Full wwPDB EM Validation Report ⓘ

Sep 16, 2021 – 03:12 pm BST

PDB ID	:	7O1V
EMDB ID	:	EMD-12697
Title	:	Structure of a Minimal Photosystem I
Authors	:	Nelson, N.; Caspy, I.; Lambrev, P.
Deposited on	:	2021-03-30
Resolution	:	4.31 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 following versions of software and data (see references ⓘ) were used in the production of this report:

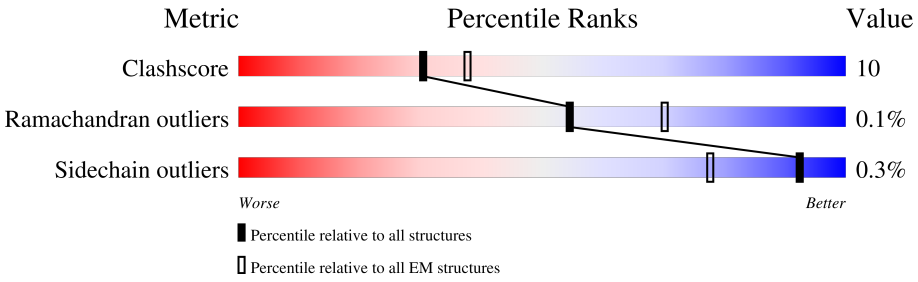
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.31 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	739	81% 19%
2	B	729	82% 17% .
3	C	80	76% 24%
4	D	141	77% 22% .
5	E	69	81% 19%
6	K	80	88% 12%
7	M	31	81% 19%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLA	A	1011	X	-	-	-
8	CLA	A	1012	X	-	-	-
8	CLA	A	1013	X	-	-	-
8	CLA	A	1101	X	-	-	-
8	CLA	A	1102	X	-	-	-
8	CLA	A	1103	X	-	-	-
8	CLA	A	1104	X	-	-	-
8	CLA	A	1105	X	-	-	-
8	CLA	A	1106	X	-	-	-
8	CLA	A	1107	X	-	-	-
8	CLA	A	1108	X	-	-	-
8	CLA	A	1109	X	-	-	-
8	CLA	A	1110	X	-	-	-
8	CLA	A	1111	X	-	-	-
8	CLA	A	1112	X	-	-	-
8	CLA	A	1113	X	-	-	-
8	CLA	A	1114	X	-	-	-
8	CLA	A	1115	X	-	-	-
8	CLA	A	1116	X	-	-	-
8	CLA	A	1117	X	-	-	-
8	CLA	A	1118	X	-	-	-
8	CLA	A	1119	X	-	-	-
8	CLA	A	1120	X	-	-	-
8	CLA	A	1121	X	-	-	-
8	CLA	A	1122	X	-	-	-
8	CLA	A	1123	X	-	-	-
8	CLA	A	1124	X	-	-	-
8	CLA	A	1125	X	-	-	-
8	CLA	A	1126	X	-	-	-
8	CLA	A	1127	X	-	-	-
8	CLA	A	1128	X	-	-	-
8	CLA	A	1129	X	-	-	-
8	CLA	A	1130	X	-	-	-
8	CLA	A	1131	X	-	-	-
8	CLA	A	1132	X	-	-	-
8	CLA	A	1133	X	-	-	-
8	CLA	A	1134	X	-	-	-
8	CLA	A	1135	X	-	-	-
8	CLA	A	1136	X	-	-	-
8	CLA	A	1137	X	-	-	-
8	CLA	A	1138	X	-	-	-
8	CLA	A	1139	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLA	A	1140	X	-	-	-
8	CLA	A	1801	X	-	-	-
8	CLA	B	1021	X	-	-	-
8	CLA	B	1022	X	-	-	-
8	CLA	B	1023	X	-	-	-
8	CLA	B	1201	X	-	-	-
8	CLA	B	1202	X	-	-	-
8	CLA	B	1203	X	-	-	-
8	CLA	B	1204	X	-	-	-
8	CLA	B	1205	X	-	-	-
8	CLA	B	1206	X	-	-	-
8	CLA	B	1207	X	-	-	-
8	CLA	B	1208	X	-	-	-
8	CLA	B	1209	X	-	-	-
8	CLA	B	1210	X	-	-	-
8	CLA	B	1211	X	-	-	-
8	CLA	B	1212	X	-	-	-
8	CLA	B	1213	X	-	-	-
8	CLA	B	1214	X	-	-	-
8	CLA	B	1215	X	-	-	-
8	CLA	B	1216	X	-	-	-
8	CLA	B	1217	X	-	-	-
8	CLA	B	1218	X	-	-	-
8	CLA	B	1219	X	-	-	-
8	CLA	B	1220	X	-	-	-
8	CLA	B	1221	X	-	-	-
8	CLA	B	1222	X	-	-	-
8	CLA	B	1223	X	-	-	-
8	CLA	B	1224	X	-	-	-
8	CLA	B	1225	X	-	-	-
8	CLA	B	1226	X	-	-	-
8	CLA	B	1227	X	-	-	-
8	CLA	B	1228	X	-	-	-
8	CLA	B	1229	X	-	-	-
8	CLA	B	1230	X	-	-	-
8	CLA	B	1231	X	-	-	-
8	CLA	B	1232	X	-	-	-
8	CLA	B	1234	X	-	-	-
8	CLA	B	1235	X	-	-	-
8	CLA	B	1236	X	-	-	-
8	CLA	B	1237	X	-	-	-
8	CLA	B	1238	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CLA	B	1239	X	-	-	-
8	CLA	B	1240	X	-	-	-
8	CLA	K	1401	X	-	-	-
8	CLA	K	1402	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 20914 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	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

- 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	141	Total	C	N	O	S	0	0
			1102	697	190	211	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			543	340	96	107		

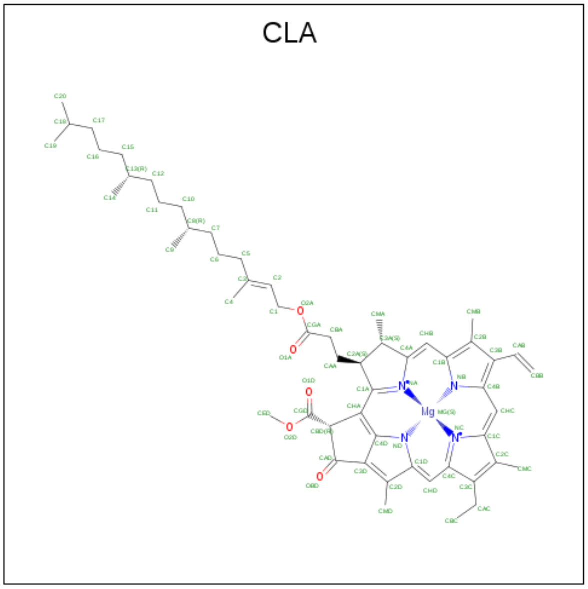
- Molecule 6 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	80	Total	C	N	O	S	1	0
			579	378	93	102	6		

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

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

- Molecule 8 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	A	1	Total 2446	C 2006	Mg 44	N 176	O 220	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0
8	B	1	Total 2482	C 2062	Mg 42	N 168	O 210	0

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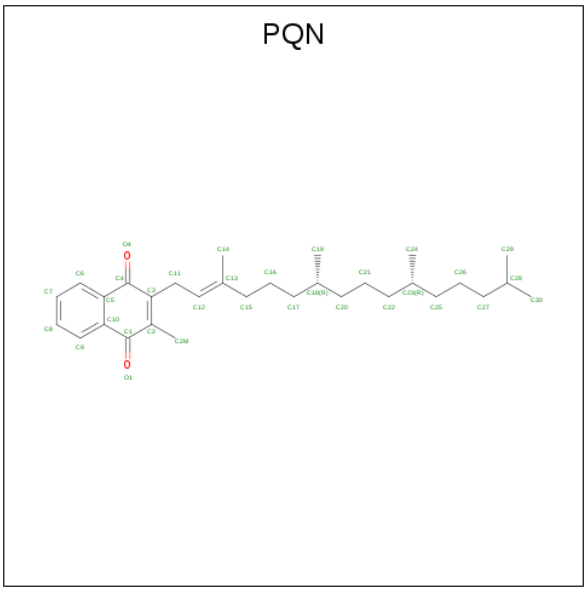
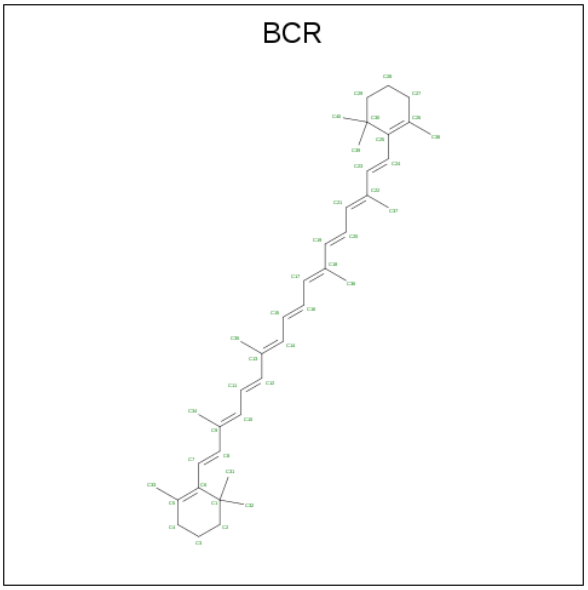
Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	B	1	Total C Mg N O 2482 2062 42 168 210	0
8	K	1	Total C Mg N O 130 110 2 8 10	0
8	K	1	Total C Mg N O 130 110 2 8 10	0

- Molecule 9 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 10 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			280	280	
10	A	1	Total	C	0
			280	280	

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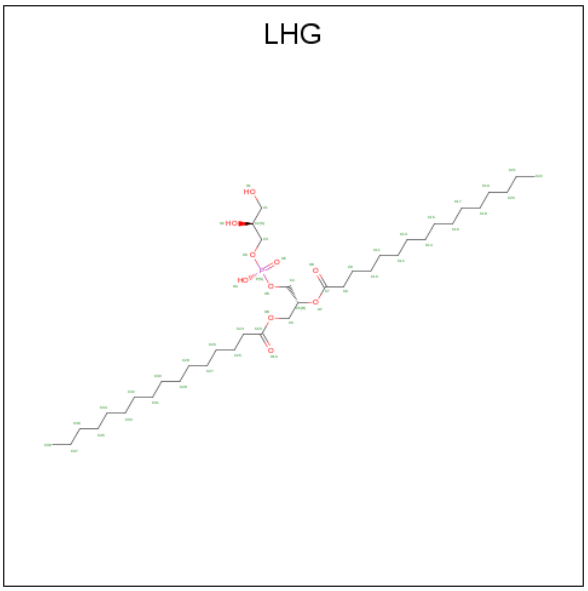
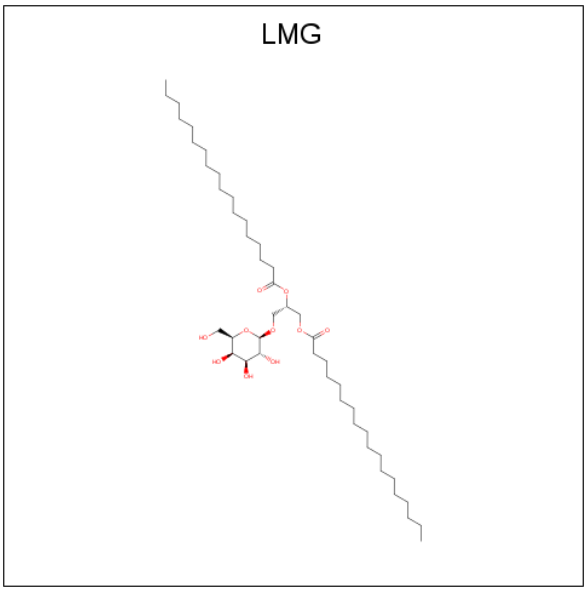
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 280 280	0
10	A	1	Total C 280 280	0
10	A	1	Total C 280 280	0
10	A	1	Total C 280 280	0
10	A	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	B	1	Total C 280 280	0
10	K	1	Total C 40 40	0

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



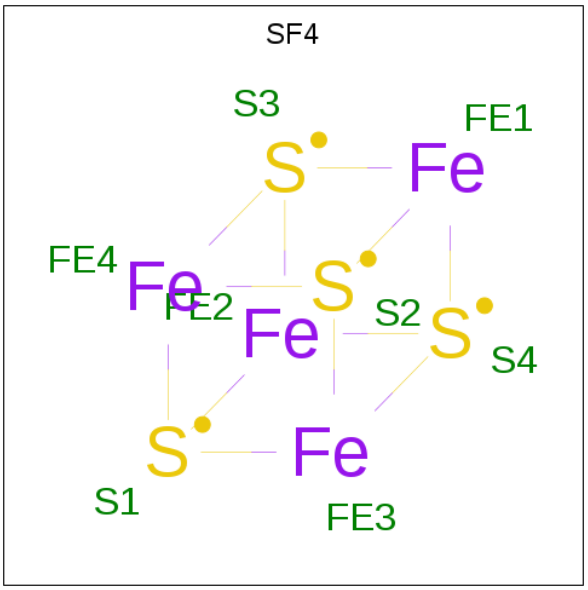
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			98	76	20	2	
11	A	1	Total	C	O	P	0
			98	76	20	2	
11	B	1	Total	C	O	P	0
			73	51	20	2	
11	B	1	Total	C	O	P	0
			73	51	20	2	
11	M	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 12 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



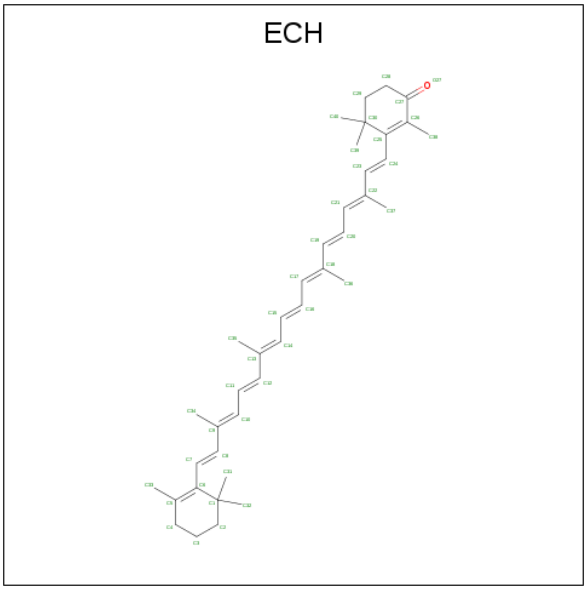
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C O 50 40 10	0
12	B	1	Total C O 86 66 20	0
12	B	1	Total C O 86 66 20	0
12	K	1	Total C O 55 45 10	0

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



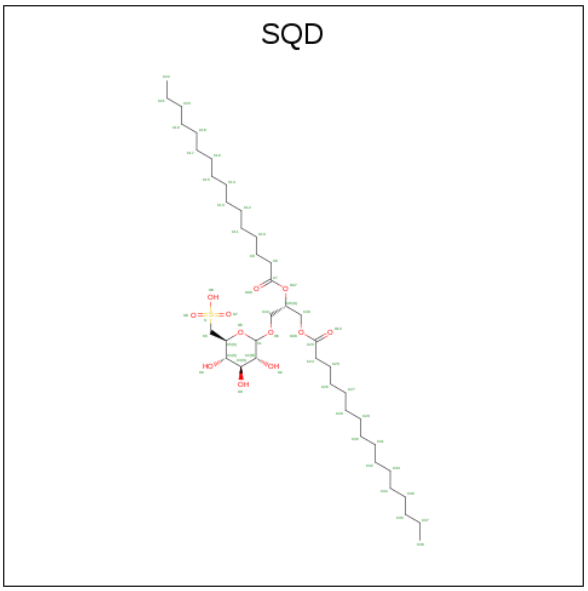
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 16 8 8	0
13	C	1	Total Fe S 16 8 8	0

- Molecule 14 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



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

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



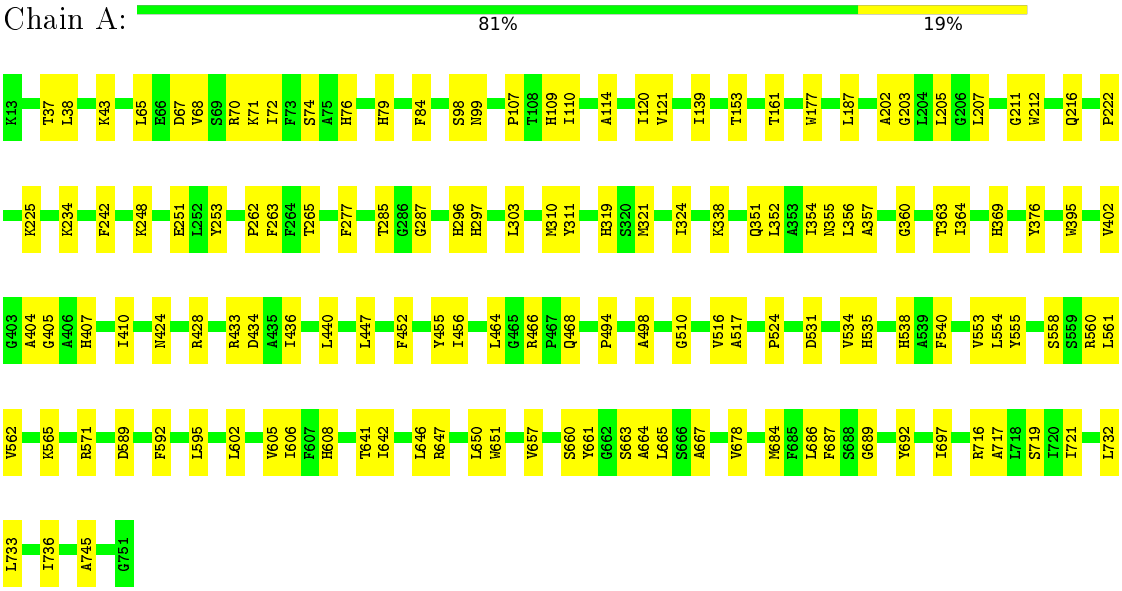
Mol	Chain	Residues	Atoms				AltConf
15	B	1	Total	C	O	S	0
			54	41	12	1	

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. 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. 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.

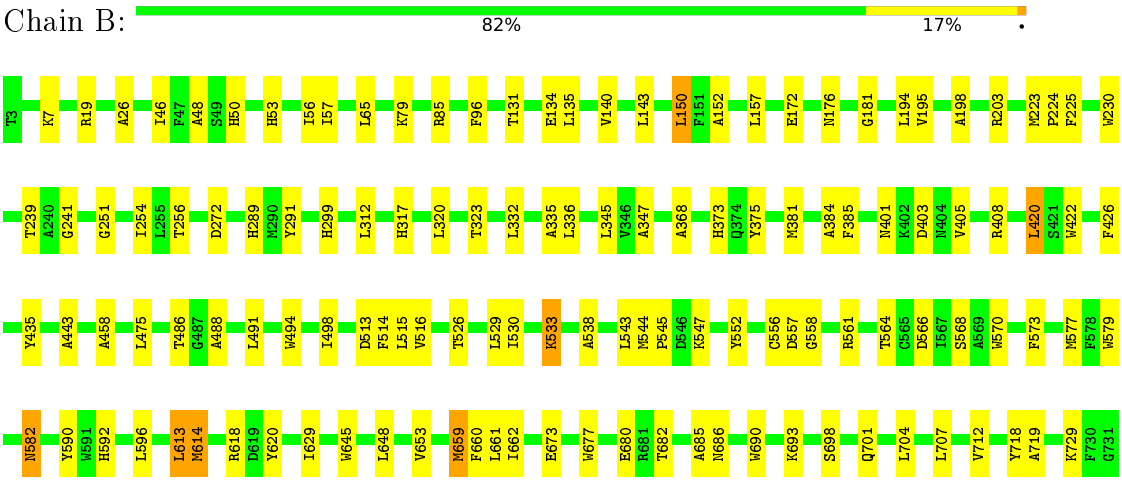
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



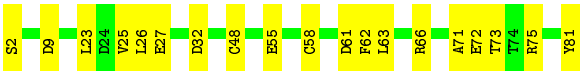
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



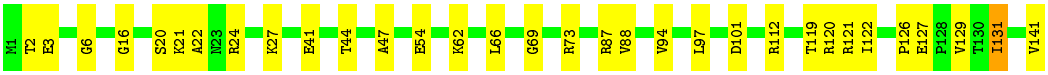
- Molecule 3: Photosystem I iron-sulfur center

Chain C:



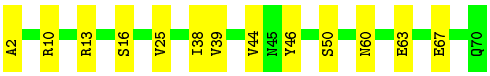
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



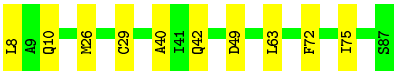
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



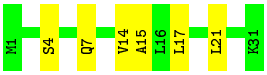
• Molecule 6: Photosystem I reaction center subunit PsaK 2

Chain K:



• Molecule 7: Photosystem I reaction center subunit XII

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74303	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/5985	0.59	2/8158 (0.0%)
2	B	0.31	0/5981	0.61	9/8178 (0.1%)
3	C	0.33	0/610	0.74	0/826
4	D	0.31	0/1126	0.67	1/1517 (0.1%)
5	E	0.27	0/552	0.59	0/745
6	K	0.30	0/590	0.64	0/797
7	M	0.29	0/241	0.80	1/326 (0.3%)
All	All	0.31	0/15085	0.61	13/20547 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	614	MET	CG-SD-CE	-7.51	88.18	100.20
2	B	150	LEU	CA-CB-CG	6.68	130.68	115.30
7	M	17	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	310	MET	CA-CB-CG	5.86	123.26	113.30
2	B	659	MET	CG-SD-CE	-5.67	91.12	100.20
2	B	381	MET	CG-SD-CE	-5.67	91.13	100.20
1	A	684	MET	CA-CB-CG	5.47	122.60	113.30
2	B	613	LEU	CA-CB-CG	5.46	127.87	115.30
4	D	131	ILE	CG1-CB-CG2	-5.42	99.48	111.40
2	B	659	MET	CB-CA-C	-5.31	99.78	110.40
2	B	475	LEU	CA-CB-CG	5.20	127.27	115.30
2	B	420	LEU	CA-CB-CG	5.18	127.22	115.30
2	B	533	LYS	CB-CG-CD	5.15	125.00	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5646	114	0
2	B	5770	0	5547	106	0
3	C	600	0	581	17	0
4	D	1102	0	1101	20	0
5	E	543	0	525	10	0
6	K	579	0	601	7	0
7	M	238	0	260	4	0
8	A	2446	0	2250	95	0
8	B	2482	0	2461	109	0
8	K	130	0	142	2	0
9	A	33	0	46	4	0
9	B	33	0	46	1	0
10	A	280	0	370	23	0
10	B	280	0	371	24	0
10	K	40	0	53	4	0
11	A	98	0	148	13	0
11	B	73	0	92	5	0
11	M	49	0	74	1	0
12	A	50	0	73	0	0
12	B	86	0	118	9	0
12	K	55	0	86	0	0
13	A	8	0	0	1	0
13	C	16	0	0	1	0
14	B	41	0	54	6	0
14	M	41	0	54	2	0
15	B	54	0	77	0	0
All	All	20914	0	20776	412	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 10.

All (412) 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)
3:C:58:CYS:HB2	13:C:3003:SF4:S4	2.03	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1220:CLA:HAB	8:B:1227:CLA:HAC1	1.59	0.84
1:A:72:ILE:HG22	1:A:76:HIS:CE1	2.14	0.82
2:B:582:ASN:C	2:B:582:ASN:HD22	1.82	0.82
8:B:1236:CLA:H43	10:B:4010:BCR:H10C	1.61	0.81
13:A:3001:SF4:S3	2:B:556:CYS:HB3	2.26	0.76
1:A:351:GLN:O	1:A:355:ASN:ND2	2.21	0.73
1:A:440:LEU:HD22	8:A:1137:CLA:HBB1	1.69	0.72
8:A:1102:CLA:HBA2	8:A:1109:CLA:H51	1.71	0.72
10:B:4010:BCR:H24C	10:B:4018:BCR:H281	1.71	0.72
2:B:385:PHE:HZ	8:B:1222:CLA:HAB	1.56	0.69
1:A:395:TRP:CD1	8:A:1126:CLA:HAB	2.27	0.69
1:A:357:ALA:HB1	10:A:4008:BCR:H343	1.75	0.68
3:C:55:GLU:HA	3:C:63:LEU:HD11	1.76	0.67
8:A:1127:CLA:H61	10:A:4003:BCR:H23C	1.76	0.66
2:B:65:LEU:HD11	2:B:135:LEU:HD22	1.78	0.66
5:E:38:ILE:HG12	5:E:60:ASN:HB3	1.78	0.65
1:A:72:ILE:HG22	1:A:76:HIS:HE1	1.58	0.65
8:A:1112:CLA:C1B	10:A:4002:BCR:H10C	2.27	0.65
2:B:150:LEU:HB3	7:M:21:LEU:HD22	1.78	0.65
8:B:1229:CLA:HBB2	8:B:1230:CLA:H11	1.78	0.64
4:D:88:VAL:HG12	4:D:94:VAL:HG12	1.78	0.64
1:A:436:ILE:HD12	8:A:1129:CLA:HBB1	1.78	0.64
8:B:1219:CLA:HBB1	10:B:4018:BCR:H323	1.80	0.64
3:C:23:LEU:HD12	3:C:48:CYS:HA	1.81	0.63
1:A:647:ARG:HB3	2:B:629:ILE:HG21	1.80	0.62
4:D:101:ASP:OD2	4:D:112:ARG:NH2	2.32	0.62
2:B:291:TYR:HA	2:B:299:HIS:H	1.64	0.62
8:B:1234:CLA:HMB2	8:B:1236:CLA:HED1	1.82	0.62
8:B:1216:CLA:HBB1	8:B:1221:CLA:H72	1.80	0.62
1:A:277:PHE:HE1	8:A:1116:CLA:HBB1	1.65	0.62
1:A:642:ILE:HD11	8:B:1022:CLA:HMA2	1.81	0.62
8:A:1124:CLA:H52	8:A:1133:CLA:HBB2	1.83	0.61
2:B:673:GLU:HG2	3:C:81:TYR:HE1	1.65	0.61
5:E:13:ARG:HH11	5:E:16:SER:HB2	1.65	0.61
8:A:1120:CLA:HMD2	10:A:4001:BCR:H24C	1.83	0.60
8:A:1103:CLA:H142	10:A:4003:BCR:H372	1.83	0.60
2:B:614:MET:O	2:B:618:ARG:HB3	2.02	0.60
2:B:577:MET:HG2	2:B:707:LEU:HD21	1.82	0.60
2:B:557:ASP:OD1	3:C:66:ARG:NH2	2.36	0.59
1:A:561:LEU:HD23	1:A:562:VAL:HG13	1.84	0.59
1:A:455:TYR:HE2	8:A:1011:CLA:H141	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:HIS:HA	1:A:410:ILE:HG22	1.85	0.59
1:A:602:LEU:HA	1:A:605:VAL:HG12	1.84	0.59
1:A:534:VAL:HG11	1:A:608:HIS:CD2	2.38	0.59
2:B:701:GLN:HG3	12:B:5002:LMG:H131	1.85	0.59
2:B:543:LEU:HD21	2:B:564:THR:HG22	1.84	0.59
8:B:1205:CLA:H8	10:B:4017:BCR:H332	1.85	0.58
8:B:1222:CLA:H51	8:B:1234:CLA:H11	1.84	0.58
1:A:405:GLY:HA2	10:A:4008:BCR:HC41	1.84	0.58
2:B:19:ARG:NH2	3:C:72:GLU:OE2	2.37	0.58
8:B:1223:CLA:H101	10:B:4010:BCR:H17C	1.85	0.58
2:B:181:GLY:HA3	8:B:1210:CLA:HBB1	1.86	0.58
1:A:595:LEU:HD21	11:A:5001:LHG:H312	1.86	0.57
8:A:1138:CLA:HBB2	8:A:1138:CLA:H172	1.85	0.57
1:A:717:ALA:HB1	9:A:2001:PQN:H6	1.86	0.57
9:B:2002:PQN:H142	10:B:4017:BCR:H393	1.86	0.57
3:C:2:SER:N	3:C:71:ALA:O	2.38	0.57
8:B:1234:CLA:H72	8:B:1235:CLA:H2	1.86	0.57
3:C:25:VAL:HG13	3:C:26:LEU:HD12	1.85	0.57
2:B:323:THR:HG21	2:B:401:ASN:HD21	1.69	0.57
6:K:75:ILE:HG22	10:K:4001:BCR:H321	1.85	0.57
8:A:1107:CLA:H2	10:A:4012:BCR:H17C	1.87	0.57
8:A:1107:CLA:H2	10:A:4012:BCR:H19C	1.86	0.57
2:B:514:PHE:HD1	2:B:515:LEU:HD22	1.70	0.56
1:A:109:HIS:HB3	1:A:110:ILE:HD12	1.87	0.56
1:A:494:PRO:HA	1:A:498:ALA:HB3	1.86	0.56
1:A:203:GLY:HA2	1:A:207:LEU:HD23	1.87	0.56
8:A:1127:CLA:H8	8:A:1127:CLA:HMD2	1.87	0.56
2:B:690:TRP:HE1	2:B:693:LYS:HD3	1.71	0.56
8:B:1211:CLA:H3A	14:B:4006:ECH:H38B	1.87	0.56
8:B:1217:CLA:H201	14:B:4006:ECH:H4	1.87	0.56
8:A:1105:CLA:H12	10:A:4019:BCR:H16C	1.88	0.56
8:A:1128:CLA:H121	11:A:5001:LHG:H362	1.88	0.55
3:C:61:ASP:OD2	5:E:16:SER:OG	2.23	0.55
3:C:27:GLU:OE2	4:D:112:ARG:NH1	2.40	0.55
1:A:216:GLN:NE2	8:A:1117:CLA:O1D	2.39	0.55
6:K:8:LEU:HD23	6:K:10:GLN:H	1.71	0.55
2:B:426:PHE:HZ	8:B:1235:CLA:HMC3	1.71	0.55
1:A:560:ARG:NH1	2:B:673:GLU:OE1	2.40	0.54
1:A:211:GLY:C	8:A:1112:CLA:HAB	2.27	0.54
8:A:1106:CLA:H143	11:A:5001:LHG:H202	1.89	0.54
3:C:23:LEU:O	4:D:62:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:SER:O	4:D:24:ARG:HB2	2.08	0.54
1:A:464:LEU:HD12	2:B:96:PHE:HA	1.88	0.54
1:A:531:ASP:O	1:A:535:HIS:ND1	2.37	0.54
1:A:79:HIS:HB2	8:A:1103:CLA:HMB2	1.89	0.54
8:A:1012:CLA:HAB	2:B:579:TRP:CH2	2.43	0.54
5:E:25:VAL:HA	5:E:39:VAL:HA	1.90	0.53
2:B:570:TRP:HZ2	2:B:704:LEU:HD12	1.73	0.53
1:A:719:SER:OG	5:E:50:SER:OG	2.27	0.53
2:B:317:HIS:HB3	2:B:320:LEU:HD12	1.89	0.53
8:B:1212:CLA:HMA1	14:B:4006:ECH:H34B	1.90	0.53
2:B:239:THR:HG23	2:B:241:GLY:H	1.73	0.53
8:B:1216:CLA:H72	11:B:5004:LHG:H223	1.89	0.53
1:A:716:ARG:HH21	5:E:46:TYR:HA	1.74	0.53
4:D:22:ALA:HA	4:D:27:LYS:HB3	1.91	0.53
1:A:65:LEU:HB2	1:A:187:LEU:HD21	1.90	0.53
1:A:697:ILE:HD11	10:B:4014:BCR:H272	1.90	0.53
8:A:1126:CLA:H12	10:B:4011:BCR:H291	1.91	0.53
2:B:46:ILE:HG21	8:B:1202:CLA:H193	1.90	0.53
2:B:385:PHE:CZ	8:B:1222:CLA:HAB	2.41	0.52
5:E:2:ALA:N	5:E:63:GLU:OE2	2.42	0.52
8:A:1104:CLA:HMA1	8:A:1128:CLA:HAB	1.92	0.52
8:A:1112:CLA:C2B	10:A:4002:BCR:H10C	2.39	0.52
2:B:558:GLY:O	2:B:564:THR:OG1	2.24	0.52
8:B:1211:CLA:HHB	14:B:4006:ECH:H24	1.89	0.52
8:B:1225:CLA:H202	10:B:4005:BCR:H352	1.92	0.52
1:A:98:SER:OG	1:A:99:ASN:N	2.42	0.52
1:A:571:ARG:NE	11:A:5001:LHG:O5	2.43	0.52
2:B:582:ASN:C	2:B:582:ASN:ND2	2.58	0.52
2:B:719:ALA:HB2	8:B:1224:CLA:HBB1	1.91	0.52
1:A:67:ASP:N	1:A:67:ASP:OD1	2.42	0.52
1:A:571:ARG:HH21	11:A:5001:LHG:HC31	1.75	0.52
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.92	0.52
8:A:1122:CLA:H2	8:A:1133:CLA:H171	1.91	0.52
2:B:458:ALA:HB2	8:B:1235:CLA:HED2	1.92	0.52
1:A:641:THR:OG1	1:A:642:ILE:N	2.42	0.51
1:A:651:TRP:HD1	8:B:1021:CLA:HBC1	1.76	0.51
2:B:486:THR:HG23	2:B:488:ALA:H	1.75	0.51
2:B:375:TYR:HB3	8:B:1224:CLA:HMC3	1.93	0.51
8:B:1239:CLA:HBB1	10:B:4017:BCR:H363	1.92	0.51
1:A:369:HIS:ND1	8:A:1116:CLA:OBD	2.43	0.51
8:A:1117:CLA:H111	8:A:1117:CLA:H193	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1215:CLA:H191	8:B:1231:CLA:H43	1.93	0.51
1:A:510:GLY:HA2	1:A:524:PRO:HB3	1.92	0.51
1:A:114:ALA:HB3	1:A:139:ILE:HD13	1.93	0.51
2:B:172:GLU:O	2:B:176:ASN:ND2	2.38	0.51
2:B:543:LEU:O	2:B:561:ARG:NH1	2.44	0.51
4:D:121:ARG:HG2	4:D:122:ILE:H	1.76	0.51
1:A:338:LYS:O	1:A:424:ASN:ND2	2.42	0.51
1:A:395:TRP:HB3	8:A:1126:CLA:HMC3	1.92	0.51
6:K:26:MET:HA	6:K:29:CYS:HB3	1.93	0.51
1:A:202:ALA:HB1	8:A:1118:CLA:HBC3	1.93	0.50
6:K:49:ASP:HB3	6:K:63:LEU:HD13	1.92	0.50
10:A:4001:BCR:H23C	6:K:72:PHE:HB2	1.94	0.50
2:B:405:VAL:HG23	8:B:1227:CLA:HMD3	1.94	0.50
2:B:140:VAL:HG23	7:M:14:VAL:HG11	1.92	0.50
2:B:544:MET:HG3	2:B:561:ARG:HH12	1.75	0.50
1:A:84:PHE:HE1	8:A:1103:CLA:H8	1.77	0.50
9:A:2001:PQN:H2M1	9:A:2001:PQN:H142	1.93	0.50
1:A:120:ILE:HG22	1:A:121:VAL:HG13	1.93	0.50
8:A:1101:CLA:HMB2	11:A:5001:LHG:H162	1.93	0.50
2:B:195:VAL:HG13	2:B:254:ILE:HG21	1.93	0.49
8:B:1214:CLA:H193	8:B:1231:CLA:H41	1.95	0.49
1:A:589:ASP:HA	1:A:592:PHE:HB3	1.94	0.49
1:A:689:GLY:HA3	2:B:566:ASP:HB2	1.95	0.49
2:B:345:LEU:HD22	8:B:1215:CLA:H43	1.94	0.49
2:B:543:LEU:HD23	2:B:544:MET:HB2	1.94	0.49
8:B:1238:CLA:H42	8:B:1239:CLA:H101	1.95	0.49
1:A:452:PHE:HD2	8:B:1023:CLA:H61	1.77	0.49
8:A:1012:CLA:HMA2	2:B:613:LEU:HD21	1.93	0.49
8:A:1011:CLA:H111	8:A:1011:CLA:H52	1.94	0.49
2:B:435:TYR:CE1	2:B:515:LEU:HB3	2.48	0.49
8:B:1220:CLA:HMD2	8:B:1221:CLA:HAB	1.94	0.48
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.93	0.48
2:B:577:MET:HE2	12:B:5002:LMG:H371	1.95	0.48
8:B:1225:CLA:H121	10:B:4005:BCR:H17C	1.94	0.48
8:A:1122:CLA:H11	10:A:4007:BCR:H351	1.95	0.48
2:B:347:ALA:HB2	2:B:373:HIS:HB2	1.95	0.48
10:B:4010:BCR:H353	11:B:5004:LHG:H192	1.95	0.48
3:C:32:ASP:OD1	3:C:32:ASP:N	2.47	0.48
4:D:20:SER:HB3	4:D:24:ARG:HE	1.77	0.48
1:A:71:LYS:NZ	8:A:1109:CLA:OBD	2.47	0.48
1:A:177:TRP:HB2	8:A:1109:CLA:HMC3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HG22	8:A:1112:CLA:HBA1	1.95	0.48
1:A:562:VAL:HG23	1:A:565:LYS:HD3	1.96	0.48
1:A:651:TRP:CD1	8:B:1021:CLA:HBC1	2.49	0.48
1:A:428:ARG:NH1	8:A:1129:CLA:O1D	2.46	0.48
8:B:1216:CLA:H41	8:B:1216:CLA:H61	1.53	0.48
8:B:1227:CLA:HAB	8:B:1236:CLA:CBB	2.44	0.48
1:A:68:VAL:O	1:A:72:ILE:HG12	2.14	0.48
1:A:296:HIS:HD2	8:A:1116:CLA:NA	2.12	0.48
1:A:296:HIS:HD1	1:A:297:HIS:HD2	1.62	0.48
8:A:1139:CLA:HBC2	9:A:2001:PQN:H171	1.96	0.48
8:B:1238:CLA:H61	8:B:1238:CLA:H41	1.48	0.48
1:A:263:PHE:HE1	8:A:1115:CLA:HBB1	1.78	0.47
8:A:1118:CLA:HBB1	10:K:4001:BCR:H342	1.96	0.47
8:B:1206:CLA:HBA1	8:B:1206:CLA:H3A	1.60	0.47
2:B:368:ALA:HB1	8:B:1224:CLA:HMA1	1.97	0.47
4:D:6:GLY:HA2	4:D:54:GLU:HB2	1.96	0.47
8:A:1135:CLA:H112	11:A:5003:LHG:H361	1.96	0.47
4:D:41:GLU:HA	4:D:47:ALA:HA	1.96	0.47
6:K:72:PHE:HA	6:K:75:ILE:HG12	1.96	0.47
1:A:447:LEU:HD21	8:A:1136:CLA:HMB3	1.96	0.47
8:B:1231:CLA:H2	8:B:1232:CLA:HMB2	1.96	0.47
8:A:1102:CLA:HMA2	8:A:1109:CLA:HMD2	1.96	0.47
2:B:225:PHE:O	2:B:230:TRP:NE1	2.39	0.47
8:B:1214:CLA:HMD3	8:B:1215:CLA:H122	1.96	0.47
8:B:1227:CLA:H62	8:B:1227:CLA:H2	1.71	0.47
8:A:1106:CLA:HBA2	8:A:1106:CLA:H3A	1.52	0.47
8:B:1205:CLA:HMC2	10:B:4017:BCR:H333	1.97	0.47
8:B:1216:CLA:H43	8:B:1223:CLA:H102	1.96	0.47
8:B:1219:CLA:H2	8:B:1219:CLA:H62	1.72	0.47
1:A:736:ILE:HG21	8:A:1126:CLA:HMC2	1.97	0.47
8:A:1131:CLA:HAB	8:A:1132:CLA:HMB2	1.97	0.47
2:B:526:THR:O	2:B:530:ILE:HG12	2.15	0.47
8:B:1202:CLA:H101	8:B:1202:CLA:HED2	1.96	0.47
1:A:571:ARG:HG2	1:A:721:ILE:HD12	1.96	0.47
1:A:733:LEU:HD13	8:A:1140:CLA:HMA1	1.97	0.47
8:A:1138:CLA:HMB2	8:B:1229:CLA:H61	1.95	0.47
4:D:126:PRO:HB2	4:D:131:ILE:HD11	1.97	0.47
1:A:212:TRP:NE1	8:A:1117:CLA:O1D	2.45	0.46
4:D:2:THR:OG1	4:D:3:GLU:N	2.47	0.46
2:B:203:ARG:NE	2:B:251:GLY:O	2.48	0.46
1:A:553:VAL:HG21	10:A:4008:BCR:HC31	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1209:CLA:H3A	8:B:1209:CLA:HBA2	1.51	0.46
1:A:262:PRO:HA	1:A:265:THR:HG22	1.97	0.46
2:B:50:HIS:CD2	8:B:1202:CLA:HAA1	2.50	0.46
1:A:395:TRP:HD1	8:A:1126:CLA:HAB	1.80	0.46
2:B:718:TYR:HD2	8:B:1021:CLA:HED3	1.81	0.46
3:C:81:TYR:HA	4:D:21:LYS:HB2	1.98	0.46
2:B:422:TRP:CE2	8:B:1228:CLA:HAB	2.50	0.46
2:B:516:VAL:HG21	2:B:590:TYR:HB2	1.98	0.46
8:B:1219:CLA:H161	8:B:1219:CLA:H202	1.77	0.46
8:A:1138:CLA:H91	8:A:1138:CLA:H112	1.79	0.46
1:A:354:ILE:HD11	10:A:4007:BCR:H321	1.98	0.46
1:A:733:LEU:HG	10:B:4011:BCR:H382	1.98	0.46
8:A:1013:CLA:HMB1	8:A:1013:CLA:HBB1	1.98	0.46
8:B:1217:CLA:H92	8:B:1217:CLA:H61	1.78	0.46
11:M:5001:LHG:H162	11:M:5001:LHG:H191	1.71	0.46
1:A:555:TYR:O	1:A:565:LYS:NZ	2.40	0.45
10:A:4002:BCR:H351	10:A:4002:BCR:H15C	1.77	0.45
4:D:120:ARG:NH2	4:D:141:VAL:O	2.49	0.45
8:A:1126:CLA:HBA2	8:A:1126:CLA:H3A	1.59	0.45
2:B:131:THR:HG23	2:B:134:GLU:H	1.81	0.45
1:A:686:LEU:HD12	2:B:662:ILE:HD12	1.99	0.45
8:A:1136:CLA:H112	8:A:1136:CLA:H71	1.73	0.45
4:D:16:GLY:O	4:D:44:THR:OG1	2.34	0.45
1:A:153:THR:O	1:A:234:LYS:NZ	2.47	0.45
1:A:466:ARG:HB2	1:A:468:GLN:HE22	1.82	0.45
1:A:554:LEU:HD21	8:A:1119:CLA:H203	1.98	0.45
8:A:1013:CLA:HBA2	8:A:1013:CLA:H12	1.77	0.45
2:B:48:ALA:HB2	2:B:157:LEU:HD21	1.98	0.45
2:B:573:PHE:HE2	12:B:5002:LMG:H361	1.81	0.45
2:B:592:HIS:ND1	2:B:620:TYR:OH	2.43	0.45
8:B:1218:CLA:HMD2	10:B:4004:BCR:H24C	1.97	0.45
11:A:5003:LHG:H212	11:A:5003:LHG:H371	1.99	0.45
2:B:336:LEU:HD21	8:B:1226:CLA:HAB	1.98	0.45
1:A:37:THR:HG23	1:A:38:LEU:HD12	1.97	0.45
2:B:557:ASP:OD1	2:B:561:ARG:NH2	2.41	0.45
2:B:712:VAL:HG23	12:B:5002:LMG:H453	1.97	0.45
8:A:1108:CLA:HBA1	8:A:1108:CLA:H3A	1.59	0.45
2:B:538:ALA:HA	2:B:547:LYS:HD2	1.98	0.45
8:B:1227:CLA:HMA2	8:B:1228:CLA:HED3	1.98	0.45
1:A:360:GLY:O	1:A:364:ILE:HG12	2.16	0.45
1:A:667:ALA:HB1	8:A:1106:CLA:HMC1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1103:CLA:H143	10:A:4002:BCR:H332	1.98	0.45
1:A:311:TYR:HA	1:A:319:HIS:H	1.81	0.45
1:A:434:ASP:OD2	1:A:434:ASP:N	2.41	0.45
1:A:678:VAL:HG22	8:A:1140:CLA:HBB1	1.99	0.45
8:A:1012:CLA:HAB	2:B:579:TRP:HH2	1.79	0.45
8:A:1124:CLA:HBA1	8:A:1124:CLA:H3A	1.57	0.45
8:B:1213:CLA:HBD	8:B:1213:CLA:HBA1	1.99	0.45
8:B:1220:CLA:H93	8:B:1220:CLA:H61	1.84	0.45
8:A:1138:CLA:HED2	2:B:422:TRP:HB2	1.99	0.45
1:A:660:SER:HB2	1:A:665:LEU:HB2	1.99	0.44
2:B:680:GLU:O	2:B:686:ASN:ND2	2.40	0.44
1:A:538:HIS:CD2	8:A:1135:CLA:HAB	2.53	0.44
2:B:332:LEU:HD11	8:B:1226:CLA:HMB3	1.99	0.44
2:B:494:TRP:O	2:B:498:ILE:HG12	2.17	0.44
8:B:1215:CLA:HMB1	8:B:1215:CLA:HBB1	1.98	0.44
1:A:360:GLY:O	1:A:363:THR:OG1	2.32	0.44
2:B:152:ALA:HB2	8:B:1208:CLA:HBC2	1.98	0.44
8:B:1230:CLA:H143	8:B:1230:CLA:H161	1.84	0.44
9:A:2001:PQN:H111	10:B:4014:BCR:H271	1.98	0.44
2:B:682:THR:HG23	2:B:685:ALA:HB3	2.00	0.44
8:B:1022:CLA:CAD	8:B:1021:CLA:HMB3	2.47	0.44
8:B:1216:CLA:HMB2	8:B:1221:CLA:HMA3	2.00	0.44
10:B:4004:BCR:H351	10:B:4004:BCR:H15C	1.58	0.44
3:C:9:ASP:HB3	4:D:119:THR:HA	1.99	0.44
4:D:127:GLU:OE1	4:D:129:VAL:HG22	2.17	0.44
1:A:222:PRO:HB2	1:A:242:PHE:HE1	1.82	0.44
8:A:1109:CLA:H61	8:A:1109:CLA:H41	1.62	0.44
2:B:223:MET:SD	2:B:224:PRO:HD3	2.57	0.44
8:B:1204:CLA:HMB3	8:B:1205:CLA:HHB	2.00	0.44
10:A:4019:BCR:H351	10:A:4019:BCR:H15C	1.66	0.44
1:A:352:LEU:HD22	1:A:407:HIS:CG	2.53	0.44
2:B:26:ALA:HB2	12:B:5002:LMG:H132	1.99	0.44
8:B:1021:CLA:HBA1	8:B:1021:CLA:H3A	1.46	0.44
1:A:356:LEU:HB3	1:A:404:ALA:HB2	2.00	0.44
8:A:1012:CLA:H61	8:A:1012:CLA:H41	1.82	0.44
4:D:66:LEU:HD23	4:D:66:LEU:HA	1.78	0.44
2:B:143:LEU:HD21	7:M:15:ALA:HB2	1.98	0.44
8:B:1217:CLA:H193	10:B:4005:BCR:H342	2.00	0.44
8:A:1106:CLA:H111	10:A:4012:BCR:H24C	1.99	0.43
8:A:1140:CLA:HBA1	11:A:5001:LHG:H192	1.98	0.43
2:B:56:ILE:HD11	14:M:4021:ECH:H23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1210:CLA:H111	8:B:1210:CLA:H152	1.68	0.43
8:B:1229:CLA:HAB	8:B:1230:CLA:HMB2	2.00	0.43
2:B:420:LEU:HB3	2:B:529:LEU:HB2	1.99	0.43
2:B:561:ARG:HH22	3:C:66:ARG:HH22	1.66	0.43
5:E:13:ARG:HD2	5:E:16:SER:HB2	1.99	0.43
8:B:1213:CLA:H201	10:B:4004:BCR:H21C	1.99	0.43
8:B:1224:CLA:H93	8:B:1224:CLA:H111	1.92	0.43
8:B:1238:CLA:H92	8:B:1238:CLA:H62	1.81	0.43
1:A:84:PHE:HZ	8:A:1111:CLA:H52	1.83	0.43
1:A:285:THR:HG23	1:A:287:GLY:H	1.83	0.43
8:A:1013:CLA:C1D	2:B:579:TRP:HE1	2.31	0.43
2:B:79:LYS:HD3	2:B:79:LYS:HA	1.82	0.43
2:B:336:LEU:HB3	2:B:384:ALA:HB2	2.00	0.43
8:B:1226:CLA:H112	12:B:5002:LMG:H421	2.00	0.43
1:A:402:VAL:HG11	1:A:595:LEU:HD12	2.01	0.43
2:B:729:LYS:HB2	2:B:729:LYS:HE2	1.88	0.43
8:B:1225:CLA:H3A	8:B:1225:CLA:HBA2	1.50	0.43
1:A:248:LYS:HA	1:A:251:GLU:HG2	1.99	0.43
3:C:73:THR:HG22	3:C:75:ARG:H	1.83	0.43
8:B:1227:CLA:H92	8:B:1227:CLA:H61	1.81	0.43
8:A:1112:CLA:HBA2	10:A:4002:BCR:H342	2.00	0.43
8:A:1123:CLA:HED2	8:A:1123:CLA:HBA1	2.01	0.43
8:A:1136:CLA:H92	8:A:1136:CLA:H61	1.76	0.43
11:A:5001:LHG:H182	11:A:5001:LHG:H151	1.75	0.43
1:A:43:LYS:HZ3	5:E:44:VAL:HG21	1.83	0.42
8:B:1202:CLA:H93	8:B:1202:CLA:H111	1.89	0.42
8:B:1234:CLA:HMB1	8:B:1234:CLA:HBB1	2.01	0.42
8:A:1105:CLA:H3A	8:A:1105:CLA:HBA2	1.61	0.42
8:B:1210:CLA:H151	8:B:1225:CLA:HMD2	2.00	0.42
8:B:1214:CLA:H13	8:B:1232:CLA:HMA2	2.00	0.42
8:B:1225:CLA:HMB1	8:B:1225:CLA:HBB1	2.01	0.42
1:A:663:SER:OG	1:A:664:ALA:N	2.53	0.42
8:A:1117:CLA:H162	8:A:1133:CLA:H72	2.00	0.42
8:B:1022:CLA:H143	8:B:1206:CLA:HBB1	2.00	0.42
4:D:69:GLY:O	4:D:73:ARG:HG3	2.19	0.42
6:K:40:ALA:O	6:K:42:GLN:NE2	2.52	0.42
14:M:4021:ECH:H15	14:M:4021:ECH:H35	1.74	0.42
2:B:545:PRO:HD3	3:C:62:PHE:CZ	2.54	0.42
10:K:4001:BCR:H351	10:K:4001:BCR:H15C	1.78	0.42
10:A:4001:BCR:H15C	10:A:4001:BCR:H351	1.63	0.42
2:B:516:VAL:HG11	2:B:590:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:LEU:HD23	2:B:596:LEU:HA	1.90	0.42
1:A:433:ARG:HA	1:A:436:ILE:HG22	2.02	0.42
8:A:1130:CLA:H41	8:A:1130:CLA:H62	1.84	0.42
8:A:1117:CLA:H111	8:A:1117:CLA:H152	1.85	0.42
8:A:1122:CLA:H141	11:A:5003:LHG:H171	2.01	0.42
1:A:456:ILE:HG22	8:A:1132:CLA:HBC2	2.01	0.42
8:B:1217:CLA:H91	8:B:1217:CLA:H112	1.77	0.42
8:B:1227:CLA:HAB	8:B:1236:CLA:HBB2	2.01	0.42
7:M:4:SER:HB2	7:M:7:GLN:HG3	2.01	0.42
1:A:516:VAL:HG22	1:A:517:ALA:H	1.84	0.42
8:A:1119:CLA:H18	10:A:4007:BCR:H332	2.01	0.42
2:B:272:ASP:HB3	8:B:1214:CLA:HMA1	2.01	0.42
8:B:1235:CLA:H41	8:B:1235:CLA:H61	1.54	0.42
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.89	0.41
2:B:653:VAL:HG22	8:B:1239:CLA:HMB3	2.02	0.41
8:B:1226:CLA:H152	12:B:5002:LMG:H441	2.02	0.41
8:B:1240:CLA:H112	8:B:1240:CLA:H91	1.82	0.41
11:B:5004:LHG:H181	11:B:5004:LHG:H212	1.86	0.41
1:A:67:ASP:HA	1:A:70:ARG:HD2	2.01	0.41
1:A:602:LEU:O	1:A:606:ILE:HG12	2.20	0.41
8:A:1124:CLA:HAB	10:A:4008:BCR:H321	2.02	0.41
8:B:1227:CLA:HBC1	10:B:4018:BCR:H24C	2.02	0.41
14:B:4006:ECH:H20	14:B:4006:ECH:H36	1.71	0.41
8:K:1402:CLA:C1B	10:K:4001:BCR:H14C	2.51	0.41
2:B:335:ALA:HB1	8:B:1202:CLA:HED3	2.02	0.41
8:B:1202:CLA:H92	8:B:1202:CLA:H61	1.79	0.41
8:B:1222:CLA:H52	8:B:1231:CLA:HBB2	2.01	0.41
8:A:1111:CLA:HED2	8:A:1111:CLA:H2A	2.01	0.41
2:B:312:LEU:HD21	11:B:5004:LHG:HC42	2.01	0.41
2:B:403:ASP:OD1	2:B:408:ARG:NH2	2.50	0.41
2:B:488:ALA:HB3	2:B:491:LEU:HD23	2.02	0.41
8:B:1234:CLA:H91	8:B:1234:CLA:H111	1.86	0.41
1:A:661:TYR:HD1	2:B:443:ALA:HA	1.84	0.41
2:B:19:ARG:HD2	2:B:698:SER:HB3	2.02	0.41
2:B:256:THR:HA	8:B:1213:CLA:HED1	2.01	0.41
2:B:435:TYR:HD2	2:B:613:LEU:HD12	1.84	0.41
8:B:1204:CLA:HHB	8:B:1205:CLA:HMB3	2.01	0.41
8:B:1214:CLA:H202	8:B:1214:CLA:H161	1.88	0.41
8:B:1221:CLA:H41	8:B:1221:CLA:H62	1.77	0.41
1:A:433:ARG:NH1	1:A:558:SER:O	2.53	0.41
1:A:646:LEU:HD22	2:B:648:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:LEU:HD22	12:B:5002:LMG:H142	2.02	0.41
10:B:4018:BCR:H15C	10:B:4018:BCR:H351	1.80	0.41
1:A:650:LEU:HD23	1:A:650:LEU:HA	1.89	0.41
1:A:687:PHE:CE1	2:B:661:LEU:HG	2.55	0.41
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.02	0.41
8:B:1021:CLA:H92	8:B:1021:CLA:H62	1.87	0.41
8:B:1227:CLA:HBB1	11:B:5004:LHG:H292	2.03	0.41
8:B:1235:CLA:H61	8:B:1235:CLA:H93	1.85	0.41
1:A:74:SER:OG	8:A:1109:CLA:HAC2	2.21	0.41
1:A:225:LYS:HZ2	1:A:253:TYR:HE1	1.68	0.41
1:A:321:MET:HA	1:A:324:ILE:HG22	2.02	0.41
1:A:732:LEU:O	1:A:736:ILE:HG12	2.20	0.41
8:A:1116:CLA:H62	8:A:1116:CLA:H41	1.87	0.41
8:A:1140:CLA:HBA1	11:A:5001:LHG:H171	2.03	0.41
2:B:53:HIS:O	2:B:57:ILE:HG12	2.21	0.41
2:B:573:PHE:CE2	12:B:5002:LMG:H361	2.56	0.41
8:B:1219:CLA:H62	8:B:1219:CLA:H92	1.81	0.41
1:A:692:TYR:OH	2:B:530:ILE:HG23	2.21	0.41
8:A:1128:CLA:H41	8:A:1128:CLA:H62	1.62	0.41
8:B:1225:CLA:H142	14:B:4006:ECH:H37A	2.02	0.41
8:B:1229:CLA:H3A	10:B:4014:BCR:H353	2.03	0.41
5:E:10:ARG:O	5:E:67:GLU:N	2.52	0.41
8:K:1401:CLA:H161	8:K:1401:CLA:H122	1.91	0.41
1:A:376:TYR:CE2	8:A:1127:CLA:HED2	2.56	0.40
8:A:1124:CLA:HAB	10:A:4008:BCR:C8	2.52	0.40
2:B:645:TRP:HZ3	10:B:4017:BCR:H322	1.85	0.40
8:B:1203:CLA:H141	8:B:1203:CLA:H162	1.85	0.40
8:B:1239:CLA:H202	8:B:1239:CLA:H162	1.95	0.40
1:A:205:LEU:HD21	8:A:1127:CLA:H192	2.02	0.40
11:A:5003:LHG:H142	11:A:5003:LHG:H112	1.70	0.40
2:B:513:ASP:HA	2:B:516:VAL:HG12	2.03	0.40
2:B:552:TYR:O	2:B:568:SER:OG	2.35	0.40
8:A:1103:CLA:HED1	8:A:1128:CLA:HBB2	2.03	0.40
8:A:1140:CLA:H141	8:A:1140:CLA:H162	1.81	0.40
2:B:289:HIS:CE1	10:B:4004:BCR:H363	2.55	0.40
8:B:1213:CLA:H92	8:B:1213:CLA:H62	1.95	0.40
1:A:560:ARG:HH22	2:B:677:TRP:HB2	1.87	0.40
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.91	0.40
1:A:376:TYR:HE2	8:A:1127:CLA:HED2	1.87	0.40
2:B:659:MET:HB3	2:B:660:PHE:H	1.70	0.40
8:B:1228:CLA:H93	8:B:1228:CLA:H111	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:ARG:NH2	4:D:97:LEU:HD21	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	737/739 (100%)	693 (94%)	43 (6%)	1 (0%)	51 85
2	B	727/729 (100%)	695 (96%)	32 (4%)	0	100 100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100 100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
5	E	67/69 (97%)	62 (92%)	5 (8%)	0	100 100
6	K	79/80 (99%)	67 (85%)	12 (15%)	0	100 100
7	M	29/31 (94%)	29 (100%)	0	0	100 100
All	All	1856/1869 (99%)	1755 (95%)	100 (5%)	1 (0%)	54 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO

5.3.2 Protein sidechains

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	593/593 (100%)	593 (100%)	0	100 100
2	B	582/582 (100%)	578 (99%)	4 (1%)	84 90
3	C	68/68 (100%)	68 (100%)	0	100 100
4	D	116/116 (100%)	116 (100%)	0	100 100
5	E	58/58 (100%)	58 (100%)	0	100 100
6	K	60/60 (100%)	60 (100%)	0	100 100
7	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1502/1502 (100%)	1498 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	LYS
2	B	85	ARG
2	B	533	LYS
2	B	582	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	HIS
1	A	608	HIS
2	B	582	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

120 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	CLA	B	1203	-	56,73,73	1.30	6 (10%)	55,113,113	1.85	7 (12%)
8	CLA	A	1139	-	37,54,73	1.59	6 (16%)	32,90,113	2.28	6 (18%)
8	CLA	K	1401	-	56,73,73	1.29	7 (12%)	55,113,113	2.00	10 (18%)
8	CLA	A	1120	-	40,57,73	1.54	6 (15%)	34,93,113	2.42	7 (20%)
8	CLA	A	1109	-	51,68,73	1.34	6 (11%)	49,107,113	2.06	10 (20%)
8	CLA	B	1235	-	51,68,73	1.32	5 (9%)	49,107,113	2.13	12 (24%)
8	CLA	A	1105	-	41,58,73	1.51	6 (14%)	37,95,113	2.26	8 (21%)
8	CLA	A	1113	-	33,53,73	1.67	7 (21%)	27,89,113	2.52	8 (29%)
8	CLA	B	1227	-	46,63,73	1.40	6 (13%)	43,101,113	2.01	9 (20%)
8	CLA	B	1237	-	56,73,73	1.29	6 (10%)	55,113,113	2.09	11 (20%)
10	BCR	B	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.38	15 (26%)
10	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	14 (25%)
8	CLA	A	1111	-	46,63,73	1.42	6 (13%)	43,101,113	2.20	10 (23%)
8	CLA	A	1112	-	41,58,73	1.48	6 (14%)	37,95,113	2.35	9 (24%)
8	CLA	B	1226	-	56,73,73	1.24	6 (10%)	55,113,113	2.12	12 (21%)
8	CLA	B	1230	-	56,73,73	1.31	6 (10%)	55,113,113	2.07	11 (20%)
8	CLA	B	1213	-	56,73,73	1.29	6 (10%)	55,113,113	2.22	13 (23%)
8	CLA	B	1223	-	51,68,73	1.37	6 (11%)	49,107,113	2.11	9 (18%)
8	CLA	B	1234	-	56,73,73	1.26	5 (8%)	55,113,113	2.09	11 (20%)
10	BCR	A	4002	-	41,41,41	1.82	4 (9%)	56,56,56	4.40	17 (30%)
8	CLA	A	1121	-	41,58,73	1.52	6 (14%)	37,95,113	2.41	10 (27%)
8	CLA	A	1124	-	46,63,73	1.43	6 (13%)	43,101,113	2.14	8 (18%)
8	CLA	B	1224	-	53,70,73	1.31	6 (11%)	51,109,113	2.06	12 (23%)
8	CLA	B	1215	-	56,73,73	1.26	5 (8%)	55,113,113	2.09	10 (18%)
8	CLA	A	1801	-	37,54,73	1.58	6 (16%)	32,90,113	2.25	6 (18%)
8	CLA	B	1202	-	56,73,73	1.27	6 (10%)	55,113,113	1.91	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CLA	A	1123	-	56,73,73	1.30	5 (8%)	55,113,113	2.14	11 (20%)
10	BCR	B	4011	-	41,41,41	1.88	4 (9%)	56,56,56	4.36	17 (30%)
8	CLA	A	1127	-	56,73,73	1.26	6 (10%)	55,113,113	2.02	14 (25%)
8	CLA	A	1129	-	37,54,73	1.57	6 (16%)	32,90,113	2.28	6 (18%)
8	CLA	B	1240	-	56,73,73	1.30	5 (8%)	55,113,113	2.03	10 (18%)
8	CLA	B	1238	-	56,73,73	1.28	6 (10%)	55,113,113	1.94	10 (18%)
8	CLA	A	1133	-	56,73,73	1.29	6 (10%)	55,113,113	1.92	7 (12%)
8	CLA	B	1211	-	37,54,73	1.56	5 (13%)	32,90,113	2.23	7 (21%)
8	CLA	B	1208	-	33,53,73	1.68	6 (18%)	27,89,113	2.32	7 (25%)
10	BCR	B	4010	-	41,41,41	1.83	4 (9%)	56,56,56	4.41	21 (37%)
10	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	17 (30%)
8	CLA	A	1104	-	56,73,73	1.28	6 (10%)	55,113,113	1.95	10 (18%)
8	CLA	B	1231	-	56,73,73	1.29	6 (10%)	55,113,113	1.93	9 (16%)
12	LMG	A	5002	-	50,50,55	1.03	5 (10%)	58,58,63	1.08	2 (3%)
8	CLA	A	1103	-	51,68,73	1.34	6 (11%)	49,107,113	2.10	11 (22%)
8	CLA	B	1219	-	56,73,73	1.29	6 (10%)	55,113,113	1.94	10 (18%)
10	BCR	A	4003	-	41,41,41	1.79	4 (9%)	56,56,56	3.95	16 (28%)
8	CLA	B	1229	-	56,73,73	1.31	7 (12%)	55,113,113	1.93	9 (16%)
10	BCR	A	4012	-	41,41,41	1.86	4 (9%)	56,56,56	4.35	16 (28%)
8	CLA	K	1402	-	56,73,73	1.30	6 (10%)	55,113,113	1.98	10 (18%)
8	CLA	B	1023	-	51,68,73	1.31	6 (11%)	49,107,113	2.13	11 (22%)
8	CLA	B	1207	-	46,63,73	1.42	6 (13%)	43,101,113	2.11	9 (20%)
10	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	17 (30%)
8	CLA	B	1209	-	56,73,73	1.30	6 (10%)	55,113,113	2.01	8 (14%)
10	BCR	A	4019	-	41,41,41	1.85	4 (9%)	56,56,56	4.40	16 (28%)
8	CLA	A	1013	-	46,63,73	1.33	5 (10%)	43,101,113	2.42	12 (27%)
10	BCR	B	4014	-	41,41,41	1.90	4 (9%)	56,56,56	4.51	18 (32%)
8	CLA	B	1214	-	56,73,73	1.29	6 (10%)	55,113,113	1.99	11 (20%)
8	CLA	B	1217	-	56,73,73	1.29	6 (10%)	55,113,113	1.98	7 (12%)
8	CLA	A	1126	-	51,68,73	1.34	6 (11%)	49,107,113	2.12	10 (20%)
14	ECH	B	4006	-	42,42,42	0.86	1 (2%)	55,58,58	2.19	16 (29%)
8	CLA	B	1228	-	56,73,73	1.31	6 (10%)	55,113,113	1.89	9 (16%)
8	CLA	A	1115	-	37,54,73	1.53	5 (13%)	32,90,113	2.33	7 (21%)
13	SF4	C	3003	3	0,12,12	0.00	-	-		
8	CLA	A	1117	-	56,73,73	1.27	6 (10%)	55,113,113	2.13	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CLA	A	1130	-	46,63,73	1.44	6 (13%)	43,101,113	2.14	9 (20%)
10	BCR	A	4007	-	41,41,41	1.82	4 (9%)	56,56,56	4.30	18 (32%)
14	ECH	M	4021	-	42,42,42	0.78	0	55,58,58	2.09	16 (29%)
8	CLA	A	1136	-	56,73,73	1.29	6 (10%)	55,113,113	1.95	9 (16%)
8	CLA	B	1220	-	48,65,73	1.39	6 (12%)	45,103,113	2.19	11 (24%)
8	CLA	A	1108	-	33,53,73	1.71	6 (18%)	27,89,113	2.38	6 (22%)
15	SQD	B	5008	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
12	LMG	B	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.04	3 (4%)
8	CLA	B	1221	-	46,63,73	1.39	5 (10%)	43,101,113	2.24	12 (27%)
8	CLA	B	1201	-	37,54,73	1.59	6 (16%)	32,90,113	2.27	5 (15%)
8	CLA	B	1218	-	41,58,73	1.48	6 (14%)	37,95,113	2.38	10 (27%)
8	CLA	A	1128	-	51,68,73	1.32	6 (11%)	49,107,113	2.14	13 (26%)
8	CLA	A	1137	-	41,58,73	1.51	6 (14%)	37,95,113	2.29	12 (32%)
8	CLA	A	1132	-	41,58,73	1.50	6 (14%)	37,95,113	2.31	8 (21%)
8	CLA	B	1222	-	46,63,73	1.41	6 (13%)	43,101,113	2.24	11 (25%)
8	CLA	A	1102	-	46,63,73	1.43	6 (13%)	43,101,113	2.33	11 (25%)
11	LHG	B	5006	-	23,23,48	0.53	0	26,29,54	1.37	3 (11%)
8	CLA	A	1011	-	51,68,73	1.33	6 (11%)	49,107,113	2.15	10 (20%)
8	CLA	A	1110	-	51,68,73	1.39	6 (11%)	49,107,113	2.12	9 (18%)
8	CLA	B	1021	-	51,68,73	1.30	6 (11%)	49,107,113	2.24	12 (24%)
11	LHG	A	5003	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
10	BCR	A	4008	-	41,41,41	1.80	4 (9%)	56,56,56	4.23	14 (25%)
8	CLA	B	1205	-	46,63,73	1.43	6 (13%)	43,101,113	2.30	9 (20%)
11	LHG	M	5001	-	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
8	CLA	A	1012	-	46,63,73	1.45	6 (13%)	43,101,113	2.13	12 (27%)
8	CLA	A	1114	-	33,53,73	1.69	6 (18%)	27,89,113	2.40	6 (22%)
8	CLA	A	1131	-	46,63,73	1.43	6 (13%)	43,101,113	2.19	9 (20%)
8	CLA	B	1210	-	56,73,73	1.29	6 (10%)	55,113,113	2.06	13 (23%)
11	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
8	CLA	B	1212	-	33,53,73	1.67	6 (18%)	27,89,113	2.44	7 (25%)
13	SF4	A	3001	1,2	0,12,12	0.00	-	-		
8	CLA	B	1239	-	56,73,73	1.30	6 (10%)	55,113,113	1.99	11 (20%)
8	CLA	B	1204	-	37,54,73	1.58	6 (16%)	32,90,113	2.19	6 (18%)
8	CLA	A	1134	-	37,54,73	1.60	6 (16%)	32,90,113	2.31	6 (18%)
8	CLA	A	1119	-	56,73,73	1.30	6 (10%)	55,113,113	1.92	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CLA	A	1138	-	56,73,73	1.30	6 (10%)	55,113,113	2.04	10 (18%)
8	CLA	B	1232	-	41,58,73	1.54	7 (17%)	37,95,113	2.32	9 (24%)
8	CLA	A	1122	-	51,68,73	1.34	6 (11%)	49,107,113	2.18	10 (20%)
8	CLA	B	1225	-	56,73,73	1.26	5 (8%)	55,113,113	2.04	13 (23%)
12	LMG	K	5009	-	55,55,55	1.14	6 (10%)	63,63,63	1.03	2 (3%)
9	PQN	A	2001	-	34,34,34	0.37	0	42,45,45	1.11	5 (11%)
11	LHG	B	5004	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
8	CLA	A	1107	-	41,58,73	1.52	6 (14%)	37,95,113	2.35	8 (21%)
8	CLA	A	1116	-	45,62,73	1.45	6 (13%)	41,99,113	2.25	13 (31%)
8	CLA	A	1106	-	51,68,73	1.31	6 (11%)	49,107,113	2.11	11 (22%)
8	CLA	A	1125	-	43,60,73	1.50	5 (11%)	39,97,113	2.39	14 (35%)
8	CLA	A	1101	-	56,73,73	1.30	6 (10%)	55,113,113	1.95	9 (16%)
10	BCR	B	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	18 (32%)
8	CLA	B	1206	-	46,63,73	1.43	6 (13%)	43,101,113	2.35	11 (25%)
8	CLA	B	1236	-	41,58,73	1.50	6 (14%)	37,95,113	2.22	11 (29%)
9	PQN	B	2002	-	34,34,34	0.36	0	42,45,45	1.17	3 (7%)
8	CLA	B	1216	-	46,63,73	1.42	6 (13%)	43,101,113	2.17	10 (23%)
12	LMG	B	5005	-	31,31,55	0.54	0	39,39,63	1.10	2 (5%)
8	CLA	A	1118	-	37,54,73	1.55	6 (16%)	32,90,113	2.33	7 (21%)
8	CLA	A	1135	-	56,73,73	1.27	6 (10%)	55,113,113	2.02	11 (20%)
8	CLA	B	1022	-	51,68,73	1.37	5 (9%)	49,107,113	2.02	10 (20%)
10	BCR	B	4017	-	41,41,41	1.86	5 (12%)	56,56,56	4.52	19 (33%)
13	SF4	C	3002	3	0,12,12	0.00	-	-		
8	CLA	A	1140	-	56,73,73	1.30	6 (10%)	55,113,113	1.95	8 (14%)

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
8	CLA	B	1203	-	1/1/15/20	16/37/115/115	-
8	CLA	A	1139	-	1/1/11/20	6/15/93/115	-
8	CLA	K	1401	-	1/1/15/20	16/37/115/115	-
8	CLA	A	1120	-	1/1/11/20	8/18/96/115	-
8	CLA	A	1109	-	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	B	1235	-	1/1/14/20	16/31/109/115	-
8	CLA	A	1105	-	1/1/12/20	7/19/97/115	-
8	CLA	A	1113	-	1/1/11/20	4/11/91/115	-
8	CLA	B	1227	-	1/1/13/20	14/25/103/115	-
8	CLA	B	1237	-	1/1/15/20	16/37/115/115	-
10	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
10	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
8	CLA	A	1111	-	1/1/13/20	12/25/103/115	-
8	CLA	A	1112	-	1/1/12/20	11/19/97/115	-
8	CLA	B	1226	-	1/1/15/20	15/37/115/115	-
8	CLA	B	1230	-	1/1/15/20	18/37/115/115	-
8	CLA	B	1213	-	1/1/15/20	12/37/115/115	-
8	CLA	B	1223	-	1/1/14/20	15/31/109/115	-
8	CLA	B	1234	-	1/1/15/20	21/37/115/115	-
10	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
8	CLA	A	1121	-	1/1/12/20	7/19/97/115	-
8	CLA	A	1124	-	1/1/13/20	5/25/103/115	-
8	CLA	B	1224	-	1/1/14/20	19/34/112/115	-
8	CLA	B	1215	-	1/1/15/20	21/37/115/115	-
8	CLA	A	1801	-	1/1/11/20	6/15/93/115	-
8	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
8	CLA	A	1123	-	1/1/15/20	24/37/115/115	-
10	BCR	B	4011	-	-	16/29/63/63	0/2/2/2
8	CLA	A	1127	-	1/1/15/20	22/37/115/115	-
8	CLA	A	1129	-	1/1/11/20	7/15/93/115	-
8	CLA	B	1240	-	1/1/15/20	17/37/115/115	-
8	CLA	B	1238	-	1/1/15/20	17/37/115/115	-
8	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
8	CLA	B	1211	-	1/1/11/20	3/15/93/115	-
8	CLA	B	1208	-	1/1/11/20	3/11/91/115	-
10	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
10	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
8	CLA	A	1104	-	1/1/15/20	18/37/115/115	-
8	CLA	B	1231	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMG	A	5002	-	-	19/45/65/70	0/1/1/1
8	CLA	A	1103	-	1/1/14/20	16/31/109/115	-
8	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
10	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
8	CLA	B	1229	-	1/1/15/20	16/37/115/115	-
10	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
8	CLA	K	1402	-	1/1/15/20	18/37/115/115	-
8	CLA	B	1023	-	1/1/14/20	13/31/109/115	-
8	CLA	B	1207	-	1/1/13/20	7/25/103/115	-
10	BCR	A	4001	-	-	11/29/63/63	0/2/2/2
8	CLA	B	1209	-	1/1/15/20	23/37/115/115	-
10	BCR	A	4019	-	-	9/29/63/63	0/2/2/2
8	CLA	A	1013	-	1/1/13/20	13/25/103/115	-
10	BCR	B	4014	-	-	12/29/63/63	0/2/2/2
8	CLA	B	1214	-	1/1/15/20	16/37/115/115	-
8	CLA	B	1217	-	1/1/15/20	17/37/115/115	-
8	CLA	A	1126	-	1/1/14/20	18/31/109/115	-
14	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
8	CLA	B	1228	-	1/1/15/20	21/37/115/115	-
8	CLA	A	1115	-	1/1/11/20	6/15/93/115	-
13	SF4	C	3003	3	-	-	0/6/5/5
8	CLA	A	1117	-	1/1/15/20	20/37/115/115	-
8	CLA	A	1130	-	1/1/13/20	11/25/103/115	-
10	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
14	ECH	M	4021	-	-	17/29/66/66	0/2/2/2
8	CLA	A	1136	-	1/1/15/20	17/37/115/115	-
8	CLA	B	1220	-	1/1/13/20	9/28/106/115	-
8	CLA	A	1108	-	1/1/11/20	7/11/91/115	-
15	SQD	B	5008	-	-	10/49/69/69	0/1/1/1
12	LMG	B	5002	-	-	13/50/70/70	0/1/1/1
8	CLA	B	1221	-	1/1/13/20	9/25/103/115	-
8	CLA	B	1201	-	1/1/11/20	13/15/93/115	-
8	CLA	B	1218	-	1/1/12/20	10/19/97/115	-
8	CLA	A	1128	-	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	A	1137	-	1/1/12/20	8/19/97/115	-
8	CLA	A	1132	-	1/1/12/20	8/19/97/115	-
8	CLA	B	1222	-	1/1/13/20	7/25/103/115	-
8	CLA	A	1102	-	1/1/13/20	7/25/103/115	-
11	LHG	B	5006	-	-	17/28/28/53	-
8	CLA	A	1011	-	1/1/14/20	16/31/109/115	-
8	CLA	A	1110	-	1/1/14/20	16/31/109/115	-
8	CLA	B	1021	-	1/1/14/20	20/31/109/115	-
11	LHG	A	5003	-	-	29/53/53/53	-
10	BCR	A	4008	-	-	17/29/63/63	0/2/2/2
8	CLA	B	1205	-	1/1/13/20	10/25/103/115	-
11	LHG	M	5001	-	-	34/53/53/53	-
8	CLA	A	1012	-	1/1/13/20	10/25/103/115	-
8	CLA	A	1114	-	1/1/11/20	5/11/91/115	-
8	CLA	A	1131	-	1/1/13/20	13/25/103/115	-
8	CLA	B	1210	-	1/1/15/20	23/37/115/115	-
11	LHG	A	5001	-	-	30/53/53/53	-
8	CLA	B	1212	-	1/1/11/20	5/11/91/115	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
8	CLA	B	1239	-	1/1/15/20	12/37/115/115	-
8	CLA	B	1204	-	1/1/11/20	6/15/93/115	-
8	CLA	A	1134	-	1/1/11/20	11/15/93/115	-
8	CLA	A	1119	-	1/1/15/20	14/37/115/115	-
8	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
8	CLA	B	1232	-	1/1/12/20	9/19/97/115	-
8	CLA	A	1122	-	1/1/14/20	14/31/109/115	-
8	CLA	B	1225	-	1/1/15/20	13/37/115/115	-
12	LMG	K	5009	-	-	16/50/70/70	0/1/1/1
9	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
11	LHG	B	5004	-	-	28/53/53/53	-
8	CLA	A	1107	-	1/1/12/20	4/19/97/115	-
8	CLA	A	1116	-	1/1/12/20	12/24/102/115	-
8	CLA	A	1106	-	1/1/14/20	13/31/109/115	-
8	CLA	A	1125	-	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	A	1101	-	1/1/15/20	15/37/115/115	-
10	BCR	B	4018	-	-	9/29/63/63	0/2/2/2
8	CLA	B	1206	-	1/1/13/20	9/25/103/115	-
8	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
9	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
8	CLA	B	1216	-	1/1/13/20	15/25/103/115	-
12	LMG	B	5005	-	-	6/26/46/70	0/1/1/1
8	CLA	A	1118	-	1/1/11/20	8/15/93/115	-
8	CLA	A	1135	-	1/1/15/20	17/37/115/115	-
8	CLA	B	1022	-	1/1/14/20	12/31/109/115	-
10	BCR	B	4017	-	-	10/29/63/63	0/2/2/2
13	SF4	C	3002	3	-	-	0/6/5/5
8	CLA	A	1140	-	1/1/15/20	14/37/115/115	-

All (599) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	4014	BCR	C10-C9	7.60	1.45	1.35
10	B	4011	BCR	C10-C9	7.41	1.45	1.35
10	A	4012	BCR	C10-C9	7.35	1.45	1.35
10	A	4019	BCR	C10-C9	7.23	1.45	1.35
10	B	4018	BCR	C10-C9	7.23	1.45	1.35
10	B	4004	BCR	C10-C9	7.15	1.45	1.35
10	B	4017	BCR	C10-C9	7.09	1.45	1.35
10	A	4001	BCR	C10-C9	7.07	1.45	1.35
10	B	4005	BCR	C10-C9	7.07	1.45	1.35
10	K	4001	BCR	C10-C9	6.86	1.44	1.35
10	A	4003	BCR	C10-C9	6.84	1.44	1.35
10	A	4002	BCR	C10-C9	6.78	1.44	1.35
10	B	4010	BCR	C10-C9	6.77	1.44	1.35
10	A	4007	BCR	C10-C9	6.76	1.44	1.35
10	A	4008	BCR	C10-C9	6.57	1.44	1.35
8	A	1108	CLA	MG-NA	6.55	2.21	2.06
8	A	1125	CLA	MG-NA	6.48	2.21	2.06
8	A	1123	CLA	MG-NA	6.44	2.21	2.06
8	B	1228	CLA	MG-NA	6.44	2.21	2.06
8	A	1139	CLA	MG-NA	6.43	2.21	2.06
8	A	1110	CLA	MG-NA	6.42	2.21	2.06
8	B	1232	CLA	MG-NA	6.42	2.21	2.06
8	B	1214	CLA	MG-NA	6.42	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1230	CLA	MG-NA	6.42	2.21	2.06
8	B	1239	CLA	MG-NA	6.41	2.21	2.06
8	A	1134	CLA	MG-NA	6.41	2.21	2.06
8	B	1223	CLA	MG-NA	6.39	2.21	2.06
8	A	1119	CLA	MG-NA	6.39	2.21	2.06
8	B	1240	CLA	MG-NA	6.38	2.21	2.06
8	A	1801	CLA	MG-NA	6.38	2.21	2.06
8	A	1121	CLA	MG-NA	6.37	2.21	2.06
8	K	1402	CLA	MG-NA	6.37	2.21	2.06
8	A	1120	CLA	MG-NA	6.37	2.21	2.06
8	B	1206	CLA	MG-NA	6.36	2.21	2.06
8	A	1130	CLA	MG-NA	6.36	2.21	2.06
8	B	1213	CLA	MG-NA	6.36	2.21	2.06
8	B	1216	CLA	MG-NA	6.35	2.21	2.06
8	A	1114	CLA	MG-NA	6.35	2.21	2.06
8	A	1116	CLA	MG-NA	6.35	2.21	2.06
8	A	1127	CLA	MG-NA	6.35	2.21	2.06
8	B	1217	CLA	MG-NA	6.35	2.21	2.06
8	A	1129	CLA	MG-NA	6.35	2.21	2.06
8	B	1207	CLA	MG-NA	6.35	2.21	2.06
8	A	1107	CLA	MG-NA	6.34	2.21	2.06
8	A	1105	CLA	MG-NA	6.34	2.21	2.06
8	B	1229	CLA	MG-NA	6.33	2.21	2.06
8	A	1011	CLA	MG-NA	6.33	2.21	2.06
8	B	1220	CLA	MG-NA	6.33	2.21	2.06
8	B	1234	CLA	MG-NA	6.33	2.21	2.06
8	A	1131	CLA	MG-NA	6.33	2.21	2.06
8	A	1140	CLA	MG-NA	6.33	2.21	2.06
8	A	1132	CLA	MG-NA	6.33	2.21	2.06
8	A	1136	CLA	MG-NA	6.32	2.21	2.06
8	B	1225	CLA	MG-NA	6.32	2.21	2.06
8	B	1210	CLA	MG-NA	6.32	2.21	2.06
8	B	1204	CLA	MG-NA	6.31	2.21	2.06
8	A	1101	CLA	MG-NA	6.31	2.21	2.06
8	A	1126	CLA	MG-NA	6.30	2.21	2.06
8	B	1203	CLA	MG-NA	6.30	2.21	2.06
8	B	1236	CLA	MG-NA	6.30	2.21	2.06
8	B	1208	CLA	MG-NA	6.30	2.21	2.06
8	A	1124	CLA	MG-NA	6.30	2.21	2.06
8	B	1219	CLA	MG-NA	6.29	2.21	2.06
8	B	1201	CLA	MG-NA	6.29	2.21	2.06
8	A	1102	CLA	MG-NA	6.29	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1205	CLA	MG-NA	6.29	2.21	2.06
8	B	1211	CLA	MG-NA	6.29	2.21	2.06
8	A	1133	CLA	MG-NA	6.28	2.21	2.06
8	A	1122	CLA	MG-NA	6.28	2.21	2.06
8	B	1209	CLA	MG-NA	6.27	2.21	2.06
8	A	1137	CLA	MG-NA	6.27	2.21	2.06
8	A	1109	CLA	MG-NA	6.27	2.21	2.06
8	A	1135	CLA	MG-NA	6.26	2.21	2.06
8	A	1138	CLA	MG-NA	6.26	2.21	2.06
8	B	1221	CLA	MG-NA	6.26	2.21	2.06
8	B	1215	CLA	MG-NA	6.26	2.21	2.06
8	B	1237	CLA	MG-NA	6.25	2.21	2.06
8	A	1112	CLA	MG-NA	6.25	2.21	2.06
8	B	1218	CLA	MG-NA	6.25	2.21	2.06
8	A	1118	CLA	MG-NA	6.25	2.21	2.06
8	B	1238	CLA	MG-NA	6.25	2.21	2.06
8	A	1113	CLA	MG-NA	6.25	2.21	2.06
8	A	1103	CLA	MG-NA	6.25	2.21	2.06
8	B	1227	CLA	MG-NA	6.24	2.21	2.06
8	A	1012	CLA	MG-NA	6.24	2.21	2.06
8	B	1224	CLA	MG-NA	6.23	2.21	2.06
8	B	1212	CLA	MG-NA	6.23	2.21	2.06
8	B	1231	CLA	MG-NA	6.22	2.21	2.06
8	K	1401	CLA	MG-NA	6.22	2.21	2.06
8	A	1104	CLA	MG-NA	6.21	2.21	2.06
8	B	1222	CLA	MG-NA	6.20	2.21	2.06
8	B	1235	CLA	MG-NA	6.19	2.21	2.06
8	B	1226	CLA	MG-NA	6.18	2.21	2.06
8	A	1117	CLA	MG-NA	6.17	2.20	2.06
8	A	1128	CLA	MG-NA	6.17	2.20	2.06
8	B	1202	CLA	MG-NA	6.17	2.20	2.06
8	A	1115	CLA	MG-NA	6.16	2.20	2.06
8	A	1111	CLA	MG-NA	6.13	2.20	2.06
8	B	1021	CLA	MG-NA	6.11	2.20	2.06
8	A	1106	CLA	MG-NA	6.06	2.20	2.06
10	A	4001	BCR	C24-C23	6.01	1.51	1.33
8	A	1013	CLA	MG-NA	6.01	2.20	2.06
8	B	1023	CLA	MG-NA	5.99	2.20	2.06
8	B	1022	CLA	MG-NA	5.95	2.20	2.06
10	A	4012	BCR	C24-C23	5.92	1.51	1.33
10	B	4011	BCR	C24-C23	5.88	1.50	1.33
10	B	4014	BCR	C24-C23	5.86	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	4018	BCR	C24-C23	5.78	1.50	1.33
10	B	4010	BCR	C24-C23	5.76	1.50	1.33
10	A	4019	BCR	C24-C23	5.75	1.50	1.33
10	B	4004	BCR	C24-C23	5.71	1.50	1.33
10	A	4007	BCR	C24-C23	5.71	1.50	1.33
10	A	4002	BCR	C24-C23	5.69	1.50	1.33
10	K	4001	BCR	C24-C23	5.68	1.50	1.33
10	B	4017	BCR	C24-C23	5.63	1.50	1.33
10	A	4003	BCR	C24-C23	5.59	1.50	1.33
10	A	4008	BCR	C24-C23	5.57	1.49	1.33
10	B	4005	BCR	C24-C23	5.52	1.49	1.33
10	A	4008	BCR	C11-C12	-5.30	1.20	1.34
10	K	4001	BCR	C11-C12	-5.29	1.21	1.34
10	A	4002	BCR	C11-C12	-5.27	1.21	1.34
10	A	4007	BCR	C11-C12	-5.24	1.21	1.34
10	B	4004	BCR	C11-C12	-5.24	1.21	1.34
10	A	4001	BCR	C11-C12	-5.17	1.21	1.34
10	B	4010	BCR	C11-C12	-5.17	1.21	1.34
10	B	4014	BCR	C11-C12	-5.16	1.21	1.34
10	B	4017	BCR	C11-C12	-5.15	1.21	1.34
10	B	4005	BCR	C11-C12	-5.14	1.21	1.34
10	B	4018	BCR	C11-C12	-5.09	1.21	1.34
10	A	4019	BCR	C11-C12	-5.06	1.21	1.34
10	A	4012	BCR	C11-C12	-5.05	1.21	1.34
10	B	4011	BCR	C11-C12	-4.99	1.21	1.34
10	A	4003	BCR	C11-C12	-4.88	1.22	1.34
10	A	4008	BCR	C16-C17	-4.34	1.30	1.43
10	K	4001	BCR	C16-C17	-4.34	1.30	1.43
10	B	4017	BCR	C16-C17	-4.33	1.30	1.43
10	A	4002	BCR	C16-C17	-4.30	1.30	1.43
10	A	4019	BCR	C16-C17	-4.30	1.30	1.43
10	B	4011	BCR	C16-C17	-4.29	1.30	1.43
10	B	4005	BCR	C16-C17	-4.28	1.30	1.43
10	A	4003	BCR	C16-C17	-4.25	1.30	1.43
10	B	4004	BCR	C16-C17	-4.21	1.30	1.43
10	A	4001	BCR	C16-C17	-4.21	1.30	1.43
10	B	4010	BCR	C16-C17	-4.21	1.30	1.43
10	B	4014	BCR	C16-C17	-4.20	1.30	1.43
10	B	4018	BCR	C16-C17	-4.19	1.30	1.43
10	A	4007	BCR	C16-C17	-4.18	1.30	1.43
10	A	4012	BCR	C16-C17	-4.15	1.30	1.43
8	A	1110	CLA	C4C-NC	4.01	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1123	CLA	C4C-NC	3.81	1.38	1.35
8	A	1108	CLA	C4C-NC	3.79	1.38	1.35
8	B	1212	CLA	C4C-NC	3.78	1.38	1.35
8	B	1230	CLA	C4C-NC	3.75	1.38	1.35
8	B	1240	CLA	C4C-NC	3.74	1.38	1.35
8	K	1401	CLA	C4C-NC	3.73	1.38	1.35
8	A	1138	CLA	C4C-NC	3.72	1.38	1.35
8	A	1801	CLA	C4C-NC	3.71	1.38	1.35
8	A	1012	CLA	C4C-NC	3.70	1.38	1.35
8	B	1209	CLA	C4C-NC	3.69	1.38	1.35
8	B	1210	CLA	C4C-NC	3.69	1.38	1.35
8	A	1130	CLA	C4C-NC	3.68	1.38	1.35
8	A	1125	CLA	C4C-NC	3.68	1.38	1.35
8	B	1213	CLA	C4C-NC	3.65	1.38	1.35
8	B	1229	CLA	C4C-NC	3.65	1.38	1.35
8	B	1205	CLA	C4C-NC	3.64	1.38	1.35
8	B	1222	CLA	C4C-NC	3.64	1.38	1.35
8	A	1131	CLA	C4C-NC	3.63	1.38	1.35
8	B	1211	CLA	C4C-NC	3.63	1.38	1.35
8	A	1121	CLA	C4C-NC	3.63	1.38	1.35
8	K	1402	CLA	C4C-NC	3.61	1.38	1.35
8	B	1238	CLA	C4C-NC	3.61	1.38	1.35
8	B	1207	CLA	C4C-NC	3.60	1.38	1.35
8	A	1114	CLA	C4C-NC	3.60	1.38	1.35
8	A	1113	CLA	C4C-NC	3.60	1.38	1.35
8	A	1103	CLA	C4C-NC	3.59	1.38	1.35
8	A	1126	CLA	C4C-NC	3.59	1.38	1.35
8	B	1203	CLA	C4C-NC	3.59	1.38	1.35
8	B	1234	CLA	C4C-NC	3.59	1.38	1.35
8	A	1111	CLA	C4C-NC	3.59	1.38	1.35
8	A	1119	CLA	C4C-NC	3.59	1.38	1.35
8	A	1137	CLA	C4C-NC	3.58	1.38	1.35
8	B	1228	CLA	C4C-NC	3.58	1.38	1.35
8	A	1120	CLA	C4C-NC	3.58	1.38	1.35
8	A	1134	CLA	C4C-NC	3.56	1.38	1.35
8	B	1232	CLA	C4C-NC	3.56	1.38	1.35
8	A	1105	CLA	C4C-NC	3.55	1.38	1.35
8	B	1231	CLA	C4C-NC	3.55	1.38	1.35
8	B	1217	CLA	C4C-NC	3.55	1.38	1.35
8	B	1215	CLA	C4C-NC	3.55	1.38	1.35
8	A	1136	CLA	C4C-NC	3.54	1.38	1.35
8	B	1206	CLA	C4C-NC	3.53	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1223	CLA	C4C-NC	3.53	1.38	1.35
8	A	1117	CLA	C4C-NC	3.52	1.38	1.35
8	B	1204	CLA	C4C-NC	3.52	1.38	1.35
8	A	1115	CLA	C4C-NC	3.52	1.38	1.35
8	A	1101	CLA	C4C-NC	3.51	1.38	1.35
8	B	1237	CLA	C4C-NC	3.51	1.38	1.35
8	B	1208	CLA	C4C-NC	3.51	1.38	1.35
8	B	1214	CLA	C4C-NC	3.51	1.38	1.35
8	A	1135	CLA	C4C-NC	3.51	1.38	1.35
8	B	1201	CLA	C4C-NC	3.51	1.38	1.35
8	A	1124	CLA	C4C-NC	3.50	1.38	1.35
8	B	1219	CLA	C4C-NC	3.50	1.38	1.35
8	B	1225	CLA	C4C-NC	3.49	1.38	1.35
8	B	1235	CLA	C4C-NC	3.49	1.38	1.35
8	B	1202	CLA	C4C-NC	3.49	1.38	1.35
8	A	1116	CLA	C4C-NC	3.49	1.38	1.35
8	A	1112	CLA	C4C-NC	3.49	1.38	1.35
8	A	1107	CLA	C4C-NC	3.49	1.38	1.35
8	A	1122	CLA	C4C-NC	3.47	1.38	1.35
8	A	1132	CLA	C4C-NC	3.47	1.38	1.35
8	A	1102	CLA	C4C-NC	3.47	1.38	1.35
8	A	1139	CLA	C4C-NC	3.46	1.38	1.35
8	B	1023	CLA	C4C-NC	3.45	1.38	1.35
8	A	1109	CLA	C4C-NC	3.43	1.38	1.35
8	B	1236	CLA	C4C-NC	3.43	1.38	1.35
8	B	1236	CLA	CBB-CAB	3.43	1.52	1.29
8	A	1140	CLA	C4C-NC	3.42	1.38	1.35
8	A	1133	CLA	C4C-NC	3.41	1.38	1.35
8	A	1125	CLA	CBB-CAB	3.39	1.51	1.29
8	B	1224	CLA	C4C-NC	3.39	1.38	1.35
8	B	1239	CLA	C4C-NC	3.39	1.38	1.35
8	B	1220	CLA	C4C-NC	3.39	1.38	1.35
8	A	1113	CLA	CBB-CAB	3.37	1.51	1.29
8	B	1023	CLA	CBB-CAB	3.37	1.51	1.29
8	B	1240	CLA	CBB-CAB	3.37	1.51	1.29
8	B	1022	CLA	C4C-NC	3.37	1.38	1.35
8	B	1209	CLA	CBB-CAB	3.37	1.51	1.29
8	B	1211	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1117	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1120	CLA	CBB-CAB	3.36	1.51	1.29
8	B	1226	CLA	CBB-CAB	3.36	1.51	1.29
8	B	1232	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	1401	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1106	CLA	C4C-NC	3.36	1.38	1.35
8	B	1221	CLA	C4C-NC	3.36	1.38	1.35
8	A	1103	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1121	CLA	CBB-CAB	3.36	1.51	1.29
8	B	1221	CLA	CBB-CAB	3.36	1.51	1.29
8	B	1238	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1114	CLA	CBB-CAB	3.36	1.51	1.29
8	B	1213	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1012	CLA	CBB-CAB	3.36	1.51	1.29
8	A	1129	CLA	CBB-CAB	3.36	1.51	1.29
8	K	1402	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1122	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1219	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1234	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1140	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1215	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1011	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1210	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1107	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1119	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1105	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1218	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1136	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1131	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1202	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1206	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1230	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1138	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1237	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1108	CLA	CBB-CAB	3.35	1.51	1.29
8	A	1127	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1208	CLA	CBB-CAB	3.35	1.51	1.29
8	B	1220	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1227	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1109	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1128	CLA	C4C-NC	3.34	1.38	1.35
8	B	1216	CLA	C4C-NC	3.34	1.38	1.35
8	A	1118	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1225	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1134	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1130	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1207	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1217	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1205	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1106	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1228	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1224	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1132	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1801	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1112	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1101	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1222	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1212	CLA	CBB-CAB	3.34	1.51	1.29
8	B	1216	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1013	CLA	CBB-CAB	3.34	1.51	1.29
8	A	1104	CLA	CBB-CAB	3.33	1.51	1.29
8	B	1231	CLA	CBB-CAB	3.33	1.51	1.29
8	B	1229	CLA	CBB-CAB	3.33	1.51	1.29
8	A	1135	CLA	CBB-CAB	3.33	1.51	1.29
8	A	1124	CLA	CBB-CAB	3.33	1.51	1.29
8	B	1204	CLA	CBB-CAB	3.33	1.51	1.29
8	B	1235	CLA	CBB-CAB	3.33	1.51	1.29
8	A	1110	CLA	CBB-CAB	3.33	1.51	1.29
8	A	1102	CLA	CBB-CAB	3.33	1.51	1.29
8	A	1128	CLA	CBB-CAB	3.33	1.51	1.29
8	B	1223	CLA	CBB-CAB	3.32	1.51	1.29
8	B	1022	CLA	C3B-C2B	-3.32	1.35	1.40
8	A	1133	CLA	CBB-CAB	3.32	1.51	1.29
8	B	1022	CLA	CBB-CAB	3.32	1.51	1.29
8	A	1126	CLA	CBB-CAB	3.32	1.51	1.29
8	A	1123	CLA	CBB-CAB	3.32	1.51	1.29
8	B	1214	CLA	CBB-CAB	3.32	1.51	1.29
8	A	1115	CLA	CBB-CAB	3.32	1.51	1.29
8	B	1021	CLA	CBB-CAB	3.32	1.51	1.29
8	B	1239	CLA	CBB-CAB	3.31	1.51	1.29
8	A	1116	CLA	CBB-CAB	3.31	1.51	1.29
8	B	1201	CLA	CBB-CAB	3.31	1.51	1.29
8	B	1203	CLA	CBB-CAB	3.31	1.51	1.29
8	A	1139	CLA	CBB-CAB	3.29	1.51	1.29
8	A	1129	CLA	C4C-NC	3.29	1.38	1.35
12	B	5002	LMG	C40-C39	-3.28	1.33	1.51
8	A	1104	CLA	C4C-NC	3.28	1.38	1.35
12	B	5002	LMG	C43-C42	-3.28	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1111	CLA	CBB-CAB	3.26	1.50	1.29
8	A	1011	CLA	C4C-NC	3.26	1.38	1.35
12	K	5009	LMG	C37-C36	-3.26	1.33	1.51
12	B	5002	LMG	C19-C18	-3.24	1.33	1.51
12	K	5009	LMG	C43-C42	-3.24	1.33	1.51
12	K	5009	LMG	C40-C39	-3.24	1.33	1.51
12	B	5002	LMG	C37-C36	-3.23	1.33	1.51
8	A	1118	CLA	C4C-NC	3.23	1.38	1.35
8	B	1021	CLA	C3B-C2B	-3.22	1.35	1.40
12	K	5009	LMG	C25-C24	-3.22	1.33	1.51
8	B	1218	CLA	C4C-NC	3.22	1.38	1.35
12	A	5002	LMG	C37-C36	-3.21	1.33	1.51
12	A	5002	LMG	C19-C18	-3.21	1.33	1.51
8	A	1127	CLA	C4C-NC	3.21	1.38	1.35
12	K	5009	LMG	C19-C18	-3.19	1.33	1.51
12	K	5009	LMG	C22-C21	-3.19	1.33	1.51
12	B	5002	LMG	C22-C21	-3.19	1.33	1.51
8	A	1137	CLA	CBB-CAB	3.18	1.50	1.29
12	B	5002	LMG	C25-C24	-3.17	1.33	1.51
12	A	5002	LMG	C43-C42	-3.16	1.33	1.51
12	A	5002	LMG	C40-C39	-3.16	1.33	1.51
8	B	1239	CLA	C3B-C2B	-3.09	1.36	1.40
8	A	1101	CLA	C3B-C2B	-3.04	1.36	1.40
8	B	1227	CLA	C4C-NC	3.03	1.37	1.35
8	A	1012	CLA	C1C-C2C	3.01	1.49	1.42
8	B	1226	CLA	C4C-NC	2.99	1.37	1.35
8	A	1013	CLA	C4C-NC	2.99	1.37	1.35
8	A	1125	CLA	C1C-C2C	2.98	1.49	1.42
8	B	1227	CLA	C3B-C2B	-2.86	1.36	1.40
8	B	1235	CLA	C1C-C2C	2.85	1.49	1.42
8	A	1111	CLA	C3B-C2B	-2.82	1.36	1.40
8	A	1119	CLA	C1C-C2C	2.82	1.48	1.42
8	B	1240	CLA	C1C-C2C	2.79	1.48	1.42
8	B	1229	CLA	C3B-C2B	-2.79	1.36	1.40
8	B	1211	CLA	C1C-C2C	2.77	1.48	1.42
8	B	1201	CLA	C3B-C2B	-2.77	1.36	1.40
8	B	1223	CLA	C1C-C2C	2.77	1.48	1.42
8	A	1133	CLA	C3B-C2B	-2.77	1.36	1.40
8	B	1203	CLA	C3B-C2B	-2.76	1.36	1.40
8	B	1220	CLA	C1C-C2C	2.76	1.48	1.42
8	B	1234	CLA	C1C-C2C	2.75	1.48	1.42
8	B	1203	CLA	C1C-C2C	2.74	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1232	CLA	C1C-C2C	2.74	1.48	1.42
8	A	1130	CLA	C1C-C2C	2.73	1.48	1.42
8	B	1201	CLA	C1C-C2C	2.72	1.48	1.42
8	A	1129	CLA	C3B-C2B	-2.72	1.36	1.40
8	A	1108	CLA	C1C-C2C	2.72	1.48	1.42
8	A	1134	CLA	C1C-C2C	2.71	1.48	1.42
8	A	1105	CLA	C1C-C2C	2.71	1.48	1.42
8	A	1107	CLA	C3B-C2B	-2.71	1.36	1.40
8	B	1218	CLA	C1C-C2C	2.71	1.48	1.42
8	B	1204	CLA	C1C-C2C	2.71	1.48	1.42
8	B	1214	CLA	C1C-C2C	2.70	1.48	1.42
8	B	1216	CLA	C1C-C2C	2.70	1.48	1.42
8	A	1129	CLA	C1C-C2C	2.70	1.48	1.42
8	B	1207	CLA	C1C-C2C	2.70	1.48	1.42
8	A	1114	CLA	C1C-C2C	2.70	1.48	1.42
8	A	1116	CLA	C1C-C2C	2.70	1.48	1.42
8	B	1237	CLA	C1C-C2C	2.70	1.48	1.42
8	A	1126	CLA	C1C-C2C	2.69	1.48	1.42
8	B	1202	CLA	C1C-C2C	2.69	1.48	1.42
8	A	1139	CLA	C1C-C2C	2.69	1.48	1.42
8	B	1222	CLA	C3B-C2B	-2.68	1.36	1.40
8	A	1110	CLA	C3B-C2B	-2.68	1.36	1.40
8	B	1208	CLA	C3B-C2B	-2.68	1.36	1.40
8	B	1221	CLA	C1C-C2C	2.67	1.48	1.42
8	B	1231	CLA	C3B-C2B	-2.67	1.36	1.40
8	A	1140	CLA	C1C-C2C	2.67	1.48	1.42
8	B	1209	CLA	C1C-C2C	2.67	1.48	1.42
8	A	1801	CLA	C1C-C2C	2.67	1.48	1.42
8	A	1128	CLA	C3B-C2B	-2.66	1.36	1.40
8	K	1402	CLA	C1C-C2C	2.66	1.48	1.42
8	B	1219	CLA	C3B-C2B	-2.66	1.36	1.40
8	A	1120	CLA	C1C-C2C	2.66	1.48	1.42
8	A	1124	CLA	C1C-C2C	2.65	1.48	1.42
8	B	1217	CLA	C1C-C2C	2.65	1.48	1.42
8	A	1139	CLA	C3B-C2B	-2.64	1.36	1.40
8	B	1229	CLA	C1C-C2C	2.64	1.48	1.42
8	B	1204	CLA	C3B-C2B	-2.64	1.36	1.40
8	A	1122	CLA	C1C-C2C	2.64	1.48	1.42
8	A	1106	CLA	C1C-C2C	2.64	1.48	1.42
8	B	1212	CLA	C1C-C2C	2.64	1.48	1.42
8	A	1123	CLA	C1C-C2C	2.63	1.48	1.42
8	B	1022	CLA	C1C-C2C	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1134	CLA	C3B-C2B	-2.63	1.36	1.40
8	A	1124	CLA	C3B-C2B	-2.63	1.36	1.40
8	A	1120	CLA	C3B-C2B	-2.63	1.36	1.40
8	B	1208	CLA	C1C-C2C	2.62	1.48	1.42
8	B	1228	CLA	C1C-C2C	2.62	1.48	1.42
8	B	1232	CLA	C3B-C2B	-2.62	1.36	1.40
8	B	1213	CLA	C1C-C2C	2.61	1.48	1.42
8	A	1131	CLA	C1C-C2C	2.61	1.48	1.42
8	A	1115	CLA	C1C-C2C	2.61	1.48	1.42
8	A	1102	CLA	C1C-C2C	2.61	1.48	1.42
8	A	1121	CLA	C3B-C2B	-2.61	1.36	1.40
8	A	1132	CLA	C1C-C2C	2.60	1.48	1.42
8	A	1133	CLA	C1C-C2C	2.60	1.48	1.42
8	A	1102	CLA	C3B-C2B	-2.59	1.36	1.40
8	B	1224	CLA	C1C-C2C	2.59	1.48	1.42
8	A	1011	CLA	C1C-C2C	2.59	1.48	1.42
8	B	1021	CLA	C4C-NC	2.59	1.37	1.35
8	B	1206	CLA	C3B-C2B	-2.58	1.36	1.40
8	A	1104	CLA	C1C-C2C	2.58	1.48	1.42
8	A	1013	CLA	C1C-C2C	2.58	1.48	1.42
8	A	1110	CLA	C1C-C2C	2.58	1.48	1.42
8	A	1136	CLA	C1C-C2C	2.57	1.48	1.42
8	B	1209	CLA	C3B-C2B	-2.57	1.36	1.40
8	A	1109	CLA	C3B-C2B	-2.57	1.36	1.40
8	A	1112	CLA	C1C-C2C	2.57	1.48	1.42
8	B	1205	CLA	C1C-C2C	2.57	1.48	1.42
8	B	1206	CLA	C1C-C2C	2.57	1.48	1.42
8	B	1231	CLA	C1C-C2C	2.56	1.48	1.42
8	A	1140	CLA	C3B-C2B	-2.56	1.36	1.40
8	A	1137	CLA	C1C-C2C	2.56	1.48	1.42
8	B	1223	CLA	C3B-C2B	-2.56	1.36	1.40
8	B	1219	CLA	C1C-C2C	2.55	1.48	1.42
8	A	1136	CLA	C3B-C2B	-2.55	1.36	1.40
8	A	1107	CLA	C1C-C2C	2.55	1.48	1.42
8	A	1118	CLA	C1C-C2C	2.55	1.48	1.42
8	B	1226	CLA	C3B-C2B	-2.55	1.36	1.40
8	B	1230	CLA	C1C-C2C	2.55	1.48	1.42
8	A	1121	CLA	C1C-C2C	2.55	1.48	1.42
8	B	1215	CLA	C1C-C2C	2.54	1.48	1.42
8	B	1230	CLA	C3B-C2B	-2.53	1.36	1.40
8	A	1113	CLA	C1C-C2C	2.53	1.48	1.42
8	A	1104	CLA	C3B-C2B	-2.52	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1023	CLA	C3B-C2B	-2.51	1.36	1.40
8	A	1111	CLA	C1C-C2C	2.51	1.48	1.42
8	B	1210	CLA	C1C-C2C	2.51	1.48	1.42
8	A	1131	CLA	C3B-C2B	-2.50	1.36	1.40
8	A	1127	CLA	C1C-C2C	2.50	1.48	1.42
8	B	1227	CLA	C1C-C2C	2.48	1.48	1.42
8	B	1238	CLA	C1C-C2C	2.48	1.48	1.42
8	A	1138	CLA	C1C-C2C	2.48	1.48	1.42
8	B	1228	CLA	C3B-C2B	-2.47	1.36	1.40
8	A	1114	CLA	C3B-C2B	-2.46	1.37	1.40
8	A	1117	CLA	C1C-C2C	2.45	1.48	1.42
8	B	1236	CLA	C1C-C2C	2.45	1.48	1.42
8	A	1105	CLA	C3B-C2B	-2.45	1.37	1.40
8	B	1239	CLA	C1C-C2C	2.44	1.48	1.42
8	A	1135	CLA	C1C-C2C	2.43	1.48	1.42
8	K	1401	CLA	C1C-C2C	2.43	1.48	1.42
8	B	1205	CLA	C3B-C2B	-2.43	1.37	1.40
8	A	1113	CLA	C3B-C2B	-2.43	1.37	1.40
8	A	1109	CLA	C1C-C2C	2.42	1.48	1.42
8	B	1237	CLA	C3B-C2B	-2.42	1.37	1.40
8	B	1238	CLA	C3B-C2B	-2.41	1.37	1.40
8	A	1132	CLA	C3B-C2B	-2.41	1.37	1.40
8	A	1103	CLA	C3B-C2B	-2.40	1.37	1.40
8	A	1116	CLA	C3B-C2B	-2.40	1.37	1.40
8	K	1401	CLA	C3B-C2B	-2.40	1.37	1.40
8	B	1225	CLA	C1C-C2C	2.40	1.48	1.42
8	B	1222	CLA	C1C-C2C	2.39	1.48	1.42
8	A	1103	CLA	C1C-C2C	2.39	1.48	1.42
8	K	1402	CLA	C3B-C2B	-2.38	1.37	1.40
8	A	1108	CLA	C3B-C2B	-2.38	1.37	1.40
8	A	1122	CLA	C3B-C2B	-2.38	1.37	1.40
8	B	1212	CLA	C3B-C2B	-2.38	1.37	1.40
8	B	1023	CLA	C1C-C2C	2.37	1.47	1.42
8	B	1224	CLA	C3B-C2B	-2.37	1.37	1.40
8	B	1218	CLA	C3B-C2B	-2.37	1.37	1.40
8	B	1210	CLA	C3B-C2B	-2.36	1.37	1.40
8	A	1128	CLA	C1C-C2C	2.35	1.47	1.42
8	A	1138	CLA	C3B-C2B	-2.35	1.37	1.40
8	A	1011	CLA	C3B-C2B	-2.35	1.37	1.40
8	B	1214	CLA	C3B-C2B	-2.35	1.37	1.40
8	B	1220	CLA	C3B-C2B	-2.35	1.37	1.40
8	A	1130	CLA	C3B-C2B	-2.34	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1108	CLA	C1A-CHA	2.34	1.52	1.43
8	B	1206	CLA	C1A-CHA	2.34	1.52	1.43
8	A	1127	CLA	C3B-C2B	-2.33	1.37	1.40
8	B	1236	CLA	C3B-C2B	-2.33	1.37	1.40
8	A	1112	CLA	C3B-C2B	-2.32	1.37	1.40
8	A	1101	CLA	C1C-C2C	2.31	1.47	1.42
8	A	1012	CLA	C3B-C2B	-2.30	1.37	1.40
8	A	1137	CLA	C3B-C2B	-2.30	1.37	1.40
8	A	1118	CLA	C3B-C2B	-2.29	1.37	1.40
8	A	1013	CLA	C1A-CHA	2.28	1.52	1.43
14	B	4006	ECH	C1-C6	-2.27	1.50	1.53
8	B	1213	CLA	C1A-CHA	2.27	1.52	1.43
8	B	1209	CLA	C1A-CHA	2.26	1.52	1.43
8	B	1230	CLA	C1A-CHA	2.25	1.52	1.43
8	A	1102	CLA	C1A-CHA	2.25	1.52	1.43
8	A	1120	CLA	C1A-CHA	2.25	1.52	1.43
8	A	1119	CLA	C3B-C2B	-2.24	1.37	1.40
8	A	1011	CLA	C1A-CHA	2.24	1.52	1.43
8	B	1201	CLA	C1A-CHA	2.24	1.52	1.43
8	B	1220	CLA	C1A-CHA	2.24	1.52	1.43
8	B	1232	CLA	C1A-CHA	2.24	1.52	1.43
8	A	1126	CLA	C3B-C2B	-2.23	1.37	1.40
8	B	1213	CLA	C3B-C2B	-2.22	1.37	1.40
8	B	1225	CLA	C1A-CHA	2.22	1.52	1.43
8	A	1134	CLA	C1A-CHA	2.22	1.52	1.43
8	A	1110	CLA	C1A-CHA	2.22	1.52	1.43
8	A	1127	CLA	C1A-CHA	2.22	1.52	1.43
8	A	1138	CLA	C1A-CHA	2.21	1.52	1.43
8	B	1021	CLA	C1A-CHA	2.21	1.52	1.43
8	A	1123	CLA	C1A-CHA	2.21	1.52	1.43
8	A	1118	CLA	C1A-CHA	2.21	1.52	1.43
8	A	1113	CLA	C1A-CHA	2.21	1.52	1.43
8	A	1132	CLA	C1A-CHA	2.20	1.52	1.43
8	B	1240	CLA	C1A-CHA	2.20	1.52	1.43
8	A	1103	CLA	C1A-CHA	2.20	1.52	1.43
8	B	1208	CLA	C1A-CHA	2.20	1.52	1.43
8	B	1216	CLA	C1A-CHA	2.20	1.52	1.43
8	B	1221	CLA	C1A-CHA	2.20	1.52	1.43
8	A	1121	CLA	C1A-CHA	2.19	1.52	1.43
8	B	1217	CLA	C3B-C2B	-2.19	1.37	1.40
8	A	1122	CLA	C1A-CHA	2.19	1.52	1.43
8	B	1218	CLA	C1A-CHA	2.19	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1226	CLA	C1A-CHA	2.19	1.52	1.43
8	A	1112	CLA	C1A-CHA	2.18	1.52	1.43
8	B	1217	CLA	C1A-CHA	2.18	1.52	1.43
8	A	1105	CLA	C1A-CHA	2.18	1.52	1.43
10	B	4017	BCR	C1-C6	-2.18	1.50	1.53
8	B	1216	CLA	C3B-C2B	-2.18	1.37	1.40
8	A	1801	CLA	C1A-CHA	2.18	1.52	1.43
8	B	1203	CLA	C1A-CHA	2.18	1.52	1.43
8	A	1109	CLA	C1A-CHA	2.17	1.52	1.43
8	K	1402	CLA	C1A-CHA	2.17	1.52	1.43
8	B	1228	CLA	C1A-CHA	2.17	1.52	1.43
8	A	1129	CLA	C1A-CHA	2.16	1.52	1.43
8	A	1119	CLA	C1A-CHA	2.16	1.52	1.43
8	B	1207	CLA	C3B-C2B	-2.16	1.37	1.40
8	A	1126	CLA	C1A-CHA	2.15	1.52	1.43
8	B	1023	CLA	C1A-CHA	2.15	1.52	1.43
8	A	1801	CLA	C3B-C2B	-2.15	1.37	1.40
8	A	1107	CLA	C1A-CHA	2.15	1.52	1.43
8	A	1131	CLA	C1A-CHA	2.15	1.52	1.43
8	B	1215	CLA	C1A-CHA	2.15	1.52	1.43
8	B	1239	CLA	C1A-CHA	2.15	1.52	1.43
8	A	1125	CLA	C1A-CHA	2.14	1.52	1.43
8	A	1135	CLA	C3B-C2B	-2.14	1.37	1.40
8	A	1117	CLA	C1A-CHA	2.14	1.52	1.43
8	A	1113	CLA	C1B-NB	2.14	1.37	1.35
8	A	1106	CLA	C3B-C2B	-2.14	1.37	1.40
8	B	1207	CLA	C1A-CHA	2.13	1.51	1.43
8	A	1116	CLA	C1A-CHA	2.13	1.51	1.43
8	A	1133	CLA	C1A-CHA	2.12	1.51	1.43
8	B	1212	CLA	C1A-CHA	2.12	1.51	1.43
8	B	1210	CLA	C1A-CHA	2.12	1.51	1.43
8	B	1237	CLA	C1A-CHA	2.12	1.51	1.43
8	B	1205	CLA	C1A-CHA	2.12	1.51	1.43
8	A	1111	CLA	C1A-CHA	2.11	1.51	1.43
8	B	1224	CLA	C1A-CHA	2.11	1.51	1.43
8	B	1214	CLA	C1A-CHA	2.11	1.51	1.43
8	A	1124	CLA	C1A-CHA	2.11	1.51	1.43
8	A	1114	CLA	C1A-CHA	2.11	1.51	1.43
8	B	1238	CLA	C1A-CHA	2.10	1.51	1.43
8	A	1140	CLA	C1A-CHA	2.10	1.51	1.43
8	K	1401	CLA	C1A-CHA	2.10	1.51	1.43
8	A	1137	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1222	CLA	C1A-CHA	2.10	1.51	1.43
8	B	1021	CLA	C1C-C2C	2.09	1.47	1.42
8	B	1223	CLA	C1A-CHA	2.09	1.51	1.43
8	A	1136	CLA	C1A-CHA	2.09	1.51	1.43
8	B	1234	CLA	C1A-CHA	2.09	1.51	1.43
8	B	1229	CLA	C1A-CHA	2.09	1.51	1.43
8	A	1101	CLA	C1A-CHA	2.09	1.51	1.43
8	B	1232	CLA	C1B-NB	2.09	1.37	1.35
8	B	1211	CLA	C1A-CHA	2.08	1.51	1.43
8	B	1235	CLA	C1A-CHA	2.08	1.51	1.43
8	B	1231	CLA	C1A-CHA	2.08	1.51	1.43
8	B	1219	CLA	C1A-CHA	2.08	1.51	1.43
8	B	1202	CLA	C3B-C2B	-2.07	1.37	1.40
8	A	1130	CLA	C1A-CHA	2.07	1.51	1.43
8	A	1104	CLA	C1A-CHA	2.07	1.51	1.43
8	B	1227	CLA	C1A-CHA	2.07	1.51	1.43
8	A	1115	CLA	C1A-CHA	2.07	1.51	1.43
8	B	1236	CLA	C1A-CHA	2.06	1.51	1.43
8	K	1401	CLA	C1B-NB	2.06	1.37	1.35
8	B	1204	CLA	C1A-CHA	2.06	1.51	1.43
8	A	1128	CLA	C1A-CHA	2.06	1.51	1.43
8	B	1226	CLA	C1C-C2C	2.06	1.47	1.42
8	A	1106	CLA	C1A-CHA	2.06	1.51	1.43
8	A	1135	CLA	C1A-CHA	2.06	1.51	1.43
8	B	1202	CLA	C1A-CHA	2.05	1.51	1.43
8	A	1012	CLA	C1A-CHA	2.05	1.51	1.43
8	B	1229	CLA	C1B-NB	2.05	1.37	1.35
8	A	1139	CLA	C1A-CHA	2.04	1.51	1.43
8	A	1117	CLA	C3B-C2B	-2.03	1.37	1.40
12	A	5002	LMG	C22-C21	-2.00	1.33	1.49

All (1164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	4017	BCR	C10-C11-C12	18.17	179.92	123.22
10	A	4008	BCR	C10-C11-C12	17.82	178.84	123.22
10	A	4001	BCR	C10-C11-C12	17.71	178.50	123.22
10	B	4011	BCR	C10-C11-C12	17.58	178.09	123.22
10	A	4019	BCR	C10-C11-C12	17.52	177.90	123.22
10	A	4007	BCR	C10-C11-C12	17.46	177.69	123.22
10	K	4001	BCR	C10-C11-C12	17.45	177.68	123.22
10	B	4005	BCR	C10-C11-C12	17.37	177.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	4002	BCR	C10-C11-C12	17.34	177.31	123.22
10	A	4012	BCR	C10-C11-C12	17.31	177.25	123.22
10	B	4014	BCR	C10-C11-C12	17.31	177.24	123.22
10	B	4004	BCR	C10-C11-C12	17.12	176.64	123.22
10	B	4018	BCR	C10-C11-C12	17.10	176.59	123.22
10	B	4010	BCR	C10-C11-C12	16.67	175.25	123.22
10	A	4003	BCR	C10-C11-C12	15.56	171.79	123.22
10	B	4014	BCR	C16-C15-C14	15.21	154.62	123.47
10	B	4017	BCR	C16-C15-C14	14.15	152.46	123.47
10	B	4011	BCR	C16-C15-C14	14.14	152.44	123.47
10	B	4005	BCR	C16-C15-C14	14.09	152.34	123.47
10	B	4004	BCR	C16-C15-C14	13.98	152.11	123.47
10	A	4012	BCR	C11-C10-C9	13.83	147.05	127.31
10	B	4010	BCR	C16-C15-C14	13.67	151.48	123.47
10	A	4019	BCR	C16-C15-C14	13.61	151.35	123.47
10	A	4012	BCR	C21-C20-C19	13.37	164.94	123.22
10	A	4002	BCR	C11-C10-C9	13.34	146.35	127.31
10	A	4001	BCR	C16-C15-C14	13.26	150.64	123.47
10	A	4003	BCR	C16-C15-C14	13.26	150.63	123.47
10	A	4008	BCR	C16-C15-C14	13.18	150.47	123.47
10	A	4002	BCR	C16-C15-C14	13.07	150.25	123.47
10	A	4019	BCR	C11-C10-C9	12.92	145.74	127.31
10	B	4010	BCR	C11-C10-C9	12.86	145.67	127.31
10	K	4001	BCR	C21-C20-C19	12.84	163.29	123.22
10	A	4002	BCR	C21-C20-C19	12.78	163.10	123.22
10	B	4014	BCR	C11-C10-C9	12.77	145.53	127.31
10	B	4010	BCR	C21-C20-C19	12.72	162.92	123.22
10	A	4007	BCR	C16-C15-C14	12.67	149.44	123.47
10	B	4004	BCR	C11-C10-C9	12.60	145.29	127.31
10	A	4001	BCR	C21-C20-C19	12.59	162.52	123.22
10	A	4008	BCR	C21-C20-C19	12.53	162.31	123.22
10	A	4001	BCR	C11-C10-C9	12.48	145.12	127.31
10	A	4007	BCR	C21-C20-C19	12.45	162.07	123.22
10	B	4018	BCR	C11-C10-C9	12.44	145.06	127.31
10	K	4001	BCR	C11-C10-C9	12.34	144.93	127.31
10	B	4004	BCR	C21-C20-C19	12.33	161.68	123.22
10	K	4001	BCR	C16-C15-C14	12.20	148.47	123.47
10	B	4017	BCR	C21-C20-C19	12.13	161.08	123.22
10	A	4003	BCR	C21-C20-C19	12.12	161.03	123.22
10	B	4005	BCR	C11-C10-C9	11.99	144.42	127.31
10	B	4017	BCR	C11-C10-C9	11.96	144.38	127.31
10	B	4011	BCR	C11-C10-C9	11.94	144.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	4005	BCR	C21-C20-C19	11.83	160.12	123.22
10	B	4018	BCR	C16-C15-C14	11.55	147.13	123.47
10	B	4014	BCR	C21-C20-C19	11.43	158.90	123.22
10	A	4012	BCR	C16-C15-C14	11.34	146.71	123.47
10	B	4018	BCR	C11-C12-C13	11.31	158.19	126.42
10	A	4007	BCR	C11-C10-C9	11.30	143.44	127.31
10	B	4005	BCR	C11-C12-C13	10.92	157.09	126.42
10	A	4007	BCR	C11-C12-C13	10.69	156.45	126.42
10	A	4002	BCR	C11-C12-C13	10.63	156.26	126.42
10	B	4017	BCR	C11-C12-C13	10.54	156.02	126.42
10	A	4008	BCR	C11-C12-C13	10.42	155.68	126.42
10	B	4011	BCR	C11-C12-C13	10.38	155.58	126.42
10	A	4019	BCR	C11-C12-C13	10.35	155.49	126.42
10	A	4019	BCR	C20-C19-C18	10.28	155.28	126.42
10	K	4001	BCR	C11-C12-C13	10.21	155.10	126.42
10	B	4004	BCR	C11-C12-C13	10.18	155.03	126.42
8	A	1013	CLA	C4A-NA-C1A	10.10	111.25	106.71
10	A	4001	BCR	C11-C12-C13	10.00	154.52	126.42
10	B	4011	BCR	C21-C20-C19	9.95	154.28	123.22
8	B	1021	CLA	C4A-NA-C1A	9.89	111.15	106.71
10	A	4019	BCR	C21-C20-C19	9.85	153.96	123.22
10	B	4018	BCR	C21-C20-C19	9.78	153.75	123.22
8	A	1011	CLA	C4A-NA-C1A	9.72	111.07	106.71
8	A	1102	CLA	C4A-NA-C1A	9.70	111.07	106.71
10	B	4014	BCR	C11-C12-C13	9.66	153.56	126.42
10	A	4012	BCR	C11-C12-C13	9.60	153.39	126.42
8	B	1205	CLA	C4A-NA-C1A	9.59	111.02	106.71
8	A	1103	CLA	C4A-NA-C1A	9.57	111.01	106.71
8	B	1201	CLA	C4A-NA-C1A	9.56	111.00	106.71
8	A	1113	CLA	C4A-NA-C1A	9.54	111.00	106.71
8	B	1213	CLA	C4A-NA-C1A	9.52	110.99	106.71
8	A	1123	CLA	C4A-NA-C1A	9.52	110.98	106.71
8	A	1120	CLA	C4A-NA-C1A	9.49	110.97	106.71
8	A	1138	CLA	C4A-NA-C1A	9.47	110.97	106.71
8	B	1215	CLA	C4A-NA-C1A	9.44	110.95	106.71
8	B	1209	CLA	C4A-NA-C1A	9.42	110.94	106.71
8	B	1217	CLA	C4A-NA-C1A	9.42	110.94	106.71
8	A	1118	CLA	C4A-NA-C1A	9.40	110.93	106.71
8	B	1226	CLA	C4A-NA-C1A	9.38	110.92	106.71
8	B	1218	CLA	C4A-NA-C1A	9.35	110.91	106.71
8	A	1129	CLA	C4A-NA-C1A	9.34	110.91	106.71
8	B	1230	CLA	C4A-NA-C1A	9.31	110.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1140	CLA	C4A-NA-C1A	9.30	110.89	106.71
8	B	1023	CLA	C4A-NA-C1A	9.29	110.88	106.71
8	B	1240	CLA	C4A-NA-C1A	9.24	110.86	106.71
8	A	1117	CLA	C4A-NA-C1A	9.24	110.86	106.71
8	A	1121	CLA	C4A-NA-C1A	9.24	110.86	106.71
10	A	4008	BCR	C11-C10-C9	9.23	140.49	127.31
8	B	1206	CLA	C4A-NA-C1A	9.23	110.85	106.71
8	A	1112	CLA	C4A-NA-C1A	9.21	110.85	106.71
8	A	1132	CLA	C4A-NA-C1A	9.21	110.84	106.71
8	B	1212	CLA	C4A-NA-C1A	9.18	110.83	106.71
8	B	1220	CLA	C4A-NA-C1A	9.17	110.83	106.71
8	A	1108	CLA	C4A-NA-C1A	9.14	110.81	106.71
8	B	1232	CLA	C4A-NA-C1A	9.13	110.81	106.71
8	B	1208	CLA	C4A-NA-C1A	9.09	110.79	106.71
8	B	1216	CLA	C4A-NA-C1A	9.08	110.79	106.71
8	B	1237	CLA	C4A-NA-C1A	9.07	110.78	106.71
8	K	1401	CLA	C4A-NA-C1A	9.07	110.78	106.71
10	B	4010	BCR	C11-C12-C13	9.07	151.88	126.42
8	A	1131	CLA	C4A-NA-C1A	9.06	110.78	106.71
8	A	1101	CLA	C4A-NA-C1A	9.01	110.75	106.71
8	B	1221	CLA	C4A-NA-C1A	9.00	110.75	106.71
8	A	1139	CLA	C4A-NA-C1A	8.98	110.74	106.71
8	A	1122	CLA	C4A-NA-C1A	8.97	110.74	106.71
8	A	1134	CLA	C4A-NA-C1A	8.97	110.74	106.71
8	A	1104	CLA	C4A-NA-C1A	8.96	110.74	106.71
8	A	1115	CLA	C4A-NA-C1A	8.96	110.73	106.71
10	A	4003	BCR	C11-C12-C13	8.95	151.55	126.42
8	B	1239	CLA	C4A-NA-C1A	8.93	110.72	106.71
8	B	1229	CLA	C4A-NA-C1A	8.91	110.71	106.71
8	A	1135	CLA	C4A-NA-C1A	8.91	110.71	106.71
8	A	1106	CLA	C4A-NA-C1A	8.89	110.70	106.71
8	A	1105	CLA	C4A-NA-C1A	8.87	110.69	106.71
8	A	1109	CLA	C4A-NA-C1A	8.85	110.68	106.71
8	K	1402	CLA	C4A-NA-C1A	8.85	110.68	106.71
8	A	1107	CLA	C4A-NA-C1A	8.85	110.68	106.71
8	A	1114	CLA	C4A-NA-C1A	8.84	110.68	106.71
8	B	1223	CLA	C4A-NA-C1A	8.83	110.68	106.71
8	B	1211	CLA	C4A-NA-C1A	8.83	110.67	106.71
8	A	1110	CLA	C4A-NA-C1A	8.80	110.66	106.71
8	B	1238	CLA	C4A-NA-C1A	8.80	110.66	106.71
8	B	1222	CLA	C4A-NA-C1A	8.80	110.66	106.71
10	B	4014	BCR	C20-C19-C18	8.78	151.09	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1136	CLA	C4A-NA-C1A	8.78	110.66	106.71
8	B	1225	CLA	C4A-NA-C1A	8.78	110.66	106.71
8	A	1124	CLA	C4A-NA-C1A	8.75	110.64	106.71
8	A	1801	CLA	C4A-NA-C1A	8.74	110.64	106.71
8	A	1111	CLA	C4A-NA-C1A	8.74	110.64	106.71
8	B	1214	CLA	C4A-NA-C1A	8.74	110.64	106.71
8	B	1219	CLA	C4A-NA-C1A	8.72	110.63	106.71
8	A	1128	CLA	C4A-NA-C1A	8.70	110.62	106.71
8	B	1231	CLA	C4A-NA-C1A	8.69	110.61	106.71
8	A	1119	CLA	C4A-NA-C1A	8.69	110.61	106.71
8	B	1203	CLA	C4A-NA-C1A	8.68	110.61	106.71
8	A	1126	CLA	C4A-NA-C1A	8.63	110.59	106.71
8	A	1127	CLA	C4A-NA-C1A	8.58	110.56	106.71
10	A	4003	BCR	C11-C10-C9	8.57	139.54	127.31
8	B	1204	CLA	C4A-NA-C1A	8.56	110.55	106.71
8	A	1137	CLA	C4A-NA-C1A	8.55	110.55	106.71
8	A	1133	CLA	C4A-NA-C1A	8.55	110.55	106.71
8	B	1207	CLA	C4A-NA-C1A	8.55	110.55	106.71
8	B	1202	CLA	C4A-NA-C1A	8.52	110.54	106.71
8	B	1210	CLA	C4A-NA-C1A	8.52	110.53	106.71
8	A	1130	CLA	C4A-NA-C1A	8.48	110.52	106.71
8	B	1234	CLA	C4A-NA-C1A	8.47	110.52	106.71
8	B	1236	CLA	C4A-NA-C1A	8.38	110.47	106.71
8	B	1235	CLA	C4A-NA-C1A	8.35	110.46	106.71
8	B	1228	CLA	C4A-NA-C1A	8.30	110.44	106.71
8	A	1125	CLA	C4A-NA-C1A	8.21	110.40	106.71
8	A	1116	CLA	C4A-NA-C1A	8.15	110.37	106.71
8	B	1227	CLA	C4A-NA-C1A	8.06	110.33	106.71
8	B	1224	CLA	C4A-NA-C1A	8.04	110.32	106.71
8	A	1012	CLA	C4A-NA-C1A	8.03	110.31	106.71
8	B	1022	CLA	C4A-NA-C1A	7.91	110.26	106.71
10	B	4005	BCR	C20-C19-C18	7.76	148.20	126.42
10	B	4017	BCR	C20-C19-C18	7.74	148.16	126.42
10	A	4003	BCR	C20-C19-C18	7.41	147.24	126.42
10	A	4001	BCR	C20-C19-C18	7.32	146.98	126.42
10	A	4007	BCR	C20-C19-C18	7.30	146.93	126.42
10	B	4004	BCR	C20-C19-C18	7.30	146.91	126.42
10	A	4008	BCR	C20-C19-C18	7.28	146.87	126.42
10	B	4010	BCR	C20-C19-C18	7.17	146.55	126.42
10	A	4002	BCR	C20-C19-C18	6.90	145.79	126.42
10	K	4001	BCR	C20-C19-C18	6.84	145.64	126.42
8	B	1206	CLA	O2D-CGD-CBD	6.65	123.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	4012	BCR	C20-C19-C18	6.53	144.76	126.42
8	B	1213	CLA	O2D-CGD-CBD	6.33	122.51	111.27
14	B	4006	ECH	C20-C21-C22	-6.30	118.32	127.31
14	M	4021	ECH	C20-C21-C22	-6.21	118.45	127.31
8	A	1123	CLA	O2D-CGD-CBD	6.20	122.29	111.27
8	B	1237	CLA	O2A-C1-C2	6.14	124.78	108.64
8	A	1110	CLA	O2D-CGD-CBD	6.10	122.11	111.27
14	B	4006	ECH	C16-C17-C18	-6.10	118.61	127.31
8	A	1102	CLA	O2D-CGD-CBD	6.06	122.03	111.27
10	B	4018	BCR	C20-C19-C18	6.04	143.38	126.42
8	A	1122	CLA	O2D-CGD-CBD	5.96	121.86	111.27
10	B	4011	BCR	C20-C19-C18	5.94	143.10	126.42
8	B	1230	CLA	O2D-CGD-CBD	5.89	121.74	111.27
8	A	1138	CLA	O2A-C1-C2	5.89	124.11	108.64
8	B	1226	CLA	O2A-C1-C2	5.88	124.09	108.64
8	A	1126	CLA	O2A-C1-C2	5.88	124.08	108.64
8	A	1134	CLA	O2D-CGD-CBD	5.87	121.70	111.27
8	B	1209	CLA	O2D-CGD-CBD	5.86	121.68	111.27
8	B	1210	CLA	O2A-C1-C2	5.85	124.00	108.64
8	B	1240	CLA	O2D-CGD-CBD	5.82	121.61	111.27
14	M	4021	ECH	C15-C14-C13	-5.78	119.06	127.31
14	B	4006	ECH	C11-C10-C9	-5.78	119.07	127.31
8	A	1117	CLA	O2A-C1-C2	5.77	123.79	108.64
8	B	1221	CLA	O2D-CGD-CBD	5.73	121.46	111.27
8	B	1226	CLA	O2D-CGD-CBD	5.71	121.42	111.27
8	A	1128	CLA	O2A-C1-C2	5.69	123.60	108.64
8	A	1111	CLA	O2D-CGD-CBD	5.62	121.26	111.27
10	B	4014	BCR	C15-C14-C13	-5.62	119.29	127.31
8	B	1230	CLA	O2A-C1-C2	5.60	123.34	108.64
8	B	1231	CLA	O2A-C1-C2	5.58	123.29	108.64
8	B	1234	CLA	O2D-CGD-CBD	5.57	121.16	111.27
8	B	1234	CLA	O2A-C1-C2	5.54	123.19	108.64
8	A	1129	CLA	O2D-CGD-CBD	5.51	121.06	111.27
8	B	1215	CLA	O2D-CGD-CBD	5.51	121.06	111.27
8	B	1222	CLA	O2A-C1-C2	5.50	123.10	108.64
8	B	1222	CLA	O2D-CGD-CBD	5.50	121.04	111.27
8	B	1228	CLA	O2A-C1-C2	5.49	123.05	108.64
8	A	1128	CLA	O2D-CGD-CBD	5.48	121.00	111.27
8	B	1229	CLA	O2D-CGD-CBD	5.47	120.99	111.27
8	A	1109	CLA	O2A-C1-C2	5.47	123.01	108.64
8	B	1235	CLA	O2D-CGD-CBD	5.46	120.97	111.27
8	K	1402	CLA	O2D-CGD-CBD	5.45	120.95	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1205	CLA	O2A-C1-C2	5.42	122.88	108.64
8	B	1238	CLA	O2A-C1-C2	5.40	122.83	108.64
8	K	1401	CLA	O2D-CGD-CBD	5.38	120.83	111.27
8	A	1127	CLA	O2A-C1-C2	5.38	122.77	108.64
8	A	1120	CLA	O2A-C1-C2	5.37	121.52	108.97
8	B	1239	CLA	O2D-CGD-CBD	5.36	120.80	111.27
8	B	1021	CLA	O2A-C1-C2	5.35	122.71	108.64
8	B	1204	CLA	O2D-CGD-CBD	5.35	120.78	111.27
8	B	1210	CLA	O2D-CGD-CBD	5.34	120.76	111.27
8	A	1121	CLA	O2A-C1-C2	5.34	122.67	108.64
8	B	1023	CLA	O2A-C1-C2	5.33	122.63	108.64
8	B	1224	CLA	O2D-CGD-CBD	5.33	120.73	111.27
8	A	1104	CLA	O2A-C1-C2	5.32	122.63	108.64
8	A	1135	CLA	O2D-CGD-CBD	5.31	120.70	111.27
8	B	1205	CLA	O2D-CGD-CBD	5.30	120.69	111.27
8	B	1232	CLA	O2A-C1-C2	5.29	122.53	108.64
8	K	1401	CLA	O2A-C1-C2	5.28	122.50	108.64
8	A	1125	CLA	O2D-CGD-CBD	5.27	120.63	111.27
8	A	1106	CLA	O2D-CGD-CBD	5.27	120.63	111.27
8	B	1212	CLA	O2D-CGD-CBD	5.26	120.61	111.27
8	A	1101	CLA	O2D-CGD-CBD	5.26	120.61	111.27
8	A	1117	CLA	O2D-CGD-CBD	5.26	120.61	111.27
8	B	1207	CLA	O2D-CGD-CBD	5.25	120.60	111.27
8	A	1110	CLA	O2A-C1-C2	5.24	122.42	108.64
8	A	1133	CLA	O2A-C1-C2	5.22	122.37	108.64
8	B	1223	CLA	O2A-C1-C2	5.22	122.36	108.64
8	A	1135	CLA	O2A-C1-C2	5.22	122.35	108.64
8	A	1124	CLA	O2A-C1-C2	5.22	122.34	108.64
8	B	1021	CLA	O2D-CGD-CBD	5.21	120.53	111.27
8	B	1214	CLA	O2D-CGD-CBD	5.21	120.52	111.27
8	A	1013	CLA	O2A-C1-C2	5.20	122.31	108.64
8	B	1220	CLA	O2A-C1-C2	5.20	122.30	108.64
8	A	1136	CLA	O2D-CGD-CBD	5.18	120.48	111.27
8	B	1213	CLA	O2A-C1-C2	5.18	122.25	108.64
8	A	1114	CLA	O2D-CGD-CBD	5.18	120.47	111.27
8	A	1122	CLA	O2A-C1-C2	5.18	122.24	108.64
8	A	1107	CLA	O2A-C1-C2	5.17	122.23	108.64
8	B	1219	CLA	O2D-CGD-CBD	5.17	120.45	111.27
8	A	1136	CLA	O2A-C1-C2	5.17	122.21	108.64
8	B	1237	CLA	O2D-CGD-CBD	5.16	120.44	111.27
8	B	1224	CLA	O2A-C1-C2	5.16	122.20	108.64
8	A	1139	CLA	O2D-CGD-CBD	5.16	120.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1119	CLA	O2A-C1-C2	5.14	122.15	108.64
8	A	1012	CLA	O2A-C1-C2	5.13	122.13	108.64
8	A	1130	CLA	O2A-C1-C2	5.13	122.12	108.64
8	A	1111	CLA	O2A-C1-C2	5.12	122.10	108.64
8	B	1219	CLA	O2A-C1-C2	5.12	122.10	108.64
8	A	1107	CLA	O2D-CGD-CBD	5.12	120.36	111.27
8	B	1216	CLA	O2A-C1-C2	5.12	122.09	108.64
8	A	1116	CLA	O2D-CGD-CBD	5.10	120.34	111.27
8	B	1225	CLA	O2A-C1-C2	5.10	122.04	108.64
8	A	1102	CLA	O2A-C1-C2	5.08	121.99	108.64
8	B	1215	CLA	O2A-C1-C2	5.08	121.97	108.64
8	B	1217	CLA	O2A-C1-C2	5.07	121.96	108.64
8	B	1217	CLA	O2D-CGD-CBD	5.06	120.27	111.27
8	B	1238	CLA	O2D-CGD-CBD	5.05	120.24	111.27
8	A	1105	CLA	O2A-C1-C2	5.04	121.89	108.64
8	B	1206	CLA	O2A-C1-C2	5.03	121.86	108.64
8	A	1140	CLA	O2D-CGD-CBD	5.03	120.21	111.27
8	B	1218	CLA	O2A-C1-C2	5.03	121.84	108.64
8	A	1112	CLA	O2A-C1-C2	5.02	121.84	108.64
8	A	1123	CLA	O2A-C1-C2	5.02	121.83	108.64
10	B	4010	BCR	C15-C14-C13	-5.02	120.15	127.31
14	M	4021	ECH	C16-C17-C18	-5.01	120.16	127.31
8	B	1220	CLA	O2D-CGD-CBD	5.01	120.17	111.27
8	A	1133	CLA	O2D-CGD-CBD	5.01	120.17	111.27
8	A	1130	CLA	O2D-CGD-CBD	5.01	120.17	111.27
8	A	1137	CLA	O2A-C1-C2	5.00	121.78	108.64
8	A	1140	CLA	O2A-C1-C2	5.00	121.78	108.64
8	A	1121	CLA	O2D-CGD-CBD	4.99	120.13	111.27
8	A	1115	CLA	O2D-CGD-CBD	4.99	120.13	111.27
8	B	1203	CLA	O2A-C1-C2	4.98	121.73	108.64
8	B	1229	CLA	O2A-C1-C2	4.98	121.72	108.64
8	B	1023	CLA	O2D-CGD-CBD	4.96	120.09	111.27
8	B	1225	CLA	O2D-CGD-CBD	4.96	120.08	111.27
8	B	1214	CLA	O2A-C1-C2	4.96	121.66	108.64
8	A	1116	CLA	O2A-C1-C2	4.94	121.62	108.64
8	A	1104	CLA	O2D-CGD-CBD	4.93	120.03	111.27
8	B	1236	CLA	O2D-CGD-CBD	4.92	120.01	111.27
8	A	1113	CLA	O2D-CGD-CBD	4.92	120.01	111.27
8	B	1235	CLA	O2A-C1-C2	4.92	121.56	108.64
8	A	1126	CLA	O2D-CGD-CBD	4.91	120.00	111.27
8	A	1138	CLA	O2D-CGD-CBD	4.91	120.00	111.27
8	B	1228	CLA	O2D-CGD-CBD	4.91	120.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1231	CLA	O2D-CGD-CBD	4.90	119.97	111.27
8	A	1101	CLA	O2A-C1-C2	4.87	121.44	108.64
8	B	1218	CLA	O2D-CGD-CBD	4.87	119.92	111.27
8	A	1011	CLA	O2D-CGD-CBD	4.86	119.91	111.27
8	A	1137	CLA	O2D-CGD-CBD	4.86	119.90	111.27
8	A	1131	CLA	O2D-CGD-CBD	4.84	119.87	111.27
8	B	1209	CLA	O2A-C1-C2	4.83	121.34	108.64
8	A	1124	CLA	O2D-CGD-CBD	4.83	119.84	111.27
8	A	1013	CLA	O2D-CGD-CBD	4.83	119.84	111.27
8	A	1120	CLA	O2D-CGD-CBD	4.82	119.84	111.27
8	A	1131	CLA	O2A-C1-C2	4.82	121.31	108.64
8	B	1202	CLA	O2A-C1-C2	4.82	121.29	108.64
8	B	1240	CLA	O2A-C1-C2	4.81	121.27	108.64
8	A	1103	CLA	O2D-CGD-CBD	4.80	119.80	111.27
8	A	1132	CLA	O2D-CGD-CBD	4.80	119.80	111.27
8	B	1239	CLA	O2A-C1-C2	4.79	121.21	108.64
8	B	1207	CLA	O2A-C1-C2	4.78	121.20	108.64
8	A	1125	CLA	O2A-C1-C2	4.78	121.20	108.64
8	A	1801	CLA	O2D-CGD-CBD	4.78	119.76	111.27
8	A	1011	CLA	O2A-C1-C2	4.77	121.17	108.64
8	A	1106	CLA	O2A-C1-C2	4.75	121.11	108.64
8	B	1202	CLA	O2D-CGD-CBD	4.72	119.66	111.27
8	B	1022	CLA	O2A-C1-C2	4.72	121.04	108.64
8	A	1112	CLA	O2D-CGD-CBD	4.72	119.65	111.27
8	B	1216	CLA	O2D-CGD-CBD	4.71	119.63	111.27
8	A	1132	CLA	O2A-C1-C2	4.70	120.97	108.64
8	A	1105	CLA	O2D-CGD-CBD	4.69	119.61	111.27
8	A	1108	CLA	O2D-CGD-CBD	4.69	119.60	111.27
10	B	4011	BCR	C34-C9-C10	-4.68	116.37	122.92
8	A	1109	CLA	O2D-CGD-CBD	4.67	119.56	111.27
8	B	1201	CLA	O2D-CGD-CBD	4.65	119.54	111.27
8	A	1103	CLA	O2A-C1-C2	4.65	120.85	108.64
14	B	4006	ECH	C33-C5-C6	-4.63	119.33	124.53
8	B	1221	CLA	O2A-C1-C2	4.62	120.78	108.64
8	B	1203	CLA	O2D-CGD-CBD	4.60	119.44	111.27
8	A	1012	CLA	O2D-CGD-CBD	4.60	119.44	111.27
8	B	1223	CLA	O2D-CGD-CBD	4.58	119.41	111.27
8	A	1118	CLA	O2D-CGD-CBD	4.55	119.36	111.27
8	B	1227	CLA	O2D-CGD-CBD	4.55	119.35	111.27
8	B	1022	CLA	O2D-CGD-CBD	4.54	119.33	111.27
14	M	4021	ECH	C24-C23-C22	-4.53	119.39	126.23
8	K	1402	CLA	O2A-C1-C2	4.52	120.52	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1236	CLA	O2A-C1-C2	4.50	120.46	108.64
8	B	1227	CLA	O2A-C1-C2	4.50	120.46	108.64
8	A	1119	CLA	O2D-CGD-CBD	4.46	119.19	111.27
8	B	1232	CLA	O2D-CGD-CBD	4.43	119.15	111.27
8	B	1208	CLA	O2D-CGD-CBD	4.39	119.07	111.27
8	A	1125	CLA	OBD-CAD-C3D	-4.39	120.70	127.98
10	B	4017	BCR	C33-C5-C4	4.36	122.00	113.62
10	B	4011	BCR	C15-C14-C13	-4.36	121.09	127.31
10	B	4011	BCR	C34-C9-C8	4.31	124.87	118.08
8	A	1127	CLA	O2D-CGD-CBD	4.31	118.93	111.27
12	A	5002	LMG	O7-C10-C11	4.25	120.67	111.50
14	B	4006	ECH	C24-C23-C22	-4.18	119.92	126.23
10	A	4008	BCR	C15-C14-C13	-4.15	121.39	127.31
12	K	5009	LMG	O7-C10-C11	4.14	120.42	111.50
11	A	5001	LHG	O7-C7-C8	4.12	120.37	111.50
11	M	5001	LHG	O7-C7-C8	4.09	120.33	111.50
11	B	5006	LHG	O7-C7-C8	4.09	120.32	111.50
8	B	1211	CLA	O2D-CGD-CBD	4.03	118.42	111.27
11	A	5003	LHG	O7-C7-C8	4.02	120.16	111.50
12	B	5005	LMG	O7-C10-C11	3.99	120.11	111.50
10	B	4017	BCR	C33-C5-C6	-3.97	120.06	124.53
8	B	1021	CLA	CMC-C2C-C3C	3.96	132.42	124.94
10	B	4018	BCR	C19-C18-C17	3.92	124.96	118.94
10	B	4004	BCR	C15-C14-C13	-3.91	121.73	127.31
8	B	1022	CLA	OBD-CAD-C3D	-3.89	121.52	127.98
10	A	4019	BCR	C15-C14-C13	-3.87	121.78	127.31
10	B	4017	BCR	C1-C6-C5	-3.82	117.24	122.61
11	B	5004	LHG	O7-C7-C8	3.81	119.72	111.50
10	B	4010	BCR	C28-C27-C26	-3.78	107.32	114.08
8	A	1117	CLA	O2A-CGA-CBA	3.78	123.78	111.91
10	B	4011	BCR	C33-C5-C6	-3.76	120.30	124.53
10	B	4018	BCR	C36-C18-C17	-3.76	117.65	122.92
14	M	4021	ECH	C7-C8-C9	-3.74	120.59	126.23
8	B	1235	CLA	CMB-C2B-C3B	3.72	131.64	124.68
8	A	1139	CLA	CMA-C3A-C4A	3.72	121.78	111.77
10	A	4007	BCR	C33-C5-C6	-3.68	120.40	124.53
10	B	4017	BCR	C15-C14-C13	-3.68	122.06	127.31
8	B	1215	CLA	C1-C2-C3	-3.67	119.69	126.04
10	A	4012	BCR	C33-C5-C6	-3.66	120.42	124.53
12	B	5002	LMG	O7-C10-C11	3.66	119.38	111.50
14	B	4006	ECH	C16-C15-C14	-3.65	116.00	123.47
8	B	1234	CLA	CMB-C2B-C3B	3.64	131.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1013	CLA	CMB-C2B-C3B	3.64	131.48	124.68
8	A	1107	CLA	C1-C2-C3	-3.63	120.88	126.75
10	A	4008	BCR	C34-C9-C10	-3.62	117.85	122.92
10	A	4012	BCR	C19-C18-C17	3.61	124.48	118.94
10	A	4001	BCR	C15-C14-C13	-3.61	122.16	127.31
10	A	4007	BCR	C33-C5-C4	3.60	120.53	113.62
10	B	4005	BCR	C23-C24-C25	-3.58	117.15	127.20
8	A	1128	CLA	C1-C2-C3	-3.55	119.91	126.04
8	A	1122	CLA	C1-C2-C3	-3.52	119.95	126.04
8	B	1226	CLA	C1-C2-C3	-3.51	119.97	126.04
10	B	4005	BCR	C15-C14-C13	-3.50	122.31	127.31
10	B	4014	BCR	C37-C22-C21	-3.46	118.08	122.92
8	B	1225	CLA	CMB-C2B-C3B	3.46	131.14	124.68
8	B	1218	CLA	C1-C2-C3	-3.45	121.17	126.75
14	M	4021	ECH	C33-C5-C6	-3.45	120.65	124.53
10	B	4010	BCR	C33-C5-C6	-3.45	120.66	124.53
10	B	4018	BCR	C27-C26-C25	-3.44	117.73	122.73
15	B	5008	SQD	O7-S-C6	-3.43	102.86	106.94
8	B	1222	CLA	C1-C2-C3	-3.43	120.11	126.04
8	B	1232	CLA	C1-C2-C3	-3.43	121.21	126.75
8	B	1236	CLA	C1-C2-C3	-3.42	121.21	126.75
8	A	1133	CLA	C1-C2-C3	-3.42	120.13	126.04
8	A	1115	CLA	CMB-C2B-C3B	3.41	131.06	124.68
8	A	1121	CLA	C1-C2-C3	-3.41	121.24	126.75
8	B	1234	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
8	A	1105	CLA	C1-C2-C3	-3.40	121.25	126.75
8	A	1104	CLA	C1-C2-C3	-3.38	120.19	126.04
8	B	1235	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
10	A	4012	BCR	C36-C18-C17	-3.37	118.20	122.92
11	B	5006	LHG	O8-C23-C24	3.34	120.14	111.38
8	B	1234	CLA	CMA-C3A-C4A	3.33	120.73	111.77
10	B	4010	BCR	C33-C5-C4	3.33	120.02	113.62
8	A	1111	CLA	C1-C2-C3	-3.31	120.31	126.04
8	A	1013	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
10	B	4017	BCR	C4-C5-C6	-3.30	117.94	122.73
14	B	4006	ECH	C28-C27-C26	-3.30	115.61	118.65
8	A	1126	CLA	CMB-C2B-C3B	3.28	130.81	124.68
14	M	4021	ECH	C20-C19-C18	-3.27	117.23	126.42
10	A	4012	BCR	C37-C22-C21	-3.27	118.35	122.92
8	A	1121	CLA	CMA-C3A-C4A	3.26	120.54	111.77
8	A	1120	CLA	CMA-C3A-C4A	3.26	120.53	111.77
8	A	1135	CLA	C1-C2-C3	-3.25	120.43	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1224	CLA	CMB-C2B-C3B	3.24	130.75	124.68
10	B	4004	BCR	C33-C5-C6	-3.24	120.89	124.53
8	B	1234	CLA	C1-C2-C3	-3.22	120.47	126.04
14	M	4021	ECH	C28-C27-C26	-3.22	115.68	118.65
8	B	1225	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
8	A	1124	CLA	CMA-C3A-C4A	3.21	120.40	111.77
8	B	1224	CLA	C1-C2-C3	-3.20	120.51	126.04
8	A	1113	CLA	CMA-C3A-C4A	3.20	120.36	111.77
10	B	4018	BCR	C33-C5-C6	-3.20	120.94	124.53
10	B	4018	BCR	C33-C5-C4	3.19	119.75	113.62
8	B	1223	CLA	OBD-CAD-C3D	-3.19	122.68	127.98
8	A	1114	CLA	CMA-C3A-C4A	3.18	120.33	111.77
8	A	1011	CLA	C1-C2-C3	-3.18	120.54	126.04
8	A	1136	CLA	C1-C2-C3	-3.18	120.55	126.04
9	B	2002	PQN	C11-C12-C13	-3.17	121.51	126.79
8	B	1213	CLA	C1-C2-C3	-3.16	120.57	126.04
8	B	1215	CLA	CMB-C2B-C3B	3.16	130.58	124.68
8	B	1206	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
8	A	1106	CLA	C1-C2-C3	-3.14	120.60	126.04
8	B	1202	CLA	C1-C2-C3	-3.14	120.61	126.04
10	A	4001	BCR	C33-C5-C6	-3.14	121.00	124.53
10	A	4012	BCR	C33-C5-C4	3.14	119.64	113.62
8	A	1127	CLA	C1-C2-C3	-3.14	120.62	126.04
8	B	1216	CLA	CMA-C3A-C4A	3.13	120.19	111.77
8	B	1237	CLA	C1-C2-C3	-3.12	120.65	126.04
8	B	1223	CLA	C1-C2-C3	-3.11	120.66	126.04
8	K	1402	CLA	CMA-C3A-C4A	3.11	120.13	111.77
8	A	1137	CLA	C1-C2-C3	-3.10	121.73	126.75
8	A	1140	CLA	CMA-C3A-C4A	3.10	120.10	111.77
8	B	1211	CLA	CMB-C2B-C3B	3.09	130.46	124.68
10	A	4003	BCR	C33-C5-C4	3.08	119.53	113.62
10	A	4001	BCR	C33-C5-C4	3.07	119.52	113.62
8	A	1126	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
8	A	1116	CLA	C1-C2-C3	-3.07	120.74	126.04
8	A	1132	CLA	C1-C2-C3	-3.06	121.80	126.75
8	A	1101	CLA	CMA-C3A-C4A	3.06	119.99	111.77
8	B	1230	CLA	CMA-C3A-C4A	3.06	119.99	111.77
8	A	1126	CLA	CMA-C3A-C4A	3.05	119.96	111.77
8	A	1102	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
8	B	1217	CLA	CMA-C3A-C4A	3.04	119.95	111.77
8	B	1209	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
8	A	1123	CLA	CMA-C3A-C4A	3.04	119.95	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1131	CLA	CMA-C3A-C4A	3.04	119.94	111.77
8	A	1110	CLA	C1-C2-C3	-3.04	120.79	126.04
10	A	4019	BCR	C33-C5-C6	-3.03	121.12	124.53
8	B	1210	CLA	C1-C2-C3	-3.03	120.80	126.04
14	B	4006	ECH	C11-C12-C13	-3.03	117.91	126.42
8	A	1126	CLA	C1-C2-C3	-3.03	120.80	126.04
8	B	1213	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	B	4006	ECH	C7-C8-C9	-3.02	121.67	126.23
8	B	1237	CLA	CMA-C3A-C4A	3.01	119.88	111.77
8	A	1801	CLA	CMA-C3A-C4A	3.01	119.87	111.77
8	B	1219	CLA	CMA-C3A-C4A	3.01	119.87	111.77
8	B	1220	CLA	CMA-C3A-C4A	3.01	119.87	111.77
8	B	1225	CLA	CMC-C2C-C3C	3.01	130.62	124.94
8	B	1223	CLA	CMA-C3A-C4A	3.01	119.85	111.77
8	B	1205	CLA	CMA-C3A-C4A	3.00	119.85	111.77
8	A	1132	CLA	CMA-C3A-C4A	3.00	119.85	111.77
8	B	1238	CLA	CMA-C3A-C4A	3.00	119.84	111.77
8	B	1237	CLA	C1-O2A-CGA	3.00	124.32	116.44
9	B	2002	PQN	C14-C13-C15	3.00	120.31	115.27
8	B	1235	CLA	C1-C2-C3	-3.00	120.86	126.04
8	A	1117	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
8	A	1127	CLA	CMA-C3A-C4A	2.98	119.79	111.77
10	A	4003	BCR	C33-C5-C6	-2.98	121.18	124.53
8	B	1204	CLA	CMA-C3A-C4A	2.98	119.78	111.77
10	B	4017	BCR	C38-C26-C25	-2.97	121.19	124.53
8	B	1225	CLA	CMA-C3A-C4A	2.97	119.77	111.77
8	A	1124	CLA	C1-C2-C3	-2.97	120.90	126.04
14	B	4006	ECH	C20-C19-C18	-2.97	118.07	126.42
8	A	1134	CLA	CMA-C3A-C4A	2.97	119.75	111.77
10	B	4014	BCR	C33-C5-C4	2.96	119.31	113.62
8	A	1013	CLA	C1-O2A-CGA	2.96	124.22	116.44
8	A	1127	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
8	B	1213	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
10	A	4001	BCR	C36-C18-C17	-2.95	118.79	122.92
8	B	1224	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
8	B	1201	CLA	CMA-C3A-C4A	2.95	119.69	111.77
8	B	1237	CLA	O2A-CGA-CBA	2.95	121.15	111.91
8	B	1240	CLA	CMA-C3A-C4A	2.94	119.69	111.77
8	A	1138	CLA	CMA-C3A-C4A	2.94	119.68	111.77
8	A	1117	CLA	CMA-C3A-C4A	2.94	119.67	111.77
8	A	1115	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
8	A	1127	CLA	CMB-C2B-C3B	2.93	130.17	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1801	CLA	CMC-C2C-C3C	2.93	130.47	124.94
8	A	1119	CLA	C1-C2-C3	-2.93	120.97	126.04
8	B	1221	CLA	CMB-C2B-C3B	2.93	130.16	124.68
10	A	4003	BCR	C15-C14-C13	-2.92	123.14	127.31
8	A	1110	CLA	CMA-C3A-C4A	2.91	119.61	111.77
10	B	4011	BCR	C33-C5-C4	2.91	119.21	113.62
8	A	1135	CLA	CMA-C3A-C4A	2.91	119.61	111.77
8	B	1023	CLA	O2A-CGA-CBA	2.91	121.05	111.91
10	A	4002	BCR	C36-C18-C17	-2.91	118.84	122.92
8	A	1109	CLA	CMA-C3A-C4A	2.91	119.59	111.77
10	B	4018	BCR	C30-C25-C26	-2.91	118.52	122.61
8	A	1012	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
8	A	1130	CLA	CMA-C3A-C4A	2.89	119.55	111.77
10	K	4001	BCR	C36-C18-C17	-2.89	118.87	122.92
8	A	1123	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
8	A	1112	CLA	CMA-C3A-C4A	2.89	119.53	111.77
8	A	1129	CLA	CMA-C3A-C4A	2.89	119.53	111.77
8	A	1136	CLA	CMA-C3A-C4A	2.88	119.53	111.77
8	A	1140	CLA	C1-C2-C3	-2.88	121.06	126.04
8	A	1122	CLA	CMA-C3A-C4A	2.88	119.51	111.77
8	A	1011	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
8	B	1022	CLA	OBD-CAD-CBD	-2.88	121.79	125.89
8	B	1212	CLA	CMA-C3A-C4A	2.87	119.48	111.77
8	A	1012	CLA	CMB-C2B-C3B	2.86	130.04	124.68
8	B	1239	CLA	CMA-C3A-C4A	2.86	119.47	111.77
8	A	1119	CLA	CMA-C3A-C4A	2.86	119.47	111.77
12	B	5002	LMG	O8-C28-C29	2.86	120.89	111.91
10	B	4005	BCR	C33-C5-C6	-2.86	121.32	124.53
8	B	1210	CLA	O2A-CGA-CBA	2.86	120.88	111.91
8	B	1201	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
8	A	1102	CLA	C1-C2-C3	-2.86	121.11	126.04
10	A	4019	BCR	C33-C5-C4	2.85	119.10	113.62
10	A	4002	BCR	C27-C26-C25	-2.85	118.59	122.73
14	M	4021	ECH	C23-C24-C25	-2.85	119.21	127.20
10	A	4003	BCR	C36-C18-C17	-2.84	118.94	122.92
8	A	1138	CLA	C1-C2-C3	-2.84	121.13	126.04
8	B	1218	CLA	CMA-C3A-C4A	2.84	119.41	111.77
8	B	1213	CLA	CMA-C3A-C4A	2.84	119.40	111.77
10	B	4010	BCR	C27-C26-C25	-2.83	118.62	122.73
8	A	1128	CLA	CMA-C3A-C4A	2.83	119.37	111.77
8	A	1013	CLA	C1-C2-C3	-2.83	121.15	126.04
11	A	5003	LHG	O8-C23-C24	2.82	120.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1205	CLA	O2A-CGA-CBA	2.82	120.75	111.91
10	B	4010	BCR	C37-C22-C21	-2.82	118.98	122.92
8	B	1238	CLA	C1-C2-C3	-2.82	121.17	126.04
8	B	1235	CLA	CMA-C3A-C4A	2.81	119.33	111.77
8	A	1110	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
10	B	4004	BCR	C28-C27-C26	-2.80	109.08	114.08
8	A	1109	CLA	C1-C2-C3	-2.79	121.21	126.04
10	A	4002	BCR	C23-C24-C25	-2.79	119.37	127.20
10	A	4007	BCR	C36-C18-C17	-2.78	119.03	122.92
10	B	4010	BCR	C8-C7-C6	-2.78	119.40	127.20
10	B	4011	BCR	C19-C18-C17	2.77	123.20	118.94
8	K	1401	CLA	CMA-C3A-C4A	2.77	119.22	111.77
8	B	1221	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
8	B	1206	CLA	C1-C2-C3	-2.76	121.28	126.04
11	M	5001	LHG	O8-C23-C24	2.75	120.53	111.91
10	B	4005	BCR	C38-C26-C27	2.75	118.89	113.62
8	B	1215	CLA	CMA-C3A-C4A	2.75	119.15	111.77
8	A	1108	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	B	4006	ECH	C23-C24-C25	-2.74	119.50	127.20
8	B	1240	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
8	B	1205	CLA	C1-C2-C3	-2.74	121.30	126.04
8	B	1229	CLA	CMA-C3A-C4A	2.74	119.14	111.77
8	B	1234	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
8	A	1123	CLA	C1-C2-C3	-2.73	121.32	126.04
10	A	4019	BCR	C34-C9-C10	-2.73	119.10	122.92
12	A	5002	LMG	O8-C28-C29	2.72	120.46	111.91
8	A	1105	CLA	CMA-C3A-C4A	2.72	119.09	111.77
8	B	1208	CLA	CMA-C3A-C4A	2.72	119.08	111.77
10	B	4004	BCR	C33-C5-C4	2.72	118.83	113.62
8	B	1214	CLA	CMA-C3A-C4A	2.72	119.07	111.77
8	B	1022	CLA	CHA-C1A-NA	-2.71	120.18	126.40
8	B	1211	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
8	B	1207	CLA	CMA-C3A-C4A	2.71	119.06	111.77
8	B	1232	CLA	CMA-C3A-C4A	2.70	119.04	111.77
8	A	1106	CLA	CMB-C2B-C3B	2.70	129.73	124.68
10	K	4001	BCR	C37-C22-C21	-2.70	119.14	122.92
8	B	1230	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
8	A	1011	CLA	CMA-C3A-C4A	2.70	119.02	111.77
8	B	1226	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
8	A	1131	CLA	C1-C2-C3	-2.69	121.39	126.04
14	M	4021	ECH	C11-C10-C9	-2.69	123.48	127.31
8	B	1239	CLA	C1-C2-C3	-2.69	121.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1136	CLA	O2A-CGA-CBA	2.68	120.32	111.91
8	A	1012	CLA	CMA-C3A-C4A	2.68	118.97	111.77
10	A	4002	BCR	C38-C26-C27	2.68	118.76	113.62
8	A	1125	CLA	CMB-C2B-C3B	2.68	129.68	124.68
8	A	1116	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
8	A	1130	CLA	C1-C2-C3	-2.67	121.42	126.04
8	B	1023	CLA	C1-C2-C3	-2.66	121.43	126.04
10	B	4014	BCR	C34-C9-C10	-2.66	119.19	122.92
10	A	4002	BCR	C34-C9-C10	-2.66	119.19	122.92
8	B	1210	CLA	CMC-C2C-C3C	2.66	129.96	124.94
10	B	4010	BCR	C30-C25-C26	-2.66	118.86	122.61
10	B	4011	BCR	C30-C25-C26	-2.66	118.87	122.61
14	B	4006	ECH	C8-C7-C6	-2.66	119.74	127.20
8	A	1123	CLA	CMB-C2B-C3B	2.65	129.64	124.68
8	B	1210	CLA	C1-O2A-CGA	2.65	123.41	116.44
8	B	1220	CLA	O2A-CGA-CBA	2.65	120.23	111.91
10	B	4017	BCR	C8-C7-C6	-2.65	119.76	127.20
8	A	1116	CLA	CMB-C2B-C3B	2.65	129.64	124.68
12	K	5009	LMG	O8-C28-C29	2.65	120.22	111.91
8	B	1224	CLA	O2A-CGA-CBA	2.65	120.21	111.91
11	B	5006	LHG	C5-O7-C7	-2.65	111.28	117.79
14	M	4021	ECH	C7-C6-C5	-2.64	115.07	121.46
8	B	1021	CLA	C1-C2-C3	-2.64	121.48	126.04
10	A	4012	BCR	C34-C9-C10	-2.64	119.23	122.92
8	A	1112	CLA	C1-C2-C3	-2.63	122.49	126.75
8	B	1222	CLA	CMC-C2C-C3C	2.63	129.90	124.94
12	B	5005	LMG	O8-C28-C29	2.63	120.16	111.91
8	A	1137	CLA	CMA-C3A-C4A	2.62	118.83	111.77
9	A	2001	PQN	C14-C13-C15	2.62	119.69	115.27
8	B	1022	CLA	O2A-CGA-CBA	2.62	120.13	111.91
8	B	1213	CLA	CBA-CAA-C2A	2.62	121.59	113.86
11	A	5001	LHG	O8-C23-C24	2.62	120.12	111.91
10	B	4014	BCR	C30-C25-C24	2.61	123.18	115.78
8	B	1226	CLA	CMC-C2C-C3C	2.61	129.87	124.94
8	A	1013	CLA	O2A-CGA-CBA	2.61	120.11	111.91
8	B	1215	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
8	A	1121	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
10	B	4014	BCR	C4-C5-C6	-2.61	118.95	122.73
8	A	1112	CLA	O2A-CGA-CBA	2.60	120.08	111.91
8	A	1117	CLA	CMB-C2B-C3B	2.60	129.54	124.68
8	B	1021	CLA	O2A-CGA-CBA	2.60	120.06	111.91
11	B	5004	LHG	C5-O7-C7	-2.59	111.41	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1127	CLA	C1-O2A-CGA	2.59	123.24	116.44
8	B	1214	CLA	C1-C2-C3	-2.59	121.57	126.04
8	B	1229	CLA	C1-C2-C3	-2.59	121.57	126.04
10	B	4018	BCR	C38-C26-C27	2.58	118.58	113.62
8	B	1210	CLA	CMA-C3A-C4A	2.58	118.71	111.77
8	B	1235	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
8	B	1207	CLA	C1-C2-C3	-2.58	121.59	126.04
8	A	1128	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
8	A	1118	CLA	CMA-C3A-C4A	2.58	118.69	111.77
8	A	1118	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
8	B	1206	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
8	B	1223	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
8	A	1122	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
8	A	1106	CLA	O2A-CGA-CBA	2.56	119.94	111.91
8	B	1240	CLA	C1-C2-C3	-2.56	121.62	126.04
8	B	1214	CLA	OBD-CAD-C3D	-2.55	123.74	127.98
8	A	1012	CLA	C1-O2A-CGA	2.55	123.14	116.44
11	B	5004	LHG	O8-C23-C24	2.55	119.91	111.91
8	B	1221	CLA	O2A-CGA-CBA	2.55	119.90	111.91
8	B	1230	CLA	C1-C2-C3	-2.54	121.64	126.04
14	M	4021	ECH	C15-C16-C17	-2.54	118.27	123.47
8	B	1222	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
10	A	4002	BCR	C19-C18-C17	2.54	122.83	118.94
10	K	4001	BCR	C38-C26-C25	-2.53	121.69	124.53
8	B	1023	CLA	CMB-C2B-C3B	2.53	129.41	124.68
10	A	4003	BCR	C34-C9-C10	-2.53	119.38	122.92
8	A	1122	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
10	A	4007	BCR	C4-C5-C6	-2.53	119.06	122.73
8	A	1116	CLA	O2A-CGA-CBA	2.52	119.83	111.91
10	A	4001	BCR	C34-C9-C10	-2.52	119.39	122.92
8	A	1113	CLA	CAA-CBA-CGA	-2.52	108.17	113.59
8	B	1204	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
8	A	1127	CLA	O2A-CGA-CBA	2.52	119.82	111.91
8	B	1236	CLA	CMA-C3A-C4A	2.52	118.55	111.77
8	B	1214	CLA	O2A-CGA-CBA	2.52	119.80	111.91
8	B	1209	CLA	C1-C2-C3	-2.52	121.69	126.04
8	A	1134	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
8	A	1125	CLA	C4D-C3D-CAD	2.51	109.87	108.47
8	A	1108	CLA	CHA-C1A-NA	-2.51	120.64	126.40
8	B	1023	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
8	B	1221	CLA	C1-C2-C3	-2.51	121.71	126.04
8	A	1101	CLA	O2A-CGA-CBA	2.51	119.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1219	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
8	B	1021	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
8	A	1129	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
8	B	1217	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
8	A	1103	CLA	C1-C2-C3	-2.50	121.72	126.04
8	B	1217	CLA	C1-O2A-CGA	2.50	123.01	116.44
8	A	1101	CLA	C1-C2-C3	-2.50	121.72	126.04
8	B	1239	CLA	CMC-C2C-C3C	2.50	129.65	124.94
8	A	1134	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
8	B	1220	CLA	C1-C2-C3	-2.49	121.73	126.04
10	A	4002	BCR	C15-C14-C13	-2.49	123.75	127.31
8	A	1012	CLA	C1-C2-C3	-2.49	121.73	126.04
10	B	4014	BCR	C33-C5-C6	-2.49	121.73	124.53
8	B	1231	CLA	C1-O2A-CGA	2.49	122.97	116.44
8	B	1239	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
8	B	1203	CLA	C1-C2-C3	-2.48	121.75	126.04
8	A	1118	CLA	OBD-CAD-C3D	-2.48	123.86	127.98
8	A	1012	CLA	CHA-C1A-NA	-2.48	120.72	126.40
8	B	1227	CLA	C1-C2-C3	-2.48	121.75	126.04
8	B	1228	CLA	O2A-CGA-CBA	2.48	119.68	111.91
8	B	1202	CLA	CMB-C2B-C3B	2.48	129.31	124.68
8	K	1401	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
8	B	1210	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
8	A	1109	CLA	O2A-CGA-CBA	2.47	119.67	111.91
8	A	1106	CLA	OBD-CAD-C3D	-2.47	123.88	127.98
8	B	1211	CLA	CMA-C3A-C4A	2.47	118.41	111.77
8	B	1022	CLA	C1-C2-C3	-2.47	121.78	126.04
8	A	1111	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
11	A	5001	LHG	C5-O7-C7	-2.46	111.73	117.79
8	A	1103	CLA	CMA-C3A-C4A	2.46	118.39	111.77
10	B	4014	BCR	C38-C26-C25	-2.46	121.76	124.53
8	B	1225	CLA	C1-C2-C3	-2.46	121.80	126.04
8	A	1120	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
8	K	1402	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
8	A	1125	CLA	OBD-CAD-CBD	-2.45	122.40	125.89
10	B	4018	BCR	C35-C13-C12	2.45	121.94	118.08
10	B	4017	BCR	C23-C24-C25	-2.45	120.33	127.20
11	M	5001	LHG	C5-O7-C7	-2.45	111.77	117.79
10	B	4005	BCR	C27-C26-C25	-2.44	119.18	122.73
10	A	4001	BCR	C30-C25-C26	-2.44	119.18	122.61
10	A	4008	BCR	C38-C26-C25	-2.44	121.79	124.53
8	A	1135	CLA	O2D-CGD-O1D	-2.44	119.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	4001	BCR	C15-C14-C13	-2.44	123.83	127.31
8	A	1125	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
8	B	1221	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
11	A	5003	LHG	C5-O7-C7	-2.43	111.82	117.79
10	K	4001	BCR	C19-C18-C17	2.43	122.67	118.94
8	B	1226	CLA	CMA-C3A-C4A	2.43	118.30	111.77
10	B	4010	BCR	C30-C25-C24	2.42	122.64	115.78
10	B	4014	BCR	C1-C6-C5	-2.42	119.20	122.61
8	A	1123	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
8	A	1119	CLA	CHA-C1A-NA	-2.42	120.85	126.40
8	A	1107	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
8	A	1138	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
10	A	4002	BCR	C37-C22-C21	-2.42	119.53	122.92
8	B	1226	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
8	B	1206	CLA	OBD-CAD-C3D	-2.42	123.96	127.98
10	B	4010	BCR	C38-C26-C27	2.42	118.26	113.62
8	B	1212	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
10	A	4007	BCR	C34-C9-C10	-2.42	119.54	122.92
8	A	1110	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
8	A	1140	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
8	B	1213	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
10	B	4004	BCR	C34-C9-C10	-2.41	119.55	122.92
10	A	4002	BCR	C33-C5-C6	-2.41	121.82	124.53
10	A	4007	BCR	C19-C18-C17	2.41	122.64	118.94
8	B	1215	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
8	A	1125	CLA	O2A-CGA-CBA	2.41	119.46	111.91
10	A	4008	BCR	C33-C5-C6	-2.41	121.83	124.53
8	B	1219	CLA	C1-C2-C3	-2.41	121.88	126.04
8	B	1023	CLA	CHA-C1A-NA	-2.40	120.90	126.40
10	A	4019	BCR	C36-C18-C19	2.40	121.86	118.08
8	A	1108	CLA	C2A-C1A-CHA	2.40	128.06	123.86
8	A	1125	CLA	C1-C2-C3	-2.40	121.89	126.04
8	B	1221	CLA	CHA-C1A-NA	-2.40	120.90	126.40
10	B	4018	BCR	C8-C7-C6	-2.40	120.47	127.20
8	B	1223	CLA	CHA-C1A-NA	-2.39	120.92	126.40
8	A	1102	CLA	CMA-C3A-C4A	2.39	118.20	111.77
8	B	1224	CLA	CHA-C1A-NA	-2.39	120.92	126.40
8	B	1229	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
8	A	1125	CLA	CHA-C1A-NA	-2.39	120.93	126.40
8	A	1103	CLA	C1-O2A-CGA	2.39	122.70	116.44
8	A	1132	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
10	A	4003	BCR	C4-C5-C6	-2.38	119.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	1402	CLA	C1-C2-C3	-2.38	121.93	126.04
8	A	1117	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
8	A	1125	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
10	B	4004	BCR	C23-C24-C25	-2.38	120.53	127.20
8	B	1206	CLA	CMA-C3A-C4A	2.37	118.15	111.77
8	B	1207	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
8	A	1125	CLA	CMA-C3A-C4A	2.37	118.15	111.77
8	B	1213	CLA	C1-O2A-CGA	2.37	122.67	116.44
8	B	1202	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
8	B	1236	CLA	O2A-CGA-CBA	2.37	119.34	111.91
8	B	1216	CLA	CMB-C2B-C3B	2.37	129.11	124.68
8	A	1137	CLA	CMB-C2B-C3B	2.37	129.10	124.68
9	A	2001	PQN	C5-C10-C1	-2.36	118.12	120.68
8	A	1115	CLA	CMA-C3A-C4A	2.36	118.12	111.77
8	B	1219	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
8	B	1228	CLA	CMA-C3A-C4A	2.36	118.11	111.77
8	A	1103	CLA	CMC-C2C-C3C	2.36	129.39	124.94
10	B	4018	BCR	C4-C5-C6	-2.36	119.31	122.73
14	B	4006	ECH	C4-C5-C6	-2.36	119.31	122.73
8	A	1111	CLA	CHA-C1A-NA	-2.36	121.00	126.40
8	A	1107	CLA	O2A-CGA-CBA	2.36	119.30	111.91
8	B	1231	CLA	C1-C2-C3	-2.36	121.97	126.04
8	B	1236	CLA	CMC-C2C-C3C	2.35	129.38	124.94
8	B	1231	CLA	CMA-C3A-C4A	2.35	118.09	111.77
8	B	1206	CLA	O2A-CGA-CBA	2.35	119.29	111.91
8	B	1240	CLA	O2A-CGA-CBA	2.35	119.28	111.91
10	B	4010	BCR	C4-C5-C6	-2.35	119.32	122.73
8	B	1210	CLA	CHA-C1A-NA	-2.35	121.02	126.40
8	A	1139	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
8	A	1103	CLA	CHA-C1A-NA	-2.35	121.03	126.40
8	A	1113	CLA	CAA-C2A-C3A	-2.35	106.36	112.78
10	B	4011	BCR	C35-C13-C14	-2.35	119.64	122.92
8	A	1130	CLA	O2A-CGA-CBA	2.34	119.26	111.91
10	B	4004	BCR	C36-C18-C17	-2.34	119.64	122.92
8	B	1230	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
14	M	4021	ECH	C29-C30-C25	-2.34	106.88	110.48
8	A	1130	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
8	B	1224	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
8	A	1134	CLA	CHA-C1A-NA	-2.33	121.06	126.40
8	B	1219	CLA	O2A-CGA-CBA	2.33	119.23	111.91
8	A	1113	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
8	A	1135	CLA	CHA-C1A-NA	-2.33	121.06	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1121	CLA	C1-O2A-CGA	2.33	122.56	116.44
8	B	1227	CLA	CBC-CAC-C3C	-2.33	106.33	112.27
8	B	1232	CLA	CHA-C1A-NA	-2.33	121.06	126.40
8	B	1231	CLA	O2A-CGA-CBA	2.33	119.22	111.91
8	A	1111	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
10	A	4007	BCR	C37-C22-C21	-2.33	119.66	122.92
8	B	1213	CLA	CHA-C1A-NA	-2.33	121.07	126.40
8	A	1117	CLA	C1-C2-C3	-2.33	122.02	126.04
8	B	1202	CLA	O2A-CGA-CBA	2.32	119.20	111.91
10	B	4005	BCR	C38-C26-C25	-2.32	121.92	124.53
8	A	1136	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
8	A	1133	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
8	B	1222	CLA	CMA-C3A-C4A	2.32	118.01	111.77
8	B	1206	CLA	CHA-C1A-NA	-2.32	121.09	126.40
8	A	1128	CLA	CMC-C2C-C3C	2.32	129.31	124.94
8	B	1223	CLA	O2A-CGA-CBA	2.32	119.18	111.91
8	B	1225	CLA	CHA-C1A-NA	-2.32	121.10	126.40
8	A	1013	CLA	C2A-C1A-CHA	2.32	127.91	123.86
10	A	4007	BCR	C38-C26-C27	2.31	118.06	113.62
8	A	1011	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
8	B	1203	CLA	CHA-C1A-NA	-2.31	121.11	126.40
8	B	1216	CLA	C1-C2-C3	-2.31	122.05	126.04
8	B	1234	CLA	CHA-C1A-NA	-2.31	121.11	126.40
8	B	1214	CLA	CHA-C1A-NA	-2.31	121.12	126.40
8	A	1139	CLA	CHA-C1A-NA	-2.31	121.12	126.40
8	B	1236	CLA	CHA-C1A-NA	-2.31	121.12	126.40
8	A	1132	CLA	O2A-CGA-CBA	2.30	119.13	111.91
8	A	1106	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
8	A	1123	CLA	CHA-C1A-NA	-2.30	121.13	126.40
8	A	1104	CLA	O2A-CGA-CBA	2.30	119.13	111.91
8	A	1124	CLA	CHA-C1A-NA	-2.30	121.14	126.40
8	A	1115	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
8	B	1023	CLA	C2A-C1A-CHA	2.30	127.88	123.86
8	A	1114	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
8	K	1401	CLA	C1-O2A-CGA	2.29	122.46	116.44
9	B	2002	PQN	C2M-C2-C3	-2.29	120.66	124.40
8	B	1219	CLA	CMC-C2C-C3C	2.29	129.26	124.94
9	A	2001	PQN	C10-C1-C2	2.29	122.22	118.95
8	B	1218	CLA	CMC-C2C-C3C	2.29	129.25	124.94
8	A	1011	CLA	O2A-CGA-CBA	2.28	119.08	111.91
8	B	1224	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
8	B	1215	CLA	O2D-CGD-O1D	-2.28	119.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1218	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
8	A	1122	CLA	CHA-C1A-NA	-2.28	121.17	126.40
10	B	4005	BCR	C35-C13-C12	2.28	121.67	118.08
8	A	1127	CLA	CMC-C2C-C3C	2.28	129.24	124.94
8	B	1239	CLA	O2A-CGA-CBA	2.28	119.06	111.91
8	A	1121	CLA	CMC-C2C-C3C	2.28	129.24	124.94
8	B	1235	CLA	O2A-CGA-CBA	2.28	119.06	111.91
8	A	1101	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
10	A	4019	BCR	C38-C26-C25	-2.28	121.97	124.53
10	B	4005	BCR	C33-C5-C4	2.28	117.99	113.62
10	B	4010	BCR	C35-C13-C14	-2.28	119.73	122.92
8	A	1112	CLA	CMB-C2B-C3B	2.28	128.94	124.68
8	A	1119	CLA	CMB-C2B-C3B	2.28	128.94	124.68
8	A	1107	CLA	CHA-C1A-NA	-2.27	121.19	126.40
8	B	1021	CLA	C1-O2A-CGA	2.27	122.41	116.44
8	A	1104	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
8	A	1011	CLA	CHA-C1A-NA	-2.27	121.19	126.40
8	A	1127	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
8	A	1124	CLA	O2A-CGA-CBA	2.27	119.03	111.91
8	B	1021	CLA	CMA-C3A-C4A	2.27	117.88	111.77
10	B	4011	BCR	C1-C6-C7	2.27	122.20	115.78
8	B	1228	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
8	A	1126	CLA	C1-O2A-CGA	2.27	122.40	116.44
8	B	1229	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
8	A	1128	CLA	O2A-CGA-CBA	2.27	119.03	111.91
8	B	1222	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
8	B	1213	CLA	C2A-C1A-CHA	2.27	127.82	123.86
8	A	1118	CLA	CMC-C2C-C3C	2.27	129.22	124.94
10	B	4017	BCR	C1-C6-C7	2.27	122.19	115.78
8	A	1116	CLA	CMA-C3A-C4A	2.27	117.86	111.77
8	B	1205	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
10	A	4008	BCR	C23-C24-C25	-2.26	120.85	127.20
10	B	4017	BCR	C37-C22-C21	-2.26	119.75	122.92
10	B	4014	BCR	C30-C25-C26	-2.26	119.43	122.61
8	B	1240	CLA	CMB-C2B-C3B	2.26	128.91	124.68
8	B	1226	CLA	O2A-CGA-CBA	2.26	119.00	111.91
10	A	4002	BCR	C35-C13-C12	2.26	121.64	118.08
8	B	1220	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
8	K	1402	CLA	O2A-CGA-CBA	2.26	119.00	111.91
8	B	1228	CLA	CHA-C1A-NA	-2.26	121.22	126.40
8	A	1112	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
8	B	1239	CLA	CHA-C1A-NA	-2.26	121.23	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1228	CLA	C1-C2-C3	-2.26	122.14	126.04
8	A	1127	CLA	CHA-C1A-NA	-2.26	121.23	126.40
8	A	1104	CLA	CMA-C3A-C4A	2.25	117.83	111.77
8	B	1220	CLA	CHA-C1A-NA	-2.25	121.23	126.40
8	B	1209	CLA	O2A-CGA-CBA	2.25	118.98	111.91
8	A	1013	CLA	CHA-C1A-NA	-2.25	121.24	126.40
8	B	1215	CLA	CHA-C1A-NA	-2.25	121.24	126.40
8	A	1801	CLA	CHA-C1A-NA	-2.25	121.24	126.40
8	A	1104	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
8	A	1126	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
8	B	1227	CLA	CHA-C1A-NA	-2.25	121.25	126.40
8	A	1128	CLA	CMB-C2B-C3B	2.25	128.88	124.68
8	A	1121	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
8	A	1137	CLA	CHA-C1A-NA	-2.25	121.25	126.40
10	B	4011	BCR	C37-C22-C23	2.24	121.61	118.08
8	B	1220	CLA	CMB-C2B-C3B	2.24	128.88	124.68
8	A	1133	CLA	CHA-C1A-NA	-2.24	121.26	126.40
8	B	1231	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
8	A	1105	CLA	O2A-CGA-CBA	2.24	118.95	111.91
10	A	4001	BCR	C4-C5-C6	-2.24	119.47	122.73
15	B	5008	SQD	O3-C3-C2	-2.24	105.17	110.35
8	B	1235	CLA	C1-O2A-CGA	2.24	122.33	116.44
8	B	1224	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
8	A	1105	CLA	CHA-C1A-NA	-2.24	121.27	126.40
8	A	1107	CLA	CMA-C3A-C4A	2.24	117.79	111.77
8	A	1131	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
8	B	1205	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
8	B	1240	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
10	A	4001	BCR	C1-C6-C5	-2.24	119.46	122.61
10	B	4014	BCR	C23-C22-C21	2.24	122.37	118.94
8	A	1103	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
8	A	1105	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
8	B	1236	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
8	A	1112	CLA	CHA-C1A-NA	-2.23	121.29	126.40
10	B	4010	BCR	C36-C18-C17	-2.23	119.80	122.92
10	K	4001	BCR	C29-C28-C27	2.23	116.36	111.38
8	B	1022	CLA	C2A-C1A-CHA	2.23	127.76	123.86
8	B	1220	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
8	A	1102	CLA	CHA-C1A-NA	-2.23	121.30	126.40
8	B	1237	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
8	B	1225	CLA	C2A-C1A-CHA	2.23	127.75	123.86
10	A	4012	BCR	C23-C22-C21	2.23	122.36	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1110	CLA	CHA-C1A-NA	-2.23	121.30	126.40
8	A	1116	CLA	CHA-C1A-NA	-2.23	121.30	126.40
8	B	1225	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
8	A	1111	CLA	O2A-CGA-CBA	2.22	118.89	111.91
8	K	1401	CLA	O2A-CGA-CBA	2.22	118.88	111.91
10	B	4010	BCR	C1-C6-C7	2.22	122.06	115.78
8	B	1208	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
8	K	1402	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
8	A	1114	CLA	CHA-C1A-NA	-2.22	121.31	126.40
8	A	1136	CLA	CHA-C1A-NA	-2.22	121.31	126.40
8	A	1124	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
8	B	1238	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
8	B	1214	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
8	B	1207	CLA	CHA-C1A-NA	-2.22	121.32	126.40
8	B	1218	CLA	CHA-C1A-NA	-2.22	121.32	126.40
8	A	1106	CLA	CHA-C1A-NA	-2.22	121.32	126.40
8	B	1202	CLA	C1-O2A-CGA	2.22	122.26	116.44
8	B	1022	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
8	A	1123	CLA	CMB-C2B-C1B	-2.22	125.06	128.46
8	A	1121	CLA	CHA-C1A-NA	-2.21	121.33	126.40
8	A	1108	CLA	CMA-C3A-C4A	2.21	117.72	111.77
8	B	1210	CLA	CMB-C2B-C3B	2.21	128.81	124.68
8	A	1131	CLA	O2A-CGA-CBA	2.21	118.84	111.91
8	B	1202	CLA	CHA-C1A-NA	-2.21	121.34	126.40
8	B	1227	CLA	CMA-C3A-C4A	2.21	117.70	111.77
8	B	1216	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
8	A	1138	CLA	O2A-CGA-CBA	2.20	118.82	111.91
10	B	4018	BCR	C34-C9-C10	-2.20	119.84	122.92
8	B	1216	CLA	CHA-C1A-NA	-2.20	121.35	126.40
8	B	1220	CLA	C2A-C1A-CHA	2.20	127.71	123.86
8	B	1222	CLA	CHA-C1A-NA	-2.20	121.36	126.40
8	A	1116	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
8	B	1208	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
8	B	1214	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
8	A	1137	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
8	A	1130	CLA	CHA-C1A-NA	-2.20	121.36	126.40
8	B	1229	CLA	CHA-C1A-NA	-2.20	121.36	126.40
8	A	1138	CLA	CHA-C1A-NA	-2.20	121.37	126.40
8	B	1230	CLA	C1-O2A-CGA	2.20	122.21	116.44
8	A	1138	CLA	C1-O2A-CGA	2.20	122.20	116.44
8	A	1129	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
10	A	4001	BCR	C37-C22-C21	-2.19	119.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1128	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
8	A	1104	CLA	CHA-C1A-NA	-2.19	121.38	126.40
8	A	1101	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
8	B	1209	CLA	CHA-C1A-NA	-2.19	121.38	126.40
14	M	4021	ECH	C8-C7-C6	-2.19	121.06	127.20
8	B	1216	CLA	O2A-CGA-CBA	2.19	118.78	111.91
8	K	1402	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
8	A	1101	CLA	CHA-C1A-NA	-2.19	121.39	126.40
10	B	4017	BCR	C34-C9-C10	-2.19	119.86	122.92
8	A	1129	CLA	CHA-C1A-NA	-2.19	121.39	126.40
8	B	1219	CLA	CHA-C1A-NA	-2.19	121.39	126.40
8	A	1120	CLA	O2A-CGA-CBA	2.19	118.77	111.91
10	A	4019	BCR	C38-C26-C27	2.19	117.81	113.62
8	B	1226	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
8	B	1239	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
8	B	1211	CLA	CHA-C1A-NA	-2.18	121.40	126.40
8	B	1226	CLA	CMB-C2B-C3B	2.18	128.76	124.68
8	B	1238	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
10	B	4010	BCR	C1-C6-C5	-2.18	119.55	122.61
8	A	1106	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
8	A	1120	CLA	CHA-C1A-NA	-2.18	121.42	126.40
8	B	1222	CLA	O2A-CGA-CBA	2.17	118.73	111.91
8	A	1109	CLA	C1-O2A-CGA	2.17	122.15	116.44
8	A	1132	CLA	CHA-C1A-NA	-2.17	121.42	126.40
8	A	1127	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
8	A	1135	CLA	CMB-C2B-C3B	2.17	128.74	124.68
8	B	1230	CLA	CHA-C1A-NA	-2.17	121.43	126.40
8	A	1801	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
8	B	1225	CLA	O2A-CGA-CBA	2.17	118.71	111.91
8	A	1103	CLA	C11-C10-C8	-2.17	108.92	115.92
9	A	2001	PQN	C26-C25-C23	-2.16	108.92	115.92
8	B	1240	CLA	CHA-C1A-NA	-2.16	121.44	126.40
8	A	1127	CLA	C2A-C1A-CHA	2.16	127.64	123.86
8	B	1234	CLA	O2A-CGA-CBA	2.16	118.69	111.91
8	A	1137	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
8	K	1402	CLA	CHA-C1A-NA	-2.16	121.45	126.40
8	A	1137	CLA	CMC-C2C-C3C	2.16	129.01	124.94
8	A	1113	CLA	CHA-C1A-NA	-2.16	121.46	126.40
8	B	1021	CLA	CHA-C1A-NA	-2.16	121.46	126.40
10	A	4002	BCR	C33-C5-C4	2.16	117.76	113.62
8	A	1102	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
8	B	1222	CLA	O1D-CGD-CBD	-2.15	120.08	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1237	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
10	A	4008	BCR	C36-C18-C17	-2.15	119.91	122.92
8	B	1206	CLA	C2A-C1A-CHA	2.15	127.62	123.86
8	K	1401	CLA	CHA-C1A-NA	-2.15	121.47	126.40
8	A	1116	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
10	A	4003	BCR	C19-C18-C17	2.15	122.24	118.94
8	B	1236	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
8	B	1224	CLA	CMA-C3A-C4A	2.14	117.53	111.77
8	A	1137	CLA	C1-O2A-CGA	2.14	122.06	116.44
10	A	4007	BCR	C1-C6-C5	-2.14	119.60	122.61
8	A	1138	CLA	CMC-C2C-C3C	2.14	128.98	124.94
10	B	4017	BCR	C36-C18-C17	-2.14	119.93	122.92
8	A	1126	CLA	CHA-C1A-NA	-2.14	121.51	126.40
8	A	1128	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
8	B	1221	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
8	A	1118	CLA	CHA-C1A-NA	-2.13	121.52	126.40
8	A	1131	CLA	CHA-C1A-NA	-2.13	121.52	126.40
8	A	1011	CLA	C2A-C1A-CHA	2.13	127.58	123.86
8	K	1401	CLA	C1-C2-C3	-2.13	122.36	126.04
8	B	1238	CLA	CHA-C1A-NA	-2.13	121.53	126.40
14	B	4006	ECH	C28-C29-C30	-2.13	109.77	113.18
8	A	1116	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
10	A	4019	BCR	C35-C13-C14	-2.13	119.95	122.92
8	B	1226	CLA	CHA-C1A-NA	-2.12	121.53	126.40
8	A	1117	CLA	CHA-C1A-NA	-2.12	121.53	126.40
8	A	1123	CLA	C2A-C1A-CHA	2.12	127.57	123.86
14	B	4006	ECH	C29-C30-C25	-2.12	107.21	110.48
10	A	4012	BCR	C28-C27-C26	-2.12	110.29	114.08
10	B	4014	BCR	C35-C13-C14	-2.12	119.95	122.92
8	B	1209	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	B	4006	ECH	C15-C14-C13	-2.12	124.29	127.31
8	B	1218	CLA	O2A-CGA-CBA	2.12	118.56	111.91
8	A	1013	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
10	A	4012	BCR	C27-C26-C25	-2.12	119.66	122.73
8	A	1109	CLA	CHA-C1A-NA	-2.12	121.55	126.40
8	A	1013	CLA	CMA-C3A-C4A	2.12	117.46	111.77
8	A	1109	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
8	B	1231	CLA	CHA-C1A-NA	-2.11	121.56	126.40
10	A	4008	BCR	C29-C28-C27	2.11	116.10	111.38
8	A	1110	CLA	O2A-CGA-CBA	2.11	118.53	111.91
8	B	1212	CLA	CHA-C1A-NA	-2.11	121.56	126.40
8	K	1401	CLA	O1D-CGD-CBD	-2.11	120.17	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1204	CLA	CHA-C1A-NA	-2.11	121.58	126.40
8	A	1128	CLA	CHA-C1A-NA	-2.10	121.58	126.40
8	A	1115	CLA	CHA-C1A-NA	-2.10	121.58	126.40
8	B	1228	CLA	C1-O2A-CGA	2.10	121.96	116.44
10	K	4001	BCR	C35-C13-C12	2.10	121.39	118.08
8	A	1119	CLA	O2A-CGA-CBA	2.10	118.50	111.91
8	A	1111	CLA	C2A-C1A-CHA	2.10	127.53	123.86
8	B	1238	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
8	A	1114	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
8	B	1221	CLA	CMA-C3A-C2A	2.10	122.29	113.83
10	A	4003	BCR	C23-C24-C25	-2.10	121.31	127.20
10	K	4001	BCR	C31-C1-C6	-2.10	106.90	110.30
8	B	1207	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
8	B	1232	CLA	O2A-CGA-CBA	2.09	118.48	111.91
8	B	1235	CLA	CHA-C1A-NA	-2.09	121.60	126.40
10	A	4007	BCR	C31-C1-C6	-2.09	106.90	110.30
8	B	1208	CLA	CHA-C1A-NA	-2.09	121.61	126.40
10	B	4018	BCR	C37-C22-C23	2.09	121.37	118.08
8	A	1102	CLA	O2A-CGA-CBA	2.09	118.47	111.91
8	A	1117	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
14	M	4021	ECH	C28-C29-C30	-2.09	109.83	113.18
8	B	1217	CLA	CHA-C1A-NA	-2.09	121.61	126.40
8	B	1232	CLA	C2A-C1A-CHA	2.09	127.51	123.86
8	A	1131	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
8	B	1218	CLA	OBD-CAD-C3D	-2.09	124.52	127.98
8	B	1227	CLA	O2A-CGA-CBA	2.09	118.45	111.91
8	A	1117	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
10	A	4007	BCR	C27-C26-C25	-2.08	119.70	122.73
8	B	1203	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
8	A	1135	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
8	A	1135	CLA	OBD-CAD-C3D	-2.08	124.52	127.98
8	B	1239	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
8	A	1136	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
8	B	1235	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
8	A	1012	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
8	A	1109	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
8	A	1140	CLA	CHA-C1A-NA	-2.08	121.64	126.40
8	B	1210	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
8	A	1012	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
8	A	1140	CLA	O2A-CGA-CBA	2.07	118.41	111.91
8	B	1237	CLA	CHA-C1A-NA	-2.07	121.65	126.40
8	A	1128	CLA	O2D-CGD-O1D	-2.07	119.79	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1210	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
8	B	1229	CLA	C6-C5-C3	-2.06	108.04	113.45
8	A	1113	CLA	CMC-C2C-C3C	2.06	128.83	124.94
8	A	1122	CLA	CMC-C2C-C3C	2.06	128.83	124.94
10	B	4011	BCR	C28-C27-C26	-2.06	110.39	114.08
10	B	4004	BCR	C19-C18-C17	2.06	122.11	118.94
8	A	1133	CLA	CMA-C3A-C4A	2.06	117.31	111.77
8	A	1116	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
8	B	1201	CLA	CHA-C1A-NA	-2.06	121.68	126.40
10	A	4019	BCR	C37-C22-C23	2.06	121.32	118.08
8	A	1122	CLA	CMB-C2B-C3B	2.06	128.53	124.68
10	B	4004	BCR	C37-C22-C21	-2.06	120.04	122.92
8	B	1212	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
8	A	1102	CLA	CMC-C2C-C3C	2.05	128.81	124.94
8	B	1021	CLA	CBC-CAC-C3C	-2.05	107.04	112.27
8	A	1125	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
8	A	1130	CLA	C1-O2A-CGA	2.05	121.82	116.44
8	B	1208	CLA	CMC-C2C-C3C	2.05	128.81	124.94
8	A	1111	CLA	CMC-C2C-C3C	2.05	128.80	124.94
9	A	2001	PQN	O1-C1-C10	-2.05	118.25	121.56
8	B	1230	CLA	CMC-C2C-C3C	2.05	128.80	124.94
8	A	1102	CLA	C2A-C1A-CHA	2.04	127.43	123.86
10	A	4007	BCR	C38-C26-C25	-2.04	122.23	124.53
8	B	1212	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
8	B	1214	CLA	CMB-C2B-C3B	2.04	128.50	124.68
8	A	1103	CLA	O2A-CGA-CBA	2.04	118.31	111.91
10	A	4019	BCR	C4-C5-C6	-2.04	119.77	122.73
8	B	1227	CLA	CMC-C2C-C3C	2.04	128.79	124.94
8	A	1139	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
8	B	1203	CLA	O2A-CGA-CBA	2.04	118.31	111.91
8	B	1204	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
8	A	1012	CLA	C2A-C1A-CHA	2.04	127.42	123.86
8	A	1104	CLA	CMC-C2C-C3C	2.04	128.78	124.94
8	B	1211	CLA	C4D-C3D-CAD	2.04	109.61	108.47
10	A	4001	BCR	C19-C18-C17	2.04	122.07	118.94
10	A	4003	BCR	C1-C6-C5	-2.04	119.75	122.61
8	B	1023	CLA	CMA-C3A-C4A	2.04	117.24	111.77
8	A	1106	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
8	A	1137	CLA	O2A-CGA-CBA	2.03	118.28	111.91
8	B	1232	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
8	B	1021	CLA	C2A-C1A-CHA	2.03	127.41	123.86
8	B	1213	CLA	CMB-C2B-C3B	2.03	128.47	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	4004	BCR	C35-C13-C14	-2.02	120.09	122.92
8	B	1023	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
8	B	1234	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
8	B	1236	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
10	A	4012	BCR	C38-C26-C27	2.02	117.50	113.62
10	A	4001	BCR	C27-C26-C25	-2.02	119.80	122.73
10	A	4003	BCR	C27-C26-C25	-2.02	119.80	122.73
14	M	4021	ECH	C33-C5-C4	2.02	117.49	113.62
8	B	1221	CLA	C2A-C1A-CHA	2.02	127.38	123.86
8	B	1238	CLA	O2A-CGA-CBA	2.02	118.23	111.91
8	B	1237	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
8	A	1135	CLA	CMC-C2C-C3C	2.01	128.74	124.94
10	A	4008	BCR	C34-C9-C8	2.01	121.25	118.08
10	B	4017	BCR	C38-C26-C27	2.01	117.48	113.62
12	B	5002	LMG	O8-C28-O10	-2.01	118.51	123.59
10	B	4004	BCR	C1-C6-C7	2.01	121.47	115.78
8	B	1205	CLA	CHA-C1A-NA	-2.01	121.79	126.40
8	B	1207	CLA	O2A-CGA-CBA	2.01	118.21	111.91
8	B	1230	CLA	O2A-CGA-CBA	2.01	118.20	111.91
8	B	1216	CLA	C1-O2A-CGA	2.01	121.71	116.44
10	B	4005	BCR	C34-C9-C10	-2.00	120.12	122.92
8	B	1225	CLA	O2D-CGD-O1D	-2.00	119.93	123.84

All (88) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1011	CLA	ND
8	A	1012	CLA	ND
8	A	1101	CLA	ND
8	A	1102	CLA	ND
8	A	1103	CLA	ND
8	A	1104	CLA	ND
8	A	1105	CLA	ND
8	A	1106	CLA	ND
8	A	1107	CLA	ND
8	A	1108	CLA	ND
8	A	1109	CLA	ND
8	A	1110	CLA	ND
8	A	1111	CLA	ND
8	A	1112	CLA	ND
8	A	1113	CLA	ND
8	A	1114	CLA	ND

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Mol	Chain	Res	Type	Atom
8	A	1115	CLA	ND
8	A	1116	CLA	ND
8	A	1117	CLA	ND
8	A	1118	CLA	ND
8	A	1119	CLA	ND
8	A	1120	CLA	ND
8	A	1121	CLA	ND
8	A	1122	CLA	ND
8	A	1123	CLA	ND
8	A	1124	CLA	ND
8	A	1125	CLA	ND
8	A	1126	CLA	ND
8	A	1127	CLA	ND
8	A	1128	CLA	ND
8	A	1129	CLA	ND
8	A	1130	CLA	ND
8	A	1131	CLA	ND
8	A	1132	CLA	ND
8	A	1133	CLA	ND
8	A	1134	CLA	ND
8	A	1135	CLA	ND
8	A	1136	CLA	ND
8	A	1137	CLA	ND
8	A	1138	CLA	ND
8	A	1139	CLA	ND
8	A	1140	CLA	ND
8	A	1801	CLA	ND
8	A	1013	CLA	ND
8	B	1022	CLA	ND
8	B	1237	CLA	ND
8	B	1021	CLA	ND
8	B	1023	CLA	ND
8	B	1201	CLA	ND
8	B	1202	CLA	ND
8	B	1203	CLA	ND
8	B	1204	CLA	ND
8	B	1205	CLA	ND
8	B	1206	CLA	ND
8	B	1207	CLA	ND
8	B	1208	CLA	ND
8	B	1209	CLA	ND
8	B	1210	CLA	ND

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Mol	Chain	Res	Type	Atom
8	B	1211	CLA	ND
8	B	1212	CLA	ND
8	B	1213	CLA	ND
8	B	1214	CLA	ND
8	B	1215	CLA	ND
8	B	1216	CLA	ND
8	B	1217	CLA	ND
8	B	1218	CLA	ND
8	B	1219	CLA	ND
8	B	1220	CLA	ND
8	B	1221	CLA	ND
8	B	1222	CLA	ND
8	B	1223	CLA	ND
8	B	1224	CLA	ND
8	B	1225	CLA	ND
8	B	1226	CLA	ND
8	B	1227	CLA	ND
8	B	1228	CLA	ND
8	B	1229	CLA	ND
8	B	1230	CLA	ND
8	B	1231	CLA	ND
8	B	1232	CLA	ND
8	B	1234	CLA	ND
8	B	1235	CLA	ND
8	B	1236	CLA	ND
8	B	1238	CLA	ND
8	B	1239	CLA	ND
8	B	1240	CLA	ND
8	K	1401	CLA	ND
8	K	1402	CLA	ND

All (1541) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1011	CLA	C2A-CAA-CBA-CGA
8	A	1011	CLA	CHA-CBD-CGD-O1D
8	A	1011	CLA	CHA-CBD-CGD-O2D
8	A	1011	CLA	CBD-CGD-O2D-CED
8	A	1101	CLA	CHA-CBD-CGD-O1D
8	A	1101	CLA	CHA-CBD-CGD-O2D
8	A	1103	CLA	C3A-C2A-CAA-CBA
8	A	1104	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	A	1104	CLA	CHA-CBD-CGD-O2D
8	A	1104	CLA	CBD-CGD-O2D-CED
8	A	1105	CLA	C1A-C2A-CAA-CBA
8	A	1106	CLA	C1A-C2A-CAA-CBA
8	A	1106	CLA	C3A-C2A-CAA-CBA
8	A	1108	CLA	C1A-C2A-CAA-CBA
8	A	1108	CLA	C3A-C2A-CAA-CBA
8	A	1108	CLA	CAD-CBD-CGD-O1D
8	A	1108	CLA	CAD-CBD-CGD-O2D
8	A	1108	CLA	CBD-CGD-O2D-CED
8	A	1109	CLA	C2-C3-C5-C6
8	A	1109	CLA	C4-C3-C5-C6
8	A	1110	CLA	CAD-CBD-CGD-O2D
8	A	1110	CLA	CBD-CGD-O2D-CED
8	A	1112	CLA	C1A-C2A-CAA-CBA
8	A	1112	CLA	C3A-C2A-CAA-CBA
8	A	1112	CLA	C2-C1-O2A-CGA
8	A	1112	CLA	CBD-CGD-O2D-CED
8	A	1115	CLA	CBD-CGD-O2D-CED
8	A	1116	CLA	C2A-CAA-CBA-CGA
8	A	1117	CLA	C2-C1-O2A-CGA
8	A	1117	CLA	CHA-CBD-CGD-O1D
8	A	1117	CLA	CHA-CBD-CGD-O2D
8	A	1117	CLA	CBD-CGD-O2D-CED
8	A	1118	CLA	CBA-CGA-O2A-C1
8	A	1118	CLA	CHA-CBD-CGD-O1D
8	A	1118	CLA	CHA-CBD-CGD-O2D
8	A	1118	CLA	CAD-CBD-CGD-O1D
8	A	1118	CLA	CAD-CBD-CGD-O2D
8	A	1119	CLA	C3A-C2A-CAA-CBA
8	A	1119	CLA	CHA-CBD-CGD-O1D
8	A	1119	CLA	CHA-CBD-CGD-O2D
8	A	1119	CLA	CBD-CGD-O2D-CED
8	A	1120	CLA	C1A-C2A-CAA-CBA
8	A	1120	CLA	C3A-C2A-CAA-CBA
8	A	1120	CLA	CBD-CGD-O2D-CED
8	A	1121	CLA	C1A-C2A-CAA-CBA
8	A	1121	CLA	CHA-CBD-CGD-O1D
8	A	1121	CLA	CHA-CBD-CGD-O2D
8	A	1121	CLA	CBD-CGD-O2D-CED
8	A	1122	CLA	CHA-CBD-CGD-O1D
8	A	1122	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	A	1123	CLA	C3A-C2A-CAA-CBA
8	A	1123	CLA	C2-C1-O2A-CGA
8	A	1123	CLA	C11-C12-C13-C14
8	A	1124	CLA	C1A-C2A-CAA-CBA
8	A	1124	CLA	C3A-C2A-CAA-CBA
8	A	1125	CLA	CBD-CGD-O2D-CED
8	A	1126	CLA	C1A-C2A-CAA-CBA
8	A	1126	CLA	C3A-C2A-CAA-CBA
8	A	1126	CLA	C2-C1-O2A-CGA
8	A	1126	CLA	CHA-CBD-CGD-O1D
8	A	1126	CLA	CHA-CBD-CGD-O2D
8	A	1126	CLA	CBD-CGD-O2D-CED
8	A	1127	CLA	CHA-CBD-CGD-O1D
8	A	1127	CLA	CHA-CBD-CGD-O2D
8	A	1129	CLA	CBA-CGA-O2A-C1
8	A	1132	CLA	CHA-CBD-CGD-O1D
8	A	1132	CLA	CHA-CBD-CGD-O2D
8	A	1133	CLA	C2A-CAA-CBA-CGA
8	A	1133	CLA	CHA-CBD-CGD-O1D
8	A	1133	CLA	CHA-CBD-CGD-O2D
8	A	1133	CLA	CBD-CGD-O2D-CED
8	A	1134	CLA	C1A-C2A-CAA-CBA
8	A	1134	CLA	C3A-C2A-CAA-CBA
8	A	1136	CLA	CHA-CBD-CGD-O1D
8	A	1136	CLA	CHA-CBD-CGD-O2D
8	A	1137	CLA	CHA-CBD-CGD-O1D
8	A	1137	CLA	CHA-CBD-CGD-O2D
8	A	1138	CLA	C2-C1-O2A-CGA
8	A	1138	CLA	CHA-CBD-CGD-O1D
8	A	1138	CLA	CHA-CBD-CGD-O2D
8	A	1140	CLA	C1A-C2A-CAA-CBA
8	A	1140	CLA	C3A-C2A-CAA-CBA
8	A	1801	CLA	C2C-C3C-CAC-CBC
8	A	1013	CLA	C1A-C2A-CAA-CBA
8	A	1013	CLA	C3A-C2A-CAA-CBA
8	A	1013	CLA	CBA-CGA-O2A-C1
8	A	1013	CLA	O1A-CGA-O2A-C1
8	A	1013	CLA	CHA-CBD-CGD-O1D
8	A	1013	CLA	CHA-CBD-CGD-O2D
8	B	1022	CLA	CHA-CBD-CGD-O1D
8	B	1022	CLA	CHA-CBD-CGD-O2D
8	B	1237	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	B	1021	CLA	C3A-C2A-CAA-CBA
8	B	1021	CLA	CBA-CGA-O2A-C1
8	B	1021	CLA	CBD-CGD-O2D-CED
8	B	1023	CLA	CHA-CBD-CGD-O1D
8	B	1023	CLA	CHA-CBD-CGD-O2D
8	B	1201	CLA	CAD-CBD-CGD-O1D
8	B	1201	CLA	CAD-CBD-CGD-O2D
8	B	1202	CLA	C2-C1-O2A-CGA
8	B	1202	CLA	CHA-CBD-CGD-O1D
8	B	1202	CLA	CHA-CBD-CGD-O2D
8	B	1203	CLA	CHA-CBD-CGD-O1D
8	B	1203	CLA	CHA-CBD-CGD-O2D
8	B	1204	CLA	CHA-CBD-CGD-O1D
8	B	1204	CLA	CHA-CBD-CGD-O2D
8	B	1206	CLA	C1A-C2A-CAA-CBA
8	B	1206	CLA	C3A-C2A-CAA-CBA
8	B	1207	CLA	C2-C1-O2A-CGA
8	B	1207	CLA	CBD-CGD-O2D-CED
8	B	1208	CLA	CBD-CGD-O2D-CED
8	B	1209	CLA	C1A-C2A-CAA-CBA
8	B	1209	CLA	C3A-C2A-CAA-CBA
8	B	1209	CLA	CBD-CGD-O2D-CED
8	B	1210	CLA	C2-C1-O2A-CGA
8	B	1211	CLA	CBA-CGA-O2A-C1
8	B	1212	CLA	CHA-CBD-CGD-O1D
8	B	1212	CLA	CHA-CBD-CGD-O2D
8	B	1213	CLA	C1A-C2A-CAA-CBA
8	B	1213	CLA	CBD-CGD-O2D-CED
8	B	1215	CLA	C3A-C2A-CAA-CBA
8	B	1215	CLA	CBD-CGD-O2D-CED
8	B	1216	CLA	C1A-C2A-CAA-CBA
8	B	1216	CLA	CHA-CBD-CGD-O1D
8	B	1216	CLA	CHA-CBD-CGD-O2D
8	B	1216	CLA	CBD-CGD-O2D-CED
8	B	1216	CLA	C2-C3-C5-C6
8	B	1216	CLA	C4-C3-C5-C6
8	B	1217	CLA	C1A-C2A-CAA-CBA
8	B	1217	CLA	C3A-C2A-CAA-CBA
8	B	1218	CLA	C1A-C2A-CAA-CBA
8	B	1218	CLA	CHA-CBD-CGD-O1D
8	B	1218	CLA	CHA-CBD-CGD-O2D
8	B	1219	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	B	1219	CLA	CHA-CBD-CGD-O2D
8	B	1220	CLA	CBD-CGD-O2D-CED
8	B	1221	CLA	C2-C1-O2A-CGA
8	B	1221	CLA	CHA-CBD-CGD-O2D
8	B	1223	CLA	CAD-CBD-CGD-O1D
8	B	1223	CLA	CAD-CBD-CGD-O2D
8	B	1223	CLA	CBD-CGD-O2D-CED
8	B	1224	CLA	CHA-CBD-CGD-O1D
8	B	1224	CLA	CHA-CBD-CGD-O2D
8	B	1224	CLA	CBD-CGD-O2D-CED
8	B	1225	CLA	C1A-C2A-CAA-CBA
8	B	1225	CLA	C3A-C2A-CAA-CBA
8	B	1226	CLA	CHA-CBD-CGD-O1D
8	B	1226	CLA	CHA-CBD-CGD-O2D
8	B	1228	CLA	C2-C1-O2A-CGA
8	B	1228	CLA	CBD-CGD-O2D-CED
8	B	1229	CLA	C2-C1-O2A-CGA
8	B	1229	CLA	CBD-CGD-O2D-CED
8	B	1230	CLA	C2-C1-O2A-CGA
8	B	1230	CLA	CHA-CBD-CGD-O2D
8	B	1231	CLA	C2-C1-O2A-CGA
8	B	1232	CLA	C1A-C2A-CAA-CBA
8	B	1235	CLA	CHA-CBD-CGD-O1D
8	B	1235	CLA	CHA-CBD-CGD-O2D
8	B	1235	CLA	C2-C3-C5-C6
8	B	1235	CLA	C4-C3-C5-C6
8	B	1236	CLA	CBD-CGD-O2D-CED
8	B	1239	CLA	C2-C1-O2A-CGA
8	B	1240	CLA	CHA-CBD-CGD-O2D
8	K	1401	CLA	CBD-CGD-O2D-CED
8	K	1402	CLA	C2-C1-O2A-CGA
9	B	2002	PQN	C12-C13-C15-C16
9	B	2002	PQN	C14-C13-C15-C16
10	A	4001	BCR	C7-C8-C9-C10
10	A	4001	BCR	C7-C8-C9-C34
10	A	4001	BCR	C11-C10-C9-C8
10	A	4001	BCR	C11-C10-C9-C34
10	A	4001	BCR	C9-C10-C11-C12
10	A	4001	BCR	C17-C18-C19-C20
10	A	4001	BCR	C36-C18-C19-C20
10	A	4002	BCR	C7-C8-C9-C10
10	A	4002	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
10	A	4002	BCR	C11-C10-C9-C8
10	A	4002	BCR	C11-C10-C9-C34
10	A	4002	BCR	C10-C11-C12-C13
10	A	4003	BCR	C7-C8-C9-C10
10	A	4003	BCR	C7-C8-C9-C34
10	A	4003	BCR	C11-C10-C9-C8
10	A	4003	BCR	C11-C10-C9-C34
10	A	4003	BCR	C17-C18-C19-C20
10	A	4003	BCR	C36-C18-C19-C20
10	A	4007	BCR	C11-C10-C9-C34
10	A	4007	BCR	C17-C18-C19-C20
10	A	4007	BCR	C36-C18-C19-C20
10	A	4007	BCR	C23-C24-C25-C30
10	A	4008	BCR	C11-C10-C9-C8
10	A	4008	BCR	C11-C10-C9-C34
10	A	4008	BCR	C10-C11-C12-C13
10	A	4008	BCR	C11-C12-C13-C14
10	A	4008	BCR	C11-C12-C13-C35
10	A	4008	BCR	C21-C22-C23-C24
10	A	4008	BCR	C37-C22-C23-C24
10	A	4008	BCR	C23-C24-C25-C26
10	A	4012	BCR	C7-C8-C9-C10
10	A	4012	BCR	C7-C8-C9-C34
10	A	4012	BCR	C11-C10-C9-C8
10	A	4012	BCR	C11-C10-C9-C34
10	A	4012	BCR	C10-C11-C12-C13
10	A	4012	BCR	C11-C12-C13-C14
10	A	4012	BCR	C11-C12-C13-C35
10	A	4019	BCR	C11-C10-C9-C8
10	A	4019	BCR	C11-C10-C9-C34
10	A	4019	BCR	C17-C18-C19-C20
10	A	4019	BCR	C36-C18-C19-C20
10	A	4019	BCR	C19-C20-C21-C22
10	B	4011	BCR	C7-C8-C9-C10
10	B	4011	BCR	C7-C8-C9-C34
10	B	4011	BCR	C11-C10-C9-C8
10	B	4011	BCR	C11-C10-C9-C34
10	B	4011	BCR	C19-C20-C21-C22
10	B	4011	BCR	C21-C22-C23-C24
10	B	4011	BCR	C37-C22-C23-C24
10	B	4011	BCR	C23-C24-C25-C26
10	B	4011	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
10	B	4004	BCR	C5-C6-C7-C8
10	B	4004	BCR	C11-C10-C9-C8
10	B	4004	BCR	C11-C10-C9-C34
10	B	4004	BCR	C10-C11-C12-C13
10	B	4004	BCR	C21-C22-C23-C24
10	B	4004	BCR	C37-C22-C23-C24
10	B	4005	BCR	C5-C6-C7-C8
10	B	4005	BCR	C7-C8-C9-C10
10	B	4005	BCR	C7-C8-C9-C34
10	B	4005	BCR	C17-C18-C19-C20
10	B	4005	BCR	C36-C18-C19-C20
10	B	4010	BCR	C11-C10-C9-C8
10	B	4010	BCR	C11-C10-C9-C34
10	B	4010	BCR	C10-C11-C12-C13
10	B	4010	BCR	C17-C18-C19-C20
10	B	4010	BCR	C36-C18-C19-C20
10	B	4010	BCR	C21-C22-C23-C24
10	B	4010	BCR	C37-C22-C23-C24
10	B	4010	BCR	C23-C24-C25-C26
10	B	4010	BCR	C23-C24-C25-C30
10	B	4014	BCR	C11-C10-C9-C8
10	B	4014	BCR	C11-C10-C9-C34
10	B	4017	BCR	C11-C10-C9-C8
10	B	4017	BCR	C11-C10-C9-C34
10	B	4017	BCR	C10-C11-C12-C13
10	B	4017	BCR	C11-C12-C13-C14
10	B	4017	BCR	C11-C12-C13-C35
10	B	4018	BCR	C21-C22-C23-C24
10	B	4018	BCR	C37-C22-C23-C24
10	K	4001	BCR	C11-C10-C9-C8
10	K	4001	BCR	C11-C10-C9-C34
10	K	4001	BCR	C10-C11-C12-C13
11	A	5001	LHG	C1-C2-C3-O3
11	A	5003	LHG	O1-C1-C2-C3
11	A	5003	LHG	C4-O6-P-O5
11	B	5004	LHG	C1-C2-C3-O3
11	B	5004	LHG	C3-O3-P-O6
11	B	5004	LHG	C4-O6-P-O3
11	B	5004	LHG	C8-C7-O7-C5
11	B	5006	LHG	O1-C1-C2-C3
11	B	5006	LHG	C1-C2-C3-O3
11	B	5006	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
11	B	5006	LHG	O9-C7-O7-C5
11	B	5006	LHG	C8-C7-O7-C5
11	M	5001	LHG	O1-C1-C2-O2
11	M	5001	LHG	C3-O3-P-O5
11	M	5001	LHG	C4-O6-P-O5
11	M	5001	LHG	O9-C7-O7-C5
12	K	5009	LMG	C2-C1-O1-C7
12	K	5009	LMG	O6-C1-O1-C7
12	K	5009	LMG	C11-C10-O7-C8
14	B	4006	ECH	C7-C8-C9-C34
14	B	4006	ECH	C21-C22-C23-C24
14	M	4021	ECH	C5-C6-C7-C8
14	M	4021	ECH	C7-C8-C9-C10
14	M	4021	ECH	C7-C8-C9-C34
14	M	4021	ECH	C11-C12-C13-C14
14	M	4021	ECH	C11-C12-C13-C35
14	M	4021	ECH	C17-C18-C19-C20
14	M	4021	ECH	C36-C18-C19-C20
14	M	4021	ECH	C21-C22-C23-C24
14	M	4021	ECH	C37-C22-C23-C24
14	M	4021	ECH	C23-C24-C25-C30
15	B	5008	SQD	C2-C1-O6-C44
15	B	5008	SQD	O5-C1-O6-C44
15	B	5008	SQD	O47-C45-C46-O48
8	A	1011	CLA	O1D-CGD-O2D-CED
8	A	1012	CLA	O1D-CGD-O2D-CED
8	A	1105	CLA	O1D-CGD-O2D-CED
8	A	1132	CLA	O1D-CGD-O2D-CED
8	A	1138	CLA	O1D-CGD-O2D-CED
8	B	1202	CLA	O1D-CGD-O2D-CED
8	B	1227	CLA	O1D-CGD-O2D-CED
8	B	1228	CLA	O1D-CGD-O2D-CED
8	A	1104	CLA	O1D-CGD-O2D-CED
8	A	1128	CLA	O1D-CGD-O2D-CED
8	A	1131	CLA	O1D-CGD-O2D-CED
8	A	1139	CLA	O1D-CGD-O2D-CED
8	A	1801	CLA	O1D-CGD-O2D-CED
8	B	1021	CLA	O1D-CGD-O2D-CED
8	B	1203	CLA	O1D-CGD-O2D-CED
8	B	1208	CLA	O1D-CGD-O2D-CED
8	B	1232	CLA	O1D-CGD-O2D-CED
8	B	1238	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	A	1012	CLA	CBD-CGD-O2D-CED
8	A	1102	CLA	CBD-CGD-O2D-CED
8	A	1103	CLA	CBD-CGD-O2D-CED
8	A	1105	CLA	CBD-CGD-O2D-CED
8	A	1107	CLA	CBD-CGD-O2D-CED
8	A	1109	CLA	CBD-CGD-O2D-CED
8	A	1111	CLA	CBD-CGD-O2D-CED
8	A	1113	CLA	CBD-CGD-O2D-CED
8	A	1114	CLA	CBD-CGD-O2D-CED
8	A	1116	CLA	CBD-CGD-O2D-CED
8	A	1118	CLA	CBD-CGD-O2D-CED
8	A	1123	CLA	CBD-CGD-O2D-CED
8	A	1124	CLA	CBD-CGD-O2D-CED
8	A	1128	CLA	CBD-CGD-O2D-CED
8	A	1130	CLA	CBD-CGD-O2D-CED
8	A	1131	CLA	CBD-CGD-O2D-CED
8	A	1132	CLA	CBD-CGD-O2D-CED
8	A	1134	CLA	CBD-CGD-O2D-CED
8	A	1135	CLA	CBD-CGD-O2D-CED
8	A	1136	CLA	CBD-CGD-O2D-CED
8	A	1137	CLA	CBD-CGD-O2D-CED
8	A	1138	CLA	CBD-CGD-O2D-CED
8	A	1139	CLA	CBD-CGD-O2D-CED
8	A	1801	CLA	CBD-CGD-O2D-CED
8	A	1013	CLA	CBD-CGD-O2D-CED
8	B	1022	CLA	CBD-CGD-O2D-CED
8	B	1237	CLA	CBD-CGD-O2D-CED
8	B	1023	CLA	CBD-CGD-O2D-CED
8	B	1202	CLA	CBD-CGD-O2D-CED
8	B	1203	CLA	CBD-CGD-O2D-CED
8	B	1204	CLA	CBD-CGD-O2D-CED
8	B	1206	CLA	CBD-CGD-O2D-CED
8	B	1210	CLA	CBD-CGD-O2D-CED
8	B	1214	CLA	CBD-CGD-O2D-CED
8	B	1217	CLA	CBD-CGD-O2D-CED
8	B	1218	CLA	CBD-CGD-O2D-CED
8	B	1219	CLA	CBD-CGD-O2D-CED
8	B	1221	CLA	CBD-CGD-O2D-CED
8	B	1222	CLA	CBD-CGD-O2D-CED
8	B	1225	CLA	CBD-CGD-O2D-CED
8	B	1227	CLA	CBD-CGD-O2D-CED
8	B	1231	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	B	1232	CLA	CBD-CGD-O2D-CED
8	B	1238	CLA	CBD-CGD-O2D-CED
8	B	1239	CLA	CBD-CGD-O2D-CED
8	B	1240	CLA	CBD-CGD-O2D-CED
8	K	1402	CLA	CBD-CGD-O2D-CED
8	A	1107	CLA	O1A-CGA-O2A-C1
8	A	1109	CLA	O1A-CGA-O2A-C1
8	A	1127	CLA	O1A-CGA-O2A-C1
8	B	1237	CLA	O1A-CGA-O2A-C1
8	B	1021	CLA	O1A-CGA-O2A-C1
8	A	1115	CLA	O1A-CGA-O2A-C1
8	A	1118	CLA	O1A-CGA-O2A-C1
8	A	1108	CLA	O1D-CGD-O2D-CED
8	A	1109	CLA	O1D-CGD-O2D-CED
8	A	1113	CLA	O1D-CGD-O2D-CED
8	A	1116	CLA	O1D-CGD-O2D-CED
8	A	1117	CLA	O1D-CGD-O2D-CED
8	A	1119	CLA	O1D-CGD-O2D-CED
8	A	1124	CLA	O1D-CGD-O2D-CED
8	A	1137	CLA	O1D-CGD-O2D-CED
8	A	1013	CLA	O1D-CGD-O2D-CED
8	B	1237	CLA	O1D-CGD-O2D-CED
8	B	1218	CLA	O1D-CGD-O2D-CED
8	B	1219	CLA	O1D-CGD-O2D-CED
8	B	1231	CLA	O1D-CGD-O2D-CED
8	A	1115	CLA	CBA-CGA-O2A-C1
8	A	1134	CLA	CBA-CGA-O2A-C1
8	A	1102	CLA	O1D-CGD-O2D-CED
8	A	1107	CLA	O1D-CGD-O2D-CED
8	A	1110	CLA	O1D-CGD-O2D-CED
8	A	1112	CLA	O1D-CGD-O2D-CED
8	A	1114	CLA	O1D-CGD-O2D-CED
8	A	1121	CLA	O1D-CGD-O2D-CED
8	A	1125	CLA	O1D-CGD-O2D-CED
8	A	1133	CLA	O1D-CGD-O2D-CED
8	A	1135	CLA	O1D-CGD-O2D-CED
8	B	1022	CLA	O1D-CGD-O2D-CED
8	B	1206	CLA	O1D-CGD-O2D-CED
8	B	1207	CLA	O1D-CGD-O2D-CED
8	B	1213	CLA	O1D-CGD-O2D-CED
8	B	1214	CLA	O1D-CGD-O2D-CED
8	B	1215	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	B	1224	CLA	O1D-CGD-O2D-CED
8	B	1229	CLA	O1D-CGD-O2D-CED
8	A	1107	CLA	CBA-CGA-O2A-C1
8	A	1109	CLA	CBA-CGA-O2A-C1
8	B	1214	CLA	CBA-CGA-O2A-C1
8	B	1221	CLA	CBA-CGA-O2A-C1
8	A	1106	CLA	CBD-CGD-O2D-CED
8	A	1122	CLA	CBD-CGD-O2D-CED
8	A	1129	CLA	CBD-CGD-O2D-CED
8	A	1140	CLA	CBD-CGD-O2D-CED
8	B	1201	CLA	CBD-CGD-O2D-CED
8	B	1205	CLA	CBD-CGD-O2D-CED
8	B	1212	CLA	CBD-CGD-O2D-CED
8	B	1226	CLA	CBD-CGD-O2D-CED
8	B	1230	CLA	CBD-CGD-O2D-CED
8	A	1102	CLA	O1A-CGA-O2A-C1
8	A	1104	CLA	O1A-CGA-O2A-C1
8	B	1206	CLA	O1A-CGA-O2A-C1
8	B	1209	CLA	O1A-CGA-O2A-C1
8	B	1214	CLA	O1A-CGA-O2A-C1
8	B	1219	CLA	O1A-CGA-O2A-C1
8	B	1221	CLA	O1A-CGA-O2A-C1
8	B	1227	CLA	O1A-CGA-O2A-C1
8	B	1228	CLA	O1A-CGA-O2A-C1
8	B	1238	CLA	O1A-CGA-O2A-C1
12	A	5002	LMG	O10-C28-O8-C9
12	B	5005	LMG	O10-C28-O8-C9
8	A	1129	CLA	O1A-CGA-O2A-C1
8	B	1211	CLA	O1A-CGA-O2A-C1
8	A	1115	CLA	O1D-CGD-O2D-CED
8	A	1120	CLA	O1D-CGD-O2D-CED
8	A	1126	CLA	O1D-CGD-O2D-CED
8	B	1216	CLA	O1D-CGD-O2D-CED
8	B	1220	CLA	O1D-CGD-O2D-CED
8	B	1223	CLA	O1D-CGD-O2D-CED
8	B	1209	CLA	O1D-CGD-O2D-CED
8	B	1225	CLA	O1D-CGD-O2D-CED
8	B	1236	CLA	O1D-CGD-O2D-CED
8	K	1401	CLA	O1D-CGD-O2D-CED
8	A	1130	CLA	O1D-CGD-O2D-CED
8	A	1134	CLA	O1D-CGD-O2D-CED
11	B	5004	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
12	K	5009	LMG	O9-C10-O7-C8
8	A	1801	CLA	O1A-CGA-O2A-C1
8	A	1123	CLA	C3-C5-C6-C7
8	A	1126	CLA	C3-C5-C6-C7
8	A	1127	CLA	C3-C5-C6-C7
8	A	1131	CLA	C3-C5-C6-C7
8	B	1021	CLA	C3-C5-C6-C7
8	B	1023	CLA	C3-C5-C6-C7
8	B	1203	CLA	C3-C5-C6-C7
8	B	1205	CLA	C3-C5-C6-C7
8	B	1206	CLA	C3-C5-C6-C7
8	B	1215	CLA	C3-C5-C6-C7
8	B	1222	CLA	C3-C5-C6-C7
8	B	1223	CLA	C3-C5-C6-C7
8	B	1226	CLA	C3-C5-C6-C7
8	B	1238	CLA	C3-C5-C6-C7
8	K	1401	CLA	C3-C5-C6-C7
8	K	1402	CLA	C3-C5-C6-C7
9	B	2002	PQN	C13-C15-C16-C17
8	A	1011	CLA	CBA-CGA-O2A-C1
8	A	1102	CLA	CBA-CGA-O2A-C1
8	A	1112	CLA	CBA-CGA-O2A-C1
8	A	1127	CLA	CBA-CGA-O2A-C1
8	A	1131	CLA	CBA-CGA-O2A-C1
8	A	1132	CLA	CBA-CGA-O2A-C1
8	B	1209	CLA	CBA-CGA-O2A-C1
8	B	1218	CLA	CBA-CGA-O2A-C1
8	B	1227	CLA	CBA-CGA-O2A-C1
8	B	1228	CLA	CBA-CGA-O2A-C1
8	B	1238	CLA	CBA-CGA-O2A-C1
12	A	5002	LMG	C29-C28-O8-C9
12	B	5005	LMG	C29-C28-O8-C9
11	M	5001	LHG	C8-C7-O7-C5
8	B	1023	CLA	O1D-CGD-O2D-CED
8	B	1217	CLA	O1D-CGD-O2D-CED
8	A	1127	CLA	CBD-CGD-O2D-CED
8	A	1134	CLA	O1A-CGA-O2A-C1
8	A	1801	CLA	CBA-CGA-O2A-C1
8	A	1012	CLA	C4-C3-C5-C6
8	A	1131	CLA	C4-C3-C5-C6
8	B	1215	CLA	C4-C3-C5-C6
8	B	1225	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	A	2001	PQN	C14-C13-C15-C16
8	A	1012	CLA	C2-C3-C5-C6
8	A	1106	CLA	C2A-CAA-CBA-CGA
8	A	1119	CLA	C2A-CAA-CBA-CGA
8	A	1130	CLA	C2A-CAA-CBA-CGA
8	B	1237	CLA	C2A-CAA-CBA-CGA
8	B	1214	CLA	C2A-CAA-CBA-CGA
8	B	1216	CLA	C2A-CAA-CBA-CGA
8	B	1229	CLA	C2A-CAA-CBA-CGA
8	B	1230	CLA	C2A-CAA-CBA-CGA
12	A	5002	LMG	C17-C18-C19-C20
12	A	5002	LMG	C38-C39-C40-C41
12	A	5002	LMG	C41-C42-C43-C44
12	B	5002	LMG	C20-C21-C22-C23
12	B	5002	LMG	C23-C24-C25-C26
12	B	5002	LMG	C35-C36-C37-C38
8	A	1109	CLA	C3-C5-C6-C7
8	A	1111	CLA	C3-C5-C6-C7
8	A	1133	CLA	C3-C5-C6-C7
8	A	1135	CLA	C3-C5-C6-C7
8	B	1209	CLA	C3-C5-C6-C7
8	B	1225	CLA	C3-C5-C6-C7
8	A	1104	CLA	CBA-CGA-O2A-C1
8	A	1110	CLA	CBA-CGA-O2A-C1
8	A	1120	CLA	CBA-CGA-O2A-C1
8	A	1138	CLA	CBA-CGA-O2A-C1
8	B	1023	CLA	CBA-CGA-O2A-C1
8	B	1206	CLA	CBA-CGA-O2A-C1
8	B	1207	CLA	CBA-CGA-O2A-C1
8	B	1210	CLA	CBA-CGA-O2A-C1
8	B	1216	CLA	CBA-CGA-O2A-C1
8	B	1219	CLA	CBA-CGA-O2A-C1
8	B	1239	CLA	CBA-CGA-O2A-C1
8	B	1222	CLA	O1D-CGD-O2D-CED
8	A	1118	CLA	O1D-CGD-O2D-CED
8	B	1204	CLA	O1D-CGD-O2D-CED
8	B	1221	CLA	O1D-CGD-O2D-CED
8	B	1240	CLA	O1D-CGD-O2D-CED
8	A	1011	CLA	O1A-CGA-O2A-C1
8	A	1112	CLA	O1A-CGA-O2A-C1
8	A	1120	CLA	O1A-CGA-O2A-C1
8	A	1130	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	A	1132	CLA	O1A-CGA-O2A-C1
8	B	1218	CLA	O1A-CGA-O2A-C1
8	B	1239	CLA	O1A-CGA-O2A-C1
10	A	4003	BCR	C13-C14-C15-C16
10	A	4008	BCR	C15-C16-C17-C18
10	A	4008	BCR	C19-C20-C21-C22
10	B	4010	BCR	C13-C14-C15-C16
10	B	4014	BCR	C19-C20-C21-C22
8	A	1111	CLA	O1D-CGD-O2D-CED
11	B	5004	LHG	O2-C2-C3-O3
8	B	1210	CLA	C3-C5-C6-C7
8	B	1216	CLA	C3-C5-C6-C7
8	B	1240	CLA	C3-C5-C6-C7
8	A	1122	CLA	CBA-CGA-O2A-C1
8	A	1130	CLA	CBA-CGA-O2A-C1
8	K	1402	CLA	CBA-CGA-O2A-C1
8	A	1131	CLA	O1A-CGA-O2A-C1
8	B	1207	CLA	O1A-CGA-O2A-C1
8	B	1216	CLA	O1A-CGA-O2A-C1
8	K	1402	CLA	O1D-CGD-O2D-CED
8	B	1234	CLA	CBD-CGD-O2D-CED
8	A	1110	CLA	O1A-CGA-O2A-C1
8	A	1138	CLA	O1A-CGA-O2A-C1
8	B	1023	CLA	O1A-CGA-O2A-C1
8	B	1235	CLA	CBD-CGD-O2D-CED
8	A	1130	CLA	C3-C5-C6-C7
8	A	1136	CLA	C3-C5-C6-C7
8	B	1224	CLA	C3-C5-C6-C7
8	A	1136	CLA	O1D-CGD-O2D-CED
8	B	1210	CLA	O1A-CGA-O2A-C1
8	K	1402	CLA	O1A-CGA-O2A-C1
8	A	1128	CLA	C4-C3-C5-C6
8	B	1238	CLA	C4-C3-C5-C6
8	B	1238	CLA	C2-C3-C5-C6
8	A	1122	CLA	C2A-CAA-CBA-CGA
8	A	1131	CLA	C2A-CAA-CBA-CGA
8	A	1136	CLA	C2A-CAA-CBA-CGA
8	B	1224	CLA	C2A-CAA-CBA-CGA
8	B	1228	CLA	C2A-CAA-CBA-CGA
8	A	1123	CLA	O1D-CGD-O2D-CED
8	A	1122	CLA	O1A-CGA-O2A-C1
8	B	1231	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	A	1103	CLA	O1D-CGD-O2D-CED
8	A	1140	CLA	O1D-CGD-O2D-CED
8	B	1202	CLA	CBA-CGA-O2A-C1
8	B	1231	CLA	CBA-CGA-O2A-C1
8	B	1239	CLA	O1D-CGD-O2D-CED
8	A	1129	CLA	O1D-CGD-O2D-CED
8	B	1201	CLA	O1D-CGD-O2D-CED
8	B	1205	CLA	O1D-CGD-O2D-CED
8	B	1210	CLA	O1D-CGD-O2D-CED
8	B	1212	CLA	O1D-CGD-O2D-CED
8	A	1101	CLA	CBD-CGD-O2D-CED
11	M	5001	LHG	C1-C2-C3-O3
8	B	1202	CLA	O1A-CGA-O2A-C1
8	A	1116	CLA	CBA-CGA-O2A-C1
8	A	1117	CLA	CBA-CGA-O2A-C1
8	A	1123	CLA	CBA-CGA-O2A-C1
8	B	1215	CLA	CBA-CGA-O2A-C1
8	B	1222	CLA	CBA-CGA-O2A-C1
8	B	1240	CLA	CBA-CGA-O2A-C1
10	A	4001	BCR	C19-C20-C21-C22
10	A	4002	BCR	C15-C16-C17-C18
10	A	4008	BCR	C9-C10-C11-C12
10	A	4008	BCR	C13-C14-C15-C16
11	B	5004	LHG	C23-C24-C25-C26
8	B	1229	CLA	C8-C10-C11-C12
11	A	5003	LHG	C13-C14-C15-C16
8	A	1102	CLA	C5-C6-C7-C8
8	A	1104	CLA	C13-C15-C16-C17
8	A	1110	CLA	C5-C6-C7-C8
8	B	1210	CLA	C10-C11-C12-C13
8	B	1229	CLA	C13-C15-C16-C17
8	B	1230	CLA	C5-C6-C7-C8
8	B	1234	CLA	C10-C11-C12-C13
8	B	1238	CLA	C15-C16-C17-C18
9	A	2001	PQN	C18-C20-C21-C22
11	A	5001	LHG	O2-C2-C3-O3
11	B	5006	LHG	O2-C2-C3-O3
11	M	5001	LHG	O2-C2-C3-O3
11	A	5001	LHG	C7-C8-C9-C10
8	B	1240	CLA	O1A-CGA-O2A-C1
8	A	1131	CLA	C2-C3-C5-C6
8	B	1215	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	A	2001	PQN	C12-C13-C15-C16
8	A	1101	CLA	C6-C7-C8-C9
8	A	1103	CLA	C6-C7-C8-C9
8	B	1021	CLA	C6-C7-C8-C9
8	B	1203	CLA	C14-C13-C15-C16
8	B	1214	CLA	C6-C7-C8-C9
8	B	1215	CLA	C6-C7-C8-C9
8	B	1228	CLA	C6-C7-C8-C9
8	B	1234	CLA	C11-C10-C8-C9
9	A	2001	PQN	C21-C22-C23-C24
8	A	1106	CLA	O1D-CGD-O2D-CED
8	A	1122	CLA	O1D-CGD-O2D-CED
8	B	1226	CLA	O1D-CGD-O2D-CED
8	B	1230	CLA	O1D-CGD-O2D-CED
8	A	1104	CLA	C10-C11-C12-C13
10	A	4002	BCR	C36-C18-C19-C20
10	A	4003	BCR	C11-C12-C13-C35
10	A	4008	BCR	C36-C18-C19-C20
10	A	4019	BCR	C37-C22-C23-C24
10	B	4004	BCR	C7-C8-C9-C34
10	B	4014	BCR	C7-C8-C9-C34
10	B	4014	BCR	C37-C22-C23-C24
10	B	4018	BCR	C11-C12-C13-C35
10	A	4002	BCR	C17-C18-C19-C20
10	A	4003	BCR	C11-C12-C13-C14
10	A	4019	BCR	C21-C22-C23-C24
10	B	4004	BCR	C7-C8-C9-C10
10	B	4014	BCR	C7-C8-C9-C10
10	B	4014	BCR	C21-C22-C23-C24
12	A	5002	LMG	C11-C10-O7-C8
11	A	5003	LHG	C11-C12-C13-C14
8	A	1116	CLA	O1A-CGA-O2A-C1
8	A	1117	CLA	O1A-CGA-O2A-C1
8	B	1022	CLA	C8-C10-C11-C12
8	B	1223	CLA	C10-C11-C12-C13
8	B	1220	CLA	C8-C10-C11-C12
8	A	1133	CLA	CBA-CGA-O2A-C1
8	A	1101	CLA	C13-C15-C16-C17
8	A	1106	CLA	C5-C6-C7-C8
8	A	1123	CLA	C13-C15-C16-C17
8	A	1127	CLA	C10-C11-C12-C13
8	A	1135	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	A	1136	CLA	C13-C15-C16-C17
8	B	1209	CLA	C15-C16-C17-C18
8	B	1210	CLA	C15-C16-C17-C18
8	B	1215	CLA	C8-C10-C11-C12
8	B	1215	CLA	C13-C15-C16-C17
8	B	1225	CLA	C5-C6-C7-C8
8	B	1238	CLA	C10-C11-C12-C13
8	K	1402	CLA	C8-C10-C11-C12
8	A	1119	CLA	C13-C15-C16-C17
8	A	1128	CLA	C10-C11-C12-C13
8	A	1136	CLA	C15-C16-C17-C18
8	B	1202	CLA	C5-C6-C7-C8
8	B	1214	CLA	C8-C10-C11-C12
8	B	1219	CLA	C15-C16-C17-C18
8	B	1223	CLA	C5-C6-C7-C8
8	B	1228	CLA	C5-C6-C7-C8
8	B	1238	CLA	C8-C10-C11-C12
9	A	2001	PQN	C15-C16-C17-C18
11	A	5001	LHG	C23-C24-C25-C26
12	B	5002	LMG	C28-C29-C30-C31
8	A	1119	CLA	C10-C11-C12-C13
8	A	1140	CLA	C13-C15-C16-C17
8	B	1216	CLA	C5-C6-C7-C8
8	B	1219	CLA	C5-C6-C7-C8
8	B	1228	CLA	C8-C10-C11-C12
8	B	1228	CLA	C15-C16-C17-C18
8	B	1234	CLA	C13-C15-C16-C17
8	A	1110	CLA	C2-C1-O2A-CGA
8	A	1120	CLA	C2-C1-O2A-CGA
8	A	1131	CLA	C2-C1-O2A-CGA
8	A	1132	CLA	C2-C1-O2A-CGA
8	A	1140	CLA	C2-C1-O2A-CGA
8	B	1237	CLA	C2-C1-O2A-CGA
8	B	1023	CLA	C2-C1-O2A-CGA
8	B	1203	CLA	C2-C1-O2A-CGA
8	B	1206	CLA	C2-C1-O2A-CGA
8	B	1209	CLA	C2-C1-O2A-CGA
8	B	1216	CLA	C2-C1-O2A-CGA
8	B	1219	CLA	C2-C1-O2A-CGA
8	B	1227	CLA	C2-C1-O2A-CGA
8	B	1236	CLA	C2-C1-O2A-CGA
8	A	1119	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	B	1217	CLA	C8-C10-C11-C12
8	B	1235	CLA	C8-C10-C11-C12
8	B	1209	CLA	C13-C15-C16-C17
8	A	1116	CLA	C4-C3-C5-C6
8	A	1126	CLA	C11-C10-C8-C7
8	A	1127	CLA	C11-C12-C13-C15
8	B	1237	CLA	C6-C7-C8-C10
8	B	1223	CLA	C6-C7-C8-C10
8	B	1229	CLA	C3-C5-C6-C7
8	A	1123	CLA	O1A-CGA-O2A-C1
8	B	1222	CLA	O1A-CGA-O2A-C1
10	B	4010	BCR	C9-C10-C11-C12
10	B	4017	BCR	C13-C14-C15-C16
8	A	1127	CLA	O1D-CGD-O2D-CED
8	A	1138	CLA	C15-C16-C17-C18
8	A	1140	CLA	C8-C10-C11-C12
8	A	1140	CLA	C10-C11-C12-C13
8	B	1207	CLA	C5-C6-C7-C8
8	B	1209	CLA	C5-C6-C7-C8
8	B	1225	CLA	C13-C15-C16-C17
8	B	1217	CLA	C5-C6-C7-C8
8	B	1231	CLA	C13-C15-C16-C17
10	A	4001	BCR	C10-C11-C12-C13
10	A	4003	BCR	C10-C11-C12-C13
10	B	4014	BCR	C10-C11-C12-C13
12	A	5002	LMG	O9-C10-O7-C8
8	B	1224	CLA	C13-C15-C16-C17
8	A	1123	CLA	C8-C10-C11-C12
8	A	1128	CLA	C8-C10-C11-C12
8	B	1022	CLA	C10-C11-C12-C13
8	B	1021	CLA	C8-C10-C11-C12
8	B	1221	CLA	C5-C6-C7-C8
8	B	1226	CLA	C10-C11-C12-C13
8	K	1402	CLA	C5-C6-C7-C8
8	B	1224	CLA	CBA-CGA-O2A-C1
8	B	1236	CLA	CBA-CGA-O2A-C1
8	A	1133	CLA	O1A-CGA-O2A-C1
8	B	1215	CLA	O1A-CGA-O2A-C1
8	A	1104	CLA	C15-C16-C17-C18
8	A	1126	CLA	C10-C11-C12-C13
8	A	1136	CLA	C10-C11-C12-C13
8	B	1217	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	B	1234	CLA	C5-C6-C7-C8
8	B	1239	CLA	C8-C10-C11-C12
11	A	5001	LHG	C8-C7-O7-C5
8	A	1103	CLA	C8-C10-C11-C12
8	B	1214	CLA	C15-C16-C17-C18
8	B	1217	CLA	C13-C15-C16-C17
11	A	5003	LHG	C3-O3-P-O6
8	A	1013	CLA	C3-C5-C6-C7
8	A	1136	CLA	C5-C6-C7-C8
11	A	5001	LHG	O9-C7-O7-C5
8	B	1225	CLA	C2-C3-C5-C6
8	B	1225	CLA	C8-C10-C11-C12
8	B	1231	CLA	C8-C10-C11-C12
8	A	1012	CLA	C2A-CAA-CBA-CGA
8	A	1117	CLA	C2A-CAA-CBA-CGA
8	B	1204	CLA	C2A-CAA-CBA-CGA
8	B	1218	CLA	C2A-CAA-CBA-CGA
8	A	1012	CLA	C6-C7-C8-C9
8	A	1108	CLA	C2A-CAA-CBA-CGA
8	A	1133	CLA	C13-C15-C16-C17
10	A	4012	BCR	C9-C10-C11-C12
14	M	4021	ECH	C9-C10-C11-C12
11	M	5001	LHG	C7-C8-C9-C10
11	A	5003	LHG	C8-C7-O7-C5
8	A	1011	CLA	C10-C11-C12-C13
10	B	4018	BCR	C11-C10-C9-C34
8	A	1110	CLA	C3-C5-C6-C7
8	B	1231	CLA	C3-C5-C6-C7
11	M	5001	LHG	C11-C12-C13-C14
8	A	1117	CLA	C16-C17-C18-C20
8	A	1127	CLA	C16-C17-C18-C19
8	B	1021	CLA	C11-C12-C13-C14
8	B	1215	CLA	C16-C17-C18-C20
8	B	1230	CLA	C16-C17-C18-C19
8	A	1136	CLA	CBA-CGA-O2A-C1
8	B	1229	CLA	CBA-CGA-O2A-C1
11	B	5004	LHG	C13-C14-C15-C16
11	A	5003	LHG	O9-C7-O7-C5
11	A	5001	LHG	C28-C29-C30-C31
12	K	5009	LMG	C32-C33-C34-C35
12	A	5002	LMG	C28-C29-C30-C31
10	A	4007	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
10	B	4018	BCR	C11-C10-C9-C8
11	B	5004	LHG	C31-C32-C33-C34
9	B	2002	PQN	C25-C26-C27-C28
8	A	1135	CLA	C16-C17-C18-C20
8	B	1203	CLA	C16-C17-C18-C19
8	B	1210	CLA	C16-C17-C18-C19
8	B	1213	CLA	C16-C17-C18-C20
8	B	1228	CLA	C16-C17-C18-C20
8	B	1235	CLA	C11-C12-C13-C15
11	M	5001	LHG	C28-C29-C30-C31
12	A	5002	LMG	C16-C17-C18-C19
12	K	5009	LMG	C29-C30-C31-C32
8	A	1122	CLA	C6-C7-C8-C9
8	A	1123	CLA	C14-C13-C15-C16
8	A	1140	CLA	C11-C10-C8-C9
8	A	1117	CLA	C15-C16-C17-C18
8	B	1210	CLA	C8-C10-C11-C12
8	K	1402	CLA	C13-C15-C16-C17
8	A	1138	CLA	C2A-CAA-CBA-CGA
8	B	1234	CLA	C2A-CAA-CBA-CGA
8	B	1240	CLA	C2A-CAA-CBA-CGA
14	B	4006	ECH	C37-C22-C23-C24
11	B	5004	LHG	C9-C10-C11-C12
11	A	5001	LHG	O1-C1-C2-C3
11	B	5004	LHG	O1-C1-C2-C3
11	M	5001	LHG	O1-C1-C2-C3
12	B	5005	LMG	O9-C10-O7-C8
8	A	1011	CLA	C5-C6-C7-C8
8	A	1128	CLA	C5-C6-C7-C8
8	B	1021	CLA	C5-C6-C7-C8
12	B	5005	LMG	C11-C10-O7-C8
11	A	5001	LHG	C31-C32-C33-C34
11	M	5001	LHG	C23-C24-C25-C26
8	A	1123	CLA	C16-C17-C18-C19
8	A	1123	CLA	C16-C17-C18-C20
8	A	1127	CLA	C16-C17-C18-C20
8	B	1022	CLA	C11-C12-C13-C15
8	B	1021	CLA	C11-C12-C13-C15
8	B	1209	CLA	C16-C17-C18-C20
8	B	1215	CLA	C16-C17-C18-C19
8	B	1217	CLA	C16-C17-C18-C19
8	A	1110	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	A	1126	CLA	C8-C10-C11-C12
8	B	1237	CLA	C5-C6-C7-C8
12	A	5002	LMG	C33-C34-C35-C36
8	A	1123	CLA	C15-C16-C17-C18
11	M	5001	LHG	C13-C14-C15-C16
8	A	1140	CLA	C3-C5-C6-C7
8	A	1012	CLA	C3A-C2A-CAA-CBA
8	A	1101	CLA	C3A-C2A-CAA-CBA
8	A	1104	CLA	C3A-C2A-CAA-CBA
8	A	1105	CLA	C3A-C2A-CAA-CBA
8	A	1111	CLA	C3A-C2A-CAA-CBA
8	A	1113	CLA	C3A-C2A-CAA-CBA
8	A	1131	CLA	C3A-C2A-CAA-CBA
8	A	1135	CLA	C3A-C2A-CAA-CBA
8	A	1139	CLA	C3A-C2A-CAA-CBA
8	B	1210	CLA	C3A-C2A-CAA-CBA
8	B	1213	CLA	C3A-C2A-CAA-CBA
8	B	1218	CLA	C3A-C2A-CAA-CBA
8	B	1219	CLA	C3A-C2A-CAA-CBA
8	B	1223	CLA	C3A-C2A-CAA-CBA
8	B	1234	CLA	C3A-C2A-CAA-CBA
8	B	1240	CLA	C3A-C2A-CAA-CBA
8	K	1402	CLA	C3A-C2A-CAA-CBA
8	A	1117	CLA	C5-C6-C7-C8
8	A	1123	CLA	C5-C6-C7-C8
8	B	1226	CLA	C5-C6-C7-C8
8	B	1238	CLA	C5-C6-C7-C8
11	B	5004	LHG	C7-C8-C9-C10
8	B	1236	CLA	O1A-CGA-O2A-C1
8	B	1237	CLA	C16-C17-C18-C19
8	B	1237	CLA	C16-C17-C18-C20
8	B	1209	CLA	C16-C17-C18-C19
8	B	1217	CLA	C16-C17-C18-C20
8	B	1230	CLA	C16-C17-C18-C20
11	A	5003	LHG	C28-C29-C30-C31
11	B	5004	LHG	C11-C12-C13-C14
11	M	5001	LHG	C9-C10-C11-C12
8	B	1224	CLA	O1A-CGA-O2A-C1
8	A	1133	CLA	C4-C3-C5-C6
8	A	1136	CLA	C4-C3-C5-C6
8	B	1209	CLA	C4-C3-C5-C6
8	B	1227	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	1128	CLA	C2-C3-C5-C6
8	A	1136	CLA	C2-C3-C5-C6
8	B	1219	CLA	C2-C3-C5-C6
8	B	1227	CLA	C2-C3-C5-C6
11	A	5003	LHG	O1-C1-C2-O2
11	B	5004	LHG	O1-C1-C2-O2
8	A	1126	CLA	C5-C6-C7-C8
11	B	5006	LHG	C7-C8-C9-C10
8	B	1229	CLA	O1A-CGA-O2A-C1
8	A	1122	CLA	C8-C10-C11-C12
8	B	1203	CLA	C10-C11-C12-C13
12	A	5002	LMG	C12-C13-C14-C15
8	B	1226	CLA	CBA-CGA-O2A-C1
11	A	5003	LHG	C26-C27-C28-C29
8	A	1011	CLA	C2-C1-O2A-CGA
8	A	1103	CLA	C2-C1-O2A-CGA
8	A	1105	CLA	C2-C1-O2A-CGA
8	A	1106	CLA	C2-C1-O2A-CGA
8	A	1111	CLA	C2-C1-O2A-CGA
8	A	1119	CLA	C2-C1-O2A-CGA
8	A	1125	CLA	C2-C1-O2A-CGA
8	A	1130	CLA	C2-C1-O2A-CGA
8	B	1022	CLA	C2-C1-O2A-CGA
8	B	1218	CLA	C2-C1-O2A-CGA
8	B	1220	CLA	C2-C1-O2A-CGA
8	B	1240	CLA	C2-C1-O2A-CGA
8	B	1214	CLA	C10-C11-C12-C13
8	B	1222	CLA	C5-C6-C7-C8
8	A	1136	CLA	O1A-CGA-O2A-C1
11	M	5001	LHG	C29-C30-C31-C32
12	B	5002	LMG	C34-C35-C36-C37
12	K	5009	LMG	C19-C20-C21-C22
8	B	1228	CLA	C16-C17-C18-C19
10	A	4002	BCR	C1-C6-C7-C8
10	A	4002	BCR	C5-C6-C7-C8
10	A	4007	BCR	C23-C24-C25-C26
10	A	4008	BCR	C1-C6-C7-C8
10	A	4008	BCR	C5-C6-C7-C8
10	A	4008	BCR	C23-C24-C25-C30
10	A	4012	BCR	C23-C24-C25-C26
10	A	4012	BCR	C23-C24-C25-C30
10	A	4019	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
10	A	4019	BCR	C23-C24-C25-C30
10	B	4004	BCR	C1-C6-C7-C8
10	B	4004	BCR	C23-C24-C25-C26
10	B	4004	BCR	C23-C24-C25-C30
10	B	4005	BCR	C1-C6-C7-C8
10	B	4014	BCR	C23-C24-C25-C26
10	B	4014	BCR	C23-C24-C25-C30
10	K	4001	BCR	C23-C24-C25-C26
10	K	4001	BCR	C23-C24-C25-C30
14	B	4006	ECH	C23-C24-C25-C26
14	B	4006	ECH	C23-C24-C25-C30
14	M	4021	ECH	C1-C6-C7-C8
14	M	4021	ECH	C23-C24-C25-C26
8	A	1011	CLA	C8-C10-C11-C12
8	A	1106	CLA	C8-C10-C11-C12
8	B	1023	CLA	C10-C11-C12-C13
8	B	1219	CLA	C4-C3-C5-C6
8	A	1101	CLA	O1D-CGD-O2D-CED
8	A	1101	CLA	C6-C7-C8-C10
8	A	1122	CLA	C6-C7-C8-C10
8	A	1123	CLA	C12-C13-C15-C16
8	A	1140	CLA	C11-C10-C8-C7
8	B	1210	CLA	C12-C13-C15-C16
8	B	1224	CLA	C2-C3-C5-C6
8	B	1226	CLA	O1A-CGA-O2A-C1
11	A	5003	LHG	C9-C10-C11-C12
8	A	1101	CLA	C5-C6-C7-C8
8	A	1135	CLA	C10-C11-C12-C13
8	B	1225	CLA	C15-C16-C17-C18
8	B	1234	CLA	C8-C10-C11-C12
8	B	1203	CLA	C16-C17-C18-C20
8	B	1235	CLA	C11-C12-C13-C14
8	A	1128	CLA	CBA-CGA-O2A-C1
11	A	5001	LHG	C25-C26-C27-C28
11	M	5001	LHG	C11-C10-C9-C8
8	A	1111	CLA	C2A-CAA-CBA-CGA
8	A	1115	CLA	C2A-CAA-CBA-CGA
8	A	1134	CLA	C2A-CAA-CBA-CGA
8	A	1013	CLA	C2A-CAA-CBA-CGA
8	B	1022	CLA	C2A-CAA-CBA-CGA
8	B	1023	CLA	C2A-CAA-CBA-CGA
8	B	1215	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
8	B	1235	CLA	O1D-CGD-O2D-CED
11	B	5004	LHG	C34-C35-C36-C37
8	B	1234	CLA	O1D-CGD-O2D-CED
8	B	1229	CLA	C5-C6-C7-C8
11	A	5003	LHG	C30-C31-C32-C33
8	B	1213	CLA	C16-C17-C18-C19
9	B	2002	PQN	C26-C27-C28-C30
15	B	5008	SQD	C8-C7-O47-C45
8	A	1116	CLA	C5-C6-C7-C8
8	B	1240	CLA	C8-C10-C11-C12
8	A	1117	CLA	C16-C17-C18-C19
8	B	1205	CLA	C5-C6-C7-C8
8	A	1116	CLA	C2-C3-C5-C6
8	A	1133	CLA	C2-C3-C5-C6
8	B	1202	CLA	C2-C3-C5-C6
8	B	1209	CLA	C2-C3-C5-C6
15	B	5008	SQD	C13-C14-C15-C16
8	A	1127	CLA	C11-C12-C13-C14
8	A	1127	CLA	C14-C13-C15-C16
8	A	1138	CLA	C11-C12-C13-C14
8	B	1237	CLA	C6-C7-C8-C9
8	B	1210	CLA	C14-C13-C15-C16
8	B	1223	CLA	C6-C7-C8-C9
8	B	1021	CLA	C2A-CAA-CBA-CGA
8	B	1207	CLA	C2A-CAA-CBA-CGA
12	A	5002	LMG	C11-C12-C13-C14
10	A	4003	BCR	C37-C22-C23-C24
10	B	4018	BCR	C36-C18-C19-C20
12	A	5002	LMG	C40-C41-C42-C43
10	A	4003	BCR	C21-C22-C23-C24
8	A	1101	CLA	C1A-C2A-CAA-CBA
8	A	1103	CLA	C1A-C2A-CAA-CBA
8	A	1104	CLA	C1A-C2A-CAA-CBA
8	A	1111	CLA	C1A-C2A-CAA-CBA
8	A	1113	CLA	C1A-C2A-CAA-CBA
8	A	1114	CLA	C1A-C2A-CAA-CBA
8	A	1117	CLA	C1A-C2A-CAA-CBA
8	A	1119	CLA	C1A-C2A-CAA-CBA
8	A	1122	CLA	C1A-C2A-CAA-CBA
8	A	1123	CLA	C1A-C2A-CAA-CBA
8	A	1127	CLA	C1A-C2A-CAA-CBA
8	A	1132	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	A	1133	CLA	C1A-C2A-CAA-CBA
8	A	1135	CLA	C1A-C2A-CAA-CBA
8	A	1139	CLA	C1A-C2A-CAA-CBA
8	B	1021	CLA	C1A-C2A-CAA-CBA
8	B	1208	CLA	C1A-C2A-CAA-CBA
8	B	1210	CLA	C1A-C2A-CAA-CBA
8	B	1215	CLA	C1A-C2A-CAA-CBA
8	B	1219	CLA	C1A-C2A-CAA-CBA
8	B	1223	CLA	C1A-C2A-CAA-CBA
8	B	1234	CLA	C1A-C2A-CAA-CBA
8	B	1236	CLA	C1A-C2A-CAA-CBA
8	B	1240	CLA	C1A-C2A-CAA-CBA
8	K	1402	CLA	C1A-C2A-CAA-CBA
8	A	1012	CLA	C6-C7-C8-C10
8	A	1109	CLA	C11-C12-C13-C14
8	B	1022	CLA	C11-C12-C13-C14
10	K	4001	BCR	C9-C10-C11-C12
8	A	1117	CLA	C13-C15-C16-C17
8	A	1123	CLA	C10-C11-C12-C13
11	A	5003	LHG	C4-O6-P-O3
8	B	1230	CLA	CBA-CGA-O2A-C1
11	A	5003	LHG	O6-C4-C5-C6
11	M	5001	LHG	O6-C4-C5-C6
12	B	5002	LMG	O6-C5-C6-O5
8	A	1135	CLA	C16-C17-C18-C19
11	A	5001	LHG	C26-C27-C28-C29
8	A	1133	CLA	C10-C11-C12-C13
11	B	5004	LHG	C28-C29-C30-C31
8	B	1224	CLA	C4-C3-C5-C6
12	A	5002	LMG	C14-C15-C16-C17
11	A	5003	LHG	C25-C26-C27-C28
8	A	1104	CLA	C5-C6-C7-C8
8	A	1122	CLA	C11-C12-C13-C15
8	B	1229	CLA	C16-C17-C18-C19
11	A	5001	LHG	C9-C10-C11-C12
11	M	5001	LHG	C4-C5-C6-O8
12	K	5009	LMG	C7-C8-C9-O8
15	B	5008	SQD	C44-C45-C46-O48
8	A	1109	CLA	C8-C10-C11-C12
8	B	1201	CLA	CBA-CGA-O2A-C1
8	B	1231	CLA	C5-C6-C7-C8
11	B	5006	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	B	1229	CLA	C15-C16-C17-C18
8	A	1128	CLA	O1A-CGA-O2A-C1
11	A	5003	LHG	C29-C30-C31-C32
12	B	5002	LMG	C29-C30-C31-C32
12	K	5009	LMG	O6-C5-C6-O5
8	A	1123	CLA	C4-C3-C5-C6
8	B	1202	CLA	C4-C3-C5-C6
8	K	1402	CLA	C4-C3-C5-C6
11	B	5004	LHG	C33-C34-C35-C36
8	A	1111	CLA	CBA-CGA-O2A-C1
11	A	5003	LHG	C35-C36-C37-C38
8	A	1121	CLA	C2-C1-O2A-CGA
8	A	1124	CLA	C2-C1-O2A-CGA
8	B	1234	CLA	C2-C1-O2A-CGA
8	K	1401	CLA	C2-C1-O2A-CGA
11	M	5001	LHG	C26-C27-C28-C29
12	B	5002	LMG	C36-C37-C38-C39
8	B	1203	CLA	CBA-CGA-O2A-C1
8	A	1109	CLA	C11-C12-C13-C15
9	B	2002	PQN	C26-C27-C28-C29
8	B	1230	CLA	O1A-CGA-O2A-C1
8	A	1138	CLA	C13-C15-C16-C17
12	B	5005	LMG	C2-C1-O1-C7
8	A	1133	CLA	C15-C16-C17-C18
8	A	1011	CLA	C6-C7-C8-C10
8	A	1103	CLA	C6-C7-C8-C10
8	A	1104	CLA	C11-C12-C13-C15
8	A	1123	CLA	C2-C3-C5-C6
8	A	1127	CLA	C12-C13-C15-C16
8	A	1135	CLA	C6-C7-C8-C10
8	A	1135	CLA	C11-C12-C13-C15
8	A	1138	CLA	C11-C12-C13-C15
8	B	1209	CLA	C12-C13-C15-C16
8	B	1210	CLA	C6-C7-C8-C10
8	B	1214	CLA	C6-C7-C8-C10
8	B	1226	CLA	C12-C13-C15-C16
8	B	1228	CLA	C6-C7-C8-C10
8	B	1228	CLA	C11-C12-C13-C15
8	B	1229	CLA	C6-C7-C8-C10
8	B	1239	CLA	C11-C12-C13-C15
8	K	1401	CLA	C6-C7-C8-C10
8	K	1402	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	B	2002	PQN	C21-C22-C23-C25
8	A	1011	CLA	C3-C5-C6-C7
8	B	1235	CLA	C3-C5-C6-C7
8	A	1101	CLA	C11-C10-C8-C9
8	A	1135	CLA	C6-C7-C8-C9
8	B	1237	CLA	C11-C12-C13-C14
8	B	1202	CLA	C11-C12-C13-C14
8	B	1210	CLA	C6-C7-C8-C9
8	B	1213	CLA	C14-C13-C15-C16
8	B	1214	CLA	C11-C12-C13-C14
8	B	1226	CLA	C14-C13-C15-C16
8	B	1228	CLA	C11-C12-C13-C14
8	B	1229	CLA	C6-C7-C8-C9
8	B	1230	CLA	C6-C7-C8-C9
8	B	1239	CLA	C11-C12-C13-C14
8	K	1401	CLA	C6-C7-C8-C9
9	B	2002	PQN	C21-C22-C23-C24
10	B	4004	BCR	C19-C20-C21-C22
10	B	4005	BCR	C13-C14-C15-C16
11	A	5001	LHG	C24-C23-O8-C6
8	B	1229	CLA	C10-C11-C12-C13
8	A	1135	CLA	C2A-CAA-CBA-CGA
8	A	1122	CLA	C11-C12-C13-C14
14	B	4006	ECH	C7-C8-C9-C10
8	B	1227	CLA	C3-C5-C6-C7
15	B	5008	SQD	O49-C7-O47-C45
9	B	2002	PQN	C18-C20-C21-C22
8	A	1139	CLA	CBA-CGA-O2A-C1
11	A	5003	LHG	C17-C18-C19-C20
8	B	1023	CLA	C5-C6-C7-C8
11	B	5004	LHG	O6-C4-C5-C6
8	B	1215	CLA	C10-C11-C12-C13
8	B	1210	CLA	C5-C6-C7-C8
8	A	1103	CLA	CBA-CGA-O2A-C1
8	A	1125	CLA	CBA-CGA-O2A-C1
8	A	1129	CLA	C3A-C2A-CAA-CBA
8	B	1205	CLA	C3A-C2A-CAA-CBA
8	B	1216	CLA	C3A-C2A-CAA-CBA
10	A	4002	BCR	C9-C10-C11-C12
10	B	4010	BCR	C19-C20-C21-C22
8	B	1214	CLA	C13-C15-C16-C17
8	A	1135	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	B	5006	LHG	C4-C5-C6-O8
8	B	1229	CLA	C16-C17-C18-C20
11	A	5001	LHG	C33-C34-C35-C36
8	A	1111	CLA	O1A-CGA-O2A-C1
8	B	1203	CLA	O1A-CGA-O2A-C1
8	B	1225	CLA	C10-C11-C12-C13
11	A	5001	LHG	O6-C4-C5-O7
11	A	5003	LHG	O6-C4-C5-O7
11	B	5006	LHG	O6-C4-C5-O7
11	M	5001	LHG	C31-C32-C33-C34
12	K	5009	LMG	O7-C8-C9-O8
10	B	4017	BCR	C9-C10-C11-C12
8	A	1104	CLA	C16-C17-C18-C20
11	A	5001	LHG	C10-C11-C12-C13
8	B	1213	CLA	C8-C10-C11-C12
8	A	1122	CLA	C11-C10-C8-C9
8	B	1217	CLA	C11-C10-C8-C9
8	B	1234	CLA	C11-C12-C13-C14
8	K	1401	CLA	C11-C12-C13-C14
8	A	1103	CLA	C10-C11-C12-C13
8	B	1203	CLA	C13-C15-C16-C17
8	B	1214	CLA	C5-C6-C7-C8
11	B	5004	LHG	C2-C3-O3-P
11	A	5001	LHG	C24-C25-C26-C27
11	A	5003	LHG	C32-C33-C34-C35
10	A	4001	BCR	C23-C24-C25-C26
10	B	4011	BCR	C1-C6-C7-C8
10	B	4011	BCR	C5-C6-C7-C8
10	B	4017	BCR	C23-C24-C25-C26
8	A	1127	CLA	C5-C6-C7-C8
8	A	1111	CLA	CAA-CBA-CGA-O2A
10	A	4008	BCR	C17-C18-C19-C20
10	B	4018	BCR	C11-C12-C13-C14
10	B	4018	BCR	C17-C18-C19-C20
8	B	1210	CLA	C16-C17-C18-C20
11	A	5001	LHG	O10-C23-O8-C6
11	B	5006	LHG	O6-C4-C5-C6
8	A	1101	CLA	C11-C10-C8-C7
8	A	1106	CLA	C11-C10-C8-C7
8	A	1117	CLA	C12-C13-C15-C16
8	A	1123	CLA	C6-C7-C8-C10
8	B	1237	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
8	B	1237	CLA	C12-C13-C15-C16
8	B	1202	CLA	C11-C12-C13-C15
8	B	1213	CLA	C12-C13-C15-C16
8	B	1214	CLA	C11-C12-C13-C15
8	B	1215	CLA	C11-C12-C13-C15
8	B	1220	CLA	C11-C10-C8-C7
8	B	1226	CLA	C6-C7-C8-C10
8	B	1230	CLA	C6-C7-C8-C10
8	B	1231	CLA	C11-C10-C8-C7
8	B	1234	CLA	C11-C12-C13-C15
8	B	1239	CLA	C6-C7-C8-C10
8	K	1401	CLA	C11-C12-C13-C15
8	A	1140	CLA	CBA-CGA-O2A-C1
8	B	1226	CLA	C8-C10-C11-C12
8	A	1110	CLA	C2A-CAA-CBA-CGA
12	K	5009	LMG	C33-C34-C35-C36
11	A	5003	LHG	C11-C10-C9-C8
8	B	1219	CLA	C8-C10-C11-C12
8	B	1202	CLA	C8-C10-C11-C12
8	A	1112	CLA	CAD-CBD-CGD-O2D
11	M	5001	LHG	C17-C18-C19-C20
11	M	5001	LHG	C33-C34-C35-C36
8	A	1140	CLA	O1A-CGA-O2A-C1
11	B	5004	LHG	O6-C4-C5-O7
8	B	1227	CLA	C5-C6-C7-C8
8	B	1225	CLA	C2A-CAA-CBA-CGA
8	A	1126	CLA	C11-C12-C13-C14
8	A	1103	CLA	CHA-CBD-CGD-O1D
8	A	1103	CLA	CHA-CBD-CGD-O2D
8	A	1116	CLA	CHA-CBD-CGD-O1D
8	A	1123	CLA	CHA-CBD-CGD-O1D
8	A	1123	CLA	CHA-CBD-CGD-O2D
8	A	1128	CLA	CHA-CBD-CGD-O1D
8	A	1128	CLA	CHA-CBD-CGD-O2D
8	A	1130	CLA	CHA-CBD-CGD-O2D
8	B	1021	CLA	CHA-CBD-CGD-O1D
8	B	1021	CLA	CHA-CBD-CGD-O2D
8	B	1205	CLA	CHA-CBD-CGD-O1D
8	B	1205	CLA	CHA-CBD-CGD-O2D
8	B	1209	CLA	CHA-CBD-CGD-O1D
8	B	1209	CLA	CHA-CBD-CGD-O2D
8	B	1210	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	B	1210	CLA	CHA-CBD-CGD-O2D
8	B	1217	CLA	CHA-CBD-CGD-O1D
8	B	1217	CLA	CHA-CBD-CGD-O2D
8	B	1221	CLA	CHA-CBD-CGD-O1D
8	B	1230	CLA	CHA-CBD-CGD-O1D
8	B	1234	CLA	CHA-CBD-CGD-O1D
8	B	1234	CLA	CHA-CBD-CGD-O2D
8	B	1240	CLA	CHA-CBD-CGD-O1D
8	K	1402	CLA	CHA-CBD-CGD-O1D
8	K	1402	CLA	CHA-CBD-CGD-O2D
8	B	1220	CLA	C3-C5-C6-C7
8	A	1103	CLA	O1A-CGA-O2A-C1
8	A	1125	CLA	O1A-CGA-O2A-C1
8	A	1135	CLA	O1A-CGA-O2A-C1
11	B	5004	LHG	C29-C30-C31-C32
8	A	1104	CLA	C16-C17-C18-C19
11	M	5001	LHG	C10-C11-C12-C13
9	A	2001	PQN	C13-C15-C16-C17
8	A	1011	CLA	C4-C3-C5-C6
8	A	1011	CLA	C2-C3-C5-C6
8	B	1021	CLA	C10-C11-C12-C13
8	B	1237	CLA	C14-C13-C15-C16
8	B	1239	CLA	C6-C7-C8-C9
8	B	1239	CLA	C14-C13-C15-C16
8	A	1117	CLA	C8-C10-C11-C12
8	A	1138	CLA	C8-C10-C11-C12
11	A	5003	LHG	C33-C34-C35-C36
8	A	1131	CLA	C1A-C2A-CAA-CBA
8	A	1137	CLA	C1A-C2A-CAA-CBA
8	A	1801	CLA	C1A-C2A-CAA-CBA
8	B	1205	CLA	C1A-C2A-CAA-CBA
8	B	1212	CLA	C1A-C2A-CAA-CBA
8	B	1238	CLA	C1A-C2A-CAA-CBA
8	A	1109	CLA	C2-C1-O2A-CGA
8	A	1137	CLA	C2-C1-O2A-CGA
8	B	1217	CLA	C2-C1-O2A-CGA
8	B	1232	CLA	C2-C1-O2A-CGA
11	B	5006	LHG	C3-O3-P-O6
11	M	5001	LHG	C4-O6-P-O3
11	A	5001	LHG	C16-C17-C18-C19
11	A	5003	LHG	C3-O3-P-O5
11	B	5004	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
11	B	5004	LHG	C4-O6-P-O4
8	A	1128	CLA	C11-C12-C13-C15
8	B	1205	CLA	C6-C7-C8-C9
8	K	1401	CLA	C16-C17-C18-C19
8	K	1401	CLA	CAA-CBA-CGA-O2A
11	M	5001	LHG	C35-C36-C37-C38
8	A	1110	CLA	CAD-CBD-CGD-O1D
8	B	1234	CLA	CAD-CBD-CGD-O1D
8	A	1109	CLA	C5-C6-C7-C8
8	B	1235	CLA	C5-C6-C7-C8
11	B	5004	LHG	C11-C10-C9-C8
8	A	1013	CLA	C4-C3-C5-C6
8	A	1117	CLA	C6-C7-C8-C10
8	A	1136	CLA	C11-C12-C13-C15
8	B	1021	CLA	C6-C7-C8-C10
8	B	1209	CLA	C11-C10-C8-C7
8	B	1215	CLA	C6-C7-C8-C10
8	B	1234	CLA	C6-C7-C8-C10
8	B	1239	CLA	C12-C13-C15-C16
11	M	5001	LHG	O6-C4-C5-O7
11	A	5003	LHG	C24-C25-C26-C27
8	B	1230	CLA	C13-C15-C16-C17
8	B	1219	CLA	C2A-CAA-CBA-CGA
12	A	5002	LMG	O1-C7-C8-C9
12	K	5009	LMG	O1-C7-C8-C9
11	B	5006	LHG	O7-C5-C6-O8
12	A	5002	LMG	O1-C7-C8-O7
12	K	5009	LMG	O1-C7-C8-O7
11	A	5001	LHG	C35-C36-C37-C38
11	A	5003	LHG	C19-C20-C21-C22
8	A	1126	CLA	C11-C12-C13-C15
11	A	5003	LHG	O8-C23-C24-C25
8	B	1202	CLA	C10-C11-C12-C13
8	A	1106	CLA	C11-C10-C8-C9
8	A	1117	CLA	C6-C7-C8-C9
8	A	1123	CLA	C6-C7-C8-C9
8	B	1023	CLA	C6-C7-C8-C9
8	B	1202	CLA	C6-C7-C8-C9
8	B	1209	CLA	C14-C13-C15-C16
8	B	1215	CLA	C11-C12-C13-C14
8	B	1219	CLA	C11-C10-C8-C9
8	B	1220	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
8	B	1226	CLA	C6-C7-C8-C9
11	A	5001	LHG	O1-C1-C2-O2
10	B	4011	BCR	C18-C19-C20-C21
10	B	4018	BCR	C18-C19-C20-C21
10	A	4003	BCR	C15-C16-C17-C18
10	B	4014	BCR	C36-C18-C19-C20
8	B	1240	CLA	C16-C17-C18-C19
8	K	1402	CLA	C15-C16-C17-C18
8	A	1126	CLA	CBA-CGA-O2A-C1
8	A	1120	CLA	C1-C2-C3-C4
8	B	1206	CLA	C2A-CAA-CBA-CGA
8	B	1210	CLA	C2A-CAA-CBA-CGA
8	K	1402	CLA	C2A-CAA-CBA-CGA
8	A	1012	CLA	C2-C1-O2A-CGA
8	A	1102	CLA	C2-C1-O2A-CGA
8	B	1213	CLA	C2-C1-O2A-CGA
8	B	1201	CLA	O1A-CGA-O2A-C1
8	A	1126	CLA	O1A-CGA-O2A-C1
11	B	5006	LHG	C2-C3-O3-P
11	A	5003	LHG	C16-C17-C18-C19
11	M	5001	LHG	C34-C35-C36-C37
8	A	1116	CLA	CAA-CBA-CGA-O2A
8	B	1224	CLA	C8-C10-C11-C12
10	A	4001	BCR	C23-C24-C25-C30
10	B	4017	BCR	C23-C24-C25-C30
11	M	5001	LHG	C16-C17-C18-C19
8	B	1210	CLA	CAA-CBA-CGA-O2A
8	B	1209	CLA	C2A-CAA-CBA-CGA
11	M	5001	LHG	O7-C5-C6-O8
11	A	5001	LHG	C3-O3-P-O6
11	A	5001	LHG	C4-O6-P-O3
11	B	5006	LHG	C4-O6-P-O3
11	M	5001	LHG	C3-O3-P-O6
11	A	5003	LHG	C10-C11-C12-C13
8	A	1133	CLA	C8-C10-C11-C12
8	B	1228	CLA	C10-C11-C12-C13
8	B	1238	CLA	C11-C12-C13-C15
8	A	1011	CLA	C6-C7-C8-C9
8	A	1126	CLA	C11-C10-C8-C9
8	A	1135	CLA	C11-C12-C13-C14
8	A	1136	CLA	C11-C12-C13-C14
11	B	5006	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	M	4021	ECH	C15-C16-C17-C18
8	A	1137	CLA	O1A-CGA-O2A-C1
8	B	1213	CLA	C15-C16-C17-C18
8	B	1205	CLA	C6-C7-C8-C10
11	A	5001	LHG	C13-C14-C15-C16
8	A	1101	CLA	C8-C10-C11-C12
8	A	1125	CLA	C4-C3-C5-C6
8	A	1127	CLA	C4-C3-C5-C6
8	A	1128	CLA	C11-C12-C13-C14
8	A	1137	CLA	CBA-CGA-O2A-C1
8	B	1203	CLA	C8-C10-C11-C12
8	B	1203	CLA	C15-C16-C17-C18
12	B	5005	LMG	C10-C11-C12-C13
10	A	4012	BCR	C13-C14-C15-C16
10	B	4017	BCR	C19-C20-C21-C22
10	K	4001	BCR	C19-C20-C21-C22
8	B	1234	CLA	C3-C5-C6-C7
8	A	1119	CLA	C3-C5-C6-C7
8	B	1201	CLA	C2A-CAA-CBA-CGA
8	A	1110	CLA	C3A-C2A-CAA-CBA
8	A	1121	CLA	C3A-C2A-CAA-CBA
8	B	1201	CLA	C3A-C2A-CAA-CBA
8	B	1232	CLA	C3A-C2A-CAA-CBA
8	A	1127	CLA	C11-C10-C8-C9
8	B	1238	CLA	C11-C10-C8-C9
8	B	1238	CLA	C14-C13-C15-C16
9	A	2001	PQN	C19-C18-C20-C21
11	B	5004	LHG	C16-C17-C18-C19
10	B	4011	BCR	C35-C13-C14-C15
10	B	4011	BCR	C16-C17-C18-C36
14	B	4006	ECH	C11-C10-C9-C34
14	B	4006	ECH	C35-C13-C14-C15
14	M	4021	ECH	C11-C10-C9-C34
8	A	1103	CLA	C3-C5-C6-C7
8	B	1221	CLA	C2A-CAA-CBA-CGA
11	B	5004	LHG	C25-C26-C27-C28
11	M	5001	LHG	C24-C25-C26-C27
8	A	1139	CLA	O1A-CGA-O2A-C1
8	K	1401	CLA	C16-C17-C18-C20
11	A	5001	LHG	C19-C20-C21-C22
8	B	1226	CLA	C13-C15-C16-C17
8	A	1012	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	A	1109	CLA	C1A-C2A-CAA-CBA
8	A	1129	CLA	C1A-C2A-CAA-CBA
8	B	1022	CLA	C1A-C2A-CAA-CBA
8	A	1103	CLA	C11-C10-C8-C7
8	A	1138	CLA	C12-C13-C15-C16
8	B	1203	CLA	C12-C13-C15-C16
8	B	1224	CLA	C6-C7-C8-C10
8	B	1224	CLA	C12-C13-C15-C16
8	B	1234	CLA	C11-C10-C8-C7
8	B	1230	CLA	C8-C10-C11-C12
8	A	1104	CLA	C4-C3-C5-C6
8	A	1013	CLA	C5-C6-C7-C8
8	B	1210	CLA	C13-C15-C16-C17
15	B	5008	SQD	C12-C13-C14-C15
10	B	4011	BCR	C12-C13-C14-C15
10	B	4011	BCR	C16-C17-C18-C19
14	B	4006	ECH	C11-C10-C9-C8
14	B	4006	ECH	C12-C13-C14-C15
14	M	4021	ECH	C11-C10-C9-C8
12	A	5002	LMG	C32-C33-C34-C35
14	M	4021	ECH	C19-C20-C21-C22
8	B	1240	CLA	C4-C3-C5-C6
8	A	1127	CLA	C2-C3-C5-C6
8	A	1135	CLA	C13-C15-C16-C17
8	A	1110	CLA	C11-C10-C8-C9
8	B	1222	CLA	C2A-CAA-CBA-CGA
8	B	1240	CLA	C16-C17-C18-C20
8	A	1105	CLA	O1A-CGA-O2A-C1
8	A	1117	CLA	CAA-CBA-CGA-O2A
8	A	1105	CLA	CBA-CGA-O2A-C1
8	B	1219	CLA	C3-C5-C6-C7
11	A	5001	LHG	O6-C4-C5-C6
8	K	1401	CLA	O1A-CGA-O2A-C1
8	A	1104	CLA	C2-C3-C5-C6
8	B	1238	CLA	C11-C10-C8-C7
8	B	1240	CLA	C2-C3-C5-C6
10	K	4001	BCR	C15-C16-C17-C18
8	B	1021	CLA	CAA-CBA-CGA-O2A
8	B	1237	CLA	C15-C16-C17-C18
8	A	1127	CLA	CAA-CBA-CGA-O2A
8	K	1401	CLA	CBA-CGA-O2A-C1
10	B	4005	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
8	A	1138	CLA	C4-C3-C5-C6
11	B	5004	LHG	C30-C31-C32-C33
8	A	1013	CLA	C2-C3-C5-C6
8	A	1101	CLA	CAA-CBA-CGA-O2A
8	A	1130	CLA	CAA-CBA-CGA-O2A
8	A	1117	CLA	C14-C13-C15-C16
8	A	1140	CLA	C11-C12-C13-C14
8	B	1209	CLA	C11-C10-C8-C9
8	B	1219	CLA	C6-C7-C8-C9
8	B	1224	CLA	C6-C7-C8-C9
8	B	1224	CLA	C14-C13-C15-C16
8	B	1228	CLA	C11-C10-C8-C9
8	B	1231	CLA	C11-C10-C8-C9
8	B	1234	CLA	C6-C7-C8-C9
8	A	1136	CLA	C3A-C2A-CAA-CBA
8	B	1022	CLA	C3A-C2A-CAA-CBA
8	B	1220	CLA	C3A-C2A-CAA-CBA
8	B	1235	CLA	C3A-C2A-CAA-CBA
8	B	1235	CLA	CAA-CBA-CGA-O2A
8	A	1103	CLA	C2A-CAA-CBA-CGA
12	B	5002	LMG	O9-C10-O7-C8
12	B	5002	LMG	O7-C10-C11-C12
11	M	5001	LHG	C12-C13-C14-C15
8	B	1201	CLA	CAA-CBA-CGA-O2A
10	B	4014	BCR	C17-C18-C19-C20
8	B	1021	CLA	C2C-C3C-CAC-CBC
15	B	5008	SQD	C24-C25-C26-C27
8	A	1125	CLA	CAA-CBA-CGA-O2A
8	A	1116	CLA	C6-C7-C8-C9
8	B	1224	CLA	C10-C11-C12-C13
8	B	1232	CLA	CAA-CBA-CGA-O2A
12	K	5009	LMG	C31-C32-C33-C34
8	A	1106	CLA	CHA-CBD-CGD-O1D
8	A	1106	CLA	CHA-CBD-CGD-O2D
8	A	1111	CLA	CHA-CBD-CGD-O1D
8	A	1114	CLA	CHA-CBD-CGD-O1D
8	A	1114	CLA	CHA-CBD-CGD-O2D
8	A	1116	CLA	CHA-CBD-CGD-O2D
8	A	1129	CLA	CHA-CBD-CGD-O2D
8	A	1130	CLA	CHA-CBD-CGD-O1D
8	A	1134	CLA	CHA-CBD-CGD-O1D
8	A	1134	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	B	1201	CLA	CHA-CBD-CGD-O1D
8	B	1201	CLA	CHA-CBD-CGD-O2D
8	B	1213	CLA	CHA-CBD-CGD-O1D
8	B	1214	CLA	CHA-CBD-CGD-O1D
8	B	1214	CLA	CHA-CBD-CGD-O2D
8	B	1223	CLA	CHA-CBD-CGD-O2D
8	B	1227	CLA	CHA-CBD-CGD-O1D
8	B	1227	CLA	CHA-CBD-CGD-O2D
8	B	1232	CLA	CHA-CBD-CGD-O1D
8	B	1232	CLA	CHA-CBD-CGD-O2D
8	B	1236	CLA	CHA-CBD-CGD-O1D
8	B	1236	CLA	CHA-CBD-CGD-O2D
8	K	1401	CLA	CHA-CBD-CGD-O1D
8	K	1401	CLA	CHA-CBD-CGD-O2D
8	B	1223	CLA	CAA-CBA-CGA-O2A
8	B	1219	CLA	C13-C15-C16-C17
11	B	5004	LHG	C12-C13-C14-C15
8	B	1215	CLA	CAA-CBA-CGA-O2A
8	B	1236	CLA	CAA-CBA-CGA-O2A
8	B	1227	CLA	CAA-CBA-CGA-O2A
8	B	1230	CLA	CAA-CBA-CGA-O2A
11	A	5001	LHG	O8-C23-C24-C25
8	A	1110	CLA	C11-C10-C8-C7
8	A	1125	CLA	C2-C3-C5-C6
8	A	1138	CLA	C2-C3-C5-C6
8	B	1228	CLA	C12-C13-C15-C16
8	A	1134	CLA	CAA-CBA-CGA-O2A
8	A	1138	CLA	C14-C13-C15-C16
8	B	1238	CLA	C11-C12-C13-C14
10	A	4007	BCR	C19-C20-C21-C22
11	A	5003	LHG	C31-C32-C33-C34
8	A	1101	CLA	CAA-CBA-CGA-O1A
8	A	1127	CLA	CAA-CBA-CGA-O1A
12	B	5002	LMG	C32-C33-C34-C35
11	A	5001	LHG	C17-C18-C19-C20
12	B	5002	LMG	C22-C23-C24-C25
8	A	1130	CLA	CAA-CBA-CGA-O1A
8	B	1201	CLA	CAA-CBA-CGA-O1A
8	A	1110	CLA	C1A-C2A-CAA-CBA
8	B	1201	CLA	C1A-C2A-CAA-CBA
8	B	1220	CLA	C1A-C2A-CAA-CBA
8	B	1224	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	B	1227	CLA	C1A-C2A-CAA-CBA
8	B	1230	CLA	C1A-C2A-CAA-CBA
11	M	5001	LHG	C19-C20-C21-C22
8	B	1219	CLA	C16-C17-C18-C20
15	B	5008	SQD	C11-C10-C9-C8
8	B	1232	CLA	CAA-CBA-CGA-O1A
8	B	1235	CLA	C2A-CAA-CBA-CGA
8	A	1125	CLA	CAA-CBA-CGA-O1A
8	B	1021	CLA	CAA-CBA-CGA-O1A
8	B	1236	CLA	CAA-CBA-CGA-O1A
8	B	1215	CLA	CAA-CBA-CGA-O1A
8	B	1223	CLA	CAA-CBA-CGA-O1A
8	B	1235	CLA	CAA-CBA-CGA-O1A
11	A	5001	LHG	O10-C23-C24-C25
8	A	1110	CLA	C10-C11-C12-C13
8	A	1119	CLA	C15-C16-C17-C18
11	B	5006	LHG	C4-O6-P-O5
8	A	1115	CLA	CAA-CBA-CGA-O2A
12	A	5002	LMG	C34-C35-C36-C37
11	M	5001	LHG	C30-C31-C32-C33
8	A	1102	CLA	C6-C7-C8-C9
8	B	1223	CLA	C11-C12-C13-C15
8	A	1111	CLA	CAA-CBA-CGA-O1A
8	B	1227	CLA	CAA-CBA-CGA-O1A
12	B	5002	LMG	O9-C10-C11-C12
8	B	1217	CLA	C4-C3-C5-C6
8	B	1209	CLA	CAD-CBD-CGD-O1D
8	B	1211	CLA	CAD-CBD-CGD-O1D
8	B	1240	CLA	CAD-CBD-CGD-O1D
8	A	1106	CLA	CAA-CBA-CGA-O2A
8	A	1104	CLA	C11-C12-C13-C14
8	B	1217	CLA	C6-C7-C8-C9
8	B	1228	CLA	C14-C13-C15-C16
11	A	5001	LHG	C11-C12-C13-C14
8	B	1235	CLA	C10-C11-C12-C13
8	B	1234	CLA	CAA-CBA-CGA-O2A
12	K	5009	LMG	O8-C28-C29-C30
8	B	1228	CLA	C13-C15-C16-C17
8	A	1112	CLA	CAA-CBA-CGA-O2A
8	A	1128	CLA	CAA-CBA-CGA-O2A
8	A	1131	CLA	CAA-CBA-CGA-O2A
12	A	5002	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	B	1230	CLA	CAA-CBA-CGA-O1A
8	A	1109	CLA	C11-C10-C8-C7
8	A	1126	CLA	C6-C7-C8-C10
8	B	1023	CLA	C6-C7-C8-C10
8	B	1228	CLA	C11-C10-C8-C7
9	A	2001	PQN	C21-C22-C23-C25
8	B	1217	CLA	CAA-CBA-CGA-O2A
8	A	1112	CLA	CAA-CBA-CGA-O1A
8	A	1134	CLA	CAA-CBA-CGA-O1A
8	B	1224	CLA	CAA-CBA-CGA-O2A
8	B	1231	CLA	CAA-CBA-CGA-O2A
8	K	1402	CLA	CAA-CBA-CGA-O2A
12	K	5009	LMG	C42-C43-C44-C45
8	A	1119	CLA	CAA-CBA-CGA-O2A
8	B	1204	CLA	CAA-CBA-CGA-O2A
8	A	1127	CLA	C15-C16-C17-C18
8	A	1128	CLA	CAA-CBA-CGA-O1A
8	A	1112	CLA	C2A-CAA-CBA-CGA
8	K	1401	CLA	C5-C6-C7-C8
8	A	1131	CLA	CAA-CBA-CGA-O1A
8	B	1216	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

104 monomers are involved in 248 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1203	CLA	1	0
8	A	1139	CLA	1	0
8	K	1401	CLA	1	0
8	A	1120	CLA	1	0
8	A	1109	CLA	6	0
8	B	1235	CLA	5	0
8	A	1105	CLA	2	0
8	B	1227	CLA	9	0
10	B	4005	BCR	3	0
10	K	4001	BCR	4	0
8	A	1111	CLA	2	0
8	A	1112	CLA	5	0
8	B	1226	CLA	4	0
8	B	1230	CLA	3	0
8	B	1213	CLA	4	0
8	B	1223	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1234	CLA	5	0
10	A	4002	BCR	5	0
8	A	1124	CLA	4	0
8	B	1224	CLA	4	0
8	B	1215	CLA	4	0
8	B	1202	CLA	6	0
8	A	1123	CLA	1	0
10	B	4011	BCR	2	0
8	A	1127	CLA	5	0
8	A	1129	CLA	2	0
8	B	1240	CLA	1	0
8	B	1238	CLA	3	0
8	A	1133	CLA	3	0
8	B	1211	CLA	2	0
8	B	1208	CLA	1	0
10	B	4010	BCR	4	0
10	B	4004	BCR	4	0
8	A	1104	CLA	1	0
8	B	1231	CLA	4	0
8	A	1103	CLA	5	0
8	B	1219	CLA	4	0
10	A	4003	BCR	2	0
8	B	1229	CLA	4	0
10	A	4012	BCR	3	0
8	K	1402	CLA	1	0
8	B	1023	CLA	1	0
10	A	4001	BCR	3	0
8	B	1209	CLA	1	0
10	A	4019	BCR	2	0
8	A	1013	CLA	3	0
10	B	4014	BCR	3	0
8	B	1214	CLA	5	0
8	B	1217	CLA	4	0
8	A	1126	CLA	6	0
14	B	4006	ECH	6	0
8	B	1228	CLA	3	0
8	A	1115	CLA	1	0
13	C	3003	SF4	1	0
8	A	1117	CLA	5	0
8	A	1130	CLA	1	0
10	A	4007	BCR	3	0
14	M	4021	ECH	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1136	CLA	3	0
8	B	1220	CLA	3	0
8	A	1108	CLA	1	0
12	B	5002	LMG	9	0
8	B	1221	CLA	4	0
8	B	1218	CLA	1	0
8	A	1128	CLA	4	0
8	A	1137	CLA	1	0
8	A	1132	CLA	2	0
8	B	1222	CLA	4	0
8	A	1102	CLA	2	0
8	A	1011	CLA	2	0
8	B	1021	CLA	6	0
11	A	5003	LHG	4	0
10	A	4008	BCR	5	0
8	B	1205	CLA	4	0
11	M	5001	LHG	1	0
8	A	1012	CLA	4	0
8	A	1131	CLA	1	0
8	B	1210	CLA	3	0
11	A	5001	LHG	9	0
8	B	1212	CLA	1	0
13	A	3001	SF4	1	0
8	B	1239	CLA	4	0
8	B	1204	CLA	2	0
8	A	1119	CLA	2	0
8	A	1138	CLA	4	0
8	B	1232	CLA	2	0
8	A	1122	CLA	3	0
8	B	1225	CLA	6	0
9	A	2001	PQN	4	0
11	B	5004	LHG	5	0
8	A	1107	CLA	2	0
8	A	1116	CLA	4	0
8	A	1106	CLA	4	0
8	A	1101	CLA	1	0
10	B	4018	BCR	4	0
8	B	1206	CLA	2	0
8	B	1236	CLA	4	0
9	B	2002	PQN	1	0
8	B	1216	CLA	5	0
8	A	1118	CLA	2	0

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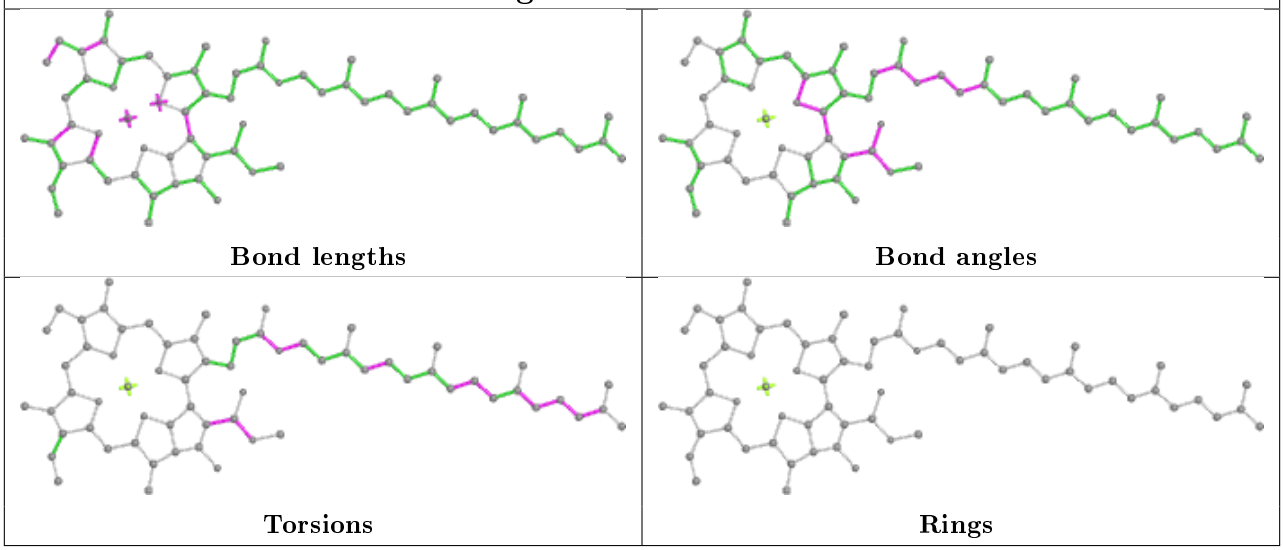
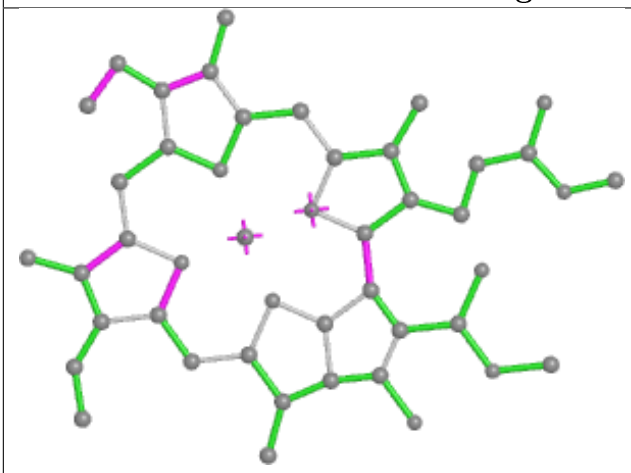
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1135	CLA	2	0
8	B	1022	CLA	3	0
10	B	4017	BCR	5	0
8	A	1140	CLA	5	0

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

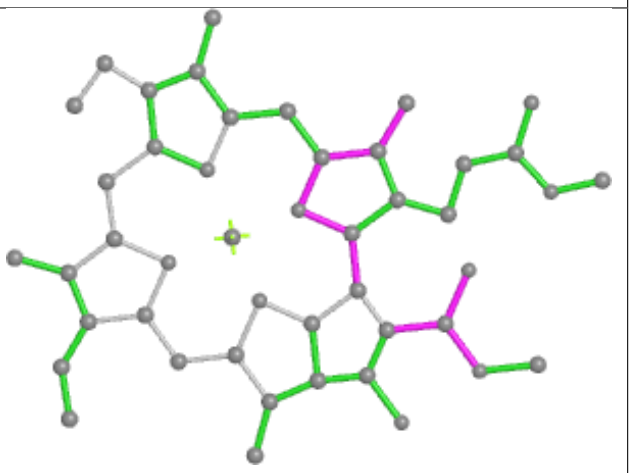
Ligand CLA B 1203



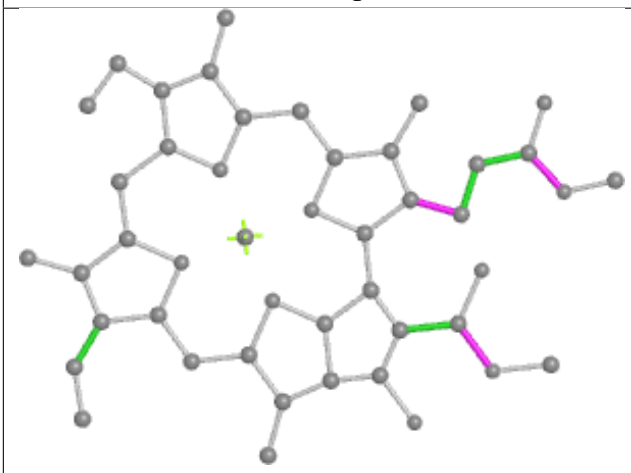
Ligand CLA A 1139



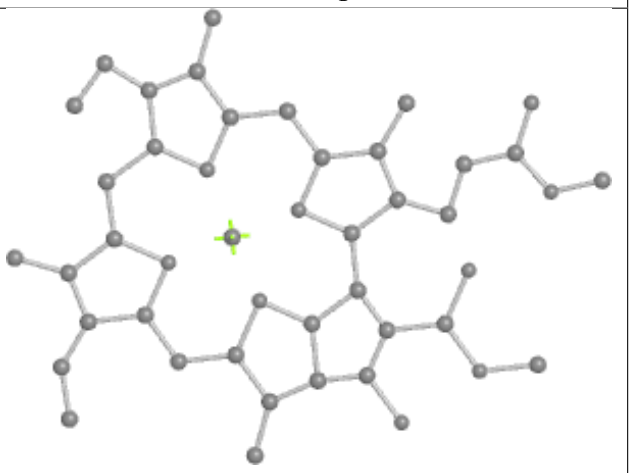
Bond lengths



Bond angles

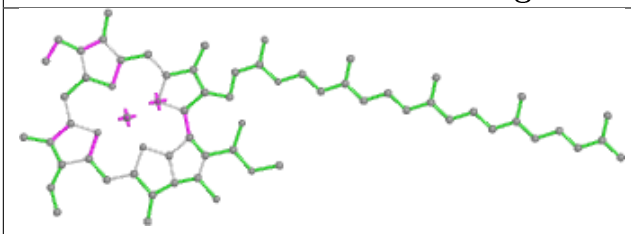


Torsions

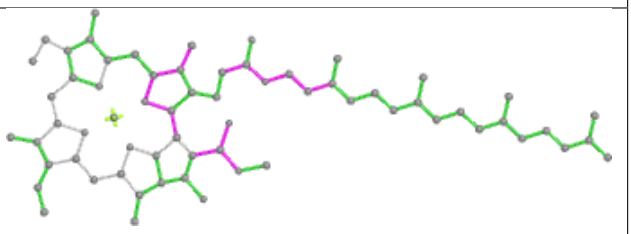


Rings

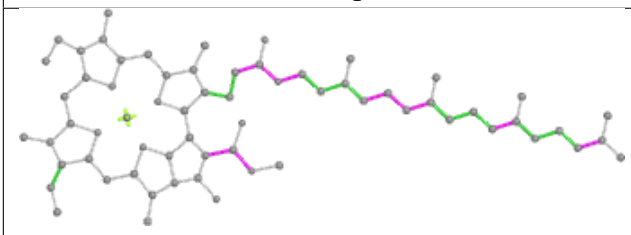
Ligand CLA K 1401



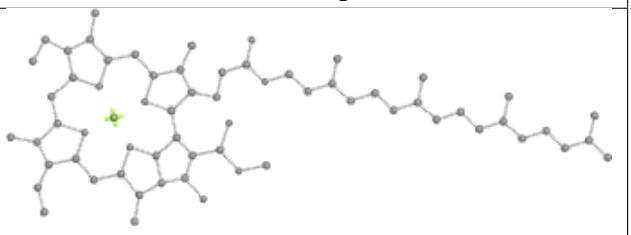
Bond lengths



Bond angles

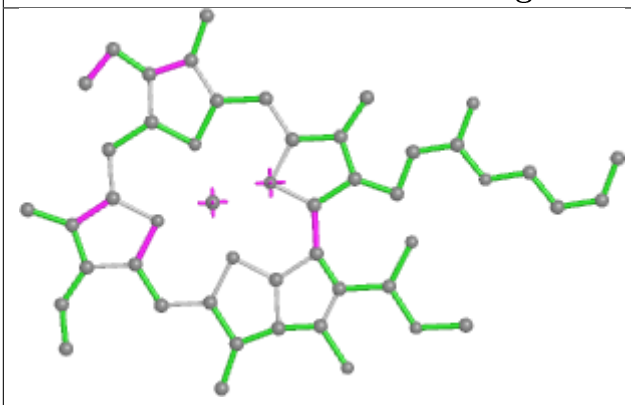


Torsions

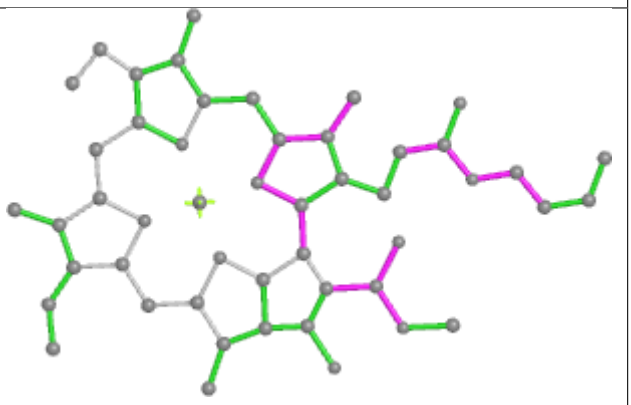


Rings

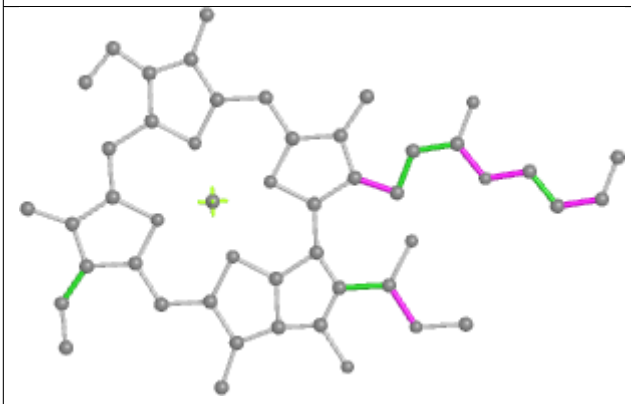
Ligand CLA A 1120



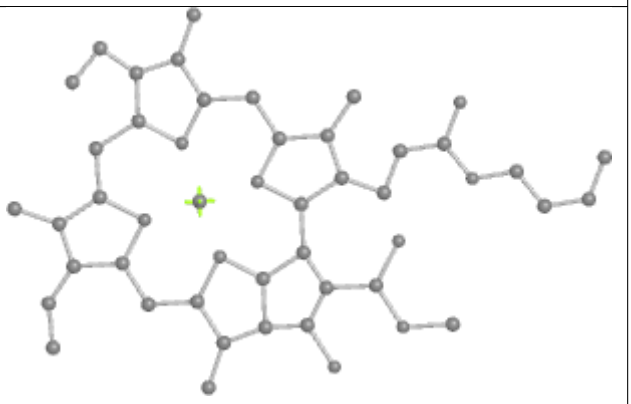
Bond lengths



Bond angles

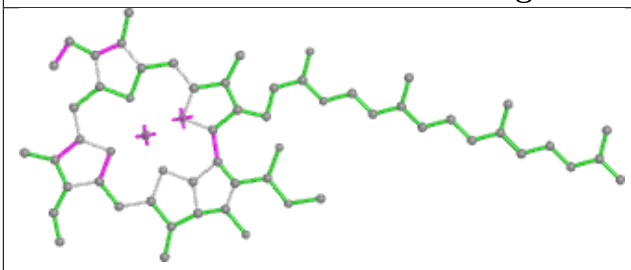


Torsions

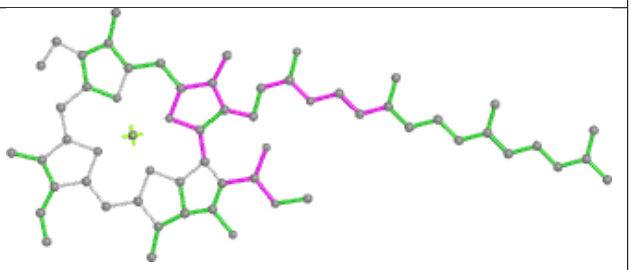


Rings

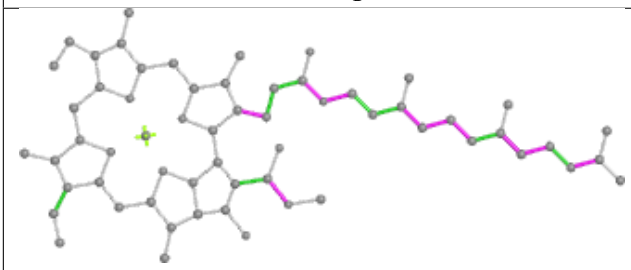
Ligand CLA A 1109



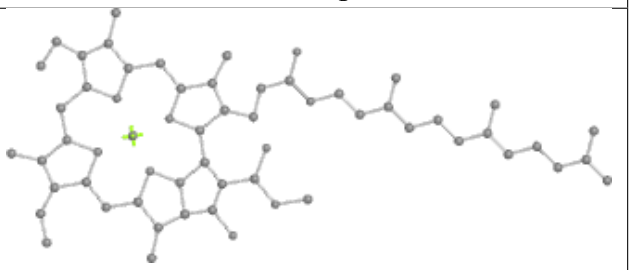
Bond lengths



Bond angles

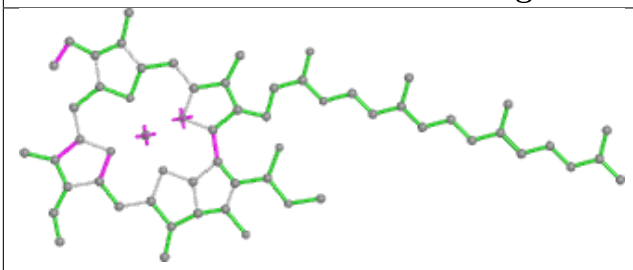


Torsions

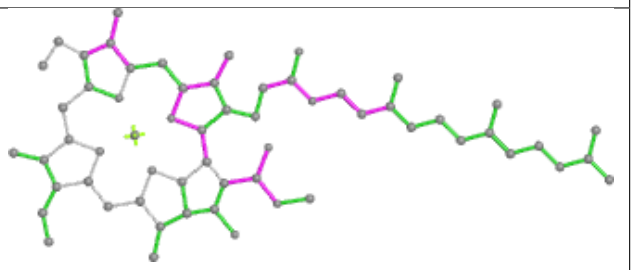


Rings

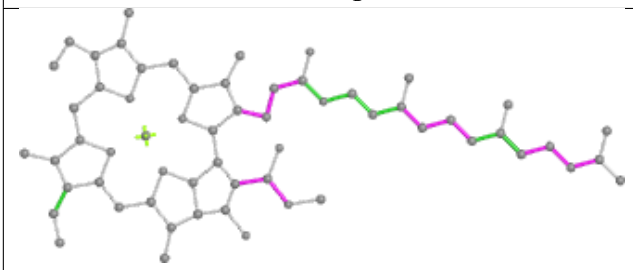
Ligand CLA B 1235



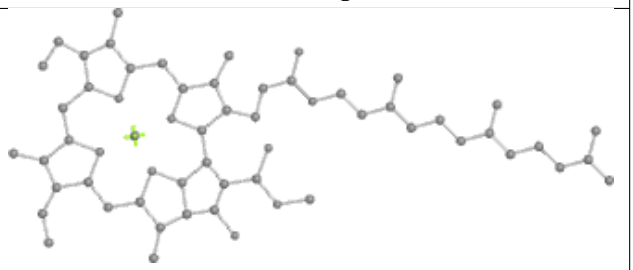
Bond lengths



Bond angles

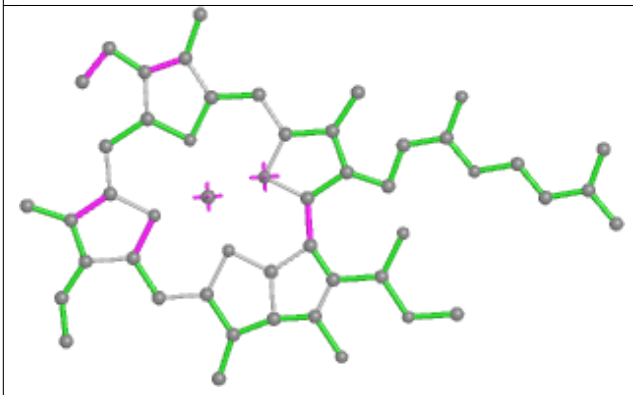


Torsions

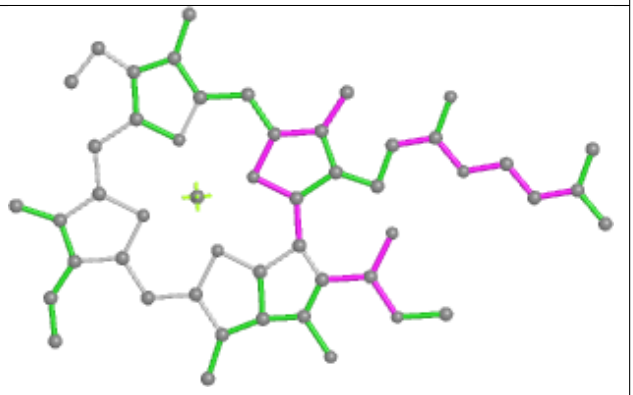


Rings

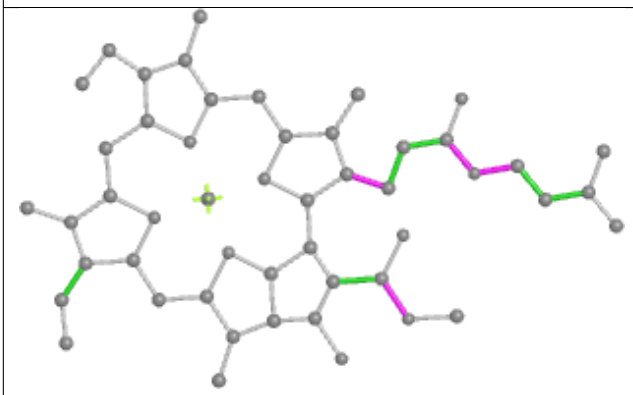
Ligand CLA A 1105



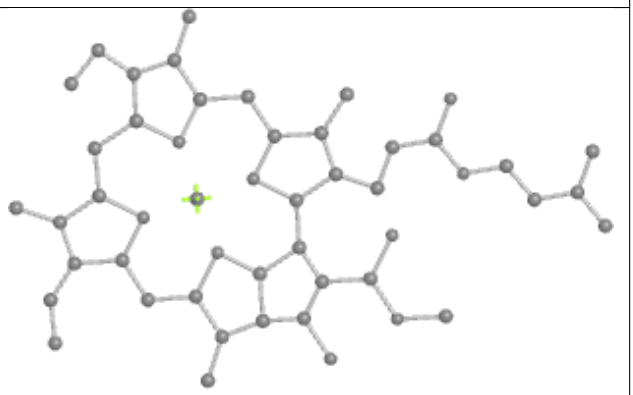
Bond lengths



Bond angles

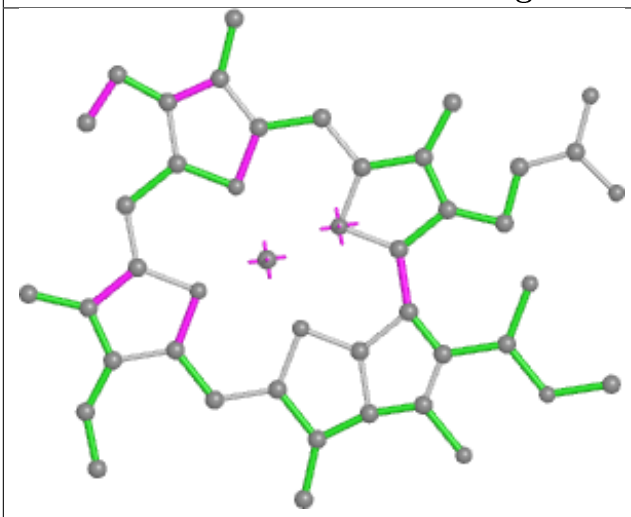


Torsions

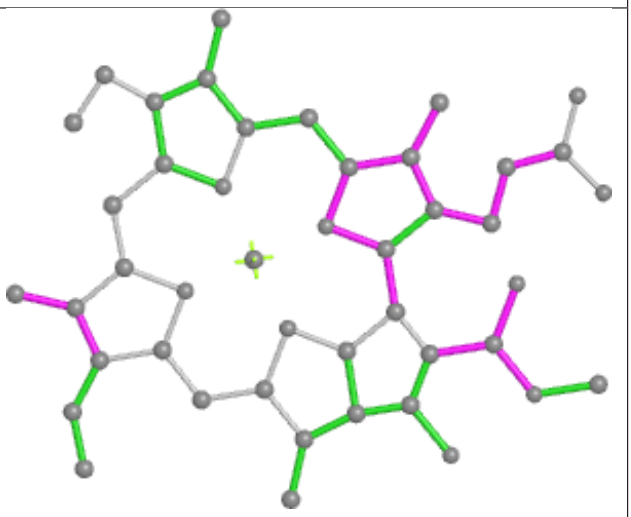


Rings

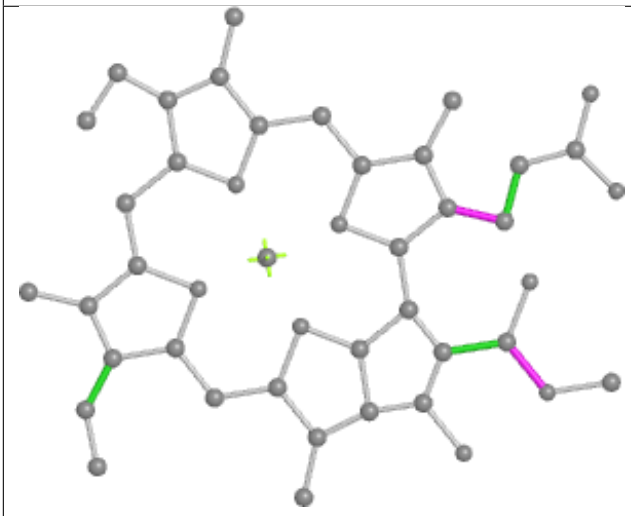
Ligand CLA A 1113



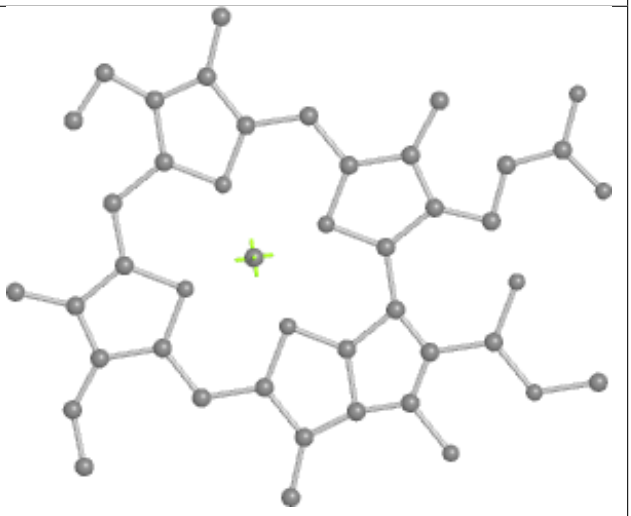
Bond lengths



Bond angles

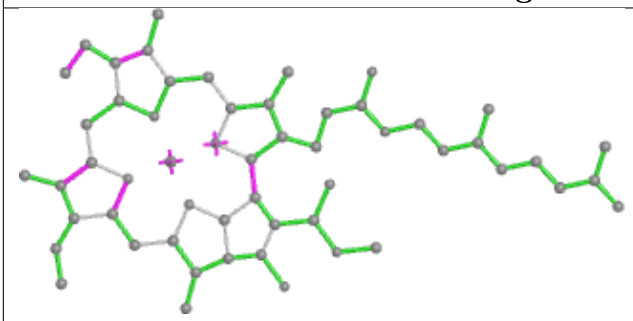


Torsions



Rings

Ligand CLA B 1227



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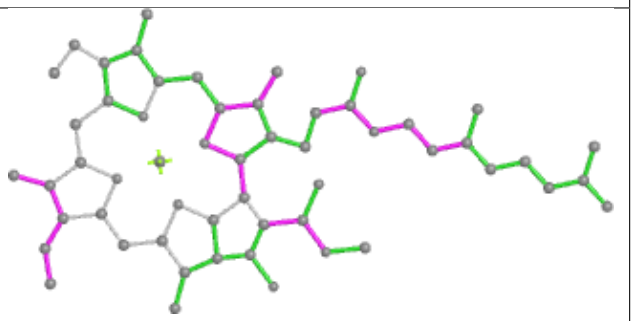
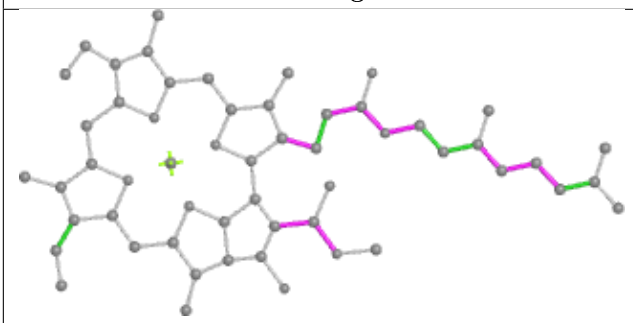
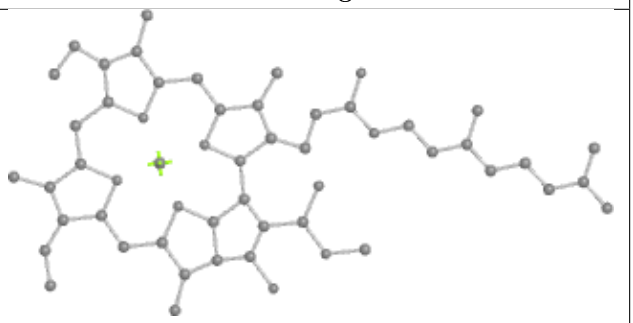


Bond angles

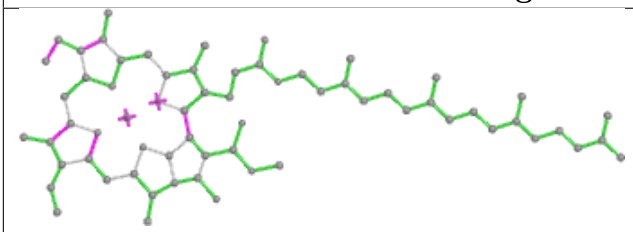


Torsions

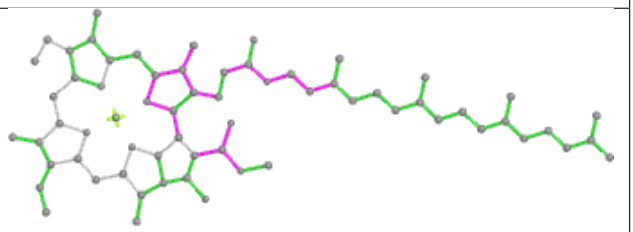


Rings

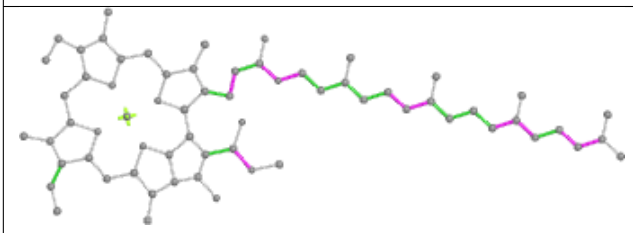
Ligand CLA B 1237



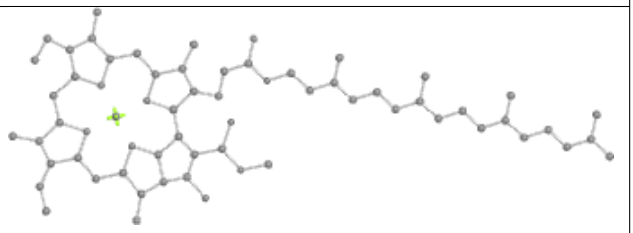
Bond lengths



Bond angles

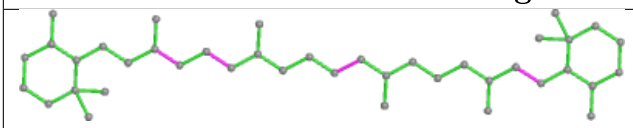


Torsions

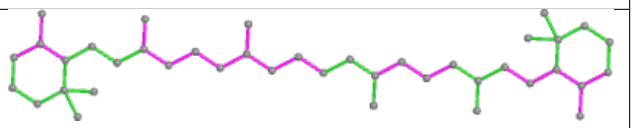


Rings

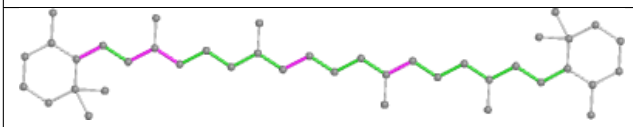
Ligand BCR B 4005



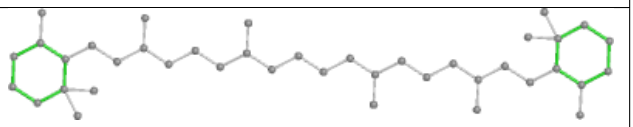
Bond lengths



Bond angles

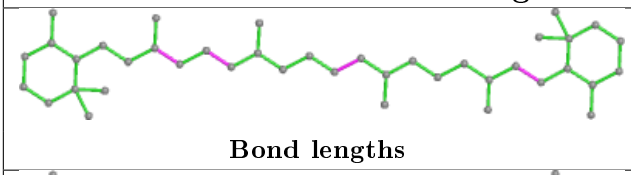


Torsions

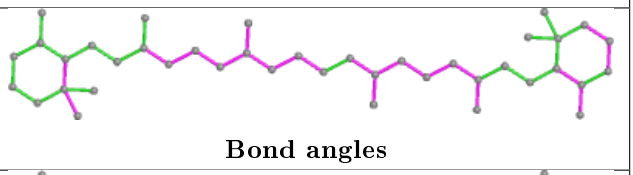


Rings

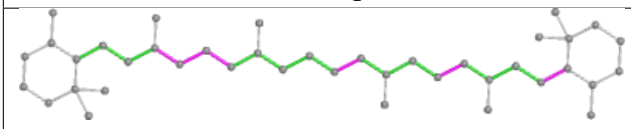
Ligand BCR K 4001



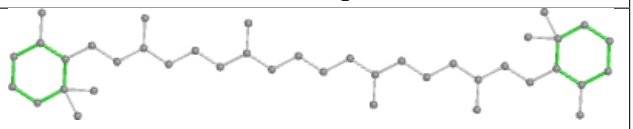
Bond lengths



Bond angles

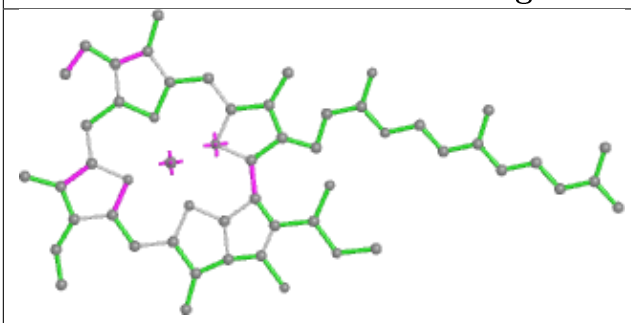


Torsions

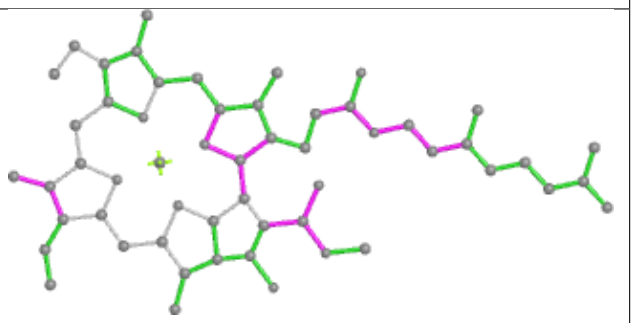


Rings

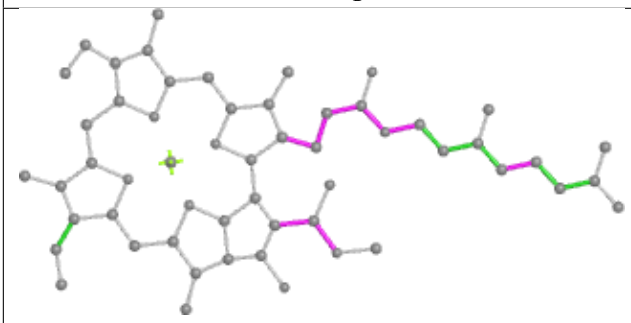
Ligand CLA A 1111



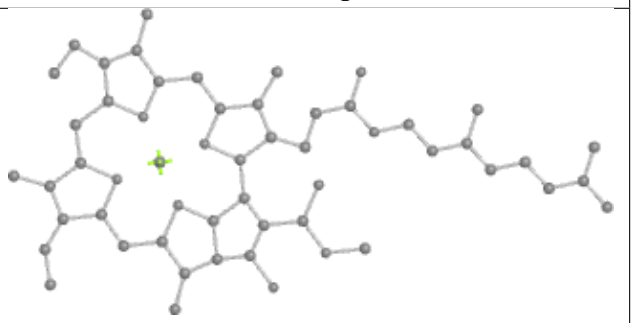
Bond lengths



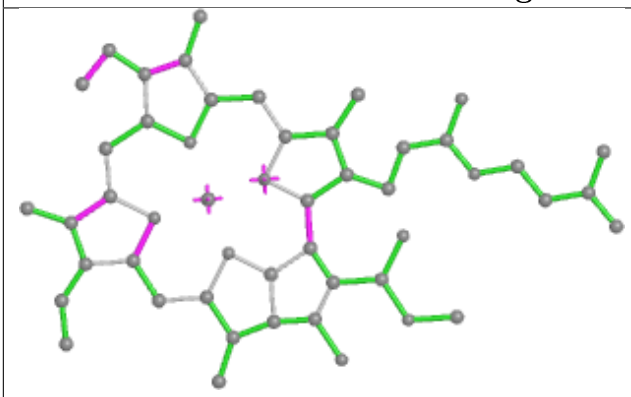
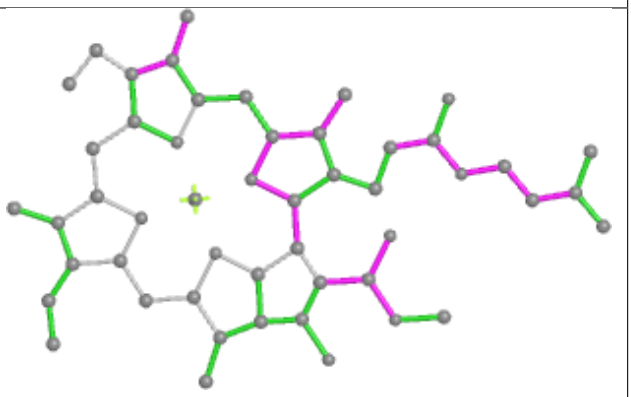
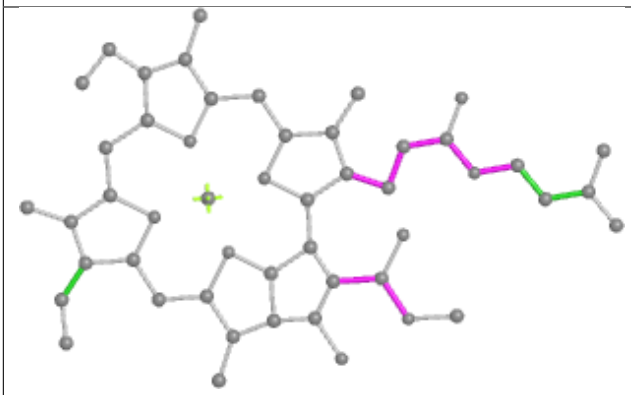
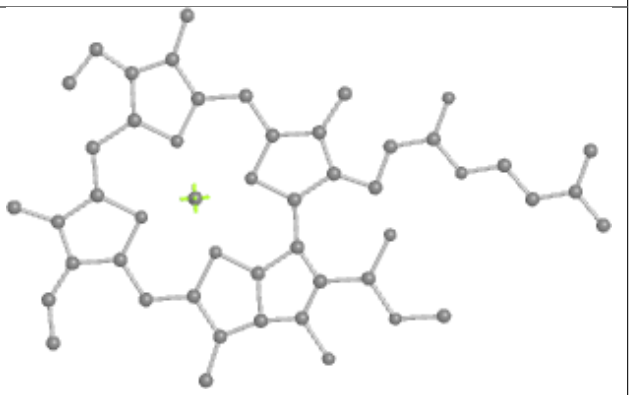
Bond angles

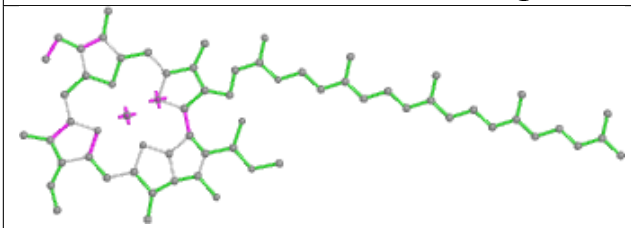
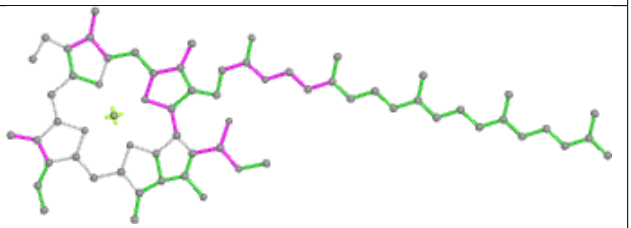
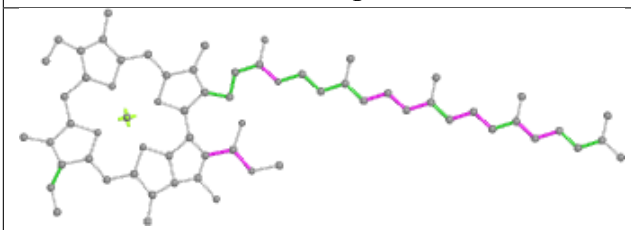
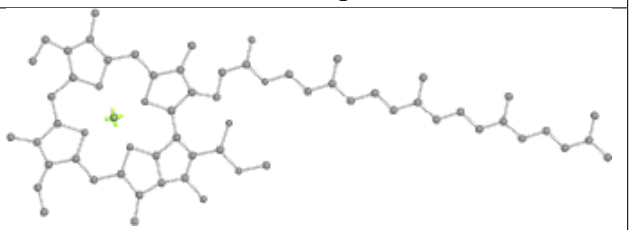


Torsions

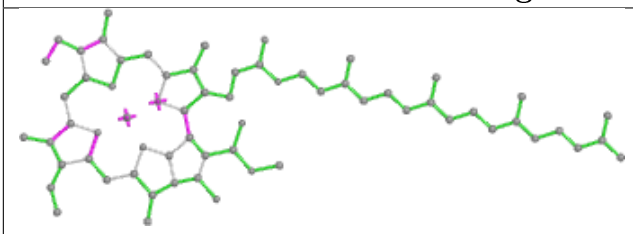


Rings

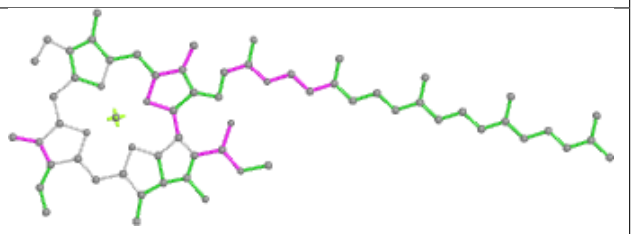
Ligand CLA A 1112	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1226	
 Bond lengths	 Bond angles
 Torsions	 Rings

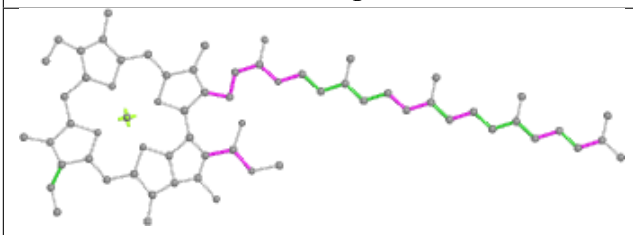
Ligand CLA B 1230



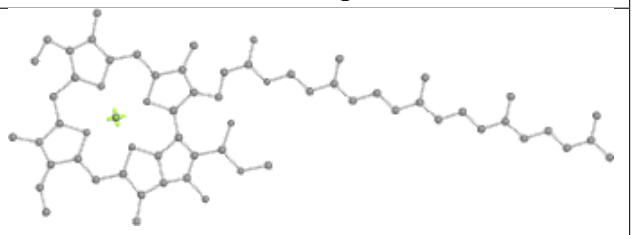
Bond lengths



Bond angles

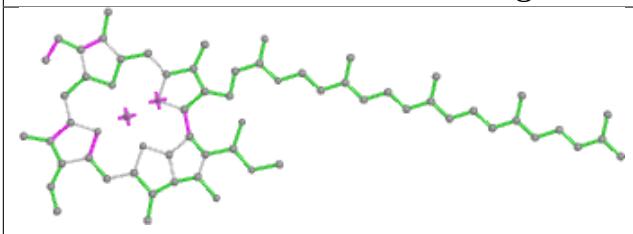


Torsions

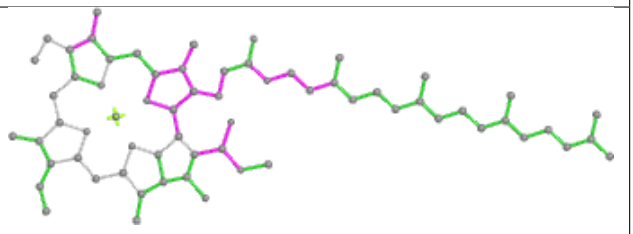


Rings

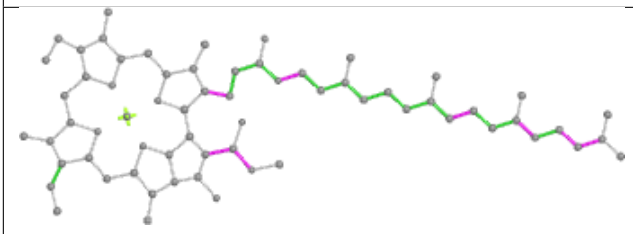
Ligand CLA B 1213



Bond lengths



Bond angles



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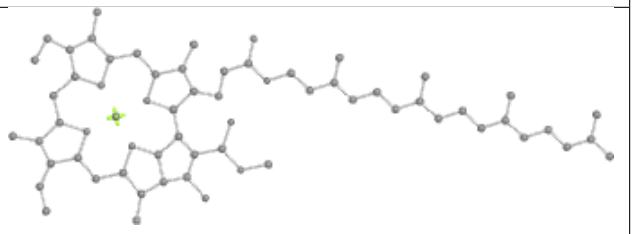
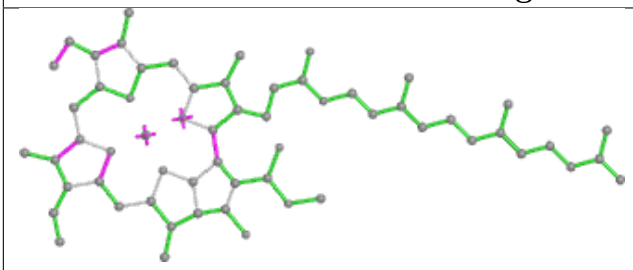
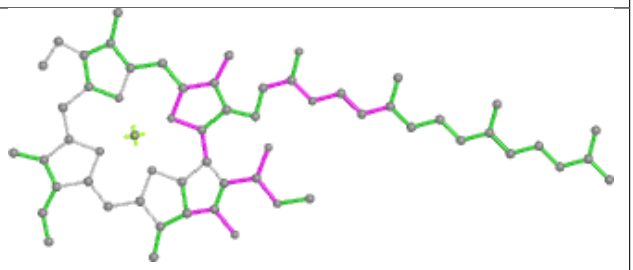


Rings

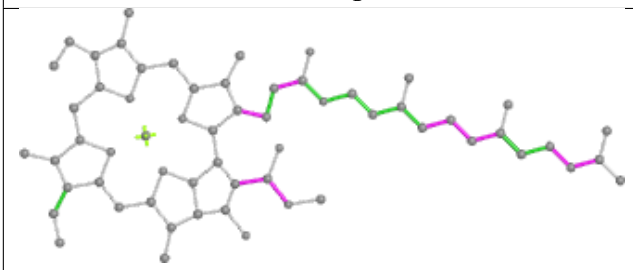
Ligand CLA B 1223



Bond lengths



Bond angles



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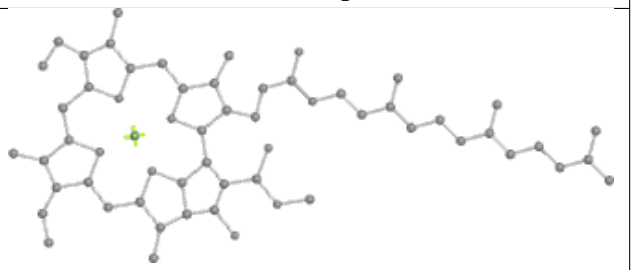
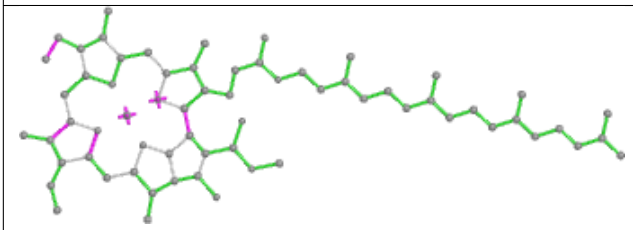
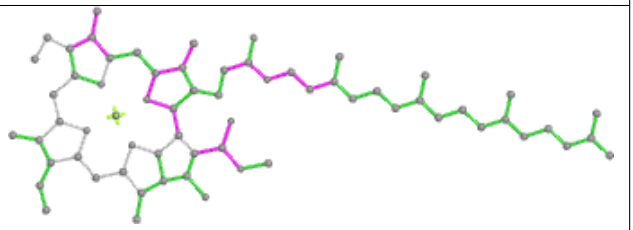


Rings

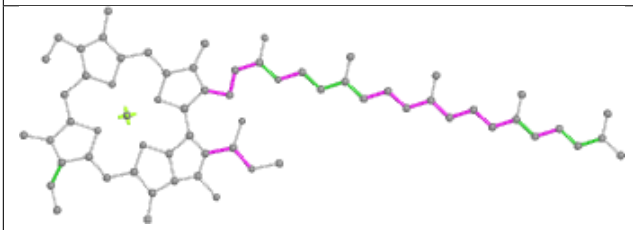
Ligand CLA B 1234



Bond lengths



Bond angles



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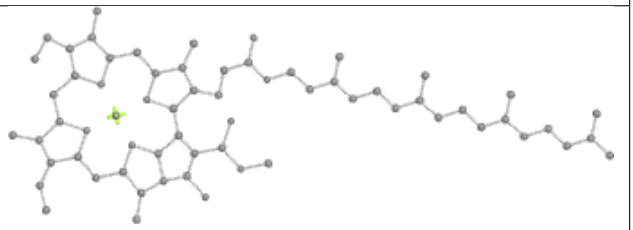
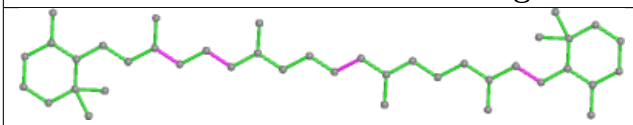


Rings

Ligand BCR A 4002



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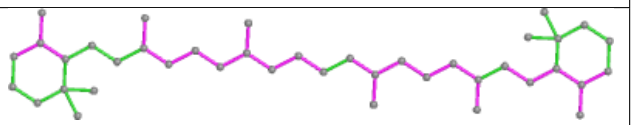
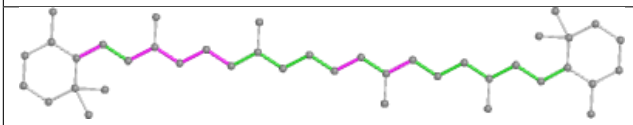


Bond angles



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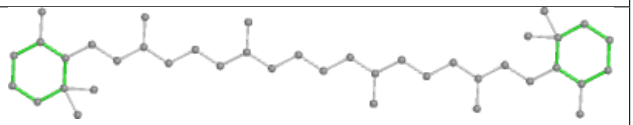
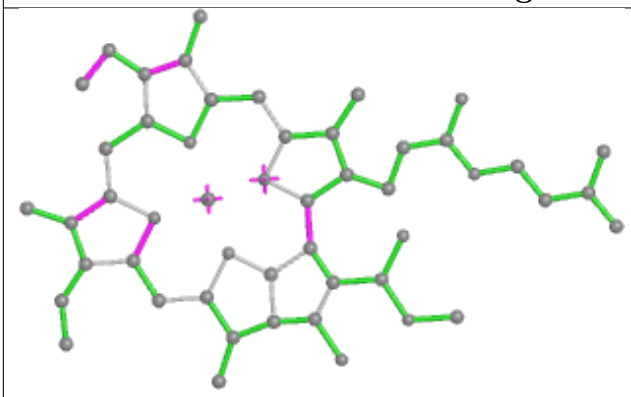
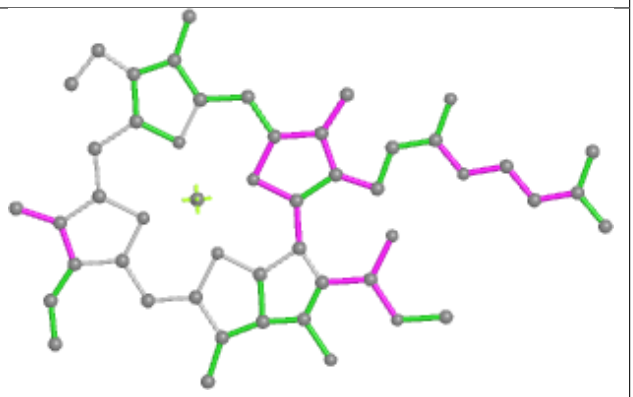


Rings

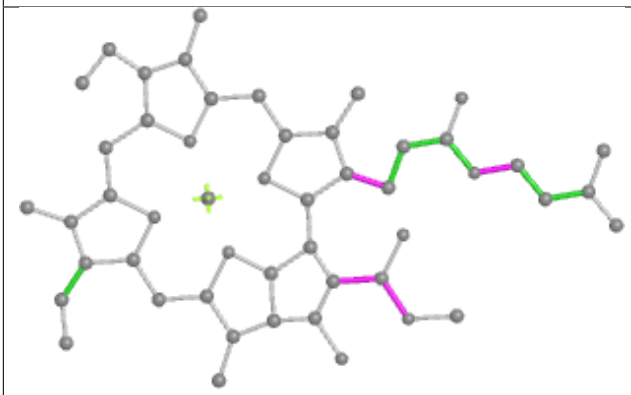
Ligand CLA A 1121



Bond lengths



Bond angles



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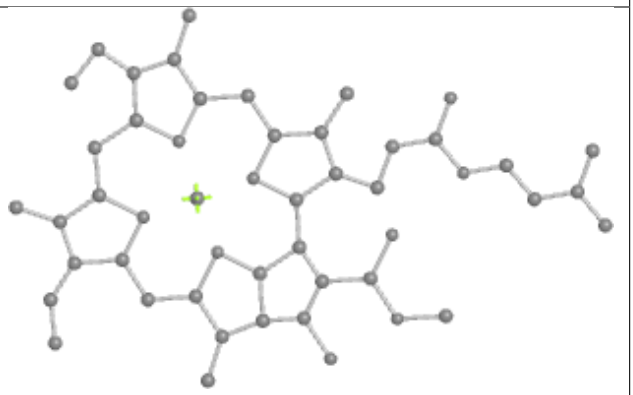
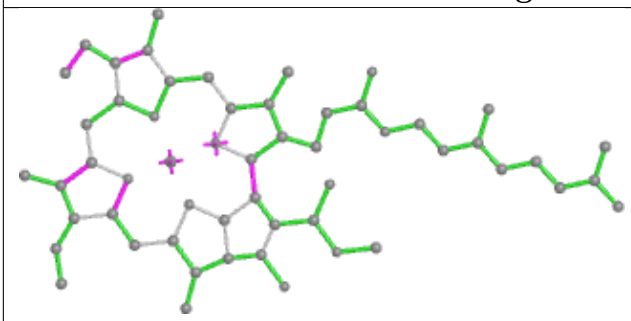
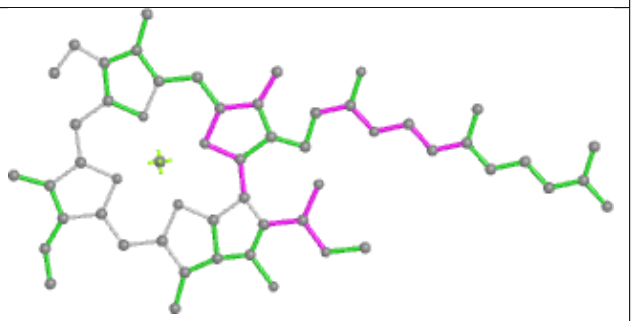


Rings

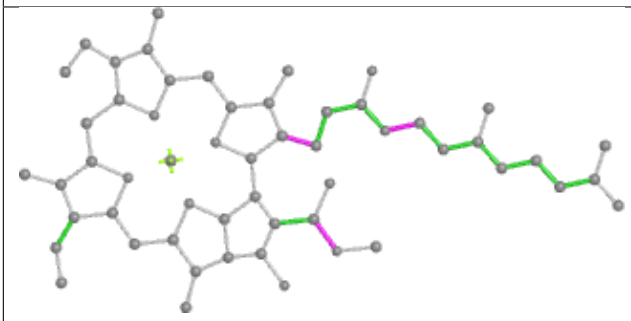
Ligand CLA A 1124



Bond lengths



Bond angles



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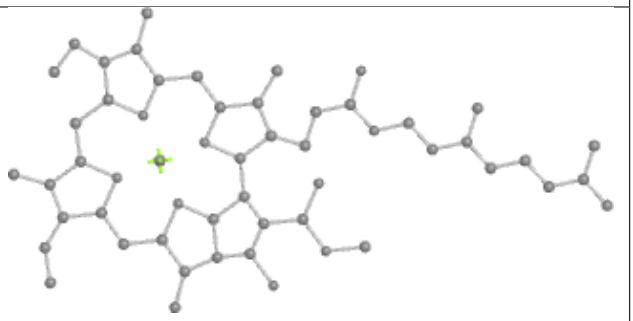
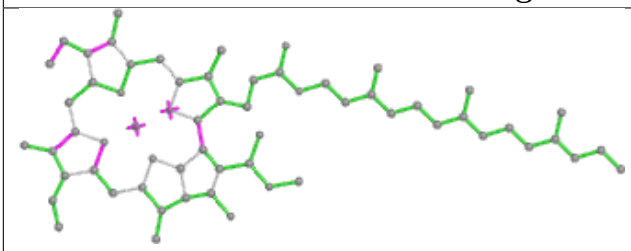
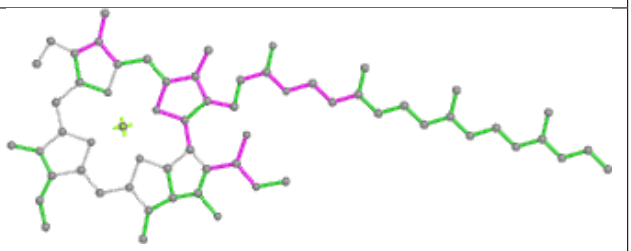
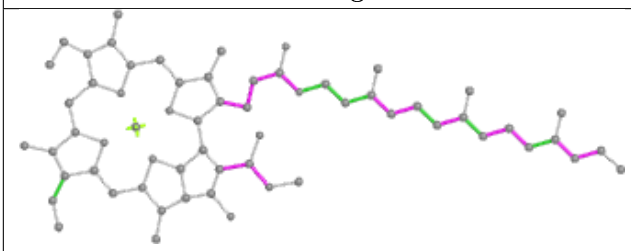
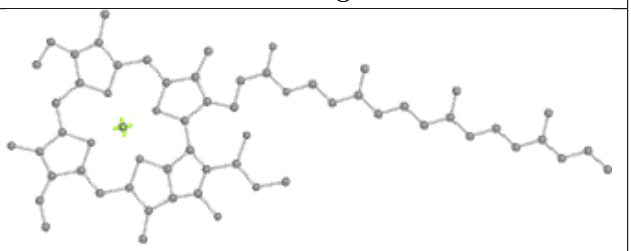
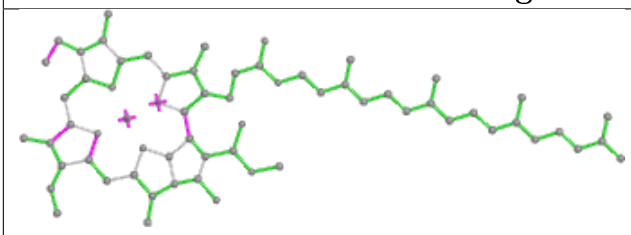
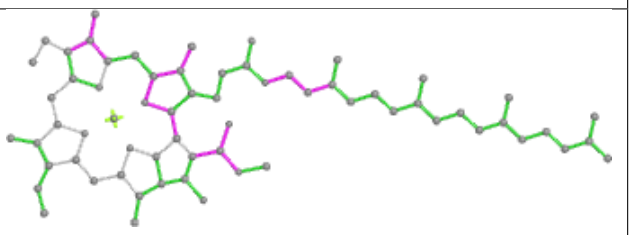
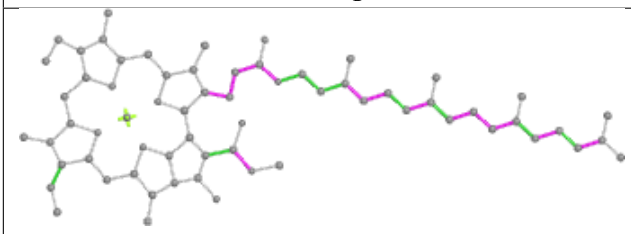
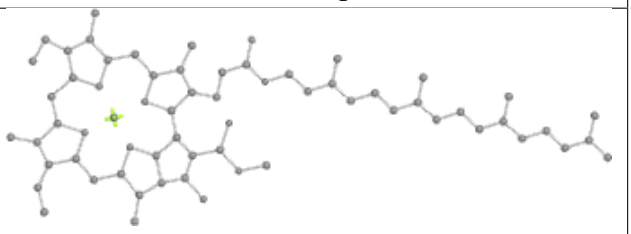
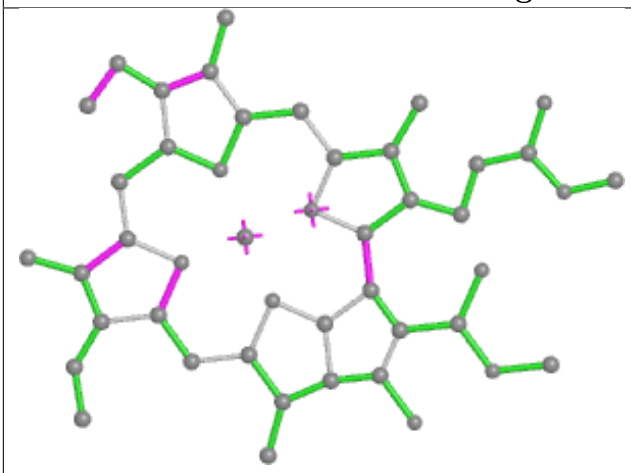


Rings

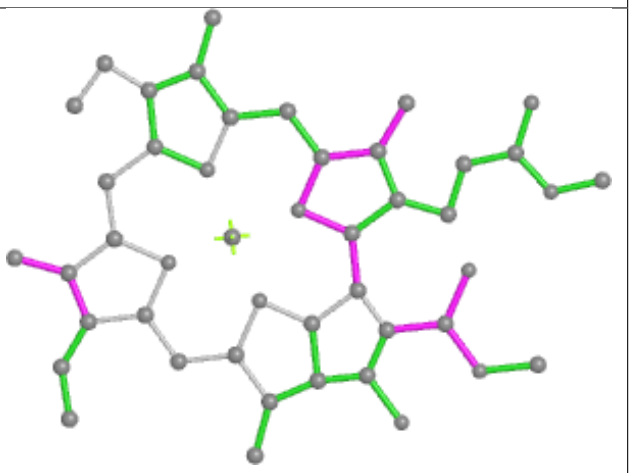
Ligand CLA B 1224	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1215	
 Bond lengths	 Bond angles
 Torsions	 Rings

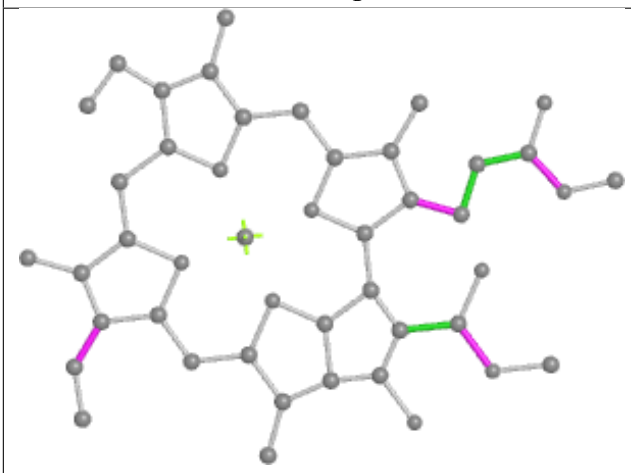
Ligand CLA A 1801



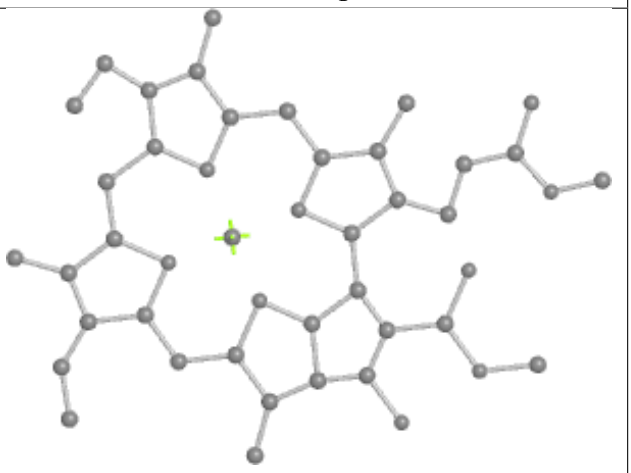
Bond lengths



Bond angles

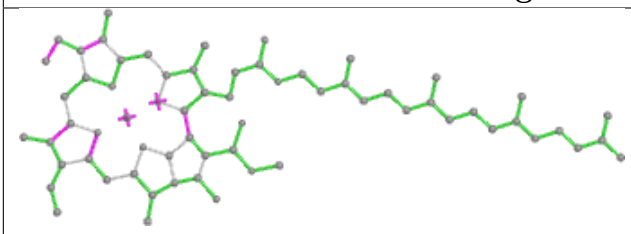


Torsions

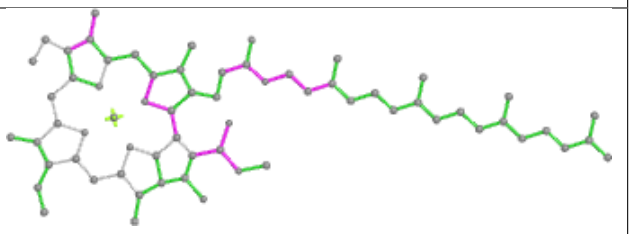


Rings

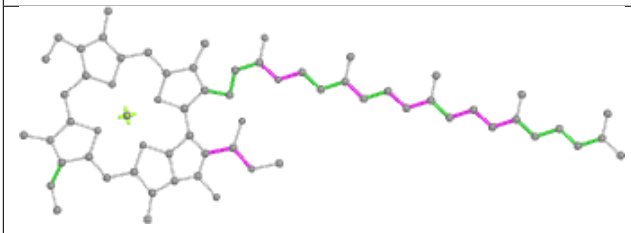
Ligand CLA B 1202



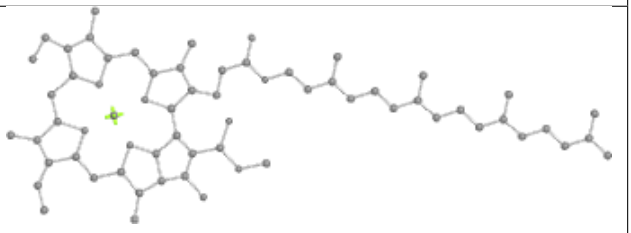
Bond lengths



Bond angles

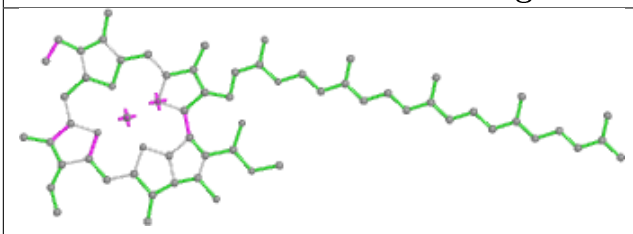


Torsions

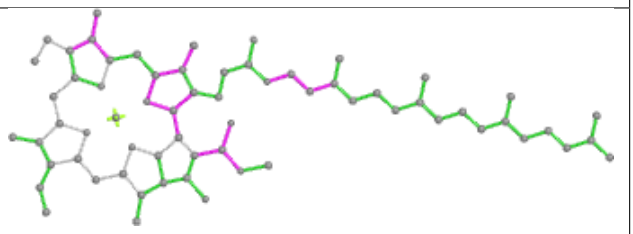


Rings

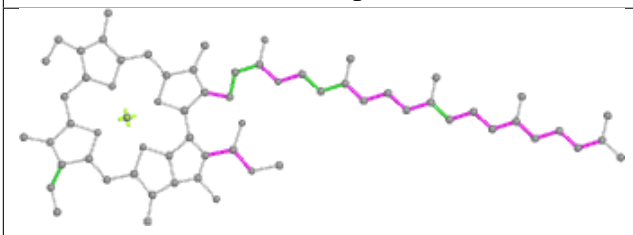
Ligand CLA A 1123



Bond lengths



Bond angles



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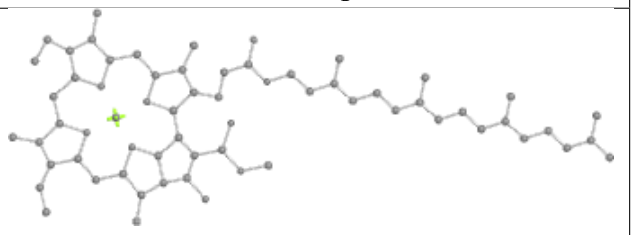
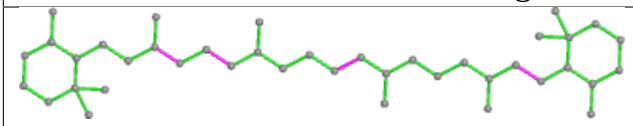
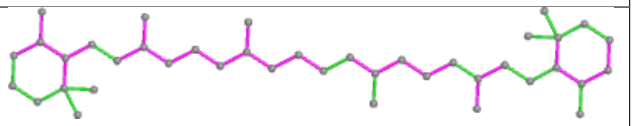


Rings

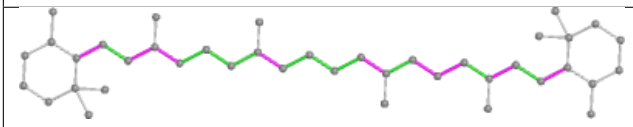
Ligand BCR B 4011



Bond lengths



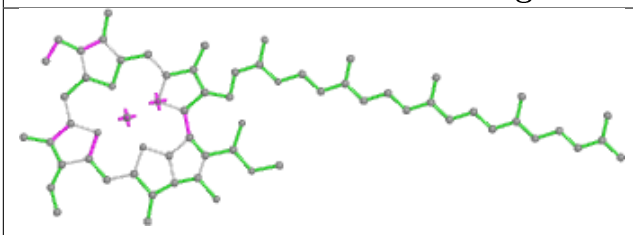
Bond angles



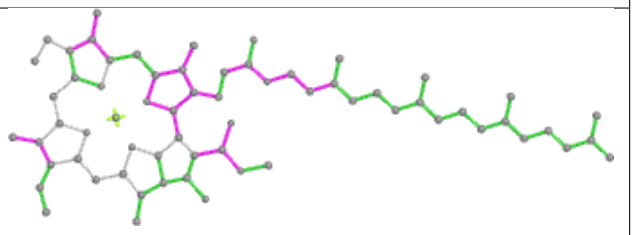
Torsions

Rings

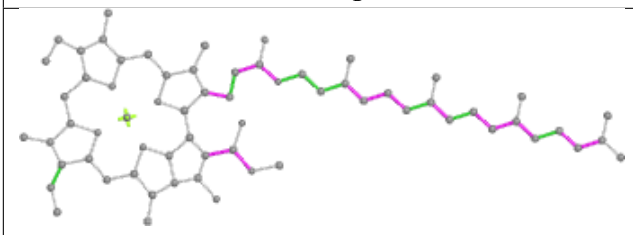
Ligand CLA A 1127



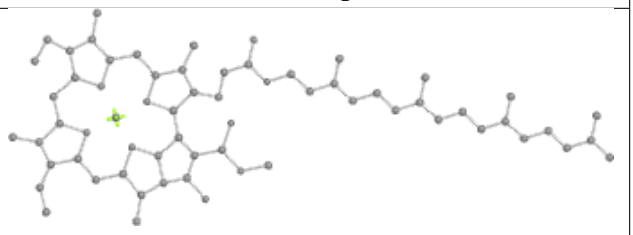
Bond lengths



Bond angles

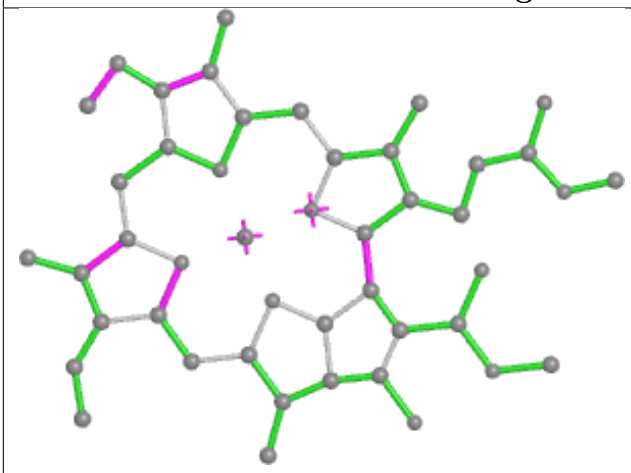


Torsions

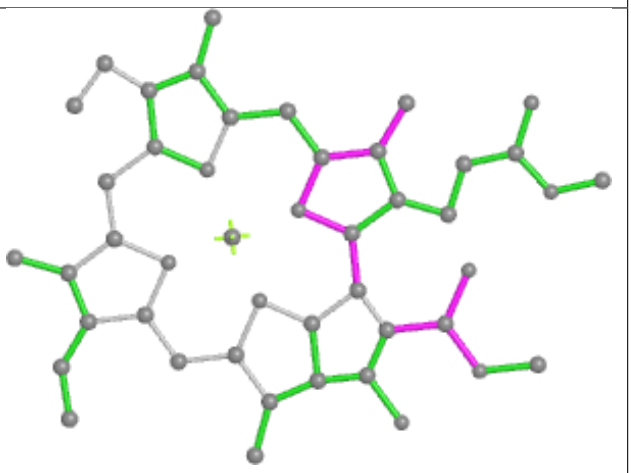


Rings

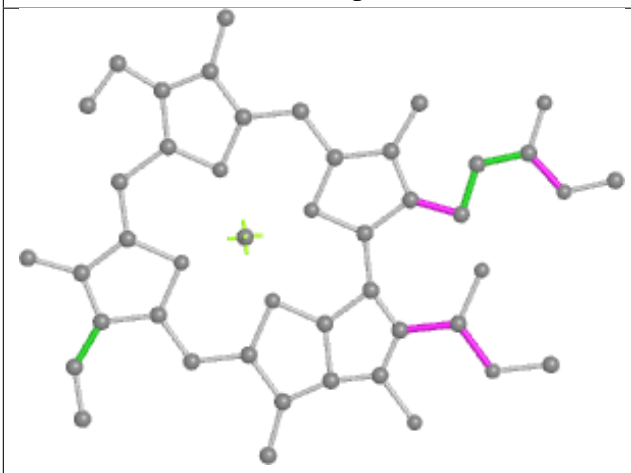
Ligand CLA A 1129



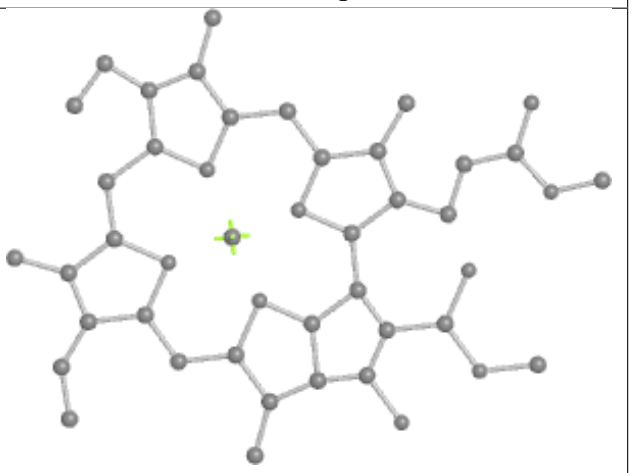
Bond lengths



Bond angles

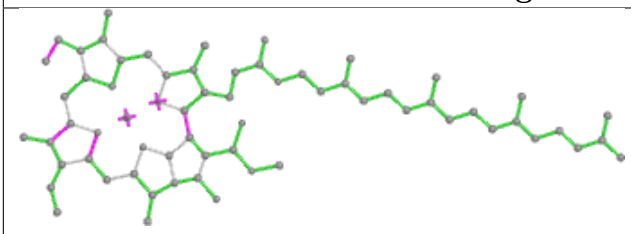


Torsions

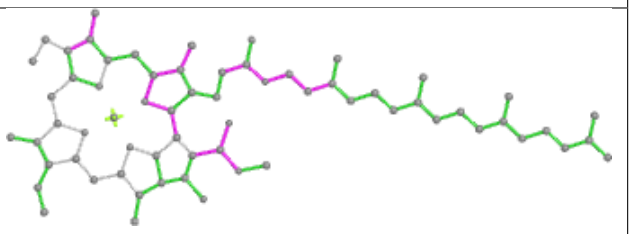


Rings

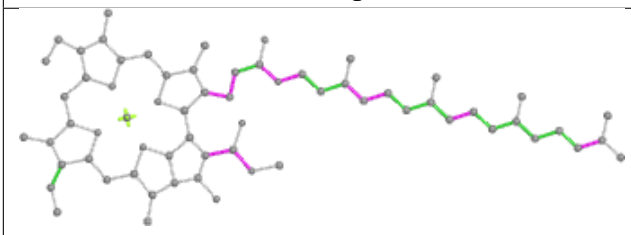
Ligand CLA B 1240



Bond lengths



Bond angles



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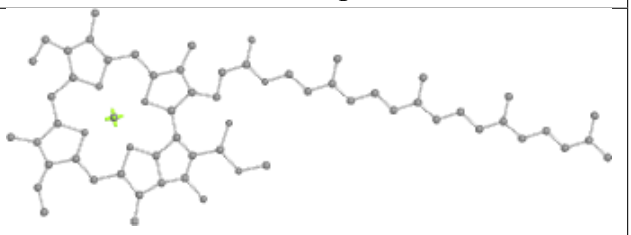
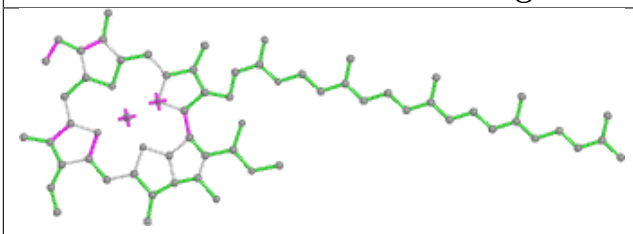
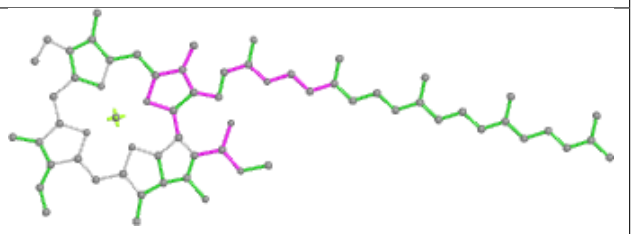


Rings

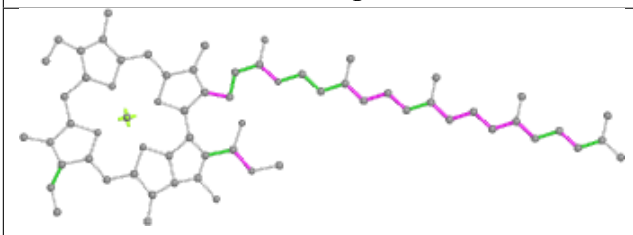
Ligand CLA B 1238



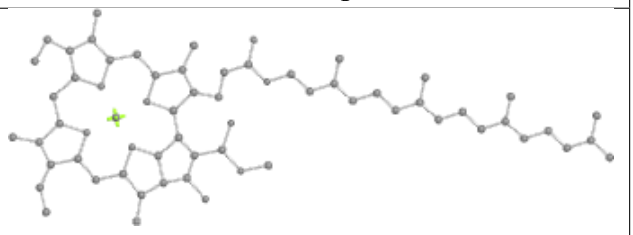
Bond lengths



Bond angles

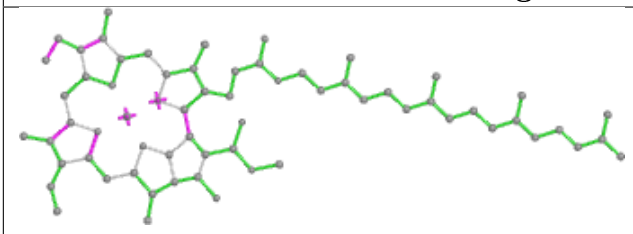


Torsions

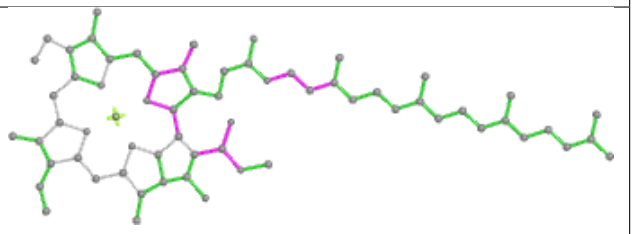


Rings

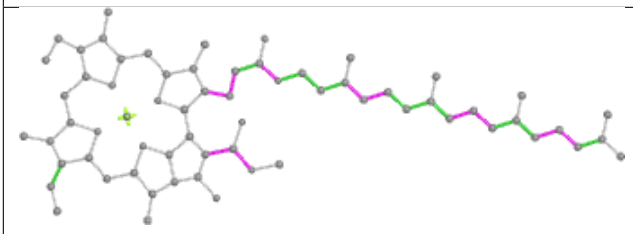
Ligand CLA A 1133



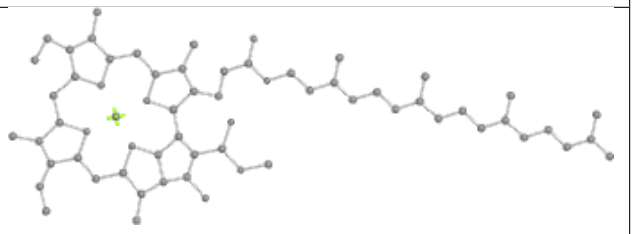
Bond lengths



Bond angles

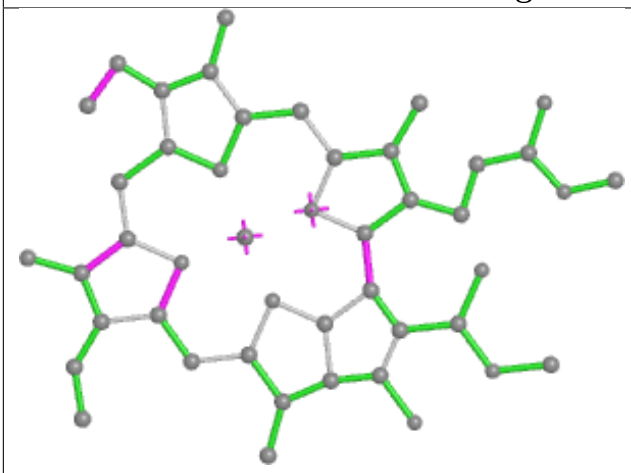


Torsions

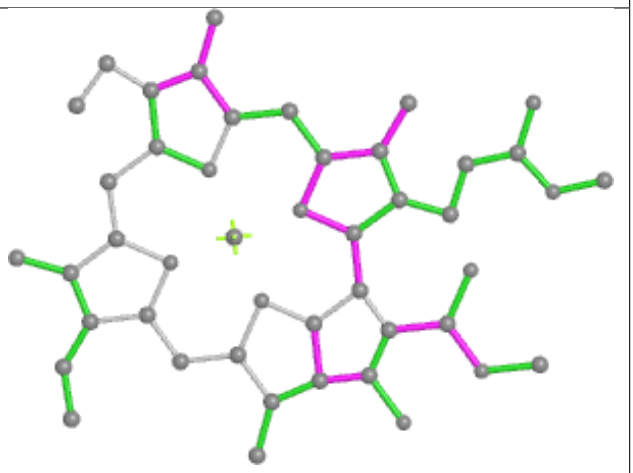


Rings

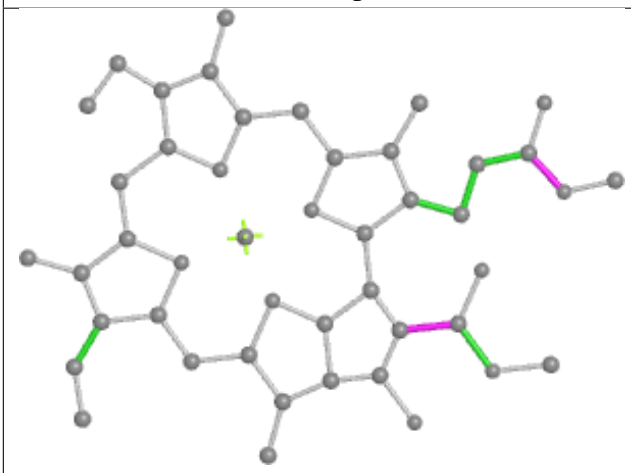
Ligand CLA B 1211



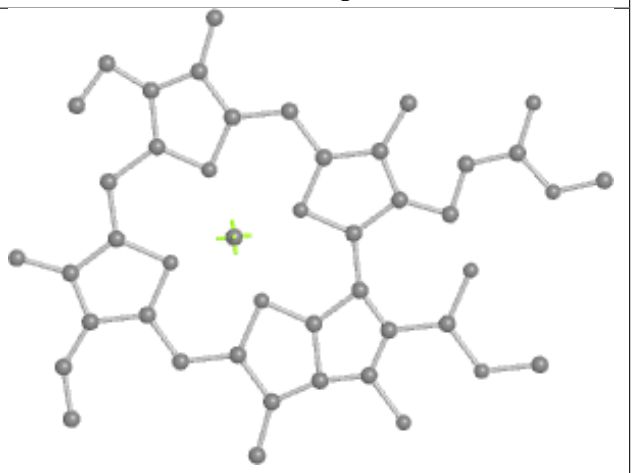
Bond lengths



Bond angles

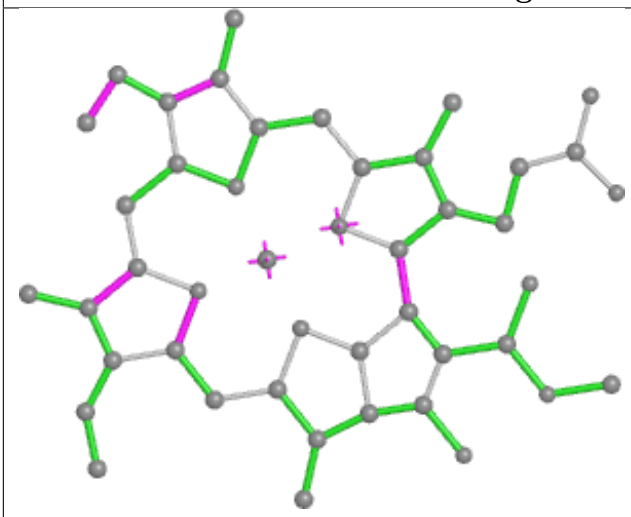


Torsions

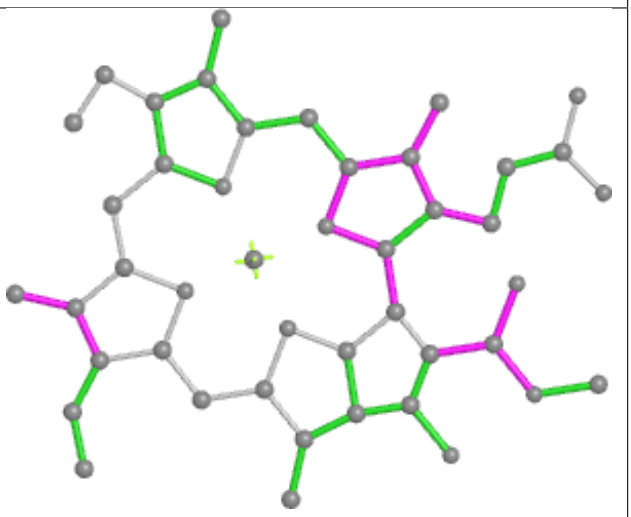


Rings

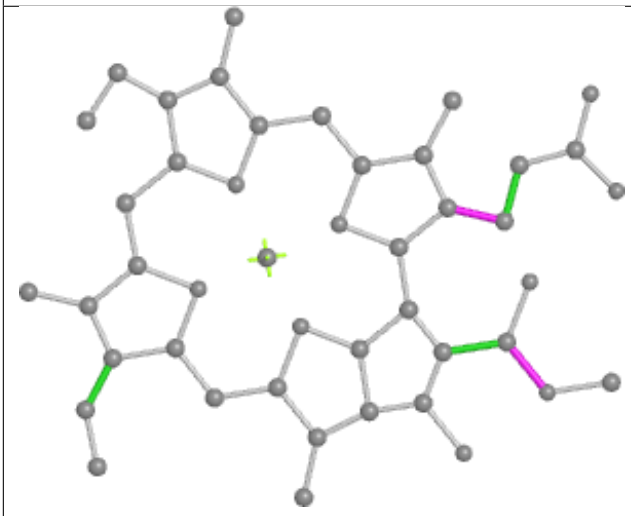
Ligand CLA B 1208



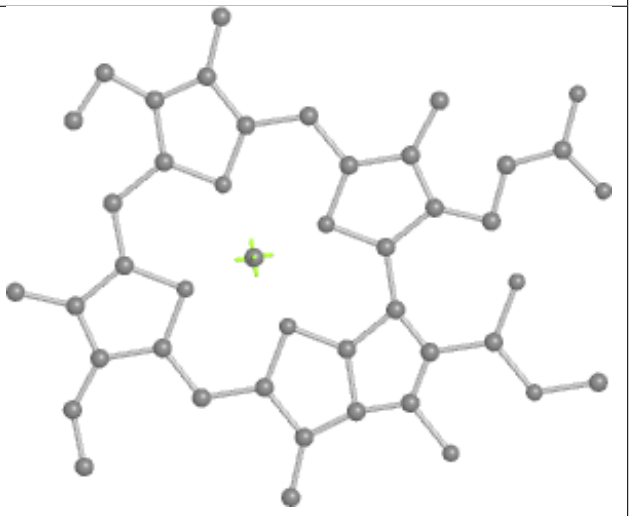
Bond lengths



Bond angles

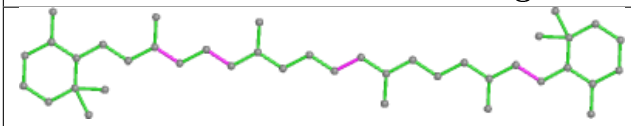


Torsions

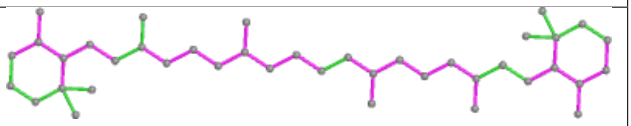


Rings

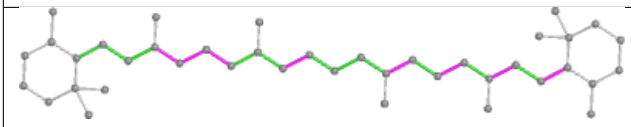
Ligand BCR B 4010



Bond lengths



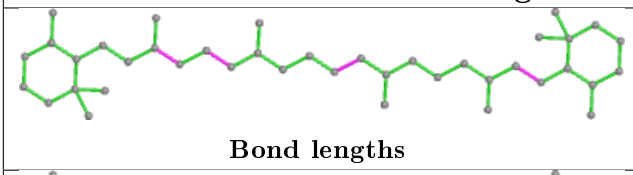
Bond angles



Torsions

Rings

Ligand BCR B 4004



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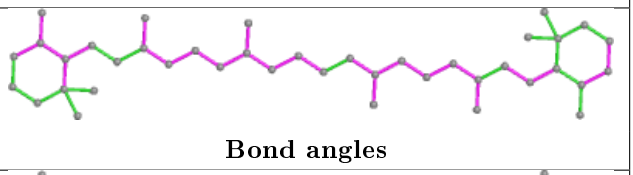
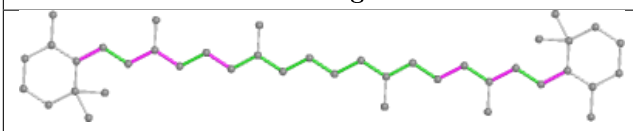
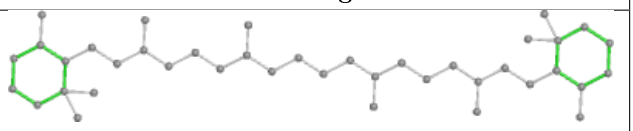


Bond angles

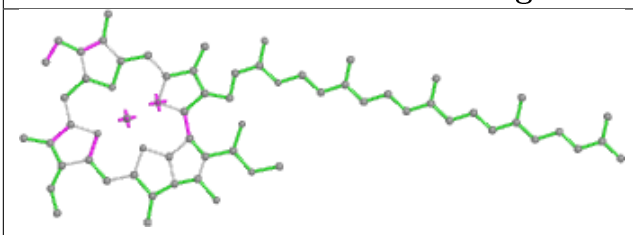


Torsions

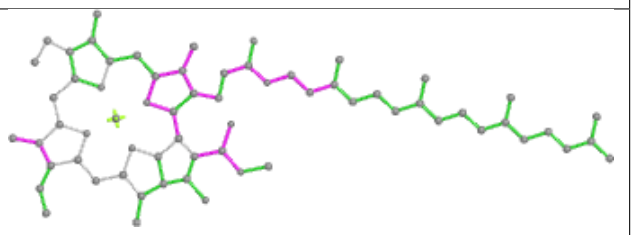


Rings

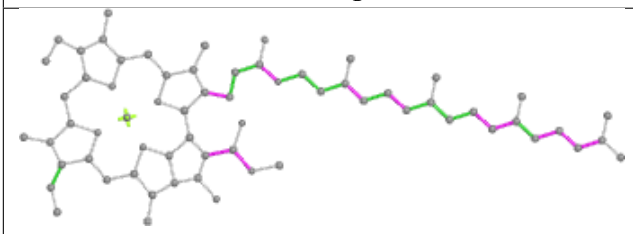
Ligand CLA A 1104



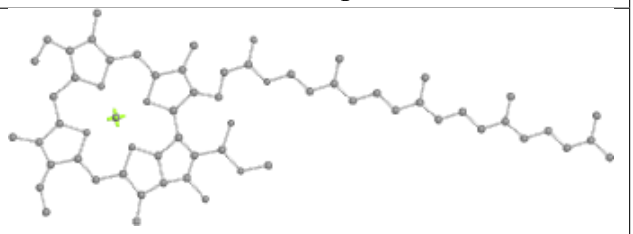
Bond lengths



Bond angles

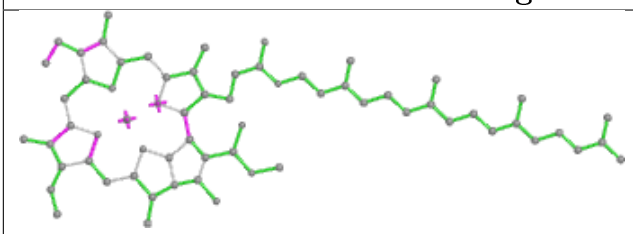


Torsions

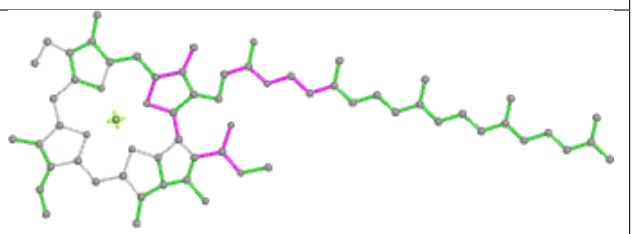


Rings

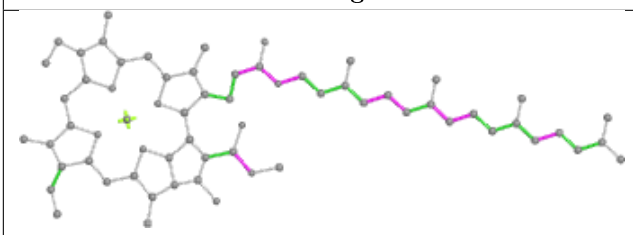
Ligand CLA B 1231



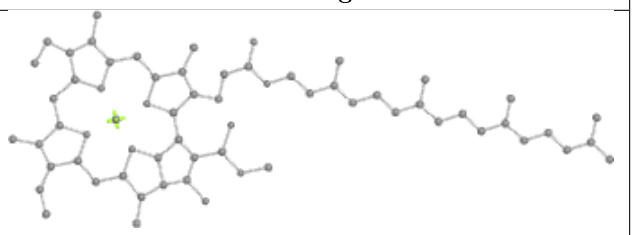
Bond lengths



Bond angles

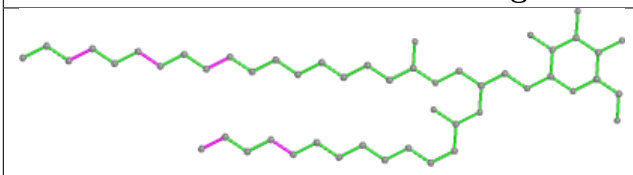


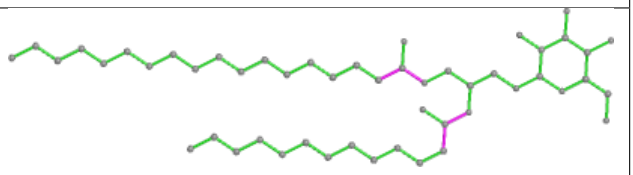
Torsions

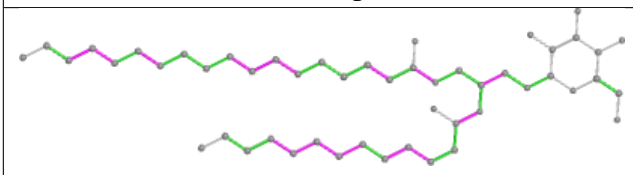


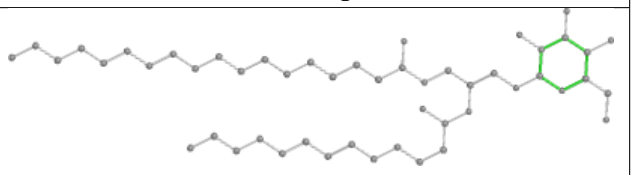
Rings

Ligand LMG A 5002

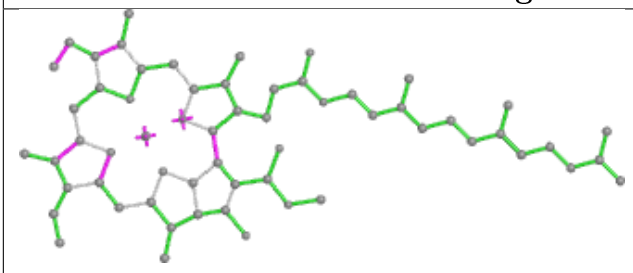

Bond lengths

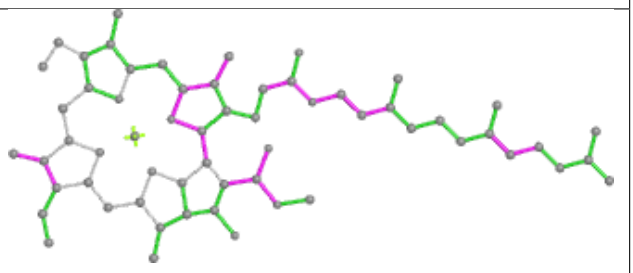

Bond angles

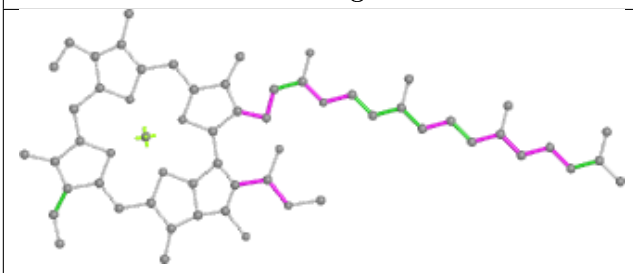

Torsions


Rings

Ligand CLA A 1103


Bond lengths


Bond angles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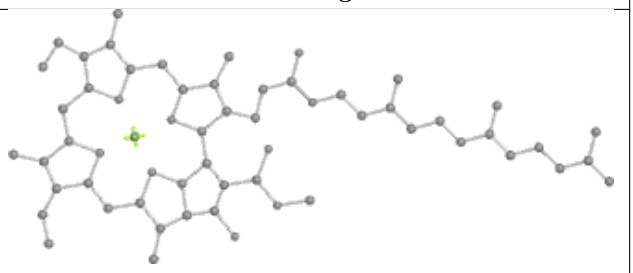
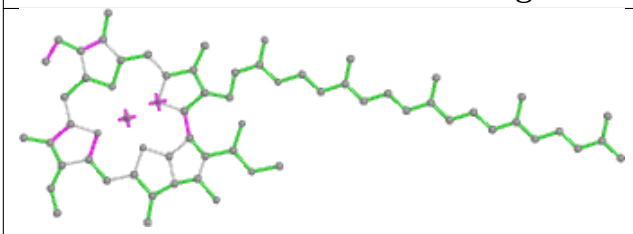
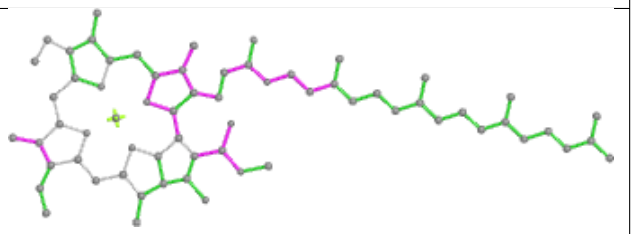
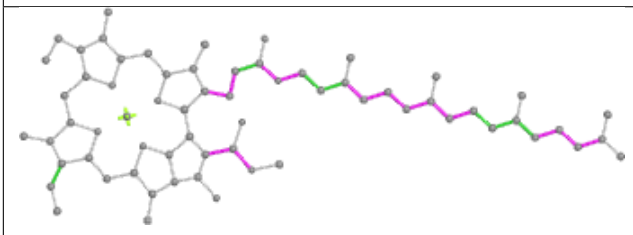

Rings

Ligand CLA B 1219


Bond lengths


Bond angles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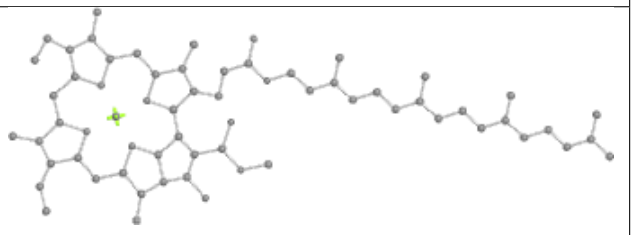
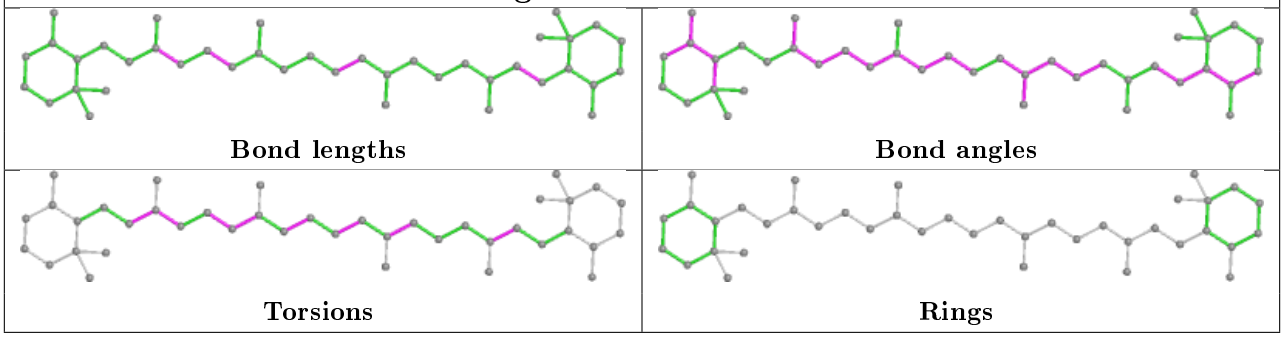
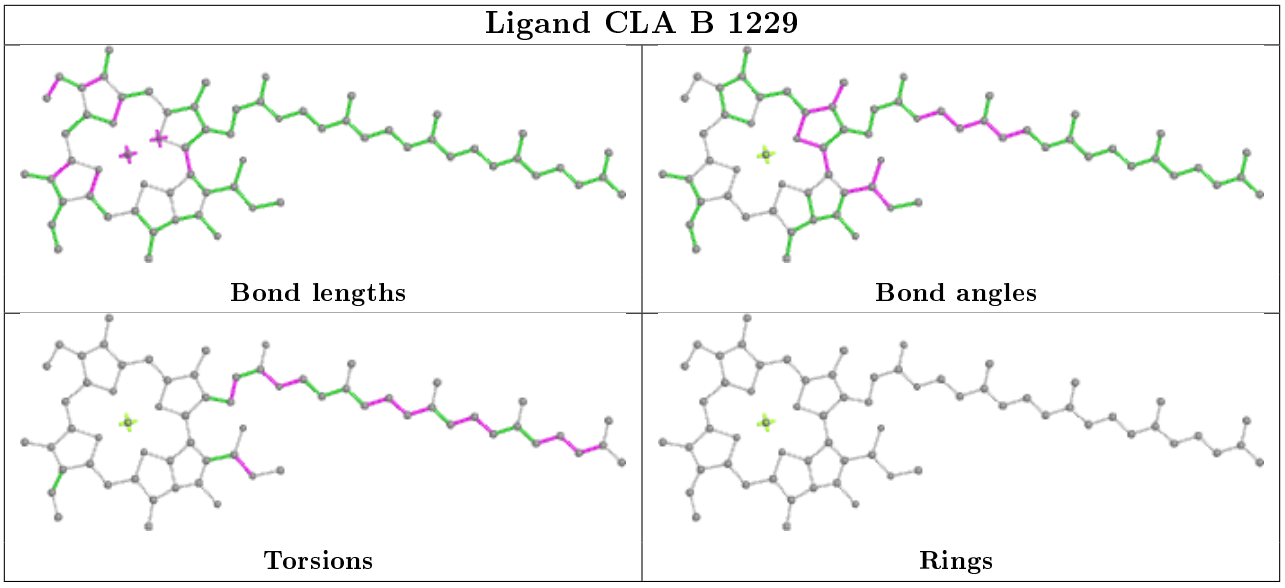

Rings

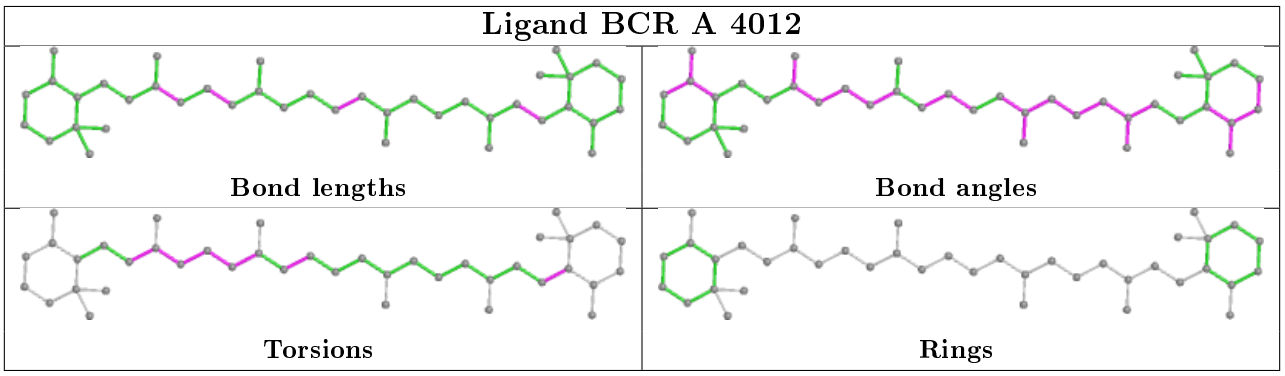
Ligand BCR A 4003

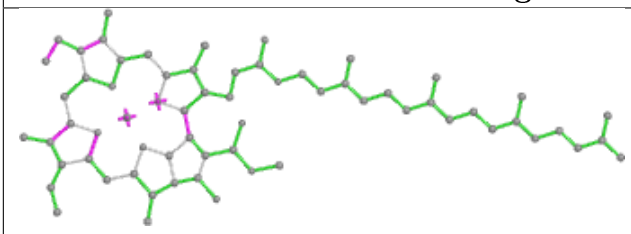
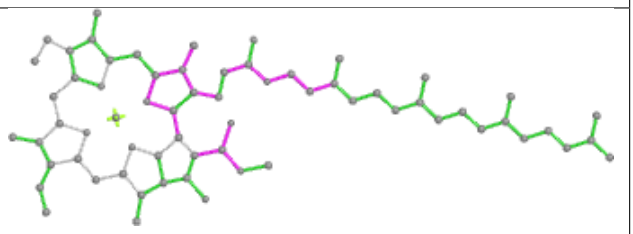
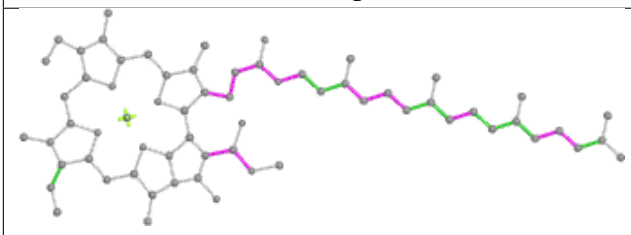
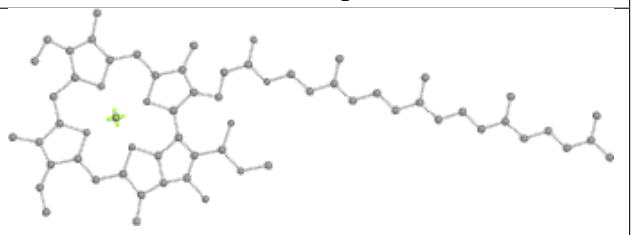


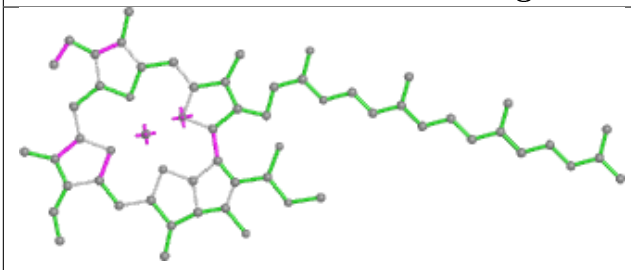
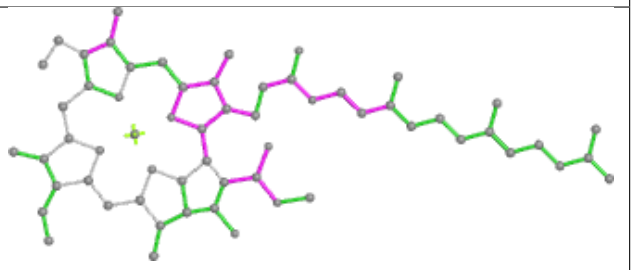
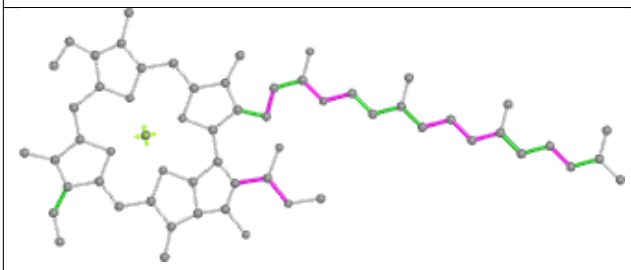
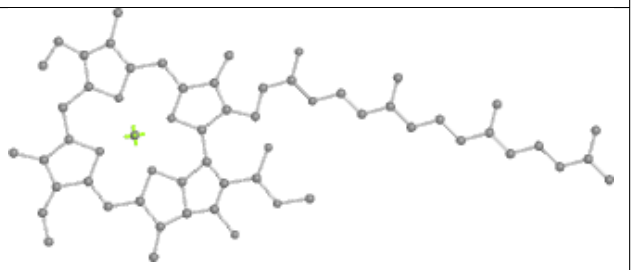
Ligand CLA B 1229



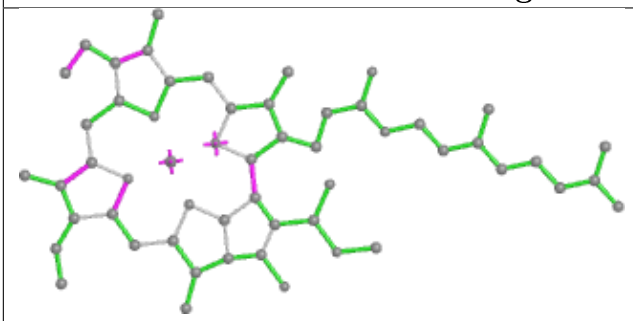
Ligand BCR A 4012



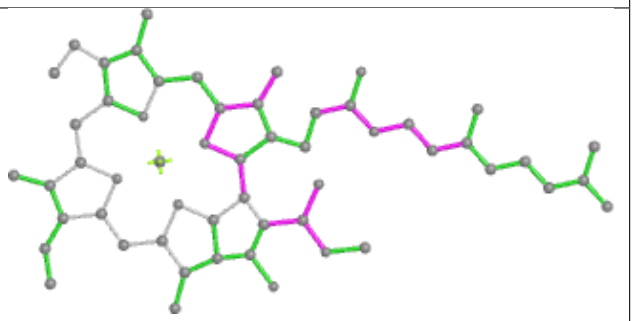
Ligand CLA K 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1023	
 Bond lengths	 Bond angles
 Torsions	 Rings

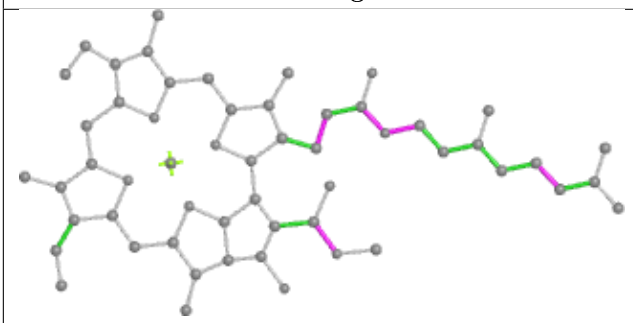
Ligand CLA B 1207



Bond lengths



Bond angles



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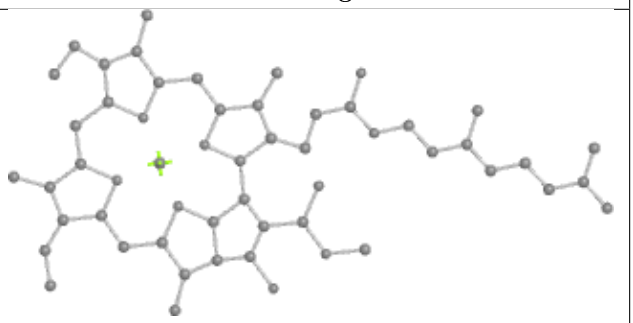
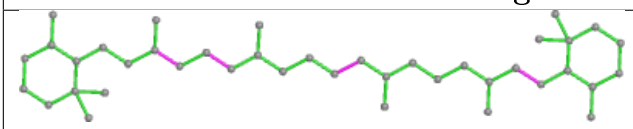


Rings

Ligand BCR A 4001



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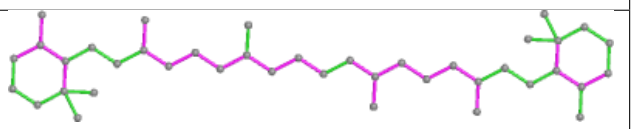
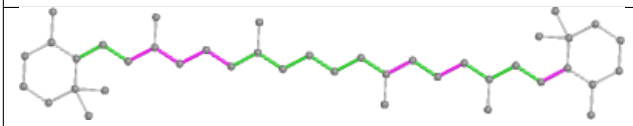


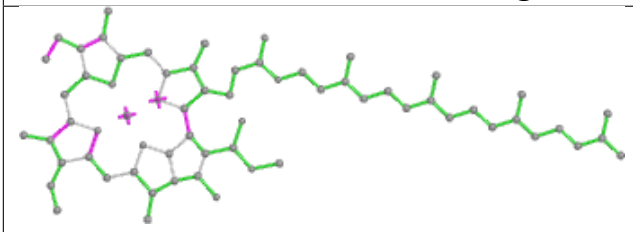
Bond angles



Torsions

Rings

Ligand CLA B 1209



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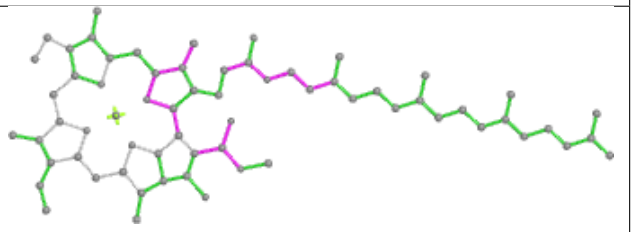

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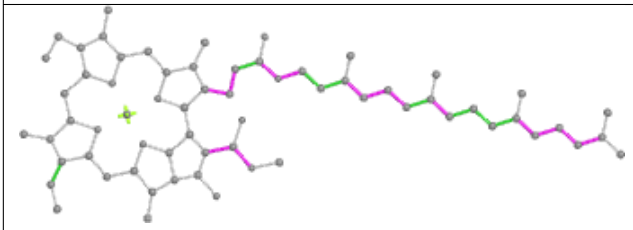

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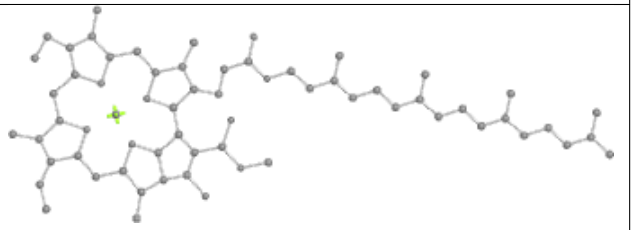
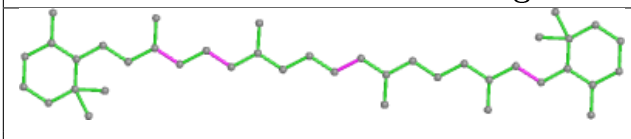


Rings

Ligand BCR A 4019



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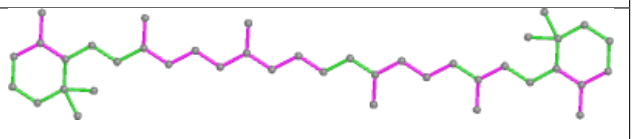

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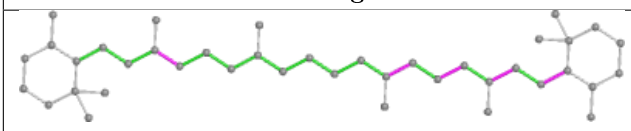

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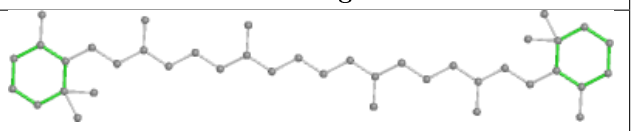
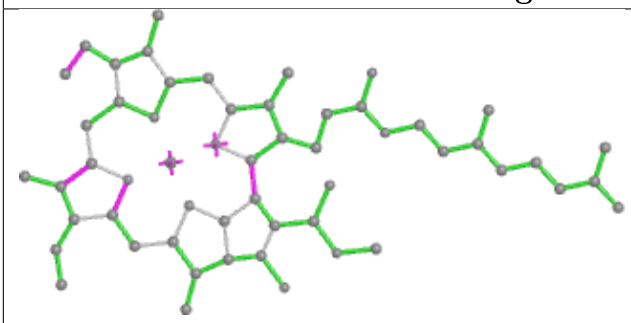


Rings

Ligand CLA A 1013



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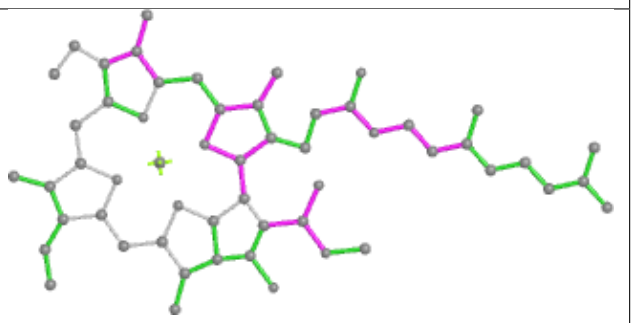
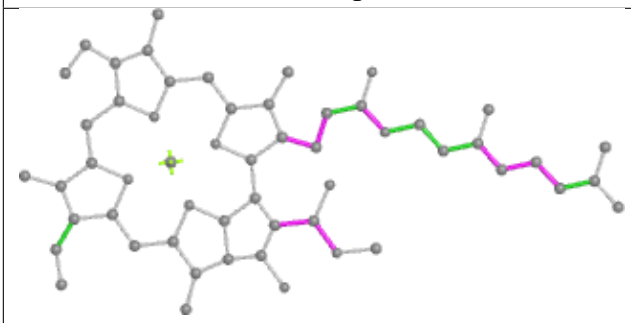


Bond angles



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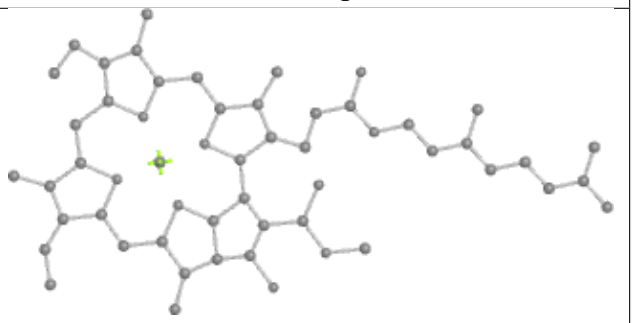
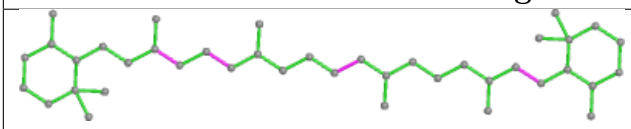


Rings

Ligand BCR B 4014



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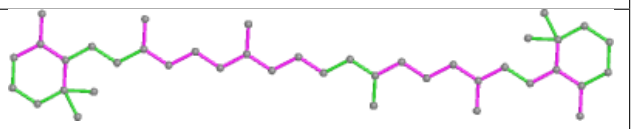

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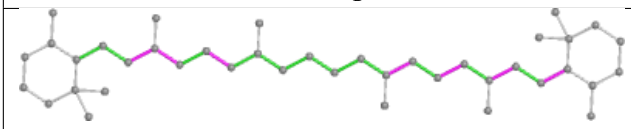
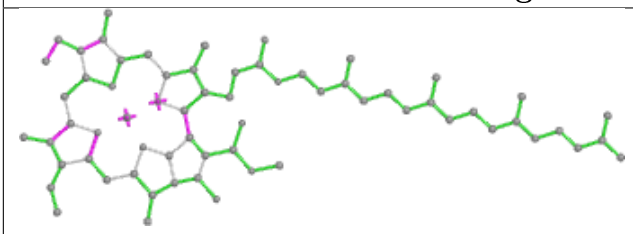


Torsions

Rings

Ligand CLA B 1214



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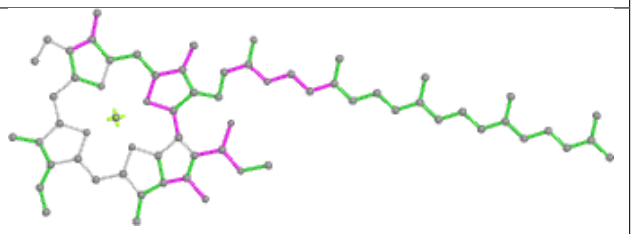

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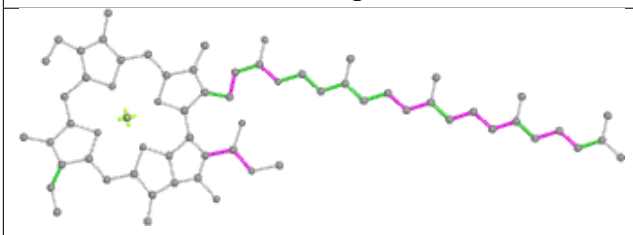

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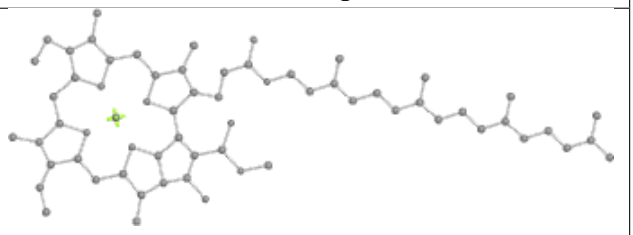
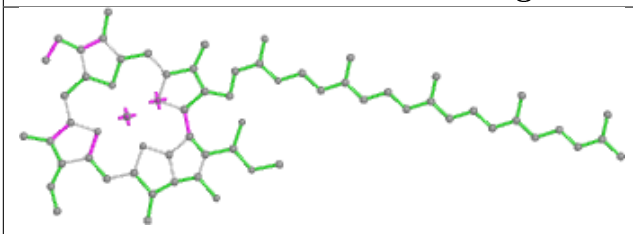


Rings

Ligand CLA B 1217



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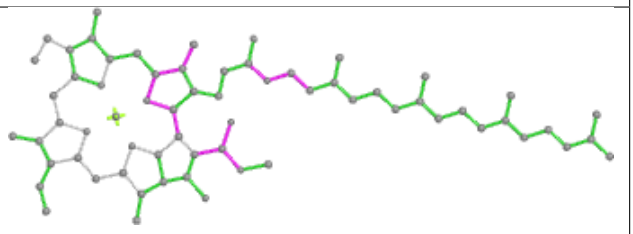

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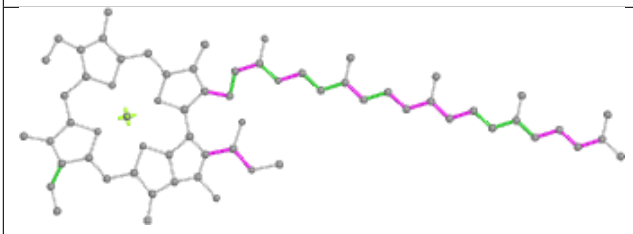

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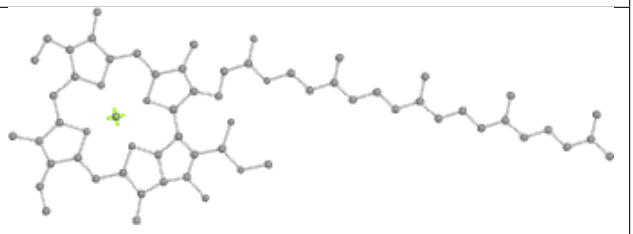
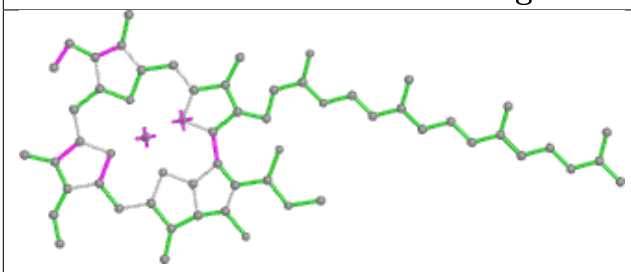


Rings

Ligand CLA A 1126



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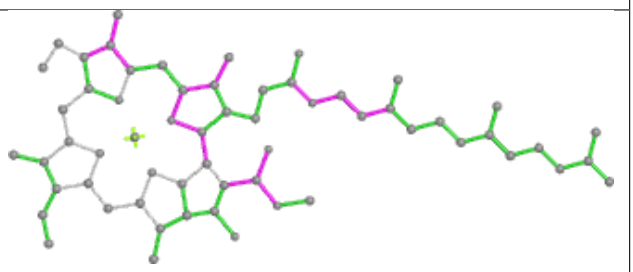
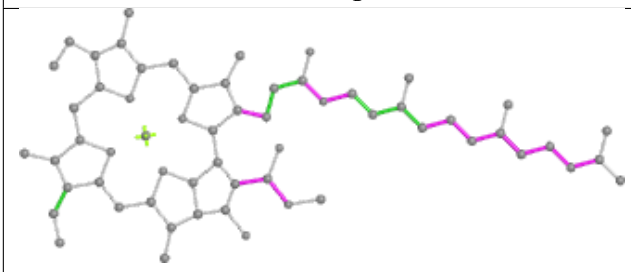


Bond angles



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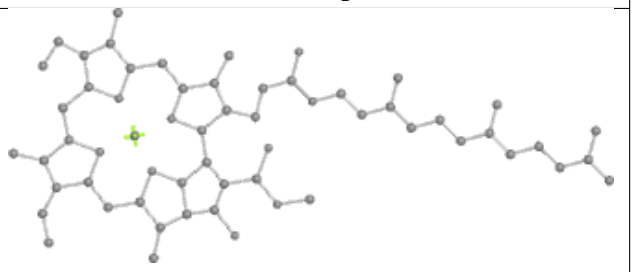
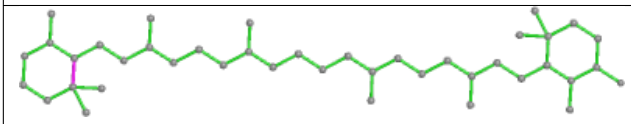


Rings

Ligand ECH B 4006



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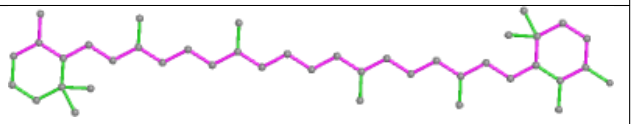
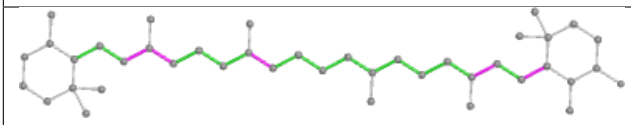


Bond angles



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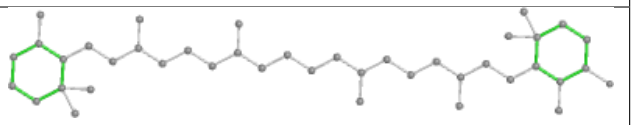
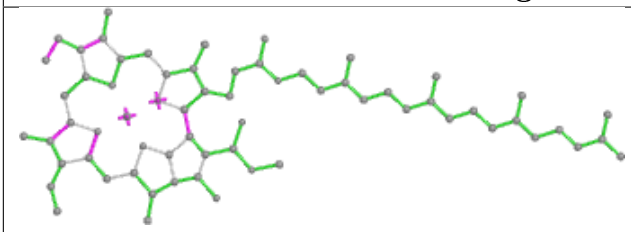


Rings

Ligand CLA B 1228



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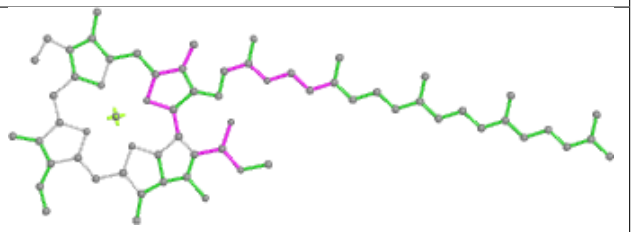
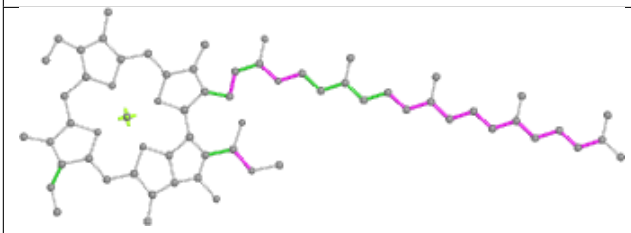


Bond angles



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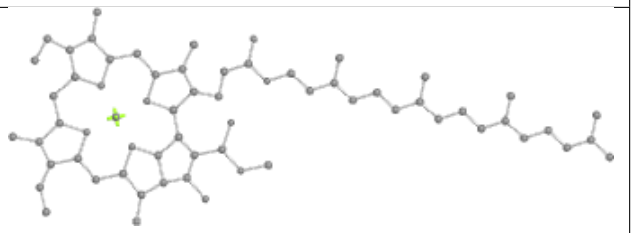
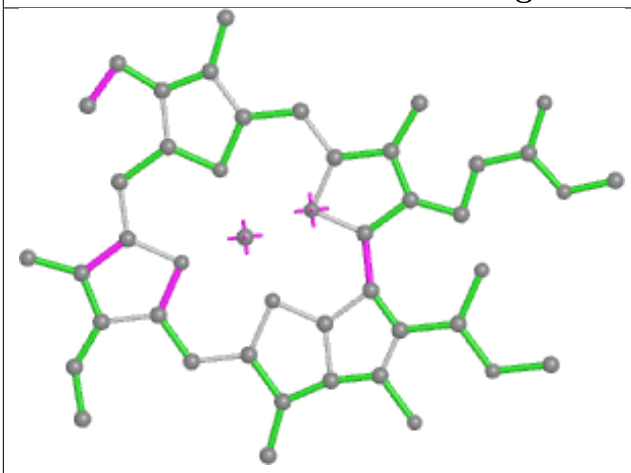


Rings

Ligand CLA A 1115



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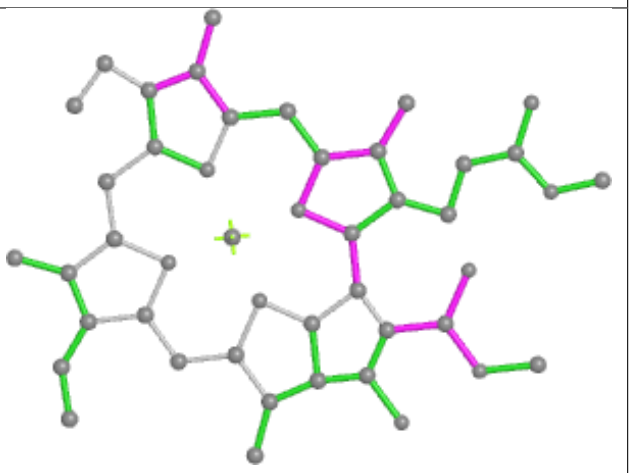
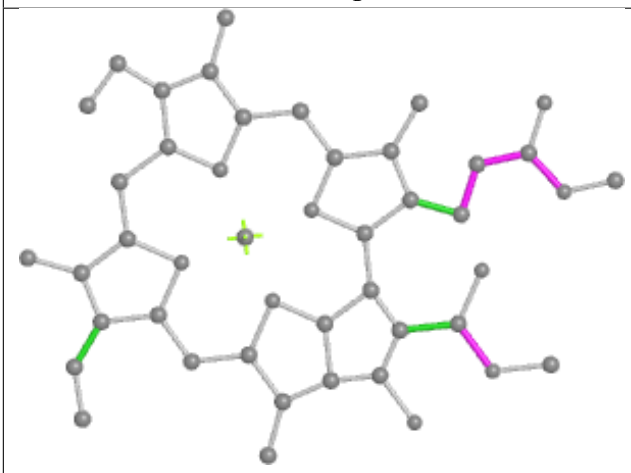


Bond angles



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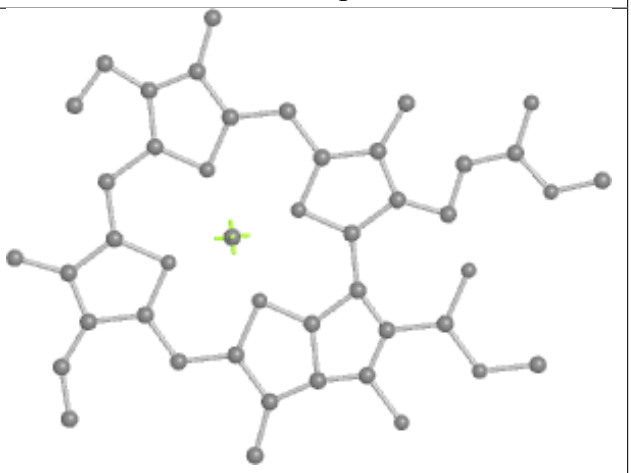
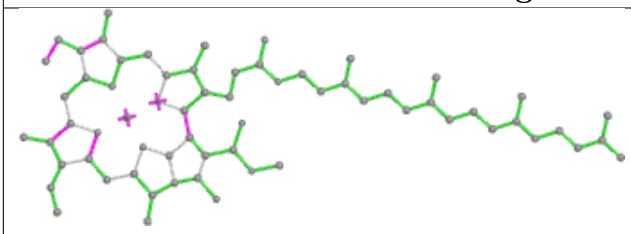


Rings

Ligand CLA A 1117



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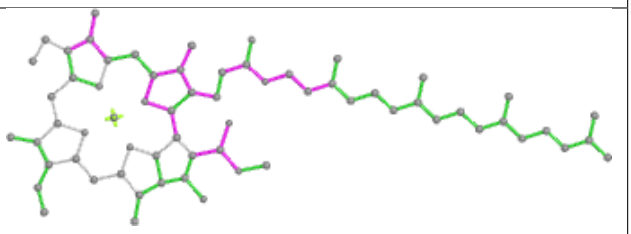
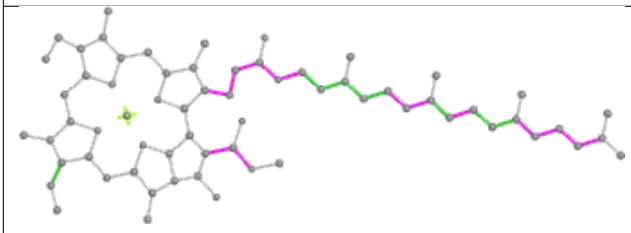


Bond angles



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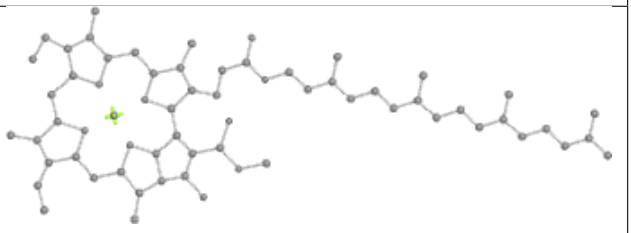
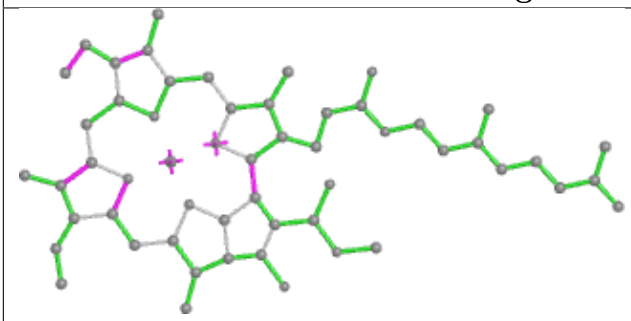
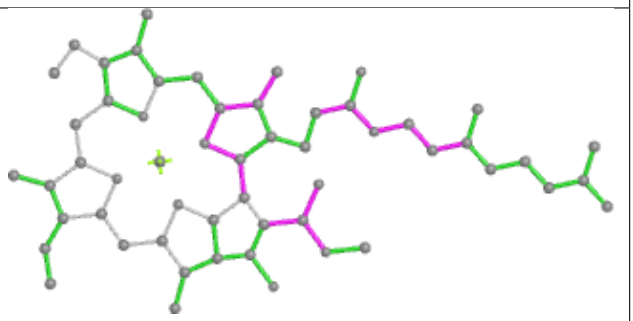


Rings

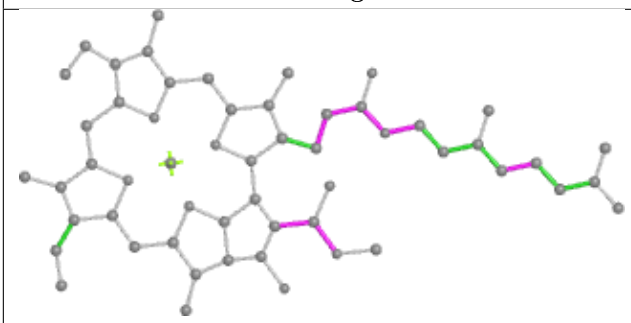
Ligand CLA A 1130



Bond lengths



Bond angles



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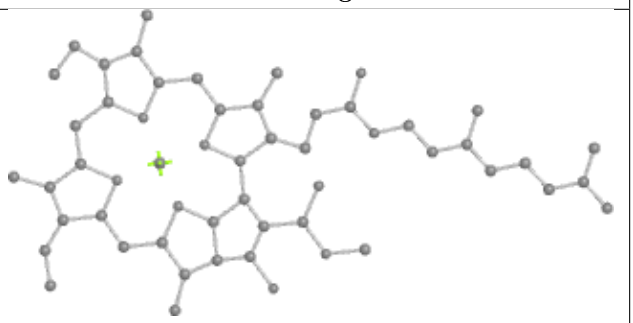
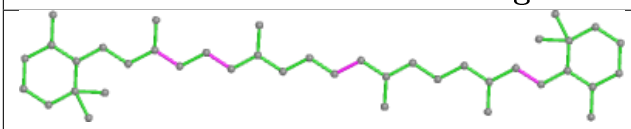
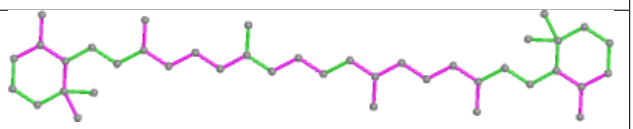


Rings

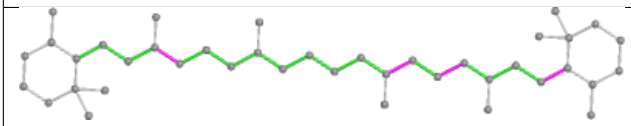
Ligand BCR A 4007



Bond lengths



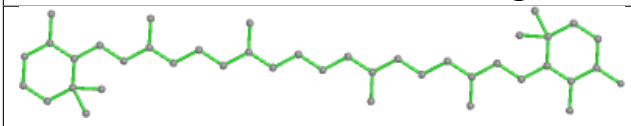
Bond angles



Torsions

Rings

Ligand ECH M 4021



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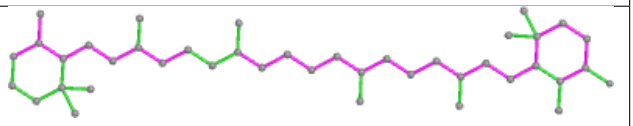
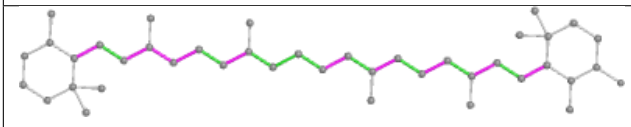
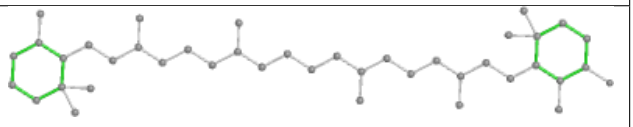


Bond angles

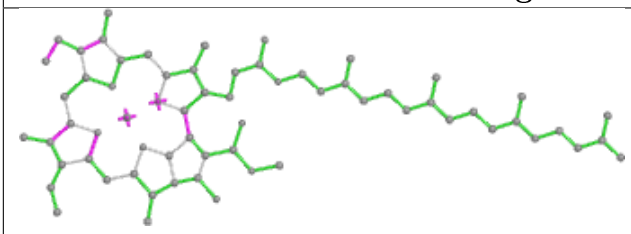


Torsions

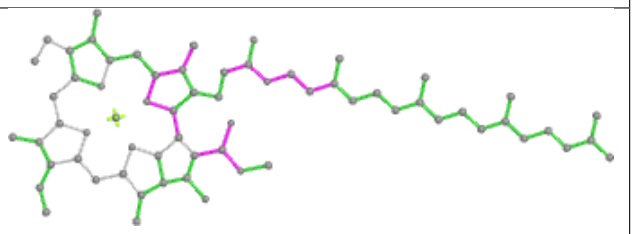


Rings

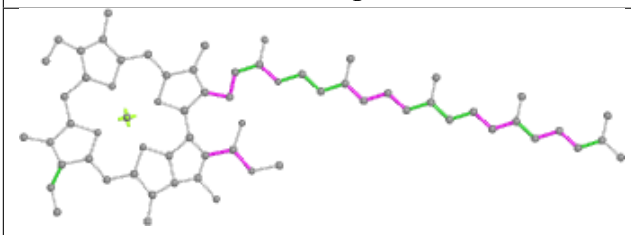
Ligand CLA A 1136



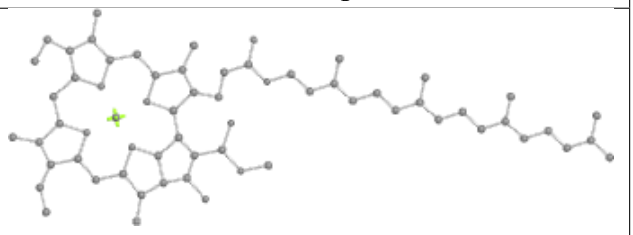
Bond lengths



Bond angles

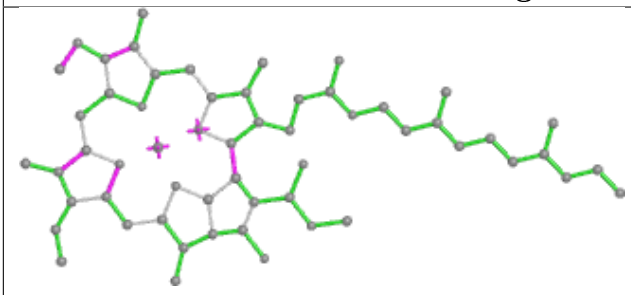


Torsions

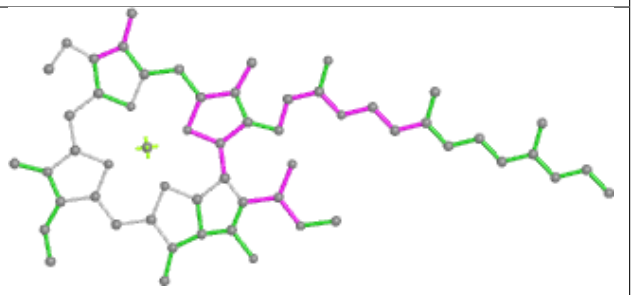


Rings

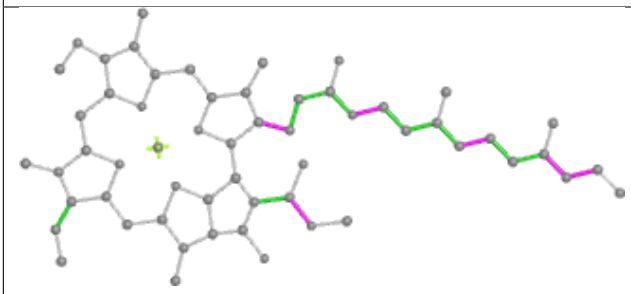
Ligand CLA B 1220



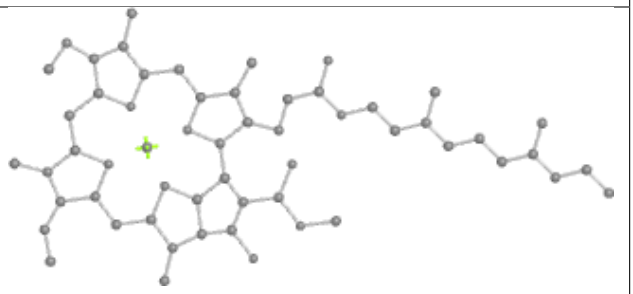
Bond lengths



Bond angles

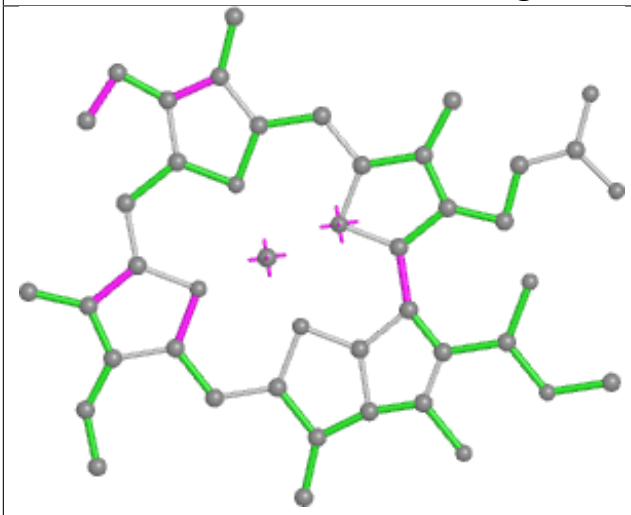


Torsions

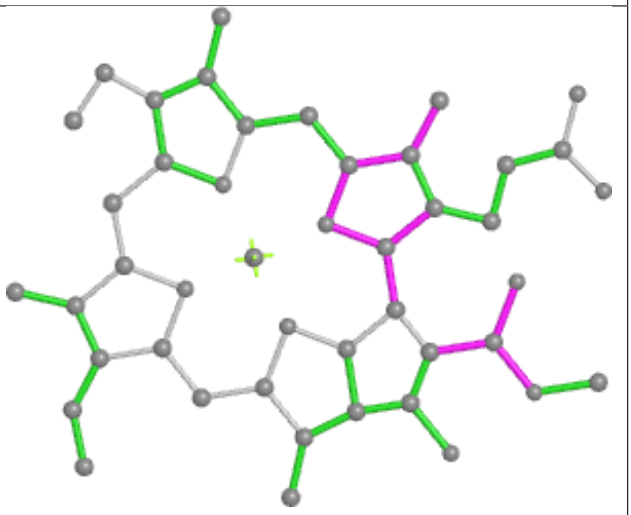


Rings

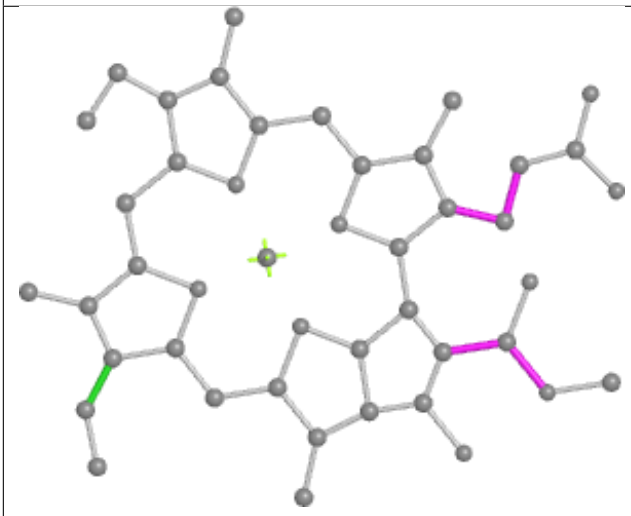
Ligand CLA A 1108



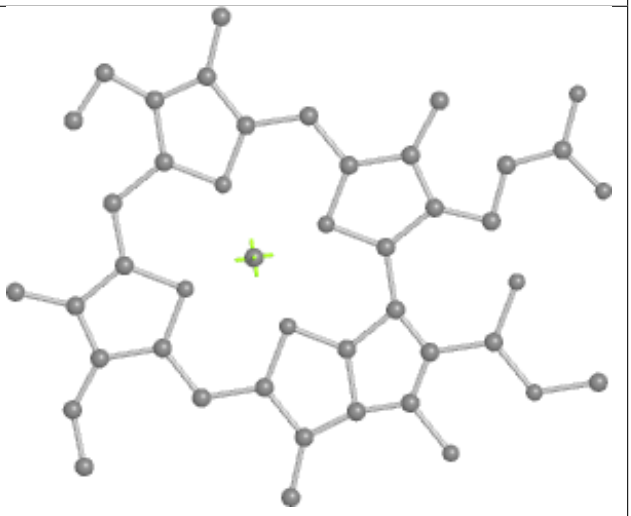
Bond lengths



Bond angles

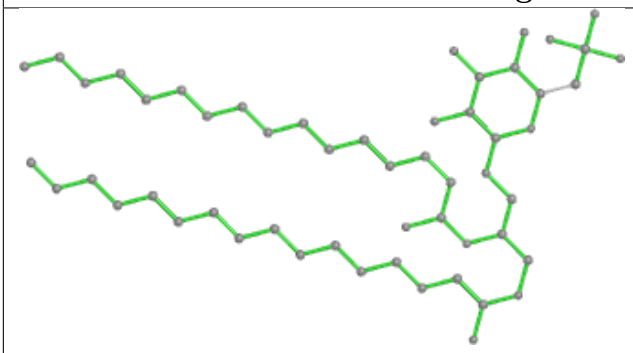


Torsions

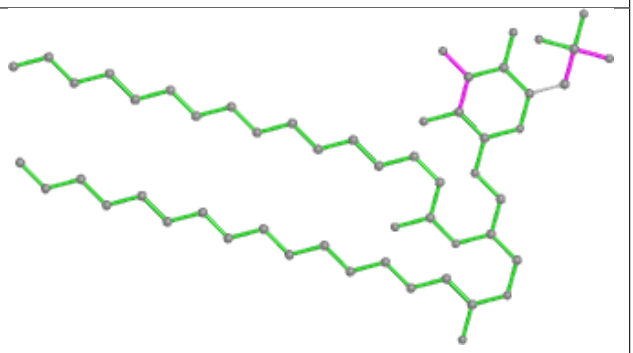


Rings

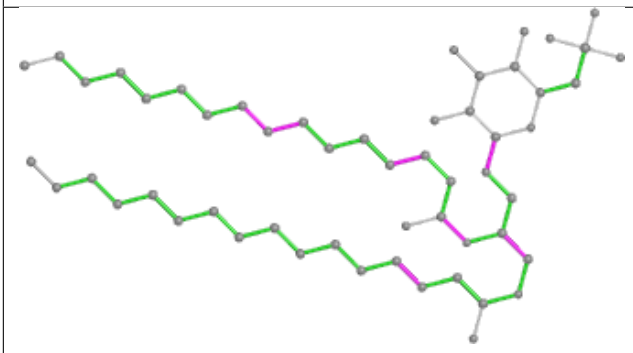
Ligand SQD B 5008



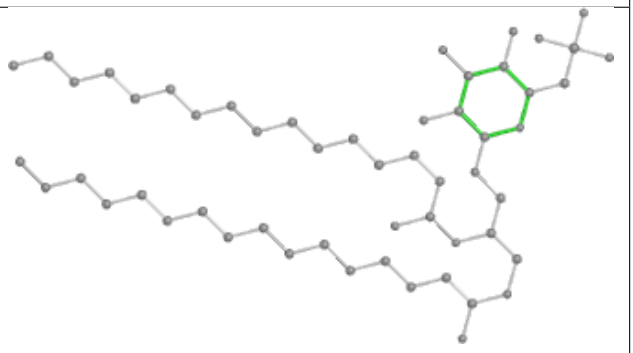
Bond lengths



Bond angles

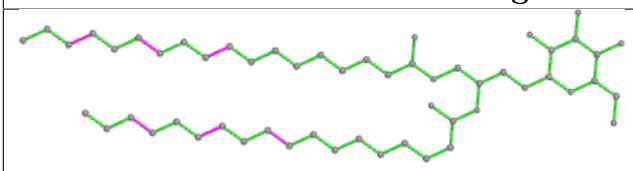


Torsions

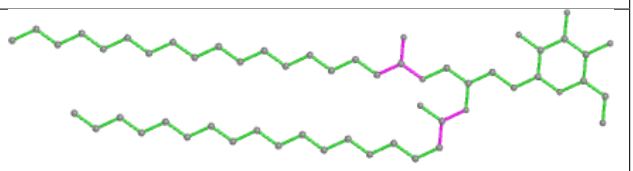


Rings

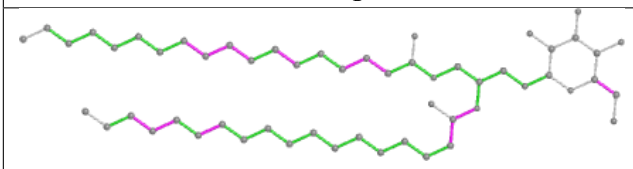
Ligand LMG B 5002



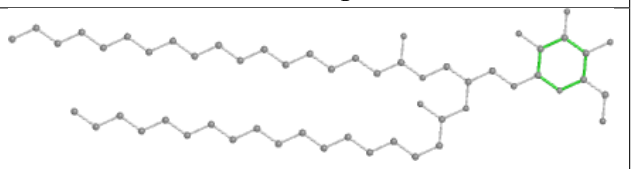
Bond lengths



Bond angles

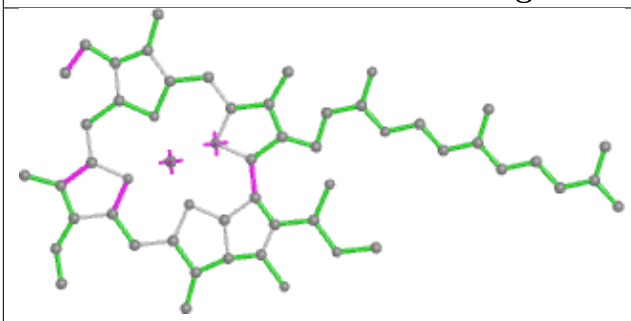


Torsions

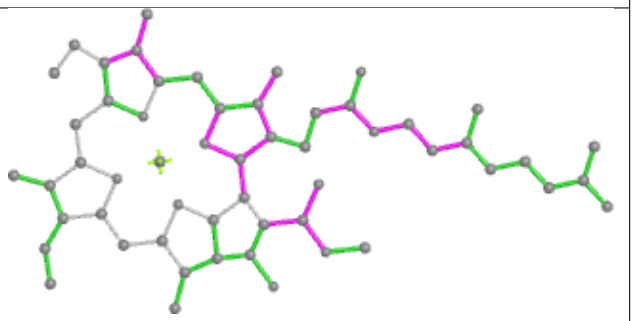


Rings

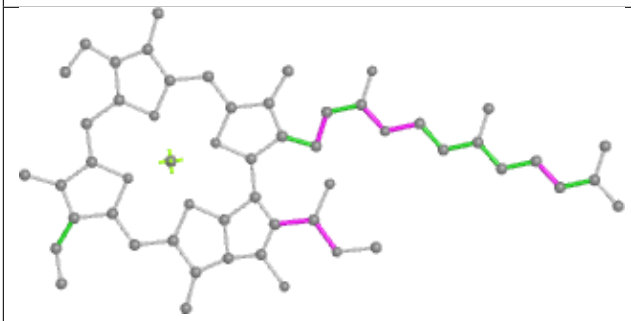
Ligand CLA B 1221



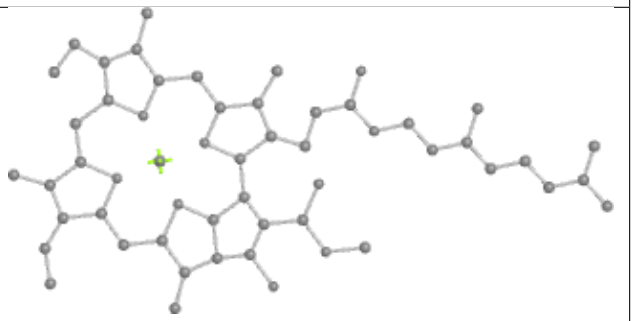
Bond lengths



Bond angles

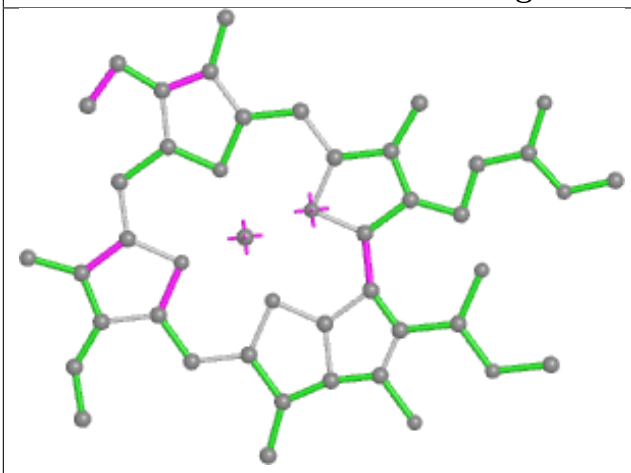


Torsions

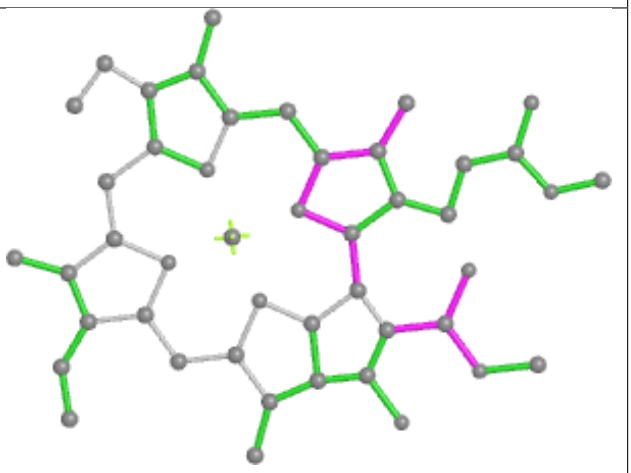


Rings

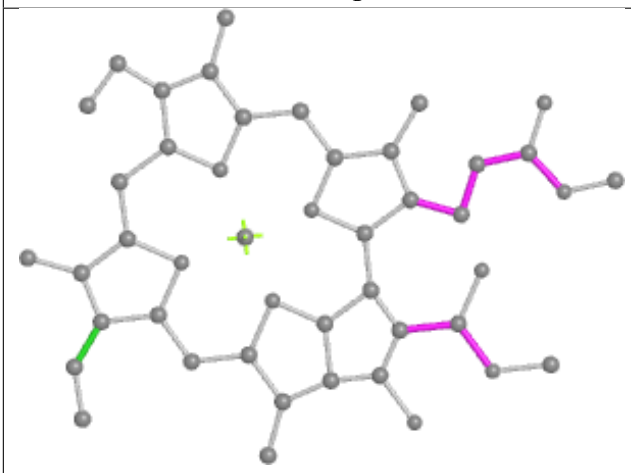
Ligand CLA B 1201



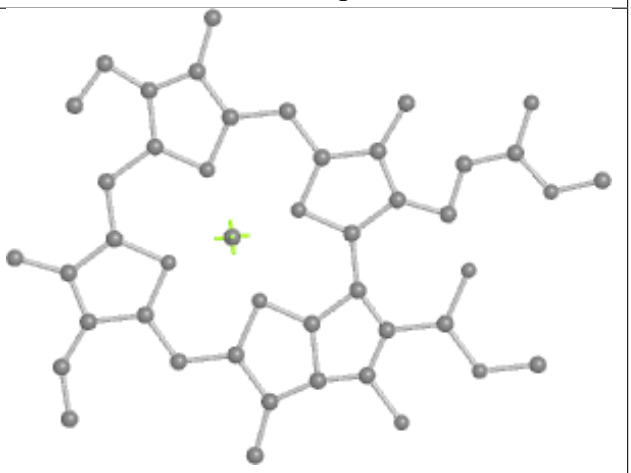
Bond lengths



Bond angles

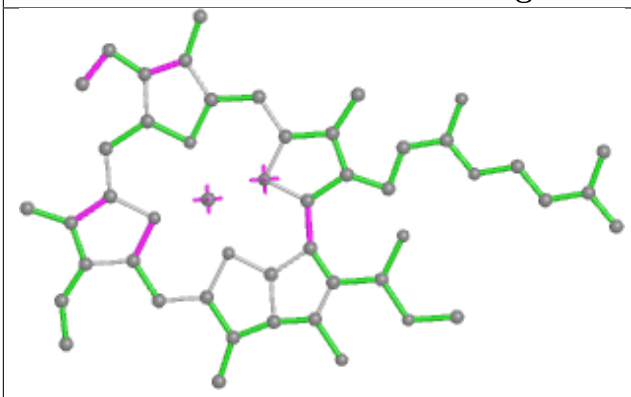


Torsions

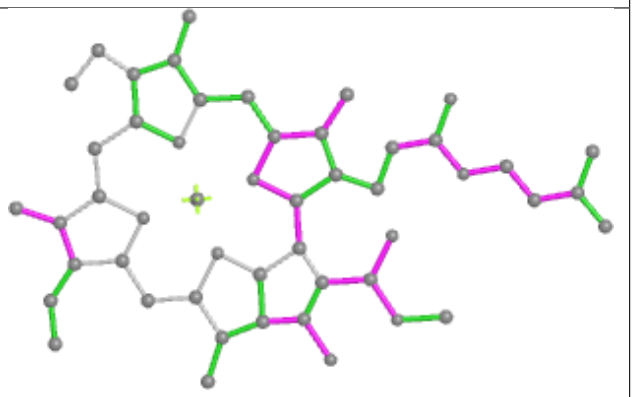


Rings

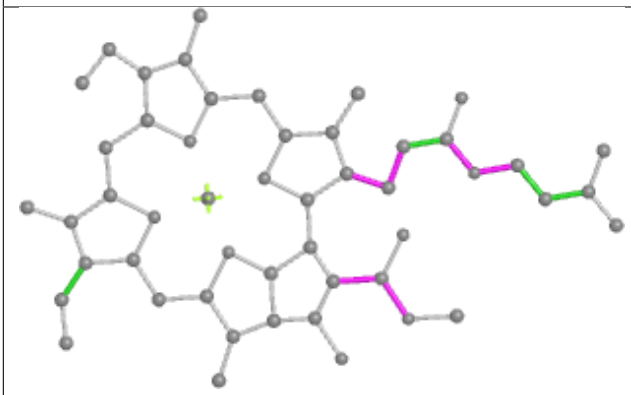
Ligand CLA B 1218



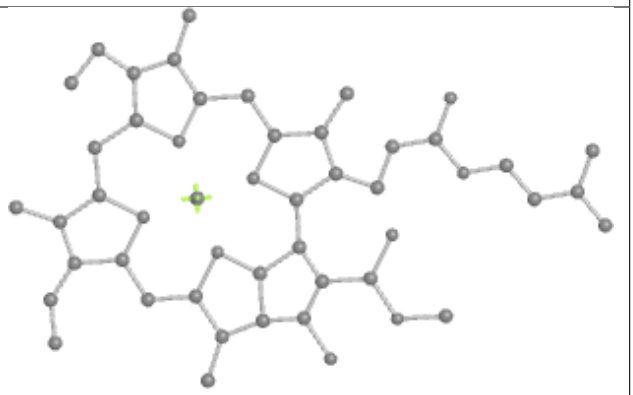
Bond lengths



Bond angles

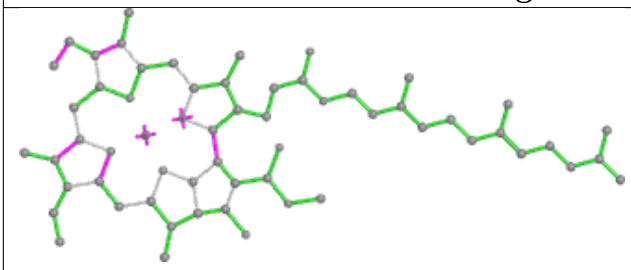


Torsions

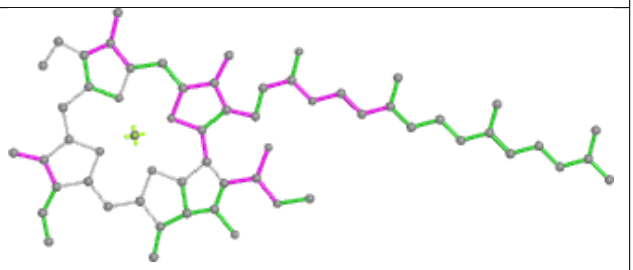


Rings

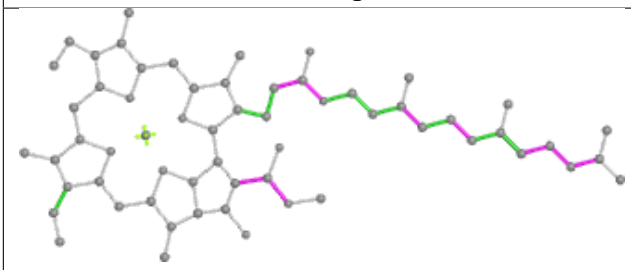
Ligand CLA A 1128



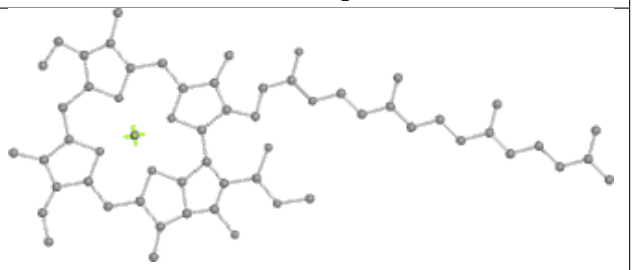
Bond lengths



Bond angles

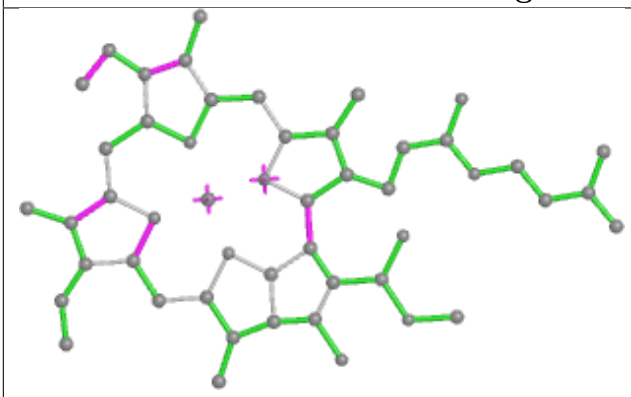


Torsions

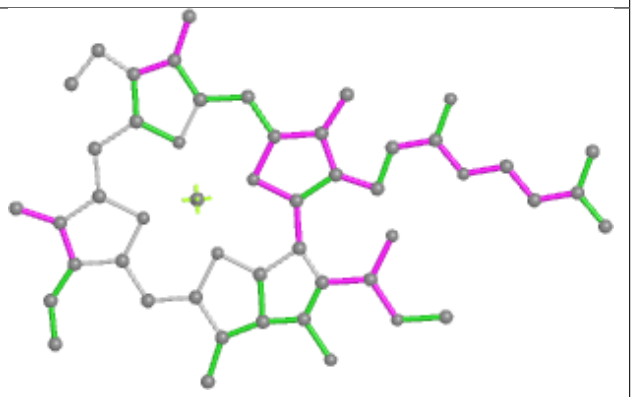


Rings

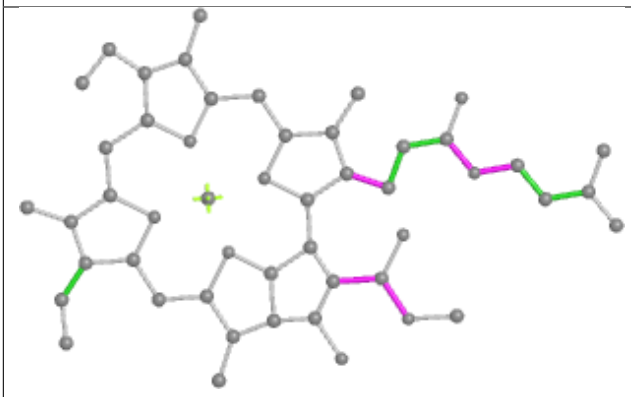
Ligand CLA A 1137



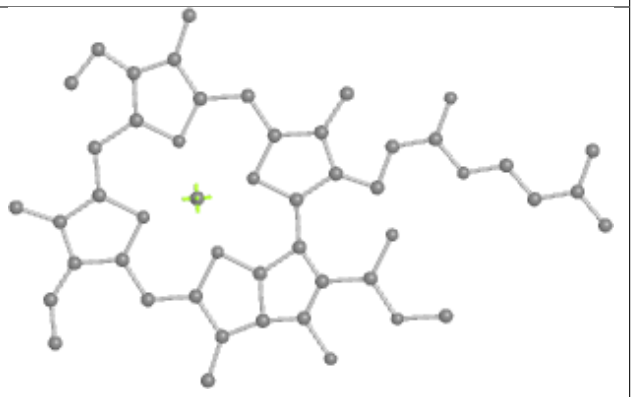
Bond lengths



Bond angles

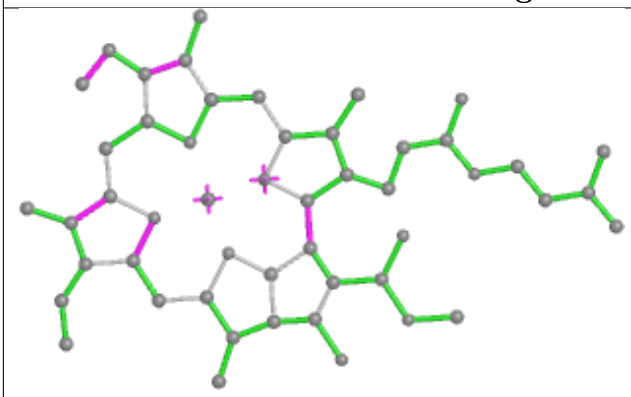


Torsions

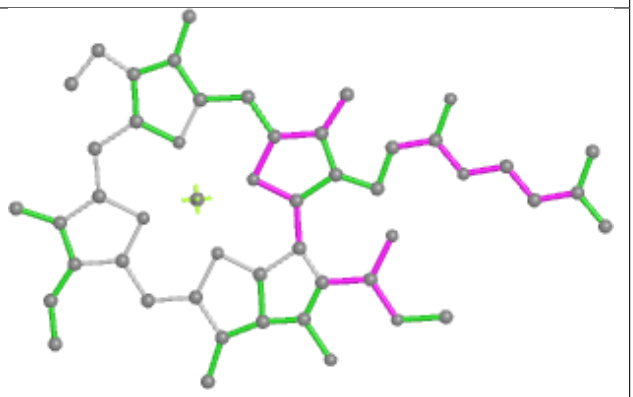


Rings

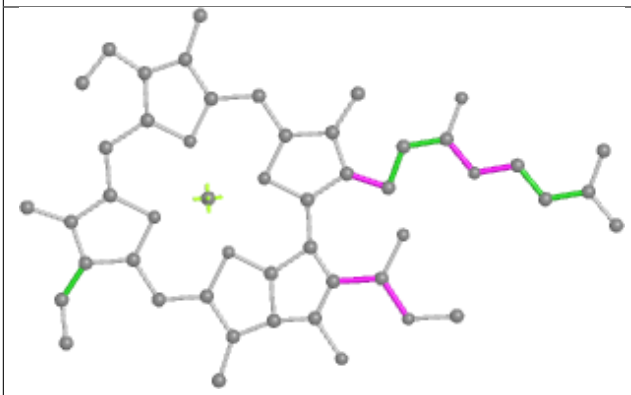
Ligand CLA A 1132



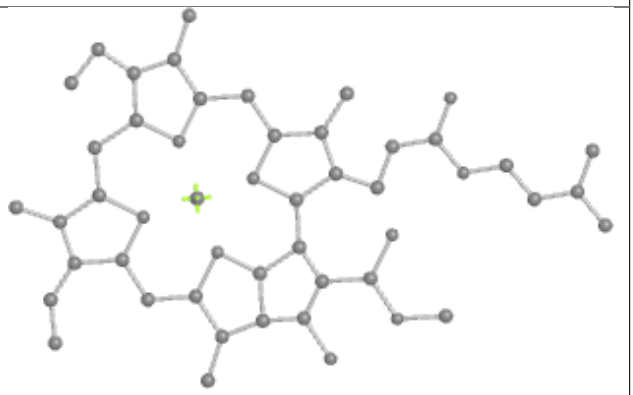
Bond lengths



Bond angles

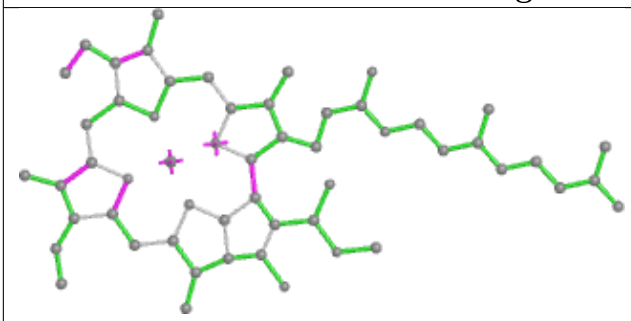


Torsions

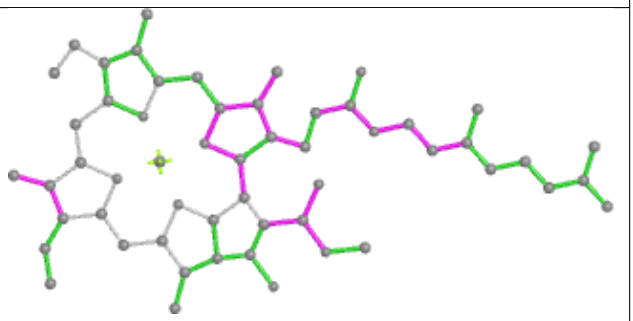


Rings

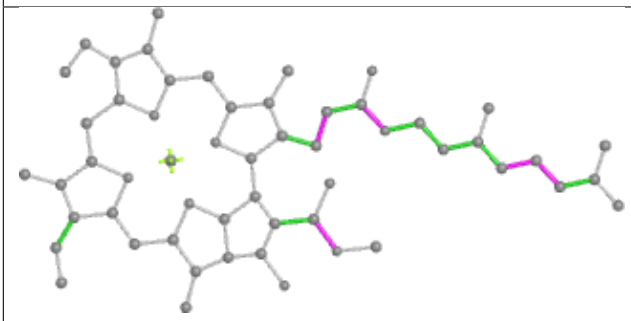
Ligand CLA B 1222



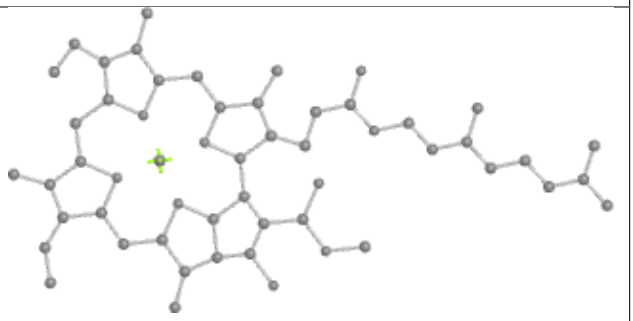
Bond lengths



Bond angles

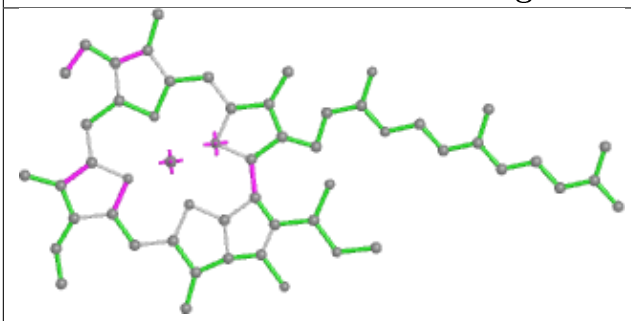


Torsions

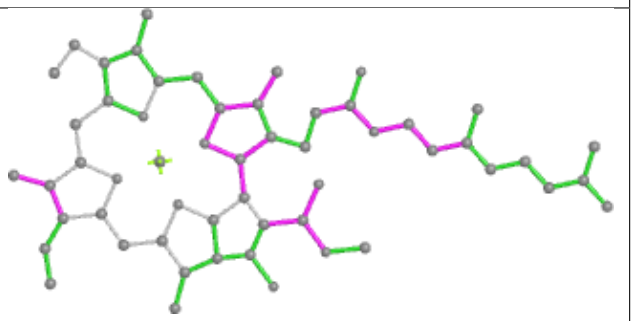


Rings

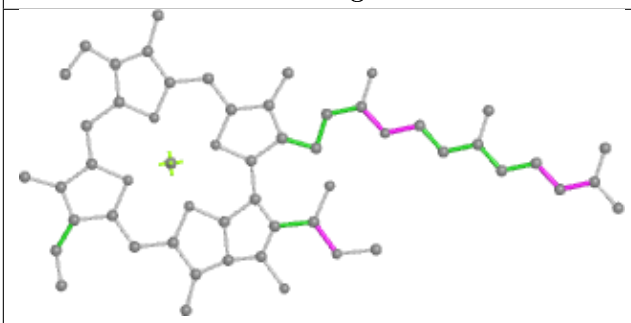
Ligand CLA A 1102



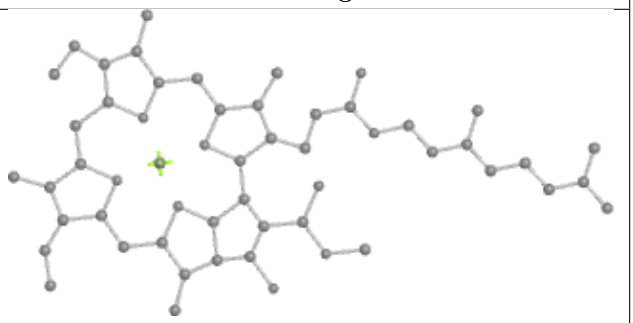
Bond lengths



Bond angles

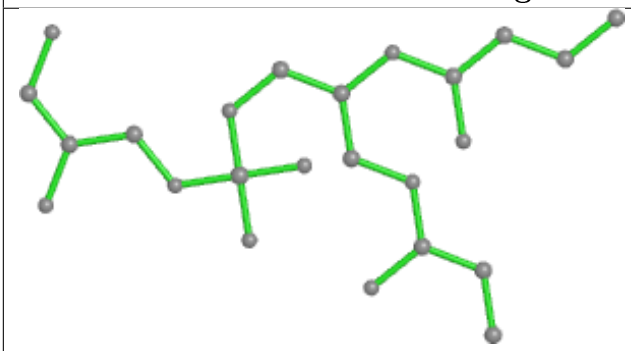


Torsions

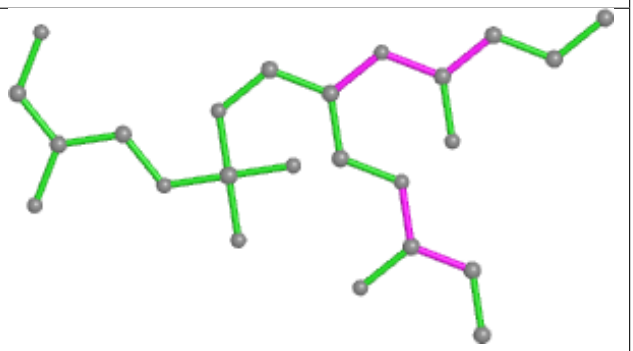


Rings

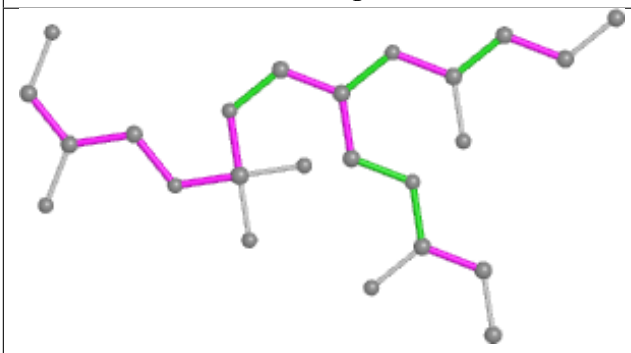
Ligand LHG B 5006



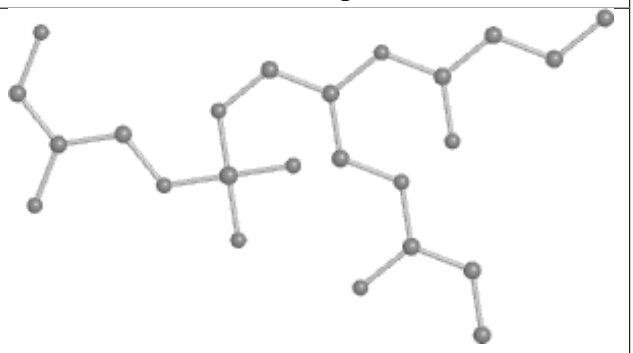
Bond lengths



Bond angles

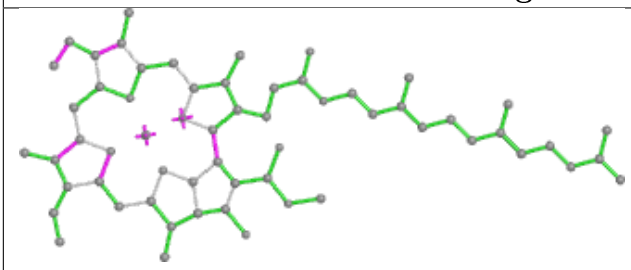


Torsions

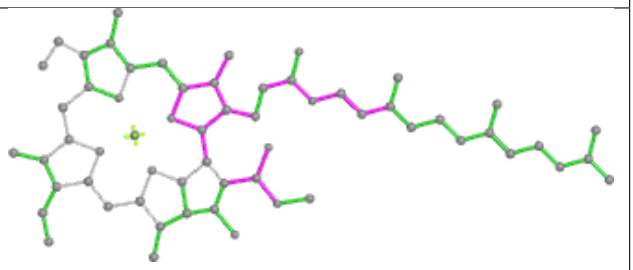


Rings

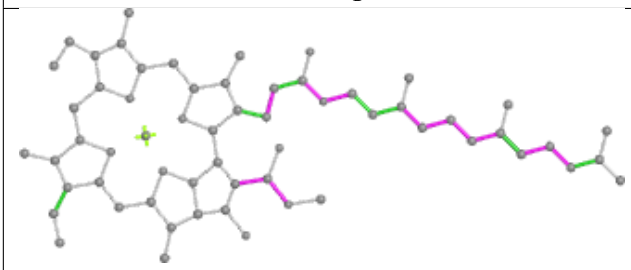
Ligand CLA A 1011



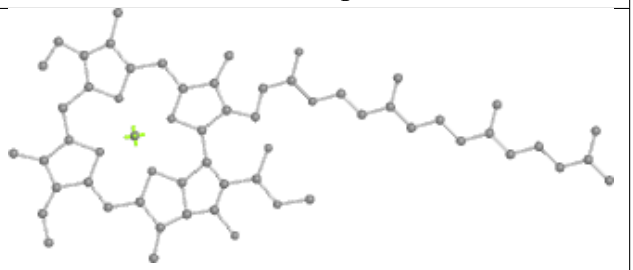
Bond lengths



Bond angles

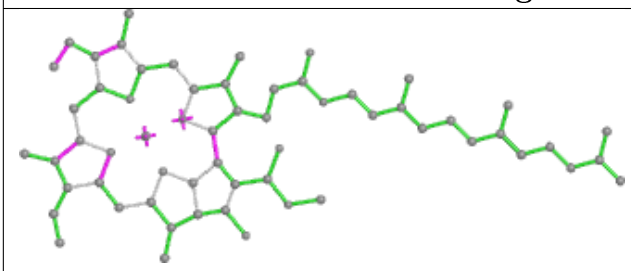


Torsions

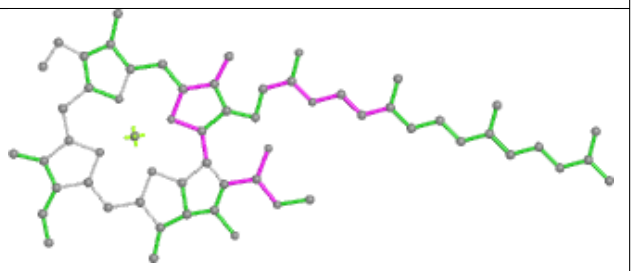


Rings

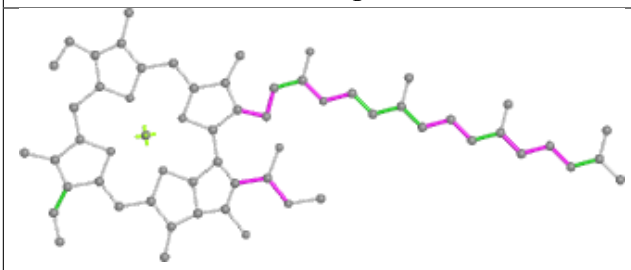
Ligand CLA A 1110



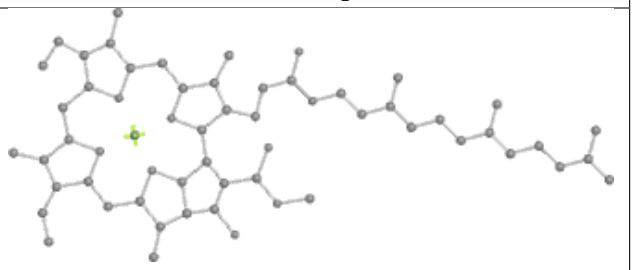
Bond lengths



Bond angles

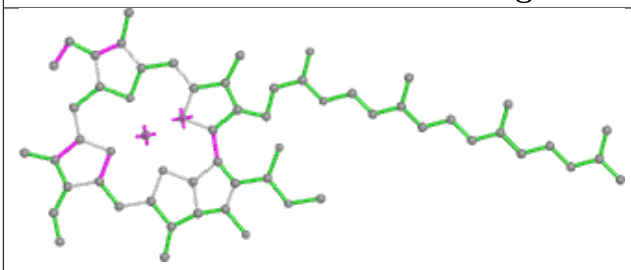


Torsions

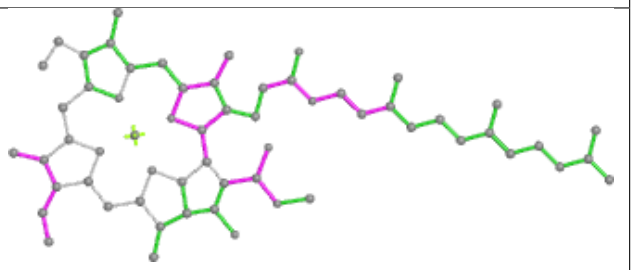


Rings

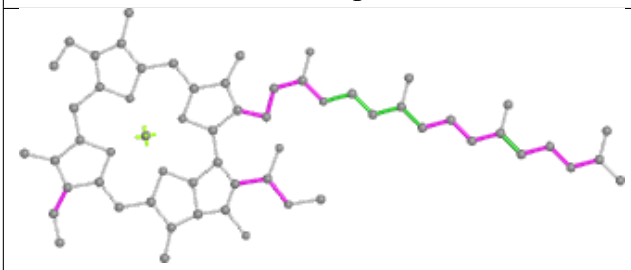
Ligand CLA B 1021



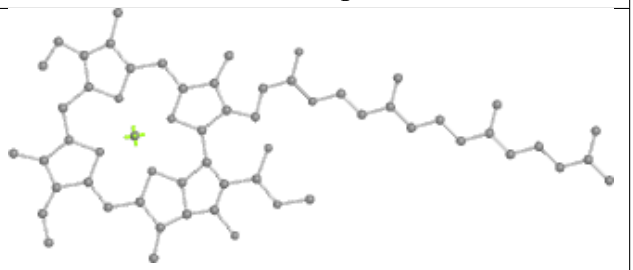
Bond lengths



Bond angles

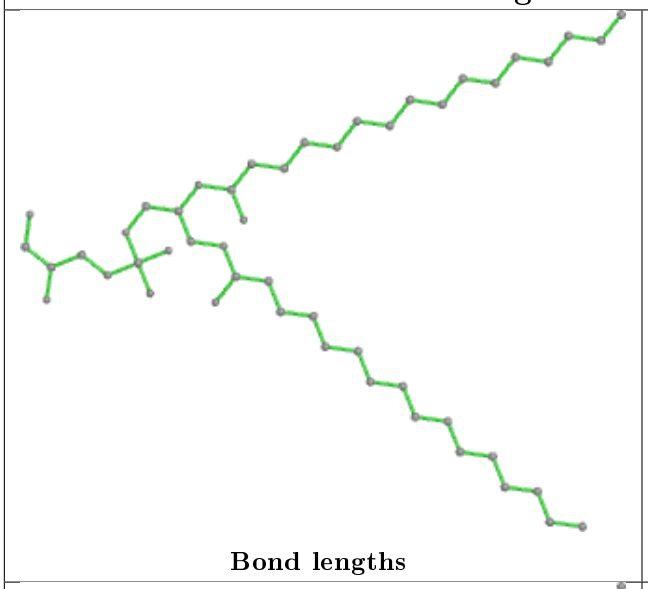


Torsions

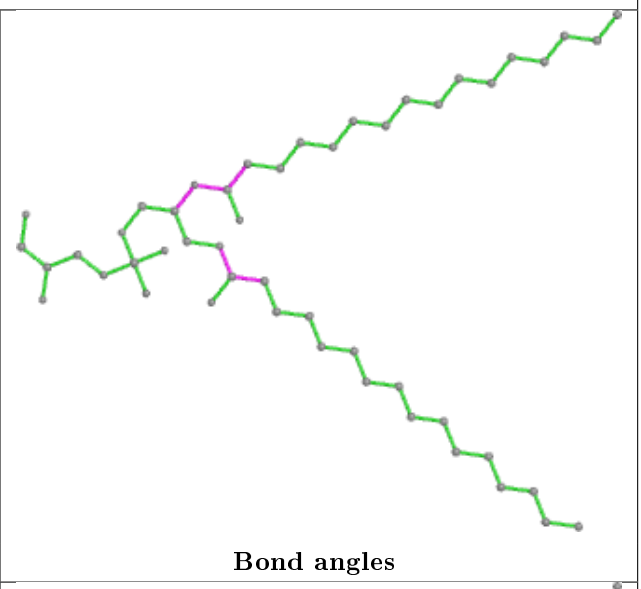


Rings

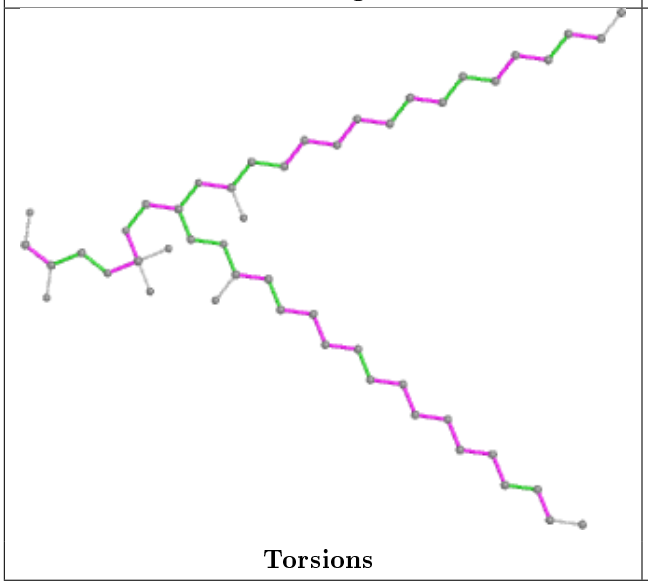
Ligand LHG A 5003



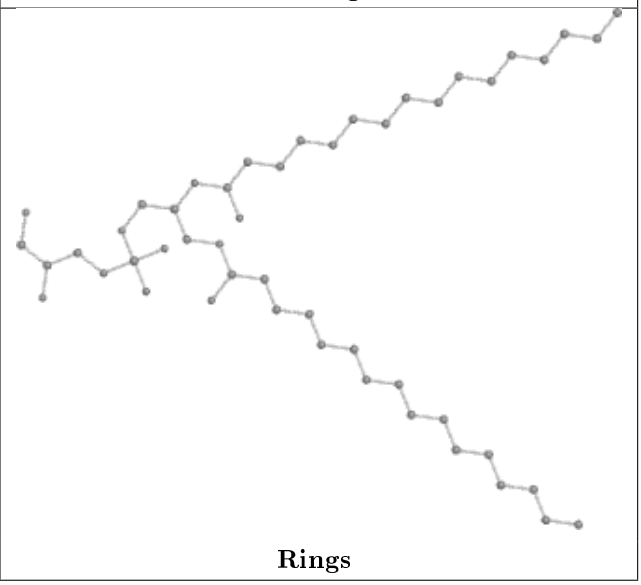
Bond lengths



Bond angles

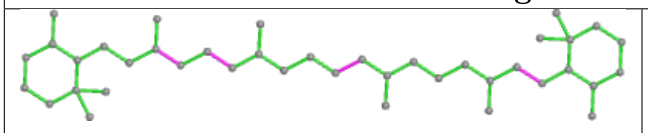


Torsions

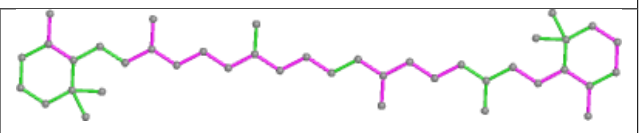


Rings

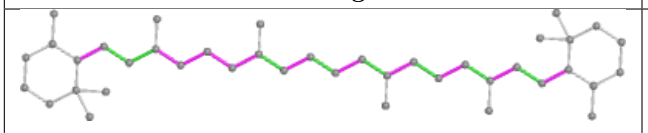
Ligand BCR A 4008



Bond lengths



Bond angles



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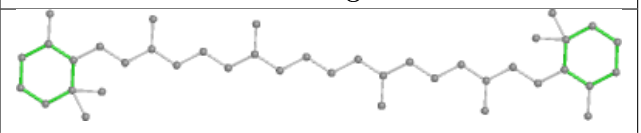
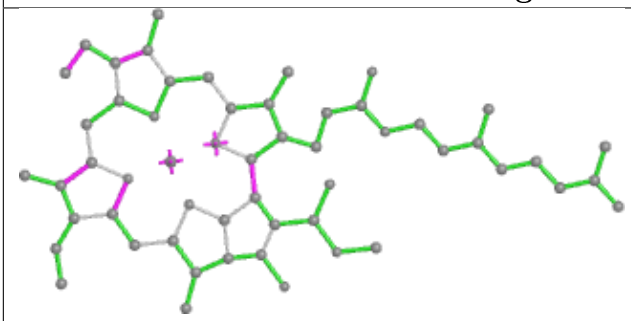
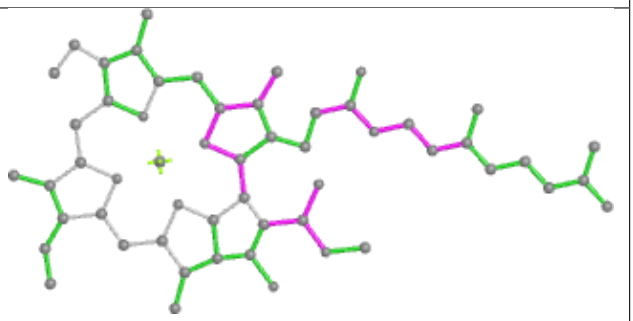


Rings

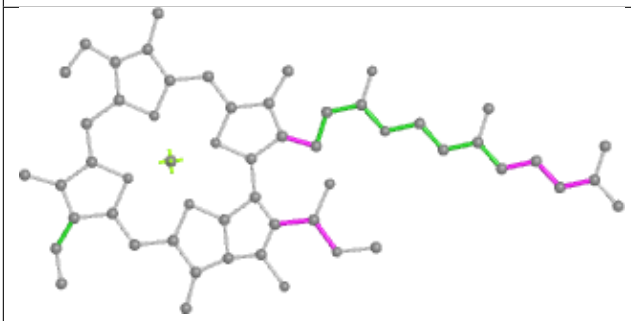
Ligand CLA B 1205



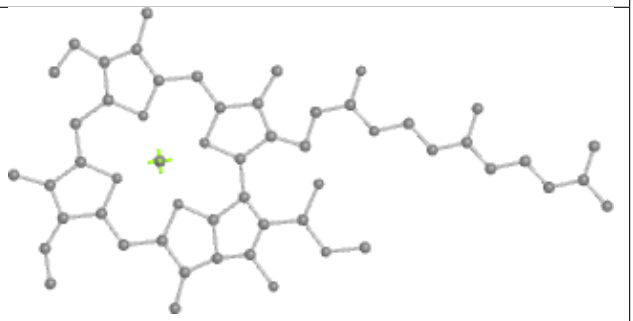
Bond lengths



Bond angles

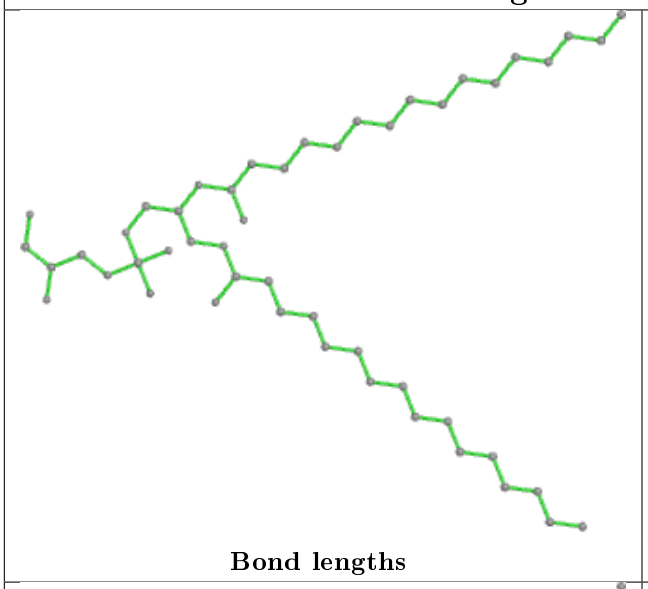


Torsions

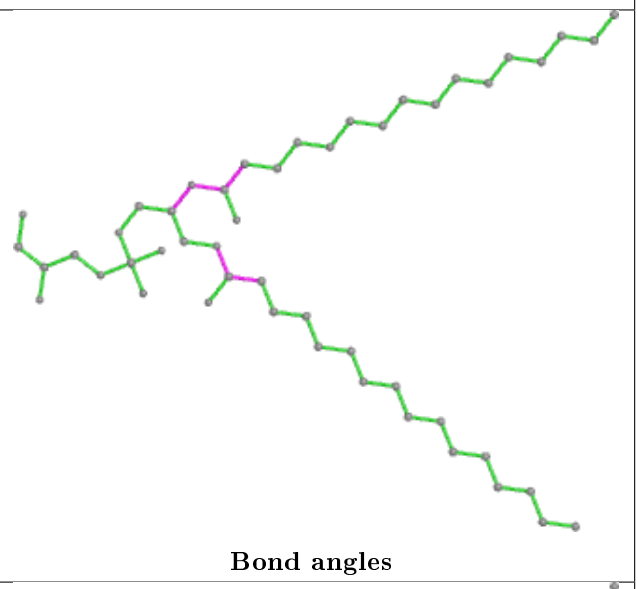


Rings

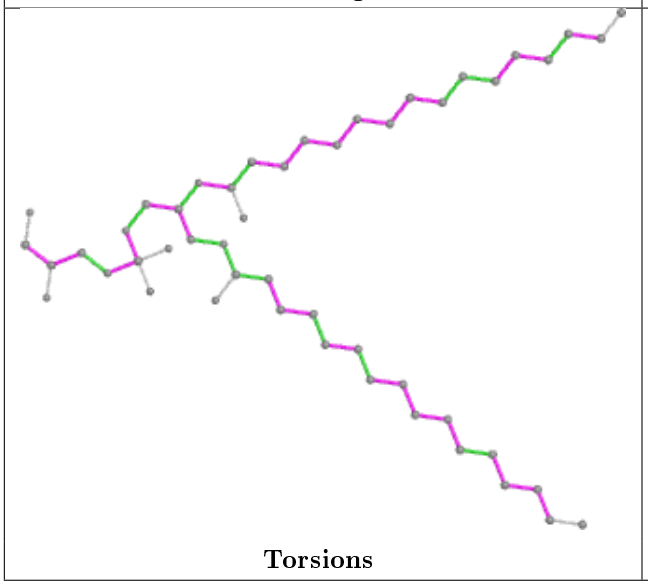
Ligand LHG M 5001



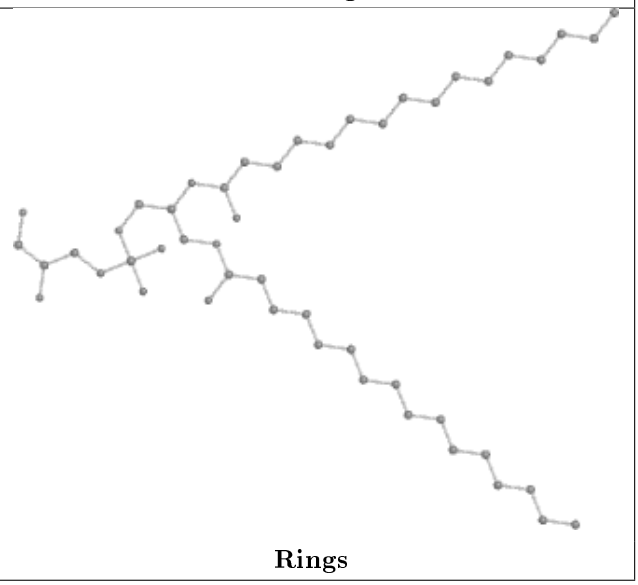
Bond lengths



Bond angles

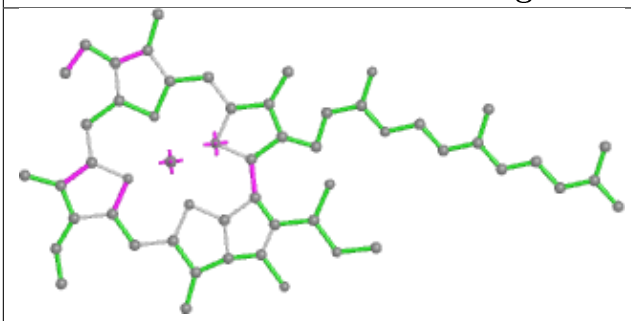


Torsions

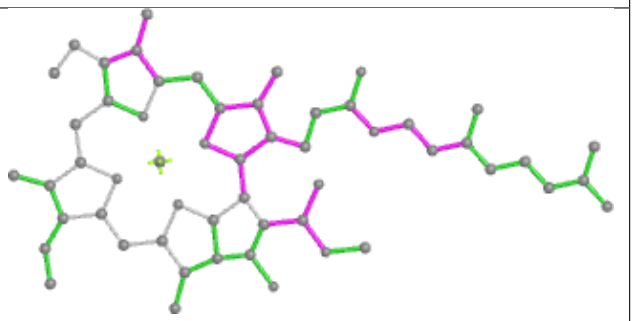


Rings

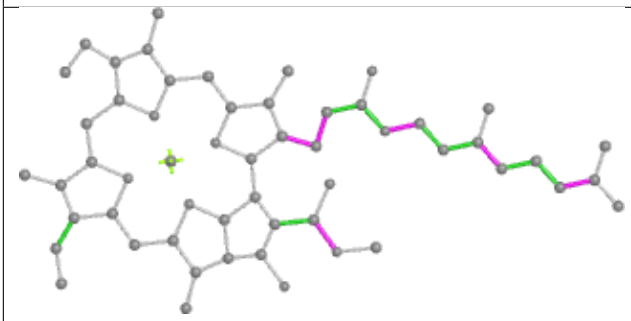
Ligand CLA A 1012



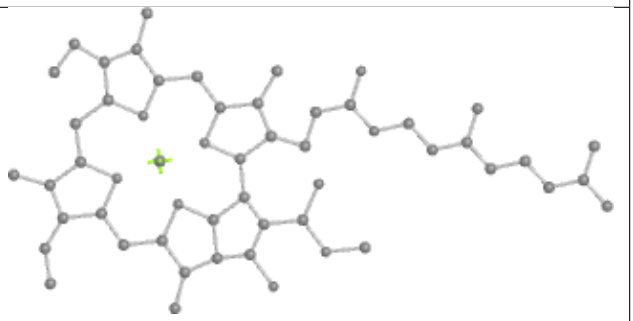
Bond lengths



Bond angles

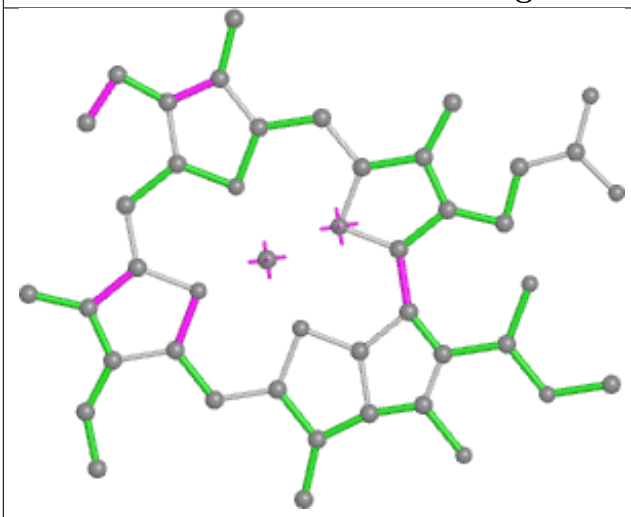


Torsions

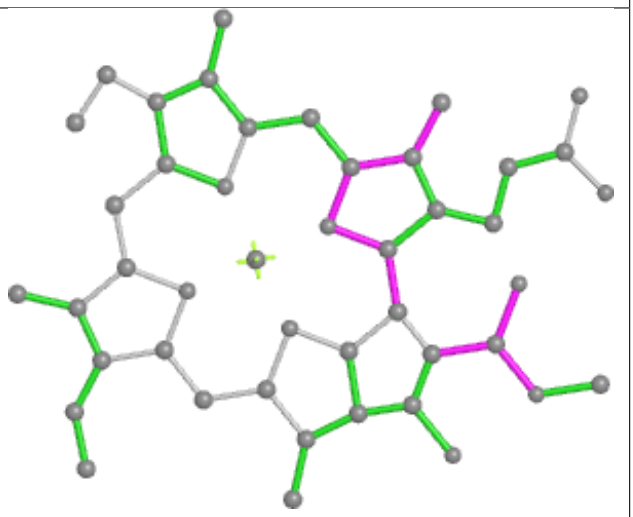


Rings

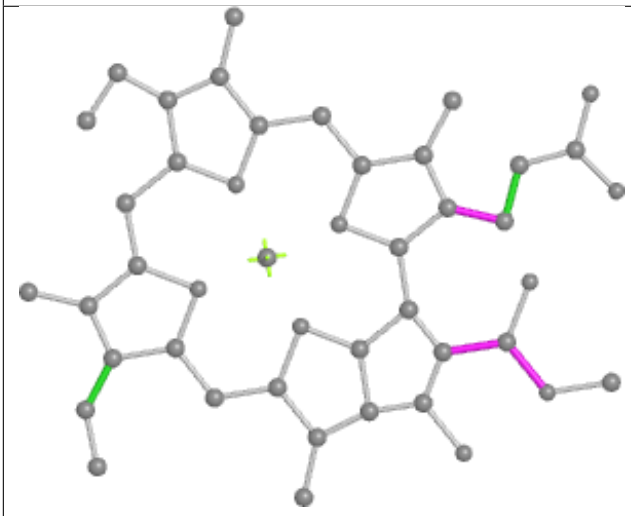
Ligand CLA A 1114



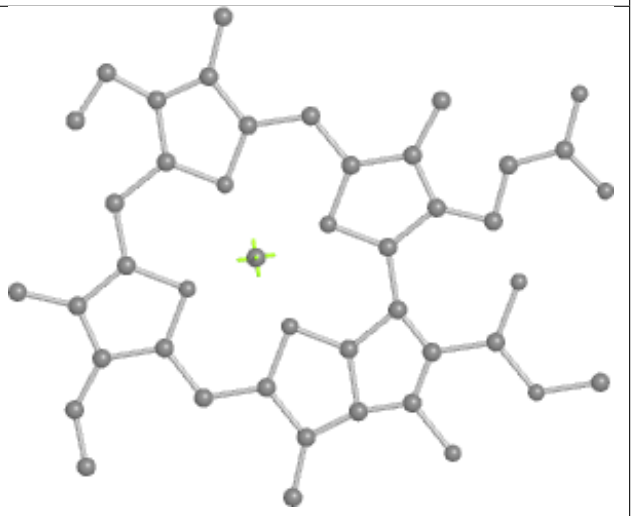
Bond lengths



Bond angles

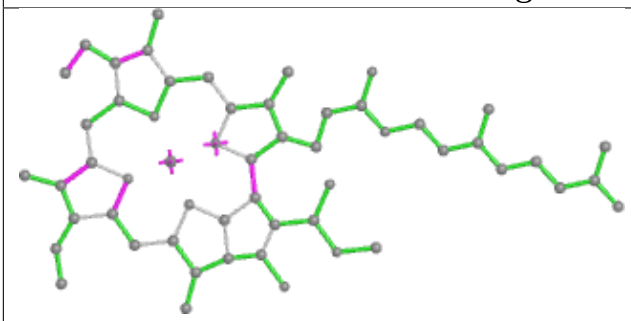


Torsions

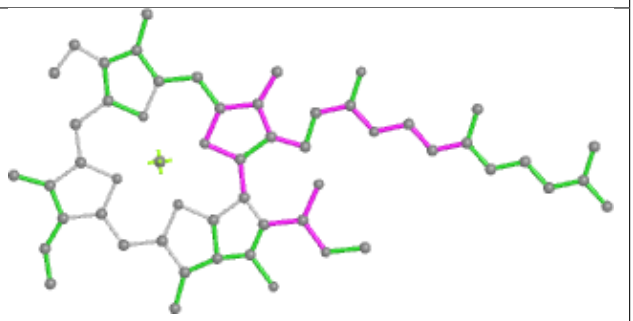


Rings

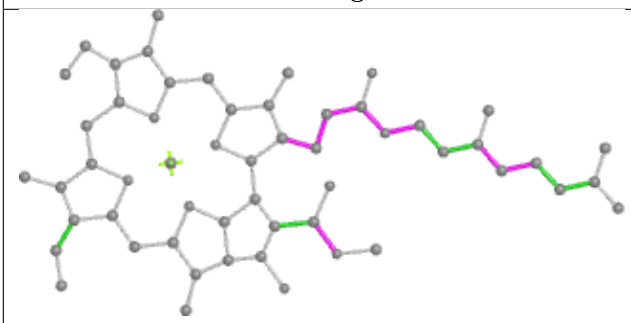
Ligand CLA A 1131



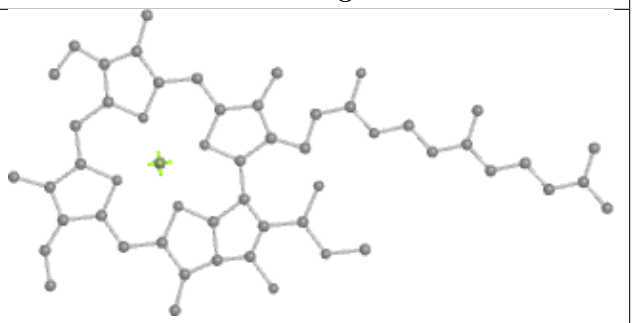
Bond lengths



Bond angles

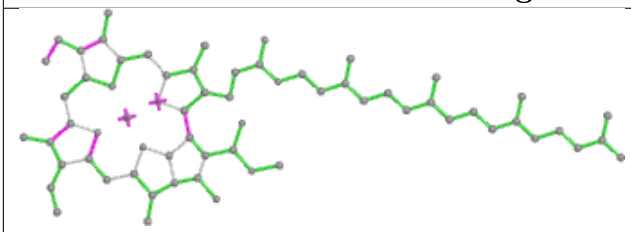


Torsions

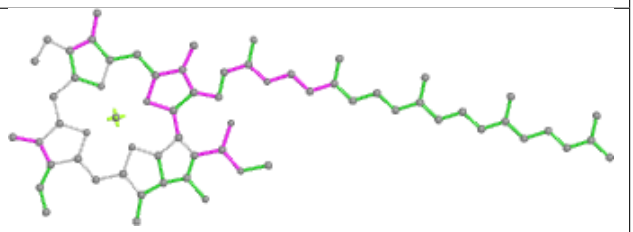


Rings

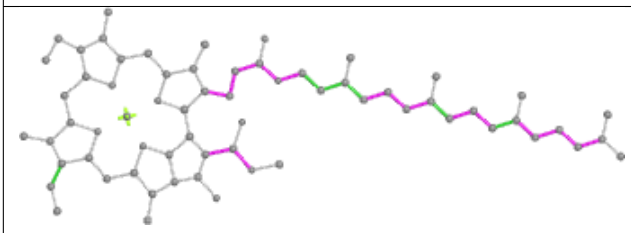
Ligand CLA B 1210



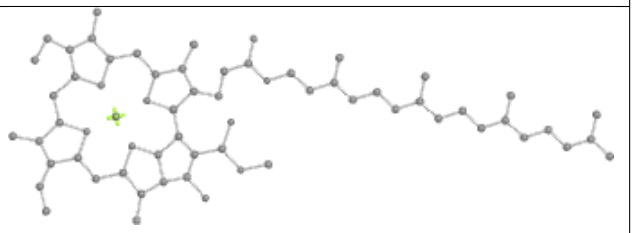
Bond lengths



Bond angles

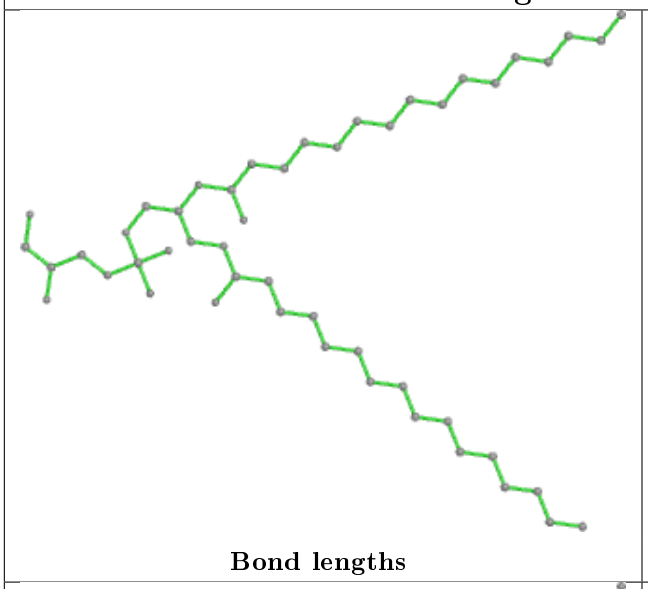


Torsions

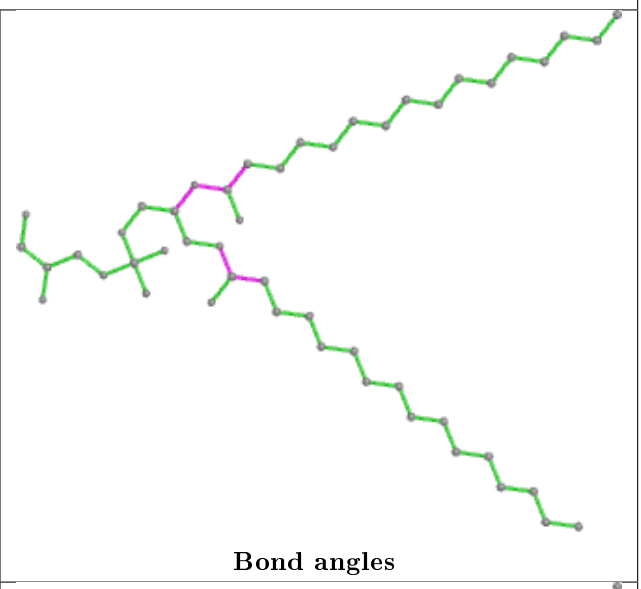


Rings

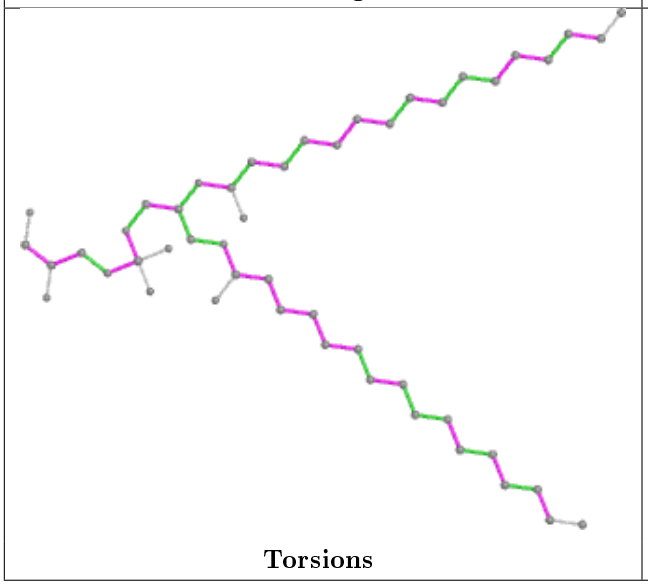
Ligand LHG A 5001



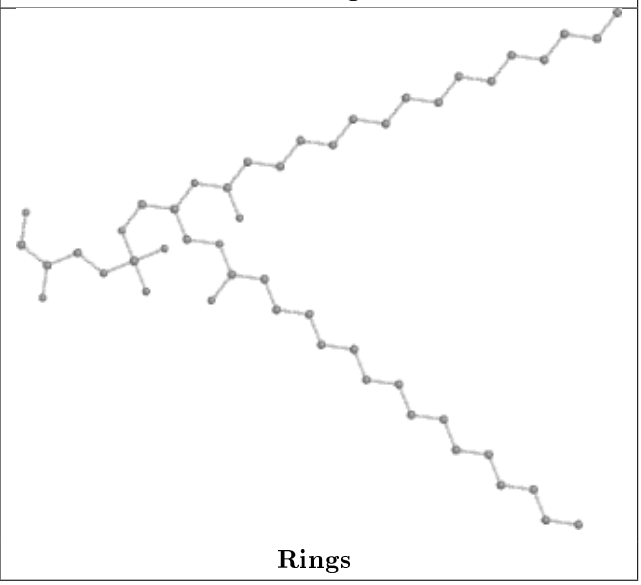
Bond lengths



Bond angles

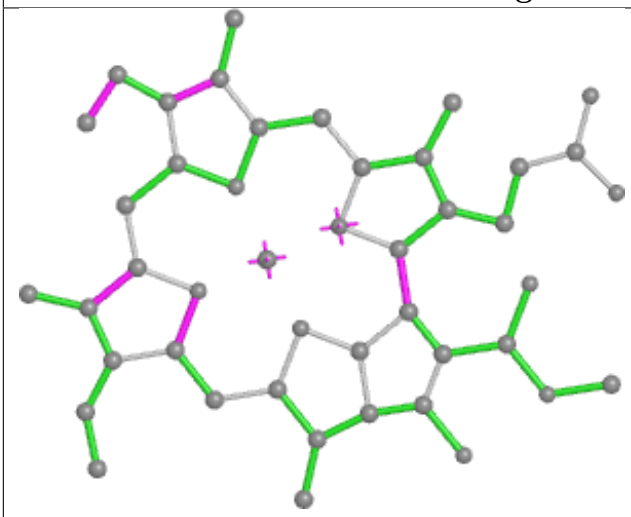


Torsions

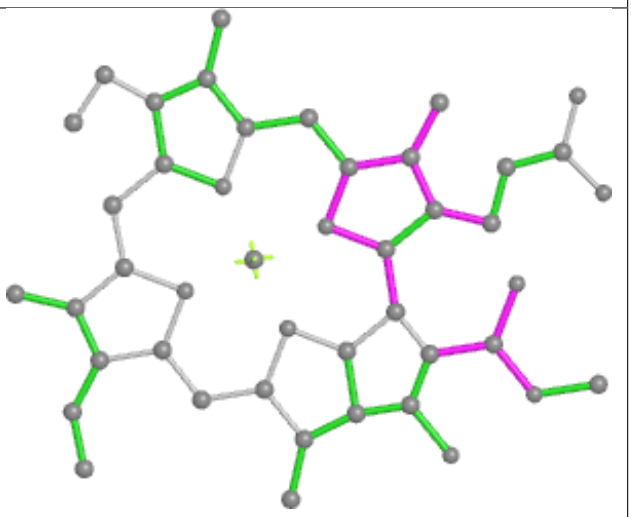


Rings

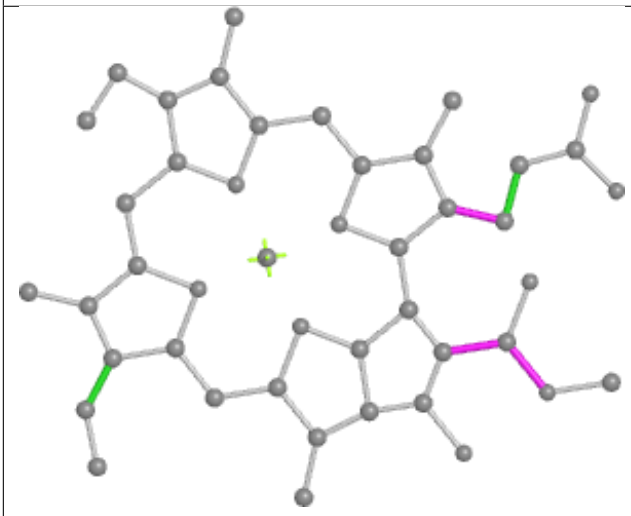
Ligand CLA B 1212



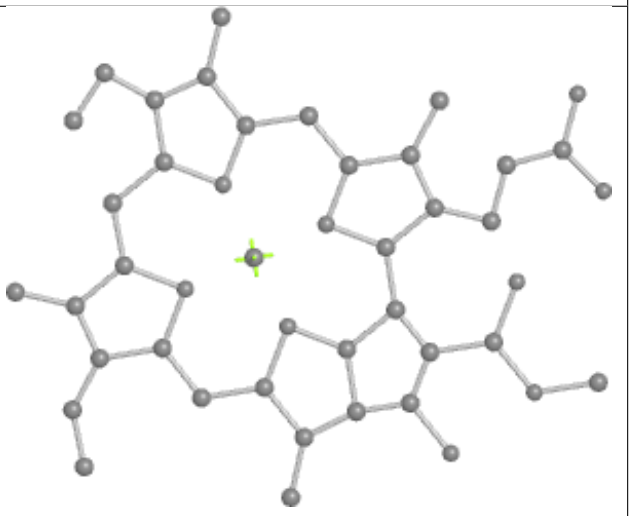
Bond lengths



Bond angles

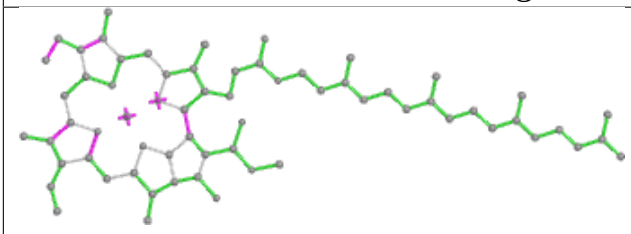


Torsions

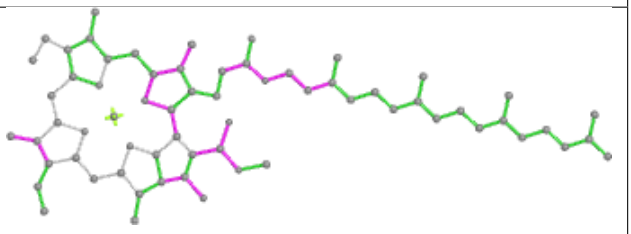


Rings

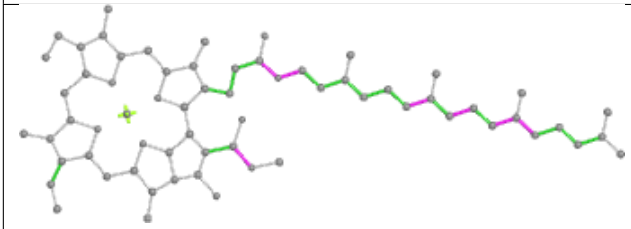
Ligand CLA B 1239



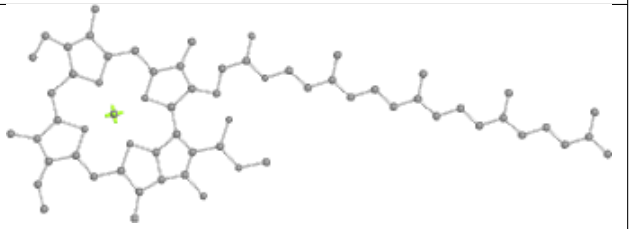
Bond lengths



Bond angles

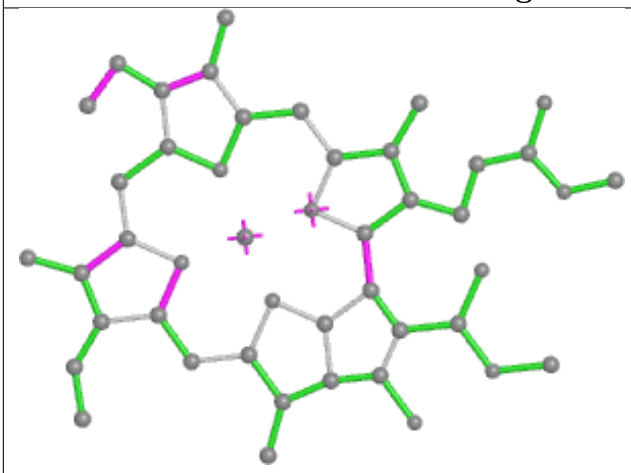


Torsions

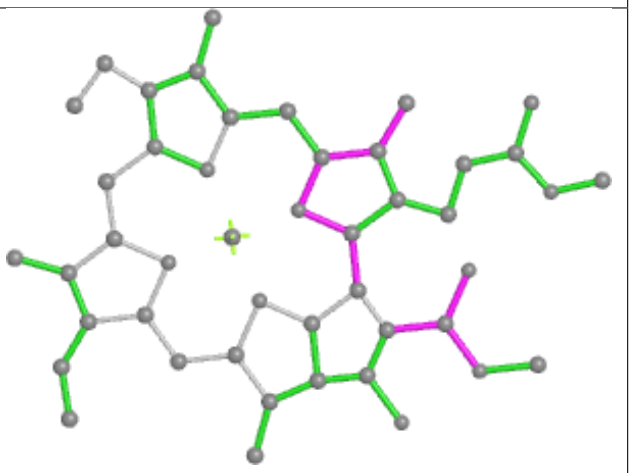


Rings

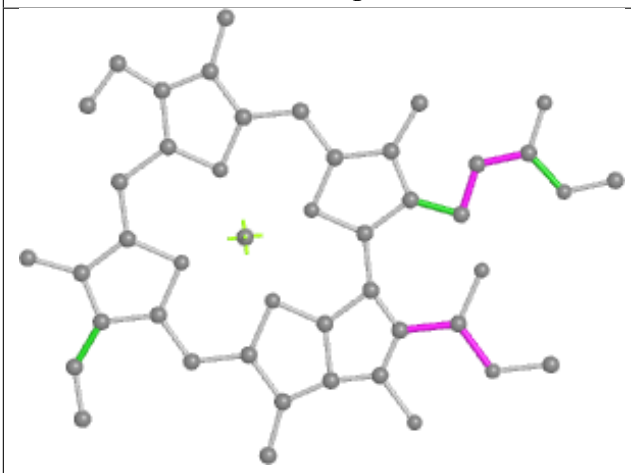
Ligand CLA B 1204



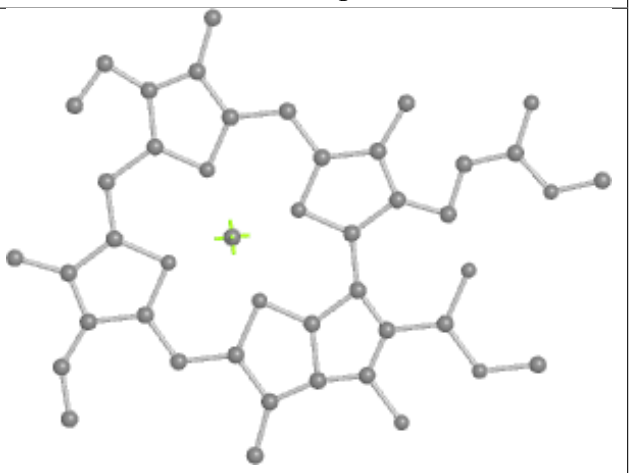
Bond lengths



Bond angles

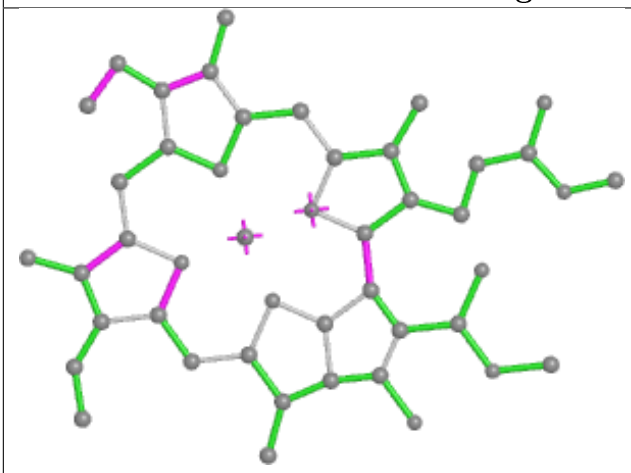


Torsions

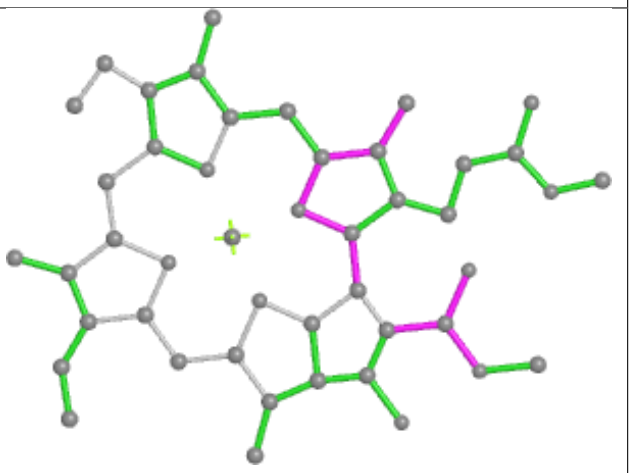


Rings

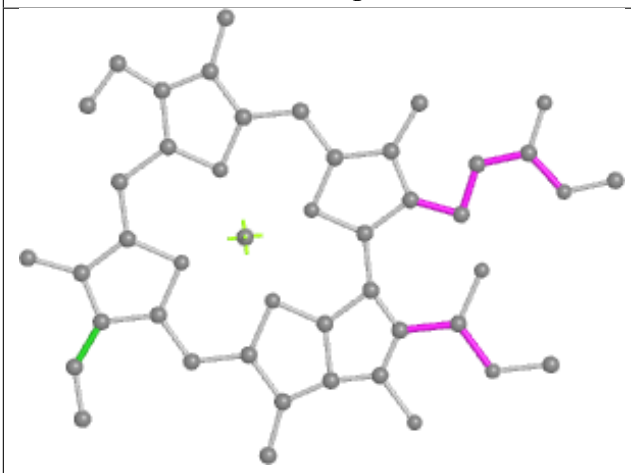
Ligand CLA A 1134



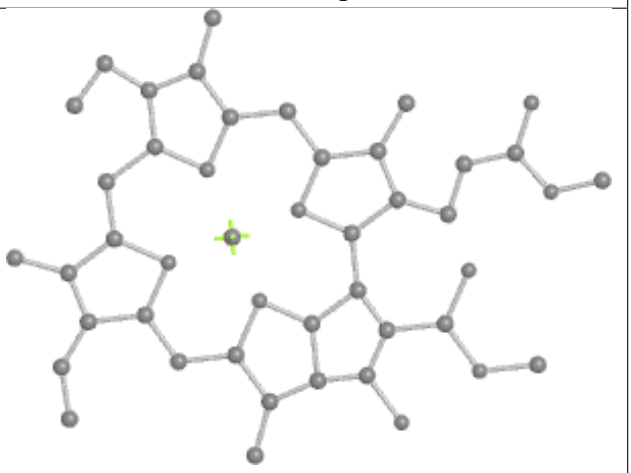
Bond lengths



Bond angles

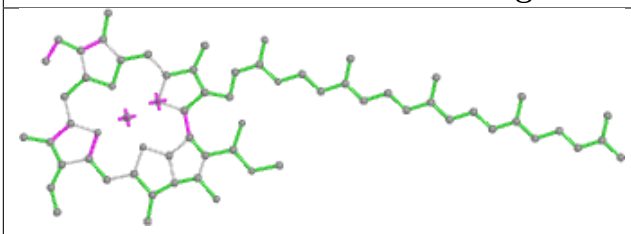


Torsions

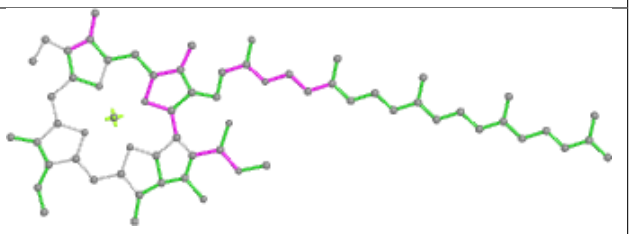


Rings

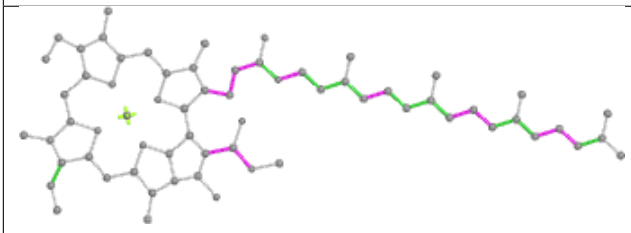
Ligand CLA A 1119



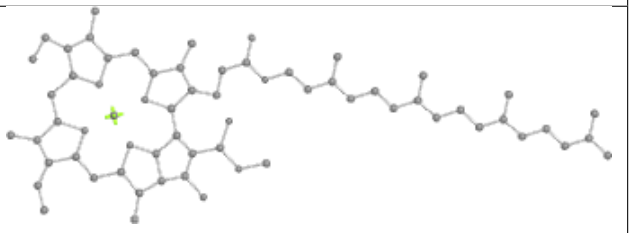
Bond lengths



Bond angles

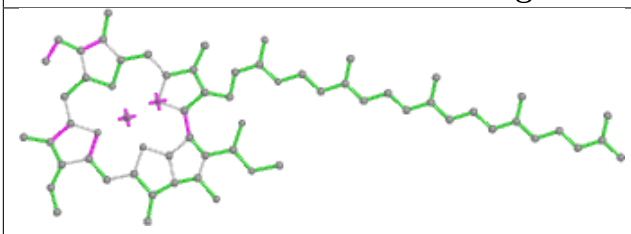


Torsions

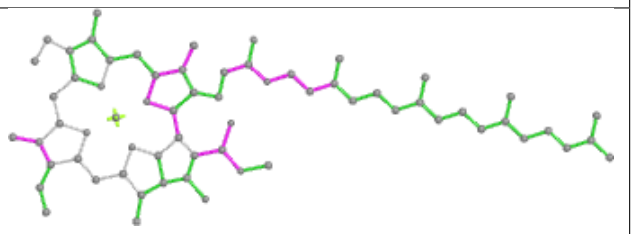


Rings

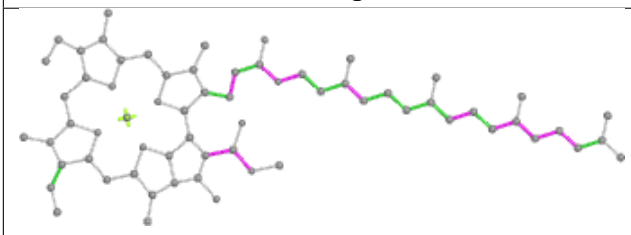
Ligand CLA A 1138



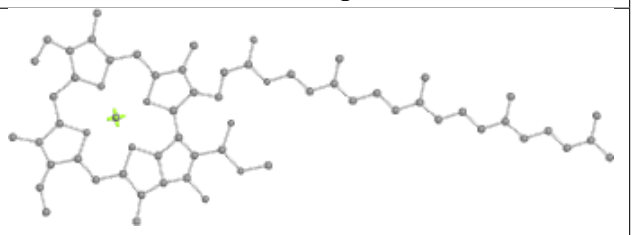
Bond lengths



Bond angles

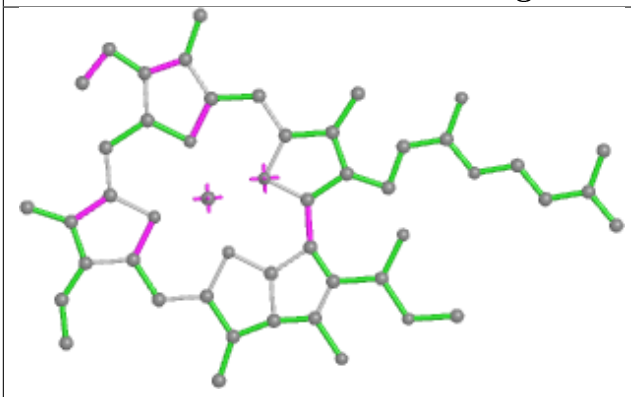


Torsions

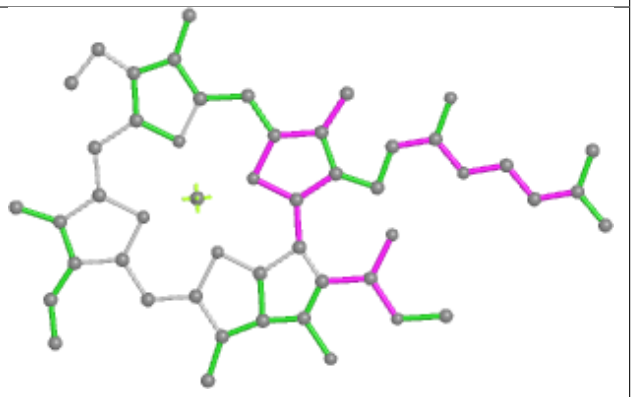


Rings

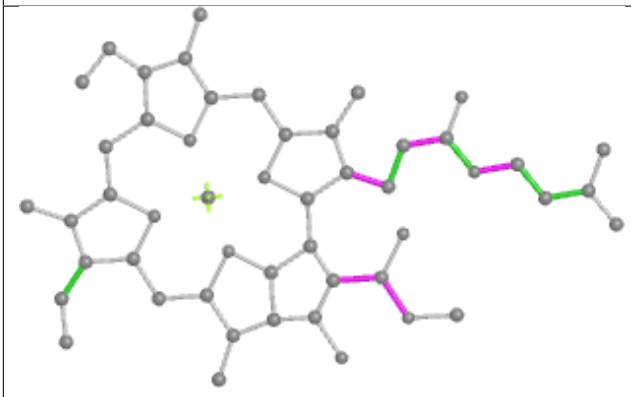
Ligand CLA B 1232



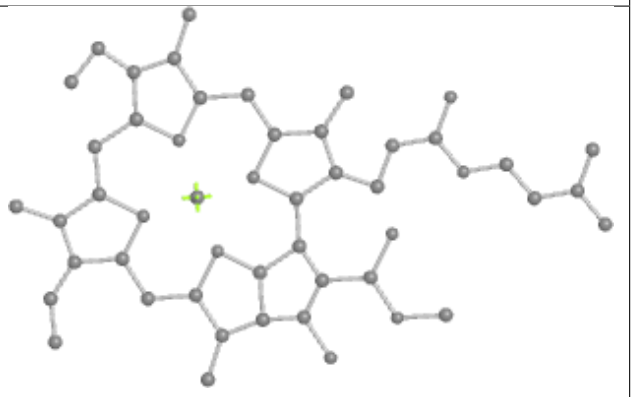
Bond lengths



Bond angles

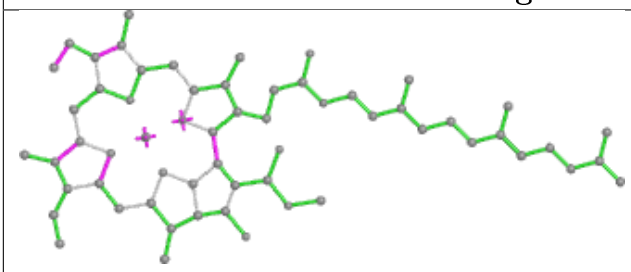


Torsions

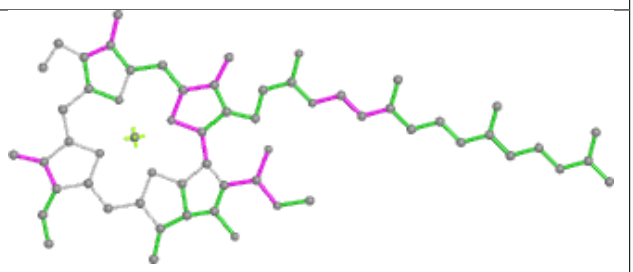


Rings

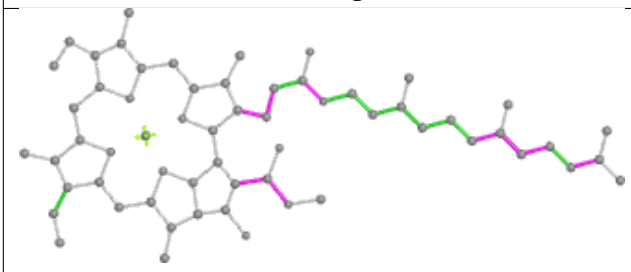
Ligand CLA A 1122



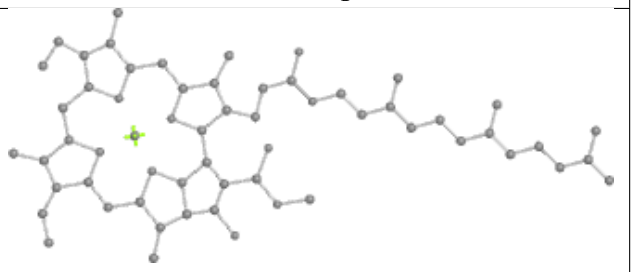
Bond lengths



Bond angles

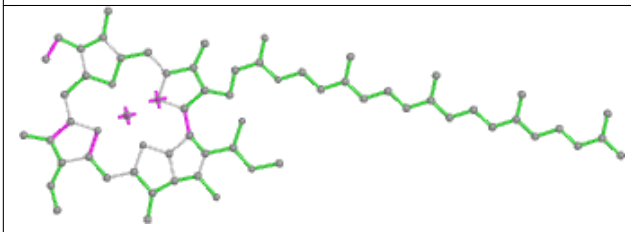


Torsions

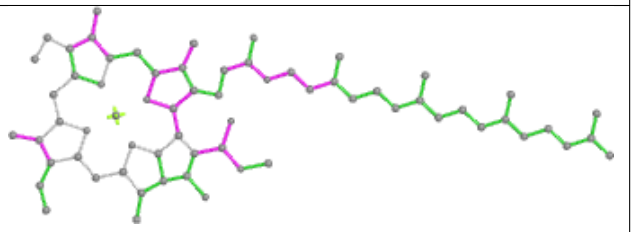


Rings

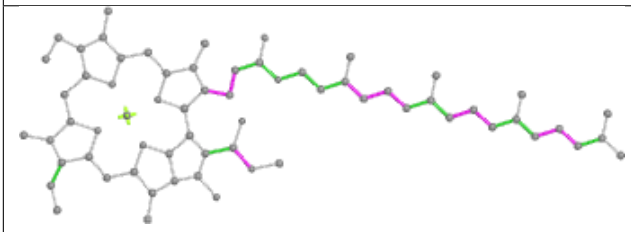
Ligand CLA B 1225



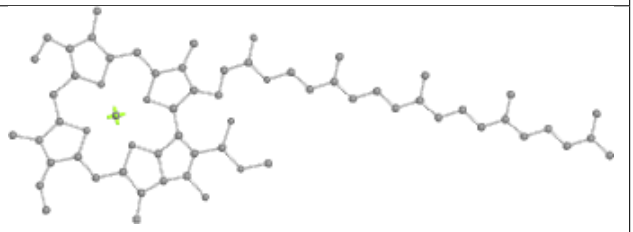
Bond lengths



Bond angles

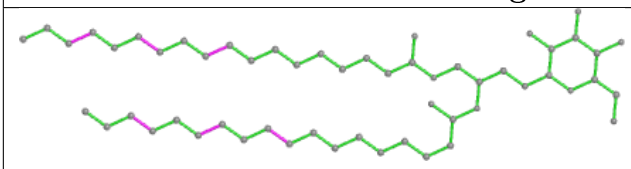


Torsions

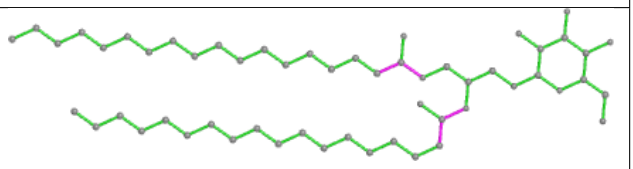


Rings

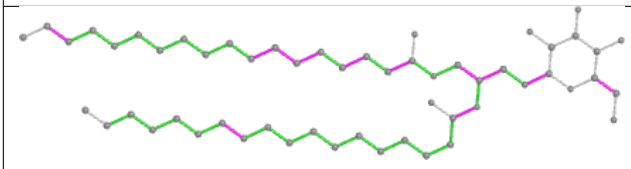
Ligand LMG K 5009



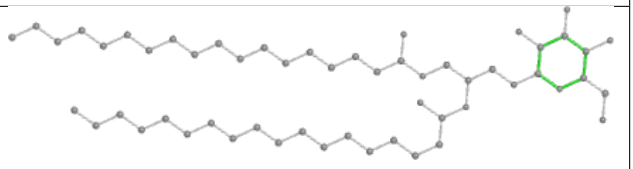
Bond lengths



Bond angles

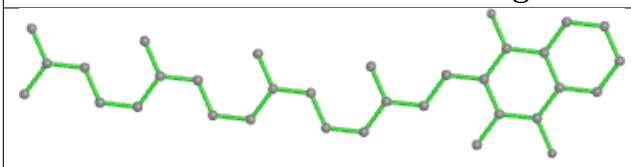


Torsions

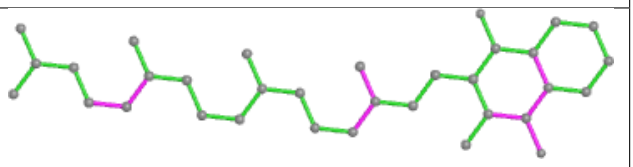


Rings

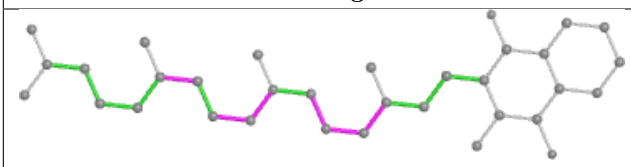
Ligand PQN A 2001



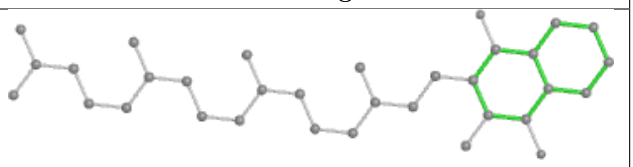
Bond lengths



Bond angles

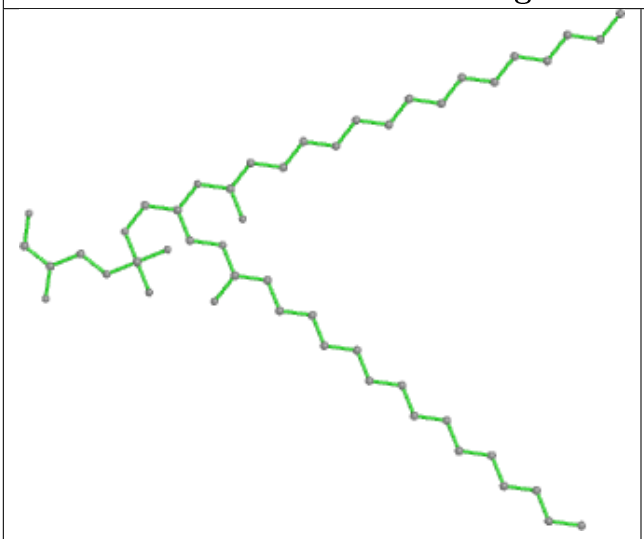


Torsions

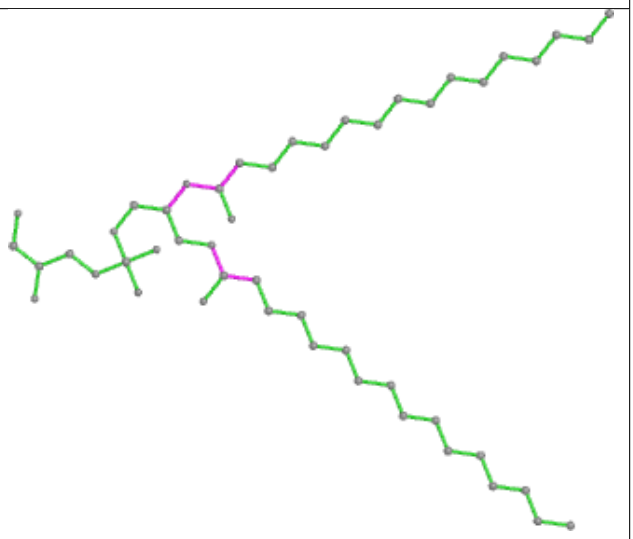


Rings

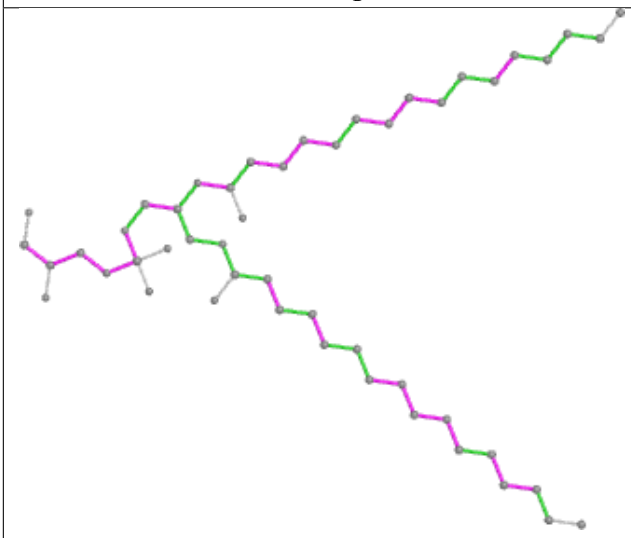
Ligand LHG B 5004



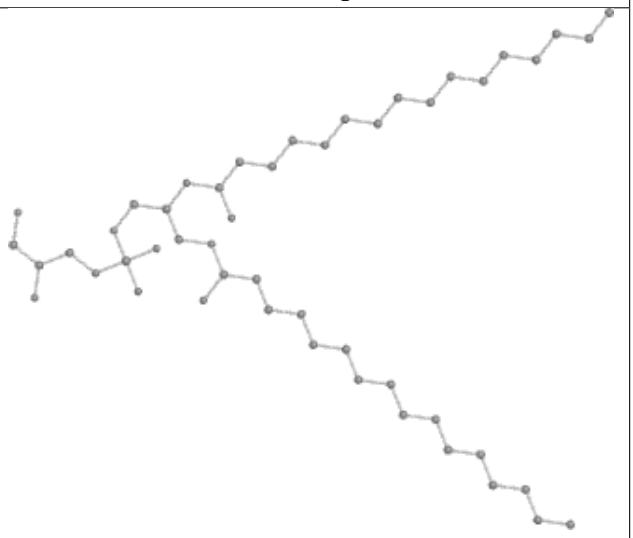
Bond lengths



Bond angles

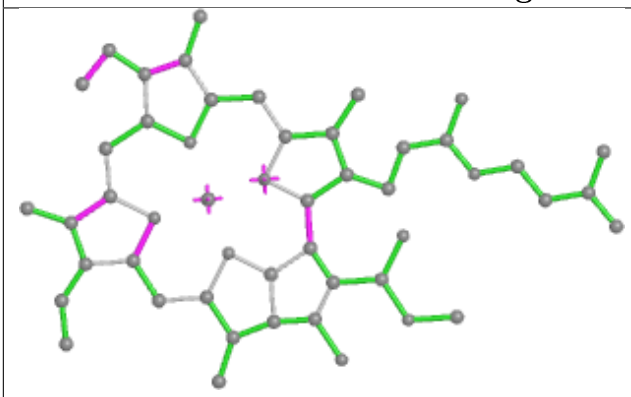


Torsions

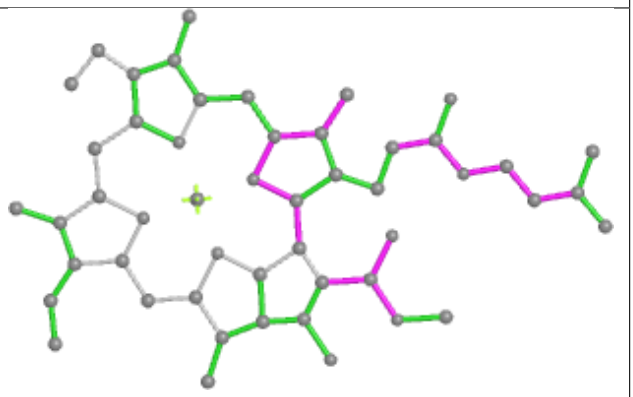


Rings

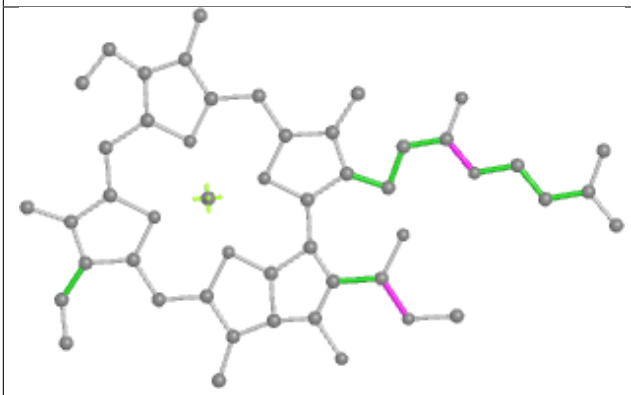
Ligand CLA A 1107



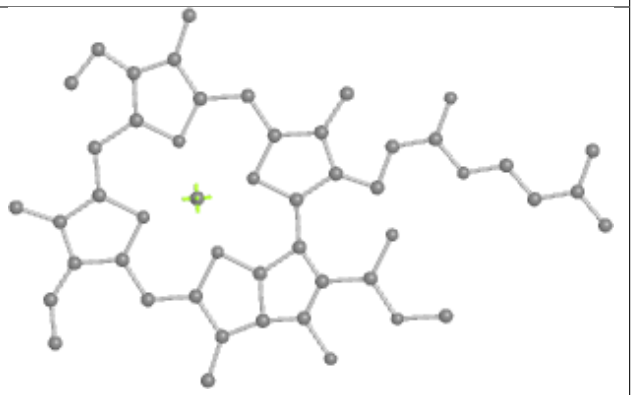
Bond lengths



Bond angles

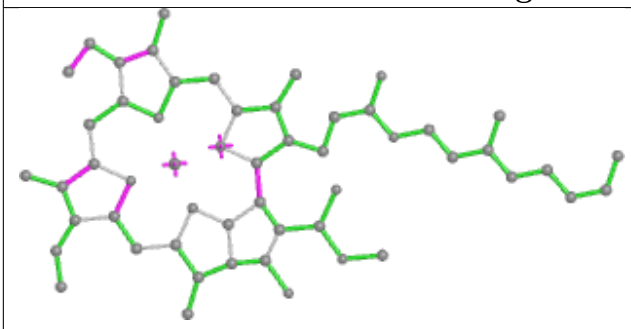


Torsions

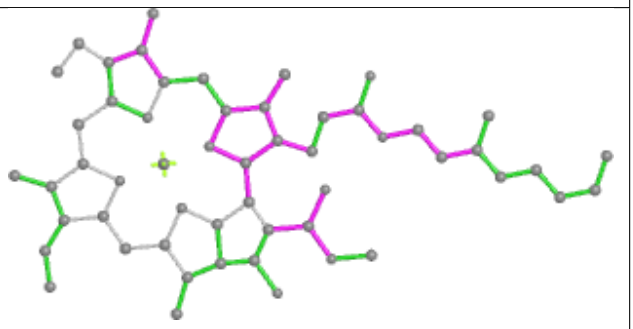


Rings

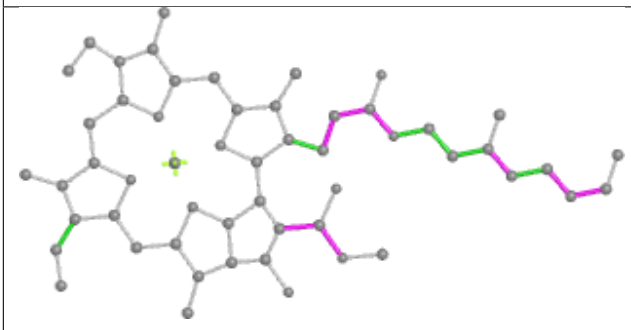
Ligand CLA A 1116



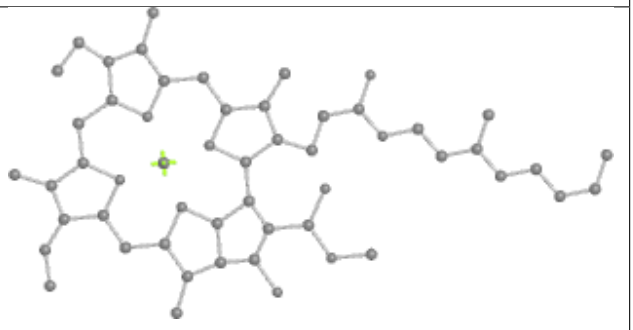
Bond lengths



Bond angles

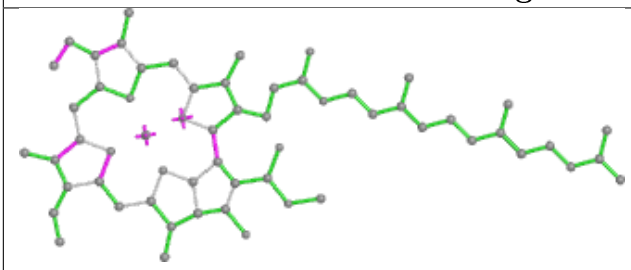


Torsions

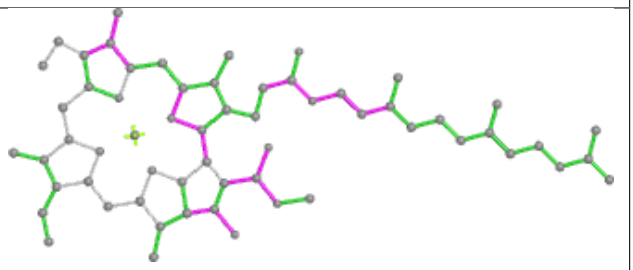


Rings

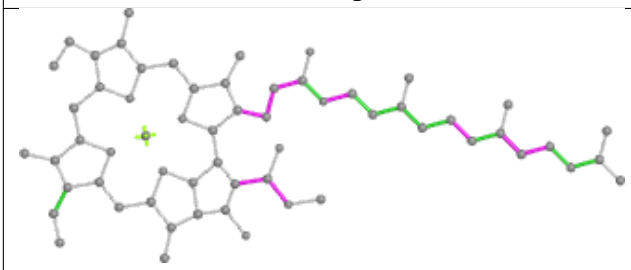
Ligand CLA A 1106



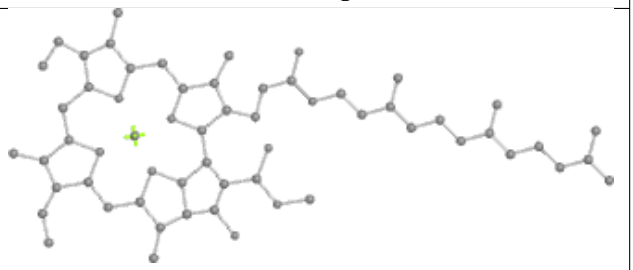
Bond lengths



Bond angles

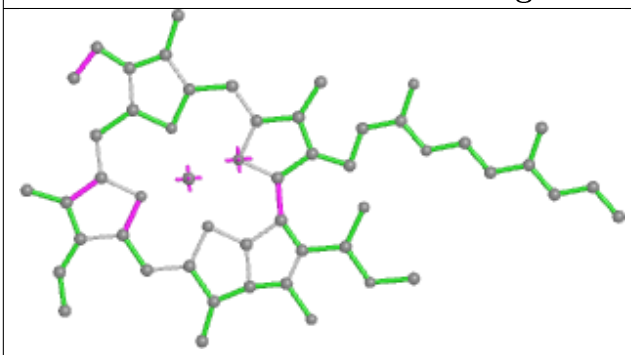


Torsions

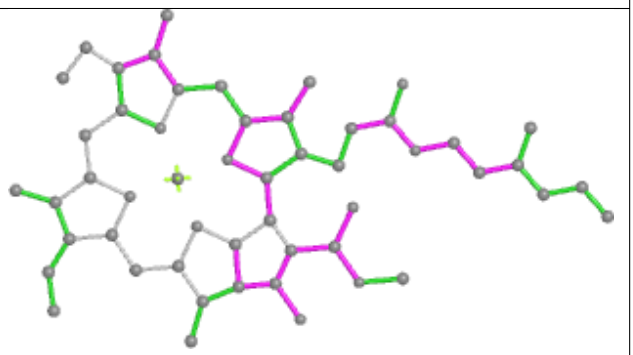


Rings

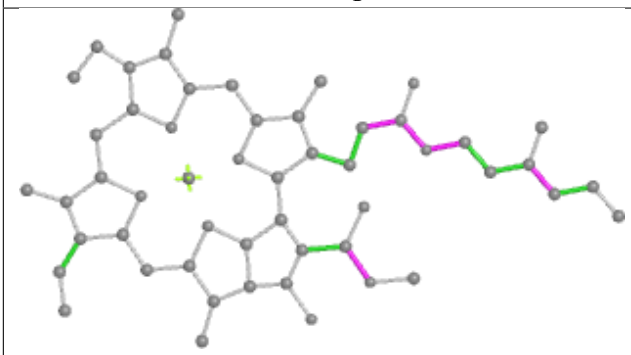
Ligand CLA A 1125



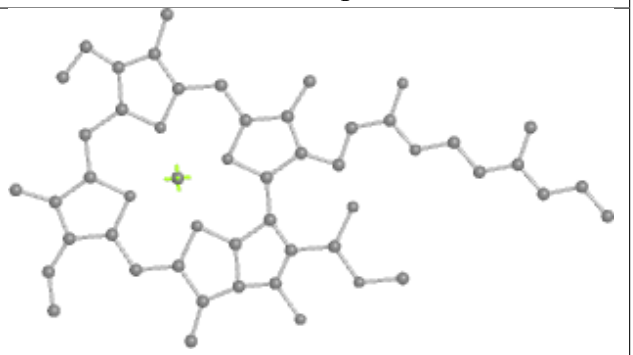
Bond lengths



Bond angles

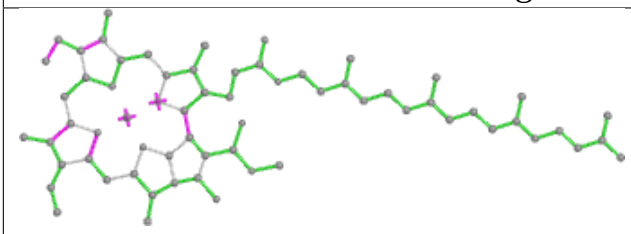


Torsions

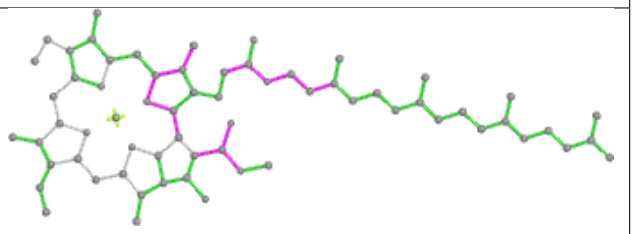


Rings

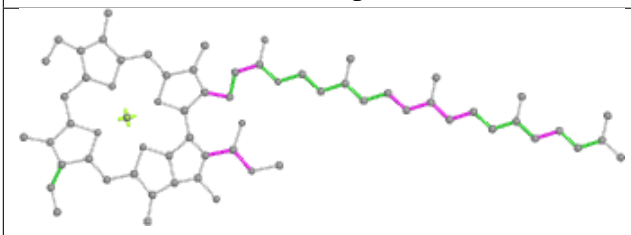
Ligand CLA A 1101



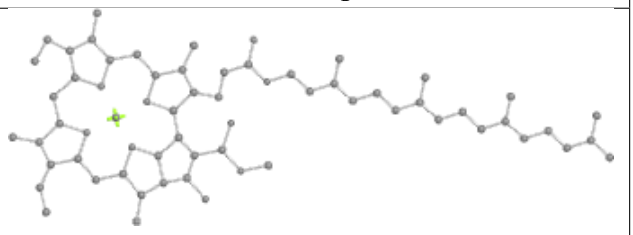
Bond lengths



Bond angles

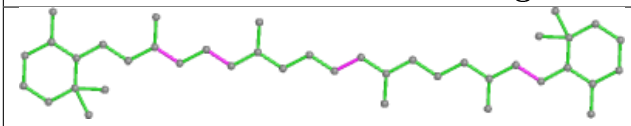


Torsions

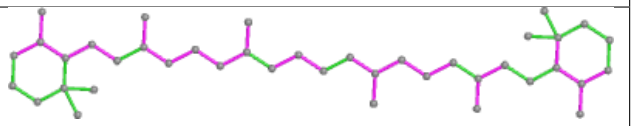


Rings

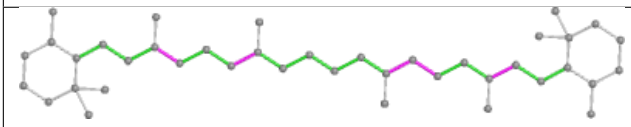
Ligand BCR B 4018



Bond lengths



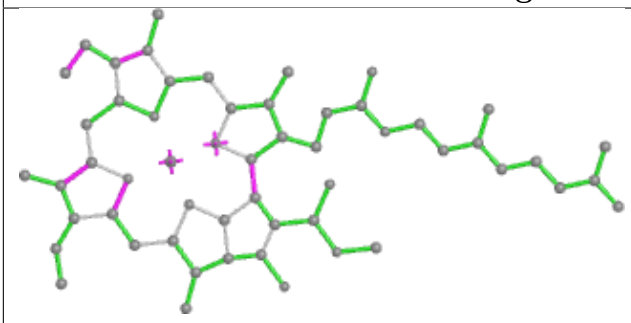
Bond angles



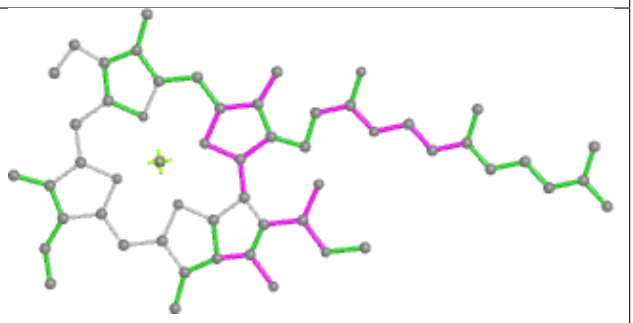
Torsions

Rings

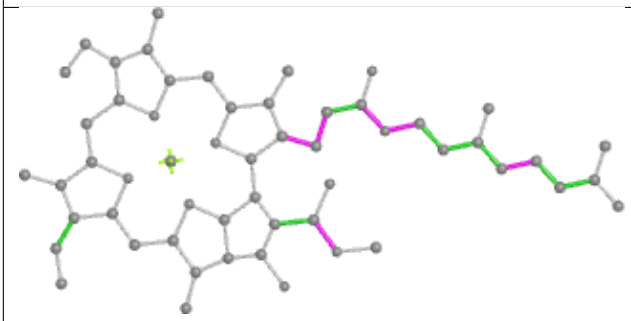
Ligand CLA B 1206



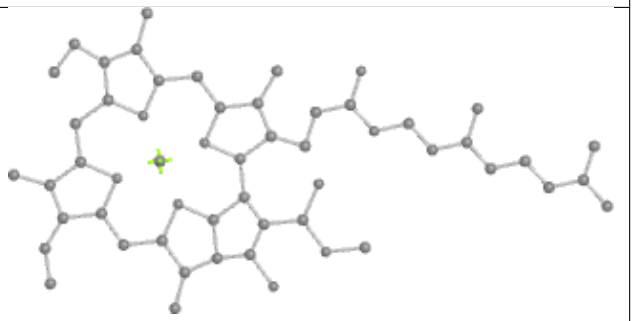
Bond lengths



Bond angles

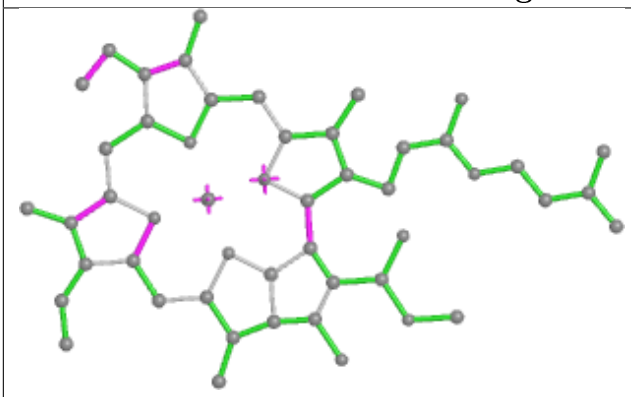


Torsions

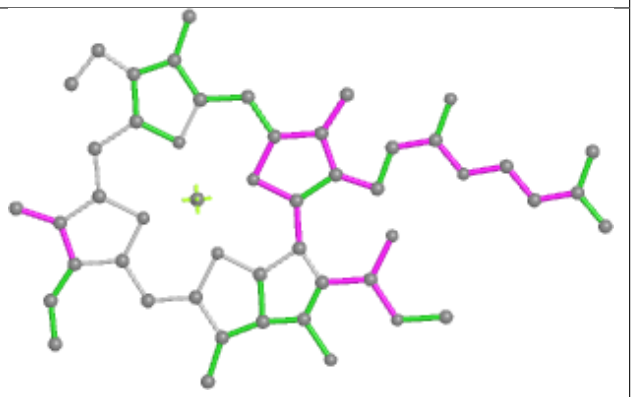


Rings

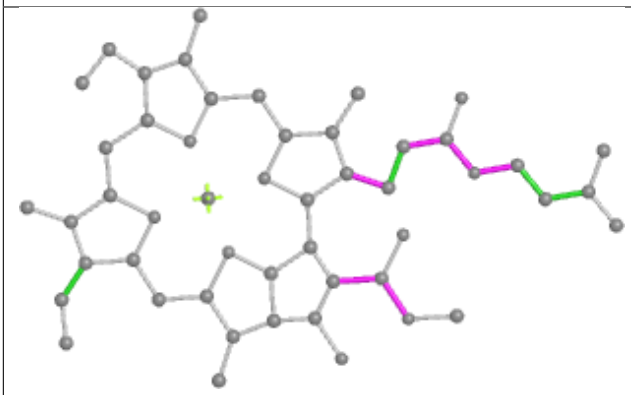
Ligand CLA B 1236



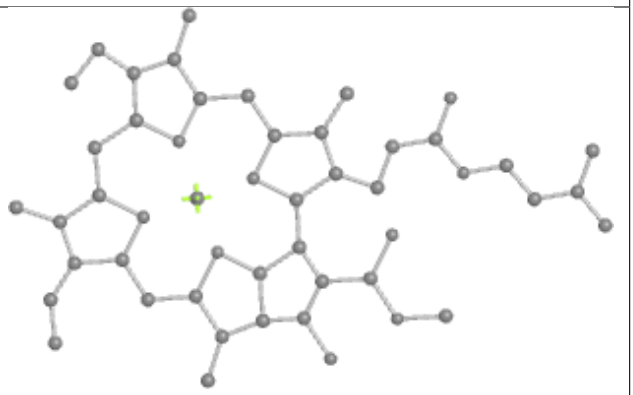
Bond lengths



Bond angles

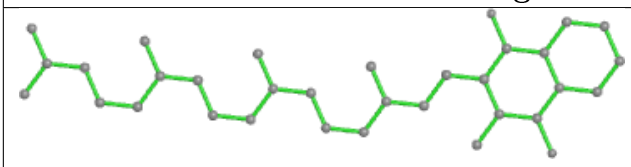


Torsions

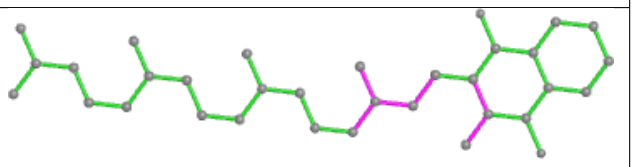


Rings

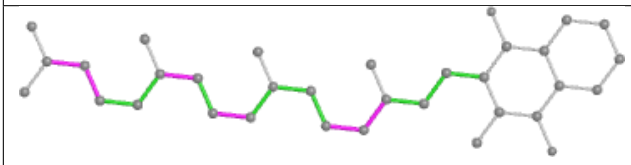
Ligand PQN B 2002



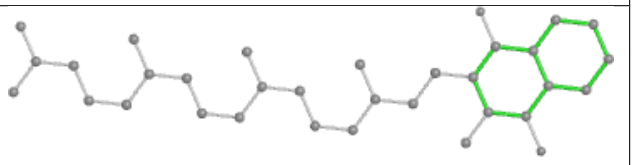
Bond lengths



Bond angles

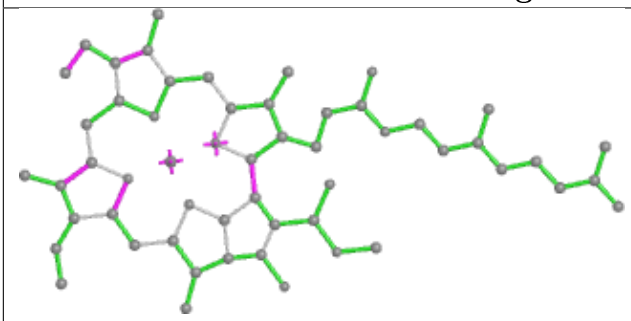


Torsions

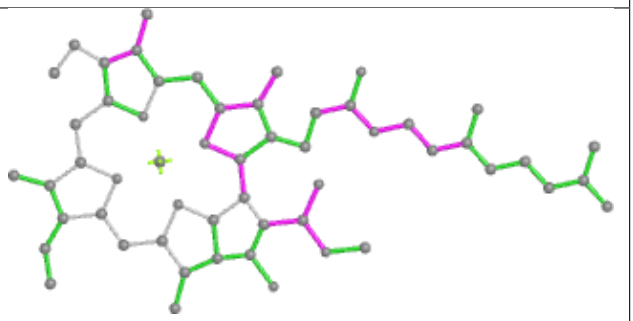


Rings

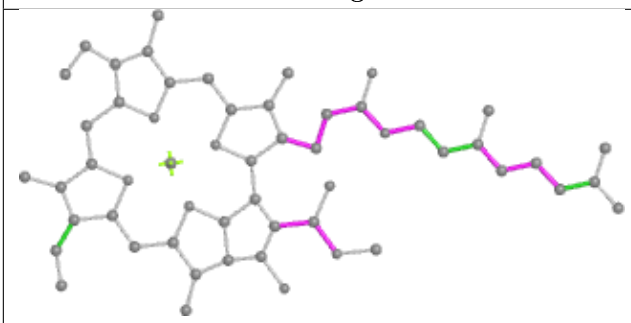
Ligand CLA B 1216



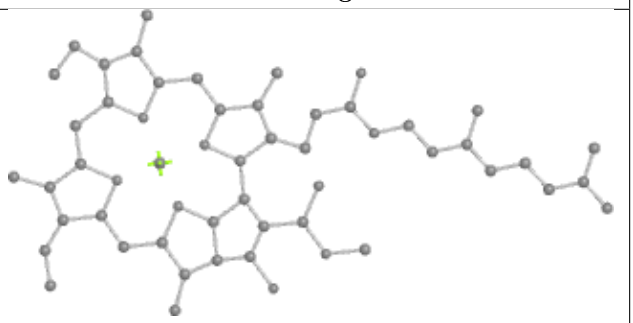
Bond lengths



Bond angles

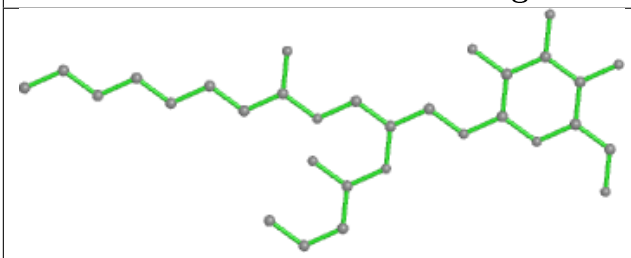


Torsions

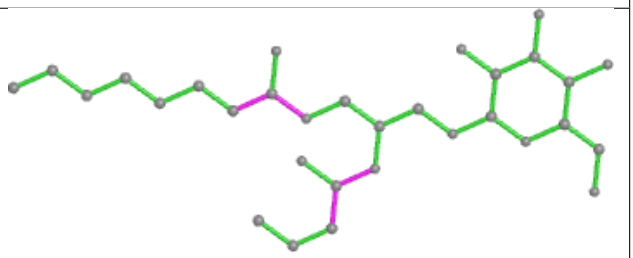


Rings

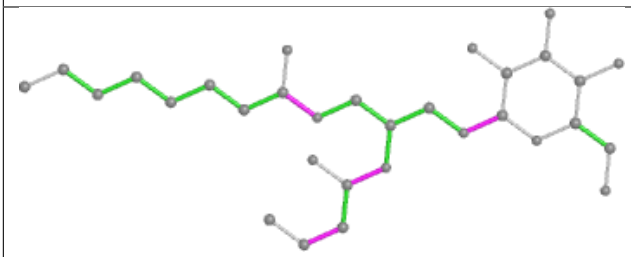
Ligand LMG B 5005



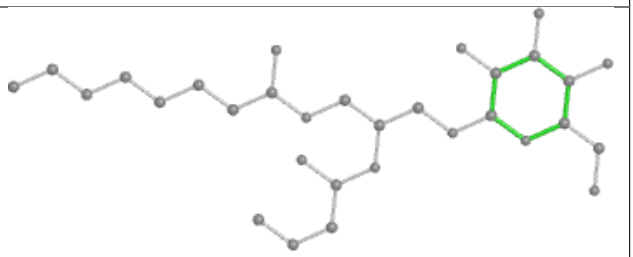
Bond lengths



Bond angles

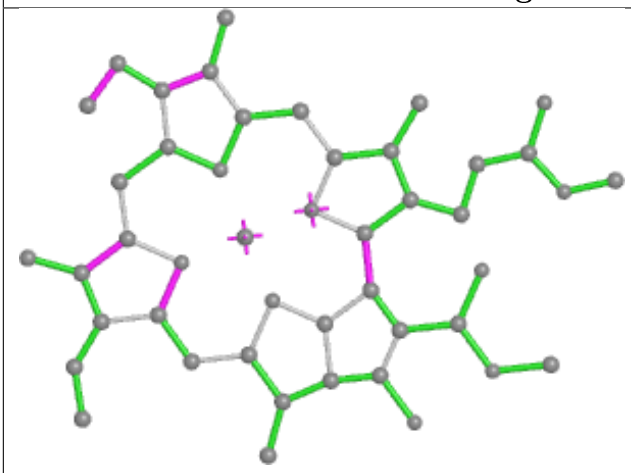


Torsions

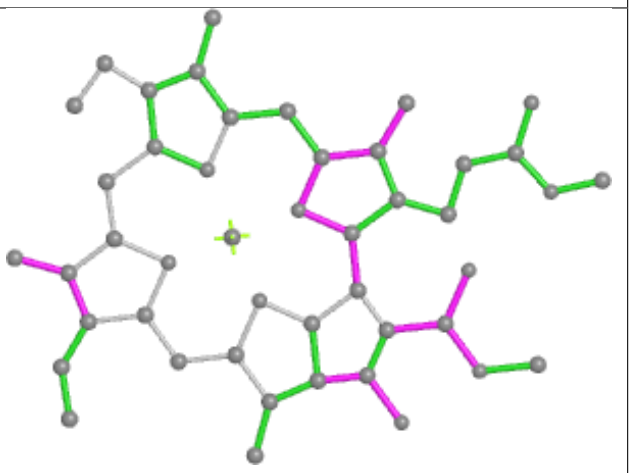


Rings

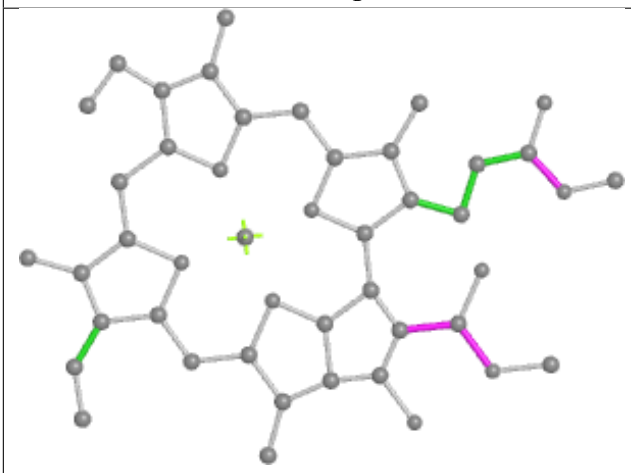
Ligand CLA A 1118



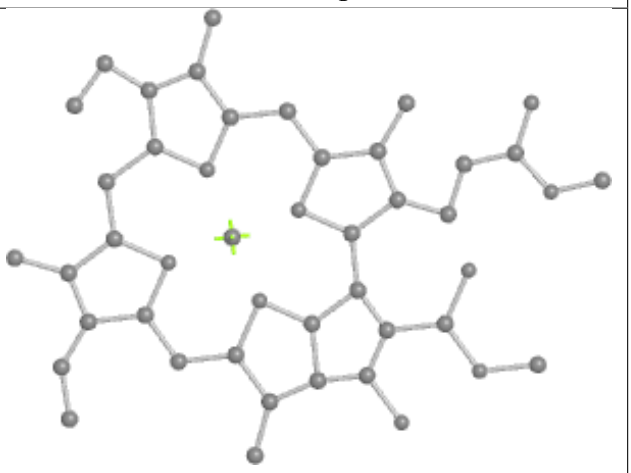
Bond lengths



Bond angles

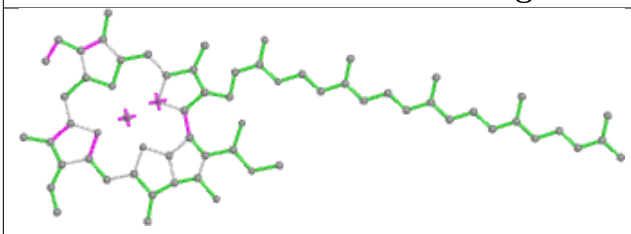


Torsions

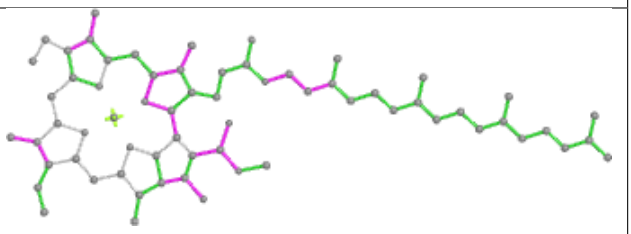


Rings

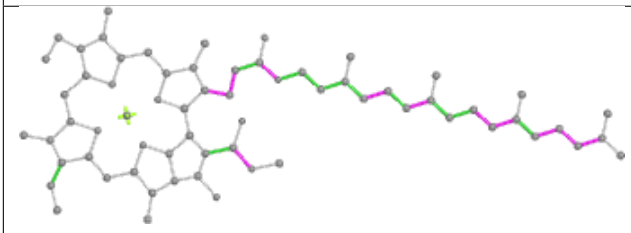
Ligand CLA A 1135



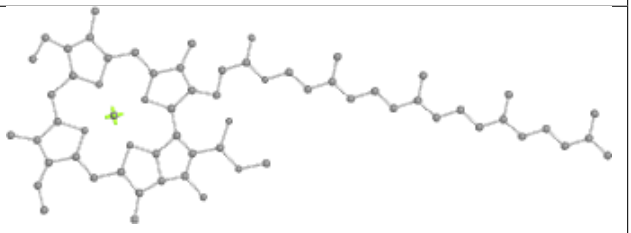
Bond lengths



Bond angles

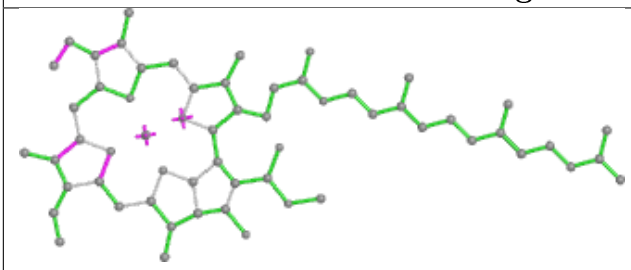


Torsions

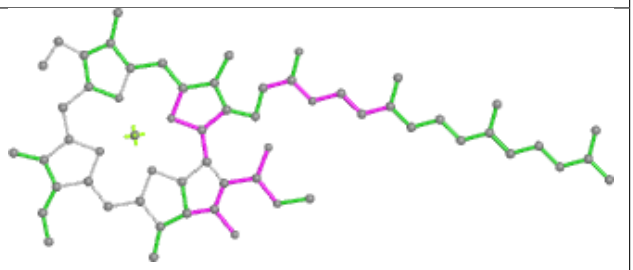


Rings

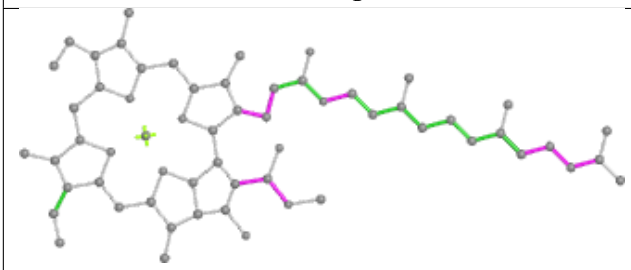
Ligand CLA B 1022



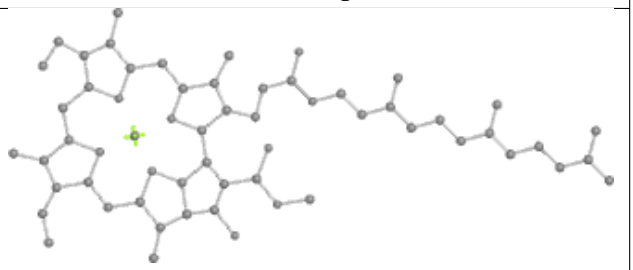
Bond lengths



Bond angles

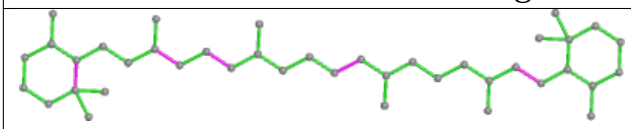


Torsions

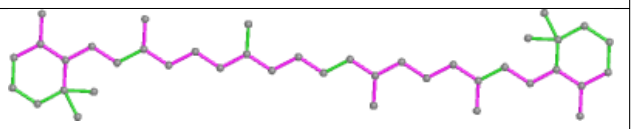


Rings

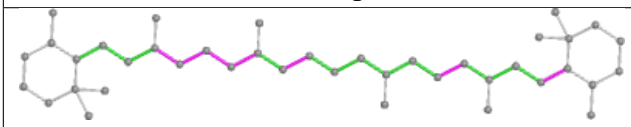
Ligand BCR B 4017



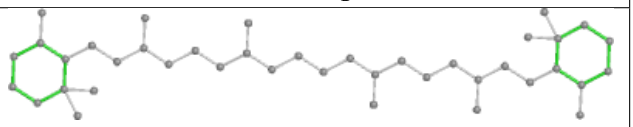
Bond lengths



Bond angles

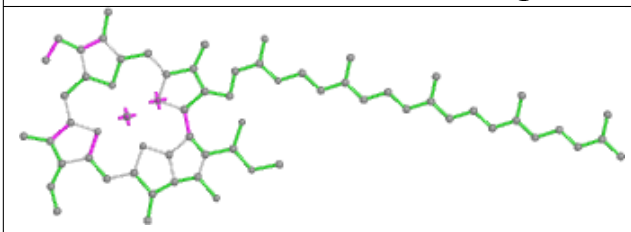


Torsions

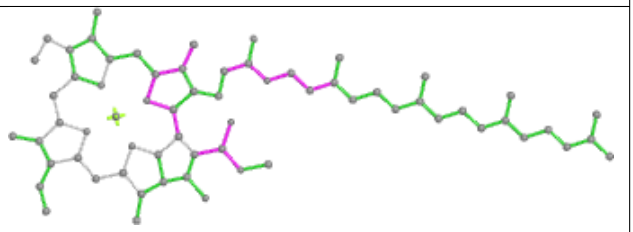


Rings

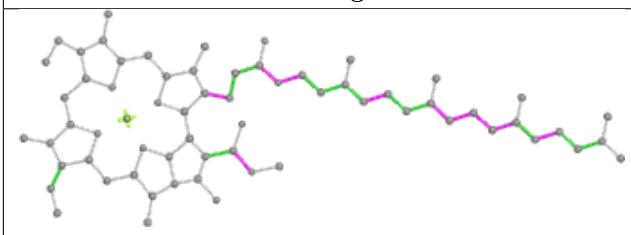
Ligand CLA A 1140



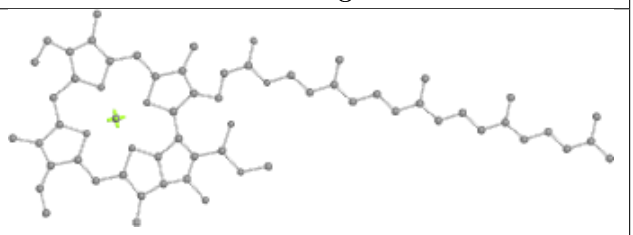
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.