Full wwPDB EM Validation Report ⓘ

Nov 3, 2026 – 12:53 PM EST

PDB ID	:	9OY9 / pdb_00009oy9
EMDB ID	:	EMD-71005
Title	:	Structure of a red shifted PSI monomer from 6803
Authors	:	Mazor, Y.; Kahtun, H.; Asido, M.; Gorski, C.; Schlau-Cohen, G.S.
Deposited on	:	2025-06-04
Resolution	:	1.76 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:

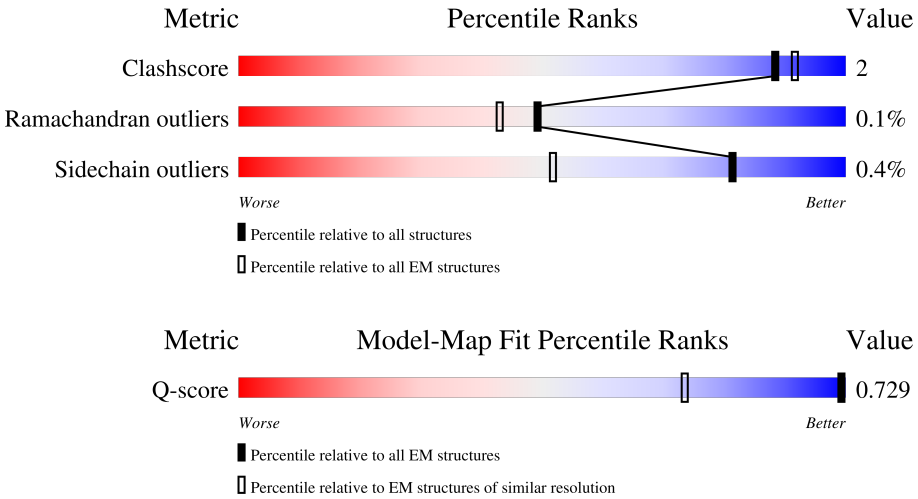
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 1.76 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.



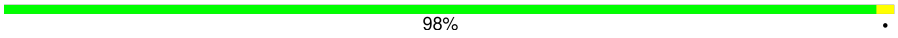
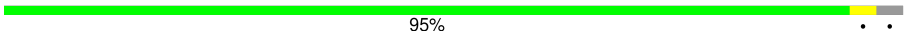
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	674 (1.27 - 2.26)

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	751	97%
2	B	735	96%
3	C	81	99%
4	D	141	98%

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Mol	Chain	Length	Quality of chain
5	E	74	
6	F	165	
7	I	40	
8	J	40	
9	K	86	
10	L	157	
11	M	31	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 25286 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	741	Total	C	N	O	S	0	0
			5801	3800	987	987	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5818	3831	974	998	15		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	GLN	HIS	engineered mutation	UNP P29255
B	486	ALA	-	linker	UNP P29255
B	487	TRP	-	linker	UNP P29255
B	488	PRO	-	linker	UNP P29255
B	489	ASN	-	linker	UNP P29255
B	490	TYR	-	linker	UNP P29255
B	491	GLY	-	linker	UNP P29255
B	492	ASN	-	linker	UNP P29255
B	493	VAL	-	linker	UNP P29255

- 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
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	40	Total	C	N	O	S	0	0
			318	215	47	53	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

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

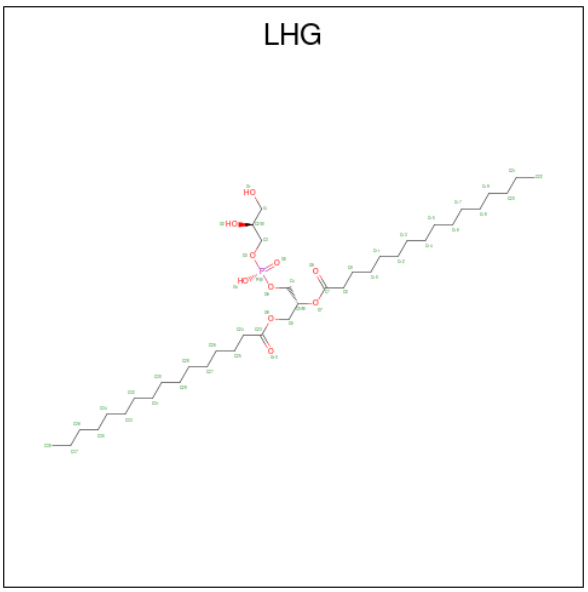
Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

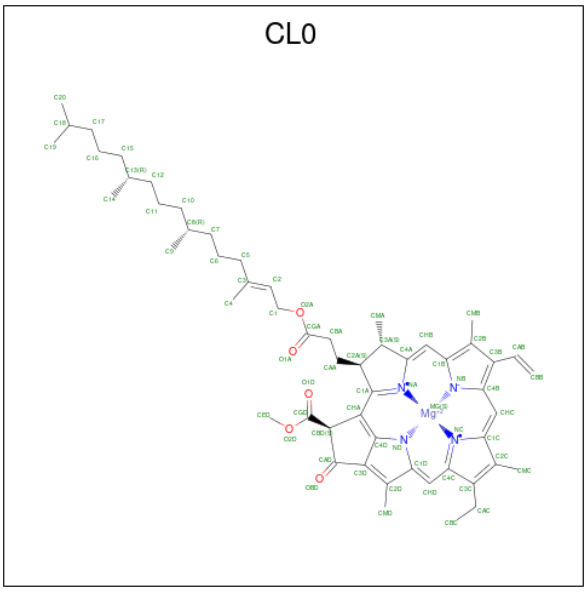
- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: $C_{38}H_{75}O_{10}P$).



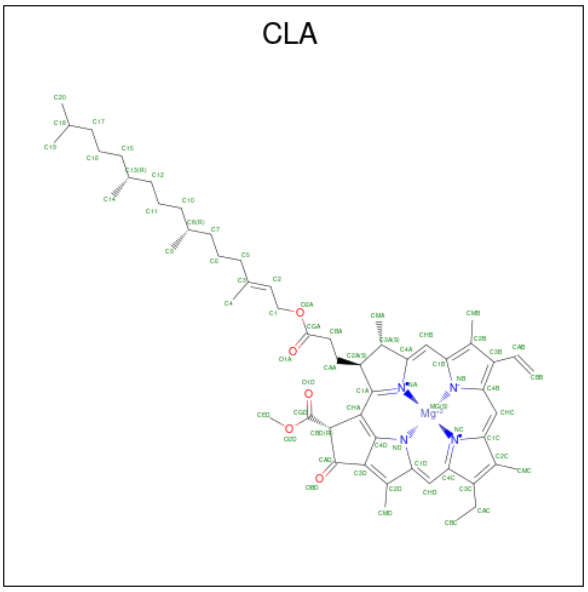
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			48	37	10	1	
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	B	1	Total	C	O	P	0
			38	27	10	1	
12	M	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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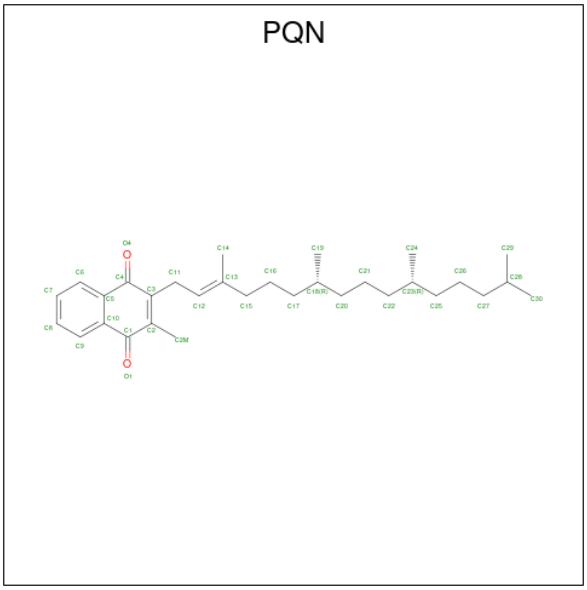
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



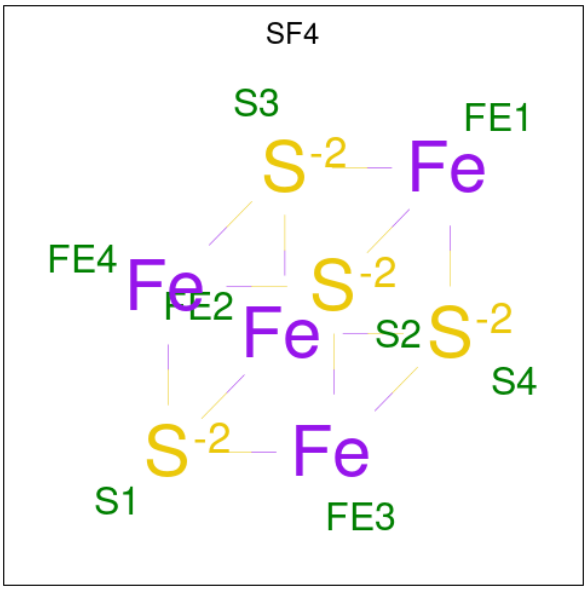
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	

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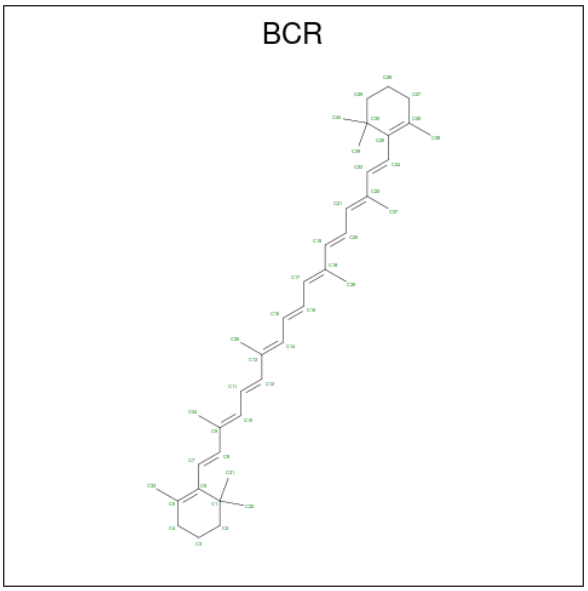
Mol	Chain	Residues	Atoms	AltConf
15	B	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



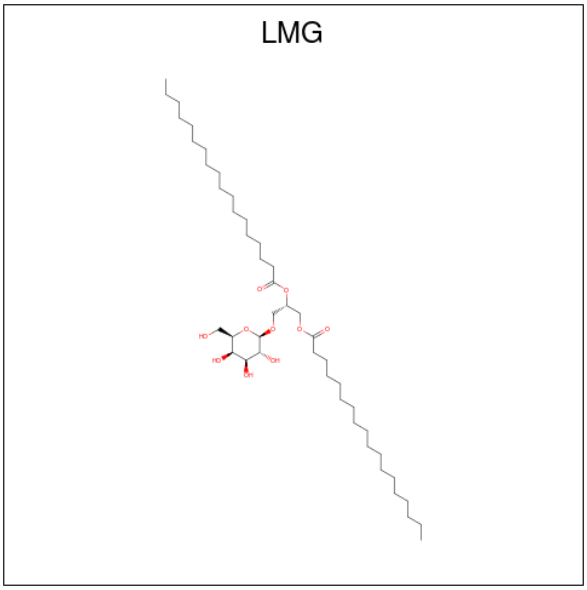
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 30 30	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	I	1	Total C 40 40	0

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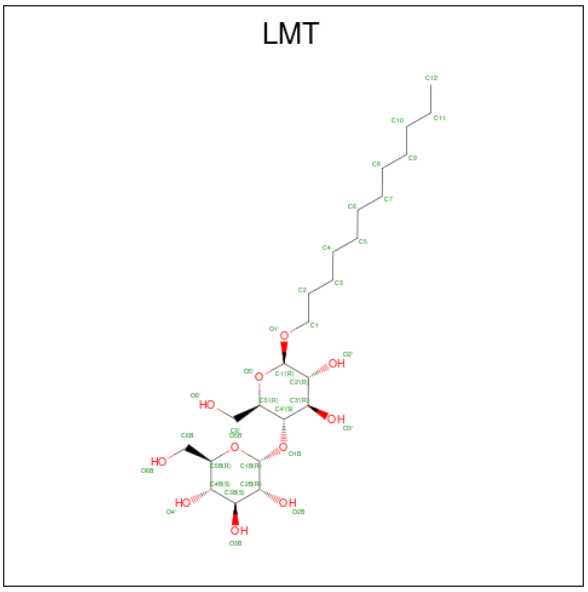
Mol	Chain	Residues	Atoms	AltConf
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O 46 36 10	0
18	B	1	Total C O 50 40 10	0
18	B	1	Total C O 38 28 10	0
18	I	1	Total C O 38 28 10	0

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

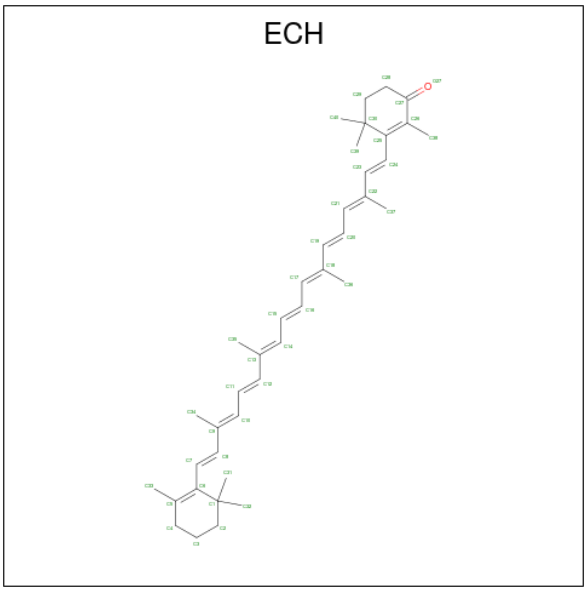


Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	F	1	Total C O 35 24 11	0
19	F	1	Total C O 35 24 11	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total Ca 1 1	0
20	L	1	Total Ca 1 1	0

- Molecule 21 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C O 41 40 1	0
21	I	1	Total C O 41 40 1	0
21	M	1	Total C O 41 40 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	A	109	Total O 109 109	0
22	B	153	Total O 153 153	0
22	C	31	Total O 31 31	0
22	D	23	Total O 23 23	0
22	E	3	Total O 3 3	0
22	F	4	Total O 4 4	0
22	I	4	Total O 4 4	0
22	J	2	Total O 2 2	0
22	K	2	Total O 2 2	0

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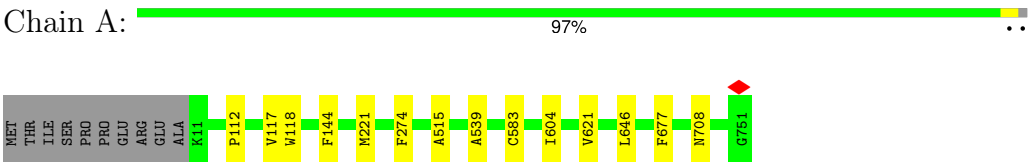
Mol	Chain	Residues	Atoms	AltConf
22	L	16	Total O 16 16	0
22	M	3	Total O 3 3	0

3 Residue-property plots (i)

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

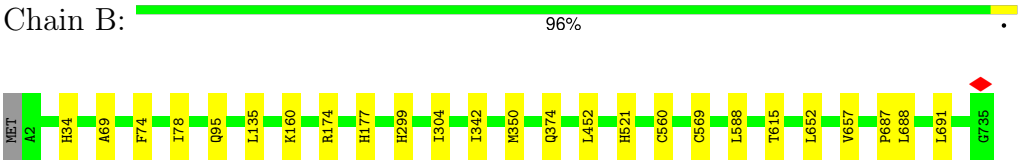
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



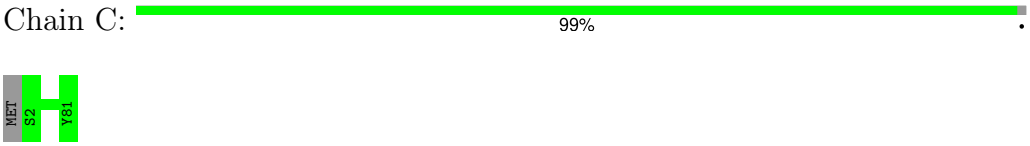
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



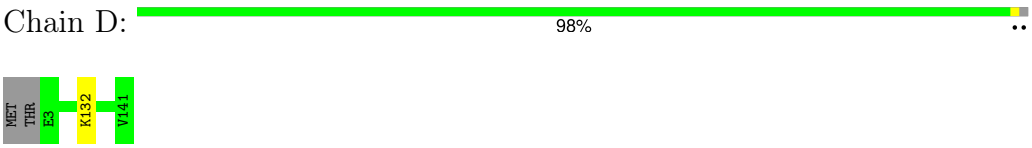
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



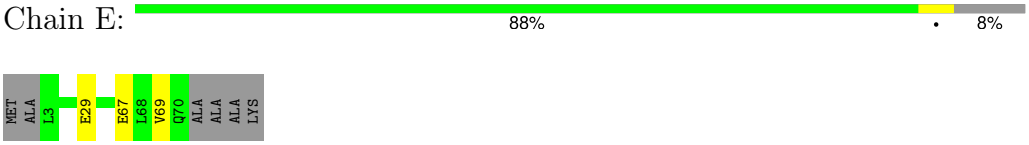
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



• Molecule 6: Photosystem I reaction center subunit III

Chain F:

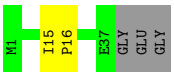




• Molecule 7: Photosystem I reaction center subunit VIII

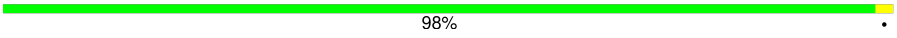
Chain I:





• Molecule 8: Photosystem I reaction center subunit IX

Chain J:





• Molecule 9: Photosystem I reaction center subunit PsaK 1

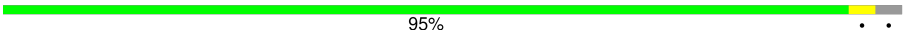
Chain K:

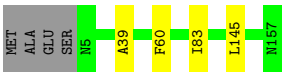




• Molecule 10: Photosystem I reaction center subunit XI

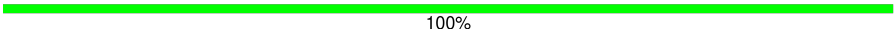
Chain L:





• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	857484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	54.034	Depositor
Minimum map value	-12.744	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	321.64, 321.64, 321.64	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMG, SF4, CLA, CA, CL0, LHG, ECH, LMT, BCR

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	0.30	0/5999	0.29	0/8176
2	B	0.31	0/6032	0.30	0/8250
3	C	0.29	0/610	0.34	0/826
4	D	0.27	0/1111	0.29	0/1497
5	E	0.23	0/546	0.28	0/738
6	F	0.22	0/1130	0.29	0/1535
7	I	0.32	0/304	0.29	0/416
8	J	0.27	0/327	0.27	0/443
9	K	0.21	0/549	0.26	0/745
10	L	0.29	0/1180	0.29	0/1603
11	M	0.29	0/241	0.24	0/326
All	All	0.29	0/18029	0.29	0/24555

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5801	0	5664	9	0
2	B	5818	0	5588	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	581	0	0
4	D	1087	0	1082	0	0
5	E	537	0	520	2	0
6	F	1100	0	1096	3	0
7	I	293	0	292	1	0
8	J	318	0	328	1	0
9	K	538	0	565	0	0
10	L	1150	0	1122	4	0
11	M	238	0	260	0	0
12	A	97	0	143	0	0
12	B	38	0	49	0	0
12	M	40	0	50	0	0
13	A	65	0	72	3	0
14	A	2708	0	2844	20	0
14	B	2455	0	2569	31	0
14	F	156	0	138	2	0
14	J	160	0	144	1	0
14	K	155	0	138	0	0
14	L	195	0	216	1	0
15	A	33	0	46	0	0
15	B	33	0	46	0	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
17	A	200	0	280	7	0
17	B	230	0	319	3	0
17	F	80	0	112	2	0
17	I	40	0	56	0	0
17	J	80	0	112	2	0
17	K	80	0	112	1	0
17	L	80	0	112	4	0
18	A	46	0	62	0	0
18	B	88	0	119	0	0
18	I	38	0	46	0	0
19	A	140	0	184	0	0
19	F	70	0	92	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	B	41	0	54	1	0
21	I	41	0	54	0	0
21	M	41	0	54	3	0
22	A	109	0	0	0	0
22	B	153	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	31	0	0	0	0
22	D	23	0	0	0	0
22	E	3	0	0	0	0
22	F	4	0	0	0	0
22	I	4	0	0	0	0
22	J	2	0	0	0	0
22	K	2	0	0	0	0
22	L	16	0	0	0	0
22	M	3	0	0	0	0
All	All	25286	0	25321	95	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 2.

All (95) 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)
14:A:804:CLA:HMB1	14:A:804:CLA:HBB1	1.74	0.69
14:A:820:CLA:HMB1	14:A:820:CLA:HBB1	1.78	0.66
14:B:837:CLA:HMB1	14:B:837:CLA:HBB1	1.77	0.66
2:B:452:LEU:HD22	2:B:615:THR:HG21	1.83	0.61
1:A:604:ILE:HD11	13:A:802:CL0:H35	1.84	0.60
1:A:677:PHE:CG	17:A:852:BCR:H363	2.37	0.59
8:J:14:MET:HA	8:J:14:MET:HE2	1.84	0.59
2:B:691:LEU:HD11	10:L:39:ALA:HB1	1.85	0.57
14:B:826:CLA:HBB1	14:B:826:CLA:HMB1	1.85	0.56
1:A:708:ASN:O	6:F:88:ILE:HD11	2.05	0.56
14:B:806:CLA:HBB1	14:B:806:CLA:HMB1	1.86	0.56
14:B:811:CLA:H42	10:L:83:ILE:HG22	1.89	0.55
17:A:852:BCR:H23C	17:A:852:BCR:H403	1.89	0.55
5:E:69:VAL:HG22	5:E:69:VAL:O	2.08	0.54
14:J:1101:CLA:HMB1	14:J:1101:CLA:HBB1	1.89	0.53
14:B:801:CLA:H201	17:J:1104:BCR:H362	1.91	0.53
14:A:828:CLA:HBB1	14:A:828:CLA:HMB1	1.89	0.53
21:M:102:ECH:H40B	21:M:102:ECH:H23	1.90	0.52
14:B:839:CLA:HMB1	14:B:839:CLA:HBB1	1.90	0.52
14:A:816:CLA:HMB1	14:A:816:CLA:HBB1	1.92	0.51
14:B:811:CLA:HED2	14:B:811:CLA:H43	1.92	0.50
10:L:145:LEU:HD13	14:L:204:CLA:H43	1.92	0.50
17:A:852:BCR:H393	17:J:1104:BCR:H322	1.94	0.50
2:B:34:HIS:HE1	14:B:805:CLA:HED1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:837:CLA:HMB2	14:B:839:CLA:HED1	1.94	0.49
14:B:819:CLA:O1A	14:B:829:CLA:HMD1	2.12	0.49
14:B:827:CLA:HMB1	14:B:827:CLA:HBB1	1.94	0.49
2:B:374:GLN:O	2:B:588:LEU:HD11	2.14	0.48
14:A:829:CLA:HMB1	14:A:829:CLA:HBB1	1.96	0.48
2:B:174:ARG:HD2	14:B:825:CLA:OBD	2.14	0.47
2:B:350:MET:HE3	22:B:1050:HOH:O	2.14	0.47
17:A:852:BCR:H381	14:F:201:CLA:HMA1	1.97	0.47
2:B:657:VAL:HG22	14:B:841:CLA:HMB3	1.95	0.47
14:B:814:CLA:HMB1	14:B:814:CLA:HBB1	1.96	0.47
14:B:819:CLA:HMB1	14:B:819:CLA:HBB1	1.97	0.47
2:B:521:HIS:CG	14:B:838:CLA:HED3	2.50	0.46
10:L:60:PHE:C	10:L:60:PHE:CD1	2.93	0.46
14:B:816:CLA:HBB1	14:B:816:CLA:HMB1	1.98	0.46
14:B:830:CLA:HBB1	14:B:830:CLA:HMB1	1.98	0.45
14:A:803:CLA:CGA	14:A:803:CLA:H3A	2.47	0.45
14:A:807:CLA:HBB1	14:A:807:CLA:HMB1	1.98	0.45
1:A:118:TRP:CD2	14:A:810:CLA:HED3	2.51	0.45
14:A:837:CLA:HMB1	17:A:851:BCR:H281	1.99	0.45
17:K:4001:BCR:C8	17:K:4001:BCR:H331	2.46	0.45
21:M:102:ECH:H24	21:M:102:ECH:H37	1.83	0.45
7:I:15:ILE:HB	7:I:16:PRO:HD3	1.97	0.45
17:L:206:BCR:C23	17:L:206:BCR:H403	2.47	0.45
14:A:826:CLA:O1D	14:A:826:CLA:H42	2.17	0.44
13:A:802:CL0:H35	13:A:802:CL0:H41	1.77	0.44
2:B:177:HIS:CG	14:B:814:CLA:HMC2	2.52	0.44
14:F:203:CLA:HBB1	14:F:203:CLA:HMB1	2.00	0.44
1:A:646:LEU:HD22	2:B:652:LEU:HD21	1.99	0.44
21:M:102:ECH:C23	21:M:102:ECH:H39A	2.47	0.44
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.53	0.43
17:F:202:BCR:C8	17:F:202:BCR:H331	2.48	0.43
13:A:802:CL0:H32	14:A:804:CLA:C1D	2.48	0.43
14:A:818:CLA:HBB1	14:A:818:CLA:HMB1	2.00	0.43
14:B:807:CLA:H41	14:B:807:CLA:H71	2.00	0.43
14:B:833:CLA:H62	14:B:833:CLA:H41	1.85	0.43
17:A:849:BCR:H383	17:A:849:BCR:H23C	2.00	0.43
14:B:810:CLA:H91	14:B:841:CLA:O1A	2.19	0.43
17:A:851:BCR:C23	17:A:851:BCR:H403	2.49	0.42
14:A:815:CLA:CHA	14:A:817:CLA:HMB3	2.49	0.42
14:A:859:CLA:H121	17:B:849:BCR:H362	2.02	0.42
1:A:112:PRO:HB3	1:A:144:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:MET:CE	22:B:1050:HOH:O	2.67	0.42
17:L:206:BCR:H20C	17:L:206:BCR:H361	1.92	0.42
1:A:221:MET:HE1	1:A:274:PHE:HB2	2.02	0.42
14:B:826:CLA:HMB2	14:B:839:CLA:HBA1	2.02	0.41
2:B:299:HIS:HB3	2:B:304:ILE:HD11	2.02	0.41
14:B:801:CLA:HBB1	14:B:801:CLA:HMB1	2.02	0.41
14:B:813:CLA:H93	17:B:845:BCR:H332	2.02	0.41
6:F:55:VAL:HG12	6:F:65:PHE:HB2	2.00	0.41
14:A:825:CLA:H91	14:A:832:CLA:CBC	2.50	0.41
14:B:837:CLA:HMB1	14:B:837:CLA:CBB	2.47	0.41
14:B:813:CLA:C9	17:B:845:BCR:H332	2.50	0.41
14:A:822:CLA:H122	14:A:825:CLA:H93	2.03	0.41
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.02	0.41
2:B:74:PHE:CE2	2:B:78:ILE:HD11	2.56	0.41
2:B:160:LYS:HD3	2:B:160:LYS:H	1.85	0.41
2:B:687:PRO:O	2:B:688:LEU:HB2	2.21	0.41
14:B:809:CLA:H203	14:B:809:CLA:H151	2.01	0.41
21:B:846:ECH:H24	21:B:846:ECH:H37	1.91	0.41
14:B:826:CLA:HMB1	14:B:827:CLA:H203	2.03	0.41
14:A:813:CLA:CGA	14:A:813:CLA:C1A	2.99	0.41
14:A:819:CLA:HED2	14:A:820:CLA:O1A	2.21	0.41
14:B:820:CLA:HMB2	14:B:825:CLA:HMA3	2.03	0.41
14:B:826:CLA:HMB1	14:B:826:CLA:CBB	2.51	0.41
5:E:69:VAL:O	5:E:69:VAL:CG2	2.69	0.41
17:L:205:BCR:H392	17:L:205:BCR:H23C	2.03	0.41
1:A:539:ALA:HB1	14:A:839:CLA:HMB3	2.01	0.40
1:A:515:ALA:HB2	1:A:621:VAL:HG21	2.01	0.40
14:A:840:CLA:HHC	14:A:840:CLA:CBB	2.51	0.40
17:L:205:BCR:C23	17:L:205:BCR:H403	2.50	0.40
6:F:72:PHE:HB2	17:F:202:BCR:H321	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	739/751 (98%)	719 (97%)	20 (3%)	0	100 100
2	B	732/735 (100%)	716 (98%)	15 (2%)	1 (0%)	48 32
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100 100
4	D	137/141 (97%)	132 (96%)	4 (3%)	1 (1%)	18 7
5	E	66/74 (89%)	60 (91%)	6 (9%)	0	100 100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100 100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100 100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100 100
9	K	75/86 (87%)	73 (97%)	2 (3%)	0	100 100
10	L	151/157 (96%)	146 (97%)	5 (3%)	0	100 100
11	M	29/31 (94%)	29 (100%)	0	0	100 100
All	All	2219/2301 (96%)	2156 (97%)	61 (3%)	2 (0%)	49 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	132	LYS
2	B	560	CYS

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	594/603 (98%)	592 (100%)	2 (0%)	86 83
2	B	587/588 (100%)	584 (100%)	3 (0%)	81 75
3	C	68/69 (99%)	68 (100%)	0	100 100
4	D	114/116 (98%)	114 (100%)	0	100 100
5	E	58/60 (97%)	56 (97%)	2 (3%)	32 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	118/137 (86%)	117 (99%)	1 (1%)	73 64
7	I	31/32 (97%)	31 (100%)	0	100 100
8	J	35/35 (100%)	35 (100%)	0	100 100
9	K	55/62 (89%)	55 (100%)	0	100 100
10	L	115/118 (98%)	115 (100%)	0	100 100
11	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1800/1845 (98%)	1792 (100%)	8 (0%)	81 80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	A	583	CYS
2	B	95	GLN
2	B	342	ILE
2	B	569	CYS
5	E	29	GLU
5	E	67	GLU
6	F	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
2	B	14	GLN
2	B	34	HIS
2	B	95	GLN
2	B	133	GLN
2	B	361	GLN
2	B	363	HIS
2	B	373	HIS
2	B	705	GLN
3	C	38	GLN
5	E	64	ASN
6	F	61	HIS
6	F	99	GLN
9	K	39	GLN
10	L	9	GLN
10	L	36	ASN

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Mol	Chain	Res	Type
10	L	122	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 141 ligands modelled in this entry, 2 are monoatomic - leaving 139 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CLA	B	821	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	4 (4%)
14	CLA	K	4002	9	49,53,73	1.15	4 (8%)	58,89,113	0.92	3 (5%)
14	CLA	A	843	1	69,73,73	0.95	4 (5%)	82,113,113	1.06	6 (7%)
17	BCR	A	850	-	41,41,41	0.32	0	56,56,56	0.50	0
14	CLA	B	817	2	64,68,73	1.00	4 (6%)	76,107,113	1.08	4 (5%)
14	CLA	L	202	10	69,73,73	0.96	3 (4%)	82,113,113	1.11	3 (3%)
21	ECH	B	846	-	42,42,42	0.39	0	55,58,58	0.65	0
14	CLA	B	827	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	A	816	1	49,53,73	1.13	4 (8%)	58,89,113	1.09	2 (3%)
14	CLA	A	811	1	49,53,73	1.15	5 (10%)	58,89,113	1.14	3 (5%)
14	CLA	B	818	2	69,73,73	0.97	4 (5%)	82,113,113	1.01	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	PQN	B	843	-	34,34,34	0.50	0	43,45,45	0.68	1 (2%)
17	BCR	J	1104	-	41,41,41	0.33	0	56,56,56	0.58	0
14	CLA	J	1103	8	54,58,73	1.10	5 (9%)	64,95,113	1.04	5 (7%)
14	CLA	B	832	2	59,63,73	1.05	3 (5%)	70,101,113	1.07	6 (8%)
14	CLA	A	834	1	69,73,73	0.96	3 (4%)	82,113,113	1.01	7 (8%)
14	CLA	B	838	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	A	825	1	69,73,73	0.98	4 (5%)	82,113,113	1.00	4 (4%)
14	CLA	A	844	22	69,73,73	0.96	4 (5%)	82,113,113	1.01	4 (4%)
14	CLA	K	4003	9	49,53,73	1.17	5 (10%)	58,89,113	1.09	2 (3%)
18	LMG	I	101	-	38,38,55	0.62	0	46,46,63	0.70	0
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	A	819	1	69,73,73	0.95	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	B	840	22	69,73,73	0.96	3 (4%)	82,113,113	0.93	5 (6%)
14	CLA	A	820	1	69,73,73	0.96	4 (5%)	82,113,113	1.18	6 (7%)
17	BCR	F	202	-	41,41,41	0.33	0	56,56,56	0.94	1 (1%)
14	CLA	B	841	2	69,73,73	0.96	4 (5%)	82,113,113	1.14	6 (7%)
14	CLA	A	808	1	69,73,73	0.95	4 (5%)	82,113,113	1.01	4 (4%)
14	CLA	B	814	2	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	B	820	22	69,73,73	0.98	6 (8%)	82,113,113	0.94	2 (2%)
14	CLA	B	813	2	59,63,73	1.04	5 (8%)	70,101,113	0.99	3 (4%)
14	CLA	B	823	2	49,53,73	1.14	4 (8%)	58,89,113	0.99	3 (5%)
14	CLA	B	835	22	49,53,73	1.15	4 (8%)	58,89,113	1.22	3 (5%)
14	CLA	J	1101	1	69,73,73	0.96	3 (4%)	82,113,113	0.90	1 (1%)
14	CLA	A	833	1	64,68,73	1.00	4 (6%)	76,107,113	0.97	3 (3%)
17	BCR	I	102	-	41,41,41	0.37	0	56,56,56	0.84	1 (1%)
21	ECH	M	102	-	42,42,42	0.39	0	55,58,58	0.70	0
14	CLA	A	822	22	69,73,73	0.97	3 (4%)	82,113,113	0.94	4 (4%)
14	CLA	B	822	2	69,73,73	0.97	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	A	806	1	69,73,73	0.99	4 (5%)	82,113,113	1.14	7 (8%)
14	CLA	B	836	22	50,54,73	1.12	5 (10%)	59,90,113	0.97	1 (1%)
18	LMG	B	802	-	50,50,55	0.59	0	58,58,63	0.64	0
14	CLA	A	827	22	64,68,73	1.01	3 (4%)	76,107,113	0.96	2 (2%)
14	CLA	A	803	-	69,73,73	0.95	4 (5%)	82,113,113	1.01	3 (3%)
14	CLA	B	808	2	69,73,73	0.97	5 (7%)	82,113,113	1.21	5 (6%)
12	LHG	M	101	-	39,39,48	0.57	0	42,45,54	0.55	0
19	LMT	A	858	-	36,36,36	0.58	0	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	A	848	-	41,41,41	0.34	0	56,56,56	0.54	0
14	CLA	A	815	1	59,63,73	1.04	4 (6%)	70,101,113	1.02	4 (5%)
14	CLA	B	801	22	69,73,73	0.95	4 (5%)	82,113,113	1.04	5 (6%)
14	CLA	B	809	2	69,73,73	0.95	3 (4%)	82,113,113	1.06	4 (4%)
14	CLA	B	828	2	69,73,73	0.96	4 (5%)	82,113,113	1.01	5 (6%)
14	CLA	B	834	22	59,63,73	1.03	4 (6%)	70,101,113	1.05	6 (8%)
14	CLA	A	810	1	54,58,73	1.10	4 (7%)	64,95,113	1.03	2 (3%)
14	CLA	A	821	1	69,73,73	0.98	4 (5%)	82,113,113	0.98	4 (4%)
19	LMT	A	854	-	36,36,36	0.64	0	47,47,47	0.66	0
14	CLA	A	859	-	69,73,73	0.97	5 (7%)	82,113,113	1.10	5 (6%)
14	CLA	B	839	2	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
14	CLA	F	203	22	49,53,73	1.14	3 (6%)	58,89,113	1.01	4 (6%)
14	CLA	A	807	1	69,73,73	0.99	4 (5%)	82,113,113	0.95	2 (2%)
14	CLA	A	840	1	69,73,73	0.96	3 (4%)	82,113,113	1.13	5 (6%)
14	CLA	B	829	-	69,73,73	0.96	4 (5%)	82,113,113	1.00	4 (4%)
14	CLA	B	826	22	69,73,73	0.97	4 (5%)	82,113,113	0.99	3 (3%)
14	CLA	A	817	22	50,54,73	1.12	5 (10%)	59,90,113	1.09	6 (10%)
14	CLA	A	828	1	69,73,73	0.96	4 (5%)	82,113,113	0.99	4 (4%)
14	CLA	A	814	1	69,73,73	0.97	5 (7%)	82,113,113	0.98	5 (6%)
14	CLA	A	835	1	69,73,73	0.96	3 (4%)	82,113,113	1.02	7 (8%)
17	BCR	B	845	-	41,41,41	0.33	0	56,56,56	0.69	0
14	CLA	B	810	2	69,73,73	0.96	3 (4%)	82,113,113	0.96	3 (3%)
18	LMG	B	851	-	38,38,55	0.59	0	46,46,63	0.61	0
14	CLA	A	838	1	55,59,73	1.07	3 (5%)	64,96,113	0.98	2 (3%)
14	CLA	B	824	2	57,61,73	1.06	4 (7%)	67,98,113	1.17	4 (5%)
14	CLA	K	4004	22	69,73,73	0.97	4 (5%)	82,113,113	1.01	2 (2%)
17	BCR	K	4001	-	41,41,41	0.35	0	56,56,56	0.83	2 (3%)
19	LMT	F	206	-	36,36,36	0.57	0	47,47,47	0.90	2 (4%)
17	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
14	CLA	B	815	2	69,73,73	0.94	3 (4%)	82,113,113	0.97	5 (6%)
13	CL0	A	802	1	69,73,73	0.98	6 (8%)	82,113,113	1.01	4 (4%)
14	CLA	A	805	1	69,73,73	0.96	5 (7%)	82,113,113	1.00	5 (6%)
14	CLA	A	837	1	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
14	CLA	A	841	1	69,73,73	0.95	4 (5%)	82,113,113	1.01	6 (7%)
17	BCR	F	205	-	41,41,41	0.31	0	56,56,56	0.56	0
14	CLA	F	204	6	50,54,73	1.12	4 (8%)	59,90,113	0.96	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	F	201	2	69,73,73	0.97	3 (4%)	82,113,113	1.00	2 (2%)
17	BCR	J	1105	-	41,41,41	0.31	0	56,56,56	0.61	0
14	CLA	A	845	12	50,54,73	1.11	3 (6%)	59,90,113	0.98	2 (3%)
17	BCR	B	852	-	41,41,41	0.31	0	56,56,56	0.55	1 (1%)
14	CLA	B	842	12	50,54,73	1.12	4 (8%)	59,90,113	1.00	3 (5%)
17	BCR	L	206	-	41,41,41	0.34	0	56,56,56	0.74	1 (1%)
21	ECH	I	103	-	42,42,42	0.42	0	55,58,58	0.58	0
14	CLA	B	804	2	69,73,73	0.98	3 (4%)	82,113,113	0.90	2 (2%)
16	SF4	A	847	1,2	0,12,12	-	-	-		
14	CLA	B	805	2	69,73,73	0.97	3 (4%)	82,113,113	0.96	4 (4%)
14	CLA	A	832	1	69,73,73	0.98	6 (8%)	82,113,113	0.98	4 (4%)
14	CLA	B	812	2	69,73,73	0.96	4 (5%)	82,113,113	1.04	3 (3%)
14	CLA	L	204	-	69,73,73	0.96	4 (5%)	82,113,113	1.00	5 (6%)
17	BCR	B	849	-	41,41,41	0.35	0	56,56,56	0.79	1 (1%)
17	BCR	A	852	-	41,41,41	0.32	0	56,56,56	0.62	1 (1%)
12	LHG	A	855	14	48,48,48	0.56	0	51,54,54	0.51	0
14	CLA	A	830	1	69,73,73	1.01	5 (7%)	82,113,113	1.05	7 (8%)
12	LHG	A	801	-	47,47,48	0.53	0	50,53,54	0.59	0
17	BCR	B	847	-	30,30,41	0.45	0	39,39,56	0.68	0
14	CLA	A	813	1	58,62,73	1.05	5 (8%)	68,99,113	0.99	2 (2%)
17	BCR	B	848	-	41,41,41	0.34	0	56,56,56	0.82	2 (3%)
14	CLA	B	806	2	69,73,73	0.95	3 (4%)	82,113,113	1.03	5 (6%)
14	CLA	B	811	2	69,73,73	0.96	4 (5%)	82,113,113	1.02	1 (1%)
14	CLA	A	836	1	69,73,73	0.95	5 (7%)	82,113,113	1.01	4 (4%)
14	CLA	B	825	22	69,73,73	0.99	4 (5%)	82,113,113	1.16	5 (6%)
14	CLA	B	807	2	69,73,73	0.98	3 (4%)	82,113,113	0.96	3 (3%)
17	BCR	B	844	-	41,41,41	0.32	0	56,56,56	0.62	0
14	CLA	J	1102	8	49,53,73	1.15	5 (10%)	58,89,113	0.97	2 (3%)
16	SF4	C	101	3	0,12,12	-	-	-		
14	CLA	B	819	2	69,73,73	0.95	4 (5%)	82,113,113	1.02	5 (6%)
18	LMG	A	853	-	46,46,55	0.58	0	54,54,63	0.68	0
14	CLA	A	824	1	55,59,73	1.07	4 (7%)	64,96,113	1.03	4 (6%)
14	CLA	A	804	22	69,73,73	0.97	3 (4%)	82,113,113	0.94	3 (3%)
12	LHG	B	850	14	37,37,48	0.59	0	40,43,54	0.57	0
17	BCR	A	851	-	41,41,41	0.34	0	56,56,56	0.71	1 (1%)
14	CLA	A	812	1	69,73,73	0.96	3 (4%)	82,113,113	0.94	2 (2%)
14	CLA	A	839	1	69,73,73	0.95	4 (5%)	82,113,113	0.99	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	830	2	69,73,73	0.97	5 (7%)	82,113,113	0.95	5 (6%)
17	BCR	L	205	-	41,41,41	0.33	0	56,56,56	0.56	0
14	CLA	A	809	1	69,73,73	0.95	4 (5%)	82,113,113	1.17	4 (4%)
14	CLA	A	818	1	69,73,73	0.96	4 (5%)	82,113,113	1.08	5 (6%)
14	CLA	B	837	2	54,58,73	1.10	4 (7%)	64,95,113	0.99	3 (4%)
14	CLA	A	826	22	69,73,73	0.97	4 (5%)	82,113,113	1.01	2 (2%)
14	CLA	B	833	2	69,73,73	0.96	5 (7%)	82,113,113	0.98	4 (4%)
19	LMT	A	857	-	36,36,36	0.55	0	47,47,47	0.78	1 (2%)
19	LMT	F	207	-	36,36,36	0.57	0	47,47,47	0.71	0
14	CLA	A	831	1	69,73,73	0.95	3 (4%)	82,113,113	0.97	2 (2%)
14	CLA	A	842	22	69,73,73	0.98	3 (4%)	82,113,113	0.98	3 (3%)
14	CLA	B	831	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	4 (4%)
17	BCR	K	4005	-	41,41,41	0.30	0	56,56,56	0.53	0
14	CLA	L	203	10	69,73,73	0.95	4 (5%)	82,113,113	1.00	2 (2%)
14	CLA	A	823	1	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	A	829	1	69,73,73	0.97	5 (7%)	82,113,113	1.04	6 (7%)
14	CLA	B	816	2	64,68,73	0.99	3 (4%)	76,107,113	1.11	4 (5%)
19	LMT	A	856	-	36,36,36	0.57	0	47,47,47	0.63	0
15	PQN	A	846	-	34,34,34	0.46	0	43,45,45	0.66	1 (2%)

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
14	CLA	B	821	2	-	9/39/115/115	-
14	CLA	K	4002	9	-	3/15/91/115	-
14	CLA	A	843	1	-	8/39/115/115	-
17	BCR	A	850	-	-	4/29/63/63	0/2/2/2
14	CLA	B	817	2	-	7/33/109/115	-
14	CLA	L	202	10	-	8/39/115/115	-
21	ECH	B	846	-	-	6/29/66/66	0/2/2/2
14	CLA	B	827	2	-	6/39/115/115	-
14	CLA	A	816	1	-	0/15/91/115	-
14	CLA	A	811	1	-	4/15/91/115	-
14	CLA	B	818	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	B	843	-	-	4/23/43/43	0/2/2/2
17	BCR	J	1104	-	-	7/29/63/63	0/2/2/2
14	CLA	J	1103	8	-	7/21/97/115	-
14	CLA	B	832	2	-	2/27/103/115	-
14	CLA	A	834	1	-	5/39/115/115	-
14	CLA	B	838	2	-	10/39/115/115	-
14	CLA	A	825	1	-	12/39/115/115	-
14	CLA	A	844	22	-	15/39/115/115	-
14	CLA	K	4003	9	-	7/15/91/115	-
18	LMG	I	101	-	-	8/33/53/70	0/1/1/1
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	819	1	-	9/39/115/115	-
14	CLA	B	840	22	-	3/39/115/115	-
14	CLA	A	820	1	-	6/39/115/115	-
17	BCR	F	202	-	-	4/29/63/63	0/2/2/2
14	CLA	B	841	2	-	12/39/115/115	-
14	CLA	A	808	1	-	9/39/115/115	-
14	CLA	B	814	2	-	9/39/115/115	-
14	CLA	B	820	22	-	9/39/115/115	-
14	CLA	B	813	2	-	9/27/103/115	-
14	CLA	B	823	2	-	3/15/91/115	-
14	CLA	B	835	22	-	1/15/91/115	-
14	CLA	J	1101	1	-	2/39/115/115	-
14	CLA	A	833	1	-	2/33/109/115	-
17	BCR	I	102	-	-	5/29/63/63	0/2/2/2
21	ECH	M	102	-	-	8/29/66/66	0/2/2/2
14	CLA	A	822	22	-	6/39/115/115	-
14	CLA	B	822	2	-	14/39/115/115	-
14	CLA	A	806	1	-	14/39/115/115	-
14	CLA	B	836	22	-	3/17/93/115	-
18	LMG	B	802	-	-	12/45/65/70	0/1/1/1
14	CLA	A	827	22	-	2/33/109/115	-
14	CLA	A	803	-	-	4/39/115/115	-
14	CLA	B	808	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LHG	M	101	-	-	9/44/44/53	-
19	LMT	A	858	-	-	7/21/61/61	0/2/2/2
17	BCR	A	848	-	-	2/29/63/63	0/2/2/2
14	CLA	A	815	1	-	6/27/103/115	-
14	CLA	B	801	22	-	7/39/115/115	-
14	CLA	B	809	2	-	7/39/115/115	-
14	CLA	B	828	2	-	7/39/115/115	-
14	CLA	B	834	22	-	6/27/103/115	-
14	CLA	A	810	1	-	4/21/97/115	-
14	CLA	A	821	1	-	5/39/115/115	-
19	LMT	A	854	-	-	5/21/61/61	0/2/2/2
14	CLA	A	859	-	-	5/39/115/115	-
14	CLA	B	839	2	-	8/39/115/115	-
14	CLA	F	203	22	-	5/15/91/115	-
14	CLA	A	807	1	-	13/39/115/115	-
14	CLA	A	840	1	-	8/39/115/115	-
14	CLA	B	829	-	-	2/39/115/115	-
14	CLA	B	826	22	-	9/39/115/115	-
14	CLA	A	817	22	-	7/17/93/115	-
14	CLA	A	828	1	-	6/39/115/115	-
14	CLA	A	814	1	-	11/39/115/115	-
14	CLA	A	835	1	-	5/39/115/115	-
17	BCR	B	845	-	-	2/29/63/63	0/2/2/2
14	CLA	B	810	2	-	7/39/115/115	-
18	LMG	B	851	-	-	10/33/53/70	0/1/1/1
14	CLA	A	838	1	-	2/23/99/115	-
14	CLA	B	824	2	-	5/25/101/115	-
14	CLA	K	4004	22	-	11/39/115/115	-
17	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
19	LMT	F	206	-	-	4/21/61/61	0/2/2/2
17	BCR	A	849	-	-	6/29/63/63	0/2/2/2
14	CLA	B	815	2	-	6/39/115/115	-
13	CL0	A	802	1	-	4/39/115/115	-
14	CLA	A	805	1	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	837	1	-	7/39/115/115	-
14	CLA	A	841	1	-	5/39/115/115	-
17	BCR	F	205	-	-	2/29/63/63	0/2/2/2
14	CLA	F	204	6	-	3/17/93/115	-
14	CLA	F	201	2	-	8/39/115/115	-
17	BCR	J	1105	-	-	5/29/63/63	0/2/2/2
14	CLA	A	845	12	-	4/17/93/115	-
17	BCR	B	852	-	-	4/29/63/63	0/2/2/2
14	CLA	B	842	12	-	1/17/93/115	-
17	BCR	L	206	-	-	7/29/63/63	0/2/2/2
21	ECH	I	103	-	-	5/29/66/66	0/2/2/2
14	CLA	B	804	2	-	4/39/115/115	-
16	SF4	A	847	1,2	-	-	0/6/5/5
14	CLA	B	805	2	-	3/39/115/115	-
14	CLA	A	832	1	-	7/39/115/115	-
14	CLA	B	812	2	-	11/39/115/115	-
14	CLA	L	204	-	-	9/39/115/115	-
17	BCR	B	849	-	-	1/29/63/63	0/2/2/2
17	BCR	A	852	-	-	11/29/63/63	0/2/2/2
12	LHG	A	855	14	-	8/53/53/53	-
14	CLA	A	830	1	-	7/39/115/115	-
12	LHG	A	801	-	-	15/52/52/53	-
17	BCR	B	847	-	-	1/24/41/63	0/1/1/2
14	CLA	A	813	1	-	6/26/102/115	-
17	BCR	B	848	-	-	2/29/63/63	0/2/2/2
14	CLA	B	806	2	-	8/39/115/115	-
14	CLA	B	811	2	-	3/39/115/115	-
14	CLA	A	836	1	-	4/39/115/115	-
14	CLA	B	825	22	-	18/39/115/115	-
14	CLA	B	807	2	-	4/39/115/115	-
17	BCR	B	844	-	-	4/29/63/63	0/2/2/2
14	CLA	J	1102	8	-	4/15/91/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	819	2	-	9/39/115/115	-
18	LMG	A	853	-	-	16/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	824	1	-	4/23/99/115	-
14	CLA	A	804	22	-	7/39/115/115	-
12	LHG	B	850	14	-	4/42/42/53	-
17	BCR	A	851	-	-	4/29/63/63	0/2/2/2
14	CLA	A	812	1	-	17/39/115/115	-
14	CLA	A	839	1	-	7/39/115/115	-
14	CLA	B	830	2	-	12/39/115/115	-
17	BCR	L	205	-	-	6/29/63/63	0/2/2/2
14	CLA	A	809	1	-	5/39/115/115	-
14	CLA	A	818	1	-	8/39/115/115	-
14	CLA	B	837	2	-	1/21/97/115	-
14	CLA	A	826	22	-	16/39/115/115	-
14	CLA	B	833	2	-	8/39/115/115	-
19	LMT	A	857	-	-	3/21/61/61	0/2/2/2
19	LMT	F	207	-	-	10/21/61/61	0/2/2/2
14	CLA	A	831	1	-	12/39/115/115	-
14	CLA	A	842	22	-	6/39/115/115	-
14	CLA	B	831	2	-	6/39/115/115	-
17	BCR	K	4005	-	-	3/29/63/63	0/2/2/2
14	CLA	L	203	10	-	6/39/115/115	-
14	CLA	A	823	1	-	14/39/115/115	-
14	CLA	A	829	1	-	12/39/115/115	-
14	CLA	B	816	2	-	13/33/109/115	-
19	LMT	A	856	-	-	5/21/61/61	0/2/2/2
15	PQN	A	846	-	-	0/23/43/43	0/2/2/2

All (386) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C1D-ND	3.13	1.42	1.37
14	J	1103	CLA	C1D-ND	3.13	1.42	1.37
14	K	4002	CLA	C1D-ND	3.12	1.42	1.37
14	A	838	CLA	C1D-ND	3.11	1.41	1.37
14	K	4003	CLA	C1D-ND	3.11	1.41	1.37
14	B	842	CLA	C1D-ND	3.10	1.41	1.37
14	A	812	CLA	C1D-ND	3.10	1.41	1.37
14	F	203	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	806	CLA	C1D-ND	3.08	1.41	1.37
14	J	1102	CLA	C1D-ND	3.08	1.41	1.37
14	F	204	CLA	C1D-ND	3.07	1.41	1.37
14	B	837	CLA	C1D-ND	3.06	1.41	1.37
14	A	813	CLA	C1D-ND	3.05	1.41	1.37
14	A	826	CLA	C1D-ND	3.05	1.41	1.37
14	B	804	CLA	C1D-ND	3.04	1.41	1.37
14	A	827	CLA	C1D-ND	3.04	1.41	1.37
14	A	829	CLA	C1D-ND	3.03	1.41	1.37
14	B	820	CLA	C1D-ND	3.03	1.41	1.37
14	B	807	CLA	C1D-ND	3.03	1.41	1.37
14	F	201	CLA	C1D-ND	3.03	1.41	1.37
14	A	821	CLA	C1D-ND	3.03	1.41	1.37
14	A	835	CLA	C1D-ND	3.03	1.41	1.37
14	B	835	CLA	C1D-ND	3.03	1.41	1.37
14	A	811	CLA	C1D-ND	3.02	1.41	1.37
14	A	815	CLA	C1D-ND	3.02	1.41	1.37
14	A	842	CLA	C1D-ND	3.01	1.41	1.37
14	B	832	CLA	C1D-ND	3.01	1.41	1.37
14	B	816	CLA	C1D-ND	3.01	1.41	1.37
14	A	840	CLA	C1D-ND	3.00	1.41	1.37
14	B	809	CLA	C1D-ND	2.99	1.41	1.37
14	B	805	CLA	C1D-ND	2.99	1.41	1.37
14	J	1101	CLA	C1D-ND	2.98	1.41	1.37
14	B	822	CLA	C1D-ND	2.98	1.41	1.37
14	B	838	CLA	C1D-ND	2.98	1.41	1.37
14	A	807	CLA	C1D-ND	2.98	1.41	1.37
14	A	824	CLA	C1D-ND	2.98	1.41	1.37
14	A	809	CLA	C1D-ND	2.96	1.41	1.37
14	A	820	CLA	C1D-ND	2.96	1.41	1.37
14	B	817	CLA	C1D-ND	2.95	1.41	1.37
14	K	4004	CLA	C1D-ND	2.95	1.41	1.37
14	B	827	CLA	C1D-ND	2.95	1.41	1.37
14	A	831	CLA	C1D-ND	2.94	1.41	1.37
14	A	817	CLA	C1D-ND	2.94	1.41	1.37
14	B	811	CLA	C1D-ND	2.94	1.41	1.37
14	A	823	CLA	C1D-ND	2.94	1.41	1.37
14	B	821	CLA	C1D-ND	2.94	1.41	1.37
14	A	822	CLA	C1D-ND	2.93	1.41	1.37
14	B	839	CLA	C1D-ND	2.93	1.41	1.37
14	A	830	CLA	C1D-ND	2.93	1.41	1.37
14	B	831	CLA	C1D-ND	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	C1D-ND	2.92	1.41	1.37
14	B	824	CLA	C1D-ND	2.92	1.41	1.37
14	B	806	CLA	C1D-ND	2.91	1.41	1.37
14	B	828	CLA	C1D-ND	2.91	1.41	1.37
14	B	801	CLA	C1D-ND	2.90	1.41	1.37
14	B	834	CLA	C1D-ND	2.89	1.41	1.37
14	A	828	CLA	C1D-ND	2.89	1.41	1.37
14	B	812	CLA	C1D-ND	2.88	1.41	1.37
14	A	810	CLA	C1D-ND	2.88	1.41	1.37
14	B	810	CLA	C1D-ND	2.87	1.41	1.37
14	A	843	CLA	C1D-ND	2.87	1.41	1.37
14	L	202	CLA	C1D-ND	2.87	1.41	1.37
14	A	816	CLA	C1D-ND	2.87	1.41	1.37
14	A	825	CLA	C1D-ND	2.87	1.41	1.37
14	A	805	CLA	C1D-ND	2.87	1.41	1.37
14	A	839	CLA	C1D-ND	2.86	1.41	1.37
14	A	804	CLA	C1D-ND	2.86	1.41	1.37
14	B	808	CLA	C1D-ND	2.86	1.41	1.37
14	A	837	CLA	C1D-ND	2.86	1.41	1.37
14	L	204	CLA	C1D-ND	2.86	1.41	1.37
14	B	830	CLA	C1D-ND	2.84	1.41	1.37
14	B	814	CLA	C1D-ND	2.84	1.41	1.37
14	B	813	CLA	C1D-ND	2.84	1.41	1.37
14	B	840	CLA	C1D-ND	2.83	1.41	1.37
14	A	814	CLA	C1D-ND	2.82	1.41	1.37
14	A	859	CLA	C1D-ND	2.82	1.41	1.37
14	B	818	CLA	C1D-ND	2.81	1.41	1.37
14	B	841	CLA	C1D-ND	2.81	1.41	1.37
14	B	829	CLA	C1D-ND	2.81	1.41	1.37
14	A	833	CLA	C1D-ND	2.81	1.41	1.37
14	B	826	CLA	C1D-ND	2.79	1.41	1.37
13	A	802	CL0	C1D-ND	2.79	1.41	1.37
14	A	845	CLA	C1D-ND	2.78	1.41	1.37
14	B	819	CLA	C1D-ND	2.78	1.41	1.37
14	A	834	CLA	C1D-ND	2.78	1.41	1.37
14	L	203	CLA	C1D-ND	2.78	1.41	1.37
14	B	823	CLA	C1D-ND	2.76	1.41	1.37
14	A	844	CLA	C1D-ND	2.75	1.41	1.37
14	A	819	CLA	C1D-ND	2.72	1.41	1.37
14	B	833	CLA	C1D-ND	2.72	1.41	1.37
14	A	836	CLA	C1D-ND	2.72	1.41	1.37
14	A	841	CLA	C1D-ND	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	815	CLA	C1D-ND	2.70	1.41	1.37
14	A	818	CLA	C1D-ND	2.66	1.41	1.37
14	A	832	CLA	C1D-ND	2.66	1.41	1.37
14	B	825	CLA	C1D-ND	2.61	1.41	1.37
14	A	803	CLA	C1D-ND	2.59	1.41	1.37
14	K	4003	CLA	C1B-C2B	2.49	1.49	1.43
14	B	835	CLA	C1B-C2B	2.45	1.48	1.43
14	J	1103	CLA	C3B-C4B	2.45	1.49	1.42
14	B	842	CLA	C1B-C2B	2.44	1.48	1.43
14	A	837	CLA	C3B-C4B	2.43	1.49	1.42
14	B	832	CLA	C1B-C2B	2.41	1.48	1.43
14	A	840	CLA	C3B-C4B	2.41	1.49	1.42
14	J	1103	CLA	C1B-C2B	2.40	1.48	1.43
14	K	4002	CLA	C1B-C2B	2.40	1.48	1.43
13	A	802	CL0	C1B-C2B	2.40	1.48	1.43
14	A	813	CLA	C3B-C4B	2.40	1.49	1.42
14	A	817	CLA	C1B-C2B	2.40	1.48	1.43
14	B	823	CLA	C1B-C2B	2.39	1.48	1.43
14	A	842	CLA	C3B-C4B	2.38	1.49	1.42
14	B	804	CLA	C1B-C2B	2.38	1.48	1.43
14	A	829	CLA	C3B-C4B	2.38	1.49	1.42
14	A	818	CLA	C1B-C2B	2.37	1.48	1.43
14	A	805	CLA	C3B-C4B	2.36	1.49	1.42
14	B	837	CLA	C3B-C4B	2.36	1.49	1.42
14	J	1101	CLA	C1B-C2B	2.35	1.48	1.43
14	J	1102	CLA	C3B-C4B	2.35	1.49	1.42
14	F	201	CLA	C1B-C2B	2.34	1.48	1.43
14	A	814	CLA	C1B-C2B	2.34	1.48	1.43
14	K	4004	CLA	C1B-C2B	2.34	1.48	1.43
14	F	204	CLA	C3B-C4B	2.34	1.49	1.42
14	A	839	CLA	C1B-C2B	2.34	1.48	1.43
14	B	836	CLA	C3B-C4B	2.34	1.49	1.42
14	A	843	CLA	C3B-C4B	2.34	1.49	1.42
14	B	820	CLA	C3B-C4B	2.34	1.49	1.42
14	B	841	CLA	C1B-C2B	2.33	1.48	1.43
14	A	828	CLA	C1B-C2B	2.33	1.48	1.43
14	A	833	CLA	C1B-C2B	2.33	1.48	1.43
14	B	816	CLA	C1B-C2B	2.32	1.48	1.43
14	B	840	CLA	C3B-C4B	2.32	1.49	1.42
14	B	826	CLA	C3B-C4B	2.31	1.49	1.42
14	J	1102	CLA	C1B-C2B	2.31	1.48	1.43
14	B	831	CLA	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	836	CLA	C3B-C4B	2.31	1.49	1.42
14	A	832	CLA	MG-ND	-2.31	2.01	2.05
14	F	203	CLA	C1B-C2B	2.31	1.48	1.43
14	B	829	CLA	C1B-C2B	2.30	1.48	1.43
14	B	822	CLA	C1B-C2B	2.30	1.48	1.43
14	B	807	CLA	C1B-C2B	2.30	1.48	1.43
14	A	823	CLA	C1B-C2B	2.30	1.48	1.43
14	L	203	CLA	C1B-C2B	2.29	1.48	1.43
14	A	815	CLA	C3B-C4B	2.29	1.49	1.42
14	B	834	CLA	C1B-C2B	2.29	1.48	1.43
14	A	827	CLA	C1B-C2B	2.29	1.48	1.43
14	A	845	CLA	C1B-C2B	2.29	1.48	1.43
14	B	827	CLA	C1B-C2B	2.29	1.48	1.43
14	B	841	CLA	C3B-C4B	2.29	1.49	1.42
14	A	812	CLA	C1B-C2B	2.28	1.48	1.43
14	A	830	CLA	MG-ND	-2.28	2.01	2.05
14	A	820	CLA	C3B-C4B	2.28	1.49	1.42
14	A	830	CLA	C3B-C4B	2.28	1.49	1.42
14	B	824	CLA	C1B-C2B	2.28	1.48	1.43
14	B	839	CLA	C1B-C2B	2.28	1.48	1.43
14	A	811	CLA	C1B-C2B	2.28	1.48	1.43
14	B	821	CLA	C1B-C2B	2.28	1.48	1.43
14	A	821	CLA	C1B-C2B	2.28	1.48	1.43
14	L	204	CLA	C3B-C4B	2.27	1.49	1.42
14	B	828	CLA	C1B-C2B	2.27	1.48	1.43
14	B	817	CLA	C1B-C2B	2.27	1.48	1.43
14	A	814	CLA	C3B-C4B	2.27	1.49	1.42
14	B	813	CLA	MG-ND	-2.27	2.01	2.05
14	A	816	CLA	C1B-C2B	2.26	1.48	1.43
14	B	830	CLA	C3B-C4B	2.26	1.49	1.42
14	A	824	CLA	C1B-C2B	2.26	1.48	1.43
14	K	4003	CLA	C3B-C4B	2.26	1.49	1.42
14	A	841	CLA	C1B-C2B	2.26	1.48	1.43
14	A	825	CLA	C1B-C2B	2.26	1.48	1.43
14	B	810	CLA	C3B-C4B	2.26	1.49	1.42
14	B	809	CLA	C1B-C2B	2.26	1.48	1.43
14	A	838	CLA	C3B-C4B	2.25	1.49	1.42
14	B	814	CLA	C1B-C2B	2.25	1.48	1.43
14	B	801	CLA	C1B-C2B	2.25	1.48	1.43
14	B	811	CLA	C1B-C2B	2.25	1.48	1.43
14	A	826	CLA	C1B-C2B	2.25	1.48	1.43
14	B	805	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	804	CLA	C1B-C2B	2.24	1.48	1.43
14	A	834	CLA	C1B-C2B	2.24	1.48	1.43
14	B	838	CLA	C1B-C2B	2.24	1.48	1.43
14	B	805	CLA	C1B-C2B	2.24	1.48	1.43
14	B	833	CLA	C1B-C2B	2.24	1.48	1.43
14	A	809	CLA	C1B-C2B	2.24	1.48	1.43
14	F	204	CLA	C1B-C2B	2.24	1.48	1.43
14	A	844	CLA	C1B-C2B	2.23	1.48	1.43
14	A	822	CLA	C3B-C4B	2.23	1.49	1.42
14	L	204	CLA	C1B-C2B	2.23	1.48	1.43
14	A	859	CLA	C1B-C2B	2.23	1.48	1.43
14	A	809	CLA	C3B-C4B	2.23	1.49	1.42
14	A	831	CLA	C3B-C4B	2.22	1.49	1.42
14	A	803	CLA	C3B-C4B	2.22	1.49	1.42
14	A	821	CLA	C3B-C4B	2.22	1.49	1.42
14	K	4002	CLA	C3B-C4B	2.22	1.49	1.42
14	A	829	CLA	C1B-C2B	2.22	1.48	1.43
14	F	201	CLA	C3B-C4B	2.21	1.49	1.42
14	A	828	CLA	C3B-C4B	2.21	1.49	1.42
14	A	808	CLA	C1B-C2B	2.21	1.48	1.43
14	L	202	CLA	C1B-C2B	2.21	1.48	1.43
14	B	823	CLA	MG-ND	-2.21	2.01	2.05
14	A	838	CLA	C1B-C2B	2.21	1.48	1.43
14	B	826	CLA	C1B-C2B	2.21	1.48	1.43
14	B	825	CLA	C3B-C4B	2.21	1.49	1.42
14	B	806	CLA	C1B-C2B	2.21	1.48	1.43
14	A	835	CLA	C1B-C2B	2.21	1.48	1.43
14	B	808	CLA	MG-ND	-2.21	2.01	2.05
14	B	806	CLA	C3B-C4B	2.21	1.49	1.42
14	B	818	CLA	C1B-C2B	2.21	1.48	1.43
14	A	811	CLA	C3B-C4B	2.20	1.49	1.42
14	A	859	CLA	MG-ND	-2.20	2.01	2.05
14	A	859	CLA	C3B-C4B	2.20	1.49	1.42
14	A	843	CLA	C1B-C2B	2.20	1.48	1.43
14	K	4004	CLA	C3B-C4B	2.20	1.49	1.42
14	A	818	CLA	MG-ND	-2.20	2.01	2.05
14	B	808	CLA	C1B-C2B	2.20	1.48	1.43
14	A	810	CLA	C3B-C4B	2.20	1.49	1.42
14	A	803	CLA	MG-ND	-2.20	2.01	2.05
14	B	812	CLA	C3B-C4B	2.20	1.49	1.42
14	A	842	CLA	C1B-C2B	2.20	1.48	1.43
14	B	815	CLA	C1B-C2B	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	810	CLA	MG-ND	-2.19	2.01	2.05
14	B	818	CLA	MG-ND	-2.19	2.01	2.05
14	A	841	CLA	C3B-C4B	2.19	1.49	1.42
14	A	810	CLA	C1B-C2B	2.19	1.48	1.43
14	B	839	CLA	C3B-C4B	2.19	1.49	1.42
14	A	835	CLA	C3B-C4B	2.19	1.49	1.42
14	A	830	CLA	C1B-C2B	2.19	1.48	1.43
14	A	806	CLA	C3B-C4B	2.19	1.49	1.42
14	B	836	CLA	C1B-C2B	2.18	1.48	1.43
14	B	830	CLA	C1B-C2B	2.18	1.48	1.43
14	A	844	CLA	C3B-C4B	2.18	1.49	1.42
14	J	1101	CLA	C3B-C4B	2.18	1.49	1.42
14	A	808	CLA	C3B-C4B	2.18	1.49	1.42
14	B	819	CLA	MG-ND	-2.18	2.01	2.05
14	B	822	CLA	C3B-C4B	2.17	1.49	1.42
14	B	809	CLA	C3B-C4B	2.17	1.49	1.42
14	A	813	CLA	C1B-C2B	2.17	1.48	1.43
14	B	824	CLA	C3B-C4B	2.17	1.49	1.42
14	A	831	CLA	C1B-C2B	2.17	1.48	1.43
14	B	833	CLA	MG-ND	-2.17	2.01	2.05
14	A	805	CLA	C1B-C2B	2.16	1.48	1.43
14	B	814	CLA	C3B-C4B	2.16	1.49	1.42
14	A	807	CLA	MG-ND	-2.16	2.01	2.05
14	A	804	CLA	C3B-C4B	2.16	1.49	1.42
14	A	815	CLA	C1B-C2B	2.16	1.48	1.43
14	A	832	CLA	C1B-C2B	2.16	1.48	1.43
14	A	832	CLA	C4B-NB	-2.16	1.35	1.37
14	A	807	CLA	C1B-C2B	2.16	1.48	1.43
14	B	821	CLA	C3B-C4B	2.16	1.49	1.42
14	B	817	CLA	C3B-C4B	2.16	1.49	1.42
14	A	816	CLA	C3B-C4B	2.15	1.49	1.42
14	K	4004	CLA	MG-ND	-2.15	2.01	2.05
14	B	811	CLA	MG-ND	-2.15	2.01	2.05
14	B	812	CLA	C1B-C2B	2.15	1.48	1.43
14	L	203	CLA	C3B-C4B	2.15	1.49	1.42
14	A	833	CLA	C3B-C4B	2.15	1.49	1.42
14	A	844	CLA	MG-ND	-2.15	2.01	2.05
14	B	842	CLA	MG-ND	-2.15	2.01	2.05
14	B	839	CLA	MG-ND	-2.14	2.01	2.05
14	A	837	CLA	MG-ND	-2.14	2.01	2.05
14	J	1103	CLA	CHC-C1C	2.14	1.42	1.38
14	B	837	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	834	CLA	C3B-C4B	2.13	1.49	1.42
14	A	824	CLA	C3B-C4B	2.13	1.49	1.42
14	B	816	CLA	C3B-C4B	2.13	1.49	1.42
14	A	829	CLA	MG-ND	-2.13	2.01	2.05
14	B	833	CLA	C3B-C4B	2.13	1.48	1.42
14	A	805	CLA	CHC-C1C	2.13	1.42	1.38
14	B	838	CLA	C3B-C4B	2.13	1.48	1.42
14	A	826	CLA	C3B-C4B	2.12	1.48	1.42
14	B	819	CLA	C3B-C4B	2.12	1.48	1.42
14	B	807	CLA	MG-ND	-2.12	2.01	2.05
14	B	828	CLA	C3B-C4B	2.12	1.48	1.42
14	F	203	CLA	C3B-C4B	2.12	1.48	1.42
14	A	841	CLA	MG-ND	-2.12	2.01	2.05
14	L	203	CLA	MG-ND	-2.12	2.01	2.05
14	A	803	CLA	C1B-C2B	2.12	1.48	1.43
14	B	815	CLA	C3B-C4B	2.12	1.48	1.42
14	A	806	CLA	C1B-C2B	2.12	1.48	1.43
14	L	202	CLA	C3B-C4B	2.12	1.48	1.42
14	A	807	CLA	C3B-C4B	2.11	1.48	1.42
14	A	814	CLA	MG-ND	-2.11	2.01	2.05
14	B	840	CLA	C1B-C2B	2.11	1.48	1.43
14	A	817	CLA	MG-ND	-2.11	2.01	2.05
14	A	833	CLA	MG-ND	-2.11	2.01	2.05
14	B	829	CLA	C3B-C4B	2.11	1.48	1.42
14	B	813	CLA	C1B-C2B	2.11	1.48	1.43
14	B	821	CLA	MG-ND	-2.11	2.01	2.05
13	A	802	CL0	MG-NB	-2.11	2.01	2.05
14	B	819	CLA	C1B-C2B	2.11	1.48	1.43
14	B	831	CLA	MG-ND	-2.11	2.01	2.05
14	A	819	CLA	MG-ND	-2.11	2.01	2.05
14	B	813	CLA	C3B-C4B	2.11	1.48	1.42
14	B	832	CLA	C3B-C4B	2.11	1.48	1.42
14	B	824	CLA	MG-ND	-2.10	2.01	2.05
14	A	822	CLA	C1B-C2B	2.10	1.48	1.43
14	A	823	CLA	C3B-C4B	2.10	1.48	1.42
14	B	834	CLA	C3B-C4B	2.10	1.48	1.42
14	A	812	CLA	C3B-C4B	2.10	1.48	1.42
14	A	819	CLA	C1B-C2B	2.10	1.48	1.43
14	B	827	CLA	C3B-C4B	2.10	1.48	1.42
14	A	806	CLA	MG-ND	-2.10	2.01	2.05
14	B	801	CLA	C3B-C4B	2.10	1.48	1.42
14	A	825	CLA	MG-ND	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	845	CLA	C3B-C4B	2.09	1.48	1.42
14	A	819	CLA	C3B-C4B	2.09	1.48	1.42
14	B	823	CLA	C3B-C4B	2.09	1.48	1.42
14	A	825	CLA	C3B-C4B	2.09	1.48	1.42
14	A	823	CLA	MG-ND	-2.08	2.01	2.05
14	J	1102	CLA	MG-ND	-2.08	2.01	2.05
14	B	831	CLA	C3B-C4B	2.08	1.48	1.42
14	A	829	CLA	CHC-C1C	2.08	1.42	1.38
14	B	827	CLA	MG-ND	-2.08	2.01	2.05
13	A	802	CL0	C4B-NB	-2.08	1.35	1.37
14	B	811	CLA	C3B-C4B	2.08	1.48	1.42
14	B	820	CLA	C1B-C2B	2.08	1.48	1.43
14	A	813	CLA	MG-ND	-2.07	2.01	2.05
14	K	4003	CLA	MG-ND	-2.07	2.01	2.05
14	B	842	CLA	C3B-C4B	2.07	1.48	1.42
14	A	817	CLA	C4B-NB	-2.07	1.35	1.37
14	A	820	CLA	MG-ND	-2.07	2.01	2.05
13	A	802	CL0	CHC-C1C	2.07	1.42	1.38
14	A	811	CLA	MG-ND	-2.07	2.01	2.05
14	F	204	CLA	CHC-C1C	2.06	1.42	1.38
14	B	801	CLA	MG-ND	-2.06	2.01	2.05
14	A	827	CLA	C3B-C4B	2.06	1.48	1.42
14	A	824	CLA	MG-ND	-2.06	2.01	2.05
14	A	821	CLA	MG-ND	-2.06	2.01	2.05
14	B	814	CLA	MG-ND	-2.06	2.01	2.05
14	A	836	CLA	MG-ND	-2.06	2.01	2.05
14	B	825	CLA	MG-ND	-2.06	2.01	2.05
14	B	836	CLA	CHC-C1C	2.06	1.42	1.38
14	A	832	CLA	MG-NB	-2.06	2.01	2.05
14	A	837	CLA	CHC-C1C	2.06	1.42	1.38
14	A	840	CLA	C1B-C2B	2.06	1.48	1.43
14	B	820	CLA	MG-ND	-2.05	2.01	2.05
14	B	822	CLA	MG-ND	-2.05	2.01	2.05
14	A	843	CLA	CHC-C1C	2.05	1.42	1.38
14	A	813	CLA	CHC-C1C	2.05	1.42	1.38
14	A	828	CLA	MG-ND	-2.05	2.01	2.05
14	B	818	CLA	C3B-C4B	2.05	1.48	1.42
14	B	813	CLA	MG-NB	-2.05	2.01	2.05
14	A	826	CLA	MG-ND	-2.04	2.01	2.05
14	B	830	CLA	MG-ND	-2.04	2.01	2.05
14	A	814	CLA	CHC-C1C	2.04	1.42	1.38
14	L	204	CLA	MG-ND	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	808	CLA	C3B-C4B	2.04	1.48	1.42
14	B	834	CLA	MG-ND	-2.04	2.01	2.05
14	A	830	CLA	CHC-C1C	2.04	1.42	1.38
14	B	830	CLA	CHC-C1C	2.04	1.42	1.38
14	A	836	CLA	CHC-C1C	2.04	1.42	1.38
14	B	817	CLA	MG-ND	-2.04	2.01	2.05
14	B	828	CLA	MG-ND	-2.04	2.01	2.05
14	B	810	CLA	C1B-C2B	2.04	1.47	1.43
14	B	804	CLA	MG-ND	-2.03	2.01	2.05
14	J	1103	CLA	MG-ND	-2.03	2.01	2.05
14	A	808	CLA	MG-ND	-2.03	2.01	2.05
14	A	816	CLA	MG-ND	-2.03	2.01	2.05
14	A	859	CLA	C4B-NB	-2.03	1.35	1.37
14	B	820	CLA	CHC-C1C	2.03	1.42	1.38
13	A	802	CL0	C3B-C4B	2.02	1.48	1.42
14	A	805	CLA	MG-ND	-2.02	2.01	2.05
14	B	835	CLA	C3B-C4B	2.02	1.48	1.42
14	A	817	CLA	MG-NB	-2.02	2.01	2.05
14	K	4002	CLA	MG-ND	-2.02	2.01	2.05
14	B	826	CLA	MG-ND	-2.02	2.01	2.05
14	A	839	CLA	MG-ND	-2.02	2.01	2.05
14	B	808	CLA	C4B-NB	-2.02	1.35	1.37
14	A	815	CLA	CHC-C1C	2.02	1.42	1.38
14	A	839	CLA	C4B-NB	-2.02	1.35	1.37
14	B	838	CLA	MG-ND	-2.02	2.01	2.05
14	B	825	CLA	C1B-C2B	2.02	1.47	1.43
14	A	832	CLA	C3B-C4B	2.01	1.48	1.42
14	A	820	CLA	C1B-C2B	2.01	1.47	1.43
14	B	835	CLA	MG-ND	-2.01	2.01	2.05
14	J	1102	CLA	CHC-C1C	2.01	1.42	1.38
14	B	841	CLA	MG-ND	-2.01	2.01	2.05
14	A	811	CLA	CHC-C1C	2.01	1.42	1.38
14	B	829	CLA	MG-ND	-2.01	2.01	2.05
14	A	818	CLA	C3B-C4B	2.01	1.48	1.42
14	B	833	CLA	C4B-NB	-2.01	1.35	1.37
14	B	837	CLA	CHC-C1C	2.01	1.42	1.38
14	A	836	CLA	C1B-C2B	2.01	1.47	1.43
14	B	836	CLA	MG-ND	-2.01	2.01	2.05
14	B	812	CLA	MG-ND	-2.01	2.01	2.05
14	A	809	CLA	MG-ND	-2.00	2.01	2.05
14	K	4003	CLA	CHC-C1C	2.00	1.42	1.38
14	B	820	CLA	MG-NB	-2.00	2.01	2.05

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	809	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	B	835	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	B	825	CLA	C4A-NA-C1A	5.73	109.30	106.68
14	L	202	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	A	859	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	B	824	CLA	C4A-NA-C1A	5.13	109.02	106.68
14	A	840	CLA	C4A-NA-C1A	5.12	109.01	106.68
14	B	816	CLA	C4A-NA-C1A	5.01	108.97	106.68
14	B	808	CLA	C4A-NA-C1A	5.01	108.96	106.68
14	B	841	CLA	C4A-NA-C1A	4.86	108.90	106.68
14	B	809	CLA	C4A-NA-C1A	4.81	108.87	106.68
14	F	201	CLA	C4A-NA-C1A	4.45	108.71	106.68
14	A	811	CLA	C4A-NA-C1A	4.43	108.70	106.68
14	B	812	CLA	C4A-NA-C1A	4.34	108.66	106.68
14	B	817	CLA	C4A-NA-C1A	4.21	108.60	106.68
14	A	843	CLA	C4A-NA-C1A	4.11	108.56	106.68
14	B	831	CLA	C4A-NA-C1A	3.91	108.46	106.68
14	A	806	CLA	C4A-NA-C1A	3.91	108.46	106.68
14	A	820	CLA	C1-C2-C3	-3.89	119.82	126.20
14	B	829	CLA	C4A-NA-C1A	3.79	108.41	106.68
14	B	828	CLA	C4A-NA-C1A	3.70	108.37	106.68
14	K	4003	CLA	C4A-NA-C1A	3.65	108.34	106.68
14	B	811	CLA	C4A-NA-C1A	3.59	108.32	106.68
14	A	816	CLA	C4A-NA-C1A	3.54	108.29	106.68
14	A	833	CLA	C4A-NA-C1A	3.40	108.23	106.68
14	B	806	CLA	C4A-NA-C1A	3.37	108.22	106.68
14	A	808	CLA	C4A-NA-C1A	3.36	108.21	106.68
14	A	818	CLA	C4A-NA-C1A	3.34	108.20	106.68
14	A	815	CLA	C4A-NA-C1A	3.32	108.19	106.68
14	A	844	CLA	C4A-NA-C1A	3.30	108.19	106.68
14	A	821	CLA	C4A-NA-C1A	3.22	108.15	106.68
13	A	802	CL0	C4A-NA-C1A	3.18	108.13	106.68
17	I	102	BCR	C24-C23-C22	-3.17	121.55	126.23
14	A	836	CLA	C4A-NA-C1A	3.11	108.10	106.68
14	A	841	CLA	C1-C2-C3	-3.10	121.12	126.20
14	A	834	CLA	C4A-NA-C1A	3.09	108.09	106.68
14	A	803	CLA	C4A-NA-C1A	3.05	108.07	106.68
14	B	808	CLA	C1-C2-C3	-2.97	121.33	126.20
14	A	839	CLA	C4A-NA-C1A	2.95	108.03	106.68
14	B	815	CLA	C4A-NA-C1A	2.93	108.02	106.68
14	B	832	CLA	C3B-C2B-C1B	-2.86	103.79	107.17
14	A	806	CLA	C1-O2A-CGA	2.86	123.58	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	801	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
14	A	828	CLA	CHD-C1D-ND	-2.85	120.80	124.80
14	A	825	CLA	C3B-C2B-C1B	-2.84	103.82	107.17
14	K	4004	CLA	C1-C2-C3	-2.84	121.55	126.20
14	B	810	CLA	CHD-C1D-ND	-2.81	120.85	124.80
14	A	806	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
14	A	820	CLA	CAA-C2A-C1A	-2.80	102.79	111.97
14	B	839	CLA	CHD-C1D-ND	-2.79	120.88	124.80
14	B	808	CLA	C2A-C1A-CHA	2.78	128.68	123.87
14	A	804	CLA	C3B-C4B-NB	-2.77	108.05	110.53
14	A	807	CLA	C4A-NA-C1A	2.77	107.94	106.68
14	A	807	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
14	A	814	CLA	CHD-C1D-ND	-2.75	120.94	124.80
14	F	203	CLA	C3B-C2B-C1B	-2.72	103.96	107.17
14	A	825	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	818	CLA	C1-C2-C3	-2.70	121.78	126.20
14	A	844	CLA	CHD-C1D-ND	-2.69	121.01	124.80
14	A	843	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	F	206	LMT	C1B-O1B-C4'	2.69	124.34	117.98
14	A	826	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
14	A	835	CLA	C4A-NA-C1A	2.67	107.90	106.68
14	B	826	CLA	CHD-C1D-ND	-2.66	121.06	124.80
15	A	846	PQN	C11-C3-C4	-2.65	115.78	118.58
14	A	831	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
17	A	851	BCR	C24-C23-C22	-2.62	122.36	126.23
14	B	840	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	821	CLA	CHD-C1D-ND	-2.61	121.14	124.80
14	B	805	CLA	CHD-C1D-ND	-2.60	121.15	124.80
14	A	840	CLA	C3B-C4B-NB	-2.59	108.22	110.53
14	A	832	CLA	CHD-C1D-ND	-2.58	121.17	124.80
14	A	835	CLA	C1-C2-C3	-2.58	121.97	126.20
14	B	833	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
14	A	805	CLA	CHD-C1D-ND	-2.56	121.20	124.80
14	B	809	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
14	B	805	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
14	A	812	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
14	A	835	CLA	CHA-C1A-NA	-2.54	120.63	126.39
17	L	206	BCR	C7-C8-C9	-2.54	122.47	126.23
14	B	841	CLA	C5-C3-C2	2.54	126.87	121.17
14	B	832	CLA	C4A-NA-C1A	2.54	107.84	106.68
14	A	832	CLA	C3B-C2B-C1B	-2.54	104.18	107.17
14	F	203	CLA	C3B-C4B-NB	-2.54	108.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	813	CLA	C4A-NA-C1A	2.53	107.83	106.68
14	B	834	CLA	CHD-C1D-ND	-2.53	121.24	124.80
14	J	1103	CLA	C1-C2-C3	-2.52	122.68	126.76
14	A	840	CLA	C3B-C2B-C1B	-2.52	104.20	107.17
15	B	843	PQN	C11-C3-C4	-2.52	115.93	118.58
14	B	816	CLA	C1-C2-C3	-2.51	122.08	126.20
14	B	807	CLA	C3B-C2B-C1B	-2.51	104.22	107.17
14	A	836	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	A	859	CLA	CHD-C1D-ND	-2.49	121.29	124.80
14	A	824	CLA	C4A-NA-C1A	2.49	107.82	106.68
14	B	839	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
14	A	817	CLA	C3B-C4B-NB	-2.48	108.32	110.53
14	A	818	CLA	C3B-C2B-C1B	-2.47	104.26	107.17
14	A	809	CLA	CHA-C1A-NA	-2.47	120.80	126.39
14	A	819	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
14	A	820	CLA	C2A-C3A-C4A	-2.46	97.89	101.87
14	B	817	CLA	CHD-C1D-ND	-2.46	121.33	124.80
14	B	807	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
14	B	830	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	B	841	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
14	A	841	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
14	J	1101	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
14	A	804	CLA	CHD-C1D-ND	-2.45	121.35	124.80
14	B	842	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
14	B	819	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
14	B	825	CLA	C5-C3-C2	2.45	126.66	121.17
14	B	832	CLA	CHD-C1D-ND	-2.44	121.36	124.80
14	A	817	CLA	C3B-C2B-C1B	-2.44	104.29	107.17
14	B	840	CLA	CHD-C1D-ND	-2.43	121.38	124.80
14	A	820	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
14	B	833	CLA	CHD-C1D-ND	-2.43	121.39	124.80
14	A	816	CLA	C3B-C2B-C1B	-2.42	104.31	107.17
14	A	842	CLA	C3B-C4B-NB	-2.42	108.37	110.53
14	B	832	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
17	B	852	BCR	C2-C1-C6	2.42	113.95	110.44
14	A	828	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
14	B	815	CLA	C1-C2-C3	-2.42	122.23	126.20
14	B	828	CLA	CHD-C1D-ND	-2.41	121.40	124.80
17	B	849	BCR	C2-C1-C6	2.41	113.95	110.44
14	A	842	CLA	C3B-C2B-C1B	-2.41	104.33	107.17
14	A	837	CLA	CHD-C1D-ND	-2.41	121.41	124.80
14	A	818	CLA	CHA-C1A-NA	-2.41	120.94	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	827	CLA	C3B-C2B-C1B	-2.41	104.33	107.17
14	A	829	CLA	CHA-C1A-NA	-2.40	120.95	126.39
14	B	831	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	B	831	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
14	A	839	CLA	CMB-C2B-C1B	2.40	129.07	125.42
14	A	845	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	B	814	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
14	A	819	CLA	CHD-C1D-ND	-2.39	121.44	124.80
14	A	823	CLA	C3B-C2B-C1B	-2.37	104.37	107.17
14	B	838	CLA	C3B-C2B-C1B	-2.37	104.37	107.17
14	A	825	CLA	C4A-NA-C1A	2.37	107.76	106.68
14	A	835	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	A	843	CLA	C3B-C4B-NB	-2.37	108.41	110.53
14	A	820	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	B	841	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	A	830	CLA	C2A-C1A-CHA	2.37	127.98	123.87
14	A	836	CLA	CMB-C2B-C1B	2.37	129.02	125.42
14	A	841	CLA	CHD-C1D-ND	-2.36	121.48	124.80
14	F	203	CLA	CHD-C1D-ND	-2.36	121.49	124.80
14	A	829	CLA	C4A-NA-C1A	2.35	107.75	106.68
14	B	823	CLA	CHD-C1D-ND	-2.35	121.49	124.80
14	A	829	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
14	J	1103	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
14	B	808	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
14	B	819	CLA	C3B-C4B-NB	-2.34	108.44	110.53
14	J	1103	CLA	CHD-C1D-ND	-2.34	121.51	124.80
14	A	820	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	A	824	CLA	C1-C2-C3	-2.34	122.37	126.20
14	A	844	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
14	B	834	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
14	B	824	CLA	C3B-C4B-NB	-2.34	108.44	110.53
14	A	840	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	B	827	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	A	805	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	L	204	CLA	C4A-NA-C1A	2.32	107.74	106.68
14	A	823	CLA	C1-C2-C3	-2.32	122.40	126.20
14	B	837	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
14	A	803	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	B	804	CLA	CHD-C1D-ND	-2.31	121.55	124.80
14	B	815	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
14	B	806	CLA	C4-C3-C5	2.31	119.24	115.23
14	A	823	CLA	CHD-C1D-ND	-2.31	121.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	803	CLA	CHD-C1D-ND	-2.31	121.56	124.80
14	A	826	CLA	C4A-NA-C1A	2.31	107.73	106.68
14	A	808	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
14	A	808	CLA	CHD-C1D-ND	-2.30	121.56	124.80
14	A	827	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
14	A	822	CLA	C7-C6-C5	-2.29	107.15	113.26
14	B	830	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	B	836	CLA	CHD-C1D-ND	-2.29	121.58	124.80
14	B	820	CLA	CHD-C1D-ND	-2.29	121.58	124.80
14	K	4002	CLA	CHD-C1D-ND	-2.29	121.58	124.80
14	B	809	CLA	C1-C2-C3	-2.29	122.44	126.20
17	K	4001	BCR	C24-C23-C22	-2.29	122.85	126.23
14	A	821	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
14	B	819	CLA	CAA-CBA-CGA	-2.28	106.73	113.21
14	B	815	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	A	857	LMT	O1B-C4'-C3'	2.28	113.03	107.23
14	B	830	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
14	A	825	CLA	CHD-C1D-ND	-2.27	121.60	124.80
14	B	838	CLA	C3B-C4B-NB	-2.27	108.50	110.53
14	B	837	CLA	CHD-C1D-ND	-2.27	121.60	124.80
19	A	858	LMT	O1B-C4'-C3'	2.26	112.98	107.23
14	B	814	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
14	B	805	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
14	B	822	CLA	CHD-C1D-ND	-2.26	121.62	124.80
14	A	806	CLA	CHD-C1D-ND	-2.26	121.62	124.80
13	A	802	CL0	CHD-C1D-ND	-2.26	121.62	124.80
14	A	811	CLA	C3B-C2B-C1B	-2.25	104.51	107.17
14	B	828	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	A	832	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	L	204	CLA	C1-C2-C3	-2.25	122.51	126.20
14	A	830	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
14	A	815	CLA	CHD-C1D-ND	-2.25	121.64	124.80
14	B	841	CLA	C4-C3-C2	-2.24	117.87	123.63
14	A	830	CLA	C3B-C4B-NB	-2.24	108.53	110.53
14	A	815	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	B	829	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
14	B	818	CLA	C4A-NA-C1A	2.24	107.70	106.68
14	B	817	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
14	B	828	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
14	A	805	CLA	C4D-CHA-C1A	-2.24	118.57	121.24
14	B	804	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
14	A	822	CLA	C3B-C2B-C1B	-2.23	104.53	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	835	CLA	O2A-CGA-O1A	-2.23	117.59	123.33
14	F	201	CLA	CHD-C1D-ND	-2.23	121.66	124.80
14	A	817	CLA	CHA-C1A-NA	-2.23	121.34	126.39
14	L	203	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	B	806	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	A	828	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	J	1103	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	A	843	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
14	B	819	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	F	204	CLA	CHD-C1D-ND	-2.23	121.67	124.80
14	B	812	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	K	4003	CLA	CHD-C1D-ND	-2.22	121.67	124.80
14	A	822	CLA	C3B-C4B-NB	-2.22	108.55	110.53
14	B	818	CLA	C3B-C2B-C1B	-2.22	104.55	107.17
14	B	830	CLA	CHA-C1A-NA	-2.22	121.37	126.39
14	A	815	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
14	A	841	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	A	828	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	A	810	CLA	C4A-NA-C1A	2.21	107.69	106.68
14	A	845	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
14	A	830	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
14	B	839	CLA	C3B-C4B-NB	-2.21	108.56	110.53
14	B	835	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
14	B	831	CLA	C3B-C4B-NB	-2.20	108.56	110.53
14	A	814	CLA	C4-C3-C5	2.20	119.05	115.23
14	L	202	CLA	CHD-C1D-ND	-2.20	121.70	124.80
14	A	831	CLA	CHA-C1A-NA	-2.20	121.41	126.39
14	B	829	CLA	CHD-C1D-ND	-2.20	121.71	124.80
14	A	830	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
14	A	844	CLA	CMB-C2B-C1B	2.20	128.76	125.42
14	B	809	CLA	CMB-C2B-C1B	2.20	128.76	125.42
14	B	821	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
14	B	820	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
14	A	817	CLA	C4A-NA-C1A	2.19	107.68	106.68
14	K	4004	CLA	CHD-C1D-ND	-2.19	121.72	124.80
14	A	812	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	B	818	CLA	C4-C3-C2	-2.18	118.02	123.63
14	B	826	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
14	A	839	CLA	C1C-C2C-C3C	-2.17	104.69	106.98
14	B	816	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
14	J	1103	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
14	A	817	CLA	CHD-C1D-ND	-2.17	121.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	832	CLA	C3B-C4B-NB	-2.17	108.60	110.53
14	B	838	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	L	204	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
14	A	836	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	J	1102	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	L	204	CLA	C1C-C2C-C3C	-2.16	104.71	106.98
14	B	810	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	B	806	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	A	840	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
14	B	807	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	A	810	CLA	CHD-C1D-ND	-2.15	121.77	124.80
14	B	813	CLA	C4A-NA-C1A	2.15	107.66	106.68
14	B	827	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	A	805	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
14	B	825	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	A	822	CLA	CHD-C1D-ND	-2.15	121.78	124.80
14	A	842	CLA	CHD-C1D-ND	-2.14	121.78	124.80
14	B	842	CLA	CHB-C4A-NA	2.14	127.50	124.40
14	B	842	CLA	CHD-C1D-ND	-2.14	121.79	124.80
14	A	805	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	A	833	CLA	CHD-C1D-ND	-2.13	121.80	124.80
14	B	818	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
14	B	829	CLA	C3B-C4B-NB	-2.13	108.63	110.53
14	B	818	CLA	CHD-C1D-ND	-2.13	121.81	124.80
14	B	827	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	A	818	CLA	CHD-C1D-ND	-2.13	121.81	124.80
14	B	832	CLA	C3B-C4B-NB	-2.13	108.63	110.53
14	A	834	CLA	CHA-C1A-NA	-2.13	121.57	126.39
14	B	837	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
14	B	819	CLA	C4-C3-C5	2.12	118.92	115.23
14	A	841	CLA	C4A-NA-C1A	2.12	107.65	106.68
14	A	841	CLA	C3B-C4B-NB	-2.12	108.63	110.53
14	A	809	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
14	B	832	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	B	833	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
14	B	841	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	A	834	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
14	A	843	CLA	C1-C2-C3	-2.11	122.73	126.20
17	A	849	BCR	C29-C30-C25	2.11	113.51	110.44
14	A	824	CLA	CHD-C1D-ND	-2.11	121.83	124.80
14	B	825	CLA	CHD-C1D-ND	-2.11	121.83	124.80
14	A	806	CLA	CAC-C3C-C4C	2.11	127.54	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	813	CLA	CHA-C1A-NA	-2.11	121.62	126.39
14	A	829	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
14	A	835	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	B	816	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
14	B	812	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	A	824	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	A	859	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
14	A	808	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
14	B	801	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	B	825	CLA	C4-C3-C2	-2.10	118.24	123.63
19	F	206	LMT	O1B-C4'-C3'	2.10	112.56	107.23
14	A	838	CLA	C4A-NA-C1A	2.10	107.64	106.68
14	B	806	CLA	C4-C3-C2	-2.09	118.25	123.63
17	F	202	BCR	C12-C13-C14	-2.09	115.72	119.01
14	B	823	CLA	C3B-C4B-NB	-2.09	108.66	110.53
14	B	824	CLA	C1-C2-C3	-2.09	122.77	126.20
14	B	838	CLA	C5-C3-C2	2.09	125.86	121.17
13	A	802	CL0	C3B-C2B-C1B	-2.09	104.71	107.17
14	B	821	CLA	C1-C2-C3	-2.09	122.78	126.20
14	A	814	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
14	B	818	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	B	813	CLA	CMB-C2B-C1B	2.08	128.59	125.42
14	A	806	CLA	C7-C6-C5	-2.08	107.72	113.26
14	A	859	CLA	C3C-C4C-NC	-2.08	107.77	110.43
14	A	837	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	A	830	CLA	C2A-C3A-C4A	-2.08	98.51	101.87
17	B	848	BCR	C16-C15-C14	-2.08	119.27	123.52
14	B	801	CLA	CHD-C1D-ND	-2.08	121.88	124.80
14	A	819	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	B	814	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	A	804	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	B	834	CLA	CAA-CBA-CGA	-2.07	107.33	113.21
14	B	840	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	A	835	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	A	834	CLA	CHD-C1D-ND	-2.07	121.89	124.80
14	A	837	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	A	821	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	B	830	CLA	C3B-C4B-NB	-2.07	108.69	110.53
14	L	202	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
14	B	834	CLA	C4A-NA-C1A	2.06	107.62	106.68
14	K	4002	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	B	801	CLA	C4-C3-C2	-2.06	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	834	CLA	C1-C2-C3	-2.06	122.82	126.20
14	A	829	CLA	C2A-C1A-CHA	2.06	127.44	123.87
14	B	805	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	A	833	CLA	C3B-C2B-C1B	-2.06	104.75	107.17
14	A	813	CLA	CHD-C1D-ND	-2.05	121.91	124.80
14	B	834	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
14	A	823	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	A	838	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	B	840	CLA	C3B-C2B-C1B	-2.05	104.76	107.17
14	B	839	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
14	B	833	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	F	203	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	A	859	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	B	815	CLA	CMB-C2B-C1B	2.04	128.52	125.42
14	J	1102	CLA	C4A-NA-C1A	2.04	107.61	106.68
14	A	814	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	A	817	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	A	809	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	A	811	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	B	839	CLA	C4A-NA-C1A	2.03	107.61	106.68
13	A	802	CL0	C3B-C4B-NB	-2.03	108.72	110.53
14	A	839	CLA	CHD-C1D-ND	-2.03	121.95	124.80
14	B	808	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
14	B	826	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
14	A	829	CLA	CHB-C4A-NA	2.02	127.32	124.40
17	A	852	BCR	C11-C10-C9	2.02	130.11	127.28
14	A	843	CLA	C7-C6-C5	-2.02	107.88	113.26
14	A	830	CLA	CHD-C1D-ND	-2.02	121.96	124.80
14	A	814	CLA	C3B-C4B-NB	-2.02	108.73	110.53
14	B	801	CLA	C3B-C4B-NB	-2.02	108.73	110.53
14	K	4002	CLA	CMB-C2B-C1B	2.02	128.49	125.42
14	A	806	CLA	CHD-C1D-C2D	2.02	129.68	125.49
17	K	4001	BCR	C24-C25-C26	2.01	126.19	121.56
14	B	822	CLA	CHB-C4A-NA	2.01	127.30	124.40
14	B	840	CLA	CHB-C4A-NA	2.01	127.30	124.40
14	B	817	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	A	835	CLA	C1C-C2C-C3C	-2.01	104.86	106.98
14	A	834	CLA	CMB-C2B-C1B	2.01	128.48	125.42
14	L	203	CLA	C4-C3-C2	-2.01	118.47	123.63
14	A	834	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
14	F	204	CLA	C4A-NA-C1A	2.01	107.59	106.68
14	B	810	CLA	CHA-C1A-NA	-2.00	121.85	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	822	CLA	C4A-NA-C1A	2.00	107.59	106.68
14	B	823	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
14	B	824	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
17	B	848	BCR	C2-C1-C6	2.00	113.35	110.44
14	A	821	CLA	C1-C2-C3	-2.00	122.92	126.20
14	A	834	CLA	C3B-C4B-NB	-2.00	108.74	110.53
14	B	828	CLA	CHA-C1A-NA	-2.00	121.86	126.39
14	L	204	CLA	CHA-C1A-NA	-2.00	121.86	126.39
14	B	821	CLA	C3B-C2B-C1B	-2.00	104.81	107.17

There are no chirality outliers.

All (905) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C3-O3-P-O5
12	A	801	LHG	C4-O6-P-O5
12	A	801	LHG	O9-C7-O7-C5
12	A	855	LHG	C3-O3-P-O5
12	B	850	LHG	C3-O3-P-O5
12	M	101	LHG	C2-C3-O3-P
12	M	101	LHG	O9-C7-O7-C5
13	A	802	CL0	C4-C3-C5-C6
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	812	CLA	C1A-C2A-CAA-CBA
14	A	813	CLA	C1A-C2A-CAA-CBA
14	A	818	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	819	CLA	C2B-C3B-CAB-CBB
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	CHA-CBD-CGD-O1D
14	A	823	CLA	CHA-CBD-CGD-O2D
14	A	824	CLA	C1A-C2A-CAA-CBA
14	A	825	CLA	C4B-C3B-CAB-CBB
14	A	825	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	826	CLA	CHA-CBD-CGD-O2D
14	A	830	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	834	CLA	C2B-C3B-CAB-CBB
14	A	834	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	836	CLA	C11-C10-C8-C9
14	A	842	CLA	C1A-C2A-CAA-CBA
14	A	844	CLA	C4B-C3B-CAB-CBB
14	A	845	CLA	CBA-CGA-O2A-C1
14	A	845	CLA	O1A-CGA-O2A-C1
14	B	806	CLA	C1A-C2A-CAA-CBA
14	B	808	CLA	C1A-C2A-CAA-CBA
14	B	809	CLA	CHA-CBD-CGD-O1D
14	B	809	CLA	CHA-CBD-CGD-O2D
14	B	812	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	C3A-C2A-CAA-CBA
14	B	812	CLA	C4-C3-C5-C6
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	CHA-CBD-CGD-O1D
14	B	816	CLA	CHA-CBD-CGD-O2D
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	819	CLA	C6-C7-C8-C9
14	B	825	CLA	CHA-CBD-CGD-O1D
14	B	825	CLA	CHA-CBD-CGD-O2D
14	B	826	CLA	CHA-CBD-CGD-O1D
14	B	826	CLA	CHA-CBD-CGD-O2D
14	B	828	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	839	CLA	C11-C10-C8-C9
14	F	201	CLA	C1A-C2A-CAA-CBA
14	F	203	CLA	C1A-C2A-CAA-CBA
14	F	203	CLA	C3A-C2A-CAA-CBA
14	J	1103	CLA	C1A-C2A-CAA-CBA
14	J	1103	CLA	C3A-C2A-CAA-CBA
14	J	1103	CLA	CBD-CGD-O2D-CED
14	K	4003	CLA	CHA-CBD-CGD-O1D
14	K	4003	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	K	4003	CLA	CBD-CGD-O2D-CED
14	K	4004	CLA	C1A-C2A-CAA-CBA
14	L	202	CLA	C1A-C2A-CAA-CBA
14	L	202	CLA	C3A-C2A-CAA-CBA
17	A	851	BCR	C23-C24-C25-C30
17	A	852	BCR	C17-C18-C19-C20
17	A	852	BCR	C23-C24-C25-C26
17	A	852	BCR	C23-C24-C25-C30
17	B	844	BCR	C21-C22-C23-C24
17	B	844	BCR	C37-C22-C23-C24
17	B	844	BCR	C23-C24-C25-C26
17	B	848	BCR	C7-C8-C9-C10
17	B	852	BCR	C23-C24-C25-C26
17	F	202	BCR	C17-C18-C19-C20
17	F	202	BCR	C21-C22-C23-C24
17	I	102	BCR	C17-C18-C19-C20
17	J	1104	BCR	C11-C12-C13-C14
17	J	1104	BCR	C11-C12-C13-C35
17	J	1105	BCR	C17-C18-C19-C20
17	K	4001	BCR	C21-C22-C23-C24
17	K	4001	BCR	C37-C22-C23-C24
17	L	205	BCR	C21-C22-C23-C24
17	L	205	BCR	C37-C22-C23-C24
17	L	205	BCR	C23-C24-C25-C30
17	L	206	BCR	C1-C6-C7-C8
17	L	206	BCR	C23-C24-C25-C26
17	L	206	BCR	C23-C24-C25-C30
18	A	853	LMG	O9-C10-O7-C8
18	B	851	LMG	O6-C1-O1-C7
18	I	101	LMG	O10-C28-O8-C9
19	A	858	LMT	C3'-C4'-O1B-C1B
19	F	206	LMT	C2'-C1'-O1'-C1
19	F	206	LMT	O5'-C1'-O1'-C1
21	M	102	ECH	C11-C12-C13-C14
21	M	102	ECH	C11-C12-C13-C35
19	A	857	LMT	C3'-C4'-O1B-C1B
19	F	206	LMT	C3'-C4'-O1B-C1B
14	J	1103	CLA	O1D-CGD-O2D-CED
14	K	4003	CLA	O1D-CGD-O2D-CED
14	K	4003	CLA	C4C-C3C-CAC-CBC
18	I	101	LMG	C29-C28-O8-C9
14	A	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	821	CLA	O1A-CGA-O2A-C1
14	A	831	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	O1A-CGA-O2A-C1
14	F	201	CLA	O1A-CGA-O2A-C1
18	B	851	LMG	O10-C28-O8-C9
14	A	817	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	C3-C5-C6-C7
14	A	826	CLA	C3-C5-C6-C7
14	B	826	CLA	C3-C5-C6-C7
14	B	834	CLA	C3-C5-C6-C7
14	B	839	CLA	C3-C5-C6-C7
14	B	841	CLA	C3-C5-C6-C7
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	821	CLA	CBA-CGA-O2A-C1
14	B	841	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	CBA-CGA-O2A-C1
18	B	851	LMG	C29-C28-O8-C9
14	B	841	CLA	CBD-CGD-O2D-CED
12	A	801	LHG	C8-C7-O7-C5
12	M	101	LHG	C8-C7-O7-C5
18	A	853	LMG	C11-C10-O7-C8
14	B	806	CLA	C4-C3-C5-C6
13	A	802	CL0	C2-C3-C5-C6
14	B	806	CLA	C2-C3-C5-C6
14	B	812	CLA	C2-C3-C5-C6
14	F	204	CLA	CBA-CGA-O2A-C1
14	B	825	CLA	C3-C5-C6-C7
12	M	101	LHG	C24-C23-O8-C6
14	A	812	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	CBA-CGA-O2A-C1
14	A	827	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	J	1103	CLA	CBA-CGA-O2A-C1
21	M	102	ECH	C9-C10-C11-C12
14	A	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	832	CLA	O1A-CGA-O2A-C1
14	B	841	CLA	O1A-CGA-O2A-C1
14	J	1103	CLA	O1A-CGA-O2A-C1
18	A	853	LMG	O10-C28-O8-C9
14	A	815	CLA	C3-C5-C6-C7
14	A	831	CLA	C3-C5-C6-C7
14	A	844	CLA	C3-C5-C6-C7
14	B	812	CLA	C3-C5-C6-C7
14	B	821	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	CBA-CGA-O2A-C1
14	B	839	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	O1A-CGA-O2A-C1
14	B	814	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1
18	B	802	LMG	C10-C11-C12-C13
18	I	101	LMG	C11-C10-O7-C8
14	B	819	CLA	C3-C5-C6-C7
14	B	810	CLA	CBA-CGA-O2A-C1
18	A	853	LMG	C29-C28-O8-C9
12	M	101	LHG	O10-C23-O8-C6
14	A	815	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	O1A-CGA-O2A-C1
14	F	204	CLA	O1A-CGA-O2A-C1
14	A	843	CLA	C2A-CAA-CBA-CGA
14	B	810	CLA	O1A-CGA-O2A-C1
14	L	203	CLA	CBA-CGA-O2A-C1
14	B	836	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	818	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	CBA-CGA-O2A-C1
14	A	830	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	CBA-CGA-O2A-C1
14	B	812	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	CBA-CGA-O2A-C1
14	B	831	CLA	CBA-CGA-O2A-C1
14	B	833	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	C6-C7-C8-C9
14	A	808	CLA	C6-C7-C8-C9
14	A	840	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	B	815	CLA	C14-C13-C15-C16
14	B	817	CLA	C11-C10-C8-C9
14	B	822	CLA	C11-C10-C8-C9
14	B	825	CLA	C14-C13-C15-C16
14	B	830	CLA	C14-C13-C15-C16
14	L	204	CLA	C11-C10-C8-C9
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	O1A-CGA-O2A-C1
17	A	850	BCR	C37-C22-C23-C24
17	A	851	BCR	C37-C22-C23-C24
17	A	852	BCR	C36-C18-C19-C20
17	B	848	BCR	C7-C8-C9-C34
17	F	202	BCR	C36-C18-C19-C20
17	F	202	BCR	C37-C22-C23-C24
17	I	102	BCR	C36-C18-C19-C20
17	I	102	BCR	C37-C22-C23-C24
17	J	1105	BCR	C36-C18-C19-C20
17	L	206	BCR	C7-C8-C9-C34
21	B	846	ECH	C7-C8-C9-C34
17	A	850	BCR	C21-C22-C23-C24
17	A	851	BCR	C21-C22-C23-C24
17	I	102	BCR	C21-C22-C23-C24
17	L	206	BCR	C7-C8-C9-C10
14	B	818	CLA	O1A-CGA-O2A-C1
18	I	101	LMG	O9-C10-O7-C8
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C13-C15-C16-C17
14	B	816	CLA	C3-C5-C6-C7
14	A	809	CLA	C13-C15-C16-C17
14	A	808	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBA-CGA-O2A-C1
19	A	856	LMT	O1'-C1-C2-C3
14	B	841	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	830	CLA	O1A-CGA-O2A-C1
14	B	831	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	C15-C16-C17-C18
14	A	809	CLA	C2A-CAA-CBA-CGA
14	A	810	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	B	840	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	B	842	CLA	C2A-CAA-CBA-CGA
14	F	203	CLA	C2A-CAA-CBA-CGA
14	A	859	CLA	C8-C10-C11-C12
14	B	812	CLA	O1A-CGA-O2A-C1
14	B	833	CLA	O1A-CGA-O2A-C1
14	A	821	CLA	C3-C5-C6-C7
14	B	821	CLA	C3-C5-C6-C7
14	B	812	CLA	CBD-CGD-O2D-CED
14	A	804	CLA	C15-C16-C17-C18
14	A	835	CLA	C15-C16-C17-C18
14	B	806	CLA	C5-C6-C7-C8
14	A	833	CLA	O1A-CGA-O2A-C1
14	L	203	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	C5-C6-C7-C8
15	B	843	PQN	C25-C26-C27-C28
14	B	806	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	C5-C6-C7-C8
14	A	841	CLA	C8-C10-C11-C12
14	A	803	CLA	C8-C10-C11-C12
14	B	831	CLA	C15-C16-C17-C18
14	B	807	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	C4-C3-C5-C6
14	A	831	CLA	C4-C3-C5-C6
14	B	833	CLA	C4-C3-C5-C6
14	A	805	CLA	C5-C6-C7-C8
19	F	207	LMT	O5B-C1B-O1B-C4'
14	A	844	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	C10-C11-C12-C13
17	A	849	BCR	C7-C8-C9-C34
17	A	852	BCR	C37-C22-C23-C24
17	J	1104	BCR	C7-C8-C9-C34
17	J	1105	BCR	C11-C12-C13-C35
21	B	846	ECH	C7-C8-C9-C10
14	B	818	CLA	C2A-CAA-CBA-CGA
14	B	822	CLA	C2A-CAA-CBA-CGA
14	B	821	CLA	C15-C16-C17-C18
14	A	806	CLA	O2A-C1-C2-C3
14	B	836	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	B	810	CLA	C16-C17-C18-C19
14	B	834	CLA	C6-C7-C8-C10
14	B	806	CLA	O1A-CGA-O2A-C1
14	B	828	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	C5-C6-C7-C8
14	B	822	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	C2-C1-O2A-CGA
14	B	805	CLA	C16-C17-C18-C19
14	B	834	CLA	C6-C7-C8-C9
14	B	839	CLA	C16-C17-C18-C20
19	A	858	LMT	C5-C6-C7-C8
13	A	802	CL0	C5-C6-C7-C8
18	A	853	LMG	C33-C34-C35-C36
14	A	819	CLA	C4B-C3B-CAB-CBB
18	B	851	LMG	C10-C11-C12-C13
14	B	810	CLA	C16-C17-C18-C20
14	B	839	CLA	C16-C17-C18-C19
14	F	201	CLA	C16-C17-C18-C19
14	F	201	CLA	C16-C17-C18-C20
12	A	801	LHG	C16-C17-C18-C19
18	A	853	LMG	C31-C32-C33-C34
14	B	822	CLA	C12-C13-C15-C16
14	B	826	CLA	O1A-CGA-O2A-C1
14	L	202	CLA	C3-C5-C6-C7
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	810	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	813	CLA	C3A-C2A-CAA-CBA
14	A	818	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C3A-C2A-CAA-CBA
14	B	806	CLA	C3A-C2A-CAA-CBA
14	B	813	CLA	C3A-C2A-CAA-CBA
14	B	825	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	C3A-C2A-CAA-CBA
14	J	1101	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	C10-C11-C12-C13
14	A	844	CLA	C16-C17-C18-C20
14	L	204	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	A	855	LHG	C27-C28-C29-C30
14	A	838	CLA	CBA-CGA-O2A-C1
14	A	844	CLA	O1A-CGA-O2A-C1
14	B	807	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	O1A-CGA-O2A-C1
17	A	849	BCR	C5-C6-C7-C8
17	A	851	BCR	C23-C24-C25-C26
17	B	844	BCR	C23-C24-C25-C30
17	B	852	BCR	C23-C24-C25-C30
17	I	102	BCR	C23-C24-C25-C30
17	K	4001	BCR	C23-C24-C25-C30
17	L	205	BCR	C23-C24-C25-C26
17	L	206	BCR	C5-C6-C7-C8
21	M	102	ECH	C23-C24-C25-C26
14	B	838	CLA	CBA-CGA-O2A-C1
14	B	807	CLA	C3-C5-C6-C7
19	A	854	LMT	C7-C8-C9-C10
14	B	834	CLA	C4-C3-C5-C6
14	A	839	CLA	C13-C15-C16-C17
14	A	829	CLA	C2-C3-C5-C6
14	A	831	CLA	C2-C3-C5-C6
14	B	833	CLA	C2-C3-C5-C6
14	A	807	CLA	C16-C17-C18-C20
18	B	851	LMG	C15-C16-C17-C18
14	A	807	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	CBA-CGA-O2A-C1
14	B	813	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	C11-C10-C8-C9
14	B	840	CLA	C14-C13-C15-C16
14	B	813	CLA	C5-C6-C7-C8
14	B	825	CLA	C10-C11-C12-C13
18	B	851	LMG	C11-C12-C13-C14
14	A	825	CLA	C15-C16-C17-C18
12	A	855	LHG	C29-C30-C31-C32
14	B	825	CLA	CBA-CGA-O2A-C1
18	B	802	LMG	C36-C37-C38-C39
14	A	842	CLA	C13-C15-C16-C17
14	B	814	CLA	C4C-C3C-CAC-CBC
14	A	838	CLA	O1A-CGA-O2A-C1
21	I	103	ECH	C7-C8-C9-C34
19	A	857	LMT	C7-C8-C9-C10
17	J	1105	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	844	CLA	C16-C17-C18-C19
12	A	801	LHG	C11-C10-C9-C8
18	B	802	LMG	C14-C15-C16-C17
14	B	821	CLA	C5-C6-C7-C8
14	A	819	CLA	C15-C16-C17-C18
14	A	806	CLA	C8-C10-C11-C12
15	B	843	PQN	C23-C25-C26-C27
14	F	201	CLA	C3-C5-C6-C7
14	B	838	CLA	O1A-CGA-O2A-C1
19	F	207	LMT	C3-C4-C5-C6
19	A	854	LMT	O5B-C5B-C6B-O6B
19	A	856	LMT	C7-C8-C9-C10
14	B	834	CLA	C2-C3-C5-C6
18	A	853	LMG	C13-C14-C15-C16
19	A	858	LMT	C7-C8-C9-C10
18	A	853	LMG	O6-C5-C6-O5
14	A	817	CLA	C1A-C2A-CAA-CBA
14	A	837	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	823	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C1A-C2A-CAA-CBA
14	B	841	CLA	C1A-C2A-CAA-CBA
14	J	1102	CLA	C1A-C2A-CAA-CBA
14	B	801	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	O1A-CGA-O2A-C1
14	B	825	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	C15-C16-C17-C18
14	A	804	CLA	C12-C13-C15-C16
14	A	820	CLA	C11-C12-C13-C15
14	A	825	CLA	C11-C10-C8-C7
14	A	840	CLA	C11-C10-C8-C7
14	B	820	CLA	C6-C7-C8-C10
14	B	826	CLA	C6-C7-C8-C10
14	B	830	CLA	C12-C13-C15-C16
14	B	838	CLA	C6-C7-C8-C10
14	B	838	CLA	C12-C13-C15-C16
14	K	4004	CLA	C11-C12-C13-C15
15	B	843	PQN	C22-C23-C25-C26
14	A	807	CLA	C5-C6-C7-C8
14	A	821	CLA	C5-C6-C7-C8
14	A	829	CLA	C13-C15-C16-C17
14	A	839	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	B	801	CLA	C2A-CAA-CBA-CGA
14	A	808	CLA	C11-C12-C13-C14
14	A	825	CLA	C11-C10-C8-C9
14	A	840	CLA	C11-C10-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	A	844	CLA	C14-C13-C15-C16
14	B	816	CLA	C11-C10-C8-C9
14	B	820	CLA	C6-C7-C8-C9
14	B	825	CLA	C11-C10-C8-C9
14	B	838	CLA	C11-C10-C8-C9
14	K	4004	CLA	C11-C10-C8-C9
14	A	814	CLA	CBA-CGA-O2A-C1
19	A	858	LMT	O5B-C5B-C6B-O6B
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C10-C11-C12-C13
18	I	101	LMG	O6-C5-C6-O5
19	A	857	LMT	O5B-C5B-C6B-O6B
17	A	849	BCR	C7-C8-C9-C10
14	A	825	CLA	C13-C15-C16-C17
19	A	854	LMT	C1-C2-C3-C4
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	CBA-CGA-O2A-C1
14	B	822	CLA	O2A-C1-C2-C3
14	A	859	CLA	C15-C16-C17-C18
14	A	807	CLA	O1A-CGA-O2A-C1
14	A	814	CLA	O1A-CGA-O2A-C1
14	A	831	CLA	C5-C6-C7-C8
12	A	801	LHG	C10-C11-C12-C13
14	A	806	CLA	C2C-C3C-CAC-CBC
14	B	834	CLA	C5-C6-C7-C8
14	A	843	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	C5-C6-C7-C8
19	A	854	LMT	C9-C10-C11-C12
19	A	856	LMT	C9-C10-C11-C12
14	A	819	CLA	CAA-CBA-CGA-O2A
12	A	801	LHG	C34-C35-C36-C37
14	A	826	CLA	C13-C15-C16-C17
18	B	802	LMG	C40-C41-C42-C43
14	B	824	CLA	CBD-CGD-O2D-CED
19	A	854	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	B	812	CLA	O1D-CGD-O2D-CED
14	B	809	CLA	C16-C17-C18-C19
14	A	812	CLA	C13-C15-C16-C17
19	F	207	LMT	C2-C1-O1'-C1'
14	A	803	CLA	C11-C12-C13-C14
14	A	804	CLA	C14-C13-C15-C16
14	A	808	CLA	C14-C13-C15-C16
14	A	820	CLA	C11-C12-C13-C14
14	A	822	CLA	C6-C7-C8-C9
14	A	831	CLA	C6-C7-C8-C9
14	A	837	CLA	C11-C12-C13-C14
14	B	801	CLA	C11-C12-C13-C14
14	B	822	CLA	C14-C13-C15-C16
14	B	826	CLA	C6-C7-C8-C9
14	B	838	CLA	C6-C7-C8-C9
14	B	838	CLA	C14-C13-C15-C16
14	K	4004	CLA	C11-C12-C13-C14
15	B	843	PQN	C24-C23-C25-C26
14	A	820	CLA	C5-C6-C7-C8
14	A	843	CLA	C4B-C3B-CAB-CBB
14	B	809	CLA	C4B-C3B-CAB-CBB
14	F	204	CLA	C4B-C3B-CAB-CBB
14	K	4003	CLA	C4B-C3B-CAB-CBB
12	A	855	LHG	C10-C11-C12-C13
12	B	850	LHG	C7-C8-C9-C10
19	A	858	LMT	O5B-C1B-O1B-C4'
12	A	855	LHG	C13-C14-C15-C16
14	A	803	CLA	C11-C12-C13-C15
14	A	808	CLA	C11-C12-C13-C15
14	A	808	CLA	C12-C13-C15-C16
14	A	812	CLA	C6-C7-C8-C10
14	A	822	CLA	C6-C7-C8-C10
14	A	831	CLA	C6-C7-C8-C10
14	A	836	CLA	C11-C10-C8-C7
14	A	841	CLA	C11-C10-C8-C7
14	A	844	CLA	C12-C13-C15-C16
14	B	825	CLA	C11-C10-C8-C7
14	B	831	CLA	C6-C7-C8-C10
14	B	838	CLA	C11-C10-C8-C7
14	K	4004	CLA	C11-C10-C8-C7
14	A	813	CLA	C6-C7-C8-C9
14	B	809	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	A	807	CLA	C3A-C2A-CAA-CBA
14	A	812	CLA	C3A-C2A-CAA-CBA
14	B	817	CLA	C4-C3-C5-C6
14	A	844	CLA	C13-C15-C16-C17
14	B	824	CLA	C5-C6-C7-C8
17	L	206	BCR	C19-C20-C21-C22
14	A	823	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	C2A-CAA-CBA-CGA
19	A	858	LMT	C1-C2-C3-C4
14	K	4004	CLA	C16-C17-C18-C19
14	B	815	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	C14-C15-C16-C17
14	A	807	CLA	C16-C17-C18-C19
14	B	813	CLA	C6-C7-C8-C9
14	A	844	CLA	C2B-C3B-CAB-CBB
17	A	849	BCR	C1-C6-C7-C8
17	B	849	BCR	C23-C24-C25-C26
17	K	4001	BCR	C23-C24-C25-C26
18	I	101	LMG	O7-C8-C9-O8
14	B	817	CLA	C2-C3-C5-C6
14	K	4004	CLA	C16-C17-C18-C20
14	B	820	CLA	C3-C5-C6-C7
14	A	844	CLA	C6-C7-C8-C9
14	B	810	CLA	C11-C10-C8-C9
14	L	204	CLA	O1D-CGD-O2D-CED
17	J	1105	BCR	C19-C20-C21-C22
14	A	828	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBA-CGA-O2A-C1
14	A	837	CLA	CBA-CGA-O2A-C1
14	A	859	CLA	C10-C11-C12-C13
14	B	827	CLA	C16-C17-C18-C20
14	A	805	CLA	C11-C10-C8-C7
14	A	812	CLA	C12-C13-C15-C16
14	A	823	CLA	C11-C10-C8-C7
14	A	825	CLA	C12-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C15
14	A	844	CLA	C6-C7-C8-C10
14	A	859	CLA	C11-C12-C13-C15
14	B	809	CLA	C12-C13-C15-C16
14	B	810	CLA	C11-C10-C8-C7
14	B	816	CLA	C11-C10-C8-C7
14	B	841	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	L	202	CLA	C6-C7-C8-C10
14	L	204	CLA	C11-C10-C8-C7
17	J	1104	BCR	C7-C8-C9-C10
14	A	843	CLA	O1A-CGA-O2A-C1
18	A	853	LMG	C8-C7-O1-C1
14	A	804	CLA	C2A-CAA-CBA-CGA
12	M	101	LHG	C30-C31-C32-C33
14	A	840	CLA	C16-C17-C18-C19
14	A	814	CLA	C13-C15-C16-C17
18	B	802	LMG	C17-C18-C19-C20
14	A	805	CLA	C11-C12-C13-C14
14	A	812	CLA	C14-C13-C15-C16
14	A	823	CLA	C11-C10-C8-C9
14	A	859	CLA	C11-C12-C13-C14
14	B	809	CLA	C14-C13-C15-C16
14	B	813	CLA	C6-C7-C8-C10
14	A	828	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	C2-C1-O2A-CGA
12	A	801	LHG	C26-C27-C28-C29
14	A	828	CLA	C16-C17-C18-C19
14	A	837	CLA	O1A-CGA-O2A-C1
18	A	853	LMG	C37-C38-C39-C40
12	M	101	LHG	C29-C30-C31-C32
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	813	CLA	C4B-C3B-CAB-CBB
14	B	836	CLA	C4B-C3B-CAB-CBB
14	J	1101	CLA	C1A-C2A-CAA-CBA
14	J	1102	CLA	C4B-C3B-CAB-CBB
14	J	1103	CLA	C4B-C3B-CAB-CBB
14	B	824	CLA	O1D-CGD-O2D-CED
17	A	852	BCR	C21-C22-C23-C24
14	B	816	CLA	C10-C11-C12-C13
12	A	801	LHG	O6-C4-C5-C6
14	A	824	CLA	C2-C3-C5-C6
14	A	808	CLA	C6-C7-C8-C10
14	A	814	CLA	C6-C7-C8-C10
14	B	822	CLA	C11-C10-C8-C7
14	B	827	CLA	C12-C13-C15-C16
14	B	828	CLA	C12-C13-C15-C16
14	K	4004	CLA	C12-C13-C15-C16
14	A	826	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	A	840	CLA	C16-C17-C18-C20
14	A	823	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	C4-C3-C5-C6
12	A	801	LHG	O6-C4-C5-O7
14	A	806	CLA	C2A-CAA-CBA-CGA
14	A	805	CLA	C11-C10-C8-C9
14	A	812	CLA	C6-C7-C8-C9
14	A	825	CLA	C14-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C14
14	B	841	CLA	C11-C12-C13-C14
14	L	202	CLA	C6-C7-C8-C9
14	A	842	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	C15-C16-C17-C18
14	K	4004	CLA	C13-C15-C16-C17
18	B	802	LMG	C16-C17-C18-C19
14	K	4003	CLA	C2C-C3C-CAC-CBC
18	A	853	LMG	O1-C7-C8-O7
14	A	834	CLA	C5-C6-C7-C8
18	A	853	LMG	O1-C7-C8-C9
19	F	207	LMT	C2-C3-C4-C5
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	845	CLA	CAD-CBD-CGD-O2D
14	B	801	CLA	CAD-CBD-CGD-O2D
14	B	818	CLA	C10-C11-C12-C13
14	A	842	CLA	O1A-CGA-O2A-C1
14	A	843	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	812	CLA	CHA-CBD-CGD-O1D
14	A	812	CLA	CHA-CBD-CGD-O2D
14	A	845	CLA	CAD-CBD-CGD-O1D
14	B	801	CLA	CAD-CBD-CGD-O1D
14	A	841	CLA	C4-C3-C5-C6
14	B	819	CLA	C4-C3-C5-C6
14	A	817	CLA	C2B-C3B-CAB-CBB
14	A	825	CLA	C2B-C3B-CAB-CBB
17	B	845	BCR	C5-C6-C7-C8
14	B	812	CLA	CAA-CBA-CGA-O2A
17	A	850	BCR	C36-C18-C19-C20
17	B	852	BCR	C7-C8-C9-C34
17	L	205	BCR	C7-C8-C9-C34
14	A	828	CLA	C16-C17-C18-C20
19	A	858	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	B	831	CLA	C3-C5-C6-C7
14	A	826	CLA	C16-C17-C18-C20
12	M	101	LHG	C6-C5-O7-C7
17	J	1104	BCR	C9-C10-C11-C12
18	B	851	LMG	C13-C14-C15-C16
14	B	831	CLA	C6-C7-C8-C9
14	B	833	CLA	C11-C12-C13-C14
14	A	840	CLA	C12-C13-C15-C16
14	A	830	CLA	C5-C6-C7-C8
14	A	822	CLA	C4-C3-C5-C6
14	A	804	CLA	C13-C15-C16-C17
13	A	802	CL0	CAA-CBA-CGA-O2A
14	B	815	CLA	C8-C10-C11-C12
14	A	805	CLA	C4-C3-C5-C6
14	B	827	CLA	C16-C17-C18-C19
17	A	849	BCR	C36-C18-C19-C20
14	A	834	CLA	C16-C17-C18-C20
14	B	814	CLA	C16-C17-C18-C20
12	A	855	LHG	C11-C12-C13-C14
14	A	818	CLA	C8-C10-C11-C12
14	B	819	CLA	C5-C6-C7-C8
21	M	102	ECH	C13-C14-C15-C16
14	B	827	CLA	C14-C13-C15-C16
14	B	820	CLA	C4B-C3B-CAB-CBB
14	B	824	CLA	C4B-C3B-CAB-CBB
14	K	4002	CLA	C4B-C3B-CAB-CBB
14	A	819	CLA	CAA-CBA-CGA-O1A
12	B	850	LHG	C16-C17-C18-C19
14	A	841	CLA	C2-C3-C5-C6
14	B	814	CLA	C11-C10-C8-C7
14	B	820	CLA	C12-C13-C15-C16
14	B	839	CLA	C11-C10-C8-C7
14	A	837	CLA	C3-C5-C6-C7
14	A	829	CLA	C3A-C2A-CAA-CBA
14	A	830	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C3A-C2A-CAA-CBA
14	A	828	CLA	C2-C3-C5-C6
14	A	829	CLA	C16-C17-C18-C19
17	A	852	BCR	C11-C10-C9-C34
17	A	852	BCR	C16-C17-C18-C36
17	F	205	BCR	C35-C13-C14-C15
21	B	846	ECH	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
21	B	846	ECH	C20-C21-C22-C37
21	I	103	ECH	C11-C10-C9-C34
21	M	102	ECH	C11-C10-C9-C34
14	B	825	CLA	C5-C6-C7-C8
14	A	825	CLA	C8-C10-C11-C12
14	A	824	CLA	C4-C3-C5-C6
19	A	856	LMT	C3-C4-C5-C6
14	A	815	CLA	C4-C3-C5-C6
14	A	829	CLA	C6-C7-C8-C9
14	A	839	CLA	C11-C12-C13-C14
14	B	840	CLA	C6-C7-C8-C9
18	B	851	LMG	C31-C32-C33-C34
14	A	807	CLA	C15-C16-C17-C18
14	B	830	CLA	C10-C11-C12-C13
14	B	830	CLA	CBD-CGD-O2D-CED
14	K	4002	CLA	CAA-CBA-CGA-O1A
14	A	829	CLA	C1A-C2A-CAA-CBA
14	B	814	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C1A-C2A-CAA-CBA
17	A	852	BCR	C11-C10-C9-C8
17	A	852	BCR	C16-C17-C18-C19
17	F	205	BCR	C12-C13-C14-C15
21	B	846	ECH	C11-C10-C9-C8
21	B	846	ECH	C20-C21-C22-C23
21	I	103	ECH	C11-C10-C9-C8
21	M	102	ECH	C11-C10-C9-C8
17	A	848	BCR	C1-C6-C7-C8
17	J	1104	BCR	C1-C6-C7-C8
17	J	1104	BCR	C5-C6-C7-C8
21	I	103	ECH	C1-C6-C7-C8
18	B	851	LMG	C11-C10-O7-C8
14	A	840	CLA	C15-C16-C17-C18
12	M	101	LHG	C24-C25-C26-C27
14	A	820	CLA	C16-C17-C18-C20
14	A	821	CLA	C4-C3-C5-C6
14	B	830	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	C2-C3-C5-C6
17	B	847	BCR	C19-C20-C21-C22
14	A	826	CLA	C12-C13-C15-C16
14	B	811	CLA	C12-C13-C15-C16
14	B	825	CLA	C12-C13-C15-C16
14	B	826	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	L	203	CLA	C12-C13-C15-C16
14	L	203	CLA	C16-C17-C18-C20
17	K	4005	BCR	C37-C22-C23-C24
19	F	206	LMT	O5'-C5'-C6'-O6'
14	B	804	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C16-C17-C18-C20
14	L	204	CLA	C16-C17-C18-C20
14	B	820	CLA	C14-C13-C15-C16
17	A	852	BCR	C19-C20-C21-C22
14	B	817	CLA	CBA-CGA-O2A-C1
14	L	202	CLA	O1A-CGA-O2A-C1
14	B	814	CLA	C4-C3-C5-C6
19	A	856	LMT	C2-C3-C4-C5
14	A	815	CLA	C2-C3-C5-C6
14	B	819	CLA	C2-C3-C5-C6
14	B	819	CLA	C8-C10-C11-C12
14	K	4002	CLA	CAA-CBA-CGA-O2A
19	F	207	LMT	C1-C2-C3-C4
14	B	817	CLA	O1A-CGA-O2A-C1
14	A	814	CLA	C2A-CAA-CBA-CGA
14	A	814	CLA	C10-C11-C12-C13
18	A	853	LMG	C14-C15-C16-C17
18	B	851	LMG	O9-C10-O7-C8
14	J	1102	CLA	CAA-CBA-CGA-O2A
14	A	823	CLA	C16-C17-C18-C19
14	B	825	CLA	C16-C17-C18-C20
14	A	823	CLA	C5-C6-C7-C8
14	A	823	CLA	C8-C10-C11-C12
14	B	821	CLA	C4B-C3B-CAB-CBB
14	K	4004	CLA	C4B-C3B-CAB-CBB
14	B	838	CLA	C13-C15-C16-C17
14	A	823	CLA	C16-C17-C18-C20
14	A	813	CLA	O1A-CGA-O2A-C1
14	B	823	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	C4-C3-C5-C6
19	F	207	LMT	C5'-C4'-O1B-C1B
14	A	814	CLA	C6-C7-C8-C9
14	A	819	CLA	C14-C13-C15-C16
14	A	822	CLA	C11-C10-C8-C9
14	B	826	CLA	C11-C12-C13-C14
14	B	827	CLA	C11-C12-C13-C14
14	B	830	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	810	CLA	C2-C1-O2A-CGA
14	A	826	CLA	C2-C1-O2A-CGA
14	B	818	CLA	C2-C1-O2A-CGA
14	A	813	CLA	CBA-CGA-O2A-C1
14	B	816	CLA	C3A-C2A-CAA-CBA
14	B	830	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	C3A-C2A-CAA-CBA
14	J	1102	CLA	CAA-CBA-CGA-O1A
14	B	807	CLA	C10-C11-C12-C13
14	F	203	CLA	CAA-CBA-CGA-O2A
14	L	202	CLA	CBA-CGA-O2A-C1
18	I	101	LMG	C7-C8-C9-O8
14	A	831	CLA	C10-C11-C12-C13
14	B	833	CLA	C8-C10-C11-C12
14	A	807	CLA	CAA-CBA-CGA-O2A
14	F	203	CLA	CAA-CBA-CGA-O1A
14	A	839	CLA	C11-C10-C8-C9
14	A	842	CLA	C6-C7-C8-C9
14	B	801	CLA	C11-C10-C8-C9
14	K	4004	CLA	C14-C13-C15-C16
14	A	805	CLA	C16-C17-C18-C19
14	B	825	CLA	C16-C17-C18-C19
17	B	852	BCR	C7-C8-C9-C10
14	B	825	CLA	CAA-CBA-CGA-O2A
14	B	833	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C6-C7-C8-C10
14	A	809	CLA	C12-C13-C15-C16
14	A	819	CLA	C11-C12-C13-C15
14	A	825	CLA	C11-C12-C13-C15
14	B	817	CLA	C11-C10-C8-C7
14	B	819	CLA	C6-C7-C8-C10
14	B	827	CLA	C11-C12-C13-C15
14	B	830	CLA	C11-C12-C13-C15
14	A	839	CLA	C2B-C3B-CAB-CBB
17	A	848	BCR	C5-C6-C7-C8
21	M	102	ECH	C23-C24-C25-C30
14	A	832	CLA	C2-C1-O2A-CGA
14	A	837	CLA	C2-C1-O2A-CGA
14	B	806	CLA	C2-C1-O2A-CGA
14	B	825	CLA	C2-C1-O2A-CGA
14	B	828	CLA	C2-C1-O2A-CGA
14	B	841	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	B	818	CLA	CAA-CBA-CGA-O2A
19	F	207	LMT	C5-C6-C7-C8
14	A	820	CLA	C16-C17-C18-C19
14	L	204	CLA	C16-C17-C18-C19
12	A	855	LHG	O7-C7-C8-C9
18	B	802	LMG	O7-C10-C11-C12
14	B	808	CLA	C2-C3-C5-C6
14	B	829	CLA	C2-C3-C5-C6
18	B	802	LMG	C11-C10-O7-C8
14	B	816	CLA	CAA-CBA-CGA-O2A
14	A	814	CLA	C16-C17-C18-C19
14	B	808	CLA	C4-C3-C5-C6
14	B	829	CLA	C4-C3-C5-C6
18	A	853	LMG	O7-C10-C11-C12
14	A	805	CLA	C2-C3-C5-C6
14	A	812	CLA	C2A-CAA-CBA-CGA
14	A	811	CLA	CAA-CBA-CGA-O2A
14	A	830	CLA	C13-C15-C16-C17
14	A	826	CLA	C14-C13-C15-C16
14	A	832	CLA	C14-C13-C15-C16
14	B	812	CLA	C11-C10-C8-C9
14	B	816	CLA	C6-C7-C8-C9
14	B	828	CLA	C14-C13-C15-C16
12	A	801	LHG	O8-C23-C24-C25
14	A	826	CLA	CAA-CBA-CGA-O2A
14	B	810	CLA	C8-C10-C11-C12
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	817	CLA	C4B-C3B-CAB-CBB
14	A	825	CLA	C1A-C2A-CAA-CBA
14	A	837	CLA	C4B-C3B-CAB-CBB
14	B	837	CLA	C1A-C2A-CAA-CBA
14	B	841	CLA	C4B-C3B-CAB-CBB
18	I	101	LMG	C33-C34-C35-C36
14	B	822	CLA	C13-C15-C16-C17
14	A	805	CLA	CAA-CBA-CGA-O2A
14	A	812	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	CAA-CBA-CGA-O2A
14	B	811	CLA	CAA-CBA-CGA-O2A
17	A	849	BCR	C17-C18-C19-C20
17	A	850	BCR	C17-C18-C19-C20
17	L	205	BCR	C7-C8-C9-C10
21	I	103	ECH	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	B	815	CLA	C16-C17-C18-C20
14	B	814	CLA	C5-C6-C7-C8
14	B	822	CLA	CAA-CBA-CGA-O2A
12	A	801	LHG	C25-C26-C27-C28
14	A	817	CLA	C2C-C3C-CAC-CBC
14	A	822	CLA	C16-C17-C18-C20
14	A	805	CLA	C8-C10-C11-C12
14	A	814	CLA	C8-C10-C11-C12
14	A	826	CLA	C11-C12-C13-C15
14	A	831	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	A	835	CLA	C11-C12-C13-C15
14	A	839	CLA	C11-C10-C8-C7
14	B	841	CLA	C11-C10-C8-C7
14	L	202	CLA	C12-C13-C15-C16
14	L	203	CLA	C11-C10-C8-C7
14	A	814	CLA	C16-C17-C18-C20
18	A	853	LMG	C9-C8-O7-C10
18	B	802	LMG	C30-C31-C32-C33
19	F	207	LMT	C2B-C1B-O1B-C4'
14	A	832	CLA	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C20
14	A	805	CLA	C13-C15-C16-C17
14	A	808	CLA	C10-C11-C12-C13
19	F	207	LMT	C3'-C4'-O1B-C1B
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	817	CLA	C3A-C2A-CAA-CBA
14	A	844	CLA	C3A-C2A-CAA-CBA
14	B	820	CLA	C4-C3-C5-C6
14	B	823	CLA	C3A-C2A-CAA-CBA
14	B	824	CLA	C3A-C2A-CAA-CBA
14	B	804	CLA	C8-C10-C11-C12
14	A	829	CLA	C16-C17-C18-C20
14	A	806	CLA	CAA-CBA-CGA-O2A
14	B	818	CLA	CAA-CBA-CGA-O1A
18	B	802	LMG	C4-C5-C6-O5
14	A	818	CLA	C14-C13-C15-C16
14	A	826	CLA	C11-C12-C13-C14
14	A	832	CLA	C11-C12-C13-C14
14	A	835	CLA	C14-C13-C15-C16
14	A	840	CLA	C14-C13-C15-C16
14	B	811	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	B	841	CLA	C11-C10-C8-C9
12	A	801	LHG	O10-C23-C24-C25
14	B	825	CLA	CAA-CBA-CGA-O1A
14	B	833	CLA	CAA-CBA-CGA-O1A
18	B	802	LMG	O9-C10-C11-C12
14	A	814	CLA	C4-C3-C5-C6
12	A	855	LHG	O9-C7-C8-C9
14	F	201	CLA	C10-C11-C12-C13
14	A	811	CLA	CAA-CBA-CGA-O1A
17	B	845	BCR	C11-C12-C13-C14
17	K	4005	BCR	C17-C18-C19-C20
17	K	4005	BCR	C21-C22-C23-C24
14	A	805	CLA	CAA-CBA-CGA-O1A
14	B	804	CLA	O1A-CGA-O2A-C1
18	B	802	LMG	O9-C10-O7-C8
14	A	843	CLA	CAA-CBA-CGA-O1A
14	A	844	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	CAD-CBD-CGD-O2D
14	B	813	CLA	CAD-CBD-CGD-O2D
14	B	815	CLA	CAD-CBD-CGD-O2D
14	A	805	CLA	C15-C16-C17-C18
14	B	822	CLA	C8-C10-C11-C12
14	B	816	CLA	CAA-CBA-CGA-O1A
14	B	821	CLA	C13-C15-C16-C17
19	F	207	LMT	C11-C10-C9-C8
14	A	818	CLA	C2-C1-O2A-CGA
14	B	813	CLA	C2-C1-O2A-CGA
14	A	806	CLA	CAA-CBA-CGA-O1A
14	A	826	CLA	CAA-CBA-CGA-O1A
12	B	850	LHG	C17-C18-C19-C20
14	A	812	CLA	CAA-CBA-CGA-O1A
14	B	822	CLA	CAA-CBA-CGA-O1A
18	A	853	LMG	O9-C10-C11-C12
14	B	838	CLA	C15-C16-C17-C18
14	B	821	CLA	CAA-CBA-CGA-O2A
14	L	203	CLA	C2C-C3C-CAC-CBC
14	B	804	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

60 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	846	ECH	1	0
14	B	827	CLA	2	0
14	A	816	CLA	1	0
17	J	1104	BCR	2	0
14	B	838	CLA	1	0
14	A	825	CLA	2	0
14	A	819	CLA	1	0
14	A	820	CLA	2	0
17	F	202	BCR	2	0
14	B	841	CLA	2	0
14	B	814	CLA	2	0
14	B	820	CLA	1	0
14	B	813	CLA	2	0
14	J	1101	CLA	1	0
21	M	102	ECH	3	0
14	A	822	CLA	1	0
14	A	803	CLA	1	0
14	A	815	CLA	1	0
14	B	801	CLA	2	0
14	B	809	CLA	1	0
14	A	810	CLA	1	0
14	A	859	CLA	1	0
14	B	839	CLA	3	0
14	F	203	CLA	1	0
14	A	807	CLA	1	0
14	A	840	CLA	1	0
14	B	829	CLA	1	0
14	B	826	CLA	4	0
14	A	817	CLA	1	0
14	A	828	CLA	1	0
17	B	845	BCR	2	0
14	B	810	CLA	1	0
17	K	4001	BCR	1	0
17	A	849	BCR	1	0
13	A	802	CL0	3	0
14	A	837	CLA	1	0
14	F	201	CLA	1	0
17	L	206	BCR	2	0
14	B	805	CLA	1	0
14	A	832	CLA	1	0
14	L	204	CLA	1	0
17	B	849	BCR	1	0
17	A	852	BCR	4	0

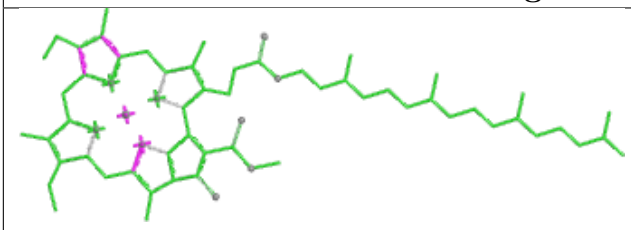
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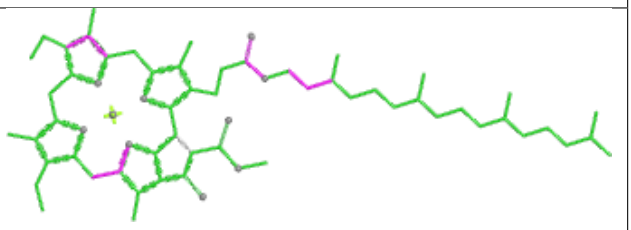
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	813	CLA	1	0
14	B	806	CLA	1	0
14	B	811	CLA	2	0
14	B	825	CLA	2	0
14	B	807	CLA	1	0
14	B	819	CLA	2	0
14	A	804	CLA	2	0
17	A	851	BCR	2	0
14	A	839	CLA	1	0
14	B	830	CLA	1	0
17	L	205	BCR	2	0
14	A	818	CLA	1	0
14	B	837	CLA	3	0
14	A	826	CLA	1	0
14	B	833	CLA	1	0
14	A	829	CLA	1	0
14	B	816	CLA	1	0

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

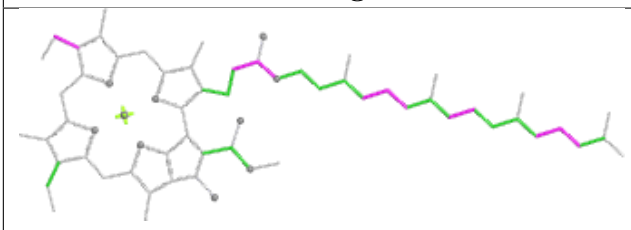
Ligand CLA B 821



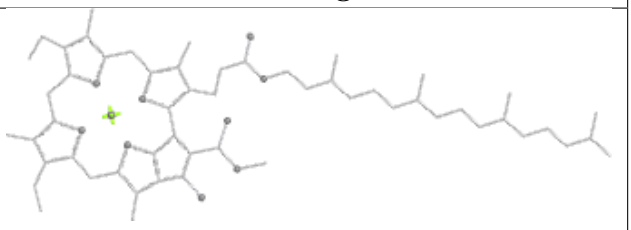
Bond lengths



Bond angles

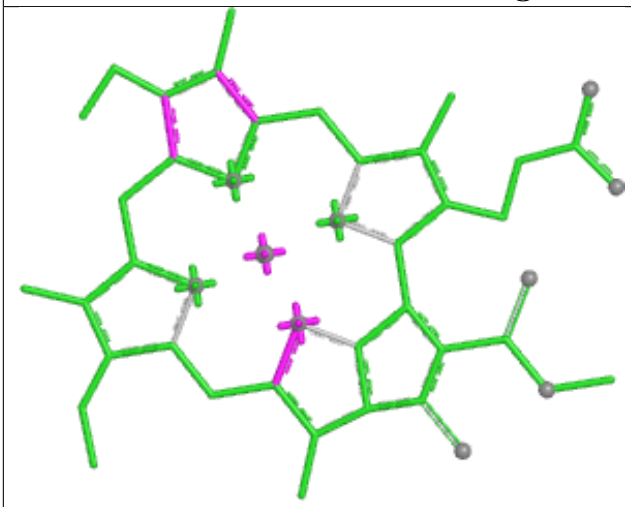


Torsions

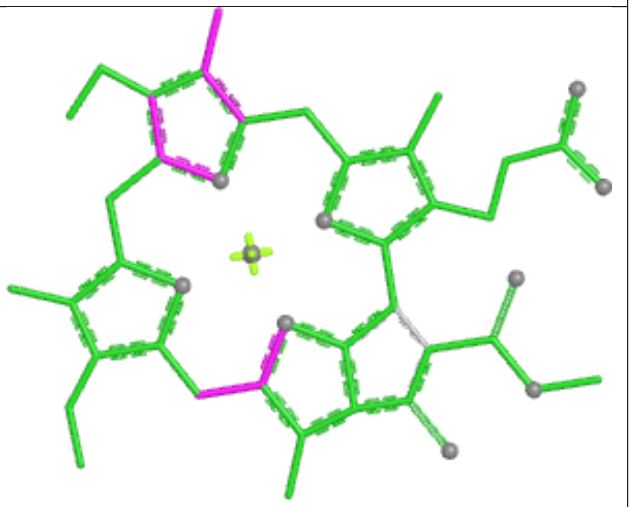


Rings

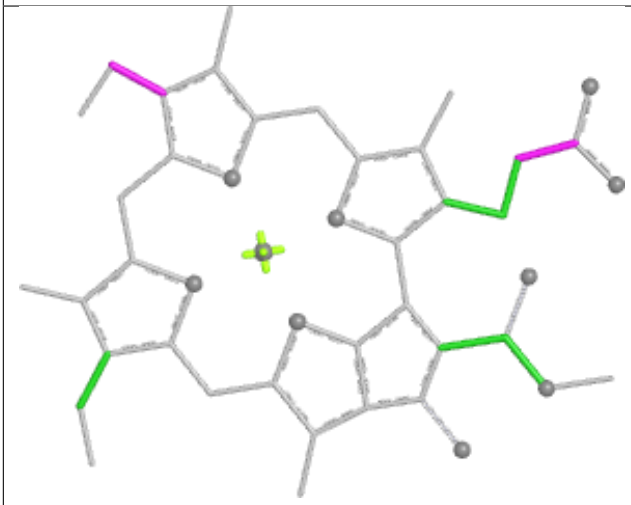
Ligand CLA K 4002



Bond lengths



Bond angles

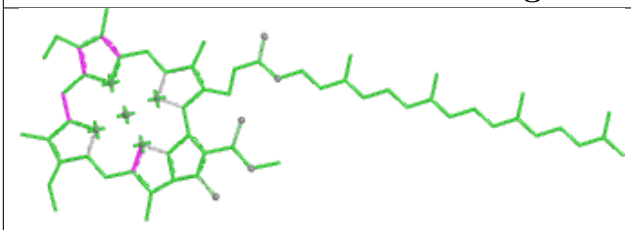


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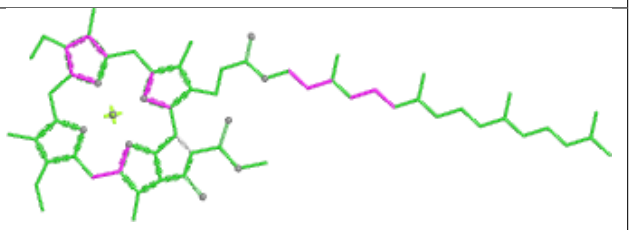


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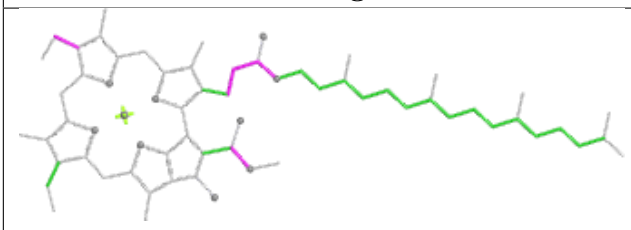
Ligand CLA A 843



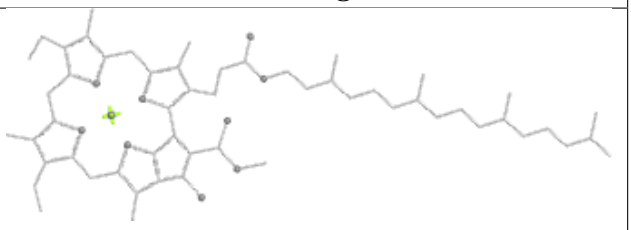
Bond lengths



Bond angles

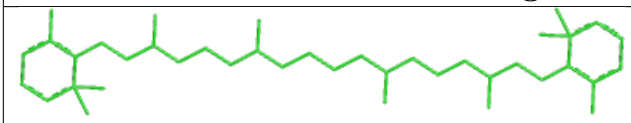


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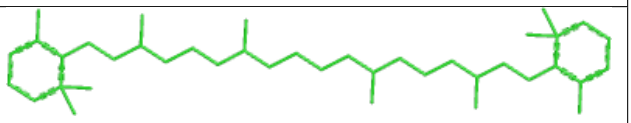


Rings

Ligand BCR A 850



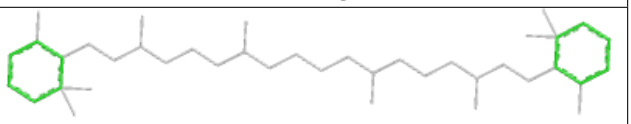
Bond lengths



Bond angles

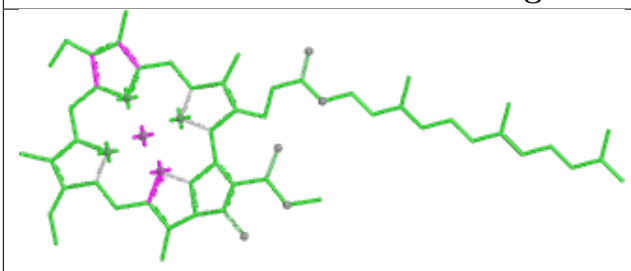


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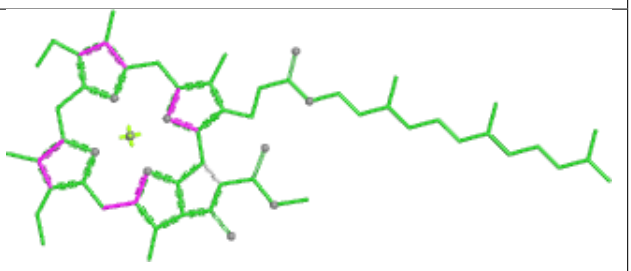


Rings

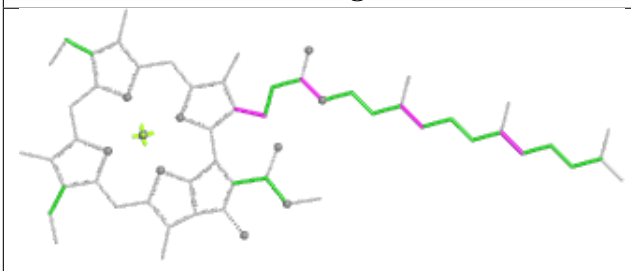
Ligand CLA B 817



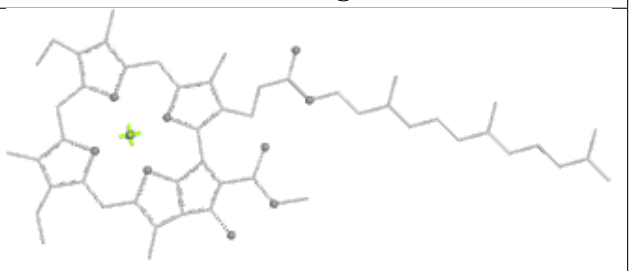
Bond lengths



Bond angles

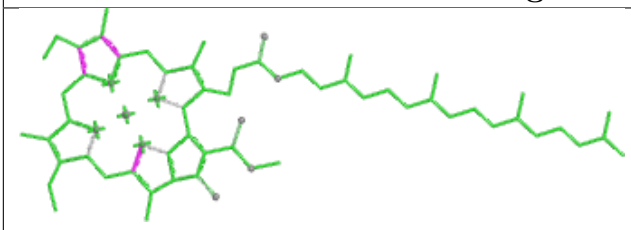


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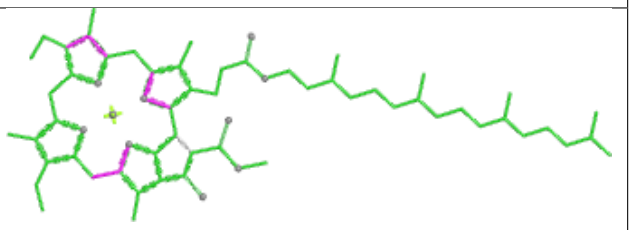


Rings

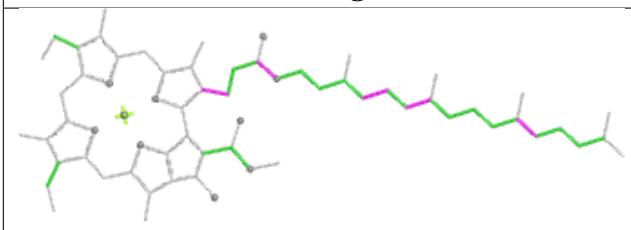
Ligand CLA L 202



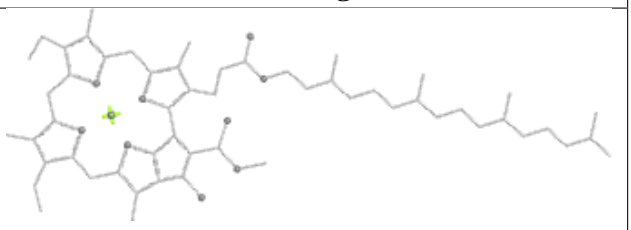
Bond lengths



Bond angles

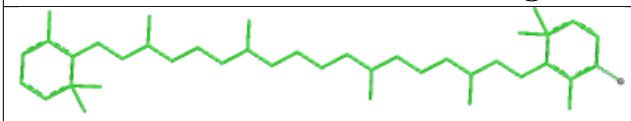


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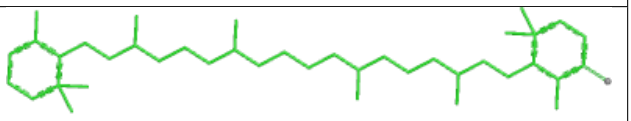


Rings

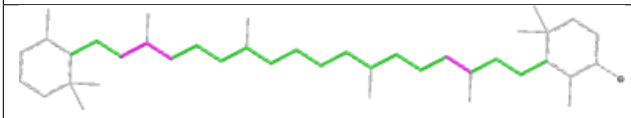
Ligand ECH B 846



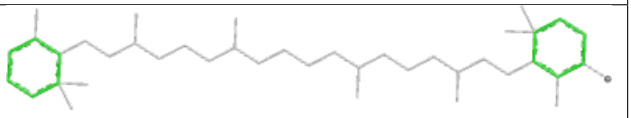
Bond lengths



Bond angles

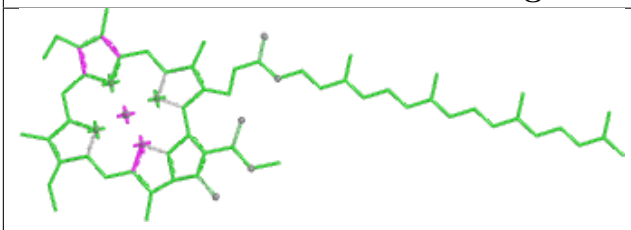


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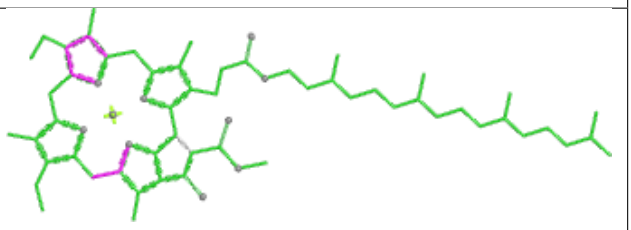


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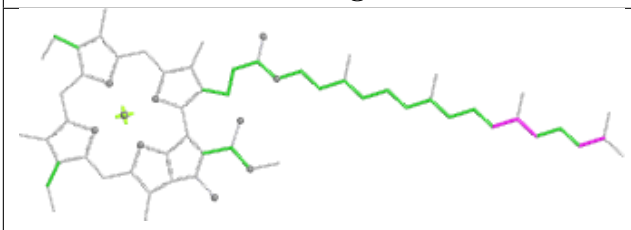
Ligand CLA B 827



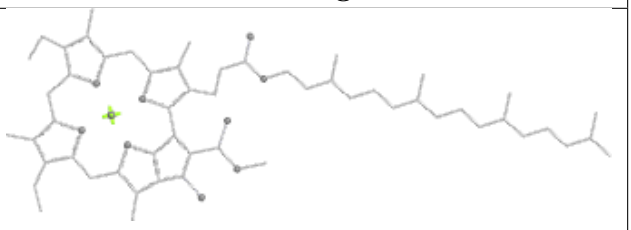
Bond lengths



Bond angles

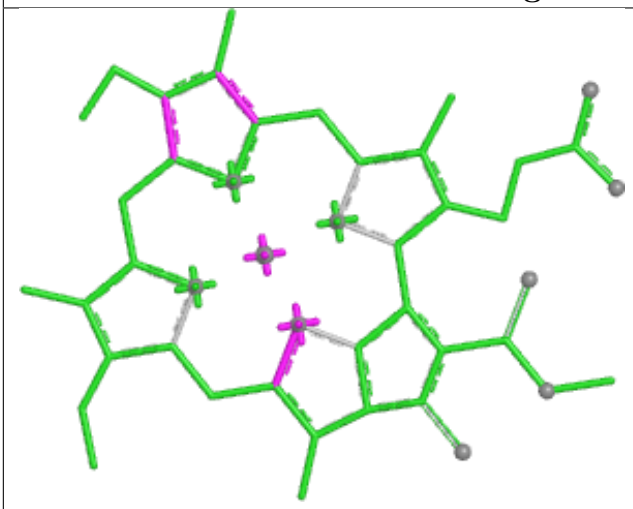


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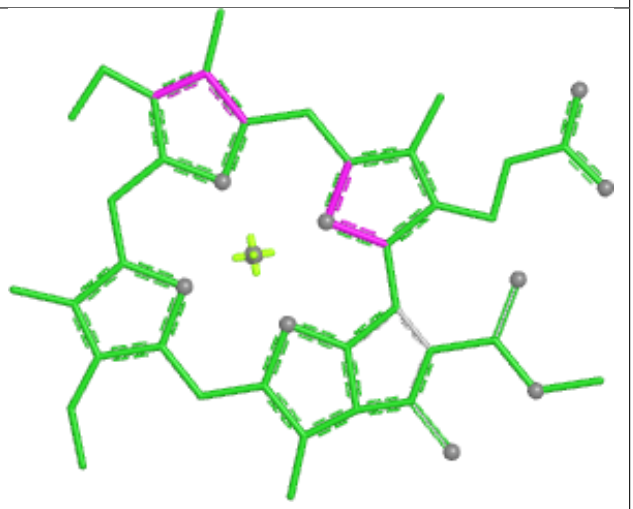


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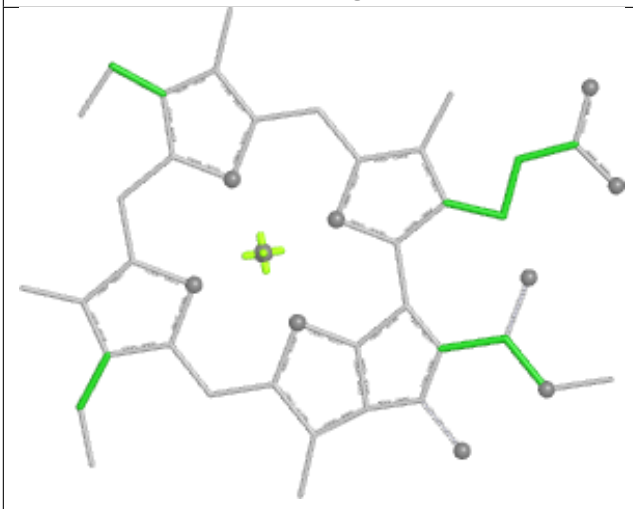
Ligand CLA A 816



Bond lengths



Bond angles

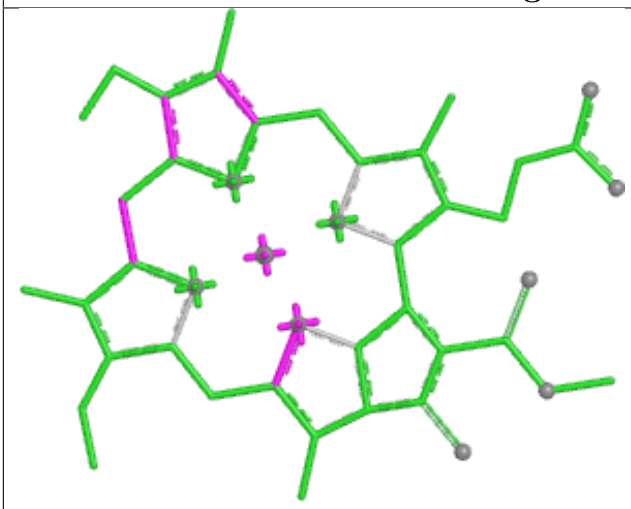


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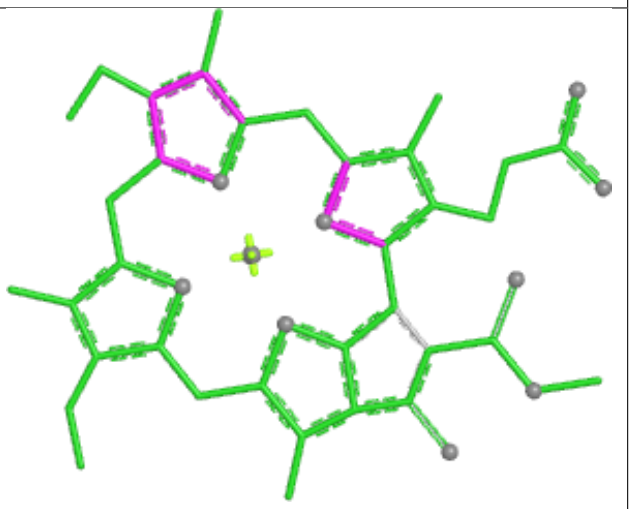


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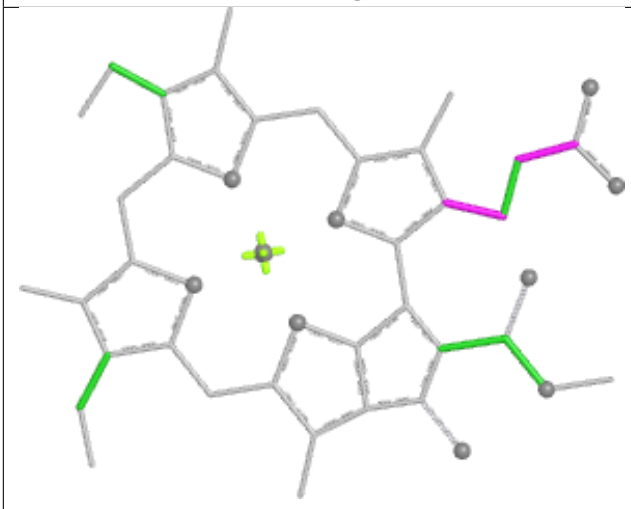
Ligand CLA A 811



Bond lengths



Bond angles

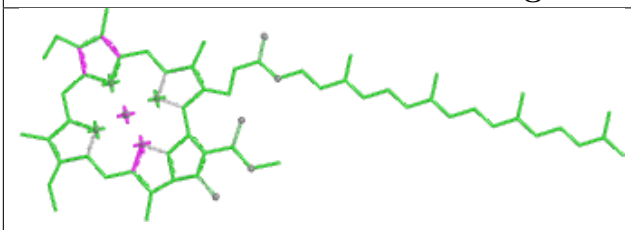


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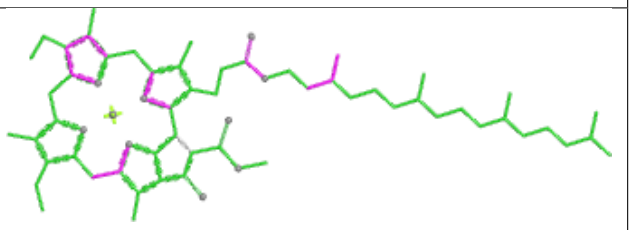


Rings

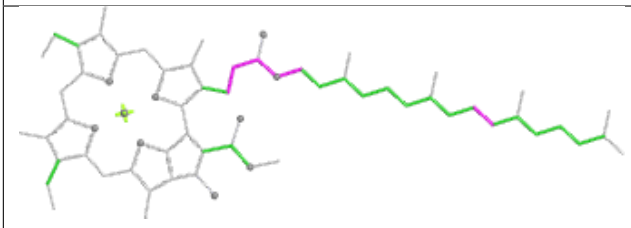
Ligand CLA B 818



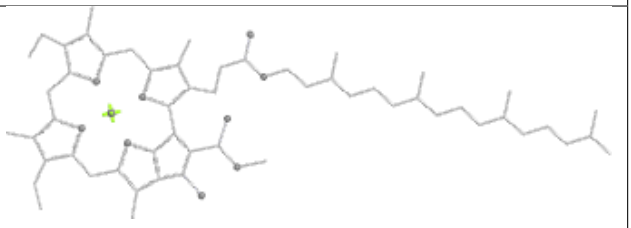
Bond lengths



Bond angles

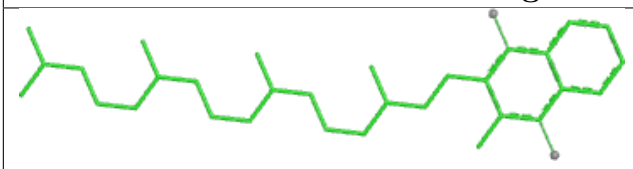


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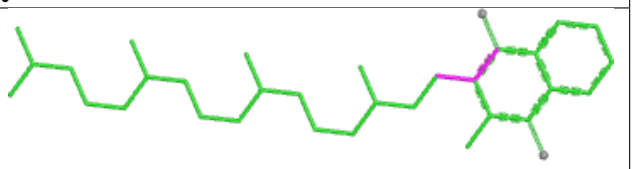


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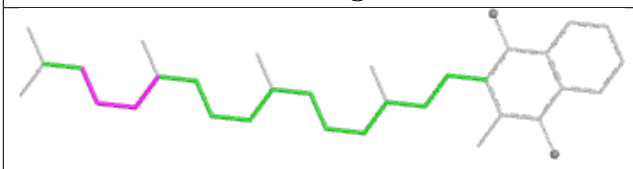
Ligand PQN B 843



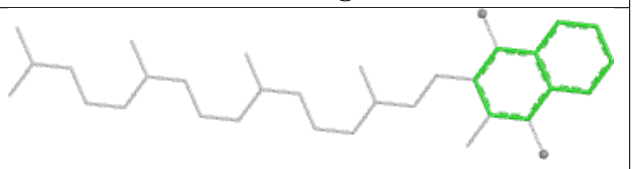
Bond lengths



Bond angles



Torsions

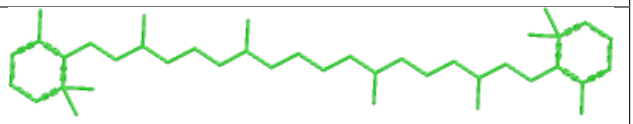


Rings

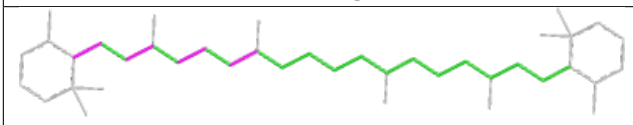
Ligand BCR J 1104



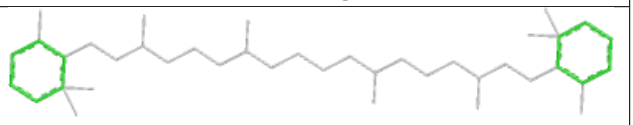
Bond lengths



Bond angles

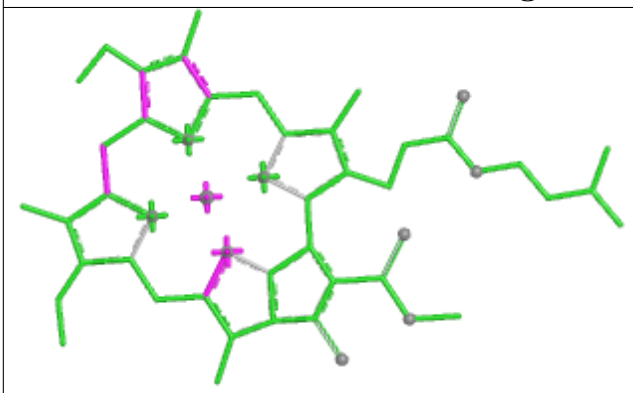


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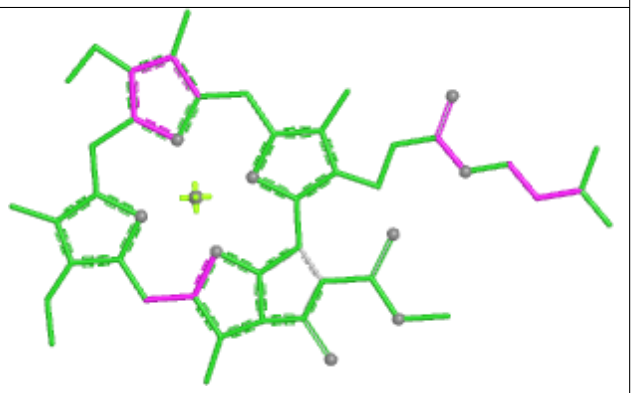


Rings

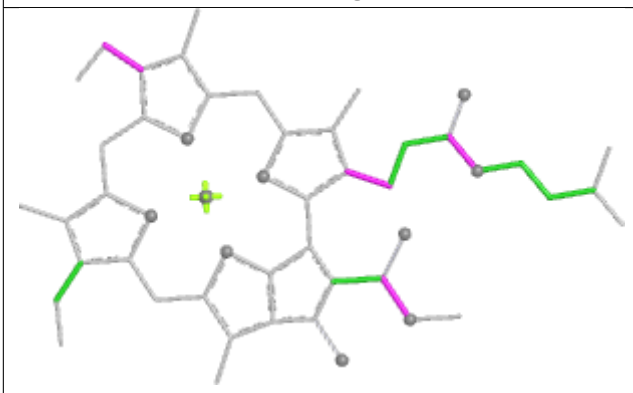
Ligand CLA J 1103



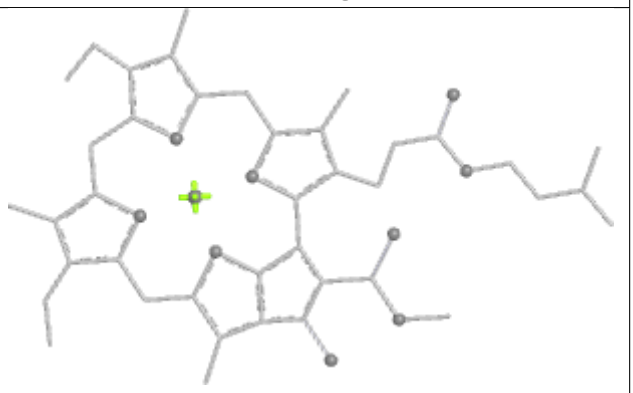
Bond lengths



Bond angles

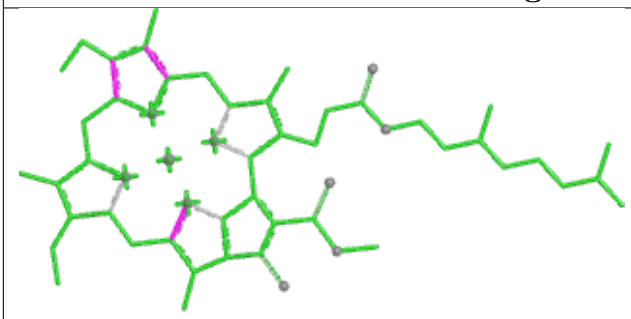


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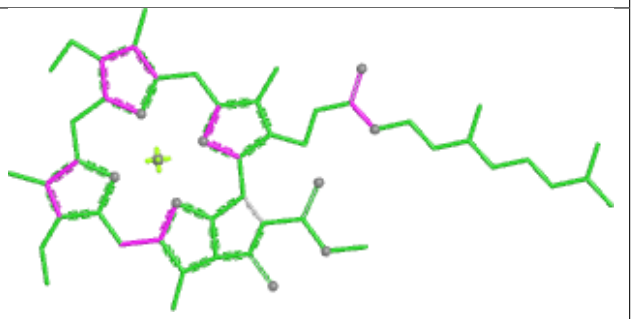


Rings

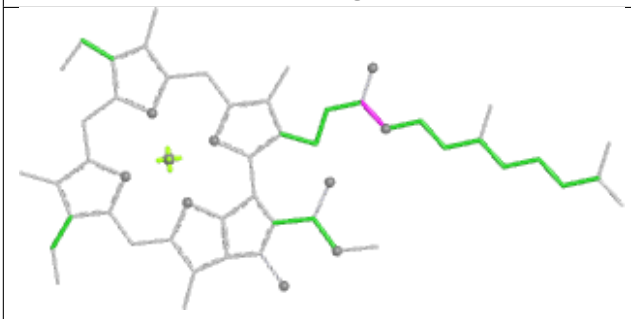
Ligand CLA B 832



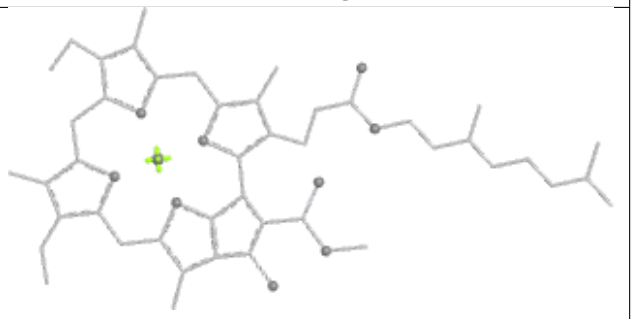
Bond lengths



Bond angles

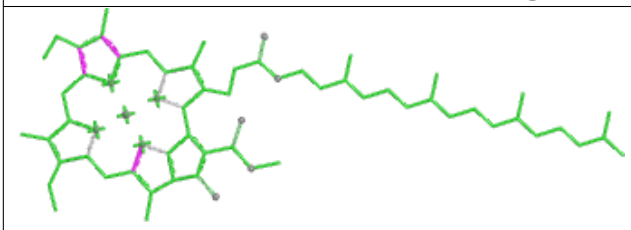


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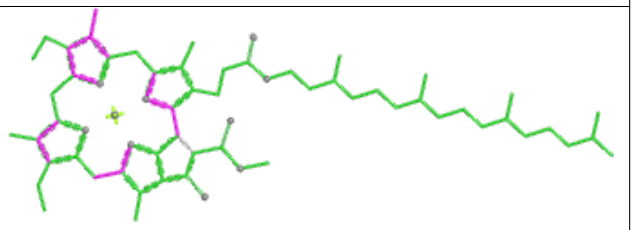


Rings

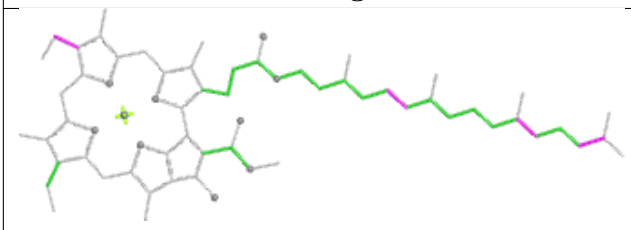
Ligand CLA A 834



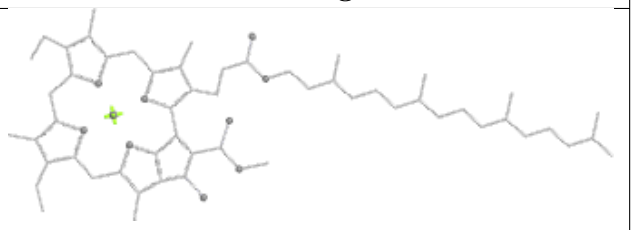
Bond lengths



Bond angles

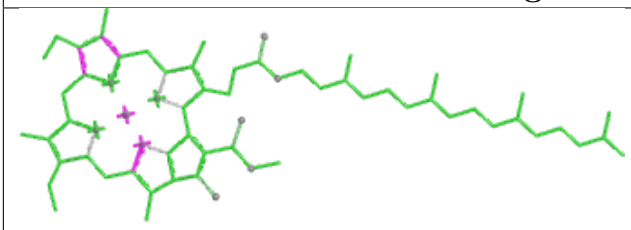


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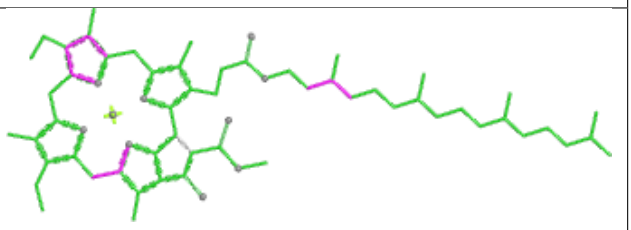


Rings

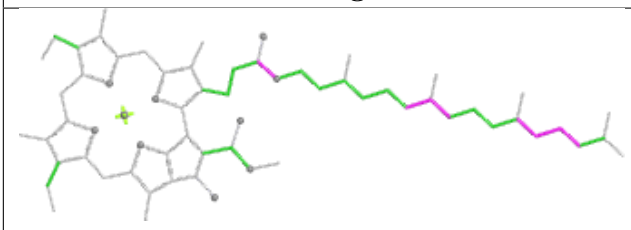
Ligand CLA B 838



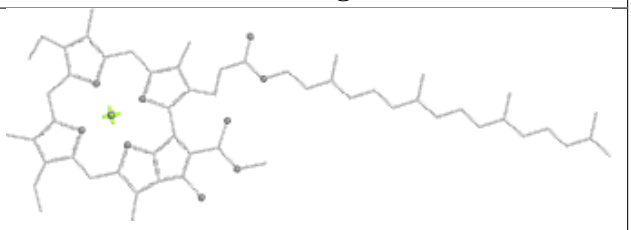
Bond lengths



Bond angles

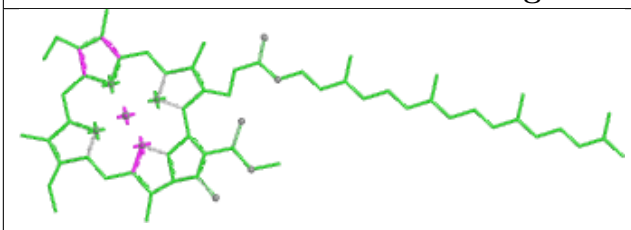


Torsions

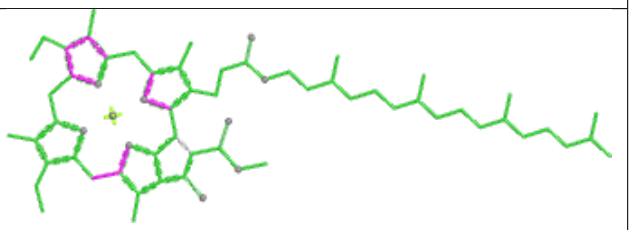


Rings

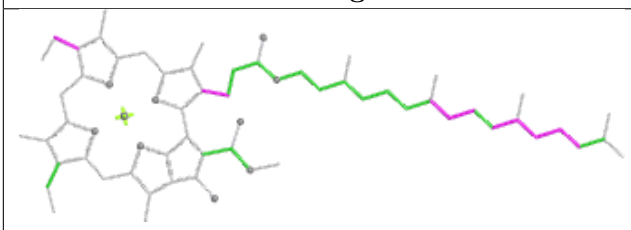
Ligand CLA A 825



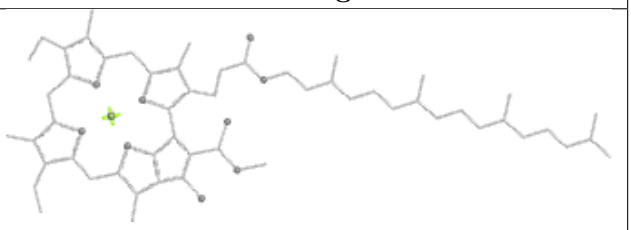
Bond lengths



Bond angles

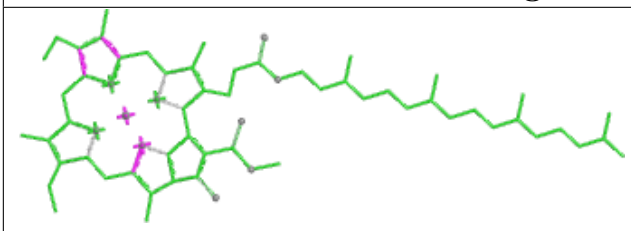


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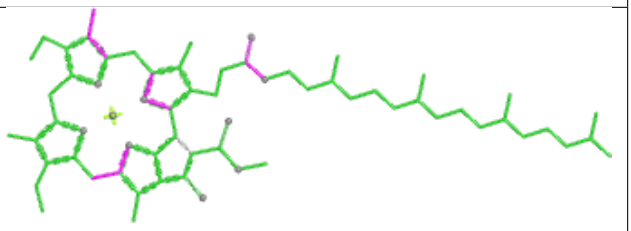


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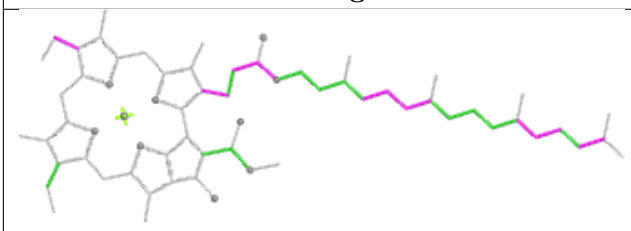
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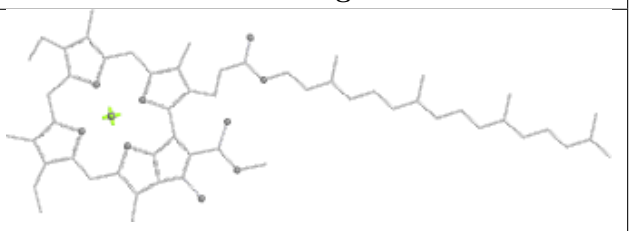
Bond lengths



Bond angles

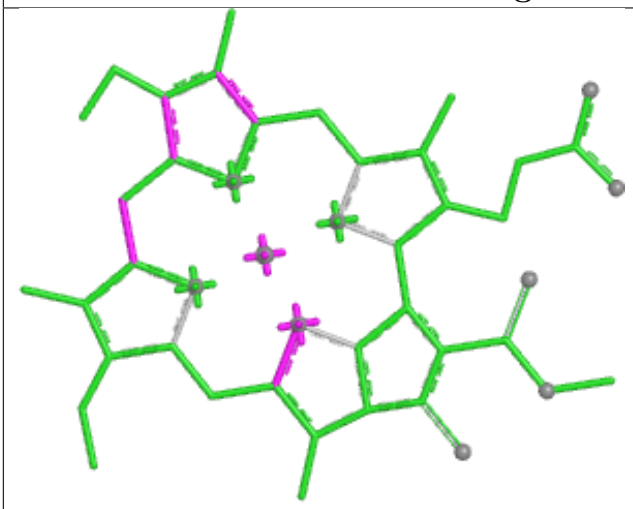


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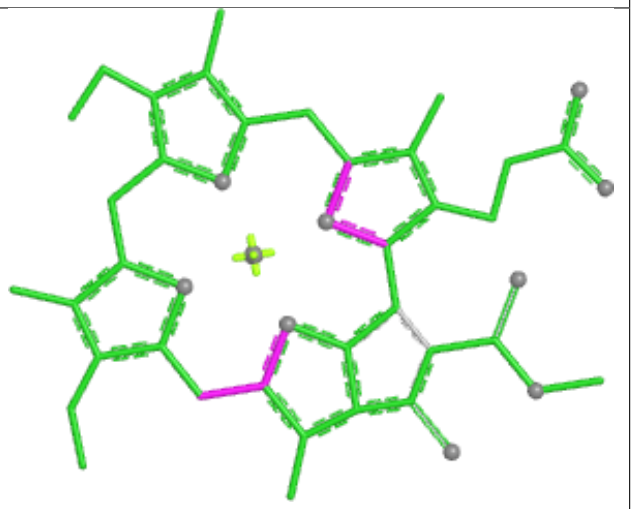


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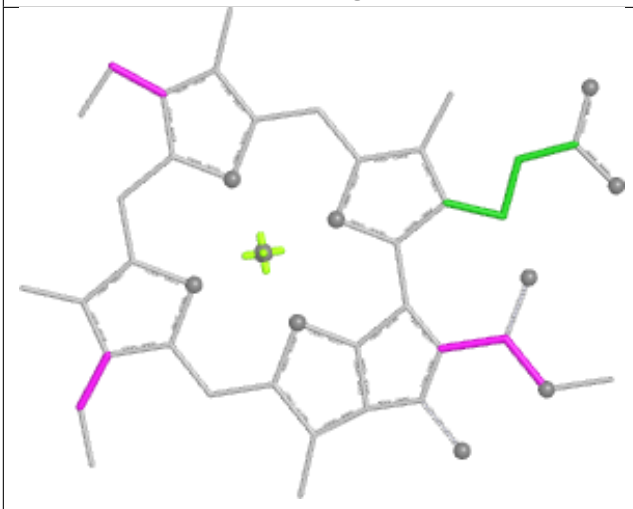
Ligand CLA K 4003



Bond lengths



Bond angles

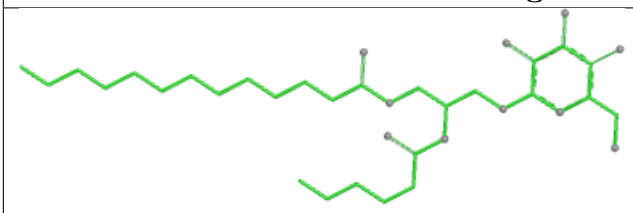


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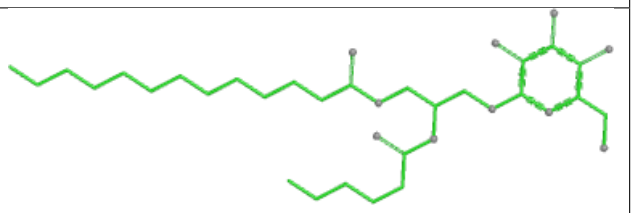


Rings

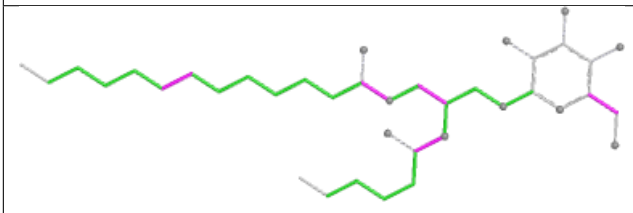
Ligand LMG I 101



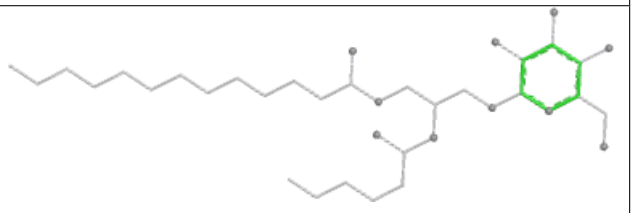
Bond lengths



Bond angles

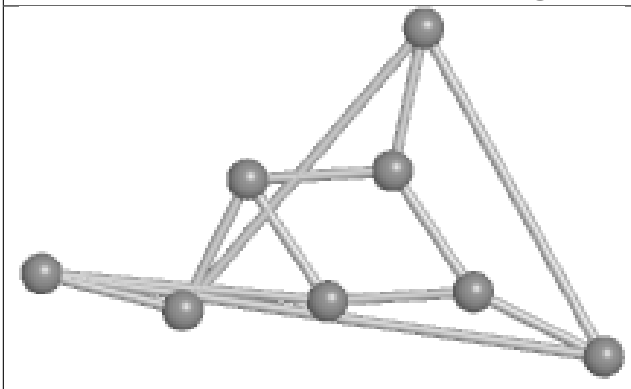


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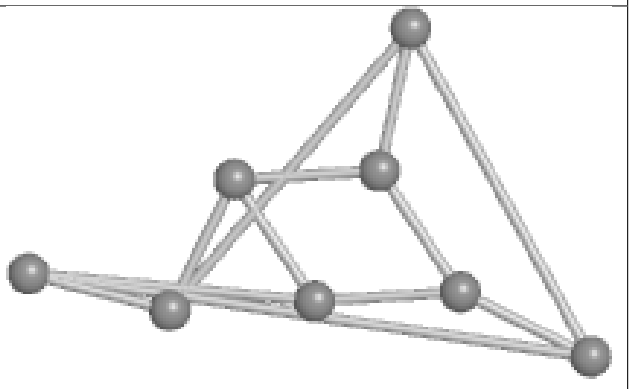


Rings

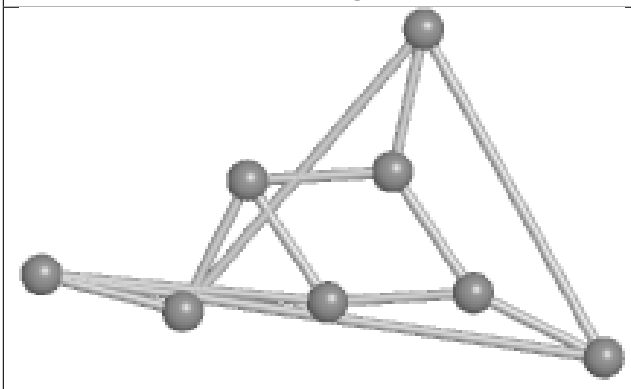
Ligand SF4 C 102



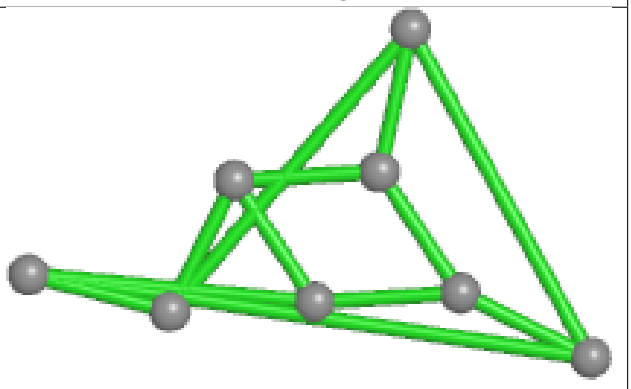
Bond lengths



Bond angles

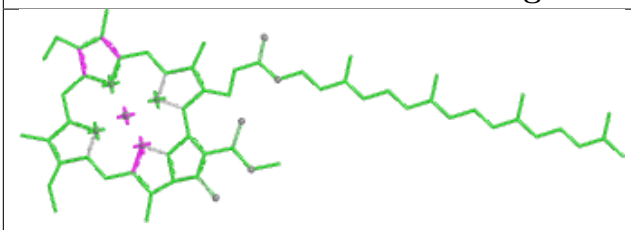


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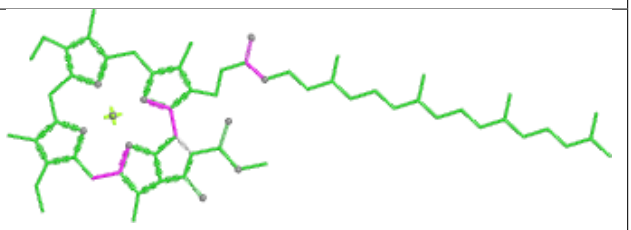


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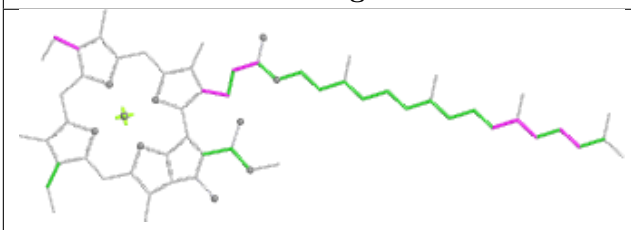
Ligand CLA A 819



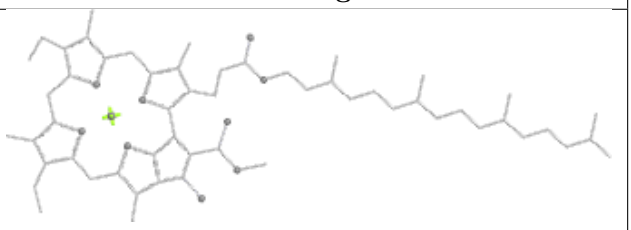
Bond lengths



Bond angles

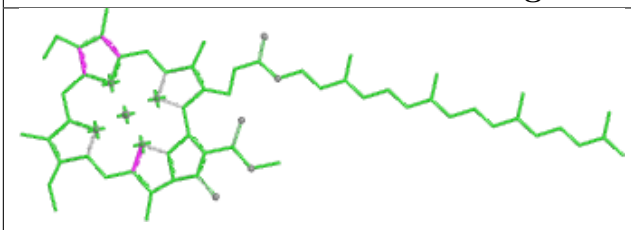


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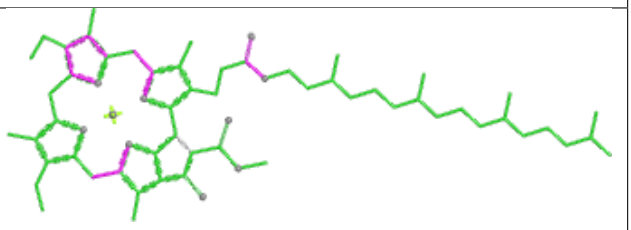


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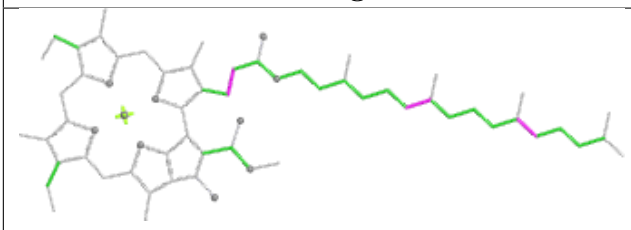
Ligand CLA B 840



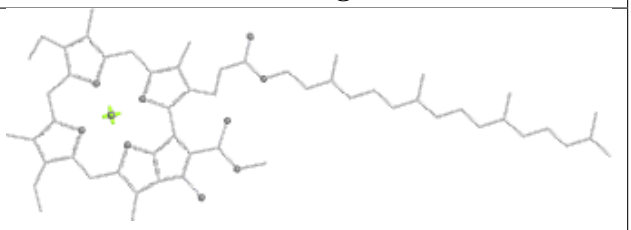
Bond lengths



Bond angles

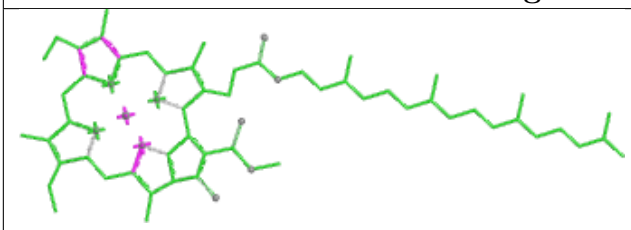


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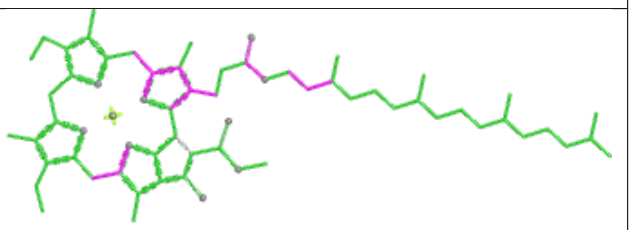


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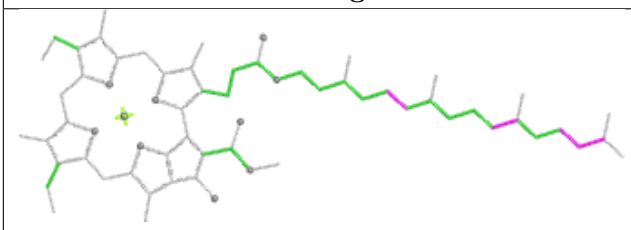
Ligand CLA A 820



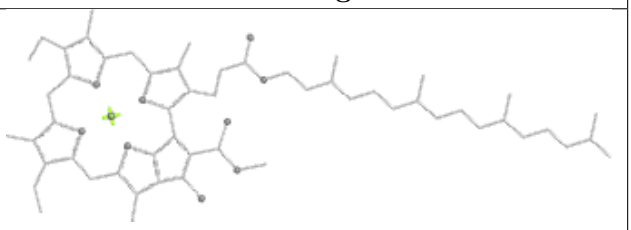
Bond lengths



Bond angles



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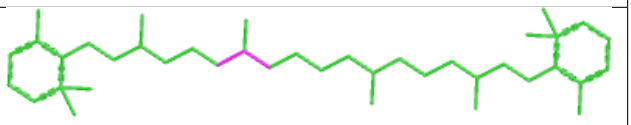


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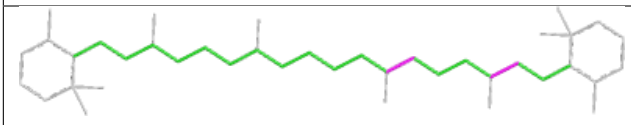
Ligand BCR F 202



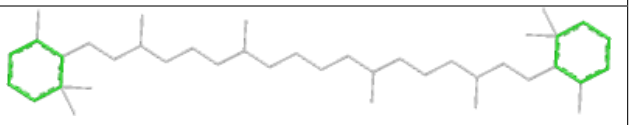
Bond lengths



Bond angles

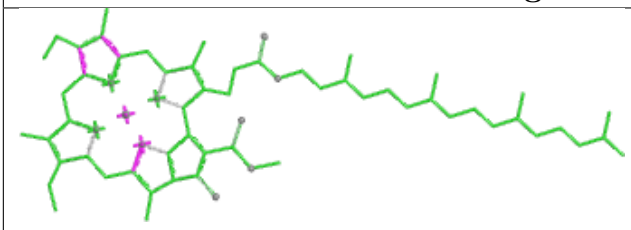


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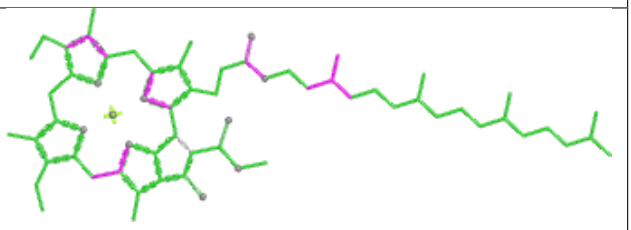


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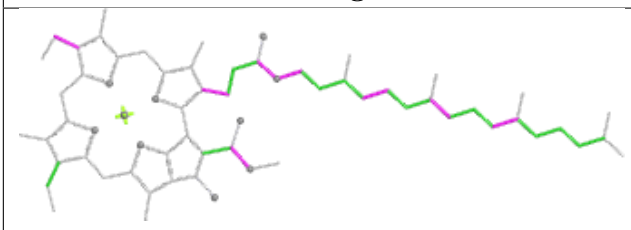
Ligand CLA B 841



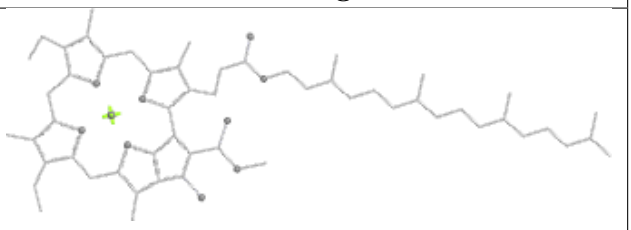
Bond lengths



Bond angles

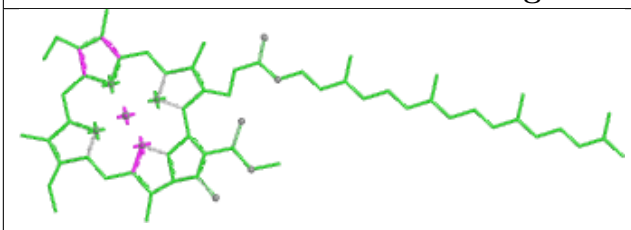


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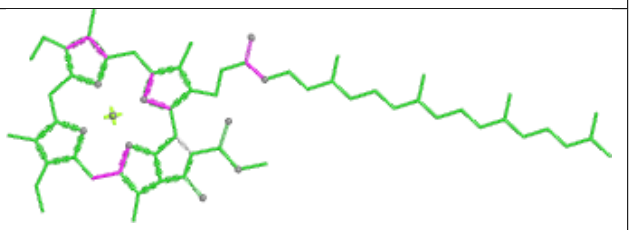


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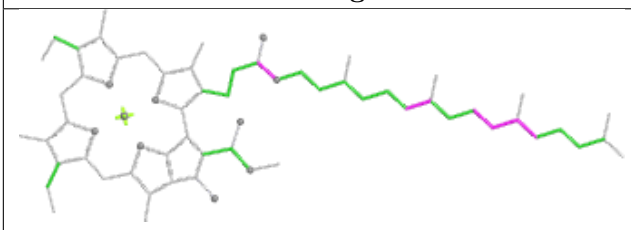
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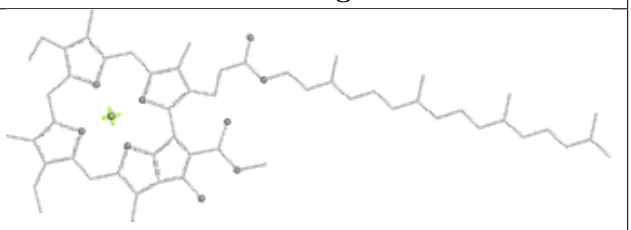
Bond lengths



Bond angles

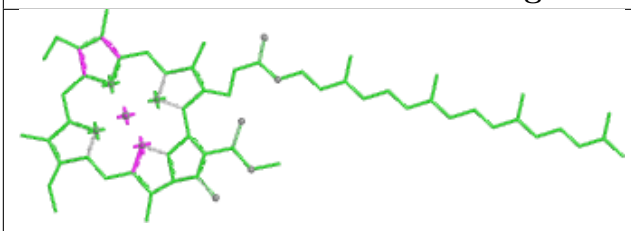


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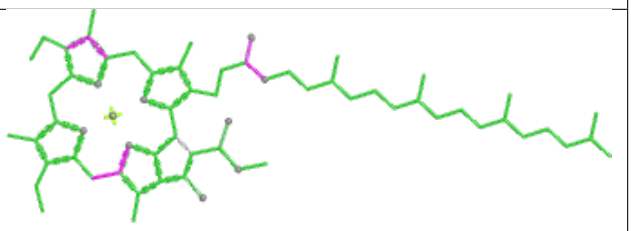


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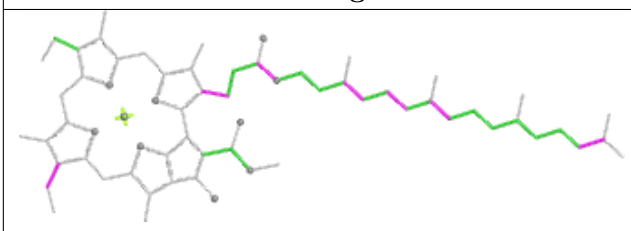
Ligand CLA B 814



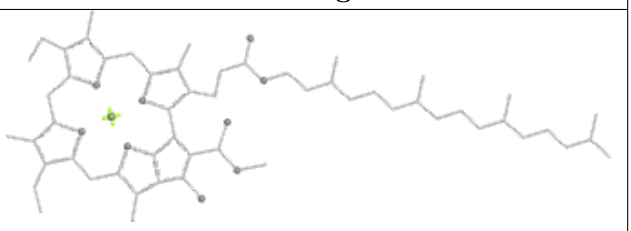
Bond lengths



Bond angles

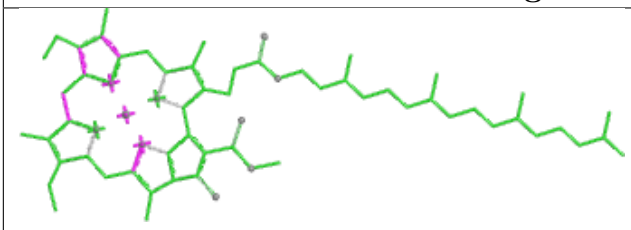


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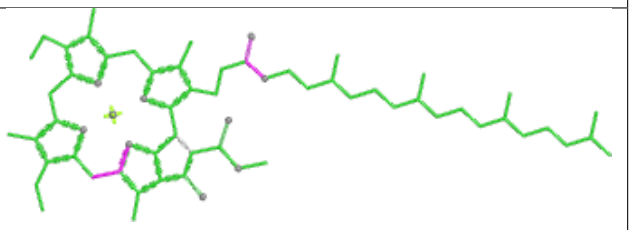


Rings

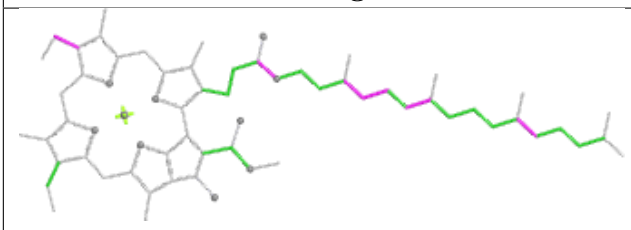
Ligand CLA B 820



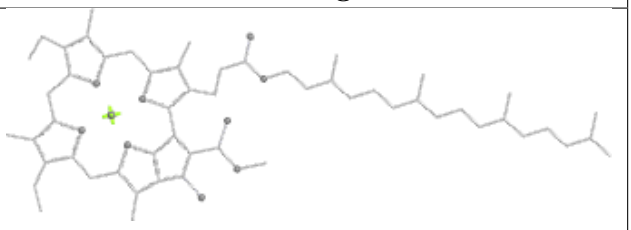
Bond lengths



Bond angles

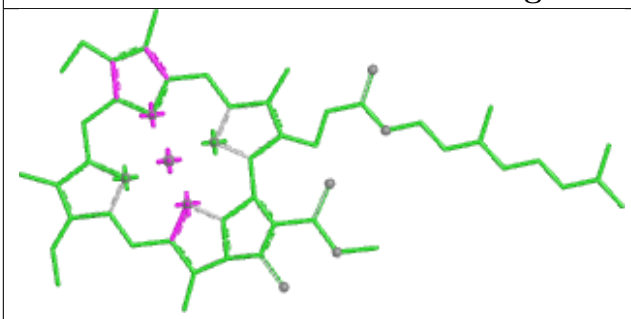


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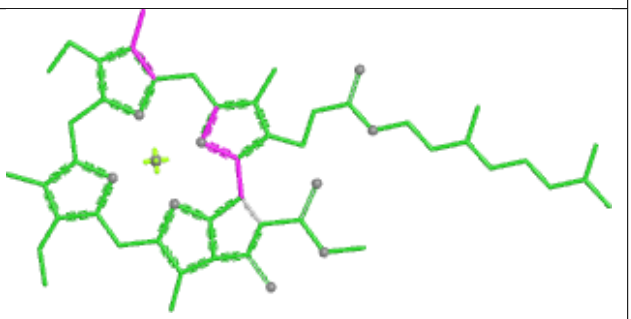


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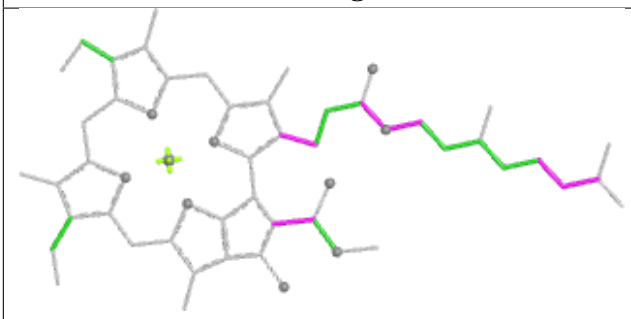
Ligand CLA B 813



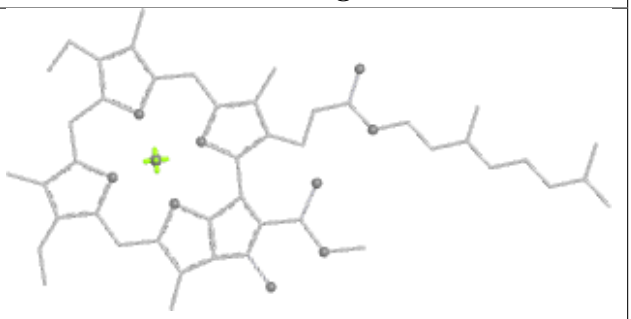
Bond lengths



Bond angles

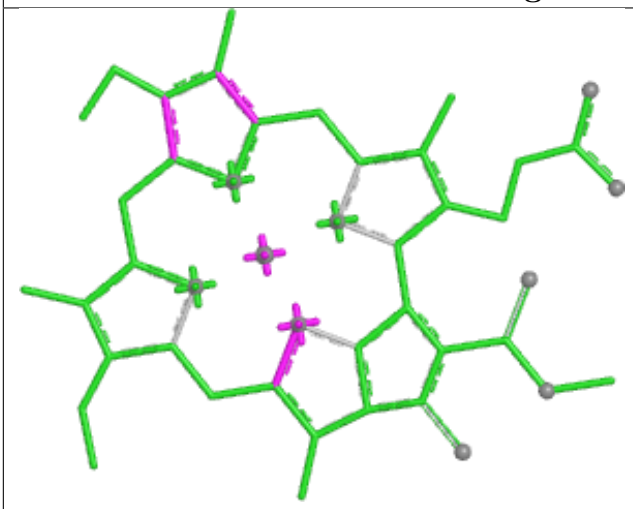


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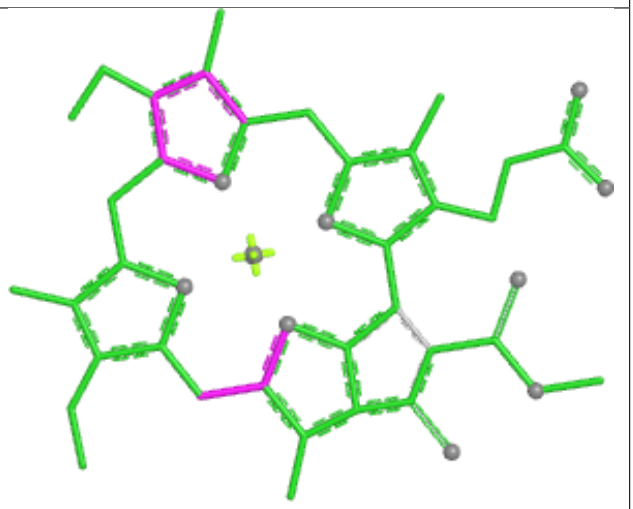


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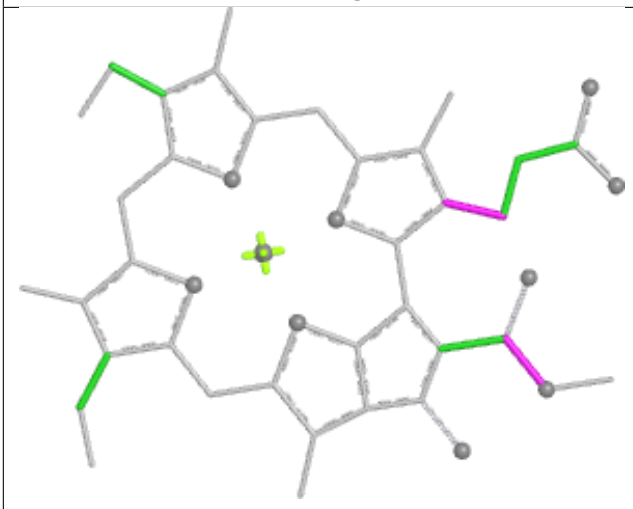
Ligand CLA B 823



Bond lengths



Bond angles

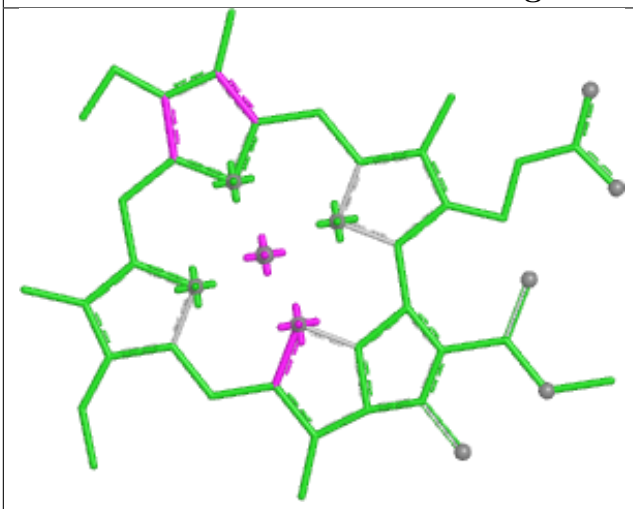


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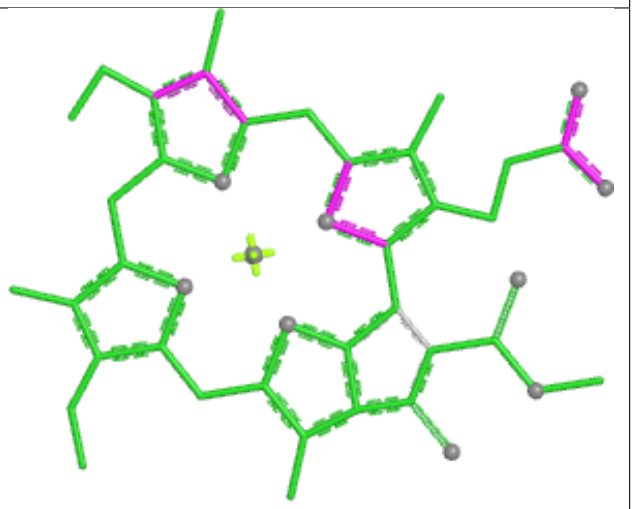


Rings

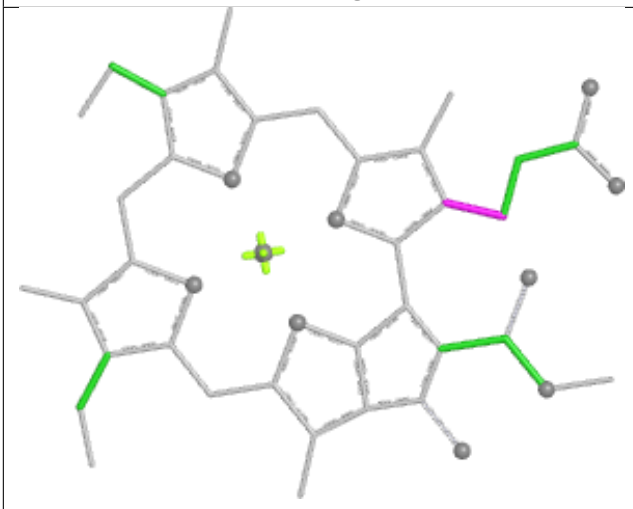
Ligand CLA B 835



Bond lengths



Bond angles

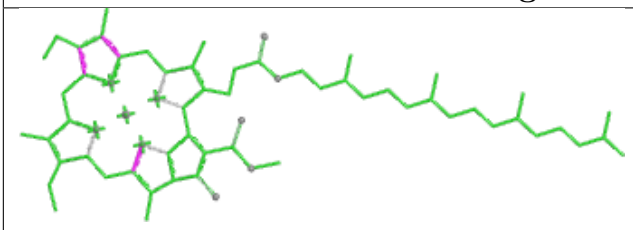


Torsions

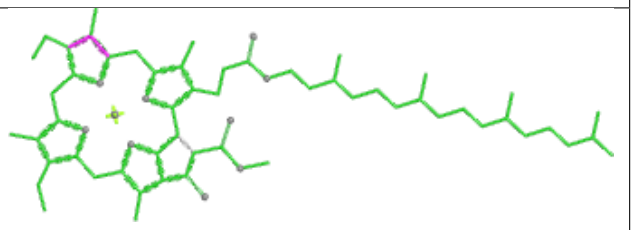


Rings

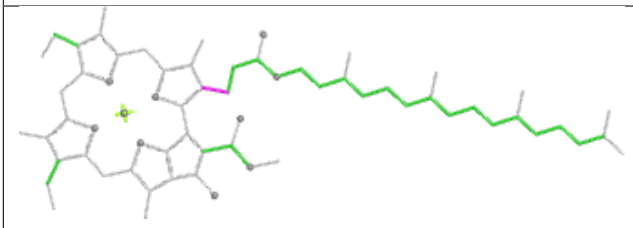
Ligand CLA J 1101



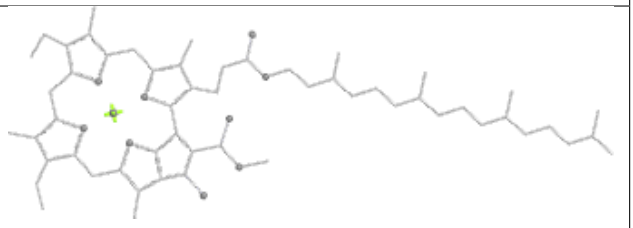
Bond lengths



Bond angles

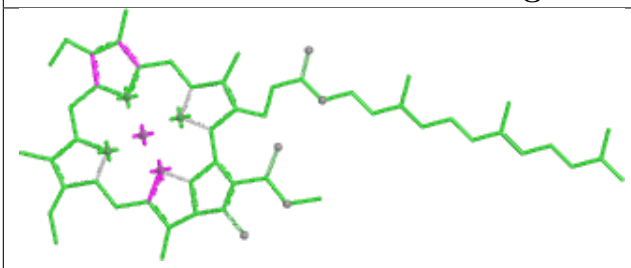


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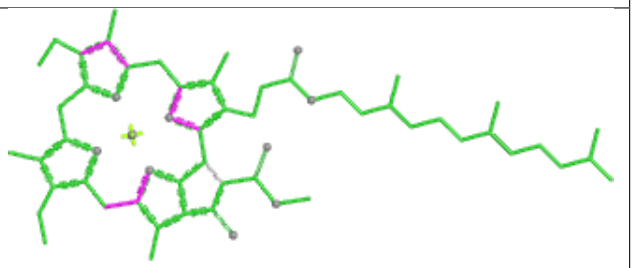


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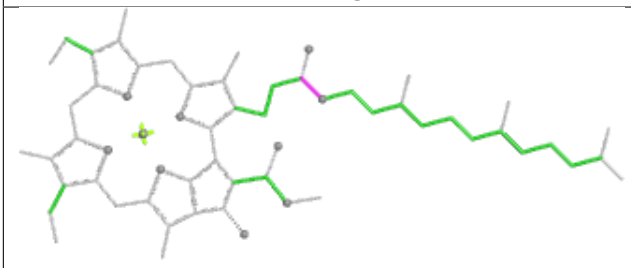
Ligand CLA A 833



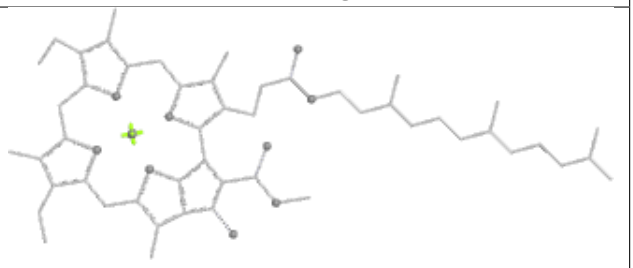
Bond lengths



Bond angles

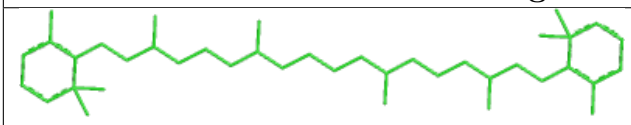


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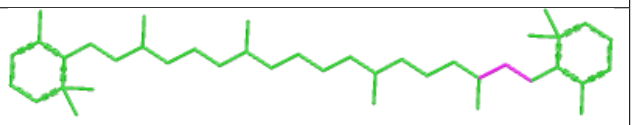


Rings

Ligand BCR I 102



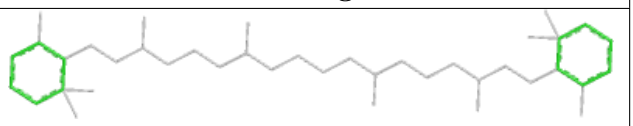
Bond lengths



Bond angles



Torsions



Rings

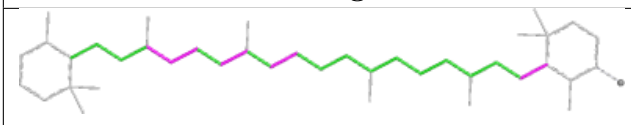
Ligand ECH M 102



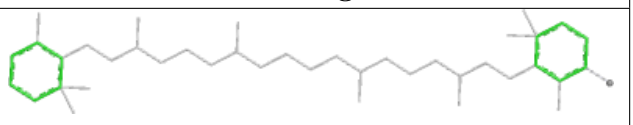
Bond lengths



Bond angles

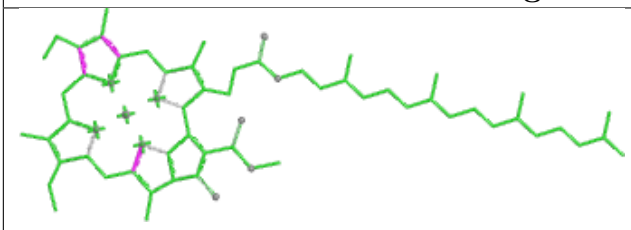


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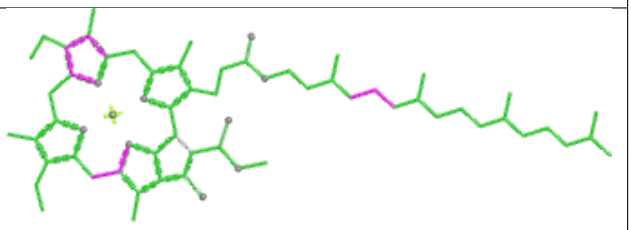


Rings

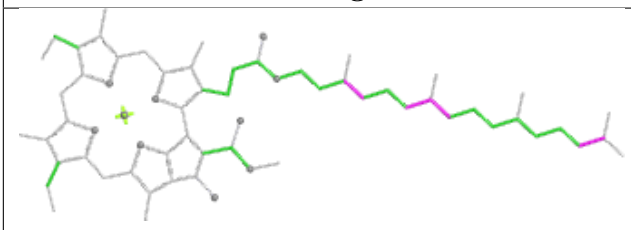
Ligand CLA A 822



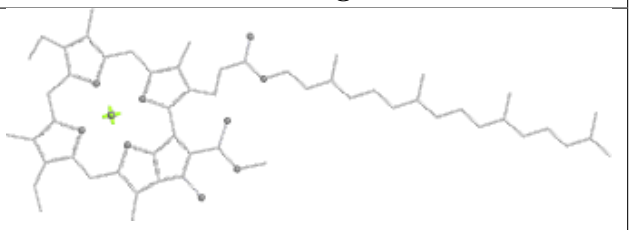
Bond lengths



Bond angles

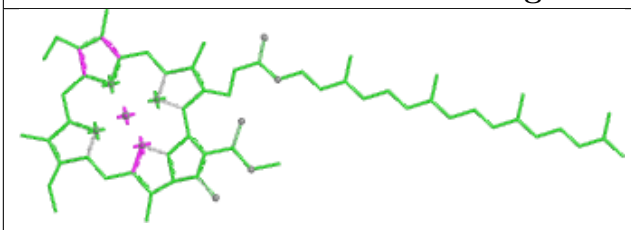


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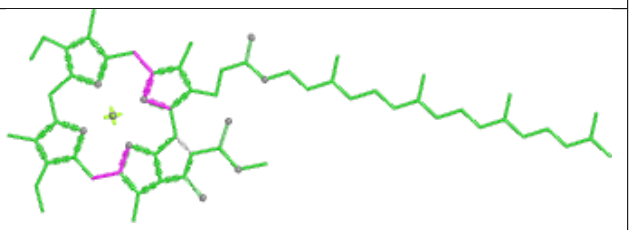


Rings

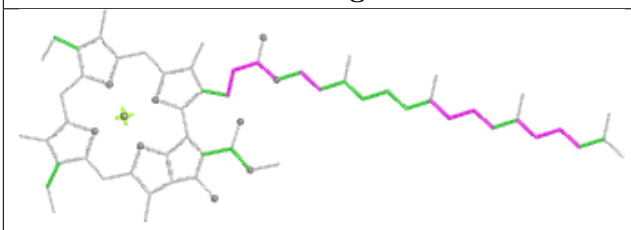
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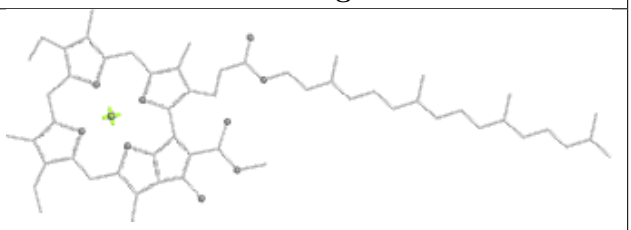
Bond lengths



Bond angles

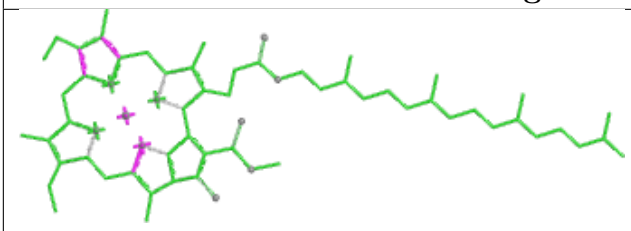


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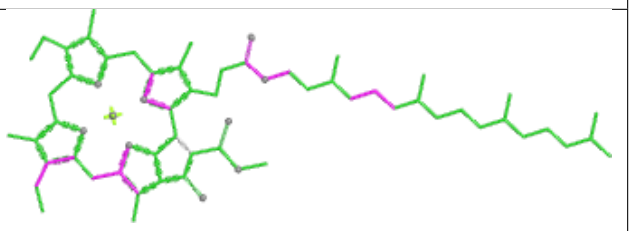


Rings

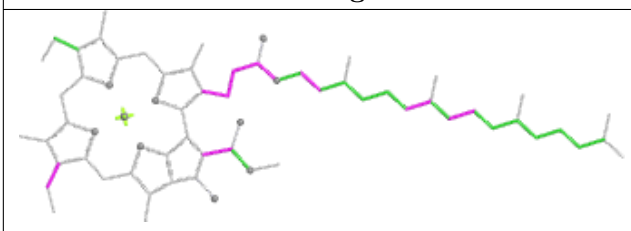
Ligand CLA A 806



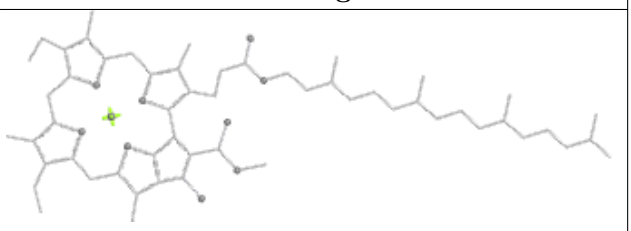
Bond lengths



Bond angles

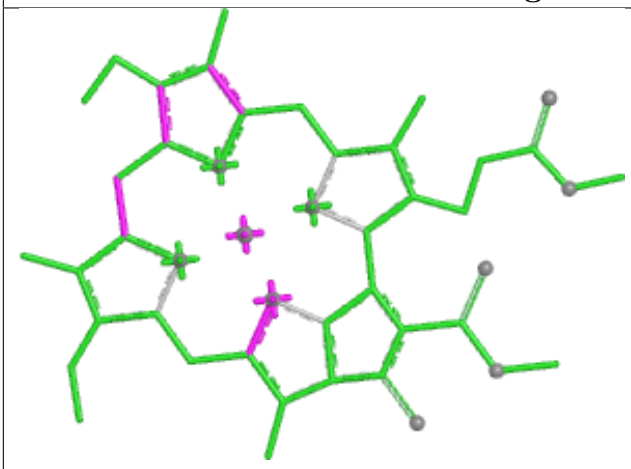


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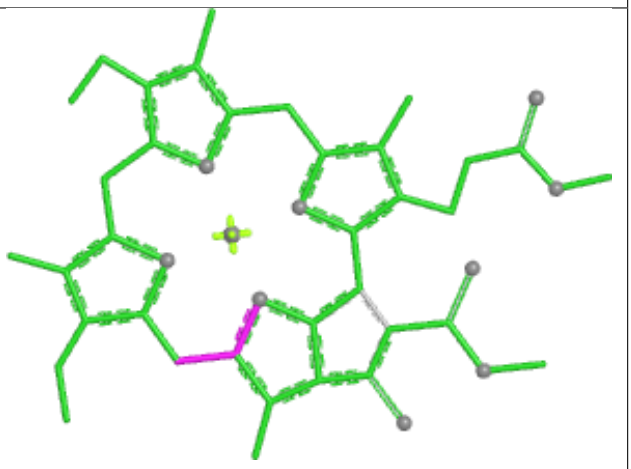


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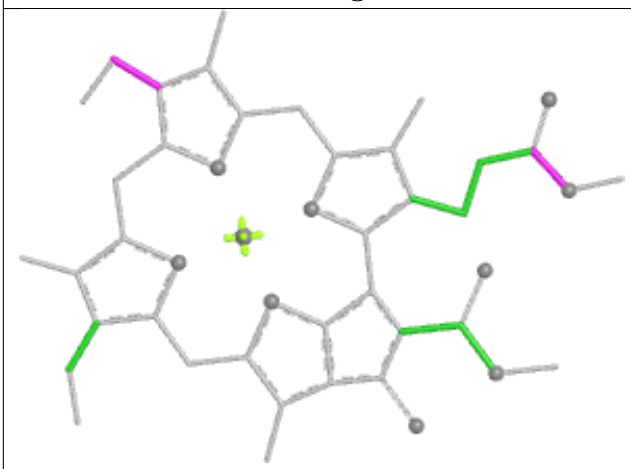
Ligand CLA B 836



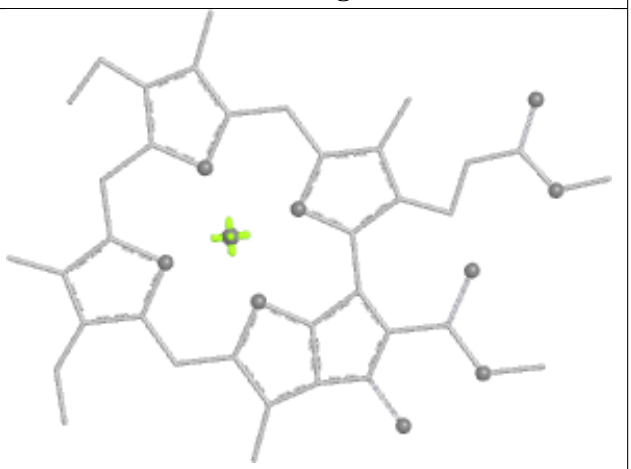
Bond lengths



Bond angles

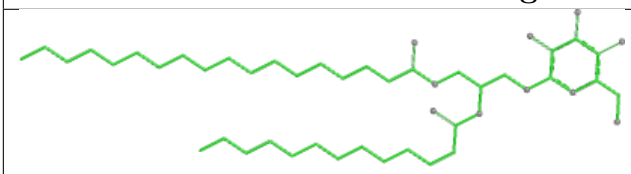


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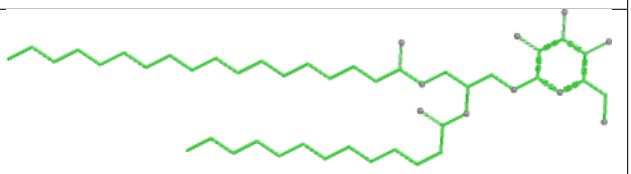


Rings

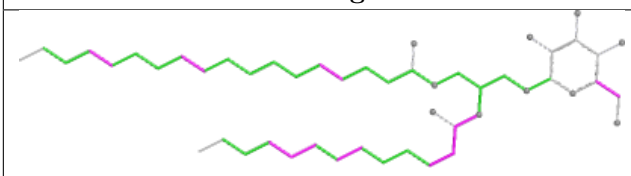
Ligand LMG B 802



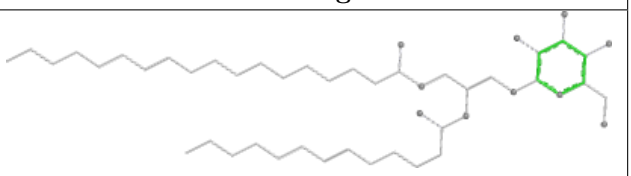
Bond lengths



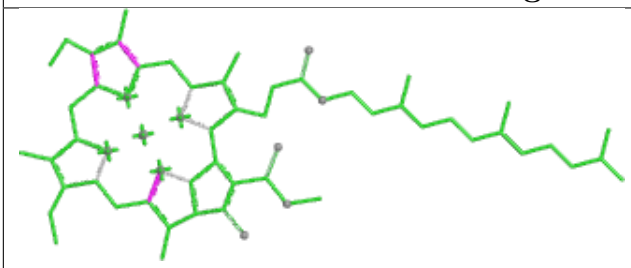
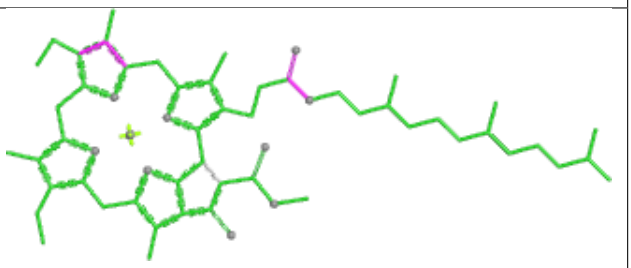
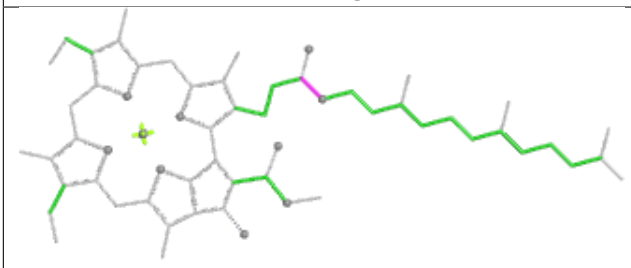
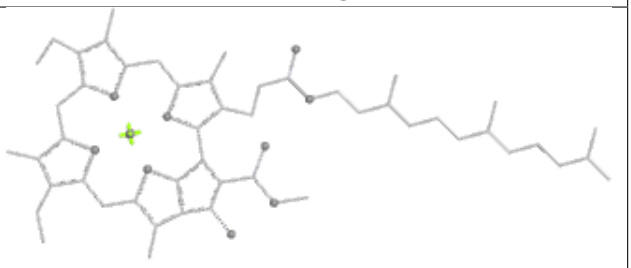
Bond angles

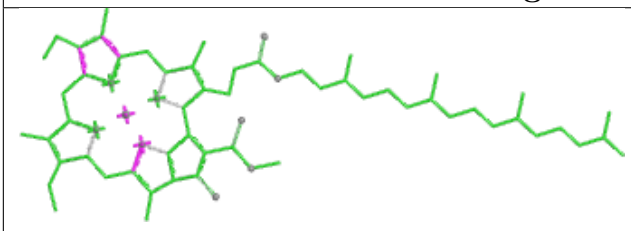
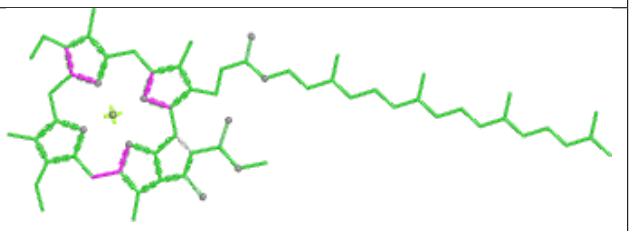
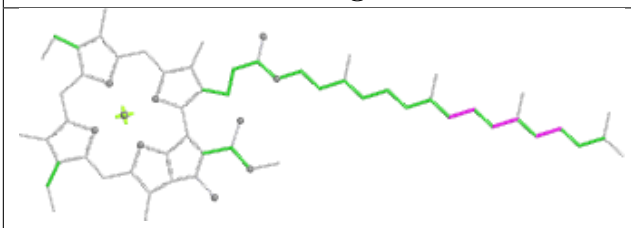
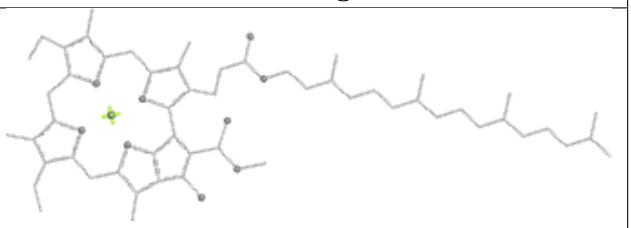


Torsions

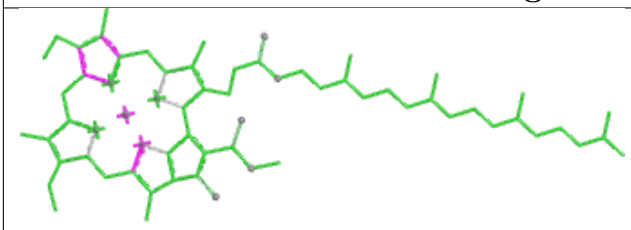


Rings

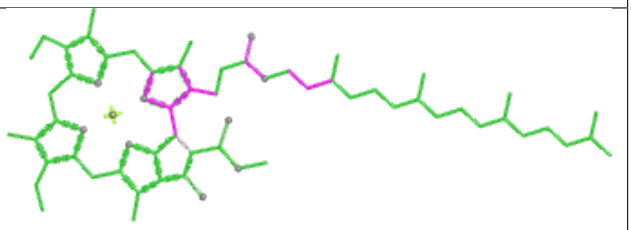
Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

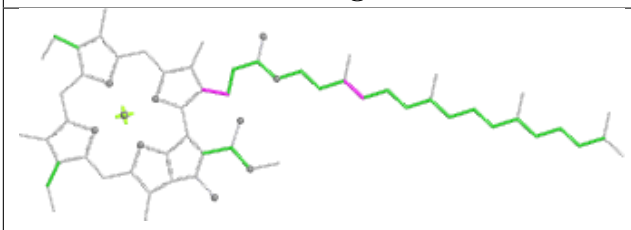
Ligand CLA B 808



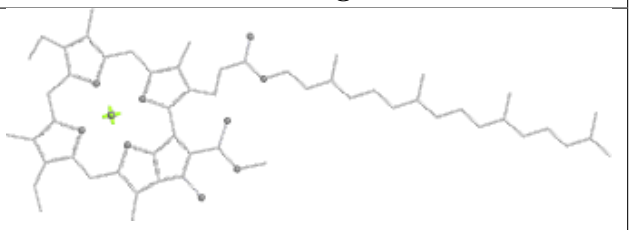
Bond lengths



Bond angles

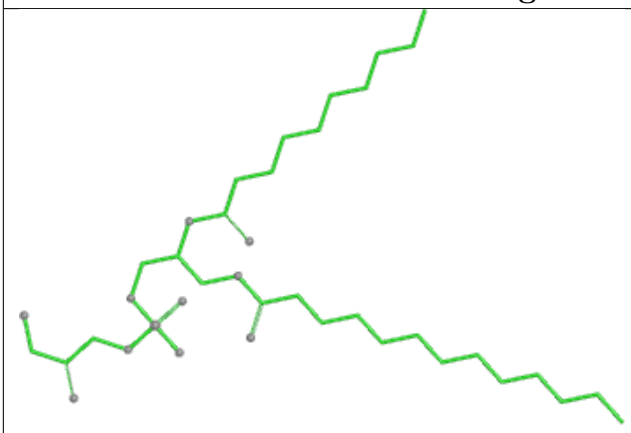


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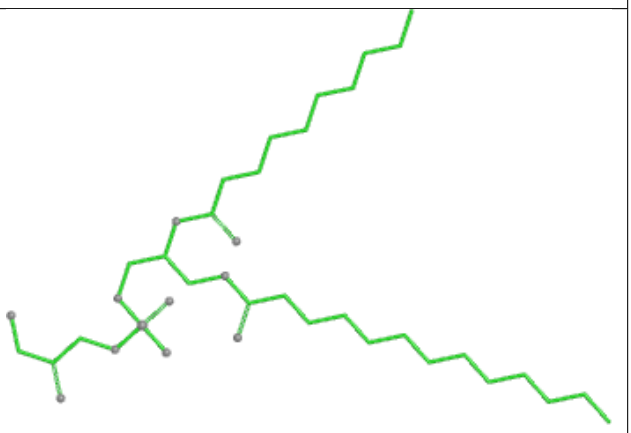


Rings

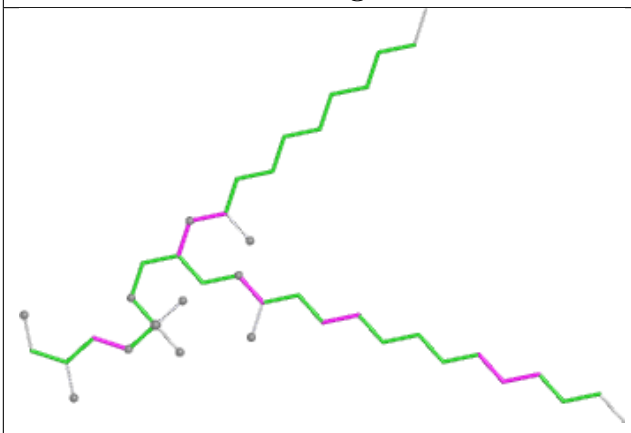
Ligand LHG M 101



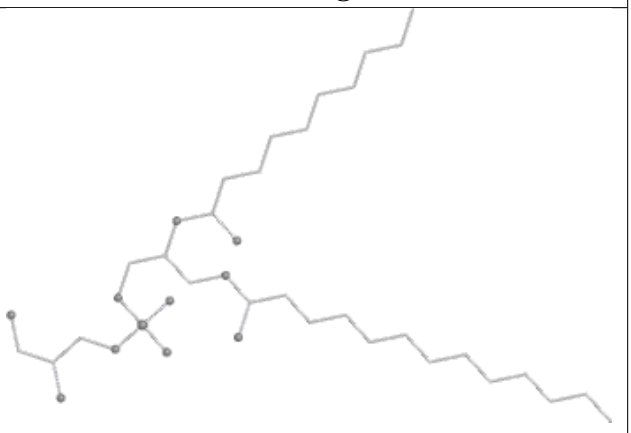
Bond lengths



Bond angles

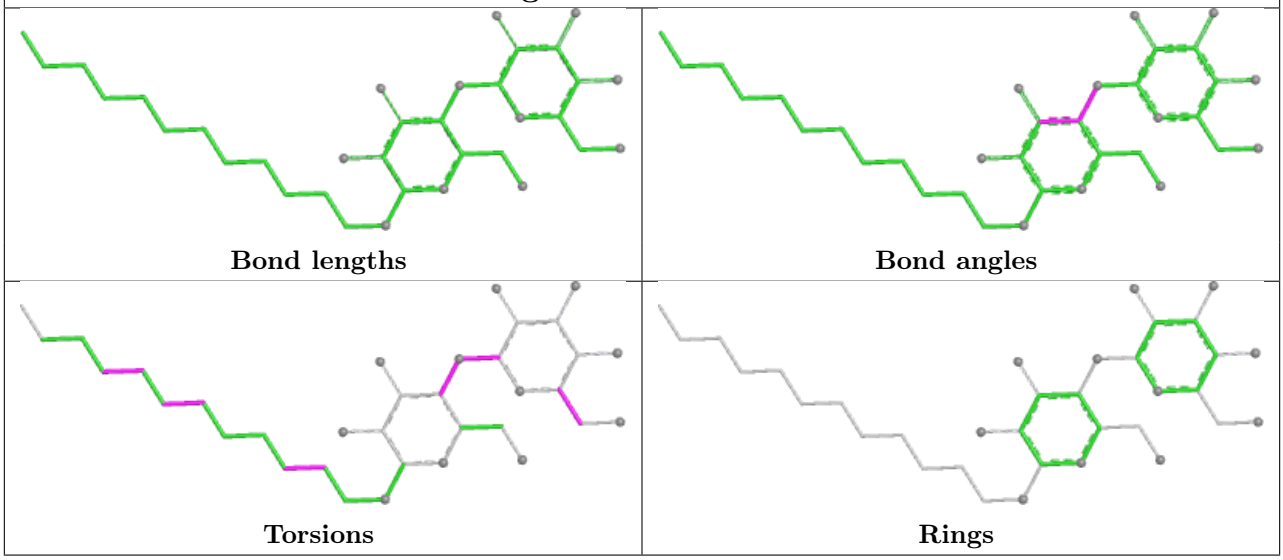


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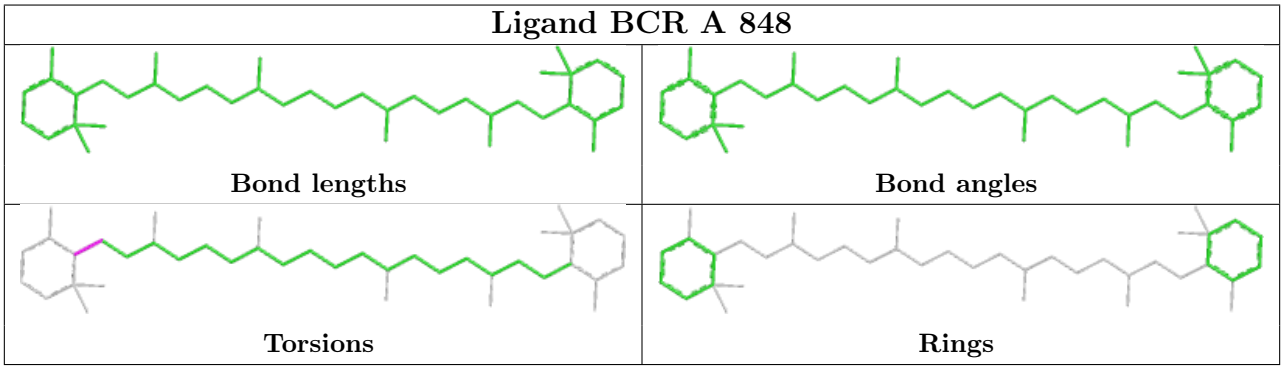


Rings

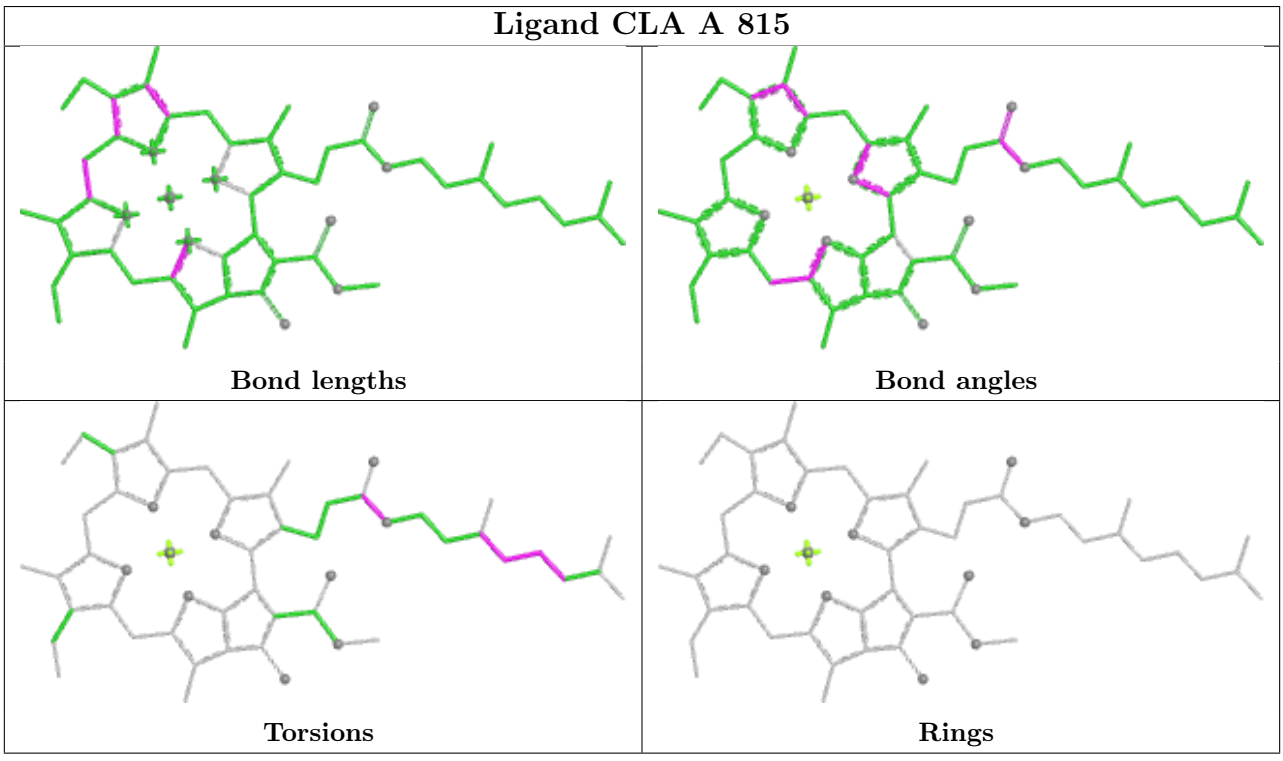
Ligand LMT A 858



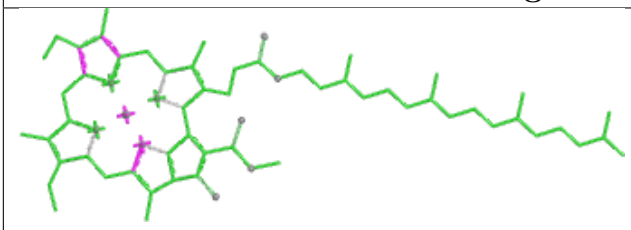
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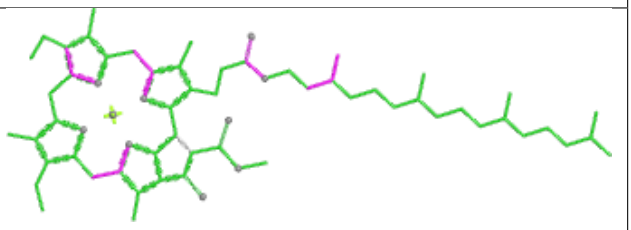
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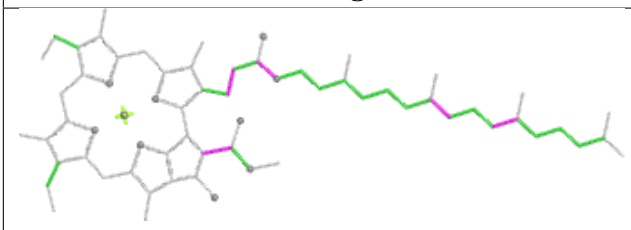
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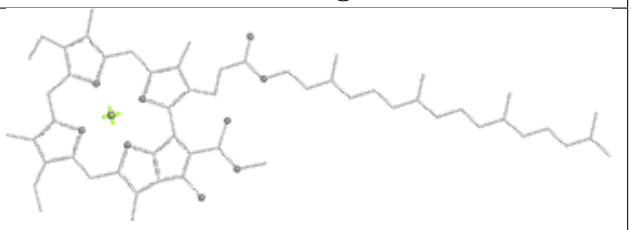
Bond lengths



Bond angles

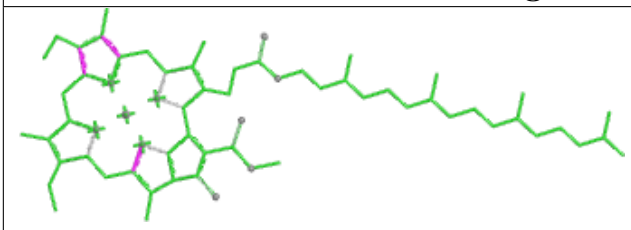


Torsions

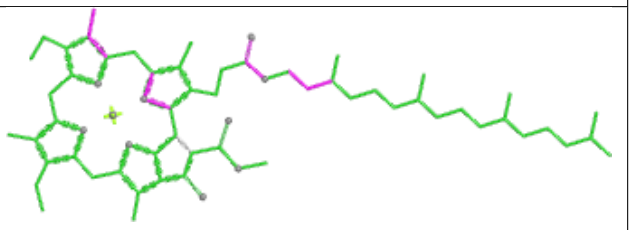


Rings

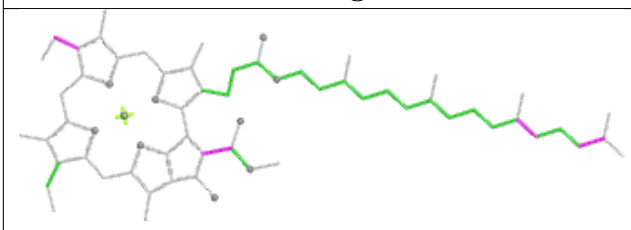
Ligand CLA B 809



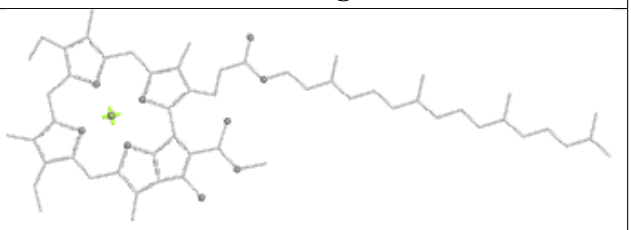
Bond lengths



Bond angles

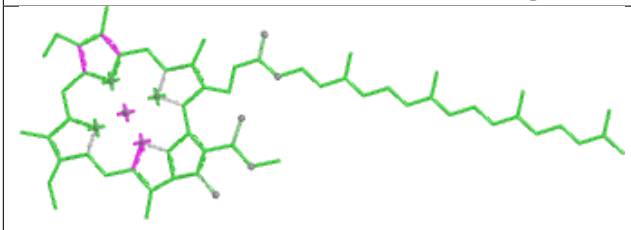


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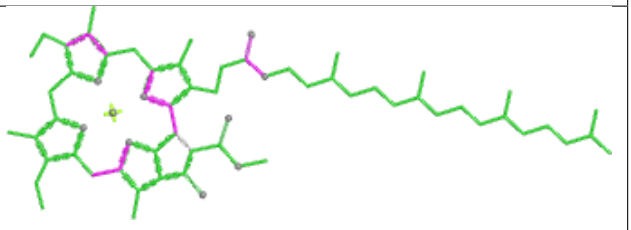


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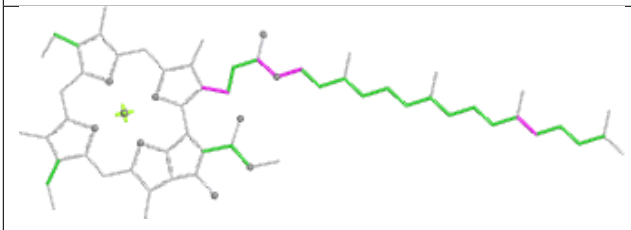
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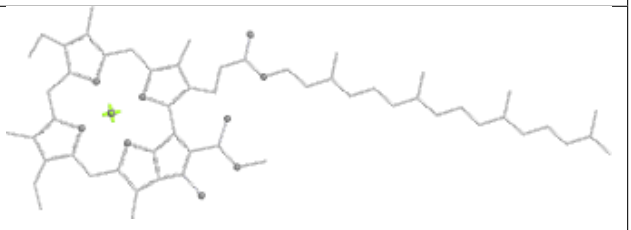
Bond lengths



Bond angles

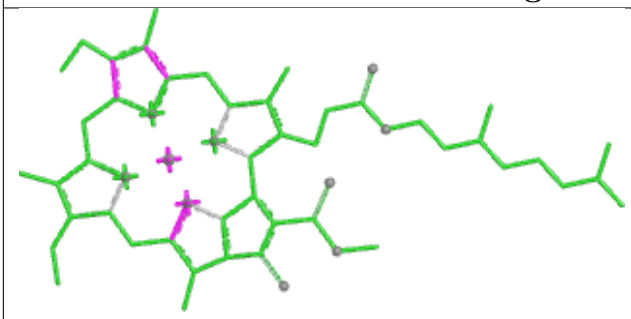


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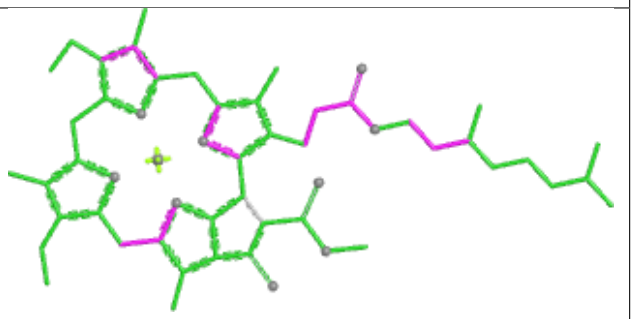


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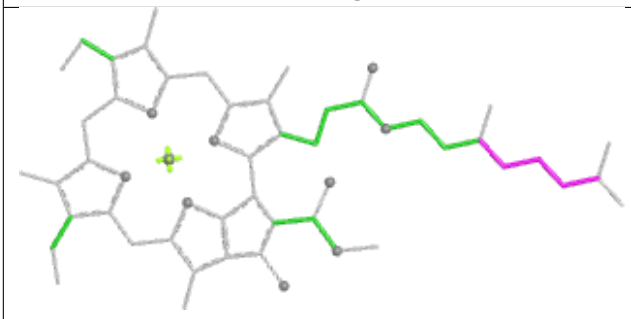
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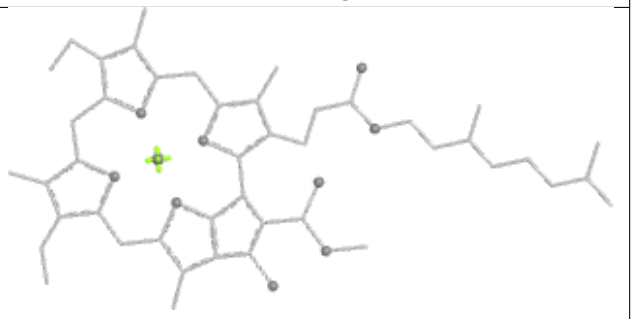
Bond lengths



Bond angles

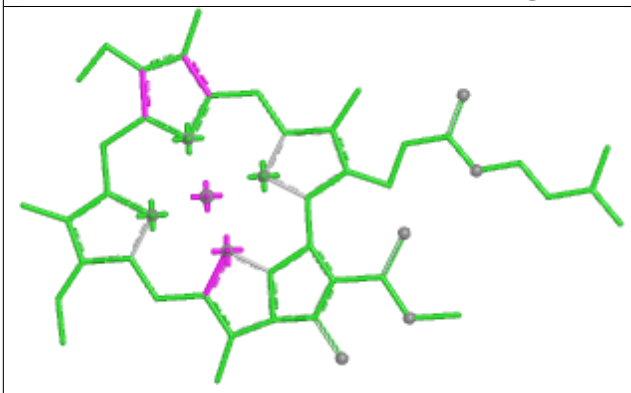


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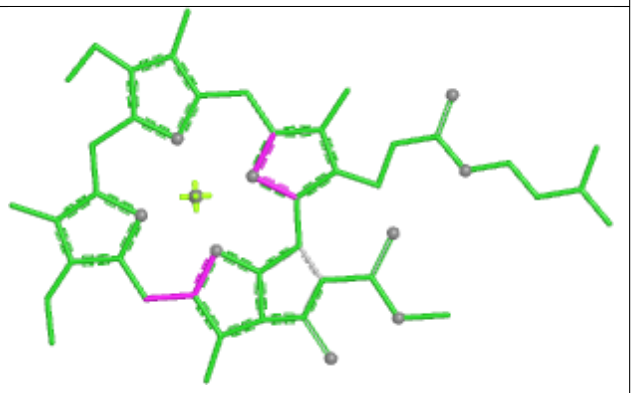


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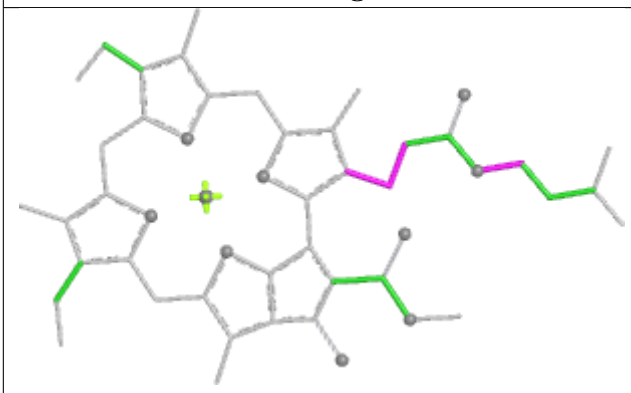
Ligand CLA A 810



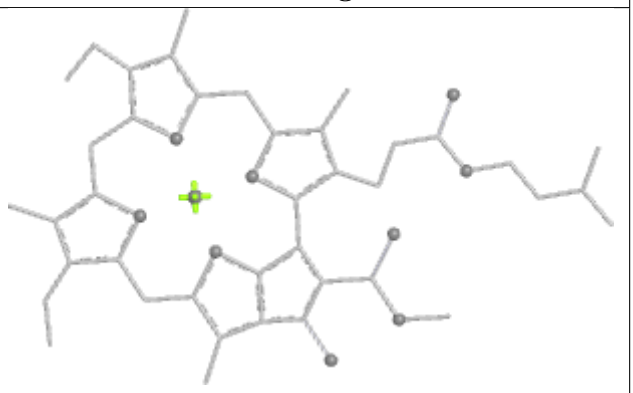
Bond lengths



Bond angles

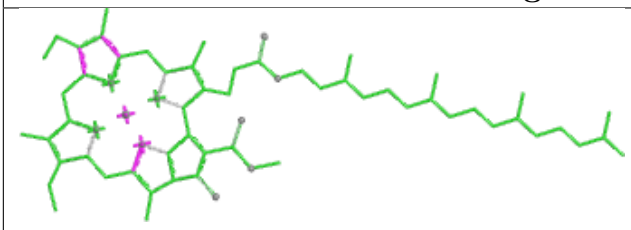


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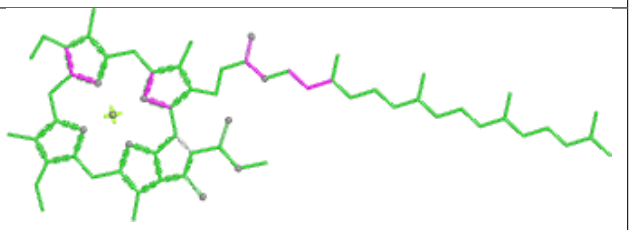


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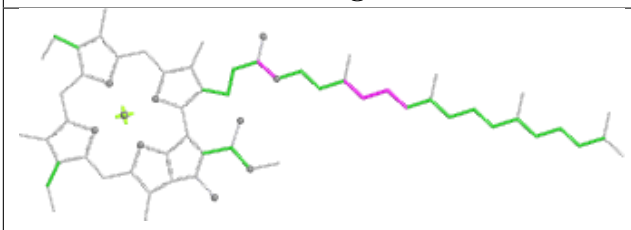
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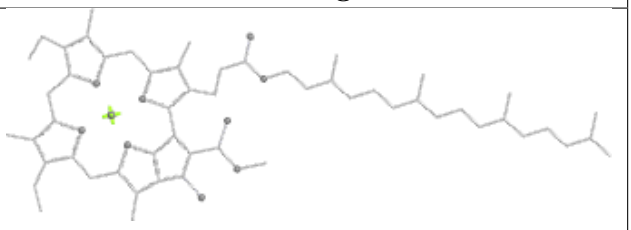
Bond lengths



Bond angles

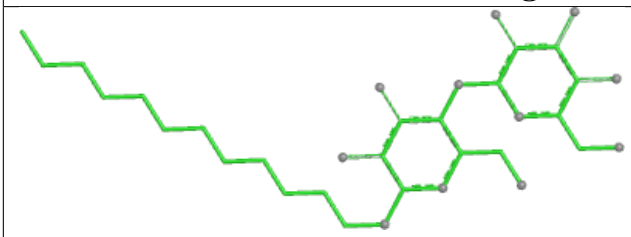


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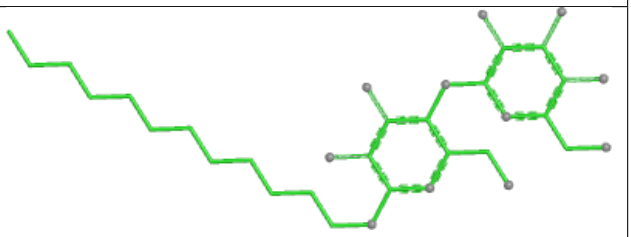


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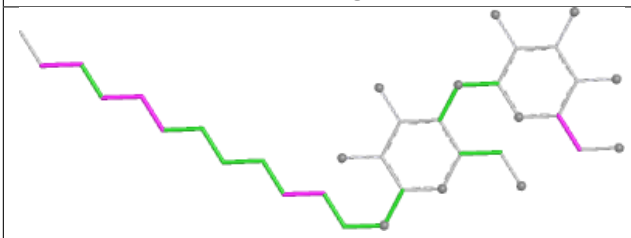
Ligand LMT A 854



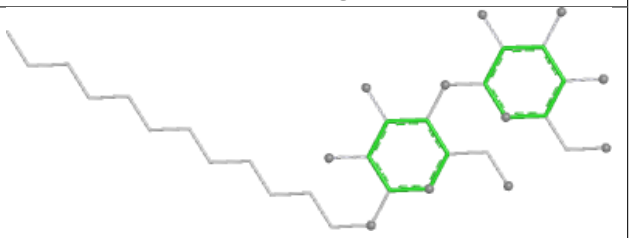
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Bond angles

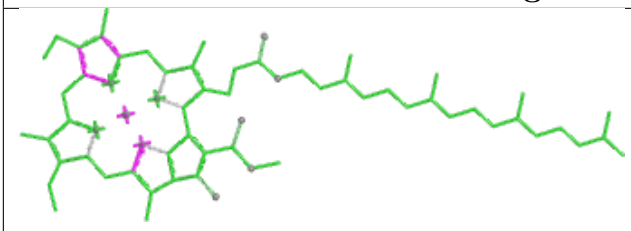


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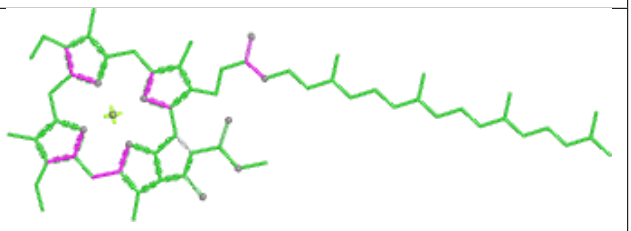


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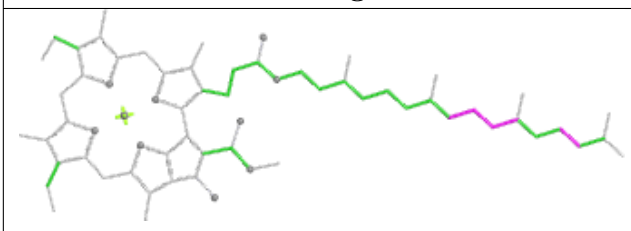
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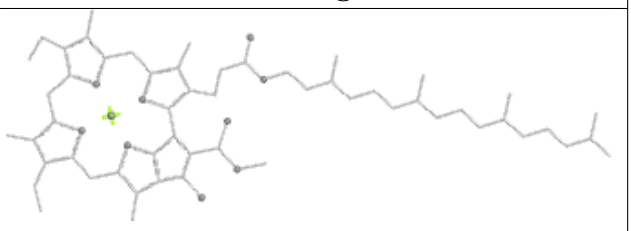
Bond lengths



Bond angles

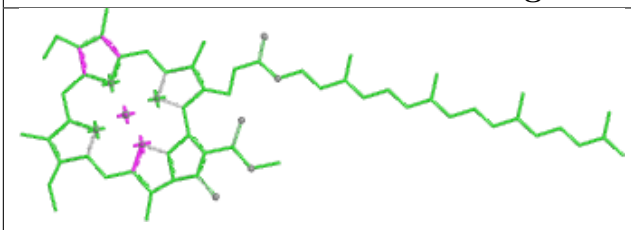


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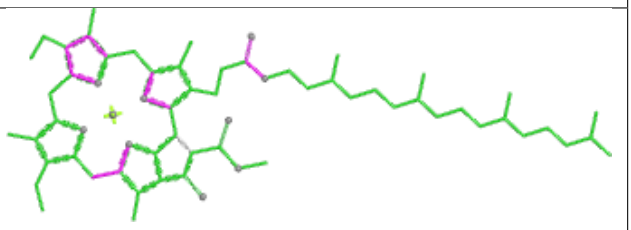


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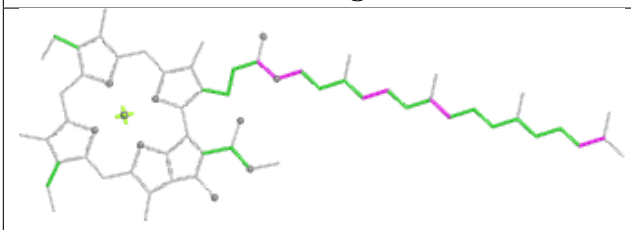
Ligand CLA B 839



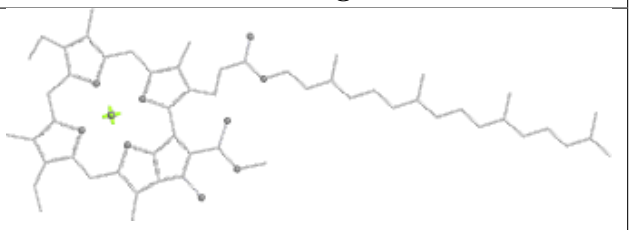
Bond lengths



Bond angles

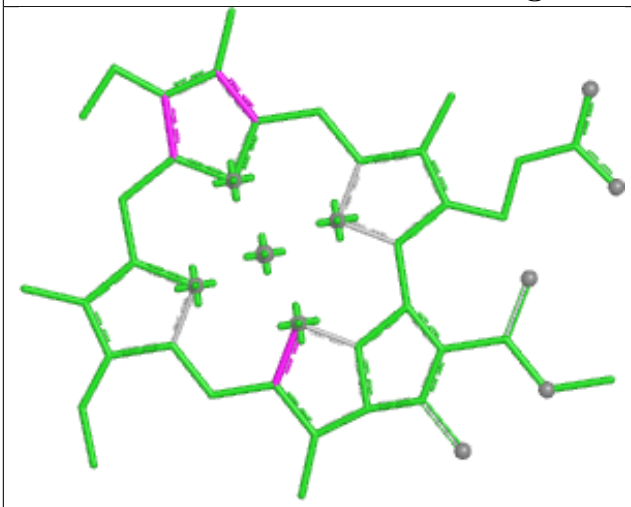


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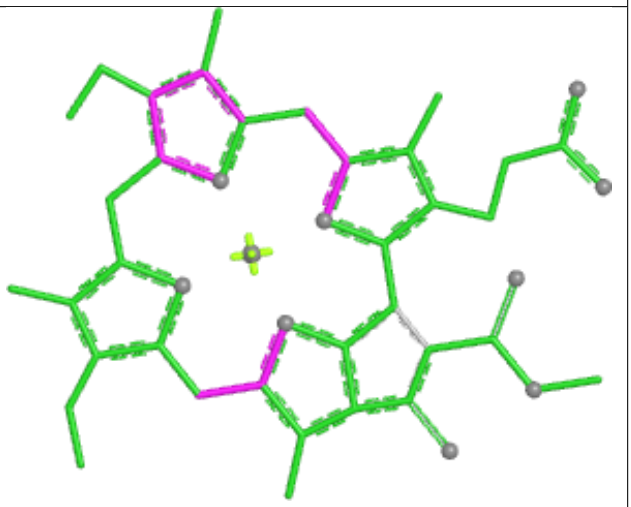


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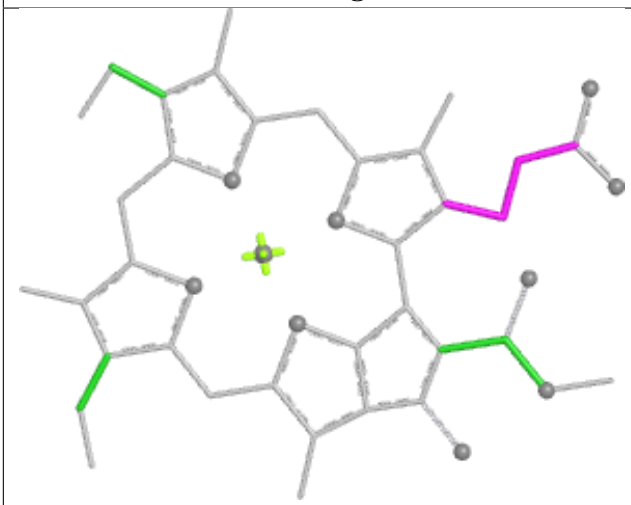
Ligand CLA F 203



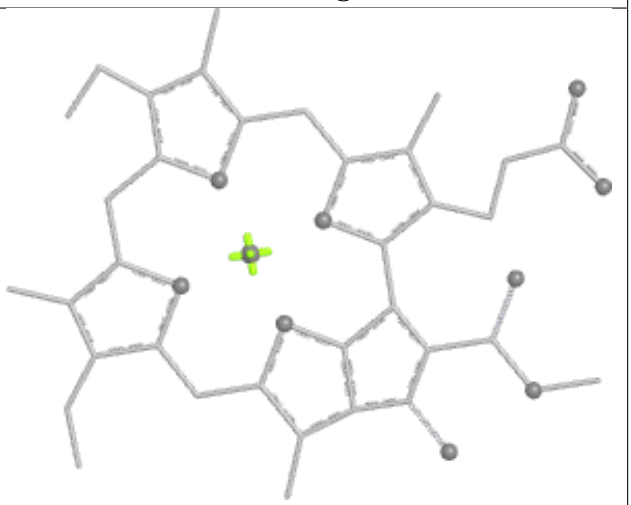
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Bond angles

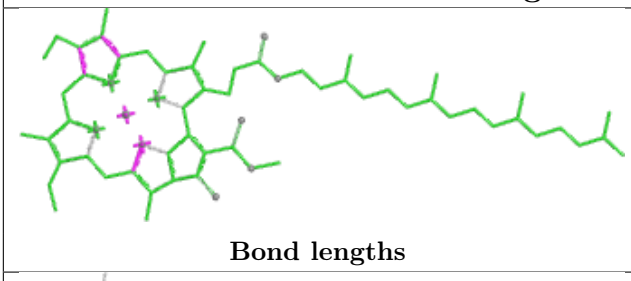


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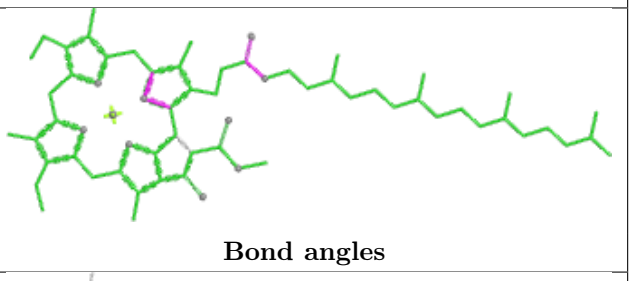


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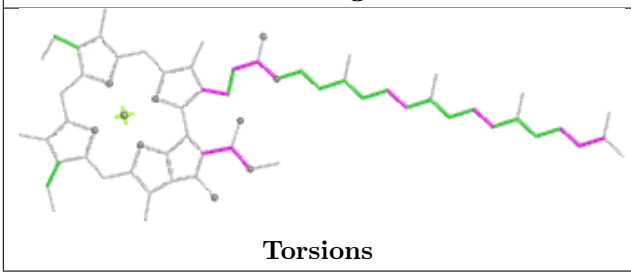
Ligand CLA A 807



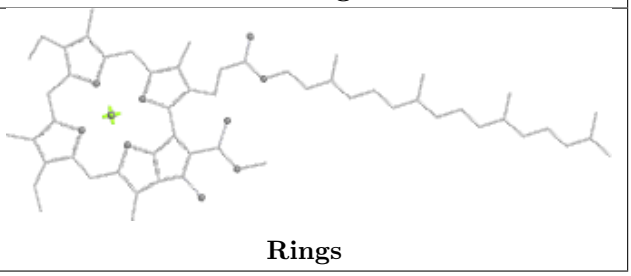
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Bond angles

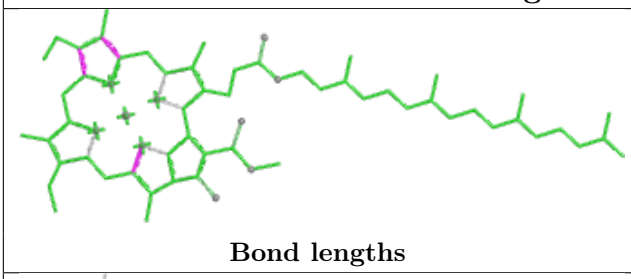


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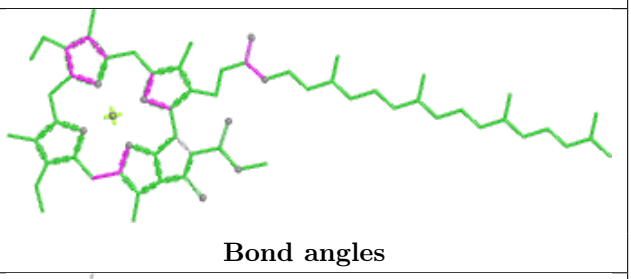


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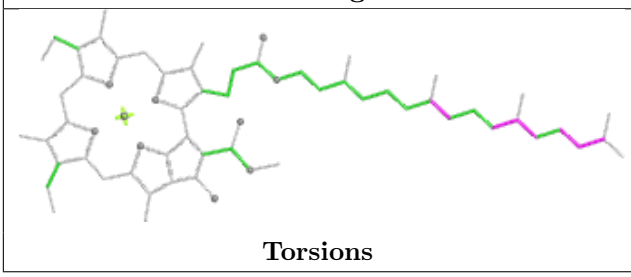
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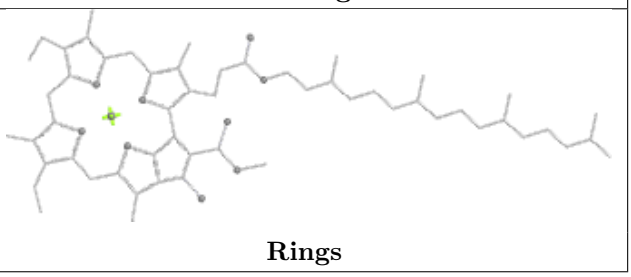
Bond lengths



Bond angles

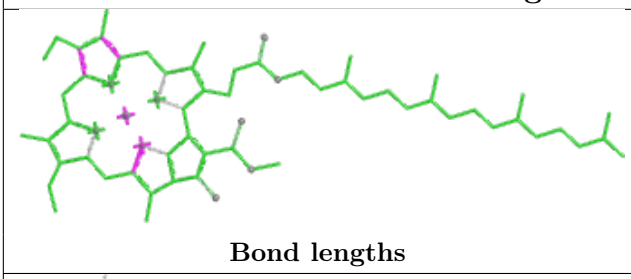


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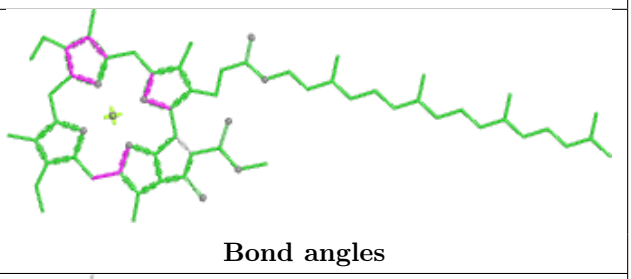


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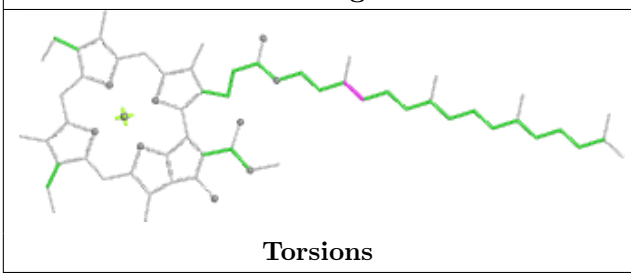
Ligand CLA B 829



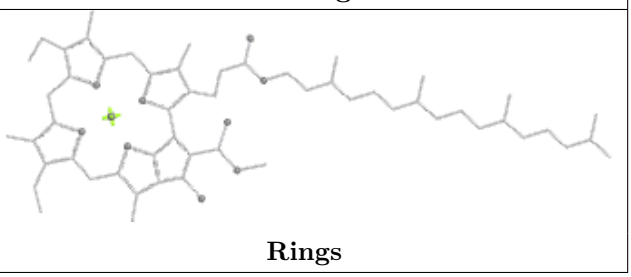
Bond lengths



Bond angles

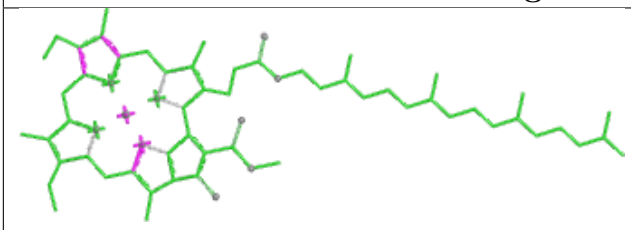


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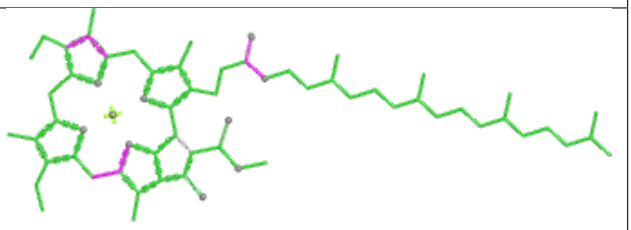


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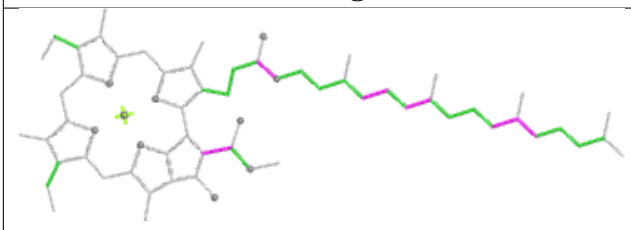
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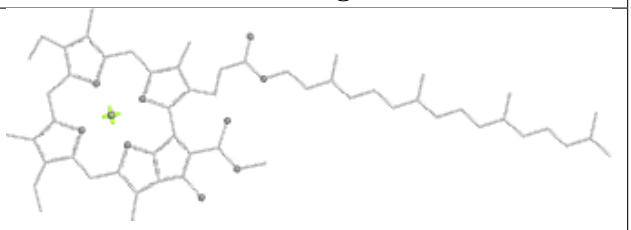
Bond lengths



Bond angles

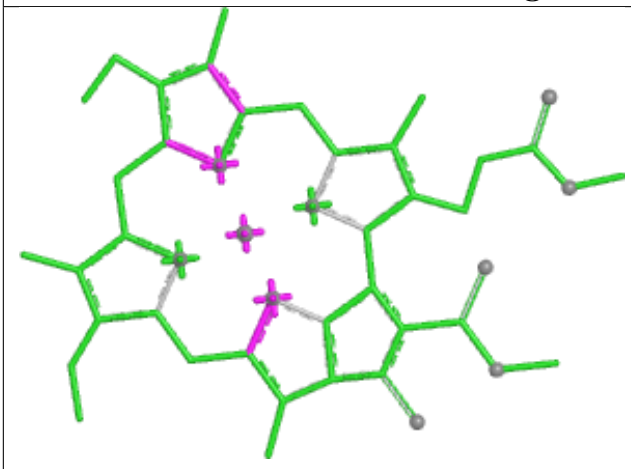


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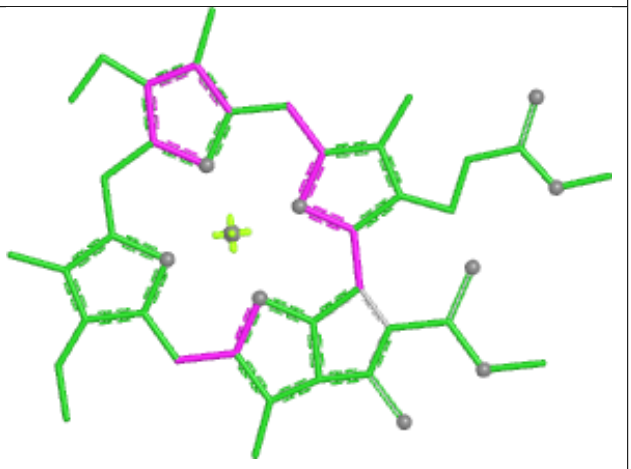


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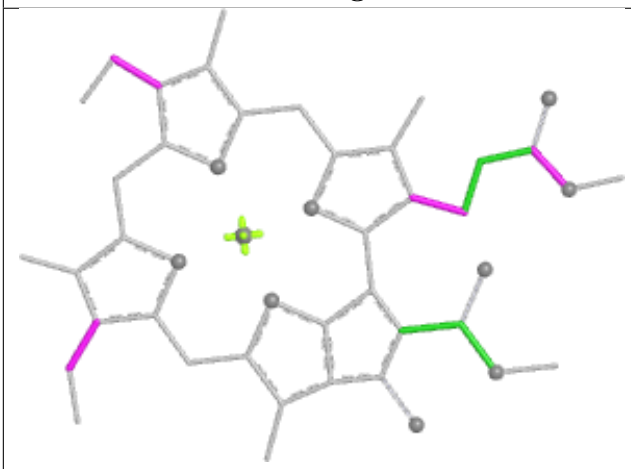
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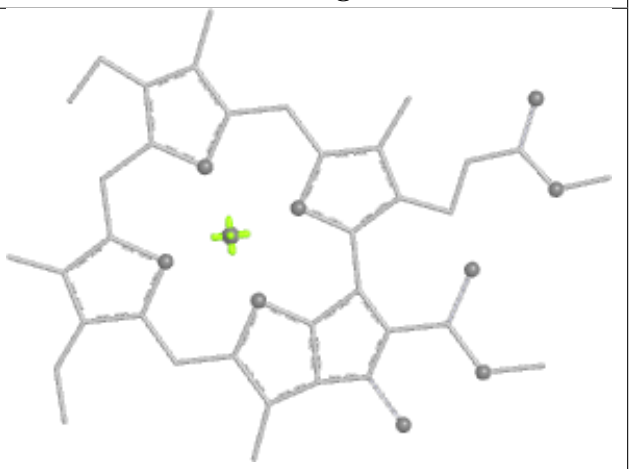
Bond lengths



Bond angles

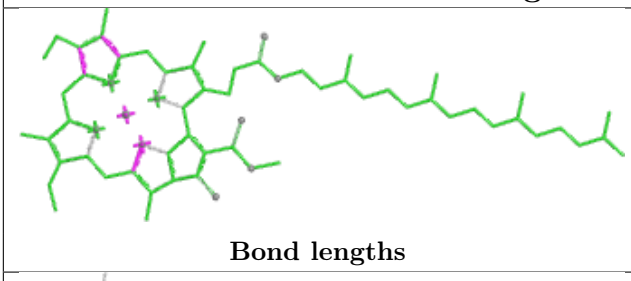


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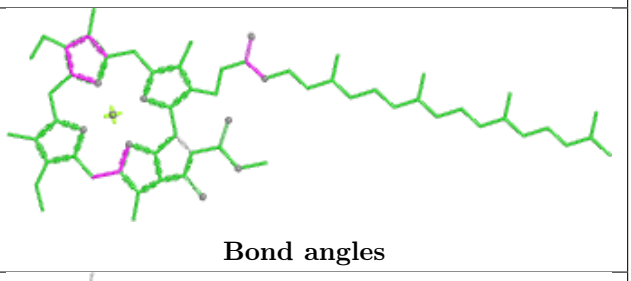


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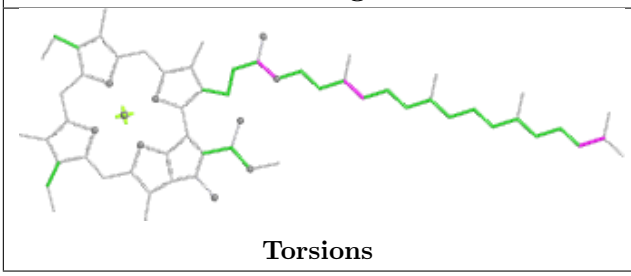
Ligand CLA A 828



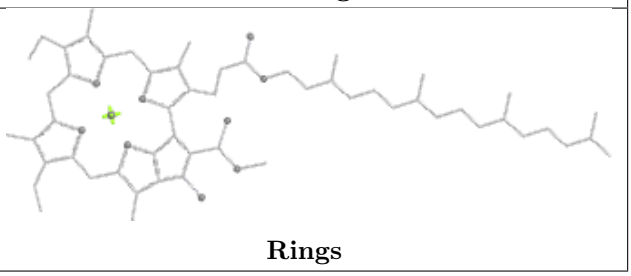
Bond lengths



Bond angles

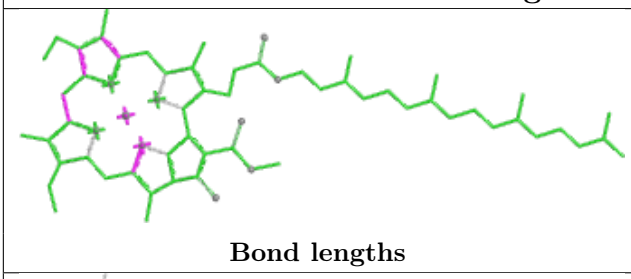


Torsions

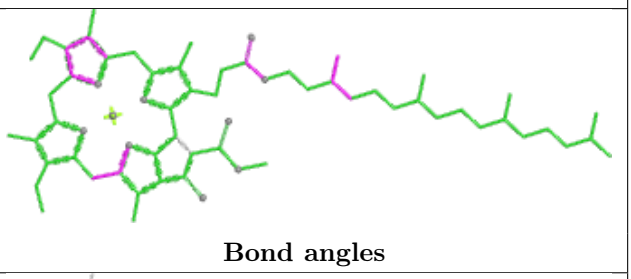


Rings

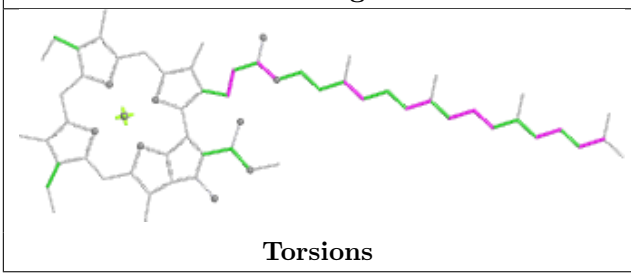
Ligand CLA A 814



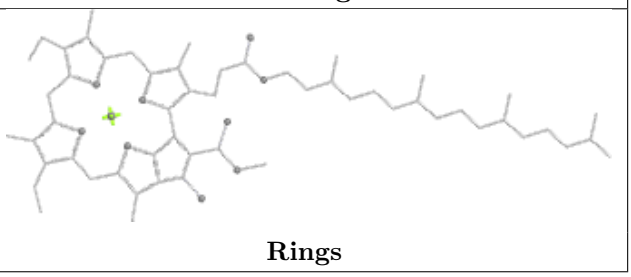
Bond lengths



Bond angles

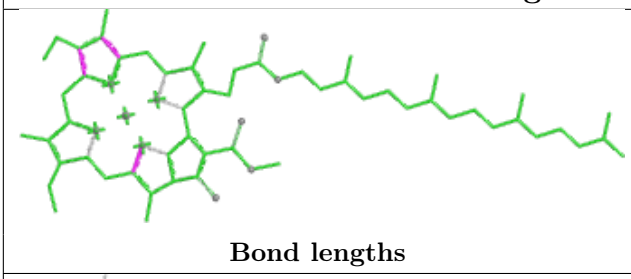


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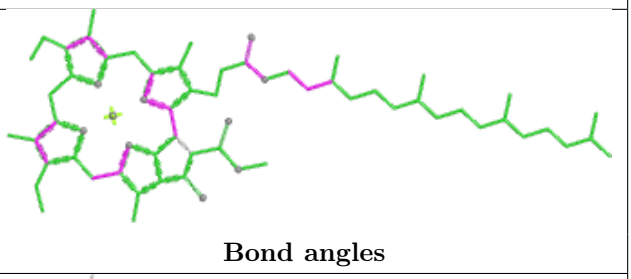


Rings

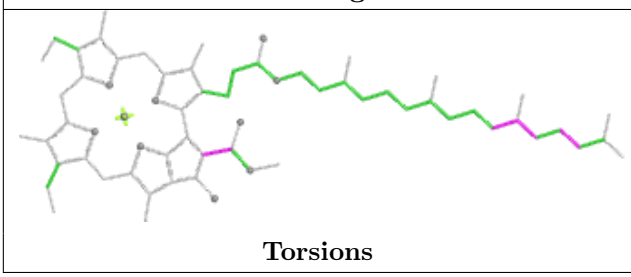
Ligand CLA A 835



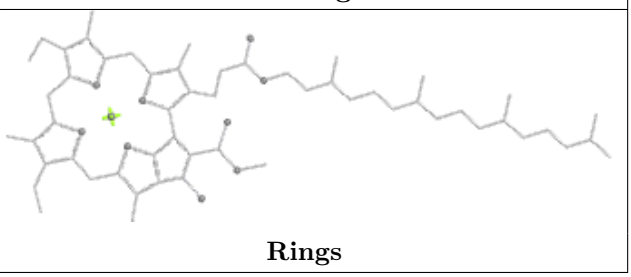
Bond lengths



Bond angles

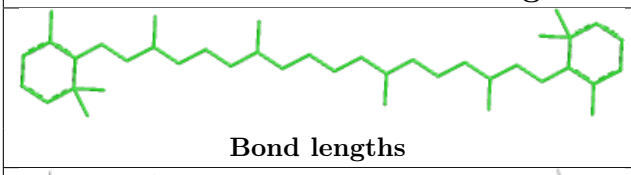


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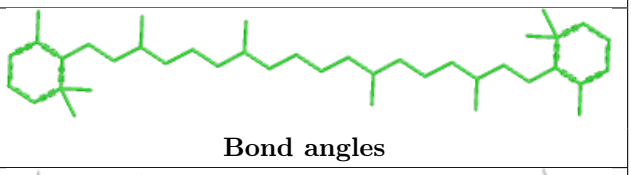


Rings

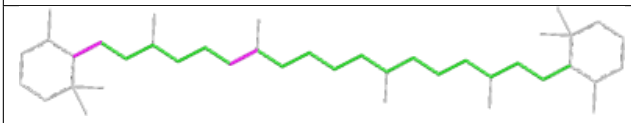
Ligand BCR B 845



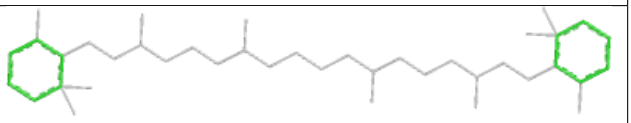
Bond lengths



Bond angles

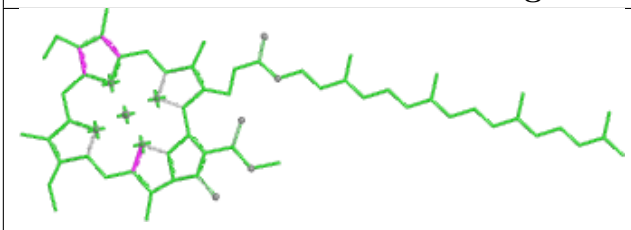


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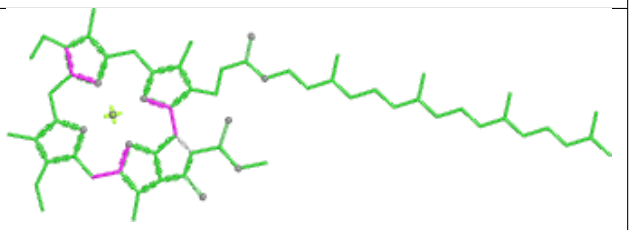


Rings

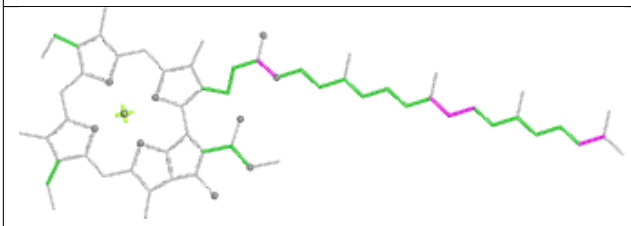
Ligand CLA B 810



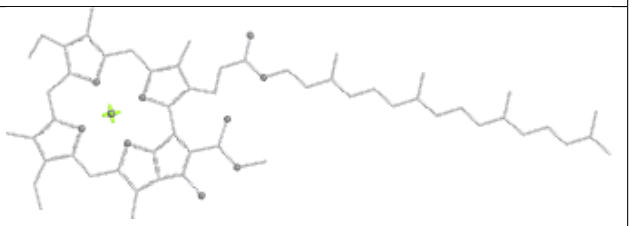
Bond lengths



Bond angles

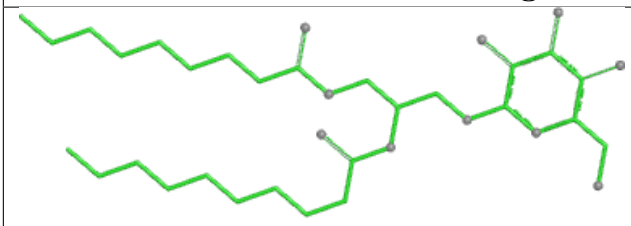


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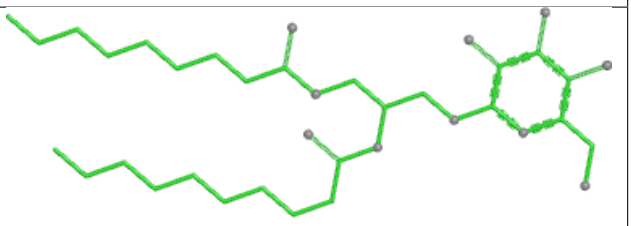


Rings

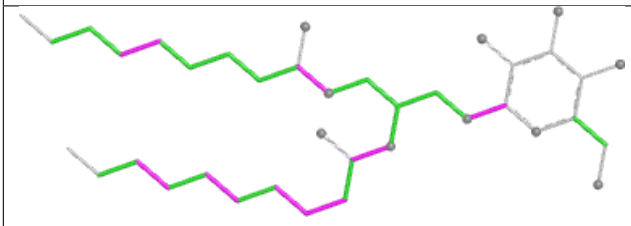
Ligand LMG B 851



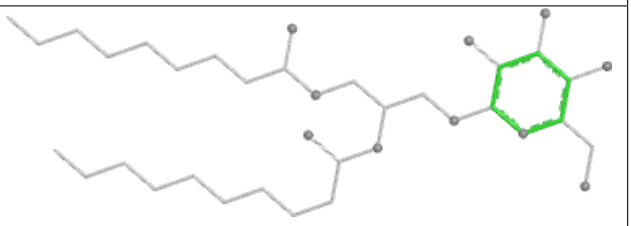
Bond lengths



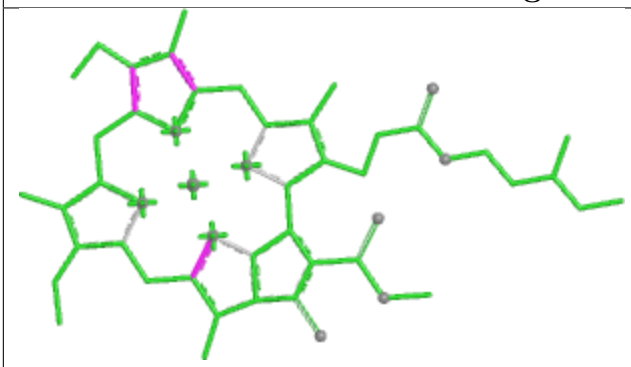
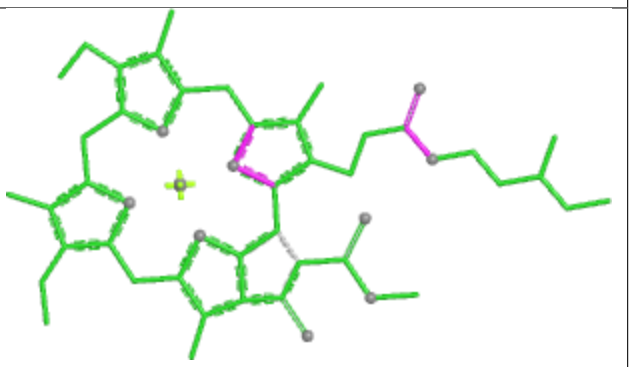
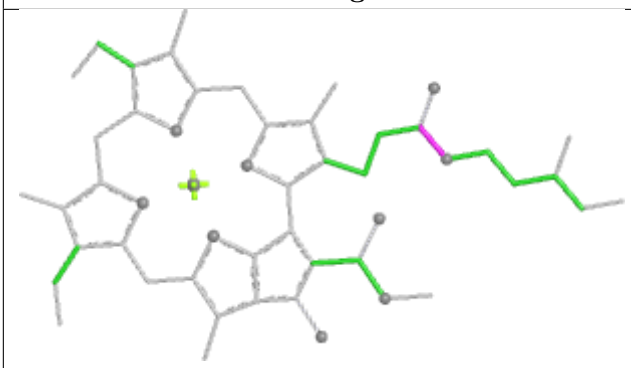
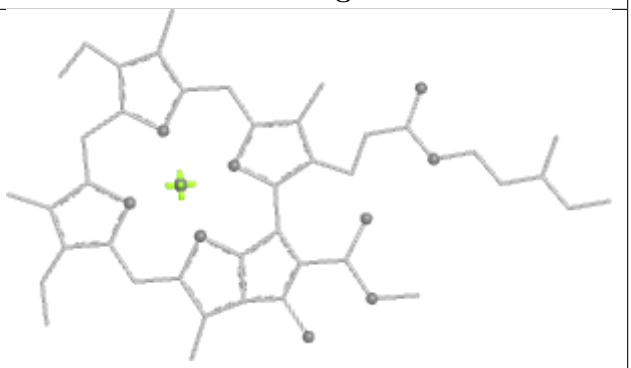
Bond angles

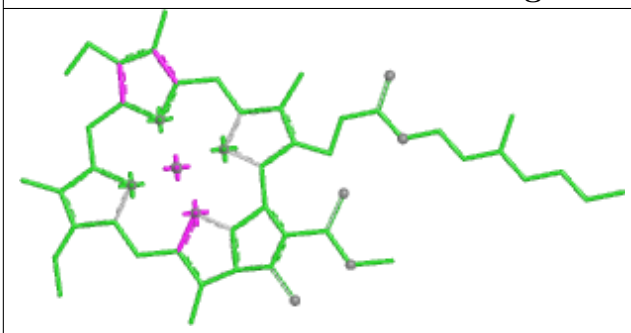
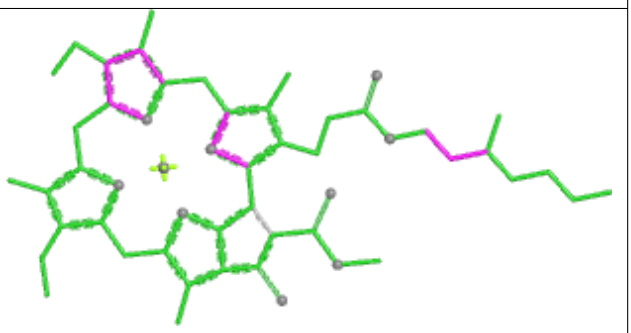
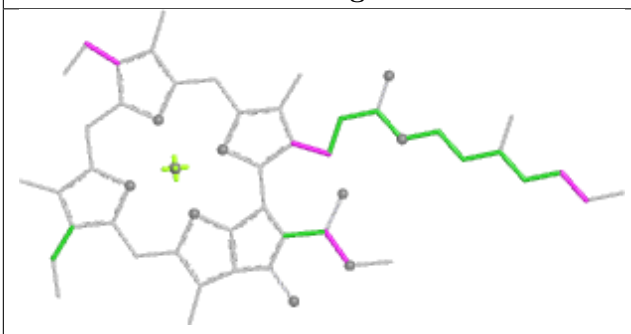
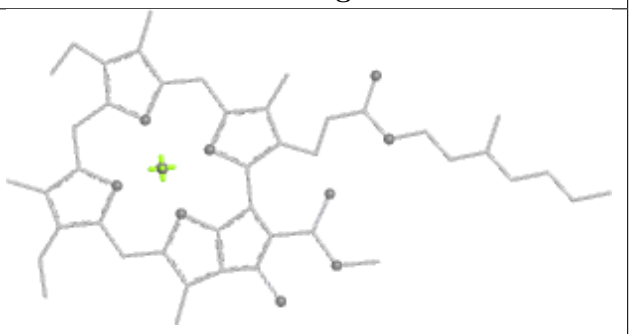


Torsions

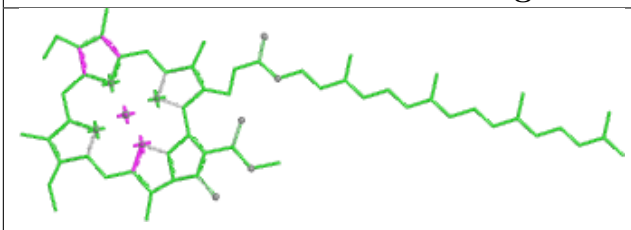


Rings

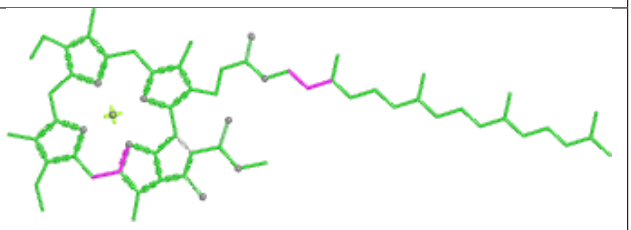
Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

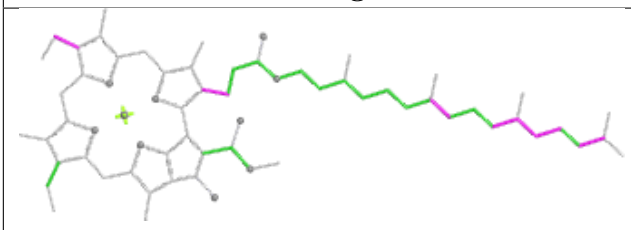
Ligand CLA K 4004



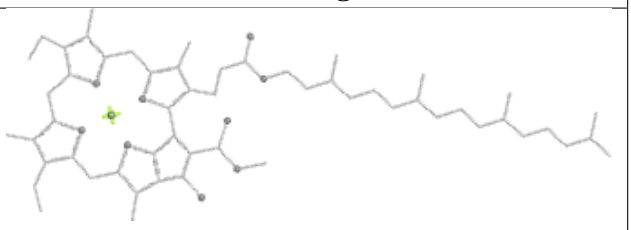
Bond lengths



Bond angles

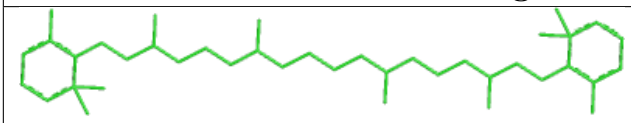


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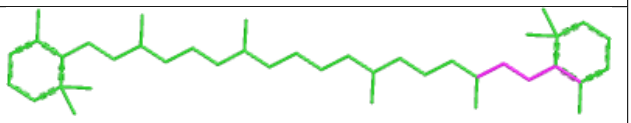


Rings

Ligand BCR K 4001



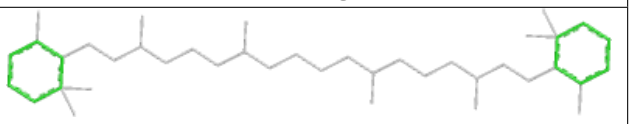
Bond lengths



Bond angles

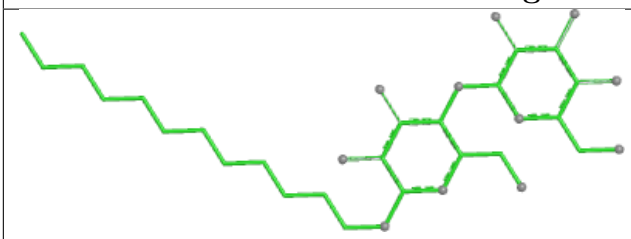


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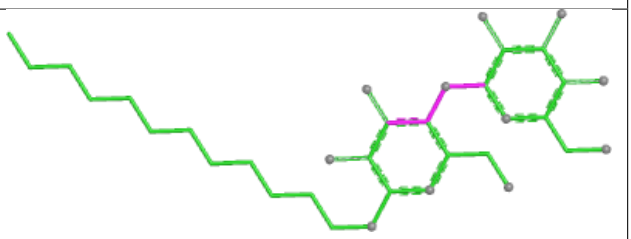


Rings

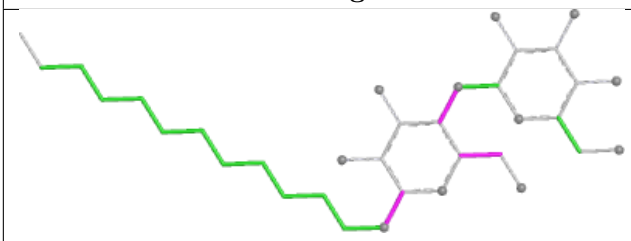
Ligand LMT F 206



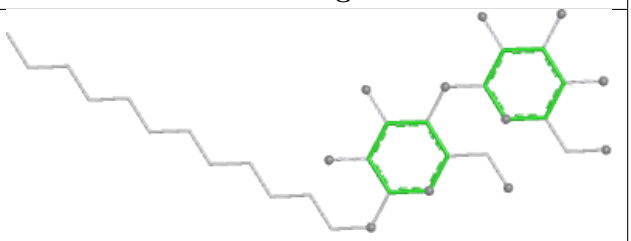
Bond lengths



Bond angles

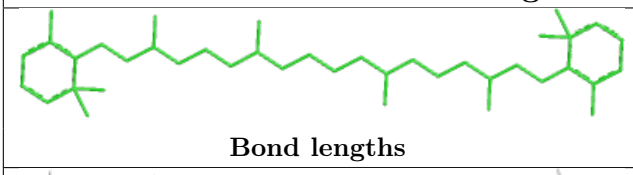


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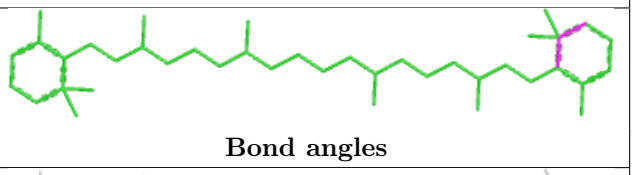


Rings

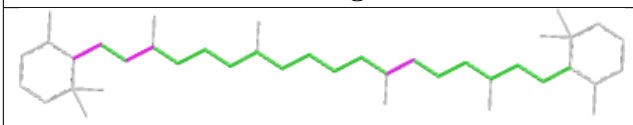
Ligand BCR A 849



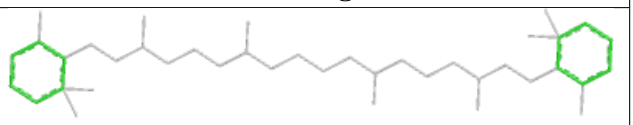
Bond lengths



Bond angles

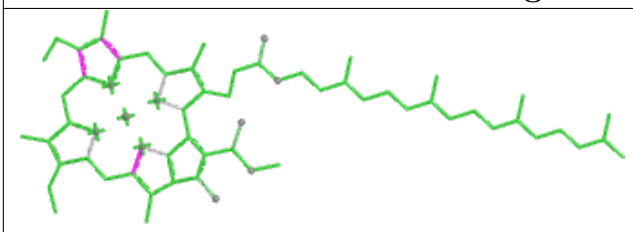


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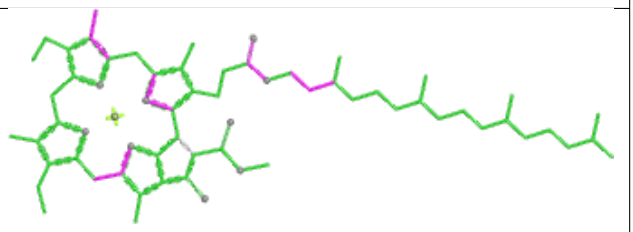


Rings

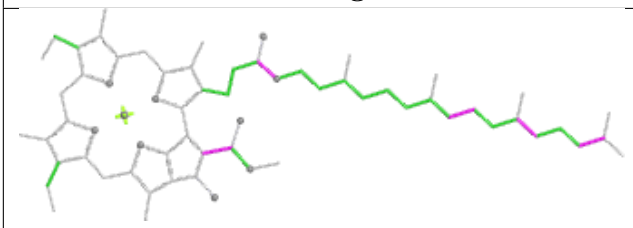
Ligand CLA B 815



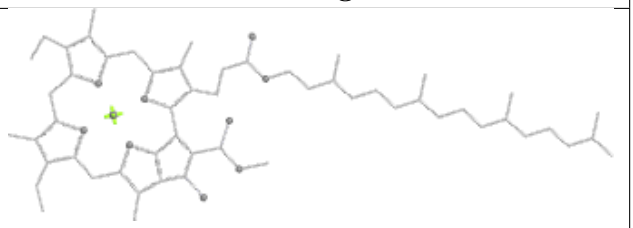
Bond lengths



Bond angles

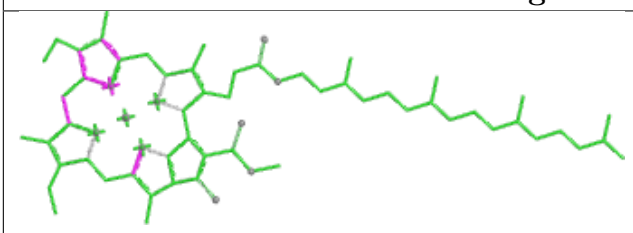


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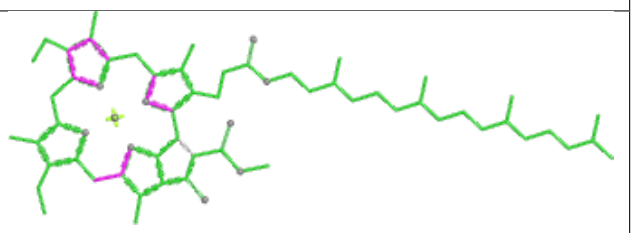


Rings

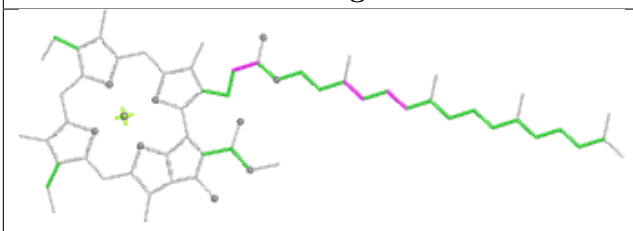
Ligand CL0 A 802



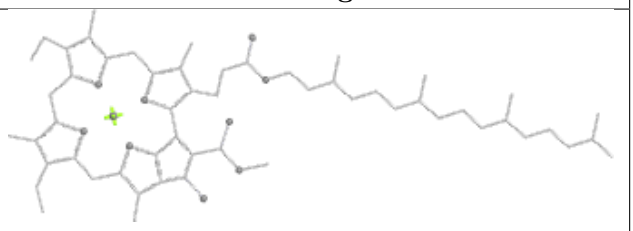
Bond lengths



Bond angles

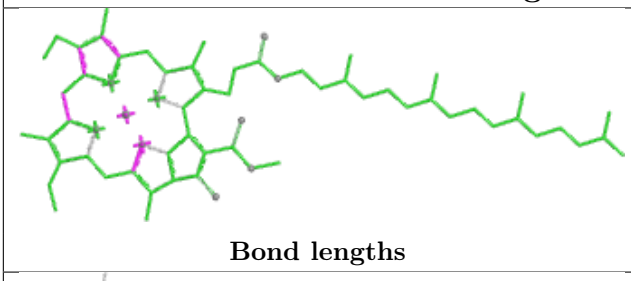


Torsions

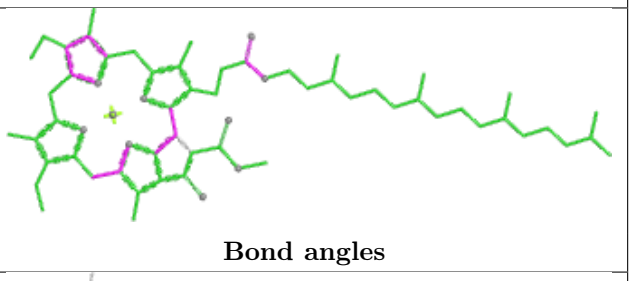


Rings

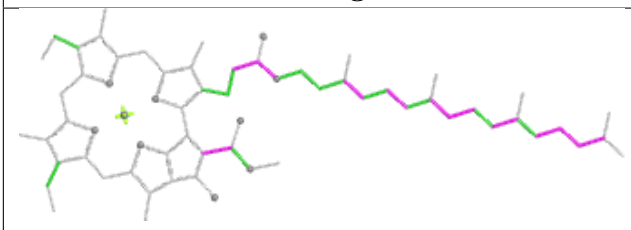
Ligand CLA A 805



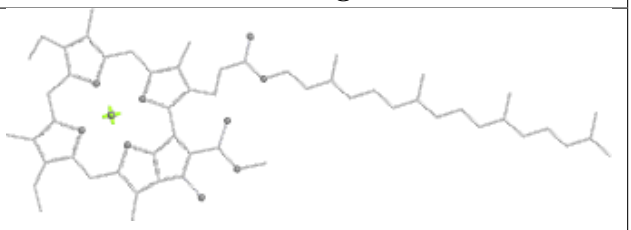
Bond lengths



Bond angles

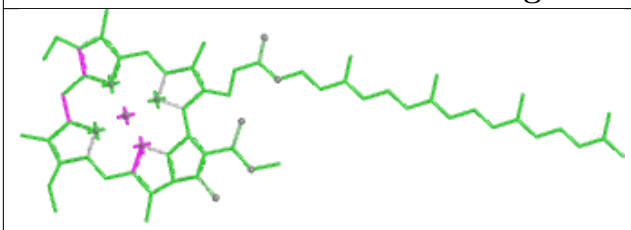


Torsions

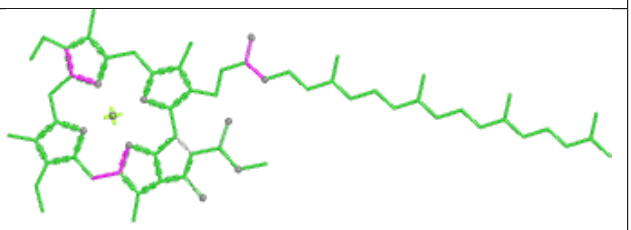


Rings

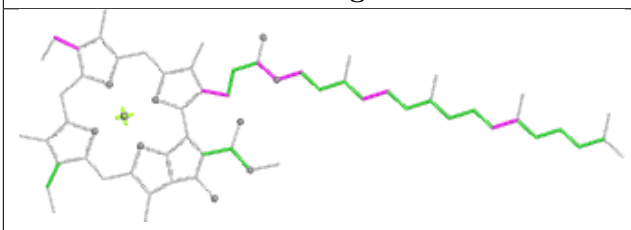
Ligand CLA A 837



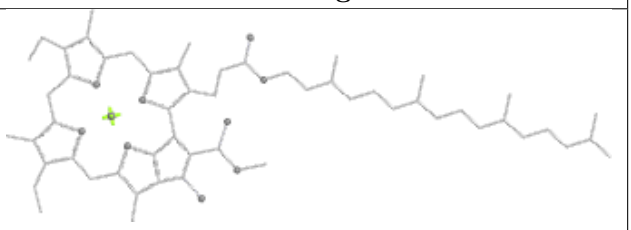
Bond lengths



Bond angles

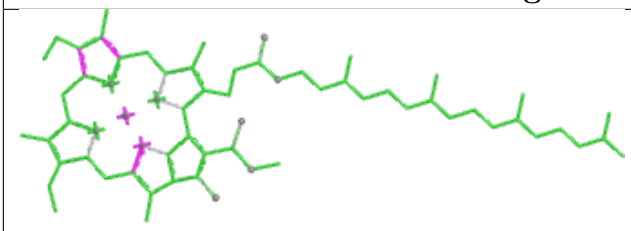


Torsions

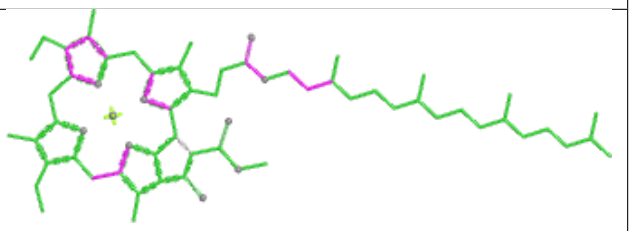


Rings

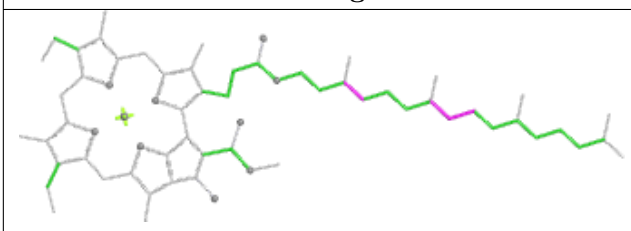
Ligand CLA A 841



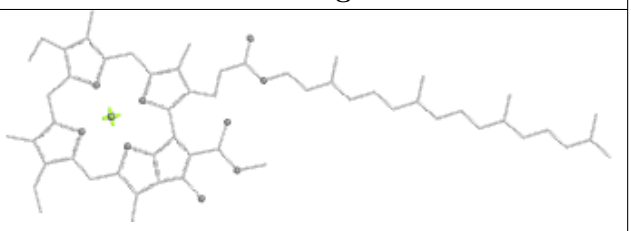
Bond lengths



Bond angles

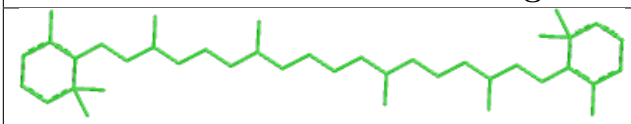


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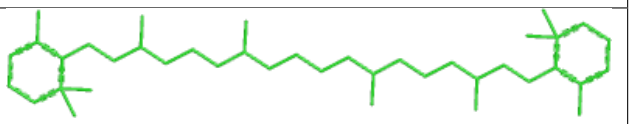


Rings

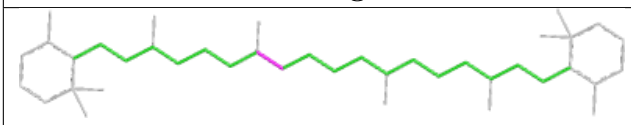
Ligand BCR F 205



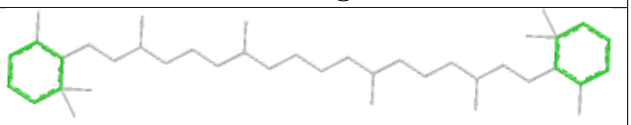
Bond lengths



Bond angles

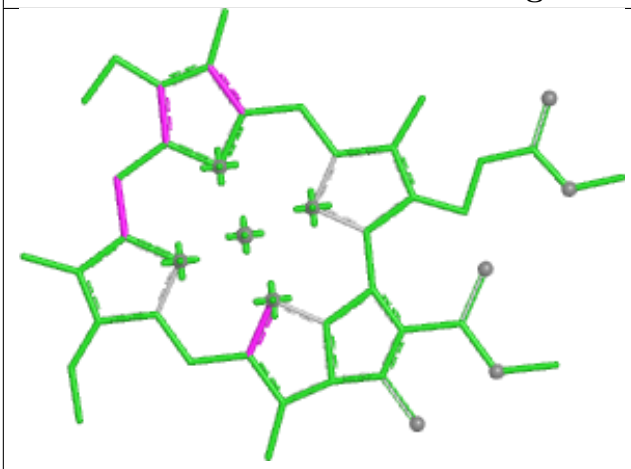


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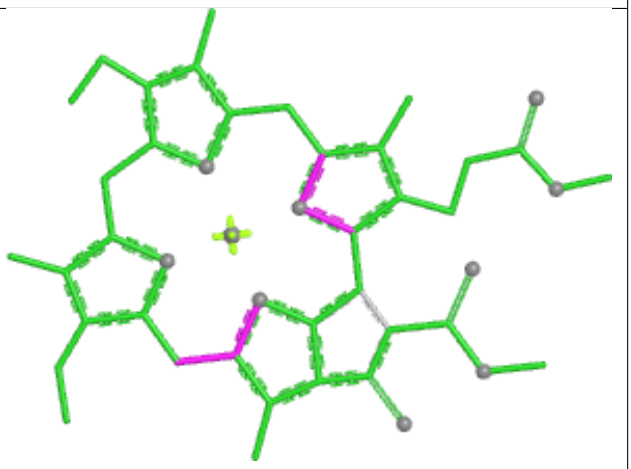


Rings

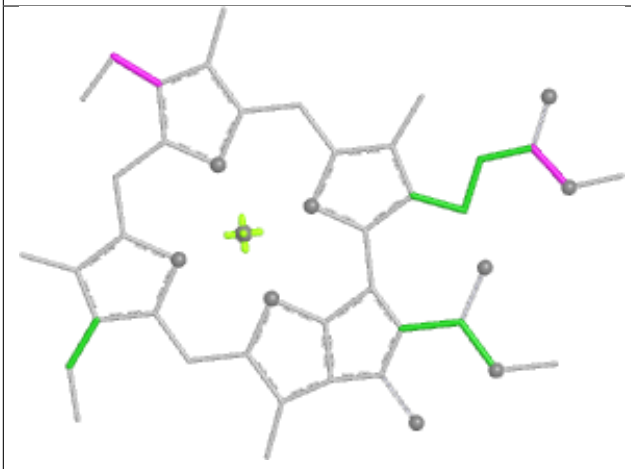
Ligand CLA F 204



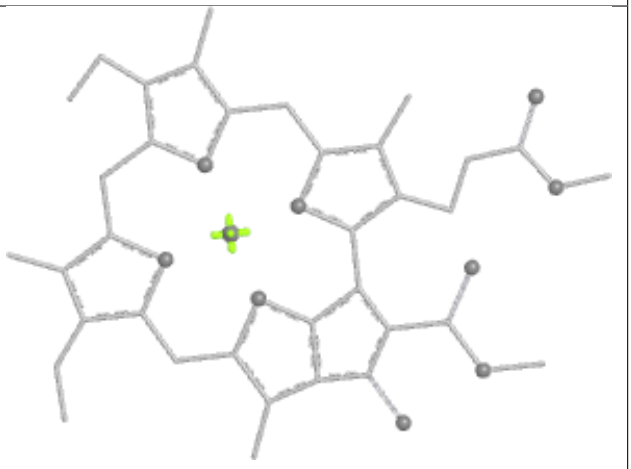
Bond lengths



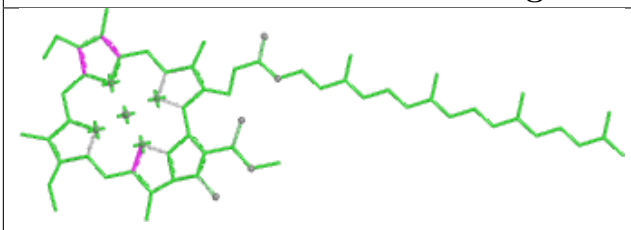
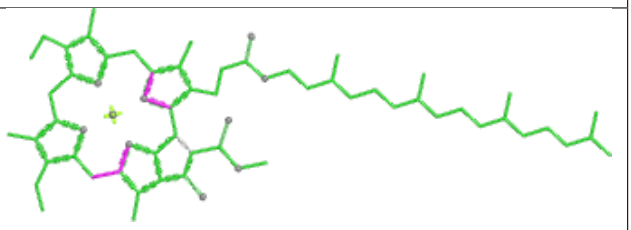
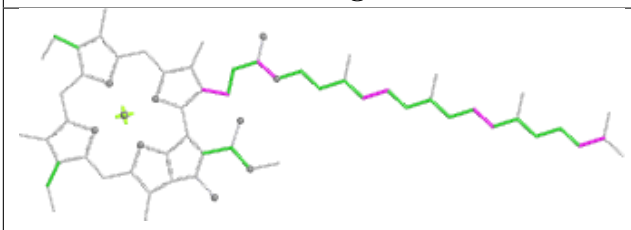
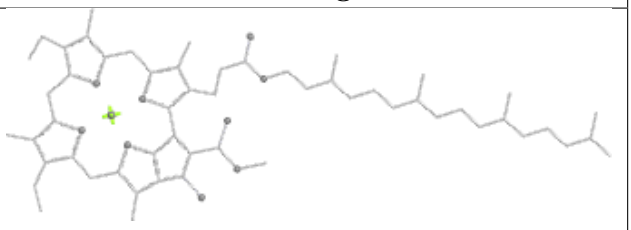
Bond angles

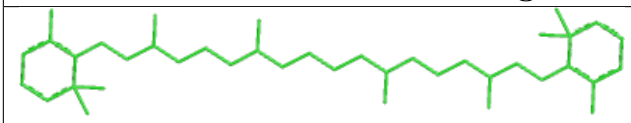
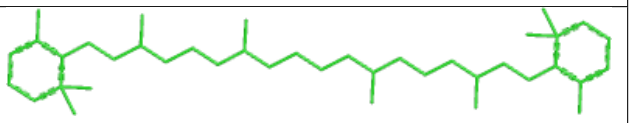
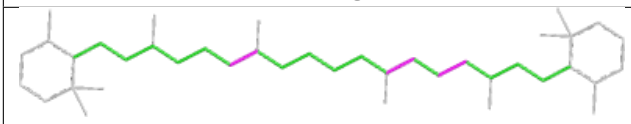
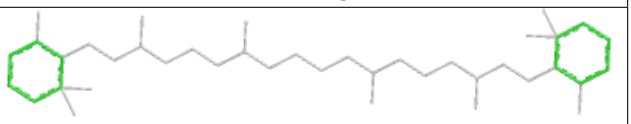


Torsions

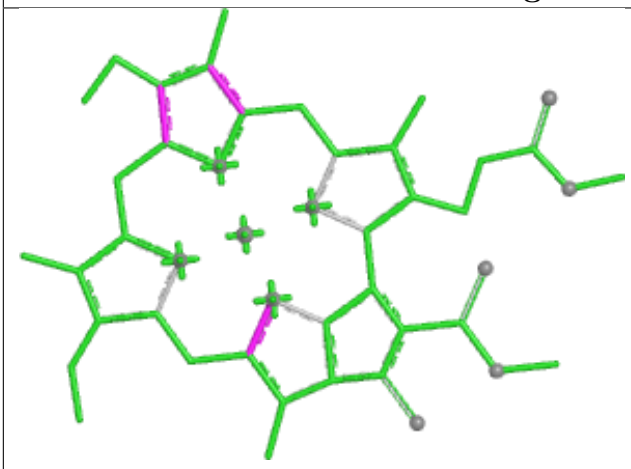


Rings

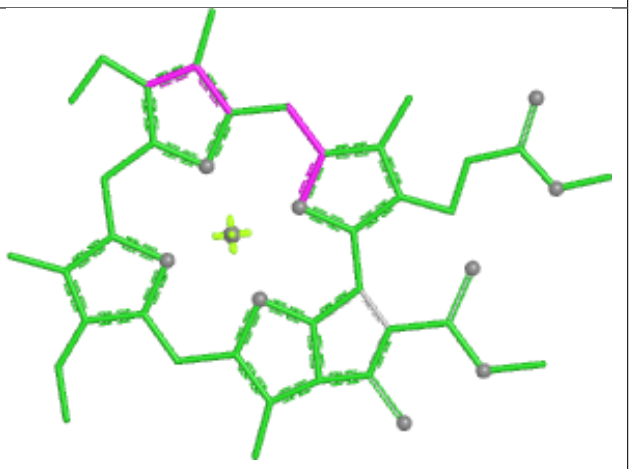
Ligand CLA F 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 1105	
	
Bond lengths	Bond angles
	
Torsions	Rings

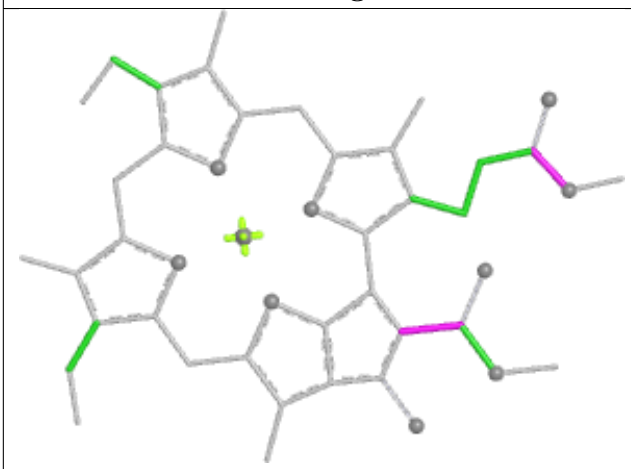
Ligand CLA A 845



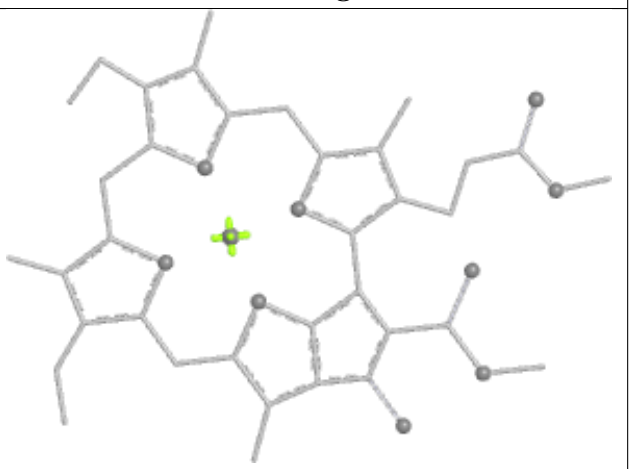
Bond lengths



Bond angles



Torsions



Rings

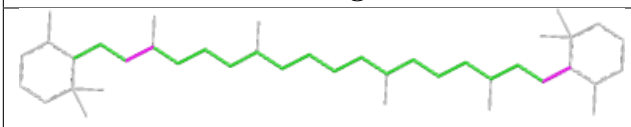
Ligand BCR B 852



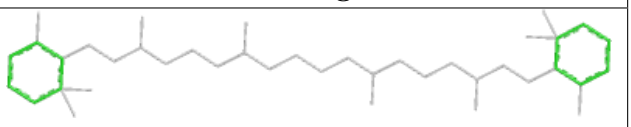
Bond lengths



Bond angles

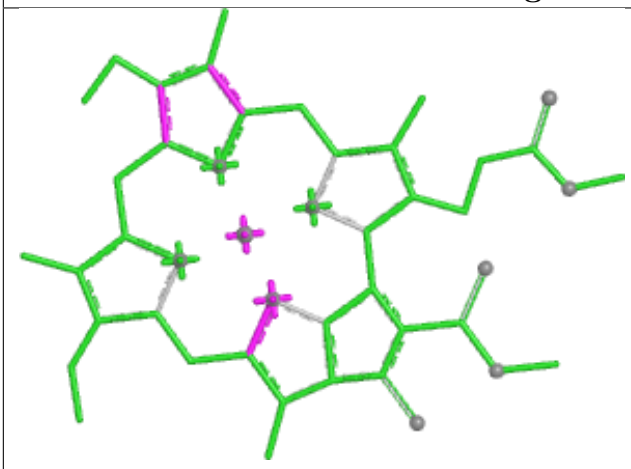


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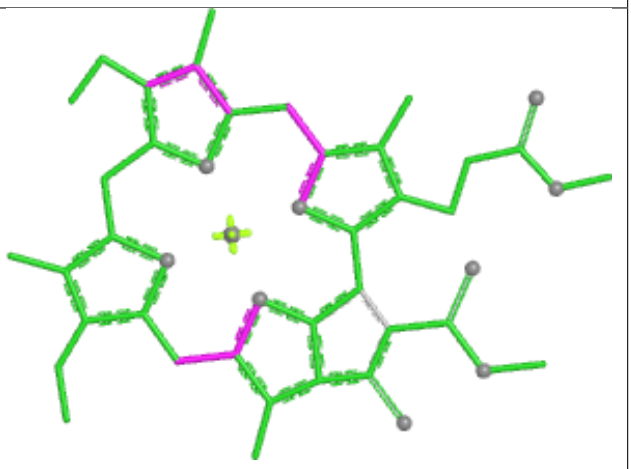


Rings

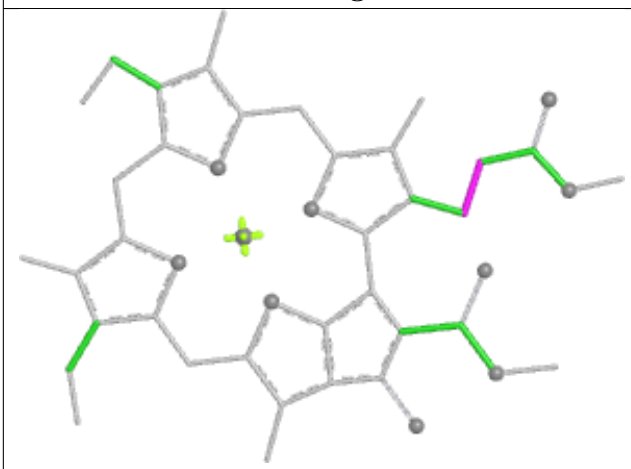
Ligand CLA B 842



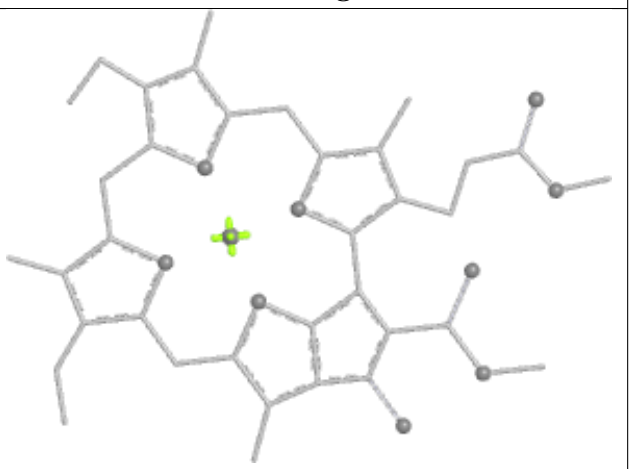
Bond lengths



Bond angles



Torsions



Rings

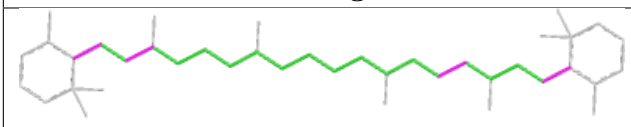
Ligand BCR L 206



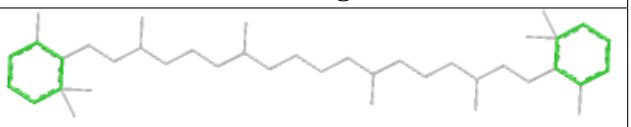
Bond lengths



Bond angles

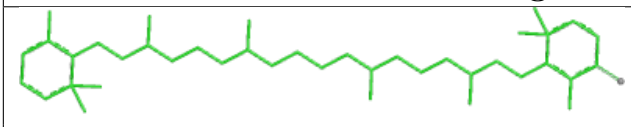


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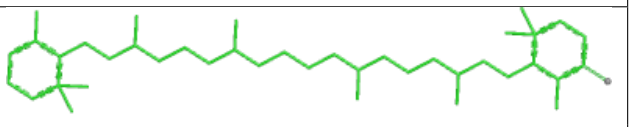


Rings

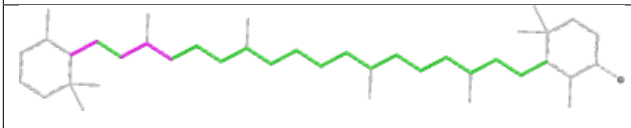
Ligand ECH I 103



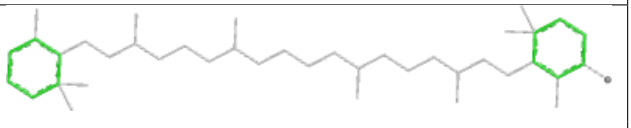
Bond lengths



Bond angles

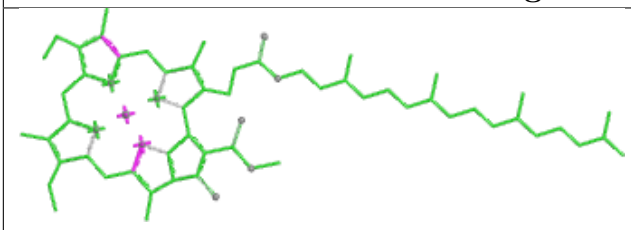


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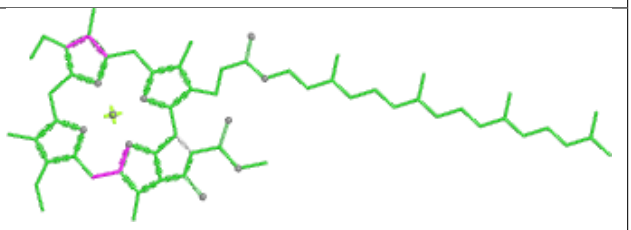


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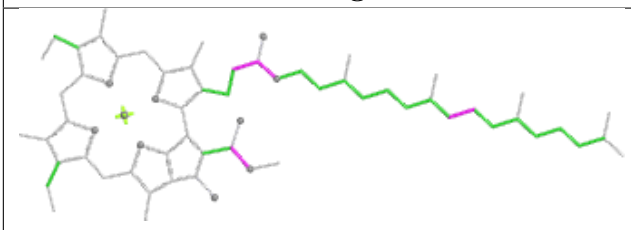
Ligand CLA B 804



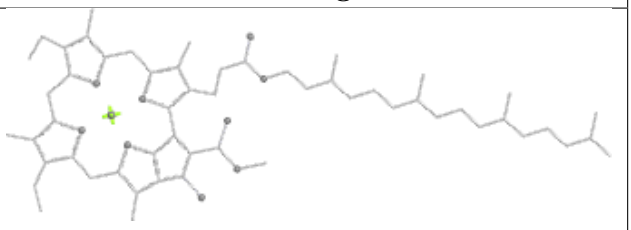
Bond lengths



Bond angles

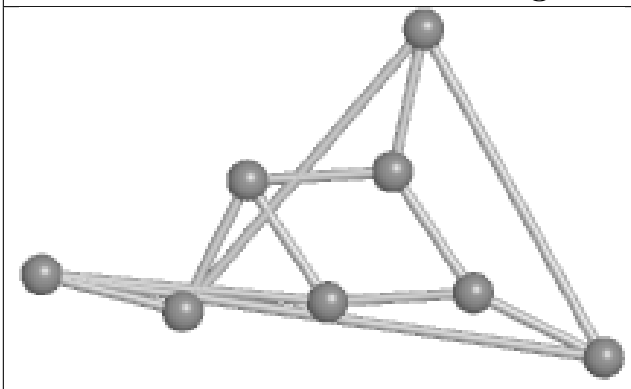


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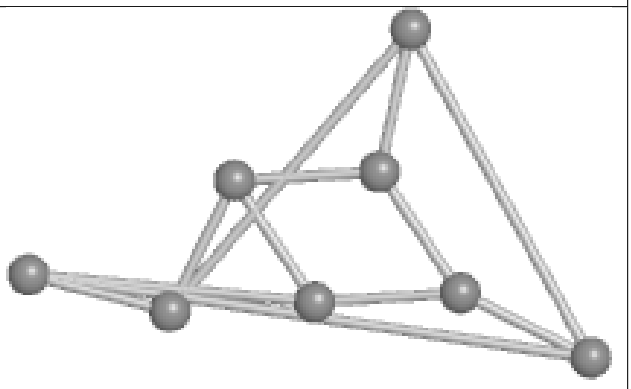


Rings

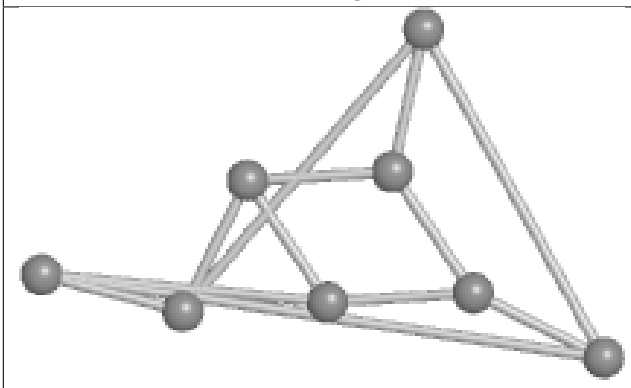
Ligand SF4 A 847



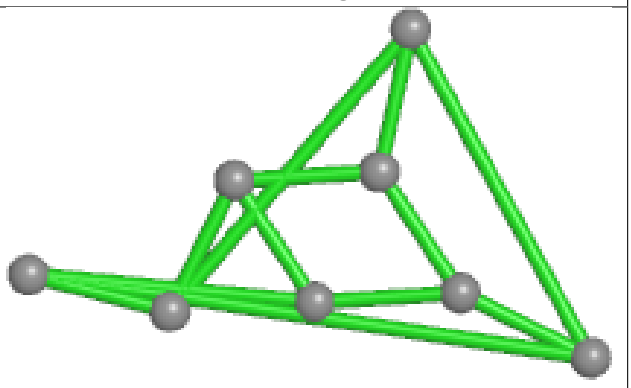
Bond lengths



Bond angles

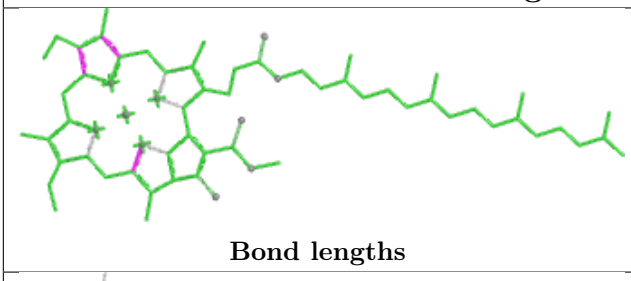


Torsions

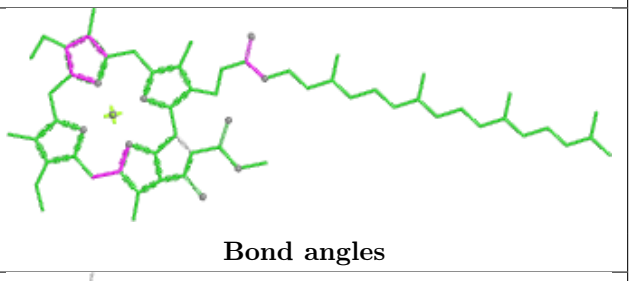


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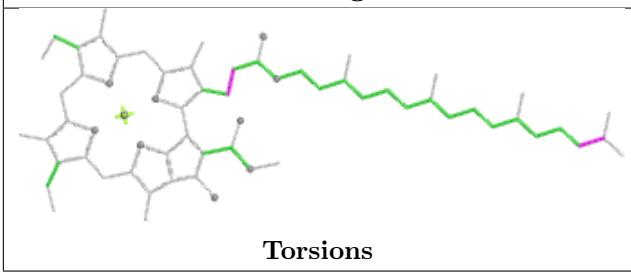
Ligand CLA B 805



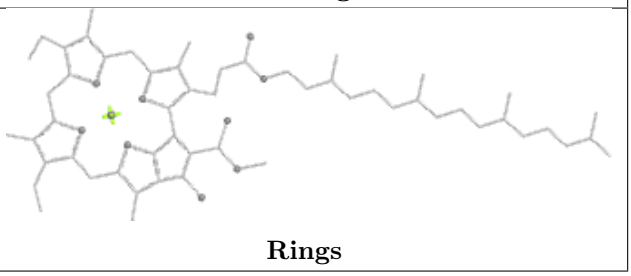
Bond lengths



Bond angles

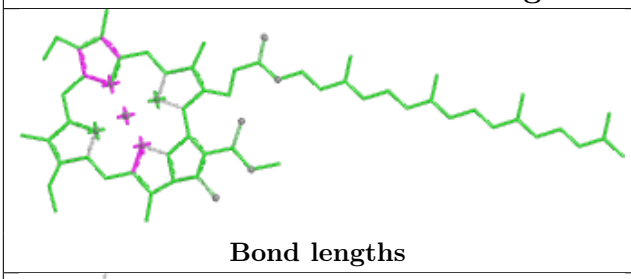


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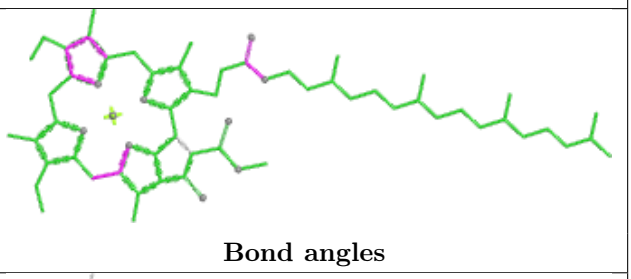


Rings

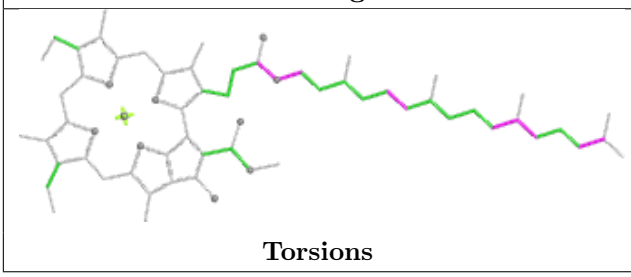
Ligand CLA A 832



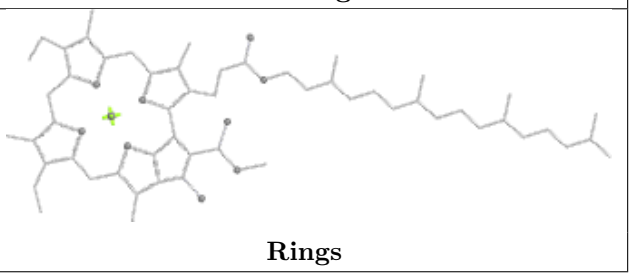
Bond lengths



Bond angles

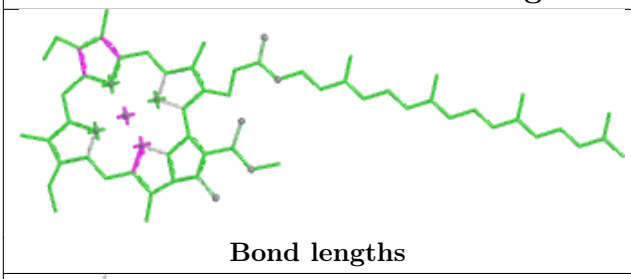


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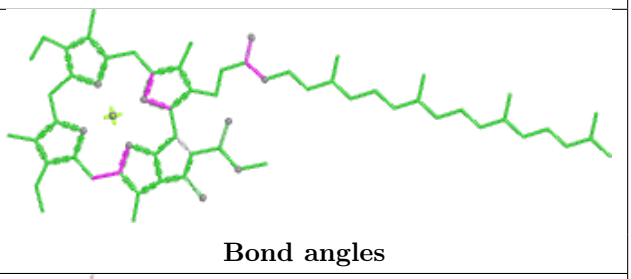


Rings

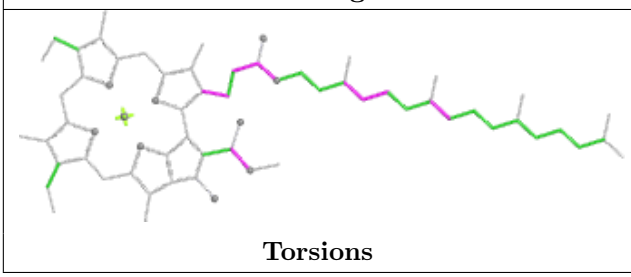
Ligand CLA B 812



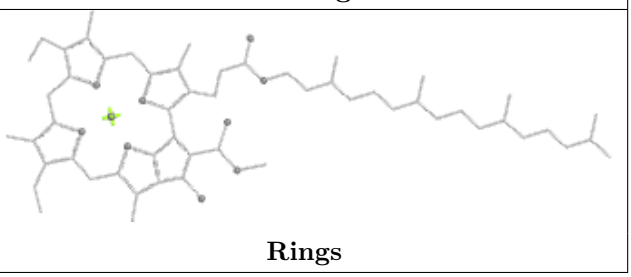
Bond lengths



Bond angles

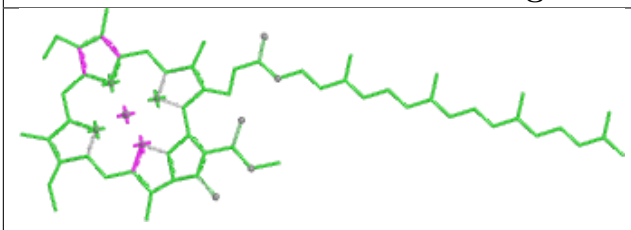


Torsions

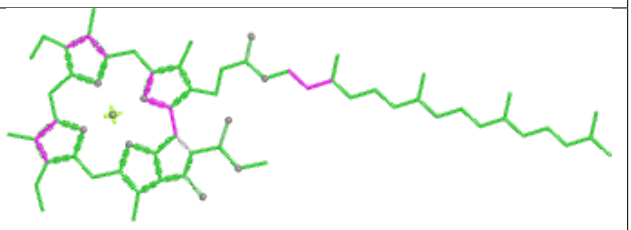


Rings

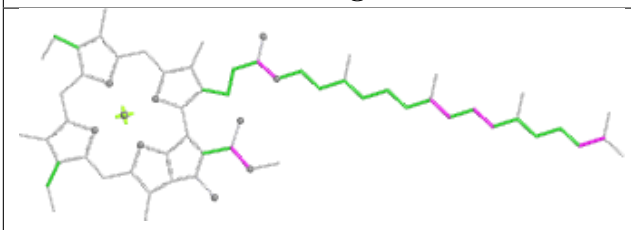
Ligand CLA L 204



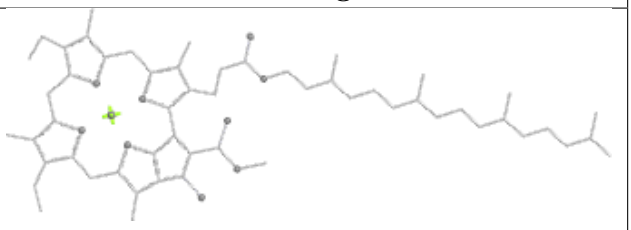
Bond lengths



Bond angles

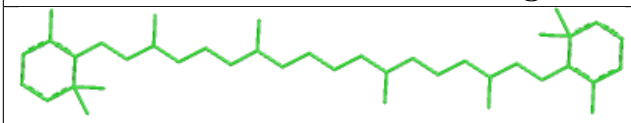


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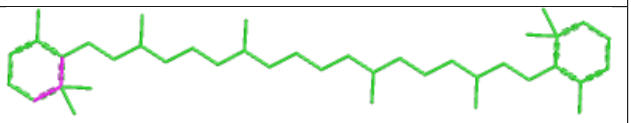


Rings

Ligand BCR B 849



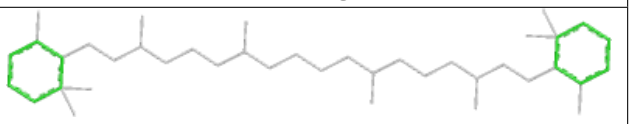
Bond lengths



Bond angles



Torsions



Rings

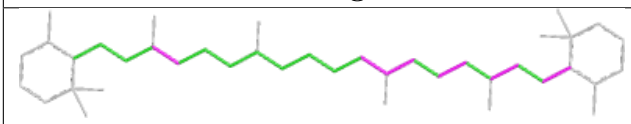
Ligand BCR A 852



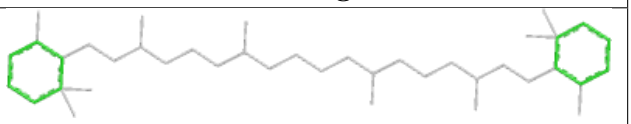
Bond lengths



Bond angles

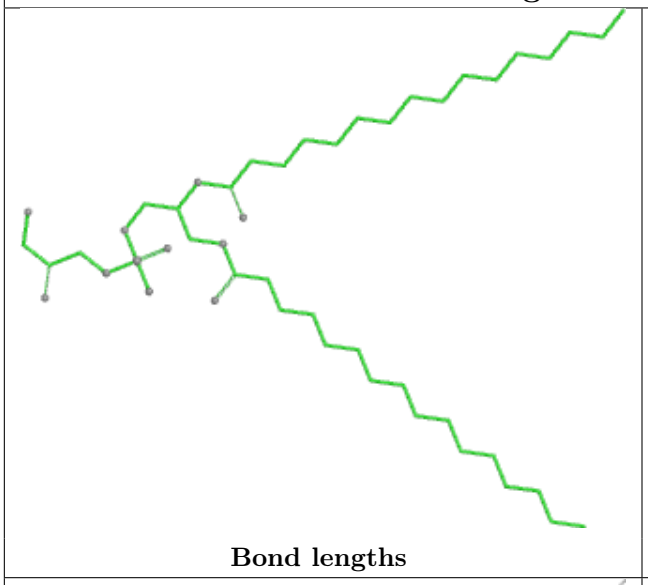


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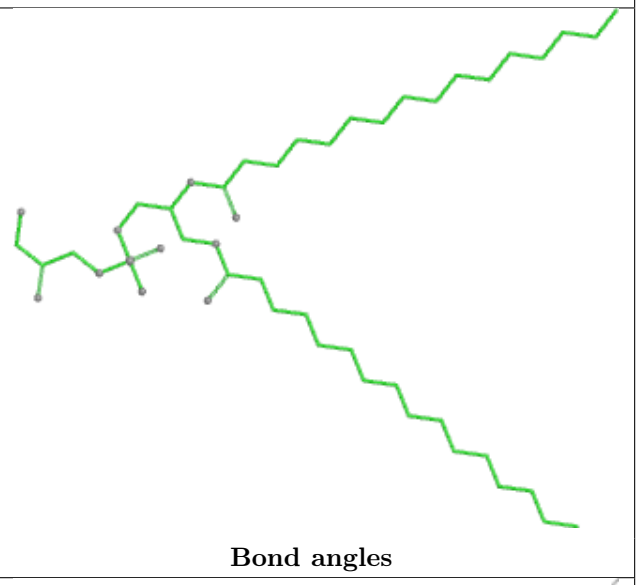


Rings

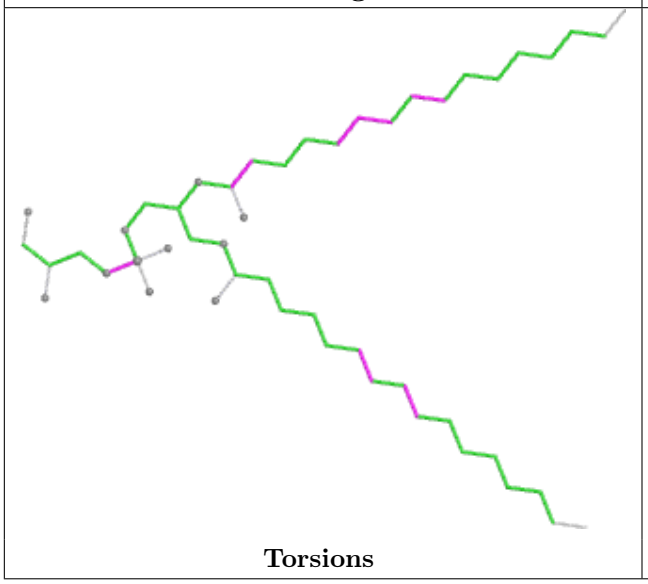
Ligand LHG A 855



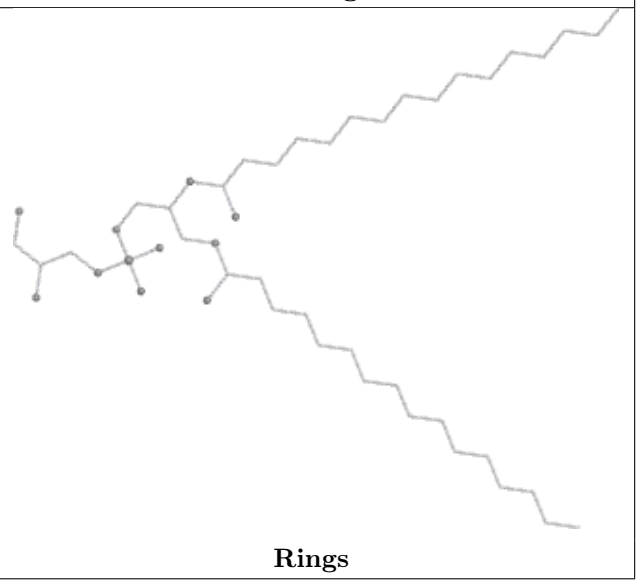
Bond lengths



Bond angles

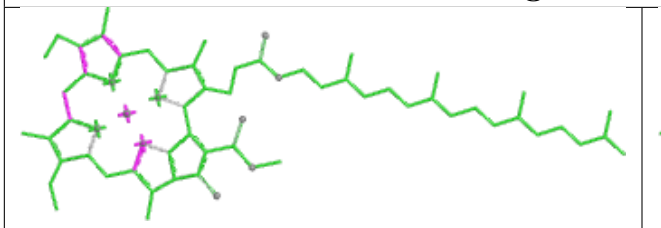


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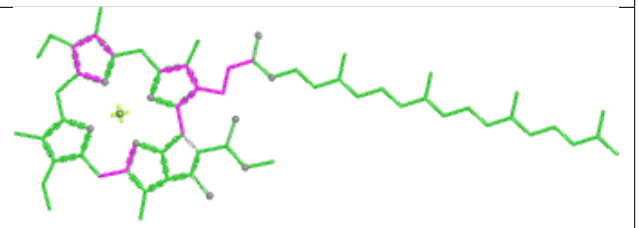


Rings

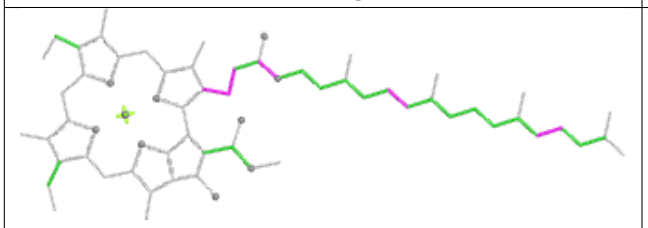
Ligand CLA A 830



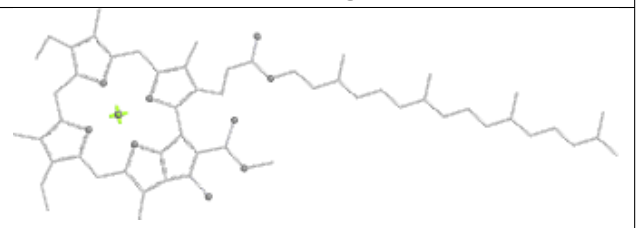
Bond lengths



Bond angles

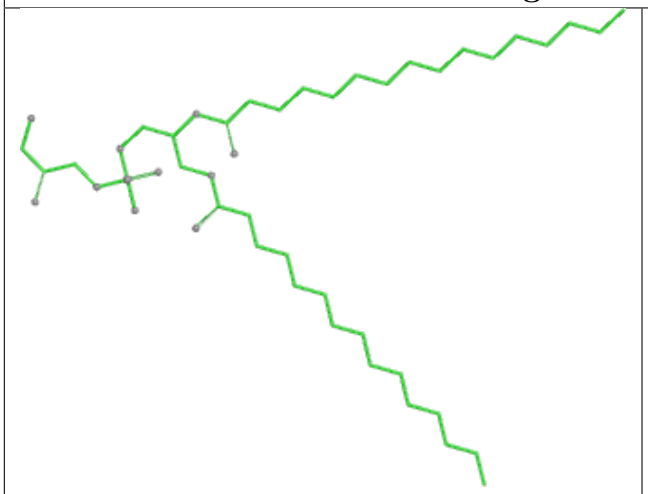


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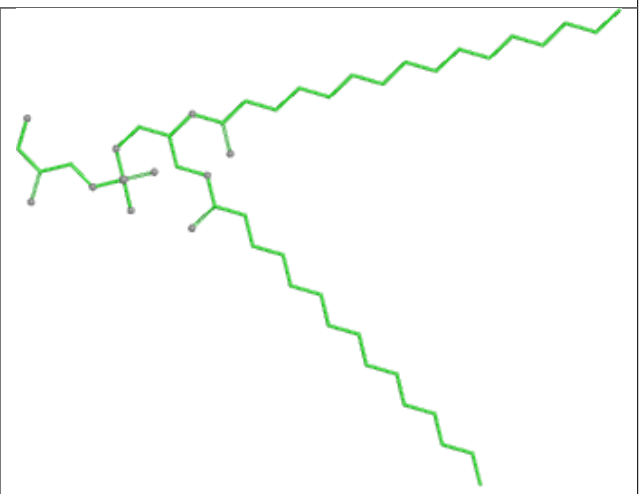


Rings

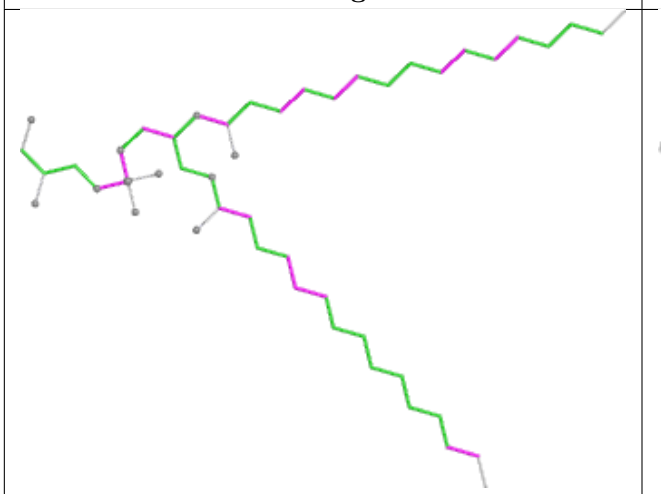
Ligand LHG A 801



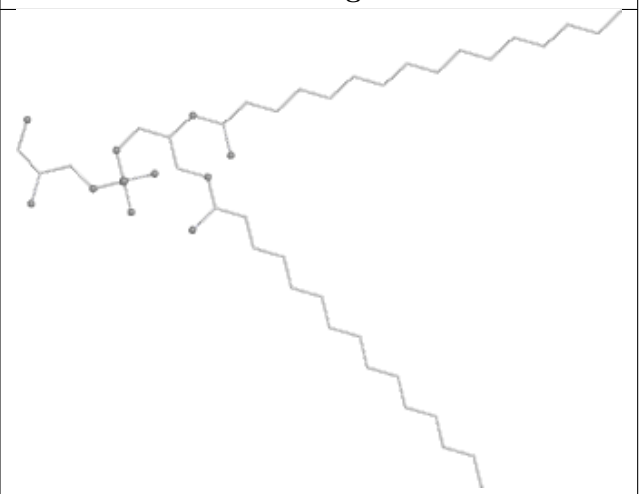
Bond lengths



Bond angles

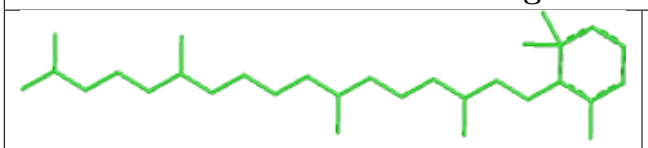


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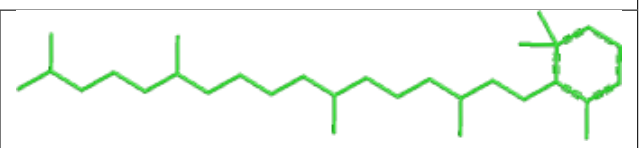


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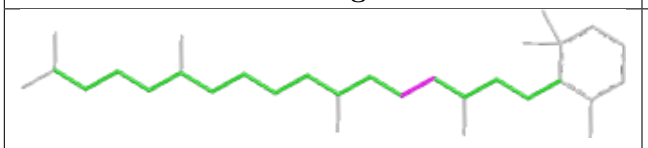
Ligand BCR B 847



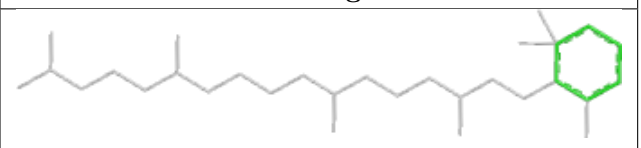
Bond lengths



Bond angles

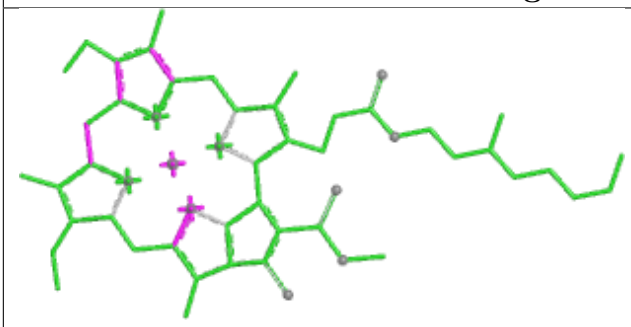


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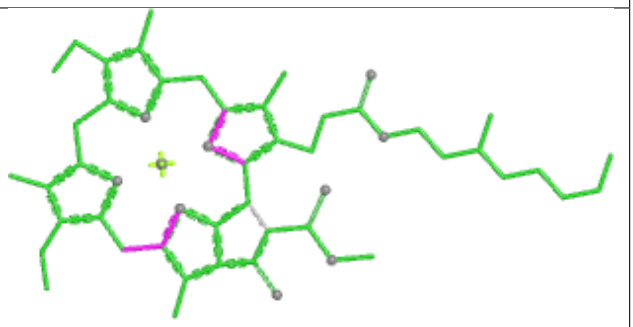


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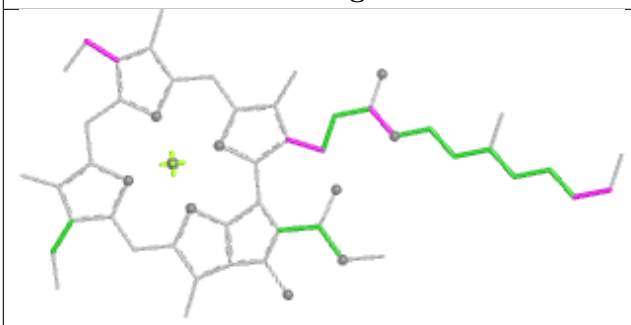
Ligand CLA A 813



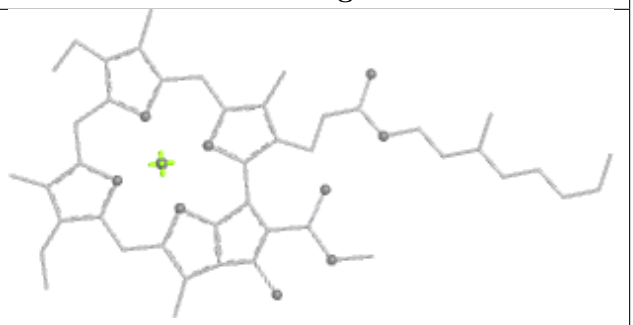
Bond lengths



Bond angles



Torsions

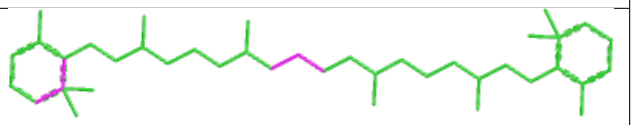


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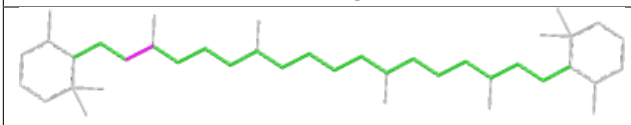
Ligand BCR B 848



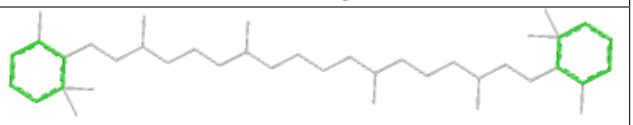
Bond lengths



Bond angles

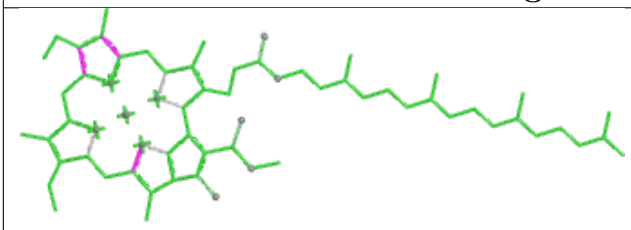


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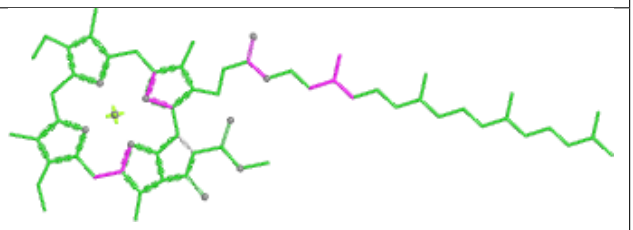


Rings

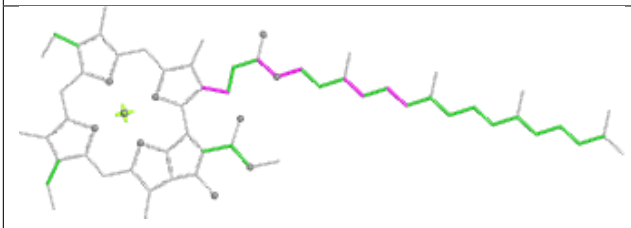
Ligand CLA B 806



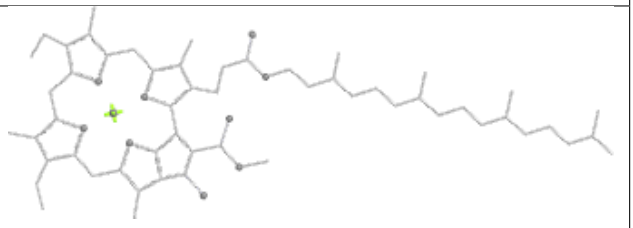
Bond lengths



Bond angles

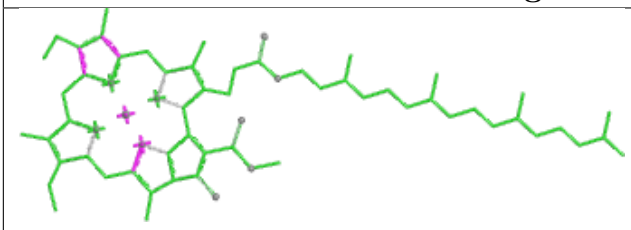


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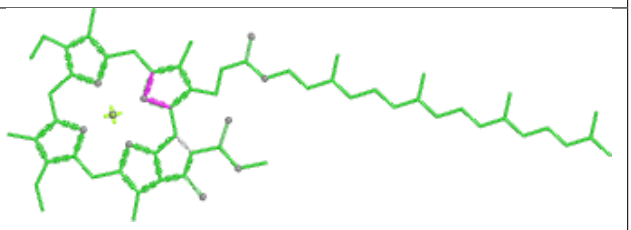


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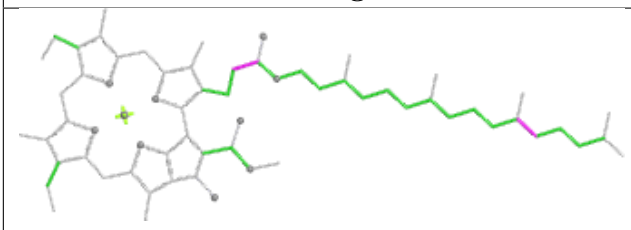
Ligand CLA B 811



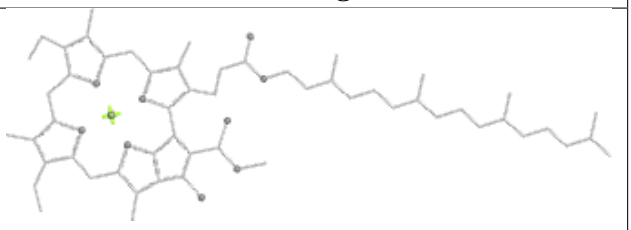
Bond lengths



Bond angles

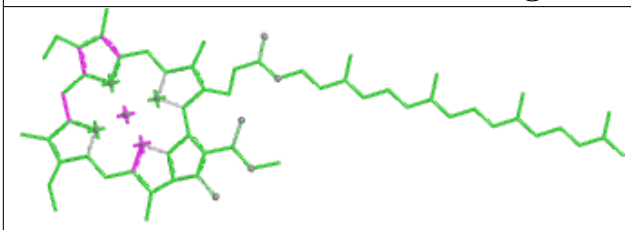


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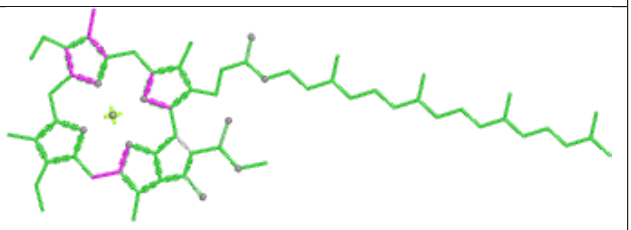


Rings

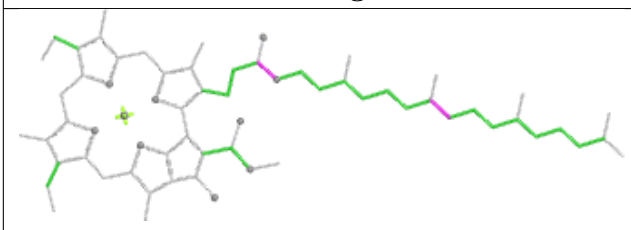
Ligand CLA A 836



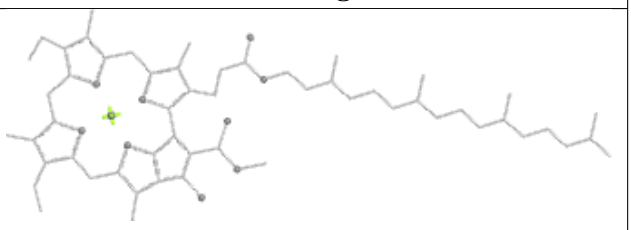
Bond lengths



Bond angles

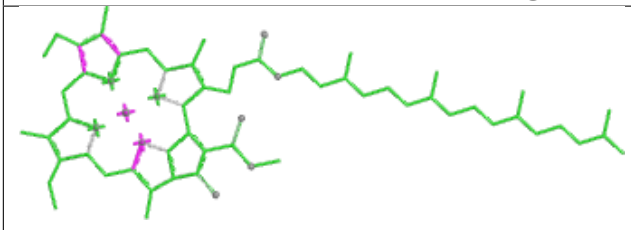


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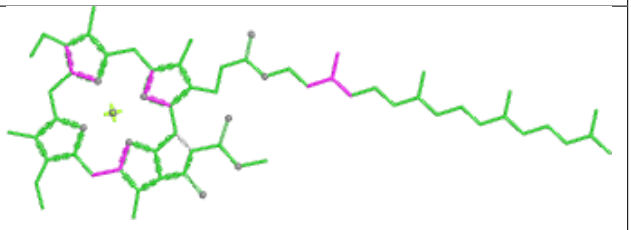


Rings

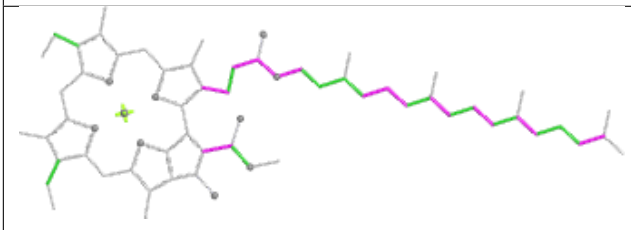
Ligand CLA B 825



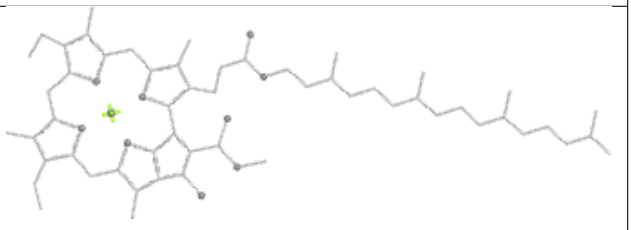
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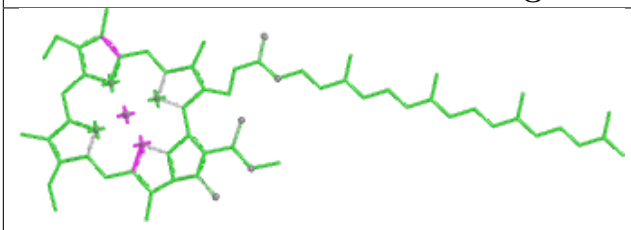
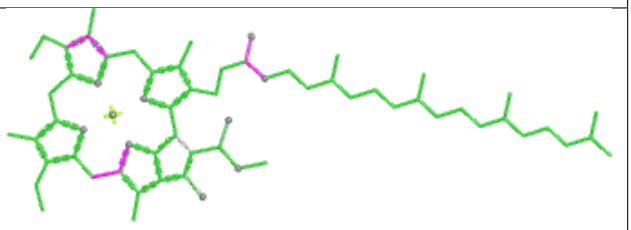
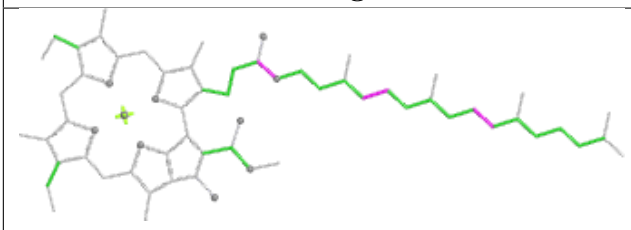
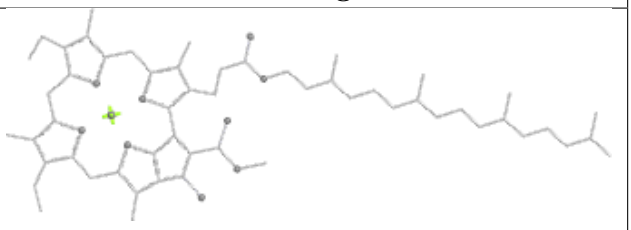
Bond angles

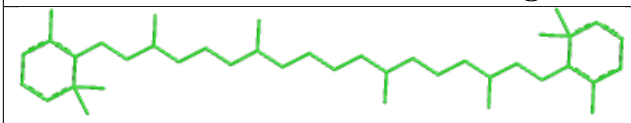
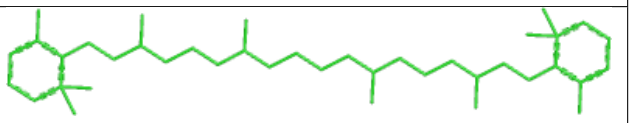
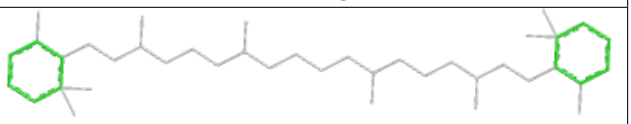


Torsions

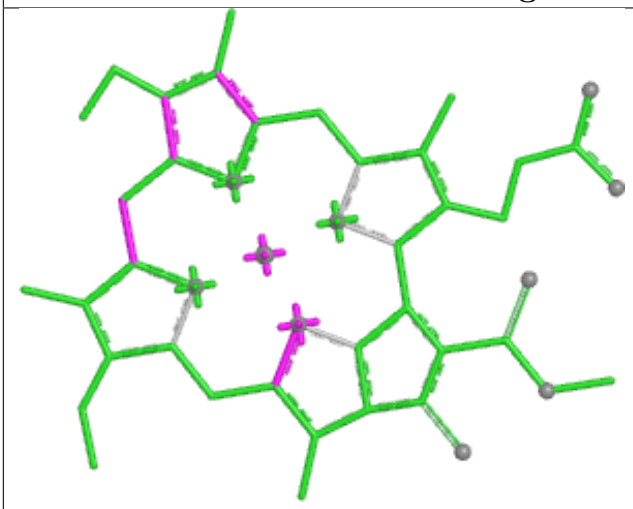


Rings

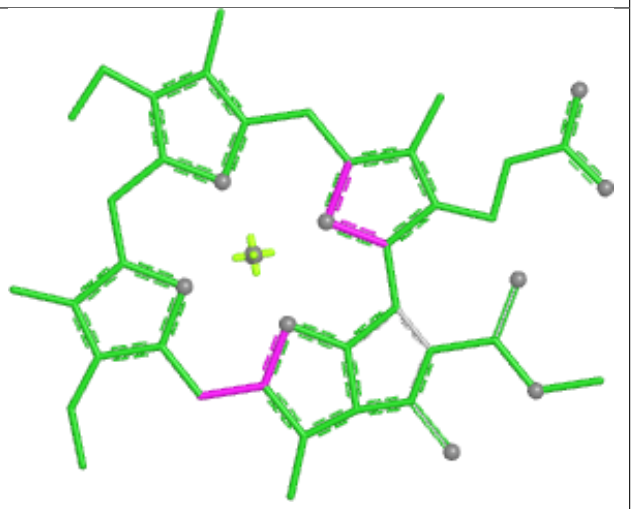
Ligand CLA B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

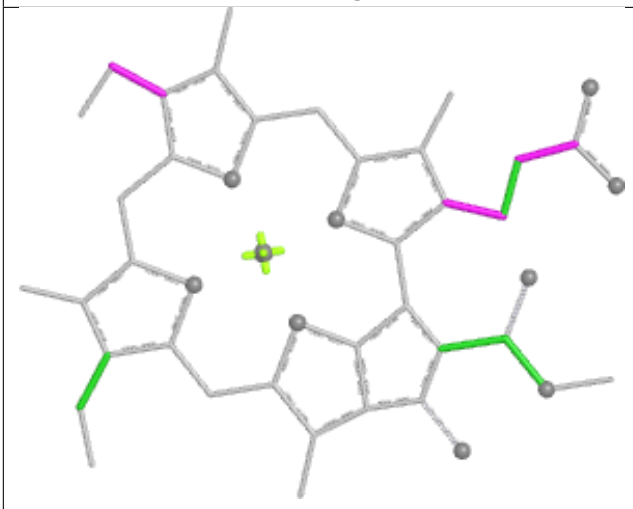
Ligand CLA J 1102



Bond lengths



Bond angles

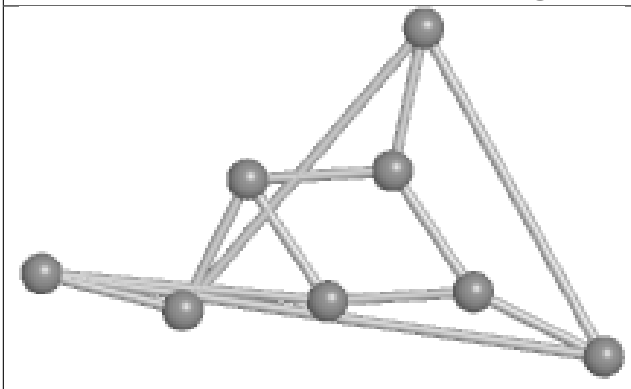


Torsions

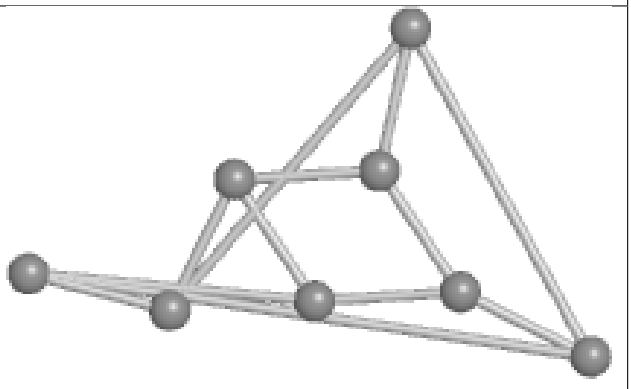


Rings

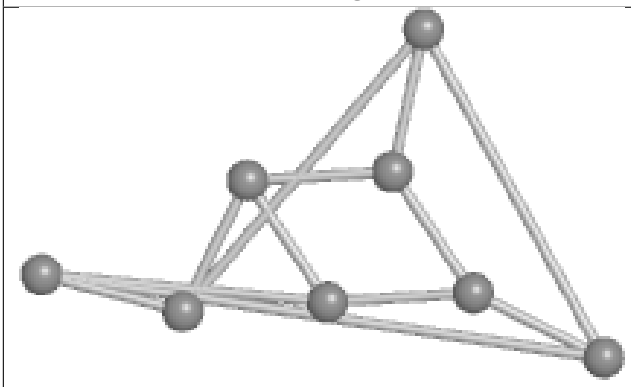
Ligand SF4 C 101



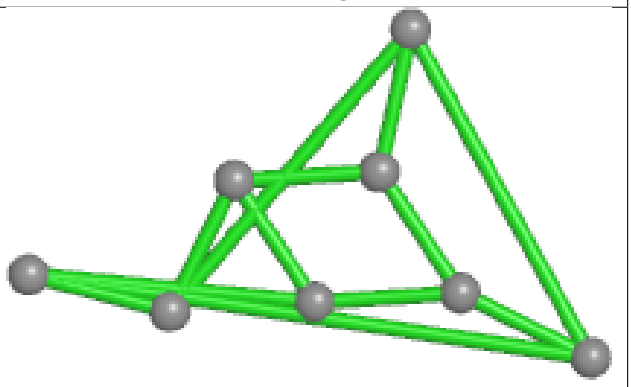
Bond lengths



Bond angles

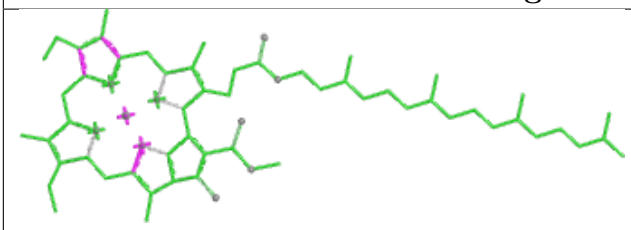


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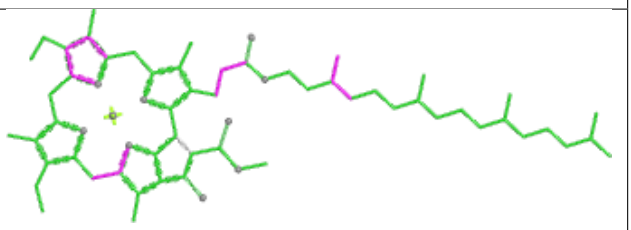


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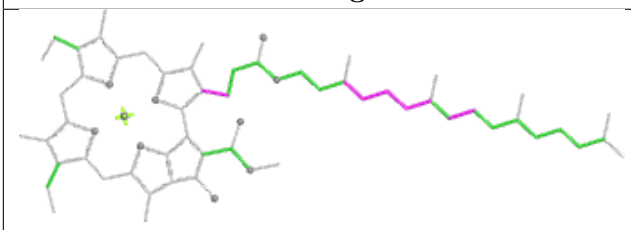
Ligand CLA B 819



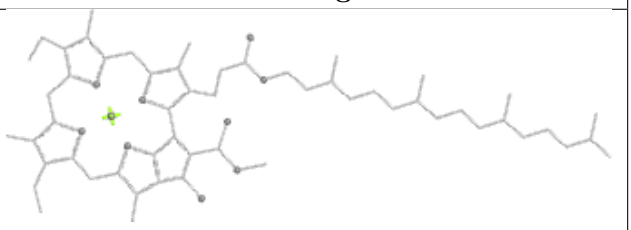
Bond lengths



Bond angles

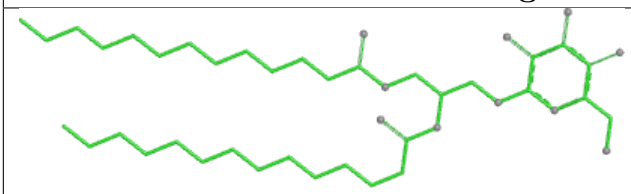


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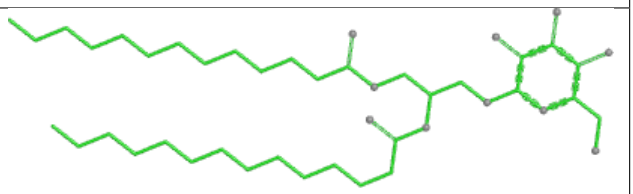


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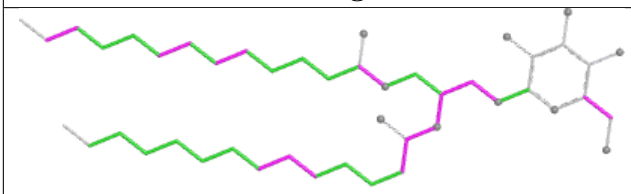
Ligand LMG A 853



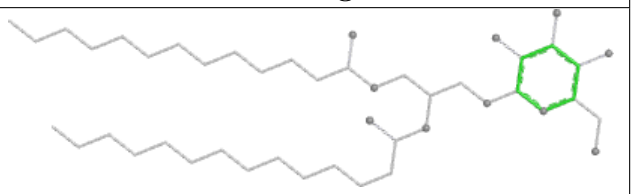
Bond lengths



Bond angles

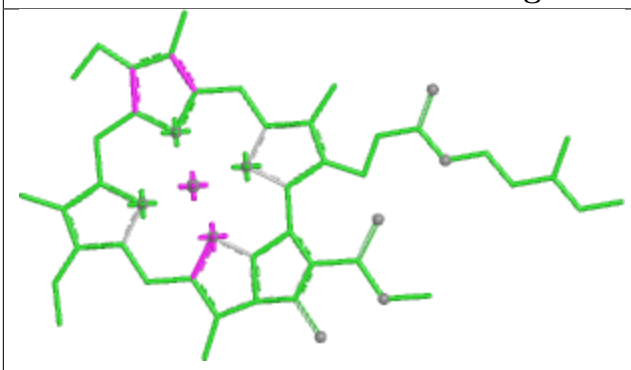


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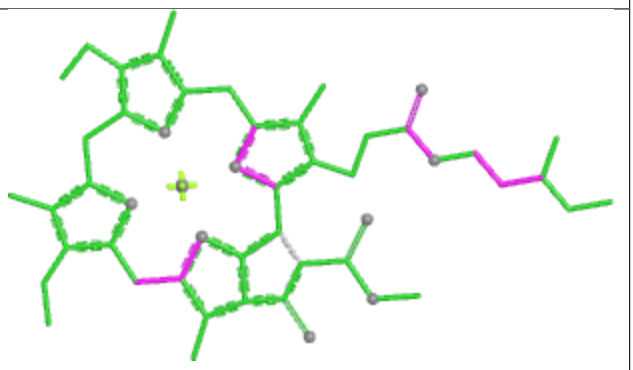


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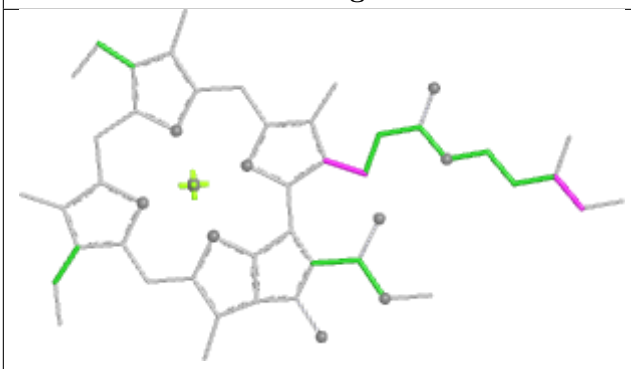
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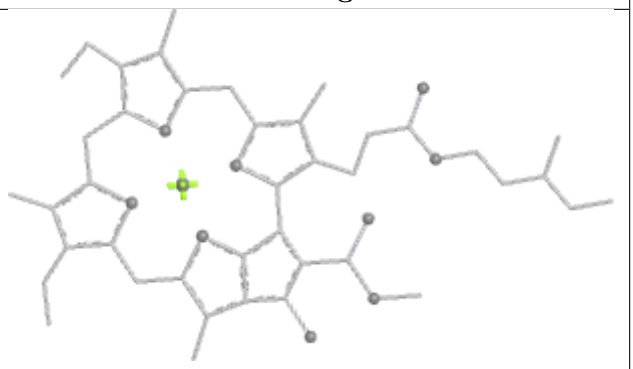
Bond lengths



Bond angles

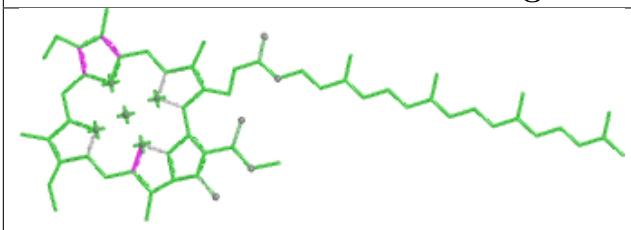


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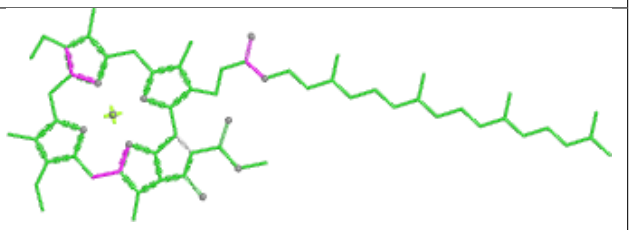


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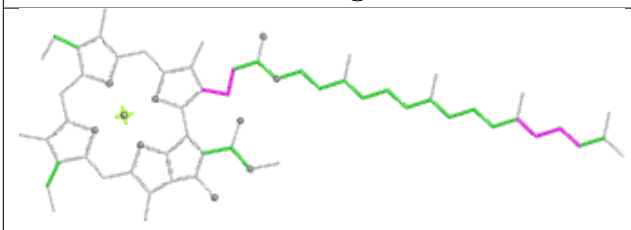
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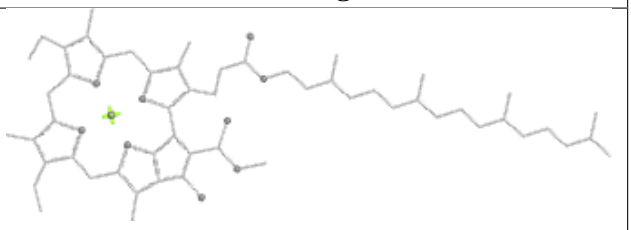
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Bond angles

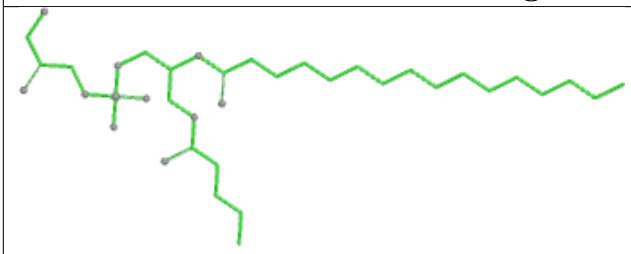


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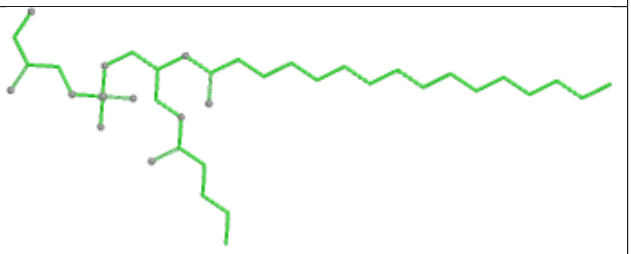


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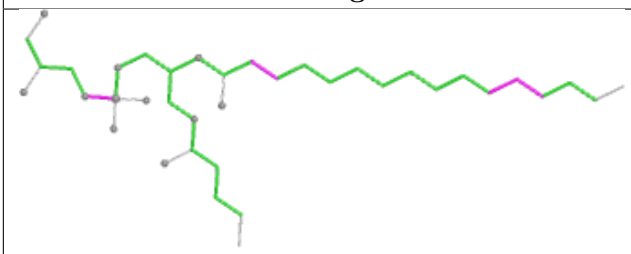
Ligand LHG B 850



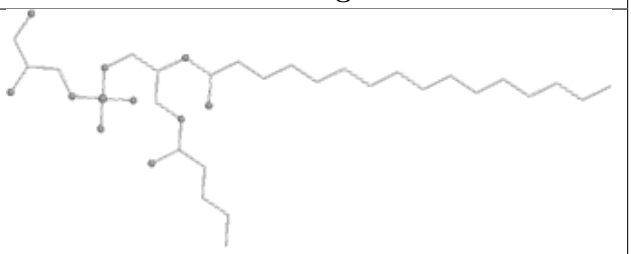
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Bond angles

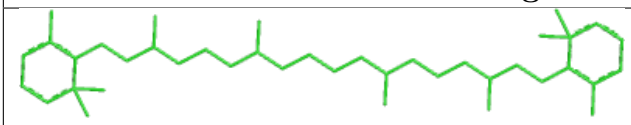


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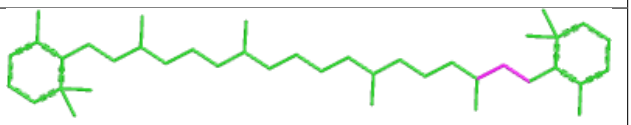


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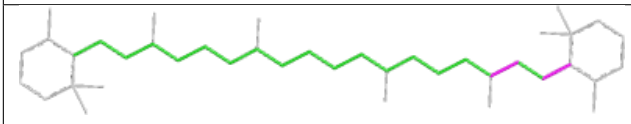
Ligand BCR A 851



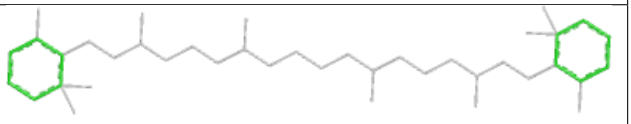
Bond lengths



Bond angles

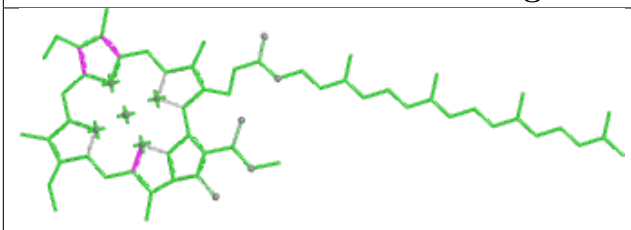


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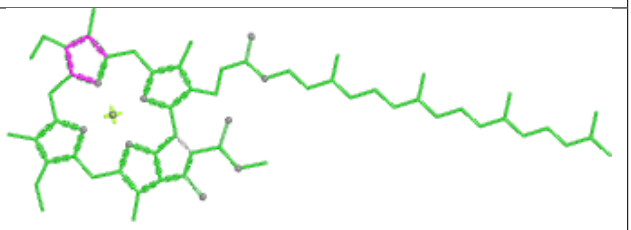


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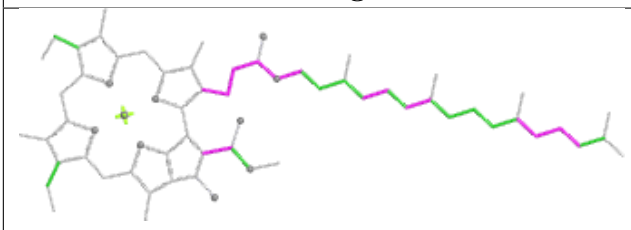
Ligand CLA A 812



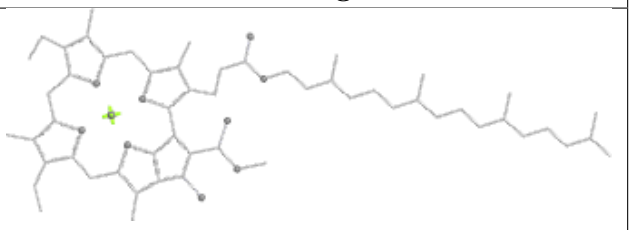
Bond lengths



Bond angles

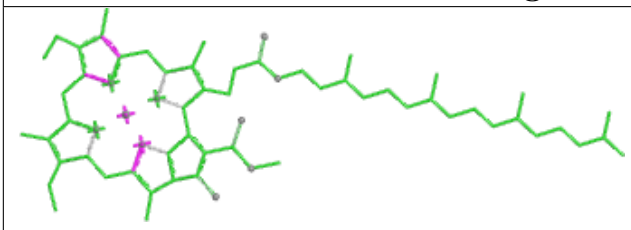


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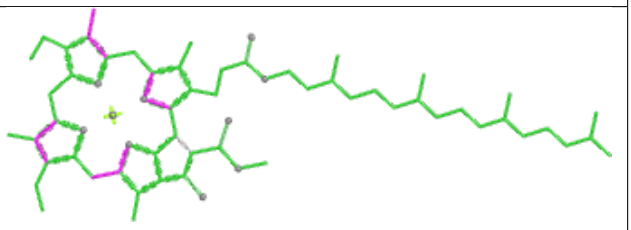


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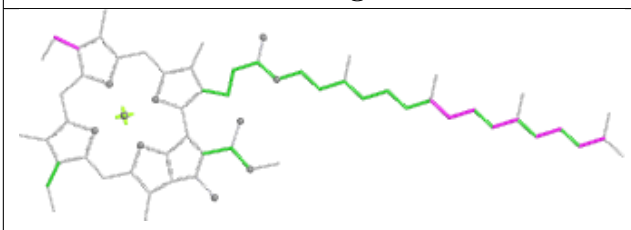
Ligand CLA A 839



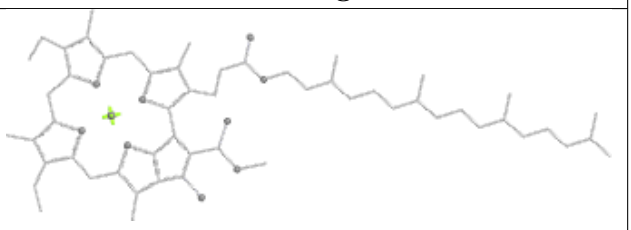
Bond lengths



Bond angles

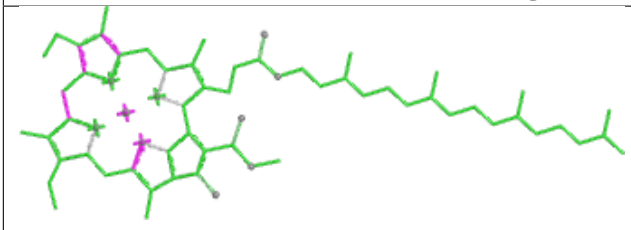


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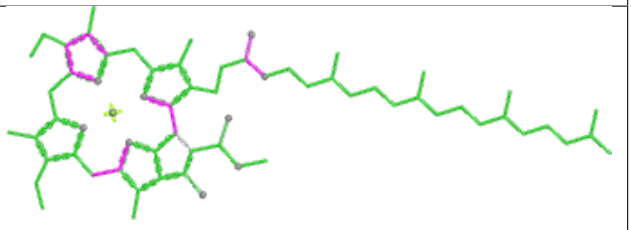


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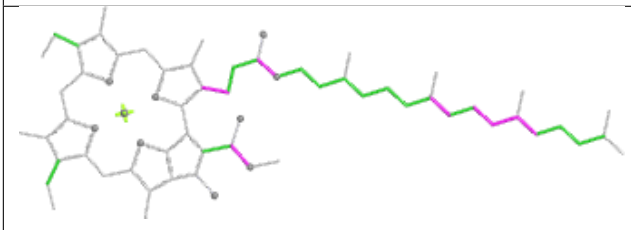
Ligand CLA B 830



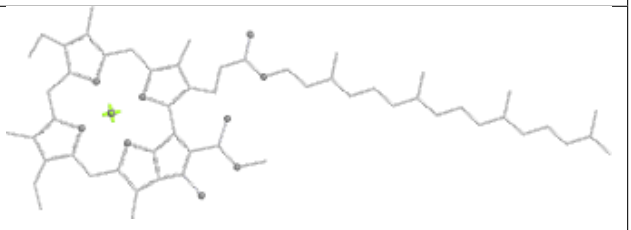
Bond lengths



Bond angles

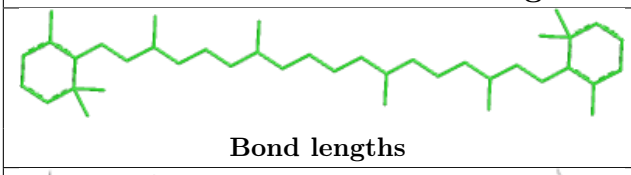


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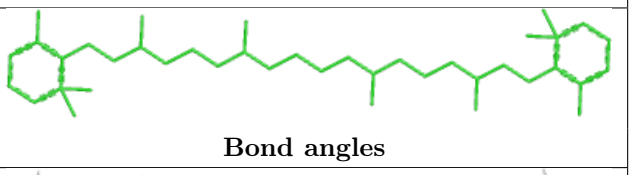


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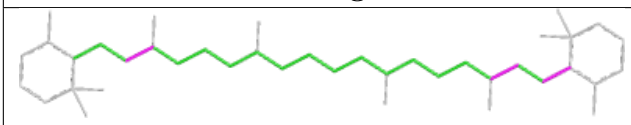
Ligand BCR L 205



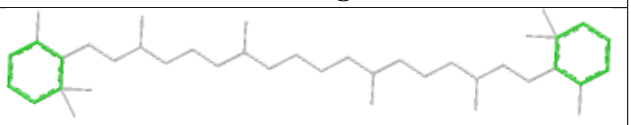
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Bond angles

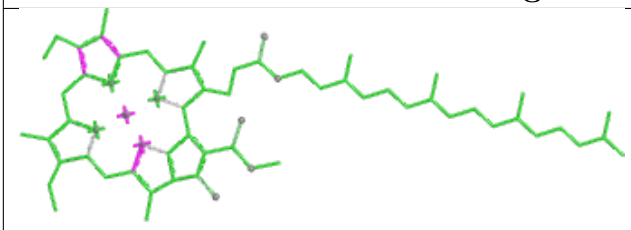


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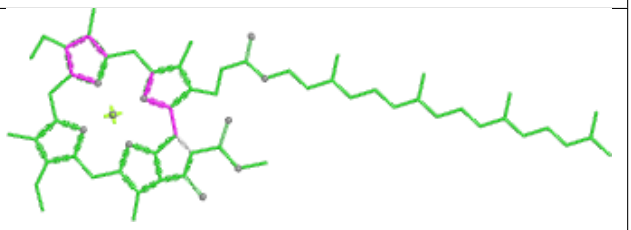


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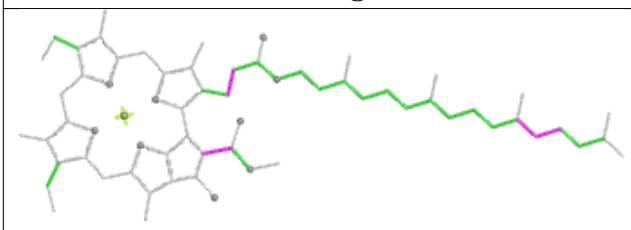
Ligand CLA A 809



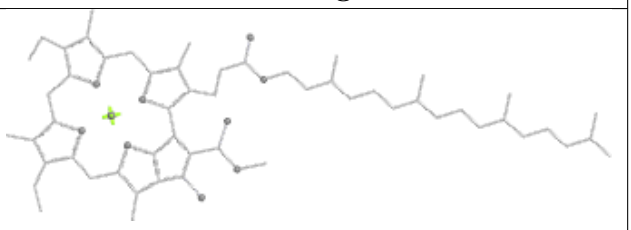
Bond lengths



Bond angles

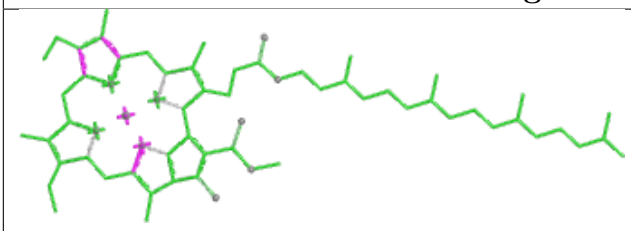


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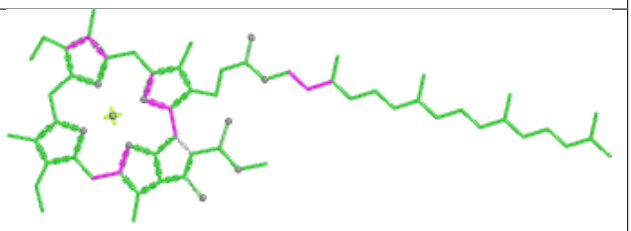


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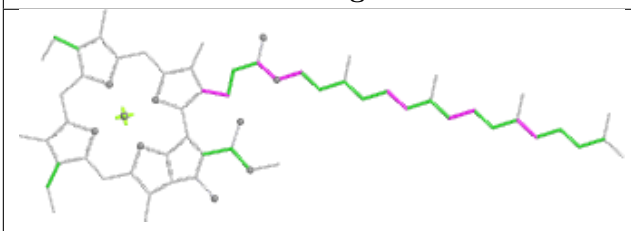
Ligand CLA A 818



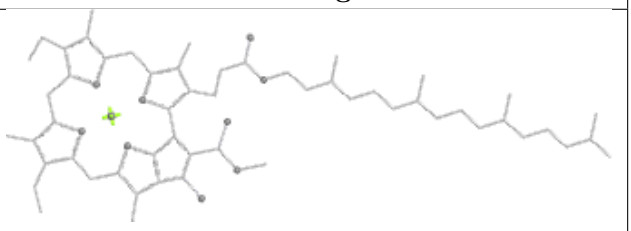
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Bond angles

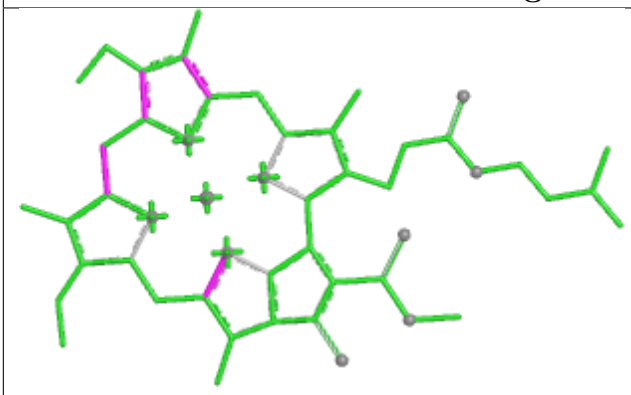


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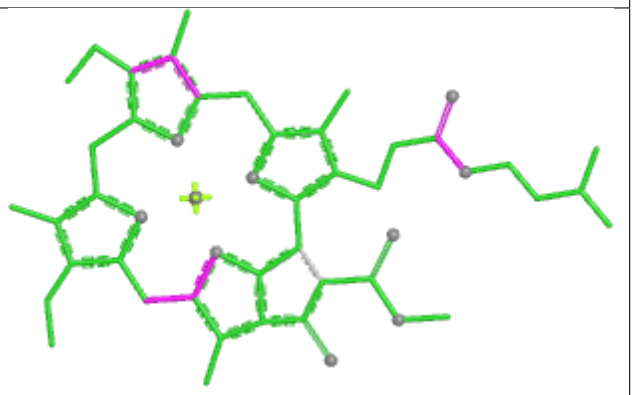


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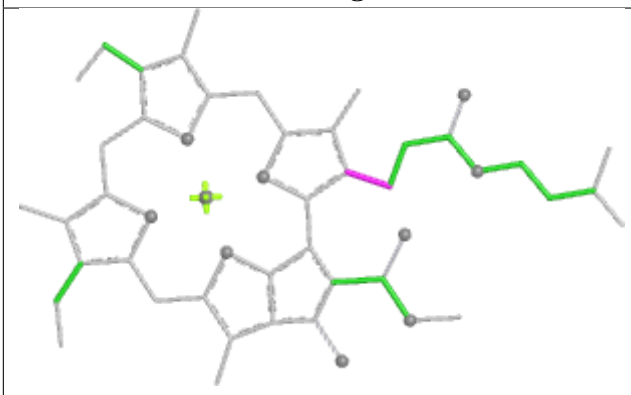
Ligand CLA B 837



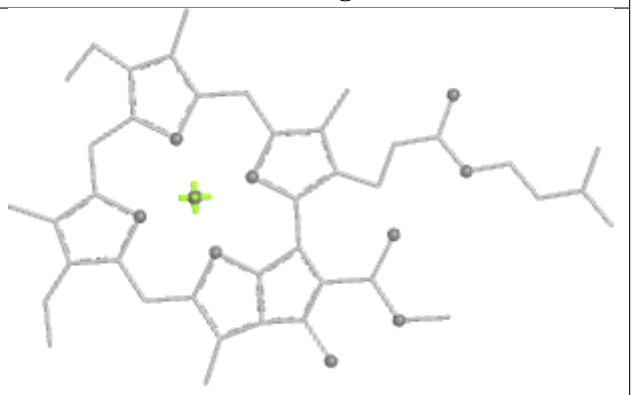
Bond lengths



Bond angles

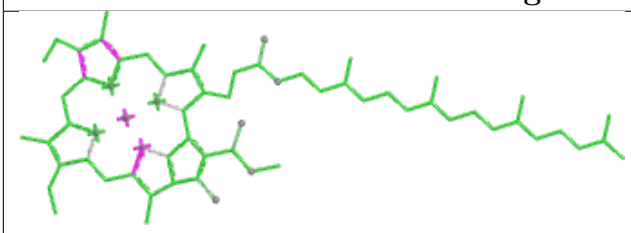


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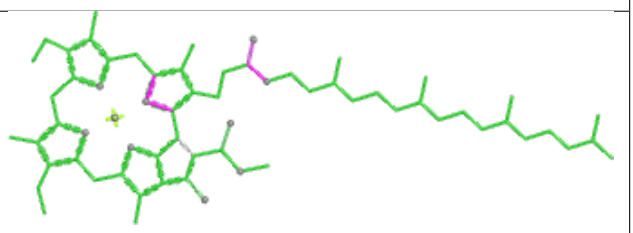


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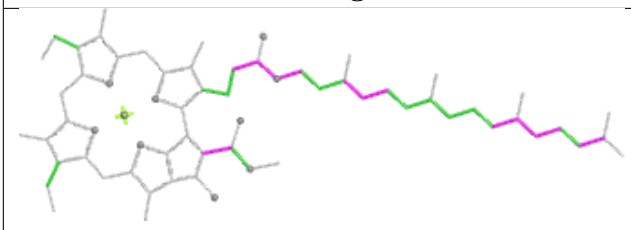
Ligand CLA A 826



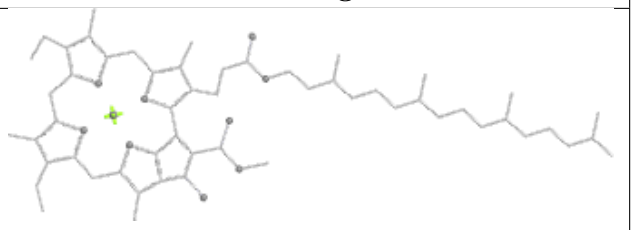
Bond lengths



Bond angles

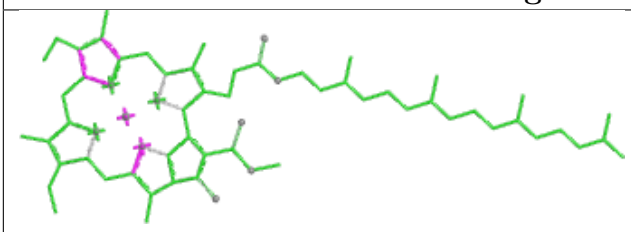


Torsions

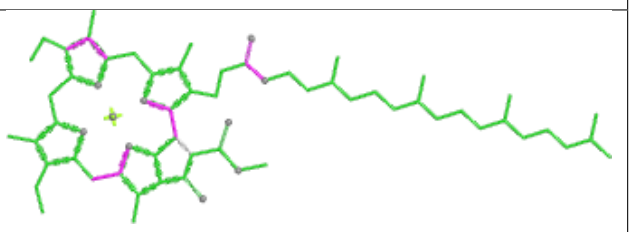


Rings

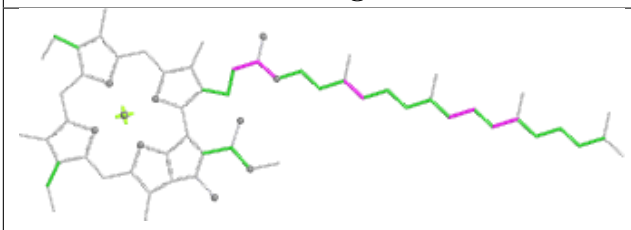
Ligand CLA B 833



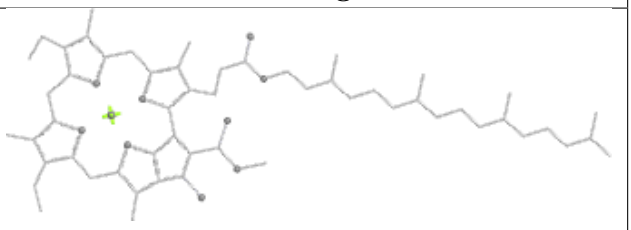
Bond lengths



Bond angles

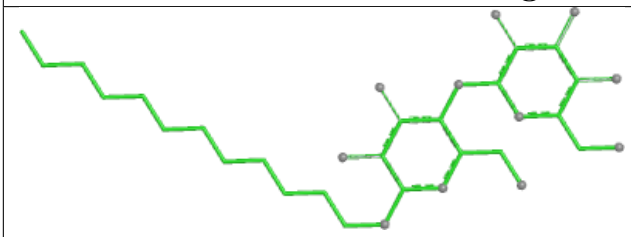


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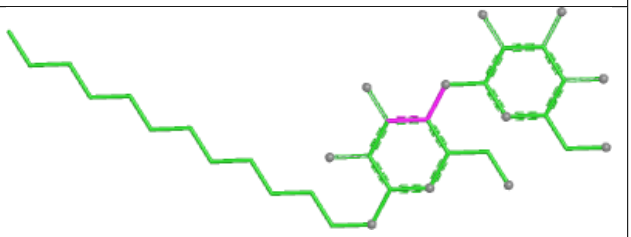


Rings

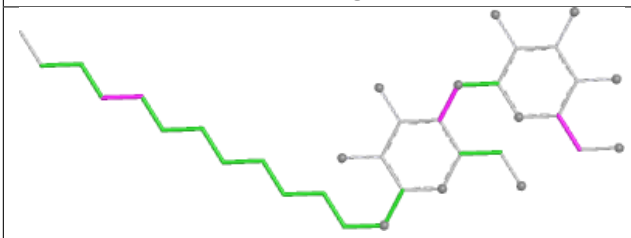
Ligand LMT A 857



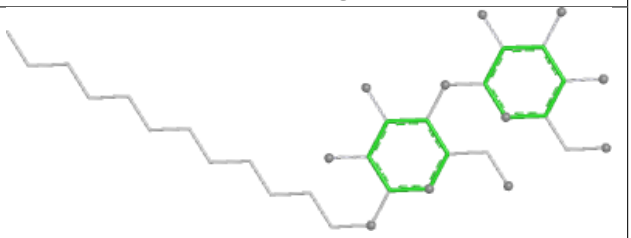
Bond lengths



Bond angles

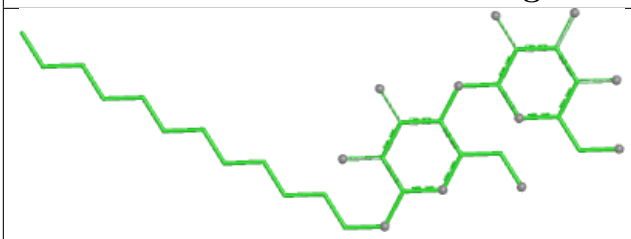


Torsions

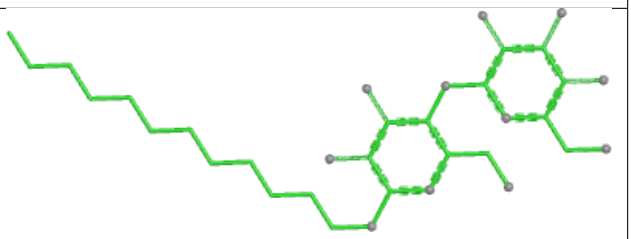


Rings

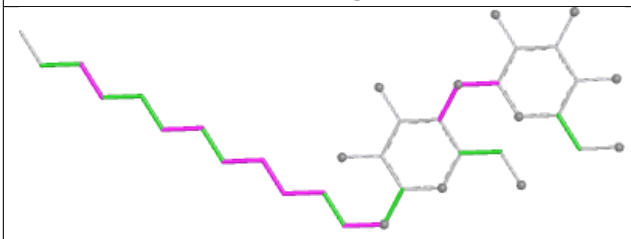
Ligand LMT F 207



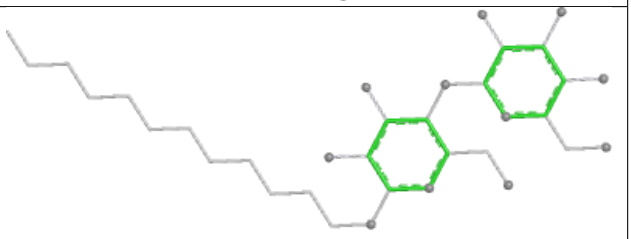
Bond lengths



Bond angles

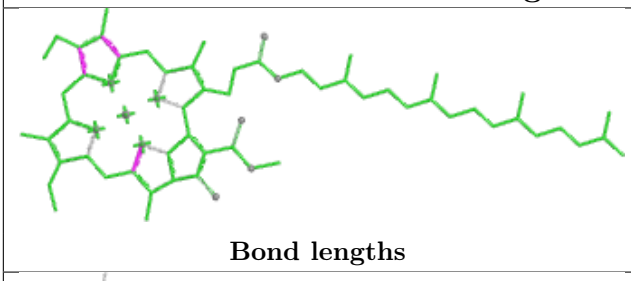


Torsions

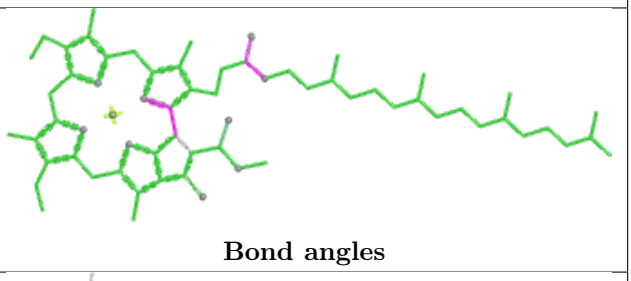


Rings

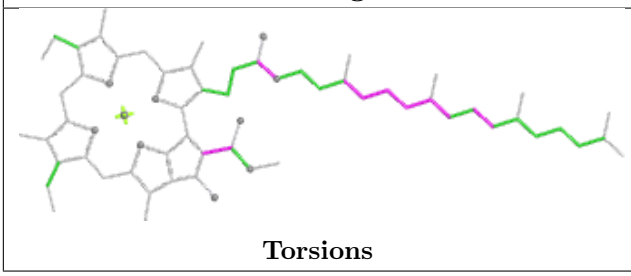
Ligand CLA A 831



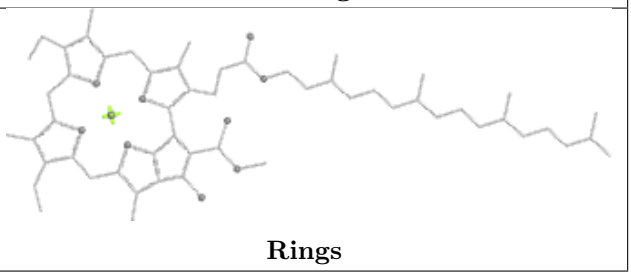
Bond lengths



Bond angles

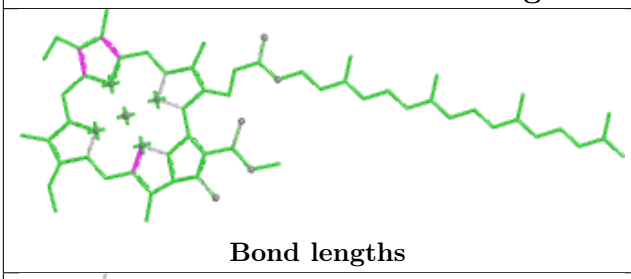


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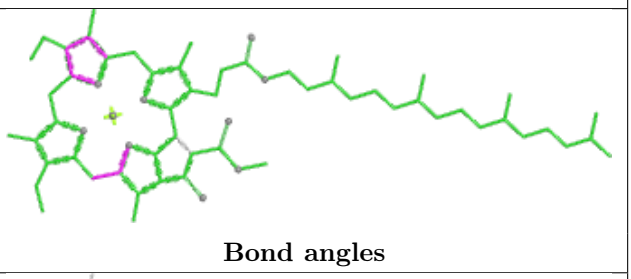


Rings

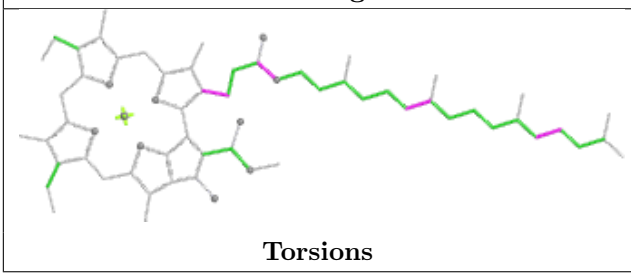
Ligand CLA A 842



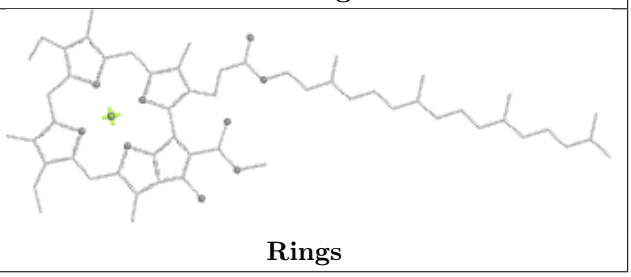
Bond lengths



Bond angles

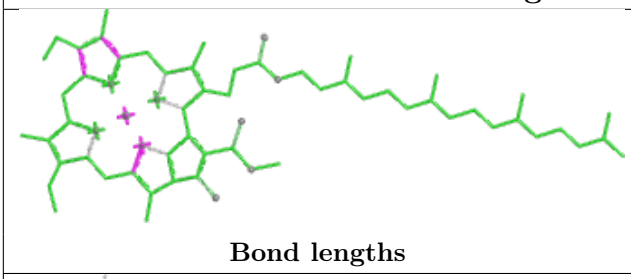


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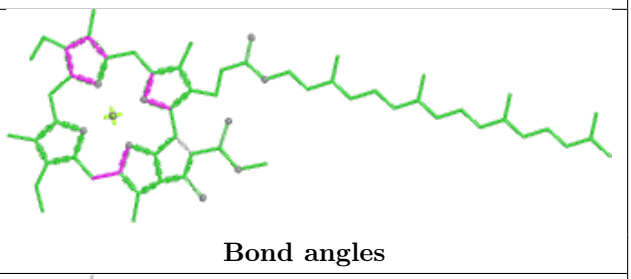


Rings

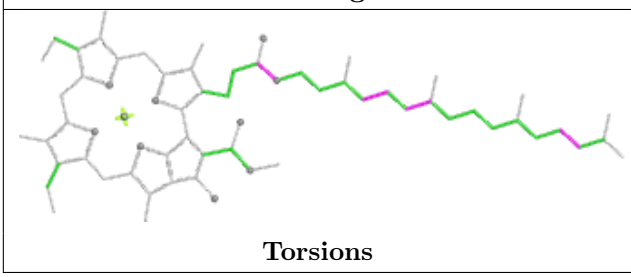
Ligand CLA B 831



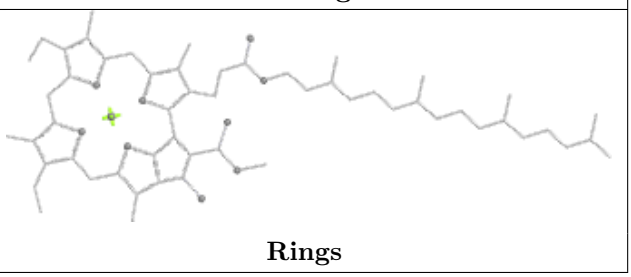
Bond lengths



Bond angles

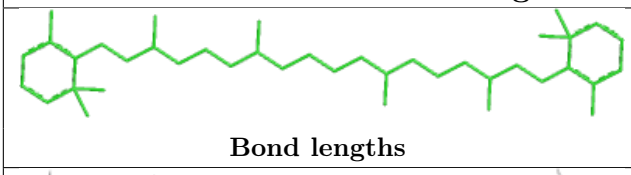


Torsions

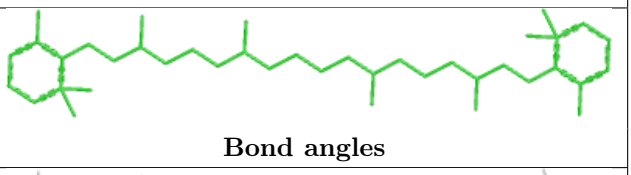


Rings

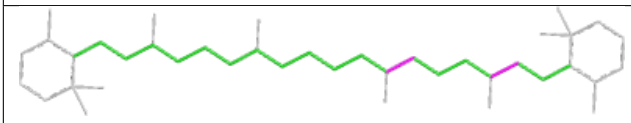
Ligand BCR K 4005



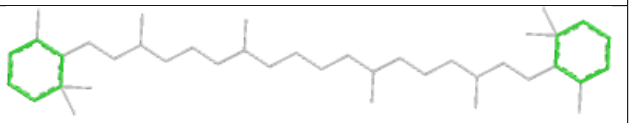
Bond lengths



Bond angles

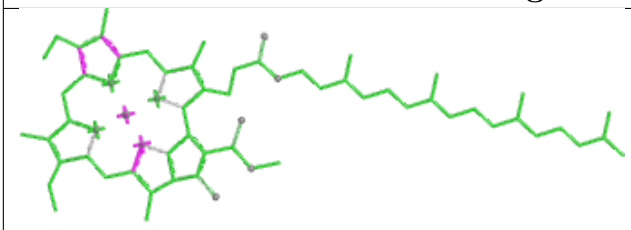


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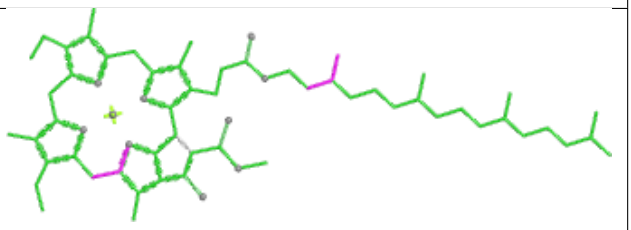


Rings

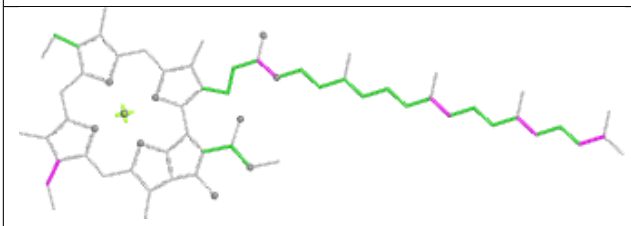
Ligand CLA L 203



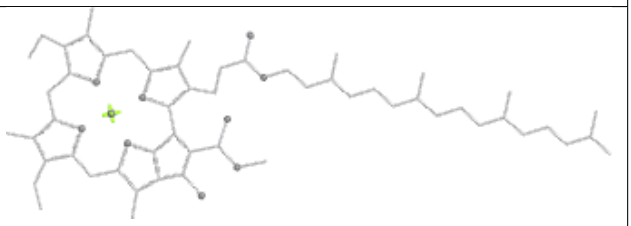
Bond lengths



Bond angles

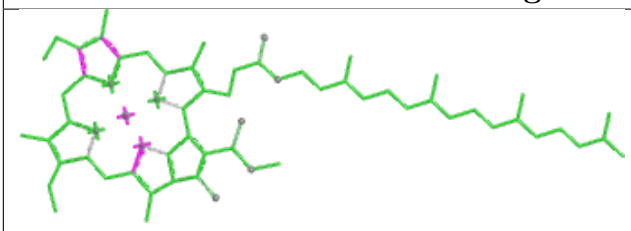


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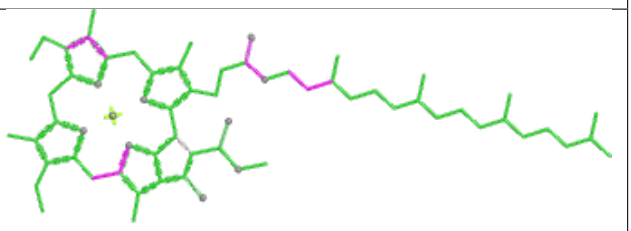


Rings

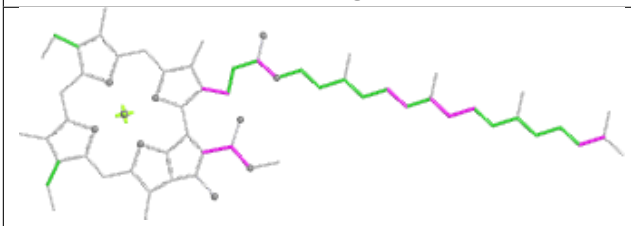
Ligand CLA A 823



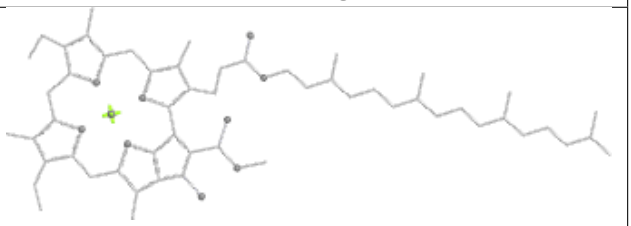
Bond lengths



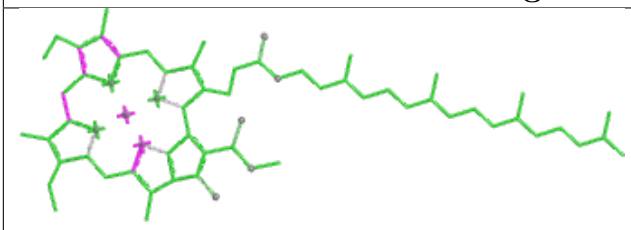
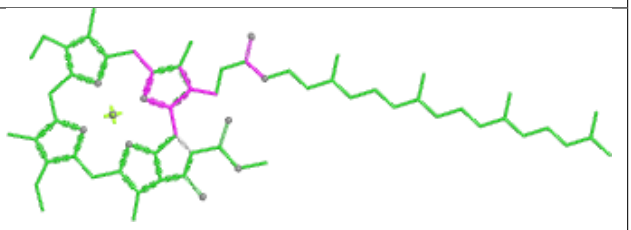
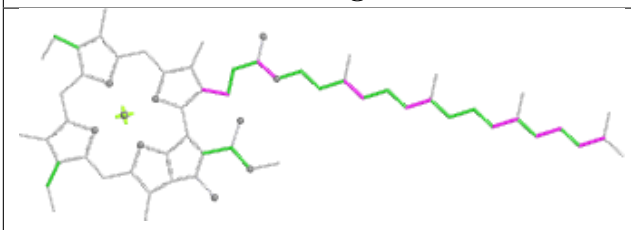
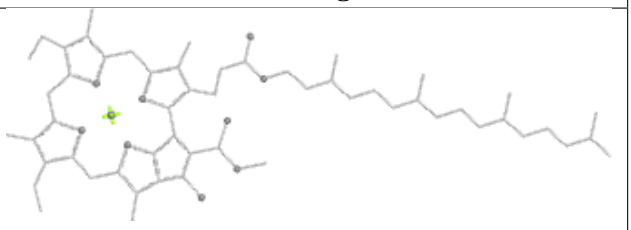
Bond angles

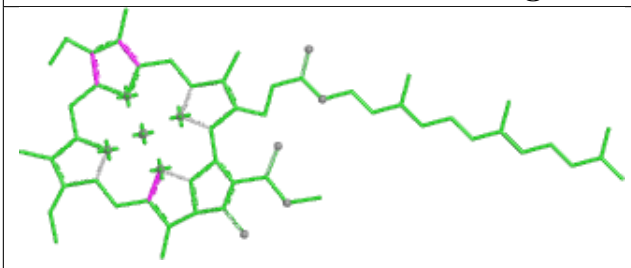
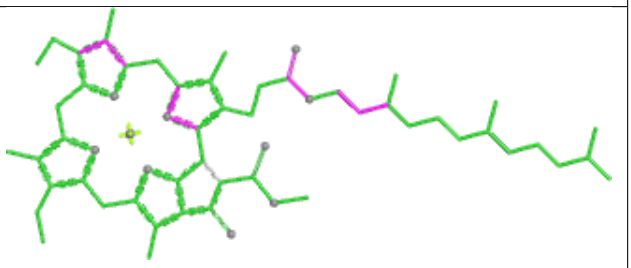
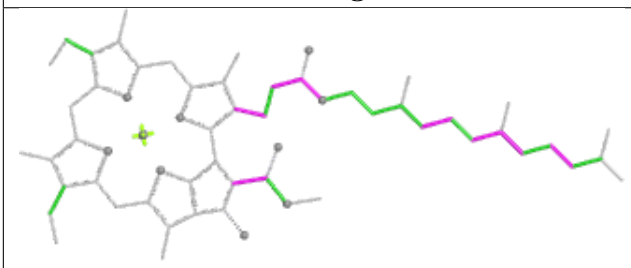
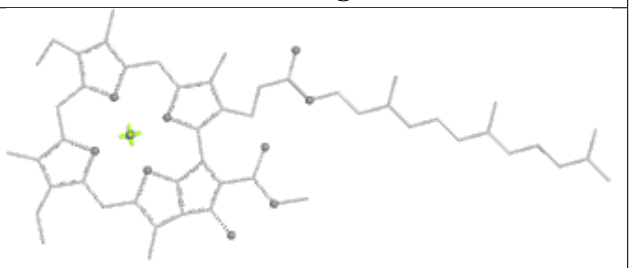


Torsions

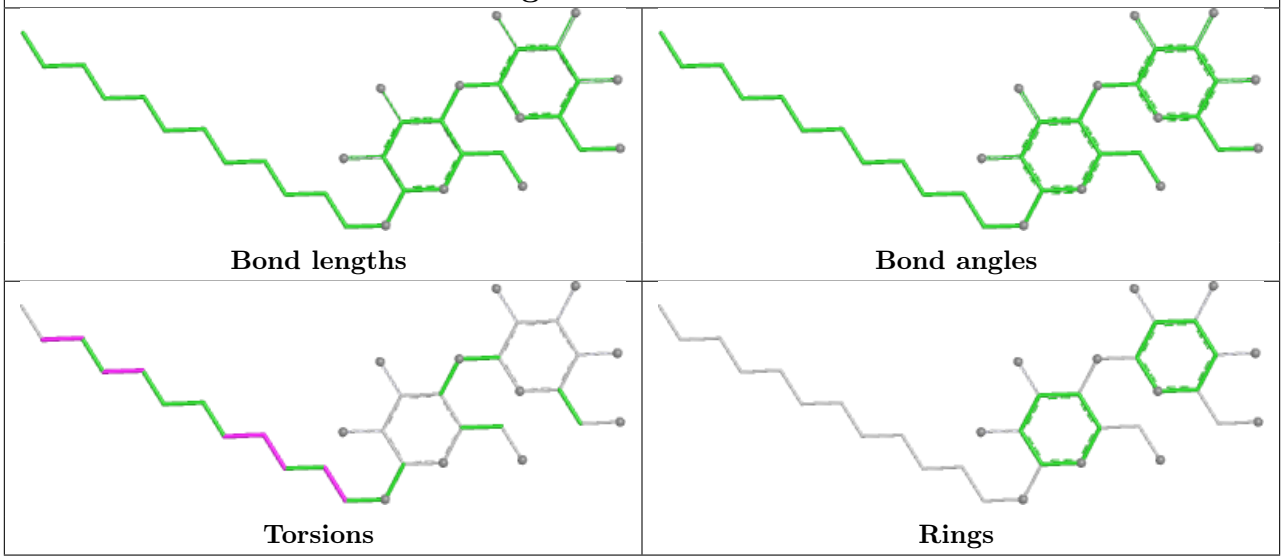


Rings

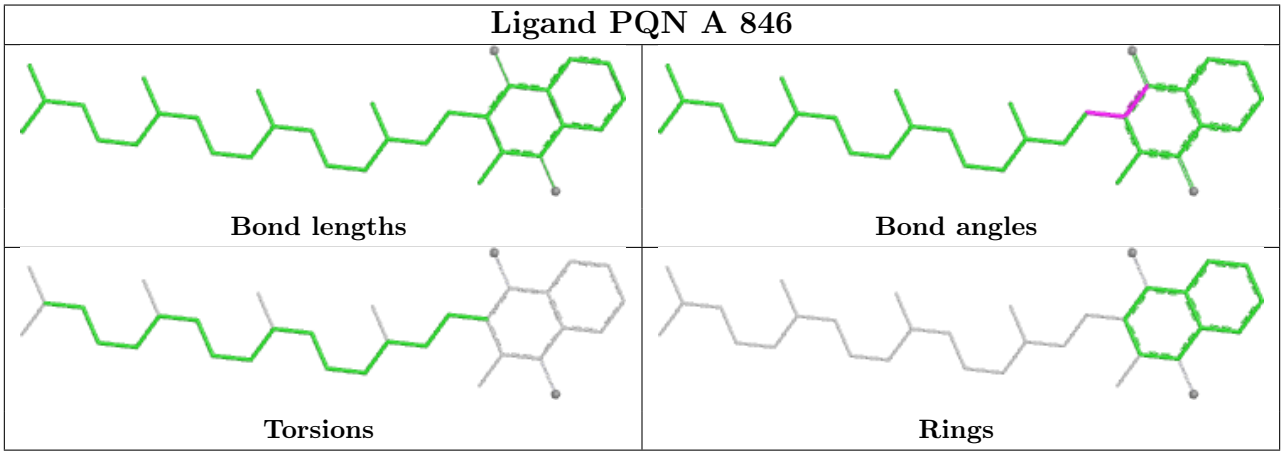
Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT A 856



Ligand PQN A 846



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

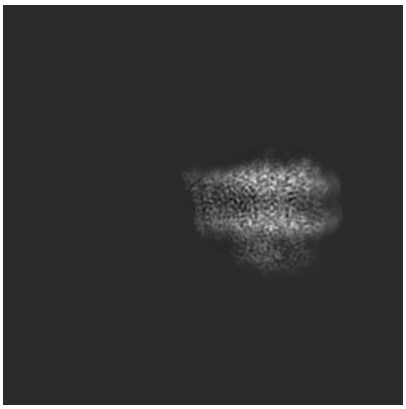
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71005. These allow visual inspection of the internal detail of the map and identification of artifacts.

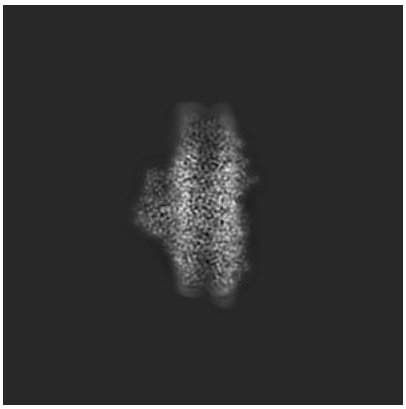
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

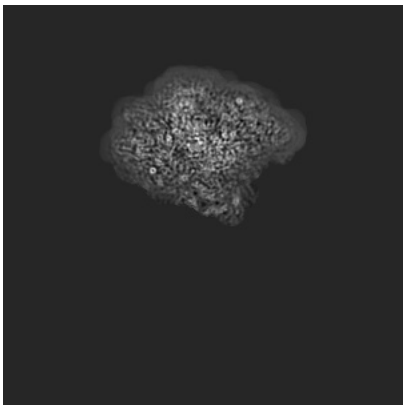
6.1.1 Primary map



X

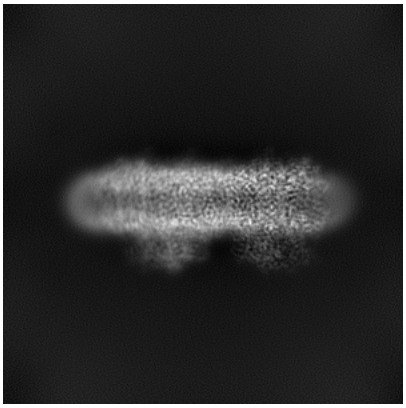


Y

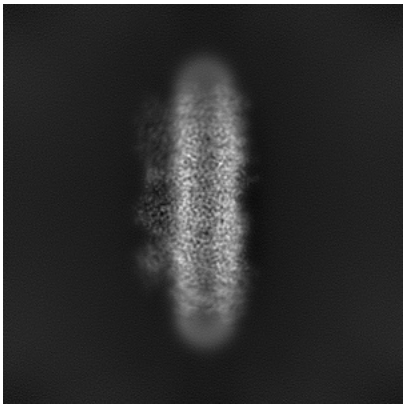


Z

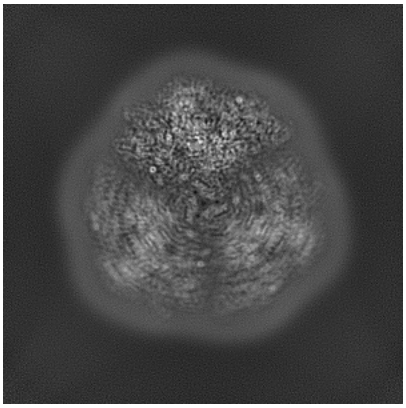
6.1.2 Raw map



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: 220

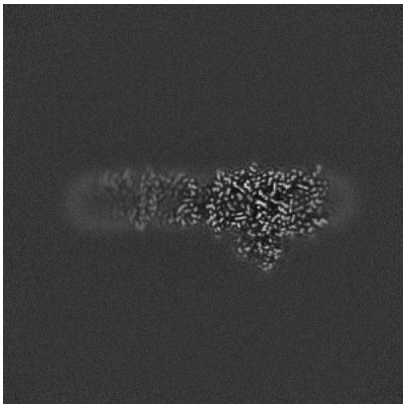


Y Index: 220

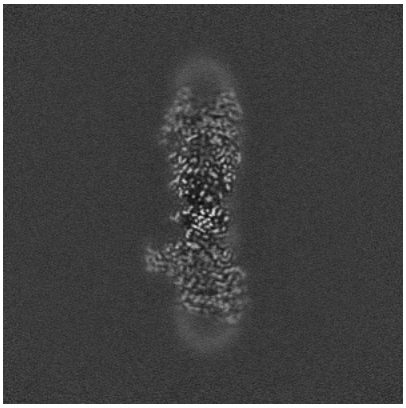


Z Index: 220

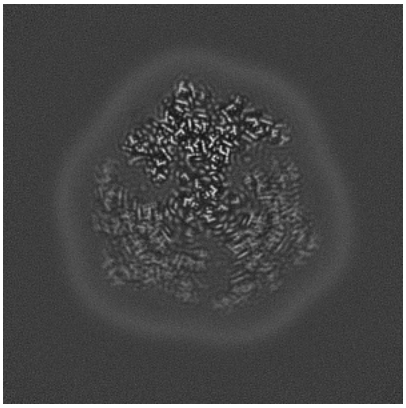
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

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

6.3 Largest variance slices (i)

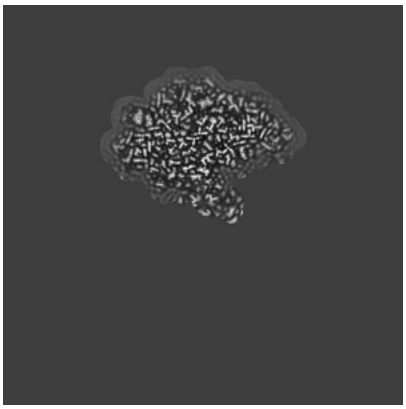
6.3.1 Primary map



X Index: 213

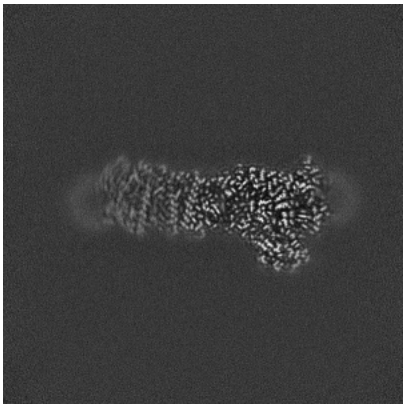


Y Index: 293

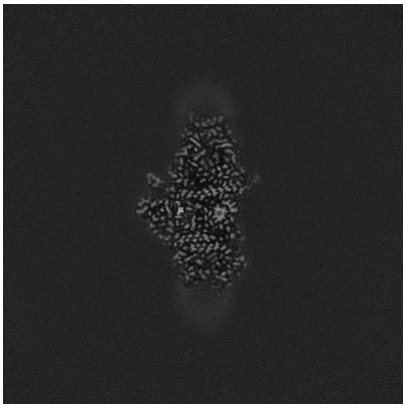


Z Index: 238

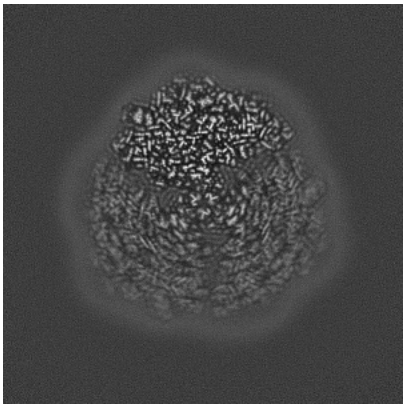
6.3.2 Raw map



X Index: 204



Y Index: 293

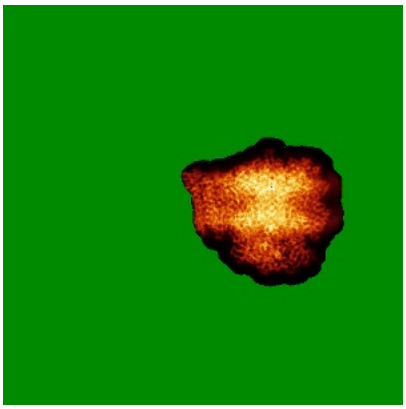


Z Index: 238

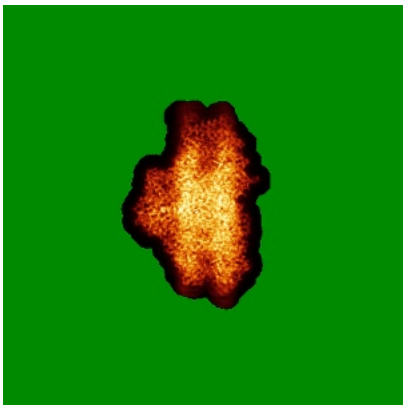
The images above show the largest variance slices of the map in three orthogonal directions.

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

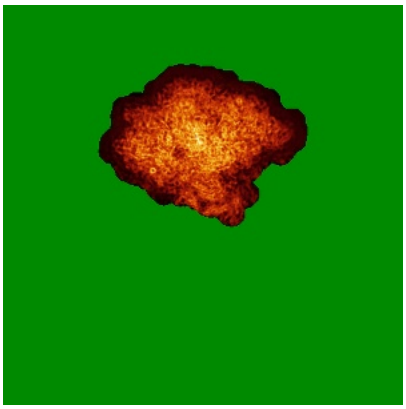
6.4.1 Primary map



X

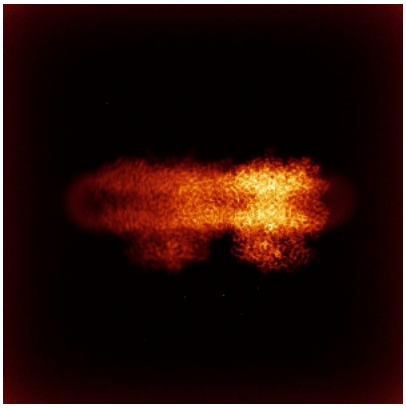


Y

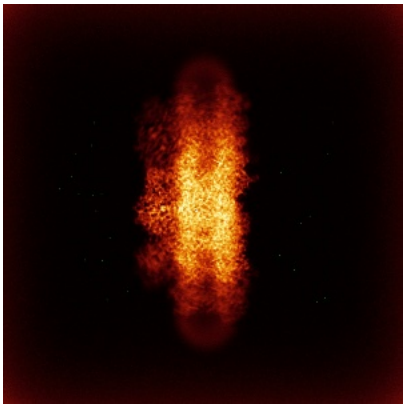


Z

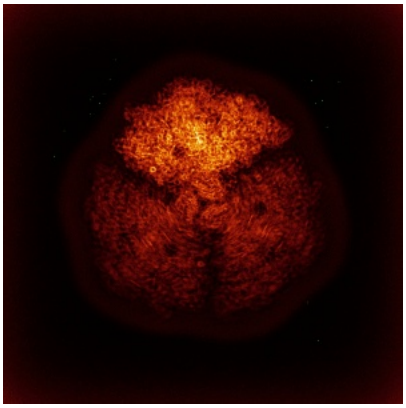
6.4.2 Raw map



X



Y

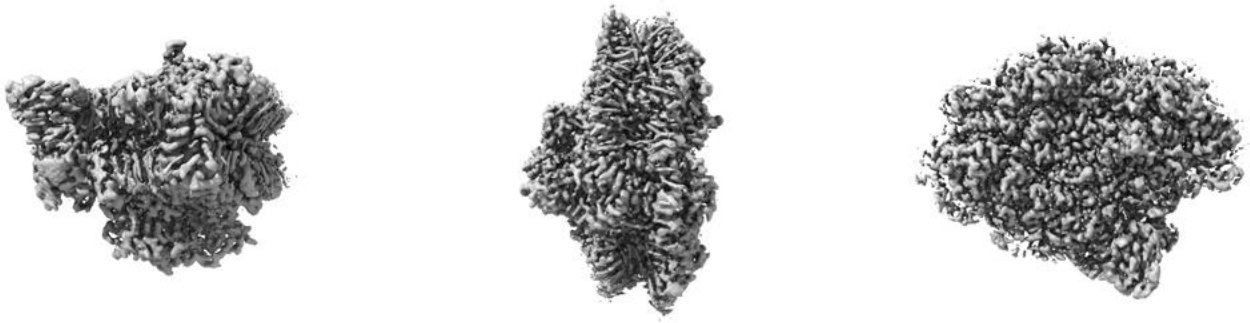


Z

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 4.4. 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.

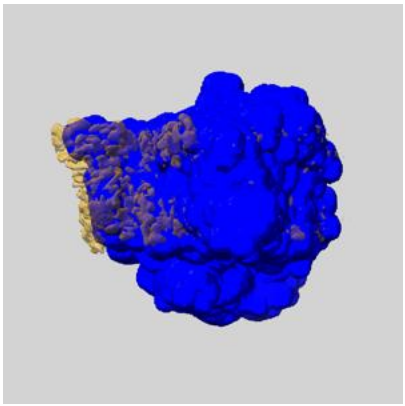
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

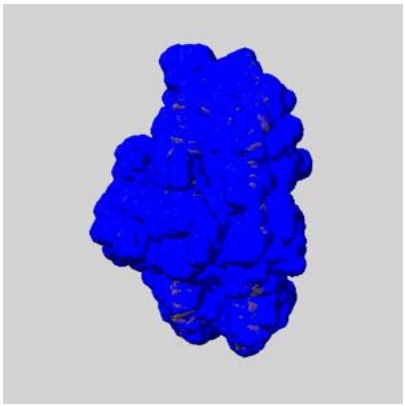
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

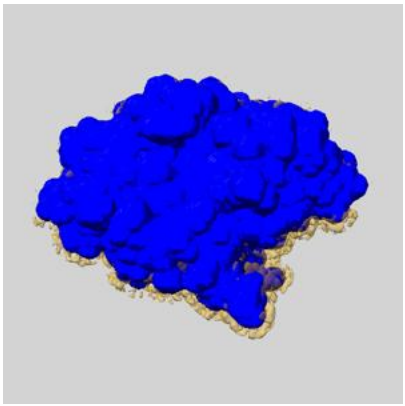
6.6.1 emd_71005_msk_1.map (i)



X



Y

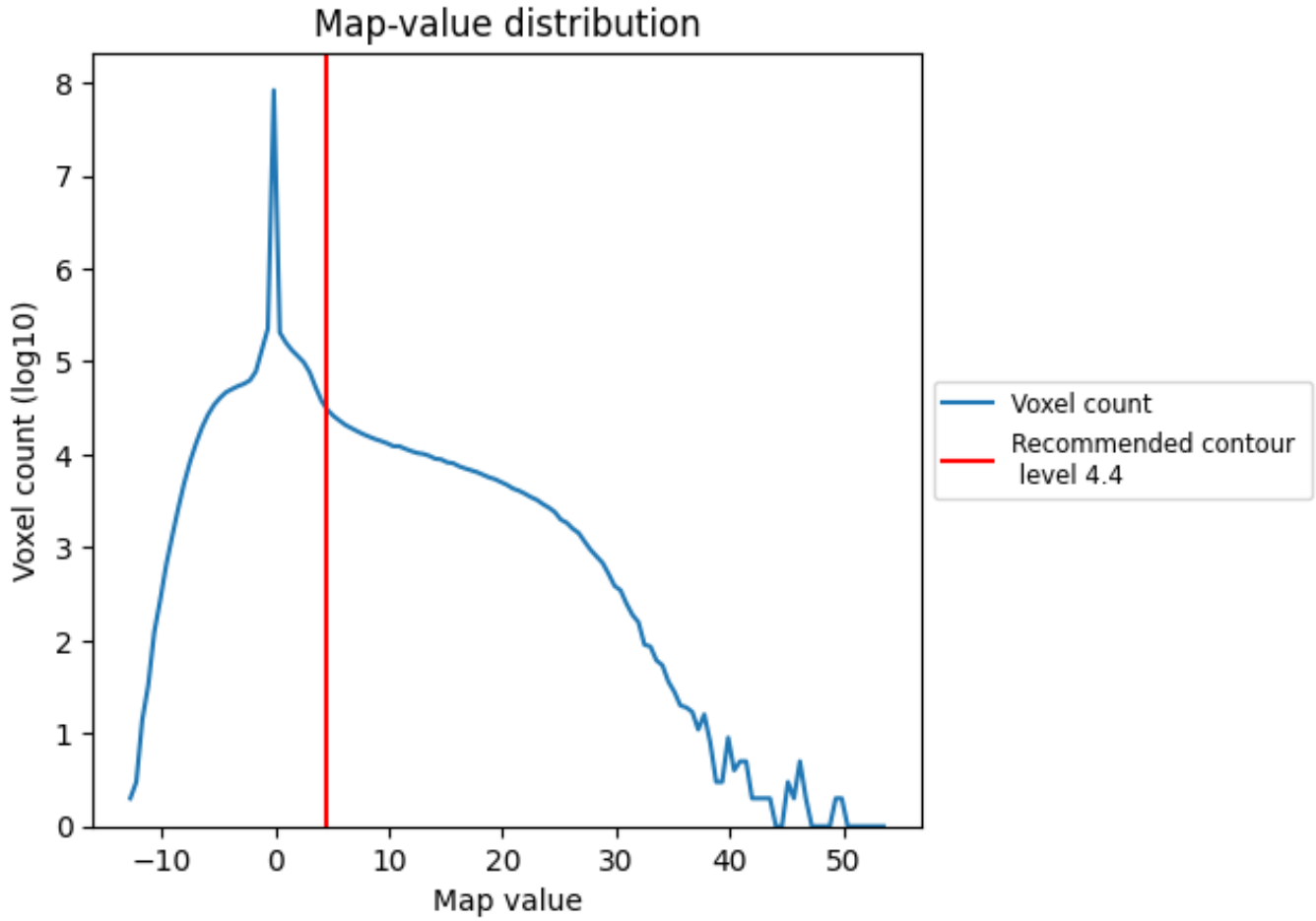


Z

7 Map analysis

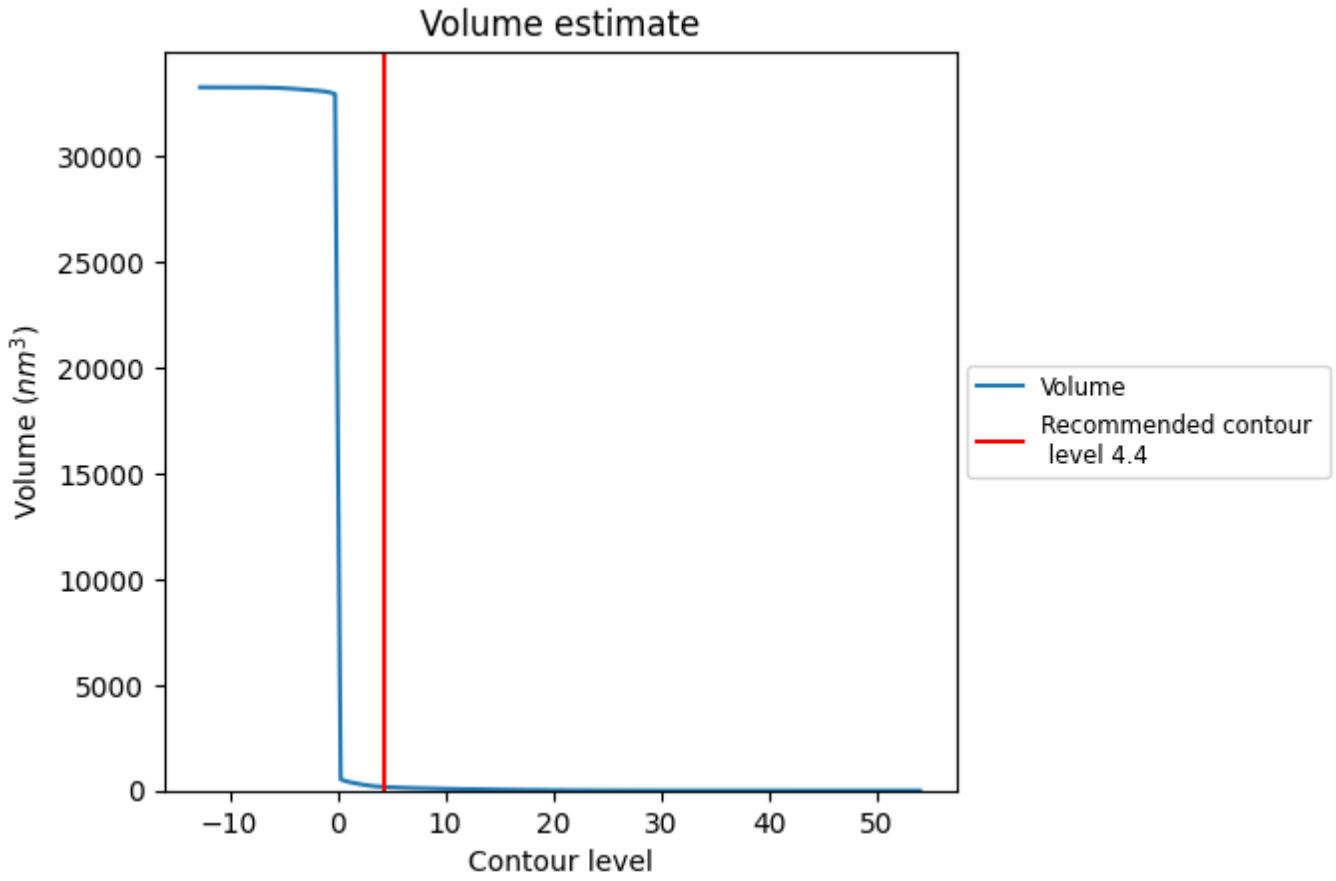
This section contains the results of statistical analysis of the map.

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.

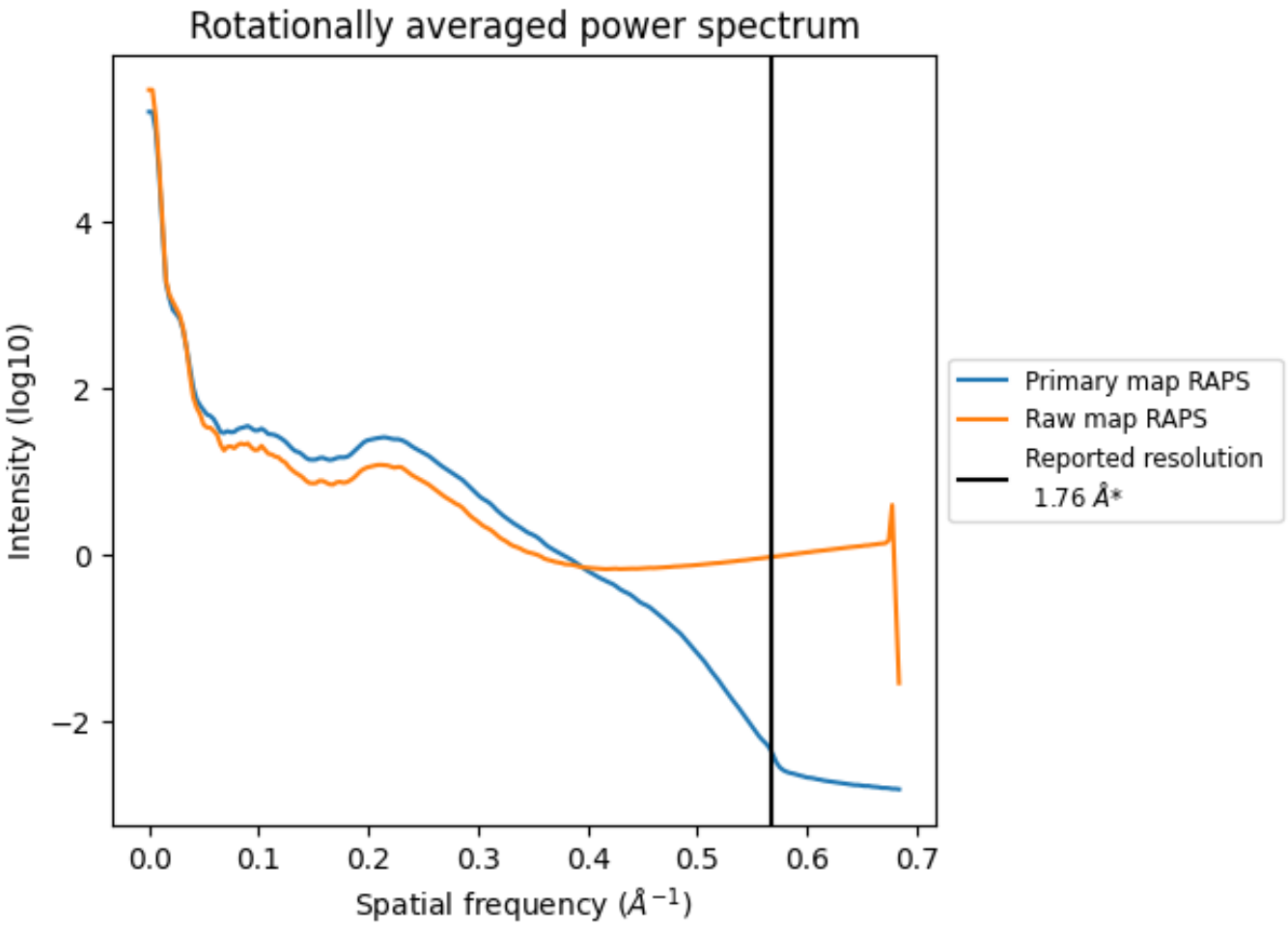
7.2 Volume estimate



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 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)

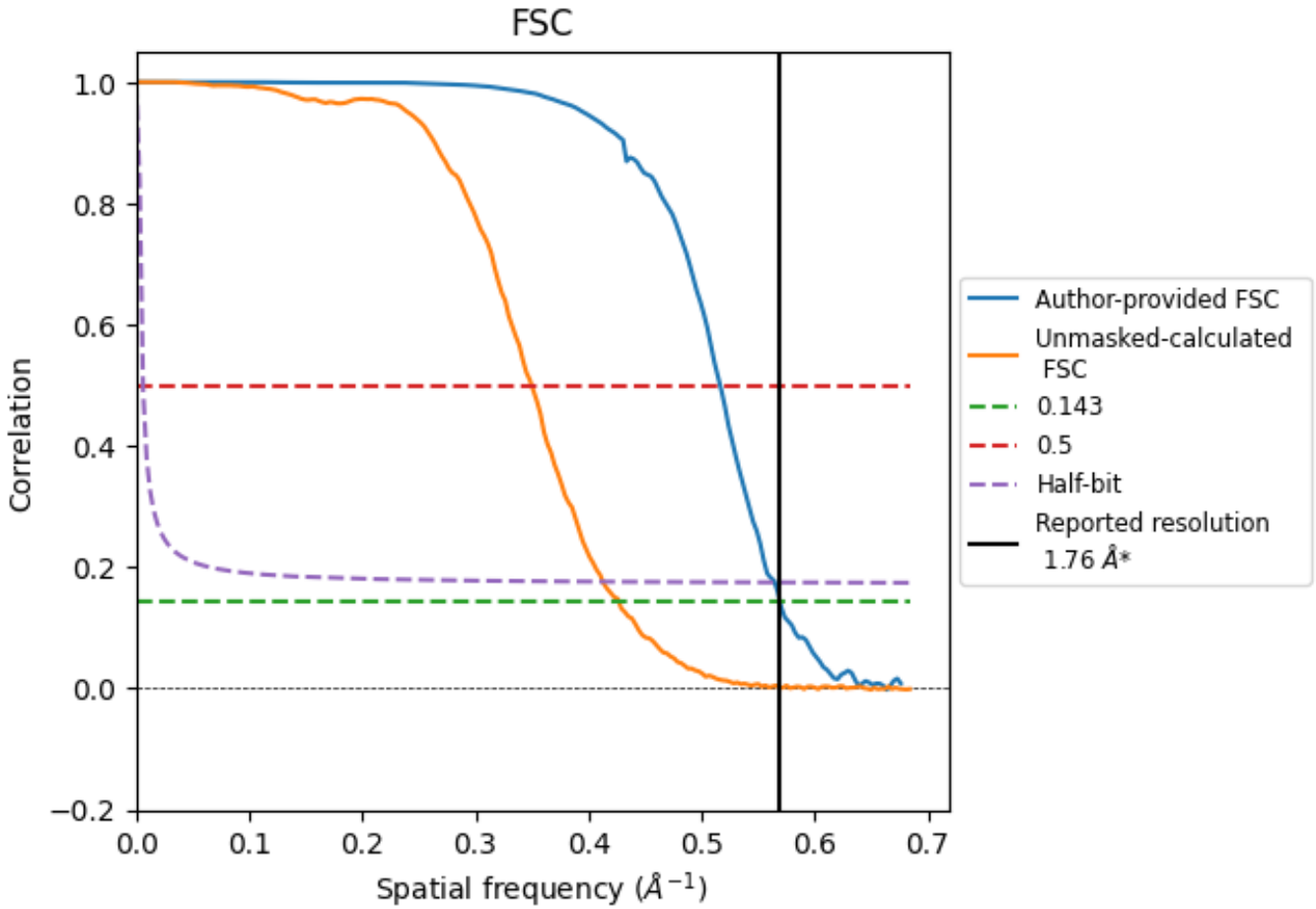


*Reported resolution corresponds to spatial frequency of 0.568 Å^{-1}

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 0.568 Å^{-1}

8.2 Resolution estimates (i)

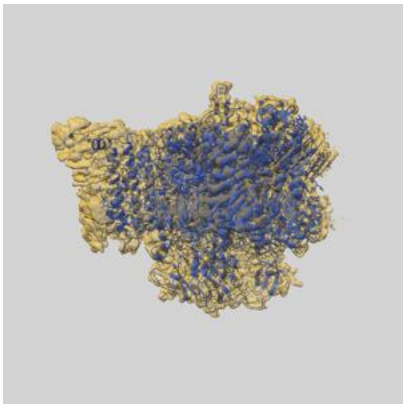
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.76	-	-
Author-provided FSC curve	1.76	1.94	1.77
Unmasked-calculated*	2.34	2.86	2.42

*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 2.34 differs from the reported value 1.76 by more than 10 %

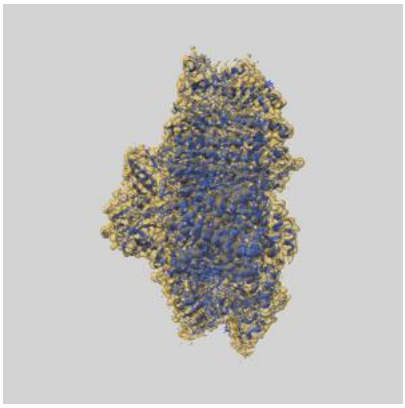
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71005 and PDB model 9OY9. Per-residue inclusion information can be found in section 3 on page 19.

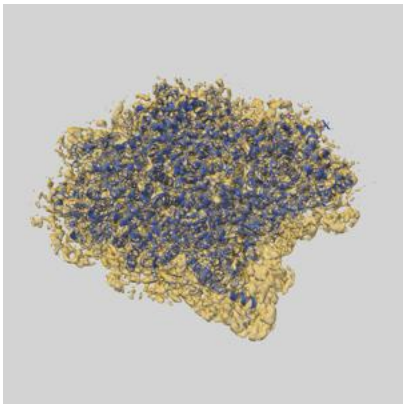
9.1 Map-model overlay



X



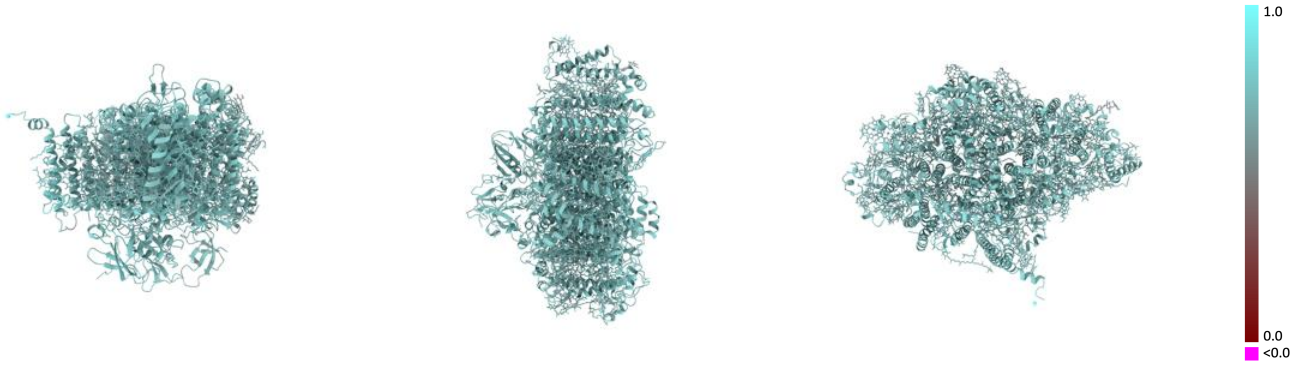
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.4 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.

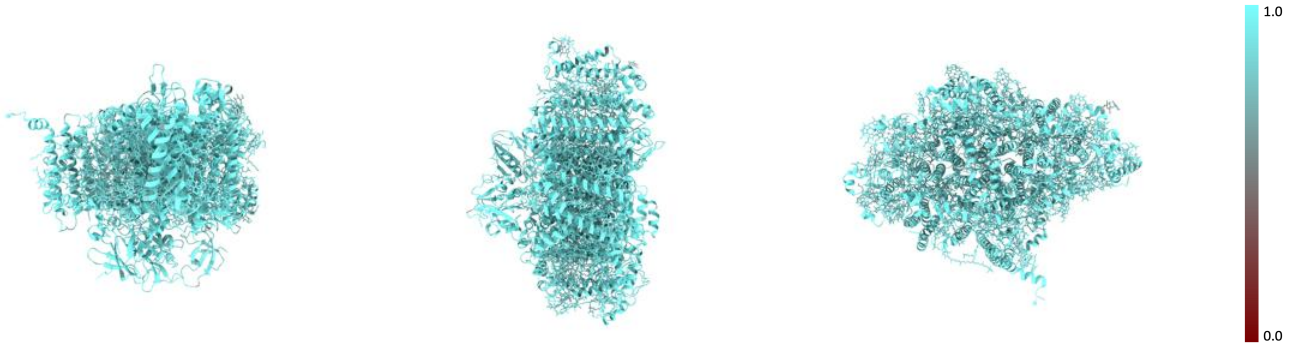
9.2 Q-score mapped to coordinate model (i)



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.

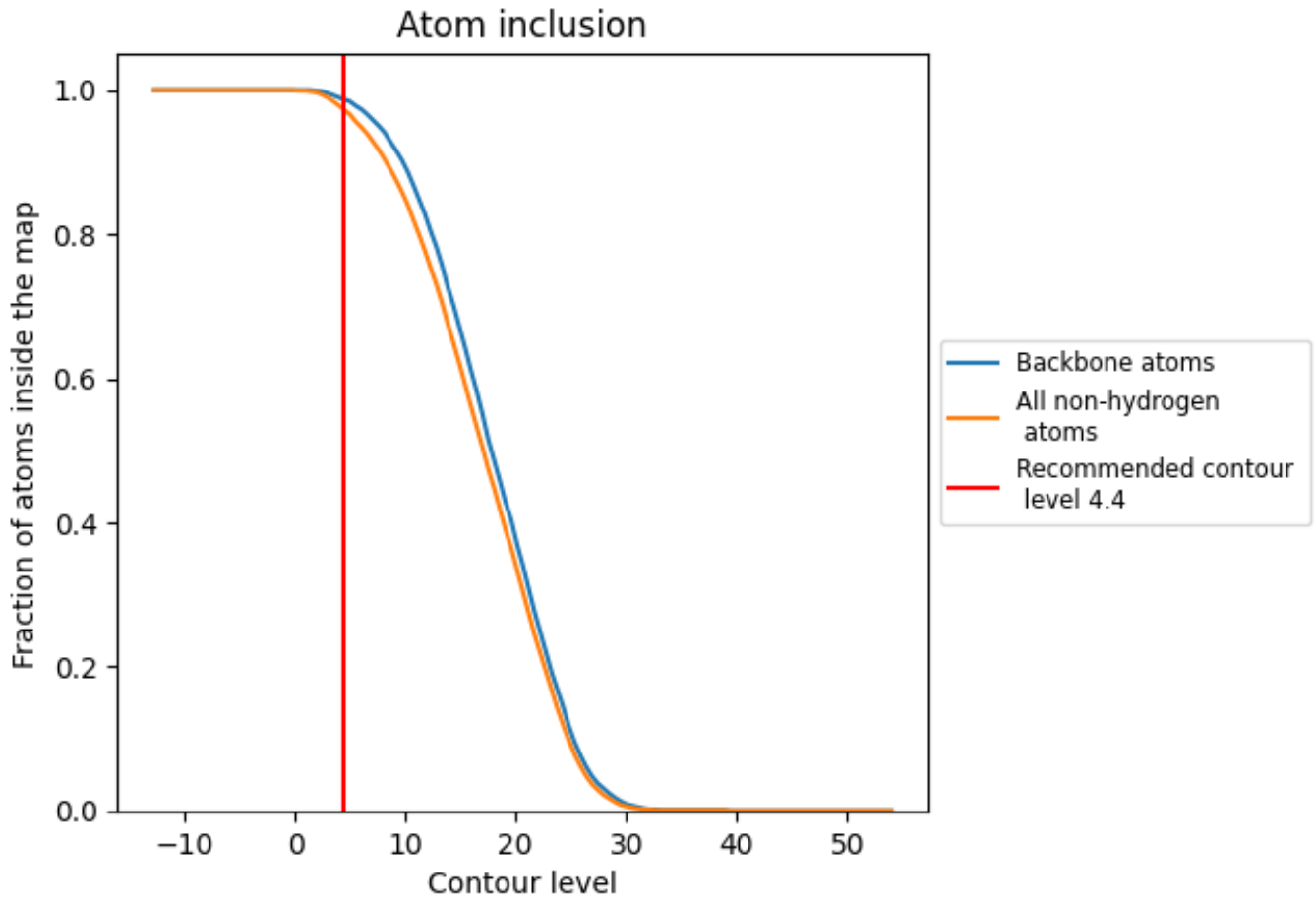
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.4).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9730	0.7290
A	0.9740	0.7330
B	0.9740	0.7350
C	0.9950	0.7480
D	0.9750	0.7270
E	0.9620	0.7060
F	0.9550	0.7020
I	0.9830	0.7350
J	0.9670	0.6990
K	0.9410	0.6910
L	0.9760	0.7320
M	0.9810	0.7270

