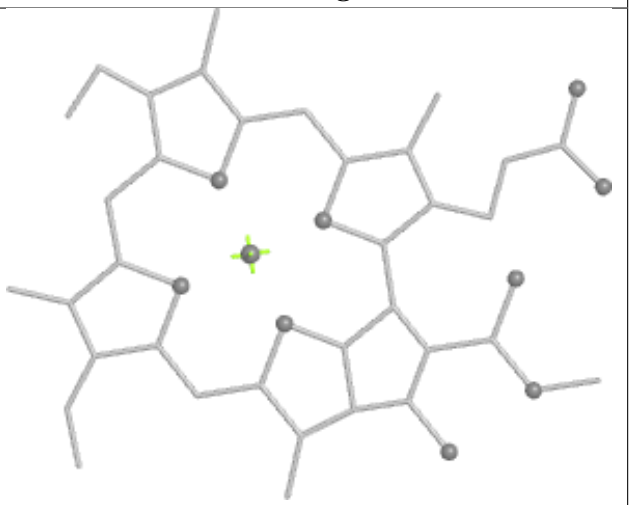
Bond lengths



Bond angles

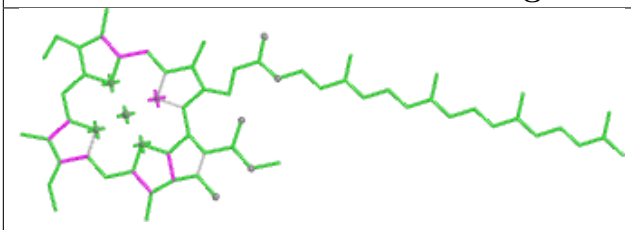


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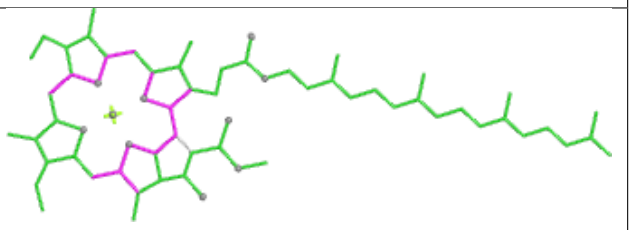


Rings

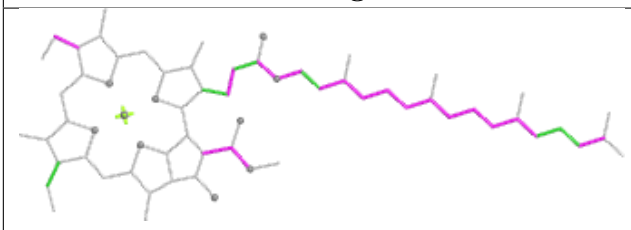
Ligand CLA A 806



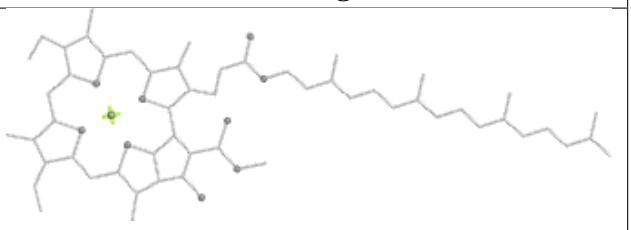
Bond lengths



Bond angles

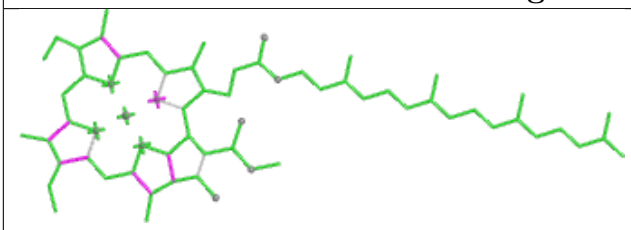


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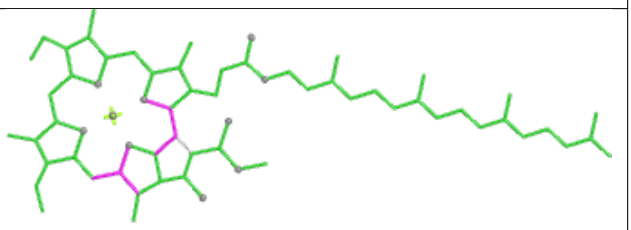


Rings

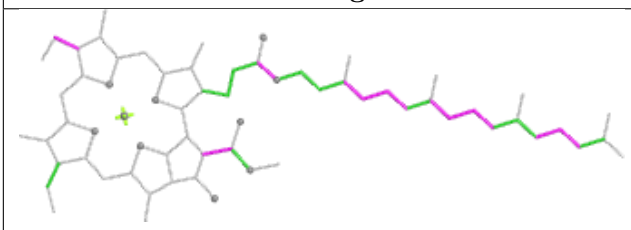
Ligand CLA b 829



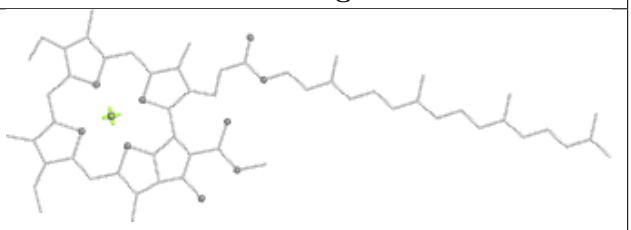
Bond lengths



Bond angles

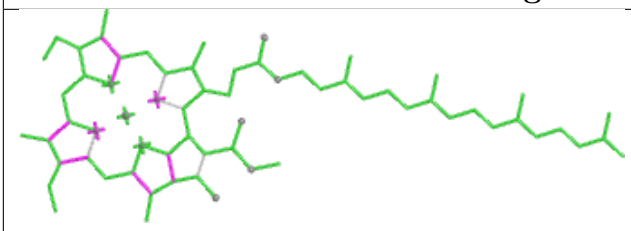


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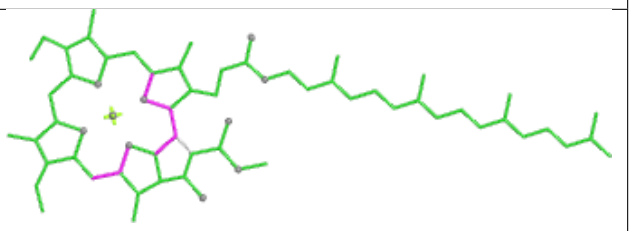


Rings

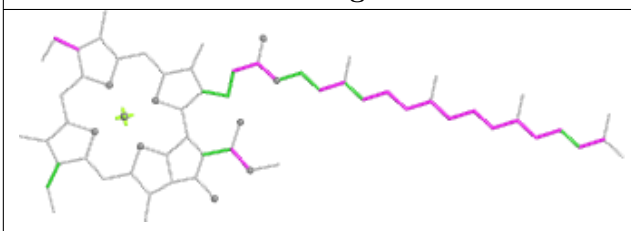
Ligand CLA A 847



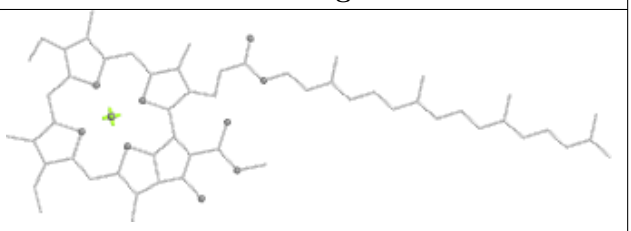
Bond lengths



Bond angles

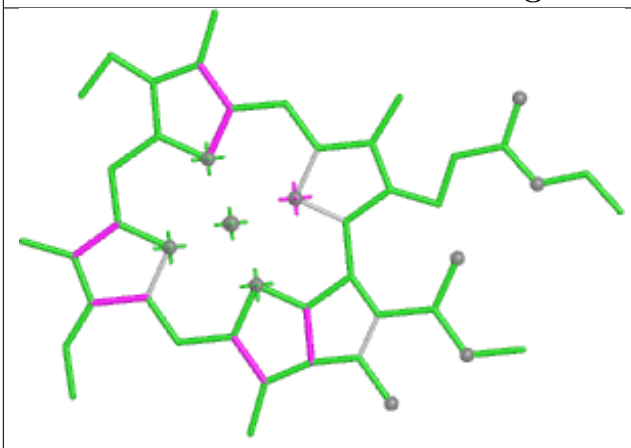


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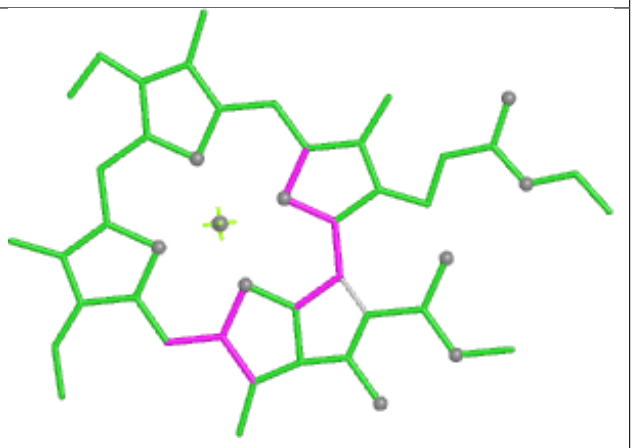


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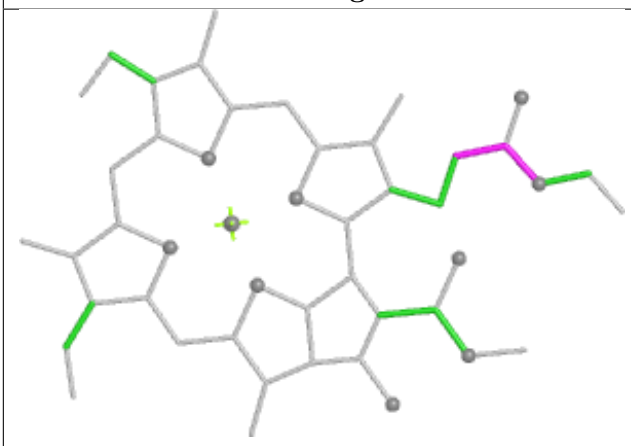
Ligand CLA B 830



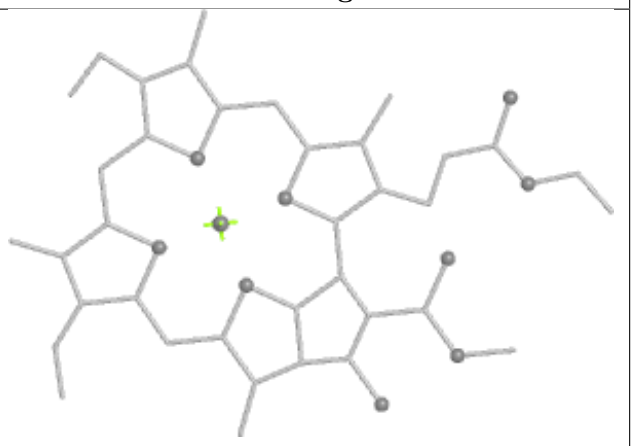
Bond lengths



Bond angles

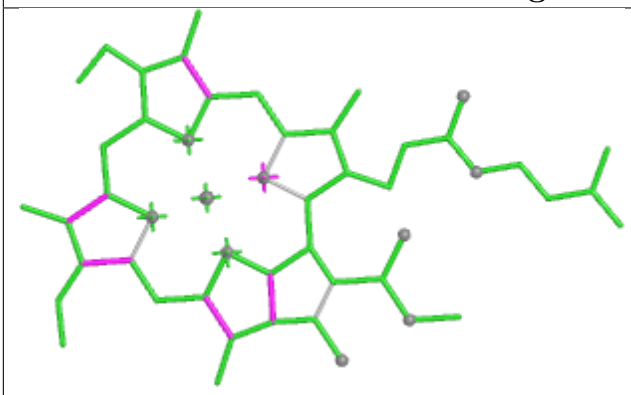


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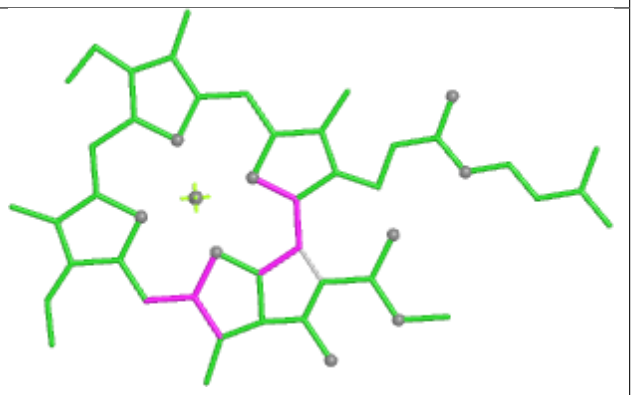


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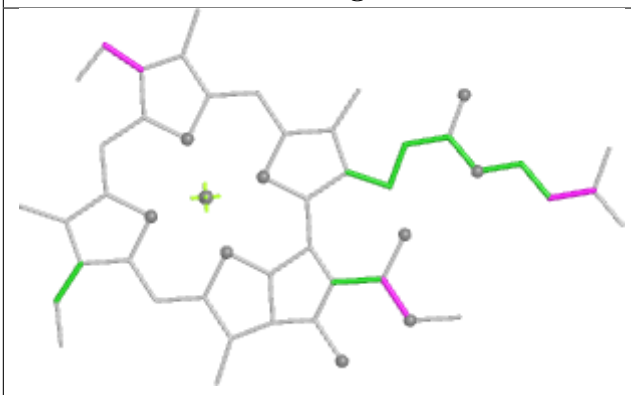
Ligand CLA a 813



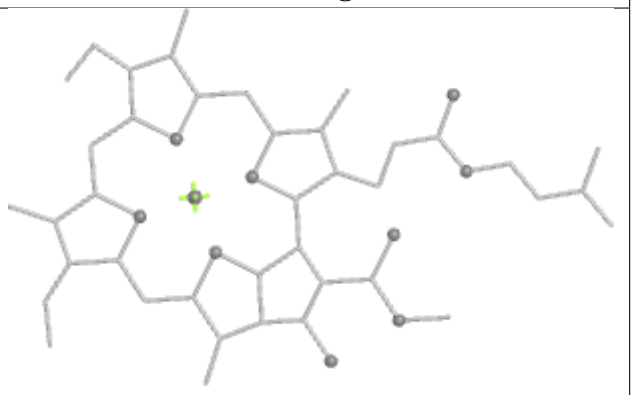
Bond lengths



Bond angles

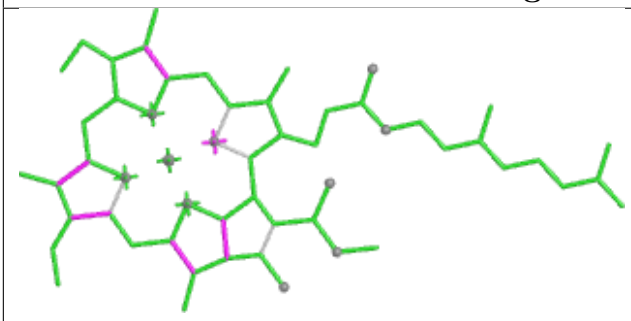


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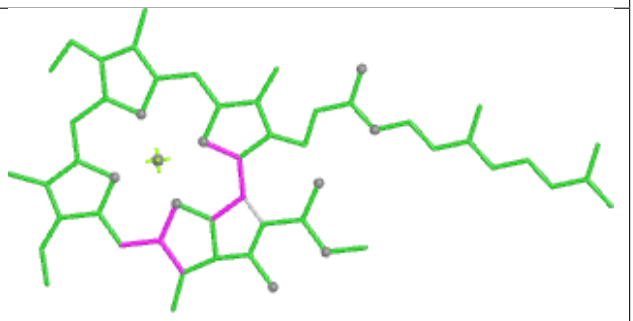


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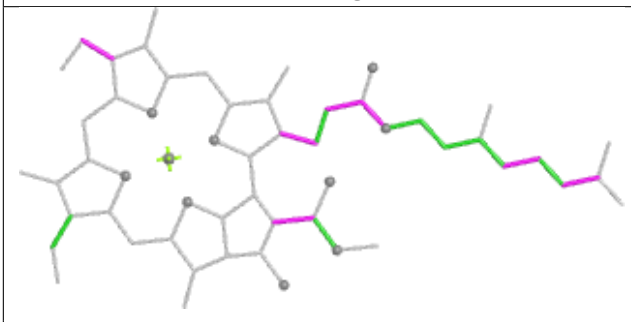
Ligand CLA A 820



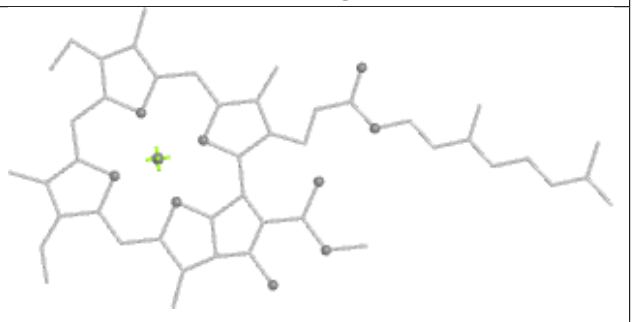
Bond lengths



Bond angles



Torsions

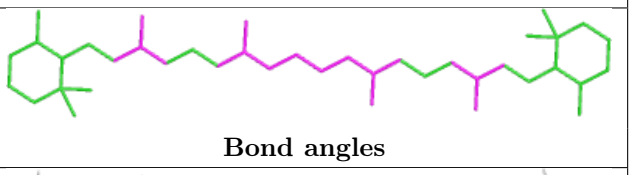


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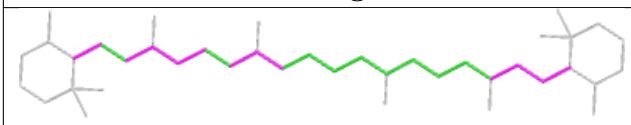
Ligand BCR B 836



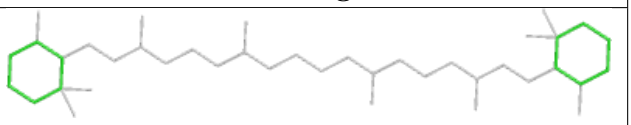
Bond lengths



Bond angles

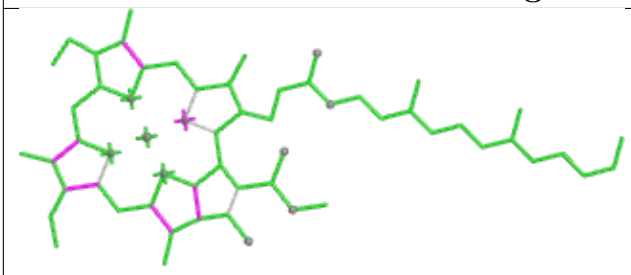


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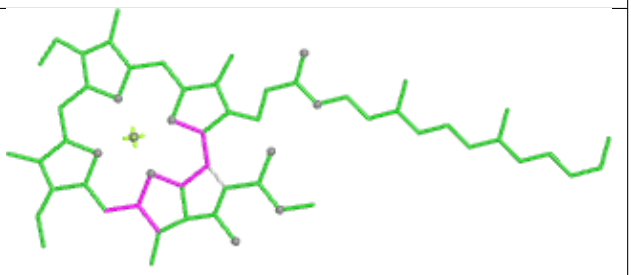


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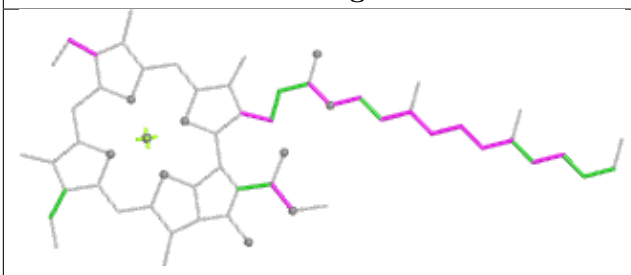
Ligand CLA B 818



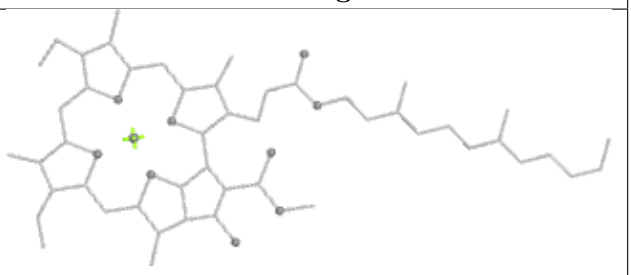
Bond lengths



Bond angles

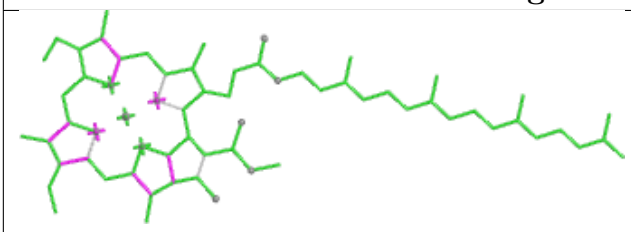


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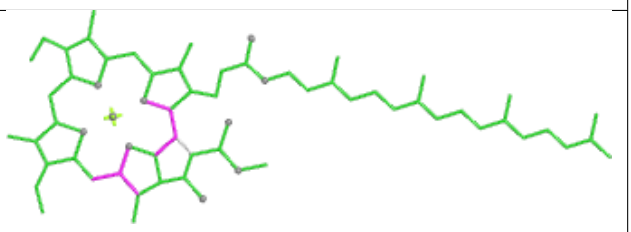


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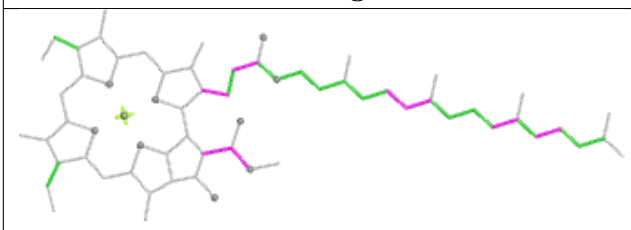
Ligand CLA b 825



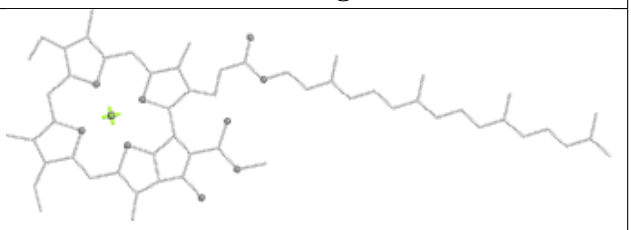
Bond lengths



Bond angles

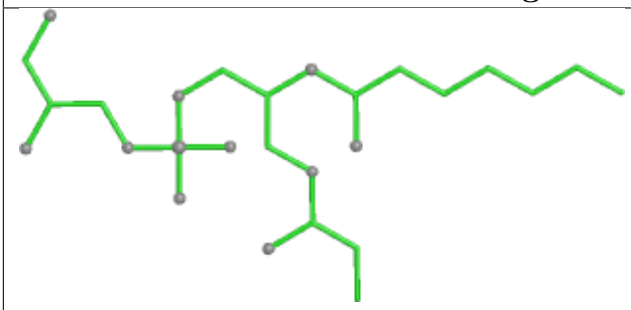


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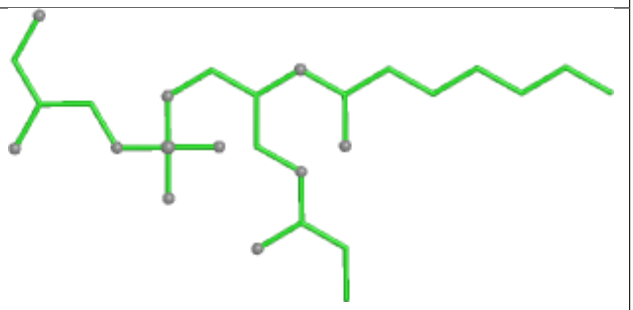


Rings

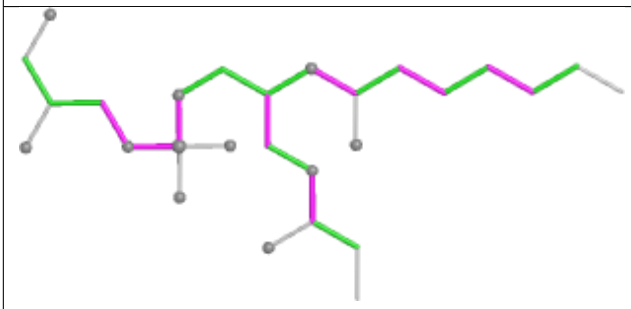
Ligand LHG A 839



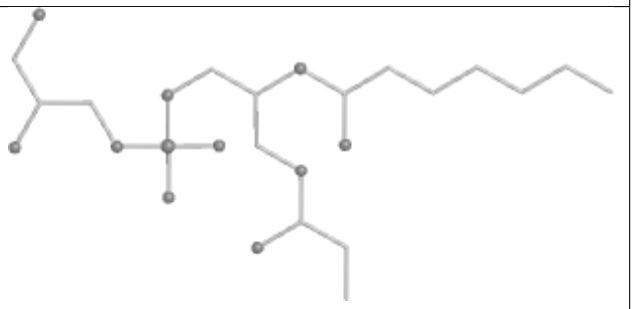
Bond lengths



Bond angles

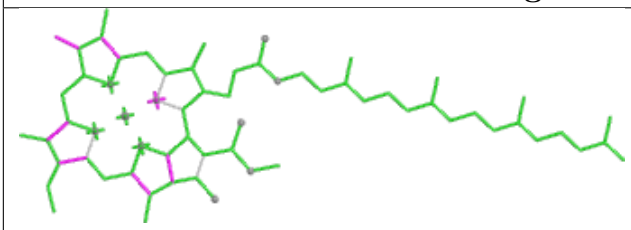


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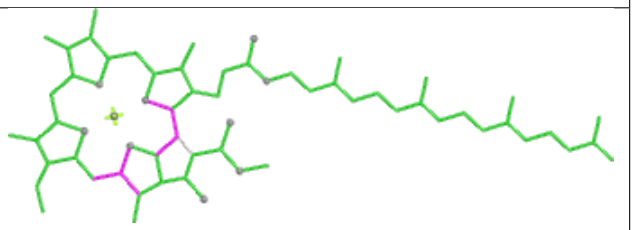


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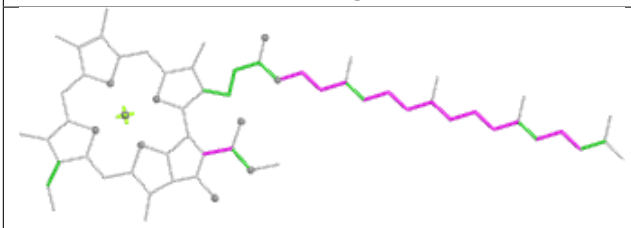
Ligand CLA B 821



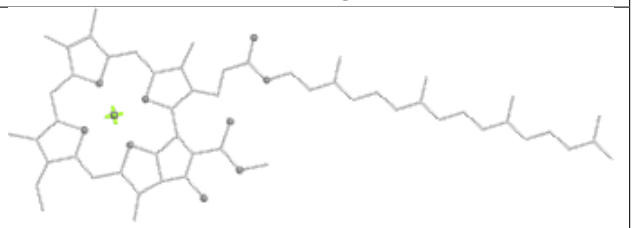
Bond lengths



Bond angles

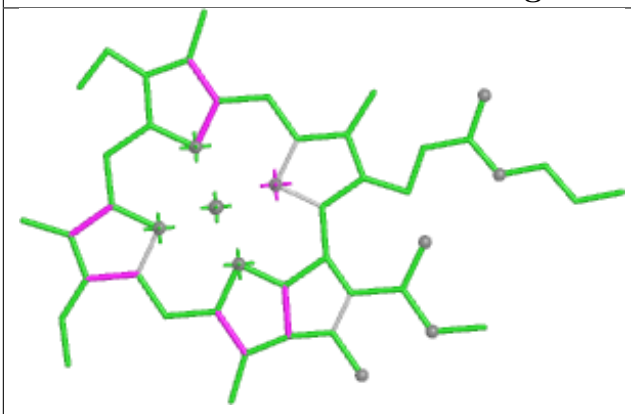


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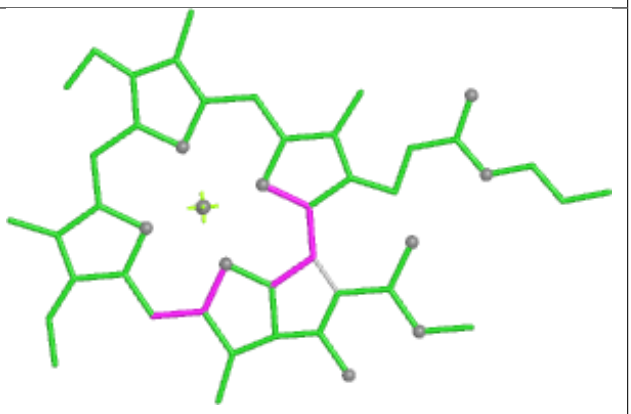


Rings

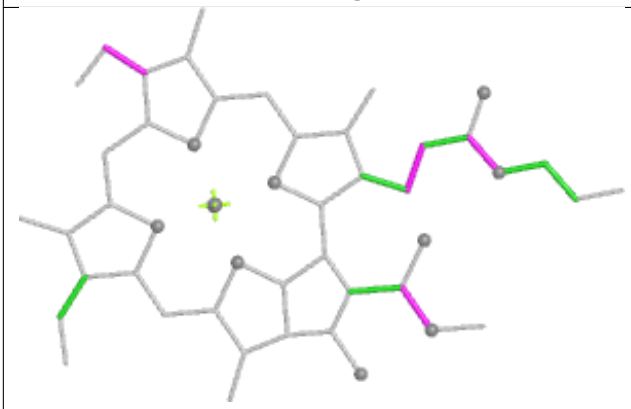
Ligand CLA B 840



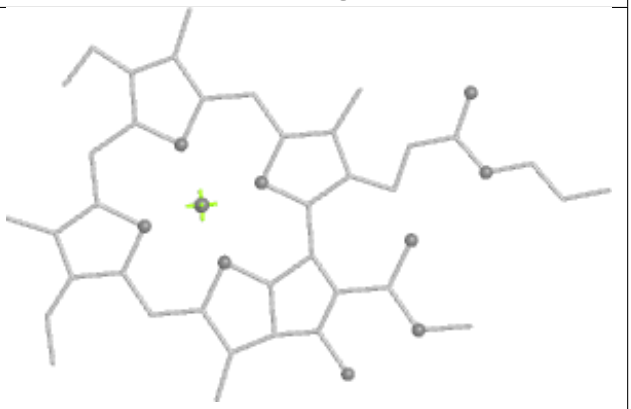
Bond lengths



Bond angles

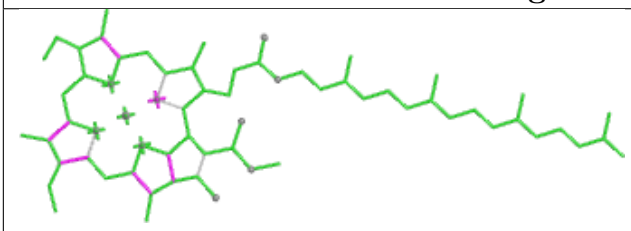


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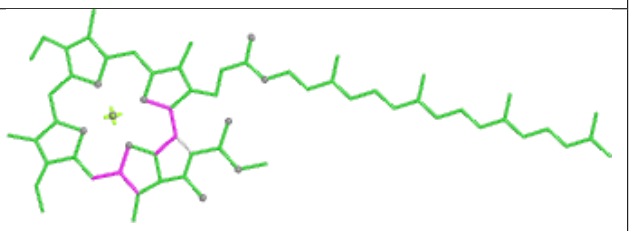


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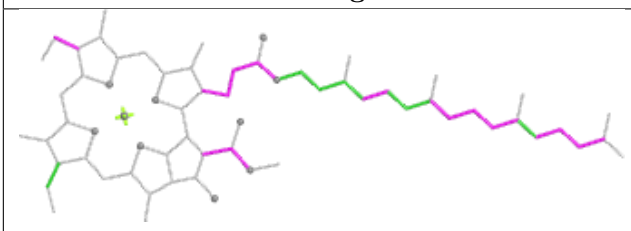
Ligand CLA a 811



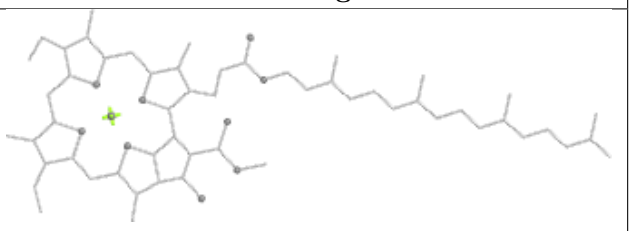
Bond lengths



Bond angles

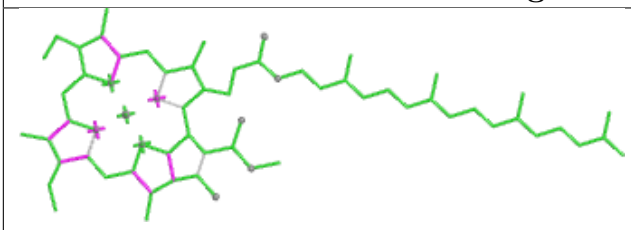


Torsions

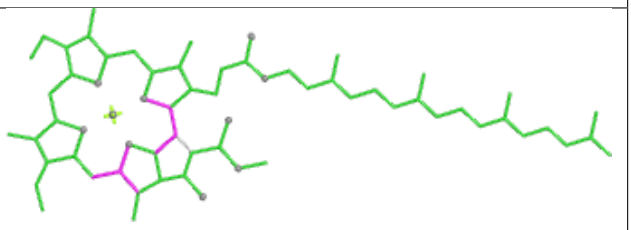


Rings

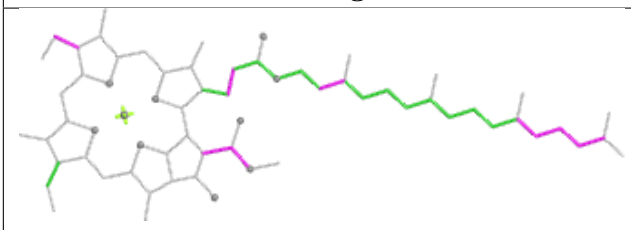
Ligand CLA b 831



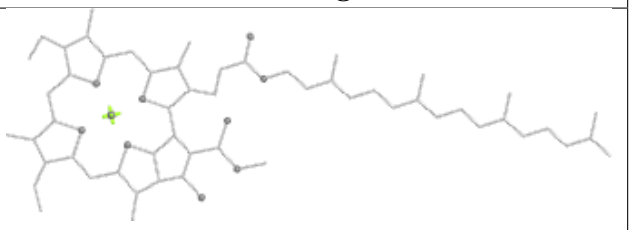
Bond lengths



Bond angles

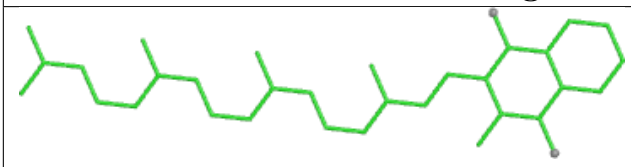


Torsions

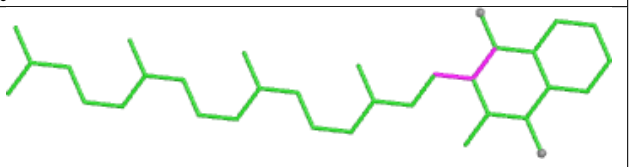


Rings

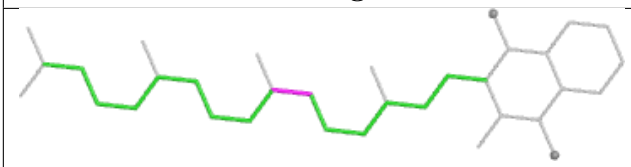
Ligand PQN B 833



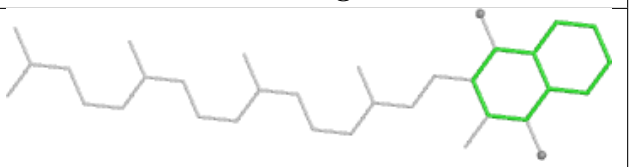
Bond lengths



Bond angles

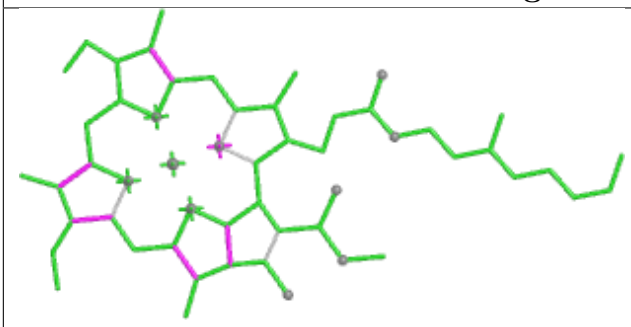


Torsions

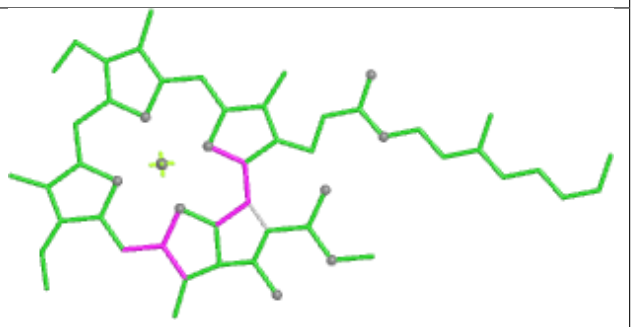


Rings

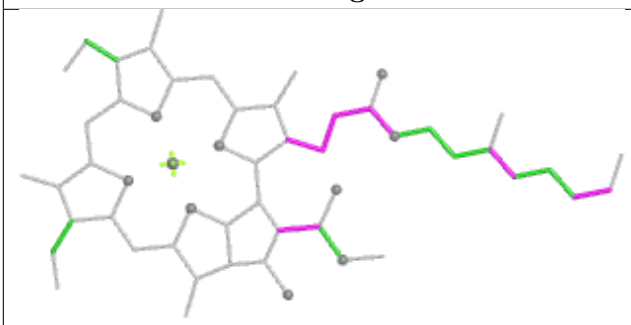
Ligand CLA A 810



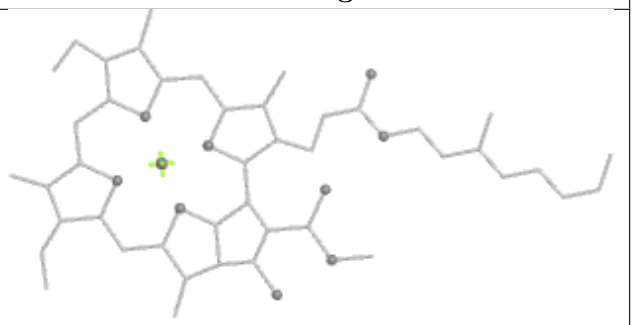
Bond lengths



Bond angles

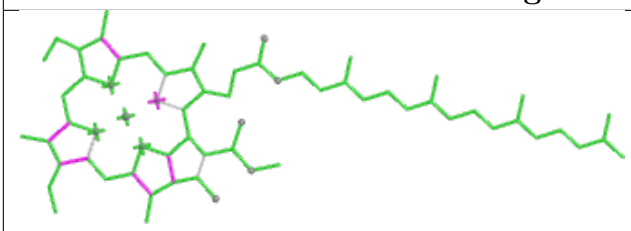


Torsions

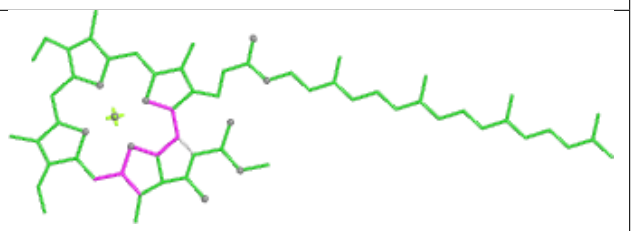


Rings

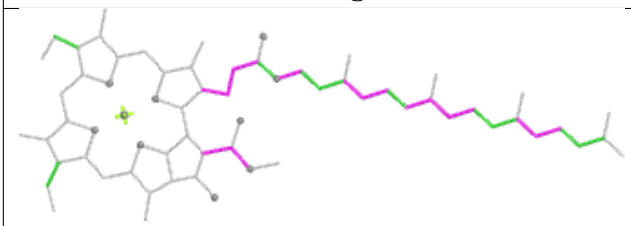
Ligand CLA A 824



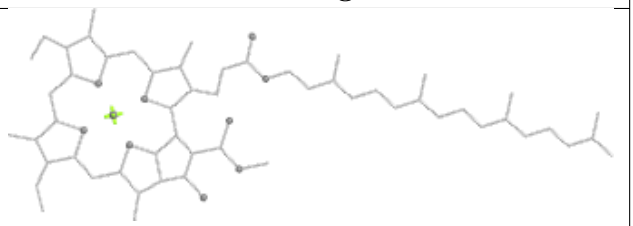
Bond lengths



Bond angles

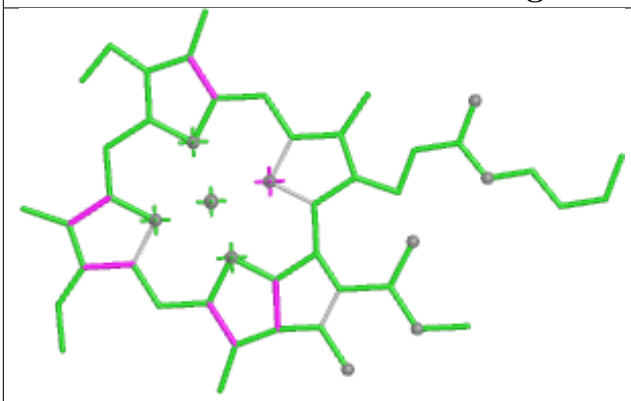


Torsions

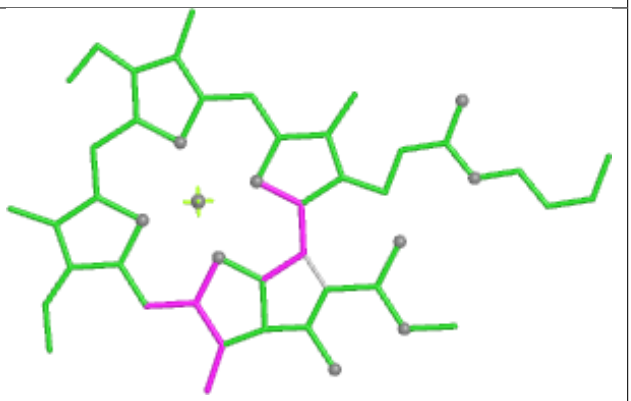


Rings

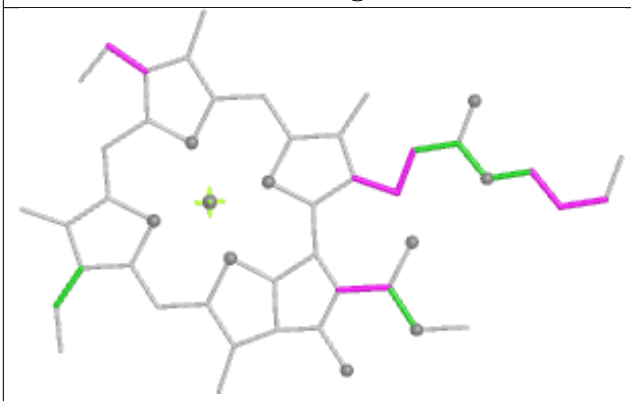
Ligand CLA L 302



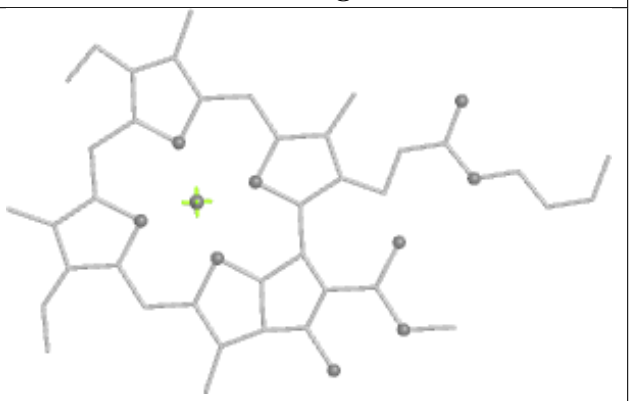
Bond lengths



Bond angles

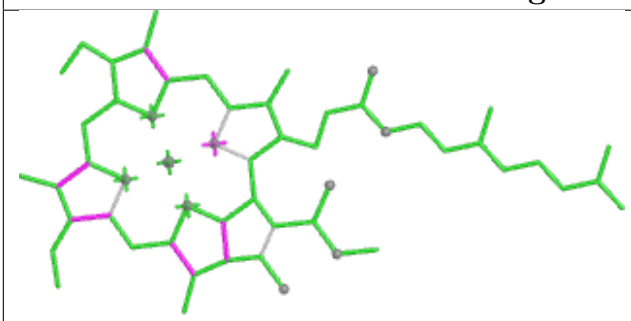


Torsions

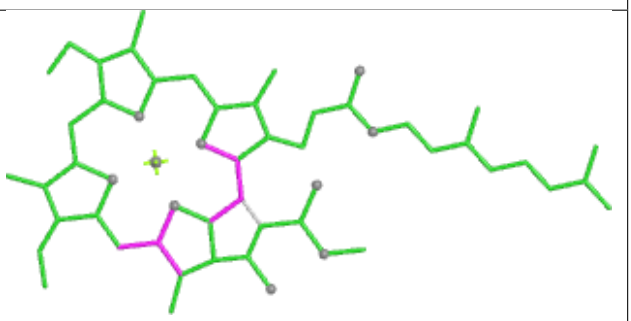


Rings

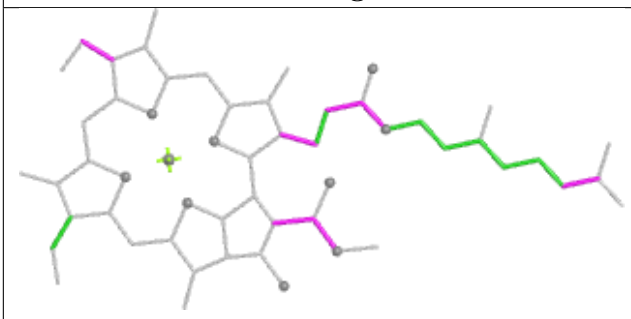
Ligand CLA a 821



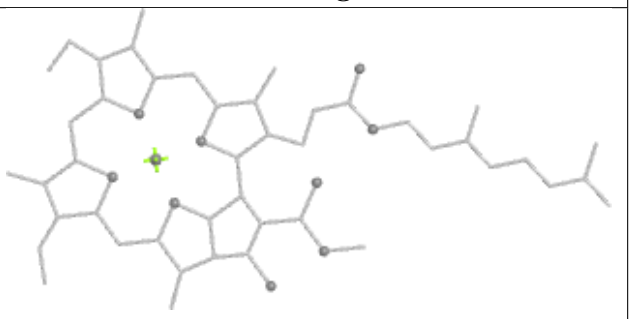
Bond lengths



Bond angles

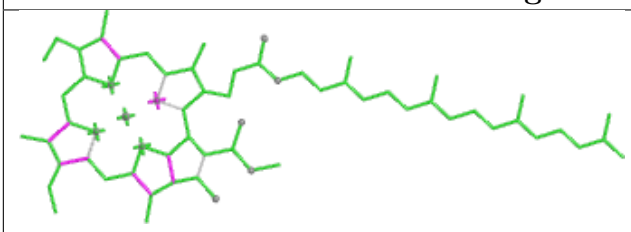


Torsions

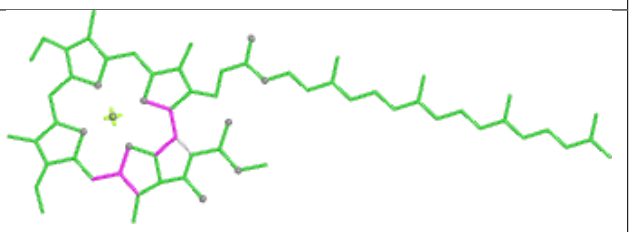


Rings

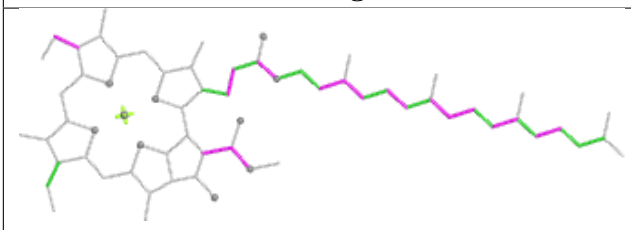
Ligand CLA B 811



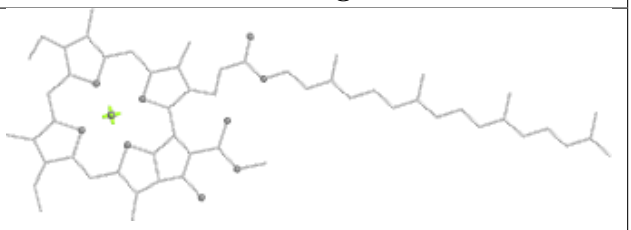
Bond lengths



Bond angles

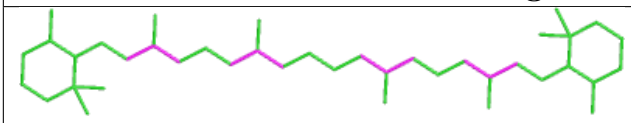


Torsions

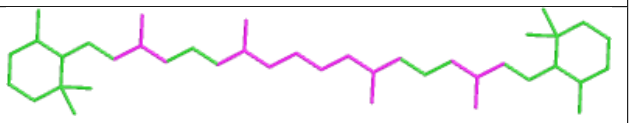


Rings

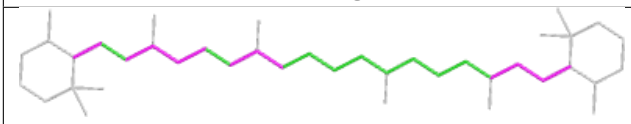
Ligand BCR b 836



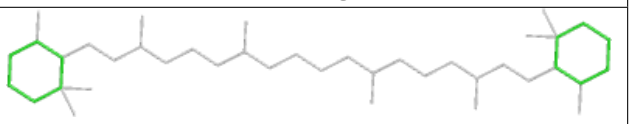
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

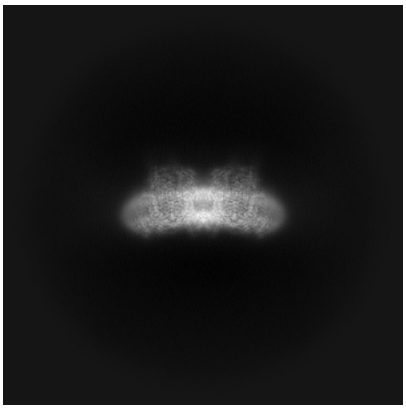
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67061. These allow visual inspection of the internal detail of the map and identification of artifacts.

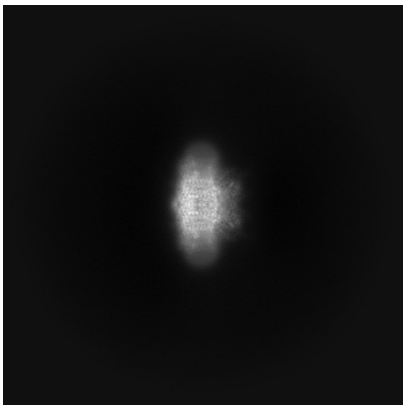
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

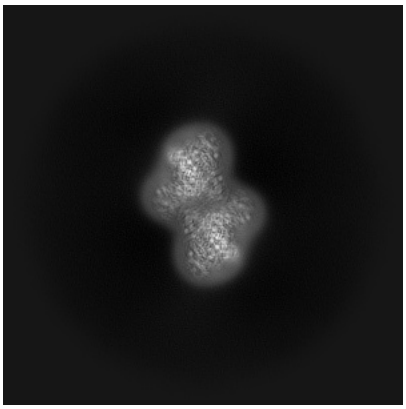
6.1.1 Primary map



X

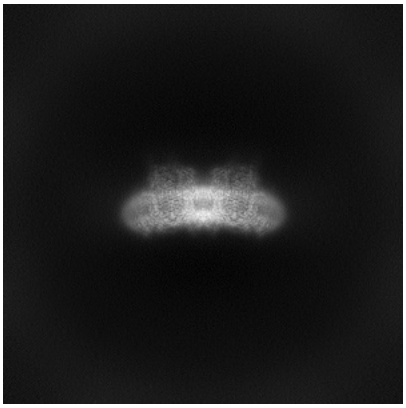


Y

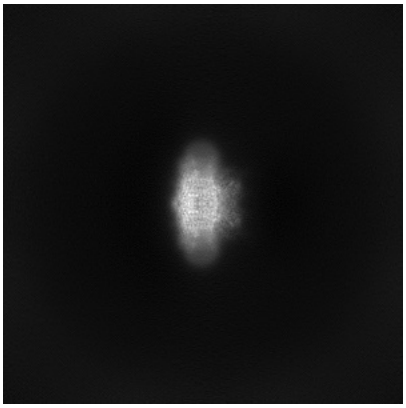


Z

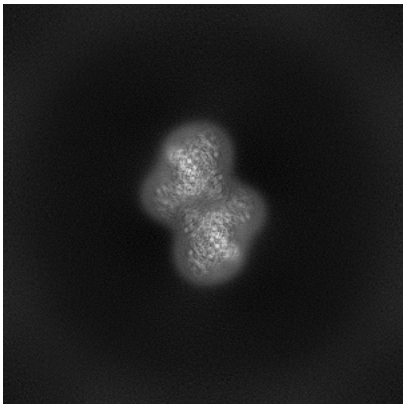
6.1.2 Raw map



X



Y

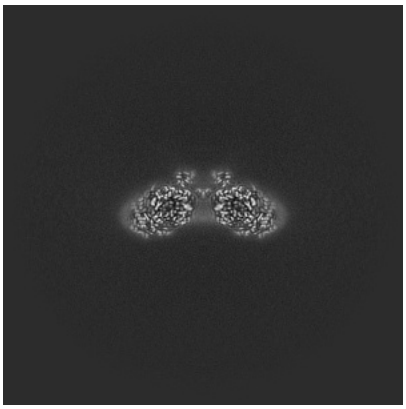


Z

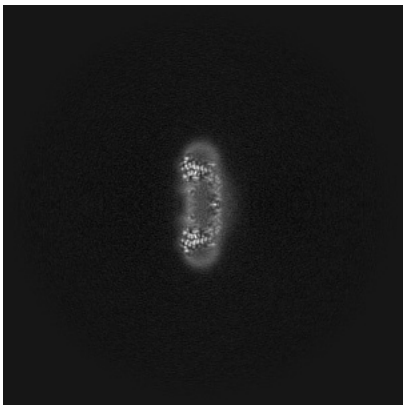
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

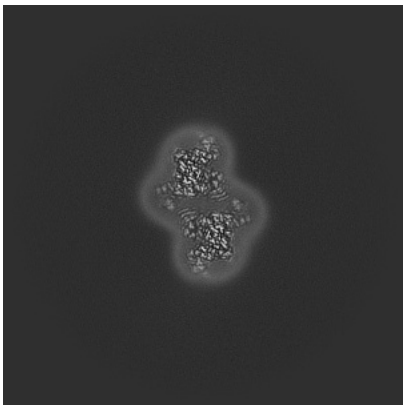
6.2.1 Primary map



X Index: 256

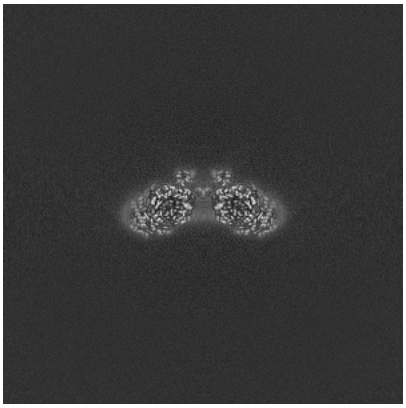


Y Index: 256

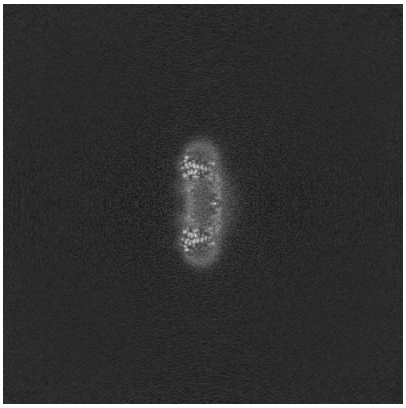


Z Index: 256

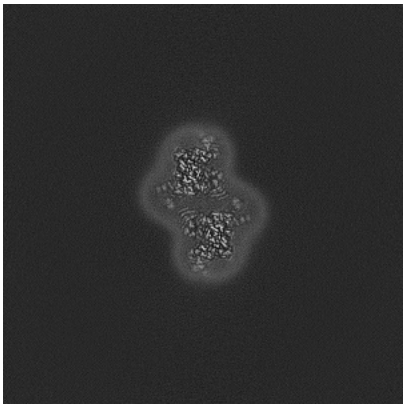
6.2.2 Raw map



X Index: 256



Y Index: 256

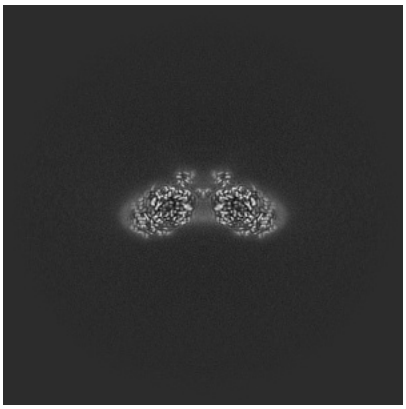


Z Index: 256

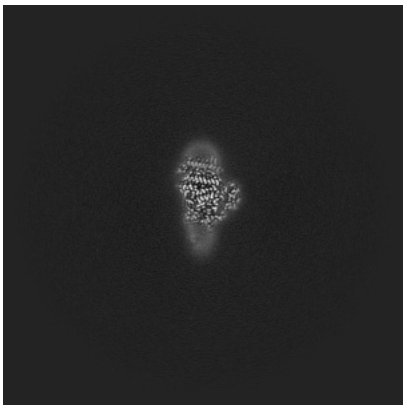
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

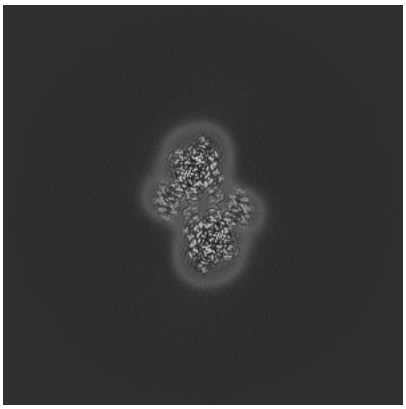
6.3.1 Primary map



X Index: 256

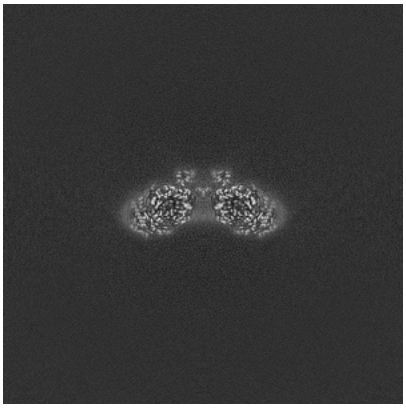


Y Index: 235

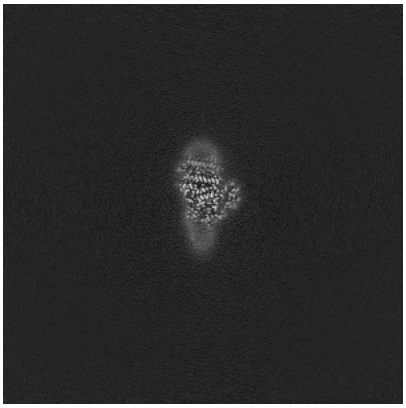


Z Index: 243

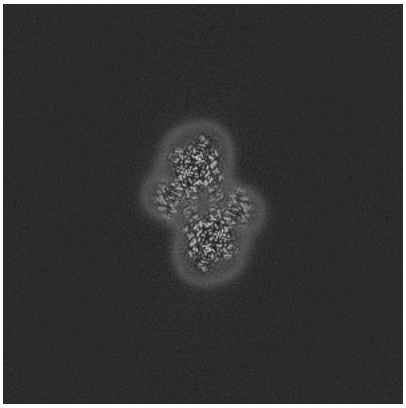
6.3.2 Raw map



X Index: 256



Y Index: 235

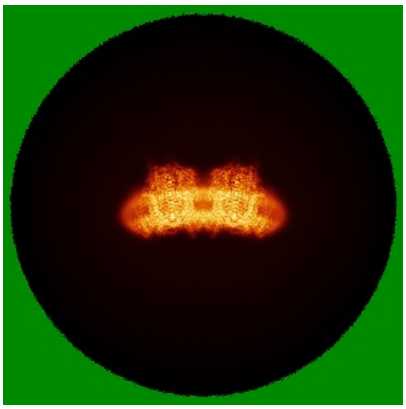


Z Index: 243

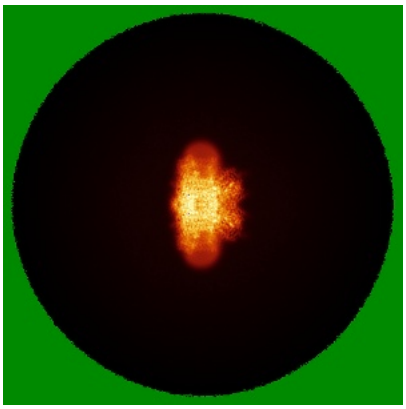
The images above show the largest variance slices of the map in three orthogonal directions.

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

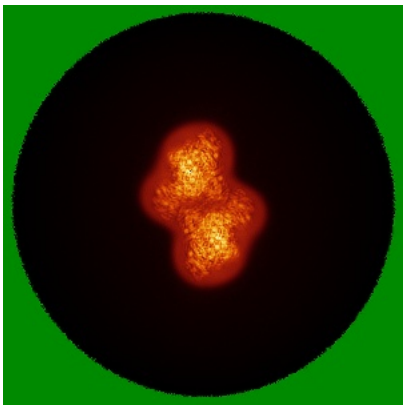
6.4.1 Primary map



X

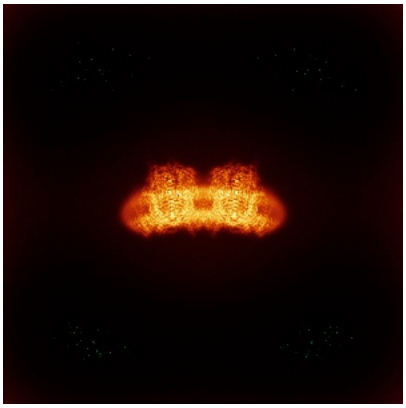


Y

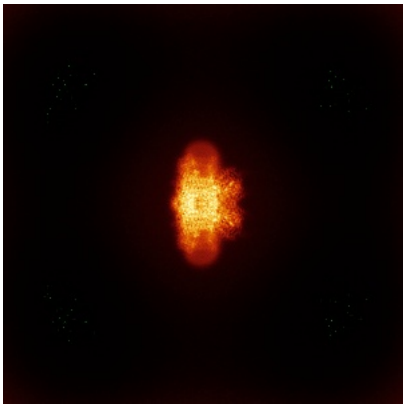


Z

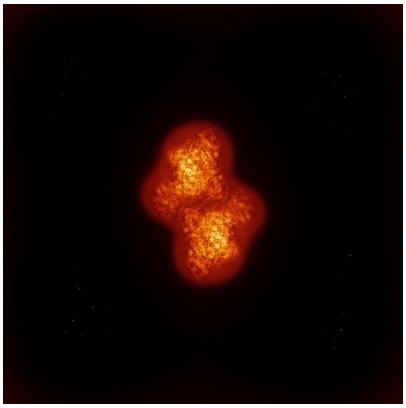
6.4.2 Raw map



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 0.0614. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

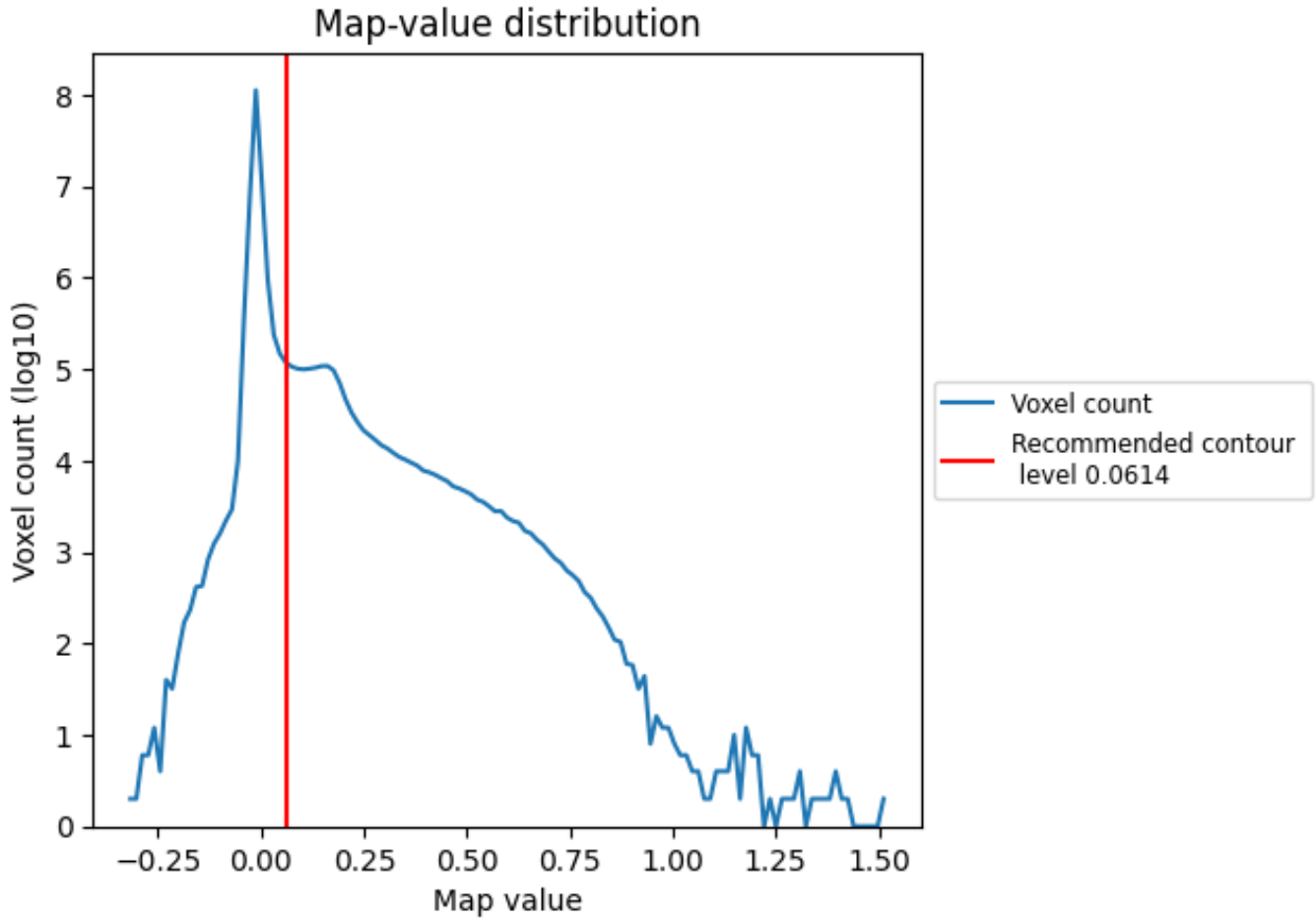
6.6 Mask visualisation (i)

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

7 Map analysis

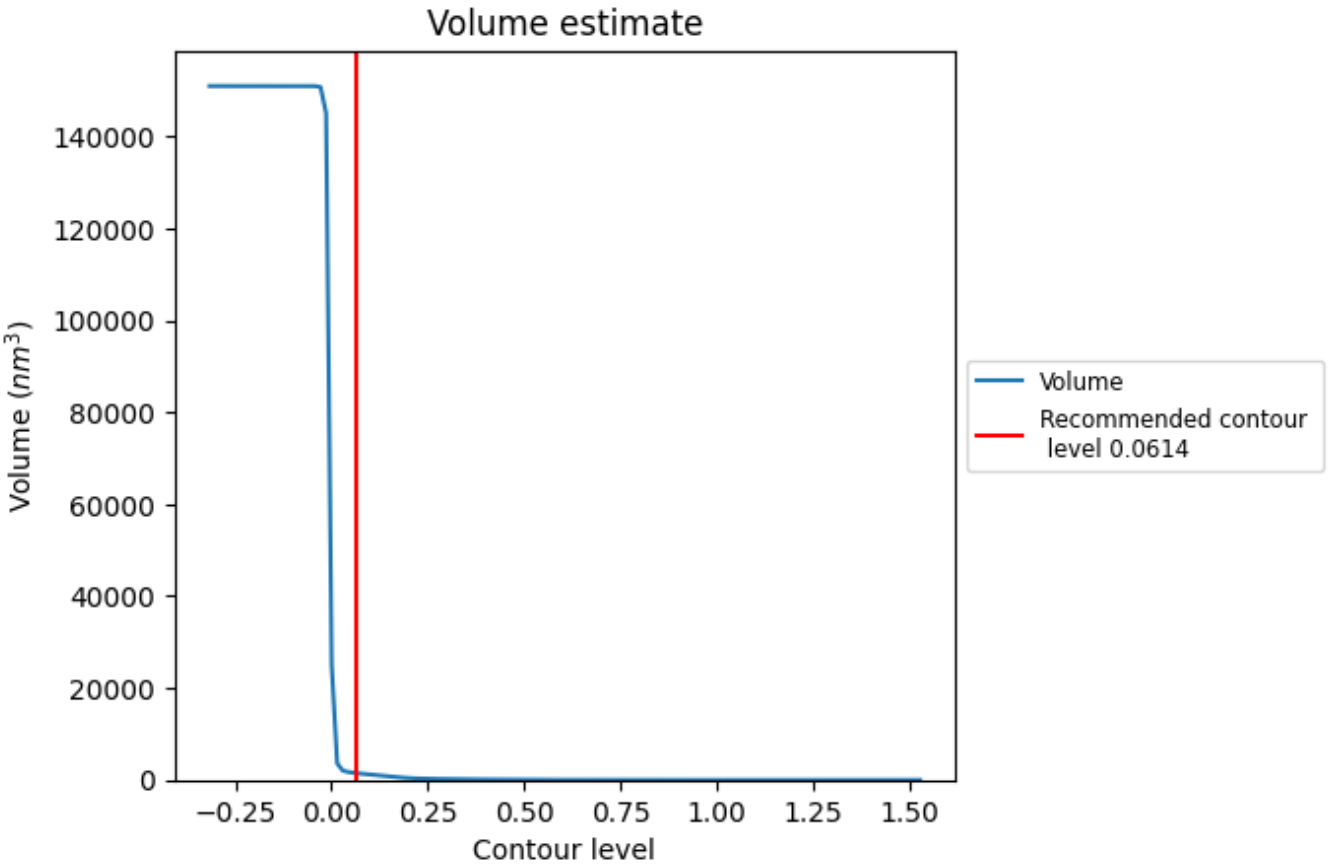
This section contains the results of statistical analysis of the map.

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.

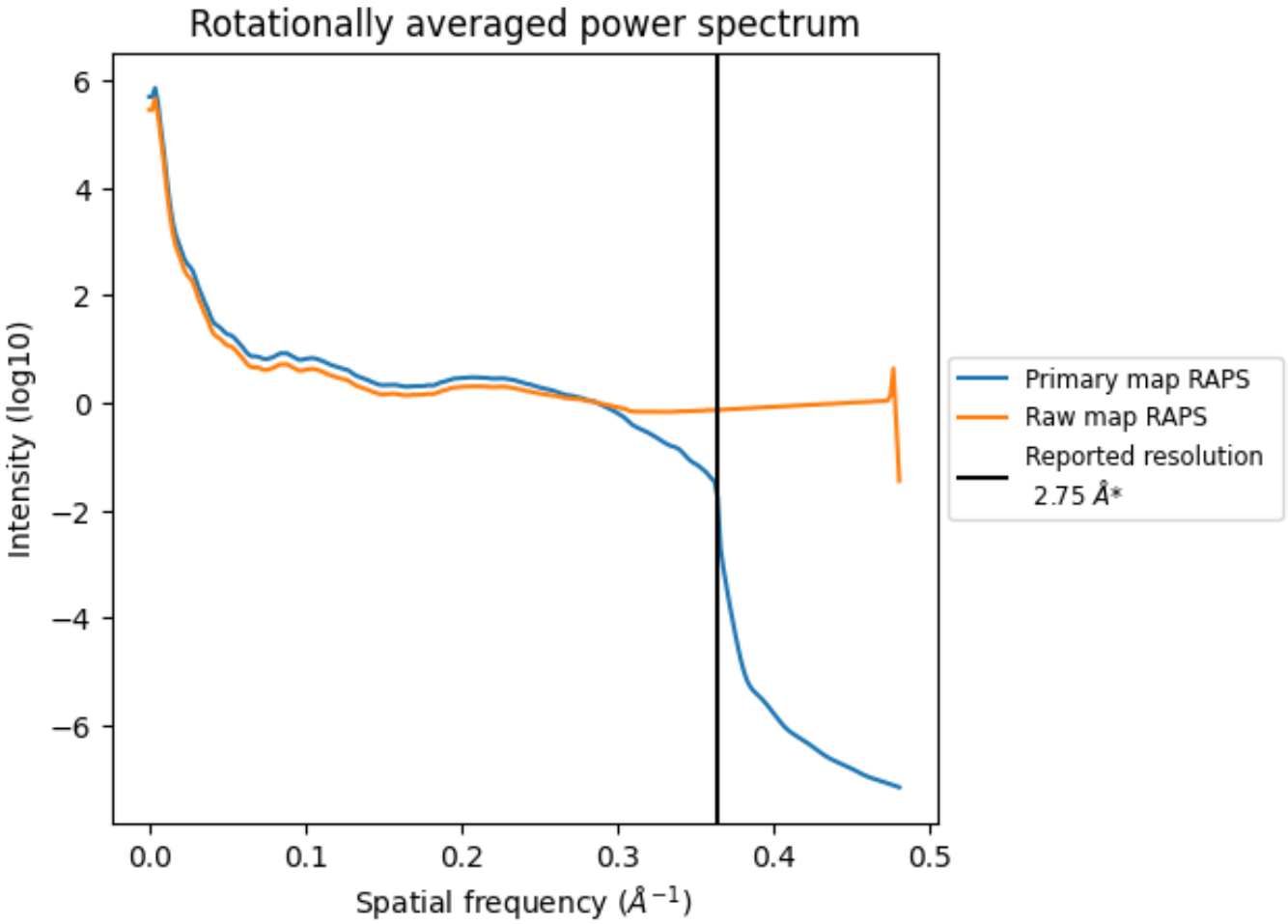
7.2 Volume estimate



The volume at the recommended contour level is 1511 nm^3; this corresponds to an approximate mass of 1365 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)

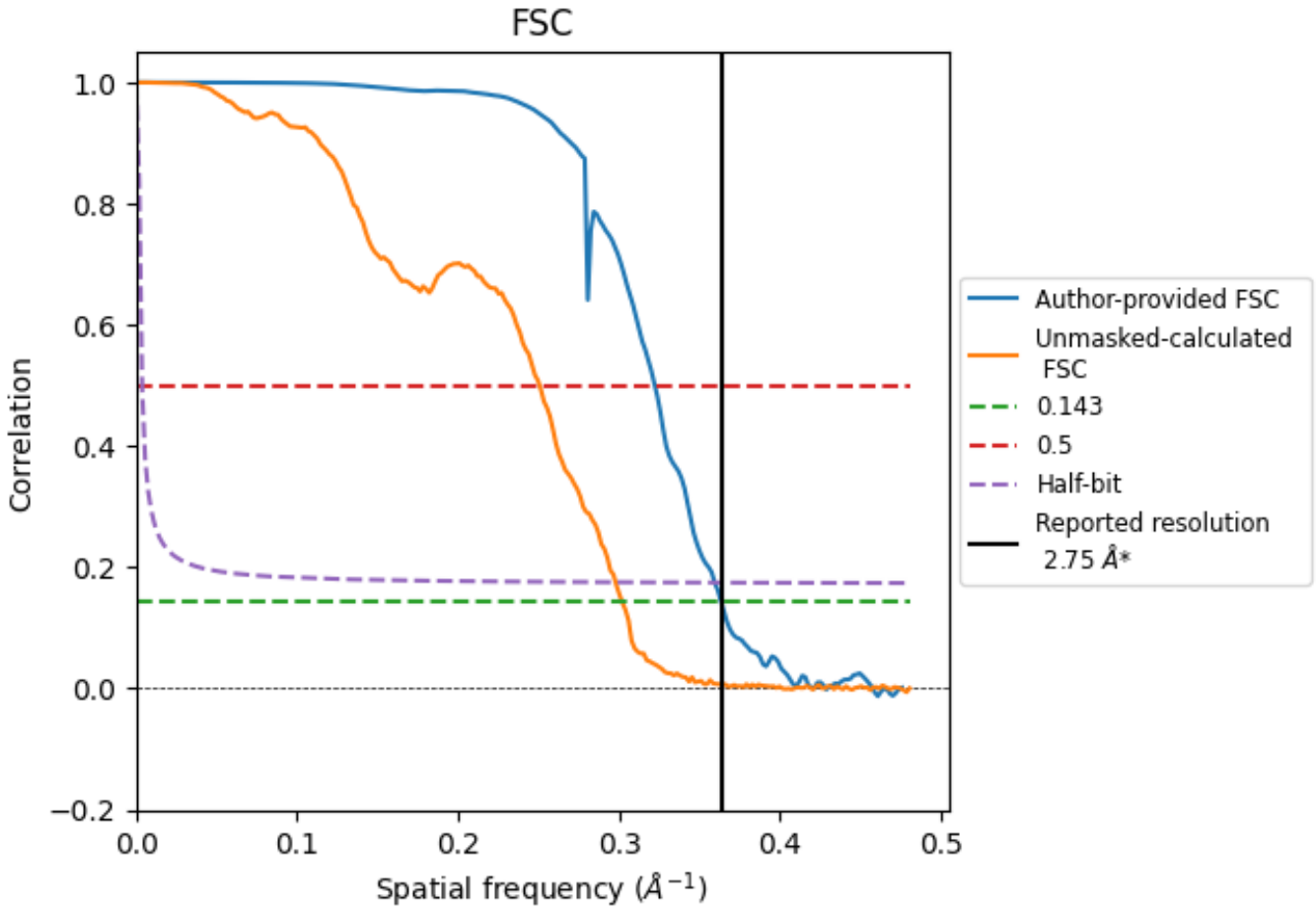


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

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 0.364 Å^{-1}

8.2 Resolution estimates (i)

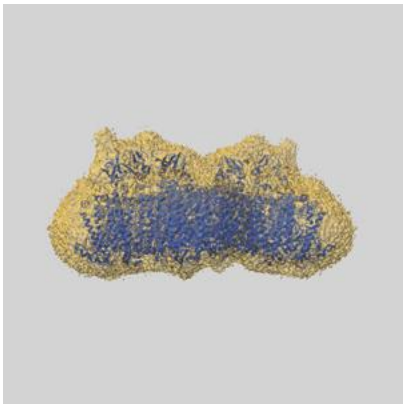
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.10	2.78
Unmasked-calculated*	3.31	3.99	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.75 by more than 10 %

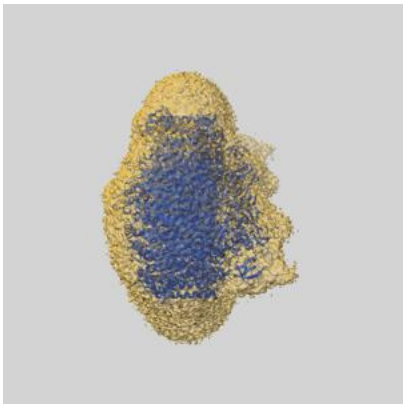
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67061 and PDB model 9XNV. Per-residue inclusion information can be found in section 3 on page 19.

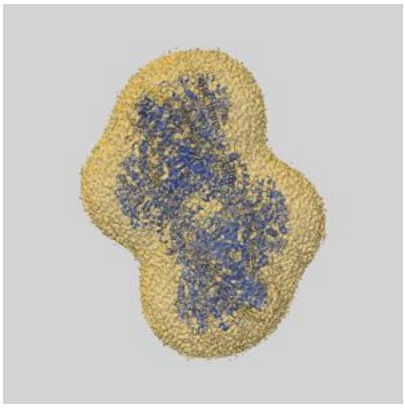
9.1 Map-model overlay



X



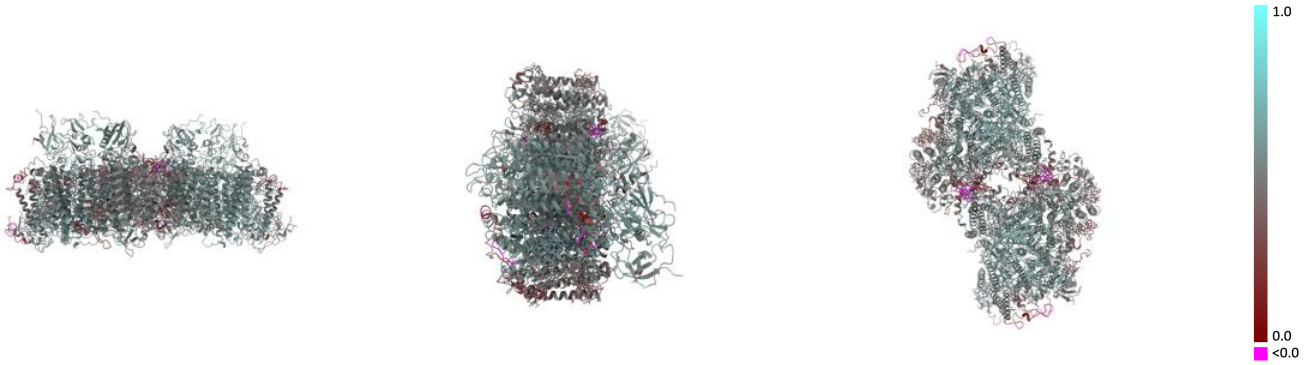
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0614 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

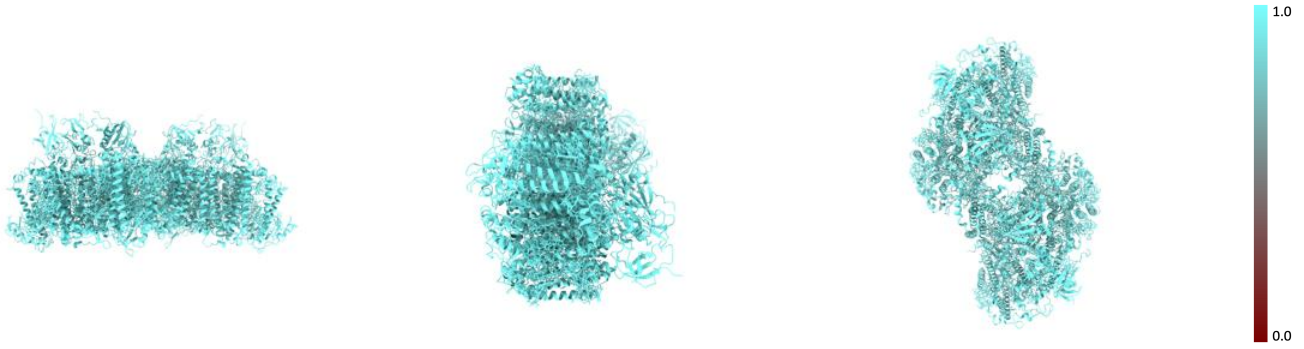
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

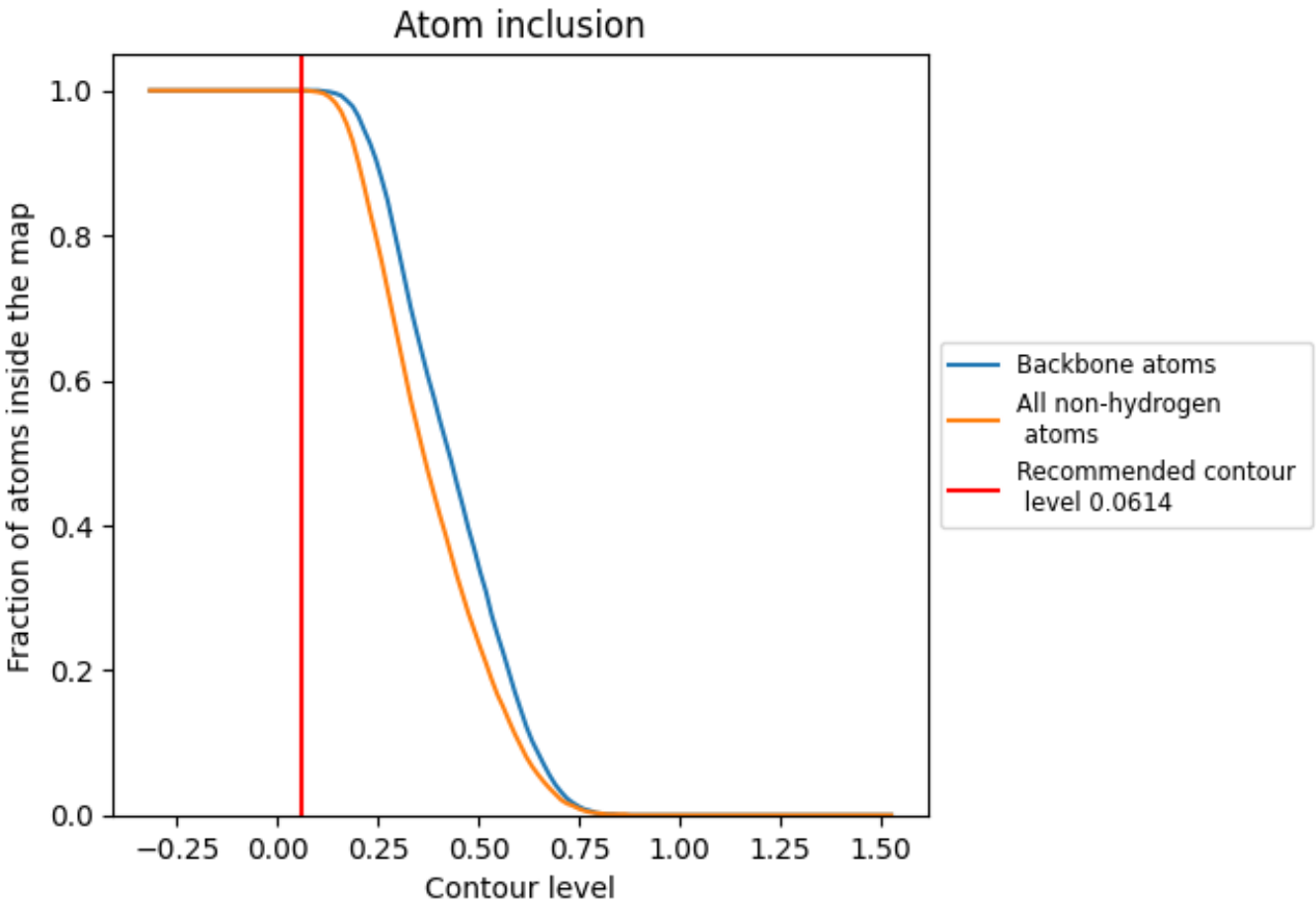
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0614).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0614) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	1.0000	0.5160
A	1.0000	0.4900
B	1.0000	0.5410
C	1.0000	0.5670
D	1.0000	0.5660
E	1.0000	0.5280
H	1.0000	0.4870
I	1.0000	0.5450
L	0.9990	0.4810
a	1.0000	0.4890
b	1.0000	0.5420
c	1.0000	0.5690
d	1.0000	0.5620
e	1.0000	0.5280
h	1.0000	0.4580
i	1.0000	0.5470
l	0.9990	0.4700

