Full wwPDB EM Validation Report

Mar 30, 2026 – 11:53 AM UTC

PDB ID	:	6ZZX / pdb_00006zzx
EMDB ID	:	EMD-11588
Title	:	Structure of low-light grown Chlorella ohadii Photosystem I
Authors	:	Caspy, I.; Nelson, N.; Nechushtai, R.; Neumann, E.; Shkolnisky, Y.
Deposited on	:	2020-08-05
Resolution	:	2.70 Å(reported)
Based on initial model	:	6IJO

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

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

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

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

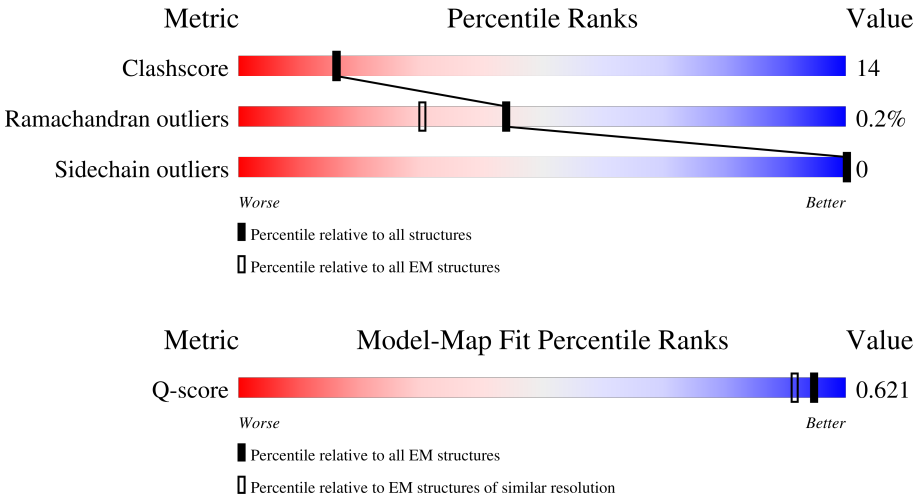
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	741	74% 26%
2	B	731	79% 21%
3	C	80	78% 22%
4	D	143	79% 21%

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Mol	Chain	Length	Quality of chain
5	E	64	80% 20%
6	F	165	82% 18%
7	G	99	84% 16%
8	H	94	5% 68% 32%
9	J	41	73% 27%
10	K	86	87% 13%
11	L	157	75% 25%
12	M	31	68% 32%
13	I	35	66% 34%
14	O	87	34% 71% 26%
15	1	192	74% 26%
15	a	192	77% 23%
16	3	241	81% 19%
17	4	207	80% 19%
18	5	229	74% 26%
19	6	231	77% 23%
20	7	221	86% 14%
21	8	219	77% 23%
22	2	215	77% 23%
23	9	183	80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CL0	A	1011	X	-	-	-
25	CLA	1	601	X	-	-	-
25	CLA	1	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	615	X	-	-	-
25	CLA	2	601	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	607	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	615	X	-	-	-
25	CLA	2	621	X	-	-	-
25	CLA	3	601	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	605	X	-	-	-
25	CLA	3	606	X	-	-	-
25	CLA	3	607	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	616	X	-	-	-
25	CLA	3	618	X	-	-	-
25	CLA	4	601	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	605	X	-	-	-
25	CLA	4	606	X	-	-	-
25	CLA	4	607	X	-	-	-
25	CLA	4	608	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	4	615	X	-	-	-
25	CLA	4	616	X	-	-	-
25	CLA	4	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	605	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	614	X	-	-	-
25	CLA	5	615	X	-	-	-
25	CLA	6	601	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	6	606	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	6	618	X	-	-	-
25	CLA	7	601	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	605	X	-	-	-
25	CLA	7	606	X	-	-	-
25	CLA	7	607	X	-	-	-
25	CLA	7	608	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	605	X	-	-	-
25	CLA	8	606	X	-	-	-
25	CLA	8	607	X	-	-	-
25	CLA	8	608	X	-	-	-
25	CLA	8	609	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	8	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	8	618	X	-	-	-
25	CLA	8	620	X	-	-	-
25	CLA	9	602	X	-	-	-
25	CLA	9	604	X	-	-	-
25	CLA	9	605	X	-	-	-
25	CLA	9	606	X	-	-	-
25	CLA	9	607	X	-	-	-
25	CLA	9	609	X	-	-	-
25	CLA	9	612	X	-	-	-
25	CLA	A	1012	X	-	-	-
25	CLA	A	1013	X	-	-	-
25	CLA	A	1101	X	-	-	-
25	CLA	A	1102	X	-	-	-
25	CLA	A	1103	X	-	-	-
25	CLA	A	1104	X	-	-	-
25	CLA	A	1105	X	-	-	-
25	CLA	A	1106	X	-	-	-
25	CLA	A	1107	X	-	-	-
25	CLA	A	1108	X	-	-	-
25	CLA	A	1109	X	-	-	-
25	CLA	A	1110	X	-	-	-
25	CLA	A	1111	X	-	-	-
25	CLA	A	1112	X	-	-	-
25	CLA	A	1113	X	-	-	-
25	CLA	A	1115	X	-	-	-
25	CLA	A	1116	X	-	-	-
25	CLA	A	1117	X	-	-	-
25	CLA	A	1118	X	-	-	-
25	CLA	A	1119	X	-	-	-
25	CLA	A	1120	X	-	-	-
25	CLA	A	1121	X	-	-	-
25	CLA	A	1122	X	-	-	-
25	CLA	A	1123	X	-	-	-
25	CLA	A	1124	X	-	-	-
25	CLA	A	1125	X	-	-	-
25	CLA	A	1126	X	-	-	-
25	CLA	A	1127	X	-	-	-
25	CLA	A	1128	X	-	-	-
25	CLA	A	1129	X	-	-	-
25	CLA	A	1130	X	-	-	-
25	CLA	A	1131	X	-	-	-
25	CLA	A	1132	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	1133	X	-	-	-
25	CLA	A	1134	X	-	-	-
25	CLA	A	1135	X	-	-	-
25	CLA	A	1136	X	-	-	-
25	CLA	A	1137	X	-	-	-
25	CLA	A	1138	X	-	-	-
25	CLA	A	1139	X	-	-	-
25	CLA	A	1140	X	-	-	-
25	CLA	A	1141	X	-	-	-
25	CLA	B	1021	X	-	-	-
25	CLA	B	1022	X	-	-	-
25	CLA	B	1023	X	-	-	-
25	CLA	B	1201	X	-	-	-
25	CLA	B	1202	X	-	-	-
25	CLA	B	1203	X	-	-	-
25	CLA	B	1204	X	-	-	-
25	CLA	B	1205	X	-	-	-
25	CLA	B	1206	X	-	-	-
25	CLA	B	1207	X	-	-	-
25	CLA	B	1208	X	-	-	-
25	CLA	B	1209	X	-	-	-
25	CLA	B	1210	X	-	-	-
25	CLA	B	1211	X	-	-	-
25	CLA	B	1212	X	-	-	-
25	CLA	B	1213	X	-	-	-
25	CLA	B	1214	X	-	-	-
25	CLA	B	1215	X	-	-	-
25	CLA	B	1216	X	-	-	-
25	CLA	B	1217	X	-	-	-
25	CLA	B	1218	X	-	-	-
25	CLA	B	1219	X	-	-	-
25	CLA	B	1220	X	-	-	-
25	CLA	B	1221	X	-	-	-
25	CLA	B	1222	X	-	-	-
25	CLA	B	1223	X	-	-	-
25	CLA	B	1224	X	-	-	-
25	CLA	B	1225	X	-	-	-
25	CLA	B	1226	X	-	-	-
25	CLA	B	1227	X	-	-	-
25	CLA	B	1228	X	-	-	-
25	CLA	B	1229	X	-	-	-
25	CLA	B	1230	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	1231	X	-	-	-
25	CLA	B	1232	X	-	-	-
25	CLA	B	1235	X	-	-	-
25	CLA	B	1236	X	-	-	-
25	CLA	B	1237	X	-	-	-
25	CLA	B	1238	X	-	-	-
25	CLA	B	1239	X	-	-	-
25	CLA	B	1240	X	-	-	-
25	CLA	F	1301	X	-	-	-
25	CLA	F	1302	X	-	-	-
25	CLA	G	1601	X	-	-	-
25	CLA	G	1602	X	-	-	-
25	CLA	G	1603	X	-	-	-
25	CLA	H	1701	X	-	-	-
25	CLA	H	1702	X	-	-	-
25	CLA	H	1703	X	-	-	-
25	CLA	J	1901	X	-	-	-
25	CLA	K	1401	X	-	-	-
25	CLA	K	1402	X	-	-	-
25	CLA	K	1403	X	-	-	-
25	CLA	K	1404	X	-	-	-
25	CLA	L	1501	X	-	-	-
25	CLA	L	1502	X	-	-	-
25	CLA	L	1503	X	-	-	-
25	CLA	L	1504	X	-	-	-
25	CLA	O	1801	X	-	-	-
25	CLA	O	1802	X	-	-	-
25	CLA	O	1803	X	-	-	-
25	CLA	a	601	X	-	-	-
25	CLA	a	602	X	-	-	-
25	CLA	a	603	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	611	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	a	615	X	-	-	-
26	CHL	1	604	X	-	-	-
26	CHL	1	609	X	-	-	-
26	CHL	1	610	X	-	-	-
26	CHL	1	611	X	-	-	-
26	CHL	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	2	609	X	-	-	-
26	CHL	2	610	X	-	-	-
26	CHL	2	613	X	-	-	-
26	CHL	3	603	X	-	-	-
26	CHL	3	604	X	-	-	-
26	CHL	3	608	X	-	-	-
26	CHL	3	611	X	-	-	-
26	CHL	4	609	X	-	-	-
26	CHL	4	613	X	-	-	-
26	CHL	4	618	X	-	-	-
26	CHL	5	610	X	-	-	-
26	CHL	5	611	X	-	-	-
26	CHL	5	613	X	-	-	-
26	CHL	5	617	X	-	-	-
26	CHL	5	618	X	-	-	-
26	CHL	6	609	X	-	-	-
26	CHL	6	610	X	-	-	-
26	CHL	6	611	X	-	-	-
26	CHL	6	613	X	-	-	-
26	CHL	6	617	X	-	-	-
26	CHL	6	619	X	-	-	-
26	CHL	7	609	X	-	-	-
26	CHL	7	611	X	-	-	-
26	CHL	7	613	X	-	-	-
26	CHL	7	615	X	-	-	-
26	CHL	7	617	X	-	-	-
26	CHL	8	601	X	-	-	-
26	CHL	8	603	X	-	-	-
26	CHL	8	604	X	-	-	-
26	CHL	8	610	X	-	-	-
26	CHL	8	613	X	-	-	-
26	CHL	9	601	X	-	-	-
26	CHL	9	603	X	-	-	-
26	CHL	9	608	X	-	-	-
26	CHL	9	610	X	-	-	-
26	CHL	9	613	X	-	-	-
26	CHL	A	1114	X	-	-	-
26	CHL	a	604	X	-	-	-
26	CHL	a	606	X	-	-	-
26	CHL	a	609	X	-	-	-
26	CHL	a	610	X	-	-	-
26	CHL	a	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	NEX	F	4001	X	-	-	-
40	RRX	3	506	X	-	-	-
40	RRX	J	4002	X	-	-	-
43	LUT	2	507	X	-	-	-
43	LUT	4	501	X	-	-	-
43	LUT	7	501	X	-	-	-
46	QTB	a	504	X	-	-	-
50	XAT	2	501	X	-	-	-
50	XAT	7	502	X	-	-	-
50	XAT	9	504	X	-	-	-
50	XAT	9	507	X	-	-	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 56369 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
			Total	C	N	O	S		
1	A	741	5824	3815	988	1001	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	SER	conflict	UNP W8SY74
A	437	ILE	MET	conflict	UNP W8SY74

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5796	3807	980	994	15	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP W8SUA3
B	5	LEU	-	insertion	UNP W8SUA3
B	241	ALA	VAL	conflict	UNP W8SUA3
B	402	ALA	GLU	conflict	UNP W8SUA3
B	403	GLN	ALA	conflict	UNP W8SUA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	601	367	104	119	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	716	196	208	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ALA	VAL	conflict	UNP A0A2P6TKF8
D	320	ILE	VAL	conflict	UNP A0A2P6TKF8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			509	323	91	95		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	GLN	THR	conflict	UNP A0A2P6U4S6
E	48	LEU	MET	conflict	UNP A0A2P6U4S6
E	96	VAL	GLU	conflict	UNP A0A2P6U4S6
E	97	ALA	GLU	conflict	UNP A0A2P6U4S6
E	98	ALA	VAL	conflict	UNP A0A2P6U4S6

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1277	830	216	228	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LEU	MET	conflict	UNP A0A2P6TPV8
F	348	ASN	LYS	conflict	UNP A0A2P6TPV8
F	351	ALA	GLU	conflict	UNP A0A2P6TPV8
F	352	ASP	GLY	conflict	UNP A0A2P6TPV8
F	360	LYS	GLN	conflict	UNP A0A2P6TPV8
F	364	ALA	ASP	conflict	UNP A0A2P6TPV8
F	367	GLU	ASN	conflict	UNP A0A2P6TPV8
F	430	ALA	SER	conflict	UNP A0A2P6TPV8
F	431	ALA	SER	conflict	UNP A0A2P6TPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	conflict	UNP A0A2P6TPV8
F	433	ALA	THR	conflict	UNP A0A2P6TPV8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	99	Total	C	N	O	S	0	0
			727	466	127	130	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	ALA	SER	conflict	UNP A0A2P6TZI8
G	1272	LEU	MET	conflict	UNP A0A2P6TZI8
G	1285	ILE	VAL	conflict	UNP A0A2P6TZI8
G	1313	ILE	LEU	conflict	UNP A0A2P6TZI8
G	1317	SER	HIS	conflict	UNP A0A2P6TZI8
G	1320	GLY	GLN	conflict	UNP A0A2P6TZI8
G	1321	LEU	VAL	conflict	UNP A0A2P6TZI8
G	1324	ASN	VAL	conflict	UNP A0A2P6TZI8

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	94	Total	C	N	O	S	0	0
			729	457	132	139	1		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	92	ILE	VAL	conflict	UNP A0A2P6TPU7
H	102	GLY	LEU	conflict	UNP A0A2P6TPU7
H	105	ALA	SER	conflict	UNP A0A2P6TPU7
H	106	ALA	SER	conflict	UNP A0A2P6TPU7
H	109	ARG	SER	conflict	UNP A0A2P6TPU7
H	?	-	ILE	deletion	UNP A0A2P6TPU7
H	113	VAL	LYS	conflict	UNP A0A2P6TPU7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			316	212	46	57	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	86	Total	C	N	O	S	0	0
			613	390	106	115	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	74	ALA	GLU	conflict	UNP A0A2P6U0J1
K	103	LEU	ILE	conflict	UNP A0A2P6U0J1
K	105	CYS	VAL	conflict	UNP A0A2P6U0J1
K	107	ILE	VAL	conflict	UNP A0A2P6U0J1
K	108	VAL	ILE	conflict	UNP A0A2P6U0J1
K	112	LYS	ARG	conflict	UNP A0A2P6U0J1
K	113	SER	GLY	conflict	UNP A0A2P6U0J1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	157	Total	C	N	O	S	0	0
			1165	758	192	211	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	350	TYR	PHE	conflict	UNP A0A2P6TC44
L	364	ASP	ASN	conflict	UNP A0A2P6TC44
L	?	-	ALA	deletion	UNP A0A2P6TC44
L	421	ASP	GLU	conflict	UNP A0A2P6TC44
L	443	LEU	ILE	conflict	UNP A0A2P6TC44

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			239	163	36	39	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	S	0	0
			270	183	37	47	3		

- Molecule 14 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	87	Total	C	N	O	S	0	0
			679	453	109	115	2		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
15	a	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	166	SER	LEU	conflict	UNP A0A2P6TT36
1	167	LYS	GLU	conflict	UNP A0A2P6TT36
1	171	THR	VAL	conflict	UNP A0A2P6TT36
1	194	THR	ASN	conflict	UNP A0A2P6TT36
1	196	ALA	GLN	conflict	UNP A0A2P6TT36
1	204	SER	ALA	conflict	UNP A0A2P6TT36
1	210	MET	LEU	conflict	UNP A0A2P6TT36
a	166	SER	LEU	conflict	UNP A0A2P6TT36
a	167	LYS	GLU	conflict	UNP A0A2P6TT36
a	171	THR	VAL	conflict	UNP A0A2P6TT36
a	194	THR	ASN	conflict	UNP A0A2P6TT36
a	196	ALA	GLN	conflict	UNP A0A2P6TT36
a	204	SER	ALA	conflict	UNP A0A2P6TT36
a	210	MET	LEU	conflict	UNP A0A2P6TT36

- Molecule 16 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	314	CYS	GLY	conflict	UNP A0A2P6TMT4
3	329	ILE	VAL	conflict	UNP A0A2P6TMT4
3	339	THR	SER	conflict	UNP A0A2P6TMT4
3	359	LYS	ASN	conflict	UNP A0A2P6TMT4
3	405	GLY	ALA	conflict	UNP A0A2P6TMT4
3	429	GLU	ALA	conflict	UNP A0A2P6TMT4
3	484	THR	ARG	conflict	UNP A0A2P6TMT4
3	485	ILE	ARG	conflict	UNP A0A2P6TMT4
3	486	LEU	ARG	conflict	UNP A0A2P6TMT4
3	487	LYS	ALA	conflict	UNP A0A2P6TMT4

- Molecule 17 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	207	Total	C	N	O	S	0	0
			1631	1056	277	294	4		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	229	Total	C	N	O	S	0	0
			1786	1146	310	317	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	32	LYS	ASP	conflict	UNP A0A2P6U4K1
5	38	VAL	ALA	conflict	UNP A0A2P6U4K1
5	40	ALA	SER	conflict	UNP A0A2P6U4K1
5	42	GLY	ALA	conflict	UNP A0A2P6U4K1
5	113	SER	GLY	conflict	UNP A0A2P6U4K1
5	127	ILE	LEU	conflict	UNP A0A2P6U4K1
5	195	VAL	ILE	conflict	UNP A0A2P6U4K1

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	231	Total	C	N	O	S	0	0
			1787	1168	295	314	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	83	CYS	ALA	conflict	UNP A0A2P6TPR7
6	94	LEU	MET	conflict	UNP A0A2P6TPR7
6	196	ILE	VAL	conflict	UNP A0A2P6TPR7
6	201	ALA	GLY	conflict	UNP A0A2P6TPR7
6	250	GLN	ASN	conflict	UNP A0A2P6TPR7

- Molecule 20 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	103	GLU	ASP	conflict	UNP A0A2P6TZ50

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	215	Total	C	N	O	S	0	0
			1666	1074	277	309	6		

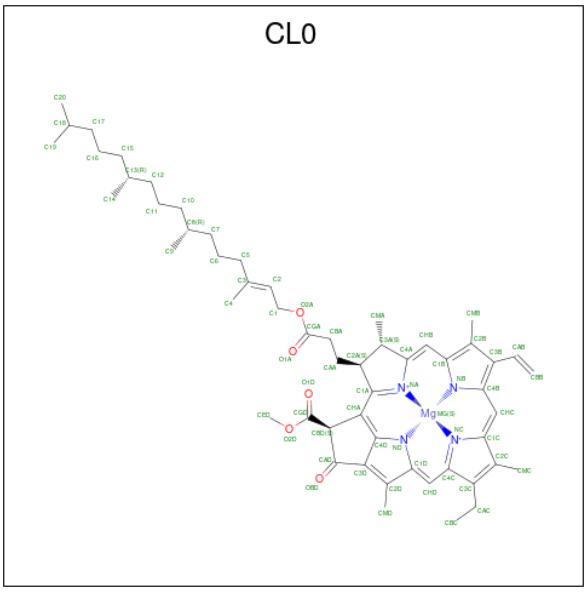
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	64	ASP	GLU	conflict	UNP A0A2P6TMX4
2	97	PRO	ASN	conflict	UNP A0A2P6TMX4

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

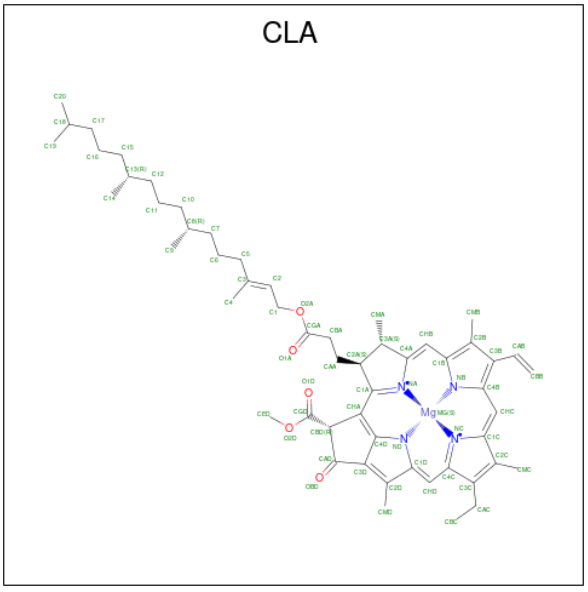
Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	183	Total	C	N	O	S	0	0
			1406	909	237	254	6		

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	N	O		0
			64	55	4	5		
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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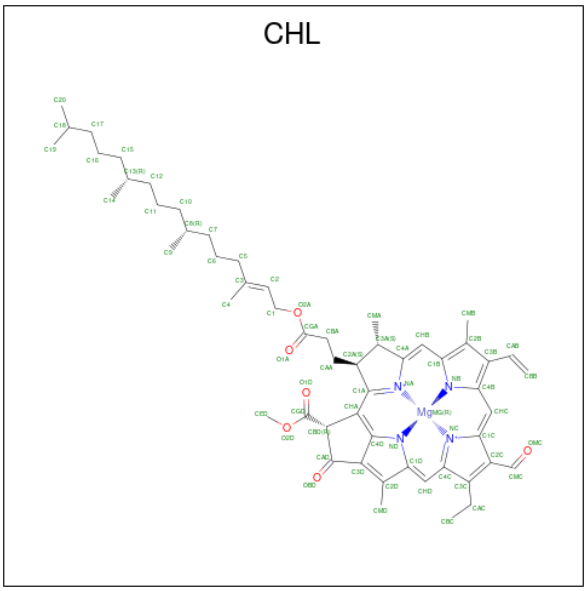
Mol	Chain	Residues	Atoms					AltConf
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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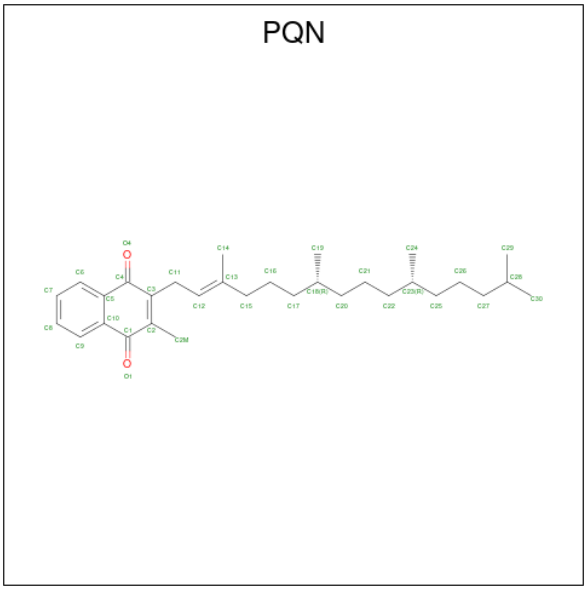
Mol	Chain	Residues	Atoms					AltConf
26	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	7	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
26	7	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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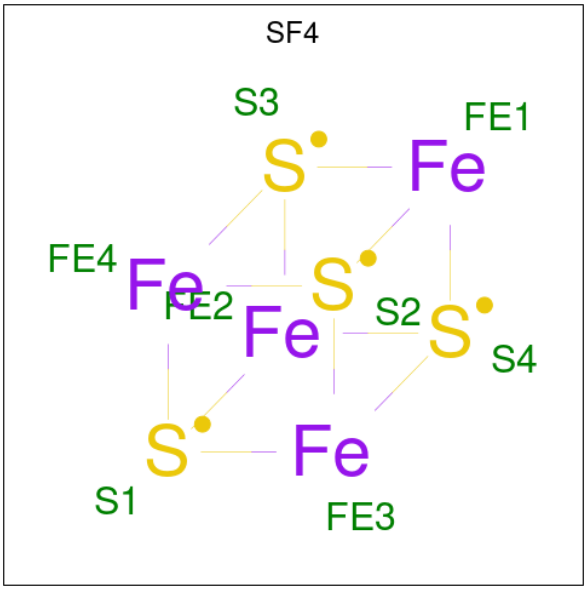
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



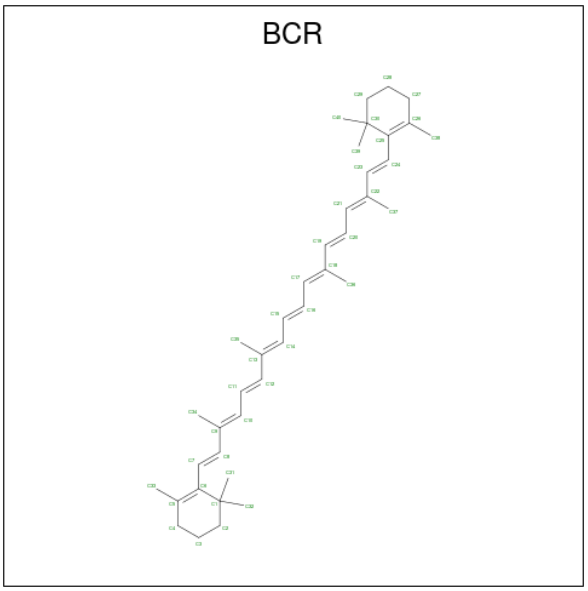
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O 33 31 2	0
27	B	1	Total C O 33 31 2	0

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



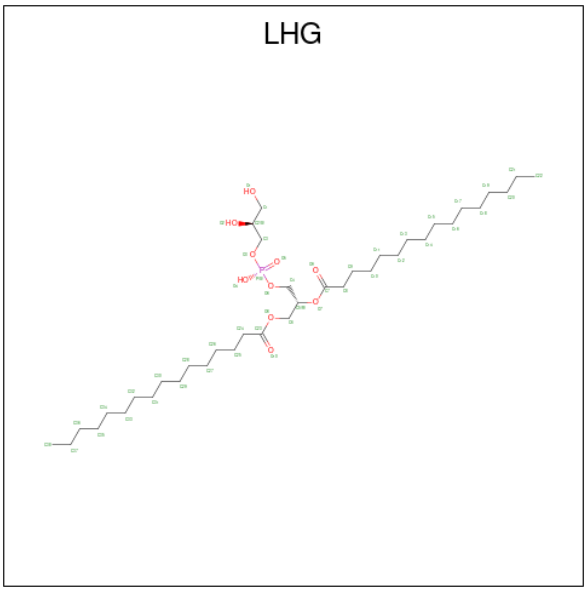
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	I	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



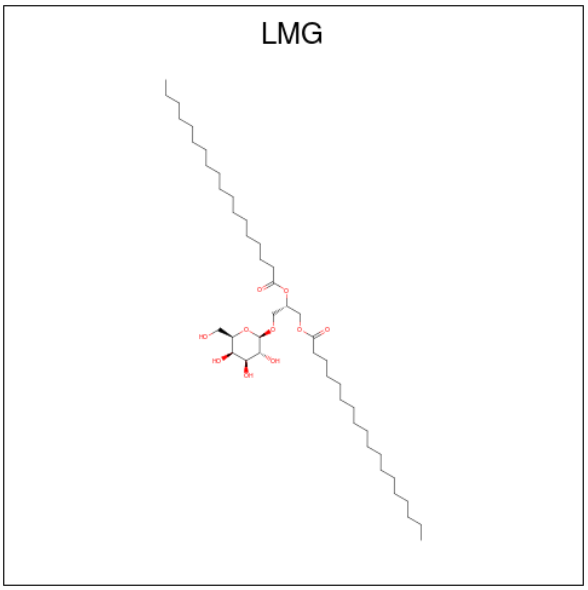
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	A	1	Total	C	O	P	0
			46	35	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	F	1	Total	C	O	P	0
			36	25	10	1	
30	F	1	Total	C	O	P	0
			43	32	10	1	
30	1	1	Total	C	O	P	0
			35	24	10	1	
30	1	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			35	24	10	1	
30	3	1	Total	C	O	P	0
			49	38	10	1	
30	4	1	Total	C	O	P	0
			32	21	10	1	
30	4	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			49	38	10	1	

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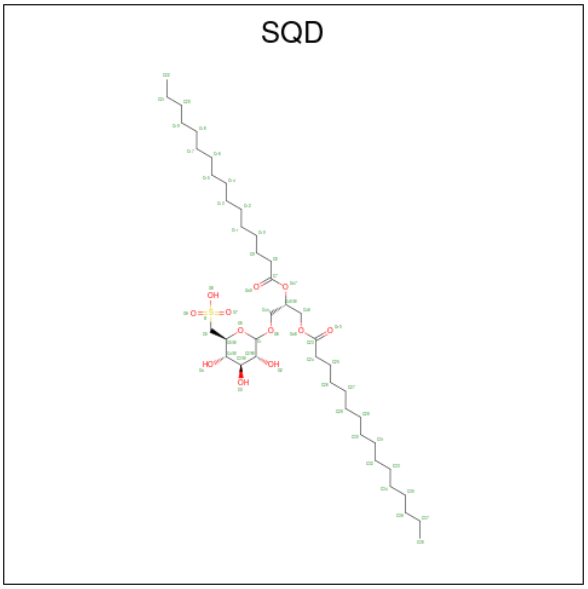
Mol	Chain	Residues	Atoms				AltConf
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	6	1	Total	C	O	P	0
			49	38	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			36	25	10	1	
30	7	1	Total	C	O	P	0
			35	24	10	1	
30	8	1	Total	C	O	P	0
			37	26	10	1	
30	2	1	Total	C	O	P	0
			49	38	10	1	
30	2	1	Total	C	O	P	0
			49	38	10	1	
30	9	1	Total	C	O	P	0
			49	38	10	1	
30	9	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



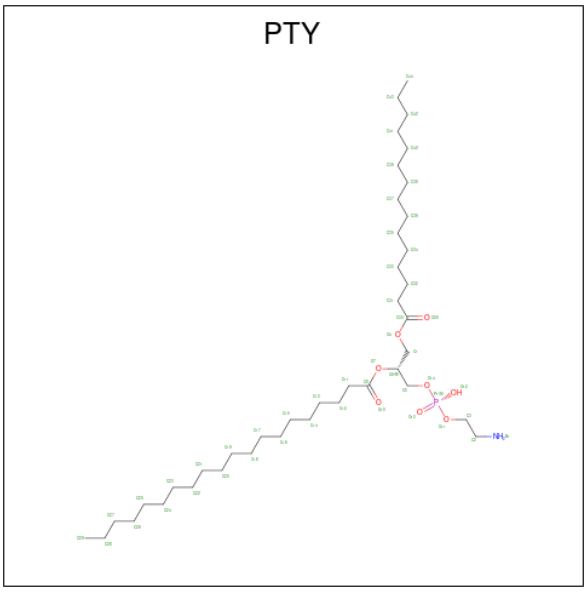
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			42	32	10	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



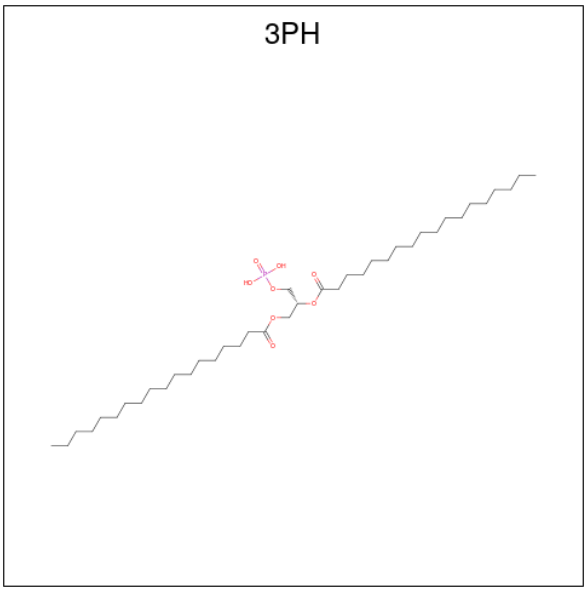
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			54	41	12	1	
32	G	1	Total	C	O	S	0
			46	33	12	1	
32	H	1	Total	C	O	S	0
			45	32	12	1	
32	I	1	Total	C	O	S	0
			54	41	12	1	
32	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



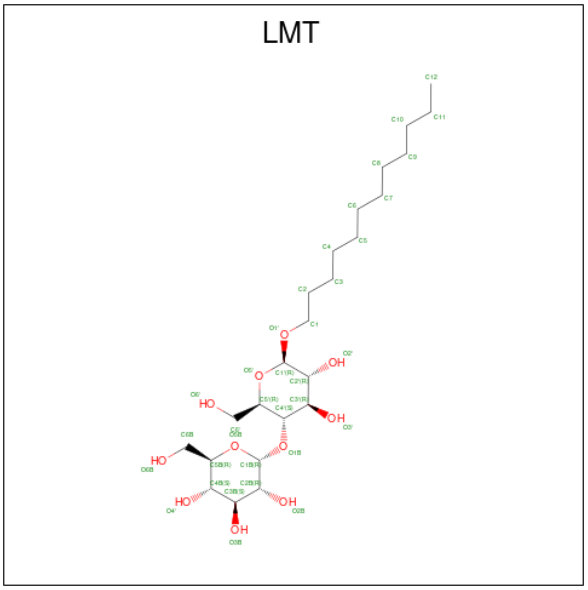
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
33	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
33	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
33	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
33	9	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



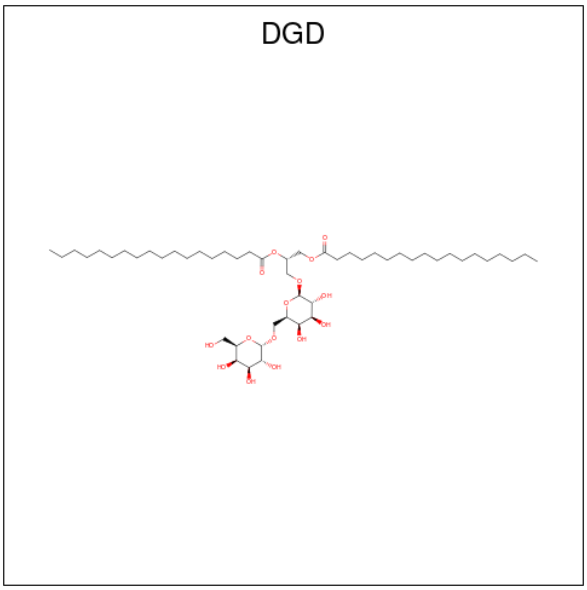
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			35	24	11	
35	B	1	Total	C	O	0
			35	24	11	
35	1	1	Total	C	O	0
			35	24	11	

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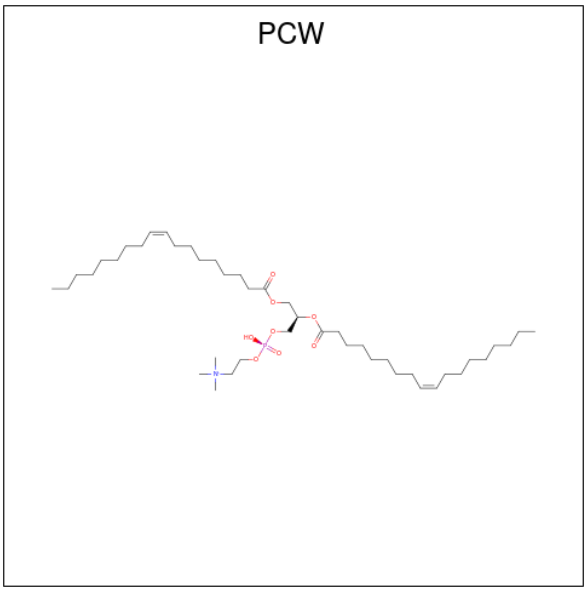
Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			35	24	11	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



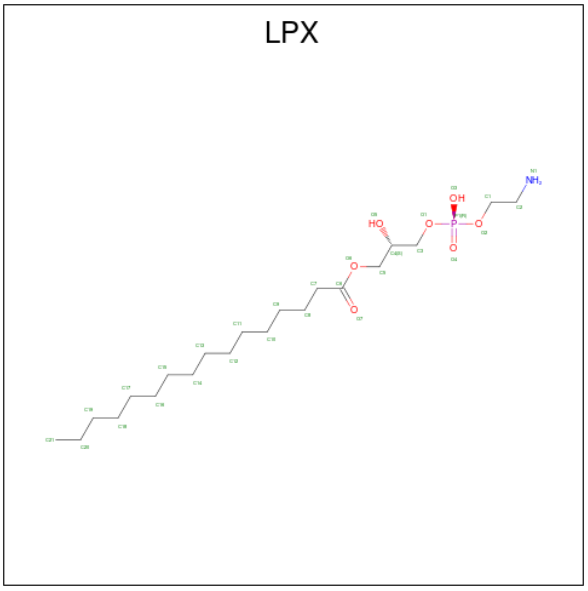
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			66	51	15	
36	7	1	Total	C	O	0
			50	35	15	
36	8	1	Total	C	O	0
			59	44	15	
36	8	1	Total	C	O	0
			46	31	15	

- Molecule 37 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



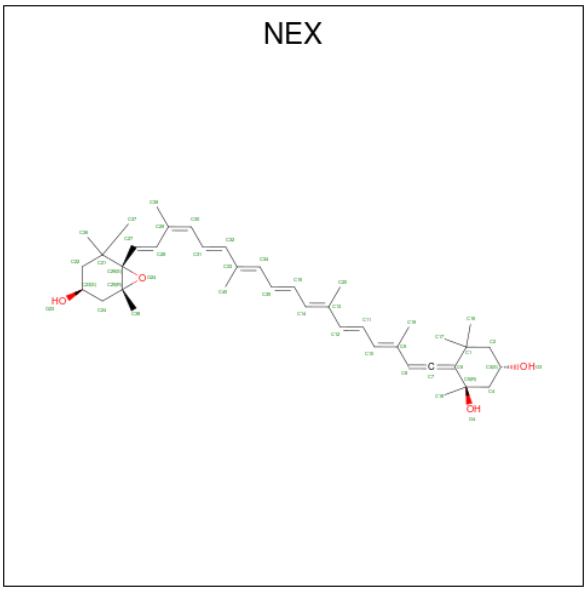
Mol	Chain	Residues	Atoms					AltConf
37	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
37	K	1	Total	C	N	O	P	0
			36	26	1	8	1	
37	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
37	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 38 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



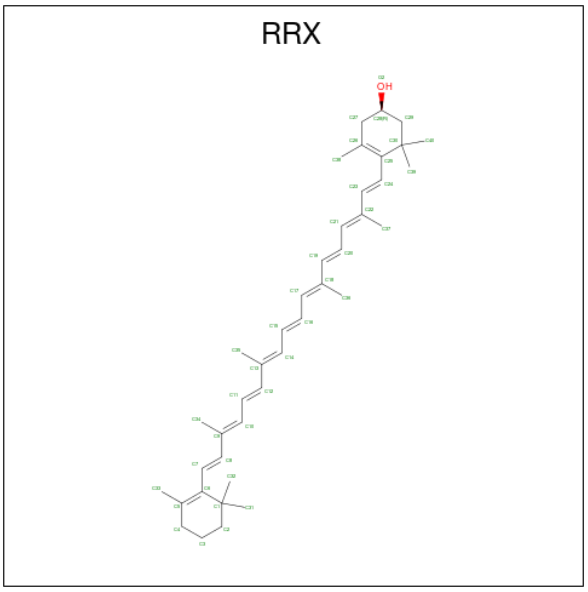
Mol	Chain	Residues	Atoms					AltConf
38	F	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 39 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



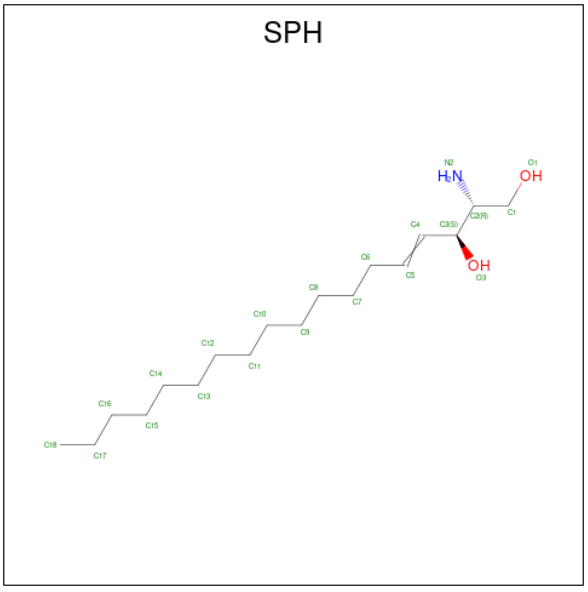
Mol	Chain	Residues	Atoms			AltConf
39	F	1	Total	C	O	0
			44	40	4	

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms	AltConf
40	J	1	Total C O 41 40 1	0
40	3	1	Total C O 41 40 1	0

- Molecule 41 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



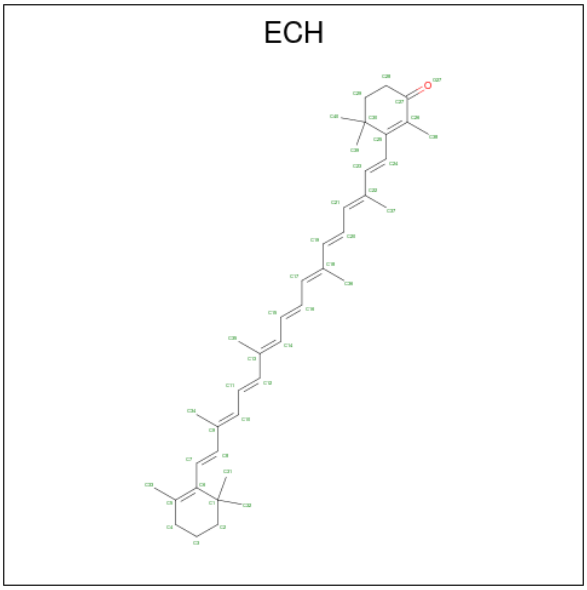
Mol	Chain	Residues	Atoms	AltConf
41	J	1	Total C N O 21 18 1 2	0
41	4	1	Total C N O 21 18 1 2	0

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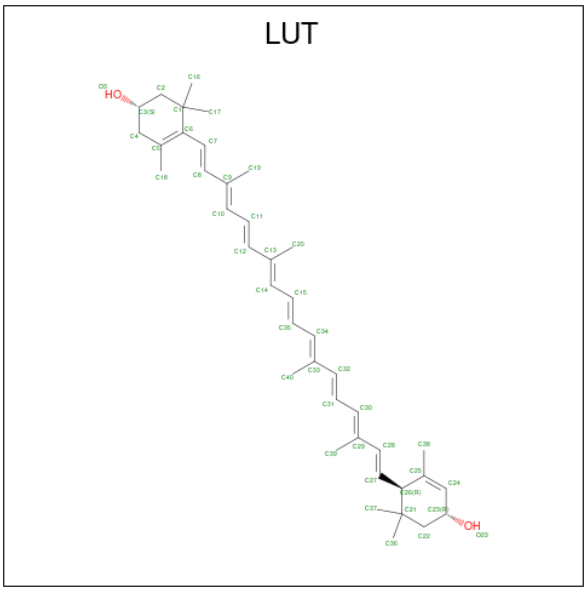
Mol	Chain	Residues	Atoms				AltConf
41	6	1	Total	C	N	O	0
			21	18	1	2	
41	9	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 42 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



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

- Molecule 43 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



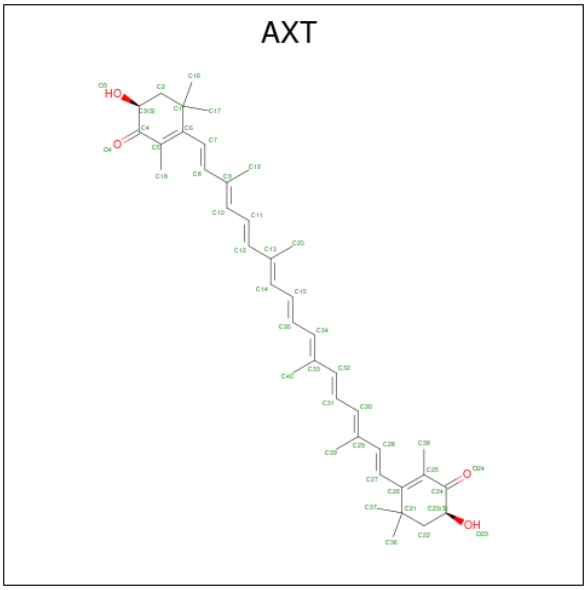
Mol	Chain	Residues	Atoms			AltConf
43	1	1	Total	C	O	0
			42	40	2	
43	1	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	

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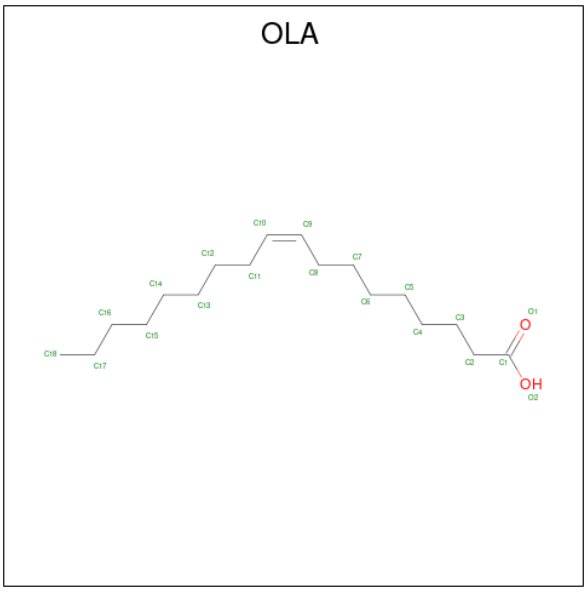
Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total C O 42 40 2	0
43	8	1	Total C O 42 40 2	0
43	8	1	Total C O 42 40 2	0
43	2	1	Total C O 42 40 2	0
43	2	1	Total C O 42 40 2	0
43	9	1	Total C O 42 40 2	0
43	9	1	Total C O 42 40 2	0

- Molecule 44 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$).



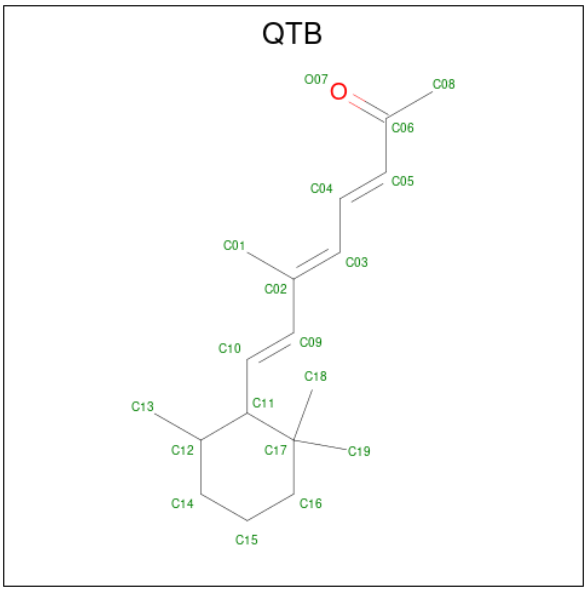
Mol	Chain	Residues	Atoms	AltConf
44	1	1	Total C O 43 40 3	0
44	7	1	Total C O 43 40 3	0

- Molecule 45 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



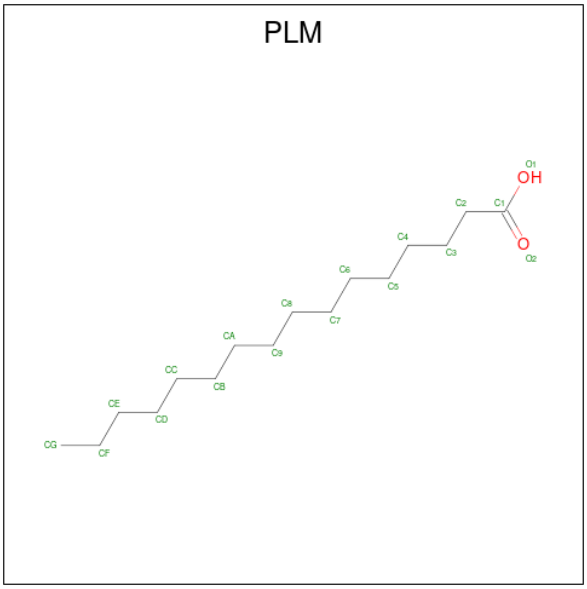
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	C	O	0
			20	18	2	
45	a	1	Total	C	O	0
			20	18	2	
45	8	1	Total	C	O	0
			20	18	2	
45	8	1	Total	C	O	0
			20	18	2	

- Molecule 46 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7 -trien-2-one (CCD ID: QTB) (formula: $C_{18}H_{28}O$).



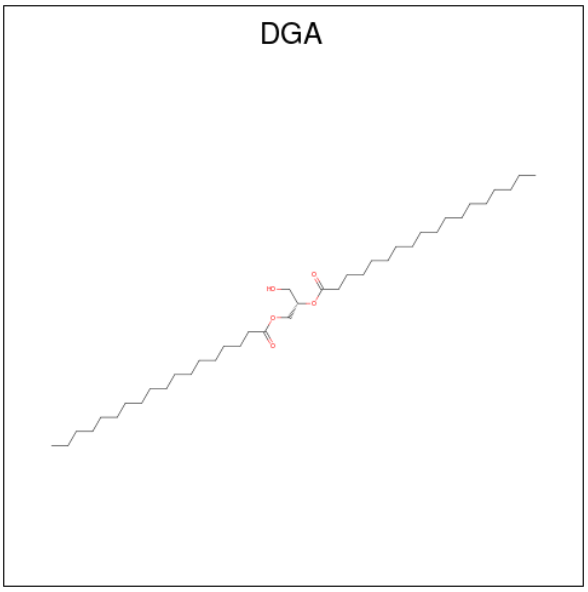
Mol	Chain	Residues	Atoms	AltConf
46	a	1	Total C O 19 18 1	0

- Molecule 47 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



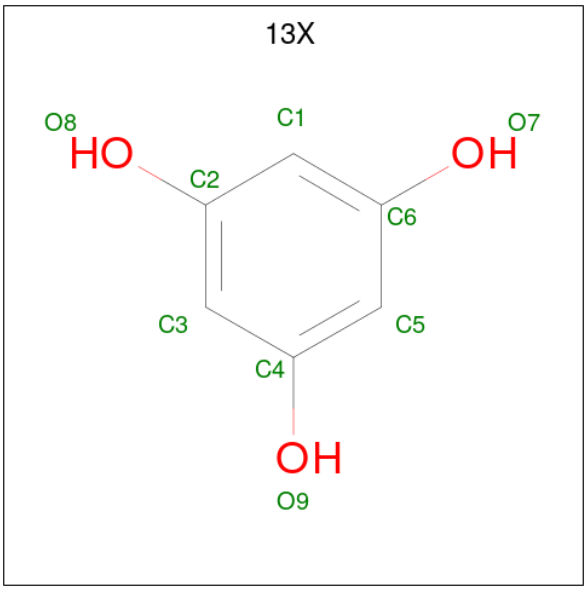
Mol	Chain	Residues	Atoms	AltConf
47	a	1	Total C O 17 16 1	0
47	4	1	Total C O 18 16 2	0
47	4	1	Total C O 17 16 1	0
47	5	1	Total C O 18 16 2	0
47	6	1	Total C O 18 16 2	0
47	8	1	Total C O 17 16 1	0
47	8	1	Total C O 18 16 2	0

- Molecule 48 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



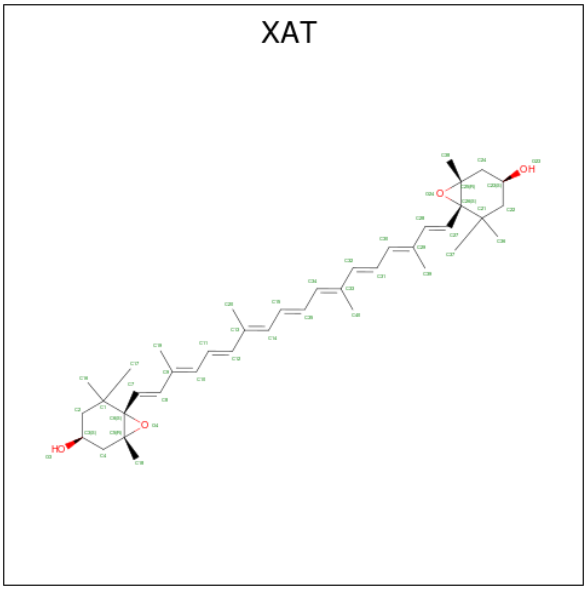
Mol	Chain	Residues	Atoms	AltConf
48	3	1	Total C O 24 19 5	0
48	5	1	Total C O 23 18 5	0
48	8	1	Total C O 40 35 5	0
48	2	1	Total C O 37 32 5	0

- Molecule 49 is benzene-1,3,5-triol (CCD ID: 13X) (formula: $C_6H_6O_3$).



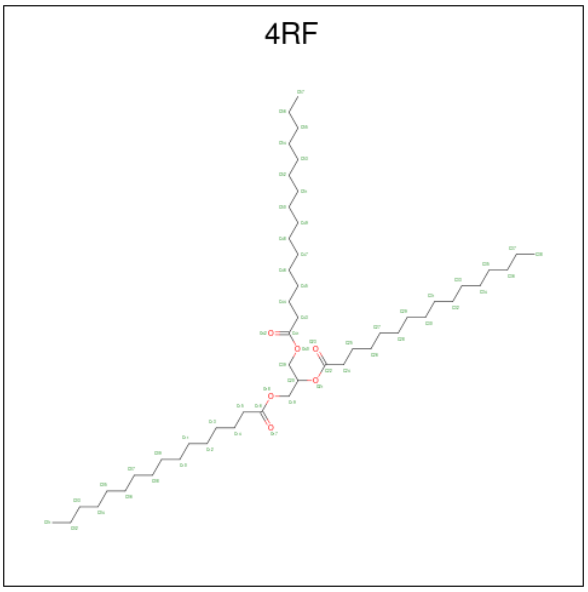
Mol	Chain	Residues	Atoms	AltConf
49	6	1	Total C O 9 6 3	0

- Molecule 50 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



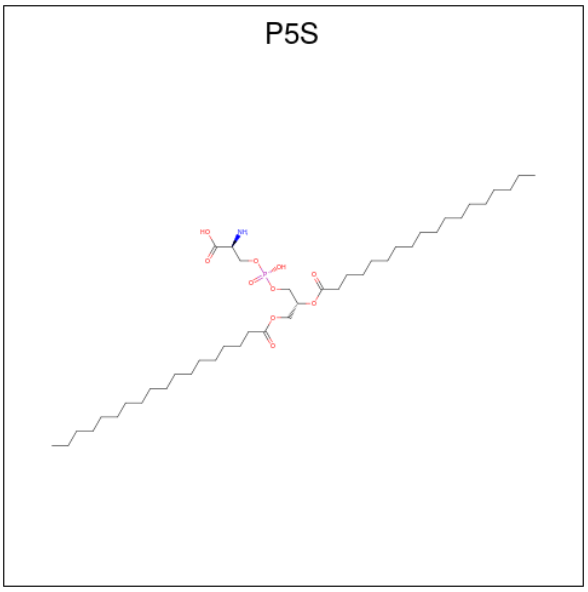
Mol	Chain	Residues	Atoms	AltConf
50	7	1	Total C O 44 40 4	0
50	2	1	Total C O 44 40 4	0
50	9	1	Total C O 44 40 4	0
50	9	1	Total C O 44 40 4	0

- Molecule 51 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



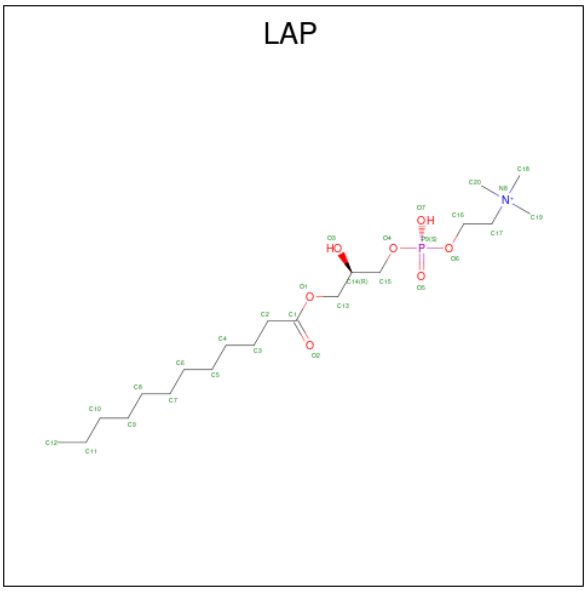
Mol	Chain	Residues	Atoms			AltConf
51	7	1	Total	C	O	0
			37	31	6	

- Molecule 52 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
52	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

- Molecule 53 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: $C_{20}H_{43}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
53	8	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	A	20	Total	O	0
			20	20	
54	A	1	Total	O	0
			1	1	
54	B	2	Total	O	0
			2	2	
54	B	2	Total	O	0
			2	2	
54	B	5	Total	O	0
			5	5	
54	B	6	Total	O	0
			6	6	
54	B	4	Total	O	0
			4	4	
54	B	3	Total	O	0
			3	3	
54	B	1	Total	O	0
			1	1	
54	B	1	Total	O	0
			1	1	
54	C	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
54	C	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	E	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	G	1	Total O 1 1	0
54	G	2	Total O 2 2	0
54	H	1	Total O 1 1	0
54	J	1	Total O 1 1	0
54	K	3	Total O 3 3	0
54	L	1	Total O 1 1	0
54	L	1	Total O 1 1	0
54	M	1	Total O 1 1	0
54	1	5	Total O 5 5	0
54	a	1	Total O 1 1	0
54	3	4	Total O 4 4	0
54	3	1	Total O 1 1	0
54	4	3	Total O 3 3	0
54	4	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
54	5	3	Total O 3 3	0
54	6	7	Total O 7 7	0
54	7	2	Total O 2 2	0
54	8	1	Total O 1 1	0
54	8	1	Total O 1 1	0
54	2	4	Total O 4 4	0
54	9	1	Total O 1 1	0
54	9	1	Total O 1 1	0

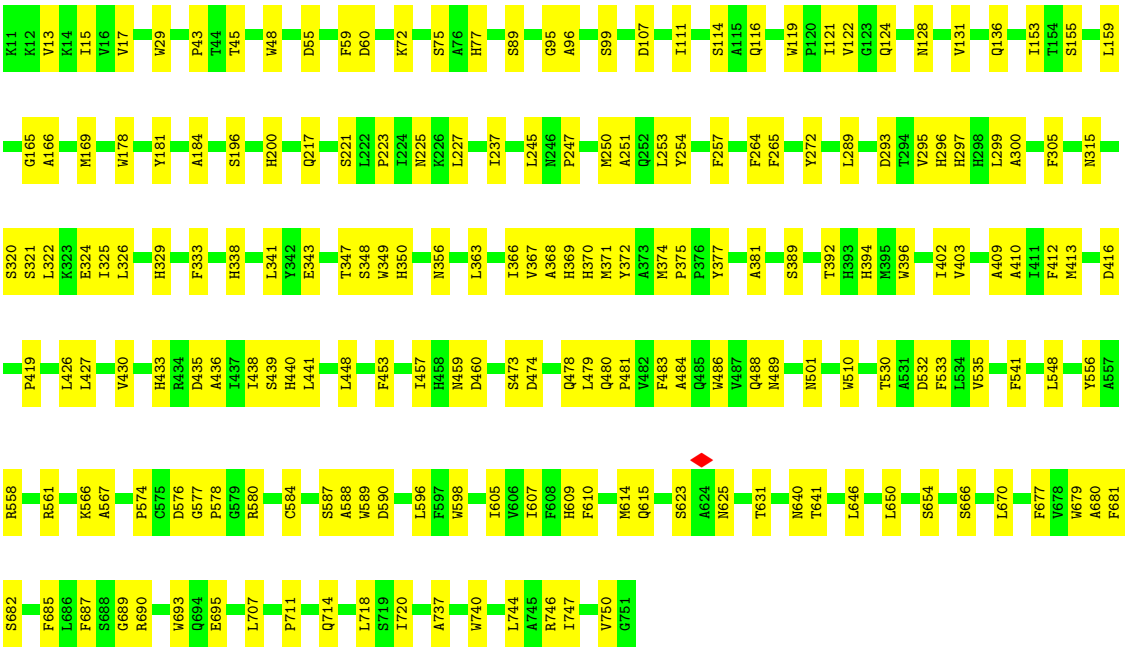
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

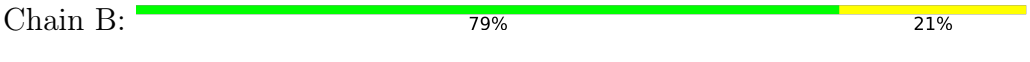
Chain A:

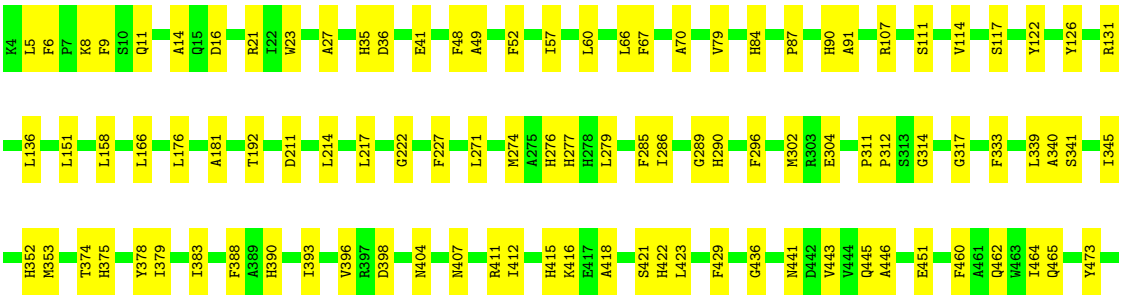


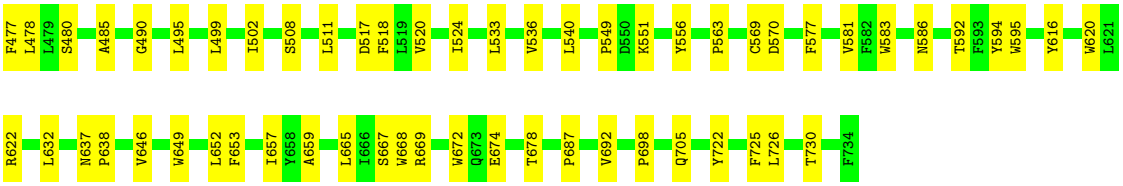


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

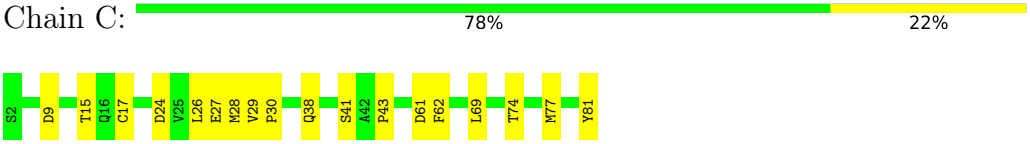
Chain B:



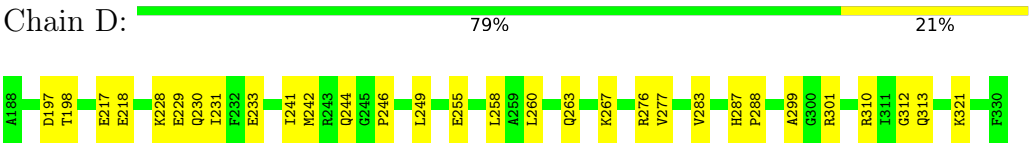




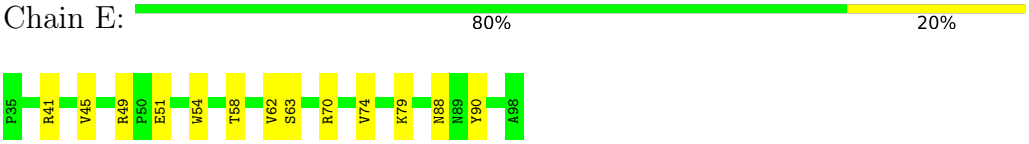
• Molecule 3: Photosystem I iron-sulfur center



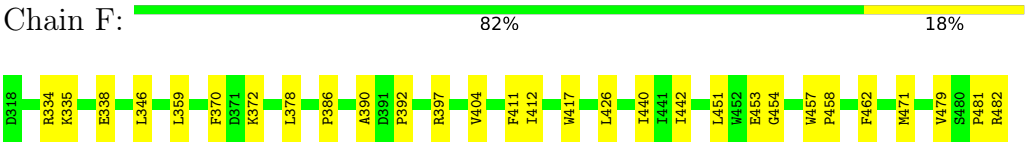
• Molecule 4: Photosystem I reaction center subunit chloroplastic



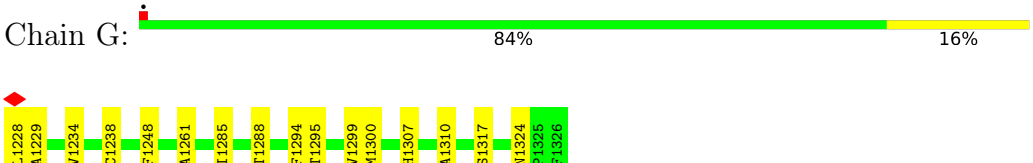
• Molecule 5: Photosystem I reaction center subunit IV



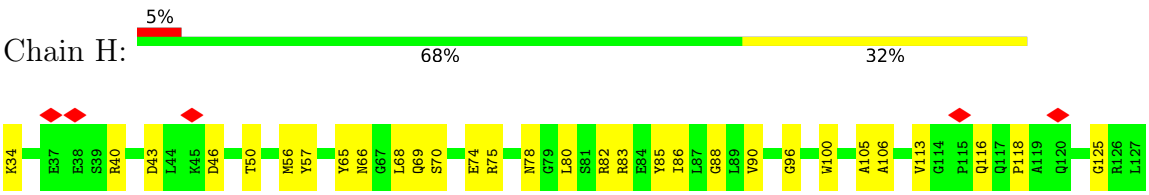
• Molecule 6: PSI-F



• Molecule 7: Photosystem I reaction center subunit chloroplastic



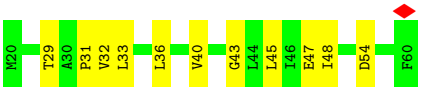
• Molecule 8: Photosystem I reaction center subunit VI-chloroplastic-like



• Molecule 9: Photosystem I reaction center subunit IX

Chain J:

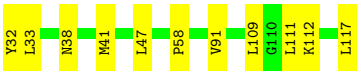




• Molecule 10: Photosystem I reaction center subunit chloroplastic

Chain K:

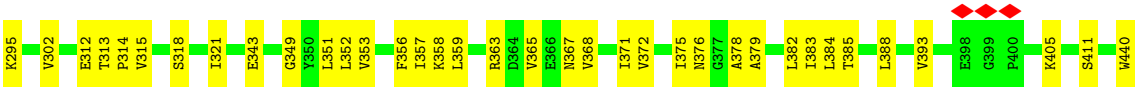


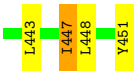


• Molecule 11: Photosystem I reaction center subunit XI

Chain L:



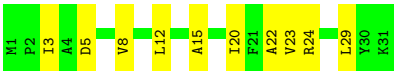




• Molecule 12: Photosystem I reaction center subunit XII

Chain M:

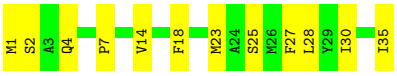




• Molecule 13: Photosystem I reaction center subunit VIII

Chain I:

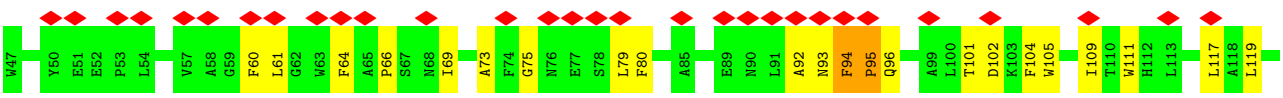




• Molecule 14: Photosystem I subunit O

Chain O:

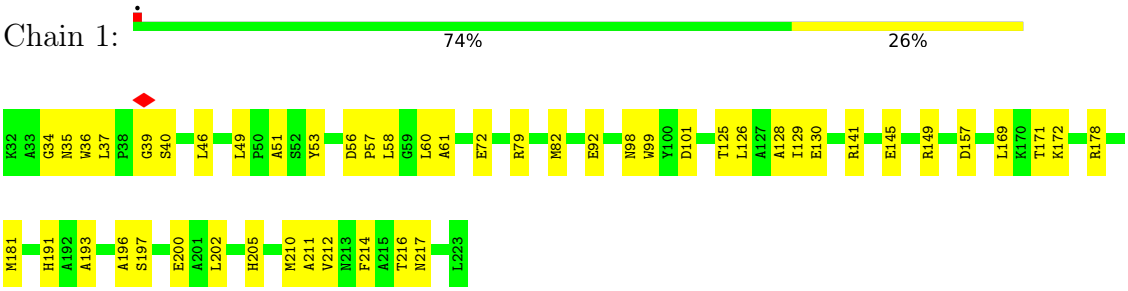






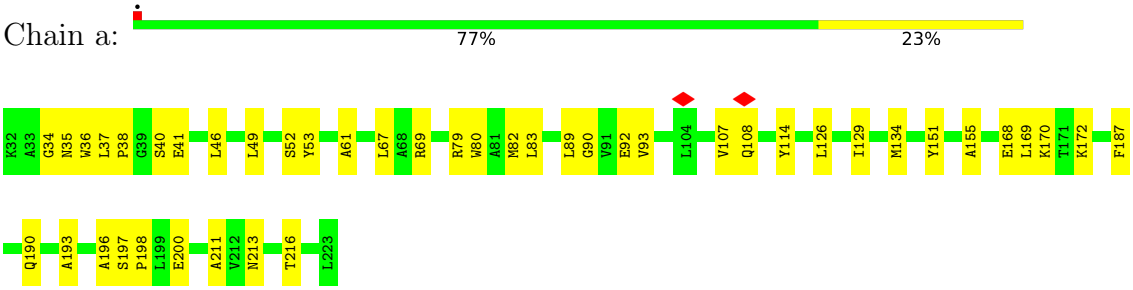
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



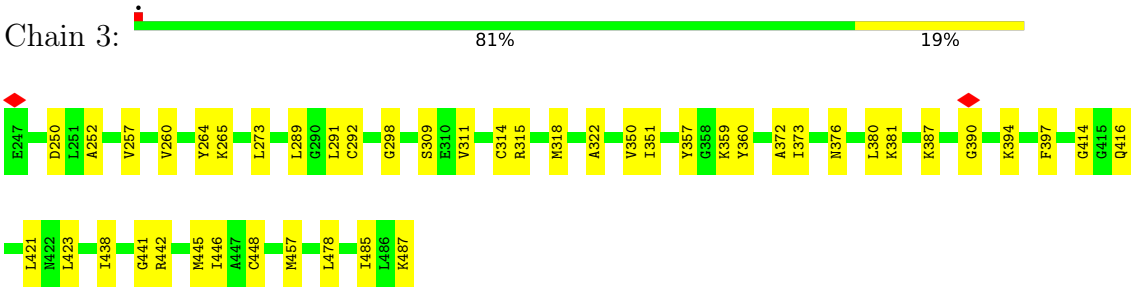
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain a:



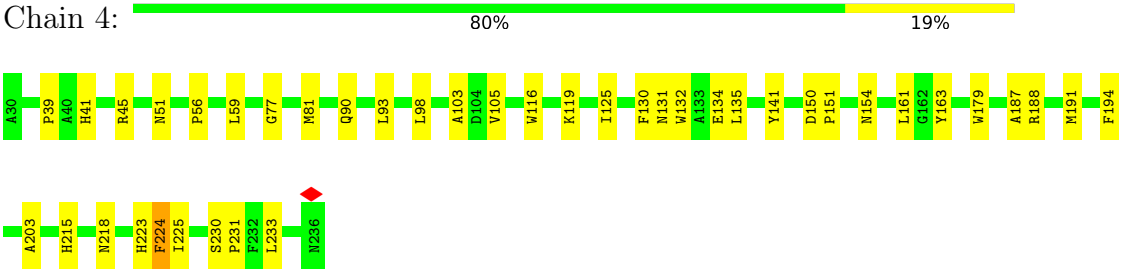
• Molecule 16: Glutathione reductase

Chain 3:



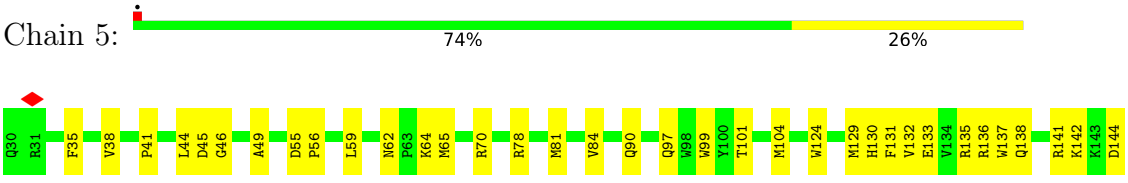
• Molecule 17: Lhca4

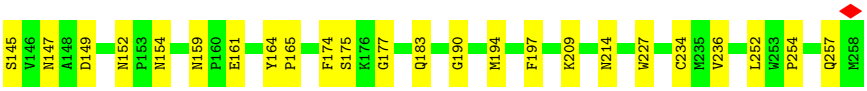
Chain 4:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:

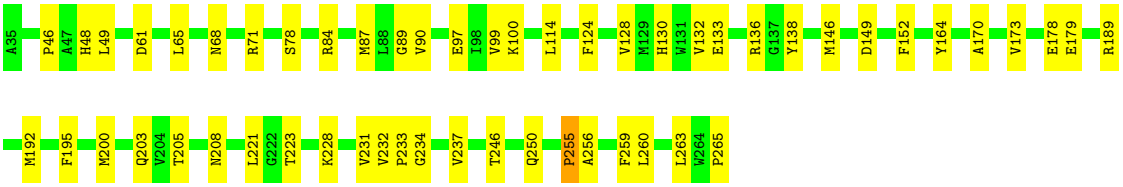




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:





• Molecule 20: Lhca7

Chain 7:

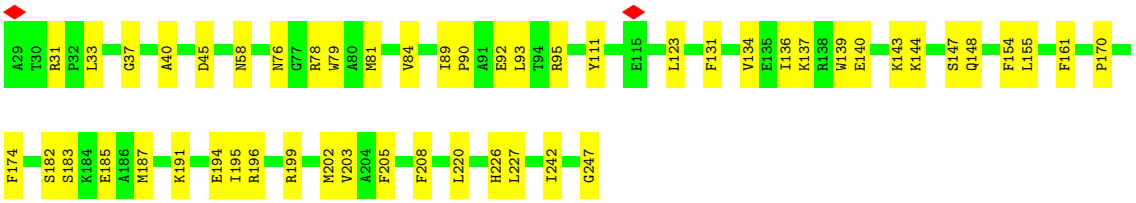




• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

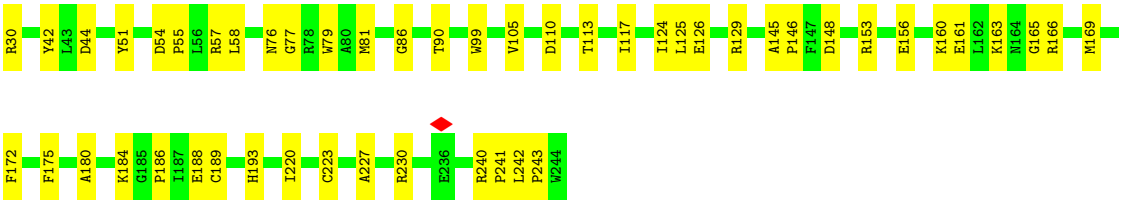




• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

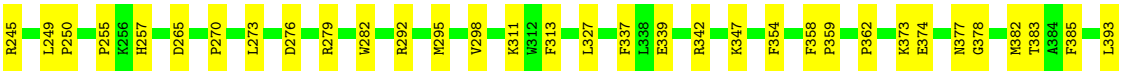




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain 9:






L394
T395
R396
M414
P423
G427

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	185138	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 ($e^-/Å^2$)	49.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size (Å)	394.56, 394.56, 394.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82199997, 0.82199997, 0.82199997	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, PLM, PCW, ECH, 4RF, LUT, SF4, LAP, BCR, 13X, SPH, 3PH, PTY, P5S, CLA, LMT, QTB, SQD, OLA, RRX, XAT, LMG, CL0, PQN, CHL, DGA, LPX, LHG, AXT, NEX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.16	0/6022	0.39	0/8215
2	B	0.16	0/6006	0.39	1/8205 (0.0%)
3	C	0.14	0/611	0.35	0/828
4	D	0.13	0/1150	0.41	0/1551
5	E	0.13	0/520	0.39	0/705
6	F	0.15	0/1309	0.36	0/1771
7	G	0.13	0/743	0.31	0/1007
8	H	0.15	0/744	0.43	0/1000
9	J	0.13	0/322	0.33	0/439
10	K	0.13	0/622	0.32	0/844
11	L	0.16	0/1195	0.40	0/1635
12	M	0.14	0/244	0.32	0/330
13	I	0.15	0/276	0.43	0/373
14	O	0.18	0/703	0.49	0/956
15	1	0.15	0/1443	0.35	0/1960
15	a	0.16	0/1443	0.41	0/1960
16	3	0.16	0/1896	0.38	0/2573
17	4	0.15	0/1681	0.39	0/2285
18	5	0.14	0/1842	0.31	0/2505
19	6	0.15	0/1845	0.37	0/2515
20	7	0.16	0/1748	0.37	0/2372
21	8	0.17	0/1717	0.36	0/2330
22	2	0.14	0/1708	0.35	0/2318
23	9	0.15	0/1444	0.32	0/1957
All	All	0.15	0/37234	0.38	1/50634 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	222	GLY	N-CA-C	5.41	119.41	110.97

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	5824	0	5675	171	0
2	B	5796	0	5576	137	0
3	C	601	0	576	15	0
4	D	1124	0	1129	21	0
5	E	509	0	507	8	0
6	F	1277	0	1296	21	0
7	G	727	0	724	14	0
8	H	729	0	705	26	0
9	J	316	0	332	9	0
10	K	613	0	639	10	0
11	L	1165	0	1181	37	0
12	M	239	0	255	10	0
13	I	270	0	287	12	0
14	O	679	0	661	26	0
15	1	1405	0	1370	43	0
15	a	1405	0	1370	41	0
16	3	1844	0	1805	37	0
17	4	1631	0	1575	35	0
18	5	1786	0	1736	50	0
19	6	1787	0	1760	43	0
20	7	1698	0	1640	28	0
21	8	1669	0	1619	50	0
22	2	1666	0	1657	48	0
23	9	1406	0	1385	34	0
24	A	65	0	72	6	0
25	1	528	0	523	41	0
25	2	615	0	568	40	0
25	3	576	0	555	31	0
25	4	768	0	685	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	5	642	0	564	29	0
25	6	624	0	591	29	0
25	7	566	0	525	30	0
25	8	573	0	480	34	0
25	9	379	0	338	22	0
25	A	2532	0	2566	196	0
25	B	2583	0	2685	168	0
25	F	105	0	88	7	0
25	G	155	0	130	8	0
25	H	156	0	130	7	0
25	J	42	0	30	2	0
25	K	200	0	161	12	0
25	L	205	0	168	11	0
25	O	134	0	95	6	0
25	a	496	0	443	22	0
26	1	284	0	248	26	0
26	2	165	0	137	7	0
26	3	236	0	223	18	0
26	4	174	0	154	15	0
26	5	271	0	217	15	0
26	6	333	0	284	23	0
26	7	296	0	267	21	0
26	8	296	0	265	19	0
26	9	273	0	233	23	0
26	A	66	0	69	8	0
26	a	264	0	205	29	0
27	A	33	0	46	7	0
27	B	33	0	46	5	0
28	A	8	0	0	0	0
28	C	16	0	0	1	0
29	3	120	0	158	11	0
29	4	40	0	53	8	0
29	5	80	0	103	8	0
29	6	80	0	106	8	0
29	7	40	0	52	9	0
29	8	40	0	53	3	0
29	A	200	0	264	23	0
29	B	280	0	371	34	0
29	G	40	0	53	5	0
29	H	40	0	53	4	0
29	I	40	0	52	2	0
29	J	40	0	53	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	80	0	106	7	0
29	L	120	0	159	6	0
29	O	40	0	52	1	0
30	1	84	0	114	5	0
30	2	98	0	148	11	0
30	3	49	0	74	1	0
30	4	81	0	108	4	0
30	5	49	0	74	2	0
30	6	86	0	118	5	0
30	7	108	0	126	3	0
30	8	37	0	44	1	0
30	9	82	0	110	7	0
30	A	144	0	213	8	0
30	B	98	0	148	6	0
30	F	79	0	101	2	0
30	a	35	0	40	2	0
31	A	42	0	54	0	0
32	7	39	0	41	1	0
32	A	54	0	77	8	0
32	G	46	0	55	4	0
32	H	45	0	53	3	0
32	I	54	0	77	4	0
33	3	38	0	49	3	0
33	5	38	0	49	3	0
33	7	33	0	39	0	0
33	9	48	0	72	4	0
33	A	34	0	41	4	0
33	B	42	0	60	2	0
33	G	56	0	62	2	0
33	J	28	0	29	2	0
33	a	76	0	98	4	0
34	A	33	0	39	3	0
35	1	35	0	46	2	0
35	2	35	0	45	5	0
35	A	35	0	45	1	0
35	B	35	0	45	2	0
36	7	50	0	58	3	0
36	8	105	0	126	7	0
36	B	66	0	96	4	0
37	6	36	0	44	3	0
37	B	39	0	50	1	0
37	K	77	0	99	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	30	0	43	2	0
39	F	44	0	54	4	0
40	3	41	0	56	1	0
40	J	41	0	56	3	0
41	4	21	0	37	0	0
41	6	21	0	37	1	0
41	9	21	0	37	2	0
41	J	21	0	37	1	0
42	M	41	0	54	5	0
43	1	84	0	110	6	0
43	2	84	0	110	11	0
43	3	84	0	110	7	0
43	4	84	0	110	10	0
43	5	126	0	165	12	0
43	6	84	0	110	10	0
43	7	42	0	55	5	0
43	8	84	0	110	11	0
43	9	84	0	110	17	0
43	a	126	0	165	13	0
44	1	43	0	52	3	0
44	7	43	0	52	10	0
45	1	20	0	33	2	0
45	8	40	0	66	1	0
45	a	20	0	33	2	0
46	a	19	0	0	0	0
47	4	35	0	62	3	0
47	5	18	0	31	3	0
47	6	18	0	31	1	0
47	8	35	0	62	6	0
47	a	17	0	31	0	0
48	2	37	0	56	6	0
48	3	24	0	30	3	0
48	5	23	0	28	3	0
48	8	40	0	65	5	0
49	6	9	0	6	0	0
50	2	44	0	56	3	0
50	7	44	0	56	3	0
50	9	88	0	112	7	0
51	7	37	0	49	6	0
52	8	37	0	40	2	0
53	8	29	0	42	4	0
54	1	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2	4	0	0	0	0
54	3	5	0	0	0	0
54	4	4	0	0	0	0
54	5	3	0	0	0	0
54	6	7	0	0	0	0
54	7	2	0	0	0	0
54	8	2	0	0	0	0
54	9	2	0	0	0	0
54	A	21	0	0	1	0
54	B	24	0	0	0	0
54	C	2	0	0	0	0
54	D	2	0	0	0	0
54	E	1	0	0	0	0
54	F	3	0	0	0	0
54	G	3	0	0	0	0
54	H	1	0	0	0	0
54	J	1	0	0	0	0
54	K	3	0	0	0	0
54	L	2	0	0	0	0
54	M	1	0	0	0	0
54	a	1	0	0	0	0
All	All	56369	0	56465	1606	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 14.

All (1606) 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)
11:L:295:LYS:N	14:O:133:TYR:HH	1.63	0.94
50:9:504:XAT:H32	50:9:507:XAT:H10	1.50	0.94
1:A:396:TRP:CD1	25:A:1126:CLA:HAB	2.04	0.92
18:5:161:GLU:OE2	18:5:183:GLN:NE2	2.05	0.89
11:L:356:PHE:HB2	11:L:372:VAL:HG13	1.55	0.89
15:a:83:LEU:HB3	26:a:606:CHL:HBB2	1.59	0.85
11:L:357:ILE:HG13	11:L:372:VAL:HG11	1.56	0.85
29:J:4001:BCR:H16C	40:J:4002:RRX:H32	1.58	0.83
25:A:1131:CLA:HBB1	25:A:1132:CLA:H2	1.59	0.83
14:O:66:PRO:HA	14:O:69:ILE:HG22	1.60	0.82
18:5:101:THR:HB	18:5:104:MET:HE2	1.58	0.82
2:B:285:PHE:HE1	25:B:1216:CLA:HAB	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:353:VAL:HG13	11:L:376:ASN:HD22	1.46	0.81
43:4:501:LUT:H30	25:4:601:CLA:H71	1.63	0.80
11:L:451:TYR:H	25:L:1504:CLA:HAB	1.46	0.80
25:A:1110:CLA:H2	16:3:289:LEU:HD23	1.62	0.80
29:H:4001:BCR:H24C	11:L:440:TRP:HE1	1.45	0.80
21:8:33:LEU:HD11	21:8:40:ALA:HB2	1.63	0.80
25:K:1403:CLA:HBA2	37:K:5002:PCW:H321	1.64	0.79
15:a:197:SER:OG	15:a:200:GLU:OE1	2.00	0.79
25:4:608:CLA:H2	26:4:609:CHL:H102	1.66	0.77
1:A:333:PHE:HB2	30:A:5001:LHG:HC41	1.66	0.77
25:5:612:CLA:H111	26:6:619:CHL:H43	1.67	0.76
22:2:184:LYS:HB3	22:2:188:GLU:HB3	1.66	0.76
1:A:489:ASN:HB3	14:O:101:THR:HG21	1.68	0.76
1:A:396:TRP:HD1	25:A:1126:CLA:HAB	1.45	0.76
11:L:349:GLY:O	11:L:376:ASN:ND2	2.18	0.76
29:7:503:BCR:H21C	26:7:613:CHL:H2	1.66	0.76
29:6:503:BCR:H19C	26:6:613:CHL:HBA2	1.67	0.75
19:6:65:LEU:HD23	20:7:160:LEU:HD21	1.68	0.75
26:a:609:CHL:HMA2	17:4:135:LEU:HD13	1.69	0.74
14:O:60:PHE:O	14:O:64:PHE:HB2	1.86	0.74
43:a:503:LUT:H41	26:a:606:CHL:H51	1.70	0.74
26:4:618:CHL:HBD	26:4:618:CHL:HBA1	1.70	0.73
29:L:4001:BCR:H10C	13:I:23:MET:HG2	1.69	0.73
25:A:1109:CLA:H102	25:A:1101:CLA:HBB2	1.71	0.73
25:B:1219:CLA:HBA1	35:B:5006:LMT:H12	1.70	0.73
25:B:1220:CLA:H72	29:B:4004:BCR:H10C	1.69	0.73
11:L:357:ILE:HA	11:L:372:VAL:HG21	1.71	0.73
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.70	0.72
29:A:4001:BCR:H362	29:A:4002:BCR:H21C	1.71	0.72
2:B:111:SER:O	8:H:116:GLN:NE2	2.22	0.72
8:H:68:LEU:HG	25:H:1701:CLA:HAC1	1.70	0.72
43:2:507:LUT:H193	25:2:601:CLA:HBC1	1.71	0.72
25:2:603:CLA:HBA1	25:2:603:CLA:HBD	1.72	0.72
25:6:603:CLA:H93	30:6:801:LHG:H322	1.71	0.72
44:7:504:AXT:H27	21:8:242:ILE:HG21	1.71	0.72
27:A:2001:PQN:H142	29:B:4006:BCR:H271	1.72	0.72
21:8:139:TRP:NE1	36:8:803:DGD:O3D	2.23	0.71
1:A:670:LEU:HB3	25:A:1012:CLA:H71	1.73	0.71
4:D:312:GLY:N	5:E:51:GLU:OE2	2.23	0.71
19:6:87:MET:SD	25:6:601:CLA:HAB	2.31	0.71
11:L:358:LYS:HE2	25:L:1503:CLA:HMA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:223:HIS:O	17:4:225:ILE:N	2.21	0.71
1:A:223:PRO:HD3	1:A:250:MET:HE1	1.71	0.71
2:B:217:LEU:HD11	23:9:423:PRO:HA	1.72	0.71
20:7:119:ILE:HA	51:7:807:4RF:H52	1.73	0.71
43:3:502:LUT:H32	26:3:604:CHL:HBB1	1.73	0.70
25:A:1101:CLA:HHC	25:A:1101:CLA:HBB1	1.73	0.70
1:A:369:HIS:HA	1:A:372:TYR:CE1	2.26	0.70
19:6:200:MET:HG3	25:6:603:CLA:HAC2	1.73	0.70
43:2:502:LUT:H12	25:2:604:CLA:HAB	1.72	0.70
25:B:1220:CLA:HBB2	25:B:1240:CLA:H52	1.74	0.70
25:4:605:CLA:HHC	25:4:605:CLA:HBB1	1.71	0.70
26:4:609:CHL:H11	30:4:801:LHG:H182	1.74	0.70
20:7:121:ASN:ND2	21:8:37:GLY:O	2.25	0.70
25:8:605:CLA:HHC	25:8:605:CLA:HBB1	1.72	0.70
25:4:610:CLA:HBA1	25:4:612:CLA:HBC3	1.73	0.70
26:5:618:CHL:HED1	30:6:801:LHG:H311	1.72	0.70
13:I:25:SER:HB3	32:I:5001:SQD:H81	1.74	0.70
29:5:504:BCR:H373	26:6:619:CHL:H12	1.73	0.70
16:3:457:MET:HG3	16:3:485:ILE:HG13	1.73	0.70
15:a:190:GLN:NE2	15:a:196:ALA:O	2.23	0.69
36:7:806:DGD:HA61	36:7:806:DGD:HB71	1.72	0.69
25:B:1209:CLA:H12	23:9:273:LEU:HD22	1.74	0.69
29:5:504:BCR:H383	26:5:610:CHL:H11	1.74	0.69
35:2:804:LMT:H5B	35:2:804:LMT:H6D	1.73	0.69
1:A:119:TRP:HE1	32:A:5005:SQD:H3	1.58	0.69
1:A:598:TRP:CH2	25:B:1022:CLA:HAB	2.28	0.69
30:4:801:LHG:H291	30:4:801:LHG:H122	1.74	0.69
25:1:602:CLA:HBB1	25:1:602:CLA:HHC	1.74	0.69
25:B:1222:CLA:H52	25:B:1231:CLA:HBB2	1.73	0.69
25:L:1504:CLA:HHC	25:L:1504:CLA:HBB1	1.75	0.69
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.25	0.68
25:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.28	0.68
25:A:1105:CLA:HBC1	32:A:5005:SQD:H361	1.75	0.68
18:5:81:MET:SD	25:5:601:CLA:HAB	2.33	0.68
26:6:609:CHL:H12	30:6:801:LHG:H141	1.75	0.68
7:G:1307:HIS:CD2	29:G:4001:BCR:H352	2.28	0.68
25:8:606:CLA:HBD	52:8:805:P5S:H3	1.74	0.68
18:5:159:ASN:HB3	18:5:165:PRO:HA	1.76	0.68
30:B:5001:LHG:H161	30:B:5001:LHG:H301	1.76	0.68
32:H:5001:SQD:H261	25:2:605:CLA:H43	1.76	0.68
25:B:1202:CLA:HHC	25:B:1202:CLA:HBB1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:503:BCR:H271	25:3:613:CLA:H71	1.76	0.67
13:I:1:MET:O	13:I:4:GLN:NE2	2.27	0.67
15:1:35:ASN:C	15:1:37:LEU:H	2.02	0.67
2:B:722:TYR:HB2	25:B:1021:CLA:HED3	1.75	0.67
2:B:388:PHE:HZ	25:B:1222:CLA:HAB	1.59	0.67
1:A:707:LEU:HD13	39:F:4001:NEX:H383	1.77	0.67
38:F:5003:LPX:H4	25:F:1301:CLA:HBA2	1.75	0.67
43:9:502:LUT:H32	25:9:604:CLA:HAB	1.77	0.67
25:B:1209:CLA:HHC	25:B:1209:CLA:HBB1	1.77	0.67
25:F:1302:CLA:HBD	51:7:807:4RF:H5	1.76	0.67
43:8:502:LUT:H32	26:8:604:CHL:HBB1	1.77	0.67
25:7:610:CLA:H13	30:7:803:LHG:H302	1.77	0.66
1:A:483:PHE:HB3	25:A:1135:CLA:H2	1.75	0.66
25:A:1138:CLA:HAB	25:A:1138:CLA:H111	1.77	0.66
15:1:82:MET:SD	25:1:601:CLA:HAB	2.35	0.66
25:B:1023:CLA:H13	29:B:4007:BCR:H16C	1.77	0.66
25:5:602:CLA:HHC	25:5:602:CLA:HBB1	1.76	0.66
16:3:318:MET:SD	25:3:601:CLA:HAB	2.35	0.66
17:4:93:LEU:HG	17:4:98:LEU:HB2	1.76	0.66
19:6:136:ARG:NH2	25:6:612:CLA:O1D	2.29	0.66
50:9:507:XAT:H32	25:9:606:CLA:HBA2	1.78	0.66
25:B:1204:CLA:HED2	13:I:7:PRO:HB3	1.77	0.66
18:5:49:ALA:O	18:5:70:ARG:NH2	2.28	0.65
43:3:502:LUT:H32	26:3:604:CHL:CBB	2.26	0.65
2:B:398:ASP:OD2	4:D:321:LYS:NZ	2.28	0.65
21:8:31:ARG:NH2	21:8:45:ASP:O	2.29	0.65
20:7:49:HIS:CE1	51:7:807:4RF:H51	2.31	0.65
26:9:610:CHL:OBD	33:9:803:PTY:N1	2.29	0.65
2:B:276:HIS:HB3	25:B:1214:CLA:HMB2	1.79	0.65
16:3:350:VAL:HG13	16:3:351:ILE:HG13	1.78	0.65
22:2:220:ILE:HG22	25:9:612:CLA:HBB1	1.79	0.65
1:A:596:LEU:HD21	25:A:1128:CLA:HBC1	1.77	0.65
2:B:41:GLU:HG2	2:B:166:LEU:HB2	1.79	0.64
22:2:58:LEU:HD21	22:2:242:LEU:HD23	1.80	0.64
25:A:1012:CLA:H41	25:A:1012:CLA:H8	1.80	0.64
25:A:1110:CLA:HHC	25:A:1110:CLA:HBB1	1.78	0.64
21:8:139:TRP:CE3	53:8:810:LAP:H193	2.33	0.64
26:4:609:CHL:O1A	19:6:130:HIS:ND1	2.31	0.64
2:B:443:VAL:HG21	25:B:1230:CLA:HAC2	1.78	0.64
29:3:504:BCR:H10C	26:3:611:CHL:HBA1	1.79	0.64
23:9:373:LYS:HG3	25:9:607:CLA:HED2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:9:393:LEU:O	23:9:396:ARG:NH1	2.31	0.64
25:B:1228:CLA:HBA1	6:F:471:MET:HE2	1.78	0.64
4:D:198:THR:HG23	4:D:246:PRO:HB2	1.80	0.64
18:5:234:CYS:SG	33:5:802:PTY:N1	2.68	0.64
43:7:501:LUT:H28	43:7:501:LUT:H361	1.80	0.63
17:4:77:GLY:HA3	17:4:187:ALA:HB1	1.80	0.63
20:7:111:VAL:HG21	29:7:503:BCR:H362	1.80	0.63
25:B:1219:CLA:HBB2	29:B:4004:BCR:H343	1.80	0.63
25:9:612:CLA:H171	25:9:612:CLA:H91	1.79	0.63
1:A:370:HIS:ND1	25:A:1116:CLA:OBD	2.31	0.63
2:B:285:PHE:CE1	25:B:1216:CLA:HAB	2.30	0.63
25:B:1212:CLA:H112	29:B:4001:BCR:H21C	1.80	0.63
15:a:82:MET:SD	25:a:601:CLA:HAB	2.38	0.63
26:6:619:CHL:HMC	37:6:803:PCW:H322	1.80	0.63
43:8:502:LUT:H32	26:8:604:CHL:CBB	2.29	0.63
35:2:804:LMT:H3'	25:2:615:CLA:HED1	1.80	0.63
30:A:5003:LHG:H201	16:3:448:CYS:HB3	1.80	0.63
25:B:1217:CLA:HHC	25:B:1217:CLA:HBB1	1.80	0.63
29:7:503:BCR:H372	26:7:613:CHL:H102	1.80	0.63
18:5:254:PRO:HA	33:5:802:PTY:HC31	1.79	0.63
43:8:501:LUT:H32	26:8:601:CHL:HBB1	1.80	0.63
25:A:1115:CLA:H51	10:K:109:LEU:HD13	1.81	0.62
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.81	0.62
23:9:394:LEU:HD12	26:9:603:CHL:HMD3	1.80	0.62
1:A:297:HIS:HB2	25:A:1116:CLA:C1B	2.29	0.62
22:2:125:LEU:HD13	43:2:507:LUT:H163	1.80	0.62
22:2:77:GLY:O	22:2:81:MET:HG3	1.99	0.62
1:A:392:THR:HB	25:A:1126:CLA:HMB2	1.82	0.62
30:B:5001:LHG:H351	47:8:807:PLM:HA1	1.81	0.62
14:O:131:GLN:HG2	25:O:1802:CLA:HBD	1.82	0.62
2:B:27:ALA:HA	25:B:1226:CLA:H43	1.80	0.62
17:4:130:PHE:HB3	25:4:612:CLA:HAB	1.82	0.62
22:2:42:TYR:OH	22:2:54:ASP:OD2	2.18	0.62
18:5:97:GLN:HG2	25:5:606:CLA:HED3	1.81	0.62
2:B:214:LEU:O	23:9:396:ARG:NH2	2.32	0.62
43:1:501:LUT:H30	25:1:601:CLA:H52	1.80	0.62
43:2:507:LUT:H182	25:2:601:CLA:HAC2	1.80	0.62
26:A:1114:CHL:HBA1	33:A:5006:PTY:H112	1.81	0.62
26:7:609:CHL:H91	25:7:603:CLA:HBC3	1.80	0.62
26:7:617:CHL:H191	36:8:802:DGD:HB71	1.82	0.62
21:8:187:MET:HG3	21:8:191:LYS:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:156:GLU:OE2	22:2:160:LYS:NZ	2.30	0.62
1:A:436:ALA:O	1:A:440:HIS:ND1	2.27	0.62
1:A:17:VAL:HG11	1:A:184:ALA:HB1	1.82	0.62
26:5:610:CHL:HHC	26:5:610:CHL:HBB1	1.82	0.62
43:1:501:LUT:H162	25:1:608:CLA:HBC1	1.82	0.61
18:5:129:MET:HG3	25:5:612:CLA:HMC3	1.82	0.61
1:A:677:PHE:CG	29:A:4005:BCR:H363	2.36	0.61
26:a:606:CHL:HHC	26:a:606:CHL:HBB1	1.83	0.61
26:2:609:CHL:HHC	26:2:609:CHL:HBB1	1.81	0.61
2:B:378:TYR:CD2	25:B:1224:CLA:HAB	2.36	0.61
19:6:46:PRO:HG2	19:6:49:LEU:HB2	1.83	0.61
11:L:302:VAL:HA	11:L:312:GLU:HG3	1.81	0.61
25:7:604:CLA:H172	25:7:605:CLA:HBB1	1.83	0.61
1:A:666:SER:HB2	2:B:446:ALA:HB1	1.83	0.61
16:3:478:LEU:HB2	26:3:603:CHL:H11	1.82	0.61
17:4:150:ASP:OD1	17:4:154:ASN:N	2.33	0.61
23:9:282:TRP:HZ2	25:9:612:CLA:HAA1	1.65	0.61
1:A:296:HIS:HB3	25:A:1116:CLA:HMB2	1.82	0.61
44:7:504:AXT:H383	21:8:247:GLY:HA3	1.82	0.61
2:B:67:PHE:HZ	12:M:8:VAL:HG13	1.65	0.61
7:G:1228:LEU:HD23	7:G:1317:SER:HB2	1.83	0.61
22:2:57:ARG:HH22	30:2:802:LHG:HC32	1.66	0.61
1:A:389:SER:HB3	25:A:1126:CLA:HMA1	1.81	0.60
4:D:287:HIS:HB3	4:D:288:PRO:HD3	1.82	0.60
13:I:28:LEU:HD12	32:I:5001:SQD:H242	1.82	0.60
26:8:603:CHL:HBC1	47:8:806:PLM:H81	1.83	0.60
25:B:1204:CLA:H12	13:I:14:VAL:HG21	1.82	0.60
15:1:35:ASN:O	15:1:37:LEU:N	2.32	0.60
25:A:1106:CLA:H71	25:A:1128:CLA:H171	1.83	0.60
43:8:502:LUT:H30	26:8:604:CHL:H72	1.83	0.60
5:E:54:TRP:NE1	5:E:79:LYS:O	2.27	0.60
47:4:804:PLM:HD2	25:8:602:CLA:H42	1.83	0.60
6:F:479:VAL:HG21	6:F:482:ARG:HH22	1.66	0.60
22:2:81:MET:SD	25:2:601:CLA:HAB	2.42	0.60
15:a:155:ALA:H	33:a:802:PTY:HN12	1.48	0.60
26:3:608:CHL:HHC	26:3:608:CHL:HBB1	1.81	0.60
26:5:617:CHL:HHC	26:5:617:CHL:HBB1	1.82	0.60
19:6:192:MET:SD	25:6:604:CLA:HBB1	2.42	0.60
25:A:1108:CLA:H12	25:A:1110:CLA:H43	1.83	0.60
25:B:1220:CLA:HAB	25:B:1227:CLA:HMD1	1.82	0.60
25:8:605:CLA:H62	36:8:803:DGD:HA51	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:604:CLA:HBC1	30:2:801:LHG:H111	1.83	0.60
1:A:72:LYS:HZ1	25:A:1109:CLA:HED2	1.66	0.60
17:4:45:ARG:O	17:4:51:ASN:ND2	2.33	0.60
1:A:486:TRP:CD1	14:O:101:THR:HG1	2.20	0.60
1:A:501:ASN:HB2	25:A:1134:CLA:HED3	1.84	0.60
1:A:598:TRP:HH2	25:B:1022:CLA:HAB	1.66	0.60
25:A:1113:CLA:H112	29:A:4002:BCR:H282	1.84	0.60
7:G:1248:PHE:HB3	43:1:503:LUT:H221	1.83	0.60
16:3:373:ILE:HG23	26:7:609:CHL:H11	1.83	0.60
26:4:609:CHL:HHC	26:4:609:CHL:HBB1	1.84	0.60
23:9:276:ASP:HB3	23:9:279:ARG:HB2	1.84	0.60
1:A:689:GLY:HA3	2:B:570:ASP:HB2	1.83	0.59
26:9:603:CHL:H142	30:9:801:LHG:H281	1.83	0.59
2:B:107:ARG:NH2	2:B:114:VAL:O	2.35	0.59
25:A:1131:CLA:H51	29:B:4007:BCR:H372	1.84	0.59
2:B:87:PRO:HB2	2:B:117:SER:HB3	1.83	0.59
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.82	0.59
2:B:692:VAL:HG11	25:B:1237:CLA:HAB	1.84	0.59
15:1:125:THR:O	15:1:129:ILE:HG13	2.02	0.59
21:8:143:LYS:HE3	36:8:803:DGD:HD3	1.83	0.59
25:A:1118:CLA:HBA1	10:K:91:VAL:HG23	1.84	0.59
8:H:83:ARG:HG3	11:L:388:LEU:HD21	1.83	0.59
26:a:613:CHL:HHC	26:a:613:CHL:HBB1	1.85	0.59
2:B:176:LEU:HD12	2:B:302:MET:HE1	1.85	0.59
26:3:604:CHL:H2	26:3:604:CHL:O1A	2.01	0.59
30:4:801:LHG:HC91	30:4:801:LHG:H271	1.85	0.59
43:9:501:LUT:H32	26:9:601:CHL:HAB	1.85	0.59
14:O:69:ILE:HD11	14:O:79:LEU:HD13	1.85	0.59
26:7:615:CHL:HHC	26:7:615:CHL:HBB1	1.84	0.59
1:A:305:PHE:HE1	25:A:1119:CLA:HAB	1.66	0.59
8:H:106:ALA:HA	8:H:113:VAL:HG21	1.82	0.59
25:4:606:CLA:HMA2	26:4:613:CHL:C3C	2.33	0.59
18:5:62:ASN:HB3	18:5:65:MET:HB2	1.85	0.59
18:5:147:ASN:ND2	18:5:159:ASN:OD1	2.32	0.59
26:6:617:CHL:HHC	26:6:617:CHL:HBB1	1.85	0.59
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.85	0.59
25:A:1102:CLA:HMB1	25:A:1102:CLA:HBB1	1.85	0.59
22:2:30:ARG:NH1	22:2:44:ASP:O	2.35	0.59
22:2:79:TRP:CZ2	43:2:507:LUT:H7	2.38	0.59
2:B:659:ALA:C	25:B:1023:CLA:HAB	2.28	0.59
43:9:502:LUT:H32	25:9:604:CLA:CAB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1023:CLA:HMA3	25:B:1023:CLA:H2	1.85	0.58
15:a:35:ASN:O	15:a:37:LEU:N	2.36	0.58
25:B:1236:CLA:HED2	25:B:1236:CLA:H2A	1.84	0.58
8:H:43:ASP:H	8:H:50:THR:HG21	1.68	0.58
26:1:611:CHL:HHC	26:1:611:CHL:HBB1	1.86	0.58
29:3:503:BCR:H383	25:3:606:CLA:HAB	1.85	0.58
26:2:610:CHL:HHC	26:2:610:CHL:HBB1	1.86	0.58
26:9:610:CHL:HMD2	33:9:803:PTY:HC52	1.85	0.58
19:6:133:GLU:OE1	19:6:136:ARG:NH1	2.35	0.58
26:9:613:CHL:HHC	26:9:613:CHL:HBB1	1.84	0.58
1:A:114:SER:HB2	1:A:131:VAL:HG11	1.85	0.58
1:A:349:TRP:HB3	25:A:1103:CLA:HAC1	1.85	0.58
10:K:38:ASN:HD21	25:K:1401:CLA:HED2	1.68	0.58
25:K:1401:CLA:HBB1	29:K:4002:BCR:H10C	1.85	0.58
15:1:178:ARG:HB3	26:1:604:CHL:HBC3	1.85	0.58
26:6:611:CHL:HHC	26:6:611:CHL:HBB1	1.86	0.58
25:A:1117:CLA:HMB1	25:A:1117:CLA:HBB1	1.85	0.58
25:B:1224:CLA:H161	36:B:5003:DGD:HAG2	1.86	0.58
16:3:292:CYS:SG	26:3:604:CHL:HAA2	2.43	0.58
4:D:229:GLU:HA	4:D:242:MET:O	2.04	0.58
19:6:90:VAL:HG11	43:6:501:LUT:H12	1.84	0.58
2:B:6:PHE:O	2:B:8:LYS:N	2.36	0.58
2:B:620:TRP:HB3	25:B:1021:CLA:H101	1.86	0.58
7:G:1307:HIS:NE2	29:G:4001:BCR:H352	2.19	0.58
15:1:39:GLY:HA3	21:8:147:SER:HB3	1.85	0.58
26:7:617:CHL:HBB1	26:7:617:CHL:HHC	1.86	0.58
36:8:802:DGD:HBT1	25:8:607:CLA:C1C	2.34	0.58
26:9:608:CHL:HHC	26:9:608:CHL:HBB1	1.85	0.58
26:9:610:CHL:HHC	26:9:610:CHL:HBB1	1.86	0.58
25:A:1106:CLA:H101	29:J:4001:BCR:H10C	1.86	0.58
2:B:151:LEU:HD22	12:M:22:ALA:HA	1.85	0.58
25:B:1237:CLA:H72	25:B:1238:CLA:H43	1.86	0.58
19:6:78:SER:HB2	25:6:612:CLA:HED2	1.85	0.58
26:8:610:CHL:HHC	26:8:610:CHL:HBB1	1.86	0.58
2:B:412:ILE:HA	2:B:415:HIS:CE1	2.38	0.58
1:A:121:ILE:HG23	1:A:122:VAL:HG22	1.84	0.57
22:2:193:HIS:CG	25:2:603:CLA:HAA1	2.39	0.57
11:L:318:SER:HB3	11:L:321:ILE:HB	1.85	0.57
18:5:132:VAL:HG11	29:5:503:BCR:H16C	1.85	0.57
22:2:126:GLU:HG3	25:2:612:CLA:C1B	2.34	0.57
2:B:60:LEU:HD12	42:M:4001:ECH:H37A	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1223:CLA:H122	29:B:4004:BCR:H373	1.86	0.57
1:A:95:GLY:O	1:A:99:SER:OG	2.22	0.57
25:A:1130:CLA:HBA1	2:B:687:PRO:HD3	1.86	0.57
43:1:503:LUT:H10	26:1:613:CHL:HBA1	1.85	0.57
2:B:549:PRO:HB3	6:F:481:PRO:HG2	1.87	0.57
15:1:92:GLU:OE2	15:1:197:SER:OG	2.19	0.57
17:4:230:SER:HB2	17:4:231:PRO:HD3	1.85	0.57
26:2:609:CHL:HBC3	30:2:801:LHG:HC5	1.85	0.57
30:2:802:LHG:H291	30:2:802:LHG:H192	1.87	0.57
1:A:305:PHE:CE1	25:A:1119:CLA:HAB	2.39	0.57
23:9:245:ARG:NH1	23:9:265:ASP:OD1	2.37	0.57
1:A:679:TRP:CE3	24:A:1011:CL0:H6	2.38	0.57
15:a:83:LEU:HB3	26:a:606:CHL:CBB	2.32	0.57
19:6:170:ALA:HB2	25:6:601:CLA:HBD	1.86	0.57
1:A:343:GLU:O	1:A:347:THR:OG1	2.20	0.57
1:A:435:ASP:OD2	1:A:561:ARG:NH1	2.36	0.57
25:B:1224:CLA:HBC3	36:B:5003:DGD:HBG3	1.86	0.57
23:9:249:LEU:HD12	23:9:250:PRO:HD2	1.85	0.57
1:A:695:GLU:OE2	2:B:551:LYS:NZ	2.33	0.57
25:H:1701:CLA:CBB	29:L:4003:BCR:H10C	2.34	0.57
15:a:52:SER:HB2	26:a:604:CHL:HED2	1.85	0.57
15:a:169:LEU:HB3	25:a:601:CLA:HMA2	1.86	0.57
23:9:378:GLY:O	23:9:382:MET:HG3	2.04	0.57
25:A:1129:CLA:HMA1	11:L:313:THR:HG21	1.87	0.57
2:B:429:PHE:CE1	25:B:1235:CLA:HAB	2.40	0.57
17:4:215:HIS:CG	25:4:603:CLA:HAA2	2.39	0.57
29:5:503:BCR:H272	47:5:804:PLM:HE1	1.87	0.57
26:8:613:CHL:HHC	26:8:613:CHL:HBB1	1.86	0.57
25:A:1106:CLA:HHC	25:A:1106:CLA:HBB1	1.87	0.56
43:7:501:LUT:H30	25:7:601:CLA:H72	1.86	0.56
25:A:1140:CLA:HHC	25:A:1140:CLA:HBB1	1.87	0.56
34:A:5007:3PH:H372	34:A:5007:3PH:H2A2	1.86	0.56
54:A:6020:HOH:O	2:B:622:ARG:NH1	2.38	0.56
2:B:304:GLU:HG3	7:G:1261:ALA:HA	1.87	0.56
25:B:1219:CLA:HBB1	25:B:1219:CLA:HMB1	1.87	0.56
25:L:1503:CLA:HBB1	25:L:1503:CLA:HMB1	1.86	0.56
15:1:51:ALA:HB2	15:1:171:THR:HA	1.86	0.56
21:8:205:PHE:CD2	43:8:502:LUT:H12	2.40	0.56
1:A:169:MET:HE1	25:A:1111:CLA:H92	1.86	0.56
25:A:1113:CLA:HBA2	16:3:485:ILE:HD13	1.87	0.56
25:A:1113:CLA:HMA2	26:A:1114:CHL:H18	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:193:ALA:HB2	25:a:615:CLA:HED3	1.86	0.56
16:3:416:GLN:NE2	18:5:55:ASP:O	2.36	0.56
19:6:132:VAL:HG11	29:6:503:BCR:H16C	1.86	0.56
25:7:606:CLA:HMA2	26:7:613:CHL:HBC3	1.87	0.56
26:9:610:CHL:HHB	41:9:804:SPH:H152	1.86	0.56
2:B:352:HIS:ND1	25:B:1214:CLA:OBD	2.37	0.56
22:2:165:GLY:O	22:2:169:MET:HG3	2.05	0.56
2:B:524:ILE:HG21	25:B:1234:CLA:HAB	1.87	0.56
25:1:612:CLA:H203	30:1:802:LHG:H321	1.88	0.56
25:a:603:CLA:HBC2	25:a:615:CLA:HMD3	1.87	0.56
16:3:446:ILE:HG22	26:3:603:CHL:HBB1	1.87	0.56
18:5:56:PRO:HD2	43:5:502:LUT:H23	1.87	0.56
44:7:504:AXT:H393	30:7:803:LHG:H131	1.86	0.56
1:A:375:PRO:HG3	1:A:381:ALA:HB2	1.88	0.56
48:2:803:DGA:HAF2	48:2:803:DGA:HBW1	1.87	0.56
1:A:746:ARG:O	1:A:750:VAL:HG22	2.06	0.56
12:M:3:ILE:O	13:I:2:SER:OG	2.19	0.56
25:B:1236:CLA:H43	29:B:4005:BCR:H10C	1.87	0.56
18:5:236:VAL:O	18:5:257:GLN:NE2	2.39	0.56
25:2:604:CLA:HMB3	25:2:604:CLA:HBB1	1.88	0.56
1:A:680:ALA:HB3	25:A:1013:CLA:HBB2	1.88	0.56
10:K:58:PRO:HG2	29:K:4001:BCR:H291	1.87	0.56
25:5:603:CLA:HBC3	30:5:801:LHG:H372	1.88	0.56
26:2:613:CHL:HHC	26:2:613:CHL:HBB1	1.88	0.56
1:A:356:ASN:ND2	25:A:1103:CLA:OBD	2.26	0.56
25:A:1012:CLA:HAB	2:B:583:TRP:HH2	1.70	0.56
15:1:193:ALA:HB2	25:1:615:CLA:HED3	1.88	0.56
15:a:37:LEU:HB3	15:a:40:SER:HB3	1.88	0.56
33:a:803:PTY:H111	45:a:805:OLA:H81	1.88	0.56
20:7:59:MET:SD	25:7:601:CLA:HAB	2.46	0.56
1:A:413:MET:HE1	1:A:427:LEU:HD11	1.87	0.55
25:A:1113:CLA:H42	29:3:505:BCR:H10C	1.86	0.55
29:A:4005:BCR:H24C	25:B:1230:CLA:HMC2	1.87	0.55
11:L:405:LYS:HG2	11:L:411:SER:HA	1.89	0.55
43:a:502:LUT:H32	26:a:604:CHL:HBB1	1.88	0.55
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.87	0.55
26:A:1114:CHL:HHC	26:A:1114:CHL:HBB1	1.87	0.55
1:A:325:ILE:O	1:A:329:HIS:ND1	2.38	0.55
1:A:474:ASP:OD1	1:A:480:GLN:NE2	2.39	0.55
25:A:1127:CLA:H2	29:A:4002:BCR:HC7	1.88	0.55
20:7:105:ILE:HG23	25:7:612:CLA:HBB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:199:ARG:HA	21:8:202:MET:HE3	1.88	0.55
43:8:501:LUT:H34	26:8:601:CHL:CBB	2.36	0.55
33:a:803:PTY:H162	45:a:805:OLA:H141	1.87	0.55
2:B:390:HIS:HA	2:B:393:ILE:HD12	1.88	0.55
15:1:197:SER:OG	15:1:200:GLU:HG3	2.06	0.55
15:1:99:TRP:HB2	44:1:502:AXT:H3	1.87	0.55
23:9:354:PHE:HD1	50:9:504:XAT:H242	1.72	0.55
1:A:484:ALA:HA	25:A:1135:CLA:HBA1	1.89	0.55
1:A:533:PHE:HA	25:A:1136:CLA:HED1	1.89	0.55
12:M:12:LEU:HB3	25:2:615:CLA:HBB2	1.88	0.55
26:4:618:CHL:HHC	26:4:618:CHL:HBB1	1.89	0.55
11:L:363:ARG:HA	11:L:368:VAL:HG21	1.88	0.55
29:4:503:BCR:H24C	26:4:613:CHL:HAA1	1.89	0.55
18:5:138:GLN:OE1	18:5:141:ARG:NH1	2.38	0.55
22:2:81:MET:HB3	50:2:501:XAT:C35	2.37	0.55
18:5:45:ASP:OD1	18:5:46:GLY:N	2.40	0.55
1:A:584:CYS:N	2:B:669:ARG:O	2.40	0.54
8:H:88:GLY:HA3	32:H:5001:SQD:H262	1.88	0.54
1:A:322:LEU:HD13	25:A:1123:CLA:HAC2	1.90	0.54
2:B:388:PHE:CZ	25:B:1222:CLA:HAB	2.42	0.54
15:a:90:GLY:HA3	26:a:606:CHL:HBC3	1.88	0.54
43:a:502:LUT:H382	26:a:604:CHL:H11	1.88	0.54
16:3:380:LEU:HD13	26:7:609:CHL:HMA2	1.89	0.54
43:4:502:LUT:H30	25:4:604:CLA:H72	1.88	0.54
25:2:605:CLA:HBC1	26:2:610:CHL:HAB	1.88	0.54
1:A:265:PHE:HA	25:K:1401:CLA:HBC3	1.88	0.54
30:B:5001:LHG:H242	15:1:60:LEU:HD21	1.89	0.54
25:1:607:CLA:HAB	25:a:612:CLA:H11	1.89	0.54
26:1:609:CHL:HHC	26:1:609:CHL:HBB1	1.89	0.54
26:3:604:CHL:H162	25:3:605:CLA:HBB1	1.89	0.54
43:4:502:LUT:H372	26:7:617:CHL:H152	1.90	0.54
29:7:503:BCR:C21	26:7:613:CHL:H2	2.35	0.54
25:2:604:CLA:CGA	25:2:604:CLA:H3A	2.38	0.54
26:5:613:CHL:HMB3	26:5:613:CHL:HBB1	1.89	0.54
26:7:611:CHL:HHC	26:7:611:CHL:HBB1	1.88	0.54
2:B:126:TYR:O	2:B:131:ARG:NH1	2.38	0.54
8:H:90:VAL:HG11	11:L:385:THR:HB	1.89	0.54
26:1:611:CHL:HBA1	45:1:803:OLA:H162	1.90	0.54
16:3:291:LEU:HD13	26:3:604:CHL:H42	1.89	0.54
16:3:390:GLY:O	16:3:394:LYS:NZ	2.32	0.54
18:5:197:PHE:CE1	43:5:502:LUT:H10	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1206:CLA:HMB1	25:B:1206:CLA:HBB1	1.88	0.54
25:B:1240:CLA:H2A	25:B:1240:CLA:HED2	1.90	0.54
26:3:603:CHL:H41	26:3:603:CHL:H72	1.89	0.54
21:8:203:VAL:HG12	26:8:603:CHL:HBB1	1.89	0.54
1:A:75:SER:OG	1:A:181:TYR:HB2	2.08	0.54
17:4:203:ALA:HB2	25:4:615:CLA:HED3	1.90	0.54
19:6:223:THR:O	19:6:228:LYS:NZ	2.34	0.54
25:8:606:CLA:HMA2	26:8:613:CHL:HBC3	1.89	0.54
43:2:502:LUT:H12	25:2:604:CLA:CAB	2.38	0.54
25:A:1138:CLA:HAA2	25:B:1228:CLA:HMB1	1.89	0.54
25:1:605:CLA:H202	25:1:605:CLA:H141	1.89	0.54
26:7:609:CHL:HHC	26:7:609:CHL:HBB1	1.89	0.54
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.90	0.54
25:B:1211:CLA:HMA3	29:B:4003:BCR:H292	1.90	0.54
8:H:86:ILE:HG23	11:L:388:LEU:HD22	1.90	0.54
25:A:1119:CLA:H41	29:A:4004:BCR:H16C	1.90	0.53
25:A:1138:CLA:H2	25:B:1229:CLA:H42	1.89	0.53
29:4:503:BCR:H271	25:4:606:CLA:NB	2.22	0.53
21:8:144:LYS:HB3	21:8:147:SER:OG	2.08	0.53
25:A:1106:CLA:HBB2	25:A:1126:CLA:H202	1.89	0.53
18:5:190:GLY:O	18:5:194:MET:HG3	2.08	0.53
19:6:233:PRO:HA	47:6:804:PLM:H71	1.90	0.53
43:8:501:LUT:H32	26:8:601:CHL:CBB	2.39	0.53
21:8:226:HIS:CG	26:8:603:CHL:HAA2	2.43	0.53
22:2:105:VAL:HG13	43:2:507:LUT:H383	1.90	0.53
1:A:250:MET:HG3	1:A:257:PHE:HD2	1.74	0.53
25:B:1229:CLA:CAB	25:B:1230:CLA:HMB2	2.38	0.53
43:a:502:LUT:H32	26:a:604:CHL:CBB	2.38	0.53
43:5:505:LUT:H371	43:5:505:LUT:H28	1.90	0.53
2:B:340:ALA:HB2	29:B:4005:BCR:H372	1.91	0.53
4:D:231:ILE:HG12	4:D:241:ILE:HG12	1.89	0.53
16:3:314:CYS:HB3	16:3:441:GLY:HA3	1.91	0.53
1:A:598:TRP:HE1	25:B:1023:CLA:C1D	2.21	0.53
25:A:1130:CLA:H72	25:L:1502:CLA:H12	1.89	0.53
2:B:341:SER:O	2:B:345:ILE:HG12	2.08	0.53
25:G:1601:CLA:C1B	29:G:4001:BCR:H353	2.39	0.53
16:3:381:LYS:HD3	26:3:611:CHL:CBB	2.39	0.53
25:B:1212:CLA:C1B	29:B:4001:BCR:H271	2.39	0.53
25:B:1218:CLA:HMD1	29:B:4001:BCR:HC7	1.91	0.53
30:B:5001:LHG:H342	47:8:807:PLM:HF1	1.90	0.53
25:1:608:CLA:H11	26:1:609:CHL:H42	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:610:CHL:HHC	26:a:610:CHL:HBB1	1.90	0.53
17:4:56:PRO:HB2	26:7:617:CHL:H42	1.91	0.53
26:4:613:CHL:HBB1	26:4:613:CHL:HHC	1.90	0.53
18:5:130:HIS:ND1	26:6:609:CHL:O1A	2.42	0.53
18:5:137:TRP:CE2	18:5:141:ARG:HD2	2.43	0.53
22:2:51:TYR:HB2	25:2:604:CLA:HMD1	1.89	0.53
22:2:180:ALA:HB2	35:2:804:LMT:H32	1.90	0.53
2:B:286:ILE:HG23	2:B:290:HIS:HE1	1.74	0.53
15:1:210:MET:HE2	25:1:608:CLA:HMA1	1.90	0.53
19:6:164:TYR:HB3	25:6:601:CLA:HED3	1.90	0.53
1:A:435:ASP:OD1	1:A:556:TYR:OH	2.25	0.53
24:A:1011:CL0:H11	24:A:1011:CL0:H15	1.91	0.53
3:C:27:GLU:OE2	3:C:43:PRO:HG3	2.08	0.53
4:D:263:GLN:O	4:D:267:LYS:HB2	2.09	0.53
6:F:453:GLU:OE2	21:8:58:ASN:ND2	2.41	0.53
15:a:34:GLY:HA3	15:a:53:TYR:CD2	2.44	0.53
15:1:57:PRO:HG3	47:8:807:PLM:H81	1.91	0.52
15:a:36:TRP:HE1	26:a:609:CHL:C2B	2.22	0.52
22:2:58:LEU:HD12	25:2:604:CLA:H12	1.91	0.52
1:A:430:VAL:HA	1:A:433:HIS:CE1	2.44	0.52
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.91	0.52
2:B:460:PHE:HB3	25:B:1234:CLA:H11	1.91	0.52
8:H:100:TRP:O	8:H:105:ALA:N	2.31	0.52
19:6:195:PHE:CD2	43:6:502:LUT:H12	2.44	0.52
19:6:265:PRO:HD2	25:6:615:CLA:HED2	1.90	0.52
20:7:101:LEU:HD21	25:7:610:CLA:H141	1.90	0.52
26:7:613:CHL:HHC	26:7:613:CHL:HBB1	1.90	0.52
1:A:610:PHE:O	1:A:614:MET:HG2	2.09	0.52
1:A:679:TRP:HZ3	25:A:1012:CLA:HMD3	1.74	0.52
2:B:659:ALA:HB3	25:B:1023:CLA:HBB2	1.92	0.52
7:G:1288:THR:HG21	7:G:1295:THR:HA	1.91	0.52
11:L:447:ILE:HG22	11:L:448:LEU:H	1.75	0.52
42:M:4001:ECH:H8	25:2:615:CLA:CBB	2.38	0.52
29:3:504:BCR:HC7	26:3:611:CHL:HMB2	1.90	0.52
25:3:606:CLA:HMA2	25:3:613:CLA:C3C	2.40	0.52
29:5:503:BCR:H282	47:5:804:PLM:HC1	1.91	0.52
2:B:374:THR:HB	25:B:1224:CLA:HMB1	1.92	0.52
32:G:5001:SQD:H242	32:G:5001:SQD:H81	1.90	0.52
15:1:214:PHE:CE1	25:1:608:CLA:HED2	2.45	0.52
17:4:132:TRP:CD1	29:4:503:BCR:H14C	2.45	0.52
18:5:84:VAL:HG11	43:5:501:LUT:H12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:802:LHG:H222	30:2:802:LHG:H302	1.92	0.52
25:A:1109:CLA:CHA	25:A:1109:CLA:HBA1	2.39	0.52
26:A:1114:CHL:HBC2	25:3:610:CLA:HAB	1.91	0.52
25:A:1139:CLA:C4C	27:A:2001:PQN:H262	2.40	0.52
25:B:1229:CLA:HBB1	29:B:4006:BCR:H323	1.90	0.52
29:L:4001:BCR:H14C	13:I:27:PHE:HB2	1.90	0.52
17:4:194:PHE:CE1	43:4:502:LUT:H10	2.44	0.52
18:5:161:GLU:HG3	18:5:164:TYR:HD2	1.74	0.52
25:A:1137:CLA:HHC	25:A:1137:CLA:HBB1	1.91	0.52
4:D:277:VAL:HG22	4:D:283:VAL:HG22	1.90	0.52
25:G:1603:CLA:HHC	25:G:1603:CLA:HBB1	1.91	0.52
15:1:37:LEU:HD23	15:1:40:SER:HB3	1.91	0.52
15:1:141:ARG:HA	26:1:611:CHL:HBC2	1.92	0.52
15:1:157:ASP:OD1	25:1:601:CLA:HBA2	2.10	0.52
1:A:580:ARG:NH1	4:D:255:GLU:OE2	2.43	0.52
25:B:1202:CLA:H2	25:B:1202:CLA:HAA2	1.92	0.52
26:3:611:CHL:HHC	26:3:611:CHL:HBB1	1.92	0.52
1:A:59:PHE:CD2	25:A:1103:CLA:HMC2	2.45	0.52
29:5:503:BCR:H343	26:5:617:CHL:HAB	1.92	0.52
25:A:1117:CLA:H92	25:A:1127:CLA:H91	1.92	0.52
2:B:404:ASN:OD1	2:B:407:ASN:ND2	2.39	0.52
25:B:1218:CLA:CMD	29:B:4001:BCR:HC7	2.40	0.52
1:A:441:LEU:HG	1:A:548:LEU:HB2	1.91	0.51
14:O:102:ASP:H	14:O:105:TRP:HD1	1.56	0.51
15:a:61:ALA:HB2	26:a:604:CHL:HBA1	1.90	0.51
25:4:616:CLA:H12	25:4:616:CLA:HBD	1.92	0.51
25:A:1125:CLA:CED	25:A:1133:CLA:HAB	2.41	0.51
12:M:5:ASP:OD1	35:2:804:LMT:O3B	2.23	0.51
14:O:69:ILE:HG23	14:O:80:PHE:HB2	1.92	0.51
25:1:605:CLA:HBC1	25:1:612:CLA:HAC1	1.92	0.51
18:5:174:PHE:HD2	25:5:601:CLA:H11	1.75	0.51
25:5:605:CLA:OBD	25:5:612:CLA:HBA2	2.10	0.51
25:A:1102:CLA:HAB	25:A:1104:CLA:CAD	2.41	0.51
25:B:1204:CLA:H102	29:I:4001:BCR:HC41	1.93	0.51
26:6:610:CHL:HHC	26:6:610:CHL:HBB1	1.92	0.51
6:F:378:LEU:HD23	6:F:386:PRO:HB3	1.93	0.51
11:L:295:LYS:N	14:O:133:TYR:OH	2.35	0.51
15:a:92:GLU:OE2	15:a:197:SER:OG	2.29	0.51
15:a:151:TYR:CZ	15:a:170:LYS:HD3	2.46	0.51
43:5:505:LUT:H183	25:7:608:CLA:HAB	1.92	0.51
25:9:609:CLA:HMB1	25:9:609:CLA:HBB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:VAL:HG21	25:B:1205:CLA:HAC1	1.92	0.51
25:B:1236:CLA:HHC	25:B:1236:CLA:HBB1	1.92	0.51
3:C:17:CYS:HB3	28:C:3003:SF4:S4	2.49	0.51
18:5:149:ASP:HB3	18:5:152:ASN:O	2.11	0.51
18:5:152:ASN:OD1	18:5:154:ASN:ND2	2.39	0.51
25:6:608:CLA:H2	26:6:609:CHL:H122	1.93	0.51
25:A:1108:CLA:HBB1	25:A:1111:CLA:H112	1.93	0.51
25:A:1126:CLA:O1D	25:A:1127:CLA:HHB	2.11	0.51
2:B:669:ARG:HB2	27:B:2002:PQN:H7	1.91	0.51
25:B:1204:CLA:H61	29:I:4001:BCR:HC31	1.92	0.51
26:5:618:CHL:HHC	26:5:618:CHL:HBB1	1.92	0.51
25:B:1023:CLA:H201	25:B:1239:CLA:H52	1.92	0.51
25:1:607:CLA:HBB1	29:8:503:BCR:HC21	1.93	0.51
7:G:1294:PHE:CE2	7:G:1299:VAL:HG22	2.46	0.51
17:4:223:HIS:C	17:4:225:ILE:H	2.14	0.51
20:7:50:ALA:HB2	25:7:612:CLA:HED2	1.91	0.51
1:A:320:SER:HB3	1:A:325:ILE:HD11	1.93	0.51
25:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.93	0.51
2:B:49:ALA:HB3	12:M:29:LEU:HD21	1.93	0.51
2:B:667:SER:HB3	2:B:672:TRP:HE1	1.76	0.51
25:B:1216:CLA:HED2	25:B:1220:CLA:HED2	1.92	0.51
15:a:114:TYR:HD1	26:a:606:CHL:HAA1	1.75	0.51
43:a:501:LUT:H32	25:a:601:CLA:CAB	2.41	0.51
22:2:230:ARG:HB2	23:9:347:LYS:HE3	1.93	0.51
25:A:1110:CLA:H12	16:3:291:LEU:HD21	1.91	0.50
2:B:374:THR:HG23	2:B:592:THR:HG21	1.93	0.50
25:B:1201:CLA:H12	25:B:1201:CLA:H121	1.92	0.50
17:4:223:HIS:HB2	25:4:608:CLA:HED3	1.93	0.50
22:2:166:ARG:HB3	25:2:604:CLA:CBC	2.42	0.50
35:2:804:LMT:H22	48:2:803:DGA:HA72	1.93	0.50
1:A:374:MET:HE1	25:A:1125:CLA:HBB1	1.93	0.50
25:B:1207:CLA:H101	11:L:378:ALA:HB2	1.92	0.50
4:D:230:GLN:HG3	4:D:242:MET:HE3	1.92	0.50
26:5:611:CHL:HHC	26:5:611:CHL:HBB1	1.93	0.50
21:8:139:TRP:CD2	25:8:612:CLA:HMA2	2.46	0.50
2:B:6:PHE:HB2	13:I:30:ILE:HA	1.92	0.50
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.93	0.50
25:B:1205:CLA:O1A	25:B:1224:CLA:HBD	2.11	0.50
25:B:1220:CLA:HMD3	25:B:1221:CLA:HAB	1.92	0.50
15:a:168:GLU:HG2	15:a:172:LYS:NZ	2.25	0.50
1:A:711:PRO:HA	6:F:426:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1012:CLA:H42	29:A:4005:BCR:H362	1.94	0.50
2:B:375:HIS:HB2	25:B:1224:CLA:C1B	2.41	0.50
8:H:66:ASN:HB3	8:H:69:GLN:HG2	1.92	0.50
11:L:371:ILE:O	11:L:375:ILE:HG12	2.11	0.50
43:6:501:LUT:H383	26:6:611:CHL:H12	1.94	0.50
1:A:679:TRP:O	1:A:682:SER:OG	2.21	0.50
25:A:1113:CLA:H92	29:A:4001:BCR:H393	1.94	0.50
3:C:24:ASP:OD1	4:D:287:HIS:HA	2.12	0.50
15:1:172:LYS:HG3	25:1:607:CLA:HED2	1.93	0.50
17:4:59:LEU:HD13	25:4:604:CLA:H42	1.93	0.50
25:A:1122:CLA:H92	29:A:4003:BCR:H15C	1.92	0.50
27:A:2001:PQN:H191	25:A:1101:CLA:H42	1.93	0.50
2:B:84:HIS:ND1	8:H:125:GLY:O	2.39	0.50
25:1:612:CLA:HBC1	26:1:613:CHL:HBB1	1.93	0.50
33:A:5006:PTY:C30	33:A:5006:PTY:H111	2.42	0.50
29:B:4002:BCR:H322	25:9:612:CLA:H141	1.93	0.50
4:D:228:LYS:HA	4:D:244:GLN:HG3	1.94	0.50
6:F:397:ARG:NH2	25:F:1301:CLA:OBD	2.45	0.50
8:H:86:ILE:HD11	11:L:384:LEU:HD21	1.92	0.50
25:1:615:CLA:HMB1	25:1:615:CLA:HBB1	1.93	0.50
15:a:107:VAL:HG12	15:a:108:GLN:HG3	1.92	0.50
43:a:503:LUT:H10	26:a:613:CHL:CGA	2.41	0.50
25:3:601:CLA:H52	25:3:602:CLA:HMA3	1.94	0.50
25:4:605:CLA:H2A	25:4:605:CLA:HED2	1.93	0.50
26:9:603:CHL:HHC	26:9:603:CHL:HBB1	1.92	0.50
1:A:679:TRP:CD2	24:A:1011:CL0:H6	2.47	0.50
25:A:1013:CLA:H121	29:A:4005:BCR:H23C	1.93	0.50
25:A:1111:CLA:H191	25:3:605:CLA:H51	1.94	0.50
14:O:61:LEU:HB2	14:O:119:LEU:HD23	1.94	0.50
14:O:69:ILE:HG21	14:O:111:TRP:HE1	1.75	0.50
25:6:615:CLA:HMC2	26:6:619:CHL:HBC3	1.93	0.50
1:A:367:VAL:O	1:A:371:MET:HG3	2.12	0.50
25:B:1208:CLA:H2A	25:B:1208:CLA:HED2	1.94	0.50
30:F:5002:LHG:H281	45:8:809:OLA:H51	1.92	0.50
33:3:802:PTY:H352	48:3:803:DGA:HB21	1.94	0.50
43:6:501:LUT:H28	25:6:601:CLA:H43	1.92	0.50
22:2:172:PHE:CZ	43:2:502:LUT:H30	2.46	0.50
25:2:607:CLA:C3C	30:2:801:LHG:HC62	2.42	0.49
15:1:169:LEU:HB3	25:1:601:CLA:HMA2	1.93	0.49
25:A:1128:CLA:H101	25:A:1139:CLA:HAA2	1.93	0.49
2:B:698:PRO:O	3:C:81:TYR:OH	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1201:CLA:H18	25:B:1204:CLA:H203	1.94	0.49
25:F:1302:CLA:H61	51:7:807:4RF:H35	1.94	0.49
44:1:502:AXT:H34	26:1:604:CHL:CBB	2.42	0.49
25:9:604:CLA:HBC2	25:9:609:CLA:HBB2	1.94	0.49
11:L:382:LEU:O	11:L:385:THR:HG22	2.13	0.49
19:6:138:TYR:HB3	19:6:146:MET:HE3	1.95	0.49
23:9:362:PRO:O	43:9:501:LUT:O23	2.28	0.49
3:C:29:VAL:HG12	4:D:301:ARG:HB2	1.95	0.49
43:4:501:LUT:H28	43:4:501:LUT:H361	1.94	0.49
21:8:196:ARG:HD2	25:8:607:CLA:O1D	2.13	0.49
1:A:43:PRO:HG3	6:F:440:ILE:HD13	1.93	0.49
1:A:247:PRO:HG2	16:3:487:LYS:HG3	1.93	0.49
1:A:459:ASN:HB3	1:A:641:THR:HG22	1.95	0.49
25:A:1129:CLA:HAB	25:A:1137:CLA:CBB	2.42	0.49
30:B:5001:LHG:H251	15:1:58:LEU:HD13	1.94	0.49
18:5:78:ARG:HA	18:5:81:MET:HE3	1.93	0.49
18:5:133:GLU:OE1	18:5:136:ARG:NH2	2.35	0.49
26:6:613:CHL:HMB1	26:6:613:CHL:HBB1	1.94	0.49
21:8:154:PHE:CE2	21:8:161:PHE:HE2	2.30	0.49
30:A:5003:LHG:H171	29:3:505:BCR:H19C	1.95	0.49
2:B:646:VAL:HA	25:B:1206:CLA:CBC	2.43	0.49
25:B:1219:CLA:HAA2	35:B:5006:LMT:H1'	1.94	0.49
10:K:111:LEU:HB3	10:K:117:LEU:HB2	1.95	0.49
25:6:601:CLA:HMB2	25:6:602:CLA:HBA2	1.93	0.49
23:9:298:VAL:HG11	43:9:501:LUT:H12	1.95	0.49
43:9:502:LUT:C11	25:9:605:CLA:HBC3	2.42	0.49
1:A:580:ARG:HA	3:C:77:MET:HA	1.94	0.49
25:A:1117:CLA:H2	25:A:1127:CLA:H92	1.94	0.49
2:B:277:HIS:HB2	25:B:1214:CLA:C1B	2.43	0.49
25:B:1224:CLA:CGA	25:B:1224:CLA:H3A	2.39	0.49
11:L:353:VAL:CG1	11:L:376:ASN:HD22	2.20	0.49
32:I:5001:SQD:H461	22:2:243:PRO:HG2	1.95	0.49
30:6:801:LHG:H341	41:6:806:SPH:H181	1.95	0.49
1:A:107:ASP:HB3	1:A:111:ILE:HD12	1.95	0.49
25:A:1119:CLA:HED2	25:A:1122:CLA:HED2	1.93	0.49
25:A:1130:CLA:HBB1	25:A:1136:CLA:H192	1.94	0.49
25:B:1231:CLA:HHC	25:B:1231:CLA:HBB1	1.95	0.49
7:G:1238:CYS:HB2	7:G:1310:ALA:HB2	1.95	0.49
15:1:202:LEU:HD13	25:1:608:CLA:HBC2	1.95	0.49
15:a:129:ILE:HG21	26:a:613:CHL:HED3	1.94	0.49
23:9:255:PRO:HB2	23:9:257:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1215:CLA:HHC	25:B:1215:CLA:HBB1	1.94	0.49
25:B:1230:CLA:H12	33:B:5005:PTY:H111	1.95	0.49
15:a:168:GLU:HG2	15:a:172:LYS:HZ2	1.78	0.49
19:6:250:GLN:HB2	29:6:504:BCR:H343	1.95	0.49
25:B:1222:CLA:H51	25:B:1234:CLA:H62	1.94	0.48
4:D:310:ARG:HB2	4:D:313:GLN:HG3	1.95	0.48
25:a:607:CLA:H61	25:a:607:CLA:H41	1.54	0.48
21:8:76:ASN:ND2	25:8:612:CLA:OBD	2.46	0.48
22:2:163:LYS:HD3	25:2:607:CLA:O1D	2.13	0.48
1:A:377:TYR:CE2	25:A:1127:CLA:HED2	2.49	0.48
25:1:612:CLA:HBA2	35:1:804:LMT:H3'	1.95	0.48
44:7:504:AXT:H171	44:7:504:AXT:H8	1.95	0.48
22:2:166:ARG:HB3	25:2:604:CLA:HBC3	1.95	0.48
2:B:5:LEU:HA	2:B:14:ALA:HB1	1.95	0.48
2:B:653:PHE:O	2:B:657:ILE:HG13	2.13	0.48
3:C:26:LEU:HA	3:C:41:SER:O	2.13	0.48
8:H:65:TYR:OH	11:L:343:GLU:OE1	2.17	0.48
15:1:217:ASN:ND2	25:1:603:CLA:OBD	2.47	0.48
25:1:605:CLA:H203	25:1:612:CLA:H13	1.96	0.48
15:1:126:LEU:HD11	26:1:613:CHL:HMD2	1.95	0.48
16:3:311:VAL:HG22	16:3:438:ILE:HD11	1.95	0.48
2:B:9:PHE:HB2	2:B:35:HIS:CG	2.48	0.48
2:B:11:GLN:N	2:B:36:ASP:OD2	2.39	0.48
2:B:353:MET:HE1	25:B:1225:CLA:O1D	2.14	0.48
2:B:478:LEU:HD11	25:B:1232:CLA:HMC2	1.94	0.48
25:B:1021:CLA:HHC	25:B:1021:CLA:HBB1	1.94	0.48
5:E:45:VAL:O	5:E:58:THR:HA	2.14	0.48
8:H:34:LYS:N	8:H:46:ASP:OD2	2.46	0.48
25:L:1503:CLA:HBA1	25:L:1503:CLA:H3A	1.64	0.48
25:1:605:CLA:HBA1	25:1:605:CLA:H3A	1.63	0.48
18:5:64:LYS:NZ	36:7:806:DGD:HD3	2.28	0.48
20:7:60:THR:HG22	25:7:606:CLA:HAB	1.96	0.48
23:9:311:LYS:HD3	23:9:313:PHE:CZ	2.49	0.48
25:A:1105:CLA:H2	40:J:4002:RRX:H31	1.94	0.48
25:A:1128:CLA:H71	30:A:5002:LHG:H202	1.95	0.48
15:1:205:HIS:CG	25:1:603:CLA:HAA2	2.49	0.48
25:7:610:CLA:H61	25:7:610:CLA:H102	1.48	0.48
26:8:601:CHL:H42	25:8:602:CLA:HBA1	1.96	0.48
1:A:584:CYS:HB2	2:B:668:TRP:HB3	1.96	0.48
25:A:1012:CLA:H172	25:A:1126:CLA:H152	1.96	0.48
2:B:286:ILE:HG23	2:B:290:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:GLY:HA3	2:B:411:ARG:HD2	1.96	0.48
3:C:15:THR:HG22	3:C:28:MET:HG3	1.94	0.48
38:F:5003:LPX:H7A	25:F:1301:CLA:ND	2.28	0.48
26:a:604:CHL:HBC1	30:a:801:LHG:H292	1.95	0.48
16:3:372:ALA:O	16:3:376:ASN:HB2	2.14	0.48
20:7:177:ARG:HD2	25:7:607:CLA:O1D	2.12	0.48
23:9:339:GLU:HG3	25:9:612:CLA:C4B	2.44	0.48
1:A:363:LEU:O	1:A:367:VAL:HG23	2.14	0.48
25:B:1219:CLA:H91	25:B:1219:CLA:H112	1.69	0.48
3:C:9:ASP:HB2	5:E:70:ARG:HD2	1.96	0.48
26:a:609:CHL:H2	17:4:132:TRP:HB2	1.95	0.48
43:3:501:LUT:H383	26:3:611:CHL:H43	1.96	0.48
18:5:175:SER:O	18:5:177:GLY:N	2.45	0.48
29:6:503:BCR:H271	25:6:606:CLA:NB	2.28	0.48
25:2:604:CLA:CHD	26:2:609:CHL:HBB2	2.43	0.48
1:A:363:LEU:HD11	25:A:1117:CLA:H71	1.95	0.48
25:A:1108:CLA:H91	25:A:1108:CLA:H111	1.69	0.48
26:A:1114:CHL:H112	26:A:1114:CHL:CBB	2.44	0.48
26:a:604:CHL:H61	25:a:605:CLA:HMA2	1.94	0.48
25:4:601:CLA:H41	25:4:601:CLA:H61	1.47	0.48
22:2:126:GLU:OE1	22:2:129:ARG:NH2	2.37	0.48
1:A:165:GLY:HA2	33:A:5006:PTY:H352	1.96	0.48
9:J:45:LEU:HD22	29:J:4001:BCR:H402	1.95	0.48
43:a:501:LUT:H11	43:a:501:LUT:H191	1.77	0.48
48:3:803:DGA:HA22	48:3:803:DGA:HA51	1.71	0.48
19:6:48:HIS:NE2	19:6:61:ASP:OD2	2.47	0.48
1:A:479:LEU:HB2	1:A:530:THR:HG23	1.96	0.47
25:A:1126:CLA:H3A	25:A:1126:CLA:HBA2	1.49	0.47
2:B:57:ILE:HD11	42:M:4001:ECH:H39A	1.97	0.47
2:B:79:VAL:HG13	2:B:126:TYR:HE1	1.79	0.47
37:B:5004:PCW:H152	37:B:5004:PCW:H121	1.55	0.47
33:G:5002:PTY:H132	15:1:128:ALA:HB1	1.96	0.47
25:K:1402:CLA:H51	25:K:1402:CLA:H11	1.70	0.47
25:1:606:CLA:HMA3	26:1:613:CHL:C2C	2.44	0.47
25:1:607:CLA:H72	25:1:607:CLA:H112	1.58	0.47
26:1:609:CHL:HBA2	25:8:618:CLA:O1D	2.12	0.47
16:3:387:LYS:NZ	33:3:802:PTY:O12	2.41	0.47
43:5:501:LUT:H30	25:5:601:CLA:H52	1.96	0.47
23:9:292:ARG:HA	23:9:295:MET:HE3	1.95	0.47
25:B:1215:CLA:HBA2	25:B:1215:CLA:H3A	1.58	0.47
15:1:34:GLY:HA3	15:1:53:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:610:CHL:HBB2	25:5:612:CLA:HBC1	1.95	0.47
22:2:227:ALA:HB2	30:9:802:LHG:H262	1.95	0.47
43:9:501:LUT:H373	26:9:601:CHL:H42	1.95	0.47
1:A:72:LYS:NZ	25:A:1109:CLA:OBD	2.39	0.47
25:A:1116:CLA:CGA	25:A:1116:CLA:H3A	2.44	0.47
25:B:1218:CLA:H43	35:1:804:LMT:H12	1.96	0.47
17:4:134:GLU:HG3	25:4:612:CLA:NB	2.29	0.47
1:A:426:LEU:HD13	25:A:1122:CLA:C1C	2.45	0.47
26:1:609:CHL:OBD	21:8:137:LYS:NZ	2.46	0.47
25:3:606:CLA:H192	25:5:604:CLA:H202	1.96	0.47
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.97	0.47
25:A:1138:CLA:H41	29:B:4006:BCR:H21C	1.96	0.47
25:B:1205:CLA:H121	25:B:1224:CLA:H193	1.94	0.47
25:B:1216:CLA:H93	25:B:1216:CLA:H111	1.75	0.47
25:B:1207:CLA:HHC	25:B:1207:CLA:HBB1	1.96	0.47
15:1:46:LEU:HA	15:1:49:LEU:HD12	1.97	0.47
25:4:610:CLA:H202	25:4:610:CLA:H161	1.71	0.47
18:5:141:ARG:HE	48:5:803:DGA:HB42	1.79	0.47
1:A:438:ILE:HG13	1:A:556:TYR:HE2	1.79	0.47
25:L:1502:CLA:H93	25:L:1502:CLA:H111	1.78	0.47
14:O:61:LEU:CD2	14:O:122:GLY:HA3	2.45	0.47
17:4:179:TRP:HB3	25:4:601:CLA:HMA2	1.97	0.47
25:A:1122:CLA:HBB1	25:A:1129:CLA:HBC2	1.96	0.47
25:A:1130:CLA:H61	25:A:1130:CLA:H41	1.40	0.47
25:A:1101:CLA:H102	25:A:1101:CLA:H13	1.65	0.47
25:B:1228:CLA:C1C	39:F:4001:NEX:H35	2.45	0.47
6:F:335:LYS:HB2	6:F:370:PHE:CD1	2.50	0.47
7:G:1300:MET:HA	29:G:4001:BCR:H14C	1.97	0.47
14:O:69:ILE:HA	29:O:4001:BCR:H313	1.97	0.47
15:1:79:ARG:HA	15:1:82:MET:HE3	1.95	0.47
16:3:260:VAL:O	30:3:801:LHG:HC11	2.14	0.47
25:3:616:CLA:H51	25:5:615:CLA:HAA2	1.96	0.47
17:4:81:MET:HE2	17:4:187:ALA:HB2	1.96	0.47
25:6:601:CLA:H91	25:6:601:CLA:H112	1.80	0.47
29:7:503:BCR:H10C	25:8:609:CLA:H52	1.97	0.47
26:8:603:CHL:H62	26:8:603:CHL:H41	1.72	0.47
30:2:801:LHG:HC61	30:2:801:LHG:H102	1.95	0.47
26:9:610:CHL:CBB	26:9:613:CHL:HBB2	2.44	0.47
1:A:29:TRP:NE1	25:A:1109:CLA:O1A	2.48	0.47
1:A:338:HIS:HB3	1:A:341:LEU:HD12	1.96	0.47
25:A:1112:CLA:HBA1	29:A:4001:BCR:H342	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ALA:HB2	2:B:289:GLY:HA3	1.97	0.47
2:B:595:TRP:CD1	25:B:1234:CLA:HBC2	2.50	0.47
25:B:1227:CLA:HBC1	29:B:4004:BCR:H21C	1.96	0.47
6:F:417:TRP:HD1	6:F:454:GLY:C	2.22	0.47
26:a:609:CHL:HAA2	17:4:135:LEU:HD12	1.97	0.47
17:4:224:PHE:CE1	25:4:608:CLA:HED2	2.49	0.47
19:6:68:ASN:HB3	19:6:71:ARG:HB2	1.97	0.47
29:7:503:BCR:H292	32:7:805:SQD:H251	1.97	0.47
48:8:804:DGA:HB42	48:8:804:DGA:HA41	1.97	0.47
1:A:119:TRP:O	1:A:124:GLN:NE2	2.35	0.47
25:A:1119:CLA:HBC3	25:A:1125:CLA:H193	1.97	0.47
25:A:1138:CLA:HED2	2:B:421:SER:HB3	1.97	0.47
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.32	0.47
25:B:1201:CLA:HMC2	25:B:1203:CLA:HED2	1.96	0.47
6:F:454:GLY:O	6:F:457:TRP:HB3	2.15	0.47
8:H:68:LEU:HD11	29:H:4001:BCR:H312	1.96	0.47
26:1:610:CHL:HAB	26:1:613:CHL:HBB2	1.97	0.47
18:5:90:GLN:NE2	18:5:99:TRP:HB3	2.30	0.47
19:6:189:ARG:HA	19:6:192:MET:HE3	1.96	0.47
21:8:131:PHE:HA	21:8:134:VAL:HG22	1.97	0.47
43:8:502:LUT:H35	43:8:502:LUT:H401	1.80	0.47
25:9:605:CLA:OBD	25:9:612:CLA:H2	2.15	0.47
25:A:1111:CLA:H61	25:A:1111:CLA:H41	1.46	0.47
25:A:1117:CLA:H203	25:A:1125:CLA:HBA2	1.97	0.47
25:B:1238:CLA:HBB2	27:B:2002:PQN:H141	1.97	0.47
26:1:609:CHL:HMA2	21:8:136:ILE:HD13	1.97	0.47
17:4:231:PRO:O	17:4:233:LEU:N	2.43	0.47
25:7:604:CLA:H162	25:7:604:CLA:H193	1.71	0.47
43:2:507:LUT:H201	43:2:507:LUT:H15	1.66	0.47
1:A:744:LEU:HD23	1:A:744:LEU:HA	1.78	0.46
25:A:1117:CLA:H3A	25:A:1117:CLA:HBA2	1.56	0.46
25:A:1119:CLA:HBA1	25:A:1123:CLA:C3B	2.45	0.46
25:A:1125:CLA:CAB	25:A:1133:CLA:HMA2	2.44	0.46
4:D:249:LEU:HD23	4:D:260:LEU:HD22	1.97	0.46
9:J:40:VAL:HA	25:J:1901:CLA:HBB2	1.97	0.46
11:L:351:LEU:HD22	25:L:1503:CLA:HBC3	1.97	0.46
25:1:612:CLA:H91	25:1:612:CLA:H111	1.64	0.46
15:a:114:TYR:CD1	26:a:606:CHL:HAA1	2.50	0.46
25:7:610:CLA:H8	25:7:610:CLA:H121	1.72	0.46
1:A:403:VAL:HG11	1:A:596:LEU:HG	1.97	0.46
25:A:1140:CLA:HMC2	29:B:4006:BCR:H381	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:4005:BCR:H15C	29:B:4005:BCR:H351	1.74	0.46
7:G:1229:ALA:HB1	7:G:1234:VAL:HG21	1.97	0.46
19:6:89:GLY:HA2	43:6:502:LUT:H181	1.97	0.46
26:7:613:CHL:HBC2	26:7:613:CHL:HHD	1.97	0.46
21:8:137:LYS:HG2	25:8:611:CLA:HMC2	1.97	0.46
22:2:223:CYS:SG	30:9:802:LHG:H272	2.55	0.46
1:A:338:HIS:CE1	30:A:5001:LHG:HC11	2.49	0.46
33:A:5006:PTY:H182	33:A:5006:PTY:H362	1.97	0.46
15:1:145:GLU:O	15:1:149:ARG:HG3	2.16	0.46
26:a:604:CHL:H61	25:a:605:CLA:CMA	2.45	0.46
25:3:606:CLA:H51	25:3:613:CLA:HBD	1.96	0.46
25:4:612:CLA:H41	25:4:612:CLA:H61	1.49	0.46
19:6:97:GLU:CD	19:6:208:ASN:HB3	2.40	0.46
25:A:1124:CLA:H51	25:A:1135:CLA:H11	1.96	0.46
25:B:1202:CLA:HBA1	25:B:1202:CLA:H3A	1.46	0.46
25:B:1220:CLA:H3A	25:B:1220:CLA:HBA2	1.60	0.46
25:B:1221:CLA:HMA2	25:B:1221:CLA:H2	1.97	0.46
25:K:1402:CLA:H2A	25:K:1402:CLA:HED2	1.97	0.46
15:a:213:ASN:OD1	15:a:216:THR:HG23	2.16	0.46
16:3:257:VAL:HG12	16:3:264:TYR:O	2.15	0.46
21:8:199:ARG:O	21:8:203:VAL:HG23	2.15	0.46
25:8:602:CLA:H51	25:8:602:CLA:H11	1.69	0.46
26:9:601:CHL:HMB3	26:9:601:CHL:HBB1	1.97	0.46
25:H:1703:CLA:H41	25:H:1703:CLA:H61	1.46	0.46
9:J:32:VAL:O	9:J:36:LEU:HD23	2.15	0.46
15:1:191:HIS:ND1	15:1:196:ALA:O	2.49	0.46
43:a:501:LUT:H15	43:a:501:LUT:H201	1.80	0.46
26:a:606:CHL:HMA2	26:a:613:CHL:HBC3	1.97	0.46
18:5:41:PRO:HD2	18:5:44:LEU:HD12	1.97	0.46
25:7:603:CLA:H171	25:7:603:CLA:H13	1.50	0.46
1:A:29:TRP:HE1	25:A:1109:CLA:CHB	2.28	0.46
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.98	0.46
1:A:460:ASP:OD1	1:A:641:THR:HB	2.15	0.46
25:A:1125:CLA:H111	25:A:1125:CLA:H152	1.44	0.46
25:B:1201:CLA:H112	25:B:1201:CLA:H142	1.77	0.46
5:E:88:ASN:HB3	5:E:90:TYR:CE1	2.51	0.46
14:O:105:TRP:O	14:O:109:ILE:HG13	2.15	0.46
25:3:602:CLA:H2A	25:3:602:CLA:HED2	1.97	0.46
25:3:610:CLA:H41	25:3:610:CLA:H62	1.57	0.46
33:3:802:PTY:H141	33:3:802:PTY:H322	1.98	0.46
17:4:135:LEU:HD23	17:4:135:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:602:CLA:H62	25:5:602:CLA:H41	1.50	0.46
25:5:603:CLA:H2	25:5:608:CLA:HMD2	1.98	0.46
22:2:113:THR:O	22:2:117:ILE:HG12	2.16	0.46
1:A:718:LEU:HD21	27:A:2001:PQN:H151	1.96	0.46
25:B:1214:CLA:H102	25:B:1214:CLA:H61	1.50	0.46
25:K:1401:CLA:HBB1	29:K:4002:BCR:C11	2.45	0.46
15:1:98:ASN:OD1	15:1:101:ASP:HB2	2.16	0.46
15:a:35:ASN:ND2	15:a:38:PRO:O	2.49	0.46
47:4:804:PLM:H22	21:8:182:SER:HB3	1.97	0.46
18:5:35:PHE:HB3	18:5:38:VAL:CG1	2.46	0.46
25:5:606:CLA:HBC3	47:5:804:PLM:HG3	1.97	0.46
44:7:504:AXT:H163	25:7:612:CLA:C1B	2.46	0.46
22:2:240:ARG:NH2	22:2:243:PRO:O	2.48	0.46
1:A:77:HIS:ND1	25:A:1111:CLA:OBD	2.46	0.46
1:A:474:ASP:O	1:A:478:GLN:NE2	2.48	0.46
1:A:687:PHE:CD1	2:B:665:LEU:HB3	2.51	0.46
25:A:1127:CLA:HHC	25:A:1127:CLA:HBB1	1.98	0.46
25:4:601:CLA:H92	25:4:601:CLA:H62	1.76	0.46
18:5:124:TRP:HA	25:6:608:CLA:O1A	2.15	0.46
19:6:256:ALA:HA	26:6:610:CHL:CGA	2.44	0.46
44:7:504:AXT:HC22	25:7:612:CLA:H2	1.97	0.46
25:7:605:CLA:HBC1	25:7:610:CLA:HBB2	1.98	0.46
1:A:178:TRP:HB2	25:A:1109:CLA:HMC2	1.98	0.46
1:A:589:TRP:NE1	25:A:1128:CLA:HMD3	2.30	0.46
25:A:1121:CLA:H143	25:A:1121:CLA:H112	1.73	0.46
26:1:610:CHL:HMB3	26:1:610:CHL:HBB1	1.98	0.46
26:3:603:CHL:HBB1	26:3:603:CHL:HHC	1.98	0.46
19:6:84:ARG:NH1	26:6:611:CHL:OBD	2.47	0.46
22:2:55:PRO:HD2	43:2:502:LUT:H3	1.98	0.46
2:B:5:LEU:HD23	2:B:5:LEU:O	2.16	0.46
25:B:1201:CLA:H203	25:B:1201:CLA:H162	1.68	0.46
25:B:1216:CLA:HMB2	25:B:1221:CLA:HMA3	1.97	0.46
25:B:1234:CLA:H62	25:B:1234:CLA:H2	1.66	0.46
6:F:462:PHE:HZ	36:8:803:DGD:HB21	1.80	0.46
26:1:613:CHL:HBB1	26:1:613:CHL:HMB1	1.97	0.46
43:a:501:LUT:H30	25:a:601:CLA:H52	1.97	0.46
25:3:601:CLA:H3A	25:3:601:CLA:HBA2	1.55	0.46
25:5:601:CLA:HMB2	25:5:602:CLA:HBA2	1.97	0.46
20:7:152:GLY:O	20:7:162:ARG:NH1	2.48	0.46
21:8:220:LEU:HD22	48:8:804:DGA:HBN2	1.98	0.46
50:9:507:XAT:H203	25:9:606:CLA:H92	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1112:CLA:H62	29:A:4001:BCR:H343	1.98	0.45
25:A:1120:CLA:H2	25:K:1403:CLA:CHB	2.45	0.45
2:B:518:PHE:HA	25:B:1235:CLA:HED1	1.98	0.45
25:B:1209:CLA:NC	25:B:1209:CLA:H51	2.31	0.45
25:B:1228:CLA:HBA2	25:B:1228:CLA:H3A	1.59	0.45
4:D:197:ASP:O	8:H:40:ARG:NE	2.48	0.45
25:3:606:CLA:H141	25:3:606:CLA:H161	1.69	0.45
25:4:604:CLA:HAC2	30:4:801:LHG:H252	1.98	0.45
20:7:124:SER:HB2	21:8:37:GLY:HA2	1.98	0.45
23:9:282:TRP:CZ2	25:9:612:CLA:HAA1	2.48	0.45
1:A:587:SER:OG	1:A:590:ASP:OD2	2.34	0.45
1:A:687:PHE:HB2	25:A:1013:CLA:HBC1	1.98	0.45
25:A:1126:CLA:C1C	29:A:4005:BCR:HC22	2.46	0.45
25:B:1205:CLA:H143	25:B:1205:CLA:H161	1.70	0.45
25:F:1302:CLA:H61	25:F:1302:CLA:H2	1.63	0.45
16:3:322:ALA:HB1	29:3:504:BCR:H21C	1.97	0.45
25:3:616:CLA:H41	25:3:616:CLA:H61	1.64	0.45
26:5:613:CHL:H41	26:5:613:CHL:H62	1.59	0.45
43:6:502:LUT:H32	25:6:604:CLA:CBB	2.46	0.45
20:7:217:VAL:HG13	20:7:223:VAL:HG21	1.99	0.45
21:8:227:LEU:HD22	48:8:804:DGA:HA62	1.97	0.45
25:8:618:CLA:HBD	47:8:807:PLM:HD2	1.97	0.45
24:A:1011:CL0:H41	24:A:1011:CL0:H49	1.66	0.45
25:A:1116:CLA:H41	25:A:1116:CLA:H61	1.75	0.45
32:A:5005:SQD:H301	32:A:5005:SQD:H272	1.51	0.45
5:E:41:ARG:HG2	5:E:63:SER:HA	1.99	0.45
25:G:1602:CLA:H101	25:G:1602:CLA:H61	1.75	0.45
15:a:69:ARG:CZ	21:8:155:LEU:HB3	2.46	0.45
43:5:505:LUT:H11	43:5:505:LUT:H191	1.70	0.45
25:2:602:CLA:HBB1	25:2:607:CLA:H152	1.98	0.45
1:A:13:VAL:N	1:A:315:ASN:OD1	2.48	0.45
25:A:1138:CLA:H203	25:A:1140:CLA:H52	1.97	0.45
2:B:296:PHE:CD2	25:B:1217:CLA:HBD	2.52	0.45
25:B:1201:CLA:CHA	25:B:1201:CLA:HBA1	2.47	0.45
25:B:1231:CLA:H122	25:B:1231:CLA:H162	1.81	0.45
6:F:346:LEU:HA	6:F:359:LEU:HD13	1.98	0.45
26:a:609:CHL:HMB3	26:a:609:CHL:HBB1	1.97	0.45
25:a:612:CLA:H102	25:a:612:CLA:H62	1.76	0.45
43:4:502:LUT:H32	25:4:604:CLA:CAB	2.47	0.45
26:6:619:CHL:HMB3	26:6:619:CHL:HBB1	1.97	0.45
1:A:196:SER:O	1:A:200:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:5005:SQD:H312	32:A:5005:SQD:H341	1.72	0.45
25:B:1225:CLA:H52	29:B:4002:BCR:H23C	1.99	0.45
8:H:80:LEU:HG	8:H:86:ILE:HD13	1.99	0.45
11:L:357:ILE:CA	11:L:372:VAL:HG21	2.44	0.45
14:O:61:LEU:HD23	25:O:1802:CLA:HMC2	1.99	0.45
15:a:46:LEU:HA	15:a:49:LEU:HD12	1.97	0.45
19:6:173:VAL:HA	25:6:601:CLA:O1A	2.16	0.45
19:6:178:GLU:HG2	19:6:179:GLU:N	2.31	0.45
25:7:605:CLA:OBD	25:7:612:CLA:HBA2	2.17	0.45
21:8:84:VAL:HG11	43:8:501:LUT:H12	1.98	0.45
6:F:390:ALA:HB2	6:F:404:VAL:HG21	1.98	0.45
23:9:270:PRO:HD2	43:9:502:LUT:H23	1.98	0.45
23:9:385:PHE:CZ	43:9:502:LUT:H10	2.51	0.45
25:A:1103:CLA:H91	25:A:1103:CLA:H111	1.67	0.45
25:A:1106:CLA:H101	29:J:4001:BCR:C10	2.47	0.45
25:A:1112:CLA:H51	26:A:1114:CHL:H42	1.99	0.45
25:A:1133:CLA:H2A	25:A:1133:CLA:HED2	1.98	0.45
2:B:441:ASN:O	2:B:445:GLN:HG2	2.17	0.45
2:B:464:ILE:HD12	25:B:1234:CLA:O1A	2.16	0.45
2:B:726:LEU:O	2:B:730:THR:HG22	2.17	0.45
25:B:1220:CLA:H41	25:B:1220:CLA:H61	1.63	0.45
12:M:5:ASP:OD2	12:M:5:ASP:N	2.49	0.45
12:M:24:ARG:HD2	30:2:802:LHG:C7	2.46	0.45
43:1:501:LUT:H35	43:1:501:LUT:H401	1.81	0.45
15:a:172:LYS:HD3	25:a:602:CLA:HBA2	1.98	0.45
29:4:503:BCR:H24C	26:4:613:CHL:CAA	2.46	0.45
18:5:144:ASP:OD1	18:5:147:ASN:ND2	2.49	0.45
19:6:260:LEU:HD22	19:6:263:LEU:HD23	1.97	0.45
1:A:72:LYS:NZ	1:A:181:TYR:OH	2.48	0.45
1:A:250:MET:HG3	1:A:257:PHE:CD2	2.50	0.45
25:A:1108:CLA:HED2	16:3:298:GLY:O	2.17	0.45
25:B:1213:CLA:H52	25:B:1213:CLA:C1C	2.46	0.45
3:C:30:PRO:HG3	4:D:299:ALA:HA	1.97	0.45
25:a:607:CLA:H101	25:a:607:CLA:H62	1.67	0.45
29:5:504:BCR:H383	26:5:610:CHL:H52	1.98	0.45
26:5:610:CHL:HBB2	25:5:612:CLA:CBC	2.46	0.45
29:6:504:BCR:H351	29:6:504:BCR:H15C	1.60	0.45
25:2:621:CLA:H192	25:2:621:CLA:H162	1.71	0.45
2:B:48:PHE:CE2	2:B:52:PHE:HE2	2.35	0.45
2:B:632:LEU:HD22	2:B:725:PHE:HA	1.98	0.45
25:B:1222:CLA:HAA2	25:B:1223:CLA:OBD	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:612:CLA:H91	25:1:612:CLA:H143	1.97	0.45
43:a:502:LUT:H15	43:a:502:LUT:H201	1.87	0.45
25:3:605:CLA:H62	25:3:605:CLA:H93	1.71	0.45
17:4:39:PRO:O	17:4:41:HIS:N	2.46	0.45
33:5:802:PTY:H402	33:5:802:PTY:H371	1.72	0.45
21:8:123:LEU:HD21	26:8:613:CHL:CHD	2.47	0.45
29:8:503:BCR:H402	25:8:606:CLA:H61	1.99	0.45
1:A:251:ALA:HA	1:A:254:TYR:O	2.17	0.45
1:A:326:LEU:O	1:A:338:HIS:HB2	2.16	0.45
25:A:1124:CLA:H3A	25:A:1124:CLA:HBA2	1.55	0.45
25:B:1212:CLA:H51	25:B:1212:CLA:H11	1.72	0.45
25:B:1231:CLA:H93	25:B:1231:CLA:H62	1.66	0.45
3:C:74:THR:HG21	4:D:217:GLU:OE1	2.17	0.45
29:H:4001:BCR:H351	29:H:4001:BCR:H15C	1.79	0.45
26:1:604:CHL:HHC	26:1:604:CHL:HBB1	1.99	0.45
15:a:36:TRP:CE3	15:a:37:LEU:HB2	2.52	0.45
25:3:601:CLA:H151	25:3:601:CLA:H18	1.74	0.45
17:4:188:ARG:HA	17:4:191:MET:HE3	1.98	0.45
21:8:208:PHE:HE1	43:8:501:LUT:H41	1.81	0.45
26:8:603:CHL:HBB1	26:8:603:CHL:HHC	1.99	0.45
25:8:620:CLA:HAA1	48:8:804:DGA:HBH1	1.98	0.45
1:A:409:ALA:HB1	29:A:4003:BCR:H271	1.99	0.44
1:A:473:SER:HB3	1:A:640:ASN:HD22	1.81	0.44
25:A:1101:CLA:H162	25:A:1101:CLA:H141	1.70	0.44
25:B:1236:CLA:HBA2	25:B:1240:CLA:H193	1.98	0.44
3:C:61:ASP:HA	3:C:62:PHE:HA	1.82	0.44
15:1:56:ASP:HA	44:1:502:AXT:O24	2.16	0.44
25:1:606:CLA:H92	25:1:606:CLA:H61	1.80	0.44
16:3:309:SER:HA	25:3:612:CLA:HED2	1.99	0.44
25:4:606:CLA:HBA2	25:4:616:CLA:HMB3	2.00	0.44
43:5:501:LUT:H35	43:5:501:LUT:H401	1.86	0.44
22:2:55:PRO:O	22:2:241:PRO:HG2	2.17	0.44
26:9:603:CHL:CGA	26:9:603:CHL:C1A	2.95	0.44
1:A:541:PHE:HZ	25:B:1022:CLA:HBB2	1.81	0.44
1:A:558:ARG:O	1:A:567:ALA:N	2.50	0.44
1:A:578:PRO:HG2	3:C:69:LEU:HD11	1.99	0.44
25:A:1013:CLA:CGA	25:A:1013:CLA:H3A	2.47	0.44
25:B:1229:CLA:H203	25:B:1235:CLA:H161	1.99	0.44
25:5:602:CLA:C1D	25:5:607:CLA:H71	2.47	0.44
19:6:259:PHE:HB2	29:6:504:BCR:H282	1.97	0.44
25:7:610:CLA:CAB	26:7:613:CHL:HBB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1133:CLA:C2D	25:A:1134:CLA:HAB	2.47	0.44
2:B:290:HIS:CD2	29:B:4001:BCR:H352	2.53	0.44
8:H:75:ARG:HG3	25:H:1703:CLA:HED2	1.98	0.44
25:B:1021:CLA:H121	25:B:1021:CLA:H161	1.55	0.44
25:B:1208:CLA:H2	25:B:1209:CLA:HMD1	1.99	0.44
25:1:612:CLA:HBA2	25:1:612:CLA:H3A	1.52	0.44
15:a:83:LEU:HG	25:a:601:CLA:HMC3	1.99	0.44
25:4:603:CLA:H2	25:4:608:CLA:HMD3	1.99	0.44
20:7:55:GLY:O	20:7:59:MET:HG3	2.18	0.44
25:8:618:CLA:HBA1	25:8:618:CLA:H3A	1.71	0.44
22:2:160:LYS:HG3	25:2:607:CLA:HED2	1.99	0.44
1:A:43:PRO:HB3	1:A:48:TRP:CE3	2.53	0.44
25:A:1105:CLA:H8	32:A:5005:SQD:H132	1.99	0.44
25:A:1122:CLA:H42	29:A:4004:BCR:H363	2.00	0.44
25:A:1130:CLA:H41	25:A:1130:CLA:H92	1.99	0.44
6:F:334:ARG:O	6:F:338:GLU:HG3	2.18	0.44
10:K:41:MET:HG3	25:K:1401:CLA:HMD3	2.00	0.44
26:4:618:CHL:H93	26:4:618:CHL:HBC3	1.99	0.44
18:5:133:GLU:HG3	25:5:612:CLA:C4B	2.48	0.44
43:7:501:LUT:H32	25:7:601:CLA:CAB	2.48	0.44
21:8:154:PHE:HE2	21:8:161:PHE:HE2	1.63	0.44
22:2:148:ASP:OD1	50:2:501:XAT:O23	2.29	0.44
25:2:604:CLA:H102	25:2:605:CLA:H91	2.00	0.44
43:9:502:LUT:H11	25:9:605:CLA:HBC3	2.00	0.44
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.48	0.44
1:A:419:PRO:HG3	4:D:233:GLU:HB2	2.00	0.44
1:A:646:LEU:HD22	2:B:652:LEU:HD21	2.00	0.44
1:A:690:ARG:H	2:B:569:CYS:HB2	1.81	0.44
2:B:211:ASP:HA	33:9:803:PTY:H312	2.00	0.44
25:B:1205:CLA:C1A	25:B:1205:CLA:CGA	2.96	0.44
30:F:5002:LHG:H312	26:8:610:CHL:H52	1.98	0.44
33:a:802:PTY:H392	33:a:802:PTY:H152	1.99	0.44
16:3:357:TYR:CZ	16:3:359:LYS:HB2	2.53	0.44
17:4:116:TRP:H	17:4:116:TRP:CD1	2.36	0.44
25:6:615:CLA:H92	25:6:615:CLA:H61	1.80	0.44
21:8:148:GLN:HG3	25:8:611:CLA:HMC2	1.98	0.44
48:8:804:DGA:HA52	48:8:804:DGA:HB91	1.99	0.44
50:2:501:XAT:H391	50:2:501:XAT:H31	1.70	0.44
25:A:1108:CLA:H13	29:A:4002:BCR:H372	1.99	0.44
32:A:5005:SQD:H461	32:A:5005:SQD:H241	1.79	0.44
2:B:345:ILE:HD12	25:B:1215:CLA:H101	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1220:CLA:CMD	25:B:1221:CLA:HAB	2.48	0.44
33:J:5001:PTY:H332	33:J:5001:PTY:H361	1.66	0.44
43:1:501:LUT:H15	43:1:501:LUT:H201	1.84	0.44
16:3:397:PHE:CE2	26:3:611:CHL:HBB2	2.52	0.44
17:4:90:GLN:NE2	17:4:105:VAL:O	2.38	0.44
21:8:170:PRO:HB3	25:8:611:CLA:HBC2	2.00	0.44
22:2:241:PRO:O	22:2:243:PRO:HD3	2.18	0.44
1:A:89:SER:HB2	1:A:166:ALA:HB3	1.99	0.44
1:A:217:GLN:HB3	1:A:295:VAL:HG22	1.99	0.44
1:A:300:ALA:HB1	25:A:1115:CLA:HBC2	2.00	0.44
1:A:677:PHE:HB2	25:A:1012:CLA:O1A	2.18	0.44
1:A:681:PHE:HZ	25:A:1139:CLA:HBC2	1.82	0.44
25:A:1115:CLA:CHD	25:A:1116:CLA:HBB2	2.48	0.44
25:A:1123:CLA:HBA1	25:A:1127:CLA:H203	2.00	0.44
2:B:5:LEU:HD22	13:I:35:ILE:HG12	2.00	0.44
2:B:436:GLY:HA3	25:B:1230:CLA:HAB	1.99	0.44
25:B:1231:CLA:H12	29:B:4005:BCR:HC42	2.00	0.44
6:F:457:TRP:CD1	6:F:458:PRO:HD3	2.53	0.44
25:G:1603:CLA:HBA2	25:G:1603:CLA:H3A	1.54	0.44
8:H:82:ARG:HB3	8:H:85:TYR:CD2	2.53	0.44
25:K:1404:CLA:H3A	25:K:1404:CLA:HBA1	1.76	0.44
12:M:20:ILE:O	12:M:23:VAL:HG12	2.17	0.44
15:a:49:LEU:HD13	26:a:604:CHL:HED1	2.00	0.44
15:a:134:MET:HG3	25:a:612:CLA:HMC3	1.99	0.44
18:5:141:ARG:HH21	48:5:803:DGA:HB51	1.83	0.44
26:6:609:CHL:HBB1	26:6:609:CHL:HMB3	1.98	0.44
1:A:299:LEU:HD21	25:A:1115:CLA:HAB	1.99	0.44
1:A:605:ILE:HD12	24:A:1011:CL0:H53	2.00	0.44
43:3:502:LUT:H391	26:3:603:CHL:H202	1.98	0.44
25:3:607:CLA:H143	25:3:607:CLA:H161	1.75	0.44
21:8:111:TYR:HB3	26:8:613:CHL:HBC1	1.99	0.44
2:B:90:HIS:ND1	2:B:91:ALA:O	2.51	0.43
2:B:429:PHE:CD1	25:B:1235:CLA:HAB	2.53	0.43
2:B:508:SER:HA	2:B:511:LEU:HD21	2.00	0.43
2:B:536:VAL:HG22	29:B:4004:BCR:H291	2.00	0.43
25:B:1240:CLA:HMB2	25:1:605:CLA:H93	2.00	0.43
11:L:379:ALA:O	11:L:383:ILE:HG12	2.18	0.43
14:O:92:ALA:O	14:O:94:PHE:N	2.51	0.43
25:O:1802:CLA:H41	25:O:1802:CLA:H62	1.37	0.43
43:a:501:LUT:H35	43:a:501:LUT:H401	1.81	0.43
17:4:141:TYR:HA	17:4:161:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:4:501:LUT:H35	43:4:501:LUT:H401	1.74	0.43
18:5:161:GLU:HG3	18:5:164:TYR:CD2	2.52	0.43
25:6:602:CLA:H51	25:6:602:CLA:H11	1.78	0.43
20:7:135:LYS:HG2	20:7:145:VAL:HG23	1.98	0.43
21:8:183:SER:OG	21:8:185:GLU:OE1	2.27	0.43
23:9:385:PHE:CE1	43:9:502:LUT:H10	2.52	0.43
30:9:801:LHG:H102	30:9:801:LHG:H132	1.86	0.43
25:A:1013:CLA:C2	25:A:1013:CLA:HMA2	2.48	0.43
25:A:1105:CLA:HHC	25:A:1105:CLA:HBB1	1.99	0.43
25:A:1108:CLA:H41	25:A:1108:CLA:H61	1.59	0.43
25:A:1115:CLA:H91	25:A:1115:CLA:H111	1.71	0.43
25:A:1120:CLA:C3D	29:K:4001:BCR:H271	2.48	0.43
25:A:1120:CLA:C4D	29:K:4001:BCR:H271	2.49	0.43
2:B:637:ASN:HB2	2:B:638:PRO:HD2	1.99	0.43
8:H:56:MET:HG2	8:H:57:TYR:CE2	2.53	0.43
15:1:61:ALA:HB2	26:1:604:CHL:HBA1	1.99	0.43
43:3:501:LUT:H15	43:3:501:LUT:H201	1.88	0.43
26:9:601:CHL:H3A	26:9:601:CHL:HBA2	1.37	0.43
25:A:1127:CLA:H61	25:A:1127:CLA:H41	1.72	0.43
2:B:646:VAL:HA	25:B:1206:CLA:HBC2	2.00	0.43
25:B:1209:CLA:H141	25:B:1209:CLA:H161	1.76	0.43
25:G:1602:CLA:H112	25:9:609:CLA:HAC1	2.01	0.43
8:H:34:LYS:HG3	8:H:50:THR:HG22	2.00	0.43
8:H:70:SER:O	8:H:74:GLU:HG2	2.18	0.43
11:L:313:THR:C	11:L:315:VAL:H	2.27	0.43
25:4:605:CLA:HMD2	25:4:610:CLA:H51	2.00	0.43
18:5:209:LYS:HB2	18:5:214:ASN:HD21	1.84	0.43
19:6:149:ASP:HB3	19:6:152:PHE:O	2.18	0.43
21:8:79:TRP:CE2	25:8:612:CLA:HBC3	2.53	0.43
48:2:803:DGA:HA52	48:2:803:DGA:HA81	1.51	0.43
1:A:245:LEU:HD21	26:A:1114:CHL:H192	2.01	0.43
1:A:689:GLY:O	1:A:693:TRP:HD1	2.01	0.43
25:A:1133:CLA:H93	25:A:1133:CLA:H112	1.82	0.43
25:A:1133:CLA:H121	25:A:1133:CLA:H161	1.69	0.43
34:A:5007:3PH:H282	48:3:803:DGA:HB62	2.00	0.43
2:B:271:LEU:HD23	2:B:274:MET:HE3	2.01	0.43
10:K:112:LYS:HB3	10:K:117:LEU:HD23	2.00	0.43
30:1:801:LHG:H271	30:1:801:LHG:H102	2.00	0.43
44:7:504:AXT:H191	44:7:504:AXT:H11	1.73	0.43
44:7:504:AXT:O3	25:7:612:CLA:H52	2.18	0.43
25:2:603:CLA:H62	25:2:603:CLA:H41	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:801:LHG:H341	23:9:337:PHE:CD2	2.54	0.43
1:A:264:PHE:HB2	1:A:272:TYR:HE2	1.84	0.43
25:B:1021:CLA:HBA2	25:B:1021:CLA:H3A	1.52	0.43
29:H:4001:BCR:H24C	11:L:440:TRP:NE1	2.22	0.43
32:H:5001:SQD:H252	25:2:612:CLA:H11	1.99	0.43
25:L:1502:CLA:HMA3	25:L:1503:CLA:HBC1	2.01	0.43
15:a:169:LEU:HD21	25:a:602:CLA:H43	1.99	0.43
25:a:612:CLA:HBA2	25:a:612:CLA:H3A	1.44	0.43
25:3:605:CLA:H2	25:3:605:CLA:H61	1.71	0.43
25:3:616:CLA:HBC3	18:5:227:TRP:CH2	2.53	0.43
19:6:265:PRO:HB2	26:6:619:CHL:HAB	1.99	0.43
37:6:803:PCW:H20	37:6:803:PCW:H171	1.66	0.43
20:7:214:THR:HG22	25:7:603:CLA:HED1	2.00	0.43
22:2:148:ASP:OD2	22:2:153:ARG:HB2	2.19	0.43
25:2:603:CLA:HBA1	25:2:603:CLA:CBD	2.46	0.43
43:9:501:LUT:H32	26:9:601:CHL:CAB	2.49	0.43
1:A:293:ASP:HB3	25:A:1116:CLA:HMA1	2.00	0.43
24:A:1011:CL0:H53	24:A:1011:CL0:H61	1.73	0.43
2:B:465:GLN:NE2	25:B:1234:CLA:OBD	2.36	0.43
2:B:517:ASP:HA	2:B:520:VAL:HG12	1.99	0.43
7:G:1324:ASN:OD1	25:G:1603:CLA:HAC2	2.18	0.43
25:H:1703:CLA:HMA3	25:2:612:CLA:HMA2	2.00	0.43
9:J:29:THR:HB	9:J:31:PRO:HD2	1.99	0.43
43:a:503:LUT:H35	43:a:503:LUT:H401	1.64	0.43
29:4:503:BCR:H351	29:4:503:BCR:H15C	1.64	0.43
29:4:503:BCR:H19C	26:4:613:CHL:O1A	2.18	0.43
18:5:64:LYS:HZ3	36:7:806:DGD:HD3	1.83	0.43
50:7:502:XAT:H31	50:7:502:XAT:H391	1.74	0.43
25:8:609:CLA:H62	25:8:609:CLA:H92	1.82	0.43
25:A:1119:CLA:H141	25:A:1119:CLA:H161	1.71	0.43
25:B:1224:CLA:H91	25:B:1224:CLA:H111	1.70	0.43
27:B:2002:PQN:H251	27:B:2002:PQN:H211	1.90	0.43
8:H:90:VAL:HG12	32:I:5001:SQD:H322	2.01	0.43
10:K:32:TYR:HB3	37:K:5001:PCW:H32	1.99	0.43
15:1:141:ARG:O	15:1:149:ARG:HG2	2.18	0.43
15:1:212:VAL:HG12	25:1:603:CLA:HED1	2.01	0.43
25:4:615:CLA:H2	25:4:615:CLA:HAA2	2.00	0.43
25:5:612:CLA:H203	25:5:612:CLA:H162	1.72	0.43
23:9:327:LEU:HD21	26:9:613:CHL:CHD	2.49	0.43
25:9:605:CLA:H112	25:9:605:CLA:H91	1.70	0.43
25:A:1106:CLA:C3D	25:A:1126:CLA:HBA1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1111:CLA:H141	25:A:1111:CLA:H161	1.79	0.43
25:A:1125:CLA:HED2	25:A:1133:CLA:HAB	1.99	0.43
25:A:1131:CLA:CAD	29:L:4002:BCR:H10C	2.49	0.43
6:F:442:ILE:HB	9:J:33:LEU:HD12	2.00	0.43
25:G:1603:CLA:ND	33:G:5003:PTY:H142	2.33	0.43
25:1:601:CLA:H92	25:1:601:CLA:H61	1.69	0.43
16:3:250:ASP:O	16:3:252:ALA:N	2.48	0.43
18:5:142:LYS:O	18:5:145:SER:OG	2.21	0.43
25:5:609:CLA:HBA2	30:5:801:LHG:HC62	2.01	0.43
26:5:618:CHL:HED1	30:6:801:LHG:H332	2.01	0.43
20:7:73:LYS:HD3	20:7:202:ASP:OD1	2.19	0.43
20:7:135:LYS:HG2	20:7:145:VAL:CG2	2.48	0.43
23:9:383:THR:HG22	26:9:603:CHL:HBB1	2.01	0.43
25:A:1129:CLA:HAB	25:A:1137:CLA:HBB2	2.00	0.43
2:B:577:PHE:O	2:B:581:VAL:HG23	2.19	0.43
2:B:649:TRP:HH2	25:B:1022:CLA:H111	1.83	0.43
25:B:1239:CLA:H161	25:B:1239:CLA:H192	1.80	0.43
25:1:608:CLA:H42	26:1:609:CHL:H12	2.01	0.43
21:8:136:ILE:HG12	53:8:810:LAP:H191	2.00	0.43
1:A:412:PHE:CD1	1:A:416:ASP:HB2	2.54	0.43
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.54	0.43
25:A:1119:CLA:H3A	25:A:1119:CLA:HBA2	1.64	0.43
25:A:1139:CLA:HBA2	25:A:1139:CLA:H3A	1.35	0.43
27:A:2001:PQN:H222	27:A:2001:PQN:H261	1.80	0.43
29:A:4003:BCR:H313	14:O:117:LEU:HA	2.01	0.43
32:A:5005:SQD:O47	32:A:5005:SQD:O2	2.28	0.43
25:B:1220:CLA:H101	29:B:4004:BCR:C11	2.48	0.43
11:L:314:PRO:O	11:L:318:SER:HB2	2.18	0.43
14:O:104:PHE:HZ	25:O:1801:CLA:HMD3	1.84	0.43
25:4:615:CLA:H91	25:4:615:CLA:H112	1.75	0.43
25:6:615:CLA:HAB	37:6:803:PCW:C37	2.49	0.43
44:7:504:AXT:H15	25:8:615:CLA:HBC1	2.01	0.43
30:9:802:LHG:H212	30:9:802:LHG:H182	1.72	0.43
1:A:439:SER:HB3	2:B:678:THR:HG22	2.01	0.42
25:A:1103:CLA:H51	25:A:1111:CLA:H12	2.01	0.42
25:A:1105:CLA:ND	32:A:5005:SQD:H142	2.33	0.42
25:A:1126:CLA:H193	25:A:1126:CLA:H162	1.72	0.42
25:B:1225:CLA:HBA2	25:B:1225:CLA:H3A	1.36	0.42
25:B:1227:CLA:HAB	25:B:1236:CLA:CBB	2.49	0.42
25:B:1230:CLA:H41	25:B:1230:CLA:H61	1.84	0.42
3:C:15:THR:HG22	3:C:28:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:372:LYS:NZ	9:J:54:ASP:O	2.39	0.42
26:a:610:CHL:CBB	26:a:613:CHL:HBB2	2.49	0.42
48:5:803:DGA:HA22	48:5:803:DGA:HG12	1.84	0.42
19:6:205:THR:HG21	25:6:603:CLA:HED3	2.00	0.42
19:6:231:VAL:HB	26:6:619:CHL:C1C	2.49	0.42
50:9:504:XAT:H391	50:9:504:XAT:H31	1.72	0.42
1:A:55:ASP:OD2	30:A:5002:LHG:O2	2.36	0.42
15:a:80:TRP:CE2	25:a:612:CLA:HBC3	2.54	0.42
16:3:257:VAL:HG21	16:3:273:LEU:HD21	2.01	0.42
16:3:421:LEU:HA	18:5:38:VAL:HG12	2.00	0.42
25:5:612:CLA:H62	25:5:612:CLA:H2	1.77	0.42
50:7:502:XAT:H15	50:7:502:XAT:H201	1.78	0.42
25:8:612:CLA:H3A	25:8:612:CLA:HBA2	1.45	0.42
1:A:245:LEU:HD11	26:A:1114:CHL:HAC1	2.01	0.42
1:A:305:PHE:HZ	25:A:1117:CLA:H112	1.84	0.42
25:A:1012:CLA:C4	29:A:4005:BCR:H362	2.49	0.42
2:B:296:PHE:HA	7:G:1285:ILE:HD13	2.01	0.42
2:B:333:PHE:CE1	29:B:4005:BCR:H291	2.54	0.42
2:B:485:ALA:H	30:1:802:LHG:H122	1.85	0.42
25:B:1217:CLA:H51	25:B:1217:CLA:C4B	2.49	0.42
25:B:1226:CLA:H201	29:B:4007:BCR:H10C	2.02	0.42
5:E:49:ARG:CD	5:E:51:GLU:HB2	2.49	0.42
14:O:73:ALA:O	14:O:75:GLY:N	2.53	0.42
15:1:211:ALA:O	15:1:216:THR:HG21	2.19	0.42
25:1:603:CLA:H102	26:1:609:CHL:H61	2.02	0.42
25:4:601:CLA:H62	25:4:602:CLA:HMA2	2.01	0.42
47:8:807:PLM:H41	53:8:810:LAP:H202	2.00	0.42
1:A:371:MET:HE2	1:A:371:MET:HB3	1.97	0.42
1:A:402:ILE:HG23	29:A:4004:BCR:H343	2.01	0.42
25:A:1132:CLA:HMA1	11:L:359:LEU:HB3	2.01	0.42
25:A:1137:CLA:H112	29:A:4003:BCR:HC41	2.01	0.42
27:A:2001:PQN:H141	25:A:1140:CLA:HBB2	2.00	0.42
25:B:1225:CLA:ND	29:B:4002:BCR:H281	2.33	0.42
15:1:60:LEU:HD12	26:1:604:CHL:H11	2.02	0.42
25:a:608:CLA:HAA2	17:4:125:ILE:HG12	2.00	0.42
30:a:801:LHG:H101	29:4:503:BCR:H313	2.01	0.42
43:3:502:LUT:H15	43:3:502:LUT:H201	1.85	0.42
25:4:611:CLA:HHC	25:4:611:CLA:HBB1	2.00	0.42
18:5:35:PHE:O	18:5:38:VAL:HG22	2.19	0.42
18:5:131:PHE:HA	26:6:609:CHL:HBA1	2.01	0.42
25:5:612:CLA:H101	26:5:618:CHL:CBB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:6:501:LUT:H35	43:6:501:LUT:H401	1.84	0.42
25:2:603:CLA:H142	25:2:603:CLA:H111	1.86	0.42
1:A:45:THR:HG22	1:A:714:GLN:HB2	2.00	0.42
1:A:221:SER:O	1:A:225:ASN:HB2	2.19	0.42
1:A:737:ALA:HA	29:A:4005:BCR:HC42	2.01	0.42
25:A:1132:CLA:H202	25:A:1132:CLA:H161	1.70	0.42
2:B:227:PHE:HB3	32:G:5001:SQD:H261	2.01	0.42
2:B:477:PHE:H	2:B:480:SER:HB2	1.84	0.42
25:B:1202:CLA:HED2	25:B:1226:CLA:HBB2	2.01	0.42
27:B:2002:PQN:H142	29:B:4007:BCR:H271	2.02	0.42
10:K:33:LEU:HD23	37:K:5001:PCW:H321	2.01	0.42
25:3:613:CLA:H91	25:3:613:CLA:H111	1.72	0.42
17:4:163:TYR:HB3	25:4:601:CLA:O1D	2.18	0.42
20:7:183:MET:SD	25:7:604:CLA:HAB	2.60	0.42
44:7:504:AXT:H201	25:8:615:CLA:HBC1	2.01	0.42
25:8:618:CLA:H143	25:8:618:CLA:H112	1.80	0.42
25:8:620:CLA:H2A	25:8:620:CLA:HED2	2.01	0.42
22:2:76:ASN:ND2	25:2:612:CLA:OBD	2.52	0.42
22:2:81:MET:HB2	25:2:601:CLA:HMC3	2.01	0.42
25:A:1115:CLA:H62	25:A:1115:CLA:H41	1.67	0.42
2:B:312:PRO:C	2:B:314:GLY:H	2.27	0.42
2:B:451:GLU:CD	2:B:451:GLU:H	2.28	0.42
25:J:1901:CLA:HMC2	40:J:4002:RRX:H27	2.01	0.42
10:K:47:LEU:HB3	25:K:1403:CLA:HMC1	2.02	0.42
29:K:4002:BCR:H15C	29:K:4002:BCR:H351	1.83	0.42
15:1:72:GLU:HG2	25:1:612:CLA:HED3	2.02	0.42
15:1:169:LEU:HB3	25:1:601:CLA:CMA	2.50	0.42
25:1:612:CLA:H111	25:1:612:CLA:H143	1.66	0.42
16:3:414:GLY:HA3	25:3:601:CLA:HED2	2.00	0.42
17:4:90:GLN:NE2	17:4:103:ALA:O	2.53	0.42
18:5:209:LYS:HB2	18:5:214:ASN:ND2	2.34	0.42
25:5:607:CLA:H41	25:5:607:CLA:H61	1.70	0.42
25:5:614:CLA:CAD	19:6:221:LEU:HD11	2.50	0.42
22:2:124:ILE:HG13	22:2:125:LEU:N	2.34	0.42
1:A:566:LYS:NZ	2:B:674:GLU:OE2	2.37	0.42
2:B:339:LEU:HD22	2:B:383:ILE:HG23	2.01	0.42
2:B:556:TYR:HD2	25:B:1226:CLA:HED2	1.84	0.42
25:B:1220:CLA:HAB	25:B:1227:CLA:CMD	2.49	0.42
25:B:1223:CLA:C3B	25:B:1231:CLA:HMA2	2.50	0.42
25:1:601:CLA:H62	25:1:601:CLA:H41	1.85	0.42
25:1:612:CLA:H192	30:1:802:LHG:H361	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:a:503:LUT:H11	43:a:503:LUT:H191	1.85	0.42
25:3:613:CLA:H11	25:3:613:CLA:H51	1.70	0.42
20:7:122:PRO:HB2	20:7:145:VAL:HG13	2.02	0.42
21:8:89:ILE:HB	21:8:90:PRO:HD3	2.01	0.42
22:2:99:TRP:NE1	48:2:803:DGA:HB22	2.35	0.42
23:9:279:ARG:HH22	30:9:802:LHG:HC42	1.85	0.42
50:9:507:XAT:H30	25:9:606:CLA:CAD	2.50	0.42
25:9:607:CLA:HBC1	30:9:801:LHG:H132	2.02	0.42
1:A:264:PHE:CZ	29:K:4001:BCR:H343	2.55	0.42
1:A:535:VAL:HG21	1:A:609:HIS:HB2	2.02	0.42
1:A:685:PHE:HA	27:A:2001:PQN:H9	2.01	0.42
25:A:1013:CLA:H151	25:A:1013:CLA:H112	1.44	0.42
25:A:1104:CLA:H193	25:A:1104:CLA:H161	1.76	0.42
25:A:1113:CLA:H122	25:A:1113:CLA:H8	1.68	0.42
2:B:91:ALA:HA	2:B:114:VAL:HG12	2.02	0.42
25:B:1021:CLA:H142	25:B:1021:CLA:H111	1.81	0.42
25:B:1234:CLA:H93	25:B:1234:CLA:H61	1.71	0.42
33:B:5005:PTY:H342	9:J:48:ILE:HD11	2.01	0.42
39:F:4001:NEX:H373	39:F:4001:NEX:H23	1.84	0.42
15:a:126:LEU:HD11	26:a:613:CHL:HMD2	2.02	0.42
25:a:602:CLA:HHC	25:a:602:CLA:HBB1	2.02	0.42
16:3:423:LEU:HB2	25:3:601:CLA:HBA1	2.02	0.42
25:3:605:CLA:HED3	25:3:605:CLA:H72	2.02	0.42
19:6:203:GLN:HE22	29:6:504:BCR:H282	1.85	0.42
25:6:604:CLA:H192	25:6:604:CLA:H161	1.68	0.42
25:2:601:CLA:H91	25:2:601:CLA:H111	1.84	0.42
23:9:414:ASN:ND2	26:9:608:CHL:HED3	2.34	0.42
41:9:804:SPH:H161	41:9:804:SPH:H132	1.82	0.42
1:A:389:SER:HB3	25:A:1126:CLA:CMA	2.49	0.42
1:A:577:GLY:HA2	2:B:563:PRO:HD3	2.02	0.42
25:A:1118:CLA:H3A	25:A:1118:CLA:HBA2	1.35	0.42
25:A:1124:CLA:HAA2	25:A:1125:CLA:OBD	2.19	0.42
25:A:1131:CLA:H11	25:A:1131:CLA:H52	1.78	0.42
25:B:1204:CLA:HBC3	12:M:15:ALA:HB2	2.01	0.42
25:B:1224:CLA:H161	25:B:1224:CLA:H141	1.72	0.42
32:G:5001:SQD:H271	32:G:5001:SQD:H302	1.79	0.42
14:O:61:LEU:HB3	14:O:119:LEU:HA	2.02	0.42
15:a:211:ALA:O	15:a:216:THR:HG21	2.19	0.42
26:4:609:CHL:H12	26:4:609:CHL:H51	1.73	0.42
25:6:608:CLA:HBC1	25:6:603:CLA:H192	2.01	0.42
25:6:602:CLA:H41	25:6:602:CLA:H62	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:615:CLA:H142	25:6:615:CLA:H111	1.82	0.42
20:7:116:LEU:HD13	25:7:612:CLA:HMA2	2.02	0.42
43:7:501:LUT:H35	43:7:501:LUT:H401	1.83	0.42
50:7:502:XAT:H35	50:7:502:XAT:H401	1.91	0.42
26:7:617:CHL:H11	36:8:802:DGD:HA72	2.02	0.42
21:8:89:ILE:O	21:8:93:LEU:HG	2.20	0.42
22:2:57:ARG:HH12	30:2:802:LHG:HC2	1.85	0.42
22:2:110:ASP:HB3	22:2:113:THR:HG23	2.01	0.42
48:2:803:DGA:HAH2	48:2:803:DGA:HAT2	1.86	0.42
26:9:603:CHL:CHC	26:9:603:CHL:H71	2.50	0.42
30:A:5002:LHG:H122	30:A:5002:LHG:H151	1.69	0.42
25:B:1206:CLA:H161	25:B:1206:CLA:H122	1.44	0.42
25:B:1216:CLA:HBC2	25:B:1221:CLA:H18	2.02	0.42
29:B:4002:BCR:H321	29:B:4002:BCR:HC8	2.02	0.42
36:B:5003:DGD:HAE2	36:B:5003:DGD:HA81	1.75	0.42
30:1:801:LHG:H111	29:8:503:BCR:H313	2.02	0.42
16:3:315:ARG:HA	16:3:318:MET:HE3	2.00	0.42
25:4:604:CLA:HED2	25:4:604:CLA:H2A	2.02	0.42
18:5:135:ARG:HD2	26:6:609:CHL:HED3	2.01	0.42
43:5:505:LUT:H15	43:5:505:LUT:H201	1.76	0.42
19:6:99:VAL:HG12	19:6:100:LYS:HG3	2.02	0.42
19:6:246:THR:HA	19:6:255:PRO:O	2.19	0.42
26:9:610:CHL:H2	33:9:803:PTY:C30	2.50	0.42
1:A:413:MET:HG3	1:A:558:ARG:HG3	2.02	0.41
25:A:1125:CLA:HBA1	25:A:1125:CLA:H3A	1.51	0.41
11:L:393:VAL:HG23	13:I:28:LEU:HD23	2.02	0.41
29:3:504:BCR:H372	25:3:613:CLA:H151	2.01	0.41
29:5:504:BCR:H332	19:6:237:VAL:HG11	2.02	0.41
25:6:608:CLA:H2	26:6:609:CHL:H151	2.01	0.41
20:7:160:LEU:HD23	20:7:160:LEU:HA	1.87	0.41
21:8:92:GLU:OE2	21:8:95:ARG:NH2	2.37	0.41
21:8:194:GLU:HB2	26:8:601:CHL:C1B	2.50	0.41
25:8:606:CLA:HED2	52:8:805:P5S:HB	2.02	0.41
26:2:609:CHL:H62	26:2:609:CHL:H41	1.76	0.41
30:2:802:LHG:H321	30:2:802:LHG:H352	1.61	0.41
43:9:501:LUT:C30	26:9:601:CHL:H8	2.50	0.41
1:A:96:ALA:HB2	1:A:159:LEU:HB2	2.02	0.41
1:A:116:GLN:NE2	25:A:1107:CLA:OBD	2.52	0.41
25:A:1113:CLA:H93	29:3:505:BCR:HC8	2.02	0.41
14:O:131:GLN:HG3	25:O:1802:CLA:HAA1	2.02	0.41
15:a:187:PHE:CD1	15:a:198:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:442:ARG:HA	16:3:445:MET:HE3	2.02	0.41
19:6:232:VAL:O	19:6:234:GLY:N	2.54	0.41
43:9:501:LUT:H35	43:9:501:LUT:H401	1.84	0.41
1:A:289:LEU:HD21	1:A:374:MET:HB3	2.00	0.41
1:A:366:ILE:HG12	25:A:1124:CLA:HED3	2.01	0.41
25:B:1230:CLA:HBA2	25:B:1230:CLA:H3A	1.73	0.41
4:D:218:GLU:OE1	4:D:276:ARG:HD3	2.20	0.41
32:G:5001:SQD:H262	32:G:5001:SQD:H111	2.01	0.41
11:L:365:VAL:HG12	11:L:367:ASN:H	1.85	0.41
40:3:506:RRX:H42	40:3:506:RRX:H47	1.76	0.41
25:4:610:CLA:H142	25:4:610:CLA:H111	1.69	0.41
25:6:603:CLA:H141	25:6:603:CLA:H161	1.85	0.41
25:7:610:CLA:CBB	26:7:613:CHL:HBB2	2.50	0.41
21:8:78:ARG:HA	21:8:81:MET:HE3	2.02	0.41
21:8:161:PHE:CZ	25:8:611:CLA:HAB	2.55	0.41
23:9:255:PRO:O	23:9:257:HIS:N	2.50	0.41
23:9:373:LYS:O	23:9:377:ASN:ND2	2.37	0.41
1:A:623:SER:C	1:A:625:ASN:H	2.28	0.41
1:A:687:PHE:HB2	25:A:1013:CLA:CBC	2.50	0.41
25:A:1115:CLA:H3A	25:A:1115:CLA:HBA2	1.80	0.41
25:A:1138:CLA:H93	25:A:1138:CLA:H61	1.90	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.94	0.41
25:G:1601:CLA:C2B	29:G:4001:BCR:H353	2.50	0.41
13:I:18:PHE:CD1	25:2:621:CLA:H151	2.56	0.41
43:4:502:LUT:H35	43:4:502:LUT:H401	1.78	0.41
47:4:804:PLM:HG1	25:8:602:CLA:HED1	2.03	0.41
18:5:252:LEU:HD23	18:5:252:LEU:HA	1.86	0.41
43:6:501:LUT:H15	43:6:501:LUT:H201	1.90	0.41
29:6:503:BCR:H351	29:6:503:BCR:H15C	1.84	0.41
29:7:503:BCR:H15C	29:7:503:BCR:H351	1.92	0.41
25:A:1138:CLA:C1B	25:B:1229:CLA:H41	2.51	0.41
25:B:1023:CLA:H62	25:B:1023:CLA:H92	1.83	0.41
25:B:1217:CLA:H62	25:B:1217:CLA:H41	1.74	0.41
25:B:1220:CLA:H101	29:B:4004:BCR:C10	2.51	0.41
9:J:43:GLY:O	9:J:47:GLU:HG2	2.19	0.41
11:L:443:LEU:O	11:L:447:ILE:HG12	2.21	0.41
25:a:603:CLA:H102	25:a:603:CLA:H62	1.48	0.41
26:a:613:CHL:HAA1	26:a:613:CHL:HBD	2.02	0.41
25:3:612:CLA:H3A	25:3:612:CLA:HBA2	1.36	0.41
43:4:502:LUT:H15	43:4:502:LUT:H201	1.87	0.41
25:7:604:CLA:H152	25:7:604:CLA:H112	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:161:GLU:HB2	25:2:601:CLA:CHB	2.51	0.41
1:A:510:TRP:CH2	25:A:1125:CLA:HBC2	2.54	0.41
25:A:1113:CLA:H3A	25:A:1113:CLA:H12	2.03	0.41
25:B:1205:CLA:HAB	25:B:1206:CLA:HAA2	2.03	0.41
25:B:1207:CLA:H111	8:H:96:GLY:HA3	2.01	0.41
11:L:383:ILE:HB	29:L:4001:BCR:H401	2.03	0.41
42:M:4001:ECH:H35	42:M:4001:ECH:H15	1.81	0.41
14:O:131:GLN:CG	25:O:1802:CLA:HBD	2.49	0.41
26:4:609:CHL:H161	26:4:609:CHL:H122	1.98	0.41
43:5:502:LUT:H32	25:5:604:CLA:CAB	2.50	0.41
19:6:195:PHE:CD1	43:6:502:LUT:H10	2.56	0.41
43:6:502:LUT:H15	43:6:502:LUT:H201	1.84	0.41
29:7:503:BCR:H332	25:8:609:CLA:H102	2.02	0.41
25:7:603:CLA:H51	25:7:603:CLA:C1C	2.50	0.41
25:2:608:CLA:HBA1	25:2:608:CLA:H3A	1.91	0.41
1:A:368:ALA:HB2	1:A:394:HIS:HB2	2.02	0.41
1:A:480:GLN:HA	1:A:481:PRO:HD3	1.89	0.41
1:A:747:ILE:HD12	1:A:747:ILE:HA	1.94	0.41
25:A:1123:CLA:HMD2	25:A:1123:CLA:H143	2.03	0.41
25:B:1213:CLA:H61	25:B:1213:CLA:H41	1.79	0.41
25:B:1215:CLA:H62	25:B:1215:CLA:H41	1.43	0.41
30:B:5002:LHG:H271	30:B:5002:LHG:H241	1.84	0.41
5:E:62:VAL:HB	5:E:74:VAL:HG12	2.02	0.41
9:J:45:LEU:HD13	29:J:4001:BCR:H24C	2.02	0.41
14:O:95:PRO:HB2	14:O:96:GLN:H	1.77	0.41
15:1:130:GLU:OE1	26:1:610:CHL:HMC	2.21	0.41
43:3:501:LUT:H11	43:3:501:LUT:H191	1.95	0.41
18:5:59:LEU:HD13	25:5:604:CLA:H42	2.02	0.41
25:6:615:CLA:H61	25:6:615:CLA:H41	1.76	0.41
21:8:170:PRO:O	21:8:174:PHE:HB2	2.21	0.41
43:2:507:LUT:H31	43:2:507:LUT:H391	1.75	0.41
23:9:385:PHE:CD2	43:9:502:LUT:H12	2.56	0.41
1:A:227:LEU:HD12	1:A:237:ILE:HG23	2.02	0.41
1:A:532:ASP:HA	1:A:535:VAL:HG12	2.03	0.41
25:A:1133:CLA:H193	25:A:1133:CLA:H162	1.87	0.41
2:B:286:ILE:O	2:B:290:HIS:ND1	2.39	0.41
2:B:445:GLN:HG3	2:B:616:TYR:CD1	2.55	0.41
25:B:1207:CLA:H93	25:B:1207:CLA:H112	1.89	0.41
7:G:1295:THR:O	7:G:1299:VAL:HG23	2.20	0.41
21:8:140:GLU:OE2	53:8:810:LAP:H192	2.21	0.41
21:8:195:ILE:HD12	21:8:195:ILE:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:175:PHE:CE1	22:2:186:PRO:HB3	2.54	0.41
43:9:501:LUT:H15	43:9:501:LUT:H201	1.84	0.41
1:A:15:ILE:HD13	25:A:1108:CLA:HAA2	2.03	0.41
1:A:486:TRP:HA	14:O:101:THR:OG1	2.21	0.41
1:A:488:GLN:HG3	1:A:510:TRP:HA	2.02	0.41
1:A:680:ALA:CB	25:A:1013:CLA:HBB2	2.51	0.41
1:A:740:TRP:CG	29:A:4005:BCR:HC41	2.56	0.41
25:A:1103:CLA:H2	25:A:1103:CLA:H62	1.80	0.41
25:A:1103:CLA:H112	25:A:1103:CLA:H152	1.62	0.41
25:A:1130:CLA:H8	25:L:1502:CLA:H91	2.02	0.41
25:A:1136:CLA:H51	25:A:1136:CLA:H11	1.77	0.41
2:B:352:HIS:HB3	25:B:1214:CLA:HED2	2.03	0.41
2:B:418:ALA:O	2:B:422:HIS:ND1	2.49	0.41
2:B:462:GLN:HG2	2:B:473:TYR:CE1	2.55	0.41
25:B:1021:CLA:H162	25:B:1021:CLA:H202	1.75	0.41
25:B:1023:CLA:H3A	25:B:1023:CLA:CGA	2.50	0.41
25:B:1220:CLA:H72	29:B:4004:BCR:C10	2.46	0.41
25:B:1226:CLA:H61	25:B:1226:CLA:H92	1.82	0.41
25:B:1229:CLA:HBB2	29:B:4006:BCR:HC41	2.02	0.41
3:C:28:MET:HE3	3:C:38:GLN:HB2	2.02	0.41
25:F:1302:CLA:O1D	20:7:116:LEU:HD11	2.21	0.41
8:H:43:ASP:N	8:H:50:THR:HG21	2.35	0.41
8:H:78:ASN:HD22	25:H:1703:CLA:HED3	1.86	0.41
42:M:4001:ECH:H20	42:M:4001:ECH:H36	1.77	0.41
14:O:61:LEU:CB	14:O:119:LEU:HD23	2.51	0.41
15:1:178:ARG:HA	15:1:181:MET:HE3	2.02	0.41
25:1:605:CLA:H52	25:1:605:CLA:H11	1.98	0.41
15:a:61:ALA:HB1	15:a:67:LEU:HD12	2.03	0.41
29:3:505:BCR:H351	29:3:505:BCR:H15C	1.81	0.41
17:4:131:ASN:HD22	26:4:618:CHL:HMA3	1.86	0.41
25:4:604:CLA:H142	25:4:604:CLA:H111	1.96	0.41
25:5:606:CLA:HMA3	26:5:613:CHL:CMC	2.51	0.41
21:8:131:PHE:HB3	25:8:612:CLA:HAB	2.02	0.41
43:8:501:LUT:H35	43:8:501:LUT:H401	1.87	0.41
25:8:609:CLA:H91	30:8:801:LHG:H311	2.03	0.41
22:2:99:TRP:CD1	48:2:803:DGA:HB22	2.55	0.41
23:9:342:ARG:HA	23:9:358:PHE:CZ	2.56	0.41
43:9:501:LUT:H11	43:9:501:LUT:H191	1.93	0.41
1:A:153:ILE:O	1:A:155:SER:N	2.49	0.41
2:B:396:VAL:HG11	2:B:556:TYR:HB2	2.03	0.41
25:B:1236:CLA:C4	29:B:4005:BCR:H10C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1294:PHE:HE2	7:G:1299:VAL:HG22	1.85	0.41
25:K:1402:CLA:H41	25:K:1402:CLA:H61	1.88	0.41
45:1:803:OLA:H81	45:1:803:OLA:H112	1.77	0.41
15:a:79:ARG:HA	15:a:82:MET:HE3	2.03	0.41
29:3:504:BCR:H362	25:3:601:CLA:H142	2.03	0.41
20:7:174:ASN:ND2	25:7:607:CLA:OBD	2.50	0.41
23:9:358:PHE:HA	23:9:359:PRO:HA	1.91	0.41
25:A:1140:CLA:H92	6:F:451:LEU:HD12	2.02	0.40
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.55	0.40
2:B:176:LEU:HD23	2:B:176:LEU:HA	1.91	0.40
25:B:1231:CLA:H121	25:B:1231:CLA:H8	1.91	0.40
6:F:411:PHE:O	6:F:412:ILE:C	2.65	0.40
33:J:5001:PTY:H312	51:7:807:4RF:H6	2.03	0.40
19:6:114:LEU:HD11	26:6:613:CHL:HHD	2.04	0.40
19:6:124:PHE:O	19:6:128:VAL:HG22	2.21	0.40
20:7:88:TYR:HB3	26:7:613:CHL:HBC1	2.03	0.40
23:9:374:GLU:HB2	26:9:601:CHL:C1B	2.51	0.40
1:A:348:SER:OG	1:A:416:ASP:OD2	2.30	0.40
1:A:448:LEU:HD11	25:A:1136:CLA:HMB2	2.03	0.40
25:A:1108:CLA:H202	25:A:1108:CLA:H161	1.79	0.40
2:B:311:PRO:HA	2:B:312:PRO:HD3	1.97	0.40
25:B:1230:CLA:H2A	25:B:1230:CLA:HED2	2.03	0.40
27:B:2002:PQN:H292	36:B:5003:DGD:HA81	2.04	0.40
6:F:392:PRO:HG3	39:F:4001:NEX:H42	2.02	0.40
11:L:352:LEU:HD23	11:L:376:ASN:OD1	2.21	0.40
15:a:89:LEU:O	15:a:93:VAL:HG22	2.21	0.40
17:4:119:LYS:HD3	25:4:610:CLA:HBC3	2.03	0.40
43:5:501:LUT:H15	43:5:501:LUT:H201	1.88	0.40
22:2:184:LYS:HB2	22:2:189:CYS:SG	2.60	0.40
50:9:507:XAT:H30	25:9:606:CLA:C3D	2.51	0.40
1:A:300:ALA:HA	25:A:1115:CLA:HMC2	2.02	0.40
25:A:1103:CLA:HBA1	25:A:1103:CLA:H3A	1.46	0.40
25:A:1131:CLA:H141	25:A:1131:CLA:H161	1.84	0.40
30:A:5001:LHG:H171	30:A:5001:LHG:H201	1.86	0.40
2:B:79:VAL:HG13	2:B:126:TYR:CE1	2.55	0.40
2:B:495:LEU:HD23	2:B:495:LEU:HA	1.77	0.40
25:H:1703:CLA:HBA2	25:H:1703:CLA:H12	1.95	0.40
15:1:178:ARG:HB3	26:1:604:CHL:CBC	2.52	0.40
26:1:609:CHL:H92	26:1:609:CHL:H62	1.79	0.40
16:3:314:CYS:CB	16:3:441:GLY:HA3	2.51	0.40
43:5:502:LUT:H35	43:5:502:LUT:H401	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:803:LHG:H102	30:7:803:LHG:H132	1.84	0.40
22:2:86:GLY:O	22:2:90:THR:HG23	2.22	0.40
25:2:602:CLA:H11	25:2:602:CLA:H51	1.87	0.40
1:A:321:SER:HB3	1:A:324:GLU:HB2	2.02	0.40
1:A:410:ALA:HB1	1:A:588:ALA:HB1	2.04	0.40
25:A:1131:CLA:OBD	29:L:4002:BCR:H10C	2.21	0.40
29:A:4005:BCR:H351	29:A:4005:BCR:H15C	1.95	0.40
35:A:5008:LMT:H31	35:A:5008:LMT:H62	1.77	0.40
2:B:66:LEU:HD11	29:B:4003:BCR:H281	2.03	0.40
2:B:416:LYS:HB2	2:B:540:LEU:HD13	2.04	0.40
2:B:490:GLY:O	2:B:495:LEU:HB2	2.21	0.40
15:a:40:SER:OG	15:a:41:GLU:N	2.54	0.40
25:a:605:CLA:HED2	25:a:605:CLA:H2A	2.03	0.40
16:3:360:TYR:CE1	25:3:606:CLA:HAA2	2.56	0.40
17:4:151:PRO:HG2	29:4:503:BCR:H333	2.04	0.40
43:4:501:LUT:H11	43:4:501:LUT:H191	1.93	0.40
20:7:46:TRP:CE2	51:7:807:4RF:H39	2.56	0.40
20:7:62:VAL:HG11	43:7:501:LUT:H12	2.03	0.40
25:8:602:CLA:H61	25:8:602:CLA:H41	1.89	0.40
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.86	0.40
1:A:615:GLN:HB3	1:A:631:THR:HG23	2.03	0.40
1:A:650:LEU:O	1:A:654:SER:HB2	2.20	0.40
25:A:1116:CLA:H3A	25:A:1116:CLA:HBA2	1.85	0.40
25:A:1130:CLA:NC	25:L:1502:CLA:H112	2.36	0.40
34:A:5007:3PH:H361	34:A:5007:3PH:H332	1.74	0.40
2:B:379:ILE:O	2:B:383:ILE:HG13	2.21	0.40
2:B:594:TYR:HA	2:B:620:TRP:HH2	1.86	0.40
4:D:258:LEU:HD12	4:D:258:LEU:HA	1.85	0.40
41:J:5002:SPH:H5	41:J:5002:SPH:H82	1.73	0.40
26:1:611:CHL:HHD	26:1:611:CHL:HBC3	2.04	0.40
25:4:611:CLA:H11	25:4:611:CLA:H51	1.73	0.40
25:5:605:CLA:HED2	25:5:605:CLA:H2A	2.04	0.40
29:7:503:BCR:H23C	26:7:613:CHL:H2	2.03	0.40
22:2:145:ALA:HB3	22:2:146:PRO:HD3	2.04	0.40
25:2:604:CLA:H11	25:2:604:CLA:H52	1.87	0.40
25:9:604:CLA:H3A	25:9:604:CLA:CGA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	739/741 (100%)	709 (96%)	30 (4%)	0	100 100
2	B	729/731 (100%)	697 (96%)	32 (4%)	0	100 100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100 100
4	D	141/143 (99%)	129 (92%)	12 (8%)	0	100 100
5	E	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
6	F	163/165 (99%)	154 (94%)	9 (6%)	0	100 100
7	G	97/99 (98%)	94 (97%)	3 (3%)	0	100 100
8	H	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	11 29
9	J	39/41 (95%)	39 (100%)	0	0	100 100
10	K	84/86 (98%)	79 (94%)	5 (6%)	0	100 100
11	L	155/157 (99%)	144 (93%)	10 (6%)	1 (1%)	21 44
12	M	29/31 (94%)	29 (100%)	0	0	100 100
13	I	33/35 (94%)	29 (88%)	4 (12%)	0	100 100
14	O	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3 6
15	1	190/192 (99%)	174 (92%)	15 (8%)	1 (0%)	24 48
15	a	190/192 (99%)	171 (90%)	19 (10%)	0	100 100
16	3	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30 54
17	4	205/207 (99%)	184 (90%)	19 (9%)	2 (1%)	12 32
18	5	227/229 (99%)	214 (94%)	13 (6%)	0	100 100
19	6	229/231 (99%)	213 (93%)	15 (7%)	1 (0%)	30 54
20	7	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	24 48
21	8	217/219 (99%)	207 (95%)	10 (5%)	0	100 100
22	2	213/215 (99%)	197 (92%)	16 (8%)	0	100 100
23	9	181/183 (99%)	171 (94%)	10 (6%)	0	100 100
All	All	4636/4684 (99%)	4348 (94%)	277 (6%)	11 (0%)	44 68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	118	PRO
14	O	93	ASN
14	O	95	PRO
15	1	36	TRP
17	4	224	PHE
14	O	94	PHE
16	3	265	LYS
19	6	255	PRO
11	L	447	ILE
20	7	164	SER
17	4	218	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/600 (100%)	600 (100%)	0	100	100
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	71 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	66/66 (100%)	66 (100%)	0	100	100
11	L	122/122 (100%)	122 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
13	I	30/30 (100%)	30 (100%)	0	100	100
14	O	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	1	134/134 (100%)	134 (100%)	0	100	100
15	a	134/134 (100%)	134 (100%)	0	100	100
16	3	186/186 (100%)	186 (100%)	0	100	100
17	4	165/165 (100%)	165 (100%)	0	100	100
18	5	185/185 (100%)	185 (100%)	0	100	100
19	6	187/187 (100%)	187 (100%)	0	100	100
20	7	176/176 (100%)	176 (100%)	0	100	100
21	8	168/168 (100%)	168 (100%)	0	100	100
22	2	173/173 (100%)	173 (100%)	0	100	100
23	9	141/141 (100%)	141 (100%)	0	100	100
All	All	3692/3692 (100%)	3692 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	182	HIS
1	A	442	ASN
1	A	451	HIS
1	A	722	GLN
2	B	77	GLN
2	B	159	GLN
2	B	171	ASN
2	B	375	HIS
2	B	491	GLN
2	B	586	ASN
3	C	38	GLN
5	E	89	ASN
8	H	78	ASN
10	K	38	ASN
10	K	101	HIS
14	O	93	ASN
14	O	131	GLN
15	a	35	ASN
15	a	165	ASN
15	a	217	ASN

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Mol	Chain	Res	Type
17	4	75	GLN
17	4	76	ASN
17	4	131	ASN
17	4	200	GLN
17	4	218	ASN
17	4	222	ASN
18	5	75	GLN
18	5	76	ASN
18	5	189	ASN
18	5	233	HIS
20	7	213	HIS
21	8	71	ASN
21	8	76	ASN
21	8	234	ASN
22	2	76	ASN
22	2	164	ASN
22	2	209	ASN
22	2	232	GLN
23	9	318	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

403 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	$\#\|Z\| > 2$
25	CLA	A	1113	-	64,68,73	1.40	6 (9%)	76,107,113	1.94	18 (23%)
25	CLA	1	608	-	64,68,73	1.39	8 (12%)	76,107,113	1.89	16 (21%)
25	CLA	K	1401	-	50,54,73	1.58	6 (12%)	59,90,113	1.98	14 (23%)
33	PTY	G	5002	-	27,27,49	1.04	2 (7%)	28,31,54	1.07	1 (3%)
25	CLA	A	1111	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	16 (19%)
45	OLA	1	803	-	19,19,19	0.57	0	19,19,19	1.02	0
29	BCR	I	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	15 (26%)
25	CLA	B	1231	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	16 (19%)
25	CLA	2	615	-	60,64,73	1.46	7 (11%)	71,102,113	2.02	19 (26%)
49	13X	6	805	-	9,9,9	0.92	0	12,12,12	0.36	0
29	BCR	A	4004	-	41,41,41	1.63	4 (9%)	56,56,56	4.47	18 (32%)
30	LHG	4	801	-	48,48,48	0.39	0	51,54,54	1.01	2 (3%)
43	LUT	8	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.75	15 (29%)
43	LUT	3	502	-	42,43,43	2.48	1 (2%)	51,60,60	1.82	15 (29%)
26	CHL	8	610	-	50,64,74	1.38	8 (16%)	46,102,114	1.85	11 (23%)
26	CHL	1	611	-	50,64,74	1.40	9 (18%)	46,102,114	1.97	12 (26%)
25	CLA	8	607	30	50,54,73	1.57	6 (12%)	59,90,113	2.04	13 (22%)
25	CLA	3	602	-	50,54,73	1.59	8 (16%)	59,90,113	2.02	17 (28%)
35	LMT	1	804	-	36,36,36	1.14	6 (16%)	47,47,47	1.03	3 (6%)
29	BCR	3	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.47	13 (23%)
25	CLA	5	606	-	54,58,73	1.53	8 (14%)	64,95,113	2.07	17 (26%)
40	RRX	J	4002	-	42,42,42	5.02	24 (57%)	56,58,58	2.71	21 (37%)
25	CLA	A	1101	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	21 (25%)
43	LUT	a	501	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	13 (25%)
25	CLA	B	1204	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	20 (24%)
26	CHL	a	610	-	42,56,74	1.53	9 (21%)	36,92,114	2.06	11 (30%)
25	CLA	B	1238	-	69,73,73	1.35	8 (11%)	82,113,113	1.87	17 (20%)
43	LUT	6	501	-	42,43,43	2.43	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	A	1106	1	69,73,73	1.34	8 (11%)	82,113,113	1.94	19 (23%)
30	LHG	F	5001	-	42,42,48	0.42	0	45,48,54	1.11	2 (4%)
25	CLA	4	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
25	CLA	A	1138	-	69,73,73	1.35	7 (10%)	82,113,113	1.78	16 (19%)
25	CLA	H	1703	-	59,63,73	1.45	7 (11%)	70,101,113	1.98	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PCW	K	5002	-	35,35,53	1.33	4 (11%)	41,43,61	1.08	2 (4%)
25	CLA	5	609	18	55,59,73	1.53	8 (14%)	64,96,113	2.02	17 (26%)
25	CLA	O	1802	-	59,63,73	1.47	7 (11%)	70,101,113	2.05	21 (30%)
33	PTY	G	5003	-	27,27,49	1.04	2 (7%)	28,31,54	1.08	1 (3%)
25	CLA	7	602	-	48,52,73	1.61	6 (12%)	57,88,113	2.02	14 (24%)
25	CLA	2	604	-	60,64,73	1.46	7 (11%)	71,102,113	2.01	17 (23%)
26	CHL	6	610	-	50,64,74	1.44	9 (18%)	46,102,114	1.85	12 (26%)
45	OLA	a	805	-	19,19,19	0.57	0	19,19,19	1.00	0
25	CLA	5	605	-	50,54,73	1.60	8 (16%)	59,90,113	2.04	15 (25%)
29	BCR	K	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	14 (25%)
25	CLA	9	605	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	19 (25%)
29	BCR	6	504	-	41,41,41	1.63	4 (9%)	56,56,56	4.59	17 (30%)
33	PTY	a	802	-	37,37,49	1.02	4 (10%)	40,42,54	1.11	2 (5%)
25	CLA	a	607	-	62,66,73	1.43	7 (11%)	73,104,113	1.96	18 (24%)
43	LUT	2	507	-	42,43,43	2.48	1 (2%)	51,60,60	2.48	15 (29%)
36	DGD	8	802	-	60,60,67	1.17	6 (10%)	74,74,81	1.09	6 (8%)
30	LHG	8	801	25	36,36,48	0.44	0	39,42,54	1.17	3 (7%)
25	CLA	B	1225	-	69,73,73	1.35	7 (10%)	82,113,113	1.81	17 (20%)
25	CLA	A	1107	1	59,63,73	1.49	7 (11%)	70,101,113	1.96	17 (24%)
25	CLA	A	1102	25	59,63,73	1.46	6 (10%)	70,101,113	2.05	16 (22%)
25	CLA	5	603	18	60,64,73	1.45	7 (11%)	71,102,113	1.98	18 (25%)
25	CLA	6	607	30	59,63,73	1.47	7 (11%)	70,101,113	1.95	17 (24%)
25	CLA	H	1702	8	50,54,73	1.58	6 (12%)	59,90,113	2.10	14 (23%)
26	CHL	8	613	-	45,59,74	1.49	9 (20%)	40,96,114	2.11	12 (30%)
25	CLA	A	1103	-	69,73,73	1.33	6 (8%)	82,113,113	1.90	16 (19%)
25	CLA	A	1121	-	64,68,73	1.41	6 (9%)	76,107,113	1.99	18 (23%)
32	SQD	A	5005	-	52,54,54	0.78	0	62,65,65	0.85	2 (3%)
25	CLA	A	1115	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	18 (23%)
25	CLA	A	1120	-	53,57,73	1.53	7 (13%)	61,93,113	2.17	19 (31%)
30	LHG	F	5002	-	35,35,48	0.43	0	38,41,54	1.21	3 (7%)
26	CHL	6	611	-	45,59,74	1.54	9 (20%)	40,96,114	2.08	12 (30%)
25	CLA	G	1601	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	19 (29%)
29	BCR	L	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	15 (26%)
25	CLA	1	606	-	61,65,73	1.43	7 (11%)	72,103,113	2.05	16 (22%)
25	CLA	a	608	-	59,63,73	1.46	7 (11%)	70,101,113	1.97	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	LUT	5	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.81	10 (19%)
25	CLA	9	607	-	51,55,73	1.57	7 (13%)	60,91,113	2.07	17 (28%)
25	CLA	L	1502	-	64,68,73	1.40	7 (10%)	76,107,113	1.96	19 (25%)
47	PLM	8	806	-	15,16,17	0.39	0	14,15,17	0.88	0
25	CLA	2	605	-	64,68,73	1.42	8 (12%)	76,107,113	1.94	22 (28%)
43	LUT	9	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.72	13 (25%)
25	CLA	3	613	-	65,69,73	1.39	7 (10%)	77,108,113	1.91	19 (24%)
47	PLM	8	807	-	17,17,17	0.57	0	17,17,17	1.12	0
32	SQD	I	5001	-	52,54,54	0.79	0	62,65,65	0.83	2 (3%)
25	CLA	A	1141	-	49,53,73	1.60	8 (16%)	58,89,113	2.10	14 (24%)
32	SQD	G	5001	-	44,46,54	0.82	0	54,57,65	0.87	2 (3%)
25	CLA	5	614	18	50,54,73	1.59	7 (14%)	59,90,113	1.99	15 (25%)
25	CLA	8	620	-	49,53,73	1.61	8 (16%)	58,89,113	2.04	16 (27%)
29	BCR	G	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	15 (26%)
27	PQN	B	2002	-	34,34,34	0.38	0	43,45,45	1.06	3 (6%)
29	BCR	5	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.50	15 (26%)
30	LHG	2	802	-	48,48,48	0.39	0	51,54,54	1.13	4 (7%)
25	CLA	A	1118	-	59,63,73	1.46	7 (11%)	70,101,113	1.98	18 (25%)
25	CLA	6	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
25	CLA	B	1229	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	21 (25%)
25	CLA	8	615	21	50,54,73	1.57	7 (14%)	59,90,113	2.10	17 (28%)
25	CLA	5	608	-	49,53,73	1.61	7 (14%)	58,89,113	1.95	13 (22%)
26	CHL	a	606	-	50,64,74	1.41	9 (18%)	46,102,114	1.88	11 (23%)
26	CHL	1	613	-	42,56,74	1.48	8 (19%)	36,92,114	2.10	12 (33%)
26	CHL	8	603	21	60,74,74	1.41	9 (15%)	58,114,114	1.75	13 (22%)
30	LHG	7	801	25	36,36,48	0.44	0	39,42,54	1.12	3 (7%)
26	CHL	4	618	-	50,64,74	1.57	9 (18%)	46,102,114	1.88	13 (28%)
29	BCR	B	4006	-	41,41,41	1.62	4 (9%)	56,56,56	4.41	13 (23%)
26	CHL	6	613	-	45,59,74	1.52	8 (17%)	40,96,114	2.03	11 (27%)
25	CLA	4	611	-	60,64,73	1.44	7 (11%)	71,102,113	2.00	20 (28%)
26	CHL	5	611	-	45,59,74	1.73	9 (20%)	40,96,114	2.02	11 (27%)
25	CLA	A	1110	-	58,62,73	1.47	8 (13%)	68,99,113	2.02	18 (26%)
25	CLA	7	610	-	64,68,73	1.41	6 (9%)	76,107,113	1.92	20 (26%)
25	CLA	B	1205	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	19 (23%)
25	CLA	8	618	21	64,68,73	1.40	6 (9%)	76,107,113	1.98	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	LUT	1	503	-	42,43,43	2.47	1 (2%)	51,60,60	2.16	17 (33%)
25	CLA	A	1137	-	64,68,73	1.40	8 (12%)	76,107,113	1.95	22 (28%)
26	CHL	6	609	19	60,74,74	1.16	7 (11%)	58,114,114	1.65	11 (18%)
50	XAT	9	507	-	41,47,47	0.70	1 (2%)	54,74,74	1.99	15 (27%)
25	CLA	B	1232	-	49,53,73	1.60	7 (14%)	58,89,113	2.01	14 (24%)
25	CLA	2	621	22	69,73,73	1.37	7 (10%)	82,113,113	1.93	17 (20%)
29	BCR	B	4005	-	41,41,41	1.61	4 (9%)	56,56,56	4.46	13 (23%)
25	CLA	1	615	15	50,54,73	1.59	6 (12%)	59,90,113	2.03	12 (20%)
43	LUT	9	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.83	13 (25%)
25	CLA	6	605	-	50,54,73	1.59	8 (16%)	59,90,113	2.04	14 (23%)
25	CLA	2	608	-	49,53,73	1.60	7 (14%)	58,89,113	2.01	13 (22%)
43	LUT	7	501	-	42,43,43	2.47	1 (2%)	51,60,60	1.96	12 (23%)
43	LUT	2	502	-	42,43,43	2.47	1 (2%)	51,60,60	1.82	13 (25%)
25	CLA	B	1207	-	64,68,73	1.40	6 (9%)	76,107,113	1.89	17 (22%)
25	CLA	3	601	16	69,73,73	1.36	6 (8%)	82,113,113	1.84	17 (20%)
43	LUT	a	503	-	42,43,43	2.45	1 (2%)	51,60,60	2.15	14 (27%)
25	CLA	7	607	30	63,67,73	1.42	7 (11%)	74,105,113	1.96	15 (20%)
25	CLA	A	1119	-	69,73,73	1.36	6 (8%)	82,113,113	1.79	15 (18%)
25	CLA	B	1209	-	69,73,73	1.35	8 (11%)	82,113,113	1.88	17 (20%)
25	CLA	A	1117	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	15 (18%)
25	CLA	6	604	19	69,73,73	1.34	7 (10%)	82,113,113	1.87	21 (25%)
48	DGA	8	804	-	39,39,43	1.18	3 (7%)	41,41,45	1.58	3 (7%)
25	CLA	4	602	-	56,60,73	1.50	6 (10%)	65,97,113	2.01	19 (29%)
25	CLA	6	601	-	64,68,73	1.40	7 (10%)	76,107,113	1.94	19 (25%)
25	CLA	4	603	17	60,64,73	1.44	8 (13%)	71,102,113	1.94	18 (25%)
25	CLA	4	607	-	59,63,73	1.47	7 (11%)	70,101,113	2.00	18 (25%)
26	CHL	1	604	-	60,74,74	1.55	9 (15%)	58,114,114	1.74	12 (20%)
26	CHL	2	613	-	45,59,74	1.40	9 (20%)	40,96,114	2.14	11 (27%)
25	CLA	B	1234	-	58,69,73	1.51	7 (12%)	55,99,113	2.18	13 (23%)
25	CLA	A	1104	1	69,73,73	1.35	8 (11%)	82,113,113	1.87	20 (24%)
25	CLA	L	1504	-	54,58,73	1.54	7 (12%)	64,95,113	2.05	16 (25%)
30	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
43	LUT	6	502	-	42,43,43	2.41	1 (2%)	51,60,60	1.86	11 (21%)
25	CLA	a	615	15	50,54,73	1.60	7 (14%)	59,90,113	2.02	14 (23%)
25	CLA	2	606	-	50,54,73	1.59	7 (14%)	59,90,113	2.02	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	1128	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	14 (17%)
25	CLA	J	1901	9	46,50,73	1.65	6 (13%)	53,85,113	2.11	14 (26%)
25	CLA	a	605	-	59,63,73	1.47	7 (11%)	70,101,113	2.01	17 (24%)
41	SPH	J	5002	-	19,20,20	0.69	1 (5%)	18,21,21	0.92	0
37	PCW	6	803	-	35,35,53	1.32	4 (11%)	41,43,61	1.14	2 (4%)
26	CHL	2	609	22	60,74,74	1.44	9 (15%)	58,114,114	1.64	12 (20%)
25	CLA	A	1108	-	69,73,73	1.35	8 (11%)	82,113,113	1.83	18 (21%)
25	CLA	B	1022	54	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
25	CLA	B	1203	2	69,73,73	1.35	6 (8%)	82,113,113	1.83	18 (21%)
36	DGD	8	803	-	47,47,67	0.82	1 (2%)	61,61,81	1.10	4 (6%)
25	CLA	L	1501	11	54,58,73	1.53	7 (12%)	64,95,113	2.07	16 (25%)
26	CHL	6	617	19	37,51,74	1.63	8 (21%)	30,86,114	2.32	10 (33%)
43	LUT	8	502	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	12 (23%)
25	CLA	1	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.91	17 (22%)
24	CL0	A	1011	-	58,73,73	3.20	17 (29%)	60,113,113	2.83	17 (28%)
28	SF4	A	3001	1,2	0,12,12	-	-	-		
25	CLA	B	1208	-	58,62,73	1.39	6 (10%)	71,100,113	2.01	18 (25%)
30	LHG	3	801	25	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
25	CLA	A	1116	-	64,68,73	1.40	8 (12%)	76,107,113	1.91	18 (23%)
25	CLA	L	1503	-	49,53,73	1.61	8 (16%)	58,89,113	2.02	14 (24%)
29	BCR	B	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.48	17 (30%)
35	LMT	A	5008	-	36,36,36	1.16	5 (13%)	47,47,47	1.01	2 (4%)
25	CLA	1	607	30	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
25	CLA	B	1236	-	57,61,73	1.48	8 (14%)	67,98,113	2.00	19 (28%)
33	PTY	B	5005	-	41,41,49	0.95	4 (9%)	44,46,54	1.14	2 (4%)
30	LHG	1	801	25	34,34,48	0.45	0	37,40,54	1.17	3 (8%)
30	LHG	6	801	25	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
29	BCR	B	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	14 (25%)
26	CHL	7	613	-	55,69,74	1.51	9 (16%)	52,108,114	1.72	9 (17%)
34	3PH	A	5007	-	32,32,47	1.03	4 (12%)	35,37,52	1.23	2 (5%)
29	BCR	5	504	-	41,41,41	1.62	4 (9%)	56,56,56	4.70	17 (30%)
25	CLA	4	617	-	49,53,73	1.60	6 (12%)	58,89,113	2.07	16 (27%)
50	XAT	9	504	-	41,47,47	0.65	1 (2%)	54,74,74	6.35	15 (27%)
50	XAT	2	501	-	41,47,47	0.69	1 (2%)	54,74,74	2.00	14 (25%)
25	CLA	4	612	17	66,70,73	1.37	6 (9%)	78,109,113	1.97	17 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	1201	-	69,73,73	1.35	7 (10%)	82,113,113	4.03	22 (26%)
25	CLA	5	615	18	50,54,73	1.59	6 (12%)	59,90,113	2.02	15 (25%)
25	CLA	A	1013	-	69,73,73	1.34	6 (8%)	82,113,113	1.78	18 (21%)
26	CHL	1	610	-	42,56,74	1.43	7 (16%)	36,92,114	2.05	10 (27%)
25	CLA	K	1404	10	49,53,73	1.60	8 (16%)	58,89,113	2.05	14 (24%)
28	SF4	C	3002	3	0,12,12	-	-	-		
26	CHL	5	617	18	41,55,74	1.51	9 (21%)	35,91,114	2.13	12 (34%)
43	LUT	3	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.81	15 (29%)
43	LUT	a	502	-	42,43,43	2.44	1 (2%)	51,60,60	1.82	13 (25%)
25	CLA	4	604	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	17 (22%)
33	PTY	3	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.11	2 (5%)
25	CLA	9	602	-	50,54,73	1.59	7 (14%)	59,90,113	2.00	16 (27%)
25	CLA	3	607	30	69,73,73	1.36	7 (10%)	82,113,113	1.82	16 (19%)
25	CLA	A	1130	-	60,64,73	1.45	7 (11%)	71,102,113	1.97	17 (23%)
25	CLA	A	1133	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	16 (19%)
26	CHL	a	604	-	55,69,74	1.67	9 (16%)	52,108,114	1.90	12 (23%)
29	BCR	A	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.59	17 (30%)
25	CLA	3	618	16	50,54,73	1.59	7 (14%)	59,90,113	2.02	15 (25%)
25	CLA	5	601	18	64,68,73	1.40	7 (10%)	76,107,113	1.97	21 (27%)
25	CLA	G	1603	-	49,53,73	1.59	6 (12%)	58,89,113	2.03	16 (27%)
43	LUT	1	501	-	42,43,43	2.45	1 (2%)	51,60,60	1.82	15 (29%)
25	CLA	B	1023	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	18 (21%)
47	PLM	6	804	-	17,17,17	0.57	0	17,17,17	1.13	1 (5%)
29	BCR	A	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.43	17 (30%)
25	CLA	8	606	-	61,65,73	1.43	7 (11%)	72,103,113	1.94	16 (22%)
43	LUT	4	502	-	42,43,43	2.43	1 (2%)	51,60,60	1.82	11 (21%)
25	CLA	4	616	-	54,58,73	1.53	6 (11%)	64,95,113	2.04	17 (26%)
25	CLA	7	612	-	64,68,73	1.42	6 (9%)	76,107,113	1.91	16 (21%)
30	LHG	9	801	-	32,32,48	0.47	0	35,38,54	1.20	3 (8%)
26	CHL	a	613	-	40,54,74	1.46	8 (20%)	34,90,114	2.17	10 (29%)
25	CLA	A	1129	-	54,58,73	1.53	7 (12%)	64,95,113	2.06	17 (26%)
25	CLA	a	611	-	54,58,73	1.54	7 (12%)	64,95,113	2.04	16 (25%)
29	BCR	L	4001	-	41,41,41	1.59	4 (9%)	56,56,56	4.46	15 (26%)
25	CLA	4	605	-	50,54,73	1.59	7 (14%)	59,90,113	2.03	15 (25%)
29	BCR	B	4007	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	9	612	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)
38	LPX	F	5003	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
25	CLA	F	1301	-	54,58,73	1.52	6 (11%)	64,95,113	2.07	17 (26%)
40	RRX	3	506	-	42,42,42	5.05	24 (57%)	56,58,58	2.83	20 (35%)
46	QTB	a	504	-	19,19,19	2.59	4 (21%)	23,26,26	2.96	10 (43%)
25	CLA	B	1230	-	62,66,73	1.42	7 (11%)	73,104,113	1.99	19 (26%)
30	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.08	2 (5%)
33	PTY	J	5001	-	27,27,49	1.17	4 (14%)	30,32,54	1.21	2 (6%)
25	CLA	8	605	-	59,63,73	1.48	8 (13%)	70,101,113	2.00	19 (27%)
25	CLA	9	604	23	64,68,73	1.42	6 (9%)	76,107,113	1.94	19 (25%)
25	CLA	B	1220	-	64,68,73	1.40	6 (9%)	76,107,113	1.89	17 (22%)
25	CLA	B	1227	-	54,58,73	1.54	7 (12%)	64,95,113	2.08	19 (29%)
25	CLA	7	604	20	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
25	CLA	B	1226	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	16 (19%)
25	CLA	2	601	-	64,68,73	1.40	7 (10%)	76,107,113	2.04	18 (23%)
26	CHL	3	608	-	37,51,74	1.70	9 (24%)	30,86,114	2.19	10 (33%)
30	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.24	3 (8%)
43	LUT	4	501	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	10 (19%)
25	CLA	B	1219	2	63,67,73	1.42	6 (9%)	74,105,113	1.93	16 (21%)
43	LUT	5	505	-	42,43,43	2.48	1 (2%)	51,60,60	2.12	11 (21%)
48	DGA	3	803	-	23,23,43	1.43	3 (13%)	25,25,45	1.36	2 (8%)
45	OLA	8	808	-	19,19,19	0.58	0	19,19,19	1.02	0
41	SPH	6	806	-	19,20,20	0.66	0	18,21,21	1.08	1 (5%)
36	DGD	B	5003	-	67,67,67	1.30	7 (10%)	81,81,81	1.03	3 (3%)
30	LHG	B	5001	25	48,48,48	0.40	0	51,54,54	0.99	3 (5%)
44	AXT	1	502	-	44,44,45	3.01	16 (36%)	54,62,64	1.91	13 (24%)
37	PCW	K	5001	-	40,40,53	1.29	4 (10%)	46,48,61	1.09	2 (4%)
25	CLA	4	608	-	55,59,73	1.52	7 (12%)	64,96,113	2.07	17 (26%)
26	CHL	3	611	-	55,69,74	1.46	9 (16%)	52,108,114	1.72	12 (23%)
47	PLM	4	804	-	17,17,17	0.58	0	17,17,17	1.06	0
25	CLA	7	608	-	59,63,73	1.46	7 (11%)	70,101,113	2.00	17 (24%)
50	XAT	7	502	-	41,47,47	0.68	1 (2%)	54,74,74	1.95	10 (18%)
26	CHL	5	610	-	60,74,74	1.19	8 (13%)	58,114,114	1.70	11 (18%)
25	CLA	B	1221	-	69,73,73	1.36	8 (11%)	82,113,113	1.91	17 (20%)
25	CLA	B	1224	-	69,73,73	1.37	8 (11%)	82,113,113	1.88	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	1	602	-	49,53,73	1.61	7 (14%)	58,89,113	2.02	16 (27%)
30	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
25	CLA	9	609	23	50,54,73	1.58	7 (14%)	59,90,113	2.04	16 (27%)
25	CLA	B	1216	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	17 (20%)
25	CLA	2	612	-	54,58,73	1.53	7 (12%)	64,95,113	2.01	16 (25%)
43	LUT	5	501	-	42,43,43	2.44	1 (2%)	51,60,60	1.79	13 (25%)
25	CLA	1	605	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	20 (24%)
25	CLA	B	1206	2	69,73,73	1.36	6 (8%)	82,113,113	1.89	14 (17%)
47	PLM	4	803	-	15,16,17	0.39	0	14,15,17	0.89	0
25	CLA	A	1012	-	69,73,73	1.37	8 (11%)	82,113,113	1.89	17 (20%)
28	SF4	C	3003	3	0,12,12	-	-	-		
25	CLA	A	1131	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	16 (19%)
25	CLA	8	611	-	54,58,73	1.52	7 (12%)	64,95,113	2.06	17 (26%)
29	BCR	L	4003	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	14 (25%)
25	CLA	A	1127	-	69,73,73	1.35	6 (8%)	82,113,113	1.81	17 (20%)
25	CLA	B	1218	-	59,63,73	1.46	6 (10%)	70,101,113	2.10	19 (27%)
25	CLA	B	1235	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	19 (23%)
29	BCR	J	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.43	14 (25%)
26	CHL	9	608	-	42,56,74	1.60	9 (21%)	36,92,114	2.09	11 (30%)
25	CLA	6	612	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	17 (26%)
25	CLA	a	602	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	19 (29%)
26	CHL	4	613	-	46,60,74	1.47	9 (19%)	40,97,114	2.08	12 (30%)
25	CLA	9	606	-	59,63,73	1.47	8 (13%)	70,101,113	1.93	17 (24%)
25	CLA	8	608	-	56,60,73	1.49	6 (10%)	65,97,113	2.04	17 (26%)
33	PTY	a	803	-	37,37,49	1.01	4 (10%)	40,42,54	1.09	2 (5%)
25	CLA	B	1217	-	60,64,73	1.45	9 (15%)	71,102,113	2.03	21 (29%)
33	PTY	5	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.17	2 (5%)
25	CLA	6	618	-	50,54,73	1.59	6 (12%)	59,90,113	2.00	15 (25%)
36	DGD	7	806	-	51,51,67	0.96	3 (5%)	65,65,81	1.04	3 (4%)
25	CLA	B	1237	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	16 (19%)
25	CLA	B	1239	-	69,73,73	1.34	8 (11%)	82,113,113	1.86	19 (23%)
25	CLA	H	1701	-	59,63,73	1.46	6 (10%)	70,101,113	2.00	16 (22%)
30	LHG	9	802	-	48,48,48	0.39	0	51,54,54	1.14	3 (5%)
25	CLA	K	1403	10	53,57,73	1.54	6 (11%)	61,93,113	2.15	17 (27%)
26	CHL	A	1114	-	60,74,74	1.23	9 (15%)	58,114,114	1.74	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	SPH	4	805	-	19,20,20	0.65	0	18,21,21	1.09	1 (5%)
25	CLA	B	1215	-	64,68,73	1.39	7 (10%)	76,107,113	1.87	16 (21%)
51	4RF	7	807	-	36,36,56	1.08	6 (16%)	39,39,59	1.16	3 (7%)
44	AXT	7	504	-	44,44,45	2.44	17 (38%)	54,62,64	2.37	18 (33%)
29	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.25	13 (23%)
25	CLA	B	1202	-	69,73,73	1.34	8 (11%)	82,113,113	1.86	18 (21%)
25	CLA	F	1302	-	59,63,73	1.47	8 (13%)	70,101,113	1.98	18 (25%)
25	CLA	1	612	15	69,73,73	1.36	6 (8%)	82,113,113	1.86	17 (20%)
26	CHL	a	609	15	47,61,74	1.41	8 (17%)	41,98,114	1.99	11 (26%)
26	CHL	3	604	16	60,74,74	1.49	9 (15%)	58,114,114	1.88	12 (20%)
29	BCR	H	4001	-	41,41,41	1.61	4 (9%)	56,56,56	7.48	21 (37%)
25	CLA	A	1125	-	69,73,73	1.35	8 (11%)	82,113,113	1.86	21 (25%)
25	CLA	4	615	17	64,68,73	1.42	7 (10%)	76,107,113	1.86	16 (21%)
53	LAP	8	810	-	28,28,28	1.25	2 (7%)	33,35,35	1.02	1 (3%)
29	BCR	6	503	-	41,41,41	1.62	4 (9%)	56,56,56	4.41	13 (23%)
31	LMG	A	5004	-	42,42,55	0.86	2 (4%)	50,50,63	1.08	2 (4%)
26	CHL	5	613	-	50,64,74	1.30	7 (14%)	46,102,114	1.98	13 (28%)
26	CHL	4	609	17	60,74,74	1.29	9 (15%)	58,114,114	1.73	12 (20%)
32	SQD	H	5001	-	43,45,54	0.84	0	53,56,65	0.90	2 (3%)
25	CLA	A	1112	-	59,63,73	1.47	6 (10%)	70,101,113	2.07	16 (22%)
25	CLA	B	1212	-	61,65,73	1.43	6 (9%)	72,103,113	2.02	20 (27%)
25	CLA	5	602	-	56,60,73	1.51	6 (10%)	65,97,113	2.00	19 (29%)
25	CLA	6	602	-	56,60,73	1.50	7 (12%)	65,97,113	2.01	17 (26%)
25	CLA	3	610	16	61,65,73	1.43	7 (11%)	72,103,113	1.97	19 (26%)
25	CLA	3	616	-	60,64,73	1.45	7 (11%)	71,102,113	2.02	20 (28%)
25	CLA	B	1228	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	19 (23%)
42	ECH	M	4001	-	42,42,42	0.85	2 (4%)	55,58,58	2.04	15 (27%)
30	LHG	5	801	-	48,48,48	0.38	0	51,54,54	1.10	3 (5%)
25	CLA	a	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	16 (19%)
25	CLA	6	608	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	17 (24%)
25	CLA	7	606	-	58,62,73	1.49	6 (10%)	69,100,113	1.95	16 (23%)
25	CLA	2	602	-	56,60,73	1.51	7 (12%)	65,97,113	2.00	18 (27%)
25	CLA	A	1136	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
25	CLA	8	609	21	64,68,73	1.40	8 (12%)	76,107,113	1.98	20 (26%)
25	CLA	a	612	15	61,65,73	1.44	7 (11%)	72,103,113	1.91	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PCW	B	5004	-	38,38,53	1.31	4 (10%)	44,46,61	1.08	2 (4%)
25	CLA	a	601	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	20 (26%)
25	CLA	B	1214	-	63,67,73	1.42	7 (11%)	74,105,113	1.98	17 (22%)
26	CHL	7	609	20	56,70,74	1.43	9 (16%)	53,109,114	1.79	11 (20%)
35	LMT	2	804	-	36,36,36	1.16	6 (16%)	47,47,47	1.07	3 (6%)
30	LHG	2	801	25	48,48,48	0.36	0	51,54,54	1.04	2 (3%)
30	LHG	7	803	-	34,34,48	0.45	0	37,40,54	1.17	3 (8%)
29	BCR	8	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.41	13 (23%)
30	LHG	1	802	-	48,48,48	0.40	0	51,54,54	1.01	4 (7%)
25	CLA	K	1402	-	64,68,73	1.42	8 (12%)	76,107,113	1.94	17 (22%)
25	CLA	7	605	-	47,52,73	1.65	7 (14%)	55,88,113	1.94	14 (25%)
45	OLA	8	809	-	19,19,19	0.58	0	19,19,19	1.00	0
26	CHL	9	613	-	36,50,74	1.65	9 (25%)	29,85,114	2.25	9 (31%)
25	CLA	B	1240	30	69,73,73	1.37	8 (11%)	82,113,113	1.90	18 (21%)
25	CLA	4	601	-	64,68,73	1.40	6 (9%)	76,107,113	1.96	20 (26%)
29	BCR	3	504	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	16 (28%)
29	BCR	B	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	14 (25%)
25	CLA	A	1140	-	59,63,73	1.47	8 (13%)	70,101,113	2.01	19 (27%)
26	CHL	3	603	16	60,74,74	1.41	9 (15%)	58,114,114	1.76	13 (22%)
27	PQN	A	2001	-	34,34,34	0.38	0	43,45,45	1.15	3 (6%)
29	BCR	A	4005	-	41,41,41	1.59	4 (9%)	56,56,56	4.39	13 (23%)
29	BCR	B	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	14 (25%)
33	PTY	9	803	-	47,47,49	0.90	4 (8%)	50,52,54	1.12	2 (4%)
26	CHL	9	610	-	45,59,74	1.52	10 (22%)	40,96,114	1.98	11 (27%)
26	CHL	8	604	21	56,70,74	1.59	9 (16%)	53,109,114	1.89	13 (24%)
25	CLA	G	1602	7	64,68,73	1.41	7 (10%)	76,107,113	1.93	19 (25%)
25	CLA	5	612	18	69,73,73	1.34	7 (10%)	82,113,113	1.87	19 (23%)
26	CHL	2	610	-	42,56,74	1.47	9 (21%)	36,92,114	2.09	11 (30%)
25	CLA	A	1124	-	59,63,73	1.48	7 (11%)	70,101,113	1.96	19 (27%)
25	CLA	8	602	-	56,60,73	1.50	6 (10%)	65,97,113	2.04	18 (27%)
25	CLA	B	1021	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
25	CLA	O	1803	-	45,49,73	1.67	7 (15%)	54,84,113	2.11	17 (31%)
25	CLA	A	1132	-	69,73,73	1.34	7 (10%)	82,113,113	1.91	18 (21%)
25	CLA	O	1801	-	41,46,73	1.77	8 (19%)	47,80,113	2.07	12 (25%)
26	CHL	6	619	19	60,74,74	1.25	8 (13%)	58,114,114	1.80	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	BCR	3	505	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	15 (26%)
30	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.26	3 (7%)
32	SQD	7	805	-	37,39,54	0.89	0	47,50,65	0.94	3 (6%)
25	CLA	5	604	18	69,73,73	1.36	7 (10%)	82,113,113	1.88	16 (19%)
25	CLA	A	1109	25	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
33	PTY	A	5006	-	33,33,49	1.07	4 (12%)	36,38,54	1.12	2 (5%)
35	LMT	B	5006	-	36,36,36	1.15	6 (16%)	47,47,47	0.96	1 (2%)
26	CHL	9	601	-	60,74,74	1.38	8 (13%)	58,114,114	1.64	11 (18%)
25	CLA	B	1223	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	19 (23%)
30	LHG	A	5003	-	45,45,48	0.40	0	48,51,54	1.05	3 (6%)
25	CLA	7	601	20	64,68,73	1.41	7 (10%)	76,107,113	1.95	18 (23%)
25	CLA	8	612	-	54,58,73	1.52	6 (11%)	64,95,113	2.01	15 (23%)
47	PLM	5	804	-	17,17,17	0.59	0	17,17,17	1.12	0
25	CLA	A	1134	1	64,68,73	1.41	8 (12%)	76,107,113	1.99	20 (26%)
25	CLA	3	606	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	15 (18%)
25	CLA	6	615	54	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
25	CLA	7	603	20	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
52	P5S	8	805	-	35,36,53	1.18	3 (8%)	37,43,60	1.22	2 (5%)
25	CLA	B	1213	-	59,63,73	1.45	7 (11%)	70,101,113	2.00	17 (24%)
26	CHL	5	618	-	45,59,74	1.47	8 (17%)	40,96,114	2.06	12 (30%)
25	CLA	2	607	30	69,73,73	1.36	6 (8%)	82,113,113	1.89	19 (23%)
29	BCR	7	503	-	41,41,41	1.59	4 (9%)	56,56,56	4.47	17 (30%)
25	CLA	A	1126	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	20 (24%)
26	CHL	8	601	21	55,69,74	1.67	9 (16%)	52,108,114	1.89	13 (25%)
29	BCR	O	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.80	15 (26%)
30	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.11	3 (5%)
25	CLA	B	1210	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	20 (24%)
25	CLA	A	1139	-	59,63,73	1.47	8 (13%)	70,101,113	1.98	17 (24%)
25	CLA	4	606	-	54,58,73	1.54	8 (14%)	64,95,113	2.08	17 (26%)
25	CLA	6	606	19	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
47	PLM	a	804	-	15,16,17	0.39	0	14,15,17	0.92	0
48	DGA	5	803	-	22,22,43	1.45	3 (13%)	24,24,45	1.34	2 (8%)
25	CLA	5	607	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	19 (25%)
33	PTY	7	804	-	32,32,49	1.07	4 (12%)	35,37,54	1.20	2 (5%)
29	BCR	K	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.46	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	3	605	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)
25	CLA	3	612	16	54,58,73	1.50	6 (11%)	64,95,113	2.06	16 (25%)
29	BCR	4	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	11 (19%)
26	CHL	9	603	-	60,74,74	1.28	9 (15%)	58,114,114	1.75	11 (18%)
26	CHL	1	609	15	60,74,74	1.25	9 (15%)	58,114,114	1.80	12 (20%)
48	DGA	2	803	-	36,36,43	1.22	3 (8%)	38,38,45	1.36	3 (7%)
26	CHL	7	611	-	50,64,74	1.38	9 (18%)	46,102,114	2.00	12 (26%)
26	CHL	7	617	20	60,74,74	1.28	9 (15%)	58,114,114	1.78	12 (20%)
25	CLA	B	1211	-	59,63,73	1.47	8 (13%)	70,101,113	2.00	19 (27%)
25	CLA	A	1135	-	55,59,73	1.53	8 (14%)	64,96,113	2.10	20 (31%)
25	CLA	A	1105	-	61,65,73	1.43	6 (9%)	72,103,113	1.97	17 (23%)
26	CHL	7	615	20	45,59,74	1.49	9 (20%)	40,96,114	2.08	12 (30%)
39	NEX	F	4001	-	40,46,46	2.71	11 (27%)	50,70,70	4.73	15 (30%)
25	CLA	A	1122	-	64,68,73	1.41	7 (10%)	76,107,113	1.89	18 (23%)
25	CLA	2	603	22	64,68,73	1.41	6 (9%)	76,107,113	2.05	21 (27%)
25	CLA	A	1123	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	17 (20%)
25	CLA	B	1222	-	62,66,73	1.42	7 (11%)	73,104,113	1.96	18 (24%)
25	CLA	1	603	-	69,73,73	1.35	8 (11%)	82,113,113	1.86	16 (19%)
30	LHG	a	801	-	34,34,48	0.46	0	37,40,54	1.12	3 (8%)
41	SPH	9	804	-	19,20,20	0.66	0	18,21,21	1.09	0

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
25	CLA	A	1113	-	1/1/14/20	14/33/109/115	-
25	CLA	1	608	-	1/1/14/20	12/33/109/115	-
25	CLA	K	1401	-	1/1/11/20	4/17/93/115	-
33	PTY	G	5002	-	-	9/30/30/53	-
25	CLA	A	1111	-	1/1/15/20	17/39/115/115	-
45	OLA	1	803	-	-	6/17/17/17	-
29	BCR	I	4001	-	-	15/29/63/63	0/2/2/2
25	CLA	B	1231	-	1/1/15/20	15/39/115/115	-
25	CLA	2	615	-	1/1/13/20	8/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	13X	6	805	-	-	-	0/1/1/1
29	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
30	LHG	4	801	-	-	30/53/53/53	-
43	LUT	8	501	-	-	1/29/67/67	0/2/2/2
43	LUT	3	502	-	-	2/29/67/67	0/2/2/2
26	CHL	8	610	-	5/5/18/26	6/27/125/137	-
26	CHL	1	611	-	4/4/18/26	4/27/125/137	-
25	CLA	8	607	30	1/1/11/20	5/17/93/115	-
25	CLA	3	602	-	1/1/11/20	5/17/93/115	-
35	LMT	1	804	-	-	12/21/61/61	0/2/2/2
29	BCR	3	503	-	-	12/29/63/63	0/2/2/2
25	CLA	5	606	-	1/1/12/20	8/21/97/115	-
40	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
25	CLA	A	1101	-	1/1/15/20	22/39/115/115	-
43	LUT	a	501	-	-	5/29/67/67	0/2/2/2
25	CLA	B	1204	-	1/1/15/20	19/39/115/115	-
26	CHL	a	610	-	3/3/16/26	2/18/116/137	-
25	CLA	B	1238	-	1/1/15/20	10/39/115/115	-
43	LUT	6	501	-	-	3/29/67/67	0/2/2/2
25	CLA	A	1106	1	1/1/15/20	18/39/115/115	-
30	LHG	F	5001	-	-	27/47/47/53	-
25	CLA	4	610	-	1/1/15/20	22/39/115/115	-
25	CLA	A	1138	-	1/1/15/20	6/39/115/115	-
25	CLA	H	1703	-	1/1/13/20	11/27/103/115	-
37	PCW	K	5002	-	-	17/39/39/57	-
25	CLA	5	609	18	1/1/12/20	9/23/99/115	-
25	CLA	O	1802	-	1/1/13/20	13/27/103/115	-
33	PTY	G	5003	-	-	13/30/30/53	-
25	CLA	7	602	-	1/1/11/20	5/13/89/115	-
25	CLA	2	604	-	1/1/13/20	11/29/105/115	-
26	CHL	6	610	-	4/4/18/26	4/27/125/137	-
45	OLA	a	805	-	-	6/17/17/17	-
25	CLA	5	605	-	1/1/11/20	2/17/93/115	-
29	BCR	K	4001	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	9	605	-	1/1/14/20	12/33/109/115	-
29	BCR	6	504	-	-	12/29/63/63	0/2/2/2
33	PTY	a	802	-	-	20/41/41/53	-
25	CLA	a	607	-	1/1/13/20	13/31/107/115	-
43	LUT	2	507	-	1/1/12/27	19/29/67/67	0/2/2/2
36	DGD	8	802	-	-	19/48/88/95	0/2/2/2
30	LHG	8	801	25	-	28/41/41/53	-
25	CLA	B	1225	-	1/1/15/20	6/39/115/115	-
25	CLA	A	1107	1	1/1/13/20	9/27/103/115	-
25	CLA	A	1102	25	1/1/13/20	9/27/103/115	-
25	CLA	5	603	18	1/1/13/20	16/29/105/115	-
25	CLA	6	607	30	1/1/13/20	10/27/103/115	-
25	CLA	H	1702	8	1/1/11/20	8/17/93/115	-
26	CHL	8	613	-	3/3/17/26	1/21/119/137	-
25	CLA	A	1103	-	1/1/15/20	17/39/115/115	-
25	CLA	A	1121	-	1/1/14/20	18/33/109/115	-
32	SQD	A	5005	-	-	21/49/69/69	0/1/1/1
25	CLA	A	1115	-	1/1/14/20	16/33/109/115	-
25	CLA	A	1120	-	1/1/11/20	6/20/96/115	-
30	LHG	F	5002	-	-	19/40/40/53	-
26	CHL	6	611	-	3/3/17/26	4/21/119/137	-
25	CLA	G	1601	-	1/1/12/20	9/21/97/115	-
29	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
25	CLA	1	606	-	1/1/13/20	11/30/106/115	-
25	CLA	a	608	-	1/1/13/20	10/27/103/115	-
43	LUT	5	502	-	-	3/29/67/67	0/2/2/2
25	CLA	9	607	-	1/1/11/20	8/18/94/115	-
25	CLA	L	1502	-	1/1/14/20	12/33/109/115	-
47	PLM	8	806	-	-	6/14/14/15	-
25	CLA	2	605	-	1/1/14/20	18/33/109/115	-
43	LUT	9	502	-	-	3/29/67/67	0/2/2/2
25	CLA	3	613	-	1/1/14/20	12/35/111/115	-
47	PLM	8	807	-	-	5/15/15/15	-
32	SQD	I	5001	-	-	23/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	1141	-	1/1/11/20	7/15/91/115	-
32	SQD	G	5001	-	-	19/41/61/69	0/1/1/1
25	CLA	5	614	18	1/1/11/20	8/17/93/115	-
25	CLA	8	620	-	1/1/11/20	8/15/91/115	-
29	BCR	G	4001	-	-	11/29/63/63	0/2/2/2
27	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
29	BCR	5	503	-	-	13/29/63/63	0/2/2/2
30	LHG	2	802	-	-	37/53/53/53	-
25	CLA	A	1118	-	1/1/13/20	10/27/103/115	-
25	CLA	6	603	-	1/1/15/20	12/39/115/115	-
25	CLA	B	1229	-	1/1/15/20	12/39/115/115	-
25	CLA	8	615	21	1/1/11/20	9/17/93/115	-
25	CLA	5	608	-	1/1/11/20	4/15/91/115	-
26	CHL	a	606	-	4/4/18/26	6/27/125/137	-
26	CHL	1	613	-	3/3/16/26	1/18/116/137	-
26	CHL	8	603	21	4/4/20/26	9/39/137/137	-
30	LHG	7	801	25	-	25/41/41/53	-
26	CHL	4	618	-	4/4/18/26	4/27/125/137	-
29	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
26	CHL	6	613	-	3/3/17/26	0/21/119/137	-
25	CLA	4	611	-	1/1/13/20	9/29/105/115	-
26	CHL	5	611	-	3/3/17/26	3/21/119/137	-
25	CLA	A	1110	-	1/1/12/20	9/26/102/115	-
25	CLA	7	610	-	1/1/14/20	13/33/109/115	-
25	CLA	B	1205	-	1/1/15/20	13/39/115/115	-
25	CLA	8	618	21	1/1/14/20	17/33/109/115	-
43	LUT	1	503	-	-	7/29/67/67	0/2/2/2
25	CLA	A	1137	-	1/1/14/20	10/33/109/115	-
26	CHL	6	609	19	4/4/20/26	9/39/137/137	-
50	XAT	9	507	-	1/1/12/26	7/31/93/93	0/4/4/4
25	CLA	B	1232	-	1/1/11/20	8/15/91/115	-
25	CLA	2	621	22	1/1/15/20	16/39/115/115	-
29	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
25	CLA	1	615	15	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LUT	9	501	-	-	2/29/67/67	0/2/2/2
25	CLA	6	605	-	1/1/11/20	6/17/93/115	-
25	CLA	2	608	-	1/1/11/20	7/15/91/115	-
43	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
43	LUT	2	502	-	-	2/29/67/67	0/2/2/2
25	CLA	B	1207	-	1/1/14/20	18/33/109/115	-
25	CLA	3	601	16	1/1/15/20	13/39/115/115	-
43	LUT	a	503	-	-	4/29/67/67	0/2/2/2
25	CLA	7	607	30	1/1/13/20	8/31/107/115	-
25	CLA	A	1119	-	1/1/15/20	18/39/115/115	-
25	CLA	B	1209	-	1/1/15/20	15/39/115/115	-
25	CLA	A	1117	-	1/1/15/20	16/39/115/115	-
25	CLA	6	604	19	1/1/15/20	14/39/115/115	-
48	DGA	8	804	-	-	23/41/41/45	-
25	CLA	4	602	-	1/1/12/20	8/24/100/115	-
25	CLA	6	601	-	1/1/14/20	11/33/109/115	-
25	CLA	4	603	17	1/1/13/20	6/29/105/115	-
25	CLA	4	607	-	1/1/13/20	11/27/103/115	-
26	CHL	1	604	-	4/4/20/26	9/39/137/137	-
26	CHL	2	613	-	3/3/17/26	1/21/119/137	-
25	CLA	B	1234	-	-	19/37/87/115	0/5/5/9
25	CLA	A	1104	1	1/1/15/20	18/39/115/115	-
25	CLA	L	1504	-	1/1/12/20	9/21/97/115	-
30	LHG	A	5002	-	-	37/53/53/53	-
43	LUT	6	502	-	-	4/29/67/67	0/2/2/2
25	CLA	a	615	15	1/1/11/20	4/17/93/115	-
25	CLA	2	606	-	1/1/11/20	4/17/93/115	-
25	CLA	A	1128	-	1/1/15/20	19/39/115/115	-
25	CLA	J	1901	9	1/1/10/20	4/12/88/115	-
25	CLA	a	605	-	1/1/13/20	10/27/103/115	-
41	SPH	J	5002	-	-	12/21/21/21	-
37	PCW	6	803	-	-	22/39/39/57	-
26	CHL	2	609	22	4/4/20/26	9/39/137/137	-
25	CLA	A	1108	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	1022	54	1/1/15/20	12/39/115/115	-
25	CLA	B	1203	2	1/1/15/20	13/39/115/115	-
36	DGD	8	803	-	-	18/35/75/95	0/2/2/2
25	CLA	L	1501	11	1/1/12/20	7/21/97/115	-
26	CHL	6	617	19	3/3/15/26	0/12/110/137	-
43	LUT	8	502	-	-	5/29/67/67	0/2/2/2
25	CLA	1	601	-	1/1/14/20	12/33/109/115	-
24	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
28	SF4	A	3001	1,2	-	-	0/6/5/5
25	CLA	B	1208	-	1/1/13/20	11/25/101/115	-
30	LHG	3	801	25	-	32/53/53/53	-
25	CLA	A	1116	-	1/1/14/20	13/33/109/115	-
25	CLA	L	1503	-	1/1/11/20	9/15/91/115	-
29	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
35	LMT	A	5008	-	-	10/21/61/61	0/2/2/2
25	CLA	1	607	30	1/1/15/20	16/39/115/115	-
25	CLA	B	1236	-	1/1/12/20	9/25/101/115	-
33	PTY	B	5005	-	-	19/45/45/53	-
30	LHG	1	801	25	-	23/39/39/53	-
30	LHG	6	801	25	-	33/53/53/53	-
29	BCR	B	4001	-	-	11/29/63/63	0/2/2/2
26	CHL	7	613	-	4/4/19/26	4/33/131/137	-
34	3PH	A	5007	-	-	17/34/34/49	-
29	BCR	5	504	-	-	12/29/63/63	0/2/2/2
25	CLA	4	617	-	1/1/11/20	6/15/91/115	-
50	XAT	9	504	-	1/1/12/26	13/31/93/93	0/4/4/4
50	XAT	2	501	-	2/2/12/26	0/31/93/93	0/4/4/4
25	CLA	4	612	17	1/1/14/20	17/36/112/115	-
25	CLA	B	1201	-	1/1/15/20	20/39/115/115	-
25	CLA	5	615	18	1/1/11/20	9/17/93/115	-
25	CLA	A	1013	-	1/1/15/20	16/39/115/115	-
26	CHL	1	610	-	3/3/16/26	1/18/116/137	-
25	CLA	K	1404	10	1/1/11/20	8/15/91/115	-
28	SF4	C	3002	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	5	617	18	3/3/16/26	0/17/115/137	-
43	LUT	3	501	-	-	2/29/67/67	0/2/2/2
43	LUT	a	502	-	-	2/29/67/67	0/2/2/2
25	CLA	4	604	-	1/1/14/20	9/33/109/115	-
33	PTY	3	802	-	-	17/41/41/53	-
25	CLA	9	602	-	1/1/11/20	4/17/93/115	-
25	CLA	3	607	30	1/1/15/20	15/39/115/115	-
25	CLA	A	1130	-	1/1/13/20	11/29/105/115	-
25	CLA	A	1133	-	1/1/15/20	23/39/115/115	-
26	CHL	a	604	-	4/4/19/26	5/33/131/137	-
29	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
25	CLA	3	618	16	1/1/11/20	4/17/93/115	-
25	CLA	5	601	18	1/1/14/20	12/33/109/115	-
25	CLA	G	1603	-	1/1/11/20	5/15/91/115	-
43	LUT	1	501	-	-	3/29/67/67	0/2/2/2
25	CLA	B	1023	-	1/1/15/20	16/39/115/115	-
47	PLM	6	804	-	-	8/15/15/15	-
29	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
25	CLA	8	606	-	1/1/13/20	13/30/106/115	-
43	LUT	4	502	-	-	1/29/67/67	0/2/2/2
25	CLA	4	616	-	1/1/12/20	8/21/97/115	-
25	CLA	7	612	-	1/1/14/20	13/33/109/115	-
30	LHG	9	801	-	-	16/37/37/53	-
26	CHL	a	613	-	3/3/16/26	7/15/113/137	-
25	CLA	A	1129	-	1/1/12/20	9/21/97/115	-
25	CLA	a	611	-	1/1/12/20	8/21/97/115	-
29	BCR	L	4001	-	-	12/29/63/63	0/2/2/2
25	CLA	4	605	-	1/1/11/20	4/17/93/115	-
29	BCR	B	4007	-	-	7/29/63/63	0/2/2/2
25	CLA	9	612	-	1/1/15/20	13/39/115/115	-
38	LPX	F	5003	-	-	11/31/31/31	-
25	CLA	F	1301	-	1/1/12/20	8/21/97/115	-
40	RRX	3	506	-	1/1/11/25	10/29/65/65	0/2/2/2
46	QTB	a	504	-	1/1/5/10	2/11/28/28	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	1230	-	1/1/13/20	11/31/107/115	-
30	LHG	7	802	-	-	19/40/40/53	-
33	PTY	J	5001	-	-	20/31/31/53	-
25	CLA	8	605	-	1/1/13/20	12/27/103/115	-
25	CLA	9	604	23	1/1/14/20	8/33/109/115	-
25	CLA	B	1220	-	1/1/14/20	14/33/109/115	-
25	CLA	B	1227	-	1/1/12/20	12/21/97/115	-
25	CLA	7	604	20	1/1/15/20	17/39/115/115	-
25	CLA	B	1226	-	1/1/15/20	11/39/115/115	-
25	CLA	2	601	-	1/1/14/20	11/33/109/115	-
26	CHL	3	608	-	3/3/15/26	0/12/110/137	-
30	LHG	4	802	-	-	22/36/36/53	-
43	LUT	4	501	-	1/1/12/27	6/29/67/67	0/2/2/2
25	CLA	B	1219	2	1/1/13/20	10/32/108/115	-
43	LUT	5	505	-	-	9/29/67/67	0/2/2/2
48	DGA	3	803	-	-	14/25/25/45	-
45	OLA	8	808	-	-	5/17/17/17	-
41	SPH	6	806	-	-	9/21/21/21	-
36	DGD	B	5003	-	-	22/55/95/95	0/2/2/2
30	LHG	B	5001	25	-	33/53/53/53	-
44	AXT	1	502	-	-	10/29/71/75	0/2/2/2
37	PCW	K	5001	-	-	20/44/44/57	-
25	CLA	4	608	-	1/1/12/20	4/23/99/115	-
26	CHL	3	611	-	4/4/19/26	11/33/131/137	-
47	PLM	4	804	-	-	9/15/15/15	-
25	CLA	7	608	-	1/1/13/20	10/27/103/115	-
50	XAT	7	502	-	2/2/12/26	0/31/93/93	0/4/4/4
26	CHL	5	610	-	4/4/20/26	11/39/137/137	-
25	CLA	B	1221	-	1/1/15/20	9/39/115/115	-
25	CLA	B	1224	-	1/1/15/20	21/39/115/115	-
25	CLA	1	602	-	1/1/11/20	6/15/91/115	-
30	LHG	B	5002	-	-	28/53/53/53	-
25	CLA	9	609	23	1/1/11/20	6/17/93/115	-
25	CLA	B	1216	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	612	-	1/1/12/20	9/21/97/115	-
43	LUT	5	501	-	-	1/29/67/67	0/2/2/2
25	CLA	1	605	-	1/1/15/20	20/39/115/115	-
25	CLA	B	1206	2	1/1/15/20	20/39/115/115	-
47	PLM	4	803	-	-	6/14/14/15	-
25	CLA	A	1012	-	1/1/15/20	13/39/115/115	-
28	SF4	C	3003	3	-	-	0/6/5/5
25	CLA	A	1131	-	1/1/15/20	14/39/115/115	-
25	CLA	8	611	-	1/1/12/20	6/21/97/115	-
29	BCR	L	4003	-	-	10/29/63/63	0/2/2/2
25	CLA	A	1127	-	1/1/15/20	13/39/115/115	-
25	CLA	B	1218	-	1/1/13/20	7/27/103/115	-
25	CLA	B	1235	-	1/1/15/20	19/39/115/115	-
29	BCR	J	4001	-	-	11/29/63/63	0/2/2/2
26	CHL	9	608	-	3/3/16/26	6/18/116/137	-
25	CLA	6	612	-	1/1/12/20	10/21/97/115	-
25	CLA	a	602	-	1/1/12/20	8/21/97/115	-
26	CHL	4	613	-	3/3/17/26	6/23/121/137	-
25	CLA	9	606	-	1/1/13/20	6/27/103/115	-
25	CLA	8	608	-	1/1/12/20	5/24/100/115	-
33	PTY	a	803	-	-	23/41/41/53	-
25	CLA	B	1217	-	1/1/13/20	12/29/105/115	-
33	PTY	5	802	-	-	22/41/41/53	-
25	CLA	6	618	-	1/1/11/20	8/17/93/115	-
36	DGD	7	806	-	-	13/39/79/95	0/2/2/2
25	CLA	B	1237	-	1/1/15/20	20/39/115/115	-
25	CLA	B	1239	-	1/1/15/20	16/39/115/115	-
25	CLA	H	1701	-	1/1/13/20	8/27/103/115	-
30	LHG	9	802	-	-	26/53/53/53	-
25	CLA	K	1403	10	1/1/11/20	9/20/96/115	-
26	CHL	A	1114	-	4/4/20/26	9/39/137/137	-
41	SPH	4	805	-	-	10/21/21/21	-
25	CLA	B	1215	-	1/1/14/20	16/33/109/115	-
51	4RF	7	807	-	-	19/39/39/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	AXT	7	504	-	-	14/29/71/75	0/2/2/2
29	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
25	CLA	B	1202	-	1/1/15/20	16/39/115/115	-
25	CLA	F	1302	-	1/1/13/20	10/27/103/115	-
25	CLA	1	612	15	1/1/15/20	18/39/115/115	-
26	CHL	a	609	15	3/3/17/26	3/24/122/137	-
26	CHL	3	604	16	4/4/20/26	8/39/137/137	-
29	BCR	H	4001	-	-	12/29/63/63	0/2/2/2
25	CLA	A	1125	-	1/1/15/20	26/39/115/115	-
25	CLA	4	615	17	1/1/14/20	12/33/109/115	-
53	LAP	8	810	-	-	15/30/30/30	-
29	BCR	6	503	-	-	16/29/63/63	0/2/2/2
31	LMG	A	5004	-	-	4/37/57/70	0/1/1/1
26	CHL	5	613	-	4/4/18/26	5/27/125/137	-
26	CHL	4	609	17	4/4/20/26	10/39/137/137	-
32	SQD	H	5001	-	-	8/40/60/69	0/1/1/1
25	CLA	A	1112	-	1/1/13/20	15/27/103/115	-
25	CLA	B	1212	-	1/1/13/20	10/30/106/115	-
25	CLA	5	602	-	1/1/12/20	10/24/100/115	-
25	CLA	6	602	-	1/1/12/20	9/24/100/115	-
25	CLA	3	610	16	1/1/13/20	13/30/106/115	-
25	CLA	3	616	-	1/1/13/20	11/29/105/115	-
25	CLA	B	1228	-	1/1/15/20	15/39/115/115	-
42	ECH	M	4001	-	-	5/29/66/66	0/2/2/2
30	LHG	5	801	-	-	33/53/53/53	-
25	CLA	a	603	-	1/1/15/20	16/39/115/115	-
25	CLA	6	608	-	1/1/13/20	9/27/103/115	-
25	CLA	7	606	-	1/1/13/20	10/25/101/115	-
25	CLA	2	602	-	1/1/12/20	14/24/100/115	-
25	CLA	A	1136	-	1/1/15/20	16/39/115/115	-
25	CLA	8	609	21	1/1/14/20	16/33/109/115	-
25	CLA	a	612	15	1/1/13/20	10/30/106/115	-
37	PCW	B	5004	-	-	23/42/42/57	-
25	CLA	a	601	-	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	1214	-	1/1/13/20	18/32/108/115	-
26	CHL	7	609	20	4/4/19/26	8/35/133/137	-
35	LMT	2	804	-	-	5/21/61/61	0/2/2/2
30	LHG	2	801	25	-	29/53/53/53	-
30	LHG	7	803	-	-	22/39/39/53	-
29	BCR	8	503	-	-	16/29/63/63	0/2/2/2
30	LHG	1	802	-	-	33/53/53/53	-
25	CLA	K	1402	-	1/1/14/20	8/33/109/115	-
25	CLA	7	605	-	1/1/11/20	3/13/89/115	-
45	OLA	8	809	-	-	11/17/17/17	-
26	CHL	9	613	-	3/3/15/26	2/10/108/137	-
25	CLA	B	1240	30	1/1/15/20	11/39/115/115	-
25	CLA	4	601	-	1/1/14/20	9/33/109/115	-
29	BCR	3	504	-	-	11/29/63/63	0/2/2/2
29	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
25	CLA	A	1140	-	1/1/13/20	10/27/103/115	-
26	CHL	3	603	16	4/4/20/26	9/39/137/137	-
27	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
29	BCR	A	4005	-	-	13/29/63/63	0/2/2/2
29	BCR	B	4002	-	-	16/29/63/63	0/2/2/2
33	PTY	9	803	-	-	27/51/51/53	-
26	CHL	9	610	-	3/3/17/26	4/21/119/137	-
26	CHL	8	604	21	4/4/19/26	11/35/133/137	-
25	CLA	G	1602	7	1/1/14/20	11/33/109/115	-
25	CLA	5	612	18	1/1/15/20	21/39/115/115	-
26	CHL	2	610	-	4/4/16/26	2/18/116/137	-
25	CLA	A	1124	-	1/1/13/20	7/27/103/115	-
25	CLA	8	602	-	1/1/12/20	5/24/100/115	-
25	CLA	B	1021	-	1/1/15/20	16/39/115/115	-
25	CLA	O	1803	-	1/1/10/20	2/10/86/115	-
25	CLA	A	1132	-	1/1/15/20	17/39/115/115	-
25	CLA	O	1801	-	1/1/9/20	0/6/78/115	-
26	CHL	6	619	19	5/5/20/26	8/39/137/137	-
29	BCR	3	505	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	6	802	-	-	25/41/41/53	-
32	SQD	7	805	-	-	10/34/54/69	0/1/1/1
25	CLA	5	604	18	1/1/15/20	11/39/115/115	-
25	CLA	A	1109	25	1/1/15/20	19/39/115/115	-
33	PTY	A	5006	-	-	12/37/37/53	-
35	LMT	B	5006	-	-	9/21/61/61	0/2/2/2
26	CHL	9	601	-	4/4/20/26	10/39/137/137	-
25	CLA	B	1223	-	1/1/15/20	12/39/115/115	-
30	LHG	A	5003	-	-	25/50/50/53	-
25	CLA	7	601	20	1/1/14/20	14/33/109/115	-
25	CLA	8	612	-	1/1/12/20	8/21/97/115	-
47	PLM	5	804	-	-	3/15/15/15	-
25	CLA	A	1134	1	1/1/14/20	14/33/109/115	-
25	CLA	3	606	-	1/1/15/20	13/39/115/115	-
25	CLA	6	615	54	1/1/15/20	16/39/115/115	-
25	CLA	7	603	20	1/1/15/20	22/39/115/115	-
52	P5S	8	805	-	-	23/42/42/59	-
25	CLA	B	1213	-	1/1/13/20	12/27/103/115	-
26	CHL	5	618	-	3/3/17/26	3/21/119/137	-
25	CLA	2	607	30	1/1/15/20	12/39/115/115	-
29	BCR	7	503	-	-	11/29/63/63	0/2/2/2
25	CLA	A	1126	-	1/1/15/20	22/39/115/115	-
26	CHL	8	601	21	4/4/19/26	5/33/131/137	-
29	BCR	O	4001	-	-	13/29/63/63	0/2/2/2
30	LHG	A	5001	-	-	32/53/53/53	-
25	CLA	B	1210	-	1/1/15/20	20/39/115/115	-
25	CLA	A	1139	-	1/1/13/20	11/27/103/115	-
25	CLA	4	606	-	1/1/12/20	7/21/97/115	-
25	CLA	6	606	19	1/1/15/20	15/39/115/115	-
47	PLM	a	804	-	-	4/14/14/15	-
48	DGA	5	803	-	-	14/24/24/45	-
25	CLA	5	607	-	1/1/14/20	12/33/109/115	-
33	PTY	7	804	-	-	14/36/36/53	-
29	BCR	K	4002	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	3	605	-	1/1/15/20	16/39/115/115	-
25	CLA	3	612	16	1/1/12/20	6/21/97/115	-
29	BCR	4	503	-	-	15/29/63/63	0/2/2/2
26	CHL	9	603	-	4/4/20/26	9/39/137/137	-
26	CHL	1	609	15	4/4/20/26	10/39/137/137	-
48	DGA	2	803	-	-	26/38/38/45	-
26	CHL	7	611	-	4/4/18/26	5/27/125/137	-
26	CHL	7	617	20	4/4/20/26	9/39/137/137	-
25	CLA	B	1211	-	1/1/13/20	11/27/103/115	-
25	CLA	A	1135	-	1/1/12/20	9/23/99/115	-
25	CLA	A	1105	-	1/1/13/20	4/30/106/115	-
26	CHL	7	615	20	3/3/17/26	6/21/119/137	-
39	NEX	F	4001	-	1/1/12/25	13/27/83/83	0/3/3/3
25	CLA	A	1122	-	1/1/14/20	19/33/109/115	-
25	CLA	2	603	22	1/1/14/20	10/33/109/115	-
25	CLA	A	1123	-	1/1/15/20	13/39/115/115	-
25	CLA	B	1222	-	1/1/13/20	8/31/107/115	-
25	CLA	1	603	-	1/1/15/20	13/39/115/115	-
30	LHG	a	801	-	-	22/39/39/53	-
41	SPH	9	804	-	-	13/21/21/21	-

All (2247) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	3	506	RRX	C26-C25	15.98	1.61	1.34
40	J	4002	RRX	C26-C25	15.93	1.61	1.34
40	3	506	RRX	C5-C6	15.36	1.60	1.34
43	3	502	LUT	C24-C25	15.36	1.51	1.33
43	7	501	LUT	C24-C25	15.32	1.51	1.33
43	2	507	LUT	C24-C25	15.29	1.51	1.33
43	2	502	LUT	C24-C25	15.26	1.51	1.33
43	5	505	LUT	C24-C25	15.25	1.51	1.33
43	1	503	LUT	C24-C25	15.24	1.51	1.33
43	a	503	LUT	C24-C25	15.18	1.51	1.33
40	J	4002	RRX	C5-C6	15.17	1.59	1.34
43	a	501	LUT	C24-C25	15.16	1.51	1.33
43	1	501	LUT	C24-C25	15.15	1.51	1.33
43	4	501	LUT	C24-C25	15.14	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	3	501	LUT	C24-C25	15.13	1.51	1.33
43	a	502	LUT	C24-C25	15.06	1.51	1.33
43	8	501	LUT	C24-C25	15.05	1.51	1.33
43	5	501	LUT	C24-C25	15.04	1.51	1.33
43	9	501	LUT	C24-C25	15.02	1.51	1.33
43	6	501	LUT	C24-C25	14.96	1.50	1.33
43	5	502	LUT	C24-C25	14.96	1.50	1.33
43	4	502	LUT	C24-C25	14.96	1.50	1.33
43	8	502	LUT	C24-C25	14.94	1.50	1.33
43	9	502	LUT	C24-C25	14.92	1.50	1.33
43	6	502	LUT	C24-C25	14.86	1.50	1.33
44	1	502	AXT	C5-C6	13.15	1.56	1.34
40	J	4002	RRX	C29-C28	-10.40	1.37	1.52
40	3	506	RRX	C29-C28	-10.29	1.37	1.52
24	A	1011	CL0	C1A-CHA	9.54	1.50	1.40
24	A	1011	CL0	C1B-C2B	8.88	1.49	1.39
24	A	1011	CL0	C1D-C2D	8.67	1.49	1.39
46	a	504	QTB	C11-C12	-8.15	1.36	1.54
40	3	506	RRX	C27-C28	8.02	1.66	1.52
40	J	4002	RRX	C27-C28	7.74	1.65	1.52
24	A	1011	CL0	C3B-C4B	7.01	1.48	1.41
26	8	601	CHL	C3B-C4B	7.00	1.48	1.41
26	8	604	CHL	C3B-C4B	6.73	1.47	1.41
40	3	506	RRX	C2-C3	-6.72	1.36	1.52
40	J	4002	RRX	C2-C3	-6.69	1.36	1.52
26	3	604	CHL	C3B-C4B	6.62	1.47	1.41
26	a	604	CHL	C3B-C4B	6.54	1.47	1.41
26	a	604	CHL	C3A-C2A	-6.53	1.49	1.54
26	5	611	CHL	C3A-C2A	-6.52	1.49	1.54
26	4	618	CHL	C3A-C2A	-6.49	1.49	1.54
39	F	4001	NEX	C35-C15	-6.49	1.18	1.36
25	L	1504	CLA	MG-NA	6.47	2.21	2.06
25	9	605	CLA	MG-NA	6.45	2.21	2.06
25	B	1240	CLA	MG-NA	6.44	2.21	2.06
25	2	621	CLA	MG-NA	6.43	2.21	2.06
25	A	1135	CLA	MG-NA	6.43	2.21	2.06
25	K	1402	CLA	MG-NA	6.43	2.21	2.06
25	4	617	CLA	MG-NA	6.43	2.21	2.06
25	8	605	CLA	MG-NA	6.42	2.21	2.06
25	A	1107	CLA	MG-NA	6.42	2.21	2.06
25	O	1801	CLA	MG-NA	6.42	2.21	2.06
25	5	609	CLA	MG-NA	6.42	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	605	CLA	MG-NA	6.41	2.21	2.06
25	4	616	CLA	MG-NA	6.41	2.21	2.06
25	2	602	CLA	MG-NA	6.40	2.21	2.06
25	3	618	CLA	MG-NA	6.39	2.21	2.06
25	O	1803	CLA	MG-NA	6.39	2.21	2.06
25	A	1125	CLA	MG-NA	6.39	2.21	2.06
25	A	1101	CLA	MG-NA	6.38	2.21	2.06
25	G	1603	CLA	MG-NA	6.38	2.21	2.06
25	A	1123	CLA	MG-NA	6.38	2.21	2.06
25	9	612	CLA	MG-NA	6.38	2.21	2.06
25	6	602	CLA	MG-NA	6.37	2.21	2.06
25	1	602	CLA	MG-NA	6.37	2.21	2.06
25	a	611	CLA	MG-NA	6.37	2.21	2.06
25	4	615	CLA	MG-NA	6.37	2.21	2.06
25	J	1901	CLA	MG-NA	6.37	2.21	2.06
25	K	1404	CLA	MG-NA	6.37	2.21	2.06
25	1	615	CLA	MG-NA	6.37	2.21	2.06
25	4	605	CLA	MG-NA	6.36	2.21	2.06
25	2	603	CLA	MG-NA	6.36	2.21	2.06
25	4	607	CLA	MG-NA	6.36	2.21	2.06
25	B	1223	CLA	MG-NA	6.36	2.21	2.06
25	6	607	CLA	MG-NA	6.36	2.21	2.06
25	6	605	CLA	MG-NA	6.36	2.21	2.06
40	3	506	RRX	C1-C6	-6.35	1.45	1.53
25	K	1403	CLA	MG-NA	6.35	2.21	2.06
40	J	4002	RRX	C1-C6	-6.35	1.45	1.53
25	2	615	CLA	MG-NA	6.35	2.21	2.06
25	A	1130	CLA	MG-NA	6.34	2.21	2.06
25	9	607	CLA	MG-NA	6.34	2.21	2.06
25	A	1136	CLA	MG-NA	6.34	2.21	2.06
25	A	1139	CLA	MG-NA	6.34	2.21	2.06
25	O	1802	CLA	MG-NA	6.34	2.21	2.06
25	4	602	CLA	MG-NA	6.34	2.21	2.06
25	9	609	CLA	MG-NA	6.34	2.21	2.06
25	9	604	CLA	MG-NA	6.34	2.21	2.06
25	4	610	CLA	MG-NA	6.34	2.21	2.06
25	5	602	CLA	MG-NA	6.34	2.21	2.06
25	G	1601	CLA	MG-NA	6.34	2.21	2.06
25	5	615	CLA	MG-NA	6.34	2.21	2.06
25	A	1140	CLA	MG-NA	6.34	2.21	2.06
25	6	606	CLA	MG-NA	6.34	2.21	2.06
25	F	1302	CLA	MG-NA	6.33	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	604	CLA	MG-NA	6.33	2.21	2.06
25	7	605	CLA	MG-NA	6.33	2.21	2.06
25	G	1602	CLA	MG-NA	6.33	2.21	2.06
25	A	1109	CLA	MG-NA	6.33	2.21	2.06
25	A	1112	CLA	MG-NA	6.33	2.21	2.06
25	7	602	CLA	MG-NA	6.33	2.21	2.06
25	9	602	CLA	MG-NA	6.33	2.21	2.06
25	H	1701	CLA	MG-NA	6.33	2.21	2.06
25	B	1239	CLA	MG-NA	6.33	2.21	2.06
25	7	607	CLA	MG-NA	6.33	2.21	2.06
25	a	607	CLA	MG-NA	6.33	2.21	2.06
25	7	603	CLA	MG-NA	6.32	2.21	2.06
25	A	1110	CLA	MG-NA	6.32	2.21	2.06
25	1	612	CLA	MG-NA	6.32	2.21	2.06
25	5	614	CLA	MG-NA	6.32	2.21	2.06
25	a	615	CLA	MG-NA	6.32	2.21	2.06
25	L	1501	CLA	MG-NA	6.32	2.21	2.06
25	A	1134	CLA	MG-NA	6.32	2.21	2.06
25	8	620	CLA	MG-NA	6.32	2.21	2.06
25	A	1137	CLA	MG-NA	6.32	2.21	2.06
25	a	602	CLA	MG-NA	6.31	2.21	2.06
25	A	1118	CLA	MG-NA	6.31	2.21	2.06
25	3	616	CLA	MG-NA	6.31	2.21	2.06
25	2	608	CLA	MG-NA	6.31	2.21	2.06
25	K	1401	CLA	MG-NA	6.31	2.21	2.06
25	5	607	CLA	MG-NA	6.31	2.21	2.06
25	H	1702	CLA	MG-NA	6.31	2.21	2.06
25	A	1124	CLA	MG-NA	6.31	2.21	2.06
25	4	603	CLA	MG-NA	6.30	2.21	2.06
25	5	605	CLA	MG-NA	6.30	2.21	2.06
25	8	602	CLA	MG-NA	6.30	2.21	2.06
25	3	607	CLA	MG-NA	6.30	2.21	2.06
25	B	1226	CLA	MG-NA	6.30	2.21	2.06
25	A	1122	CLA	MG-NA	6.30	2.21	2.06
25	A	1141	CLA	MG-NA	6.30	2.21	2.06
25	A	1126	CLA	MG-NA	6.30	2.21	2.06
25	3	605	CLA	MG-NA	6.30	2.21	2.06
25	B	1209	CLA	MG-NA	6.29	2.21	2.06
25	8	609	CLA	MG-NA	6.29	2.21	2.06
25	3	602	CLA	MG-NA	6.29	2.21	2.06
25	6	618	CLA	MG-NA	6.29	2.21	2.06
25	B	1214	CLA	MG-NA	6.29	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1227	CLA	MG-NA	6.29	2.21	2.06
25	B	1229	CLA	MG-NA	6.29	2.21	2.06
25	5	606	CLA	MG-NA	6.29	2.21	2.06
25	5	608	CLA	MG-NA	6.29	2.21	2.06
25	B	1237	CLA	MG-NA	6.29	2.21	2.06
25	6	612	CLA	MG-NA	6.29	2.21	2.06
25	B	1238	CLA	MG-NA	6.29	2.21	2.06
25	2	606	CLA	MG-NA	6.29	2.21	2.06
25	a	603	CLA	MG-NA	6.29	2.21	2.06
25	9	606	CLA	MG-NA	6.28	2.21	2.06
25	7	610	CLA	MG-NA	6.28	2.21	2.06
25	A	1127	CLA	MG-NA	6.28	2.21	2.06
25	B	1022	CLA	MG-NA	6.28	2.21	2.06
25	1	607	CLA	MG-NA	6.28	2.21	2.06
25	A	1105	CLA	MG-NA	6.28	2.21	2.06
25	B	1218	CLA	MG-NA	6.28	2.21	2.06
25	a	605	CLA	MG-NA	6.28	2.21	2.06
25	2	607	CLA	MG-NA	6.28	2.21	2.06
25	B	1225	CLA	MG-NA	6.28	2.21	2.06
39	F	4001	NEX	C11-C12	-6.28	1.18	1.34
25	5	603	CLA	MG-NA	6.28	2.21	2.06
25	6	615	CLA	MG-NA	6.27	2.21	2.06
25	A	1129	CLA	MG-NA	6.27	2.21	2.06
25	A	1115	CLA	MG-NA	6.27	2.21	2.06
25	5	604	CLA	MG-NA	6.27	2.21	2.06
25	a	612	CLA	MG-NA	6.27	2.21	2.06
25	B	1213	CLA	MG-NA	6.27	2.21	2.06
25	4	611	CLA	MG-NA	6.27	2.21	2.06
25	8	618	CLA	MG-NA	6.27	2.21	2.06
25	a	608	CLA	MG-NA	6.27	2.21	2.06
25	7	606	CLA	MG-NA	6.27	2.21	2.06
25	B	1221	CLA	MG-NA	6.27	2.21	2.06
25	7	608	CLA	MG-NA	6.26	2.21	2.06
25	A	1108	CLA	MG-NA	6.26	2.21	2.06
25	B	1224	CLA	MG-NA	6.26	2.21	2.06
25	A	1012	CLA	MG-NA	6.26	2.21	2.06
25	B	1219	CLA	MG-NA	6.26	2.21	2.06
25	A	1131	CLA	MG-NA	6.26	2.21	2.06
25	1	603	CLA	MG-NA	6.26	2.21	2.06
25	8	615	CLA	MG-NA	6.25	2.21	2.06
25	A	1128	CLA	MG-NA	6.25	2.21	2.06
25	B	1201	CLA	MG-NA	6.25	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	607	CLA	MG-NA	6.25	2.21	2.06
25	A	1120	CLA	MG-NA	6.25	2.21	2.06
25	B	1232	CLA	MG-NA	6.25	2.21	2.06
25	3	613	CLA	MG-NA	6.25	2.21	2.06
25	A	1116	CLA	MG-NA	6.25	2.21	2.06
25	B	1210	CLA	MG-NA	6.25	2.21	2.06
25	B	1208	CLA	MG-NA	6.24	2.21	2.06
25	B	1217	CLA	MG-NA	6.24	2.21	2.06
25	1	605	CLA	MG-NA	6.24	2.21	2.06
25	B	1235	CLA	MG-NA	6.24	2.21	2.06
25	L	1503	CLA	MG-NA	6.24	2.21	2.06
25	7	604	CLA	MG-NA	6.24	2.21	2.06
25	A	1104	CLA	MG-NA	6.24	2.21	2.06
25	A	1117	CLA	MG-NA	6.24	2.21	2.06
25	B	1220	CLA	MG-NA	6.24	2.21	2.06
25	6	603	CLA	MG-NA	6.24	2.21	2.06
25	3	610	CLA	MG-NA	6.23	2.21	2.06
25	B	1228	CLA	MG-NA	6.23	2.21	2.06
25	B	1236	CLA	MG-NA	6.23	2.21	2.06
25	4	604	CLA	MG-NA	6.23	2.21	2.06
25	B	1203	CLA	MG-NA	6.23	2.21	2.06
25	2	612	CLA	MG-NA	6.23	2.21	2.06
25	F	1301	CLA	MG-NA	6.23	2.21	2.06
39	F	4001	NEX	C31-C32	-6.23	1.18	1.34
25	A	1121	CLA	MG-NA	6.23	2.21	2.06
25	4	601	CLA	MG-NA	6.22	2.21	2.06
25	8	608	CLA	MG-NA	6.22	2.21	2.06
26	1	604	CHL	C3B-C4B	6.22	1.47	1.41
25	5	612	CLA	MG-NA	6.22	2.21	2.06
25	4	608	CLA	MG-NA	6.21	2.21	2.06
25	2	601	CLA	MG-NA	6.21	2.21	2.06
25	A	1111	CLA	MG-NA	6.21	2.21	2.06
25	B	1215	CLA	MG-NA	6.21	2.21	2.06
25	a	601	CLA	MG-NA	6.21	2.21	2.06
25	B	1207	CLA	MG-NA	6.20	2.21	2.06
25	4	606	CLA	MG-NA	6.20	2.21	2.06
25	B	1206	CLA	MG-NA	6.20	2.21	2.06
25	B	1202	CLA	MG-NA	6.20	2.21	2.06
25	3	601	CLA	MG-NA	6.20	2.21	2.06
25	A	1138	CLA	MG-NA	6.19	2.21	2.06
25	B	1230	CLA	MG-NA	6.19	2.21	2.06
25	B	1212	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	601	CLA	MG-NA	6.18	2.21	2.06
25	8	606	CLA	MG-NA	6.18	2.21	2.06
25	A	1102	CLA	MG-NA	6.18	2.20	2.06
25	A	1113	CLA	MG-NA	6.17	2.20	2.06
25	B	1204	CLA	MG-NA	6.17	2.20	2.06
25	6	601	CLA	MG-NA	6.17	2.20	2.06
26	3	603	CHL	C3B-C4B	6.17	1.47	1.41
25	B	1211	CLA	MG-NA	6.17	2.20	2.06
25	A	1106	CLA	MG-NA	6.16	2.20	2.06
25	8	611	CLA	MG-NA	6.16	2.20	2.06
25	1	601	CLA	MG-NA	6.15	2.20	2.06
25	6	608	CLA	MG-NA	6.15	2.20	2.06
26	9	601	CHL	C3A-C2A	-6.15	1.49	1.54
25	7	612	CLA	MG-NA	6.15	2.20	2.06
25	A	1103	CLA	MG-NA	6.14	2.20	2.06
25	A	1133	CLA	MG-NA	6.14	2.20	2.06
25	A	1132	CLA	MG-NA	6.14	2.20	2.06
25	B	1021	CLA	MG-NA	6.14	2.20	2.06
25	A	1119	CLA	MG-NA	6.13	2.20	2.06
25	2	604	CLA	MG-NA	6.13	2.20	2.06
25	B	1222	CLA	MG-NA	6.13	2.20	2.06
25	H	1703	CLA	MG-NA	6.12	2.20	2.06
26	1	604	CHL	C3A-C2A	-6.12	1.49	1.54
25	7	601	CLA	MG-NA	6.11	2.20	2.06
25	4	612	CLA	MG-NA	6.11	2.20	2.06
25	B	1231	CLA	MG-NA	6.11	2.20	2.06
25	3	606	CLA	MG-NA	6.11	2.20	2.06
25	L	1502	CLA	MG-NA	6.11	2.20	2.06
25	1	606	CLA	MG-NA	6.11	2.20	2.06
25	B	1216	CLA	MG-NA	6.10	2.20	2.06
25	B	1023	CLA	MG-NA	6.10	2.20	2.06
25	3	612	CLA	MG-NA	6.08	2.20	2.06
25	B	1205	CLA	MG-NA	6.07	2.20	2.06
25	B	1234	CLA	C1D-C2D	6.06	1.46	1.39
25	A	1013	CLA	MG-NA	6.06	2.20	2.06
25	1	608	CLA	MG-NA	6.01	2.20	2.06
25	8	612	CLA	MG-NA	6.01	2.20	2.06
26	8	603	CHL	C3B-C4B	5.98	1.47	1.41
29	G	4001	BCR	C24-C23	5.94	1.50	1.33
40	3	506	RRX	C30-C25	-5.92	1.46	1.53
29	B	4003	BCR	C24-C23	5.91	1.50	1.33
29	L	4003	BCR	C24-C23	5.87	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	503	BCR	C24-C23	5.87	1.50	1.33
29	6	503	BCR	C24-C23	5.86	1.50	1.33
29	B	4002	BCR	C24-C23	5.84	1.50	1.33
29	K	4002	BCR	C24-C23	5.82	1.50	1.33
29	3	504	BCR	C24-C23	5.81	1.50	1.33
29	4	503	BCR	C24-C23	5.81	1.50	1.33
29	H	4001	BCR	C24-C23	5.79	1.50	1.33
29	6	504	BCR	C24-C23	5.79	1.50	1.33
29	O	4001	BCR	C24-C23	5.79	1.50	1.33
29	B	4005	BCR	C24-C23	5.77	1.50	1.33
29	B	4006	BCR	C24-C23	5.77	1.50	1.33
29	3	505	BCR	C24-C23	5.77	1.50	1.33
29	L	4001	BCR	C24-C23	5.75	1.50	1.33
29	5	504	BCR	C24-C23	5.75	1.50	1.33
44	7	504	AXT	C26-C25	5.75	1.43	1.35
29	A	4001	BCR	C24-C23	5.73	1.50	1.33
29	K	4001	BCR	C24-C23	5.73	1.50	1.33
29	A	4003	BCR	C24-C23	5.71	1.50	1.33
29	J	4001	BCR	C24-C23	5.71	1.50	1.33
29	B	4007	BCR	C24-C23	5.68	1.50	1.33
29	L	4002	BCR	C24-C23	5.67	1.50	1.33
29	B	4001	BCR	C24-C23	5.67	1.50	1.33
39	F	4001	NEX	C7-C8	5.67	1.41	1.31
29	3	503	BCR	C24-C23	5.66	1.49	1.33
26	7	613	CHL	C3A-C2A	-5.65	1.49	1.54
29	A	4004	BCR	C24-C23	5.65	1.49	1.33
29	5	503	BCR	C24-C23	5.62	1.49	1.33
29	A	4002	BCR	C24-C23	5.60	1.49	1.33
29	A	4005	BCR	C24-C23	5.60	1.49	1.33
29	B	4004	BCR	C24-C23	5.60	1.49	1.33
26	2	609	CHL	C3B-C4B	5.59	1.46	1.41
26	2	609	CHL	C3A-C2A	-5.58	1.49	1.54
29	I	4001	BCR	C24-C23	5.55	1.49	1.33
29	7	503	BCR	C24-C23	5.49	1.49	1.33
26	8	601	CHL	C3A-C2A	-5.48	1.50	1.54
29	A	4002	BCR	C11-C12	-5.46	1.20	1.34
39	F	4001	NEX	C28-C29	-5.43	1.34	1.46
46	a	504	QTB	C17-C11	-5.39	1.50	1.55
29	B	4001	BCR	C11-C12	-5.36	1.20	1.34
29	A	4004	BCR	C11-C12	-5.35	1.20	1.34
40	J	4002	RRX	C30-C25	-5.34	1.47	1.53
24	A	1011	CL0	O2A-C1	5.31	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	4006	BCR	C11-C12	-5.31	1.20	1.34
29	6	504	BCR	C11-C12	-5.31	1.20	1.34
29	5	503	BCR	C11-C12	-5.27	1.20	1.34
40	J	4002	RRX	C19-C18	5.26	1.57	1.46
29	A	4001	BCR	C11-C12	-5.26	1.21	1.34
26	7	609	CHL	C3A-C2A	-5.24	1.50	1.54
29	3	503	BCR	C11-C12	-5.24	1.21	1.34
29	A	4003	BCR	C11-C12	-5.22	1.21	1.34
29	5	504	BCR	C11-C12	-5.22	1.21	1.34
26	3	608	CHL	C3A-C2A	-5.22	1.50	1.54
26	5	611	CHL	C3B-C4B	5.22	1.46	1.41
29	B	4005	BCR	C11-C12	-5.21	1.21	1.34
40	3	506	RRX	C2-C1	5.21	1.66	1.54
29	K	4001	BCR	C11-C12	-5.21	1.21	1.34
24	A	1011	CL0	CHB-C1B	5.21	1.48	1.39
29	B	4004	BCR	C11-C12	-5.21	1.21	1.34
29	7	503	BCR	C11-C12	-5.19	1.21	1.34
26	9	608	CHL	C3B-C4B	5.19	1.46	1.41
29	J	4001	BCR	C11-C12	-5.19	1.21	1.34
40	J	4002	RRX	C2-C1	5.16	1.65	1.54
26	7	613	CHL	C3B-C4B	5.16	1.46	1.41
29	B	4007	BCR	C11-C12	-5.16	1.21	1.34
24	A	1011	CL0	CHC-C4B	5.15	1.48	1.39
29	6	503	BCR	C11-C12	-5.14	1.21	1.34
26	a	606	CHL	C3B-C4B	5.14	1.46	1.41
26	7	609	CHL	C3B-C4B	5.14	1.46	1.41
29	I	4001	BCR	C11-C12	-5.14	1.21	1.34
26	4	613	CHL	C3B-C4B	5.14	1.46	1.41
29	L	4002	BCR	C11-C12	-5.14	1.21	1.34
29	L	4003	BCR	C11-C12	-5.13	1.21	1.34
29	K	4002	BCR	C11-C12	-5.12	1.21	1.34
26	a	610	CHL	C3B-C4B	5.12	1.46	1.41
29	L	4001	BCR	C11-C12	-5.11	1.21	1.34
29	8	503	BCR	C11-C12	-5.11	1.21	1.34
26	8	604	CHL	C3A-C2A	-5.10	1.50	1.54
29	B	4003	BCR	C11-C12	-5.10	1.21	1.34
29	3	504	BCR	C11-C12	-5.10	1.21	1.34
26	6	611	CHL	C3B-C4B	5.10	1.46	1.41
26	9	603	CHL	C3B-C4B	5.10	1.46	1.41
26	6	613	CHL	C3A-C2A	-5.09	1.50	1.54
29	3	505	BCR	C11-C12	-5.08	1.21	1.34
29	B	4002	BCR	C11-C12	-5.08	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	4005	BCR	C11-C12	-5.08	1.21	1.34
26	8	610	CHL	C3B-C4B	5.08	1.46	1.41
40	3	506	RRX	C19-C18	5.07	1.56	1.46
29	O	4001	BCR	C11-C12	-5.05	1.21	1.34
29	4	503	BCR	C11-C12	-5.05	1.21	1.34
29	H	4001	BCR	C11-C12	-5.04	1.21	1.34
24	A	1011	CL0	O2D-CGD	5.02	1.45	1.33
26	7	615	CHL	C3B-C4B	5.02	1.46	1.41
44	7	504	AXT	C28-C29	4.99	1.56	1.46
26	2	610	CHL	C3B-C4B	4.99	1.46	1.41
26	3	611	CHL	C3A-C2A	-4.99	1.50	1.54
24	A	1011	CL0	OBD-CAD	4.97	1.28	1.22
44	7	504	AXT	C32-C33	4.96	1.56	1.46
24	A	1011	CL0	C3B-C2B	4.96	1.47	1.40
26	4	618	CHL	C3B-C4B	4.95	1.46	1.41
25	B	1234	CLA	C3B-C4B	4.95	1.46	1.41
26	7	611	CHL	C3B-C4B	4.92	1.46	1.41
26	9	613	CHL	C3B-C4B	4.92	1.46	1.41
44	7	504	AXT	C5-C6	4.92	1.42	1.34
40	3	506	RRX	C8-C9	4.91	1.56	1.46
26	6	617	CHL	C3B-C4B	4.91	1.46	1.41
26	1	609	CHL	C3B-C4B	4.90	1.46	1.41
40	J	4002	RRX	C8-C9	4.89	1.56	1.46
29	G	4001	BCR	C11-C12	-4.89	1.21	1.34
26	6	610	CHL	C3A-C2A	-4.88	1.50	1.54
24	A	1011	CL0	CHD-C1D	4.88	1.47	1.39
26	8	613	CHL	C3B-C4B	4.87	1.46	1.41
26	3	611	CHL	C3B-C4B	4.84	1.46	1.41
26	2	613	CHL	C3B-C4B	4.83	1.46	1.41
26	a	613	CHL	C3B-C4B	4.83	1.46	1.41
26	7	617	CHL	C3B-C4B	4.79	1.46	1.41
24	A	1011	CL0	C3D-C4D	-4.77	1.34	1.41
26	4	609	CHL	C3B-C4B	4.77	1.46	1.41
44	1	502	AXT	C8-C9	4.73	1.56	1.46
44	1	502	AXT	C28-C29	4.72	1.56	1.46
26	1	613	CHL	C3B-C4B	4.70	1.46	1.41
26	3	604	CHL	C3A-C2A	-4.70	1.50	1.54
26	9	608	CHL	C3A-C2A	-4.69	1.50	1.54
26	8	603	CHL	C3A-C2A	-4.65	1.50	1.54
24	A	1011	CL0	CHD-C4C	4.64	1.48	1.39
44	1	502	AXT	C26-C25	4.62	1.42	1.35
26	5	618	CHL	C3B-C4B	4.61	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	617	CHL	C3B-C4B	4.61	1.45	1.41
44	1	502	AXT	C21-C26	4.60	1.59	1.53
26	9	601	CHL	C3B-C4B	4.58	1.45	1.41
26	a	609	CHL	C3A-C2A	-4.57	1.50	1.54
24	A	1011	CL0	C3D-C2D	4.57	1.47	1.39
26	6	610	CHL	C3B-C4B	4.56	1.45	1.41
26	9	610	CHL	C3A-C2A	-4.55	1.50	1.54
26	3	608	CHL	C3B-C4B	4.52	1.45	1.41
44	1	502	AXT	C12-C13	4.51	1.55	1.46
26	9	610	CHL	C3B-C4B	4.50	1.45	1.41
44	1	502	AXT	C32-C33	4.50	1.55	1.46
26	5	613	CHL	C3B-C4B	4.48	1.45	1.41
26	1	611	CHL	C3A-C2A	-4.45	1.50	1.54
25	8	620	CLA	CBB-CAB	4.44	1.51	1.30
26	6	619	CHL	C3A-C2A	-4.44	1.50	1.54
46	a	504	QTB	C11-C10	-4.43	1.44	1.50
25	L	1504	CLA	CBB-CAB	4.43	1.51	1.30
40	3	506	RRX	C12-C13	4.43	1.55	1.46
25	1	602	CLA	CBB-CAB	4.42	1.51	1.30
26	1	610	CHL	C3A-C2A	-4.42	1.50	1.54
25	J	1901	CLA	CBB-CAB	4.42	1.51	1.30
25	a	607	CLA	CBB-CAB	4.42	1.51	1.30
44	7	504	AXT	C8-C9	4.42	1.55	1.46
25	a	602	CLA	CBB-CAB	4.42	1.51	1.30
25	A	1102	CLA	CBB-CAB	4.41	1.51	1.30
25	L	1501	CLA	CBB-CAB	4.41	1.51	1.30
25	5	607	CLA	CBB-CAB	4.41	1.51	1.30
25	L	1502	CLA	CBB-CAB	4.41	1.51	1.30
25	O	1803	CLA	CBB-CAB	4.41	1.51	1.30
25	1	615	CLA	CBB-CAB	4.41	1.51	1.30
25	5	602	CLA	CBB-CAB	4.41	1.51	1.30
25	2	621	CLA	CBB-CAB	4.41	1.51	1.30
40	J	4002	RRX	C27-C26	-4.41	1.44	1.51
25	L	1503	CLA	CBB-CAB	4.41	1.51	1.30
25	A	1128	CLA	CBB-CAB	4.41	1.51	1.30
25	5	608	CLA	CBB-CAB	4.41	1.51	1.30
25	G	1602	CLA	CBB-CAB	4.41	1.51	1.30
25	4	617	CLA	CBB-CAB	4.41	1.51	1.30
24	A	1011	CL0	CHC-C1C	4.41	1.47	1.39
25	2	606	CLA	CBB-CAB	4.41	1.51	1.30
25	A	1111	CLA	CBB-CAB	4.41	1.51	1.30
25	B	1210	CLA	CBB-CAB	4.41	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1207	CLA	CBB-CAB	4.41	1.51	1.30
26	1	611	CHL	C3B-C4B	4.41	1.45	1.41
25	a	605	CLA	CBB-CAB	4.41	1.51	1.30
25	7	612	CLA	CBB-CAB	4.41	1.51	1.30
26	6	611	CHL	C3A-C2A	-4.40	1.50	1.54
25	B	1230	CLA	CBB-CAB	4.40	1.51	1.30
25	G	1601	CLA	CBB-CAB	4.40	1.51	1.30
25	4	611	CLA	CBB-CAB	4.40	1.51	1.30
25	a	615	CLA	CBB-CAB	4.40	1.51	1.30
25	4	605	CLA	CBB-CAB	4.40	1.51	1.30
25	8	605	CLA	CBB-CAB	4.40	1.51	1.30
25	3	618	CLA	CBB-CAB	4.40	1.51	1.30
25	6	607	CLA	CBB-CAB	4.40	1.51	1.30
25	2	612	CLA	CBB-CAB	4.40	1.51	1.30
25	9	606	CLA	CBB-CAB	4.40	1.51	1.30
25	B	1221	CLA	CBB-CAB	4.40	1.51	1.30
25	5	606	CLA	CBB-CAB	4.40	1.51	1.30
25	K	1401	CLA	CBB-CAB	4.40	1.51	1.30
25	4	610	CLA	CBB-CAB	4.40	1.51	1.30
25	4	615	CLA	CBB-CAB	4.40	1.51	1.30
40	J	4002	RRX	C12-C13	4.40	1.55	1.46
25	B	1219	CLA	CBB-CAB	4.40	1.51	1.30
25	1	606	CLA	CBB-CAB	4.40	1.51	1.30
25	a	608	CLA	CBB-CAB	4.40	1.51	1.30
25	7	610	CLA	CBB-CAB	4.40	1.51	1.30
25	B	1227	CLA	CBB-CAB	4.40	1.51	1.30
25	7	606	CLA	CBB-CAB	4.39	1.51	1.30
25	B	1217	CLA	CBB-CAB	4.39	1.51	1.30
25	O	1802	CLA	CBB-CAB	4.39	1.51	1.30
25	9	602	CLA	CBB-CAB	4.39	1.51	1.30
25	3	602	CLA	CBB-CAB	4.39	1.51	1.30
25	6	601	CLA	CBB-CAB	4.39	1.51	1.30
25	8	608	CLA	CBB-CAB	4.39	1.51	1.30
25	B	1206	CLA	CBB-CAB	4.39	1.51	1.30
25	6	608	CLA	CBB-CAB	4.39	1.51	1.30
25	A	1123	CLA	CBB-CAB	4.39	1.51	1.30
25	6	615	CLA	CBB-CAB	4.39	1.51	1.30
25	2	608	CLA	CBB-CAB	4.39	1.51	1.30
25	A	1117	CLA	CBB-CAB	4.39	1.51	1.30
25	9	607	CLA	CBB-CAB	4.39	1.51	1.30
25	5	604	CLA	CBB-CAB	4.39	1.51	1.30
25	A	1124	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	602	CLA	CBB-CAB	4.39	1.51	1.30
25	4	608	CLA	CBB-CAB	4.39	1.51	1.30
25	a	612	CLA	CBB-CAB	4.39	1.51	1.30
25	K	1402	CLA	CBB-CAB	4.39	1.51	1.30
25	5	605	CLA	CBB-CAB	4.39	1.51	1.30
25	B	1224	CLA	CBB-CAB	4.39	1.51	1.30
25	B	1201	CLA	CBB-CAB	4.39	1.51	1.30
25	8	615	CLA	CBB-CAB	4.39	1.51	1.30
25	1	603	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1223	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1107	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1240	CLA	CBB-CAB	4.38	1.51	1.30
25	a	603	CLA	CBB-CAB	4.38	1.51	1.30
25	4	601	CLA	CBB-CAB	4.38	1.51	1.30
25	7	601	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1235	CLA	CBB-CAB	4.38	1.51	1.30
29	5	503	BCR	C16-C17	-4.38	1.29	1.43
25	3	610	CLA	CBB-CAB	4.38	1.51	1.30
25	4	606	CLA	CBB-CAB	4.38	1.51	1.30
25	5	603	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1228	CLA	CBB-CAB	4.38	1.51	1.30
25	6	618	CLA	CBB-CAB	4.38	1.51	1.30
25	F	1302	CLA	CBB-CAB	4.38	1.51	1.30
25	O	1801	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1109	CLA	CBB-CAB	4.38	1.51	1.30
25	3	613	CLA	CBB-CAB	4.38	1.51	1.30
25	6	602	CLA	CBB-CAB	4.38	1.51	1.30
25	F	1301	CLA	CBB-CAB	4.38	1.51	1.30
25	1	605	CLA	CBB-CAB	4.38	1.51	1.30
25	2	602	CLA	CBB-CAB	4.38	1.51	1.30
25	1	612	CLA	CBB-CAB	4.38	1.51	1.30
25	a	601	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1226	CLA	CBB-CAB	4.38	1.51	1.30
25	K	1404	CLA	CBB-CAB	4.38	1.51	1.30
25	3	607	CLA	CBB-CAB	4.38	1.51	1.30
25	K	1403	CLA	CBB-CAB	4.38	1.51	1.30
25	7	607	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1013	CLA	CBB-CAB	4.38	1.51	1.30
25	7	603	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1215	CLA	CBB-CAB	4.38	1.51	1.30
25	4	604	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1012	CLA	CBB-CAB	4.38	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	612	CLA	CBB-CAB	4.38	1.51	1.30
25	9	605	CLA	CBB-CAB	4.38	1.51	1.30
29	7	503	BCR	C16-C17	-4.38	1.29	1.43
25	5	612	CLA	CBB-CAB	4.38	1.51	1.30
25	2	603	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1212	CLA	CBB-CAB	4.38	1.51	1.30
25	G	1603	CLA	CBB-CAB	4.38	1.51	1.30
25	a	611	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1110	CLA	CBB-CAB	4.38	1.51	1.30
25	3	601	CLA	CBB-CAB	4.38	1.51	1.30
25	8	606	CLA	CBB-CAB	4.38	1.51	1.30
25	A	1138	CLA	CBB-CAB	4.38	1.51	1.30
25	6	605	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1209	CLA	CBB-CAB	4.38	1.51	1.30
25	6	612	CLA	CBB-CAB	4.38	1.51	1.30
25	B	1239	CLA	CBB-CAB	4.38	1.51	1.30
25	8	618	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1211	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1213	CLA	CBB-CAB	4.37	1.51	1.30
25	1	607	CLA	CBB-CAB	4.37	1.51	1.30
25	8	602	CLA	CBB-CAB	4.37	1.51	1.30
25	5	614	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1119	CLA	CBB-CAB	4.37	1.51	1.30
25	8	611	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1103	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1134	CLA	CBB-CAB	4.37	1.51	1.30
25	5	609	CLA	CBB-CAB	4.37	1.51	1.30
25	H	1701	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1126	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1231	CLA	CBB-CAB	4.37	1.51	1.30
25	4	616	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1023	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1232	CLA	CBB-CAB	4.37	1.51	1.30
25	3	606	CLA	CBB-CAB	4.37	1.51	1.30
25	2	604	CLA	CBB-CAB	4.37	1.51	1.30
25	4	607	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1132	CLA	CBB-CAB	4.37	1.51	1.30
25	A	1139	CLA	CBB-CAB	4.37	1.51	1.30
25	7	602	CLA	CBB-CAB	4.37	1.51	1.30
25	B	1222	CLA	CBB-CAB	4.37	1.51	1.30
25	7	608	CLA	CBB-CAB	4.37	1.51	1.30
39	F	4001	NEX	C10-C9	-4.37	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	607	CLA	CBB-CAB	4.37	1.51	1.30
25	9	612	CLA	CBB-CAB	4.37	1.51	1.30
25	5	601	CLA	CBB-CAB	4.36	1.51	1.30
25	8	612	CLA	CBB-CAB	4.36	1.51	1.30
25	2	607	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1121	CLA	CBB-CAB	4.36	1.51	1.30
25	8	609	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1140	CLA	CBB-CAB	4.36	1.51	1.30
25	B	1203	CLA	CBB-CAB	4.36	1.51	1.30
25	6	606	CLA	CBB-CAB	4.36	1.51	1.30
25	7	605	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1118	CLA	CBB-CAB	4.36	1.51	1.30
25	3	605	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1141	CLA	CBB-CAB	4.36	1.51	1.30
25	B	1229	CLA	CBB-CAB	4.36	1.51	1.30
25	H	1703	CLA	CBB-CAB	4.36	1.51	1.30
26	5	610	CHL	C3B-C4B	4.36	1.45	1.41
25	A	1106	CLA	CBB-CAB	4.36	1.51	1.30
25	H	1702	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1113	CLA	CBB-CAB	4.36	1.51	1.30
25	9	604	CLA	CBB-CAB	4.36	1.51	1.30
25	1	608	CLA	CBB-CAB	4.36	1.51	1.30
25	B	1204	CLA	CBB-CAB	4.36	1.51	1.30
25	B	1236	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1108	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1136	CLA	CBB-CAB	4.36	1.51	1.30
25	A	1101	CLA	CBB-CAB	4.36	1.51	1.30
25	1	601	CLA	CBB-CAB	4.36	1.51	1.30
39	F	4001	NEX	C34-C33	-4.36	1.25	1.35
25	B	1216	CLA	CBB-CAB	4.36	1.51	1.30
25	B	1238	CLA	CBB-CAB	4.35	1.51	1.30
25	6	603	CLA	CBB-CAB	4.35	1.51	1.30
25	A	1105	CLA	CBB-CAB	4.35	1.51	1.30
25	A	1120	CLA	CBB-CAB	4.35	1.51	1.30
29	B	4004	BCR	C16-C17	-4.35	1.29	1.43
25	B	1205	CLA	CBB-CAB	4.35	1.51	1.30
25	5	615	CLA	CBB-CAB	4.35	1.51	1.30
25	B	1022	CLA	CBB-CAB	4.35	1.51	1.30
25	A	1129	CLA	CBB-CAB	4.35	1.51	1.30
25	7	604	CLA	CBB-CAB	4.35	1.51	1.30
29	B	4001	BCR	C16-C17	-4.35	1.29	1.43
25	A	1116	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1122	CLA	CBB-CAB	4.35	1.51	1.30
25	A	1137	CLA	CBB-CAB	4.35	1.51	1.30
25	A	1131	CLA	CBB-CAB	4.34	1.51	1.30
25	3	612	CLA	CBB-CAB	4.34	1.51	1.30
25	9	609	CLA	CBB-CAB	4.34	1.51	1.30
25	3	616	CLA	CBB-CAB	4.34	1.51	1.30
25	2	605	CLA	CBB-CAB	4.34	1.51	1.30
29	A	4004	BCR	C16-C17	-4.34	1.29	1.43
25	2	615	CLA	CBB-CAB	4.34	1.51	1.30
25	B	1214	CLA	CBB-CAB	4.34	1.51	1.30
25	B	1220	CLA	CBB-CAB	4.34	1.51	1.30
40	3	506	RRX	C27-C26	-4.33	1.44	1.51
25	B	1237	CLA	CBB-CAB	4.33	1.51	1.30
25	B	1225	CLA	CBB-CAB	4.33	1.51	1.30
25	B	1218	CLA	CBB-CAB	4.33	1.51	1.30
25	2	601	CLA	CBB-CAB	4.33	1.51	1.30
40	J	4002	RRX	C3-C4	4.33	1.66	1.52
25	A	1133	CLA	CBB-CAB	4.32	1.51	1.30
25	B	1202	CLA	CBB-CAB	4.32	1.51	1.30
36	8	802	DGD	O1G-C1A	4.32	1.45	1.33
29	B	4005	BCR	C16-C17	-4.32	1.29	1.43
29	A	4002	BCR	C16-C17	-4.32	1.29	1.43
25	A	1104	CLA	CBB-CAB	4.32	1.51	1.30
25	B	1021	CLA	CBB-CAB	4.32	1.51	1.30
29	B	4006	BCR	C16-C17	-4.32	1.29	1.43
29	I	4001	BCR	C16-C17	-4.31	1.29	1.43
25	A	1112	CLA	CBB-CAB	4.31	1.51	1.30
36	8	803	DGD	O1G-C1A	4.31	1.45	1.33
25	4	603	CLA	CBB-CAB	4.30	1.51	1.30
36	7	806	DGD	O1G-C1A	4.30	1.45	1.33
40	J	4002	RRX	C20-C21	4.30	1.56	1.43
44	7	504	AXT	C12-C13	4.29	1.55	1.46
25	A	1130	CLA	CBB-CAB	4.29	1.51	1.30
25	A	1115	CLA	CBB-CAB	4.29	1.51	1.30
26	9	613	CHL	C2A-C3A	-4.29	1.51	1.54
25	A	1127	CLA	CBB-CAB	4.28	1.51	1.30
29	A	4003	BCR	C16-C17	-4.28	1.29	1.43
29	A	4001	BCR	C16-C17	-4.28	1.29	1.43
25	6	604	CLA	CBB-CAB	4.27	1.50	1.30
25	A	1135	CLA	CBB-CAB	4.26	1.50	1.30
39	F	4001	NEX	C30-C29	-4.26	1.25	1.35
40	3	506	RRX	C3-C4	4.26	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	617	CHL	C3A-C2A	-4.26	1.51	1.54
39	F	4001	NEX	C14-C13	-4.26	1.26	1.35
29	3	503	BCR	C16-C17	-4.26	1.30	1.43
26	7	617	CHL	C3A-C2A	-4.25	1.51	1.54
29	6	503	BCR	C16-C17	-4.25	1.30	1.43
26	A	1114	CHL	C3B-C4B	4.25	1.45	1.41
29	G	4001	BCR	C10-C9	4.25	1.45	1.35
29	J	4001	BCR	C16-C17	-4.23	1.30	1.43
29	L	4002	BCR	C16-C17	-4.22	1.30	1.43
36	B	5003	DGD	O1G-C1A	4.21	1.45	1.33
40	J	4002	RRX	C23-C22	4.21	1.55	1.46
26	1	613	CHL	C3A-C2A	-4.21	1.51	1.54
26	6	619	CHL	C3B-C4B	4.21	1.45	1.41
29	8	503	BCR	C16-C17	-4.20	1.30	1.43
29	B	4007	BCR	C16-C17	-4.20	1.30	1.43
29	5	504	BCR	C16-C17	-4.20	1.30	1.43
29	K	4002	BCR	C16-C17	-4.19	1.30	1.43
29	H	4001	BCR	C10-C9	4.19	1.45	1.35
29	B	4003	BCR	C16-C17	-4.19	1.30	1.43
26	7	615	CHL	C3A-C2A	-4.18	1.51	1.54
25	B	1234	CLA	C1B-C2B	4.18	1.44	1.39
29	B	4002	BCR	C16-C17	-4.17	1.30	1.43
25	A	1125	CLA	CBB-CAB	4.16	1.50	1.30
29	A	4005	BCR	C16-C17	-4.16	1.30	1.43
29	4	503	BCR	C10-C9	4.16	1.45	1.35
29	K	4001	BCR	C16-C17	-4.15	1.30	1.43
29	3	505	BCR	C16-C17	-4.15	1.30	1.43
29	6	504	BCR	C16-C17	-4.14	1.30	1.43
29	O	4001	BCR	C10-C9	4.14	1.45	1.35
29	O	4001	BCR	C16-C17	-4.14	1.30	1.43
29	H	4001	BCR	C16-C17	-4.13	1.30	1.43
26	a	609	CHL	C3B-C4B	4.13	1.45	1.41
29	L	4001	BCR	C16-C17	-4.11	1.30	1.43
26	6	613	CHL	C3B-C4B	4.11	1.45	1.41
29	4	503	BCR	C16-C17	-4.11	1.30	1.43
29	B	4002	BCR	C10-C9	4.11	1.45	1.35
40	3	506	RRX	C20-C21	4.11	1.55	1.43
29	3	504	BCR	C16-C17	-4.10	1.30	1.43
29	L	4003	BCR	C16-C17	-4.10	1.30	1.43
29	3	504	BCR	C10-C9	4.09	1.45	1.35
40	3	506	RRX	C23-C22	4.09	1.54	1.46
29	L	4003	BCR	C10-C9	4.08	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	503	BCR	C10-C9	4.08	1.45	1.35
29	G	4001	BCR	C16-C17	-4.08	1.30	1.43
25	A	1128	CLA	MG-ND	-4.07	1.97	2.05
29	A	4005	BCR	C10-C9	4.07	1.45	1.35
29	B	4003	BCR	C10-C9	4.07	1.45	1.35
29	I	4001	BCR	C10-C9	4.07	1.45	1.35
29	L	4001	BCR	C10-C9	4.05	1.45	1.35
29	3	505	BCR	C10-C9	4.05	1.45	1.35
25	B	1226	CLA	MG-ND	-4.04	1.97	2.05
40	3	506	RRX	C15-C14	4.03	1.55	1.43
29	B	4007	BCR	C10-C9	4.03	1.45	1.35
26	a	610	CHL	C3A-C2A	-4.02	1.51	1.54
29	K	4002	BCR	C10-C9	4.02	1.45	1.35
29	K	4001	BCR	C10-C9	4.02	1.45	1.35
26	3	603	CHL	C3A-C2A	-4.02	1.51	1.54
25	9	605	CLA	MG-ND	-4.01	1.97	2.05
29	L	4002	BCR	C10-C9	4.01	1.45	1.35
25	A	1012	CLA	MG-ND	-4.01	1.97	2.05
29	6	503	BCR	C10-C9	4.01	1.45	1.35
25	B	1022	CLA	MG-ND	-4.00	1.97	2.05
29	A	4003	BCR	C10-C9	3.99	1.45	1.35
29	3	503	BCR	C10-C9	3.99	1.45	1.35
29	B	4005	BCR	C10-C9	3.98	1.45	1.35
29	J	4001	BCR	C10-C9	3.97	1.45	1.35
25	B	1224	CLA	MG-ND	-3.96	1.97	2.05
29	6	504	BCR	C10-C9	3.95	1.44	1.35
29	7	503	BCR	C10-C9	3.95	1.44	1.35
26	4	613	CHL	C3A-C2A	-3.94	1.51	1.54
25	A	1126	CLA	MG-ND	-3.93	1.98	2.05
40	J	4002	RRX	C15-C14	3.93	1.55	1.43
29	B	4004	BCR	C10-C9	3.93	1.44	1.35
26	4	609	CHL	C3A-C2A	-3.92	1.51	1.54
25	a	615	CLA	MG-ND	-3.92	1.98	2.05
29	A	4001	BCR	C10-C9	3.91	1.44	1.35
29	5	504	BCR	C10-C9	3.91	1.44	1.35
25	4	615	CLA	MG-ND	-3.91	1.98	2.05
25	A	1127	CLA	MG-ND	-3.91	1.98	2.05
25	A	1123	CLA	MG-ND	-3.91	1.98	2.05
25	B	1023	CLA	MG-ND	-3.90	1.98	2.05
25	7	605	CLA	MG-ND	-3.90	1.98	2.05
25	2	621	CLA	MG-ND	-3.90	1.98	2.05
25	A	1131	CLA	MG-ND	-3.90	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1021	CLA	MG-ND	-3.89	1.98	2.05
25	B	1221	CLA	MG-ND	-3.88	1.98	2.05
29	5	503	BCR	C10-C9	3.88	1.44	1.35
25	A	1112	CLA	MG-ND	-3.87	1.98	2.05
25	A	1133	CLA	MG-ND	-3.87	1.98	2.05
25	J	1901	CLA	MG-ND	-3.86	1.98	2.05
25	K	1402	CLA	MG-ND	-3.86	1.98	2.05
26	5	617	CHL	C3A-C2A	-3.85	1.51	1.54
25	A	1129	CLA	MG-ND	-3.85	1.98	2.05
25	6	607	CLA	MG-ND	-3.85	1.98	2.05
25	A	1141	CLA	MG-ND	-3.85	1.98	2.05
25	5	608	CLA	MG-ND	-3.85	1.98	2.05
29	B	4006	BCR	C10-C9	3.84	1.44	1.35
25	2	615	CLA	MG-ND	-3.84	1.98	2.05
25	8	620	CLA	MG-ND	-3.84	1.98	2.05
25	6	615	CLA	MG-ND	-3.84	1.98	2.05
25	1	615	CLA	MG-ND	-3.83	1.98	2.05
29	B	4001	BCR	C10-C9	3.83	1.44	1.35
25	B	1206	CLA	MG-ND	-3.83	1.98	2.05
25	5	605	CLA	MG-ND	-3.83	1.98	2.05
26	8	601	CHL	C1A-CHA	-3.82	1.35	1.40
25	A	1013	CLA	MG-ND	-3.82	1.98	2.05
25	B	1211	CLA	MG-ND	-3.82	1.98	2.05
25	A	1107	CLA	MG-ND	-3.82	1.98	2.05
25	A	1115	CLA	MG-ND	-3.82	1.98	2.05
25	B	1223	CLA	MG-ND	-3.82	1.98	2.05
26	5	618	CHL	C3A-C2A	-3.82	1.51	1.54
25	7	612	CLA	MG-ND	-3.82	1.98	2.05
25	5	614	CLA	MG-ND	-3.82	1.98	2.05
25	8	611	CLA	MG-ND	-3.82	1.98	2.05
25	A	1102	CLA	MG-ND	-3.82	1.98	2.05
25	1	612	CLA	MG-ND	-3.81	1.98	2.05
25	B	1214	CLA	MG-ND	-3.81	1.98	2.05
25	B	1210	CLA	MG-ND	-3.81	1.98	2.05
25	B	1232	CLA	MG-ND	-3.81	1.98	2.05
25	6	608	CLA	MG-ND	-3.81	1.98	2.05
25	B	1219	CLA	MG-ND	-3.81	1.98	2.05
25	3	607	CLA	MG-ND	-3.81	1.98	2.05
25	2	607	CLA	MG-ND	-3.80	1.98	2.05
25	A	1113	CLA	MG-ND	-3.80	1.98	2.05
25	9	612	CLA	MG-ND	-3.80	1.98	2.05
25	A	1134	CLA	MG-ND	-3.80	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	612	CLA	MG-ND	-3.80	1.98	2.05
25	K	1401	CLA	MG-ND	-3.80	1.98	2.05
25	B	1225	CLA	MG-ND	-3.80	1.98	2.05
25	1	602	CLA	MG-ND	-3.79	1.98	2.05
25	5	609	CLA	MG-ND	-3.79	1.98	2.05
25	6	612	CLA	MG-ND	-3.79	1.98	2.05
29	A	4004	BCR	C10-C9	3.79	1.44	1.35
25	8	607	CLA	MG-ND	-3.79	1.98	2.05
25	2	606	CLA	MG-ND	-3.79	1.98	2.05
25	A	1117	CLA	MG-ND	-3.79	1.98	2.05
25	9	602	CLA	MG-ND	-3.79	1.98	2.05
25	A	1121	CLA	MG-ND	-3.79	1.98	2.05
25	B	1212	CLA	MG-ND	-3.79	1.98	2.05
25	A	1119	CLA	MG-ND	-3.79	1.98	2.05
25	F	1302	CLA	MG-ND	-3.79	1.98	2.05
25	a	601	CLA	MG-ND	-3.79	1.98	2.05
25	9	604	CLA	MG-ND	-3.79	1.98	2.05
25	A	1104	CLA	MG-ND	-3.79	1.98	2.05
25	4	607	CLA	MG-ND	-3.79	1.98	2.05
25	6	606	CLA	MG-ND	-3.79	1.98	2.05
25	B	1240	CLA	MG-ND	-3.78	1.98	2.05
25	3	606	CLA	MG-ND	-3.78	1.98	2.05
25	B	1201	CLA	MG-ND	-3.78	1.98	2.05
25	A	1118	CLA	MG-ND	-3.78	1.98	2.05
26	6	609	CHL	C3A-C2A	-3.78	1.51	1.54
25	2	604	CLA	MG-ND	-3.78	1.98	2.05
25	A	1135	CLA	MG-ND	-3.78	1.98	2.05
25	3	605	CLA	MG-ND	-3.78	1.98	2.05
25	9	609	CLA	MG-ND	-3.78	1.98	2.05
25	8	615	CLA	MG-ND	-3.78	1.98	2.05
25	H	1703	CLA	MG-ND	-3.78	1.98	2.05
25	L	1503	CLA	MG-ND	-3.78	1.98	2.05
25	6	605	CLA	MG-ND	-3.78	1.98	2.05
25	B	1228	CLA	MG-ND	-3.78	1.98	2.05
39	F	4001	NEX	C7-C6	-3.77	1.26	1.30
25	O	1802	CLA	MG-ND	-3.77	1.98	2.05
25	9	607	CLA	MG-ND	-3.77	1.98	2.05
25	5	615	CLA	MG-ND	-3.77	1.98	2.05
25	A	1103	CLA	MG-ND	-3.77	1.98	2.05
25	F	1301	CLA	MG-ND	-3.77	1.98	2.05
25	B	1227	CLA	MG-ND	-3.77	1.98	2.05
25	B	1235	CLA	MG-ND	-3.77	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	602	CLA	MG-ND	-3.77	1.98	2.05
25	2	605	CLA	MG-ND	-3.77	1.98	2.05
25	A	1124	CLA	MG-ND	-3.77	1.98	2.05
25	B	1239	CLA	MG-ND	-3.77	1.98	2.05
25	7	607	CLA	MG-ND	-3.77	1.98	2.05
25	A	1132	CLA	MG-ND	-3.77	1.98	2.05
25	A	1139	CLA	MG-ND	-3.77	1.98	2.05
25	B	1208	CLA	MG-ND	-3.77	1.98	2.05
26	8	613	CHL	C3A-C2A	-3.77	1.51	1.54
25	A	1136	CLA	MG-ND	-3.77	1.98	2.05
25	2	608	CLA	MG-ND	-3.76	1.98	2.05
26	6	609	CHL	C3B-C4B	3.76	1.45	1.41
25	6	618	CLA	MG-ND	-3.76	1.98	2.05
25	K	1404	CLA	MG-ND	-3.76	1.98	2.05
25	4	605	CLA	MG-ND	-3.76	1.98	2.05
25	L	1502	CLA	MG-ND	-3.76	1.98	2.05
25	A	1109	CLA	MG-ND	-3.76	1.98	2.05
25	A	1138	CLA	MG-ND	-3.76	1.98	2.05
25	7	608	CLA	MG-ND	-3.76	1.98	2.05
25	A	1125	CLA	MG-ND	-3.76	1.98	2.05
25	7	603	CLA	MG-ND	-3.76	1.98	2.05
25	A	1140	CLA	MG-ND	-3.76	1.98	2.05
25	a	611	CLA	MG-ND	-3.76	1.98	2.05
25	3	601	CLA	MG-ND	-3.76	1.98	2.05
25	8	602	CLA	MG-ND	-3.76	1.98	2.05
25	8	605	CLA	MG-ND	-3.75	1.98	2.05
36	B	5003	DGD	CAA-C9A	-3.75	1.33	1.51
25	3	610	CLA	MG-ND	-3.75	1.98	2.05
25	6	602	CLA	MG-ND	-3.75	1.98	2.05
25	7	610	CLA	MG-ND	-3.75	1.98	2.05
25	3	616	CLA	MG-ND	-3.75	1.98	2.05
25	7	602	CLA	MG-ND	-3.75	1.98	2.05
25	4	608	CLA	MG-ND	-3.75	1.98	2.05
25	2	602	CLA	MG-ND	-3.75	1.98	2.05
25	A	1130	CLA	MG-ND	-3.75	1.98	2.05
25	B	1230	CLA	MG-ND	-3.75	1.98	2.05
25	1	601	CLA	MG-ND	-3.75	1.98	2.05
26	8	610	CHL	C3A-C2A	-3.75	1.51	1.54
25	4	610	CLA	MG-ND	-3.75	1.98	2.05
25	L	1501	CLA	MG-ND	-3.75	1.98	2.05
25	B	1204	CLA	MG-ND	-3.75	1.98	2.05
26	1	610	CHL	C3B-C4B	3.75	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1116	CLA	MG-ND	-3.75	1.98	2.05
25	B	1220	CLA	MG-ND	-3.75	1.98	2.05
25	7	604	CLA	MG-ND	-3.75	1.98	2.05
25	2	603	CLA	MG-ND	-3.75	1.98	2.05
25	H	1702	CLA	MG-ND	-3.74	1.98	2.05
25	G	1602	CLA	MG-ND	-3.74	1.98	2.05
25	8	606	CLA	MG-ND	-3.74	1.98	2.05
25	8	618	CLA	MG-ND	-3.74	1.98	2.05
25	A	1120	CLA	MG-ND	-3.74	1.98	2.05
25	B	1213	CLA	MG-ND	-3.74	1.98	2.05
25	2	601	CLA	MG-ND	-3.74	1.98	2.05
25	B	1205	CLA	MG-ND	-3.74	1.98	2.05
25	1	606	CLA	MG-ND	-3.74	1.98	2.05
25	G	1601	CLA	MG-ND	-3.74	1.98	2.05
25	a	607	CLA	MG-ND	-3.74	1.98	2.05
25	6	603	CLA	MG-ND	-3.74	1.98	2.05
25	B	1207	CLA	MG-ND	-3.74	1.98	2.05
25	4	602	CLA	MG-ND	-3.73	1.98	2.05
25	7	606	CLA	MG-ND	-3.73	1.98	2.05
25	B	1238	CLA	MG-ND	-3.73	1.98	2.05
25	B	1218	CLA	MG-ND	-3.73	1.98	2.05
25	K	1403	CLA	MG-ND	-3.73	1.98	2.05
25	2	612	CLA	MG-ND	-3.73	1.98	2.05
25	a	603	CLA	MG-ND	-3.73	1.98	2.05
25	A	1111	CLA	MG-ND	-3.73	1.98	2.05
25	3	613	CLA	MG-ND	-3.73	1.98	2.05
25	B	1203	CLA	MG-ND	-3.73	1.98	2.05
25	4	604	CLA	MG-ND	-3.73	1.98	2.05
25	5	606	CLA	MG-ND	-3.73	1.98	2.05
25	4	601	CLA	MG-ND	-3.72	1.98	2.05
25	L	1504	CLA	MG-ND	-3.72	1.98	2.05
25	5	601	CLA	MG-ND	-3.72	1.98	2.05
25	B	1237	CLA	MG-ND	-3.72	1.98	2.05
36	B	5003	DGD	CDB-CCB	-3.72	1.33	1.51
25	O	1801	CLA	MG-ND	-3.72	1.98	2.05
25	B	1216	CLA	MG-ND	-3.72	1.98	2.05
25	a	602	CLA	MG-ND	-3.72	1.98	2.05
25	4	611	CLA	MG-ND	-3.72	1.98	2.05
25	4	617	CLA	MG-ND	-3.72	1.98	2.05
25	9	606	CLA	MG-ND	-3.72	1.98	2.05
25	a	605	CLA	MG-ND	-3.72	1.98	2.05
25	5	607	CLA	MG-ND	-3.72	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CLA	MG-ND	-3.72	1.98	2.05
25	B	1217	CLA	MG-ND	-3.72	1.98	2.05
25	O	1803	CLA	MG-ND	-3.72	1.98	2.05
36	B	5003	DGD	CGB-CFB	-3.72	1.33	1.51
25	3	602	CLA	MG-ND	-3.71	1.98	2.05
31	A	5004	LMG	C37-C36	-3.71	1.33	1.51
25	7	601	CLA	MG-ND	-3.71	1.98	2.05
36	8	802	DGD	CDA-CCA	-3.71	1.33	1.51
36	8	802	DGD	CAB-C9B	-3.71	1.33	1.51
25	B	1202	CLA	MG-ND	-3.71	1.98	2.05
25	1	603	CLA	MG-ND	-3.71	1.98	2.05
25	4	612	CLA	MG-ND	-3.71	1.98	2.05
25	H	1701	CLA	MG-ND	-3.71	1.98	2.05
25	4	616	CLA	MG-ND	-3.70	1.98	2.05
25	B	1215	CLA	MG-ND	-3.70	1.98	2.05
25	A	1122	CLA	MG-ND	-3.70	1.98	2.05
36	8	802	DGD	CAA-C9A	-3.70	1.33	1.51
25	8	609	CLA	MG-ND	-3.70	1.98	2.05
25	5	603	CLA	MG-ND	-3.70	1.98	2.05
26	1	604	CHL	C1A-CHA	-3.70	1.35	1.40
25	A	1137	CLA	MG-ND	-3.70	1.98	2.05
53	8	810	LAP	P9-O6	3.70	1.73	1.59
25	1	607	CLA	MG-ND	-3.69	1.98	2.05
25	3	618	CLA	MG-ND	-3.69	1.98	2.05
25	4	603	CLA	MG-ND	-3.69	1.98	2.05
25	8	612	CLA	MG-ND	-3.69	1.98	2.05
25	B	1236	CLA	MG-ND	-3.69	1.98	2.05
36	B	5003	DGD	CAB-C9B	-3.68	1.33	1.51
36	B	5003	DGD	CGA-CFA	-3.68	1.33	1.51
25	A	1108	CLA	MG-ND	-3.68	1.98	2.05
25	6	601	CLA	MG-ND	-3.68	1.98	2.05
25	B	1222	CLA	MG-ND	-3.68	1.98	2.05
25	G	1603	CLA	MG-ND	-3.68	1.98	2.05
26	7	611	CHL	C3A-C2A	-3.68	1.51	1.54
25	5	612	CLA	MG-ND	-3.67	1.98	2.05
40	3	506	RRX	C11-C10	3.67	1.54	1.43
25	A	1110	CLA	MG-ND	-3.67	1.98	2.05
26	8	604	CHL	C1A-CHA	-3.67	1.35	1.40
26	7	613	CHL	C1A-CHA	-3.66	1.35	1.40
25	4	606	CLA	MG-ND	-3.66	1.98	2.05
25	5	604	CLA	MG-ND	-3.66	1.98	2.05
25	A	1105	CLA	MG-ND	-3.65	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	7	806	DGD	CAA-C9A	-3.65	1.33	1.51
25	1	605	CLA	MG-ND	-3.65	1.98	2.05
36	B	5003	DGD	CDA-CCA	-3.64	1.33	1.51
44	7	504	AXT	C21-C26	3.64	1.58	1.53
25	a	608	CLA	MG-ND	-3.64	1.98	2.05
40	J	4002	RRX	C24-C25	3.64	1.57	1.45
25	A	1106	CLA	MG-ND	-3.63	1.98	2.05
25	A	1101	CLA	MG-ND	-3.63	1.98	2.05
25	8	608	CLA	MG-ND	-3.62	1.98	2.05
25	B	1209	CLA	MG-ND	-3.62	1.98	2.05
25	B	1231	CLA	MG-ND	-3.62	1.98	2.05
25	6	604	CLA	MG-ND	-3.61	1.98	2.05
25	B	1229	CLA	MG-ND	-3.61	1.98	2.05
26	3	604	CHL	C1A-CHA	-3.59	1.35	1.40
25	3	612	CLA	MG-ND	-3.58	1.98	2.05
26	3	611	CHL	C3B-C2B	-3.58	1.35	1.40
40	J	4002	RRX	C11-C10	3.58	1.54	1.43
44	7	504	AXT	C31-C30	3.56	1.54	1.43
26	9	601	CHL	CBB-CAB	3.56	1.51	1.29
26	a	609	CHL	CBB-CAB	3.55	1.51	1.29
26	6	619	CHL	CBB-CAB	3.55	1.51	1.29
29	A	4002	BCR	C10-C9	3.55	1.44	1.35
24	A	1011	CL0	C3A-C2A	-3.55	1.51	1.54
26	1	613	CHL	CBB-CAB	3.53	1.51	1.29
26	6	617	CHL	CBB-CAB	3.53	1.51	1.29
26	5	613	CHL	CBB-CAB	3.53	1.51	1.29
26	6	609	CHL	CBB-CAB	3.52	1.51	1.29
26	3	608	CHL	CBB-CAB	3.52	1.51	1.29
26	7	615	CHL	CBB-CAB	3.52	1.51	1.29
26	1	611	CHL	CBB-CAB	3.51	1.51	1.29
26	2	610	CHL	CBB-CAB	3.51	1.51	1.29
26	9	608	CHL	CBB-CAB	3.51	1.51	1.29
26	7	617	CHL	CBB-CAB	3.50	1.51	1.29
40	J	4002	RRX	C29-C30	3.50	1.65	1.54
40	J	4002	RRX	C16-C17	3.50	1.54	1.43
26	9	610	CHL	CBB-CAB	3.49	1.51	1.29
48	5	803	DGA	OG2-CB1	3.49	1.44	1.34
40	3	506	RRX	C16-C17	3.48	1.54	1.43
26	4	609	CHL	CBB-CAB	3.48	1.51	1.29
26	a	604	CHL	C1A-CHA	-3.48	1.36	1.40
40	3	506	RRX	C24-C25	3.48	1.57	1.45
26	8	610	CHL	CBB-CAB	3.47	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	610	CHL	CBB-CAB	3.47	1.51	1.29
25	B	1234	CLA	CBB-CAB	3.47	1.51	1.29
26	a	613	CHL	CBB-CAB	3.46	1.51	1.29
26	7	611	CHL	CBB-CAB	3.46	1.51	1.29
26	a	610	CHL	CBB-CAB	3.45	1.51	1.29
26	5	617	CHL	CBB-CAB	3.45	1.50	1.29
48	8	804	DGA	OG2-CB1	3.45	1.44	1.34
26	5	611	CHL	C3B-C2B	-3.44	1.35	1.40
26	4	613	CHL	CBB-CAB	3.44	1.50	1.29
26	A	1114	CHL	CBB-CAB	3.44	1.50	1.29
26	4	618	CHL	CBB-CAB	3.43	1.50	1.29
26	9	613	CHL	CBB-CAB	3.43	1.50	1.29
26	6	613	CHL	CBB-CAB	3.43	1.50	1.29
26	5	610	CHL	CBB-CAB	3.42	1.50	1.29
26	6	610	CHL	CBB-CAB	3.42	1.50	1.29
48	3	803	DGA	OG2-CB1	3.41	1.43	1.34
37	K	5002	PCW	O3-C11	3.41	1.43	1.33
37	B	5004	PCW	O3-C11	3.41	1.43	1.33
40	3	506	RRX	C29-C30	3.40	1.65	1.54
25	B	1230	CLA	C1C-NC	-3.40	1.32	1.37
26	8	613	CHL	CBB-CAB	3.40	1.50	1.29
37	K	5001	PCW	O3-C11	3.39	1.43	1.33
26	7	609	CHL	CBB-CAB	3.39	1.50	1.29
44	7	504	AXT	C35-C34	3.39	1.53	1.43
48	2	803	DGA	OG2-CB1	3.39	1.43	1.34
26	1	609	CHL	CBB-CAB	3.38	1.50	1.29
37	6	803	PCW	O3-C11	3.38	1.43	1.33
26	5	618	CHL	CBB-CAB	3.38	1.50	1.29
26	2	613	CHL	CBB-CAB	3.37	1.50	1.29
26	9	603	CHL	CBB-CAB	3.37	1.50	1.29
48	3	803	DGA	OG1-CA1	3.37	1.43	1.33
48	5	803	DGA	OG1-CA1	3.36	1.43	1.33
48	8	804	DGA	OG1-CA1	3.36	1.43	1.33
48	2	803	DGA	OG1-CA1	3.35	1.43	1.33
25	A	1128	CLA	C1C-NC	-3.35	1.32	1.37
26	a	606	CHL	C3A-C2A	-3.35	1.51	1.54
26	a	604	CHL	CBB-CAB	3.35	1.50	1.29
26	6	611	CHL	CBB-CAB	3.35	1.50	1.29
26	7	613	CHL	CBB-CAB	3.34	1.50	1.29
25	B	1212	CLA	C1C-NC	-3.33	1.32	1.37
26	1	604	CHL	CBB-CAB	3.33	1.50	1.29
26	a	606	CHL	CBB-CAB	3.33	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	502	AXT	C15-C14	3.33	1.53	1.43
25	B	1206	CLA	C1C-NC	-3.33	1.32	1.37
44	1	502	AXT	C31-C30	3.32	1.53	1.43
25	4	611	CLA	C1C-NC	-3.31	1.32	1.37
25	B	1215	CLA	C1C-NC	-3.31	1.32	1.37
26	9	603	CHL	C1A-CHA	-3.31	1.36	1.40
25	B	1210	CLA	C1C-NC	-3.31	1.32	1.37
26	8	601	CHL	C3B-C2B	-3.30	1.35	1.40
26	3	603	CHL	CBB-CAB	3.30	1.50	1.29
25	4	605	CLA	C1C-NC	-3.30	1.32	1.37
44	7	504	AXT	C15-C14	3.30	1.53	1.43
25	3	606	CLA	C1C-NC	-3.29	1.32	1.37
26	8	603	CHL	CBB-CAB	3.29	1.49	1.29
25	7	601	CLA	C1C-NC	-3.29	1.32	1.37
25	B	1204	CLA	C1C-NC	-3.28	1.32	1.37
25	A	1133	CLA	C1C-NC	-3.28	1.32	1.37
25	B	1023	CLA	C1C-NC	-3.28	1.32	1.37
25	A	1106	CLA	C1C-NC	-3.28	1.32	1.37
25	B	1223	CLA	C1C-NC	-3.28	1.32	1.37
25	A	1111	CLA	C1C-NC	-3.28	1.32	1.37
25	A	1124	CLA	C1C-NC	-3.28	1.32	1.37
25	A	1101	CLA	C1C-NC	-3.27	1.32	1.37
25	8	612	CLA	C1C-NC	-3.27	1.32	1.37
25	A	1105	CLA	C1C-NC	-3.27	1.32	1.37
25	K	1401	CLA	C1C-NC	-3.27	1.32	1.37
44	1	502	AXT	C35-C34	3.26	1.53	1.43
25	A	1113	CLA	C1C-NC	-3.26	1.32	1.37
44	1	502	AXT	C11-C10	3.26	1.53	1.43
26	3	603	CHL	C1A-CHA	-3.26	1.36	1.40
25	B	1226	CLA	C1C-NC	-3.26	1.32	1.37
25	5	605	CLA	C1C-NC	-3.26	1.32	1.37
25	B	1225	CLA	C1C-NC	-3.26	1.32	1.37
26	3	604	CHL	CBB-CAB	3.26	1.49	1.29
25	F	1301	CLA	C1C-NC	-3.26	1.32	1.37
25	B	1207	CLA	C1C-NC	-3.26	1.32	1.37
25	A	1122	CLA	C1C-NC	-3.26	1.32	1.37
40	J	4002	RRX	C4-C5	-3.25	1.44	1.51
26	8	604	CHL	CBB-CAB	3.25	1.49	1.29
25	A	1112	CLA	C1C-NC	-3.25	1.32	1.37
25	B	1227	CLA	C1C-NC	-3.25	1.32	1.37
26	8	604	CHL	C3B-C2B	-3.25	1.36	1.40
25	B	1205	CLA	C1C-NC	-3.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1214	CLA	C1C-NC	-3.25	1.32	1.37
25	A	1140	CLA	C1C-NC	-3.24	1.32	1.37
26	3	611	CHL	CBB-CAB	3.24	1.49	1.29
25	7	612	CLA	C1C-NC	-3.24	1.32	1.37
25	B	1218	CLA	C1C-NC	-3.24	1.32	1.37
26	5	611	CHL	CBB-CAB	3.23	1.49	1.29
25	6	603	CLA	C1C-NC	-3.23	1.32	1.37
25	2	604	CLA	C1C-NC	-3.23	1.32	1.37
25	7	610	CLA	C1C-NC	-3.23	1.32	1.37
25	L	1502	CLA	C1C-NC	-3.23	1.32	1.37
25	A	1127	CLA	C1C-NC	-3.23	1.32	1.37
25	B	1222	CLA	C1C-NC	-3.23	1.32	1.37
25	2	605	CLA	C1C-NC	-3.22	1.32	1.37
25	B	1203	CLA	C1C-NC	-3.22	1.32	1.37
25	4	612	CLA	C1C-NC	-3.22	1.32	1.37
25	B	1220	CLA	C1C-NC	-3.22	1.32	1.37
25	B	1238	CLA	C1C-NC	-3.22	1.32	1.37
25	B	1229	CLA	C1C-NC	-3.21	1.32	1.37
25	8	605	CLA	C1C-NC	-3.21	1.32	1.37
25	A	1121	CLA	C1C-NC	-3.21	1.32	1.37
25	A	1109	CLA	C1C-NC	-3.21	1.32	1.37
25	A	1108	CLA	C1C-NC	-3.21	1.32	1.37
25	A	1138	CLA	C1C-NC	-3.20	1.32	1.37
25	A	1118	CLA	C1C-NC	-3.20	1.32	1.37
25	7	604	CLA	C1C-NC	-3.20	1.32	1.37
25	3	601	CLA	C1C-NC	-3.20	1.32	1.37
25	A	1107	CLA	C1C-NC	-3.20	1.32	1.37
25	B	1021	CLA	C1C-NC	-3.20	1.32	1.37
25	B	1219	CLA	C1C-NC	-3.20	1.32	1.37
25	K	1403	CLA	C1C-NC	-3.20	1.32	1.37
25	3	618	CLA	C1C-NC	-3.19	1.32	1.37
25	B	1232	CLA	C1C-NC	-3.19	1.32	1.37
25	B	1236	CLA	C1C-NC	-3.19	1.32	1.37
25	B	1237	CLA	C1C-NC	-3.19	1.32	1.37
25	A	1013	CLA	C1C-NC	-3.19	1.32	1.37
25	A	1137	CLA	C1C-NC	-3.19	1.32	1.37
25	A	1135	CLA	C1C-NC	-3.19	1.32	1.37
25	1	602	CLA	C1C-NC	-3.19	1.32	1.37
25	B	1209	CLA	C1C-NC	-3.19	1.32	1.37
25	4	608	CLA	C1C-NC	-3.19	1.32	1.37
25	7	603	CLA	C1C-NC	-3.19	1.32	1.37
25	3	612	CLA	C1C-NC	-3.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	1701	CLA	C1C-NC	-3.18	1.32	1.37
25	5	602	CLA	C1C-NC	-3.18	1.32	1.37
25	4	601	CLA	C1C-NC	-3.18	1.32	1.37
25	5	615	CLA	C1C-NC	-3.18	1.32	1.37
25	G	1601	CLA	C1C-NC	-3.18	1.32	1.37
25	B	1231	CLA	C1C-NC	-3.18	1.32	1.37
25	A	1115	CLA	C1C-NC	-3.18	1.32	1.37
25	A	1132	CLA	C1C-NC	-3.18	1.32	1.37
25	a	602	CLA	C1C-NC	-3.18	1.32	1.37
25	B	1202	CLA	C1C-NC	-3.18	1.32	1.37
26	8	601	CHL	CBB-CAB	3.18	1.49	1.29
25	6	608	CLA	C1C-NC	-3.18	1.32	1.37
25	5	601	CLA	C1C-NC	-3.17	1.32	1.37
26	2	609	CHL	CBB-CAB	3.17	1.49	1.29
25	4	607	CLA	C1C-NC	-3.17	1.32	1.37
25	3	616	CLA	C1C-NC	-3.17	1.32	1.37
25	7	608	CLA	C1C-NC	-3.17	1.32	1.37
25	2	608	CLA	C1C-NC	-3.17	1.32	1.37
25	A	1139	CLA	C1C-NC	-3.17	1.32	1.37
25	6	618	CLA	C1C-NC	-3.17	1.32	1.37
25	B	1208	CLA	C1C-NC	-3.17	1.32	1.37
25	L	1501	CLA	C1C-NC	-3.17	1.32	1.37
25	A	1120	CLA	C1C-NC	-3.17	1.32	1.37
25	J	1901	CLA	C1C-NC	-3.17	1.32	1.37
25	a	608	CLA	C1C-NC	-3.17	1.32	1.37
25	6	606	CLA	C1C-NC	-3.17	1.32	1.37
25	A	1130	CLA	C1C-NC	-3.16	1.32	1.37
25	3	607	CLA	C1C-NC	-3.16	1.32	1.37
40	3	506	RRX	C7-C6	3.16	1.55	1.45
25	a	601	CLA	C1C-NC	-3.16	1.32	1.37
25	6	602	CLA	C1C-NC	-3.16	1.32	1.37
26	2	609	CHL	C3B-C2B	-3.16	1.36	1.40
25	3	605	CLA	C1C-NC	-3.16	1.32	1.37
25	B	1228	CLA	C1C-NC	-3.16	1.32	1.37
25	a	603	CLA	C1C-NC	-3.16	1.32	1.37
25	A	1116	CLA	C1C-NC	-3.16	1.32	1.37
25	1	607	CLA	C1C-NC	-3.16	1.32	1.37
25	2	612	CLA	C1C-NC	-3.16	1.32	1.37
25	8	602	CLA	C1C-NC	-3.16	1.32	1.37
25	2	615	CLA	C1C-NC	-3.16	1.32	1.37
25	B	1211	CLA	C1C-NC	-3.16	1.32	1.37
25	A	1117	CLA	C1C-NC	-3.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1110	CLA	C1C-NC	-3.15	1.32	1.37
25	B	1239	CLA	C1C-NC	-3.15	1.32	1.37
25	a	607	CLA	C1C-NC	-3.15	1.32	1.37
25	B	1224	CLA	C1C-NC	-3.15	1.32	1.37
25	3	610	CLA	C1C-NC	-3.15	1.32	1.37
25	3	613	CLA	C1C-NC	-3.15	1.32	1.37
40	3	506	RRX	C4-C5	-3.15	1.45	1.51
25	G	1603	CLA	C1C-NC	-3.15	1.32	1.37
25	A	1103	CLA	C1C-NC	-3.15	1.32	1.37
25	2	601	CLA	C1C-NC	-3.15	1.32	1.37
25	B	1216	CLA	C1C-NC	-3.15	1.32	1.37
25	8	609	CLA	C1C-NC	-3.14	1.32	1.37
25	8	611	CLA	C1C-NC	-3.14	1.32	1.37
25	7	605	CLA	C1C-NC	-3.14	1.32	1.37
25	1	612	CLA	C1C-NC	-3.14	1.32	1.37
25	6	607	CLA	C1C-NC	-3.14	1.32	1.37
25	1	608	CLA	C1C-NC	-3.14	1.32	1.37
25	5	609	CLA	C1C-NC	-3.14	1.32	1.37
25	B	1217	CLA	C1C-NC	-3.13	1.32	1.37
25	L	1504	CLA	C1C-NC	-3.13	1.32	1.37
26	2	610	CHL	C3A-C2A	-3.13	1.52	1.54
25	1	601	CLA	C1C-NC	-3.13	1.33	1.37
25	A	1129	CLA	C1C-NC	-3.13	1.33	1.37
25	8	615	CLA	C1C-NC	-3.13	1.33	1.37
25	a	615	CLA	C1C-NC	-3.13	1.33	1.37
25	4	610	CLA	C1C-NC	-3.13	1.33	1.37
25	A	1104	CLA	C1C-NC	-3.13	1.33	1.37
25	4	604	CLA	C1C-NC	-3.13	1.33	1.37
25	B	1240	CLA	C1C-NC	-3.13	1.33	1.37
25	8	608	CLA	C1C-NC	-3.13	1.33	1.37
25	A	1136	CLA	C1C-NC	-3.13	1.33	1.37
25	4	602	CLA	C1C-NC	-3.13	1.33	1.37
40	J	4002	RRX	C7-C6	3.12	1.55	1.45
25	1	606	CLA	C1C-NC	-3.12	1.33	1.37
25	L	1503	CLA	C1C-NC	-3.12	1.33	1.37
25	7	606	CLA	C1C-NC	-3.12	1.33	1.37
26	6	613	CHL	C1A-CHA	-3.12	1.36	1.40
25	5	603	CLA	C1C-NC	-3.12	1.33	1.37
25	A	1125	CLA	C1C-NC	-3.12	1.33	1.37
25	5	612	CLA	C1C-NC	-3.12	1.33	1.37
25	4	606	CLA	C1C-NC	-3.12	1.33	1.37
25	2	603	CLA	C1C-NC	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	608	CLA	C1C-NC	-3.12	1.33	1.37
25	8	606	CLA	C1C-NC	-3.12	1.33	1.37
25	A	1102	CLA	C1C-NC	-3.11	1.33	1.37
25	H	1702	CLA	C1C-NC	-3.11	1.33	1.37
25	a	611	CLA	C1C-NC	-3.11	1.33	1.37
25	5	607	CLA	C1C-NC	-3.11	1.33	1.37
25	B	1235	CLA	C1C-NC	-3.11	1.33	1.37
26	1	609	CHL	C3A-C2A	-3.11	1.52	1.54
25	2	606	CLA	C1C-NC	-3.11	1.33	1.37
25	6	615	CLA	C1C-NC	-3.11	1.33	1.37
25	7	607	CLA	C1C-NC	-3.11	1.33	1.37
25	B	1201	CLA	C1C-NC	-3.11	1.33	1.37
25	2	607	CLA	C1C-NC	-3.11	1.33	1.37
25	9	602	CLA	C1C-NC	-3.11	1.33	1.37
25	9	604	CLA	C1C-NC	-3.11	1.33	1.37
25	A	1141	CLA	C1C-NC	-3.11	1.33	1.37
25	O	1803	CLA	C1C-NC	-3.11	1.33	1.37
25	a	605	CLA	C1C-NC	-3.10	1.33	1.37
25	4	603	CLA	C1C-NC	-3.10	1.33	1.37
25	8	618	CLA	C1C-NC	-3.10	1.33	1.37
25	G	1602	CLA	C1C-NC	-3.10	1.33	1.37
25	2	621	CLA	C1C-NC	-3.10	1.33	1.37
25	H	1703	CLA	C1C-NC	-3.10	1.33	1.37
25	6	601	CLA	C1C-NC	-3.10	1.33	1.37
25	A	1012	CLA	C1C-NC	-3.10	1.33	1.37
25	F	1302	CLA	C1C-NC	-3.10	1.33	1.37
25	7	602	CLA	C1C-NC	-3.09	1.33	1.37
25	a	612	CLA	C1C-NC	-3.09	1.33	1.37
25	4	615	CLA	C1C-NC	-3.09	1.33	1.37
25	A	1131	CLA	C1C-NC	-3.09	1.33	1.37
25	4	616	CLA	C1C-NC	-3.09	1.33	1.37
25	9	612	CLA	C1C-NC	-3.09	1.33	1.37
26	3	608	CHL	C1A-CHA	-3.09	1.36	1.40
25	1	605	CLA	C1C-NC	-3.09	1.33	1.37
25	K	1402	CLA	C1C-NC	-3.08	1.33	1.37
26	5	618	CHL	C3B-C2B	-3.08	1.36	1.40
26	8	603	CHL	C3B-C2B	-3.08	1.36	1.40
25	A	1119	CLA	C1C-NC	-3.08	1.33	1.37
25	1	603	CLA	C1C-NC	-3.08	1.33	1.37
25	5	614	CLA	C1C-NC	-3.07	1.33	1.37
25	9	609	CLA	C1C-NC	-3.07	1.33	1.37
26	5	613	CHL	C3A-C2A	-3.07	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1134	CLA	C1C-NC	-3.07	1.33	1.37
25	O	1802	CLA	C1C-NC	-3.07	1.33	1.37
25	5	606	CLA	C1C-NC	-3.07	1.33	1.37
25	9	605	CLA	C1C-NC	-3.07	1.33	1.37
25	A	1123	CLA	C1C-NC	-3.07	1.33	1.37
25	A	1126	CLA	C1C-NC	-3.07	1.33	1.37
25	9	607	CLA	C1C-NC	-3.07	1.33	1.37
25	4	617	CLA	C1C-NC	-3.07	1.33	1.37
25	6	612	CLA	C1C-NC	-3.07	1.33	1.37
25	K	1404	CLA	C1C-NC	-3.06	1.33	1.37
25	5	604	CLA	C1C-NC	-3.06	1.33	1.37
25	6	605	CLA	C1C-NC	-3.06	1.33	1.37
25	8	620	CLA	C1C-NC	-3.06	1.33	1.37
26	5	610	CHL	C3A-C2A	-3.06	1.52	1.54
25	2	602	CLA	C1C-NC	-3.06	1.33	1.37
25	O	1801	CLA	C1C-NC	-3.06	1.33	1.37
26	A	1114	CHL	C3B-C2B	-3.05	1.36	1.40
26	8	601	CHL	CHB-C4A	-3.05	1.35	1.38
25	1	615	CLA	C1C-NC	-3.05	1.33	1.37
25	B	1022	CLA	C1C-NC	-3.04	1.33	1.37
25	8	607	CLA	C1C-NC	-3.03	1.33	1.37
26	4	609	CHL	C1A-CHA	-3.03	1.36	1.40
25	9	606	CLA	C1C-NC	-3.03	1.33	1.37
25	B	1221	CLA	C1C-NC	-3.02	1.33	1.37
26	a	606	CHL	C3B-C2B	-3.02	1.36	1.40
25	3	602	CLA	C1C-NC	-3.02	1.33	1.37
25	B	1213	CLA	C1C-NC	-3.01	1.33	1.37
24	A	1011	CL0	CHB-C4A	-3.00	1.35	1.38
44	7	504	AXT	C11-C10	3.00	1.52	1.43
25	B	1234	CLA	C3B-C2B	-3.00	1.36	1.40
25	1	608	CLA	C4B-NB	-2.99	1.33	1.37
31	A	5004	LMG	C19-C18	-2.97	1.33	1.51
52	8	805	P5S	O37-C38	2.97	1.42	1.34
25	6	604	CLA	C1C-NC	-2.96	1.33	1.37
26	3	604	CHL	C3B-C2B	-2.96	1.36	1.40
26	a	604	CHL	CHB-C4A	-2.94	1.35	1.38
26	3	603	CHL	C3B-C2B	-2.93	1.36	1.40
25	a	603	CLA	C4B-NB	-2.92	1.34	1.37
25	A	1107	CLA	C4B-NB	-2.92	1.34	1.37
53	8	810	LAP	P9-O4	2.91	1.70	1.59
44	7	504	AXT	C24-C25	2.91	1.53	1.47
26	2	609	CHL	CHB-C4A	-2.90	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	612	CLA	C4B-NB	-2.89	1.34	1.37
50	2	501	XAT	O24-C25	-2.89	1.42	1.46
26	3	611	CHL	C1A-CHA	-2.88	1.36	1.40
25	B	1206	CLA	C4B-NB	-2.88	1.34	1.37
26	6	613	CHL	CHB-C4A	-2.88	1.35	1.38
26	2	613	CHL	C3B-C2B	-2.88	1.36	1.40
40	3	506	RRX	C32-C1	2.88	1.59	1.53
40	J	4002	RRX	C32-C1	2.87	1.59	1.53
25	7	606	CLA	C4B-NB	-2.87	1.34	1.37
26	a	604	CHL	C3B-C2B	-2.87	1.36	1.40
25	3	606	CLA	C4B-NB	-2.87	1.34	1.37
25	2	601	CLA	C4B-NB	-2.86	1.34	1.37
25	B	1227	CLA	C4B-NB	-2.86	1.34	1.37
25	A	1112	CLA	C4B-NB	-2.85	1.34	1.37
25	A	1132	CLA	C4B-NB	-2.85	1.34	1.37
26	3	604	CHL	CHB-C4A	-2.85	1.35	1.38
25	3	605	CLA	C4B-NB	-2.85	1.34	1.37
26	A	1114	CHL	C3A-C2A	-2.85	1.52	1.54
25	B	1023	CLA	C4B-NB	-2.85	1.34	1.37
25	7	601	CLA	C4B-NB	-2.85	1.34	1.37
25	A	1113	CLA	C4B-NB	-2.85	1.34	1.37
25	9	604	CLA	C4B-NB	-2.85	1.34	1.37
25	7	605	CLA	C4B-NB	-2.84	1.34	1.37
25	B	1204	CLA	C4B-NB	-2.83	1.34	1.37
25	L	1503	CLA	C4B-NB	-2.83	1.34	1.37
25	A	1117	CLA	C4B-NB	-2.83	1.34	1.37
25	B	1212	CLA	C4B-NB	-2.82	1.34	1.37
25	A	1126	CLA	C4B-NB	-2.82	1.34	1.37
25	B	1218	CLA	C4B-NB	-2.82	1.34	1.37
25	1	601	CLA	C4B-NB	-2.82	1.34	1.37
25	B	1216	CLA	C4B-NB	-2.82	1.34	1.37
25	B	1224	CLA	C4B-NB	-2.82	1.34	1.37
26	1	604	CHL	CHB-C4A	-2.82	1.35	1.38
25	9	606	CLA	C4B-NB	-2.82	1.34	1.37
44	1	502	AXT	C1-C6	2.81	1.57	1.53
26	5	613	CHL	CHB-C4A	-2.81	1.35	1.38
25	B	1221	CLA	C4B-NB	-2.81	1.34	1.37
25	4	606	CLA	C4B-NB	-2.81	1.34	1.37
26	1	604	CHL	C1D-C2D	2.81	1.42	1.39
25	3	601	CLA	C4B-NB	-2.81	1.34	1.37
25	B	1222	CLA	C4B-NB	-2.81	1.34	1.37
25	2	604	CLA	C4B-NB	-2.81	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	606	CLA	C4B-NB	-2.81	1.34	1.37
25	a	601	CLA	C4B-NB	-2.81	1.34	1.37
25	8	606	CLA	C4B-NB	-2.80	1.34	1.37
25	3	610	CLA	C4B-NB	-2.80	1.34	1.37
44	7	504	AXT	C27-C26	2.80	1.54	1.45
26	8	604	CHL	CHB-C4A	-2.80	1.35	1.38
25	6	615	CLA	C4B-NB	-2.80	1.34	1.37
25	5	609	CLA	C4B-NB	-2.80	1.34	1.37
26	3	611	CHL	CHB-C4A	-2.79	1.35	1.38
25	3	616	CLA	C4B-NB	-2.79	1.34	1.37
25	4	601	CLA	C4B-NB	-2.79	1.34	1.37
25	5	604	CLA	C4B-NB	-2.79	1.34	1.37
38	F	5003	LPX	P1-O1	2.79	1.70	1.59
26	a	606	CHL	C1D-C2D	2.79	1.42	1.39
26	5	611	CHL	CHB-C4A	-2.79	1.35	1.38
25	2	606	CLA	C4B-NB	-2.78	1.34	1.37
25	2	607	CLA	C4B-NB	-2.78	1.34	1.37
25	A	1129	CLA	C4B-NB	-2.78	1.34	1.37
25	A	1102	CLA	C4B-NB	-2.78	1.34	1.37
26	8	601	CHL	C1D-C2D	2.78	1.42	1.39
25	7	610	CLA	C4B-NB	-2.78	1.34	1.37
37	K	5002	PCW	O2-C2	-2.78	1.40	1.46
25	6	605	CLA	C4B-NB	-2.78	1.34	1.37
25	4	612	CLA	C4B-NB	-2.77	1.34	1.37
26	6	609	CHL	C1B-C2B	2.77	1.42	1.39
26	6	619	CHL	C1D-C2D	2.77	1.42	1.39
26	6	610	CHL	CHB-C4A	-2.77	1.35	1.38
25	1	603	CLA	C4B-NB	-2.77	1.34	1.37
25	B	1210	CLA	C4B-NB	-2.77	1.34	1.37
26	2	610	CHL	C1D-C2D	2.77	1.42	1.39
26	A	1114	CHL	C1A-CHA	-2.77	1.36	1.40
25	3	602	CLA	C4B-NB	-2.77	1.34	1.37
25	A	1124	CLA	C4B-NB	-2.77	1.34	1.37
26	a	609	CHL	C1D-C2D	2.77	1.42	1.39
25	a	605	CLA	C4B-NB	-2.77	1.34	1.37
26	9	608	CHL	C1D-C2D	2.77	1.42	1.39
25	B	1022	CLA	C4B-NB	-2.77	1.34	1.37
25	6	603	CLA	C4B-NB	-2.77	1.34	1.37
25	7	604	CLA	C4B-NB	-2.77	1.34	1.37
25	A	1119	CLA	C4B-NB	-2.77	1.34	1.37
25	8	611	CLA	C4B-NB	-2.77	1.34	1.37
25	7	607	CLA	C4B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	609	CHL	C1D-C2D	2.76	1.42	1.39
25	B	1240	CLA	C4B-NB	-2.76	1.34	1.37
26	7	609	CHL	CHB-C4A	-2.76	1.35	1.38
26	8	603	CHL	CHB-C4A	-2.76	1.35	1.38
25	B	1230	CLA	C4B-NB	-2.76	1.34	1.37
26	9	608	CHL	CHB-C4A	-2.76	1.35	1.38
26	6	617	CHL	C1D-C2D	2.76	1.42	1.39
26	7	613	CHL	CHB-C4A	-2.75	1.35	1.38
25	B	1228	CLA	C4B-NB	-2.75	1.34	1.37
25	B	1211	CLA	C4B-NB	-2.75	1.34	1.37
26	6	617	CHL	C1B-C2B	2.75	1.42	1.39
25	1	612	CLA	C4B-NB	-2.75	1.34	1.37
26	2	613	CHL	CHB-C4A	-2.75	1.35	1.38
26	9	601	CHL	C1A-CHA	-2.75	1.36	1.40
26	6	611	CHL	C3B-C2B	-2.75	1.36	1.40
26	6	611	CHL	CHB-C4A	-2.75	1.35	1.38
25	A	1111	CLA	C4B-NB	-2.75	1.34	1.37
25	4	604	CLA	C4B-NB	-2.75	1.34	1.37
25	9	609	CLA	C4B-NB	-2.75	1.34	1.37
25	A	1013	CLA	C4B-NB	-2.74	1.34	1.37
25	A	1109	CLA	C4B-NB	-2.74	1.34	1.37
25	2	608	CLA	C4B-NB	-2.74	1.34	1.37
25	B	1226	CLA	C4B-NB	-2.74	1.34	1.37
25	B	1220	CLA	C4B-NB	-2.74	1.34	1.37
25	H	1702	CLA	C4B-NB	-2.74	1.34	1.37
26	1	610	CHL	CHB-C4A	-2.74	1.35	1.38
26	a	604	CHL	C1D-C2D	2.74	1.42	1.39
26	4	609	CHL	C1D-C2D	2.74	1.42	1.39
25	1	615	CLA	C4B-NB	-2.74	1.34	1.37
26	9	603	CHL	C1B-C2B	2.74	1.42	1.39
26	3	611	CHL	C1D-C2D	2.73	1.42	1.39
33	G	5003	PTY	O7-C6	-2.73	1.40	1.46
25	A	1123	CLA	C4B-NB	-2.73	1.34	1.37
25	9	602	CLA	C4B-NB	-2.73	1.34	1.37
25	A	1121	CLA	C4B-NB	-2.73	1.34	1.37
26	a	610	CHL	CHB-C4A	-2.73	1.35	1.38
25	a	611	CLA	C4B-NB	-2.73	1.34	1.37
25	3	613	CLA	C4B-NB	-2.73	1.34	1.37
26	a	606	CHL	CHB-C4A	-2.72	1.35	1.38
26	4	618	CHL	C1D-C2D	2.72	1.42	1.39
26	7	615	CHL	C1B-C2B	2.72	1.42	1.39
25	5	607	CLA	C4B-NB	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1219	CLA	C4B-NB	-2.72	1.34	1.37
26	3	604	CHL	C1D-C2D	2.72	1.42	1.39
26	6	610	CHL	C3B-C2B	-2.72	1.36	1.40
26	3	603	CHL	CHB-C4A	-2.72	1.35	1.38
37	6	803	PCW	O2-C2	-2.72	1.40	1.46
26	6	613	CHL	C1D-C2D	2.72	1.42	1.39
25	5	615	CLA	C4B-NB	-2.72	1.34	1.37
37	K	5001	PCW	O2-C2	-2.72	1.40	1.46
33	B	5005	PTY	O7-C6	-2.72	1.40	1.46
26	5	613	CHL	C1D-C2D	2.71	1.42	1.39
25	L	1501	CLA	C4B-NB	-2.71	1.34	1.37
33	A	5006	PTY	O7-C6	-2.71	1.40	1.46
25	8	618	CLA	C4B-NB	-2.71	1.34	1.37
25	4	607	CLA	C4B-NB	-2.71	1.34	1.37
26	7	617	CHL	CHB-C4A	-2.71	1.35	1.38
26	6	611	CHL	C1D-C2D	2.71	1.42	1.39
26	7	611	CHL	C1D-C2D	2.71	1.42	1.39
25	F	1302	CLA	C4B-NB	-2.71	1.34	1.37
26	5	610	CHL	C1B-C2B	2.71	1.42	1.39
26	4	609	CHL	C1B-C2B	2.71	1.42	1.39
26	8	604	CHL	C1D-C2D	2.71	1.42	1.39
26	9	601	CHL	CHB-C4A	-2.71	1.35	1.38
25	5	608	CLA	C4B-NB	-2.70	1.34	1.37
25	8	612	CLA	C4B-NB	-2.70	1.34	1.37
26	6	619	CHL	C1A-CHA	-2.70	1.36	1.40
26	1	610	CHL	C1D-C2D	2.70	1.42	1.39
25	B	1201	CLA	C4B-NB	-2.70	1.34	1.37
26	a	609	CHL	CHB-C4A	-2.70	1.35	1.38
25	9	605	CLA	C4B-NB	-2.70	1.34	1.37
25	2	615	CLA	C4B-NB	-2.70	1.34	1.37
26	5	617	CHL	C1B-C2B	2.70	1.42	1.39
26	5	617	CHL	CHB-C4A	-2.70	1.35	1.38
25	A	1012	CLA	C4B-NB	-2.70	1.34	1.37
26	5	611	CHL	C1D-C2D	2.70	1.42	1.39
25	9	612	CLA	C4B-NB	-2.70	1.34	1.37
26	7	609	CHL	C1D-C2D	2.70	1.42	1.39
26	8	610	CHL	CHB-C4A	-2.70	1.35	1.38
26	4	613	CHL	C1D-C2D	2.70	1.42	1.39
26	1	613	CHL	C1D-C2D	2.69	1.42	1.39
25	O	1801	CLA	C4B-NB	-2.69	1.34	1.37
26	9	601	CHL	C1D-C2D	2.69	1.42	1.39
26	8	603	CHL	C1A-CHA	-2.69	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	613	CHL	C1B-C2B	2.69	1.42	1.39
25	H	1701	CLA	C4B-NB	-2.69	1.34	1.37
25	3	607	CLA	C4B-NB	-2.69	1.34	1.37
26	8	613	CHL	C1D-C2D	2.69	1.42	1.39
33	a	802	PTY	O7-C6	-2.69	1.40	1.46
26	a	609	CHL	C1B-C2B	2.69	1.42	1.39
26	a	610	CHL	C1D-C2D	2.68	1.42	1.39
25	a	615	CLA	C4B-NB	-2.68	1.34	1.37
25	4	615	CLA	C4B-NB	-2.68	1.34	1.37
26	6	610	CHL	C1D-C2D	2.68	1.42	1.39
26	6	619	CHL	CHB-C4A	-2.68	1.35	1.38
25	6	608	CLA	C4B-NB	-2.68	1.34	1.37
25	A	1131	CLA	C4B-NB	-2.68	1.34	1.37
25	5	606	CLA	C4B-NB	-2.68	1.34	1.37
25	6	601	CLA	C4B-NB	-2.68	1.34	1.37
26	8	613	CHL	C3B-C2B	-2.68	1.36	1.40
26	5	618	CHL	CHB-C4A	-2.68	1.35	1.38
26	A	1114	CHL	C1D-C2D	2.68	1.42	1.39
33	a	803	PTY	O7-C6	-2.68	1.40	1.46
25	8	620	CLA	C4B-NB	-2.68	1.34	1.37
26	8	613	CHL	CHB-C4A	-2.67	1.35	1.38
26	2	609	CHL	C1D-C2D	2.67	1.42	1.39
25	a	607	CLA	C4B-NB	-2.67	1.34	1.37
26	3	608	CHL	C1D-C2D	2.67	1.42	1.39
37	B	5004	PCW	O2-C2	-2.67	1.40	1.46
26	6	619	CHL	C1B-C2B	2.67	1.42	1.39
34	A	5007	3PH	O21-C2	-2.67	1.40	1.46
26	7	615	CHL	CHB-C4A	-2.67	1.35	1.38
26	8	610	CHL	C1B-C2B	2.67	1.42	1.39
26	1	604	CHL	C3B-C2B	-2.67	1.36	1.40
50	7	502	XAT	O24-C25	-2.67	1.42	1.46
26	1	610	CHL	C1B-C2B	2.67	1.42	1.39
33	J	5001	PTY	O7-C6	-2.67	1.40	1.46
26	3	608	CHL	C1B-C2B	2.66	1.42	1.39
51	7	807	4RF	O21-C20	-2.66	1.40	1.46
25	A	1128	CLA	C4B-NB	-2.66	1.34	1.37
25	K	1402	CLA	C4B-NB	-2.66	1.34	1.37
25	1	605	CLA	C4B-NB	-2.66	1.34	1.37
26	9	610	CHL	C1B-C2B	2.66	1.42	1.39
25	B	1213	CLA	C4B-NB	-2.66	1.34	1.37
33	G	5002	PTY	O7-C6	-2.66	1.40	1.46
26	9	610	CHL	C1D-C2D	2.66	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	618	CHL	CHB-C4A	-2.66	1.35	1.38
25	A	1141	CLA	C4B-NB	-2.66	1.34	1.37
26	A	1114	CHL	C1B-C2B	2.66	1.42	1.39
25	O	1802	CLA	C4B-NB	-2.66	1.34	1.37
26	1	609	CHL	C1B-C2B	2.65	1.42	1.39
25	5	612	CLA	C4B-NB	-2.65	1.34	1.37
25	2	603	CLA	C4B-NB	-2.65	1.34	1.37
26	4	618	CHL	C1B-C2B	2.65	1.42	1.39
25	4	608	CLA	C4B-NB	-2.65	1.34	1.37
26	8	603	CHL	C1D-C2D	2.65	1.42	1.39
25	5	614	CLA	C4B-NB	-2.65	1.34	1.37
26	1	609	CHL	CHB-C4A	-2.65	1.35	1.38
26	5	617	CHL	C1D-C2D	2.65	1.42	1.39
26	9	613	CHL	C1D-C2D	2.65	1.42	1.39
26	6	617	CHL	CHB-C4A	-2.65	1.35	1.38
26	6	611	CHL	C1B-C2B	2.65	1.42	1.39
25	2	621	CLA	C4B-NB	-2.64	1.34	1.37
26	2	613	CHL	C1D-C2D	2.64	1.42	1.39
26	9	608	CHL	C1B-C2B	2.64	1.42	1.39
26	9	603	CHL	C3B-C2B	-2.64	1.36	1.40
26	7	613	CHL	C1D-C2D	2.64	1.42	1.39
25	A	1138	CLA	C4B-NB	-2.64	1.34	1.37
25	5	601	CLA	C4B-NB	-2.64	1.34	1.37
26	1	613	CHL	C1B-C2B	2.64	1.42	1.39
26	2	610	CHL	C1B-C2B	2.64	1.42	1.39
25	5	603	CLA	C4B-NB	-2.64	1.34	1.37
26	9	601	CHL	C1B-C2B	2.64	1.42	1.39
25	L	1502	CLA	C4B-NB	-2.64	1.34	1.37
50	9	507	XAT	O24-C25	-2.64	1.42	1.46
26	9	610	CHL	CHB-C4A	-2.64	1.35	1.38
26	a	613	CHL	C1B-C2B	2.64	1.42	1.39
26	a	613	CHL	C1D-C2D	2.64	1.42	1.39
26	8	613	CHL	C1B-C2B	2.64	1.42	1.39
26	4	613	CHL	C1B-C2B	2.64	1.42	1.39
26	6	610	CHL	C1B-C2B	2.63	1.42	1.39
25	G	1602	CLA	C4B-NB	-2.63	1.34	1.37
25	9	607	CLA	C4B-NB	-2.63	1.34	1.37
25	A	1122	CLA	C4B-NB	-2.63	1.34	1.37
25	K	1404	CLA	C4B-NB	-2.63	1.34	1.37
26	9	603	CHL	C1D-C2D	2.63	1.42	1.39
26	9	603	CHL	CHB-C4A	-2.63	1.35	1.38
52	8	805	P5S	O19-C17	2.63	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	618	CHL	C1B-C2B	2.63	1.42	1.39
26	7	617	CHL	C1B-C2B	2.63	1.42	1.39
25	A	1133	CLA	C4B-NB	-2.63	1.34	1.37
26	7	611	CHL	CHB-C4A	-2.63	1.35	1.38
26	6	609	CHL	CHB-C4A	-2.63	1.35	1.38
26	1	611	CHL	C1D-C2D	2.63	1.42	1.39
26	7	617	CHL	C1D-C2D	2.62	1.42	1.39
26	5	610	CHL	C3B-C2B	-2.62	1.36	1.40
26	A	1114	CHL	CHB-C4A	-2.62	1.35	1.38
26	a	610	CHL	C1B-C2B	2.61	1.42	1.39
26	7	609	CHL	C1B-C2B	2.61	1.42	1.39
26	3	608	CHL	CHB-C4A	-2.61	1.35	1.38
26	5	610	CHL	C1D-C2D	2.61	1.42	1.39
25	A	1104	CLA	C4B-NB	-2.61	1.34	1.37
25	B	1235	CLA	C4B-NB	-2.61	1.34	1.37
26	5	613	CHL	C1B-C2B	2.61	1.42	1.39
25	H	1703	CLA	C4B-NB	-2.60	1.34	1.37
25	6	618	CLA	C4B-NB	-2.60	1.34	1.37
26	9	613	CHL	CHB-C4A	-2.60	1.35	1.38
25	K	1403	CLA	C4B-NB	-2.60	1.34	1.37
26	2	613	CHL	C1B-C2B	2.60	1.42	1.39
26	7	609	CHL	C3B-C2B	-2.60	1.36	1.40
26	1	609	CHL	C1D-C2D	2.60	1.42	1.39
26	1	611	CHL	C1B-C2B	2.60	1.42	1.39
26	7	611	CHL	C1B-C2B	2.60	1.42	1.39
26	8	610	CHL	C1D-C2D	2.60	1.42	1.39
25	A	1103	CLA	C4B-NB	-2.60	1.34	1.37
25	A	1136	CLA	C4B-NB	-2.59	1.34	1.37
26	7	609	CHL	C1A-CHA	-2.59	1.37	1.40
25	a	612	CLA	C4B-NB	-2.59	1.34	1.37
26	5	618	CHL	C1D-C2D	2.59	1.42	1.39
25	8	602	CLA	C4B-NB	-2.58	1.34	1.37
25	B	1232	CLA	C4B-NB	-2.58	1.34	1.37
25	a	608	CLA	C4B-NB	-2.58	1.34	1.37
33	9	803	PTY	O7-C6	-2.58	1.40	1.46
26	3	611	CHL	C1B-C2B	2.58	1.42	1.39
25	A	1134	CLA	C4B-NB	-2.58	1.34	1.37
26	7	615	CHL	C1D-C2D	2.58	1.42	1.39
26	1	613	CHL	CHB-C4A	-2.58	1.35	1.38
25	A	1135	CLA	C4B-NB	-2.57	1.34	1.37
25	7	608	CLA	C4B-NB	-2.57	1.34	1.37
26	a	606	CHL	C1B-C2B	2.57	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	611	CHL	CHB-C4A	-2.57	1.35	1.38
26	4	613	CHL	CHB-C4A	-2.57	1.35	1.38
26	4	609	CHL	CHB-C4A	-2.57	1.35	1.38
26	a	613	CHL	CHB-C4A	-2.57	1.35	1.38
26	2	609	CHL	C1A-CHA	-2.57	1.37	1.40
25	6	612	CLA	C4B-NB	-2.57	1.34	1.37
26	3	603	CHL	C1B-C2B	2.56	1.42	1.39
26	3	603	CHL	C1D-C2D	2.56	1.42	1.39
26	5	611	CHL	C1A-CHA	-2.56	1.37	1.40
25	B	1203	CLA	C4B-NB	-2.56	1.34	1.37
25	6	602	CLA	C4B-NB	-2.56	1.34	1.37
25	B	1208	CLA	C4B-NB	-2.56	1.34	1.37
26	5	611	CHL	C1B-C2B	2.56	1.42	1.39
26	6	613	CHL	C1B-C2B	2.56	1.42	1.39
25	O	1803	CLA	C4B-NB	-2.55	1.34	1.37
26	2	609	CHL	C1B-C2B	2.55	1.42	1.39
26	5	610	CHL	CHB-C4A	-2.55	1.35	1.38
26	2	610	CHL	CHB-C4A	-2.55	1.35	1.38
25	5	605	CLA	C4B-NB	-2.55	1.34	1.37
25	7	602	CLA	C4B-NB	-2.55	1.34	1.37
25	B	1238	CLA	C4B-NB	-2.55	1.34	1.37
44	1	502	AXT	C27-C26	2.54	1.53	1.45
25	O	1801	CLA	C1A-CHA	2.54	1.51	1.42
26	3	604	CHL	C1B-C2B	2.54	1.42	1.39
35	B	5006	LMT	O3'-C3'	-2.54	1.36	1.43
25	B	1214	CLA	C4B-NB	-2.54	1.34	1.37
25	7	603	CLA	C4B-NB	-2.54	1.34	1.37
25	8	607	CLA	C4B-NB	-2.53	1.34	1.37
25	B	1205	CLA	C4B-NB	-2.53	1.34	1.37
26	a	604	CHL	C1B-C2B	2.53	1.42	1.39
26	7	613	CHL	C3B-C2B	-2.53	1.36	1.40
26	a	606	CHL	C1A-CHA	-2.53	1.37	1.40
25	4	610	CLA	C4B-NB	-2.52	1.34	1.37
26	7	613	CHL	C1B-C2B	2.52	1.42	1.39
26	9	603	CHL	C3A-C2A	-2.52	1.52	1.54
25	4	616	CLA	C4B-NB	-2.52	1.34	1.37
26	1	604	CHL	C1B-C2B	2.51	1.42	1.39
25	6	606	CLA	C4B-NB	-2.51	1.34	1.37
25	A	1116	CLA	C4B-NB	-2.51	1.34	1.37
25	2	612	CLA	C4B-NB	-2.51	1.34	1.37
35	2	804	LMT	O3'-C3'	-2.50	1.36	1.43
25	4	605	CLA	C4B-NB	-2.50	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1115	CLA	C4B-NB	-2.50	1.34	1.37
40	3	506	RRX	C35-C13	2.50	1.55	1.50
25	4	603	CLA	C4B-NB	-2.50	1.34	1.37
25	F	1301	CLA	C4B-NB	-2.50	1.34	1.37
25	8	608	CLA	C4B-NB	-2.50	1.34	1.37
35	A	5008	LMT	O3'-C3'	-2.49	1.36	1.43
26	1	609	CHL	C3B-C2B	-2.49	1.37	1.40
26	8	603	CHL	C1B-C2B	2.49	1.42	1.39
25	8	615	CLA	C4B-NB	-2.49	1.34	1.37
26	8	604	CHL	C1B-C2B	2.49	1.42	1.39
26	8	613	CHL	C1A-CHA	-2.48	1.37	1.40
25	1	607	CLA	C4B-NB	-2.48	1.34	1.37
25	2	602	CLA	C4B-NB	-2.48	1.34	1.37
25	A	1120	CLA	C4B-NB	-2.48	1.34	1.37
25	4	602	CLA	C4B-NB	-2.48	1.34	1.37
25	K	1401	CLA	C4B-NB	-2.48	1.34	1.37
25	6	607	CLA	C4B-NB	-2.47	1.34	1.37
25	G	1601	CLA	C4B-NB	-2.47	1.34	1.37
25	3	612	CLA	C4B-NB	-2.47	1.34	1.37
25	A	1118	CLA	C4B-NB	-2.47	1.34	1.37
25	8	609	CLA	C4B-NB	-2.46	1.34	1.37
25	A	1139	CLA	C4B-NB	-2.46	1.34	1.37
25	B	1229	CLA	C4B-NB	-2.46	1.34	1.37
25	B	1225	CLA	C4B-NB	-2.45	1.34	1.37
35	1	804	LMT	O3'-C3'	-2.45	1.36	1.43
25	4	617	CLA	C4B-NB	-2.45	1.34	1.37
25	2	605	CLA	C4B-NB	-2.45	1.34	1.37
25	A	1130	CLA	C4B-NB	-2.45	1.34	1.37
33	3	802	PTY	O7-C6	-2.45	1.40	1.46
26	9	610	CHL	C3B-C2B	-2.44	1.37	1.40
25	B	1236	CLA	C4B-NB	-2.44	1.34	1.37
40	J	4002	RRX	C35-C13	2.44	1.55	1.50
25	B	1237	CLA	C4B-NB	-2.44	1.34	1.37
26	4	618	CHL	C3B-C2B	-2.43	1.37	1.40
25	3	618	CLA	C4B-NB	-2.42	1.34	1.37
25	J	1901	CLA	C4B-NB	-2.42	1.34	1.37
33	3	802	PTY	O4-C30	2.42	1.40	1.33
25	B	1207	CLA	C4B-NB	-2.42	1.34	1.37
33	9	803	PTY	O4-C30	2.42	1.40	1.33
25	1	602	CLA	C4B-NB	-2.41	1.34	1.37
25	A	1105	CLA	C4B-NB	-2.41	1.34	1.37
25	4	611	CLA	C4B-NB	-2.41	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1215	CLA	C4B-NB	-2.41	1.34	1.37
37	K	5001	PCW	O2-C31	2.40	1.41	1.34
25	B	1223	CLA	C4B-NB	-2.40	1.34	1.37
33	a	802	PTY	O4-C30	2.40	1.40	1.33
33	J	5001	PTY	O4-C30	2.40	1.40	1.33
38	F	5003	LPX	P1-O2	2.40	1.68	1.59
33	A	5006	PTY	O4-C30	2.39	1.40	1.33
44	7	504	AXT	C1-C6	2.39	1.56	1.53
26	7	611	CHL	C1A-CHA	-2.38	1.37	1.40
26	9	608	CHL	C1A-CHA	-2.38	1.37	1.40
52	8	805	P5S	O37-C2	-2.38	1.41	1.46
25	A	1140	CLA	C4B-NB	-2.38	1.34	1.37
36	8	802	DGD	CDB-CCB	-2.38	1.33	1.50
26	a	613	CHL	C3A-C2A	-2.38	1.52	1.54
25	A	1108	CLA	C4B-NB	-2.38	1.34	1.37
33	7	804	PTY	O4-C30	2.38	1.40	1.33
51	7	807	4RF	O40-C41	2.38	1.40	1.33
25	5	602	CLA	C4B-NB	-2.38	1.34	1.37
26	4	613	CHL	C3B-C2B	-2.38	1.37	1.40
37	B	5004	PCW	O2-C31	2.37	1.41	1.34
25	A	1106	CLA	C4B-NB	-2.37	1.34	1.37
26	7	617	CHL	C1A-CHA	-2.37	1.37	1.40
25	B	1021	CLA	C4B-NB	-2.37	1.34	1.37
26	8	610	CHL	C3B-C2B	-2.36	1.37	1.40
33	a	803	PTY	O4-C30	2.36	1.40	1.33
33	5	802	PTY	O4-C30	2.36	1.40	1.33
36	8	802	DGD	CGA-CFA	-2.36	1.33	1.50
25	a	602	CLA	C4B-NB	-2.36	1.34	1.37
26	a	613	CHL	C3B-C2B	-2.36	1.37	1.40
25	A	1127	CLA	C4B-NB	-2.36	1.34	1.37
25	B	1217	CLA	C4B-NB	-2.35	1.34	1.37
25	B	1239	CLA	C4B-NB	-2.34	1.34	1.37
33	7	804	PTY	O7-C6	-2.34	1.41	1.46
37	K	5002	PCW	O2-C31	2.34	1.40	1.34
33	B	5005	PTY	O4-C30	2.34	1.40	1.33
42	M	4001	ECH	C1-C6	-2.34	1.50	1.53
25	B	1234	CLA	C3A-C2A	-2.34	1.52	1.54
33	5	802	PTY	O7-C6	-2.34	1.41	1.46
51	7	807	4RF	O18-C16	2.34	1.40	1.33
26	a	610	CHL	C1A-CHA	-2.33	1.37	1.40
25	A	1110	CLA	C4B-NB	-2.33	1.34	1.37
26	7	615	CHL	C1A-CHA	-2.33	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	601	CHL	C1B-C2B	2.33	1.42	1.39
26	1	611	CHL	C1A-CHA	-2.33	1.37	1.40
33	7	804	PTY	O7-C8	2.32	1.40	1.34
26	9	610	CHL	C2C-C3C	2.32	1.38	1.36
35	1	804	LMT	O2B-C2B	-2.32	1.37	1.43
44	7	504	AXT	C37-C21	2.32	1.58	1.53
25	8	605	CLA	C4B-NB	-2.32	1.34	1.37
44	1	502	AXT	C37-C21	2.32	1.58	1.53
35	1	804	LMT	O2'-C2'	-2.31	1.37	1.43
26	1	611	CHL	C3B-C2B	-2.31	1.37	1.40
37	6	803	PCW	O2-C31	2.31	1.40	1.34
25	A	1137	CLA	C4B-NB	-2.31	1.34	1.37
25	B	1231	CLA	C4B-NB	-2.31	1.34	1.37
26	9	613	CHL	C3B-C2B	-2.30	1.37	1.40
34	A	5007	3PH	O31-C31	2.30	1.40	1.33
26	6	611	CHL	C1A-CHA	-2.29	1.37	1.40
25	A	1125	CLA	C4B-NB	-2.29	1.34	1.37
50	9	504	XAT	O24-C25	-2.29	1.43	1.46
33	5	802	PTY	O7-C8	2.28	1.40	1.34
35	2	804	LMT	O2B-C2B	-2.28	1.37	1.43
25	A	1101	CLA	C4B-NB	-2.28	1.34	1.37
48	2	803	DGA	OG2-CG2	-2.27	1.41	1.46
51	7	807	4RF	O18-C19	-2.27	1.40	1.45
33	3	802	PTY	O7-C8	2.27	1.40	1.34
35	2	804	LMT	O2'-C2'	-2.26	1.37	1.43
25	2	603	CLA	C1A-CHA	2.26	1.52	1.43
25	B	1209	CLA	C4B-NB	-2.26	1.34	1.37
25	G	1603	CLA	C4B-NB	-2.26	1.34	1.37
25	B	1202	CLA	C4B-NB	-2.25	1.34	1.37
35	2	804	LMT	O3B-C3B	-2.25	1.37	1.43
51	7	807	4RF	O40-C39	-2.25	1.40	1.45
25	6	604	CLA	C4B-NB	-2.25	1.34	1.37
25	L	1504	CLA	C4B-NB	-2.25	1.34	1.37
25	B	1234	CLA	C4B-NB	-2.24	1.34	1.38
26	a	613	CHL	CHA-CBD	2.23	1.54	1.51
26	a	609	CHL	C1A-CHA	-2.23	1.37	1.40
25	A	1125	CLA	C1C-C2C	2.23	1.49	1.44
35	A	5008	LMT	O2B-C2B	-2.22	1.37	1.43
48	8	804	DGA	OG2-CG2	-2.22	1.41	1.46
44	7	504	AXT	C17-C1	2.22	1.58	1.53
26	5	613	CHL	CHA-CBD	2.22	1.54	1.51
26	4	609	CHL	C3B-C2B	-2.21	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	608	CHL	C3B-C2B	-2.21	1.37	1.40
26	6	610	CHL	CHA-CBD	2.21	1.54	1.51
25	2	607	CLA	C1A-CHA	2.21	1.52	1.43
26	5	611	CHL	CHA-CBD	2.21	1.54	1.51
35	A	5008	LMT	O3B-C3B	-2.20	1.37	1.43
48	3	803	DGA	OG2-CG2	-2.20	1.41	1.46
25	5	605	CLA	C3D-C4D	-2.20	1.39	1.44
26	1	609	CHL	CHA-CBD	2.20	1.54	1.51
26	7	609	CHL	CHA-CBD	2.20	1.54	1.51
26	7	611	CHL	CHA-CBD	2.20	1.54	1.51
26	2	613	CHL	CHA-CBD	2.20	1.54	1.51
26	5	610	CHL	CHA-CBD	2.20	1.54	1.51
26	4	613	CHL	C1A-CHA	-2.20	1.37	1.40
26	a	609	CHL	CHA-CBD	2.20	1.54	1.51
26	5	617	CHL	C1A-CHA	-2.20	1.37	1.40
25	6	604	CLA	C1C-C2C	2.20	1.49	1.44
44	7	504	AXT	C23-C24	2.19	1.57	1.52
35	A	5008	LMT	O1'-C1'	-2.19	1.36	1.40
26	9	603	CHL	CHA-CBD	2.19	1.54	1.51
26	1	610	CHL	CHA-CBD	2.19	1.54	1.51
26	8	604	CHL	CHA-CBD	2.19	1.54	1.51
26	9	608	CHL	CHA-CBD	2.19	1.54	1.51
25	4	612	CLA	C1A-CHA	2.19	1.52	1.43
33	a	803	PTY	O7-C8	2.19	1.40	1.34
35	1	804	LMT	O3B-C3B	-2.19	1.37	1.43
25	A	1121	CLA	C3D-C4D	-2.19	1.39	1.44
25	9	605	CLA	C3D-C4D	-2.19	1.39	1.44
26	a	606	CHL	CHA-CBD	2.19	1.54	1.51
25	B	1022	CLA	C3D-C4D	-2.19	1.39	1.44
26	7	617	CHL	CHA-CBD	2.19	1.54	1.51
33	a	802	PTY	O7-C8	2.19	1.40	1.34
26	8	610	CHL	CHA-CBD	2.19	1.54	1.51
34	A	5007	3PH	O31-C3	-2.19	1.40	1.45
25	A	1109	CLA	C1A-CHA	2.18	1.52	1.43
25	A	1141	CLA	C1A-CHA	2.18	1.52	1.43
48	5	803	DGA	OG2-CG2	-2.18	1.41	1.46
37	K	5001	PCW	P-O4P	2.18	1.67	1.59
26	1	613	CHL	C1A-CHA	-2.18	1.37	1.40
25	A	1134	CLA	C1A-CHA	2.18	1.52	1.43
35	B	5006	LMT	O2B-C2B	-2.18	1.37	1.43
33	9	803	PTY	O4-C1	-2.18	1.40	1.45
25	B	1231	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	611	CHL	CHA-CBD	2.18	1.54	1.51
26	6	619	CHL	CHA-CBD	2.18	1.54	1.51
26	8	613	CHL	CHA-CBD	2.18	1.54	1.51
26	6	609	CHL	CHA-CBD	2.18	1.54	1.51
25	K	1404	CLA	C1A-CHA	2.18	1.52	1.43
33	A	5006	PTY	O7-C8	2.17	1.40	1.34
25	8	607	CLA	C1A-CHA	2.17	1.52	1.43
25	B	1201	CLA	C1A-CHA	2.17	1.52	1.43
37	K	5002	PCW	P-O4P	2.17	1.67	1.59
26	4	618	CHL	CHA-CBD	2.17	1.54	1.51
26	6	617	CHL	CHA-CBD	2.17	1.54	1.51
25	7	604	CLA	C3D-C4D	-2.16	1.39	1.44
51	7	807	4RF	O21-C22	2.16	1.40	1.34
35	B	5006	LMT	O1'-C1'	-2.16	1.36	1.40
25	5	615	CLA	C1A-CHA	2.16	1.52	1.43
26	5	617	CHL	CHA-CBD	2.16	1.54	1.51
25	A	1117	CLA	C1A-CHA	2.16	1.52	1.43
25	2	605	CLA	C3D-C4D	-2.16	1.39	1.44
34	A	5007	3PH	O21-C21	2.16	1.40	1.34
26	A	1114	CHL	CHA-CBD	2.16	1.54	1.51
25	4	610	CLA	C1A-CHA	2.16	1.52	1.43
26	5	618	CHL	CHA-CBD	2.16	1.54	1.51
26	4	609	CHL	CHA-CBD	2.16	1.54	1.51
33	9	803	PTY	O7-C8	2.16	1.40	1.34
44	1	502	AXT	C24-C25	2.16	1.51	1.47
25	4	617	CLA	C1A-CHA	2.15	1.52	1.43
26	9	610	CHL	C1A-CHA	-2.15	1.37	1.40
25	B	1226	CLA	C3D-C4D	-2.15	1.39	1.44
25	2	615	CLA	C1C-C2C	2.15	1.48	1.44
33	B	5005	PTY	O4-C1	-2.15	1.40	1.45
37	6	803	PCW	P-O4P	2.15	1.67	1.59
26	6	617	CHL	C3B-C2B	-2.15	1.37	1.40
25	A	1123	CLA	C1A-CHA	2.15	1.52	1.43
25	H	1702	CLA	C1A-CHA	2.15	1.52	1.43
26	9	613	CHL	CHA-CBD	2.15	1.54	1.51
25	8	609	CLA	C1C-C2C	2.15	1.48	1.44
33	5	802	PTY	O4-C1	-2.15	1.40	1.45
25	A	1112	CLA	C1A-CHA	2.15	1.51	1.43
35	B	5006	LMT	O3B-C3B	-2.15	1.37	1.43
26	1	604	CHL	CHA-CBD	2.15	1.54	1.51
26	7	615	CHL	CHA-CBD	2.15	1.54	1.51
25	H	1701	CLA	C1A-CHA	2.15	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	5004	PCW	P-O4P	2.15	1.67	1.59
26	a	610	CHL	C3B-C2B	-2.15	1.37	1.40
25	7	605	CLA	C3D-C4D	-2.15	1.39	1.44
25	5	607	CLA	C1A-CHA	2.15	1.51	1.43
25	B	1221	CLA	C1A-CHA	2.14	1.51	1.43
25	A	1102	CLA	C1A-CHA	2.14	1.51	1.43
25	3	607	CLA	C1A-CHA	2.14	1.51	1.43
26	2	610	CHL	C3B-C2B	-2.14	1.37	1.40
26	7	611	CHL	C3B-C2B	-2.14	1.37	1.40
35	A	5008	LMT	O2'-C2'	-2.14	1.37	1.43
25	a	608	CLA	C1A-CHA	2.14	1.51	1.43
25	6	615	CLA	C1A-CHA	2.14	1.51	1.43
25	7	607	CLA	C1A-CHA	2.14	1.51	1.43
25	B	1223	CLA	C3D-C4D	-2.14	1.39	1.44
35	B	5006	LMT	O2'-C2'	-2.14	1.37	1.43
33	J	5001	PTY	O4-C1	-2.14	1.40	1.45
26	1	613	CHL	CHA-CBD	2.14	1.54	1.51
26	2	610	CHL	CHA-CBD	2.14	1.54	1.51
26	a	610	CHL	CHA-CBD	2.13	1.54	1.51
25	9	607	CLA	C1A-CHA	2.13	1.51	1.43
25	8	618	CLA	C3D-C4D	-2.13	1.39	1.44
33	7	804	PTY	O4-C1	-2.13	1.40	1.45
25	9	612	CLA	C1A-CHA	2.13	1.51	1.43
25	K	1403	CLA	C1A-CHA	2.13	1.51	1.43
33	a	802	PTY	O4-C1	-2.13	1.40	1.45
25	B	1216	CLA	C3D-C4D	-2.13	1.39	1.44
33	G	5002	PTY	O7-C8	2.13	1.40	1.34
26	4	613	CHL	CHA-CBD	2.13	1.54	1.51
33	J	5001	PTY	O7-C8	2.13	1.40	1.34
25	B	1235	CLA	C1A-CHA	2.13	1.51	1.43
25	1	615	CLA	C1A-CHA	2.13	1.51	1.43
26	6	611	CHL	CHA-CBD	2.13	1.54	1.51
25	a	612	CLA	C1A-CHA	2.13	1.51	1.43
26	2	613	CHL	C3A-C2A	-2.13	1.52	1.54
25	a	615	CLA	C1A-CHA	2.12	1.51	1.43
25	a	605	CLA	C3D-C4D	-2.12	1.39	1.44
26	8	601	CHL	CHA-CBD	2.12	1.54	1.51
25	7	610	CLA	C1A-CHA	2.12	1.51	1.43
25	A	1116	CLA	C1C-C2C	2.12	1.48	1.44
25	O	1802	CLA	C1A-CHA	2.12	1.51	1.43
25	A	1123	CLA	MG-NC	2.12	2.11	2.06
25	B	1208	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1235	CLA	C1C-C2C	2.12	1.48	1.44
26	1	609	CHL	C1A-CHA	-2.12	1.37	1.40
25	a	603	CLA	C1A-CHA	2.12	1.51	1.43
25	B	1209	CLA	C3D-C4D	-2.12	1.39	1.44
26	8	603	CHL	CHA-CBD	2.12	1.54	1.51
25	4	615	CLA	C1A-CHA	2.12	1.51	1.43
25	B	1223	CLA	C1A-CHA	2.12	1.51	1.43
25	A	1122	CLA	C1A-CHA	2.12	1.51	1.43
25	4	601	CLA	C1A-CHA	2.12	1.51	1.43
25	4	616	CLA	C1A-CHA	2.12	1.51	1.43
25	4	605	CLA	C3D-C4D	-2.12	1.39	1.44
25	4	606	CLA	C1C-C2C	2.12	1.48	1.44
25	G	1602	CLA	C1C-C2C	2.12	1.48	1.44
25	6	607	CLA	C1A-CHA	2.12	1.51	1.43
35	1	804	LMT	O1'-C1'	-2.11	1.36	1.40
25	B	1224	CLA	C1A-CHA	2.11	1.51	1.43
26	2	610	CHL	C1A-CHA	-2.11	1.37	1.40
25	A	1140	CLA	C1A-CHA	2.11	1.51	1.43
25	B	1206	CLA	C1A-CHA	2.11	1.51	1.43
25	1	612	CLA	C1A-CHA	2.11	1.51	1.43
25	9	605	CLA	C1A-CHA	2.11	1.51	1.43
25	G	1601	CLA	C1A-CHA	2.11	1.51	1.43
26	3	604	CHL	CHA-CBD	2.11	1.54	1.51
25	1	606	CLA	C1A-CHA	2.11	1.51	1.43
25	8	611	CLA	C1A-CHA	2.11	1.51	1.43
33	a	803	PTY	O4-C1	-2.11	1.40	1.45
25	F	1302	CLA	C1A-CHA	2.11	1.51	1.43
25	L	1504	CLA	C1A-CHA	2.11	1.51	1.43
25	7	608	CLA	C1A-CHA	2.11	1.51	1.43
25	B	1229	CLA	C1C-C2C	2.11	1.48	1.44
42	M	4001	ECH	C30-C25	-2.10	1.51	1.53
25	B	1219	CLA	C1A-CHA	2.10	1.51	1.43
25	5	604	CLA	C3D-C4D	-2.10	1.39	1.44
25	a	615	CLA	C1C-C2C	2.10	1.48	1.44
25	B	1208	CLA	C1C-C2C	2.10	1.48	1.44
25	8	615	CLA	C1A-CHA	2.10	1.51	1.43
25	A	1140	CLA	C1C-C2C	2.10	1.48	1.44
25	O	1803	CLA	C1C-C2C	2.10	1.48	1.44
25	A	1124	CLA	C1C-C2C	2.10	1.48	1.44
25	O	1803	CLA	C1A-CHA	2.10	1.51	1.43
25	A	1012	CLA	C1C-C2C	2.10	1.48	1.44
25	3	618	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	608	CHL	C3B-C2B	-2.10	1.37	1.40
25	6	607	CLA	C1C-C2C	2.10	1.48	1.44
36	7	806	DGD	O3G-C1D	2.10	1.43	1.40
26	9	610	CHL	CHA-CBD	2.10	1.54	1.51
25	4	611	CLA	C1A-CHA	2.10	1.51	1.43
44	1	502	AXT	C17-C1	2.10	1.57	1.53
25	A	1113	CLA	C1A-CHA	2.10	1.51	1.43
26	7	615	CHL	C3B-C2B	-2.10	1.37	1.40
39	F	4001	NEX	O24-C25	-2.10	1.43	1.46
25	K	1401	CLA	C1A-CHA	2.10	1.51	1.43
26	7	613	CHL	CHA-CBD	2.09	1.54	1.51
25	B	1214	CLA	C1A-CHA	2.09	1.51	1.43
25	5	614	CLA	C1A-CHA	2.09	1.51	1.43
26	2	613	CHL	C1A-CHA	-2.09	1.37	1.40
25	5	608	CLA	C1A-CHA	2.09	1.51	1.43
25	B	1240	CLA	C1A-CHA	2.09	1.51	1.43
25	3	616	CLA	C1A-CHA	2.09	1.51	1.43
25	a	607	CLA	C1A-CHA	2.09	1.51	1.43
25	A	1134	CLA	C1C-C2C	2.09	1.48	1.44
25	F	1301	CLA	C1A-CHA	2.09	1.51	1.43
25	2	602	CLA	C1C-C2C	2.09	1.48	1.44
25	B	1214	CLA	C3D-C4D	-2.09	1.39	1.44
25	2	615	CLA	C1A-CHA	2.09	1.51	1.43
25	B	1023	CLA	C1A-CHA	2.09	1.51	1.43
25	5	614	CLA	C1C-C2C	2.09	1.48	1.44
25	8	605	CLA	C3D-C4D	-2.09	1.39	1.44
25	B	1217	CLA	C3D-C4D	-2.09	1.39	1.44
25	2	621	CLA	C1A-CHA	2.09	1.51	1.43
25	8	620	CLA	C1A-CHA	2.09	1.51	1.43
25	A	1120	CLA	C1C-C2C	2.09	1.48	1.44
25	A	1139	CLA	C1C-C2C	2.09	1.48	1.44
25	B	1232	CLA	C1A-CHA	2.09	1.51	1.43
25	B	1217	CLA	C1A-CHA	2.09	1.51	1.43
25	6	612	CLA	C1A-CHA	2.09	1.51	1.43
25	6	605	CLA	C3D-C4D	-2.09	1.39	1.44
25	7	606	CLA	C1A-CHA	2.09	1.51	1.43
25	A	1119	CLA	C3D-C4D	-2.09	1.39	1.44
25	B	1218	CLA	C3D-C4D	-2.09	1.39	1.44
25	B	1217	CLA	C1C-C2C	2.09	1.48	1.44
26	7	617	CHL	C3B-C2B	-2.09	1.37	1.40
25	4	603	CLA	C1C-C2C	2.09	1.48	1.44
25	3	602	CLA	C1A-CHA	2.08	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	606	CLA	C3D-C4D	-2.08	1.39	1.44
25	3	610	CLA	C1A-CHA	2.08	1.51	1.43
25	2	608	CLA	C1A-CHA	2.08	1.51	1.43
25	B	1226	CLA	CHD-C1D	2.08	1.42	1.38
25	B	1203	CLA	C3D-C4D	-2.08	1.39	1.44
25	B	1210	CLA	C1A-CHA	2.08	1.51	1.43
25	A	1126	CLA	C3D-C4D	-2.08	1.39	1.44
25	1	601	CLA	C3D-C4D	-2.08	1.39	1.44
25	6	606	CLA	C1A-CHA	2.08	1.51	1.43
26	3	611	CHL	CHA-CBD	2.08	1.54	1.51
25	2	604	CLA	C1C-C2C	2.08	1.48	1.44
25	9	604	CLA	C3D-C4D	-2.08	1.39	1.44
25	4	615	CLA	C1C-C2C	2.08	1.48	1.44
25	8	620	CLA	C1C-C2C	2.08	1.48	1.44
25	4	603	CLA	C1A-CHA	2.08	1.51	1.43
35	2	804	LMT	O1'-C1'	-2.08	1.36	1.40
25	7	601	CLA	C3D-C4D	-2.08	1.39	1.44
25	4	604	CLA	C3D-C4D	-2.08	1.39	1.44
26	3	603	CHL	CHA-CBD	2.08	1.54	1.51
25	B	1228	CLA	C1A-CHA	2.08	1.51	1.43
25	1	603	CLA	C1A-CHA	2.08	1.51	1.43
33	A	5006	PTY	O4-C1	-2.08	1.40	1.45
25	4	605	CLA	C1A-CHA	2.08	1.51	1.43
33	G	5003	PTY	O7-C8	2.08	1.40	1.34
26	6	613	CHL	CHA-CBD	2.08	1.54	1.51
25	B	1207	CLA	C3D-C4D	-2.08	1.39	1.44
25	A	1130	CLA	C1C-C2C	2.08	1.48	1.44
25	5	603	CLA	C3D-C4D	-2.08	1.39	1.44
25	A	1109	CLA	C3D-C4D	-2.08	1.39	1.44
25	3	605	CLA	C3D-C4D	-2.08	1.39	1.44
25	A	1139	CLA	C1A-CHA	2.08	1.51	1.43
25	5	601	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1107	CLA	C3D-C4D	-2.07	1.39	1.44
25	L	1504	CLA	C1C-C2C	2.07	1.48	1.44
25	J	1901	CLA	C1A-CHA	2.07	1.51	1.43
25	1	605	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1012	CLA	C3D-C4D	-2.07	1.39	1.44
25	7	612	CLA	C1A-CHA	2.07	1.51	1.43
25	4	607	CLA	C1A-CHA	2.07	1.51	1.43
25	B	1204	CLA	C3D-C4D	-2.07	1.39	1.44
25	O	1801	CLA	C1C-C2C	2.07	1.48	1.44
25	2	601	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	1402	CLA	C1A-CHA	2.07	1.51	1.43
25	7	603	CLA	C1A-CHA	2.07	1.51	1.43
25	B	1211	CLA	C3D-C4D	-2.07	1.39	1.44
25	6	608	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1101	CLA	C1A-CHA	2.07	1.51	1.43
25	1	607	CLA	C1A-CHA	2.07	1.51	1.43
25	3	605	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1118	CLA	C1A-CHA	2.07	1.51	1.43
25	B	1239	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1125	CLA	C1A-CHA	2.07	1.51	1.43
25	a	602	CLA	C1A-CHA	2.07	1.51	1.43
25	A	1133	CLA	C3D-C4D	-2.07	1.39	1.44
25	B	1227	CLA	C1A-CHA	2.07	1.51	1.43
25	B	1211	CLA	C1C-C2C	2.07	1.48	1.44
25	O	1801	CLA	C3D-C4D	-2.07	1.39	1.44
25	A	1136	CLA	C1A-CHA	2.07	1.51	1.43
25	B	1236	CLA	C1C-C2C	2.06	1.48	1.44
25	2	605	CLA	C1C-C2C	2.06	1.48	1.44
26	2	609	CHL	CHA-CBD	2.06	1.54	1.51
25	A	1115	CLA	C1A-CHA	2.06	1.51	1.43
25	B	1228	CLA	C3D-C4D	-2.06	1.39	1.44
25	4	606	CLA	C1A-CHA	2.06	1.51	1.43
25	B	1213	CLA	C1C-C2C	2.06	1.48	1.44
25	A	1111	CLA	C1A-CHA	2.06	1.51	1.43
25	A	1108	CLA	C3D-C4D	-2.06	1.39	1.44
25	B	1202	CLA	C3D-C4D	-2.06	1.39	1.44
26	9	601	CHL	CHA-CBD	2.06	1.54	1.51
25	8	608	CLA	C3D-C4D	-2.06	1.39	1.44
25	B	1202	CLA	C1C-C2C	2.06	1.48	1.44
25	a	612	CLA	C1C-C2C	2.06	1.48	1.44
25	G	1602	CLA	C1A-CHA	2.06	1.51	1.43
25	2	604	CLA	C3D-C4D	-2.06	1.39	1.44
25	a	607	CLA	C1C-C2C	2.06	1.48	1.44
25	1	608	CLA	C3D-C4D	-2.06	1.39	1.44
25	a	601	CLA	C3D-C4D	-2.06	1.39	1.44
33	3	802	PTY	O4-C1	-2.06	1.40	1.45
25	A	1124	CLA	C1A-CHA	2.06	1.51	1.43
25	A	1126	CLA	C1A-CHA	2.06	1.51	1.43
25	B	1212	CLA	C1A-CHA	2.06	1.51	1.43
25	8	612	CLA	C3D-C4D	-2.06	1.39	1.44
26	5	617	CHL	C3B-C2B	-2.06	1.37	1.40
25	a	611	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	605	CLA	C1A-CHA	2.06	1.51	1.43
25	B	1221	CLA	C3D-C4D	-2.06	1.39	1.44
25	L	1502	CLA	C1C-C2C	2.06	1.48	1.44
25	A	1120	CLA	C1A-CHA	2.06	1.51	1.43
25	8	605	CLA	C1A-CHA	2.06	1.51	1.43
25	6	605	CLA	C1A-CHA	2.06	1.51	1.43
25	5	612	CLA	C1A-CHA	2.06	1.51	1.43
25	9	609	CLA	C1A-CHA	2.06	1.51	1.43
25	A	1122	CLA	C3D-C4D	-2.06	1.39	1.44
25	B	1213	CLA	C1A-CHA	2.06	1.51	1.43
25	A	1132	CLA	C1A-CHA	2.05	1.51	1.43
25	3	602	CLA	C3D-C4D	-2.05	1.39	1.44
25	L	1503	CLA	C1A-CHA	2.05	1.51	1.43
25	2	621	CLA	C3D-C4D	-2.05	1.39	1.44
25	A	1101	CLA	C1C-C2C	2.05	1.48	1.44
25	5	608	CLA	C1C-C2C	2.05	1.48	1.44
25	A	1103	CLA	C1A-CHA	2.05	1.51	1.43
25	B	1201	CLA	C1C-C2C	2.05	1.48	1.44
25	5	606	CLA	C1C-C2C	2.05	1.48	1.44
26	3	608	CHL	CHA-CBD	2.05	1.54	1.51
25	A	1132	CLA	C3D-C4D	-2.05	1.39	1.44
25	B	1220	CLA	C1A-CHA	2.05	1.51	1.43
25	A	1126	CLA	C1C-C2C	2.05	1.48	1.44
25	4	607	CLA	C1C-C2C	2.05	1.48	1.44
25	6	604	CLA	C3D-C4D	-2.05	1.39	1.44
25	G	1603	CLA	C1A-CHA	2.05	1.51	1.43
25	4	602	CLA	C1A-CHA	2.05	1.51	1.43
25	A	1115	CLA	C1C-C2C	2.05	1.48	1.44
25	5	601	CLA	C1C-C2C	2.05	1.48	1.44
25	6	605	CLA	C1C-C2C	2.05	1.48	1.44
25	A	1125	CLA	C3D-C4D	-2.05	1.39	1.44
25	B	1225	CLA	C3D-C4D	-2.05	1.39	1.44
25	9	607	CLA	C1C-C2C	2.05	1.48	1.44
25	A	1110	CLA	C1A-CHA	2.05	1.51	1.43
26	4	618	CHL	C1A-CHA	-2.05	1.37	1.40
25	5	607	CLA	C1C-C2C	2.05	1.48	1.44
25	7	601	CLA	C1C-C2C	2.05	1.48	1.44
25	B	1205	CLA	C3D-C4D	-2.05	1.39	1.44
25	B	1227	CLA	C3D-C4D	-2.05	1.39	1.44
25	1	607	CLA	C3D-C4D	-2.05	1.39	1.44
25	6	608	CLA	C3D-C4D	-2.05	1.39	1.44
41	J	5002	SPH	C3-C4	2.05	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1236	CLA	C3D-C4D	-2.04	1.39	1.44
25	3	606	CLA	C3D-C4D	-2.04	1.39	1.44
25	A	1104	CLA	C3D-C4D	-2.04	1.39	1.44
25	K	1402	CLA	C3D-C4D	-2.04	1.39	1.44
25	9	602	CLA	C1A-CHA	2.04	1.51	1.43
26	a	604	CHL	CHA-CBD	2.04	1.54	1.51
35	1	804	LMT	O4'-C4B	-2.04	1.37	1.43
25	6	612	CLA	C1C-C2C	2.04	1.48	1.44
25	L	1501	CLA	C1A-CHA	2.04	1.51	1.43
25	6	601	CLA	C1C-C2C	2.04	1.48	1.44
25	9	606	CLA	C1C-C2C	2.04	1.48	1.44
35	B	5006	LMT	O4'-C4B	-2.04	1.37	1.43
25	A	1129	CLA	C1A-CHA	2.04	1.51	1.43
25	5	606	CLA	C1A-CHA	2.04	1.51	1.43
25	A	1128	CLA	C1A-CHA	2.04	1.51	1.43
25	5	609	CLA	C1A-CHA	2.04	1.51	1.43
25	A	1134	CLA	C3D-C4D	-2.04	1.39	1.44
25	A	1141	CLA	C1C-C2C	2.04	1.48	1.44
25	B	1205	CLA	C1A-CHA	2.04	1.51	1.43
25	K	1404	CLA	C3D-C4D	-2.04	1.39	1.44
25	B	1229	CLA	C1A-CHA	2.04	1.51	1.43
25	8	615	CLA	C1C-C2C	2.04	1.48	1.44
25	7	602	CLA	C3D-C4D	-2.04	1.39	1.44
25	L	1501	CLA	C1C-C2C	2.04	1.48	1.44
25	3	612	CLA	C1A-CHA	2.04	1.51	1.43
25	L	1502	CLA	C1A-CHA	2.04	1.51	1.43
25	1	606	CLA	C3D-C4D	-2.04	1.39	1.44
25	A	1107	CLA	C1A-CHA	2.04	1.51	1.43
25	5	602	CLA	C1A-CHA	2.04	1.51	1.43
25	L	1503	CLA	C1C-C2C	2.04	1.48	1.44
25	A	1129	CLA	C3D-C4D	-2.04	1.39	1.44
25	B	1202	CLA	C1A-CHA	2.04	1.51	1.43
25	A	1116	CLA	C3D-C4D	-2.04	1.39	1.44
25	4	604	CLA	C1A-CHA	2.04	1.51	1.43
25	A	1135	CLA	C3D-C4D	-2.04	1.39	1.44
35	2	804	LMT	O4'-C4B	-2.03	1.37	1.43
25	a	605	CLA	C1A-CHA	2.03	1.51	1.43
25	A	1131	CLA	C3D-C4D	-2.03	1.39	1.44
25	A	1135	CLA	C1C-C2C	2.03	1.48	1.44
25	A	1138	CLA	C3D-C4D	-2.03	1.39	1.44
25	B	1209	CLA	C1C-C2C	2.03	1.48	1.44
25	1	608	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	1215	CLA	C3D-C4D	-2.03	1.39	1.44
25	5	605	CLA	C1A-CHA	2.03	1.51	1.43
25	B	1224	CLA	C1C-C2C	2.03	1.48	1.44
25	1	605	CLA	C3D-C4D	-2.03	1.39	1.44
25	5	606	CLA	C3D-C4D	-2.03	1.39	1.44
25	B	1236	CLA	C1A-CHA	2.03	1.51	1.43
25	3	613	CLA	C1A-CHA	2.03	1.51	1.43
25	K	1404	CLA	C1C-C2C	2.03	1.48	1.44
25	5	603	CLA	C1A-CHA	2.03	1.51	1.43
25	A	1108	CLA	C1C-C2C	2.03	1.48	1.44
25	B	1230	CLA	C1A-CHA	2.03	1.51	1.43
25	7	603	CLA	C3D-C4D	-2.03	1.39	1.44
25	2	612	CLA	C3D-C4D	-2.03	1.39	1.44
25	B	1240	CLA	C1C-C2C	2.03	1.48	1.44
25	A	1118	CLA	C3D-C4D	-2.03	1.39	1.44
25	B	1223	CLA	C1C-C2C	2.03	1.48	1.44
25	B	1021	CLA	C3D-C4D	-2.03	1.39	1.44
25	A	1110	CLA	C3D-C4D	-2.03	1.39	1.44
25	6	602	CLA	C1A-CHA	2.03	1.51	1.43
25	B	1238	CLA	C1C-C2C	2.03	1.48	1.44
25	A	1137	CLA	C1C-C2C	2.03	1.48	1.44
26	9	613	CHL	C1A-CHA	-2.03	1.37	1.40
25	G	1601	CLA	C1C-C2C	2.03	1.48	1.44
25	2	606	CLA	C1A-CHA	2.03	1.51	1.43
25	4	608	CLA	C3D-C4D	-2.03	1.39	1.44
25	A	1106	CLA	C1C-C2C	2.03	1.48	1.44
25	8	605	CLA	C1C-C2C	2.03	1.48	1.44
25	A	1131	CLA	C1A-CHA	2.03	1.51	1.43
25	B	1211	CLA	C1A-CHA	2.03	1.51	1.43
25	1	608	CLA	C1A-CHA	2.03	1.51	1.43
25	A	1128	CLA	C3D-C4D	-2.03	1.39	1.44
25	3	610	CLA	C3D-C4D	-2.03	1.39	1.44
25	F	1302	CLA	C1C-C2C	2.03	1.48	1.44
25	B	1239	CLA	C1C-C2C	2.03	1.48	1.44
25	5	605	CLA	C1C-C2C	2.03	1.48	1.44
25	A	1137	CLA	C3D-C4D	-2.02	1.39	1.44
25	K	1402	CLA	C1C-C2C	2.02	1.48	1.44
25	B	1237	CLA	C3D-C4D	-2.02	1.39	1.44
25	A	1106	CLA	C1A-CHA	2.02	1.51	1.43
25	A	1123	CLA	C3D-C4D	-2.02	1.39	1.44
33	B	5005	PTY	O7-C8	2.02	1.40	1.34
25	a	611	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	606	CLA	C1A-CHA	2.02	1.51	1.43
25	2	602	CLA	C1A-CHA	2.02	1.51	1.43
25	1	602	CLA	C3D-C4D	-2.02	1.39	1.44
25	6	603	CLA	C1A-CHA	2.02	1.51	1.43
25	8	620	CLA	MG-NC	2.02	2.11	2.06
25	1	602	CLA	C1A-CHA	2.02	1.51	1.43
25	B	1221	CLA	MG-NC	2.02	2.11	2.06
25	6	601	CLA	C1A-CHA	2.02	1.51	1.43
25	A	1110	CLA	C1C-C2C	2.02	1.48	1.44
25	6	603	CLA	C3D-C4D	-2.02	1.39	1.44
25	a	601	CLA	C1A-CHA	2.02	1.51	1.43
25	5	609	CLA	C1C-C2C	2.02	1.48	1.44
25	A	1135	CLA	C1A-CHA	2.02	1.51	1.43
25	3	602	CLA	C1C-C2C	2.02	1.48	1.44
25	A	1116	CLA	C1A-CHA	2.02	1.51	1.43
25	8	602	CLA	C3D-C4D	-2.02	1.39	1.44
25	A	1138	CLA	C1A-CHA	2.02	1.51	1.43
25	8	609	CLA	C1A-CHA	2.02	1.51	1.43
25	2	605	CLA	C1A-CHA	2.02	1.51	1.43
25	2	606	CLA	C1C-C2C	2.02	1.48	1.44
25	B	1238	CLA	C1A-CHA	2.02	1.51	1.43
25	B	1238	CLA	C3D-C4D	-2.02	1.39	1.44
25	4	608	CLA	C1C-C2C	2.02	1.48	1.44
25	B	1217	CLA	MG-NC	2.02	2.11	2.06
25	A	1105	CLA	C3D-C4D	-2.02	1.39	1.44
25	3	607	CLA	C3D-C4D	-2.02	1.39	1.44
25	5	612	CLA	C3D-C4D	-2.02	1.39	1.44
25	A	1012	CLA	C1A-CHA	2.02	1.51	1.43
25	B	1215	CLA	C1A-CHA	2.02	1.51	1.43
46	a	504	QTB	C14-C12	-2.02	1.48	1.53
25	3	618	CLA	C1C-C2C	2.02	1.48	1.44
25	9	602	CLA	C1C-C2C	2.02	1.48	1.44
25	A	1139	CLA	C3D-C4D	-2.02	1.39	1.44
25	B	1210	CLA	C3D-C4D	-2.02	1.39	1.44
25	a	602	CLA	C1C-C2C	2.01	1.48	1.44
25	A	1013	CLA	C1A-CHA	2.01	1.51	1.43
25	L	1503	CLA	C3D-C4D	-2.01	1.39	1.44
25	O	1802	CLA	C1C-C2C	2.01	1.48	1.44
25	9	609	CLA	C1C-C2C	2.01	1.48	1.44
25	A	1137	CLA	C1A-CHA	2.01	1.51	1.43
25	2	612	CLA	C1A-CHA	2.01	1.51	1.43
25	a	608	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1127	CLA	C1A-CHA	2.01	1.51	1.43
25	6	602	CLA	C3D-C4D	-2.01	1.39	1.44
25	3	613	CLA	C3D-C4D	-2.01	1.39	1.44
25	8	609	CLA	C3D-C4D	-2.01	1.39	1.44
25	5	604	CLA	C1C-C2C	2.01	1.48	1.44
25	A	1106	CLA	C3D-C4D	-2.01	1.39	1.44
25	B	1230	CLA	C3D-C4D	-2.01	1.39	1.44
25	3	601	CLA	C1A-CHA	2.01	1.51	1.43
25	1	603	CLA	C3D-C4D	-2.01	1.39	1.44
25	9	606	CLA	C3D-C4D	-2.01	1.39	1.44
25	A	1111	CLA	C3D-C4D	-2.01	1.39	1.44
25	F	1302	CLA	C3D-C4D	-2.01	1.39	1.44
25	7	607	CLA	C1C-C2C	2.01	1.48	1.44
25	B	1240	CLA	C3D-C4D	-2.01	1.39	1.44
25	3	616	CLA	C3D-C4D	-2.01	1.39	1.44
25	9	606	CLA	C1A-CHA	2.01	1.51	1.43
25	B	1232	CLA	C3D-C4D	-2.01	1.39	1.44
25	a	603	CLA	C1C-C2C	2.01	1.48	1.44
25	8	606	CLA	C3D-C4D	-2.01	1.39	1.44
25	A	1104	CLA	C1C-C2C	2.01	1.48	1.44
25	1	603	CLA	C1C-C2C	2.01	1.48	1.44
25	8	611	CLA	C3D-C4D	-2.01	1.39	1.44
26	6	610	CHL	C1A-CHA	-2.01	1.37	1.40
25	A	1130	CLA	C3D-C4D	-2.01	1.39	1.44
25	B	1021	CLA	C1A-CHA	2.01	1.51	1.43
25	4	603	CLA	C3D-C4D	-2.00	1.39	1.44
25	B	1225	CLA	C1A-CHA	2.00	1.51	1.43
25	A	1141	CLA	MG-NC	2.00	2.11	2.06
25	B	1222	CLA	C3D-C4D	-2.00	1.39	1.44
25	B	1239	CLA	C3D-C4D	-2.00	1.39	1.44
25	5	609	CLA	C3D-C4D	-2.00	1.39	1.44
25	7	608	CLA	C3D-C4D	-2.00	1.39	1.44
25	A	1117	CLA	C3D-C4D	-2.00	1.39	1.44
25	6	618	CLA	C3D-C4D	-2.00	1.39	1.44
25	B	1022	CLA	MG-NC	2.00	2.11	2.06
25	9	612	CLA	MG-NC	2.00	2.11	2.06
25	1	601	CLA	C1A-CHA	2.00	1.51	1.43
25	2	608	CLA	C1C-C2C	2.00	1.48	1.44
25	B	1224	CLA	C3D-C4D	-2.00	1.39	1.44
25	A	1108	CLA	C1A-CHA	2.00	1.51	1.43
25	A	1140	CLA	C3D-C4D	-2.00	1.39	1.44
25	H	1703	CLA	C3D-C4D	-2.00	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	1703	CLA	C1C-C2C	2.00	1.48	1.44
25	4	610	CLA	C1C-C2C	2.00	1.48	1.44
25	4	611	CLA	C3D-C4D	-2.00	1.39	1.44
25	2	601	CLA	C3D-C4D	-2.00	1.39	1.44
25	A	1104	CLA	C1A-CHA	2.00	1.51	1.43
25	B	1222	CLA	C1A-CHA	2.00	1.51	1.43
25	B	1209	CLA	C1A-CHA	2.00	1.51	1.43

All (5239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	H	4001	BCR	C23-C22-C21	26.56	160.78	119.01
50	9	504	XAT	C20-C13-C14	-26.26	80.27	122.82
50	9	504	XAT	C12-C13-C14	26.16	160.15	119.01
39	F	4001	NEX	C17-C1-C6	-26.13	87.08	110.47
29	H	4001	BCR	C37-C22-C21	-26.11	80.51	122.82
50	9	504	XAT	C20-C13-C12	-24.98	79.93	118.09
29	H	4001	BCR	C37-C22-C23	-24.59	80.53	118.09
25	B	1201	CLA	C4-C3-C5	-21.76	77.46	115.23
29	6	504	BCR	C10-C11-C12	19.59	179.95	123.20
29	H	4001	BCR	C10-C11-C12	19.08	178.50	123.20
29	L	4003	BCR	C10-C11-C12	18.97	178.18	123.20
29	B	4005	BCR	C10-C11-C12	18.94	178.07	123.20
29	O	4001	BCR	C10-C11-C12	18.91	178.00	123.20
29	4	503	BCR	C10-C11-C12	18.90	177.96	123.20
29	5	503	BCR	C10-C11-C12	18.90	177.96	123.20
29	L	4001	BCR	C10-C11-C12	18.88	177.90	123.20
29	3	504	BCR	C10-C11-C12	18.83	177.77	123.20
29	3	503	BCR	C10-C11-C12	18.82	177.73	123.20
29	5	504	BCR	C10-C11-C12	18.80	177.67	123.20
29	K	4002	BCR	C10-C11-C12	18.75	177.52	123.20
29	K	4001	BCR	C10-C11-C12	18.72	177.46	123.20
29	A	4003	BCR	C10-C11-C12	18.68	177.34	123.20
29	B	4007	BCR	C10-C11-C12	18.67	177.31	123.20
29	6	503	BCR	C10-C11-C12	18.64	177.20	123.20
29	B	4002	BCR	C10-C11-C12	18.62	177.14	123.20
29	7	503	BCR	C10-C11-C12	18.60	177.09	123.20
29	3	505	BCR	C10-C11-C12	18.58	177.04	123.20
29	G	4001	BCR	C10-C11-C12	18.55	176.94	123.20
29	8	503	BCR	C10-C11-C12	18.40	176.53	123.20
29	B	4004	BCR	C10-C11-C12	18.35	176.37	123.20
29	J	4001	BCR	C10-C11-C12	18.28	176.15	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	4001	BCR	C10-C11-C12	18.25	176.09	123.20
29	A	4004	BCR	C10-C11-C12	18.25	176.07	123.20
29	B	4006	BCR	C10-C11-C12	18.18	175.87	123.20
29	A	4001	BCR	C10-C11-C12	17.89	175.03	123.20
29	L	4002	BCR	C10-C11-C12	17.86	174.95	123.20
29	B	4001	BCR	C10-C11-C12	17.79	174.74	123.20
29	B	4003	BCR	C10-C11-C12	17.65	174.33	123.20
29	A	4005	BCR	C10-C11-C12	17.51	173.93	123.20
29	O	4001	BCR	C16-C15-C14	17.48	159.29	123.52
29	A	4002	BCR	C10-C11-C12	17.35	173.48	123.20
25	B	1201	CLA	C5-C3-C2	17.00	159.33	121.17
29	5	504	BCR	C16-C15-C14	16.82	157.93	123.52
25	B	1201	CLA	C4-C3-C2	-16.26	81.87	123.63
29	G	4001	BCR	C16-C15-C14	14.63	153.45	123.52
29	B	4003	BCR	C11-C10-C9	14.57	147.72	127.28
29	A	4003	BCR	C21-C20-C19	14.51	165.23	123.20
29	4	503	BCR	C16-C15-C14	14.23	152.64	123.52
24	A	1011	CL0	C1B-CHB-C4A	14.12	130.40	121.32
29	A	4005	BCR	C11-C10-C9	13.99	146.90	127.28
29	5	503	BCR	C16-C15-C14	13.90	151.95	123.52
29	B	4002	BCR	C11-C10-C9	13.87	146.74	127.28
29	L	4002	BCR	C11-C10-C9	13.87	146.73	127.28
29	K	4002	BCR	C21-C20-C19	13.75	163.05	123.20
29	I	4001	BCR	C11-C10-C9	13.73	146.53	127.28
29	K	4001	BCR	C21-C20-C19	13.71	162.93	123.20
29	3	504	BCR	C21-C20-C19	13.56	162.49	123.20
29	G	4001	BCR	C21-C20-C19	13.55	162.46	123.20
29	L	4003	BCR	C11-C10-C9	13.52	146.23	127.28
29	J	4001	BCR	C11-C10-C9	13.50	146.21	127.28
29	3	505	BCR	C11-C10-C9	13.48	146.18	127.28
29	B	4007	BCR	C16-C15-C14	13.46	151.06	123.52
29	8	503	BCR	C11-C10-C9	13.41	146.08	127.28
29	B	4001	BCR	C11-C10-C9	13.39	146.05	127.28
29	A	4001	BCR	C11-C10-C9	13.37	146.02	127.28
29	3	504	BCR	C11-C10-C9	13.35	146.01	127.28
29	K	4001	BCR	C11-C10-C9	13.30	145.94	127.28
29	A	4001	BCR	C21-C20-C19	13.29	161.70	123.20
29	4	503	BCR	C11-C10-C9	13.28	145.90	127.28
29	L	4001	BCR	C16-C15-C14	13.26	150.65	123.52
29	3	503	BCR	C16-C15-C14	13.26	150.64	123.52
29	3	505	BCR	C21-C20-C19	13.24	161.57	123.20
29	B	4006	BCR	C11-C10-C9	13.20	145.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	4003	BCR	C11-C10-C9	13.20	145.79	127.28
29	B	4001	BCR	C21-C20-C19	13.19	161.41	123.20
29	6	504	BCR	C16-C15-C14	13.16	150.45	123.52
29	A	4002	BCR	C16-C15-C14	13.15	150.42	123.52
29	O	4001	BCR	C11-C10-C9	13.14	145.71	127.28
29	L	4003	BCR	C16-C15-C14	13.06	150.23	123.52
29	B	4005	BCR	C11-C10-C9	13.03	145.56	127.28
29	B	4007	BCR	C11-C10-C9	13.03	145.56	127.28
29	A	4003	BCR	C16-C15-C14	13.00	150.12	123.52
29	B	4006	BCR	C16-C15-C14	12.98	150.07	123.52
29	L	4002	BCR	C21-C20-C19	12.95	160.72	123.20
29	B	4006	BCR	C21-C20-C19	12.90	160.57	123.20
29	6	503	BCR	C11-C10-C9	12.90	145.36	127.28
29	A	4004	BCR	C11-C10-C9	12.89	145.36	127.28
29	B	4005	BCR	C16-C15-C14	12.88	149.88	123.52
29	6	504	BCR	C21-C20-C19	12.86	160.47	123.20
29	B	4004	BCR	C11-C10-C9	12.84	145.29	127.28
29	H	4001	BCR	C16-C15-C14	12.82	149.75	123.52
29	H	4001	BCR	C11-C10-C9	12.82	145.26	127.28
29	O	4001	BCR	C21-C20-C19	12.72	160.05	123.20
29	J	4001	BCR	C21-C20-C19	12.69	159.98	123.20
29	7	503	BCR	C11-C10-C9	12.66	145.03	127.28
29	L	4001	BCR	C11-C10-C9	12.57	144.91	127.28
29	L	4001	BCR	C21-C20-C19	12.56	159.60	123.20
29	B	4001	BCR	C11-C12-C13	12.47	160.56	126.36
29	6	503	BCR	C16-C15-C14	12.46	149.01	123.52
29	B	4002	BCR	C16-C15-C14	12.41	148.91	123.52
29	A	4005	BCR	C11-C12-C13	12.37	160.29	126.36
29	L	4003	BCR	C21-C20-C19	12.36	159.02	123.20
29	H	4001	BCR	C21-C20-C19	12.33	158.93	123.20
29	K	4002	BCR	C11-C10-C9	12.32	144.56	127.28
29	L	4002	BCR	C11-C12-C13	12.32	160.13	126.36
29	A	4002	BCR	C21-C20-C19	12.30	158.84	123.20
29	A	4004	BCR	C21-C20-C19	12.29	158.81	123.20
29	B	4003	BCR	C11-C12-C13	12.29	160.05	126.36
29	6	504	BCR	C11-C10-C9	12.25	144.46	127.28
29	B	4003	BCR	C21-C20-C19	12.21	158.58	123.20
29	3	503	BCR	C11-C10-C9	12.12	144.28	127.28
29	K	4001	BCR	C16-C15-C14	12.07	148.23	123.52
29	B	4007	BCR	C21-C20-C19	12.07	158.18	123.20
29	B	4005	BCR	C21-C20-C19	12.00	157.97	123.20
29	5	503	BCR	C11-C10-C9	12.00	144.10	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	505	BCR	C16-C15-C14	11.99	148.06	123.52
29	5	504	BCR	C11-C10-C9	11.98	144.08	127.28
29	B	4002	BCR	C21-C20-C19	11.96	157.85	123.20
29	6	503	BCR	C21-C20-C19	11.94	157.79	123.20
29	7	503	BCR	C16-C15-C14	11.91	147.89	123.52
29	K	4002	BCR	C16-C15-C14	11.90	147.88	123.52
29	8	503	BCR	C21-C20-C19	11.88	157.63	123.20
29	A	4004	BCR	C11-C12-C13	11.82	158.78	126.36
29	B	4004	BCR	C11-C12-C13	11.80	158.72	126.36
29	3	504	BCR	C16-C15-C14	11.79	147.65	123.52
29	B	4004	BCR	C16-C15-C14	11.75	147.56	123.52
29	B	4004	BCR	C21-C20-C19	11.75	157.24	123.20
29	A	4001	BCR	C11-C12-C13	11.75	158.57	126.36
29	I	4001	BCR	C16-C15-C14	11.74	147.55	123.52
29	4	503	BCR	C21-C20-C19	11.65	156.96	123.20
29	8	503	BCR	C16-C15-C14	11.65	147.36	123.52
29	A	4004	BCR	C16-C15-C14	11.61	147.27	123.52
29	L	4002	BCR	C16-C15-C14	11.47	147.00	123.52
29	J	4001	BCR	C16-C15-C14	11.45	146.95	123.52
29	G	4001	BCR	C11-C10-C9	11.45	143.34	127.28
29	5	503	BCR	C21-C20-C19	11.33	156.04	123.20
29	5	504	BCR	C21-C20-C19	11.30	155.95	123.20
29	3	503	BCR	C21-C20-C19	11.29	155.90	123.20
29	3	503	BCR	C11-C12-C13	11.28	157.30	126.36
29	K	4002	BCR	C11-C12-C13	11.27	157.26	126.36
29	J	4001	BCR	C11-C12-C13	11.26	157.24	126.36
29	A	4005	BCR	C21-C20-C19	11.13	155.45	123.20
29	B	4001	BCR	C16-C15-C14	11.11	146.25	123.52
29	5	504	BCR	C11-C12-C13	11.11	156.82	126.36
29	8	503	BCR	C11-C12-C13	11.08	156.75	126.36
39	F	4001	NEX	C16-C1-C6	11.04	120.36	110.47
29	B	4007	BCR	C11-C12-C13	11.04	156.62	126.36
29	K	4001	BCR	C11-C12-C13	10.99	156.50	126.36
29	7	503	BCR	C11-C12-C13	10.99	156.49	126.36
29	I	4001	BCR	C11-C12-C13	10.97	156.44	126.36
29	B	4003	BCR	C16-C15-C14	10.95	145.92	123.52
29	I	4001	BCR	C21-C20-C19	10.88	154.74	123.20
29	6	504	BCR	C11-C12-C13	10.88	156.19	126.36
29	3	504	BCR	C11-C12-C13	10.81	156.00	126.36
29	H	4001	BCR	C11-C12-C13	10.78	155.93	126.36
29	A	4002	BCR	C11-C10-C9	10.71	142.31	127.28
29	B	4002	BCR	C11-C12-C13	10.64	155.53	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	4005	BCR	C16-C15-C14	10.62	145.24	123.52
29	A	4001	BCR	C16-C15-C14	10.59	145.20	123.52
29	L	4001	BCR	C11-C12-C13	10.54	155.26	126.36
29	3	505	BCR	C11-C12-C13	10.49	155.14	126.36
29	6	503	BCR	C11-C12-C13	10.49	155.13	126.36
29	A	4002	BCR	C11-C12-C13	10.43	154.97	126.36
29	5	503	BCR	C11-C12-C13	10.37	154.80	126.36
29	A	4003	BCR	C11-C12-C13	10.25	154.47	126.36
29	O	4001	BCR	C11-C12-C13	10.14	154.18	126.36
29	4	503	BCR	C11-C12-C13	10.11	154.09	126.36
29	B	4005	BCR	C11-C12-C13	10.08	154.00	126.36
29	L	4003	BCR	C11-C12-C13	10.03	153.86	126.36
29	B	4006	BCR	C11-C12-C13	9.89	153.49	126.36
29	7	503	BCR	C20-C19-C18	9.74	153.06	126.36
29	7	503	BCR	C21-C20-C19	9.66	151.19	123.20
29	5	504	BCR	C20-C19-C18	9.63	152.76	126.36
29	A	4005	BCR	C20-C19-C18	9.60	152.69	126.36
40	J	4002	RRX	C15-C14-C13	-9.57	113.86	127.28
25	B	1206	CLA	C4A-NA-C1A	9.42	110.98	106.68
29	4	503	BCR	C20-C19-C18	9.42	152.19	126.36
25	B	1205	CLA	C4A-NA-C1A	9.39	110.96	106.68
29	G	4001	BCR	C11-C12-C13	9.37	152.06	126.36
29	I	4001	BCR	C20-C19-C18	9.32	151.92	126.36
40	3	506	RRX	C15-C14-C13	-9.28	114.26	127.28
25	A	1141	CLA	C4A-NA-C1A	9.22	110.89	106.68
29	3	503	BCR	C20-C19-C18	9.21	151.62	126.36
25	2	603	CLA	C4A-NA-C1A	9.21	110.88	106.68
25	B	1221	CLA	C4A-NA-C1A	9.19	110.87	106.68
25	A	1123	CLA	C4A-NA-C1A	9.18	110.87	106.68
25	4	612	CLA	C4A-NA-C1A	9.18	110.87	106.68
29	5	503	BCR	C20-C19-C18	9.15	151.46	126.36
25	2	615	CLA	C4A-NA-C1A	9.11	110.84	106.68
25	5	615	CLA	C4A-NA-C1A	9.09	110.83	106.68
25	B	1235	CLA	C4A-NA-C1A	9.09	110.82	106.68
25	8	615	CLA	C4A-NA-C1A	9.08	110.82	106.68
39	F	4001	NEX	C17-C1-C16	-9.07	82.65	108.63
25	B	1228	CLA	C4A-NA-C1A	9.07	110.81	106.68
25	A	1103	CLA	C4A-NA-C1A	9.04	110.80	106.68
29	B	4005	BCR	C20-C19-C18	9.03	151.13	126.36
25	B	1201	CLA	C4A-NA-C1A	9.03	110.80	106.68
25	5	612	CLA	C4A-NA-C1A	9.00	110.79	106.68
25	A	1118	CLA	C4A-NA-C1A	8.99	110.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1109	CLA	C4A-NA-C1A	8.98	110.78	106.68
25	A	1102	CLA	C4A-NA-C1A	8.97	110.77	106.68
25	1	606	CLA	C4A-NA-C1A	8.95	110.76	106.68
25	6	612	CLA	C4A-NA-C1A	8.95	110.76	106.68
29	O	4001	BCR	C20-C19-C18	8.95	150.89	126.36
25	2	607	CLA	C4A-NA-C1A	8.94	110.76	106.68
25	8	609	CLA	C4A-NA-C1A	8.93	110.75	106.68
25	A	1117	CLA	C4A-NA-C1A	8.91	110.74	106.68
25	a	615	CLA	C4A-NA-C1A	8.91	110.74	106.68
25	B	1230	CLA	C4A-NA-C1A	8.90	110.74	106.68
25	B	1212	CLA	C4A-NA-C1A	8.88	110.73	106.68
25	1	608	CLA	C4A-NA-C1A	8.88	110.73	106.68
25	5	607	CLA	C4A-NA-C1A	8.88	110.73	106.68
25	B	1021	CLA	C4A-NA-C1A	8.88	110.73	106.68
25	B	1222	CLA	C4A-NA-C1A	8.87	110.72	106.68
25	9	612	CLA	C4A-NA-C1A	8.86	110.72	106.68
25	A	1106	CLA	C4A-NA-C1A	8.85	110.72	106.68
25	H	1701	CLA	C4A-NA-C1A	8.85	110.72	106.68
25	H	1702	CLA	C4A-NA-C1A	8.84	110.71	106.68
25	a	603	CLA	C4A-NA-C1A	8.84	110.71	106.68
25	8	607	CLA	C4A-NA-C1A	8.84	110.71	106.68
25	F	1301	CLA	C4A-NA-C1A	8.83	110.71	106.68
25	A	1111	CLA	C4A-NA-C1A	8.80	110.70	106.68
25	1	612	CLA	C4A-NA-C1A	8.80	110.69	106.68
25	B	1217	CLA	C4A-NA-C1A	8.79	110.69	106.68
25	K	1404	CLA	C4A-NA-C1A	8.79	110.69	106.68
25	3	606	CLA	C4A-NA-C1A	8.78	110.69	106.68
25	3	616	CLA	C4A-NA-C1A	8.78	110.69	106.68
25	J	1901	CLA	C4A-NA-C1A	8.77	110.68	106.68
25	6	615	CLA	C4A-NA-C1A	8.77	110.68	106.68
29	B	4004	BCR	C20-C19-C18	8.77	150.40	126.36
29	L	4003	BCR	C20-C19-C18	8.77	150.40	126.36
25	A	1112	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	a	608	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	6	608	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	1	615	CLA	C4A-NA-C1A	8.75	110.67	106.68
25	A	1131	CLA	C4A-NA-C1A	8.74	110.67	106.68
25	4	610	CLA	C4A-NA-C1A	8.74	110.67	106.68
25	A	1136	CLA	C4A-NA-C1A	8.73	110.66	106.68
25	8	611	CLA	C4A-NA-C1A	8.73	110.66	106.68
29	B	4002	BCR	C20-C19-C18	8.73	150.31	126.36
25	L	1502	CLA	C4A-NA-C1A	8.73	110.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	607	CLA	C4A-NA-C1A	8.72	110.66	106.68
25	1	603	CLA	C4A-NA-C1A	8.71	110.66	106.68
25	3	613	CLA	C4A-NA-C1A	8.71	110.65	106.68
25	B	1234	CLA	O2D-CGD-CBD	8.71	120.51	110.95
25	L	1501	CLA	C4A-NA-C1A	8.71	110.65	106.68
25	7	612	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	7	608	CLA	C4A-NA-C1A	8.70	110.65	106.68
25	B	1214	CLA	C4A-NA-C1A	8.69	110.64	106.68
25	8	612	CLA	C4A-NA-C1A	8.69	110.64	106.68
25	B	1023	CLA	C4A-NA-C1A	8.68	110.64	106.68
25	7	610	CLA	C4A-NA-C1A	8.68	110.64	106.68
25	B	1224	CLA	C4A-NA-C1A	8.68	110.64	106.68
25	F	1302	CLA	C4A-NA-C1A	8.68	110.64	106.68
25	7	607	CLA	C4A-NA-C1A	8.67	110.64	106.68
25	B	1239	CLA	C4A-NA-C1A	8.67	110.64	106.68
25	4	617	CLA	C4A-NA-C1A	8.67	110.63	106.68
25	3	610	CLA	C4A-NA-C1A	8.66	110.63	106.68
25	3	618	CLA	C4A-NA-C1A	8.66	110.63	106.68
25	6	603	CLA	C4A-NA-C1A	8.64	110.62	106.68
25	a	612	CLA	C4A-NA-C1A	8.63	110.62	106.68
25	1	605	CLA	C4A-NA-C1A	8.63	110.62	106.68
25	5	601	CLA	C4A-NA-C1A	8.63	110.62	106.68
25	8	618	CLA	C4A-NA-C1A	8.62	110.61	106.68
25	A	1139	CLA	C4A-NA-C1A	8.61	110.61	106.68
25	7	603	CLA	C4A-NA-C1A	8.61	110.61	106.68
25	4	601	CLA	C4A-NA-C1A	8.60	110.60	106.68
25	2	608	CLA	C4A-NA-C1A	8.60	110.60	106.68
25	K	1401	CLA	C4A-NA-C1A	8.59	110.60	106.68
25	3	612	CLA	C4A-NA-C1A	8.59	110.60	106.68
25	4	608	CLA	C4A-NA-C1A	8.59	110.60	106.68
29	6	503	BCR	C20-C19-C18	8.59	149.91	126.36
25	2	601	CLA	C4A-NA-C1A	8.58	110.59	106.68
25	L	1503	CLA	C4A-NA-C1A	8.57	110.59	106.68
25	A	1120	CLA	C4A-NA-C1A	8.57	110.59	106.68
25	K	1403	CLA	C4A-NA-C1A	8.56	110.58	106.68
25	9	602	CLA	C4A-NA-C1A	8.56	110.58	106.68
25	A	1134	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	O	1803	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	A	1132	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	A	1126	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	8	620	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	B	1202	CLA	C4A-NA-C1A	8.53	110.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	611	CLA	C4A-NA-C1A	8.53	110.57	106.68
25	B	1223	CLA	C4A-NA-C1A	8.53	110.57	106.68
25	3	607	CLA	C4A-NA-C1A	8.53	110.57	106.68
25	a	602	CLA	C4A-NA-C1A	8.52	110.57	106.68
25	4	606	CLA	C4A-NA-C1A	8.52	110.57	106.68
29	8	503	BCR	C20-C19-C18	8.52	149.72	126.36
25	B	1213	CLA	C4A-NA-C1A	8.51	110.56	106.68
25	3	602	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	A	1128	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	B	1219	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	5	606	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	5	608	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	B	1232	CLA	C4A-NA-C1A	8.50	110.56	106.68
25	2	621	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	B	1237	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	G	1601	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	A	1140	CLA	C4A-NA-C1A	8.49	110.55	106.68
25	B	1227	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	B	1215	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	A	1115	CLA	C4A-NA-C1A	8.48	110.55	106.68
25	4	607	CLA	C4A-NA-C1A	8.47	110.55	106.68
25	B	1204	CLA	C4A-NA-C1A	8.47	110.54	106.68
25	O	1802	CLA	C4A-NA-C1A	8.47	110.54	106.68
25	G	1602	CLA	C4A-NA-C1A	8.46	110.54	106.68
25	a	611	CLA	C4A-NA-C1A	8.46	110.54	106.68
25	7	601	CLA	C4A-NA-C1A	8.45	110.54	106.68
25	A	1122	CLA	C4A-NA-C1A	8.45	110.53	106.68
25	B	1210	CLA	C4A-NA-C1A	8.45	110.53	106.68
25	8	606	CLA	C4A-NA-C1A	8.45	110.53	106.68
25	a	607	CLA	C4A-NA-C1A	8.45	110.53	106.68
25	6	606	CLA	C4A-NA-C1A	8.45	110.53	106.68
25	A	1012	CLA	C4A-NA-C1A	8.44	110.53	106.68
25	A	1137	CLA	C4A-NA-C1A	8.44	110.53	106.68
25	O	1801	CLA	C4A-NA-C1A	8.44	110.53	106.68
25	B	1220	CLA	C4A-NA-C1A	8.43	110.53	106.68
25	4	604	CLA	C4A-NA-C1A	8.43	110.52	106.68
25	3	601	CLA	C4A-NA-C1A	8.42	110.52	106.68
25	K	1402	CLA	C4A-NA-C1A	8.42	110.52	106.68
25	9	609	CLA	C4A-NA-C1A	8.42	110.52	106.68
25	2	612	CLA	C4A-NA-C1A	8.40	110.51	106.68
29	A	4004	BCR	C20-C19-C18	8.39	149.37	126.36
25	6	607	CLA	C4A-NA-C1A	8.39	110.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	601	CLA	C4A-NA-C1A	8.39	110.51	106.68
25	B	1236	CLA	C4A-NA-C1A	8.38	110.50	106.68
25	A	1013	CLA	C4A-NA-C1A	8.37	110.50	106.68
25	A	1127	CLA	C4A-NA-C1A	8.37	110.50	106.68
25	5	614	CLA	C4A-NA-C1A	8.37	110.50	106.68
25	A	1133	CLA	C4A-NA-C1A	8.37	110.50	106.68
29	B	4003	BCR	C20-C19-C18	8.35	149.26	126.36
25	7	605	CLA	C4A-NA-C1A	8.35	110.49	106.68
25	5	609	CLA	C4A-NA-C1A	8.34	110.48	106.68
25	1	602	CLA	C4A-NA-C1A	8.33	110.48	106.68
25	A	1101	CLA	C4A-NA-C1A	8.33	110.48	106.68
25	3	605	CLA	C4A-NA-C1A	8.32	110.47	106.68
25	5	604	CLA	C4A-NA-C1A	8.31	110.47	106.68
25	a	605	CLA	C4A-NA-C1A	8.30	110.47	106.68
25	9	604	CLA	C4A-NA-C1A	8.30	110.47	106.68
25	B	1238	CLA	C4A-NA-C1A	8.30	110.47	106.68
25	2	606	CLA	C4A-NA-C1A	8.29	110.46	106.68
25	8	602	CLA	C4A-NA-C1A	8.29	110.46	106.68
25	A	1124	CLA	C4A-NA-C1A	8.27	110.45	106.68
25	7	604	CLA	C4A-NA-C1A	8.27	110.45	106.68
25	4	602	CLA	C4A-NA-C1A	8.27	110.45	106.68
25	8	605	CLA	C4A-NA-C1A	8.27	110.45	106.68
25	B	1208	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	A	1011	CL0	O2D-CGD-CBD	8.26	120.03	110.95
25	A	1138	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	5	605	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	2	604	CLA	C4A-NA-C1A	8.25	110.44	106.68
25	A	1116	CLA	C4A-NA-C1A	8.25	110.44	106.68
25	7	606	CLA	C4A-NA-C1A	8.24	110.44	106.68
25	B	1229	CLA	C4A-NA-C1A	8.24	110.44	106.68
25	2	602	CLA	C4A-NA-C1A	8.23	110.44	106.68
25	B	1211	CLA	C4A-NA-C1A	8.23	110.44	106.68
25	9	605	CLA	C4A-NA-C1A	8.23	110.43	106.68
25	H	1703	CLA	C4A-NA-C1A	8.22	110.43	106.68
25	A	1121	CLA	C4A-NA-C1A	8.22	110.43	106.68
25	B	1240	CLA	C4A-NA-C1A	8.22	110.43	106.68
25	4	615	CLA	C4A-NA-C1A	8.21	110.43	106.68
25	B	1218	CLA	C4A-NA-C1A	8.21	110.42	106.68
25	4	603	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	A	1113	CLA	C4A-NA-C1A	8.20	110.42	106.68
25	B	1207	CLA	C4A-NA-C1A	8.19	110.42	106.68
25	6	618	CLA	C4A-NA-C1A	8.19	110.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	603	CLA	C4A-NA-C1A	8.19	110.42	106.68
25	1	607	CLA	C4A-NA-C1A	8.18	110.41	106.68
25	A	1107	CLA	C4A-NA-C1A	8.17	110.41	106.68
25	G	1603	CLA	C4A-NA-C1A	8.17	110.41	106.68
25	A	1105	CLA	C4A-NA-C1A	8.17	110.41	106.68
25	1	601	CLA	C4A-NA-C1A	8.17	110.41	106.68
25	A	1135	CLA	C4A-NA-C1A	8.16	110.40	106.68
25	6	602	CLA	C4A-NA-C1A	8.16	110.40	106.68
25	A	1129	CLA	C4A-NA-C1A	8.16	110.40	106.68
26	1	609	CHL	C1B-CHB-C4A	8.14	126.56	121.32
25	A	1108	CLA	C4A-NA-C1A	8.14	110.39	106.68
29	B	4007	BCR	C20-C19-C18	8.13	148.66	126.36
25	A	1110	CLA	C4A-NA-C1A	8.13	110.39	106.68
25	4	605	CLA	C4A-NA-C1A	8.13	110.39	106.68
25	4	616	CLA	C4A-NA-C1A	8.12	110.39	106.68
25	B	1216	CLA	C4A-NA-C1A	8.11	110.38	106.68
25	A	1104	CLA	C4A-NA-C1A	8.11	110.38	106.68
25	7	602	CLA	C4A-NA-C1A	8.11	110.38	106.68
25	6	601	CLA	C4A-NA-C1A	8.10	110.38	106.68
25	5	602	CLA	C4A-NA-C1A	8.09	110.37	106.68
29	A	4002	BCR	C20-C19-C18	8.08	148.53	126.36
26	9	603	CHL	C1B-CHB-C4A	8.07	126.52	121.32
29	L	4001	BCR	C20-C19-C18	8.07	148.49	126.36
25	B	1203	CLA	C4A-NA-C1A	8.07	110.36	106.68
25	6	605	CLA	C4A-NA-C1A	8.05	110.35	106.68
26	2	613	CHL	C1B-CHB-C4A	8.05	126.50	121.32
43	7	501	LUT	C21-C26-C27	8.04	122.07	112.83
25	9	606	CLA	C4A-NA-C1A	8.04	110.35	106.68
25	L	1504	CLA	C4A-NA-C1A	8.02	110.34	106.68
25	A	1130	CLA	C4A-NA-C1A	8.02	110.34	106.68
25	B	1225	CLA	C4A-NA-C1A	8.00	110.33	106.68
25	A	1119	CLA	C4A-NA-C1A	7.99	110.32	106.68
25	8	608	CLA	C4A-NA-C1A	7.97	110.31	106.68
29	H	4001	BCR	C20-C19-C18	7.94	148.15	126.36
26	7	611	CHL	C1B-CHB-C4A	7.89	126.40	121.32
25	2	605	CLA	C4A-NA-C1A	7.89	110.28	106.68
26	7	617	CHL	C1B-CHB-C4A	7.87	126.38	121.32
29	J	4001	BCR	C20-C19-C18	7.85	147.89	126.36
25	A	1125	CLA	C4A-NA-C1A	7.84	110.26	106.68
29	6	504	BCR	C20-C19-C18	7.84	147.85	126.36
29	B	4006	BCR	C20-C19-C18	7.78	147.70	126.36
29	L	4002	BCR	C20-C19-C18	7.75	147.61	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1231	CLA	C4A-NA-C1A	7.74	110.21	106.68
25	B	1209	CLA	C4A-NA-C1A	7.70	110.19	106.68
29	G	4001	BCR	C20-C19-C18	7.68	147.42	126.36
26	8	613	CHL	C1B-CHB-C4A	7.65	126.25	121.32
26	3	603	CHL	C1B-CHB-C4A	7.63	126.23	121.32
26	1	611	CHL	C1B-CHB-C4A	7.63	126.23	121.32
29	3	505	BCR	C20-C19-C18	7.63	147.28	126.36
25	6	604	CLA	C4A-NA-C1A	7.56	110.13	106.68
25	B	1226	CLA	C4A-NA-C1A	7.52	110.11	106.68
25	B	1022	CLA	C4A-NA-C1A	7.50	110.10	106.68
26	4	613	CHL	C1B-CHB-C4A	7.48	126.13	121.32
26	8	603	CHL	C1B-CHB-C4A	7.43	126.10	121.32
39	F	4001	NEX	C2-C1-C6	7.40	116.41	109.21
29	B	4001	BCR	C20-C19-C18	7.39	146.62	126.36
29	3	504	BCR	C20-C19-C18	7.33	146.45	126.36
39	F	4001	NEX	O24-C25-C38	-7.32	106.86	115.05
26	6	617	CHL	C1B-CHB-C4A	7.31	126.03	121.32
26	5	613	CHL	C1B-CHB-C4A	7.30	126.02	121.32
29	A	4001	BCR	C20-C19-C18	7.29	146.35	126.36
26	a	613	CHL	C1B-CHB-C4A	7.22	125.97	121.32
29	K	4001	BCR	C20-C19-C18	7.21	146.14	126.36
43	4	501	LUT	C21-C26-C27	7.20	121.11	112.83
26	4	609	CHL	C1B-CHB-C4A	7.20	125.95	121.32
44	7	504	AXT	C1-C6-C5	-7.12	112.91	122.64
29	K	4002	BCR	C20-C19-C18	7.12	145.87	126.36
26	8	604	CHL	C1B-CHB-C4A	7.11	125.90	121.32
43	2	507	LUT	C21-C26-C27	7.03	120.91	112.83
26	a	609	CHL	C1B-CHB-C4A	7.03	125.84	121.32
26	6	611	CHL	C1B-CHB-C4A	6.98	125.81	121.32
26	3	604	CHL	C1B-CHB-C4A	6.98	125.81	121.32
26	9	613	CHL	C1B-CHB-C4A	6.98	125.81	121.32
26	7	609	CHL	C1B-CHB-C4A	6.96	125.80	121.32
26	7	615	CHL	C1B-CHB-C4A	6.89	125.76	121.32
26	a	604	CHL	C1B-CHB-C4A	6.81	125.70	121.32
43	2	507	LUT	C31-C30-C29	-6.80	117.74	127.28
40	3	506	RRX	C20-C21-C22	-6.76	117.79	127.28
26	1	613	CHL	C1B-CHB-C4A	6.74	125.66	121.32
48	8	804	DGA	CDB-CCB-CBB	-6.68	80.61	114.37
26	5	618	CHL	C1B-CHB-C4A	6.66	125.61	121.32
29	G	4001	BCR	C15-C14-C13	-6.66	117.94	127.28
26	6	613	CHL	C1B-CHB-C4A	6.64	125.60	121.32
25	A	1117	CLA	O2D-CGD-CBD	6.64	122.84	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	617	CHL	C1B-CHB-C4A	6.63	125.59	121.32
26	A	1114	CHL	C1B-CHB-C4A	6.61	125.58	121.32
26	8	601	CHL	C1B-CHB-C4A	6.59	125.56	121.32
26	9	608	CHL	C1B-CHB-C4A	6.58	125.56	121.32
25	B	1218	CLA	O2D-CGD-CBD	6.54	122.67	111.23
26	2	610	CHL	C1B-CHB-C4A	6.51	125.51	121.32
26	5	611	CHL	C1B-CHB-C4A	6.51	125.51	121.32
29	A	4003	BCR	C20-C19-C18	6.46	144.09	126.36
26	1	604	CHL	C1B-CHB-C4A	6.44	125.47	121.32
43	1	503	LUT	C15-C35-C34	-6.42	110.38	123.52
26	7	613	CHL	C1B-CHB-C4A	6.41	125.45	121.32
26	4	618	CHL	C1B-CHB-C4A	6.41	125.45	121.32
25	4	612	CLA	O2D-CGD-CBD	6.38	122.38	111.23
26	5	610	CHL	C1B-CHB-C4A	6.37	125.42	121.32
43	a	503	LUT	C35-C34-C33	-6.36	118.36	127.28
50	9	507	XAT	C15-C14-C13	-6.30	118.44	127.28
25	1	606	CLA	O2D-CGD-CBD	6.28	122.21	111.23
26	3	604	CHL	C1-O2A-CGA	6.28	131.86	116.65
43	5	505	LUT	C21-C26-C27	6.27	120.03	112.83
26	a	610	CHL	C1B-CHB-C4A	6.25	125.35	121.32
25	B	1205	CLA	O2D-CGD-CBD	6.24	122.14	111.23
25	B	1201	CLA	O2D-CGD-CBD	6.21	122.09	111.23
25	A	1106	CLA	O2D-CGD-CBD	6.21	122.08	111.23
29	7	503	BCR	C23-C24-C25	-6.15	110.56	127.00
25	8	618	CLA	CMD-C2D-C1D	6.12	135.51	124.73
43	a	503	LUT	C21-C26-C27	6.11	119.85	112.83
25	A	1128	CLA	O2D-CGD-CBD	6.10	121.89	111.23
25	H	1702	CLA	O2D-CGD-CBD	6.08	121.86	111.23
25	A	1132	CLA	O2D-CGD-CBD	6.06	121.83	111.23
25	A	1121	CLA	CMD-C2D-C1D	6.05	135.39	124.73
25	B	1221	CLA	O2D-CGD-CBD	6.05	121.81	111.23
25	A	1112	CLA	O2D-CGD-CBD	6.05	121.80	111.23
26	6	619	CHL	C1B-CHB-C4A	6.03	125.20	121.32
25	A	1101	CLA	O2D-CGD-CBD	6.02	121.75	111.23
43	2	507	LUT	C11-C10-C9	-6.01	118.84	127.28
25	B	1231	CLA	CMD-C2D-C1D	6.00	135.29	124.73
25	B	1240	CLA	O2D-CGD-CBD	5.96	121.66	111.23
26	a	606	CHL	C1B-CHB-C4A	5.96	125.16	121.32
25	1	605	CLA	O2D-CGD-CBD	5.95	121.63	111.23
25	B	1230	CLA	O2D-CGD-CBD	5.94	121.61	111.23
25	A	1120	CLA	O2D-CGD-CBD	5.93	121.60	111.23
25	2	604	CLA	CMD-C2D-C1D	5.91	135.14	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1129	CLA	O2D-CGD-CBD	5.91	121.56	111.23
25	A	1115	CLA	O2D-CGD-CBD	5.90	121.55	111.23
25	B	1211	CLA	O2D-CGD-CBD	5.88	121.52	111.23
26	9	610	CHL	C1B-CHB-C4A	5.87	125.10	121.32
25	8	609	CLA	O2D-CGD-CBD	5.87	121.48	111.23
25	B	1212	CLA	O2D-CGD-CBD	5.86	121.48	111.23
26	6	609	CHL	C1B-CHB-C4A	5.85	125.09	121.32
25	6	608	CLA	CMD-C2D-C1D	5.85	135.03	124.73
25	2	605	CLA	CMD-C2D-C1D	5.83	135.00	124.73
25	6	605	CLA	CMD-C2D-C1D	5.83	135.00	124.73
25	2	615	CLA	O2D-CGD-CBD	5.83	121.41	111.23
25	A	1134	CLA	O2D-CGD-CBD	5.81	121.39	111.23
25	7	604	CLA	CMD-C2D-C1D	5.81	134.95	124.73
25	4	606	CLA	O2D-CGD-CBD	5.81	121.38	111.23
25	A	1102	CLA	O2D-CGD-CBD	5.79	121.35	111.23
25	B	1226	CLA	CMD-C2D-C1D	5.77	134.89	124.73
25	5	604	CLA	CMD-C2D-C1D	5.75	134.86	124.73
25	B	1208	CLA	O2D-CGD-CBD	5.75	121.28	111.23
25	B	1227	CLA	O2D-CGD-CBD	5.75	121.28	111.23
25	B	1210	CLA	O2D-CGD-CBD	5.74	121.27	111.23
25	A	1109	CLA	CMD-C2D-C1D	5.74	134.83	124.73
25	A	1113	CLA	O2D-CGD-CBD	5.73	121.25	111.23
25	6	606	CLA	O2D-CGD-CBD	5.72	121.23	111.23
25	5	603	CLA	CMD-C2D-C1D	5.71	134.79	124.73
25	7	601	CLA	CMD-C2D-C1D	5.71	134.78	124.73
26	3	611	CHL	C1B-CHB-C4A	5.69	124.98	121.32
25	A	1103	CLA	O2D-CGD-CBD	5.67	121.14	111.23
25	A	1123	CLA	O2D-CGD-CBD	5.67	121.14	111.23
25	O	1802	CLA	O2D-CGD-CBD	5.66	121.13	111.23
25	a	605	CLA	O2D-CGD-CBD	5.65	121.11	111.23
40	3	506	RRX	C15-C16-C17	-5.65	111.95	123.52
25	1	605	CLA	CMD-C2D-C1D	5.64	134.66	124.73
25	a	605	CLA	CMD-C2D-C1D	5.64	134.66	124.73
26	1	610	CHL	C1B-CHB-C4A	5.64	124.95	121.32
25	2	607	CLA	O2D-CGD-CBD	5.63	121.07	111.23
25	8	607	CLA	O2D-CGD-CBD	5.63	121.07	111.23
25	9	605	CLA	CMD-C2D-C1D	5.62	134.63	124.73
25	6	604	CLA	CMD-C2D-C1D	5.62	134.62	124.73
25	A	1125	CLA	O2D-CGD-CBD	5.62	121.05	111.23
25	4	608	CLA	O2D-CGD-CBD	5.62	121.05	111.23
25	B	1223	CLA	O2D-CGD-CBD	5.62	121.05	111.23
25	6	604	CLA	O2D-CGD-CBD	5.62	121.05	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	601	CLA	CMD-C2D-C1D	5.62	134.62	124.73
25	A	1141	CLA	CMD-C2D-C1D	5.61	134.61	124.73
25	A	1111	CLA	CMD-C2D-C1D	5.61	134.61	124.73
25	A	1121	CLA	O2D-CGD-CBD	5.61	121.03	111.23
25	4	606	CLA	CMD-C2D-C1D	5.61	134.60	124.73
25	7	606	CLA	CMD-C2D-C1D	5.60	134.59	124.73
25	A	1101	CLA	CMD-C2D-C1D	5.59	134.58	124.73
25	O	1802	CLA	CMD-C2D-C1D	5.59	134.57	124.73
40	J	4002	RRX	C15-C16-C17	5.59	134.95	123.52
25	L	1503	CLA	O2D-CGD-CBD	5.58	120.99	111.23
25	B	1217	CLA	CMD-C2D-C1D	5.58	134.56	124.73
25	B	1229	CLA	O2D-CGD-CBD	5.58	120.99	111.23
25	1	606	CLA	CMD-C2D-C1D	5.58	134.55	124.73
25	B	1217	CLA	O2D-CGD-CBD	5.58	120.98	111.23
25	B	1202	CLA	O2D-CGD-CBD	5.57	120.97	111.23
25	8	620	CLA	CMD-C2D-C1D	5.57	134.54	124.73
25	B	1209	CLA	CMD-C2D-C1D	5.57	134.54	124.73
25	A	1126	CLA	CMD-C2D-C1D	5.56	134.52	124.73
25	5	601	CLA	CMD-C2D-C1D	5.56	134.52	124.73
25	8	602	CLA	CMD-C2D-C1D	5.56	134.52	124.73
25	A	1113	CLA	CMD-C2D-C1D	5.56	134.52	124.73
25	4	617	CLA	CMD-C2D-C1D	5.56	134.51	124.73
25	B	1218	CLA	CMD-C2D-C1D	5.55	134.51	124.73
40	J	4002	RRX	C24-C23-C22	-5.55	118.02	126.23
25	B	1211	CLA	CMD-C2D-C1D	5.55	134.50	124.73
25	a	601	CLA	CMD-C2D-C1D	5.55	134.50	124.73
43	1	503	LUT	C21-C26-C27	5.55	119.20	112.83
25	7	607	CLA	O2A-C1-C2	5.55	122.19	108.99
26	a	604	CHL	C1-C2-C3	-5.54	117.11	126.20
25	3	610	CLA	O2D-CGD-CBD	5.54	120.92	111.23
25	B	1228	CLA	CMD-C2D-C1D	5.54	134.49	124.73
25	3	602	CLA	CMD-C2D-C1D	5.54	134.49	124.73
25	5	605	CLA	CMD-C2D-C1D	5.54	134.48	124.73
25	3	613	CLA	O2D-CGD-CBD	5.53	120.91	111.23
25	4	604	CLA	CMD-C2D-C1D	5.53	134.46	124.73
46	a	504	QTB	C04-C03-C02	5.53	135.03	127.28
25	4	605	CLA	CMD-C2D-C1D	5.53	134.46	124.73
25	a	603	CLA	CMD-C2D-C1D	5.53	134.46	124.73
25	B	1203	CLA	CMD-C2D-C1D	5.52	134.46	124.73
25	4	610	CLA	CMD-C2D-C1D	5.52	134.46	124.73
26	2	609	CHL	C1B-CHB-C4A	5.52	124.88	121.32
25	6	606	CLA	CMD-C2D-C1D	5.52	134.45	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	O	1801	CLA	CMD-C2D-C1D	5.52	134.45	124.73
25	6	601	CLA	CMD-C2D-C1D	5.52	134.44	124.73
25	9	604	CLA	CMD-C2D-C1D	5.51	134.44	124.73
25	A	1132	CLA	CMD-C2D-C1D	5.51	134.43	124.73
25	A	1106	CLA	CMD-C2D-C1D	5.51	134.43	124.73
25	4	603	CLA	CMD-C2D-C1D	5.51	134.43	124.73
25	4	604	CLA	O2D-CGD-CBD	5.51	120.86	111.23
25	A	1136	CLA	CMD-C2D-C1D	5.51	134.43	124.73
44	7	504	AXT	C8-C9-C10	5.50	127.67	119.01
25	8	605	CLA	CMD-C2D-C1D	5.50	134.42	124.73
25	B	1229	CLA	CMD-C2D-C1D	5.50	134.41	124.73
25	4	602	CLA	O2D-CGD-CBD	5.50	120.84	111.23
25	3	605	CLA	CMD-C2D-C1D	5.50	134.41	124.73
25	2	606	CLA	CMD-C2D-C1D	5.50	134.41	124.73
25	A	1105	CLA	CMD-C2D-C1D	5.50	134.41	124.73
25	G	1602	CLA	CMD-C2D-C1D	5.50	134.41	124.73
25	A	1138	CLA	CMD-C2D-C1D	5.49	134.40	124.73
50	2	501	XAT	C38-C25-C24	5.49	120.41	114.24
25	8	602	CLA	O2D-CGD-CBD	5.49	120.83	111.23
25	A	1120	CLA	O2A-C1-C2	5.49	122.06	108.99
25	A	1134	CLA	CMD-C2D-C1D	5.49	134.40	124.73
25	O	1803	CLA	CMD-C2D-C1D	5.49	134.40	124.73
25	5	606	CLA	CMD-C2D-C1D	5.49	134.40	124.73
25	A	1125	CLA	CMD-C2D-C1D	5.49	134.39	124.73
25	9	604	CLA	O2D-CGD-CBD	5.49	120.82	111.23
25	A	1102	CLA	CMD-C2D-C1D	5.49	134.39	124.73
25	4	611	CLA	CMD-C2D-C1D	5.48	134.39	124.73
25	B	1235	CLA	O2D-CGD-CBD	5.48	120.82	111.23
25	7	603	CLA	CMD-C2D-C1D	5.48	134.38	124.73
25	K	1404	CLA	CMD-C2D-C1D	5.48	134.38	124.73
25	G	1603	CLA	CMD-C2D-C1D	5.48	134.38	124.73
25	A	1110	CLA	O2D-CGD-CBD	5.48	120.81	111.23
25	6	615	CLA	O2D-CGD-CBD	5.48	120.81	111.23
25	A	1103	CLA	CMD-C2D-C1D	5.48	134.38	124.73
25	B	1238	CLA	CMD-C2D-C1D	5.48	134.37	124.73
25	A	1140	CLA	CMD-C2D-C1D	5.48	134.37	124.73
25	9	606	CLA	CMD-C2D-C1D	5.47	134.37	124.73
25	3	606	CLA	CMD-C2D-C1D	5.47	134.37	124.73
25	3	610	CLA	CMD-C2D-C1D	5.47	134.37	124.73
25	B	1209	CLA	O2D-CGD-CBD	5.47	120.80	111.23
25	9	609	CLA	CMD-C2D-C1D	5.47	134.37	124.73
25	B	1221	CLA	CMD-C2D-C1D	5.47	134.36	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	605	CLA	CMD-C2D-C1D	5.47	134.36	124.73
25	L	1503	CLA	CMD-C2D-C1D	5.47	134.36	124.73
25	B	1222	CLA	CMD-C2D-C1D	5.47	134.36	124.73
25	8	606	CLA	CMD-C2D-C1D	5.47	134.35	124.73
25	A	1130	CLA	CMD-C2D-C1D	5.47	134.35	124.73
25	B	1231	CLA	O2D-CGD-CBD	5.47	120.78	111.23
25	2	601	CLA	CMD-C2D-C1D	5.46	134.35	124.73
25	2	603	CLA	CMD-C2D-C1D	5.46	134.35	124.73
25	A	1122	CLA	CMD-C2D-C1D	5.46	134.35	124.73
46	a	504	QTB	C13-C12-C11	5.46	122.90	112.57
25	L	1504	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	8	608	CLA	O2D-CGD-CBD	5.46	120.77	111.23
25	B	1213	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	B	1239	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	A	1116	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	K	1403	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	B	1216	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	F	1301	CLA	CMD-C2D-C1D	5.46	134.34	124.73
25	4	616	CLA	CMD-C2D-C1D	5.45	134.33	124.73
25	B	1021	CLA	O2D-CGD-CBD	5.45	120.76	111.23
25	a	611	CLA	CMD-C2D-C1D	5.45	134.32	124.73
25	B	1208	CLA	CMD-C2D-C1D	5.45	134.32	124.73
25	H	1703	CLA	CMD-C2D-C1D	5.45	134.32	124.73
25	7	604	CLA	O2D-CGD-CBD	5.44	120.75	111.23
25	B	1223	CLA	CMD-C2D-C1D	5.44	134.31	124.73
46	a	504	QTB	C09-C02-C03	5.44	127.57	119.01
25	8	611	CLA	CMD-C2D-C1D	5.44	134.31	124.73
25	B	1220	CLA	CMD-C2D-C1D	5.44	134.31	124.73
25	1	612	CLA	CMD-C2D-C1D	5.44	134.31	124.73
25	B	1210	CLA	CMD-C2D-C1D	5.44	134.30	124.73
25	H	1702	CLA	CMD-C2D-C1D	5.44	134.30	124.73
25	B	1224	CLA	CMD-C2D-C1D	5.43	134.30	124.73
25	A	1105	CLA	O2D-CGD-CBD	5.43	120.73	111.23
25	1	607	CLA	CMD-C2D-C1D	5.43	134.30	124.73
25	8	615	CLA	CMD-C2D-C1D	5.43	134.30	124.73
25	L	1501	CLA	CMD-C2D-C1D	5.43	134.30	124.73
25	B	1214	CLA	CMD-C2D-C1D	5.43	134.29	124.73
25	A	1135	CLA	CMD-C2D-C1D	5.43	134.29	124.73
25	A	1137	CLA	CMD-C2D-C1D	5.43	134.29	124.73
25	8	618	CLA	O2D-CGD-CBD	5.43	120.72	111.23
25	H	1701	CLA	CMD-C2D-C1D	5.43	134.29	124.73
26	3	608	CHL	C1B-CHB-C4A	5.43	124.81	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1235	CLA	CMD-C2D-C1D	5.43	134.29	124.73
25	A	1117	CLA	CMD-C2D-C1D	5.43	134.28	124.73
25	A	1129	CLA	CMD-C2D-C1D	5.43	134.28	124.73
25	3	612	CLA	CMD-C2D-C1D	5.42	134.27	124.73
25	A	1139	CLA	CMD-C2D-C1D	5.42	134.27	124.73
25	1	603	CLA	CMD-C2D-C1D	5.42	134.27	124.73
25	7	602	CLA	CMD-C2D-C1D	5.42	134.27	124.73
25	B	1232	CLA	CMD-C2D-C1D	5.42	134.27	124.73
25	A	1110	CLA	CMD-C2D-C1D	5.41	134.26	124.73
25	B	1207	CLA	CMD-C2D-C1D	5.41	134.26	124.73
25	K	1402	CLA	CMD-C2D-C1D	5.41	134.25	124.73
25	7	610	CLA	CMD-C2D-C1D	5.41	134.25	124.73
25	A	1108	CLA	CMD-C2D-C1D	5.41	134.25	124.73
25	9	606	CLA	O2D-CGD-CBD	5.40	120.67	111.23
25	A	1104	CLA	CMD-C2D-C1D	5.40	134.24	124.73
25	J	1901	CLA	CMD-C2D-C1D	5.39	134.23	124.73
25	8	608	CLA	CMD-C2D-C1D	5.39	134.23	124.73
44	1	502	AXT	C1-C6-C5	-5.39	115.27	122.64
25	4	601	CLA	CMD-C2D-C1D	5.39	134.22	124.73
25	L	1502	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	2	621	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	B	1212	CLA	CMD-C2D-C1D	5.38	134.21	124.73
43	3	502	LUT	C21-C26-C27	5.38	119.01	112.83
25	B	1202	CLA	CMD-C2D-C1D	5.38	134.21	124.73
25	1	602	CLA	CMD-C2D-C1D	5.38	134.21	124.73
40	J	4002	RRX	C7-C8-C9	-5.38	118.27	126.23
25	A	1107	CLA	CMD-C2D-C1D	5.38	134.20	124.73
25	A	1119	CLA	CMD-C2D-C1D	5.38	134.20	124.73
25	9	609	CLA	O2D-CGD-CBD	5.38	120.63	111.23
25	A	1107	CLA	O2D-CGD-CBD	5.38	120.63	111.23
25	3	602	CLA	O2D-CGD-CBD	5.37	120.62	111.23
25	B	1234	CLA	C2D-C1D-ND	5.37	113.31	109.43
25	a	608	CLA	CMD-C2D-C1D	5.37	134.19	124.73
25	6	603	CLA	CMD-C2D-C1D	5.37	134.19	124.73
25	8	609	CLA	CMD-C2D-C1D	5.37	134.19	124.73
25	6	602	CLA	O2D-CGD-CBD	5.37	120.62	111.23
25	a	607	CLA	O2D-CGD-CBD	5.37	120.62	111.23
25	A	1139	CLA	O2D-CGD-CBD	5.36	120.61	111.23
25	K	1403	CLA	O2D-CGD-CBD	5.36	120.61	111.23
25	B	1215	CLA	O2D-CGD-CBD	5.36	120.60	111.23
25	A	1137	CLA	O2D-CGD-CBD	5.36	120.60	111.23
25	9	605	CLA	O2D-CGD-CBD	5.36	120.59	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	1402	CLA	O2D-CGD-CBD	5.35	120.59	111.23
25	B	1227	CLA	CMD-C2D-C1D	5.35	134.15	124.73
25	B	1236	CLA	CMD-C2D-C1D	5.35	134.15	124.73
25	3	607	CLA	CMD-C2D-C1D	5.35	134.14	124.73
25	6	618	CLA	CMD-C2D-C1D	5.35	134.14	124.73
26	6	610	CHL	C1B-CHB-C4A	5.34	124.76	121.32
25	3	613	CLA	CMD-C2D-C1D	5.34	134.14	124.73
25	a	612	CLA	CMD-C2D-C1D	5.34	134.14	124.73
25	2	608	CLA	CMD-C2D-C1D	5.34	134.14	124.73
25	A	1112	CLA	CMD-C2D-C1D	5.34	134.13	124.73
25	A	1131	CLA	CMD-C2D-C1D	5.34	134.13	124.73
25	5	615	CLA	CMD-C2D-C1D	5.34	134.13	124.73
25	1	615	CLA	CMD-C2D-C1D	5.34	134.13	124.73
25	B	1230	CLA	CMD-C2D-C1D	5.34	134.13	124.73
25	1	607	CLA	O2D-CGD-CBD	5.34	120.56	111.23
25	2	621	CLA	CMD-C2D-C1D	5.33	134.12	124.73
25	6	605	CLA	O2D-CGD-CBD	5.33	120.55	111.23
25	9	607	CLA	CMD-C2D-C1D	5.33	134.11	124.73
25	2	606	CLA	O2D-CGD-CBD	5.33	120.54	111.23
25	3	618	CLA	CMD-C2D-C1D	5.33	134.11	124.73
26	8	601	CHL	C1-C2-C3	-5.33	117.47	126.20
25	2	612	CLA	CMD-C2D-C1D	5.32	134.10	124.73
25	B	1204	CLA	CMD-C2D-C1D	5.32	134.09	124.73
25	2	601	CLA	O2D-CGD-CBD	5.32	120.53	111.23
25	4	601	CLA	O2D-CGD-CBD	5.32	120.53	111.23
25	2	607	CLA	CMD-C2D-C1D	5.32	134.09	124.73
26	6	619	CHL	C1-O2A-CGA	5.32	129.52	116.65
25	4	602	CLA	CMD-C2D-C1D	5.31	134.08	124.73
25	K	1403	CLA	O2A-C1-C2	5.31	121.63	108.99
24	A	1011	CL0	O2A-CGA-O1A	-5.31	110.34	123.63
25	6	602	CLA	CMD-C2D-C1D	5.31	134.07	124.73
26	9	601	CHL	C1B-CHB-C4A	5.31	124.74	121.32
25	A	1111	CLA	O2D-CGD-CBD	5.31	120.51	111.23
25	5	609	CLA	CMD-C2D-C1D	5.30	134.06	124.73
25	B	1022	CLA	CMD-C2D-C1D	5.30	134.06	124.73
25	B	1205	CLA	CMD-C2D-C1D	5.30	134.06	124.73
25	5	612	CLA	CMD-C2D-C1D	5.30	134.06	124.73
25	5	605	CLA	O2D-CGD-CBD	5.30	120.49	111.23
25	5	601	CLA	O2D-CGD-CBD	5.29	120.48	111.23
46	a	504	QTB	C01-C02-C09	-5.29	110.00	118.09
25	B	1226	CLA	O2D-CGD-CBD	5.29	120.48	111.23
43	5	505	LUT	C15-C14-C13	-5.29	119.86	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	608	CLA	O2D-CGD-CBD	5.29	120.48	111.23
25	6	608	CLA	O2D-CGD-CBD	5.29	120.48	111.23
25	a	607	CLA	CMD-C2D-C1D	5.29	134.04	124.73
25	K	1404	CLA	O2D-CGD-CBD	5.29	120.47	111.23
25	A	1118	CLA	CMD-C2D-C1D	5.29	134.04	124.73
25	3	616	CLA	CMD-C2D-C1D	5.28	134.03	124.73
25	a	611	CLA	O2D-CGD-CBD	5.28	120.46	111.23
25	4	607	CLA	CMD-C2D-C1D	5.27	134.01	124.73
25	a	602	CLA	CMD-C2D-C1D	5.27	134.01	124.73
25	B	1204	CLA	O2D-CGD-CBD	5.27	120.44	111.23
42	M	4001	ECH	C20-C21-C22	-5.27	119.89	127.28
25	B	1201	CLA	CMD-C2D-C1D	5.27	134.00	124.73
25	B	1237	CLA	CMD-C2D-C1D	5.26	134.00	124.73
25	5	614	CLA	CMD-C2D-C1D	5.26	133.99	124.73
25	B	1224	CLA	O2D-CGD-CBD	5.26	120.43	111.23
25	B	1214	CLA	O2D-CGD-CBD	5.26	120.42	111.23
25	2	605	CLA	O2D-CGD-CBD	5.26	120.42	111.23
43	5	505	LUT	C11-C10-C9	-5.25	119.91	127.28
25	A	1131	CLA	O2D-CGD-CBD	5.25	120.41	111.23
25	6	601	CLA	O2D-CGD-CBD	5.25	120.41	111.23
25	5	602	CLA	O2D-CGD-CBD	5.25	120.41	111.23
25	A	1104	CLA	O2D-CGD-CBD	5.25	120.40	111.23
25	B	1234	CLA	C4D-ND-C1D	-5.24	102.59	108.87
25	6	603	CLA	O2D-CGD-CBD	5.24	120.40	111.23
25	7	602	CLA	O2D-CGD-CBD	5.24	120.39	111.23
25	A	1135	CLA	O2D-CGD-CBD	5.24	120.39	111.23
25	9	602	CLA	CMD-C2D-C1D	5.24	133.96	124.73
25	9	612	CLA	CMD-C2D-C1D	5.24	133.95	124.73
25	4	605	CLA	O2D-CGD-CBD	5.24	120.39	111.23
25	3	601	CLA	CMD-C2D-C1D	5.24	133.95	124.73
25	G	1603	CLA	O2D-CGD-CBD	5.23	120.38	111.23
42	M	4001	ECH	C11-C10-C9	-5.23	119.94	127.28
25	8	612	CLA	CMD-C2D-C1D	5.23	133.94	124.73
25	7	608	CLA	CMD-C2D-C1D	5.23	133.93	124.73
25	5	607	CLA	CMD-C2D-C1D	5.22	133.93	124.73
25	B	1219	CLA	CMD-C2D-C1D	5.22	133.93	124.73
25	3	616	CLA	O2D-CGD-CBD	5.22	120.36	111.23
25	A	1136	CLA	O2D-CGD-CBD	5.22	120.35	111.23
25	B	1207	CLA	O2D-CGD-CBD	5.22	120.35	111.23
25	A	1124	CLA	CMD-C2D-C1D	5.21	133.91	124.73
25	F	1302	CLA	CMD-C2D-C1D	5.21	133.91	124.73
25	A	1116	CLA	O2D-CGD-CBD	5.21	120.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	607	CLA	O2D-CGD-CBD	5.21	120.34	111.23
25	5	604	CLA	O2D-CGD-CBD	5.21	120.34	111.23
25	6	615	CLA	CMD-C2D-C1D	5.21	133.90	124.73
43	2	507	LUT	C35-C34-C33	-5.21	119.97	127.28
25	A	1140	CLA	O2D-CGD-CBD	5.21	120.33	111.23
25	A	1133	CLA	CMD-C2D-C1D	5.20	133.89	124.73
25	B	1240	CLA	CMD-C2D-C1D	5.20	133.89	124.73
25	B	1239	CLA	O2D-CGD-CBD	5.20	120.33	111.23
50	7	502	XAT	C31-C30-C29	-5.20	119.98	127.28
50	2	501	XAT	C31-C30-C29	-5.20	119.98	127.28
25	4	607	CLA	O2D-CGD-CBD	5.20	120.31	111.23
25	7	603	CLA	O2D-CGD-CBD	5.19	120.31	111.23
25	A	1126	CLA	O2D-CGD-CBD	5.19	120.31	111.23
25	H	1703	CLA	O2D-CGD-CBD	5.19	120.30	111.23
25	3	612	CLA	O2D-CGD-CBD	5.18	120.29	111.23
25	6	607	CLA	CMD-C2D-C1D	5.18	133.85	124.73
25	B	1215	CLA	CMD-C2D-C1D	5.17	133.84	124.73
25	B	1238	CLA	O2D-CGD-CBD	5.17	120.27	111.23
25	B	1236	CLA	O2D-CGD-CBD	5.17	120.27	111.23
43	3	501	LUT	C21-C26-C27	5.17	118.77	112.83
25	B	1225	CLA	CMD-C2D-C1D	5.17	133.83	124.73
25	2	602	CLA	O2D-CGD-CBD	5.17	120.26	111.23
40	3	506	RRX	C24-C23-C22	-5.16	118.60	126.23
25	3	618	CLA	O2D-CGD-CBD	5.16	120.26	111.23
25	B	1219	CLA	O2D-CGD-CBD	5.16	120.25	111.23
25	5	614	CLA	O2D-CGD-CBD	5.16	120.25	111.23
25	1	602	CLA	O2D-CGD-CBD	5.15	120.24	111.23
25	9	602	CLA	O2D-CGD-CBD	5.15	120.24	111.23
25	A	1120	CLA	CMD-C2D-C1D	5.15	133.80	124.73
25	B	1213	CLA	O2D-CGD-CBD	5.15	120.24	111.23
25	5	602	CLA	CMD-C2D-C1D	5.14	133.79	124.73
25	A	1130	CLA	O2D-CGD-CBD	5.14	120.22	111.23
25	B	1228	CLA	O2D-CGD-CBD	5.14	120.22	111.23
25	J	1901	CLA	O2D-CGD-CBD	5.14	120.22	111.23
25	4	612	CLA	CMD-C2D-C1D	5.14	133.78	124.73
25	L	1501	CLA	O2D-CGD-CBD	5.14	120.21	111.23
25	G	1601	CLA	CMD-C2D-C1D	5.13	133.77	124.73
26	8	610	CHL	C1B-CHB-C4A	5.13	124.62	121.32
25	A	1124	CLA	O2D-CGD-CBD	5.13	120.20	111.23
25	1	608	CLA	CMD-C2D-C1D	5.13	133.76	124.73
50	9	504	XAT	C31-C30-C29	-5.13	120.09	127.28
25	7	607	CLA	CMD-C2D-C1D	5.12	133.75	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	1602	CLA	O2D-CGD-CBD	5.12	120.19	111.23
25	4	615	CLA	CMD-C2D-C1D	5.12	133.75	124.73
25	2	602	CLA	CMD-C2D-C1D	5.12	133.75	124.73
25	A	1123	CLA	CMD-C2D-C1D	5.12	133.74	124.73
50	7	502	XAT	C38-C25-C24	5.12	119.99	114.24
26	8	604	CHL	C1-C2-C3	-5.12	117.82	126.20
25	A	1141	CLA	O2D-CGD-CBD	5.12	120.17	111.23
40	J	4002	RRX	C11-C10-C9	-5.11	120.11	127.28
25	7	607	CLA	O2D-CGD-CBD	5.11	120.17	111.23
25	a	602	CLA	O2D-CGD-CBD	5.11	120.17	111.23
25	2	604	CLA	O2D-CGD-CBD	5.11	120.16	111.23
25	8	605	CLA	O2D-CGD-CBD	5.10	120.15	111.23
25	9	612	CLA	O2D-CGD-CBD	5.10	120.15	111.23
25	a	601	CLA	O2D-CGD-CBD	5.09	120.14	111.23
50	9	507	XAT	C38-C25-C24	5.09	119.96	114.24
25	5	608	CLA	O2D-CGD-CBD	5.09	120.13	111.23
25	B	1022	CLA	O2D-CGD-CBD	5.08	120.12	111.23
25	8	607	CLA	CMD-C2D-C1D	5.08	133.68	124.73
43	2	507	LUT	C15-C14-C13	-5.08	120.16	127.28
25	B	1023	CLA	CMD-C2D-C1D	5.07	133.65	124.73
25	4	608	CLA	CMD-C2D-C1D	5.06	133.64	124.73
40	3	506	RRX	C7-C8-C9	-5.06	118.75	126.23
25	7	612	CLA	CMD-C2D-C1D	5.06	133.64	124.73
25	6	612	CLA	O2D-CGD-CBD	5.06	120.07	111.23
25	5	606	CLA	O2D-CGD-CBD	5.05	120.07	111.23
25	4	611	CLA	O2D-CGD-CBD	5.05	120.06	111.23
25	B	1225	CLA	O2D-CGD-CBD	5.05	120.05	111.23
25	K	1401	CLA	O2D-CGD-CBD	5.04	120.04	111.23
25	A	1133	CLA	O2D-CGD-CBD	5.04	120.04	111.23
25	a	615	CLA	O2D-CGD-CBD	5.03	120.03	111.23
25	8	615	CLA	O2D-CGD-CBD	5.03	120.02	111.23
25	3	606	CLA	O2D-CGD-CBD	5.03	120.02	111.23
25	1	601	CLA	O2D-CGD-CBD	5.02	120.01	111.23
25	6	612	CLA	CMD-C2D-C1D	5.02	133.56	124.73
25	5	609	CLA	O2D-CGD-CBD	5.02	120.00	111.23
25	A	1012	CLA	O2D-CGD-CBD	5.02	120.00	111.23
25	B	1206	CLA	O2D-CGD-CBD	5.01	119.99	111.23
25	L	1504	CLA	O2D-CGD-CBD	5.01	119.99	111.23
25	3	607	CLA	O2D-CGD-CBD	5.01	119.98	111.23
25	B	1023	CLA	O2D-CGD-CBD	5.01	119.98	111.23
42	M	4001	ECH	C15-C14-C13	-5.00	120.26	127.28
25	B	1203	CLA	O2D-CGD-CBD	5.00	119.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	1701	CLA	O2D-CGD-CBD	4.99	119.96	111.23
25	1	615	CLA	O2D-CGD-CBD	4.99	119.96	111.23
25	4	615	CLA	O2D-CGD-CBD	4.98	119.93	111.23
25	A	1115	CLA	CMD-C2D-C1D	4.97	133.49	124.73
25	B	1237	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	G	1601	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	B	1216	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	6	607	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	3	601	CLA	O2D-CGD-CBD	4.96	119.90	111.23
25	F	1301	CLA	O2D-CGD-CBD	4.96	119.90	111.23
25	7	601	CLA	O2D-CGD-CBD	4.96	119.90	111.23
25	B	1206	CLA	CMD-C2D-C1D	4.96	133.46	124.73
25	5	608	CLA	CMD-C2D-C1D	4.95	133.45	124.73
25	4	610	CLA	O2D-CGD-CBD	4.95	119.88	111.23
25	L	1502	CLA	CMD-C2D-C1D	4.94	133.43	124.73
25	5	603	CLA	O2D-CGD-CBD	4.93	119.86	111.23
25	5	612	CLA	O2D-CGD-CBD	4.93	119.84	111.23
43	5	505	LUT	C7-C8-C9	-4.91	118.96	126.23
25	6	618	CLA	O2D-CGD-CBD	4.91	119.82	111.23
25	7	610	CLA	O2D-CGD-CBD	4.91	119.81	111.23
25	2	608	CLA	O2D-CGD-CBD	4.90	119.80	111.23
29	I	4001	BCR	C23-C24-C25	-4.90	113.91	127.00
30	2	802	LHG	O7-C7-C8	4.90	122.08	111.48
25	3	605	CLA	O2D-CGD-CBD	4.90	119.80	111.23
25	K	1401	CLA	CMD-C2D-C1D	4.90	133.35	124.73
25	4	617	CLA	O2D-CGD-CBD	4.89	119.79	111.23
25	9	607	CLA	O2D-CGD-CBD	4.89	119.79	111.23
26	8	610	CHL	C1C-CHC-C4B	4.89	133.58	116.07
25	A	1127	CLA	O2D-CGD-CBD	4.88	119.75	111.23
25	A	1119	CLA	O2D-CGD-CBD	4.86	119.73	111.23
25	B	1021	CLA	CMD-C2D-C1D	4.86	133.29	124.73
25	8	620	CLA	O2D-CGD-CBD	4.86	119.72	111.23
25	F	1302	CLA	O2D-CGD-CBD	4.86	119.72	111.23
40	J	4002	RRX	C16-C15-C14	4.85	133.44	123.52
25	7	612	CLA	O2D-CGD-CBD	4.85	119.70	111.23
25	8	612	CLA	O2D-CGD-CBD	4.84	119.70	111.23
25	a	608	CLA	O2D-CGD-CBD	4.84	119.69	111.23
25	2	612	CLA	O2D-CGD-CBD	4.84	119.69	111.23
50	9	504	XAT	C18-C5-C4	4.83	119.67	114.24
25	8	611	CLA	O2D-CGD-CBD	4.83	119.67	111.23
26	3	608	CHL	C1C-CHC-C4B	4.83	133.34	116.07
25	4	616	CLA	O2D-CGD-CBD	4.82	119.65	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	O	1803	CLA	O2D-CGD-CBD	4.81	119.65	111.23
25	1	603	CLA	O2D-CGD-CBD	4.81	119.64	111.23
26	6	610	CHL	C1C-CHC-C4B	4.81	133.27	116.07
25	4	603	CLA	O2D-CGD-CBD	4.80	119.62	111.23
25	a	603	CLA	O2D-CGD-CBD	4.80	119.62	111.23
25	B	1021	CLA	C1-C2-C3	-4.80	118.34	126.20
25	a	615	CLA	CMD-C2D-C1D	4.80	133.17	124.73
43	9	501	LUT	C21-C26-C27	4.80	118.34	112.83
26	9	601	CHL	C1C-CHC-C4B	4.79	133.22	116.07
25	B	1232	CLA	O2D-CGD-CBD	4.79	119.60	111.23
25	1	612	CLA	O2D-CGD-CBD	4.79	119.60	111.23
26	1	610	CHL	C1C-CHC-C4B	4.78	133.19	116.07
43	a	502	LUT	C21-C26-C27	4.78	118.32	112.83
26	7	613	CHL	C1C-CHC-C4B	4.77	133.15	116.07
40	3	506	RRX	C33-C5-C6	-4.77	119.28	124.48
25	a	612	CLA	O2D-CGD-CBD	4.76	119.56	111.23
25	2	615	CLA	CMD-C2D-C1D	4.76	133.11	124.73
43	5	502	LUT	C21-C26-C27	4.73	118.27	112.83
26	2	610	CHL	C1C-CHC-C4B	4.73	132.98	116.07
43	a	501	LUT	C15-C14-C13	-4.73	120.65	127.28
26	9	610	CHL	C1C-CHC-C4B	4.72	132.97	116.07
26	2	609	CHL	C1C-CHC-C4B	4.72	132.97	116.07
26	6	609	CHL	C1C-CHC-C4B	4.72	132.96	116.07
43	4	501	LUT	C35-C34-C33	-4.71	120.67	127.28
25	A	1013	CLA	CMD-C2D-C1D	4.71	133.03	124.73
44	7	504	AXT	C10-C11-C12	4.71	136.85	123.20
26	6	619	CHL	C1C-CHC-C4B	4.71	132.91	116.07
43	6	502	LUT	C21-C26-C27	4.70	118.23	112.83
25	A	1121	CLA	C1-C2-C3	-4.70	118.49	126.20
26	5	610	CHL	C1C-CHC-C4B	4.70	132.88	116.07
26	a	610	CHL	C1C-CHC-C4B	4.70	132.88	116.07
25	A	1118	CLA	O2D-CGD-CBD	4.70	119.44	111.23
43	8	502	LUT	C21-C26-C27	4.70	118.22	112.83
25	1	608	CLA	O2D-CGD-CBD	4.69	119.44	111.23
26	9	608	CHL	C1C-CHC-C4B	4.68	132.82	116.07
43	6	501	LUT	C21-C26-C27	4.68	118.20	112.83
25	A	1109	CLA	O2D-CGD-CBD	4.68	119.41	111.23
25	A	1013	CLA	O2D-CGD-CBD	4.68	119.41	111.23
25	7	606	CLA	O2D-CGD-CBD	4.67	119.40	111.23
25	8	606	CLA	O2D-CGD-CBD	4.67	119.40	111.23
25	A	1012	CLA	CMD-C2D-C1D	4.66	132.94	124.73
25	2	603	CLA	O2D-CGD-CBD	4.66	119.37	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	603	CLA	CAA-C2A-C3A	-4.66	100.42	113.00
26	a	606	CHL	C1C-CHC-C4B	4.65	132.72	116.07
26	a	613	CHL	C1C-CHC-C4B	4.65	132.71	116.07
25	2	601	CLA	O2A-C1-C2	4.65	125.99	108.11
25	A	1127	CLA	CMD-C2D-C1D	4.64	132.89	124.73
25	A	1128	CLA	CMD-C2D-C1D	4.63	132.89	124.73
43	a	503	LUT	C31-C30-C29	-4.63	120.78	127.28
26	3	611	CHL	C1C-CHC-C4B	4.62	132.62	116.07
40	3	506	RRX	C11-C12-C13	-4.62	113.69	126.36
29	7	503	BCR	C23-C22-C21	-4.62	111.74	119.01
26	6	613	CHL	C1C-CHC-C4B	4.62	132.61	116.07
26	5	617	CHL	C1C-CHC-C4B	4.62	132.61	116.07
50	7	502	XAT	C18-C5-C4	4.62	119.43	114.24
26	1	604	CHL	C1-C2-C3	-4.61	118.64	126.20
43	6	502	LUT	C7-C8-C9	-4.61	119.42	126.23
40	3	506	RRX	C20-C19-C18	-4.61	113.73	126.36
26	1	613	CHL	C1C-CHC-C4B	4.60	132.54	116.07
25	B	1222	CLA	O2D-CGD-CBD	4.60	119.27	111.23
30	6	802	LHG	O7-C7-C8	4.60	121.43	111.48
39	F	4001	NEX	C17-C1-C2	-4.60	87.28	109.06
25	A	1012	CLA	C1-C2-C3	-4.60	118.67	126.20
26	7	615	CHL	C1C-CHC-C4B	4.59	132.51	116.07
26	9	613	CHL	C1C-CHC-C4B	4.59	132.50	116.07
26	5	618	CHL	C1C-CHC-C4B	4.59	132.48	116.07
26	a	609	CHL	C1C-CHC-C4B	4.57	132.44	116.07
26	4	618	CHL	C1C-CHC-C4B	4.57	132.41	116.07
36	8	803	DGD	O2G-C1B-C2B	4.56	121.33	111.48
50	2	501	XAT	C18-C5-C4	4.55	119.36	114.24
26	6	611	CHL	C1C-CHC-C4B	4.55	132.36	116.07
26	4	609	CHL	C1C-CHC-C4B	4.55	132.35	116.07
26	A	1114	CHL	C1C-CHC-C4B	4.55	132.34	116.07
26	6	617	CHL	C1C-CHC-C4B	4.54	132.33	116.07
26	1	604	CHL	C1C-CHC-C4B	4.54	132.31	116.07
26	4	613	CHL	C1C-CHC-C4B	4.53	132.28	116.07
25	A	1108	CLA	O2D-CGD-CBD	4.52	119.13	111.23
26	5	613	CHL	C1C-CHC-C4B	4.52	132.24	116.07
26	a	604	CHL	C1C-CHC-C4B	4.51	132.22	116.07
26	7	609	CHL	C1C-CHC-C4B	4.51	132.21	116.07
43	a	501	LUT	C18-C5-C6	-4.51	119.56	124.48
26	5	611	CHL	C1C-CHC-C4B	4.50	132.18	116.07
43	a	501	LUT	C11-C10-C9	-4.50	120.97	127.28
26	8	613	CHL	C1C-CHC-C4B	4.50	132.16	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	606	CLA	C1-C2-C3	-4.48	119.51	126.76
26	3	604	CHL	C1C-CHC-C4B	4.48	132.10	116.07
25	4	610	CLA	O2A-C1-C2	4.48	125.34	108.11
25	A	1126	CLA	C1-C2-C3	-4.47	118.87	126.20
26	1	611	CHL	C1C-CHC-C4B	4.47	132.07	116.07
50	9	504	XAT	C15-C14-C13	-4.47	121.01	127.28
44	7	504	AXT	C40-C33-C34	-4.46	115.58	122.82
26	9	603	CHL	C1C-CHC-C4B	4.46	132.03	116.07
40	J	4002	RRX	C20-C19-C18	-4.45	114.15	126.36
43	8	502	LUT	C7-C8-C9	-4.45	119.65	126.23
26	1	609	CHL	C1C-CHC-C4B	4.44	131.96	116.07
25	A	1122	CLA	O2D-CGD-CBD	4.44	118.99	111.23
26	7	617	CHL	C1C-CHC-C4B	4.44	131.96	116.07
43	2	507	LUT	C18-C5-C6	-4.44	119.64	124.48
33	5	802	PTY	O7-C8-C11	4.43	121.07	111.48
26	8	601	CHL	C1C-CHC-C4B	4.43	131.93	116.07
30	F	5002	LHG	O7-C7-C8	4.43	121.06	111.48
26	8	604	CHL	C1C-CHC-C4B	4.43	131.91	116.07
43	5	505	LUT	C35-C34-C33	-4.43	121.07	127.28
30	A	5001	LHG	O7-C7-C8	4.42	121.05	111.48
30	9	802	LHG	O7-C7-C8	4.42	121.05	111.48
26	7	611	CHL	C1C-CHC-C4B	4.42	131.89	116.07
26	8	603	CHL	C1C-CHC-C4B	4.41	131.86	116.07
25	2	621	CLA	C1-C2-C3	-4.40	118.98	126.20
25	5	615	CLA	O2D-CGD-CBD	4.40	118.92	111.23
43	a	503	LUT	C15-C14-C13	-4.40	121.11	127.28
26	3	603	CHL	C1C-CHC-C4B	4.40	131.80	116.07
25	A	1127	CLA	C1-C2-C3	-4.39	119.00	126.20
43	2	502	LUT	C21-C26-C27	4.39	117.87	112.83
26	2	613	CHL	C1C-CHC-C4B	4.38	131.74	116.07
30	5	801	LHG	O7-C7-C8	4.37	120.94	111.48
25	1	605	CLA	O2A-C1-C2	4.37	124.92	108.11
25	3	605	CLA	C1-C2-C3	-4.36	119.05	126.20
25	2	604	CLA	O2A-C1-C2	4.36	124.90	108.11
43	4	502	LUT	C35-C34-C33	-4.36	121.16	127.28
25	7	603	CLA	C1-C2-C3	-4.36	119.05	126.20
24	A	1011	CL0	O2A-CGA-CBA	4.36	125.12	111.83
44	7	504	AXT	C19-C9-C10	-4.35	115.76	122.82
25	4	601	CLA	C1-C2-C3	-4.35	119.07	126.20
46	a	504	QTB	C17-C11-C10	4.33	120.14	113.07
44	7	504	AXT	C8-C7-C6	4.32	138.55	127.00
25	8	606	CLA	C1-C2-C3	-4.32	119.12	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	801	LHG	O7-C7-C8	4.32	120.82	111.48
29	L	4002	BCR	C33-C5-C6	-4.31	119.78	124.48
25	A	1130	CLA	C1-C2-C3	-4.31	119.14	126.20
29	3	503	BCR	C33-C5-C6	-4.29	119.80	124.48
40	3	506	RRX	C19-C18-C17	4.28	125.74	119.01
25	H	1703	CLA	C1-C2-C3	-4.28	119.19	126.20
46	a	504	QTB	C19-C17-C11	-4.28	104.56	110.58
43	a	501	LUT	C35-C34-C33	-4.27	121.28	127.28
26	A	1114	CHL	C1-O2A-CGA	4.27	126.99	116.65
40	3	506	RRX	C1-C6-C5	-4.27	116.81	122.64
30	B	5002	LHG	O7-C7-C8	4.26	120.71	111.48
42	M	4001	ECH	C24-C23-C22	-4.26	119.93	126.23
43	1	501	LUT	C21-C26-C27	4.26	117.72	112.83
42	M	4001	ECH	C16-C17-C18	-4.26	121.30	127.28
25	A	1128	CLA	C1-C2-C3	-4.26	119.22	126.20
25	B	1220	CLA	O2D-CGD-CBD	4.26	118.67	111.23
30	F	5001	LHG	O7-C7-C8	4.26	120.69	111.48
43	a	502	LUT	C7-C8-C9	-4.26	119.94	126.23
43	5	501	LUT	C21-C26-C27	4.25	117.71	112.83
53	8	810	LAP	O7-P9-O5	4.25	132.22	112.44
24	A	1011	CL0	CHA-C1A-C2A	-4.25	123.33	133.31
29	G	4001	BCR	C33-C5-C6	-4.25	119.85	124.48
40	3	506	RRX	C38-C26-C25	-4.25	119.85	124.48
33	7	804	PTY	O7-C8-C11	4.24	120.65	111.48
25	B	1234	CLA	C3D-C4D-ND	4.24	113.14	107.71
25	A	1136	CLA	C1-C2-C3	-4.23	119.26	126.20
39	F	4001	NEX	C26-C27-C28	-4.23	117.05	125.99
25	8	605	CLA	C1-C2-C3	-4.22	119.29	126.20
43	6	502	LUT	C26-C27-C28	-4.21	118.02	124.58
29	8	503	BCR	C33-C5-C6	-4.21	119.89	124.48
25	B	1229	CLA	C1-C2-C3	-4.21	119.30	126.20
26	5	613	CHL	C3D-C4D-CHA	4.20	114.93	108.54
26	4	618	CHL	C3D-C4D-CHA	4.20	114.93	108.54
43	1	501	LUT	C35-C34-C33	-4.19	121.39	127.28
26	2	613	CHL	C3D-C4D-CHA	4.19	114.92	108.54
24	A	1011	CL0	C1-C2-C3	-4.19	119.33	126.20
43	9	501	LUT	C18-C5-C6	-4.18	119.92	124.48
26	1	609	CHL	C3D-C4D-CHA	4.18	114.89	108.54
29	L	4003	BCR	C33-C5-C6	-4.18	119.93	124.48
25	a	601	CLA	C1-C2-C3	-4.17	119.36	126.20
29	7	503	BCR	C33-C5-C6	-4.17	119.93	124.48
25	B	1204	CLA	C1-C2-C3	-4.17	119.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	615	CLA	C1-C2-C3	-4.17	119.37	126.20
37	B	5004	PCW	O2-C31-C32	4.16	120.49	111.48
26	5	610	CHL	C3D-C4D-CHA	4.16	114.87	108.54
25	7	604	CLA	C1-C2-C3	-4.16	119.39	126.20
43	5	502	LUT	C26-C27-C28	-4.15	118.12	124.58
25	A	1112	CLA	C1-C2-C3	-4.15	119.39	126.20
26	8	603	CHL	C3D-C4D-CHA	4.15	114.85	108.54
26	6	617	CHL	C3D-C4D-CHA	4.15	114.84	108.54
30	6	801	LHG	O7-C7-C8	4.14	120.45	111.48
26	7	609	CHL	C3D-C4D-CHA	4.14	114.84	108.54
26	6	610	CHL	C3D-C4D-CHA	4.14	114.83	108.54
40	J	4002	RRX	C4-C5-C6	-4.14	117.11	122.70
25	B	1224	CLA	C1-C2-C3	-4.14	119.42	126.20
26	3	603	CHL	C3D-C4D-CHA	4.14	114.83	108.54
26	6	609	CHL	C3D-C4D-CHA	4.13	114.82	108.54
43	2	507	LUT	C27-C28-C29	-4.13	117.44	126.32
26	6	611	CHL	C3D-C4D-CHA	4.13	114.81	108.54
26	7	615	CHL	C3D-C4D-CHA	4.13	114.81	108.54
26	9	608	CHL	C3D-C4D-CHA	4.12	114.81	108.54
25	7	606	CLA	C1-C2-C3	-4.12	119.44	126.20
26	5	611	CHL	C3D-C4D-CHA	4.12	114.80	108.54
26	5	618	CHL	C3D-C4D-CHA	4.12	114.80	108.54
26	1	611	CHL	C3D-C4D-CHA	4.12	114.80	108.54
26	7	611	CHL	C3D-C4D-CHA	4.12	114.80	108.54
25	B	1238	CLA	O2A-C1-C2	4.12	123.95	108.11
26	a	613	CHL	C3D-C4D-CHA	4.12	114.80	108.54
50	7	502	XAT	C15-C14-C13	-4.12	121.51	127.28
37	6	803	PCW	O2-C31-C32	4.12	120.38	111.48
33	9	803	PTY	O7-C8-C11	4.11	120.37	111.48
43	4	501	LUT	C7-C8-C9	-4.11	120.16	126.23
29	B	4002	BCR	C33-C5-C6	-4.11	120.00	124.48
43	1	503	LUT	C10-C11-C12	-4.10	111.31	123.20
26	a	606	CHL	C3D-C4D-CHA	4.10	114.78	108.54
26	2	609	CHL	C3D-C4D-CHA	4.10	114.78	108.54
48	3	803	DGA	OG2-CB1-CB2	4.10	120.35	111.48
43	2	502	LUT	C26-C27-C28	-4.10	118.20	124.58
25	B	1214	CLA	O2A-C1-C2	4.10	123.88	108.11
43	a	501	LUT	C21-C26-C27	4.10	117.54	112.83
25	A	1137	CLA	O2A-C1-C2	4.10	123.87	108.11
25	3	606	CLA	C1-C2-C3	-4.09	119.49	126.20
30	9	801	LHG	O7-C7-C8	4.09	120.33	111.48
43	4	502	LUT	C7-C8-C9	-4.09	120.19	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	613	CHL	C3D-C4D-CHA	4.09	114.75	108.54
26	8	610	CHL	C3D-C4D-CHA	4.09	114.75	108.54
26	a	609	CHL	C3D-C4D-CHA	4.08	114.75	108.54
26	7	617	CHL	C3D-C4D-CHA	4.08	114.73	108.54
52	8	805	P5S	O37-C38-C39	4.07	120.29	111.48
26	a	610	CHL	C3D-C4D-CHA	4.07	114.73	108.54
51	7	807	4RF	O21-C22-C24	4.07	120.29	111.48
26	A	1114	CHL	C3D-C4D-CHA	4.07	114.73	108.54
25	A	1109	CLA	C1-C2-C3	-4.07	119.53	126.20
34	A	5007	3PH	O21-C21-C22	4.07	120.28	111.48
26	3	611	CHL	C3D-C4D-CHA	4.06	114.71	108.54
26	5	617	CHL	C3D-C4D-CHA	4.06	114.71	108.54
25	5	601	CLA	C1-C2-C3	-4.06	119.55	126.20
46	a	504	QTB	C10-C09-C02	-4.05	117.60	126.32
43	2	502	LUT	C15-C14-C13	-4.05	121.59	127.28
26	2	610	CHL	C3D-C4D-CHA	4.05	114.70	108.54
26	1	610	CHL	C3D-C4D-CHA	4.05	114.69	108.54
25	B	1201	CLA	C1-C2-C3	-4.05	119.56	126.20
26	6	619	CHL	C3D-C4D-CHA	4.04	114.69	108.54
30	7	803	LHG	O7-C7-C8	4.04	120.23	111.48
25	A	1131	CLA	C1-C2-C3	-4.04	119.57	126.20
30	8	801	LHG	O7-C7-C8	4.04	120.23	111.48
26	4	613	CHL	C3D-C4D-CHA	4.04	114.68	108.54
25	B	1228	CLA	O2A-C1-C2	4.04	123.65	108.11
26	8	601	CHL	C3D-C4D-CHA	4.04	114.68	108.54
25	1	606	CLA	C1-C2-C3	-4.04	119.58	126.20
50	2	501	XAT	C15-C14-C13	-4.04	121.62	127.28
25	3	612	CLA	C1-C2-C3	-4.04	120.23	126.76
29	6	504	BCR	C33-C5-C6	-4.04	120.08	124.48
25	A	1012	CLA	O2A-C1-C2	4.03	123.63	108.11
30	1	801	LHG	O7-C7-C8	4.03	120.19	111.48
26	3	604	CHL	C3D-C4D-CHA	4.02	114.66	108.54
25	L	1502	CLA	O2A-C1-C2	4.02	123.57	108.11
33	J	5001	PTY	O7-C8-C11	4.01	120.16	111.48
25	A	1108	CLA	C1-C2-C3	-4.01	119.63	126.20
26	8	604	CHL	C3D-C4D-CHA	4.01	114.63	108.54
26	9	610	CHL	C3D-C4D-CHA	4.01	114.63	108.54
25	3	601	CLA	O2A-C1-C2	4.00	123.52	108.11
26	9	603	CHL	C3D-C4D-CHA	4.00	114.62	108.54
26	1	613	CHL	C3D-C4D-CHA	4.00	114.62	108.54
29	A	4003	BCR	C28-C27-C26	-4.00	106.93	114.06
40	J	4002	RRX	C38-C26-C25	-4.00	120.12	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	M	4001	ECH	C33-C5-C6	-4.00	120.12	124.48
25	A	1140	CLA	C1-C2-C3	-3.99	119.65	126.20
33	B	5005	PTY	O7-C8-C11	3.99	120.11	111.48
25	L	1504	CLA	C1-C2-C3	-3.98	120.31	126.76
43	4	502	LUT	C21-C26-C27	3.98	117.41	112.83
37	K	5001	PCW	O2-C31-C32	3.98	120.10	111.48
25	B	1209	CLA	O2A-C1-C2	3.98	123.43	108.11
25	A	1138	CLA	O2D-CGD-CBD	3.98	118.19	111.23
43	8	502	LUT	C35-C34-C33	-3.98	121.70	127.28
31	A	5004	LMG	O7-C10-C11	3.98	120.08	111.48
25	2	601	CLA	C1-C2-C3	-3.97	119.69	126.20
25	F	1301	CLA	C1-C2-C3	-3.97	120.33	126.76
43	8	501	LUT	C21-C26-C27	3.97	117.39	112.83
36	8	802	DGD	O2G-C1B-C2B	3.97	120.07	111.48
29	5	503	BCR	C33-C5-C6	-3.97	120.16	124.48
25	2	612	CLA	C1-C2-C3	-3.97	120.35	126.76
25	8	608	CLA	C1-C2-C3	-3.96	119.70	126.20
26	8	613	CHL	C3D-C4D-CHA	3.96	114.56	108.54
25	B	1203	CLA	C1-C2-C3	-3.96	119.71	126.20
26	9	601	CHL	C3D-C4D-CHA	3.96	114.56	108.54
43	9	502	LUT	C26-C27-C28	-3.96	118.42	124.58
30	4	802	LHG	O7-C7-C8	3.95	120.04	111.48
48	5	803	DGA	OG2-CB1-CB2	3.95	120.02	111.48
33	G	5002	PTY	O7-C8-C11	3.95	120.02	111.48
25	2	601	CLA	C1-O2A-CGA	3.94	126.20	116.65
25	B	1218	CLA	C1-C2-C3	-3.94	119.74	126.20
43	2	502	LUT	C7-C8-C9	-3.94	120.40	126.23
26	1	604	CHL	C3D-C4D-CHA	3.94	114.53	108.54
26	4	609	CHL	C3D-C4D-CHA	3.94	114.53	108.54
25	B	1222	CLA	C1-C2-C3	-3.94	119.75	126.20
26	1	604	CHL	CHA-C1A-C2A	-3.94	124.06	133.31
25	K	1402	CLA	C1-C2-C3	-3.93	119.75	126.20
36	B	5003	DGD	O2G-C1B-C2B	3.93	119.98	111.48
25	A	1109	CLA	O2A-C1-C2	3.93	123.22	108.11
26	3	608	CHL	CHA-C1A-C2A	-3.93	124.09	133.31
30	A	5002	LHG	O7-C7-C8	3.92	119.97	111.48
25	A	1130	CLA	O2A-C1-C2	3.92	123.21	108.11
25	6	606	CLA	C1-C2-C3	-3.92	119.77	126.20
25	A	1134	CLA	C1-C2-C3	-3.92	119.77	126.20
25	8	611	CLA	C1-C2-C3	-3.92	120.42	126.76
29	B	4007	BCR	C33-C5-C6	-3.92	120.21	124.48
25	G	1601	CLA	C1-C2-C3	-3.92	120.42	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1116	CLA	C1-C2-C3	-3.92	119.78	126.20
29	6	504	BCR	C15-C14-C13	-3.92	121.78	127.28
50	7	502	XAT	O4-C5-C18	-3.91	110.67	115.05
25	A	1119	CLA	O2A-C1-C2	3.91	123.17	108.11
24	A	1011	CL0	C1C-CHC-C4B	3.91	130.07	116.07
25	B	1216	CLA	O2A-C1-C2	3.91	123.16	108.11
29	I	4001	BCR	C27-C26-C25	-3.91	117.42	122.70
25	2	621	CLA	O2A-C1-C2	3.90	123.13	108.11
43	6	501	LUT	C18-C5-C6	-3.90	120.23	124.48
25	4	616	CLA	C1-C2-C3	-3.90	120.45	126.76
25	a	603	CLA	O2A-C1-C2	3.90	123.12	108.11
30	1	802	LHG	O7-C7-C8	3.90	119.92	111.48
25	B	1023	CLA	O2A-C1-C2	3.90	123.10	108.11
26	3	608	CHL	C3D-C4D-CHA	3.90	114.46	108.54
48	2	803	DGA	OG2-CB1-CB2	3.89	119.91	111.48
30	3	801	LHG	O7-C7-C8	3.89	119.90	111.48
43	6	502	LUT	C35-C34-C33	-3.89	121.82	127.28
25	3	616	CLA	C1-C2-C3	-3.89	119.82	126.20
48	2	803	DGA	CDB-CCB-CBB	-3.89	81.15	115.25
40	J	4002	RRX	C33-C5-C6	-3.89	120.24	124.48
26	6	619	CHL	CHA-C1A-C2A	-3.89	124.18	133.31
25	K	1402	CLA	O2A-C1-C2	3.89	123.07	108.11
25	B	1225	CLA	O2A-C1-C2	3.89	123.06	108.11
43	5	501	LUT	C18-C5-C6	-3.88	120.25	124.48
48	8	804	DGA	OG2-CB1-CB2	3.88	119.88	111.48
25	A	1135	CLA	C1-C2-C3	-3.88	119.84	126.20
33	G	5003	PTY	O7-C8-C11	3.88	119.87	111.48
43	a	503	LUT	C18-C5-C6	-3.88	120.25	124.48
25	H	1703	CLA	O2A-C1-C2	3.88	123.03	108.11
25	A	1111	CLA	C1-C2-C3	-3.88	119.85	126.20
26	8	604	CHL	CHA-C1A-C2A	-3.87	124.21	133.31
25	B	1209	CLA	C1-C2-C3	-3.87	119.85	126.20
25	F	1302	CLA	C1-C2-C3	-3.87	119.85	126.20
26	a	604	CHL	C3D-C4D-CHA	3.87	114.42	108.54
25	A	1119	CLA	C1-C2-C3	-3.87	119.86	126.20
43	4	502	LUT	C26-C27-C28	-3.87	118.56	124.58
43	4	501	LUT	C18-C5-C6	-3.87	120.26	124.48
43	3	502	LUT	C15-C14-C13	-3.86	121.86	127.28
43	4	502	LUT	C18-C5-C6	-3.86	120.27	124.48
25	A	1104	CLA	C1-C2-C3	-3.86	119.87	126.20
25	a	603	CLA	C1-C2-C3	-3.86	119.87	126.20
40	3	506	RRX	C30-C25-C26	-3.86	117.37	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	613	CHL	CHA-C1A-C2A	-3.85	124.27	133.31
30	a	801	LHG	O7-C7-C8	3.85	119.81	111.48
25	7	601	CLA	C1-C2-C3	-3.85	119.89	126.20
43	7	501	LUT	C35-C34-C33	-3.85	121.88	127.28
25	B	1227	CLA	O2A-C1-C2	3.85	122.91	108.11
25	O	1802	CLA	O2A-C1-C2	3.84	122.89	108.11
25	A	1112	CLA	O2A-C1-C2	3.84	122.87	108.11
30	A	5003	LHG	O7-C7-C8	3.83	119.78	111.48
30	7	801	LHG	O7-C7-C8	3.83	119.78	111.48
43	9	502	LUT	C21-C26-C27	3.83	117.23	112.83
33	a	802	PTY	O7-C8-C11	3.83	119.76	111.48
43	a	502	LUT	C35-C34-C33	-3.82	121.91	127.28
25	a	601	CLA	O2A-C1-C2	3.82	122.82	108.11
25	A	1115	CLA	O2A-C1-C2	3.82	122.82	108.11
29	A	4005	BCR	C23-C24-C25	-3.82	116.79	127.00
25	B	1208	CLA	O2A-C1-C2	3.82	122.81	108.11
50	9	507	XAT	C18-C5-C4	3.82	118.53	114.24
25	B	1235	CLA	O2A-C1-C2	3.82	122.80	108.11
25	B	1240	CLA	O2A-C1-C2	3.82	122.80	108.11
26	9	601	CHL	CHA-C1A-C2A	-3.82	124.34	133.31
25	8	602	CLA	C1-C2-C3	-3.82	119.94	126.20
25	2	605	CLA	O2A-C1-C2	3.81	122.79	108.11
25	B	1240	CLA	C1-C2-C3	-3.81	119.95	126.20
26	6	613	CHL	C3D-C4D-CHA	3.81	114.33	108.54
25	A	1136	CLA	O2A-C1-C2	3.81	122.76	108.11
33	A	5006	PTY	O7-C8-C11	3.81	119.71	111.48
43	8	501	LUT	C18-C5-C6	-3.80	120.34	124.48
25	5	603	CLA	O2A-C1-C2	3.80	122.73	108.11
25	A	1013	CLA	O2A-C1-C2	3.80	122.72	108.11
25	5	606	CLA	O2A-C1-C2	3.80	122.72	108.11
29	A	4003	BCR	C33-C5-C6	-3.80	120.34	124.48
26	A	1114	CHL	CHA-C1A-C2A	-3.79	124.40	133.31
25	B	1220	CLA	C1-C2-C3	-3.79	119.98	126.20
25	A	1128	CLA	O2A-C1-C2	3.79	122.70	108.11
33	3	802	PTY	O7-C8-C11	3.79	119.68	111.48
25	A	1125	CLA	O2A-C1-C2	3.79	122.69	108.11
25	2	602	CLA	O2A-C1-C2	3.78	122.66	108.11
25	4	606	CLA	C1-C2-C3	-3.78	120.65	126.76
25	3	605	CLA	O2A-C1-C2	3.78	122.64	108.11
25	1	606	CLA	O2A-C1-C2	3.77	122.63	108.11
29	A	4004	BCR	C23-C24-C25	-3.77	116.93	127.00
44	7	504	AXT	C11-C10-C9	-3.77	122.00	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	611	CHL	CHA-C1A-C2A	-3.77	124.46	133.31
26	3	604	CHL	CHA-C1A-C2A	-3.77	124.47	133.31
30	4	801	LHG	O7-C7-C8	3.76	119.62	111.48
43	6	501	LUT	C35-C34-C33	-3.76	122.00	127.28
25	B	1211	CLA	C1-C2-C3	-3.76	120.03	126.20
25	A	1117	CLA	C1-C2-C3	-3.76	120.03	126.20
25	7	610	CLA	O2A-C1-C2	3.76	122.58	108.11
26	4	609	CHL	CHA-C1A-C2A	-3.76	124.48	133.31
25	L	1501	CLA	C1-C2-C3	-3.76	120.68	126.76
26	7	613	CHL	C3D-C4D-CHA	3.76	114.25	108.54
33	a	803	PTY	O7-C8-C11	3.76	119.61	111.48
43	1	501	LUT	C15-C14-C13	-3.75	122.01	127.28
25	F	1302	CLA	O2A-C1-C2	3.75	122.54	108.11
26	6	609	CHL	CHA-C1A-C2A	-3.75	124.50	133.31
25	B	1201	CLA	O2A-C1-C2	3.75	122.54	108.11
26	a	606	CHL	CHA-C1A-C2A	-3.75	124.51	133.31
26	3	603	CHL	CHA-C1A-C2A	-3.75	124.51	133.31
25	A	1135	CLA	O2A-C1-C2	3.75	122.52	108.11
25	L	1502	CLA	C1-C2-C3	-3.74	120.06	126.20
43	5	501	LUT	C35-C34-C33	-3.74	122.03	127.28
25	A	1133	CLA	O2A-C1-C2	3.74	122.51	108.11
25	B	1225	CLA	C1-C2-C3	-3.74	120.07	126.20
25	3	606	CLA	O2A-C1-C2	3.74	122.49	108.11
25	7	601	CLA	O2A-C1-C2	3.74	122.49	108.11
25	7	606	CLA	O2A-C1-C2	3.73	122.48	108.11
25	9	607	CLA	O2A-C1-C2	3.73	121.79	108.40
25	B	1212	CLA	O2A-C1-C2	3.73	122.46	108.11
43	7	501	LUT	C18-C5-C6	-3.73	120.42	124.48
26	9	610	CHL	CHA-C1A-C2A	-3.72	124.57	133.31
44	1	502	AXT	C8-C9-C10	3.72	124.86	119.01
29	A	4004	BCR	C33-C5-C6	-3.72	120.43	124.48
43	1	501	LUT	C18-C5-C6	-3.72	120.43	124.48
25	6	601	CLA	C1-C2-C3	-3.72	120.11	126.20
25	A	1132	CLA	O2A-C1-C2	3.71	122.40	108.11
25	4	615	CLA	O2A-C1-C2	3.71	122.40	108.11
29	O	4001	BCR	C33-C5-C6	-3.71	120.43	124.48
25	B	1234	CLA	O2A-C1-C2	3.71	122.38	108.11
43	5	502	LUT	C7-C8-C9	-3.71	120.75	126.23
25	A	1117	CLA	O2A-C1-C2	3.70	122.36	108.11
29	6	503	BCR	C33-C5-C6	-3.70	120.44	124.48
25	F	1301	CLA	O2A-C1-C2	3.70	122.35	108.11
29	B	4001	BCR	C33-C5-C6	-3.70	120.44	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	607	CLA	C1-C2-C3	-3.70	120.13	126.20
25	B	1211	CLA	O2A-C1-C2	3.70	122.35	108.11
25	4	604	CLA	C1-C2-C3	-3.70	120.13	126.20
25	B	1218	CLA	O2A-C1-C2	3.70	122.35	108.11
25	6	603	CLA	C1-C2-C3	-3.70	120.14	126.20
37	K	5002	PCW	O2-C31-C32	3.70	119.48	111.48
43	6	502	LUT	C18-C5-C6	-3.70	120.45	124.48
25	6	612	CLA	C1-C2-C3	-3.69	120.79	126.76
43	1	503	LUT	C27-C28-C29	-3.69	118.39	126.32
26	a	604	CHL	CHA-C1A-C2A	-3.69	124.64	133.31
25	A	1129	CLA	C1-C2-C3	-3.69	120.79	126.76
25	A	1123	CLA	C1-C2-C3	-3.69	120.15	126.20
43	9	501	LUT	C35-C34-C33	-3.69	122.11	127.28
50	9	504	XAT	O24-C25-C24	3.69	116.95	113.49
25	A	1106	CLA	C1-C2-C3	-3.69	120.16	126.20
25	4	611	CLA	O2A-C1-C2	3.68	122.29	108.11
25	4	601	CLA	O2A-C1-C2	3.68	122.27	108.11
25	6	604	CLA	C1-C2-C3	-3.68	120.17	126.20
25	3	613	CLA	C1-C2-C3	-3.68	120.17	126.20
29	B	4005	BCR	C33-C5-C6	-3.67	120.48	124.48
25	2	603	CLA	O2A-C1-C2	3.66	122.21	108.11
25	4	607	CLA	O2A-C1-C2	3.66	122.20	108.11
26	2	609	CHL	CHA-C1A-C2A	-3.66	124.71	133.31
25	5	602	CLA	O2A-C1-C2	3.66	122.20	108.11
25	8	618	CLA	C1-C2-C3	-3.66	120.20	126.20
50	7	502	XAT	C7-C8-C9	-3.66	119.85	125.53
26	8	610	CHL	C1A-CHA-C4D	3.66	125.09	118.98
25	A	1134	CLA	O2A-C1-C2	3.66	122.19	108.11
25	G	1602	CLA	O2A-C1-C2	3.66	122.19	108.11
25	1	612	CLA	O2A-C1-C2	3.66	122.18	108.11
25	A	1121	CLA	O2A-C1-C2	3.66	122.18	108.11
26	9	603	CHL	CHA-C1A-C2A	-3.66	124.72	133.31
26	8	603	CHL	CHA-C1A-C2A	-3.66	124.72	133.31
25	B	1206	CLA	O2A-C1-C2	3.65	122.17	108.11
25	a	605	CLA	C1-C2-C3	-3.65	120.21	126.20
25	O	1801	CLA	C3A-C2A-C1A	-3.65	102.57	106.30
25	2	603	CLA	C1-C2-C3	-3.65	120.22	126.20
25	a	608	CLA	O2A-C1-C2	3.65	122.15	108.11
50	9	504	XAT	C7-C8-C9	-3.65	119.87	125.53
43	3	501	LUT	C35-C34-C33	-3.65	122.17	127.28
26	2	610	CHL	CHA-C1A-C2A	-3.64	124.75	133.31
25	8	609	CLA	O2A-C1-C2	3.64	122.13	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	601	CLA	C1-C2-C3	-3.64	120.23	126.20
43	6	501	LUT	C26-C27-C28	-3.64	118.91	124.58
25	B	1212	CLA	C1-C2-C3	-3.64	120.23	126.20
25	5	604	CLA	C1-C2-C3	-3.64	120.23	126.20
26	6	610	CHL	CHA-C1A-C2A	-3.64	124.76	133.31
25	A	1113	CLA	O2A-C1-C2	3.64	122.11	108.11
25	3	616	CLA	O2A-C1-C2	3.64	122.11	108.11
44	7	504	AXT	C39-C29-C30	-3.64	116.93	122.82
29	I	4001	BCR	C33-C5-C6	-3.63	120.52	124.48
25	B	1223	CLA	C1-C2-C3	-3.63	120.24	126.20
25	A	1140	CLA	O2A-C1-C2	3.63	122.09	108.11
26	3	608	CHL	C1A-CHA-C4D	3.63	125.04	118.98
26	1	610	CHL	C1A-CHA-C4D	3.63	125.04	118.98
43	5	502	LUT	C35-C34-C33	-3.63	122.19	127.28
25	B	1204	CLA	O2A-C1-C2	3.63	122.07	108.11
44	1	502	AXT	C39-C29-C30	-3.63	116.94	122.82
26	7	615	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
26	6	613	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
30	B	5001	LHG	O7-C7-C8	3.63	119.33	111.48
25	a	607	CLA	C1-C2-C3	-3.63	120.25	126.20
26	1	613	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
25	O	1802	CLA	C1-C2-C3	-3.63	120.26	126.20
25	5	607	CLA	O2A-C1-C2	3.63	122.06	108.11
25	a	607	CLA	O2A-C1-C2	3.62	122.06	108.11
43	9	502	LUT	C18-C5-C6	-3.62	120.53	124.48
29	H	4001	BCR	C4-C5-C6	-3.62	117.82	122.70
26	a	610	CHL	CHA-C1A-C2A	-3.62	124.82	133.31
25	6	601	CLA	O2A-C1-C2	3.61	122.02	108.11
26	5	610	CHL	C1-C2-C3	-3.61	120.28	126.20
25	B	1239	CLA	O2A-C1-C2	3.61	122.01	108.11
25	A	1127	CLA	O2A-C1-C2	3.61	122.00	108.11
25	A	1105	CLA	O2A-C1-C2	3.61	121.99	108.11
43	9	501	LUT	C7-C8-C9	-3.61	120.90	126.23
50	9	507	XAT	C26-C27-C28	-3.60	118.37	125.99
25	2	604	CLA	C1-C2-C3	-3.60	120.29	126.20
25	B	1224	CLA	O2A-C1-C2	3.60	121.98	108.11
29	7	503	BCR	C37-C22-C23	3.60	123.59	118.09
25	B	1234	CLA	C1-C2-C3	-3.60	120.29	126.20
30	7	802	LHG	O7-C7-C8	3.60	119.27	111.48
25	B	1208	CLA	C1-C2-C3	-3.60	120.30	126.20
25	A	1102	CLA	C1-C2-C3	-3.60	120.30	126.20
25	9	604	CLA	C1-C2-C3	-3.60	120.30	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1122	CLA	O2A-C1-C2	3.60	121.96	108.11
25	3	613	CLA	O2A-C1-C2	3.60	121.94	108.11
44	7	504	AXT	C32-C33-C34	3.60	124.66	119.01
43	3	501	LUT	C18-C5-C6	-3.59	120.56	124.48
25	B	1022	CLA	O2A-C1-C2	3.59	121.94	108.11
25	B	1213	CLA	O2A-C1-C2	3.59	121.92	108.11
25	8	608	CLA	O2A-C1-C2	3.59	121.92	108.11
25	A	1125	CLA	C1-C2-C3	-3.59	120.32	126.20
25	H	1701	CLA	C1-C2-C3	-3.58	120.33	126.20
25	A	1106	CLA	O2A-C1-C2	3.58	121.89	108.11
26	4	613	CHL	CHA-C1A-C2A	-3.58	124.90	133.31
25	8	606	CLA	O2A-C1-C2	3.58	121.88	108.11
25	6	615	CLA	O2A-C1-C2	3.58	121.88	108.11
25	B	1220	CLA	O2A-C1-C2	3.58	121.87	108.11
25	7	610	CLA	C1-C2-C3	-3.58	120.34	126.20
26	1	610	CHL	CHA-C1A-C2A	-3.58	124.91	133.31
25	5	601	CLA	O2A-C1-C2	3.58	121.87	108.11
25	B	1219	CLA	O2A-C1-C2	3.58	121.87	108.11
25	A	1138	CLA	C1-C2-C3	-3.57	120.34	126.20
26	9	608	CHL	CHA-C1A-C2A	-3.57	124.91	133.31
40	J	4002	RRX	C11-C12-C13	-3.57	116.56	126.36
43	5	502	LUT	C18-C5-C6	-3.57	120.58	124.48
25	B	1203	CLA	O2A-C1-C2	3.57	121.85	108.11
25	3	601	CLA	C1-C2-C3	-3.57	120.34	126.20
25	G	1601	CLA	O2A-C1-C2	3.57	121.85	108.11
29	5	503	BCR	C23-C24-C25	-3.57	117.46	127.00
25	B	1213	CLA	C1-C2-C3	-3.57	120.35	126.20
25	4	608	CLA	O2A-C1-C2	3.57	121.84	108.11
26	5	617	CHL	CHA-C1A-C2A	-3.57	124.93	133.31
29	B	4003	BCR	C33-C5-C6	-3.57	120.59	124.48
44	1	502	AXT	C40-C33-C34	-3.57	117.04	122.82
25	A	1132	CLA	C1-C2-C3	-3.57	120.36	126.20
43	8	502	LUT	C18-C5-C6	-3.57	120.59	124.48
25	A	1111	CLA	O2A-C1-C2	3.56	121.82	108.11
29	L	4001	BCR	C33-C5-C6	-3.56	120.60	124.48
25	A	1122	CLA	C1-C2-C3	-3.56	120.36	126.20
25	1	608	CLA	O2A-C1-C2	3.56	121.82	108.11
29	B	4007	BCR	C23-C24-C25	-3.56	117.48	127.00
26	7	611	CHL	CHA-C1A-C2A	-3.56	124.94	133.31
25	7	608	CLA	C1-C2-C3	-3.56	120.36	126.20
24	A	1011	CL0	CBC-CAC-C3C	-3.55	107.78	112.87
26	1	611	CHL	CHA-C1A-C2A	-3.55	124.97	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	601	CLA	O2A-C1-C2	3.55	121.77	108.11
25	L	1504	CLA	O2A-C1-C2	3.55	121.76	108.11
25	B	1229	CLA	O2A-C1-C2	3.55	121.76	108.11
25	B	1206	CLA	C1-C2-C3	-3.55	120.39	126.20
25	a	612	CLA	O2A-C1-C2	3.55	121.75	108.11
25	L	1501	CLA	O2A-C1-C2	3.54	121.75	108.11
29	A	4004	BCR	C27-C26-C25	-3.54	117.92	122.70
25	A	1104	CLA	O2A-C1-C2	3.54	121.74	108.11
25	B	1230	CLA	O2A-C1-C2	3.54	121.73	108.11
25	4	604	CLA	O2A-C1-C2	3.54	121.73	108.11
25	4	608	CLA	C1-C2-C3	-3.53	120.41	126.20
25	B	1205	CLA	O2A-C1-C2	3.53	121.71	108.11
26	5	611	CHL	CHA-C1A-C2A	-3.53	125.01	133.31
25	4	611	CLA	C1-C2-C3	-3.53	120.41	126.20
25	4	606	CLA	O2A-C1-C2	3.53	121.70	108.11
25	6	602	CLA	O2A-C1-C2	3.52	121.67	108.11
25	7	612	CLA	O2A-C1-C2	3.52	121.67	108.11
25	B	1207	CLA	C1-C2-C3	-3.52	120.43	126.20
43	7	501	LUT	C15-C14-C13	-3.52	122.34	127.28
25	6	606	CLA	O2A-C1-C2	3.52	121.66	108.11
25	A	1110	CLA	O2A-C1-C2	3.52	121.65	108.11
43	6	502	LUT	C15-C14-C13	-3.52	122.34	127.28
25	B	1210	CLA	O2A-C1-C2	3.52	121.64	108.11
44	1	502	AXT	C19-C9-C10	-3.52	117.12	122.82
25	A	1131	CLA	O2A-C1-C2	3.52	121.64	108.11
43	9	502	LUT	C35-C34-C33	-3.52	122.35	127.28
25	B	1223	CLA	O2A-C1-C2	3.51	121.63	108.11
26	8	610	CHL	CHA-C1A-C2A	-3.51	125.06	133.31
25	4	616	CLA	O2A-C1-C2	3.51	121.63	108.11
25	B	1219	CLA	C1-C2-C3	-3.51	120.44	126.20
25	5	602	CLA	C1-C2-C3	-3.51	120.44	126.20
43	1	503	LUT	C35-C15-C14	3.51	130.70	123.52
25	2	607	CLA	O2A-C1-C2	3.51	121.61	108.11
25	8	605	CLA	O2A-C1-C2	3.50	121.59	108.11
25	A	1123	CLA	O2A-C1-C2	3.50	121.58	108.11
25	A	1125	CLA	C3B-C4B-NB	-3.50	107.41	110.53
25	B	1021	CLA	O2A-C1-C2	3.50	121.58	108.11
25	a	602	CLA	C1-C2-C3	-3.50	121.10	126.76
29	4	503	BCR	C15-C14-C13	-3.50	122.37	127.28
29	A	4002	BCR	C23-C24-C25	-3.50	117.65	127.00
43	a	502	LUT	C18-C5-C6	-3.50	120.67	124.48
26	a	609	CHL	CHA-C1A-C2A	-3.49	125.10	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	607	CLA	C1-C2-C3	-3.49	120.47	126.20
25	A	1139	CLA	C1-C2-C3	-3.49	120.48	126.20
26	7	609	CHL	CHA-C1A-C2A	-3.49	125.11	133.31
25	A	1139	CLA	O2A-C1-C2	3.49	121.52	108.11
25	A	1115	CLA	C1-C2-C3	-3.49	120.49	126.20
25	H	1701	CLA	O2A-C1-C2	3.48	121.52	108.11
29	G	4001	BCR	C12-C13-C14	3.48	124.49	119.01
43	9	501	LUT	C15-C14-C13	-3.48	122.39	127.28
50	2	501	XAT	C6-C7-C8	-3.48	118.63	125.99
25	B	1222	CLA	O2A-C1-C2	3.48	121.51	108.11
25	4	610	CLA	C1-O2A-CGA	3.48	125.08	116.65
25	4	602	CLA	O2A-C1-C2	3.48	121.50	108.11
25	A	1116	CLA	O2A-C1-C2	3.48	121.49	108.11
43	8	502	LUT	C26-C27-C28	-3.48	119.17	124.58
25	B	1210	CLA	C1-C2-C3	-3.48	120.50	126.20
25	A	1124	CLA	O2A-C1-C2	3.48	121.48	108.11
25	3	612	CLA	O2A-C1-C2	3.48	121.48	108.11
26	6	617	CHL	CHA-C1A-C2A	-3.47	125.15	133.31
29	H	4001	BCR	C1-C6-C5	-3.47	117.89	122.64
25	6	602	CLA	C1-C2-C3	-3.47	120.51	126.20
36	7	806	DGD	O2G-C1B-C2B	3.47	118.99	111.48
44	1	502	AXT	C20-C13-C14	-3.47	117.20	122.82
25	8	612	CLA	O2A-C1-C2	3.47	121.44	108.11
25	2	612	CLA	O2A-C1-C2	3.47	121.44	108.11
26	8	613	CHL	CHA-C1A-C2A	-3.46	125.17	133.31
25	B	1214	CLA	C1-C2-C3	-3.46	120.53	126.20
25	3	610	CLA	O2A-C1-C2	3.46	121.42	108.11
25	A	1107	CLA	O2A-C1-C2	3.46	121.41	108.11
43	9	502	LUT	C15-C14-C13	-3.46	122.43	127.28
24	A	1011	CL0	O2A-C1-C2	3.46	121.41	108.11
26	4	609	CHL	C1-C2-C3	-3.45	120.54	126.20
29	3	505	BCR	C33-C5-C6	-3.45	120.72	124.48
25	A	1103	CLA	O2A-C1-C2	3.45	121.39	108.11
25	a	605	CLA	O2A-C1-C2	3.44	121.36	108.11
26	6	611	CHL	CHA-C1A-C2A	-3.44	125.22	133.31
25	B	1226	CLA	O2A-C1-C2	3.44	121.35	108.11
44	7	504	AXT	C28-C29-C30	3.44	124.42	119.01
25	5	604	CLA	O2A-C1-C2	3.44	121.34	108.11
25	B	1231	CLA	O2A-C1-C2	3.44	121.34	108.11
50	9	504	XAT	C38-C25-C24	3.44	118.10	114.24
40	3	506	RRX	C12-C13-C14	3.44	124.42	119.01
25	1	603	CLA	O2A-C1-C2	3.44	121.33	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	602	CLA	O2A-C1-C2	3.44	121.33	108.11
25	B	1230	CLA	C1-C2-C3	-3.43	120.57	126.20
43	3	502	LUT	C7-C8-C9	-3.43	121.16	126.23
26	8	601	CHL	CHA-C1A-C2A	-3.43	125.25	133.31
25	8	618	CLA	O2A-C1-C2	3.43	121.31	108.11
29	B	4001	BCR	C23-C24-C25	-3.43	117.84	127.00
25	B	1206	CLA	C2C-C1C-NC	3.43	113.58	109.98
25	6	607	CLA	O2A-C1-C2	3.42	121.28	108.11
29	4	503	BCR	C33-C5-C6	-3.42	120.75	124.48
25	A	1124	CLA	C1-C2-C3	-3.42	120.59	126.20
26	7	615	CHL	C1-C2-C3	-3.42	121.23	126.76
25	9	605	CLA	O2A-C1-C2	3.42	121.27	108.11
25	1	607	CLA	O2A-C1-C2	3.42	121.26	108.11
25	A	1118	CLA	O2A-C1-C2	3.42	121.26	108.11
25	a	602	CLA	O2A-C1-C2	3.42	121.25	108.11
25	B	1239	CLA	C1-C2-C3	-3.41	120.61	126.20
25	B	1237	CLA	C1-C2-C3	-3.41	120.61	126.20
43	3	502	LUT	C18-C5-C6	-3.41	120.77	124.48
25	A	1103	CLA	C1-C2-C3	-3.41	120.61	126.20
25	B	1221	CLA	O2A-C1-C2	3.41	121.21	108.11
25	7	604	CLA	O2A-C1-C2	3.41	121.21	108.11
25	B	1222	CLA	CMA-C3A-C4A	3.40	120.92	111.77
25	B	1227	CLA	C1-C2-C3	-3.40	121.26	126.76
26	5	610	CHL	CHA-C1A-C2A	-3.40	125.33	133.31
26	1	609	CHL	CHA-C1A-C2A	-3.40	125.33	133.31
29	K	4002	BCR	C33-C5-C6	-3.39	120.78	124.48
50	2	501	XAT	O4-C6-C7	-3.39	107.16	116.88
25	a	611	CLA	O2A-C1-C2	3.39	121.16	108.11
25	3	610	CLA	C1-C2-C3	-3.39	120.64	126.20
25	B	1237	CLA	O2A-C1-C2	3.39	121.16	108.11
29	5	504	BCR	C28-C27-C26	-3.39	108.02	114.06
25	B	1217	CLA	O2A-C1-C2	3.39	121.14	108.11
25	6	612	CLA	O2A-C1-C2	3.38	121.12	108.11
29	A	4005	BCR	C33-C5-C6	-3.38	120.80	124.48
25	A	1101	CLA	O2A-C1-C2	3.38	121.12	108.11
26	7	617	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
43	5	502	LUT	C15-C14-C13	-3.38	122.54	127.28
25	6	604	CLA	C3B-C4B-NB	-3.38	107.51	110.53
26	9	601	CHL	C1A-CHA-C4D	3.38	124.62	118.98
29	3	504	BCR	C27-C26-C25	-3.38	118.14	122.70
25	7	603	CLA	O2A-C1-C2	3.38	121.11	108.11
43	a	503	LUT	C11-C10-C9	-3.38	122.54	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1	501	LUT	C26-C27-C28	-3.38	119.33	124.58
25	A	1108	CLA	O2A-C1-C2	3.38	121.10	108.11
25	6	607	CLA	C1-C2-C3	-3.37	120.68	126.20
25	2	615	CLA	O2A-C1-C2	3.37	121.07	108.11
25	B	1205	CLA	C1-C2-C3	-3.37	120.68	126.20
25	9	604	CLA	O2A-C1-C2	3.36	121.05	108.11
25	B	1236	CLA	O2A-C1-C2	3.36	121.04	108.11
25	6	608	CLA	O2A-C1-C2	3.36	121.04	108.11
29	A	4001	BCR	C33-C5-C6	-3.36	120.82	124.48
25	6	604	CLA	O2A-C1-C2	3.36	121.03	108.11
26	6	609	CHL	C1A-CHA-C4D	3.36	124.58	118.98
26	9	610	CHL	C1A-CHA-C4D	3.36	124.58	118.98
26	a	604	CHL	C1A-CHA-C4D	3.35	124.58	118.98
44	1	502	AXT	C28-C29-C30	3.35	124.28	119.01
25	7	608	CLA	O2A-C1-C2	3.35	120.99	108.11
25	6	608	CLA	C1-C2-C3	-3.35	120.71	126.20
25	5	609	CLA	O2A-C1-C2	3.34	120.96	108.11
43	8	501	LUT	C7-C8-C9	-3.34	121.30	126.23
26	9	608	CHL	C1A-CHA-C4D	3.33	124.55	118.98
25	B	1202	CLA	O2A-C1-C2	3.33	120.93	108.11
39	F	4001	NEX	C28-C29-C30	3.33	124.25	119.01
25	1	607	CLA	C1-C2-C3	-3.33	120.74	126.20
29	B	4004	BCR	C23-C24-C25	-3.33	118.11	127.00
25	2	605	CLA	C1-C2-C3	-3.33	120.75	126.20
26	9	601	CHL	C1-C2-C3	-3.32	120.75	126.20
26	6	610	CHL	C1A-CHA-C4D	3.32	124.53	118.98
40	3	506	RRX	C36-C18-C17	-3.32	117.44	122.82
29	A	4003	BCR	C27-C26-C25	-3.31	118.22	122.70
25	A	1138	CLA	O2A-C1-C2	3.31	120.85	108.11
26	5	618	CHL	CHA-C1A-C2A	-3.31	125.53	133.31
25	B	1206	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
25	4	615	CLA	C1-C2-C3	-3.31	120.78	126.20
43	2	502	LUT	C18-C5-C6	-3.31	120.88	124.48
25	8	612	CLA	C1-C2-C3	-3.30	121.42	126.76
29	5	504	BCR	C4-C5-C6	-3.30	118.24	122.70
44	1	502	AXT	C32-C33-C34	3.30	124.21	119.01
25	5	612	CLA	O2A-C1-C2	3.30	120.81	108.11
42	M	4001	ECH	C28-C27-C26	-3.30	115.68	118.64
26	1	604	CHL	C3C-C4C-NC	-3.30	106.59	114.65
25	6	615	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	B	1217	CLA	C1-C2-C3	-3.29	120.80	126.20
25	A	1113	CLA	C1-C2-C3	-3.29	120.81	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1022	CLA	C1-C2-C3	-3.29	120.81	126.20
26	5	618	CHL	C1A-CHA-C4D	3.29	124.47	118.98
26	2	609	CHL	C1A-CHA-C4D	3.29	124.46	118.98
26	1	609	CHL	C1-C2-C3	-3.28	120.82	126.20
43	a	501	LUT	C7-C8-C9	-3.28	121.38	126.23
25	B	1022	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	8	611	CLA	O2A-C1-C2	3.28	120.73	108.11
25	A	1129	CLA	O2A-C1-C2	3.28	120.72	108.11
26	8	601	CHL	C3C-C4C-NC	-3.28	106.64	114.65
25	a	603	CLA	CMA-C3A-C4A	3.27	120.58	111.77
25	A	1118	CLA	C1-C2-C3	-3.27	120.83	126.20
44	7	504	AXT	C15-C14-C13	3.27	131.87	127.28
26	3	611	CHL	C3C-C4C-NC	-3.27	106.65	114.65
25	A	1137	CLA	C1-C2-C3	-3.27	120.84	126.20
25	B	1235	CLA	C1-C2-C3	-3.27	120.84	126.20
26	2	613	CHL	CHA-C1A-C2A	-3.27	125.63	133.31
43	a	502	LUT	C26-C27-C28	-3.27	119.50	124.58
29	3	503	BCR	C23-C24-C25	-3.26	118.28	127.00
43	5	501	LUT	C26-C27-C28	-3.26	119.50	124.58
25	9	606	CLA	O2A-C1-C2	3.26	120.66	108.11
25	B	1236	CLA	C1-C2-C3	-3.26	120.86	126.20
25	1	608	CLA	C1-C2-C3	-3.26	120.86	126.20
50	2	501	XAT	O4-C5-C4	-3.26	110.44	113.49
25	A	1102	CLA	O2A-C1-C2	3.25	120.62	108.11
26	5	617	CHL	C3C-C4C-NC	-3.25	106.71	114.65
25	A	1110	CLA	C1-O2A-CGA	3.25	124.51	116.65
25	5	609	CLA	C1-C2-C3	-3.25	120.88	126.20
25	B	1207	CLA	O2A-C1-C2	3.24	120.59	108.11
25	4	603	CLA	C1-C2-C3	-3.24	120.88	126.20
26	7	613	CHL	C3C-C4C-NC	-3.24	106.72	114.65
26	9	601	CHL	C3C-C4C-NC	-3.24	106.73	114.65
35	2	804	LMT	C1'-O5'-C5'	-3.24	107.39	113.72
50	9	507	XAT	C31-C30-C29	-3.24	122.73	127.28
26	1	611	CHL	C3C-C4C-NC	-3.23	106.75	114.65
43	1	503	LUT	C18-C5-C6	-3.23	120.96	124.48
26	5	613	CHL	CHA-C1A-C2A	-3.23	125.72	133.31
26	7	609	CHL	C3C-C4C-NC	-3.23	106.75	114.65
26	5	617	CHL	C1A-CHA-C4D	3.23	124.37	118.98
26	4	609	CHL	C3C-C4C-NC	-3.23	106.76	114.65
26	a	613	CHL	CHA-C1A-C2A	-3.23	125.73	133.31
25	a	608	CLA	C1-C2-C3	-3.23	120.91	126.20
25	5	612	CLA	C1-C2-C3	-3.23	120.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	4002	BCR	C23-C24-C25	-3.23	118.38	127.00
29	G	4001	BCR	C8-C9-C10	3.22	124.08	119.01
25	1	603	CLA	C1-C2-C3	-3.22	120.92	126.20
26	3	611	CHL	C1A-CHA-C4D	3.22	124.35	118.98
29	H	4001	BCR	C33-C5-C4	3.22	120.45	113.60
29	3	504	BCR	C33-C5-C6	-3.21	120.98	124.48
26	3	604	CHL	C3C-C4C-NC	-3.21	106.80	114.65
26	8	603	CHL	C3C-C4C-NC	-3.21	106.81	114.65
26	a	610	CHL	C1A-CHA-C4D	3.21	124.33	118.98
26	a	606	CHL	C1A-CHA-C4D	3.20	124.33	118.98
26	5	611	CHL	C1-C2-C3	-3.20	121.58	126.76
50	7	502	XAT	C26-C27-C28	-3.20	119.22	125.99
25	B	1237	CLA	CMA-C3A-C4A	3.20	120.38	111.77
43	4	502	LUT	C15-C14-C13	-3.20	122.79	127.28
25	9	612	CLA	O2A-C1-C2	3.20	120.42	108.11
39	F	4001	NEX	C38-C25-C24	3.20	117.83	114.24
44	1	502	AXT	C12-C13-C14	3.20	124.04	119.01
42	M	4001	ECH	C23-C24-C25	-3.20	118.46	127.00
26	5	613	CHL	C1A-CHA-C4D	3.20	124.31	118.98
25	4	602	CLA	C1-C2-C3	-3.20	120.96	126.20
26	5	611	CHL	C3C-C4C-NC	-3.19	106.84	114.65
26	6	609	CHL	C3C-C4C-NC	-3.19	106.85	114.65
26	a	609	CHL	C3C-C4C-NC	-3.19	106.85	114.65
26	9	613	CHL	C1A-CHA-C4D	3.19	124.30	118.98
26	a	604	CHL	C3C-C4C-NC	-3.19	106.86	114.65
50	9	507	XAT	O4-C5-C4	-3.19	110.50	113.49
43	5	501	LUT	C15-C14-C13	-3.19	122.81	127.28
26	A	1114	CHL	C3C-C4C-NC	-3.19	106.86	114.65
26	8	613	CHL	C3C-C4C-NC	-3.19	106.86	114.65
25	a	611	CLA	C1-C2-C3	-3.18	121.61	126.76
43	2	507	LUT	C20-C13-C12	3.18	122.95	118.09
25	A	1101	CLA	C1-C2-C3	-3.18	120.98	126.20
26	7	611	CHL	C3C-C4C-NC	-3.18	106.88	114.65
26	2	610	CHL	C1A-CHA-C4D	3.17	124.28	118.98
29	6	504	BCR	C33-C5-C4	3.17	120.36	113.60
25	7	612	CLA	C1-C2-C3	-3.17	121.00	126.20
26	6	619	CHL	C3C-C4C-NC	-3.17	106.91	114.65
26	8	604	CHL	C3C-C4C-NC	-3.16	106.92	114.65
29	A	4002	BCR	C33-C5-C6	-3.16	121.03	124.48
25	6	603	CLA	O2A-C1-C2	3.16	120.27	108.11
29	B	4005	BCR	C23-C24-C25	-3.16	118.56	127.00
25	B	1216	CLA	C1-C2-C3	-3.16	121.02	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	504	BCR	C19-C18-C17	3.16	123.97	119.01
25	B	1218	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
26	6	613	CHL	C3C-C4C-NC	-3.15	106.94	114.65
26	3	608	CHL	C3C-C4C-NC	-3.15	106.94	114.65
29	5	504	BCR	C33-C5-C4	3.15	120.32	113.60
26	9	603	CHL	C1-C2-C3	-3.15	121.03	126.20
26	a	606	CHL	C3C-C4C-NC	-3.15	106.95	114.65
26	2	609	CHL	C3C-C4C-NC	-3.15	106.95	114.65
26	6	611	CHL	C3C-C4C-NC	-3.15	106.96	114.65
25	a	612	CLA	C1-C2-C3	-3.15	121.04	126.20
26	4	618	CHL	C3C-C4C-NC	-3.15	106.96	114.65
26	5	618	CHL	C1-C2-C3	-3.14	121.67	126.76
43	3	501	LUT	C15-C14-C13	-3.14	122.87	127.28
25	7	606	CLA	C1C-C2C-C3C	-3.14	104.16	107.09
25	4	612	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
26	6	611	CHL	C1A-CHA-C4D	3.14	124.22	118.98
25	a	608	CLA	CMA-C3A-C4A	3.14	120.21	111.77
26	2	610	CHL	C3C-C4C-NC	-3.14	106.98	114.65
25	A	1117	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	1	603	CLA	CMA-C3A-C4A	3.14	120.21	111.77
25	A	1105	CLA	C1-C2-C3	-3.13	121.06	126.20
26	a	606	CHL	C1-O2A-CGA	3.13	124.24	116.65
26	9	608	CHL	C3C-C4C-NC	-3.13	107.00	114.65
25	A	1012	CLA	C3B-C4B-NB	-3.13	107.74	110.53
25	4	617	CLA	CMA-C3A-C4A	3.13	120.19	111.77
25	4	603	CLA	O2A-C1-C2	3.13	120.15	108.11
26	9	610	CHL	C1-C2-C3	-3.13	121.70	126.76
26	5	613	CHL	C1-O2A-CGA	3.13	124.22	116.65
43	7	501	LUT	C35-C15-C14	-3.13	117.12	123.52
25	B	1228	CLA	C1-C2-C3	-3.12	121.08	126.20
29	K	4001	BCR	C33-C5-C6	-3.12	121.08	124.48
40	J	4002	RRX	C1-C6-C5	-3.12	118.37	122.64
43	5	501	LUT	C7-C8-C9	-3.12	121.62	126.23
26	6	617	CHL	C3C-C4C-NC	-3.12	107.02	114.65
43	a	502	LUT	C15-C14-C13	-3.12	122.90	127.28
29	A	4001	BCR	C23-C24-C25	-3.12	118.67	127.00
43	8	501	LUT	C35-C34-C33	-3.12	122.91	127.28
26	a	606	CHL	C1-C2-C3	-3.12	121.09	126.20
29	B	4001	BCR	C12-C13-C14	-3.12	114.11	119.01
43	5	502	LUT	C10-C11-C12	-3.11	114.18	123.20
26	8	613	CHL	C1-O2A-CGA	3.11	124.18	116.65
26	2	613	CHL	C1-C2-C3	-3.11	121.73	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	501	LUT	C7-C8-C9	-3.11	121.64	126.23
25	L	1504	CLA	CMA-C3A-C4A	3.11	120.12	111.77
29	B	4006	BCR	C33-C5-C6	-3.11	121.09	124.48
26	4	613	CHL	C1A-CHA-C4D	3.11	124.16	118.98
26	6	619	CHL	C1A-CHA-C4D	3.11	124.16	118.98
26	2	613	CHL	C3C-C4C-NC	-3.11	107.06	114.65
26	9	613	CHL	C3C-C4C-NC	-3.10	107.07	114.65
25	A	1127	CLA	C3B-C4B-NB	-3.10	107.76	110.53
26	7	617	CHL	C3C-C4C-NC	-3.10	107.07	114.65
26	5	618	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
25	7	603	CLA	CMA-C3A-C4A	3.10	120.11	111.77
25	A	1141	CLA	CMA-C3A-C4A	3.10	120.11	111.77
25	B	1229	CLA	C3B-C4B-NB	-3.10	107.76	110.53
26	A	1114	CHL	C1A-CHA-C4D	3.10	124.16	118.98
25	6	604	CLA	CMA-C3A-C4A	3.10	120.11	111.77
25	2	601	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
43	2	502	LUT	C11-C10-C9	-3.10	122.93	127.28
27	A	2001	PQN	C14-C13-C15	3.10	120.60	115.23
29	B	4001	BCR	C35-C13-C12	3.10	122.82	118.09
26	5	613	CHL	C3C-C4C-NC	-3.09	107.09	114.65
26	5	610	CHL	C1A-CHA-C4D	3.09	124.14	118.98
25	B	1215	CLA	O2A-C1-C2	3.09	120.01	108.11
43	9	502	LUT	C7-C8-C9	-3.09	121.66	126.23
26	1	610	CHL	C3C-C4C-NC	-3.09	107.09	114.65
25	A	1126	CLA	O2A-C1-C2	3.09	120.00	108.11
25	O	1801	CLA	C1C-C2C-C3C	-3.09	104.21	107.09
26	1	613	CHL	C3C-C4C-NC	-3.09	107.10	114.65
25	A	1123	CLA	C2C-C1C-NC	3.09	113.22	109.98
25	2	602	CLA	C1-C2-C3	-3.08	121.14	126.20
26	6	610	CHL	C3C-C4C-NC	-3.08	107.12	114.65
43	1	503	LUT	C12-C13-C14	-3.08	114.16	119.01
43	3	502	LUT	C35-C34-C33	-3.08	122.96	127.28
25	1	606	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
26	a	610	CHL	C3C-C4C-NC	-3.08	107.12	114.65
26	4	613	CHL	C3C-C4C-NC	-3.08	107.12	114.65
25	6	603	CLA	CMA-C3A-C4A	3.08	120.04	111.77
26	1	613	CHL	C1A-CHA-C4D	3.08	124.11	118.98
26	4	618	CHL	C1A-CHA-C4D	3.08	124.11	118.98
43	6	501	LUT	C15-C14-C13	-3.08	122.97	127.28
25	K	1404	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
26	6	613	CHL	C1-C2-C3	-3.07	121.79	126.76
25	L	1501	CLA	CMA-C3A-C4A	3.07	120.03	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	2002	PQN	C11-C12-C13	-3.07	121.54	126.83
25	A	1135	CLA	C3B-C4B-NB	-3.07	107.79	110.53
26	5	610	CHL	C3C-C4C-NC	-3.07	107.16	114.65
26	8	610	CHL	C3C-C4C-NC	-3.06	107.16	114.65
26	5	611	CHL	C1A-CHA-C4D	3.06	124.09	118.98
25	O	1803	CLA	CAA-C2A-C3A	-3.06	109.21	116.23
26	7	609	CHL	C1-C2-C3	-3.06	121.19	126.20
26	5	618	CHL	C3C-C4C-NC	-3.05	107.18	114.65
26	3	603	CHL	C3C-C4C-NC	-3.05	107.19	114.65
26	8	610	CHL	C1-O2A-CGA	3.05	124.04	116.65
26	4	618	CHL	CHA-C1A-C2A	-3.05	126.16	133.31
26	6	619	CHL	C1-C2-C3	-3.04	121.21	126.20
25	B	1221	CLA	C1-C2-C3	-3.04	121.22	126.20
25	1	605	CLA	C1-O2A-CGA	3.04	124.01	116.65
25	A	1136	CLA	CMA-C3A-C4A	3.04	119.94	111.77
25	A	1141	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
43	8	501	LUT	C15-C14-C13	-3.04	123.02	127.28
43	8	501	LUT	C26-C27-C28	-3.04	119.86	124.58
25	B	1202	CLA	C1-C2-C3	-3.03	121.23	126.20
29	B	4004	BCR	C33-C5-C6	-3.03	121.18	124.48
43	3	502	LUT	C10-C11-C12	-3.02	114.44	123.20
25	A	1115	CLA	C3B-C4B-NB	-3.02	107.83	110.53
25	H	1702	CLA	CMA-C3A-C4A	3.02	119.90	111.77
26	8	603	CHL	C1-C2-C3	-3.02	121.24	126.20
25	O	1803	CLA	CMA-C3A-C4A	3.02	119.90	111.77
43	1	503	LUT	C20-C13-C12	3.02	122.71	118.09
44	1	502	AXT	C15-C35-C34	3.02	129.71	123.52
26	7	613	CHL	C1-O2A-CGA	3.02	123.97	116.65
29	A	4001	BCR	C35-C13-C12	3.02	122.70	118.09
43	6	501	LUT	C35-C15-C14	-3.02	117.34	123.52
25	4	611	CLA	CMA-C3A-C4A	3.02	119.89	111.77
25	5	603	CLA	C1-C2-C3	-3.02	121.25	126.20
25	a	615	CLA	CMA-C3A-C4A	3.02	119.89	111.77
25	2	615	CLA	C1-C2-C3	-3.02	121.25	126.20
25	G	1603	CLA	CMA-C3A-C4A	3.02	119.89	111.77
25	6	618	CLA	CMA-C3A-C4A	3.02	119.88	111.77
25	4	603	CLA	CMA-C3A-C4A	3.02	119.88	111.77
25	3	607	CLA	O2A-C1-C2	3.02	119.72	108.11
26	7	615	CHL	C3C-C4C-NC	-3.02	107.28	114.65
25	A	1109	CLA	CMA-C3A-C4A	3.01	119.87	111.77
25	9	604	CLA	CMA-C3A-C4A	3.01	119.86	111.77
25	7	602	CLA	C1C-C2C-C3C	-3.01	104.29	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	603	CHL	C3C-C4C-NC	-3.01	107.30	114.65
29	L	4003	BCR	C27-C26-C25	-3.01	118.64	122.70
43	8	501	LUT	C35-C15-C14	-3.00	117.38	123.52
25	B	1218	CLA	CMA-C3A-C4A	3.00	119.84	111.77
25	G	1602	CLA	O2A-CGA-CBA	3.00	120.98	111.83
26	a	613	CHL	C1A-CHA-C4D	3.00	123.99	118.98
25	A	1012	CLA	O2A-CGA-CBA	3.00	120.98	111.83
25	G	1601	CLA	CMA-C3A-C4A	3.00	119.83	111.77
25	a	607	CLA	CMA-C3A-C4A	3.00	119.83	111.77
25	A	1128	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
25	2	605	CLA	C3B-C4B-NB	-3.00	107.86	110.53
50	2	501	XAT	C7-C8-C9	-2.99	120.88	125.53
25	4	612	CLA	O2A-C1-C2	2.99	119.63	108.11
25	A	1102	CLA	O2A-CGA-CBA	2.99	120.96	111.83
27	A	2001	PQN	C11-C12-C13	-2.99	121.67	126.83
30	3	801	LHG	C5-O7-C7	-2.99	110.63	117.80
29	A	4003	BCR	C36-C18-C17	-2.99	117.97	122.82
50	2	501	XAT	C26-C27-C28	-2.99	119.67	125.99
25	9	606	CLA	C1-C2-C3	-2.99	121.30	126.20
25	B	1239	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
25	A	1116	CLA	C3B-C4B-NB	-2.99	107.86	110.53
26	7	617	CHL	C1-O2A-CGA	2.99	123.88	116.65
50	9	507	XAT	C38-C25-C26	-2.99	117.39	122.30
26	3	604	CHL	C1A-CHA-C4D	2.98	123.96	118.98
29	J	4001	BCR	C33-C5-C6	-2.98	121.23	124.48
25	A	1130	CLA	C3B-C4B-NB	-2.98	107.87	110.53
26	6	617	CHL	C1A-CHA-C4D	2.98	123.95	118.98
25	3	616	CLA	C2C-C1C-NC	2.98	113.11	109.98
40	J	4002	RRX	C30-C25-C26	-2.98	118.56	122.64
25	8	609	CLA	C1-C2-C3	-2.98	121.32	126.20
26	9	610	CHL	C3C-C4C-NC	-2.98	107.38	114.65
25	A	1112	CLA	C2C-C1C-NC	2.98	113.11	109.98
26	a	613	CHL	C3C-C4C-NC	-2.98	107.38	114.65
26	6	613	CHL	C1A-CHA-C4D	2.98	123.95	118.98
25	A	1103	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
25	K	1402	CLA	CMA-C3A-C4A	2.98	119.77	111.77
43	a	502	LUT	C11-C10-C9	-2.97	123.11	127.28
25	2	615	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
25	a	602	CLA	CMA-C3A-C4A	2.97	119.76	111.77
25	1	612	CLA	C1-C2-C3	-2.97	121.33	126.20
26	a	613	CHL	C4D-CHA-CBD	-2.97	105.97	108.97
25	9	607	CLA	CMA-C3A-C4A	2.97	119.75	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	607	CLA	C1-C2-C3	-2.97	121.33	126.20
25	B	1226	CLA	CMA-C3A-C4A	2.97	119.74	111.77
30	2	802	LHG	O8-C23-C24	2.97	120.88	111.83
25	A	1135	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	5	604	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	B	1238	CLA	CMA-C3A-C4A	2.96	119.74	111.77
29	A	4003	BCR	C19-C18-C17	2.96	123.67	119.01
29	G	4001	BCR	C35-C13-C14	-2.96	118.02	122.82
26	7	611	CHL	C1-C2-C3	-2.96	121.34	126.20
25	A	1137	CLA	C3B-C4B-NB	-2.96	107.89	110.53
43	1	503	LUT	C40-C33-C32	2.96	122.61	118.09
25	9	609	CLA	CMA-C3A-C4A	2.96	119.73	111.77
25	A	1125	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
29	O	4001	BCR	C27-C26-C25	-2.96	118.71	122.70
25	5	603	CLA	CMA-C3A-C4A	2.96	119.72	111.77
25	K	1403	CLA	CMA-C3A-C4A	2.96	119.72	111.77
25	B	1226	CLA	C1-C2-C3	-2.96	121.36	126.20
25	B	1223	CLA	C3B-C4B-NB	-2.96	107.89	110.53
25	A	1107	CLA	C1-C2-C3	-2.95	121.36	126.20
25	8	609	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
25	A	1131	CLA	C2C-C1C-NC	2.95	113.08	109.98
25	a	611	CLA	CMA-C3A-C4A	2.95	119.70	111.77
25	B	1238	CLA	C1-C2-C3	-2.95	121.36	126.20
43	5	505	LUT	C31-C30-C29	-2.95	123.14	127.28
25	2	621	CLA	C2C-C1C-NC	2.95	113.08	109.98
25	A	1133	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
25	J	1901	CLA	C2C-C1C-NC	2.95	113.08	109.98
26	1	609	CHL	C3C-C4C-NC	-2.95	107.45	114.65
25	4	616	CLA	CMA-C3A-C4A	2.95	119.69	111.77
25	B	1214	CLA	C1-O2A-CGA	2.94	123.78	116.65
25	B	1209	CLA	C3B-C4B-NB	-2.94	107.90	110.53
25	B	1202	CLA	C3B-C4B-NB	-2.94	107.90	110.53
29	A	4001	BCR	C12-C13-C14	-2.94	114.38	119.01
25	3	616	CLA	CMA-C3A-C4A	2.94	119.67	111.77
40	3	506	RRX	C35-C13-C14	-2.94	118.06	122.82
25	L	1504	CLA	C2C-C1C-NC	2.94	113.07	109.98
25	A	1104	CLA	C3B-C4B-NB	-2.94	107.91	110.53
25	A	1140	CLA	C3B-C4B-NB	-2.94	107.91	110.53
26	7	615	CHL	C1A-CHA-C4D	2.94	123.88	118.98
29	B	4006	BCR	C35-C13-C12	2.94	122.57	118.09
25	B	1234	CLA	O2A-CGA-CBA	2.93	120.78	111.83
26	7	615	CHL	C1-O2A-CGA	2.93	123.75	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	620	CLA	CMA-C3A-C4A	2.93	119.64	111.77
25	A	1110	CLA	C1-C2-C3	-2.93	121.40	126.20
25	B	1231	CLA	C1-C2-C3	-2.93	121.40	126.20
25	7	607	CLA	CMA-C3A-C4A	2.93	119.64	111.77
25	9	612	CLA	C2C-C1C-NC	2.93	113.06	109.98
25	B	1021	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	A	1108	CLA	CMA-C3A-C4A	2.92	119.63	111.77
25	2	615	CLA	CMA-C3A-C4A	2.92	119.63	111.77
25	B	1238	CLA	C3B-C4B-NB	-2.92	107.92	110.53
25	5	609	CLA	CMA-C3A-C4A	2.92	119.63	111.77
44	7	504	AXT	C15-C35-C34	2.92	129.50	123.52
44	7	504	AXT	C30-C31-C32	2.92	131.66	123.20
25	A	1117	CLA	CMA-C3A-C4A	2.92	119.62	111.77
25	A	1101	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	B	1202	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
25	4	607	CLA	O2A-CGA-CBA	2.92	120.74	111.83
31	A	5004	LMG	O8-C28-C29	2.92	120.73	111.83
25	2	607	CLA	CMA-C3A-C4A	2.92	119.62	111.77
26	5	610	CHL	C4D-CHA-CBD	-2.92	106.03	108.97
25	5	607	CLA	CMA-C3A-C4A	2.92	119.61	111.77
43	7	501	LUT	C7-C8-C9	-2.92	121.92	126.23
29	3	504	BCR	C36-C18-C17	-2.92	118.09	122.82
29	B	4003	BCR	C33-C5-C4	2.92	119.81	113.60
25	4	605	CLA	C2C-C1C-NC	2.92	113.05	109.98
25	A	1107	CLA	CMA-C3A-C4A	2.92	119.61	111.77
25	A	1128	CLA	C2C-C1C-NC	2.92	113.04	109.98
25	B	1226	CLA	C2C-C1C-NC	2.92	113.04	109.98
25	A	1126	CLA	C3B-C4B-NB	-2.91	107.93	110.53
29	B	4006	BCR	C23-C24-C25	-2.91	119.21	127.00
25	8	602	CLA	C3B-C4B-NB	-2.91	107.93	110.53
43	4	501	LUT	C31-C32-C33	-2.91	118.37	126.36
25	B	1220	CLA	CMA-C3A-C4A	2.91	119.60	111.77
25	H	1701	CLA	C2C-C1C-NC	2.91	113.04	109.98
25	1	605	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
51	7	807	4RF	O18-C16-C15	2.91	120.71	111.83
27	B	2002	PQN	C14-C13-C15	2.91	120.28	115.23
29	H	4001	BCR	C28-C27-C26	-2.91	108.86	114.06
29	B	4003	BCR	C23-C22-C21	2.91	123.58	119.01
25	O	1802	CLA	CMA-C3A-C4A	2.91	119.59	111.77
25	4	604	CLA	CMA-C3A-C4A	2.91	119.59	111.77
26	8	604	CHL	C1A-CHA-C4D	2.91	123.83	118.98
25	A	1123	CLA	CMA-C3A-C4A	2.91	119.58	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	607	CLA	CMA-C3A-C4A	2.91	119.58	111.77
25	8	609	CLA	CMA-C3A-C4A	2.91	119.58	111.77
35	A	5008	LMT	C1'-O5'-C5'	-2.90	108.05	113.72
43	3	502	LUT	C11-C10-C9	-2.90	123.20	127.28
30	4	802	LHG	O8-C23-C24	2.90	120.69	111.83
25	4	617	CLA	C2C-C1C-NC	2.90	113.03	109.98
25	9	612	CLA	CMA-C3A-C4A	2.90	119.58	111.77
30	2	801	LHG	O8-C23-C24	2.90	120.68	111.83
25	7	607	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
43	8	502	LUT	C35-C15-C14	-2.90	117.59	123.52
25	A	1110	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	5	615	CLA	CMA-C3A-C4A	2.90	119.56	111.77
43	5	501	LUT	C35-C15-C14	-2.90	117.59	123.52
26	7	613	CHL	C1A-CHA-C4D	2.90	123.82	118.98
43	6	501	LUT	C7-C8-C9	-2.90	121.95	126.23
25	B	1223	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	B	1205	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	A	1101	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	4	607	CLA	CMA-C3A-C4A	2.89	119.55	111.77
25	A	1110	CLA	CMA-C3A-C4A	2.89	119.55	111.77
40	J	4002	RRX	C38-C26-C27	2.89	119.74	114.42
43	5	505	LUT	C22-C23-C24	-2.89	106.89	111.18
25	1	612	CLA	C2C-C1C-NC	2.89	113.02	109.98
25	2	607	CLA	C2C-C1C-NC	2.89	113.02	109.98
25	1	608	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
25	B	1202	CLA	O2A-CGA-CBA	2.89	120.64	111.83
25	B	1221	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
29	A	4001	BCR	C27-C26-C25	-2.89	118.80	122.70
25	A	1106	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
39	F	4001	NEX	O24-C25-C24	2.88	116.19	113.49
25	8	609	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	A	1106	CLA	C4B-CHC-C1C	2.88	133.03	126.25
26	7	611	CHL	C1A-CHA-C4D	2.88	123.79	118.98
25	A	1122	CLA	CMA-C3A-C4A	2.88	119.52	111.77
29	J	4001	BCR	C27-C26-C25	-2.88	118.82	122.70
25	4	603	CLA	C3B-C4B-NB	-2.87	107.96	110.53
25	K	1404	CLA	C2C-C1C-NC	2.87	113.00	109.98
40	3	506	RRX	C4-C5-C6	-2.87	118.82	122.70
25	1	602	CLA	C2C-C1C-NC	2.87	113.00	109.98
25	8	615	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
43	4	501	LUT	C15-C14-C13	-2.87	123.25	127.28
25	7	608	CLA	C2C-C1C-NC	2.87	113.00	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	9	504	XAT	C38-C25-C26	-2.87	117.58	122.30
25	8	607	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	2	621	CLA	CMA-C3A-C4A	2.87	119.48	111.77
25	1	607	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	B	1226	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
25	2	607	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	a	608	CLA	C2C-C1C-NC	2.87	112.99	109.98
43	5	505	LUT	C18-C5-C6	-2.87	121.36	124.48
26	5	613	CHL	C4D-CHA-CBD	-2.86	106.08	108.97
25	B	1231	CLA	C3B-C4B-NB	-2.86	107.97	110.53
43	8	502	LUT	C10-C11-C12	-2.86	114.90	123.20
25	5	603	CLA	O2A-CGA-CBA	2.86	120.57	111.83
25	B	1215	CLA	CMA-C3A-C4A	2.86	119.47	111.77
30	9	801	LHG	O8-C23-C24	2.86	120.56	111.83
25	B	1231	CLA	CHD-C1D-ND	-2.86	120.78	124.80
25	A	1117	CLA	C2C-C1C-NC	2.86	112.98	109.98
25	2	603	CLA	CMA-C3A-C4A	2.86	119.46	111.77
25	H	1702	CLA	C2C-C1C-NC	2.86	112.98	109.98
25	5	602	CLA	C2C-C1C-NC	2.86	112.98	109.98
38	F	5003	LPX	O3-P1-O4	2.86	125.74	112.44
25	B	1225	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	5	605	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	A	1115	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
25	A	1132	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
25	4	616	CLA	C2C-C1C-NC	2.86	112.98	109.98
25	8	608	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
25	B	1201	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	J	1901	CLA	CMA-C3A-C4A	2.85	119.44	111.77
25	B	1022	CLA	OBD-CAD-C3D	-2.85	121.75	128.42
26	7	609	CHL	C1A-CHA-C4D	2.85	123.74	118.98
25	B	1023	CLA	C3B-C4B-NB	-2.85	107.98	110.53
25	9	612	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
25	3	607	CLA	C1-C2-C3	-2.85	121.53	126.20
25	B	1226	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
43	a	501	LUT	C26-C27-C28	-2.85	120.15	124.58
25	7	612	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
25	4	610	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	8	618	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
25	1	602	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	B	1225	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	B	1209	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
25	1	605	CLA	C1C-C2C-C3C	-2.84	103.99	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	6	501	LUT	C10-C11-C12	-2.84	114.97	123.20
36	7	806	DGD	O1G-C1A-C2A	2.84	120.50	111.83
25	3	607	CLA	CMA-C3A-C4A	2.84	119.41	111.77
25	K	1403	CLA	C2C-C1C-NC	2.84	112.97	109.98
25	B	1215	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
25	4	605	CLA	C4B-CHC-C1C	2.84	132.92	126.25
25	H	1702	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
43	9	502	LUT	C35-C15-C14	-2.84	117.72	123.52
26	8	610	CHL	C4D-CHA-CBD	-2.84	106.11	108.97
33	9	803	PTY	O4-C30-C31	2.83	120.48	111.83
25	K	1403	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
43	9	501	LUT	C26-C27-C28	-2.83	120.17	124.58
30	9	802	LHG	O8-C23-C24	2.83	120.48	111.83
26	7	617	CHL	C1A-CHA-C4D	2.83	123.71	118.98
25	A	1110	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	B	1235	CLA	CMA-C3A-C4A	2.83	119.38	111.77
26	1	611	CHL	C1-C2-C3	-2.83	121.56	126.20
25	B	1223	CLA	CMA-C3A-C4A	2.83	119.38	111.77
30	F	5001	LHG	O8-C23-C24	2.83	120.47	111.83
34	A	5007	3PH	O31-C31-C32	2.83	120.46	111.83
25	A	1120	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	B	1235	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
25	9	605	CLA	C2C-C1C-NC	2.83	112.95	109.98
25	B	1234	CLA	O1D-CGD-CBD	-2.83	120.44	124.72
40	J	4002	RRX	C12-C13-C14	2.82	123.45	119.01
26	6	610	CHL	C1-C2-C3	-2.82	121.57	126.20
25	4	608	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
25	1	615	CLA	C2C-C1C-NC	2.82	112.95	109.98
25	A	1108	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	B	1218	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
25	B	1235	CLA	O2A-CGA-CBA	2.82	120.44	111.83
29	B	4006	BCR	C12-C13-C14	-2.82	114.57	119.01
25	6	604	CLA	O2A-CGA-CBA	2.82	120.43	111.83
25	A	1121	CLA	CMD-C2D-C3D	-2.82	121.22	127.69
25	a	611	CLA	C2C-C1C-NC	2.82	112.94	109.98
25	8	605	CLA	C4B-CHC-C1C	2.82	132.88	126.25
25	B	1236	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	B	1230	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
37	K	5001	PCW	O3-C11-C12	2.82	120.42	111.83
25	7	612	CLA	C2C-C1C-NC	2.82	112.94	109.98
30	A	5001	LHG	O8-C23-C24	2.82	120.42	111.83
51	7	807	4RF	O40-C41-C43	2.82	120.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1118	CLA	C2C-C1C-NC	2.82	112.94	109.98
30	F	5002	LHG	O8-C23-C24	2.82	120.42	111.83
25	B	1217	CLA	C2C-C1C-NC	2.82	112.94	109.98
25	a	612	CLA	C2C-C1C-NC	2.82	112.94	109.98
25	A	1129	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
25	G	1602	CLA	C1-O2A-CGA	2.81	123.46	116.65
25	A	1112	CLA	CMA-C3A-C4A	2.81	119.34	111.77
30	B	5002	LHG	O8-C23-C24	2.81	120.42	111.83
25	8	605	CLA	CMA-C3A-C4A	2.81	119.34	111.77
25	1	601	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
36	B	5003	DGD	O1G-C1A-C2A	2.81	120.41	111.83
26	1	604	CHL	C1A-CHA-C4D	2.81	123.68	118.98
25	4	612	CLA	C2C-C1C-NC	2.81	112.94	109.98
25	H	1703	CLA	C3B-C4B-NB	-2.81	108.02	110.53
25	2	603	CLA	C2C-C1C-NC	2.81	112.94	109.98
25	B	1221	CLA	C2C-C1C-NC	2.81	112.93	109.98
25	B	1220	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
25	F	1302	CLA	CMA-C3A-C4A	2.81	119.33	111.77
25	O	1803	CLA	C2C-C1C-NC	2.81	112.93	109.98
25	6	602	CLA	C2C-C1C-NC	2.81	112.93	109.98
25	5	607	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
25	B	1205	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
25	A	1135	CLA	C2C-C1C-NC	2.81	112.93	109.98
25	6	606	CLA	C2C-C1C-NC	2.81	112.93	109.98
25	4	610	CLA	C1-C2-C3	-2.81	121.60	126.20
25	3	607	CLA	C2C-C1C-NC	2.80	112.93	109.98
25	B	1217	CLA	O2A-CGA-CBA	2.80	120.38	111.83
43	2	507	LUT	C19-C9-C8	2.80	122.37	118.09
25	7	603	CLA	C2C-C1C-NC	2.80	112.93	109.98
25	2	602	CLA	C3B-C4B-NB	-2.80	108.03	110.53
25	B	1232	CLA	C3B-C4B-NB	-2.80	108.03	110.53
50	7	502	XAT	C38-C25-C26	-2.80	117.69	122.30
25	a	603	CLA	O2A-CGA-CBA	2.80	120.38	111.83
26	6	611	CHL	C1-C2-C3	-2.80	122.23	126.76
25	5	612	CLA	CMA-C3A-C4A	2.80	119.30	111.77
25	A	1140	CLA	C4B-CHC-C1C	2.80	132.83	126.25
26	5	613	CHL	C1-C2-C3	-2.80	121.61	126.20
25	4	606	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
29	6	504	BCR	C27-C26-C25	-2.80	118.92	122.70
25	B	1227	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
25	8	618	CLA	CMD-C2D-C3D	-2.80	121.27	127.69
30	9	802	LHG	C5-O7-C7	-2.80	111.10	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	610	CHL	C1-O2A-CGA	2.80	123.42	116.65
25	2	608	CLA	CMA-C3A-C4A	2.80	119.29	111.77
25	A	1141	CLA	C2C-C1C-NC	2.80	112.92	109.98
25	B	1204	CLA	C2C-C1C-NC	2.80	112.92	109.98
25	4	607	CLA	C2C-C1C-NC	2.80	112.92	109.98
25	5	608	CLA	C2C-C1C-NC	2.80	112.92	109.98
26	7	611	CHL	C1-O2A-CGA	2.79	123.42	116.65
25	4	602	CLA	C2C-C1C-NC	2.79	112.92	109.98
25	1	615	CLA	CMA-C3A-C4A	2.79	119.28	111.77
25	A	1139	CLA	CMA-C3A-C4A	2.79	119.28	111.77
25	O	1801	CLA	C2C-C1C-NC	2.79	112.92	109.98
25	A	1131	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
25	L	1502	CLA	CMA-C3A-C4A	2.79	119.28	111.77
25	7	607	CLA	C2C-C1C-NC	2.79	112.92	109.98
50	9	504	XAT	C18-C5-C6	-2.79	117.71	122.30
25	2	601	CLA	CMA-C3A-C4A	2.79	119.27	111.77
25	B	1215	CLA	C1-C2-C3	-2.79	121.63	126.20
25	B	1240	CLA	CMA-C3A-C4A	2.79	119.27	111.77
25	A	1110	CLA	C4B-CHC-C1C	2.79	132.81	126.25
25	4	611	CLA	C2C-C1C-NC	2.79	112.91	109.98
25	4	615	CLA	C2C-C1C-NC	2.79	112.91	109.98
25	7	608	CLA	CMA-C3A-C4A	2.79	119.27	111.77
29	B	4004	BCR	C35-C13-C12	2.79	122.35	118.09
26	2	610	CHL	CMA-C3A-C4A	2.79	120.62	114.61
25	5	603	CLA	C1-O2A-CGA	2.79	123.40	116.65
29	5	504	BCR	C33-C5-C6	-2.79	121.44	124.48
25	B	1215	CLA	C2C-C1C-NC	2.79	112.91	109.98
25	L	1504	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
25	B	1212	CLA	CMA-C3A-C4A	2.79	119.26	111.77
25	5	612	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
32	I	5001	SQD	O7-S-C6	-2.78	102.60	106.76
29	L	4002	BCR	C35-C13-C12	2.78	122.34	118.09
26	8	613	CHL	C1A-CHA-C4D	2.78	123.63	118.98
26	6	611	CHL	C4D-CHA-CBD	-2.78	106.16	108.97
25	B	1219	CLA	C2C-C1C-NC	2.78	112.91	109.98
29	B	4003	BCR	C37-C22-C21	-2.78	118.31	122.82
25	A	1106	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	2	603	CLA	O2A-CGA-CBA	2.78	120.32	111.83
29	6	503	BCR	C36-C18-C17	-2.78	118.31	122.82
25	A	1013	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
26	6	613	CHL	C1-O2A-CGA	2.78	123.39	116.65
33	3	802	PTY	O4-C30-C31	2.78	120.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	610	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	8	611	CLA	CMA-C3A-C4A	2.78	119.25	111.77
30	1	801	LHG	O8-C23-C24	2.78	120.31	111.83
48	3	803	DGA	OG1-CA1-CA2	2.78	120.31	111.83
25	2	621	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
25	5	615	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	2	602	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	8	615	CLA	CMA-C3A-C4A	2.78	119.24	111.77
25	A	1132	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	B	1214	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	a	607	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	4	612	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
26	8	603	CHL	C1A-CHA-C4D	2.78	123.62	118.98
43	1	503	LUT	C32-C33-C34	-2.78	114.64	119.01
25	B	1240	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	5	607	CLA	C2C-C1C-NC	2.78	112.90	109.98
25	a	608	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
25	8	609	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
43	2	502	LUT	C39-C29-C28	2.78	122.33	118.09
25	6	618	CLA	C2C-C1C-NC	2.77	112.90	109.98
25	A	1124	CLA	CMA-C3A-C4A	2.77	119.23	111.77
25	O	1802	CLA	C2C-C1C-NC	2.77	112.89	109.98
25	B	1211	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
42	M	4001	ECH	C8-C7-C6	-2.77	119.59	127.00
25	5	602	CLA	C4B-CHC-C1C	2.77	132.76	126.25
26	a	609	CHL	C1-C2-C3	-2.77	121.66	126.20
25	B	1210	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	A	4004	BCR	C38-C26-C27	2.77	119.50	113.60
25	A	1115	CLA	CMA-C3A-C4A	2.77	119.22	111.77
29	K	4001	BCR	C19-C18-C17	2.77	123.37	119.01
25	A	1105	CLA	C4B-CHC-C1C	2.77	132.76	126.25
25	6	608	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
26	8	601	CHL	C1A-CHA-C4D	2.77	123.60	118.98
26	8	610	CHL	CMA-C3A-C4A	2.77	120.58	114.61
33	7	804	PTY	O4-C30-C31	2.77	120.27	111.83
25	1	602	CLA	C4B-CHC-C1C	2.77	132.75	126.25
25	B	1203	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
25	A	1109	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
25	G	1602	CLA	C1-C2-C3	-2.77	121.67	126.20
25	K	1401	CLA	C2C-C1C-NC	2.77	112.89	109.98
25	B	1228	CLA	O2A-CGA-CBA	2.77	120.27	111.83
25	H	1701	CLA	CMA-C3A-C4A	2.77	119.20	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	1601	CLA	C2C-C1C-NC	2.76	112.89	109.98
25	B	1209	CLA	O2A-CGA-CBA	2.76	120.27	111.83
25	B	1209	CLA	C4B-CHC-C1C	2.76	132.75	126.25
25	3	618	CLA	C2C-C1C-NC	2.76	112.88	109.98
25	6	607	CLA	C2C-C1C-NC	2.76	112.88	109.98
26	1	611	CHL	C1A-CHA-C4D	2.76	123.59	118.98
25	7	602	CLA	C2C-C1C-NC	2.76	112.88	109.98
25	9	606	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
25	B	1239	CLA	C2C-C1C-NC	2.76	112.88	109.98
25	A	1105	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	G	1603	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	3	618	CLA	C3B-C4B-NB	-2.76	108.07	110.53
26	1	609	CHL	C4D-CHA-CBD	-2.76	106.19	108.97
33	5	802	PTY	O4-C30-C31	2.76	120.25	111.83
25	A	1013	CLA	C1-C2-C3	-2.76	121.68	126.20
25	1	603	CLA	C2C-C1C-NC	2.76	112.88	109.98
25	A	1118	CLA	CMA-C3A-C4A	2.76	119.18	111.77
25	6	601	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
25	a	602	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	B	1231	CLA	CMD-C2D-C3D	-2.75	121.37	127.69
25	L	1501	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
33	B	5005	PTY	O4-C30-C31	2.75	120.23	111.83
25	B	1207	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
25	A	1101	CLA	C4B-CHC-C1C	2.75	132.72	126.25
25	3	612	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
25	L	1503	CLA	C2C-C1C-NC	2.75	112.87	109.98
25	7	612	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
25	A	1120	CLA	C3B-C4B-NB	-2.75	108.07	110.53
25	B	1217	CLA	CMA-C3A-C4A	2.75	119.17	111.77
25	A	1134	CLA	C3B-C4B-NB	-2.75	108.08	110.53
25	7	608	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
25	B	1223	CLA	C4B-CHC-C1C	2.75	132.71	126.25
29	A	4004	BCR	C12-C13-C14	-2.75	114.69	119.01
36	8	803	DGD	O1G-C1A-C2A	2.75	120.21	111.83
25	B	1208	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
25	8	606	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
43	4	501	LUT	C35-C15-C14	-2.75	117.90	123.52
26	6	619	CHL	CMA-C3A-C4A	2.75	120.53	114.61
48	5	803	DGA	OG1-CA1-CA2	2.75	120.21	111.83
29	B	4004	BCR	C33-C5-C4	2.75	119.45	113.60
25	2	608	CLA	C2C-C1C-NC	2.74	112.86	109.98
25	B	1219	CLA	CMA-C3A-C4A	2.74	119.15	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	3	501	LUT	C35-C15-C14	-2.74	117.90	123.52
25	4	611	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
25	5	609	CLA	C2C-C1C-NC	2.74	112.86	109.98
29	3	505	BCR	C36-C18-C17	-2.74	118.37	122.82
30	A	5002	LHG	O8-C23-C24	2.74	120.20	111.83
25	2	621	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
25	B	1229	CLA	CMA-C3A-C4A	2.74	119.14	111.77
43	6	502	LUT	C11-C10-C9	-2.74	123.44	127.28
25	B	1232	CLA	CMA-C3A-C4A	2.74	119.14	111.77
25	B	1221	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
25	1	612	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
33	a	802	PTY	O4-C30-C31	2.74	120.18	111.83
25	3	606	CLA	C2C-C1C-NC	2.74	112.86	109.98
25	7	601	CLA	O2A-CGA-CBA	2.74	120.18	111.83
25	A	1104	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
25	9	607	CLA	C2C-C1C-NC	2.74	112.86	109.98
29	A	4005	BCR	C35-C13-C12	2.74	122.27	118.09
29	K	4002	BCR	C19-C18-C17	2.74	123.31	119.01
26	4	618	CHL	C4D-CHA-CBD	-2.74	106.21	108.97
26	6	617	CHL	C4D-CHA-CBD	-2.73	106.21	108.97
25	6	608	CLA	C2C-C1C-NC	2.73	112.85	109.98
29	I	4001	BCR	C35-C13-C12	2.73	122.27	118.09
25	A	1105	CLA	CMA-C3A-C4A	2.73	119.12	111.77
25	a	601	CLA	O2A-CGA-CBA	2.73	120.17	111.83
25	H	1701	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
25	G	1603	CLA	C2C-C1C-NC	2.73	112.85	109.98
25	6	602	CLA	C3B-C4B-NB	-2.73	108.09	110.53
48	8	804	DGA	OG1-CA1-CA2	2.73	120.17	111.83
32	G	5001	SQD	O7-S-C6	-2.73	102.68	106.76
26	6	609	CHL	C4D-CHA-CBD	-2.73	106.21	108.97
25	a	603	CLA	C2C-C1C-NC	2.73	112.85	109.98
25	9	609	CLA	C2C-C1C-NC	2.73	112.85	109.98
25	6	601	CLA	C1-O2A-CGA	2.73	123.27	116.65
35	1	804	LMT	C1'-O5'-C5'	-2.73	108.39	113.72
25	B	1216	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
25	B	1212	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	L	1503	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
25	B	1213	CLA	O2A-CGA-CBA	2.73	120.16	111.83
25	B	1210	CLA	O2A-CGA-CBA	2.73	120.16	111.83
25	K	1402	CLA	C2C-C1C-NC	2.73	112.85	109.98
26	2	613	CHL	C1A-CHA-C4D	2.73	123.54	118.98
25	B	1208	CLA	CMA-C3A-C4A	2.73	119.11	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1215	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
44	1	502	AXT	C8-C7-C6	2.73	134.29	127.00
42	M	4001	ECH	C7-C8-C9	-2.73	122.20	126.23
25	6	608	CLA	O2A-CGA-CBA	2.73	120.15	111.83
29	J	4001	BCR	C19-C18-C17	2.73	123.30	119.01
25	8	618	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
25	8	605	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	6	612	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
25	H	1702	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
25	B	1226	CLA	CMD-C2D-C3D	-2.73	121.44	127.69
25	A	1121	CLA	CMA-C3A-C4A	2.72	119.10	111.77
40	J	4002	RRX	C33-C5-C4	2.72	119.41	113.60
25	6	606	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
25	H	1703	CLA	OBD-CAD-C3D	-2.72	122.05	128.42
25	2	612	CLA	C2C-C1C-NC	2.72	112.84	109.98
43	4	502	LUT	C10-C11-C12	-2.72	115.31	123.20
25	B	1224	CLA	C2C-C1C-NC	2.72	112.84	109.98
29	J	4001	BCR	C36-C18-C17	-2.72	118.41	122.82
43	a	503	LUT	C7-C8-C9	-2.72	122.21	126.23
25	a	611	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
25	9	605	CLA	O2A-CGA-CBA	2.72	120.13	111.83
25	6	615	CLA	C2C-C1C-NC	2.72	112.84	109.98
43	1	503	LUT	C22-C23-C24	-2.72	107.14	111.18
50	9	504	XAT	O4-C6-C7	-2.72	109.08	116.88
25	A	1122	CLA	C3B-C4B-NB	-2.72	108.10	110.53
25	B	1203	CLA	C3B-C4B-NB	-2.72	108.10	110.53
25	L	1504	CLA	C4B-CHC-C1C	2.72	132.64	126.25
25	9	602	CLA	C2C-C1C-NC	2.72	112.84	109.98
25	B	1225	CLA	C2C-C1C-NC	2.72	112.84	109.98
26	a	609	CHL	C1A-CHA-C4D	2.72	123.52	118.98
37	B	5004	PCW	O3-C11-C12	2.72	120.12	111.83
25	A	1103	CLA	CMA-C3A-C4A	2.72	119.08	111.77
25	B	1217	CLA	C3B-C4B-NB	-2.72	108.10	110.53
50	9	504	XAT	C6-C7-C8	-2.72	120.25	125.99
25	B	1214	CLA	CMA-C3A-C4A	2.72	119.08	111.77
50	9	507	XAT	C7-C8-C9	-2.72	121.32	125.53
25	9	605	CLA	C1-C2-C3	-2.72	121.75	126.20
25	5	602	CLA	C3B-C4B-NB	-2.72	108.11	110.53
25	8	609	CLA	C2C-C1C-NC	2.72	112.83	109.98
25	4	617	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
25	2	601	CLA	C1C-C2C-C3C	-2.71	104.12	106.98
25	a	602	CLA	C4B-CHC-C1C	2.71	132.63	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1227	CLA	C2C-C1C-NC	2.71	112.83	109.98
25	A	1134	CLA	CMA-C3A-C4A	2.71	119.06	111.77
30	4	802	LHG	C5-O7-C7	-2.71	111.30	117.80
25	a	612	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
29	A	4004	BCR	C35-C13-C12	2.71	122.23	118.09
25	A	1116	CLA	O2A-CGA-CBA	2.71	120.10	111.83
25	2	604	CLA	CHD-C1D-ND	-2.71	120.99	124.80
25	L	1504	CLA	C3B-C4B-NB	-2.71	108.11	110.53
26	1	610	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
25	B	1204	CLA	O2A-CGA-CBA	2.71	120.10	111.83
25	A	1130	CLA	CMA-C3A-C4A	2.71	119.06	111.77
25	A	1123	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
26	6	610	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
25	B	1240	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
25	L	1502	CLA	C1D-ND-C4D	-2.71	104.41	106.31
25	6	612	CLA	C2C-C1C-NC	2.71	112.83	109.98
25	K	1404	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
26	a	604	CHL	CMA-C3A-C4A	2.71	120.44	114.61
25	B	1207	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
25	7	604	CLA	O2A-CGA-CBA	2.71	120.09	111.83
25	A	1117	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
25	B	1203	CLA	C2C-C1C-NC	2.71	112.82	109.98
25	6	604	CLA	C1D-ND-C4D	-2.71	104.41	106.31
25	a	602	CLA	C2C-C1C-NC	2.70	112.82	109.98
26	2	609	CHL	C1-C2-C3	-2.70	121.77	126.20
25	8	615	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	A	1113	CLA	O2A-CGA-CBA	2.70	120.08	111.83
25	8	608	CLA	C2C-C1C-NC	2.70	112.82	109.98
29	B	4003	BCR	C35-C13-C12	2.70	122.22	118.09
32	H	5001	SQD	O7-S-C6	-2.70	102.72	106.76
30	a	801	LHG	O8-C23-C24	2.70	120.07	111.83
25	B	1022	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
25	1	615	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
48	2	803	DGA	OG1-CA1-CA2	2.70	120.07	111.83
25	B	1231	CLA	C4B-CHC-C1C	2.70	132.60	126.25
25	a	605	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
25	7	608	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	7	610	CLA	C2C-C1C-NC	2.70	112.82	109.98
43	1	501	LUT	C10-C11-C12	-2.70	115.38	123.20
25	A	1102	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	B	1207	CLA	C2C-C1C-NC	2.70	112.82	109.98
25	A	1139	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1012	CLA	C2C-C1C-NC	2.70	112.82	109.98
25	A	1113	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
25	B	1022	CLA	C2C-C1C-NC	2.70	112.81	109.98
26	A	1114	CHL	CMA-C3A-C4A	2.70	120.42	114.61
25	6	602	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
25	B	1217	CLA	C4B-CHC-C1C	2.70	132.59	126.25
25	A	1137	CLA	C4B-CHC-C1C	2.70	132.59	126.25
25	1	607	CLA	C2C-C1C-NC	2.70	112.81	109.98
25	B	1202	CLA	C4B-CHC-C1C	2.70	132.59	126.25
25	8	608	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
25	7	604	CLA	CMA-C3A-C4A	2.69	119.02	111.77
25	2	615	CLA	C3B-C4B-NB	-2.69	108.12	110.53
25	2	601	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
25	B	1228	CLA	C2C-C1C-NC	2.69	112.81	109.98
25	G	1603	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
25	A	1105	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	A	1011	CL0	CMB-C2B-C3B	2.69	130.06	124.68
25	B	1234	CLA	OBD-CAD-C3D	-2.69	123.69	127.89
25	B	1239	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	9	613	CHL	C4D-CHA-CBD	-2.69	106.25	108.97
25	B	1207	CLA	C4B-CHC-C1C	2.69	132.58	126.25
39	F	4001	NEX	C39-C29-C30	-2.69	118.45	122.82
25	4	610	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
25	A	1129	CLA	C2C-C1C-NC	2.69	112.81	109.98
25	L	1501	CLA	C2C-C1C-NC	2.69	112.81	109.98
25	7	605	CLA	C2C-C1C-NC	2.69	112.81	109.98
25	A	1136	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
25	A	1127	CLA	CMA-C3A-C4A	2.69	119.01	111.77
29	L	4002	BCR	C36-C18-C17	-2.69	118.46	122.82
25	2	612	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	a	607	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
25	B	1205	CLA	C2C-C1C-NC	2.69	112.81	109.98
25	7	602	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	9	605	CLA	CHA-C4D-ND	2.69	138.09	132.55
25	3	602	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
25	2	607	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
25	7	605	CLA	CMA-C3A-C4A	2.69	119.00	111.77
25	3	613	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
25	9	604	CLA	O2A-CGA-CBA	2.69	120.03	111.83
25	3	602	CLA	C2C-C1C-NC	2.69	112.80	109.98
25	B	1236	CLA	C4B-CHC-C1C	2.69	132.56	126.25
26	6	610	CHL	C1-O2A-CGA	2.69	123.15	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	616	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	2	604	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	8	605	CLA	C2C-C1C-NC	2.68	112.80	109.98
26	3	603	CHL	C1A-CHA-C4D	2.68	123.46	118.98
26	8	601	CHL	C1-O2A-CGA	2.68	123.15	116.65
25	A	1134	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	A	1121	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
25	A	1129	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	A	1128	CLA	CMA-C3A-C4A	2.68	118.98	111.77
25	3	616	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	2	612	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	A	1111	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	A	1134	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	7	606	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	2	604	CLA	CMA-C3A-C4A	2.68	118.98	111.77
26	5	617	CHL	C4D-CHA-CBD	-2.68	106.27	108.97
25	A	1013	CLA	C3B-C4B-NB	-2.68	108.14	110.53
25	5	604	CLA	O2A-CGA-CBA	2.68	120.00	111.83
30	5	801	LHG	O8-C23-C24	2.68	120.00	111.83
25	9	609	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	B	1218	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	6	603	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	9	604	CLA	C2C-C1C-NC	2.68	112.80	109.98
25	5	601	CLA	CHD-C1D-ND	-2.68	121.03	124.80
29	4	503	BCR	C38-C26-C25	-2.68	121.56	124.48
50	7	502	XAT	C6-C7-C8	-2.68	120.33	125.99
43	1	503	LUT	C31-C30-C29	-2.68	123.52	127.28
25	a	602	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	7	604	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
25	G	1601	CLA	C3B-C4B-NB	-2.68	108.14	110.53
43	a	503	LUT	C35-C15-C14	-2.68	118.04	123.52
25	7	603	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
43	2	507	LUT	C20-C13-C14	-2.68	118.48	122.82
25	A	1133	CLA	C2C-C1C-NC	2.68	112.79	109.98
25	K	1401	CLA	CMA-C3A-C4A	2.68	118.97	111.77
26	1	609	CHL	C1A-CHA-C4D	2.68	123.45	118.98
25	O	1803	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
25	B	1205	CLA	O2A-CGA-CBA	2.68	119.99	111.83
29	7	503	BCR	C27-C26-C25	-2.68	119.09	122.70
25	A	1104	CLA	C2C-C1C-NC	2.67	112.79	109.98
29	A	4005	BCR	C12-C13-C14	-2.67	114.80	119.01
30	7	803	LHG	O8-C23-C24	2.67	119.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	1401	CLA	C3B-C4B-NB	-2.67	108.14	110.53
25	A	1118	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
25	A	1130	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
25	A	1134	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
25	A	1107	CLA	C2C-C1C-NC	2.67	112.79	109.98
30	8	801	LHG	O8-C23-C24	2.67	119.99	111.83
25	5	607	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
25	7	603	CLA	C3B-C4B-NB	-2.67	108.14	110.53
25	2	605	CLA	C4B-CHC-C1C	2.67	132.53	126.25
25	K	1403	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
25	4	601	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
26	8	613	CHL	C1-C2-C3	-2.67	122.44	126.76
50	2	501	XAT	O24-C25-C38	-2.67	112.06	115.05
25	6	612	CLA	CMA-C3A-C4A	2.67	118.95	111.77
25	B	1220	CLA	C2C-C1C-NC	2.67	112.78	109.98
42	M	4001	ECH	C29-C30-C25	-2.67	106.56	110.44
25	A	1136	CLA	C2C-C1C-NC	2.67	112.78	109.98
25	6	601	CLA	CMA-C3A-C4A	2.67	118.94	111.77
25	1	602	CLA	C3B-C4B-NB	-2.67	108.15	110.53
43	3	501	LUT	C22-C23-C24	-2.67	107.23	111.18
25	A	1105	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
25	7	602	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
33	A	5006	PTY	O4-C30-C31	2.66	119.96	111.83
25	B	1208	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	1	603	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	4	616	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	5	608	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	1	606	CLA	C2C-C1C-NC	2.66	112.78	109.98
25	A	1107	CLA	O2A-CGA-CBA	2.66	119.96	111.83
25	B	1229	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	F	1302	CLA	C2C-C1C-NC	2.66	112.78	109.98
25	A	1141	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
37	6	803	PCW	O3-C11-C12	2.66	119.95	111.83
25	B	1229	CLA	C4B-CHC-C1C	2.66	132.51	126.25
25	2	606	CLA	C2C-C1C-NC	2.66	112.78	109.98
25	A	1132	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	7	607	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	L	1503	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	4	607	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	5	608	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
50	2	501	XAT	O4-C5-C18	-2.66	112.08	115.05
25	4	607	CLA	C1C-C2C-C3C	-2.66	104.18	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	a	502	LUT	C10-C11-C12	-2.66	115.50	123.20
25	L	1502	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	1	602	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
25	B	1236	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
30	A	5003	LHG	O8-C23-C24	2.66	119.94	111.83
25	1	607	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
25	8	620	CLA	C2C-C1C-NC	2.66	112.77	109.98
25	B	1219	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
25	8	618	CLA	CMA-C3A-C4A	2.66	118.91	111.77
26	7	617	CHL	C1-C2-C3	-2.66	121.85	126.20
30	6	802	LHG	O8-C23-C24	2.66	119.93	111.83
26	1	611	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
25	1	605	CLA	C1-C2-C3	-2.66	121.85	126.20
25	1	607	CLA	C3B-C4B-NB	-2.65	108.16	110.53
25	A	1108	CLA	C4B-CHC-C1C	2.65	132.49	126.25
25	B	1217	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
29	5	503	BCR	C33-C5-C4	2.65	119.25	113.60
25	6	607	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
25	8	607	CLA	C2C-C1C-NC	2.65	112.77	109.98
25	2	604	CLA	CMD-C2D-C3D	-2.65	121.60	127.69
26	A	1114	CHL	C4D-CHA-CBD	-2.65	106.29	108.97
25	2	602	CLA	CMA-C3A-C4A	2.65	118.90	111.77
25	3	606	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
25	6	605	CLA	CMA-C3A-C4A	2.65	118.90	111.77
25	4	615	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
26	6	611	CHL	C1-O2A-CGA	2.65	123.07	116.65
43	7	501	LUT	C10-C11-C12	-2.65	115.52	123.20
25	B	1022	CLA	CHD-C1D-ND	-2.65	121.07	124.80
25	6	605	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
25	9	602	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
25	F	1301	CLA	C2C-C1C-NC	2.65	112.77	109.98
25	B	1237	CLA	C3B-C4B-NB	-2.65	108.16	110.53
26	6	609	CHL	CMA-C3A-C4A	2.65	120.32	114.61
25	A	1121	CLA	CHD-C1D-ND	-2.65	121.07	124.80
25	A	1120	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
33	a	803	PTY	O4-C30-C31	2.65	119.91	111.83
25	3	610	CLA	C2C-C1C-NC	2.65	112.77	109.98
25	A	1136	CLA	C3B-C4B-NB	-2.65	108.17	110.53
25	B	1216	CLA	C2C-C1C-NC	2.65	112.76	109.98
25	5	614	CLA	C2C-C1C-NC	2.65	112.76	109.98
25	L	1502	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	8	602	CLA	O2D-CGD-O1D	-2.65	118.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	611	CLA	C4B-CHC-C1C	2.65	132.47	126.25
52	8	805	P5S	O19-C17-C20	2.65	119.91	111.83
25	B	1204	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
25	B	1227	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
25	9	607	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
32	A	5005	SQD	O7-S-C6	-2.65	102.80	106.76
43	a	501	LUT	C35-C15-C14	-2.65	118.10	123.52
43	a	502	LUT	C35-C15-C14	-2.65	118.10	123.52
43	1	501	LUT	C7-C8-C9	-2.65	122.32	126.23
25	A	1012	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
25	4	608	CLA	C2C-C1C-NC	2.64	112.76	109.98
43	2	507	LUT	C18-C5-C4	2.64	119.28	114.42
25	3	612	CLA	CHD-C1D-ND	-2.64	121.08	124.80
25	4	604	CLA	O2A-CGA-CBA	2.64	119.90	111.83
25	4	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
25	B	1203	CLA	C4B-CHC-C1C	2.64	132.46	126.25
25	B	1021	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	2	602	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
26	2	613	CHL	C1-O2A-CGA	2.64	123.05	116.65
25	A	1101	CLA	CMA-C3A-C4A	2.64	118.87	111.77
25	7	602	CLA	CMA-C3A-C4A	2.64	118.87	111.77
25	2	603	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	8	606	CLA	C2C-C1C-NC	2.64	112.76	109.98
30	5	801	LHG	C5-O7-C7	-2.64	111.48	117.80
25	5	605	CLA	CHA-C4D-ND	2.64	138.00	132.55
25	1	601	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	6	618	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	8	602	CLA	C2C-C1C-NC	2.64	112.75	109.98
25	A	1109	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	A	1140	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
25	A	1126	CLA	C2C-C1C-NC	2.64	112.75	109.98
25	G	1603	CLA	C4B-CHC-C1C	2.64	132.45	126.25
25	B	1204	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
37	K	5002	PCW	O3-C11-C12	2.64	119.88	111.83
25	B	1217	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	4	602	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	8	612	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
25	9	607	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
43	3	501	LUT	C10-C11-C12	-2.64	115.56	123.20
29	7	503	BCR	C35-C13-C12	2.64	122.12	118.09
25	A	1133	CLA	C3B-C4B-NB	-2.64	108.17	110.53
25	G	1601	CLA	C1C-C2C-C3C	-2.64	104.21	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1209	CLA	CMA-C3A-C4A	2.64	118.86	111.77
25	B	1236	CLA	C2C-C1C-NC	2.64	112.75	109.98
25	8	605	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
25	8	612	CLA	CHD-C1D-ND	-2.64	121.09	124.80
26	8	610	CHL	C1-C2-C3	-2.63	121.88	126.20
25	3	618	CLA	C4B-CHC-C1C	2.63	132.44	126.25
50	9	507	XAT	C6-C7-C8	-2.63	120.42	125.99
25	8	607	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	6	604	CLA	CHD-C1D-ND	-2.63	121.09	124.80
25	B	1210	CLA	C2C-C1C-NC	2.63	112.75	109.98
25	9	604	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	B	1240	CLA	O2A-CGA-CBA	2.63	119.86	111.83
25	B	1215	CLA	C4B-CHC-C1C	2.63	132.44	126.25
25	8	618	CLA	C2C-C1C-NC	2.63	112.75	109.98
25	B	1204	CLA	C1D-ND-C4D	-2.63	104.47	106.31
25	6	603	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	G	1603	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	B	1228	CLA	CMA-C3A-C4A	2.63	118.84	111.77
25	F	1302	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	3	601	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	a	605	CLA	C2C-C1C-NC	2.63	112.75	109.98
25	A	1131	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	4	604	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
25	4	601	CLA	C2C-C1C-NC	2.63	112.74	109.98
25	5	606	CLA	C2C-C1C-NC	2.63	112.74	109.98
25	6	605	CLA	C2C-C1C-NC	2.63	112.74	109.98
25	5	601	CLA	O2A-CGA-CBA	2.63	119.85	111.83
25	4	602	CLA	C4B-CHC-C1C	2.63	132.43	126.25
25	8	618	CLA	CHD-C1D-ND	-2.63	121.10	124.80
26	1	613	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
25	5	612	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	7	601	CLA	C4B-CHC-C1C	2.63	132.43	126.25
25	8	607	CLA	C3B-C4B-NB	-2.63	108.18	110.53
25	5	602	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
25	B	1223	CLA	CHA-C4D-ND	2.63	137.97	132.55
25	4	604	CLA	C2C-C1C-NC	2.63	112.74	109.98
39	F	4001	NEX	C16-C1-C2	2.63	121.51	109.06
43	2	502	LUT	C15-C35-C34	-2.63	118.14	123.52
25	6	602	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	6	801	LHG	O8-C23-C24	2.63	119.84	111.83
25	B	1222	CLA	CHD-C1D-ND	-2.63	121.11	124.80
25	a	601	CLA	C1C-C2C-C3C	-2.63	104.22	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	3	506	RRX	C16-C15-C14	2.63	128.89	123.52
25	6	618	CLA	C3B-C4B-NB	-2.63	108.19	110.53
25	3	618	CLA	CMA-C3A-C4A	2.63	118.83	111.77
25	A	1107	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
25	3	605	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
25	6	615	CLA	CMA-C3A-C4A	2.62	118.83	111.77
33	J	5001	PTY	O4-C30-C31	2.62	119.84	111.83
26	9	610	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
25	B	1218	CLA	O2A-CGA-CBA	2.62	119.84	111.83
25	8	615	CLA	C2C-C1C-NC	2.62	112.74	109.98
25	A	1139	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
25	8	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
25	2	605	CLA	O2A-CGA-CBA	2.62	119.83	111.83
25	B	1231	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
30	B	5002	LHG	C5-O7-C7	-2.62	111.52	117.80
25	A	1135	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
25	3	618	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
25	5	615	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
25	2	621	CLA	O2A-CGA-CBA	2.62	119.83	111.83
25	a	615	CLA	C2C-C1C-NC	2.62	112.74	109.98
25	7	604	CLA	C2C-C1C-NC	2.62	112.74	109.98
25	2	615	CLA	C2C-C1C-NC	2.62	112.74	109.98
26	7	609	CHL	C1-O2A-CGA	2.62	123.00	116.65
25	F	1302	CLA	O2A-CGA-CBA	2.62	119.83	111.83
26	4	613	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
25	B	1201	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
25	9	602	CLA	CMA-C3A-C4A	2.62	118.81	111.77
25	B	1209	CLA	C1-O2A-CGA	2.62	122.99	116.65
46	a	504	QTB	C03-C04-C05	-2.62	115.61	123.20
25	B	1238	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
25	1	606	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
25	K	1402	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
25	B	1232	CLA	C2C-C1C-NC	2.62	112.73	109.98
25	6	606	CLA	O2A-CGA-CBA	2.62	119.81	111.83
25	A	1135	CLA	C4B-CHC-C1C	2.62	132.40	126.25
25	7	601	CLA	CMA-C3A-C4A	2.62	118.80	111.77
29	K	4001	BCR	C36-C18-C17	-2.62	118.58	122.82
29	J	4001	BCR	C28-C27-C26	-2.62	109.39	114.06
25	B	1207	CLA	C3B-C4B-NB	-2.62	108.19	110.53
25	6	606	CLA	C3B-C4B-NB	-2.62	108.19	110.53
25	7	605	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
25	B	1222	CLA	O2D-CGD-O1D	-2.61	118.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	612	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
26	8	613	CHL	C4D-CHA-CBD	-2.61	106.33	108.97
25	A	1102	CLA	C2C-C1C-NC	2.61	112.73	109.98
25	5	612	CLA	C2C-C1C-NC	2.61	112.73	109.98
29	3	503	BCR	C33-C5-C4	2.61	119.17	113.60
25	A	1120	CLA	CMA-C3A-C4A	2.61	118.80	111.77
25	A	1138	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	a	603	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	A	1012	CLA	OBD-CAD-C3D	-2.61	122.31	128.42
25	8	615	CLA	CHD-C1D-ND	-2.61	121.12	124.80
25	A	1122	CLA	O2A-CGA-CBA	2.61	119.80	111.83
25	3	610	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	A	1128	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	A	1129	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	2	606	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
29	L	4002	BCR	C19-C18-C17	2.61	123.12	119.01
25	A	1118	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	A	1102	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	a	607	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
25	A	1121	CLA	C2C-C1C-NC	2.61	112.72	109.98
29	A	4002	BCR	C36-C18-C17	-2.61	118.59	122.82
25	6	607	CLA	C3B-C4B-NB	-2.61	108.20	110.53
43	9	501	LUT	C10-C11-C12	-2.61	115.64	123.20
43	1	503	LUT	C8-C7-C6	-2.61	120.03	127.00
25	4	602	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	B	1237	CLA	C2C-C1C-NC	2.61	112.72	109.98
25	A	1116	CLA	CMA-C3A-C4A	2.61	118.78	111.77
25	2	605	CLA	CMA-C3A-C4A	2.61	118.78	111.77
25	6	604	CLA	C4B-CHC-C1C	2.61	132.38	126.25
25	K	1402	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
25	4	615	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	3	605	CLA	C2C-C1C-NC	2.61	112.72	109.98
25	A	1123	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	1	607	CLA	CMA-C3A-C4A	2.61	118.78	111.77
25	B	1224	CLA	C3B-C4B-NB	-2.61	108.20	110.53
40	J	4002	RRX	C24-C25-C26	-2.61	115.55	121.56
25	B	1023	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
25	4	608	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
25	7	601	CLA	C1D-ND-C4D	-2.61	104.48	106.31
25	5	614	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
25	2	604	CLA	C2C-C1C-NC	2.60	112.72	109.98
25	2	605	CLA	C2C-C1C-NC	2.60	112.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	608	CLA	O2A-CGA-CBA	2.60	119.78	111.83
25	3	612	CLA	C3B-C4B-NB	-2.60	108.20	110.53
25	B	1236	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
29	K	4002	BCR	C36-C18-C17	-2.60	118.60	122.82
25	A	1101	CLA	C2C-C1C-NC	2.60	112.72	109.98
25	3	601	CLA	C2C-C1C-NC	2.60	112.72	109.98
25	9	605	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
26	3	604	CHL	CMA-C3A-C4A	2.60	120.22	114.61
25	3	616	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
25	A	1113	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
26	a	609	CHL	C1-O2A-CGA	2.60	122.95	116.65
25	A	1109	CLA	C2C-C1C-NC	2.60	112.72	109.98
25	B	1218	CLA	CHD-C1D-ND	-2.60	121.14	124.80
25	B	1238	CLA	C1-O2A-CGA	2.60	122.95	116.65
25	2	615	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	2	601	CLA	C2C-C1C-NC	2.60	112.71	109.98
25	4	606	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	5	606	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	B	1201	CLA	C2C-C1C-NC	2.60	112.71	109.98
25	B	1215	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	5	601	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
43	6	502	LUT	C10-C11-C12	-2.60	115.67	123.20
25	A	1112	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
25	B	1224	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	A	1119	CLA	CHD-C1D-ND	-2.60	121.15	124.80
29	3	504	BCR	C23-C24-C25	-2.60	120.06	127.00
25	a	608	CLA	C3B-C4B-NB	-2.60	108.21	110.53
25	B	1231	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	2	608	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
25	5	603	CLA	C2C-C1C-NC	2.60	112.71	109.98
29	B	4003	BCR	C34-C9-C10	-2.60	118.61	122.82
25	6	601	CLA	CHD-C1D-ND	-2.60	121.15	124.80
25	1	601	CLA	O2A-CGA-CBA	2.60	119.75	111.83
25	A	1112	CLA	O1D-CGD-CBD	-2.60	119.40	124.52
25	5	609	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
26	2	613	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
26	a	613	CHL	CMA-C3A-C4A	2.60	120.20	114.61
30	6	801	LHG	C5-O7-C7	-2.59	111.59	117.80
25	A	1112	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	7	610	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
26	1	610	CHL	C1-O2A-CGA	2.59	124.04	116.67
25	B	1202	CLA	C2C-C1C-NC	2.59	112.71	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	605	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	B	1212	CLA	C2C-C1C-NC	2.59	112.71	109.98
25	a	611	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	A	1130	CLA	C4B-CHC-C1C	2.59	132.34	126.25
25	A	1136	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	L	1502	CLA	C2D-C1D-ND	2.59	112.69	110.13
25	B	1228	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	9	605	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	A	1141	CLA	CHA-C4D-ND	2.59	137.90	132.55
25	B	1237	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	3	607	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
25	A	1124	CLA	C2C-C1C-NC	2.59	112.70	109.98
25	6	602	CLA	C4B-CHC-C1C	2.59	132.34	126.25
25	A	1104	CLA	O2A-CGA-CBA	2.59	119.73	111.83
25	A	1117	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
25	A	1126	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
29	I	4001	BCR	C38-C26-C27	2.59	119.12	113.60
25	A	1116	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	4	604	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
26	3	603	CHL	C1C-C2C-CMC	2.59	131.47	126.80
25	4	605	CLA	CHA-C4D-ND	2.59	137.89	132.55
25	B	1229	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	7	605	CLA	CHA-C4D-ND	2.59	137.88	132.55
25	A	1126	CLA	CMA-C3A-C4A	2.59	118.72	111.77
29	B	4002	BCR	C33-C5-C4	2.59	119.11	113.60
25	G	1602	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
25	8	611	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
29	O	4001	BCR	C30-C25-C26	-2.59	119.10	122.64
25	A	1124	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
25	2	604	CLA	C4B-CHC-C1C	2.59	132.33	126.25
25	4	608	CLA	O2A-CGA-CBA	2.59	119.72	111.83
25	A	1137	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
25	4	603	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
25	A	1120	CLA	C2C-C1C-NC	2.58	112.70	109.98
43	1	501	LUT	C22-C23-C24	-2.58	107.35	111.18
25	7	604	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
32	7	805	SQD	O7-S-C6	-2.58	102.90	106.76
25	L	1501	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
25	A	1111	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
43	7	501	LUT	C31-C32-C33	-2.58	119.28	126.36
25	L	1502	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
25	6	603	CLA	O2D-CGD-O1D	-2.58	118.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	1401	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
25	6	615	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
25	B	1205	CLA	C3B-C4B-NB	-2.58	108.23	110.53
26	4	609	CHL	C1A-CHA-C4D	2.58	123.29	118.98
25	9	612	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	A	1105	CLA	C2C-C1C-NC	2.58	112.69	109.98
26	4	613	CHL	CMA-C3A-C4A	2.58	120.17	114.61
25	7	603	CLA	O2A-CGA-CBA	2.58	119.70	111.83
25	1	603	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	A	1131	CLA	CMA-C3A-C4A	2.58	118.70	111.77
25	7	604	CLA	CHD-C1D-ND	-2.58	121.18	124.80
25	A	1104	CLA	C4B-CHC-C1C	2.58	132.30	126.25
25	B	1225	CLA	C4B-CHC-C1C	2.58	132.30	126.25
25	G	1601	CLA	C4B-CHC-C1C	2.58	132.30	126.25
25	5	605	CLA	C4B-CHC-C1C	2.58	132.30	126.25
43	2	502	LUT	C22-C23-C24	-2.58	107.36	111.18
30	1	802	LHG	C5-O7-C7	-2.58	111.63	117.80
25	O	1802	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
25	9	609	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
29	B	4004	BCR	C38-C26-C25	-2.57	121.68	124.48
25	6	601	CLA	C3B-C4B-NB	-2.57	108.23	110.53
25	G	1601	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
36	7	806	DGD	O6D-C5D-C6D	2.57	111.80	106.69
25	5	604	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
25	2	605	CLA	CHA-C4D-ND	2.57	137.86	132.55
25	B	1238	CLA	C4B-CHC-C1C	2.57	132.30	126.25
25	B	1203	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
30	7	802	LHG	O8-C23-C24	2.57	119.68	111.83
25	A	1101	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
25	3	601	CLA	C4B-CHC-C1C	2.57	132.29	126.25
25	A	1140	CLA	C2C-C1C-NC	2.57	112.68	109.98
30	3	801	LHG	O8-C23-C24	2.57	119.67	111.83
26	5	611	CHL	CMA-C3A-C4A	2.57	120.15	114.61
25	6	601	CLA	O2A-CGA-CBA	2.57	119.67	111.83
25	A	1106	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
25	6	608	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
25	2	602	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	3	612	CLA	C4B-CHC-C1C	2.57	132.29	126.25
25	B	1216	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	2	605	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
25	4	601	CLA	O2A-CGA-CBA	2.57	119.66	111.83
25	A	1138	CLA	C2C-C1C-NC	2.57	112.68	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1223	CLA	C2C-C1C-NC	2.57	112.68	109.98
26	5	611	CHL	C4D-CHA-CBD	-2.57	106.38	108.97
25	7	610	CLA	CMA-C3A-C4A	2.57	118.67	111.77
25	A	1138	CLA	CHD-C1D-ND	-2.57	121.19	124.80
25	3	612	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	6	604	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
26	6	611	CHL	CMA-C3A-C4A	2.57	120.14	114.61
25	4	603	CLA	C4B-CHC-C1C	2.57	132.28	126.25
25	A	1104	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
25	6	606	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
25	F	1301	CLA	C3B-C4B-NB	-2.56	108.24	110.53
25	8	608	CLA	C4B-CHC-C1C	2.56	132.28	126.25
25	B	1230	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
25	H	1703	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	A	1124	CLA	C4B-CHC-C1C	2.56	132.27	126.25
30	1	802	LHG	O8-C23-C24	2.56	119.65	111.83
25	8	609	CLA	C1D-ND-C4D	-2.56	104.51	106.31
25	7	604	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	A	1120	CLA	C4B-CHC-C1C	2.56	132.27	126.25
25	5	614	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	6	608	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
26	8	603	CHL	CMA-C3A-C4A	2.56	120.13	114.61
43	5	501	LUT	C10-C11-C12	-2.56	115.78	123.20
25	A	1122	CLA	C2C-C1C-NC	2.56	112.67	109.98
25	a	611	CLA	O2A-CGA-CBA	2.56	119.64	111.83
29	6	504	BCR	C36-C18-C17	-2.56	118.67	122.82
25	1	608	CLA	CHD-C1D-ND	-2.56	121.20	124.80
25	5	604	CLA	CHD-C1D-ND	-2.56	121.20	124.80
25	A	1124	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	2	606	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	B	1222	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
25	A	1115	CLA	C4B-CHC-C1C	2.56	132.27	126.25
25	1	607	CLA	C4B-CHC-C1C	2.56	132.27	126.25
25	B	1225	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
25	B	1206	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	5	604	CLA	C2C-C1C-NC	2.56	112.67	109.98
29	5	503	BCR	C27-C26-C25	-2.56	119.25	122.70
25	7	608	CLA	C3B-C4B-NB	-2.56	108.25	110.53
29	O	4001	BCR	C23-C24-C25	-2.56	120.17	127.00
25	6	607	CLA	C4B-CHC-C1C	2.56	132.26	126.25
25	B	1224	CLA	O2A-CGA-CBA	2.56	119.63	111.83
25	A	1013	CLA	C1C-C2C-C3C	-2.56	104.29	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1240	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
25	A	1118	CLA	C4B-CHC-C1C	2.56	132.26	126.25
25	A	1133	CLA	CHD-C1D-ND	-2.56	121.20	124.80
25	A	1130	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	5	602	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	5	605	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
30	7	801	LHG	O8-C23-C24	2.56	119.63	111.83
25	A	1119	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
25	a	601	CLA	C2C-C1C-NC	2.56	112.67	109.98
25	6	612	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
25	K	1403	CLA	C3B-C4B-NB	-2.56	108.25	110.53
25	B	1202	CLA	C1C-C2C-C3C	-2.55	104.29	106.98
25	A	1109	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
25	G	1602	CLA	C2C-C1C-NC	2.55	112.67	109.98
25	K	1401	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
25	1	603	CLA	O2A-CGA-CBA	2.55	119.62	111.83
25	1	606	CLA	CHA-C4D-ND	2.55	137.82	132.55
25	K	1401	CLA	C4B-CHC-C1C	2.55	132.25	126.25
26	4	609	CHL	C1-O2A-CGA	2.55	122.83	116.65
25	B	1223	CLA	OBD-CAD-C3D	-2.55	122.45	128.42
24	A	1011	CL0	O2D-CGD-O1D	-2.55	118.88	123.85
25	A	1012	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
26	1	604	CHL	CMA-C3A-C4A	2.55	120.11	114.61
25	B	1230	CLA	O2A-CGA-CBA	2.55	119.62	111.83
25	4	608	CLA	CMA-C3A-C4A	2.55	118.63	111.77
25	A	1131	CLA	O2A-CGA-CBA	2.55	119.62	111.83
25	B	1204	CLA	CHD-C1D-ND	-2.55	121.21	124.80
25	A	1108	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
25	4	602	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
25	B	1219	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	3	610	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	A	1113	CLA	C2C-C1C-NC	2.55	112.66	109.98
25	B	1208	CLA	C1-O2A-CGA	2.55	122.82	116.65
26	7	617	CHL	C4D-CHA-CBD	-2.55	106.40	108.97
25	B	1230	CLA	C2C-C1C-NC	2.55	112.66	109.98
25	1	601	CLA	C2C-C1C-NC	2.55	112.66	109.98
25	B	1021	CLA	C4B-CHC-C1C	2.55	132.24	126.25
25	K	1403	CLA	C4B-CHC-C1C	2.55	132.24	126.25
25	8	609	CLA	O2A-CGA-CBA	2.55	119.60	111.83
25	7	601	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
25	6	606	CLA	CMA-C3A-C4A	2.55	118.62	111.77
25	8	602	CLA	C1C-C2C-C3C	-2.55	104.30	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	605	CLA	O2A-CGA-CBA	2.55	119.60	111.83
25	B	1229	CLA	O2A-CGA-CBA	2.55	119.60	111.83
25	B	1224	CLA	O1D-CGD-CBD	-2.55	119.50	124.52
25	K	1404	CLA	CHA-C4D-ND	2.55	137.80	132.55
25	8	605	CLA	CHA-C4D-ND	2.55	137.80	132.55
29	G	4001	BCR	C34-C9-C10	-2.55	118.69	122.82
25	1	602	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	B	1022	CLA	CHA-C4D-ND	2.55	137.80	132.55
25	B	1023	CLA	O2A-CGA-CBA	2.55	119.60	111.83
25	4	605	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
50	9	507	XAT	C27-C28-C29	2.55	129.48	125.53
25	L	1502	CLA	C2C-C1C-NC	2.54	112.66	109.98
25	3	612	CLA	C2C-C1C-NC	2.54	112.66	109.98
25	9	606	CLA	C2C-C1C-NC	2.54	112.66	109.98
25	K	1403	CLA	O2A-CGA-CBA	2.54	119.59	111.83
25	8	618	CLA	CHA-C4D-ND	2.54	137.80	132.55
25	B	1209	CLA	C1C-C2C-C3C	-2.54	104.30	106.98
25	B	1022	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
25	B	1205	CLA	CMA-C3A-C4A	2.54	118.61	111.77
43	8	501	LUT	C10-C11-C12	-2.54	115.83	123.20
25	7	612	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
29	J	4001	BCR	C23-C24-C25	-2.54	120.20	127.00
25	A	1111	CLA	O2A-CGA-CBA	2.54	119.59	111.83
25	1	608	CLA	O2A-CGA-CBA	2.54	119.59	111.83
25	B	1229	CLA	C2C-C1C-NC	2.54	112.65	109.98
29	B	4003	BCR	C36-C18-C17	-2.54	118.70	122.82
25	A	1109	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
25	6	605	CLA	CHA-C4D-ND	2.54	137.79	132.55
25	A	1130	CLA	C2C-C1C-NC	2.54	112.65	109.98
26	a	610	CHL	C4D-CHA-CBD	-2.54	106.41	108.97
25	8	602	CLA	C4B-CHC-C1C	2.54	132.22	126.25
25	B	1238	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
25	5	601	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	B	1214	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
25	3	606	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
25	B	1235	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
25	J	1901	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	3	618	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
25	B	1226	CLA	CHA-C4D-ND	2.54	137.78	132.55
25	A	1139	CLA	C4B-CHC-C1C	2.54	132.21	126.25
26	1	611	CHL	C4C-CHD-C1D	2.54	125.15	116.07
25	7	603	CLA	C1-O2A-CGA	2.54	122.79	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1127	CLA	C4B-CHC-C1C	2.54	132.21	126.25
46	a	504	QTB	C11-C10-C09	2.54	130.67	125.25
50	9	507	XAT	O4-C6-C7	-2.54	109.61	116.88
25	B	1228	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
25	A	1125	CLA	C4B-CHC-C1C	2.54	132.21	126.25
25	A	1012	CLA	CHA-C4D-ND	2.54	137.78	132.55
25	A	1125	CLA	CMA-C3A-C4A	2.54	118.59	111.77
25	7	601	CLA	C3B-C4B-NB	-2.54	108.27	110.53
25	B	1229	CLA	CHD-C1D-ND	-2.53	121.23	124.80
25	B	1237	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
25	B	1211	CLA	C1C-C2C-C3C	-2.53	104.31	106.98
25	4	601	CLA	C4B-CHC-C1C	2.53	132.21	126.25
25	6	605	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
25	A	1140	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	A	1116	CLA	C4B-CHC-C1C	2.53	132.21	126.25
25	B	1214	CLA	C3B-C4B-NB	-2.53	108.27	110.53
25	B	1207	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	H	1703	CLA	CHD-C1D-ND	-2.53	121.24	124.80
29	A	4001	BCR	C19-C18-C17	2.53	122.99	119.01
25	B	1220	CLA	CHD-C1D-ND	-2.53	121.24	124.80
44	7	504	AXT	C38-C25-C26	-2.53	120.04	124.11
25	A	1119	CLA	C2C-C1C-NC	2.53	112.64	109.98
26	9	608	CHL	C4D-CHA-CBD	-2.53	106.41	108.97
25	A	1115	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
25	J	1901	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
25	A	1110	CLA	C2C-C1C-NC	2.53	112.64	109.98
25	B	1208	CLA	C2C-C1C-NC	2.53	112.64	109.98
29	O	4001	BCR	C33-C5-C4	2.53	118.99	113.60
29	8	503	BCR	C33-C5-C4	2.53	118.99	113.60
25	B	1213	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	7	603	CLA	C4B-CHC-C1C	2.53	132.19	126.25
25	B	1021	CLA	CHA-C4D-ND	2.53	137.76	132.55
43	a	503	LUT	C31-C32-C33	-2.53	119.43	126.36
25	B	1213	CLA	C1-O2A-CGA	2.53	122.77	116.65
25	3	605	CLA	CHA-C4D-ND	2.53	137.76	132.55
25	8	608	CLA	CHD-C1D-ND	-2.53	121.25	124.80
25	A	1110	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
25	8	602	CLA	CMA-C3A-C4A	2.53	118.56	111.77
25	A	1113	CLA	CHD-C1D-ND	-2.53	121.25	124.80
26	9	603	CHL	C1A-CHA-C4D	2.53	123.20	118.98
25	A	1118	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
25	a	603	CLA	O2D-CGD-O1D	-2.52	118.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	612	CLA	CMA-C3A-C4A	2.52	118.56	111.77
25	B	1232	CLA	C4B-CHC-C1C	2.52	132.18	126.25
25	A	1137	CLA	C2C-C1C-NC	2.52	112.63	109.98
25	5	604	CLA	C4B-CHC-C1C	2.52	132.18	126.25
25	6	606	CLA	C4B-CHC-C1C	2.52	132.18	126.25
25	B	1208	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	2	615	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	2	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
36	8	802	DGD	O1G-C1A-C2A	2.52	119.53	111.83
25	3	607	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	A	1109	CLA	CHD-C1D-ND	-2.52	121.25	124.80
25	a	601	CLA	CHD-C1D-ND	-2.52	121.25	124.80
25	2	604	CLA	C1-O2A-CGA	2.52	122.76	116.65
29	H	4001	BCR	C33-C5-C6	-2.52	121.73	124.48
43	9	501	LUT	C27-C28-C29	-2.52	120.90	126.32
25	8	615	CLA	C2D-C1D-ND	2.52	112.62	110.13
24	A	1011	CL0	CAA-C2A-C3A	-2.52	106.19	113.00
25	7	601	CLA	CHD-C1D-ND	-2.52	121.25	124.80
25	9	604	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
25	7	606	CLA	C4B-CHC-C1C	2.52	132.17	126.25
25	A	1108	CLA	CHD-C1D-ND	-2.52	121.26	124.80
25	3	606	CLA	C4B-CHC-C1C	2.52	132.17	126.25
26	1	611	CHL	CMA-C3A-C4A	2.52	120.04	114.61
25	B	1204	CLA	C4B-CHC-C1C	2.52	132.17	126.25
25	B	1216	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
25	B	1213	CLA	CMA-C3A-C4A	2.52	118.54	111.77
43	3	502	LUT	C30-C31-C32	-2.52	115.91	123.20
26	2	610	CHL	C4D-CHA-CBD	-2.52	106.43	108.97
25	B	1226	CLA	CHD-C1D-ND	-2.52	121.26	124.80
25	A	1113	CLA	C1C-C2C-C3C	-2.51	104.33	106.98
25	J	1901	CLA	CHA-C4D-ND	2.51	137.74	132.55
29	6	504	BCR	C28-C27-C26	-2.51	109.57	114.06
25	A	1122	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
25	A	1137	CLA	CHD-C1D-ND	-2.51	121.27	124.80
25	6	601	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
29	L	4003	BCR	C30-C25-C26	-2.51	119.20	122.64
25	A	1125	CLA	CHA-C4D-ND	2.51	137.73	132.55
25	8	612	CLA	C3B-C4B-NB	-2.51	108.29	110.53
26	8	603	CHL	C4D-CHA-CBD	-2.51	106.43	108.97
26	6	610	CHL	CMA-C3A-C4A	2.51	120.02	114.61
26	4	613	CHL	C1-C2-C3	-2.51	122.08	126.20
25	A	1140	CLA	CMA-C3A-C4A	2.51	118.52	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	608	CLA	C4B-CHC-C1C	2.51	132.15	126.25
30	A	5003	LHG	C5-O7-C7	-2.51	111.79	117.80
25	B	1239	CLA	C4B-CHC-C1C	2.51	132.15	126.25
25	A	1104	CLA	CHA-C4D-ND	2.51	137.73	132.55
25	3	602	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
25	B	1022	CLA	CMA-C3A-C4A	2.51	118.52	111.77
26	7	615	CHL	C4D-CHA-CBD	-2.51	106.44	108.97
25	B	1210	CLA	C4B-CHC-C1C	2.51	132.15	126.25
43	2	507	LUT	C22-C23-C24	-2.51	107.46	111.18
25	4	603	CLA	C2C-C1C-NC	2.51	112.62	109.98
26	7	611	CHL	C4D-CHA-CBD	-2.51	106.44	108.97
25	4	606	CLA	CHA-C4D-ND	2.51	137.72	132.55
29	A	4003	BCR	C23-C24-C25	-2.51	120.30	127.00
25	B	1021	CLA	C2C-C1C-NC	2.51	112.61	109.98
43	1	503	LUT	C19-C9-C8	2.51	121.92	118.09
25	B	1214	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
25	B	1223	CLA	O2A-CGA-CBA	2.51	119.48	111.83
43	2	502	LUT	C40-C33-C32	2.51	121.92	118.09
25	B	1213	CLA	CHD-C1D-ND	-2.51	121.28	124.80
25	6	603	CLA	O2A-CGA-CBA	2.51	119.47	111.83
25	5	604	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
25	1	615	CLA	CHA-C4D-ND	2.51	137.72	132.55
25	A	1139	CLA	C2C-C1C-NC	2.50	112.61	109.98
25	2	607	CLA	CHA-C4D-ND	2.50	137.72	132.55
43	4	502	LUT	C35-C15-C14	-2.50	118.40	123.52
25	7	610	CLA	C4B-CHC-C1C	2.50	132.13	126.25
43	9	502	LUT	C10-C11-C12	-2.50	115.95	123.20
25	9	602	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
25	B	1240	CLA	C4B-CHC-C1C	2.50	132.13	126.25
25	B	1231	CLA	O2A-CGA-CBA	2.50	119.46	111.83
43	5	501	LUT	C11-C10-C9	-2.50	123.77	127.28
26	5	618	CHL	CMA-C3A-C4A	2.50	120.00	114.61
29	5	504	BCR	C27-C26-C25	-2.50	119.33	122.70
25	a	601	CLA	C4B-CHC-C1C	2.50	132.13	126.25
30	9	801	LHG	C5-O7-C7	-2.50	111.81	117.80
43	8	501	LUT	C11-C10-C9	-2.50	123.77	127.28
25	5	604	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
26	6	617	CHL	CMA-C3A-C4A	2.50	120.00	114.61
25	4	603	CLA	C1-O2A-CGA	2.50	122.70	116.65
25	B	1230	CLA	C1D-ND-C4D	-2.50	104.56	106.31
25	2	602	CLA	C4B-CHC-C1C	2.50	132.12	126.25
25	a	605	CLA	O2D-CGD-O1D	-2.50	118.98	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	604	CHL	C1C-C2C-CMC	2.50	131.31	126.80
25	B	1221	CLA	CHA-C4D-ND	2.50	137.70	132.55
25	B	1208	CLA	CHD-C1D-ND	-2.50	121.29	124.80
25	2	604	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
25	4	617	CLA	C4B-CHC-C1C	2.50	132.12	126.25
25	7	607	CLA	O2A-CGA-CBA	2.50	119.45	111.83
25	O	1802	CLA	C1-O2A-CGA	2.50	122.69	116.65
25	4	617	CLA	C3B-C4B-NB	-2.50	108.30	110.53
26	1	609	CHL	CMA-C3A-C4A	2.50	119.99	114.61
29	5	503	BCR	C36-C18-C17	-2.50	118.77	122.82
29	J	4001	BCR	C35-C13-C12	2.50	121.90	118.09
25	J	1901	CLA	C4B-CHC-C1C	2.50	132.12	126.25
25	7	602	CLA	C4B-CHC-C1C	2.50	132.12	126.25
25	O	1802	CLA	C1C-C2C-C3C	-2.50	104.36	106.98
25	7	612	CLA	O2A-CGA-CBA	2.50	119.44	111.83
25	A	1126	CLA	CHD-C1D-ND	-2.50	121.29	124.80
25	B	1239	CLA	O2A-CGA-CBA	2.49	119.44	111.83
25	B	1232	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
25	a	605	CLA	CHA-C4D-ND	2.49	137.70	132.55
25	4	601	CLA	CHD-C1D-ND	-2.49	121.29	124.80
25	4	612	CLA	CHA-C4D-ND	2.49	137.69	132.55
25	A	1102	CLA	CHA-C4D-ND	2.49	137.69	132.55
25	K	1403	CLA	CHA-C4D-ND	2.49	137.69	132.55
24	A	1011	CL0	C4-C3-C5	2.49	119.56	115.23
25	B	1231	CLA	CHA-C4D-ND	2.49	137.69	132.55
25	H	1702	CLA	CHA-C4D-ND	2.49	137.69	132.55
40	J	4002	RRX	C20-C21-C22	-2.49	123.78	127.28
25	B	1201	CLA	CMA-C3A-C4A	2.49	118.47	111.77
25	6	608	CLA	CHA-C4D-ND	2.49	137.69	132.55
26	1	613	CHL	CMA-C3A-C4A	2.49	119.98	114.61
25	A	1119	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	4	611	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	6	607	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	B	1206	CLA	CMA-C3A-C4A	2.49	118.47	111.77
25	A	1134	CLA	O2A-CGA-CBA	2.49	119.43	111.83
25	A	1122	CLA	CHD-C1D-ND	-2.49	121.30	124.80
25	7	612	CLA	CMA-C3A-C4A	2.49	118.47	111.77
25	A	1105	CLA	CHD-C1D-ND	-2.49	121.30	124.80
25	A	1103	CLA	C2C-C1C-NC	2.49	112.60	109.98
25	B	1238	CLA	C2C-C1C-NC	2.49	112.60	109.98
25	B	1215	CLA	CHD-C1D-ND	-2.49	121.30	124.80
26	8	603	CHL	C1C-C2C-CMC	2.49	131.29	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1137	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
25	A	1106	CLA	C1D-ND-C4D	-2.49	104.57	106.31
25	8	605	CLA	C1D-ND-C4D	-2.49	104.57	106.31
35	1	804	LMT	O5B-C5B-C4B	2.49	114.18	109.70
25	3	616	CLA	O2A-CGA-CBA	2.49	119.42	111.83
25	6	618	CLA	C4B-CHC-C1C	2.49	132.10	126.25
25	A	1108	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
25	A	1126	CLA	CHA-C4D-ND	2.49	137.68	132.55
29	6	503	BCR	C38-C26-C25	-2.49	121.77	124.48
25	5	605	CLA	CMA-C3A-C4A	2.49	118.46	111.77
25	B	1229	CLA	C1D-ND-C4D	-2.49	104.57	106.31
25	2	606	CLA	C4B-CHC-C1C	2.49	132.09	126.25
25	A	1132	CLA	C3B-C4B-NB	-2.49	108.31	110.53
25	B	1201	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
25	B	1239	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
26	3	611	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
25	9	604	CLA	C4B-CHC-C1C	2.49	132.09	126.25
25	2	605	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
26	3	603	CHL	CMA-C3A-C4A	2.48	119.97	114.61
25	B	1240	CLA	C3B-C4B-NB	-2.48	108.31	110.53
25	7	612	CLA	C3B-C4B-NB	-2.48	108.31	110.53
25	A	1132	CLA	CHA-C4D-ND	2.48	137.68	132.55
25	L	1503	CLA	CHA-C4D-ND	2.48	137.68	132.55
25	B	1236	CLA	O2A-CGA-CBA	2.48	119.41	111.83
25	B	1218	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	a	603	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	B	1220	CLA	O2A-CGA-CBA	2.48	119.41	111.83
43	a	501	LUT	C22-C23-C24	-2.48	107.50	111.18
26	3	604	CHL	C1C-C2C-CMC	2.48	131.28	126.80
25	A	1107	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	6	608	CLA	CHD-C1D-ND	-2.48	121.31	124.80
29	B	4003	BCR	C12-C13-C14	-2.48	115.11	119.01
25	A	1124	CLA	C3B-C4B-NB	-2.48	108.31	110.53
25	3	610	CLA	CHD-C1D-ND	-2.48	121.31	124.80
25	G	1602	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
25	4	616	CLA	C4B-CHC-C1C	2.48	132.08	126.25
26	a	606	CHL	C4D-CHA-CBD	-2.48	106.47	108.97
25	A	1101	CLA	CHA-C4D-ND	2.48	137.66	132.55
25	2	621	CLA	CHA-C4D-ND	2.48	137.66	132.55
43	3	502	LUT	C22-C23-C24	-2.48	107.50	111.18
25	4	606	CLA	C4B-CHC-C1C	2.48	132.07	126.25
25	1	608	CLA	C2C-C1C-NC	2.48	112.58	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	611	CHL	C1-C2-C3	-2.48	122.14	126.20
25	K	1402	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	B	1211	CLA	CHA-C4D-ND	2.48	137.66	132.55
25	A	1137	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
43	5	502	LUT	C35-C15-C14	-2.48	118.45	123.52
25	B	1203	CLA	CHA-C4D-ND	2.48	137.66	132.55
25	1	608	CLA	C4B-CHC-C1C	2.48	132.07	126.25
25	1	601	CLA	CHD-C1D-ND	-2.48	121.32	124.80
25	A	1139	CLA	C1C-C2C-C3C	-2.48	104.38	106.98
25	F	1301	CLA	C1C-C2C-C3C	-2.48	104.38	106.98
25	A	1133	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
25	B	1213	CLA	C3B-C4B-NB	-2.48	108.32	110.53
25	a	607	CLA	O2A-CGA-CBA	2.48	119.38	111.83
25	8	609	CLA	C4B-CHC-C1C	2.48	132.07	126.25
25	A	1117	CLA	CHA-C4D-ND	2.48	137.66	132.55
26	9	601	CHL	CMA-C3A-C4A	2.48	119.94	114.61
25	A	1111	CLA	CHA-C4D-ND	2.47	137.66	132.55
25	1	605	CLA	C2C-C1C-NC	2.47	112.58	109.98
25	7	603	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
25	H	1701	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
26	7	609	CHL	C4D-CHA-CBD	-2.47	106.47	108.97
25	A	1121	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
25	A	1138	CLA	O2A-CGA-CBA	2.47	119.37	111.83
29	B	4004	BCR	C4-C5-C6	-2.47	119.36	122.70
25	9	606	CLA	C4B-CHC-C1C	2.47	132.06	126.25
25	4	610	CLA	CHA-C4D-ND	2.47	137.65	132.55
25	5	603	CLA	C3B-C4B-NB	-2.47	108.32	110.53
25	B	1205	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
25	7	601	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
25	B	1216	CLA	CHD-C1D-ND	-2.47	121.32	124.80
25	8	606	CLA	CHD-C1D-ND	-2.47	121.32	124.80
25	5	614	CLA	CMA-C3A-C4A	2.47	118.42	111.77
25	1	601	CLA	C4B-CHC-C1C	2.47	132.06	126.25
25	a	615	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
25	B	1236	CLA	CHA-C4D-ND	2.47	137.65	132.55
25	6	602	CLA	CMA-C3A-C4A	2.47	118.41	111.77
25	A	1107	CLA	CHA-C4D-ND	2.47	137.65	132.55
25	B	1214	CLA	C4B-CHC-C1C	2.47	132.06	126.25
25	5	604	CLA	C1D-ND-C4D	-2.47	104.58	106.31
25	2	612	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	6	606	CLA	CHA-C4D-ND	2.47	137.64	132.55
26	1	609	CHL	C1-O2A-CGA	2.47	122.63	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	4007	BCR	C19-C18-C17	2.47	122.89	119.01
25	6	618	CLA	CHD-C1D-ND	-2.47	121.33	124.80
26	4	618	CHL	C1-C2-C3	-2.47	122.15	126.20
29	3	503	BCR	C35-C13-C12	2.47	121.86	118.09
43	a	501	LUT	C8-C7-C6	-2.47	120.41	127.00
25	A	1129	CLA	CHA-C4D-ND	2.47	137.64	132.55
30	4	801	LHG	O8-C23-C24	2.47	119.36	111.83
25	4	615	CLA	O2A-CGA-CBA	2.47	119.36	111.83
25	L	1503	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	5	612	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	B	1234	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	B	1227	CLA	C4B-CHC-C1C	2.47	132.05	126.25
25	4	617	CLA	CHA-C4D-ND	2.47	137.64	132.55
25	B	1236	CLA	CHD-C1D-ND	-2.47	121.33	124.80
25	4	603	CLA	CHD-C1D-ND	-2.47	121.33	124.80
30	B	5001	LHG	O8-C23-C24	2.47	119.35	111.83
25	2	608	CLA	C3B-C4B-NB	-2.47	108.33	110.53
25	3	613	CLA	C2C-C1C-NC	2.46	112.57	109.98
25	8	607	CLA	CHA-C4D-ND	2.46	137.63	132.55
25	4	606	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
25	8	615	CLA	C1D-ND-C4D	-2.46	104.58	106.31
29	L	4002	BCR	C12-C13-C14	-2.46	115.13	119.01
25	1	602	CLA	CHA-C4D-ND	2.46	137.63	132.55
25	1	612	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
25	7	610	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
25	L	1502	CLA	CHD-C1D-ND	-2.46	121.34	124.80
30	A	5001	LHG	C5-O7-C7	-2.46	111.90	117.80
26	3	603	CHL	C1-O2A-CGA	2.46	122.61	116.65
25	3	618	CLA	CHA-C4D-ND	2.46	137.63	132.55
25	a	615	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	B	1219	CLA	O2A-CGA-CBA	2.46	119.34	111.83
25	2	601	CLA	C4B-CHC-C1C	2.46	132.03	126.25
25	5	602	CLA	CHA-C4D-ND	2.46	137.63	132.55
25	8	620	CLA	CHA-C4D-ND	2.46	137.63	132.55
25	L	1504	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	4	607	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	4	615	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	2	603	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	5	603	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
25	A	1125	CLA	C2D-C1D-ND	2.46	112.56	110.13
25	B	1235	CLA	C2C-C1C-NC	2.46	112.56	109.98
29	3	505	BCR	C27-C26-C25	-2.46	119.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	613	CHL	C4C-CHD-C1D	2.46	124.87	116.07
25	4	608	CLA	C3B-C4B-NB	-2.46	108.33	110.53
43	a	503	LUT	C22-C23-C24	-2.46	107.53	111.18
25	4	606	CLA	C2C-C1C-NC	2.46	112.56	109.98
25	4	616	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
29	A	4003	BCR	C33-C5-C4	2.46	118.84	113.60
25	A	1113	CLA	CMA-C3A-C4A	2.46	118.38	111.77
25	8	618	CLA	O2A-CGA-CBA	2.46	119.33	111.83
40	3	506	RRX	C33-C5-C4	2.46	118.83	113.60
29	8	503	BCR	C38-C26-C25	-2.46	121.80	124.48
25	F	1301	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	2	612	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	B	1228	CLA	CHD-C1D-ND	-2.46	121.34	124.80
25	B	1235	CLA	C3B-C4B-NB	-2.46	108.34	110.53
25	A	1134	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	1	606	CLA	C4B-CHC-C1C	2.46	132.02	126.25
26	2	609	CHL	C4D-CHA-CBD	-2.46	106.49	108.97
25	5	601	CLA	C2C-C1C-NC	2.46	112.56	109.98
25	4	604	CLA	CHA-C4D-ND	2.46	137.62	132.55
25	3	610	CLA	CMA-C3A-C4A	2.46	118.37	111.77
43	4	501	LUT	C31-C30-C29	-2.46	123.83	127.28
25	B	1212	CLA	C4B-CHC-C1C	2.45	132.02	126.25
25	B	1023	CLA	CAA-C2A-C3A	-2.45	106.36	113.00
25	A	1121	CLA	CHA-C4D-ND	2.45	137.61	132.55
30	8	801	LHG	C5-O7-C7	-2.45	111.92	117.80
25	B	1239	CLA	CHD-C1D-ND	-2.45	121.35	124.80
25	5	603	CLA	CHD-C1D-ND	-2.45	121.35	124.80
25	A	1122	CLA	C4B-CHC-C1C	2.45	132.02	126.25
25	8	602	CLA	CHA-C4D-ND	2.45	137.61	132.55
25	5	603	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
25	K	1402	CLA	CHA-C4D-ND	2.45	137.61	132.55
25	4	615	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
25	B	1220	CLA	C1D-ND-C4D	-2.45	104.59	106.31
25	F	1301	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
25	B	1212	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
29	6	503	BCR	C8-C7-C6	-2.45	120.45	127.00
29	5	504	BCR	C1-C6-C5	-2.45	119.29	122.64
25	1	605	CLA	CMA-C3A-C4A	2.45	118.36	111.77
25	2	606	CLA	CMA-C3A-C4A	2.45	118.36	111.77
25	a	612	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	9	605	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	A	1106	CLA	O1D-CGD-CBD	-2.45	119.68	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	H	4001	BCR	C15-C14-C13	-2.45	123.84	127.28
25	O	1801	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
25	A	1109	CLA	CHA-C4D-ND	2.45	137.60	132.55
25	A	1132	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
25	F	1301	CLA	C4B-CHC-C1C	2.45	132.01	126.25
25	4	605	CLA	CMA-C3A-C4A	2.45	118.36	111.77
25	8	612	CLA	C2C-C1C-NC	2.45	112.55	109.98
25	8	620	CLA	C3B-C4B-NB	-2.45	108.34	110.53
26	9	613	CHL	CMA-C3A-C4A	2.45	119.89	114.61
25	a	602	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
43	6	502	LUT	C31-C30-C29	-2.45	123.84	127.28
25	A	1108	CLA	C2C-C1C-NC	2.45	112.55	109.98
25	4	605	CLA	C3B-C4B-NB	-2.45	108.34	110.53
25	1	605	CLA	C1D-ND-C4D	-2.45	104.59	106.31
25	a	612	CLA	CHA-C4D-ND	2.45	137.60	132.55
25	6	618	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
43	8	502	LUT	C31-C30-C29	-2.45	123.85	127.28
25	A	1115	CLA	C2C-C1C-NC	2.45	112.55	109.98
25	B	1211	CLA	C2C-C1C-NC	2.45	112.55	109.98
26	1	611	CHL	C1-O2A-CGA	2.45	122.57	116.65
25	B	1219	CLA	CHD-C1D-ND	-2.45	121.36	124.80
25	3	616	CLA	C1-O2A-CGA	2.45	122.57	116.65
25	H	1701	CLA	CHA-C4D-ND	2.45	137.59	132.55
25	B	1211	CLA	C4B-CHC-C1C	2.45	132.00	126.25
30	7	803	LHG	C5-O7-C7	-2.45	111.94	117.80
25	B	1209	CLA	C2C-C1C-NC	2.44	112.55	109.98
25	A	1119	CLA	C4B-CHC-C1C	2.44	132.00	126.25
25	B	1213	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
25	5	614	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	B	1223	CLA	C2D-C1D-ND	2.44	112.55	110.13
25	A	1136	CLA	CHD-C1D-ND	-2.44	121.36	124.80
29	3	504	BCR	C30-C25-C26	-2.44	119.30	122.64
25	4	610	CLA	C4B-CHC-C1C	2.44	131.99	126.25
25	A	1123	CLA	CHA-C4D-ND	2.44	137.59	132.55
25	7	603	CLA	CHA-C4D-ND	2.44	137.59	132.55
25	4	602	CLA	CHA-C4D-ND	2.44	137.59	132.55
26	3	608	CHL	C4D-CHA-CBD	-2.44	106.50	108.97
25	5	612	CLA	O2A-CGA-CBA	2.44	119.28	111.83
25	8	609	CLA	CHA-C4D-ND	2.44	137.59	132.55
25	9	612	CLA	CHA-C4D-ND	2.44	137.59	132.55
25	B	1214	CLA	CHA-C4D-ND	2.44	137.59	132.55
25	9	606	CLA	C1C-C2C-C3C	-2.44	104.41	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	608	CLA	C4B-CHC-C1C	2.44	131.99	126.25
26	5	618	CHL	C1-O2A-CGA	2.44	122.56	116.65
40	J	4002	RRX	C35-C13-C14	-2.44	118.86	122.82
25	B	1209	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
25	O	1801	CLA	C4B-CHC-C1C	2.44	131.99	126.25
25	7	606	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
25	A	1113	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	9	604	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	A	1135	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
25	3	605	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
25	3	613	CLA	C3B-C4B-NB	-2.44	108.35	110.53
25	3	607	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	B	1210	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	A	1138	CLA	C4B-CHC-C1C	2.44	131.98	126.25
25	O	1803	CLA	C4B-CHC-C1C	2.44	131.98	126.25
25	5	606	CLA	C4B-CHC-C1C	2.44	131.98	126.25
25	B	1209	CLA	CHD-C1D-ND	-2.44	121.37	124.80
25	a	605	CLA	C4B-CHC-C1C	2.44	131.98	126.25
25	A	1139	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	5	606	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	6	602	CLA	CHA-C4D-ND	2.44	137.58	132.55
25	L	1502	CLA	C3B-C4B-NB	-2.44	108.36	110.53
25	6	605	CLA	C4B-CHC-C1C	2.44	131.98	126.25
25	A	1128	CLA	CHA-C4D-ND	2.44	137.57	132.55
25	a	601	CLA	CMA-C3A-C4A	2.44	118.32	111.77
25	2	612	CLA	C4B-CHC-C1C	2.44	131.97	126.25
25	A	1110	CLA	CHD-C1D-ND	-2.44	121.38	124.80
25	2	601	CLA	CHD-C1D-ND	-2.44	121.38	124.80
25	O	1802	CLA	C4B-CHC-C1C	2.44	131.97	126.25
25	a	605	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
25	9	612	CLA	C3B-C4B-NB	-2.44	108.36	110.53
25	a	612	CLA	CMA-C3A-C4A	2.44	118.32	111.77
25	2	602	CLA	CHA-C4D-ND	2.44	137.57	132.55
25	B	1023	CLA	CHD-C1D-ND	-2.43	121.38	124.80
25	B	1222	CLA	C1D-ND-C4D	-2.43	104.60	106.31
25	7	601	CLA	CHA-C4D-ND	2.43	137.57	132.55
24	A	1011	CL0	CMC-C2C-C1C	2.43	129.11	124.73
25	A	1116	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
25	L	1502	CLA	C4B-CHC-C1C	2.43	131.97	126.25
25	3	605	CLA	C4B-CHC-C1C	2.43	131.97	126.25
40	J	4002	RRX	C2-C1-C6	2.43	113.97	110.44
25	7	604	CLA	C4B-CHC-C1C	2.43	131.97	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	610	CLA	CHA-C4D-ND	2.43	137.57	132.55
25	A	1127	CLA	C2C-C1C-NC	2.43	112.54	109.98
25	8	611	CLA	C2C-C1C-NC	2.43	112.54	109.98
25	A	1127	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
25	5	609	CLA	O2A-CGA-CBA	2.43	119.25	111.83
25	A	1135	CLA	CHA-C4D-ND	2.43	137.57	132.55
25	B	1213	CLA	CHA-C4D-ND	2.43	137.57	132.55
25	7	606	CLA	CHA-C4D-ND	2.43	137.57	132.55
25	B	1231	CLA	C1D-ND-C4D	-2.43	104.61	106.31
25	B	1201	CLA	C4B-CHC-C1C	2.43	131.96	126.25
25	1	603	CLA	C4B-CHC-C1C	2.43	131.96	126.25
25	O	1801	CLA	CHA-C4D-ND	2.43	137.56	132.55
29	B	4005	BCR	C37-C22-C23	2.43	121.80	118.09
25	A	1131	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	G	1602	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	3	602	CLA	CHA-C4D-ND	2.43	137.56	132.55
43	3	502	LUT	C31-C30-C29	-2.43	123.87	127.28
36	8	802	DGD	C3G-O3G-C1D	-2.43	108.59	113.80
25	1	601	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	6	603	CLA	CHD-C1D-ND	-2.43	121.38	124.80
25	A	1105	CLA	C1D-ND-C4D	-2.43	104.61	106.31
25	6	612	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	B	1223	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
25	O	1802	CLA	CHD-C1D-ND	-2.43	121.39	124.80
26	a	610	CHL	CMA-C3A-C4A	2.43	119.84	114.61
25	A	1140	CLA	O2A-CGA-CBA	2.43	119.24	111.83
25	G	1603	CLA	CHD-C1D-ND	-2.43	121.39	124.80
25	A	1109	CLA	O2A-CGA-CBA	2.43	119.23	111.83
25	1	612	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	5	603	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	5	607	CLA	O2A-CGA-CBA	2.43	119.23	111.83
25	5	607	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	1	607	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	9	607	CLA	CHA-C4D-ND	2.43	137.56	132.55
25	1	607	CLA	CHD-C1D-ND	-2.43	121.39	124.80
29	O	4001	BCR	C38-C26-C27	2.43	118.77	113.60
25	9	605	CLA	CMA-C3A-C4A	2.43	118.29	111.77
25	A	1140	CLA	CHA-C4D-ND	2.43	137.55	132.55
25	4	604	CLA	C4B-CHC-C1C	2.42	131.95	126.25
25	O	1803	CLA	CHA-C4D-ND	2.42	137.55	132.55
25	A	1116	CLA	CHA-C4D-ND	2.42	137.55	132.55
25	2	606	CLA	CHA-C4D-ND	2.42	137.55	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	606	CLA	CHA-C4D-ND	2.42	137.55	132.55
25	G	1601	CLA	CHA-C4D-ND	2.42	137.55	132.55
25	2	608	CLA	CHA-C4D-ND	2.42	137.55	132.55
25	8	609	CLA	C2D-C1D-ND	2.42	112.52	110.13
25	2	608	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
29	H	4001	BCR	C36-C18-C17	-2.42	118.89	122.82
25	6	605	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	a	603	CLA	C4B-CHC-C1C	2.42	131.94	126.25
25	B	1205	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	7	607	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	5	606	CLA	CMA-C3A-C4A	2.42	118.28	111.77
25	6	615	CLA	C3B-C4B-NB	-2.42	108.37	110.53
25	5	609	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	5	608	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	B	1224	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	a	615	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	B	1222	CLA	C4B-CHC-C1C	2.42	131.94	126.25
25	4	608	CLA	C4B-CHC-C1C	2.42	131.94	126.25
25	1	605	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	B	1239	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	9	602	CLA	CHA-C4D-ND	2.42	137.54	132.55
26	1	609	CHL	C4C-CHD-C1D	2.42	124.72	116.07
25	3	606	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	9	612	CLA	O2A-CGA-CBA	2.42	119.21	111.83
25	6	601	CLA	C4B-CHC-C1C	2.42	131.93	126.25
25	B	1212	CLA	CHA-C4D-ND	2.42	137.54	132.55
26	1	604	CHL	C1-O2A-CGA	2.42	122.50	116.65
25	B	1203	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	1	605	CLA	CHA-C4D-ND	2.42	137.54	132.55
25	B	1202	CLA	CMA-C3A-C4A	2.42	118.27	111.77
25	4	615	CLA	CMA-C3A-C4A	2.42	118.27	111.77
43	1	501	LUT	C11-C10-C9	-2.42	123.89	127.28
25	2	605	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	5	614	CLA	CHA-C4D-ND	2.42	137.54	132.55
29	B	4005	BCR	C8-C7-C6	-2.42	120.54	127.00
25	8	620	CLA	CHD-C1D-ND	-2.42	121.40	124.80
25	3	612	CLA	CHA-C4D-ND	2.42	137.53	132.55
25	4	616	CLA	CHA-C4D-ND	2.42	137.53	132.55
25	1	615	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
25	B	1240	CLA	CHA-C4D-ND	2.42	137.53	132.55
43	7	501	LUT	C22-C23-C24	-2.42	107.60	111.18
25	3	613	CLA	C1C-C2C-C3C	-2.42	104.44	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	605	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
43	8	501	LUT	C22-C23-C24	-2.42	107.60	111.18
25	4	607	CLA	CHA-C4D-ND	2.41	137.53	132.55
25	2	604	CLA	CHA-C4D-ND	2.41	137.53	132.55
25	3	601	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	2	606	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	5	601	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
29	5	503	BCR	C15-C14-C13	-2.41	123.89	127.28
25	B	1224	CLA	CHA-C4D-ND	2.41	137.53	132.55
25	4	611	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	7	612	CLA	CHA-C4D-ND	2.41	137.53	132.55
43	8	502	LUT	C15-C14-C13	-2.41	123.89	127.28
26	a	609	CHL	C4D-CHA-CBD	-2.41	106.53	108.97
29	A	4002	BCR	C27-C26-C25	-2.41	119.44	122.70
25	L	1501	CLA	C4B-CHC-C1C	2.41	131.92	126.25
29	3	505	BCR	C19-C18-C17	2.41	122.80	119.01
25	B	1230	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	B	1232	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	B	1207	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	6	612	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	A	1107	CLA	C4B-CHC-C1C	2.41	131.92	126.25
25	5	601	CLA	C4B-CHC-C1C	2.41	131.92	126.25
25	A	1111	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	A	1118	CLA	O2A-CGA-CBA	2.41	119.19	111.83
25	B	1235	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	8	620	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
25	A	1108	CLA	C1D-ND-C4D	-2.41	104.62	106.31
25	B	1240	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
25	A	1119	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
25	5	609	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
25	8	605	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
25	A	1110	CLA	O2A-CGA-CBA	2.41	119.18	111.83
25	7	605	CLA	C4B-CHC-C1C	2.41	131.91	126.25
25	B	1226	CLA	O2A-CGA-CBA	2.41	119.18	111.83
43	1	501	LUT	C35-C15-C14	-2.41	118.59	123.52
25	7	602	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	B	1216	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	7	604	CLA	CHA-C4D-ND	2.41	137.52	132.55
25	A	1132	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	7	612	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	B	1208	CLA	C4B-CHC-C1C	2.41	131.91	126.25
25	A	1115	CLA	CHA-C4D-ND	2.41	137.52	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	606	CLA	C4B-CHC-C1C	2.41	131.91	126.25
25	A	1137	CLA	C1D-ND-C4D	-2.41	104.62	106.31
25	1	606	CLA	O2A-CGA-CBA	2.41	119.17	111.83
25	A	1116	CLA	C2C-C1C-NC	2.41	112.51	109.98
25	5	605	CLA	C2C-C1C-NC	2.41	112.51	109.98
25	3	613	CLA	C4B-CHC-C1C	2.41	131.91	126.25
25	9	609	CLA	CHA-C4D-ND	2.41	137.51	132.55
25	8	615	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
25	B	1217	CLA	CHD-C1D-ND	-2.41	121.42	124.80
26	a	604	CHL	C4D-CHA-CBD	-2.41	106.54	108.97
25	B	1217	CLA	CHA-C4D-ND	2.41	137.51	132.55
25	4	611	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
25	A	1103	CLA	CHA-C4D-ND	2.41	137.51	132.55
25	K	1402	CLA	C4B-CHC-C1C	2.41	131.90	126.25
25	G	1602	CLA	C3B-C4B-NB	-2.41	108.38	110.53
25	a	611	CLA	CHA-C4D-ND	2.41	137.51	132.55
25	1	612	CLA	CHD-C1D-ND	-2.40	121.42	124.80
25	B	1225	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
25	A	1130	CLA	CHD-C1D-ND	-2.40	121.42	124.80
29	8	503	BCR	C36-C18-C17	-2.40	118.92	122.82
25	a	612	CLA	O2A-CGA-CBA	2.40	119.17	111.83
25	1	606	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
25	B	1220	CLA	C3B-C4B-NB	-2.40	108.38	110.53
46	a	504	QTB	C13-C12-C14	2.40	115.55	111.06
24	A	1011	CL0	C4C-CHD-C1D	2.40	124.67	116.07
25	L	1503	CLA	CMA-C3A-C4A	2.40	118.23	111.77
25	A	1130	CLA	CHA-C4D-ND	2.40	137.51	132.55
25	G	1602	CLA	C4B-CHC-C1C	2.40	131.90	126.25
25	a	608	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
25	A	1129	CLA	C4B-CHC-C1C	2.40	131.90	126.25
25	B	1023	CLA	CHA-C4D-ND	2.40	137.51	132.55
25	1	601	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
25	8	615	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	A	1117	CLA	CHD-C1D-ND	-2.40	121.42	124.80
25	A	1121	CLA	C4B-CHC-C1C	2.40	131.89	126.25
25	B	1216	CLA	C4B-CHC-C1C	2.40	131.89	126.25
25	8	612	CLA	C4B-CHC-C1C	2.40	131.89	126.25
25	K	1404	CLA	CMA-C3A-C4A	2.40	118.23	111.77
25	A	1106	CLA	C2C-C1C-NC	2.40	112.50	109.98
25	A	1111	CLA	C4B-CHC-C1C	2.40	131.89	126.25
25	5	603	CLA	C4B-CHC-C1C	2.40	131.89	126.25
25	B	1238	CLA	CHD-C1D-ND	-2.40	121.42	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	617	CHL	CMA-C3A-C4A	2.40	119.78	114.61
25	A	1137	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	5	615	CLA	C3B-C4B-NB	-2.40	108.39	110.53
25	8	612	CLA	O2A-CGA-CBA	2.40	119.15	111.83
25	8	606	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
25	5	605	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
26	9	603	CHL	C4C-CHD-C1D	2.40	124.65	116.07
25	5	601	CLA	C6-C5-C3	-2.40	107.62	113.47
26	1	610	CHL	CMA-C3A-C4A	2.40	119.78	114.61
25	B	1209	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	B	1219	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	B	1228	CLA	CHA-C4D-ND	2.40	137.50	132.55
25	a	612	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
25	A	1139	CLA	CHD-C1D-ND	-2.40	121.43	124.80
25	G	1602	CLA	CHD-C1D-ND	-2.40	121.43	124.80
25	H	1701	CLA	C4B-CHC-C1C	2.40	131.88	126.25
25	A	1102	CLA	CHD-C1D-ND	-2.40	121.43	124.80
24	A	1011	CL0	O1D-CGD-CBD	-2.40	121.09	124.72
25	A	1106	CLA	CHA-C4D-ND	2.40	137.49	132.55
25	B	1227	CLA	CHA-C4D-ND	2.40	137.49	132.55
25	B	1211	CLA	CMD-C2D-C3D	-2.40	122.20	127.69
25	4	605	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
30	1	801	LHG	C5-O7-C7	-2.40	112.06	117.80
26	3	611	CHL	C1-O2A-CGA	2.39	122.45	116.65
25	A	1136	CLA	CHA-C4D-ND	2.39	137.49	132.55
25	B	1204	CLA	CMA-C3A-C4A	2.39	118.21	111.77
25	F	1302	CLA	C4B-CHC-C1C	2.39	131.88	126.25
25	5	605	CLA	C1C-C2C-C3C	-2.39	104.46	106.98
25	9	607	CLA	C3B-C4B-NB	-2.39	108.39	110.53
25	5	609	CLA	C4B-CHC-C1C	2.39	131.88	126.25
29	A	4002	BCR	C19-C18-C17	2.39	122.77	119.01
25	3	606	CLA	CHA-C4D-ND	2.39	137.49	132.55
26	8	604	CHL	C4C-CHD-C1D	2.39	124.63	116.07
25	a	603	CLA	CHA-C4D-ND	2.39	137.49	132.55
25	a	608	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	A	1113	CLA	C3B-C4B-NB	-2.39	108.39	110.53
25	K	1404	CLA	C3B-C4B-NB	-2.39	108.39	110.53
25	6	603	CLA	C3B-C4B-NB	-2.39	108.39	110.53
25	B	1238	CLA	CHA-C4D-ND	2.39	137.49	132.55
25	6	607	CLA	CHA-C4D-ND	2.39	137.49	132.55
25	5	601	CLA	CHA-C4D-ND	2.39	137.48	132.55
25	B	1239	CLA	CMA-C3A-C4A	2.39	118.20	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1218	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	5	606	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
25	5	607	CLA	CHA-C4D-ND	2.39	137.48	132.55
26	3	603	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
25	8	606	CLA	CHA-C4D-ND	2.39	137.48	132.55
25	9	602	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	B	1202	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	A	1134	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	a	602	CLA	C1D-ND-C4D	-2.39	104.64	106.31
25	a	607	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	B	1222	CLA	C2C-C1C-NC	2.39	112.49	109.98
25	A	1102	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	6	603	CLA	C4B-CHC-C1C	2.39	131.87	126.25
25	B	1220	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	A	1133	CLA	CHA-C4D-ND	2.39	137.48	132.55
25	B	1229	CLA	CHA-C4D-ND	2.39	137.48	132.55
25	O	1802	CLA	O2A-CGA-CBA	2.39	119.12	111.83
25	O	1803	CLA	C3B-C4B-NB	-2.39	108.40	110.53
25	A	1112	CLA	CHA-C4D-ND	2.39	137.48	132.55
25	A	1136	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	4	607	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	9	609	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	A	1124	CLA	O2A-CGA-CBA	2.39	119.11	111.83
43	a	503	LUT	C27-C28-C29	-2.39	121.19	126.32
25	B	1236	CLA	C1D-ND-C4D	-2.39	104.64	106.31
25	4	601	CLA	CMA-C3A-C4A	2.39	118.19	111.77
25	6	601	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
25	H	1703	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	6	618	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
25	A	1119	CLA	CHA-C4D-ND	2.39	137.47	132.55
25	O	1802	CLA	CHA-C4D-ND	2.39	137.47	132.55
26	3	604	CHL	C4C-CHD-C1D	2.39	124.61	116.07
25	7	606	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	J	1901	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
25	3	613	CLA	CHA-C4D-ND	2.39	137.47	132.55
25	5	608	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	2	608	CLA	C4B-CHC-C1C	2.39	131.86	126.25
25	B	1208	CLA	CHA-C4D-ND	2.39	137.47	132.55
26	7	609	CHL	C4C-CHD-C1D	2.39	124.60	116.07
25	H	1702	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
25	A	1121	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
25	8	608	CLA	CHA-C4D-ND	2.39	137.47	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	604	CLA	CHD-C1D-ND	-2.39	121.45	124.80
25	B	1023	CLA	C2C-C1C-NC	2.38	112.49	109.98
25	1	601	CLA	C3B-C4B-NB	-2.38	108.40	110.53
25	8	620	CLA	C4B-CHC-C1C	2.38	131.85	126.25
25	A	1131	CLA	C3B-C4B-NB	-2.38	108.40	110.53
25	A	1127	CLA	CHA-C4D-ND	2.38	137.47	132.55
25	4	612	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
25	B	1201	CLA	CHA-C4D-ND	2.38	137.47	132.55
25	a	602	CLA	CHA-C4D-ND	2.38	137.47	132.55
25	a	607	CLA	CHA-C4D-ND	2.38	137.47	132.55
25	6	615	CLA	CHA-C4D-ND	2.38	137.47	132.55
25	7	601	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
25	B	1202	CLA	CHA-C4D-ND	2.38	137.46	132.55
25	L	1501	CLA	CHD-C1D-ND	-2.38	121.45	124.80
26	5	610	CHL	C1-O2A-CGA	2.38	122.42	116.65
25	6	601	CLA	C2C-C1C-NC	2.38	112.48	109.98
25	A	1137	CLA	O2A-CGA-CBA	2.38	119.10	111.83
29	6	504	BCR	C8-C7-C6	-2.38	120.64	127.00
25	6	601	CLA	CHA-C4D-ND	2.38	137.46	132.55
25	3	616	CLA	C4B-CHC-C1C	2.38	131.85	126.25
25	7	612	CLA	C4B-CHC-C1C	2.38	131.85	126.25
29	B	4004	BCR	C12-C13-C14	-2.38	115.26	119.01
25	7	603	CLA	CHD-C1D-ND	-2.38	121.45	124.80
25	5	615	CLA	CHA-C4D-ND	2.38	137.46	132.55
29	8	503	BCR	C35-C13-C12	2.38	121.72	118.09
25	B	1211	CLA	CHD-C1D-ND	-2.38	121.45	124.80
25	G	1603	CLA	CHA-C4D-ND	2.38	137.46	132.55
25	6	618	CLA	CHA-C4D-ND	2.38	137.46	132.55
25	5	612	CLA	CHA-C4D-ND	2.38	137.46	132.55
25	A	1111	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
25	A	1106	CLA	CHD-C1D-ND	-2.38	121.45	124.80
29	L	4003	BCR	C38-C26-C27	2.38	118.67	113.60
29	3	504	BCR	C38-C26-C27	2.38	118.67	113.60
25	3	606	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
43	3	502	LUT	C35-C15-C14	-2.38	118.65	123.52
25	B	1227	CLA	CHD-C1D-ND	-2.38	121.46	124.80
25	3	612	CLA	O2A-CGA-CBA	2.38	119.08	111.83
25	5	615	CLA	C4B-CHC-C1C	2.38	131.84	126.25
25	7	602	CLA	CHA-C4D-ND	2.38	137.45	132.55
25	7	604	CLA	C6-C5-C3	-2.38	107.68	113.47
25	A	1116	CLA	C1D-ND-C4D	-2.38	104.64	106.31
25	A	1124	CLA	CHD-C1D-ND	-2.38	121.46	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	601	CLA	CHA-C4D-ND	2.38	137.45	132.55
25	4	608	CLA	CHA-C4D-ND	2.38	137.45	132.55
25	5	604	CLA	CHA-C4D-ND	2.38	137.45	132.55
25	6	606	CLA	CHD-C1D-ND	-2.38	121.46	124.80
50	7	502	XAT	O4-C6-C7	-2.38	110.07	116.88
25	4	605	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
25	B	1021	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
25	A	1111	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
25	A	1121	CLA	O2A-CGA-CBA	2.37	119.08	111.83
25	6	612	CLA	CHD-C1D-ND	-2.37	121.46	124.80
25	a	615	CLA	C4B-CHC-C1C	2.37	131.83	126.25
25	F	1302	CLA	CHA-C4D-ND	2.37	137.44	132.55
25	L	1503	CLA	C4B-CHC-C1C	2.37	131.83	126.25
25	3	610	CLA	C4B-CHC-C1C	2.37	131.83	126.25
25	5	609	CLA	CHA-C4D-ND	2.37	137.44	132.55
29	K	4001	BCR	C2-C1-C6	2.37	113.89	110.44
25	9	604	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
25	H	1703	CLA	CHA-C4D-ND	2.37	137.44	132.55
29	A	4005	BCR	C34-C9-C10	-2.37	118.97	122.82
25	9	607	CLA	C4B-CHC-C1C	2.37	131.82	126.25
25	A	1134	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	B	1235	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	4	606	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	A	1013	CLA	O2A-CGA-CBA	2.37	119.06	111.83
25	A	1104	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	3	605	CLA	CMA-C3A-C4A	2.37	118.14	111.77
25	A	1117	CLA	C4B-CHC-C1C	2.37	131.82	126.25
25	A	1138	CLA	CHA-C4D-ND	2.37	137.44	132.55
25	4	603	CLA	CHA-C4D-ND	2.37	137.44	132.55
25	B	1207	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	4	610	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
25	7	607	CLA	C4B-CHC-C1C	2.37	131.82	126.25
25	B	1203	CLA	C1D-ND-C4D	-2.37	104.65	106.31
25	9	606	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	2	607	CLA	C4B-CHC-C1C	2.37	131.82	126.25
25	A	1120	CLA	CHA-C4D-ND	2.37	137.44	132.55
26	1	604	CHL	C4C-CHD-C1D	2.37	124.54	116.07
25	F	1302	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
25	a	615	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
25	5	607	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	3	601	CLA	C3B-C4B-NB	-2.37	108.42	110.53
25	6	608	CLA	C4B-CHC-C1C	2.37	131.81	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1105	CLA	CHA-C4D-ND	2.37	137.43	132.55
25	3	601	CLA	CHA-C4D-ND	2.37	137.43	132.55
35	1	804	LMT	C3'-C4'-C5'	-2.37	105.68	110.93
25	7	605	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
25	A	1133	CLA	C1-O2A-CGA	2.37	122.38	116.65
25	B	1225	CLA	CHA-C4D-ND	2.37	137.43	132.55
26	7	615	CHL	C4C-CHD-C1D	2.37	124.53	116.07
25	8	620	CLA	C1D-ND-C4D	-2.37	104.65	106.31
25	5	603	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
25	3	602	CLA	CMA-C3A-C4A	2.37	118.13	111.77
25	a	612	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	7	610	CLA	CAA-C2A-C3A	-2.37	106.61	113.00
25	B	1221	CLA	CMA-C3A-C4A	2.36	118.13	111.77
25	7	608	CLA	CHA-C4D-ND	2.36	137.43	132.55
26	7	617	CHL	C4C-CHD-C1D	2.36	124.53	116.07
25	1	603	CLA	CHA-C4D-ND	2.36	137.43	132.55
25	4	603	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
39	F	4001	NEX	C11-C10-C9	2.36	130.59	127.28
25	B	1204	CLA	C2D-C1D-ND	2.36	112.47	110.13
25	5	601	CLA	C1D-ND-C4D	-2.36	104.65	106.31
36	B	5003	DGD	O6D-C5D-C6D	2.36	111.38	106.69
25	H	1702	CLA	C3B-C4B-NB	-2.36	108.42	110.53
26	6	613	CHL	C4D-CHA-CBD	-2.36	106.58	108.97
29	6	503	BCR	C19-C18-C17	2.36	122.72	119.01
25	8	620	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
25	4	610	CLA	CHD-C1D-ND	-2.36	121.48	124.80
43	4	502	LUT	C31-C30-C29	-2.36	123.97	127.28
25	7	610	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	a	611	CLA	C4B-CHC-C1C	2.36	131.80	126.25
36	8	802	DGD	C2G-O2G-C1B	-2.36	112.15	117.80
25	A	1131	CLA	CHD-C1D-ND	-2.36	121.48	124.80
42	M	4001	ECH	C11-C12-C13	-2.36	119.89	126.36
25	7	608	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	9	604	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	3	610	CLA	CHA-C4D-ND	2.36	137.42	132.55
25	6	608	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	5	614	CLA	C4B-CHC-C1C	2.36	131.79	126.25
25	A	1112	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	4	608	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	A	1103	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	3	602	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	B	1222	CLA	C3B-C4B-NB	-2.36	108.42	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	606	CLA	C3B-C4B-NB	-2.36	108.42	110.53
25	4	611	CLA	CHA-C4D-ND	2.36	137.41	132.55
25	8	611	CLA	CHD-C1D-ND	-2.36	121.48	124.80
25	K	1401	CLA	CHA-C4D-ND	2.36	137.41	132.55
25	L	1501	CLA	CHA-C4D-ND	2.36	137.41	132.55
43	a	503	LUT	C8-C7-C6	-2.36	120.70	127.00
26	a	610	CHL	C1-O2A-CGA	2.36	123.36	116.67
25	8	611	CLA	CHA-C4D-ND	2.36	137.41	132.55
50	9	507	XAT	C11-C10-C9	2.36	130.58	127.28
25	A	1112	CLA	O2A-CGA-CBA	2.36	119.02	111.83
25	L	1501	CLA	C3B-C4B-NB	-2.36	108.43	110.53
25	5	615	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
25	A	1113	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
25	B	1208	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
25	A	1110	CLA	CHA-C4D-ND	2.35	137.41	132.55
25	A	1116	CLA	CHD-C1D-ND	-2.35	121.49	124.80
29	L	4002	BCR	C33-C5-C4	2.35	118.61	113.60
25	B	1216	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
25	A	1133	CLA	C4B-CHC-C1C	2.35	131.78	126.25
25	B	1230	CLA	C4B-CHC-C1C	2.35	131.78	126.25
43	9	501	LUT	C35-C15-C14	-2.35	118.71	123.52
25	B	1237	CLA	CHA-C4D-ND	2.35	137.40	132.55
25	3	607	CLA	O2A-CGA-CBA	2.35	119.01	111.83
26	8	601	CHL	C4C-CHD-C1D	2.35	124.48	116.07
25	A	1013	CLA	CHD-C1D-ND	-2.35	121.49	124.80
25	A	1125	CLA	C1D-ND-C4D	-2.35	104.66	106.31
25	7	604	CLA	C1D-ND-C4D	-2.35	104.66	106.31
25	1	601	CLA	CMA-C3A-C4A	2.35	118.09	111.77
30	6	802	LHG	C6-C5-C4	-2.35	106.30	111.78
25	B	1231	CLA	C2C-C1C-NC	2.35	112.45	109.98
29	A	4001	BCR	C36-C18-C17	-2.35	119.01	122.82
25	6	612	CLA	C4B-CHC-C1C	2.35	131.77	126.25
25	1	603	CLA	CHD-C1D-ND	-2.35	121.50	124.80
25	B	1202	CLA	C1D-ND-C4D	-2.35	104.66	106.31
25	4	612	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
25	8	602	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
25	7	606	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
25	B	1201	CLA	CHD-C1D-ND	-2.35	121.50	124.80
25	B	1235	CLA	C4B-CHC-C1C	2.35	131.77	126.25
25	B	1227	CLA	CMA-C3A-C4A	2.35	118.09	111.77
25	a	615	CLA	C2D-C1D-ND	2.35	112.45	110.13
25	B	1234	CLA	CAA-CBA-CGA	-2.35	106.54	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1132	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
25	9	609	CLA	CHD-C1D-ND	-2.35	121.50	124.80
25	A	1138	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
29	6	504	BCR	C19-C18-C17	2.35	122.70	119.01
25	A	1141	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
29	5	504	BCR	C37-C22-C23	2.35	121.67	118.09
25	A	1122	CLA	C1D-ND-C4D	-2.35	104.67	106.31
25	2	605	CLA	C1D-ND-C4D	-2.35	104.67	106.31
25	A	1103	CLA	C1-O2A-CGA	2.35	122.33	116.65
25	A	1120	CLA	CHD-C1D-ND	-2.35	121.50	124.80
26	4	609	CHL	C4D-CHA-CBD	-2.35	106.60	108.97
26	7	617	CHL	CMA-C3A-C4A	2.35	119.67	114.61
25	H	1703	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
25	6	604	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
25	B	1227	CLA	O2A-CGA-CBA	2.35	118.99	111.83
25	A	1103	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
25	A	1118	CLA	CHA-C4D-ND	2.35	137.39	132.55
25	3	616	CLA	CHA-C4D-ND	2.34	137.39	132.55
25	A	1012	CLA	CHA-C1A-NA	-2.34	121.08	126.39
25	B	1205	CLA	C4B-CHC-C1C	2.34	131.76	126.25
43	6	501	LUT	C20-C13-C12	2.34	121.67	118.09
25	B	1209	CLA	C1D-ND-C4D	-2.34	104.67	106.31
25	7	601	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
25	A	1125	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
25	B	1237	CLA	CHD-C1D-ND	-2.34	121.50	124.80
25	F	1301	CLA	CHD-C1D-ND	-2.34	121.50	124.80
25	8	615	CLA	C4B-CHC-C1C	2.34	131.76	126.25
25	L	1504	CLA	O2A-CGA-CBA	2.34	118.98	111.83
26	6	613	CHL	C4C-CHD-C1D	2.34	124.45	116.07
25	8	612	CLA	CHA-C4D-ND	2.34	137.38	132.55
25	B	1224	CLA	CMA-C3A-C4A	2.34	118.07	111.77
25	B	1237	CLA	C4B-CHC-C1C	2.34	131.76	126.25
25	2	606	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
25	6	615	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	4	616	CLA	O2A-CGA-CBA	2.34	118.98	111.83
26	3	608	CHL	CMA-C3A-C4A	2.34	119.66	114.61
25	5	612	CLA	C4B-CHC-C1C	2.34	131.75	126.25
25	8	606	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
25	a	608	CLA	CHA-C4D-ND	2.34	137.38	132.55
25	a	603	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
26	4	609	CHL	C4C-CHD-C1D	2.34	124.44	116.07
43	2	502	LUT	C38-C25-C24	-2.34	117.82	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	4002	BCR	C33-C5-C4	2.34	118.59	113.60
29	3	503	BCR	C38-C26-C25	-2.34	121.93	124.48
25	H	1703	CLA	C1D-ND-C4D	-2.34	104.67	106.31
26	3	603	CHL	C4C-CHD-C1D	2.34	124.44	116.07
25	a	612	CLA	C4B-CHC-C1C	2.34	131.75	126.25
25	A	1013	CLA	CHA-C4D-ND	2.34	137.38	132.55
25	B	1206	CLA	CHA-C4D-ND	2.34	137.38	132.55
25	O	1801	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	A	1113	CLA	C4B-CHC-C1C	2.34	131.75	126.25
25	a	605	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
26	a	609	CHL	C4C-CHD-C1D	2.34	124.44	116.07
25	B	1204	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	O	1802	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	1	612	CLA	C3B-C4B-NB	-2.34	108.44	110.53
25	a	605	CLA	C1D-ND-C4D	-2.34	104.67	106.31
25	4	611	CLA	C1D-ND-C4D	-2.34	104.67	106.31
26	8	603	CHL	C4C-CHD-C1D	2.34	124.44	116.07
25	B	1205	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	a	605	CLA	CHD-C1D-ND	-2.34	121.51	124.80
25	4	602	CLA	O2A-CGA-CBA	2.34	118.96	111.83
25	8	618	CLA	C4B-CHC-C1C	2.34	131.74	126.25
25	B	1215	CLA	CHA-C4D-ND	2.34	137.37	132.55
25	A	1129	CLA	CHD-C1D-ND	-2.34	121.52	124.80
25	9	612	CLA	C1-C2-C3	-2.34	122.37	126.20
29	8	503	BCR	C19-C18-C17	2.34	122.68	119.01
29	7	503	BCR	C33-C5-C4	2.34	118.58	113.60
25	2	603	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
25	K	1404	CLA	C4B-CHC-C1C	2.33	131.74	126.25
25	B	1223	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
25	2	615	CLA	C2D-C1D-ND	2.33	112.44	110.13
25	B	1224	CLA	C4B-CHC-C1C	2.33	131.74	126.25
25	1	615	CLA	C4B-CHC-C1C	2.33	131.74	126.25
29	B	4002	BCR	C3-C4-C5	-2.33	109.89	114.06
25	B	1230	CLA	CMA-C3A-C4A	2.33	118.05	111.77
25	7	605	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	8	618	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	6	606	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
25	A	1101	CLA	C1D-ND-C4D	-2.33	104.67	106.31
26	9	603	CHL	CMA-C3A-C4A	2.33	119.64	114.61
25	6	615	CLA	C4B-CHC-C1C	2.33	131.73	126.25
25	6	603	CLA	CHA-C4D-ND	2.33	137.36	132.55
25	3	602	CLA	C4B-CHC-C1C	2.33	131.73	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	4003	BCR	C37-C22-C21	-2.33	119.04	122.82
25	4	611	CLA	O2A-CGA-CBA	2.33	118.94	111.83
25	1	606	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
25	a	601	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	7	610	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	2	615	CLA	CHA-C4D-ND	2.33	137.36	132.55
25	A	1120	CLA	C1D-ND-C4D	-2.33	104.68	106.31
25	B	1217	CLA	C1D-ND-C4D	-2.33	104.68	106.31
25	B	1021	CLA	O2A-CGA-CBA	2.33	118.94	111.83
35	A	5008	LMT	C3'-C4'-C5'	-2.33	105.77	110.93
25	B	1204	CLA	CHA-C4D-ND	2.33	137.36	132.55
25	6	601	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
25	6	606	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
29	6	504	BCR	C4-C5-C6	-2.33	119.56	122.70
25	B	1218	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
25	4	601	CLA	CHA-C4D-ND	2.33	137.35	132.55
25	A	1135	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	A	1118	CLA	C1D-ND-C4D	-2.33	104.68	106.31
25	2	603	CLA	CHA-C1A-NA	-2.33	121.12	126.39
25	5	606	CLA	CHD-C1D-ND	-2.33	121.53	124.80
43	6	502	LUT	C35-C15-C14	-2.33	118.76	123.52
25	1	601	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
25	A	1106	CLA	CMA-C3A-C4A	2.33	118.03	111.77
40	3	506	RRX	C2-C1-C6	2.33	113.82	110.44
25	1	606	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	2	608	CLA	CHD-C1D-ND	-2.33	121.53	124.80
25	5	607	CLA	C4B-CHC-C1C	2.33	131.72	126.25
25	4	615	CLA	C4B-CHC-C1C	2.33	131.72	126.25
25	1	612	CLA	C4B-CHC-C1C	2.33	131.72	126.25
29	3	505	BCR	C23-C24-C25	-2.33	120.78	127.00
25	G	1603	CLA	C1D-ND-C4D	-2.33	104.68	106.31
25	B	1230	CLA	CHA-C4D-ND	2.33	137.35	132.55
25	4	604	CLA	C3B-C4B-NB	-2.33	108.45	110.53
25	J	1901	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
29	B	4007	BCR	C35-C13-C12	2.33	121.64	118.09
29	B	4001	BCR	C36-C18-C17	-2.33	119.05	122.82
25	4	612	CLA	C4B-CHC-C1C	2.32	131.71	126.25
25	3	616	CLA	CHD-C1D-ND	-2.32	121.53	124.80
25	5	601	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
25	2	603	CLA	C4B-CHC-C1C	2.32	131.71	126.25
25	H	1702	CLA	C4B-CHC-C1C	2.32	131.71	126.25
25	A	1118	CLA	CHD-C1D-ND	-2.32	121.53	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	607	CLA	CHD-C1D-ND	-2.32	121.53	124.80
43	3	501	LUT	C27-C28-C29	-2.32	121.33	126.32
29	A	4004	BCR	C34-C9-C10	-2.32	119.05	122.82
29	A	4001	BCR	C38-C26-C27	2.32	118.55	113.60
29	B	4007	BCR	C36-C18-C17	-2.32	119.05	122.82
25	8	607	CLA	C4B-CHC-C1C	2.32	131.71	126.25
25	9	612	CLA	C4B-CHC-C1C	2.32	131.71	126.25
25	B	1212	CLA	CHD-C1D-ND	-2.32	121.53	124.80
25	B	1219	CLA	C4B-CHC-C1C	2.32	131.71	126.25
26	8	604	CHL	C1-O2A-CGA	2.32	122.27	116.65
25	5	602	CLA	CMA-C3A-C4A	2.32	118.01	111.77
26	8	613	CHL	C4C-CHD-C1D	2.32	124.37	116.07
25	6	604	CLA	CHA-C4D-ND	2.32	137.34	132.55
25	5	602	CLA	C1D-ND-C4D	-2.32	104.68	106.31
43	1	503	LUT	C30-C31-C32	-2.32	116.48	123.20
25	4	606	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
43	9	501	LUT	C11-C10-C9	-2.32	124.02	127.28
29	B	4005	BCR	C33-C5-C4	2.32	118.54	113.60
25	3	607	CLA	C4B-CHC-C1C	2.32	131.70	126.25
25	2	603	CLA	CBA-CAA-C2A	2.32	120.69	113.79
26	7	611	CHL	CMA-C3A-C4A	2.32	119.61	114.61
25	L	1504	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
25	B	1210	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	A	1103	CLA	C4B-CHC-C1C	2.32	131.70	126.25
32	A	5005	SQD	O3-C3-C2	-2.32	104.91	110.38
25	B	1225	CLA	O2A-CGA-CBA	2.32	118.91	111.83
43	5	502	LUT	C39-C29-C28	2.32	121.63	118.09
25	7	605	CLA	O2D-CGD-O1D	-2.32	118.82	124.08
25	2	607	CLA	O2A-CGA-CBA	2.32	118.90	111.83
43	3	502	LUT	C27-C28-C29	-2.32	121.34	126.32
25	2	601	CLA	CHA-C4D-ND	2.32	137.33	132.55
26	9	601	CHL	C4D-CHA-CBD	-2.32	106.63	108.97
25	5	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	B	1221	CLA	C4B-CHC-C1C	2.31	131.69	126.25
25	A	1138	CLA	CMA-C3A-C4A	2.31	117.99	111.77
25	8	602	CLA	C1D-ND-C4D	-2.31	104.69	106.31
43	3	501	LUT	C31-C30-C29	-2.31	124.03	127.28
26	8	604	CHL	CMA-C3A-C4A	2.31	119.60	114.61
25	9	605	CLA	CHA-C1A-NA	-2.31	121.15	126.39
25	B	1221	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	3	605	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	5	605	CLA	C1D-ND-C4D	-2.31	104.69	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	612	CLA	O2A-CGA-CBA	2.31	118.89	111.83
26	6	617	CHL	C4C-CHD-C1D	2.31	124.34	116.07
25	A	1112	CLA	CHA-C1A-NA	-2.31	121.16	126.39
29	L	4002	BCR	C34-C9-C10	-2.31	119.07	122.82
25	4	601	CLA	C1D-ND-C4D	-2.31	104.69	106.31
25	6	601	CLA	C1D-ND-C4D	-2.31	104.69	106.31
26	9	608	CHL	CMA-C3A-C4A	2.31	119.59	114.61
25	2	604	CLA	O2A-CGA-CBA	2.31	118.88	111.83
25	B	1221	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
43	2	502	LUT	C30-C31-C32	-2.31	116.50	123.20
25	A	1108	CLA	CHA-C4D-ND	2.31	137.32	132.55
35	B	5006	LMT	C1'-O5'-C5'	-2.31	109.21	113.72
43	2	502	LUT	C35-C34-C33	-2.31	124.04	127.28
25	A	1137	CLA	CMA-C3A-C4A	2.31	117.98	111.77
25	A	1126	CLA	C4B-CHC-C1C	2.31	131.68	126.25
26	3	603	CHL	C1-C2-C3	-2.31	122.41	126.20
25	B	1236	CLA	C2D-C1D-ND	2.31	112.41	110.13
25	5	604	CLA	C3B-C4B-NB	-2.31	108.47	110.53
25	7	604	CLA	C3B-C4B-NB	-2.31	108.47	110.53
25	A	1122	CLA	CHA-C4D-ND	2.31	137.31	132.55
26	9	610	CHL	CMA-C3A-C4A	2.31	119.58	114.61
25	A	1134	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
25	F	1302	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	B	1201	CLA	O2A-CGA-CBA	2.31	118.87	111.83
25	H	1703	CLA	C2C-C1C-NC	2.31	112.41	109.98
25	A	1138	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	7	613	CHL	C4C-CHD-C1D	2.31	124.32	116.07
25	A	1132	CLA	C4B-CHC-C1C	2.31	131.67	126.25
43	3	501	LUT	C26-C27-C28	-2.31	120.99	124.58
25	3	613	CLA	CHD-C1D-ND	-2.31	121.56	124.80
25	4	604	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
25	8	605	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
26	4	618	CHL	C4C-CHD-C1D	2.31	124.32	116.07
25	A	1128	CLA	O2A-CGA-CBA	2.31	118.86	111.83
25	8	607	CLA	CHD-C1D-ND	-2.31	121.56	124.80
50	9	507	XAT	O24-C26-C27	-2.31	110.27	116.88
43	3	501	LUT	C11-C10-C9	-2.30	124.05	127.28
39	F	4001	NEX	C11-C12-C13	2.30	132.68	126.36
26	2	609	CHL	CMA-C3A-C4A	2.30	119.58	114.61
25	B	1238	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
25	4	603	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
26	a	604	CHL	C1C-C2C-CMC	2.30	130.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	4001	BCR	C37-C22-C21	-2.30	119.08	122.82
25	4	617	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
25	B	1213	CLA	C4B-CHC-C1C	2.30	131.66	126.25
25	7	607	CLA	C3B-C4B-NB	-2.30	108.47	110.53
25	6	605	CLA	CHD-C1D-ND	-2.30	121.56	124.80
26	7	611	CHL	C4C-CHD-C1D	2.30	124.31	116.07
25	A	1109	CLA	C4B-CHC-C1C	2.30	131.66	126.25
30	F	5002	LHG	C5-O7-C7	-2.30	112.29	117.80
25	B	1212	CLA	C3B-C4B-NB	-2.30	108.47	110.53
25	4	616	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	A	1127	CLA	C1D-ND-C4D	-2.30	104.70	106.31
29	B	4003	BCR	C4-C5-C6	-2.30	119.59	122.70
25	O	1802	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
29	4	503	BCR	C33-C5-C4	2.30	118.50	113.60
25	B	1220	CLA	CHA-C4D-ND	2.30	137.30	132.55
26	2	609	CHL	C4C-CHD-C1D	2.30	124.30	116.07
25	A	1123	CLA	C4B-CHC-C1C	2.30	131.66	126.25
25	9	605	CLA	C4B-CHC-C1C	2.30	131.66	126.25
25	2	621	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	5	608	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	3	605	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
25	4	602	CLA	CMA-C3A-C4A	2.30	117.95	111.77
25	2	621	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	2	602	CLA	O2A-CGA-CBA	2.30	118.84	111.83
25	3	618	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	B	1212	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
25	5	606	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
43	1	503	LUT	C39-C29-C30	-2.30	119.09	122.82
25	A	1124	CLA	CHA-C4D-ND	2.30	137.29	132.55
25	6	615	CLA	O2A-CGA-CBA	2.30	118.84	111.83
25	1	605	CLA	C4B-CHC-C1C	2.30	131.65	126.25
25	A	1121	CLA	C3B-C4B-NB	-2.30	108.48	110.53
25	4	602	CLA	C1D-ND-C4D	-2.30	104.70	106.31
25	9	612	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	B	1228	CLA	C4B-CHC-C1C	2.30	131.65	126.25
25	A	1119	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
25	B	1221	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
25	G	1602	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
25	A	1131	CLA	C4B-CHC-C1C	2.30	131.65	126.25
25	B	1229	CLA	C2D-C1D-ND	2.30	112.40	110.13
25	3	607	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	8	602	CLA	CHD-C1D-ND	-2.30	121.57	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	4001	BCR	C37-C22-C23	2.30	121.59	118.09
25	A	1140	CLA	CHD-C1D-ND	-2.29	121.57	124.80
25	9	607	CLA	CHD-C1D-ND	-2.29	121.57	124.80
25	B	1203	CLA	O2A-CGA-CBA	2.29	118.83	111.83
25	9	606	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
25	B	1221	CLA	O2A-CGA-CBA	2.29	118.83	111.83
29	6	503	BCR	C35-C13-C12	2.29	121.59	118.09
26	a	604	CHL	C4C-CHD-C1D	2.29	124.27	116.07
25	2	615	CLA	C4B-CHC-C1C	2.29	131.64	126.25
25	3	601	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
29	6	503	BCR	C33-C5-C4	2.29	118.48	113.60
26	a	613	CHL	C4C-CHD-C1D	2.29	124.27	116.07
25	a	611	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	O	1801	CLA	C3B-C4B-NB	-2.29	108.48	110.53
26	5	611	CHL	C4C-CHD-C1D	2.29	124.27	116.07
25	B	1226	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
25	A	1132	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
25	a	602	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
25	4	601	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
25	O	1803	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	B	1213	CLA	C2C-C1C-NC	2.29	112.39	109.98
25	1	605	CLA	C3B-C4B-NB	-2.29	108.49	110.53
29	B	4007	BCR	C34-C9-C10	-2.29	119.11	122.82
25	8	608	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
25	4	611	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
25	8	611	CLA	O2A-CGA-CBA	2.29	118.81	111.83
43	9	502	LUT	C31-C32-C33	-2.29	120.09	126.36
25	6	603	CLA	C1-O2A-CGA	2.29	122.19	116.65
43	8	501	LUT	C20-C13-C12	2.29	121.58	118.09
25	8	609	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	7	602	CLA	C1D-ND-C4D	-2.29	104.71	106.31
25	B	1023	CLA	CAC-C3C-C4C	2.29	127.77	124.79
25	A	1117	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
25	B	1225	CLA	CHD-C1D-ND	-2.29	121.58	124.80
25	B	1217	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
25	B	1228	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
29	L	4003	BCR	C23-C24-C25	-2.29	120.89	127.00
25	A	1126	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
25	B	1218	CLA	CHA-C4D-ND	2.29	137.26	132.55
25	A	1112	CLA	C4B-CHC-C1C	2.29	131.62	126.25
25	B	1232	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
25	B	1203	CLA	CMD-C2D-C3D	-2.29	122.45	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	607	CLA	C3B-C4B-NB	-2.29	108.49	110.53
25	3	605	CLA	O2A-CGA-CBA	2.28	118.80	111.83
25	A	1130	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
25	B	1240	CLA	CHA-C1A-NA	-2.28	121.22	126.39
25	8	611	CLA	C4B-CHC-C1C	2.28	131.62	126.25
25	5	606	CLA	C3B-C4B-NB	-2.28	108.49	110.53
25	B	1207	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
29	L	4001	BCR	C28-C27-C26	-2.28	109.98	114.06
26	2	610	CHL	C1-O2A-CGA	2.28	123.16	116.67
25	A	1140	CLA	C1D-ND-C4D	-2.28	104.71	106.31
25	A	1101	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
50	9	507	XAT	C20-C13-C14	-2.28	119.12	122.82
25	B	1021	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
25	a	611	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
29	I	4001	BCR	C12-C13-C14	-2.28	115.42	119.01
25	B	1227	CLA	C1-O2A-CGA	2.28	122.17	116.65
39	F	4001	NEX	C40-C33-C34	-2.28	119.12	122.82
25	2	603	CLA	CHD-C1D-ND	-2.28	121.59	124.80
25	3	610	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
25	a	601	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
25	A	1103	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
25	B	1222	CLA	CHA-C4D-ND	2.28	137.25	132.55
26	8	603	CHL	C1-O2A-CGA	2.28	122.17	116.65
25	L	1503	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
25	4	611	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
25	1	607	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
25	2	621	CLA	C4B-CHC-C1C	2.28	131.60	126.25
25	A	1105	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
29	3	504	BCR	C2-C1-C6	2.28	113.75	110.44
25	2	601	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
25	A	1122	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
25	H	1703	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
50	2	501	XAT	C38-C25-C26	-2.28	118.56	122.30
25	B	1232	CLA	CHD-C1D-ND	-2.28	121.60	124.80
25	1	615	CLA	CHD-C1D-ND	-2.28	121.60	124.80
25	B	1230	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
25	A	1101	CLA	CHD-C1D-ND	-2.28	121.60	124.80
25	B	1022	CLA	O2A-CGA-CBA	2.27	118.77	111.83
25	L	1501	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	A	1141	CLA	C4B-CHC-C1C	2.27	131.60	126.25
25	A	1125	CLA	CHD-C1D-ND	-2.27	121.60	124.80
43	8	502	LUT	C11-C10-C9	-2.27	124.09	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	617	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
25	B	1211	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
42	M	4001	ECH	C28-C29-C30	-2.27	109.89	113.21
25	9	609	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
25	A	1105	CLA	O2A-CGA-CBA	2.27	118.76	111.83
25	4	616	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
25	L	1502	CLA	CHA-C4D-ND	2.27	137.24	132.55
25	8	611	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
25	A	1116	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
25	O	1802	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
25	A	1013	CLA	C4B-CHC-C1C	2.27	131.59	126.25
25	B	1207	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	6	615	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	B	1206	CLA	CHD-C1D-ND	-2.27	121.61	124.80
25	A	1136	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
25	8	620	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
32	7	805	SQD	O3-C3-C2	-2.27	105.03	110.38
25	B	1218	CLA	C3B-C4B-NB	-2.27	108.50	110.53
25	2	607	CLA	CHD-C1D-ND	-2.27	121.61	124.80
25	2	612	CLA	O2A-CGA-CBA	2.27	118.75	111.83
25	A	1121	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	B	1208	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	B	1206	CLA	O2A-CGA-CBA	2.27	118.75	111.83
25	5	606	CLA	O2A-CGA-CBA	2.27	118.75	111.83
25	9	602	CLA	CHD-C1D-ND	-2.27	121.61	124.80
29	H	4001	BCR	C34-C9-C10	-2.27	119.14	122.82
25	G	1602	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	B	1210	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
26	8	601	CHL	C1C-C2C-CMC	2.27	130.89	126.80
25	4	607	CLA	CHD-C1D-ND	-2.27	121.61	124.80
43	9	501	LUT	C20-C13-C12	2.27	121.55	118.09
29	L	4003	BCR	C8-C7-C6	-2.27	120.94	127.00
25	B	1225	CLA	C1D-ND-C4D	-2.27	104.72	106.31
25	4	608	CLA	C1D-ND-C4D	-2.27	104.72	106.31
43	1	501	LUT	C31-C30-C29	-2.27	124.10	127.28
29	5	503	BCR	C35-C13-C12	2.26	121.55	118.09
25	F	1301	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
25	a	601	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
25	2	605	CLA	OBD-CAD-C3D	-2.26	123.12	128.42
25	H	1701	CLA	O2A-CGA-CBA	2.26	118.73	111.83
25	3	612	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
25	A	1129	CLA	O2A-CGA-CBA	2.26	118.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1106	CLA	C2D-C1D-ND	2.26	112.36	110.13
25	A	1120	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
26	6	619	CHL	C4D-CHA-CBD	-2.26	106.69	108.97
25	6	607	CLA	CHD-C1D-ND	-2.26	121.62	124.80
25	G	1602	CLA	CMA-C3A-C4A	2.26	117.85	111.77
25	6	604	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
25	1	602	CLA	C1D-ND-C4D	-2.26	104.72	106.31
25	A	1102	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
25	A	1126	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
25	A	1102	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
25	2	621	CLA	C6-C5-C3	-2.26	107.96	113.47
25	a	601	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
43	4	501	LUT	C11-C10-C9	-2.26	124.11	127.28
25	6	615	CLA	C2D-C1D-ND	2.26	112.36	110.13
26	8	613	CHL	CMA-C3A-C4A	2.26	119.48	114.61
25	A	1108	CLA	O2A-CGA-CBA	2.26	118.72	111.83
25	L	1501	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
25	A	1141	CLA	C3B-C4B-NB	-2.26	108.51	110.53
25	A	1129	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
25	8	607	CLA	CMA-C3A-C4A	2.26	117.84	111.77
25	A	1110	CLA	C1D-ND-C4D	-2.26	104.73	106.31
25	4	601	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	8	615	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
25	B	1211	CLA	CMA-C3A-C4A	2.26	117.84	111.77
25	H	1701	CLA	CHD-C1D-ND	-2.26	121.62	124.80
25	A	1117	CLA	C1-O2A-CGA	2.26	122.12	116.65
50	9	504	XAT	O4-C5-C4	-2.26	111.38	113.49
25	8	612	CLA	C1D-ND-C4D	-2.26	104.73	106.31
25	A	1125	CLA	C1C-C2C-C3C	-2.26	104.61	106.98
25	L	1502	CLA	O2A-CGA-CBA	2.26	118.72	111.83
25	7	605	CLA	OBD-CAD-C3D	-2.26	123.14	128.42
25	O	1803	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
25	a	615	CLA	C1D-ND-C4D	-2.26	104.73	106.31
41	4	805	SPH	C3-C4-C5	-2.26	120.02	124.69
25	A	1129	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
29	L	4001	BCR	C15-C14-C13	-2.26	124.11	127.28
25	G	1603	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
32	H	5001	SQD	O3-C3-C2	-2.25	105.06	110.38
25	B	1214	CLA	O2A-CGA-CBA	2.25	118.71	111.83
25	A	1013	CLA	C2C-C1C-NC	2.25	112.35	109.98
25	L	1504	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
26	1	613	CHL	C1-O2A-CGA	2.25	123.07	116.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	603	CLA	C1D-ND-C4D	-2.25	104.73	106.31
25	9	606	CLA	CMA-C3A-C4A	2.25	117.83	111.77
25	6	604	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
29	K	4002	BCR	C35-C13-C12	2.25	121.53	118.09
32	I	5001	SQD	O3-C3-C2	-2.25	105.07	110.38
25	L	1504	CLA	CHA-C1A-NA	-2.25	121.29	126.39
25	B	1023	CLA	C4B-CHC-C1C	2.25	131.54	126.25
29	7	503	BCR	C31-C1-C6	-2.25	106.71	110.24
25	J	1901	CLA	CHD-C1D-ND	-2.25	121.63	124.80
25	K	1403	CLA	CHD-C1D-ND	-2.25	121.63	124.80
25	3	605	CLA	C1D-ND-C4D	-2.25	104.73	106.31
25	8	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
25	6	612	CLA	O2A-CGA-CBA	2.25	118.70	111.83
25	A	1101	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
25	2	612	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
26	8	601	CHL	C4D-CHA-CBD	-2.25	106.70	108.97
25	B	1211	CLA	O2A-CGA-CBA	2.25	118.69	111.83
25	6	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
25	A	1137	CLA	C1-O2A-CGA	2.25	122.09	116.65
25	B	1232	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
25	B	1210	CLA	C6-C5-C3	-2.25	107.99	113.47
25	1	603	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
26	8	601	CHL	CMA-C3A-C4A	2.25	119.45	114.61
29	L	4003	BCR	C36-C18-C17	-2.25	119.18	122.82
25	1	608	CLA	CHA-C4D-ND	2.25	137.18	132.55
25	2	603	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
25	K	1402	CLA	CHD-C1D-ND	-2.25	121.64	124.80
26	4	613	CHL	C4C-CHD-C1D	2.25	124.11	116.07
43	a	502	LUT	C31-C30-C29	-2.25	124.13	127.28
25	A	1128	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
25	B	1211	CLA	C3B-C4B-NB	-2.25	108.53	110.53
25	8	611	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
25	9	612	CLA	CHA-C1A-NA	-2.25	121.31	126.39
25	A	1123	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
25	L	1502	CLA	C1-O2A-CGA	2.25	122.09	116.65
25	3	602	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
25	9	605	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
25	a	601	CLA	C1D-ND-C4D	-2.24	104.74	106.31
25	4	602	CLA	CHD-C1D-ND	-2.24	121.64	124.80
25	3	601	CLA	C1-O2A-CGA	2.24	122.08	116.65
25	A	1140	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
25	B	1204	CLA	CAA-C2A-C3A	-2.24	106.94	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	607	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	B	1201	CLA	C3B-C4B-NB	-2.24	108.53	110.53
25	B	1220	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
25	H	1701	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
25	4	610	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
26	6	619	CHL	C4C-CHD-C1D	2.24	124.09	116.07
25	2	602	CLA	CHD-C1D-ND	-2.24	121.65	124.80
43	a	502	LUT	C22-C23-C24	-2.24	107.85	111.18
25	4	617	CLA	CHD-C1D-ND	-2.24	121.65	124.80
25	2	605	CLA	CHD-C1D-ND	-2.24	121.65	124.80
29	3	505	BCR	C33-C5-C4	2.24	118.38	113.60
25	4	617	CLA	CHA-C1A-NA	-2.24	121.32	126.39
26	6	611	CHL	C4C-CHD-C1D	2.24	124.09	116.07
25	6	602	CLA	O2A-CGA-CBA	2.24	118.67	111.83
25	A	1139	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
26	7	615	CHL	CMA-C3A-C4A	2.24	119.44	114.61
25	A	1139	CLA	O2A-CGA-CBA	2.24	118.67	111.83
25	A	1122	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
25	A	1108	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
25	B	1210	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
25	A	1133	CLA	C1D-ND-C4D	-2.24	104.74	106.31
25	B	1205	CLA	C1D-ND-C4D	-2.24	104.74	106.31
25	B	1235	CLA	C1D-ND-C4D	-2.24	104.74	106.31
25	3	601	CLA	C1D-ND-C4D	-2.24	104.74	106.31
29	A	4003	BCR	C35-C13-C12	2.24	121.51	118.09
25	6	618	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
29	A	4004	BCR	C36-C18-C17	-2.24	119.19	122.82
26	1	613	CHL	C4C-CHD-C1D	2.24	124.07	116.07
25	K	1401	CLA	C1D-ND-C4D	-2.24	104.74	106.31
25	B	1230	CLA	C2D-C1D-ND	2.24	112.34	110.13
25	1	608	CLA	C3B-C4B-NB	-2.24	108.53	110.53
29	B	4002	BCR	C29-C28-C27	2.24	116.19	111.28
25	A	1107	CLA	CHD-C1D-ND	-2.24	121.66	124.80
25	A	1137	CLA	C6-C5-C3	-2.24	108.02	113.47
25	L	1504	CLA	CHD-C1D-ND	-2.24	121.66	124.80
29	K	4002	BCR	C34-C9-C10	-2.24	119.19	122.82
25	8	620	CLA	C2D-C1D-ND	2.23	112.34	110.13
25	O	1802	CLA	C1D-ND-C4D	-2.23	104.74	106.31
25	9	612	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
25	A	1115	CLA	C1-O2A-CGA	2.23	122.06	116.65
25	a	605	CLA	CMA-C3A-C4A	2.23	117.78	111.77
25	A	1107	CLA	CMD-C2D-C3D	-2.23	122.57	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	1403	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
25	A	1129	CLA	CHA-C1A-NA	-2.23	121.33	126.39
43	2	507	LUT	C39-C29-C30	-2.23	119.20	122.82
25	A	1012	CLA	C4B-CHC-C1C	2.23	131.50	126.25
40	3	506	RRX	C38-C26-C27	2.23	118.53	114.42
25	1	602	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
25	2	607	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	B	1216	CLA	C1-O2A-CGA	2.23	122.05	116.65
25	7	610	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
25	A	1130	CLA	C1D-ND-C4D	-2.23	104.75	106.31
25	4	606	CLA	C1D-ND-C4D	-2.23	104.75	106.31
25	a	602	CLA	O2A-CGA-CBA	2.23	118.64	111.83
26	5	618	CHL	C4C-CHD-C1D	2.23	124.05	116.07
25	5	615	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	9	609	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	H	1702	CLA	CHD-C1D-ND	-2.23	121.66	124.80
43	5	505	LUT	C11-C12-C13	-2.23	120.25	126.36
25	B	1205	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
25	B	1236	CLA	CMA-C3A-C4A	2.23	117.77	111.77
25	a	602	CLA	CHD-C1D-ND	-2.23	121.66	124.80
29	K	4001	BCR	C37-C22-C21	-2.23	119.20	122.82
25	B	1239	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
25	B	1214	CLA	CHD-C1D-ND	-2.23	121.67	124.80
25	B	1222	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
25	K	1404	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
36	8	802	DGD	C3G-C2G-C1G	-2.23	106.59	111.78
25	7	601	CLA	C2C-C1C-NC	2.23	112.32	109.98
25	B	1022	CLA	C4B-CHC-C1C	2.23	131.49	126.25
50	2	501	XAT	O24-C26-C27	-2.23	110.49	116.88
25	4	601	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	2	601	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	B	1214	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
25	2	601	CLA	O2A-CGA-CBA	2.23	118.62	111.83
25	2	601	CLA	C1D-ND-C4D	-2.23	104.75	106.31
29	B	4005	BCR	C23-C22-C21	-2.23	115.51	119.01
25	B	1213	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
26	8	604	CHL	C4D-CHA-CBD	-2.23	106.72	108.97
26	9	608	CHL	C1-O2A-CGA	2.22	122.99	116.67
25	7	608	CLA	O2A-CGA-CBA	2.22	118.62	111.83
25	A	1106	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
25	A	1123	CLA	O2A-CGA-CBA	2.22	118.61	111.83
25	B	1237	CLA	CMD-C2D-C3D	-2.22	122.59	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	604	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	1	612	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
43	1	503	LUT	C18-C5-C4	2.22	118.51	114.42
43	5	501	LUT	C8-C7-C6	-2.22	121.06	127.00
25	7	603	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
25	F	1302	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	K	1402	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
25	B	1207	CLA	O2A-CGA-CBA	2.22	118.60	111.83
25	F	1301	CLA	O2A-CGA-CBA	2.22	118.60	111.83
25	3	605	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	A	1119	CLA	C1D-ND-C4D	-2.22	104.75	106.31
25	B	1218	CLA	C1D-ND-C4D	-2.22	104.75	106.31
25	2	604	CLA	C1D-ND-C4D	-2.22	104.75	106.31
25	A	1110	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
25	A	1115	CLA	CHD-C1D-ND	-2.22	121.68	124.80
25	A	1134	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
25	B	1238	CLA	O2A-CGA-CBA	2.22	118.60	111.83
25	B	1227	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	5	612	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	7	602	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
29	A	4004	BCR	C30-C25-C26	-2.22	119.61	122.64
26	5	617	CHL	C4C-CHD-C1D	2.22	124.00	116.07
26	3	604	CHL	C4D-CHA-CBD	-2.22	106.73	108.97
25	O	1803	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
25	A	1133	CLA	O2A-CGA-CBA	2.22	118.59	111.83
25	L	1501	CLA	O2A-CGA-CBA	2.22	118.59	111.83
25	2	604	CLA	C3B-C4B-NB	-2.22	108.55	110.53
43	5	501	LUT	C22-C23-C24	-2.22	107.89	111.18
25	F	1302	CLA	C1D-ND-C4D	-2.21	104.76	106.31
25	a	608	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
25	A	1113	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
43	2	507	LUT	C3-C4-C5	-2.21	106.67	112.18
25	4	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	a	605	CLA	C3B-C4B-NB	-2.21	108.55	110.53
25	A	1135	CLA	C1D-ND-C4D	-2.21	104.76	106.31
25	8	606	CLA	C1D-ND-C4D	-2.21	104.76	106.31
26	5	613	CHL	C4C-CHD-C1D	2.21	123.99	116.07
43	9	501	LUT	C31-C30-C29	-2.21	124.17	127.28
26	9	613	CHL	C4C-CHD-C1D	2.21	123.98	116.07
25	A	1111	CLA	C1-O2A-CGA	2.21	122.00	116.65
43	5	505	LUT	C31-C32-C33	-2.21	120.30	126.36
25	B	1211	CLA	CAA-C2A-C3A	-2.21	107.02	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	607	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
42	M	4001	ECH	C37-C22-C23	-2.21	114.71	118.09
25	8	609	CLA	C1-O2A-CGA	2.21	122.00	116.65
25	6	602	CLA	CHD-C1D-ND	-2.21	121.69	124.80
26	6	609	CHL	C1-C2-C3	-2.21	122.58	126.20
25	A	1115	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
29	O	4001	BCR	C35-C13-C12	2.21	121.46	118.09
25	A	1141	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	F	1301	CLA	C1D-ND-C4D	-2.21	104.76	106.31
25	6	607	CLA	O2A-CGA-CBA	2.21	118.57	111.83
43	5	501	LUT	C39-C29-C28	2.21	121.46	118.09
43	9	502	LUT	C38-C25-C24	-2.21	118.14	123.36
25	4	612	CLA	CMA-C3A-C4A	2.21	117.70	111.77
25	A	1108	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
25	H	1702	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
25	A	1135	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
25	B	1201	CLA	C1D-ND-C4D	-2.21	104.76	106.31
25	B	1240	CLA	CHD-C1D-ND	-2.21	121.70	124.80
29	K	4002	BCR	C38-C26-C25	-2.21	122.08	124.48
25	B	1229	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
25	4	601	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
43	8	501	LUT	C31-C30-C29	-2.21	124.19	127.28
25	3	613	CLA	CMA-C3A-C4A	2.21	117.70	111.77
25	2	602	CLA	C1D-ND-C4D	-2.20	104.77	106.31
25	A	1101	CLA	C2D-C1D-ND	2.20	112.31	110.13
25	5	609	CLA	C3B-C4B-NB	-2.20	108.56	110.53
25	B	1212	CLA	C1-O2A-CGA	2.20	121.99	116.65
25	4	612	CLA	O2A-CGA-CBA	2.20	118.56	111.83
25	B	1235	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
43	a	501	LUT	C11-C12-C13	-2.20	120.32	126.36
25	B	1234	CLA	C2B-C1B-NB	2.20	111.02	109.43
25	1	615	CLA	CHA-C1A-NA	-2.20	121.40	126.39
25	6	603	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
25	B	1206	CLA	C4B-CHC-C1C	2.20	131.43	126.25
25	B	1023	CLA	C1-C2-C3	-2.20	122.59	126.20
26	4	618	CHL	C1-O2A-CGA	2.20	121.98	116.65
26	7	613	CHL	C4D-CHA-CBD	-2.20	106.75	108.97
25	K	1401	CLA	C2D-C1D-ND	2.20	112.31	110.13
25	9	605	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
25	8	612	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
25	A	1101	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
25	5	607	CLA	CAA-C2A-C3A	-2.20	107.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	608	CLA	C1D-ND-C4D	-2.20	104.77	106.31
25	B	1224	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
29	6	504	BCR	C34-C9-C10	-2.20	119.25	122.82
26	a	606	CHL	C4C-CHD-C1D	2.20	123.94	116.07
25	A	1104	CLA	C1-O2A-CGA	2.20	121.97	116.65
25	5	603	CLA	C1D-ND-C4D	-2.20	104.77	106.31
25	1	605	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
25	4	604	CLA	C1D-ND-C4D	-2.20	104.77	106.31
32	G	5001	SQD	O3-C3-C2	-2.20	105.20	110.38
29	B	4001	BCR	C33-C5-C4	2.20	118.28	113.60
25	6	608	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
25	B	1234	CLA	CMA-C3A-C4A	2.20	119.34	114.61
25	K	1402	CLA	O2A-CGA-CBA	2.20	118.53	111.83
25	A	1136	CLA	C1D-ND-C4D	-2.20	104.77	106.31
25	6	602	CLA	C1D-ND-C4D	-2.20	104.77	106.31
25	A	1127	CLA	C2D-C1D-ND	2.20	112.30	110.13
26	1	609	CHL	CMD-C2D-C3D	2.20	129.07	124.68
25	3	610	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
43	3	502	LUT	C26-C27-C28	-2.20	121.16	124.58
25	O	1801	CLA	O2D-CGD-O1D	-2.19	119.10	124.08
25	A	1013	CLA	C1D-ND-C4D	-2.19	104.77	106.31
25	3	602	CLA	C1D-ND-C4D	-2.19	104.77	106.31
25	A	1012	CLA	CHD-C1D-ND	-2.19	121.71	124.80
25	A	1107	CLA	CHA-C1A-NA	-2.19	121.42	126.39
25	2	621	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
25	9	604	CLA	C1D-ND-C4D	-2.19	104.77	106.31
25	2	603	CLA	C3B-C4B-NB	-2.19	108.57	110.53
25	B	1223	CLA	CHA-C1A-NA	-2.19	121.42	126.39
25	5	612	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
25	B	1022	CLA	CHA-C1A-NA	-2.19	121.43	126.39
25	A	1137	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
25	9	602	CLA	C1D-ND-C4D	-2.19	104.77	106.31
43	6	501	LUT	C39-C29-C28	2.19	121.44	118.09
25	6	604	CLA	C2D-C1D-ND	2.19	112.30	110.13
25	a	608	CLA	O2A-CGA-CBA	2.19	118.52	111.83
25	3	612	CLA	CHA-C1A-NA	-2.19	121.43	126.39
25	a	607	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
29	L	4001	BCR	C34-C9-C10	-2.19	119.27	122.82
43	6	502	LUT	C39-C29-C28	2.19	121.43	118.09
25	9	607	CLA	O2A-CGA-CBA	2.19	118.51	111.83
25	2	615	CLA	C1D-ND-C4D	-2.19	104.78	106.31
25	5	609	CLA	CMD-C2D-C3D	-2.19	122.67	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1229	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
25	1	602	CLA	CHD-C1D-ND	-2.19	121.72	124.80
25	A	1104	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
25	A	1013	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
25	K	1404	CLA	CHD-C1D-ND	-2.19	121.72	124.80
44	1	502	AXT	C30-C31-C32	2.19	129.53	123.20
25	B	1023	CLA	CHA-C1A-NA	-2.19	121.44	126.39
25	A	1137	CLA	C2D-C1D-ND	2.18	112.29	110.13
25	2	606	CLA	C3B-C4B-NB	-2.18	108.58	110.53
29	6	504	BCR	C38-C26-C27	2.18	118.25	113.60
25	B	1208	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
25	B	1022	CLA	C6-C5-C3	-2.18	108.15	113.47
25	B	1023	CLA	C1C-C2C-C3C	-2.18	104.68	106.98
25	A	1128	CLA	C4B-CHC-C1C	2.18	131.38	126.25
26	9	603	CHL	C4D-CHA-CBD	-2.18	106.77	108.97
29	5	503	BCR	C37-C22-C23	2.18	121.42	118.09
29	3	505	BCR	C38-C26-C27	2.18	118.25	113.60
25	4	606	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
29	3	503	BCR	C29-C28-C27	2.18	116.07	111.28
25	K	1402	CLA	CHA-C1A-NA	-2.18	121.45	126.39
25	A	1101	CLA	CHA-C1A-NA	-2.18	121.46	126.39
25	A	1013	CLA	C2D-C1D-ND	2.18	112.28	110.13
25	5	602	CLA	C2D-C1D-ND	2.18	112.28	110.13
26	5	610	CHL	C4C-CHD-C1D	2.18	123.86	116.07
25	B	1220	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
25	4	615	CLA	CHA-C1A-NA	-2.18	121.46	126.39
25	A	1120	CLA	C2D-C1D-ND	2.18	112.28	110.13
25	B	1202	CLA	C2D-C1D-ND	2.18	112.28	110.13
25	B	1228	CLA	C1-O2A-CGA	2.18	121.92	116.65
25	2	608	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
29	5	503	BCR	C38-C26-C27	2.18	118.23	113.60
25	7	602	CLA	CHA-C1A-NA	-2.18	121.47	126.39
25	A	1127	CLA	O2A-CGA-CBA	2.17	118.47	111.83
25	1	615	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
26	9	608	CHL	C4C-CHD-C1D	2.17	123.85	116.07
25	9	609	CLA	C1D-ND-C4D	-2.17	104.79	106.31
26	5	613	CHL	CMA-C3A-C4A	2.17	119.29	114.61
25	4	605	CLA	CHA-C1A-NA	-2.17	121.47	126.39
26	3	611	CHL	CMA-C3A-C4A	2.17	119.29	114.61
25	9	604	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
29	I	4001	BCR	C34-C9-C10	-2.17	119.30	122.82
25	B	1230	CLA	CAA-CBA-CGA	-2.17	107.04	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	1022	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
25	a	612	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
25	8	605	CLA	CHD-C1D-ND	-2.17	121.75	124.80
25	B	1215	CLA	C1D-ND-C4D	-2.17	104.79	106.31
29	L	4001	BCR	C27-C26-C25	-2.17	119.77	122.70
29	K	4002	BCR	C37-C22-C21	-2.17	119.30	122.82
26	3	603	CHL	CMD-C2D-C3D	2.17	129.02	124.68
25	J	1901	CLA	CHA-C1A-NA	-2.17	121.48	126.39
25	8	608	CLA	C1D-ND-C4D	-2.17	104.79	106.31
43	1	501	LUT	C30-C31-C32	-2.17	116.92	123.20
43	1	501	LUT	C38-C25-C24	-2.17	118.23	123.36
25	3	601	CLA	CMA-C3A-C4A	2.17	117.60	111.77
26	A	1114	CHL	C4C-CHD-C1D	2.17	123.82	116.07
25	9	606	CLA	C1D-ND-C4D	-2.17	104.79	106.31
25	A	1112	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
25	B	1227	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
25	1	601	CLA	C1D-ND-C4D	-2.16	104.79	106.31
25	5	608	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	H	1703	CLA	O2A-CGA-CBA	2.16	118.43	111.83
25	A	1105	CLA	C2D-C1D-ND	2.16	112.27	110.13
25	8	620	CLA	CHA-C1A-NA	-2.16	121.49	126.39
25	A	1134	CLA	C1D-ND-C4D	-2.16	104.79	106.31
25	B	1229	CLA	CAA-C2A-C3A	-2.16	107.15	113.00
25	A	1107	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	A	1011	CL0	C4C-C3C-C2C	-2.16	104.83	113.37
25	6	602	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
25	a	602	CLA	C2D-C1D-ND	2.16	112.27	110.13
25	B	1021	CLA	CHA-C1A-NA	-2.16	121.50	126.39
29	B	4003	BCR	C19-C18-C17	2.16	122.41	119.01
25	B	1217	CLA	C2D-C1D-ND	2.16	112.27	110.13
25	4	601	CLA	CHA-C1A-NA	-2.16	121.50	126.39
30	A	5002	LHG	C5-O7-C7	-2.16	112.63	117.80
25	9	602	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	3	610	CLA	O2A-CGA-CBA	2.16	118.42	111.83
25	B	1223	CLA	C1D-ND-C4D	-2.16	104.80	106.31
25	A	1116	CLA	C2D-C1D-ND	2.16	112.26	110.13
25	A	1102	CLA	CHA-C1A-NA	-2.16	121.50	126.39
25	A	1131	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
25	7	606	CLA	CHA-C1A-NA	-2.16	121.50	126.39
25	B	1227	CLA	C1D-ND-C4D	-2.16	104.80	106.31
25	a	607	CLA	C1D-ND-C4D	-2.16	104.80	106.31
25	1	607	CLA	O2A-CGA-CBA	2.16	118.41	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	616	CLA	C3B-C4B-NB	-2.16	108.60	110.53
25	A	1109	CLA	C3B-C4B-NB	-2.16	108.61	110.53
25	7	603	CLA	C1D-ND-C4D	-2.16	104.80	106.31
25	8	606	CLA	O2A-CGA-CBA	2.16	118.41	111.83
25	B	1202	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
43	a	502	LUT	C20-C13-C12	2.15	121.38	118.09
25	7	610	CLA	C1D-ND-C4D	-2.15	104.80	106.31
25	G	1601	CLA	CHD-C1D-ND	-2.15	121.77	124.80
43	1	501	LUT	C8-C7-C6	-2.15	121.25	127.00
25	A	1118	CLA	C2D-C1D-ND	2.15	112.26	110.13
25	B	1222	CLA	C2D-C1D-ND	2.15	112.26	110.13
25	A	1123	CLA	CHA-C1A-NA	-2.15	121.52	126.39
25	B	1224	CLA	CHA-C1A-NA	-2.15	121.52	126.39
25	A	1120	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
25	2	602	CLA	C2D-C1D-ND	2.15	112.26	110.13
26	4	613	CHL	C1-O2A-CGA	2.15	121.86	116.65
26	3	611	CHL	C4C-CHD-C1D	2.15	123.77	116.07
36	8	803	DGD	O2G-C1B-O1B	-2.15	118.67	123.70
29	A	4004	BCR	C34-C9-C8	2.15	121.38	118.09
25	8	605	CLA	CHA-C1A-NA	-2.15	121.52	126.39
25	F	1301	CLA	CHA-C1A-NA	-2.15	121.52	126.39
25	A	1115	CLA	C1D-ND-C4D	-2.15	104.80	106.31
25	B	1238	CLA	C1D-ND-C4D	-2.15	104.80	106.31
25	3	613	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
43	4	502	LUT	C31-C32-C33	-2.15	120.47	126.36
25	B	1210	CLA	CHA-C1A-NA	-2.15	121.52	126.39
25	5	601	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
25	3	618	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
25	4	616	CLA	CHA-C1A-NA	-2.15	121.52	126.39
29	O	4001	BCR	C34-C9-C10	-2.15	119.33	122.82
25	B	1237	CLA	O2A-CGA-CBA	2.15	118.39	111.83
25	B	1210	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
25	A	1125	CLA	C2C-C1C-NC	2.15	112.24	109.98
25	A	1135	CLA	CHA-C1A-NA	-2.15	121.53	126.39
25	3	606	CLA	O2A-CGA-CBA	2.15	118.38	111.83
25	3	610	CLA	C1D-ND-C4D	-2.15	104.81	106.31
25	B	1230	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
25	O	1802	CLA	C2D-C1D-ND	2.15	112.25	110.13
25	A	1127	CLA	C1C-C2C-C3C	-2.15	104.72	106.98
25	G	1601	CLA	C1-O2A-CGA	2.15	121.84	116.65
25	B	1212	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
25	3	601	CLA	CMD-C2D-C3D	-2.15	122.77	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	605	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
29	A	4003	BCR	C31-C1-C6	-2.15	106.88	110.24
29	A	4005	BCR	C37-C22-C23	2.14	121.36	118.09
25	4	610	CLA	CHA-C1A-NA	-2.14	121.53	126.39
25	6	615	CLA	CAA-CBA-CGA	-2.14	107.12	113.21
25	B	1216	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	A	1119	CLA	O2A-CGA-CBA	2.14	118.37	111.83
29	I	4001	BCR	C33-C5-C4	2.14	118.17	113.60
25	4	608	CLA	C1-O2A-CGA	2.14	121.84	116.65
25	B	1225	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
25	A	1135	CLA	O2A-CGA-CBA	2.14	118.37	111.83
25	B	1221	CLA	CHA-C1A-NA	-2.14	121.54	126.39
26	2	610	CHL	C4C-CHD-C1D	2.14	123.74	116.07
43	6	501	LUT	C31-C30-C29	-2.14	124.27	127.28
25	5	615	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	6	607	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	A	1132	CLA	O2A-CGA-CBA	2.14	118.37	111.83
43	a	503	LUT	C26-C27-C28	-2.14	121.25	124.58
25	4	602	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	4	606	CLA	C3B-C4B-NB	-2.14	108.62	110.53
30	a	801	LHG	C5-O7-C7	-2.14	112.67	117.80
25	A	1111	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	K	1401	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	2	621	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	7	605	CLA	C1D-ND-C4D	-2.14	104.81	106.31
29	B	4006	BCR	C33-C5-C4	2.14	118.16	113.60
25	4	602	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
25	2	602	CLA	CHA-C1A-NA	-2.14	121.55	126.39
25	A	1126	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	5	612	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
25	A	1128	CLA	CHD-C1D-ND	-2.14	121.79	124.80
25	4	605	CLA	CHD-C1D-ND	-2.14	121.79	124.80
43	4	502	LUT	C11-C10-C9	-2.14	124.28	127.28
25	5	615	CLA	C2D-C1D-ND	2.14	112.24	110.13
43	3	501	LUT	C8-C7-C6	-2.14	121.28	127.00
25	A	1106	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
25	A	1134	CLA	CHA-C1A-NA	-2.14	121.55	126.39
29	H	4001	BCR	C38-C26-C25	-2.14	122.15	124.48
25	B	1237	CLA	C1D-ND-C4D	-2.14	104.81	106.31
25	B	1239	CLA	C1D-ND-C4D	-2.14	104.81	106.31
25	6	618	CLA	C1D-ND-C4D	-2.14	104.81	106.31
25	A	1133	CLA	C1-C2-C3	-2.14	122.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	605	CLA	C1-O2A-CGA	2.14	121.82	116.65
25	B	1220	CLA	C2D-C1D-ND	2.14	112.24	110.13
43	9	502	LUT	C39-C29-C28	2.14	121.35	118.09
25	B	1226	CLA	C4B-CHC-C1C	2.14	131.27	126.25
25	6	603	CLA	C1D-ND-C4D	-2.14	104.81	106.31
25	A	1129	CLA	CMA-C3A-C4A	2.14	117.52	111.77
25	8	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	5	608	CLA	CMA-C3A-C4A	2.14	117.51	111.77
26	7	611	CHL	CMD-C2D-C3D	2.14	128.95	124.68
26	6	610	CHL	C4C-CHD-C1D	2.14	123.71	116.07
25	B	1222	CLA	O2A-CGA-CBA	2.14	118.35	111.83
26	3	608	CHL	CMD-C2D-C3D	2.14	128.95	124.68
25	B	1236	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
25	A	1138	CLA	C1D-ND-C4D	-2.13	104.81	106.31
25	B	1217	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
25	2	615	CLA	CHD-C1D-ND	-2.13	121.80	124.80
25	B	1219	CLA	C3B-C4B-NB	-2.13	108.62	110.53
43	9	502	LUT	C22-C23-C24	-2.13	108.02	111.18
25	9	609	CLA	CHA-C1A-NA	-2.13	121.56	126.39
26	1	604	CHL	C4D-CHA-CBD	-2.13	106.82	108.97
25	B	1216	CLA	O2A-CGA-CBA	2.13	118.34	111.83
25	L	1503	CLA	CHA-C1A-NA	-2.13	121.56	126.39
25	6	602	CLA	CHA-C1A-NA	-2.13	121.56	126.39
25	4	601	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
25	B	1201	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
25	4	607	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
26	8	610	CHL	CMD-C2D-C3D	2.13	128.94	124.68
25	F	1302	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
25	9	602	CLA	C2D-C1D-ND	2.13	112.23	110.13
25	3	605	CLA	CHA-C1A-NA	-2.13	121.57	126.39
25	5	602	CLA	CHA-C1A-NA	-2.13	121.57	126.39
43	7	501	LUT	C38-C25-C24	-2.13	118.32	123.36
25	B	1235	CLA	C2D-C1D-ND	2.13	112.23	110.13
26	1	610	CHL	CMD-C2D-C3D	2.13	128.94	124.68
25	O	1801	CLA	C1D-ND-C4D	-2.13	104.82	106.31
25	4	605	CLA	C1D-ND-C4D	-2.13	104.82	106.31
25	A	1012	CLA	CMA-C3A-C4A	2.13	117.50	111.77
25	8	609	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
25	B	1227	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
25	A	1103	CLA	C1D-ND-C4D	-2.13	104.82	106.31
26	5	618	CHL	CMD-C2D-C3D	2.13	128.94	124.68
43	8	501	LUT	C27-C28-C29	-2.13	121.75	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	617	CHL	C1-O2A-CGA	2.13	122.88	116.07
41	6	806	SPH	C3-C4-C5	-2.13	120.28	124.69
25	A	1133	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
25	5	602	CLA	CHD-C1D-ND	-2.13	121.81	124.80
25	8	618	CLA	C1D-ND-C4D	-2.13	104.82	106.31
25	2	606	CLA	CHA-C1A-NA	-2.13	121.58	126.39
26	a	610	CHL	C4C-CHD-C1D	2.12	123.67	116.07
25	2	603	CLA	C2A-C1A-CHA	2.12	127.55	123.87
25	A	1140	CLA	C2D-C1D-ND	2.12	112.23	110.13
26	4	609	CHL	CMA-C3A-C4A	2.12	119.19	114.61
25	5	609	CLA	CHA-C1A-NA	-2.12	121.58	126.39
25	4	604	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
50	9	504	XAT	C32-C33-C34	2.12	122.35	119.01
25	B	1208	CLA	C3B-C4B-NB	-2.12	108.12	110.33
25	9	607	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
26	1	604	CHL	C1C-C2C-CMC	2.12	130.63	126.80
25	a	602	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
25	A	1121	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
43	5	505	LUT	C38-C25-C24	-2.12	118.34	123.36
25	5	608	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	7	608	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	5	607	CLA	C2D-C1D-ND	2.12	112.22	110.13
25	3	616	CLA	C1D-ND-C4D	-2.12	104.82	106.31
25	5	606	CLA	C1D-ND-C4D	-2.12	104.82	106.31
25	5	614	CLA	C1D-ND-C4D	-2.12	104.82	106.31
25	B	1204	CLA	C1-O2A-CGA	2.12	121.78	116.65
25	6	605	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	9	607	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	2	607	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
26	4	618	CHL	CMA-C3A-C4A	2.12	119.18	114.61
29	B	4007	BCR	C27-C26-C25	-2.12	119.84	122.70
25	5	607	CLA	C1D-ND-C4D	-2.12	104.83	106.31
25	L	1503	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
25	8	602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	A	1118	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
25	G	1602	CLA	CHA-C1A-NA	-2.12	121.59	126.39
29	B	4003	BCR	C8-C9-C10	2.12	122.34	119.01
25	2	605	CLA	CHA-C1A-NA	-2.12	121.59	126.39
25	1	607	CLA	C1D-ND-C4D	-2.12	104.83	106.31
25	B	1021	CLA	C2D-C1D-ND	2.12	112.22	110.13
26	9	601	CHL	C4C-CHD-C1D	2.12	123.64	116.07
25	a	611	CLA	C3B-C4B-NB	-2.12	108.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	602	CLA	CHA-C1A-NA	-2.12	121.60	126.39
29	O	4001	BCR	C30-C25-C24	2.12	121.39	115.65
26	8	601	CHL	CMD-C2D-C3D	2.12	128.91	124.68
26	9	610	CHL	CMD-C2D-C3D	2.12	128.91	124.68
25	B	1239	CLA	C2D-C1D-ND	2.12	112.22	110.13
30	2	802	LHG	O7-C7-O9	-2.12	118.76	123.70
25	9	605	CLA	CHD-C1D-ND	-2.12	121.83	124.80
25	A	1120	CLA	O2A-CGA-CBA	2.11	118.28	111.83
25	3	607	CLA	CHA-C1A-NA	-2.11	121.60	126.39
29	K	4001	BCR	C33-C5-C4	2.11	118.10	113.60
26	5	613	CHL	CMD-C2D-C3D	2.11	128.91	124.68
26	6	617	CHL	CMD-C2D-C3D	2.11	128.91	124.68
25	A	1139	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	a	607	CLA	CHA-C1A-NA	-2.11	121.61	126.39
43	1	501	LUT	C39-C29-C28	2.11	121.32	118.09
25	6	606	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
25	6	612	CLA	C2D-C1D-ND	2.11	112.22	110.13
29	A	4001	BCR	C33-C5-C4	2.11	118.10	113.60
25	5	601	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
25	B	1023	CLA	C1-O2A-CGA	2.11	121.76	116.65
25	A	1125	CLA	CHA-C1A-NA	-2.11	121.61	126.39
25	A	1107	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
25	L	1502	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
25	9	612	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
25	B	1021	CLA	CHD-C1D-ND	-2.11	121.83	124.80
25	B	1021	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	B	1240	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
25	O	1803	CLA	CHA-C1A-NA	-2.11	121.62	126.39
25	A	1013	CLA	CHA-C1A-NA	-2.11	121.62	126.39
25	H	1701	CLA	C3B-C4B-NB	-2.11	108.65	110.53
25	3	606	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	3	613	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	5	612	CLA	C1D-ND-C4D	-2.11	104.83	106.31
29	B	4001	BCR	C37-C22-C23	2.11	121.31	118.09
25	B	1214	CLA	CHA-C1A-NA	-2.11	121.62	126.39
25	4	615	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
32	7	805	SQD	O5-C1-O6	-2.11	105.06	110.04
43	4	501	LUT	C10-C11-C12	-2.11	117.09	123.20
25	5	615	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
25	8	605	CLA	C2D-C1D-ND	2.11	112.21	110.13
25	a	603	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
26	a	613	CHL	CMD-C2D-C3D	2.11	128.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	4002	BCR	C38-C26-C25	-2.11	122.19	124.48
25	B	1201	CLA	CHA-C1A-NA	-2.11	121.62	126.39
25	3	607	CLA	C3B-C4B-NB	-2.11	108.65	110.53
25	3	610	CLA	C3B-C4B-NB	-2.11	108.65	110.53
25	B	1229	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
25	B	1212	CLA	C1D-ND-C4D	-2.11	104.83	106.31
25	B	1210	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
25	K	1403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	B	1212	CLA	C2D-C1D-ND	2.10	112.21	110.13
44	7	504	AXT	C11-C12-C13	-2.10	120.59	126.36
25	2	602	CLA	C1-O2A-CGA	2.10	121.74	116.65
25	3	601	CLA	O2A-CGA-CBA	2.10	118.25	111.83
25	3	613	CLA	O2A-CGA-CBA	2.10	118.25	111.83
29	K	4002	BCR	C23-C24-C25	-2.10	121.38	127.00
25	A	1123	CLA	CHD-C1D-ND	-2.10	121.84	124.80
25	6	606	CLA	C1D-ND-C4D	-2.10	104.84	106.31
25	B	1201	CLA	C2D-C1D-ND	2.10	112.21	110.13
25	3	618	CLA	CHA-C1A-NA	-2.10	121.63	126.39
25	1	608	CLA	C3B-C2B-C1B	-2.10	104.69	107.17
25	4	612	CLA	C3B-C4B-NB	-2.10	108.66	110.53
43	3	501	LUT	C38-C25-C24	-2.10	118.39	123.36
29	K	4001	BCR	C35-C13-C12	2.10	121.30	118.09
25	4	602	CLA	C2D-C1D-ND	2.10	112.20	110.13
44	7	504	AXT	C4-C5-C6	-2.10	116.44	120.76
25	A	1101	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
25	1	603	CLA	C1D-ND-C4D	-2.10	104.84	106.31
26	2	610	CHL	CMD-C2D-C3D	2.10	128.88	124.68
26	8	603	CHL	CMD-C2D-C3D	2.10	128.88	124.68
25	3	602	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	A	1120	CLA	C1-O2A-CGA	2.10	121.73	116.65
25	3	616	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
25	B	1218	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	4	603	CLA	O2A-CGA-CBA	2.10	118.23	111.83
25	1	602	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	2	603	CLA	C2D-C1D-ND	2.10	112.20	110.13
25	A	1115	CLA	O2A-CGA-CBA	2.10	118.23	111.83
25	O	1802	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	a	611	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	5	602	CLA	O2A-CGA-CBA	2.10	118.23	111.83
25	6	612	CLA	CHA-C1A-NA	-2.10	121.64	126.39
25	9	605	CLA	C2D-C1D-ND	2.10	112.20	110.13
25	5	614	CLA	CMD-C2D-C3D	-2.10	122.88	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	612	CLA	C1D-ND-C4D	-2.10	104.84	106.31
25	4	607	CLA	C1-O2A-CGA	2.10	121.72	116.65
26	3	611	CHL	CMD-C2D-C3D	2.10	128.87	124.68
29	3	504	BCR	C34-C9-C10	-2.10	119.42	122.82
25	F	1302	CLA	CHA-C1A-NA	-2.10	121.65	126.39
25	6	601	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
25	8	620	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
43	5	501	LUT	C20-C13-C12	2.09	121.29	118.09
25	9	604	CLA	C1-O2A-CGA	2.09	121.72	116.65
26	6	609	CHL	C4C-CHD-C1D	2.09	123.56	116.07
25	G	1603	CLA	C2D-C1D-ND	2.09	112.20	110.13
25	2	612	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	1	607	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
25	8	609	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
25	3	602	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
29	L	4001	BCR	C38-C26-C25	-2.09	122.20	124.48
25	A	1113	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	2	612	CLA	C1D-ND-C4D	-2.09	104.84	106.31
25	3	616	CLA	C2D-C1D-ND	2.09	112.20	110.13
25	5	601	CLA	C2D-C1D-ND	2.09	112.20	110.13
25	a	612	CLA	CHA-C1A-NA	-2.09	121.65	126.39
25	6	606	CLA	CHA-C1A-NA	-2.09	121.65	126.39
43	8	502	LUT	C38-C25-C24	-2.09	118.41	123.36
25	B	1203	CLA	C2D-C1D-ND	2.09	112.20	110.13
26	7	609	CHL	CMD-C2D-C3D	2.09	128.86	124.68
25	6	605	CLA	C1D-ND-C4D	-2.09	104.84	106.31
25	7	604	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
25	4	611	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	7	612	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	1	603	CLA	C3B-C4B-NB	-2.09	108.66	110.53
25	A	1132	CLA	CMA-C3A-C4A	2.09	117.39	111.77
29	5	504	BCR	C36-C18-C19	2.09	121.28	118.09
25	A	1126	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
26	a	610	CHL	CMD-C2D-C3D	2.09	128.86	124.68
25	K	1401	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	2	607	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
25	B	1219	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
25	7	603	CLA	C2D-C1D-ND	2.09	112.19	110.13
25	6	608	CLA	C1D-ND-C4D	-2.09	104.85	106.31
25	A	1123	CLA	C3B-C4B-NB	-2.09	108.67	110.53
25	3	602	CLA	C3B-C4B-NB	-2.09	108.67	110.53
25	A	1106	CLA	C3D-C2D-C1D	-2.09	102.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	5001	LHG	C5-O7-C7	-2.09	112.80	117.80
26	1	613	CHL	C1C-C2C-CMC	2.09	130.57	126.80
43	a	503	LUT	C19-C9-C8	2.09	121.28	118.09
29	B	4006	BCR	C36-C18-C17	-2.09	119.43	122.82
25	B	1229	CLA	CHA-C1A-NA	-2.09	121.66	126.39
25	4	612	CLA	CHA-C1A-NA	-2.09	121.66	126.39
26	A	1114	CHL	CMD-C2D-C3D	2.09	128.85	124.68
25	A	1103	CLA	C3B-C4B-NB	-2.09	108.67	110.53
26	9	613	CHL	CMD-C2D-C3D	2.09	128.85	124.68
25	A	1131	CLA	CHA-C1A-NA	-2.09	121.67	126.39
26	9	608	CHL	CMD-C2D-C3D	2.08	128.85	124.68
25	B	1228	CLA	C3B-C4B-NB	-2.08	108.67	110.53
25	3	602	CLA	C2D-C1D-ND	2.08	112.19	110.13
29	L	4001	BCR	C36-C18-C17	-2.08	119.44	122.82
25	7	608	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
26	6	611	CHL	CMD-C2D-C3D	2.08	128.85	124.68
25	B	1212	CLA	O2A-CGA-CBA	2.08	118.19	111.83
25	A	1109	CLA	CHA-C1A-NA	-2.08	121.67	126.39
25	K	1404	CLA	CHA-C1A-NA	-2.08	121.67	126.39
25	3	602	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
26	4	618	CHL	CMD-C2D-C3D	2.08	128.85	124.68
26	3	604	CHL	CMD-C2D-C3D	2.08	128.84	124.68
25	B	1204	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
25	5	615	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
25	A	1124	CLA	C1D-ND-C4D	-2.08	104.85	106.31
25	J	1901	CLA	C1D-ND-C4D	-2.08	104.85	106.31
25	3	612	CLA	C1D-ND-C4D	-2.08	104.85	106.31
26	6	610	CHL	CMD-C2D-C3D	2.08	128.84	124.68
26	a	606	CHL	CMD-C2D-C3D	2.08	128.84	124.68
25	A	1125	CLA	O2A-CGA-CBA	2.08	118.18	111.83
25	B	1219	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	5	601	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	8	609	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
25	B	1204	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
25	A	1104	CLA	CHA-C1A-NA	-2.08	121.68	126.39
26	7	617	CHL	CMD-C2D-C3D	2.08	128.84	124.68
43	9	501	LUT	C30-C31-C32	-2.08	117.17	123.20
26	5	610	CHL	CMD-C2D-C3D	2.08	128.84	124.68
26	6	609	CHL	CMD-C2D-C3D	2.08	128.84	124.68
25	B	1210	CLA	CMA-C3A-C4A	2.08	117.36	111.77
25	2	608	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	B	1217	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	615	CLA	CHD-C1D-ND	-2.08	121.88	124.80
26	a	609	CHL	CMD-C2D-C3D	2.08	128.84	124.68
29	5	504	BCR	C38-C26-C27	2.08	118.03	113.60
43	3	501	LUT	C20-C13-C12	2.08	121.26	118.09
25	A	1124	CLA	C2D-C1D-ND	2.08	112.18	110.13
25	7	606	CLA	C3B-C4B-NB	-2.08	108.67	110.53
26	2	609	CHL	CMD-C2D-C3D	2.08	128.84	124.68
25	B	1215	CLA	C2D-C1D-ND	2.08	112.18	110.13
25	4	610	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
25	A	1104	CLA	C1D-ND-C4D	-2.08	104.86	106.31
25	5	614	CLA	C2D-C1D-ND	2.08	112.18	110.13
29	B	4002	BCR	C28-C27-C26	-2.08	110.35	114.06
29	7	503	BCR	C3-C4-C5	-2.08	110.35	114.06
25	2	615	CLA	CHA-C1A-NA	-2.08	121.69	126.39
25	1	605	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
25	B	1235	CLA	C1-O2A-CGA	2.08	121.67	116.65
29	A	4002	BCR	C38-C26-C27	2.08	118.02	113.60
25	7	601	CLA	C2D-C1D-ND	2.08	112.18	110.13
25	4	605	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
25	a	608	CLA	C1D-ND-C4D	-2.08	104.86	106.31
25	B	1236	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
25	A	1134	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
25	O	1803	CLA	C1D-ND-C4D	-2.07	104.86	106.31
25	4	616	CLA	C1D-ND-C4D	-2.07	104.86	106.31
25	5	601	CLA	CMA-C3A-C4A	2.07	117.35	111.77
43	8	501	LUT	C30-C31-C32	-2.07	117.19	123.20
25	H	1701	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	7	610	CLA	O2A-CGA-CBA	2.07	118.16	111.83
29	K	4001	BCR	C31-C1-C6	-2.07	106.99	110.24
25	8	611	CLA	C1D-ND-C4D	-2.07	104.86	106.31
26	a	604	CHL	CMD-C2D-C3D	2.07	128.82	124.68
29	A	4004	BCR	C33-C5-C4	2.07	118.01	113.60
25	7	607	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	8	607	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	A	1102	CLA	C3B-C4B-NB	-2.07	108.68	110.53
25	5	607	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
25	G	1603	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	9	602	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
25	a	601	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
25	3	613	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	A	1134	CLA	C2D-C1D-ND	2.07	112.17	110.13
25	1	605	CLA	C2D-C1D-ND	2.07	112.17	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	619	CHL	CMD-C2D-C3D	2.07	128.82	124.68
25	2	605	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	A	1130	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	a	615	CLA	CHD-C1D-ND	-2.07	121.89	124.80
26	2	609	CHL	C1-O2A-CGA	2.07	121.66	116.65
25	9	607	CLA	C2D-C1D-ND	2.07	112.17	110.13
25	2	605	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
25	A	1126	CLA	CHA-C1A-NA	-2.07	121.71	126.39
29	K	4002	BCR	C38-C26-C27	2.07	118.00	113.60
25	A	1127	CLA	CHD-C1D-ND	-2.07	121.89	124.80
26	5	611	CHL	CMD-C2D-C3D	2.07	128.81	124.68
26	5	617	CHL	CMD-C2D-C3D	2.07	128.81	124.68
25	8	615	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	A	1141	CLA	C2D-C1D-ND	2.07	112.17	110.13
25	5	603	CLA	CAA-C2A-C3A	-2.07	107.42	113.00
25	B	1206	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	5	602	CLA	C1-O2A-CGA	2.07	121.65	116.65
25	5	605	CLA	CHD-C1D-ND	-2.07	121.90	124.80
25	A	1115	CLA	C2D-C1D-ND	2.07	112.17	110.13
25	8	615	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
25	O	1802	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
25	B	1226	CLA	CHA-C1A-NA	-2.06	121.72	126.39
25	1	612	CLA	CHA-C1A-NA	-2.06	121.72	126.39
25	4	602	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
25	a	601	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
25	2	615	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
25	6	607	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
29	A	4004	BCR	C8-C7-C6	-2.06	121.49	127.00
25	A	1122	CLA	C2D-C1D-ND	2.06	112.17	110.13
25	B	1224	CLA	C2D-C1D-ND	2.06	112.17	110.13
25	2	605	CLA	C2D-C1D-ND	2.06	112.17	110.13
29	L	4001	BCR	C38-C26-C27	2.06	117.99	113.60
44	7	504	AXT	C35-C15-C14	2.06	127.74	123.52
29	B	4006	BCR	C37-C22-C23	2.06	121.24	118.09
25	8	606	CLA	C3B-C4B-NB	-2.06	108.69	110.53
29	K	4002	BCR	C27-C26-C25	-2.06	119.92	122.70
25	2	606	CLA	C1D-ND-C4D	-2.06	104.87	106.31
25	B	1210	CLA	CAC-C3C-C4C	2.06	127.47	124.79
25	7	610	CLA	C1-O2A-CGA	2.06	121.64	116.65
26	4	613	CHL	CMD-C2D-C3D	2.06	128.80	124.68
26	8	604	CHL	CMD-C2D-C3D	2.06	128.80	124.68
25	4	607	CLA	CHA-C1A-NA	-2.06	121.73	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1104	CLA	C6-C5-C3	-2.06	108.45	113.47
25	4	608	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
25	B	1239	CLA	CHA-C1A-NA	-2.06	121.73	126.39
26	1	613	CHL	CMD-C2D-C3D	2.06	128.79	124.68
25	B	1212	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
25	7	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
25	A	1135	CLA	C2D-C1D-ND	2.06	112.16	110.13
25	a	601	CLA	C2D-C1D-ND	2.06	112.16	110.13
29	B	4007	BCR	C33-C5-C4	2.06	117.98	113.60
25	B	1236	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	3	606	CLA	C3B-C4B-NB	-2.06	108.69	110.53
29	H	4001	BCR	C19-C18-C17	2.06	122.24	119.01
29	7	503	BCR	C12-C13-C14	-2.06	115.77	119.01
25	9	606	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	A	1126	CLA	C6-C5-C3	-2.06	108.46	113.47
25	B	1023	CLA	C2D-C1D-ND	2.06	112.16	110.13
25	5	609	CLA	C1D-ND-C4D	-2.06	104.87	106.31
25	A	1125	CLA	CMD-C2D-C3D	-2.06	122.98	127.69
25	A	1136	CLA	O2A-CGA-CBA	2.06	118.10	111.83
25	6	604	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	5	612	CLA	CBC-CAC-C3C	-2.05	106.85	112.42
35	2	804	LMT	O1'-C1'-C2'	2.05	111.39	108.27
43	6	501	LUT	C8-C7-C6	-2.05	121.51	127.00
25	9	605	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
25	5	606	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	1	608	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
25	B	1211	CLA	C1D-ND-C4D	-2.05	104.87	106.31
25	4	617	CLA	C1D-ND-C4D	-2.05	104.87	106.31
25	A	1110	CLA	C2D-C1D-ND	2.05	112.16	110.13
25	3	618	CLA	C2D-C1D-ND	2.05	112.16	110.13
25	6	615	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
25	4	612	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
25	B	1231	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	G	1602	CLA	C2D-C1D-ND	2.05	112.16	110.13
25	3	618	CLA	C1D-ND-C4D	-2.05	104.87	106.31
25	8	602	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	8	608	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	A	1127	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	A	1137	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	5	614	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	A	1101	CLA	O2A-CGA-CBA	2.05	118.08	111.83
25	3	613	CLA	O1D-CGD-CBD	-2.05	120.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	1601	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	8	611	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	3	610	CLA	CHA-C1A-NA	-2.05	121.75	126.39
25	B	1230	CLA	C3B-C4B-NB	-2.05	108.70	110.53
25	5	605	CLA	CHA-C1A-NA	-2.05	121.76	126.39
29	4	503	BCR	C30-C25-C24	2.05	121.20	115.65
25	A	1140	CLA	CHA-C1A-NA	-2.05	121.76	126.39
29	L	4003	BCR	C33-C5-C4	2.05	117.96	113.60
43	a	501	LUT	C39-C29-C28	2.05	121.21	118.09
25	7	610	CLA	CHA-C1A-NA	-2.05	121.76	126.39
25	6	607	CLA	C1D-ND-C4D	-2.05	104.88	106.31
25	5	605	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
25	K	1404	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
25	A	1125	CLA	C1-O2A-CGA	2.04	121.60	116.65
25	a	602	CLA	CHA-C1A-NA	-2.04	121.76	126.39
29	5	504	BCR	C23-C22-C21	-2.04	115.79	119.01
25	B	1228	CLA	C1D-ND-C4D	-2.04	104.88	106.31
25	A	1136	CLA	C1-O2A-CGA	2.04	121.60	116.65
26	2	613	CHL	CMD-C2D-C3D	2.04	128.77	124.68
25	B	1218	CLA	C1-O2A-CGA	2.04	121.60	116.65
35	2	804	LMT	O5B-C5B-C4B	2.04	113.38	109.70
25	7	605	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	A	1109	CLA	C1D-ND-C4D	-2.04	104.88	106.31
26	7	615	CHL	CMD-C2D-C3D	2.04	128.76	124.68
25	B	1210	CLA	C3B-C4B-NB	-2.04	108.71	110.53
25	1	606	CLA	C3B-C4B-NB	-2.04	108.71	110.53
29	3	504	BCR	C37-C22-C21	-2.04	119.51	122.82
25	B	1225	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	B	1202	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
26	1	611	CHL	CMD-C2D-C3D	2.04	128.76	124.68
25	A	1132	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	A	1137	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
25	G	1601	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
25	A	1136	CLA	C2D-C1D-ND	2.04	112.14	110.13
29	H	4001	BCR	C27-C26-C25	-2.04	119.95	122.70
29	5	504	BCR	C15-C14-C13	-2.04	124.42	127.28
25	L	1503	CLA	C3B-C4B-NB	-2.04	108.71	110.53
43	3	502	LUT	C40-C33-C32	2.04	121.20	118.09
25	8	605	CLA	O2A-CGA-CBA	2.04	118.05	111.83
25	5	607	CLA	CHA-C1A-NA	-2.04	121.78	126.39
26	4	609	CHL	CMD-C2D-C3D	2.04	128.75	124.68
25	A	1124	CLA	CMD-C2D-C3D	-2.04	123.02	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	606	CLA	C1D-ND-C4D	-2.04	104.88	106.31
25	A	1135	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
50	2	501	XAT	C24-C23-C22	-2.03	106.98	110.79
25	2	607	CLA	CHA-C1A-NA	-2.03	121.78	126.39
29	A	4001	BCR	C31-C1-C6	-2.03	107.05	110.24
25	B	1211	CLA	CHA-C1A-NA	-2.03	121.78	126.39
25	A	1126	CLA	O2A-CGA-CBA	2.03	118.04	111.83
29	3	505	BCR	C28-C27-C26	-2.03	110.43	114.06
26	4	618	CHL	CAA-C2A-C3A	-2.03	107.50	113.00
25	B	1232	CLA	C1D-ND-C4D	-2.03	104.89	106.31
26	9	601	CHL	CMD-C2D-C3D	2.03	128.75	124.68
25	H	1703	CLA	C2D-C1D-ND	2.03	112.14	110.13
25	A	1130	CLA	O2A-CGA-CBA	2.03	118.03	111.83
25	6	604	CLA	C2C-C1C-NC	2.03	112.12	109.98
29	J	4001	BCR	C38-C26-C27	2.03	117.93	113.60
25	B	1224	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
25	A	1125	CLA	C6-C5-C3	-2.03	108.52	113.47
25	1	605	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
25	4	611	CLA	C2D-C1D-ND	2.03	112.14	110.13
25	B	1221	CLA	C3B-C4B-NB	-2.03	108.72	110.53
29	3	503	BCR	C36-C18-C17	-2.03	119.53	122.82
29	L	4002	BCR	C29-C28-C27	2.03	115.74	111.28
43	3	502	LUT	C38-C25-C24	-2.03	118.56	123.36
25	1	602	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
25	9	606	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
29	G	4001	BCR	C33-C5-C4	2.03	117.92	113.60
25	2	615	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
29	3	505	BCR	C35-C13-C12	2.03	121.19	118.09
25	4	601	CLA	C2D-C1D-ND	2.03	112.13	110.13
30	2	802	LHG	C5-O7-C7	-2.03	112.94	117.80
25	A	1138	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
25	8	618	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	4	611	CLA	C1-O2A-CGA	2.03	121.56	116.65
47	6	804	PLM	C3-C2-C1	-2.03	109.22	114.51
25	O	1803	CLA	C2D-C1D-ND	2.03	112.13	110.13
25	A	1120	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
25	B	1215	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
25	B	1232	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	B	1222	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
25	B	1228	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
25	7	605	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	B	1205	CLA	CAA-C2A-C3A	-2.03	107.52	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	F	1301	CLA	C2D-C1D-ND	2.03	112.13	110.13
25	7	610	CLA	C2D-C1D-ND	2.03	112.13	110.13
44	7	504	AXT	C20-C13-C14	-2.03	119.53	122.82
25	8	615	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
25	a	603	CLA	C1D-ND-C4D	-2.03	104.89	106.31
43	a	501	LUT	C38-C25-C24	-2.03	118.57	123.36
25	7	607	CLA	CMD-C2D-C3D	-2.03	123.05	127.69
25	4	610	CLA	C2D-C1D-ND	2.02	112.13	110.13
25	a	615	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	A	1124	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	6	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
30	7	801	LHG	C6-C5-C4	-2.02	107.06	111.78
25	8	606	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	a	607	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
25	H	1702	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	9	607	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	5	608	CLA	C1D-ND-C4D	-2.02	104.89	106.31
25	A	1104	CLA	C2D-C1D-ND	2.02	112.13	110.13
25	3	610	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
25	A	1012	CLA	C2D-C1D-ND	2.02	112.13	110.13
25	A	1126	CLA	C2D-C1D-ND	2.02	112.13	110.13
25	1	606	CLA	C1D-ND-C4D	-2.02	104.89	106.31
25	B	1216	CLA	CHA-C1A-NA	-2.02	121.81	126.39
50	9	507	XAT	C24-C23-C22	-2.02	107.01	110.79
25	9	609	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
43	5	502	LUT	C30-C31-C32	-2.02	117.34	123.20
27	B	2002	PQN	C2M-C2-C3	-2.02	121.13	124.45
43	a	502	LUT	C30-C31-C32	-2.02	117.35	123.20
29	A	4003	BCR	C38-C26-C27	2.02	117.90	113.60
25	B	1217	CLA	C1-O2A-CGA	2.02	121.54	116.65
25	8	607	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
25	B	1227	CLA	C2D-C1D-ND	2.02	112.12	110.13
25	4	607	CLA	C1D-ND-C4D	-2.02	104.89	106.31
25	A	1013	CLA	C1-O2A-CGA	2.02	121.54	116.65
25	A	1124	CLA	CHA-C1A-NA	-2.02	121.82	126.39
25	4	606	CLA	CHA-C1A-NA	-2.02	121.82	126.39
25	7	606	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
25	B	1213	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	3	613	CLA	C2D-C1D-ND	2.02	112.12	110.13
26	5	613	CHL	C3D-C4D-ND	-2.02	109.70	112.94
29	B	4002	BCR	C36-C18-C17	-2.02	119.55	122.82
29	B	4007	BCR	C15-C14-C13	-2.02	124.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	4001	BCR	C29-C28-C27	2.02	115.71	111.28
43	9	502	LUT	C8-C7-C6	-2.02	121.61	127.00
25	A	1135	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	B	1235	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	4	617	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	2	607	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	6	604	CLA	C6-C5-C3	-2.02	108.56	113.47
25	6	615	CLA	CMD-C2D-C3D	-2.02	123.07	127.69
25	F	1302	CLA	C2D-C1D-ND	2.02	112.12	110.13
25	8	602	CLA	C2D-C1D-ND	2.02	112.12	110.13
29	L	4001	BCR	C33-C5-C4	2.02	117.89	113.60
25	G	1601	CLA	C2D-C1D-ND	2.01	112.12	110.13
27	A	2001	PQN	C2M-C2-C3	-2.01	121.14	124.45
25	3	616	CLA	CHA-C1A-NA	-2.01	121.83	126.39
25	7	603	CLA	CHA-C1A-NA	-2.01	121.83	126.39
43	2	507	LUT	C38-C25-C24	-2.01	118.59	123.36
25	G	1601	CLA	O2A-CGA-CBA	2.01	117.98	111.83
25	A	1139	CLA	CHA-C1A-NA	-2.01	121.83	126.39
25	B	1207	CLA	CHA-C1A-NA	-2.01	121.83	126.39
25	A	1123	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
43	8	502	LUT	C22-C23-C24	-2.01	108.19	111.18
25	1	608	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
25	B	1205	CLA	C2D-C1D-ND	2.01	112.12	110.13
29	A	4005	BCR	C38-C26-C25	-2.01	122.29	124.48
25	A	1116	CLA	CHA-C1A-NA	-2.01	121.83	126.39
26	6	613	CHL	CMA-C3A-C4A	2.01	118.95	114.61
25	B	1239	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
25	A	1111	CLA	CMA-C3A-C4A	2.01	117.18	111.77
25	2	607	CLA	C2D-C1D-ND	2.01	112.12	110.13
29	A	4001	BCR	C30-C25-C26	-2.01	119.89	122.64
29	H	4001	BCR	C38-C26-C27	2.01	117.88	113.60
25	5	612	CLA	CHA-C1A-NA	-2.01	121.84	126.39
25	7	608	CLA	C1D-ND-C4D	-2.01	104.90	106.31
25	A	1140	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
25	9	609	CLA	C2D-C1D-ND	2.01	112.12	110.13
25	5	602	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
25	B	1203	CLA	CHA-C1A-NA	-2.01	121.84	126.39
25	O	1803	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
40	J	4002	RRX	C30-C25-C24	2.01	121.10	115.65
29	8	503	BCR	C29-C28-C27	2.01	115.70	111.28
25	A	1141	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	B	4001	BCR	C38-C26-C25	-2.01	122.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	618	CLA	CHA-C1A-NA	-2.01	121.84	126.39
26	9	603	CHL	CMD-C2D-C3D	2.01	128.70	124.68
25	4	603	CLA	C2D-C1D-ND	2.01	112.11	110.13
25	3	616	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
25	B	1223	CLA	CHD-C1D-ND	-2.01	121.98	124.80
29	B	4005	BCR	C35-C13-C12	2.01	121.16	118.09
25	B	1240	CLA	C1D-ND-C4D	-2.01	104.90	106.31
25	G	1601	CLA	C1D-ND-C4D	-2.01	104.90	106.31
25	2	603	CLA	C1D-ND-C4D	-2.01	104.90	106.31
26	3	608	CHL	C4C-CHD-C1D	2.01	123.25	116.07
25	A	1118	CLA	CHA-C1A-NA	-2.01	121.84	126.39
26	5	617	CHL	C1C-C2C-CMC	2.01	130.42	126.80
25	A	1136	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
25	A	1108	CLA	C2D-C1D-ND	2.01	112.11	110.13
25	1	607	CLA	CHA-C1A-NA	-2.01	121.84	126.39
43	7	501	LUT	C20-C13-C12	2.01	121.15	118.09
29	B	4004	BCR	C3-C4-C5	-2.01	110.48	114.06
29	B	4002	BCR	C7-C6-C5	-2.01	116.93	121.56
25	4	617	CLA	C2D-C1D-ND	2.01	112.11	110.13
25	A	1104	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	7	503	BCR	C7-C6-C5	-2.01	116.94	121.56
25	B	1217	CLA	CHA-C1A-NA	-2.01	121.85	126.39
43	7	501	LUT	C8-C7-C6	-2.01	121.64	127.00
43	8	501	LUT	C39-C29-C28	2.01	121.15	118.09
25	1	602	CLA	C2D-C1D-ND	2.01	112.11	110.13
25	9	604	CLA	CHA-C1A-NA	-2.01	121.85	126.39
25	B	1203	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
36	8	803	DGD	C2G-O2G-C1B	-2.00	113.00	117.80
30	1	802	LHG	O7-C7-O9	-2.00	119.02	123.70
25	K	1403	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
25	K	1402	CLA	C1D-ND-C4D	-2.00	104.91	106.31
25	K	1403	CLA	C2D-C1D-ND	2.00	112.11	110.13
26	8	613	CHL	CMD-C2D-C3D	2.00	128.69	124.68
25	G	1603	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
25	9	602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
29	K	4002	BCR	C33-C5-C4	2.00	117.86	113.60
25	A	1122	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
44	1	502	AXT	O3-C3-C4	2.00	114.22	109.71
36	8	802	DGD	O2G-C1B-O1B	-2.00	119.03	123.70
25	1	612	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
25	B	1228	CLA	CHA-C1A-NA	-2.00	121.86	126.39
42	M	4001	ECH	C20-C19-C18	-2.00	120.88	126.36

All (394) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	1011	CL0	ND
24	A	1011	CL0	NA
24	A	1011	CL0	NC
25	A	1012	CLA	ND
25	A	1013	CLA	ND
25	A	1102	CLA	ND
25	A	1103	CLA	ND
25	A	1104	CLA	ND
25	A	1105	CLA	ND
25	A	1106	CLA	ND
25	A	1107	CLA	ND
25	A	1108	CLA	ND
25	A	1109	CLA	ND
25	A	1110	CLA	ND
25	A	1111	CLA	ND
25	A	1112	CLA	ND
25	A	1113	CLA	ND
25	A	1115	CLA	ND
25	A	1116	CLA	ND
25	A	1117	CLA	ND
25	A	1118	CLA	ND
25	A	1119	CLA	ND
25	A	1120	CLA	ND
25	A	1121	CLA	ND
25	A	1122	CLA	ND
25	A	1123	CLA	ND
25	A	1124	CLA	ND
25	A	1125	CLA	ND
25	A	1126	CLA	ND
25	A	1127	CLA	ND
25	A	1128	CLA	ND
25	A	1129	CLA	ND
25	A	1130	CLA	ND
25	A	1131	CLA	ND
25	A	1132	CLA	ND
25	A	1133	CLA	ND
25	A	1134	CLA	ND
25	A	1135	CLA	ND
25	A	1136	CLA	ND
25	A	1137	CLA	ND
25	A	1138	CLA	ND
25	A	1139	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	1140	CLA	ND
25	A	1101	CLA	ND
25	A	1141	CLA	ND
25	B	1237	CLA	ND
25	B	1021	CLA	ND
25	B	1022	CLA	ND
25	B	1023	CLA	ND
25	B	1201	CLA	ND
25	B	1202	CLA	ND
25	B	1203	CLA	ND
25	B	1204	CLA	ND
25	B	1205	CLA	ND
25	B	1206	CLA	ND
25	B	1208	CLA	ND
25	B	1209	CLA	ND
25	B	1210	CLA	ND
25	B	1211	CLA	ND
25	B	1212	CLA	ND
25	B	1213	CLA	ND
25	B	1214	CLA	ND
25	B	1215	CLA	ND
25	B	1216	CLA	ND
25	B	1217	CLA	ND
25	B	1218	CLA	ND
25	B	1219	CLA	ND
25	B	1220	CLA	ND
25	B	1221	CLA	ND
25	B	1222	CLA	ND
25	B	1223	CLA	ND
25	B	1224	CLA	ND
25	B	1225	CLA	ND
25	B	1226	CLA	ND
25	B	1227	CLA	ND
25	B	1228	CLA	ND
25	B	1229	CLA	ND
25	B	1230	CLA	ND
25	B	1231	CLA	ND
25	B	1232	CLA	ND
25	B	1235	CLA	ND
25	B	1236	CLA	ND
25	B	1238	CLA	ND
25	B	1239	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	1240	CLA	ND
25	B	1207	CLA	ND
25	F	1301	CLA	ND
25	F	1302	CLA	ND
25	G	1601	CLA	ND
25	G	1602	CLA	ND
25	G	1603	CLA	ND
25	H	1701	CLA	ND
25	H	1702	CLA	ND
25	H	1703	CLA	ND
25	J	1901	CLA	ND
25	K	1401	CLA	ND
25	K	1402	CLA	ND
25	K	1403	CLA	ND
25	K	1404	CLA	ND
25	L	1501	CLA	ND
25	L	1502	CLA	ND
25	L	1503	CLA	ND
25	L	1504	CLA	ND
25	O	1801	CLA	ND
25	O	1802	CLA	ND
25	O	1803	CLA	ND
25	1	601	CLA	ND
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	605	CLA	ND
25	1	606	CLA	ND
25	1	607	CLA	ND
25	1	608	CLA	ND
25	1	612	CLA	ND
25	1	615	CLA	ND
25	a	601	CLA	ND
25	a	602	CLA	ND
25	a	603	CLA	ND
25	a	605	CLA	ND
25	a	607	CLA	ND
25	a	608	CLA	ND
25	a	611	CLA	ND
25	a	612	CLA	ND
25	a	615	CLA	ND
25	3	601	CLA	ND
25	3	602	CLA	ND

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Mol	Chain	Res	Type	Atom
25	3	605	CLA	ND
25	3	606	CLA	ND
25	3	607	CLA	ND
25	3	610	CLA	ND
25	3	612	CLA	ND
25	3	613	CLA	ND
25	3	618	CLA	ND
25	3	616	CLA	ND
25	4	601	CLA	ND
25	4	602	CLA	ND
25	4	603	CLA	ND
25	4	604	CLA	ND
25	4	605	CLA	ND
25	4	606	CLA	ND
25	4	607	CLA	ND
25	4	608	CLA	ND
25	4	610	CLA	ND
25	4	611	CLA	ND
25	4	612	CLA	ND
25	4	615	CLA	ND
25	4	616	CLA	ND
25	4	617	CLA	ND
25	5	601	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	605	CLA	ND
25	5	606	CLA	ND
25	5	607	CLA	ND
25	5	608	CLA	ND
25	5	609	CLA	ND
25	5	612	CLA	ND
25	5	614	CLA	ND
25	5	615	CLA	ND
25	6	608	CLA	ND
25	6	601	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	604	CLA	ND
25	6	605	CLA	ND
25	6	606	CLA	ND
25	6	607	CLA	ND

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Mol	Chain	Res	Type	Atom
25	6	612	CLA	ND
25	6	615	CLA	ND
25	6	618	CLA	ND
25	7	601	CLA	ND
25	7	602	CLA	ND
25	7	603	CLA	ND
25	7	604	CLA	ND
25	7	605	CLA	ND
25	7	606	CLA	ND
25	7	607	CLA	ND
25	7	608	CLA	ND
25	7	610	CLA	ND
25	7	612	CLA	ND
25	8	602	CLA	ND
25	8	605	CLA	ND
25	8	606	CLA	ND
25	8	607	CLA	ND
25	8	608	CLA	ND
25	8	609	CLA	ND
25	8	611	CLA	ND
25	8	612	CLA	ND
25	8	615	CLA	ND
25	8	618	CLA	ND
25	8	620	CLA	ND
25	2	601	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	604	CLA	ND
25	2	605	CLA	ND
25	2	606	CLA	ND
25	2	607	CLA	ND
25	2	608	CLA	ND
25	2	612	CLA	ND
25	2	615	CLA	ND
25	2	621	CLA	ND
25	9	602	CLA	ND
25	9	604	CLA	ND
25	9	605	CLA	ND
25	9	606	CLA	ND
25	9	607	CLA	ND
25	9	609	CLA	ND
25	9	612	CLA	ND

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Mol	Chain	Res	Type	Atom
26	A	1114	CHL	ND
26	A	1114	CHL	C8
26	A	1114	CHL	NA
26	A	1114	CHL	NC
26	1	604	CHL	ND
26	1	604	CHL	C8
26	1	604	CHL	NA
26	1	604	CHL	NC
26	1	610	CHL	ND
26	1	610	CHL	NA
26	1	610	CHL	NC
26	1	611	CHL	ND
26	1	611	CHL	C8
26	1	611	CHL	NA
26	1	611	CHL	NC
26	1	613	CHL	ND
26	1	613	CHL	NA
26	1	613	CHL	NC
26	1	609	CHL	ND
26	1	609	CHL	C8
26	1	609	CHL	NA
26	1	609	CHL	NC
26	a	604	CHL	ND
26	a	604	CHL	C8
26	a	604	CHL	NA
26	a	604	CHL	NC
26	a	606	CHL	ND
26	a	606	CHL	C8
26	a	606	CHL	NA
26	a	606	CHL	NC
26	a	609	CHL	ND
26	a	609	CHL	NA
26	a	609	CHL	NC
26	a	610	CHL	ND
26	a	610	CHL	NA
26	a	610	CHL	NC
26	a	613	CHL	ND
26	a	613	CHL	NA
26	a	613	CHL	NC
26	3	603	CHL	ND
26	3	603	CHL	C8
26	3	603	CHL	NA

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Mol	Chain	Res	Type	Atom
26	3	603	CHL	NC
26	3	604	CHL	ND
26	3	604	CHL	C8
26	3	604	CHL	NA
26	3	604	CHL	NC
26	3	608	CHL	ND
26	3	608	CHL	NA
26	3	608	CHL	NC
26	3	611	CHL	ND
26	3	611	CHL	C8
26	3	611	CHL	NA
26	3	611	CHL	NC
26	4	613	CHL	ND
26	4	613	CHL	NA
26	4	613	CHL	NC
26	4	618	CHL	ND
26	4	618	CHL	C8
26	4	618	CHL	NA
26	4	618	CHL	NC
26	4	609	CHL	ND
26	4	609	CHL	C8
26	4	609	CHL	NA
26	4	609	CHL	NC
26	5	610	CHL	ND
26	5	610	CHL	C8
26	5	610	CHL	NA
26	5	610	CHL	NC
26	5	611	CHL	ND
26	5	611	CHL	NA
26	5	611	CHL	NC
26	5	613	CHL	ND
26	5	613	CHL	C8
26	5	613	CHL	NA
26	5	613	CHL	NC
26	5	617	CHL	ND
26	5	617	CHL	NA
26	5	617	CHL	NC
26	5	618	CHL	ND
26	5	618	CHL	NA
26	5	618	CHL	NC
26	6	609	CHL	ND
26	6	609	CHL	C8

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Mol	Chain	Res	Type	Atom
26	6	609	CHL	NA
26	6	609	CHL	NC
26	6	610	CHL	ND
26	6	610	CHL	C8
26	6	610	CHL	NA
26	6	610	CHL	NC
26	6	611	CHL	ND
26	6	611	CHL	NA
26	6	611	CHL	NC
26	6	613	CHL	ND
26	6	613	CHL	NA
26	6	613	CHL	NC
26	6	617	CHL	ND
26	6	617	CHL	NA
26	6	617	CHL	NC
26	6	619	CHL	ND
26	6	619	CHL	NC
26	6	619	CHL	C3A
26	6	619	CHL	C8
26	6	619	CHL	NA
26	7	609	CHL	ND
26	7	609	CHL	C8
26	7	609	CHL	NA
26	7	609	CHL	NC
26	7	611	CHL	ND
26	7	611	CHL	C8
26	7	611	CHL	NA
26	7	611	CHL	NC
26	7	613	CHL	ND
26	7	613	CHL	C8
26	7	613	CHL	NA
26	7	613	CHL	NC
26	7	615	CHL	ND
26	7	615	CHL	NA
26	7	615	CHL	NC
26	7	617	CHL	ND
26	7	617	CHL	C8
26	7	617	CHL	NA
26	7	617	CHL	NC
26	8	601	CHL	ND
26	8	601	CHL	C8
26	8	601	CHL	NA

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Mol	Chain	Res	Type	Atom
26	8	601	CHL	NC
26	8	603	CHL	ND
26	8	603	CHL	C8
26	8	603	CHL	NA
26	8	603	CHL	NC
26	8	604	CHL	ND
26	8	604	CHL	C8
26	8	604	CHL	NA
26	8	604	CHL	NC
26	8	610	CHL	ND
26	8	610	CHL	NC
26	8	610	CHL	C3A
26	8	610	CHL	C8
26	8	610	CHL	NA
26	8	613	CHL	ND
26	8	613	CHL	NA
26	8	613	CHL	NC
26	2	609	CHL	ND
26	2	609	CHL	C8
26	2	609	CHL	NA
26	2	609	CHL	NC
26	2	610	CHL	C3A
26	2	610	CHL	ND
26	2	610	CHL	NA
26	2	610	CHL	NC
26	2	613	CHL	ND
26	2	613	CHL	NA
26	2	613	CHL	NC
26	9	601	CHL	ND
26	9	601	CHL	C8
26	9	601	CHL	NA
26	9	601	CHL	NC
26	9	603	CHL	ND
26	9	603	CHL	C8
26	9	603	CHL	NA
26	9	603	CHL	NC
26	9	608	CHL	ND
26	9	608	CHL	NA
26	9	608	CHL	NC
26	9	610	CHL	ND
26	9	610	CHL	NA
26	9	610	CHL	NC

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Mol	Chain	Res	Type	Atom
26	9	613	CHL	ND
26	9	613	CHL	NA
26	9	613	CHL	NC
39	F	4001	NEX	C25
40	J	4002	RRX	C28
40	3	506	RRX	C28
43	4	501	LUT	C26
43	7	501	LUT	C26
43	2	507	LUT	C26
46	a	504	QTB	C12
50	7	502	XAT	C26
50	7	502	XAT	C6
50	2	501	XAT	C26
50	2	501	XAT	C6
50	9	504	XAT	C6
50	9	507	XAT	C26

All (4645) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1102	CLA	C1A-C2A-CAA-CBA
25	A	1102	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	CAD-CBD-CGD-O1D
25	A	1103	CLA	CAD-CBD-CGD-O2D
25	A	1106	CLA	C3A-C2A-CAA-CBA
25	A	1106	CLA	CHA-CBD-CGD-O1D
25	A	1106	CLA	CHA-CBD-CGD-O2D
25	A	1108	CLA	C4-C3-C5-C6
25	A	1109	CLA	C1A-C2A-CAA-CBA
25	A	1109	CLA	CBD-CGD-O2D-CED
25	A	1111	CLA	CBD-CGD-O2D-CED
25	A	1111	CLA	C11-C10-C8-C9
25	A	1113	CLA	C2-C1-O2A-CGA
25	A	1115	CLA	CHA-CBD-CGD-O1D
25	A	1115	CLA	CHA-CBD-CGD-O2D
25	A	1116	CLA	C1A-C2A-CAA-CBA
25	A	1116	CLA	C3A-C2A-CAA-CBA
25	A	1116	CLA	CBD-CGD-O2D-CED
25	A	1117	CLA	C1A-C2A-CAA-CBA
25	A	1117	CLA	C3A-C2A-CAA-CBA
25	A	1117	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	A	1117	CLA	CHA-CBD-CGD-O2D
25	A	1118	CLA	C3A-C2A-CAA-CBA
25	A	1118	CLA	CBD-CGD-O2D-CED
25	A	1119	CLA	C1A-C2A-CAA-CBA
25	A	1119	CLA	C3A-C2A-CAA-CBA
25	A	1119	CLA	CBD-CGD-O2D-CED
25	A	1121	CLA	CBD-CGD-O2D-CED
25	A	1122	CLA	C3A-C2A-CAA-CBA
25	A	1123	CLA	C2-C1-O2A-CGA
25	A	1125	CLA	C1A-C2A-CAA-CBA
25	A	1125	CLA	C3A-C2A-CAA-CBA
25	A	1125	CLA	C2-C1-O2A-CGA
25	A	1125	CLA	CAD-CBD-CGD-O2D
25	A	1126	CLA	C1A-C2A-CAA-CBA
25	A	1126	CLA	C2-C1-O2A-CGA
25	A	1126	CLA	CBD-CGD-O2D-CED
25	A	1128	CLA	CHA-CBD-CGD-O1D
25	A	1128	CLA	CHA-CBD-CGD-O2D
25	A	1128	CLA	C6-C7-C8-C9
25	A	1129	CLA	C2-C1-O2A-CGA
25	A	1130	CLA	C1A-C2A-CAA-CBA
25	A	1131	CLA	C1A-C2A-CAA-CBA
25	A	1131	CLA	C3A-C2A-CAA-CBA
25	A	1131	CLA	CBD-CGD-O2D-CED
25	A	1132	CLA	CHA-CBD-CGD-O1D
25	A	1132	CLA	CHA-CBD-CGD-O2D
25	A	1133	CLA	C1A-C2A-CAA-CBA
25	A	1136	CLA	C4-C3-C5-C6
25	A	1137	CLA	C2-C1-O2A-CGA
25	A	1139	CLA	C1A-C2A-CAA-CBA
25	A	1139	CLA	C3A-C2A-CAA-CBA
25	A	1139	CLA	CBD-CGD-O2D-CED
25	A	1140	CLA	CBD-CGD-O2D-CED
25	A	1101	CLA	C1A-C2A-CAA-CBA
25	A	1101	CLA	CHA-CBD-CGD-O1D
25	A	1101	CLA	CHA-CBD-CGD-O2D
25	A	1141	CLA	C1A-C2A-CAA-CBA
25	A	1141	CLA	C3A-C2A-CAA-CBA
25	A	1141	CLA	CAD-CBD-CGD-O1D
25	A	1141	CLA	CAD-CBD-CGD-O2D
25	B	1237	CLA	C2-C1-O2A-CGA
25	B	1021	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	1022	CLA	CBD-CGD-O2D-CED
25	B	1023	CLA	C2-C1-O2A-CGA
25	B	1023	CLA	CBD-CGD-O2D-CED
25	B	1201	CLA	C1A-C2A-CAA-CBA
25	B	1201	CLA	CBA-CGA-O2A-C1
25	B	1202	CLA	C3A-C2A-CAA-CBA
25	B	1202	CLA	CAD-CBD-CGD-O1D
25	B	1202	CLA	CAD-CBD-CGD-O2D
25	B	1203	CLA	CBD-CGD-O2D-CED
25	B	1203	CLA	C6-C7-C8-C9
25	B	1205	CLA	CHA-CBD-CGD-O1D
25	B	1205	CLA	CHA-CBD-CGD-O2D
25	B	1210	CLA	C1A-C2A-CAA-CBA
25	B	1210	CLA	C3A-C2A-CAA-CBA
25	B	1212	CLA	CHA-CBD-CGD-O1D
25	B	1212	CLA	CHA-CBD-CGD-O2D
25	B	1214	CLA	C3A-C2A-CAA-CBA
25	B	1214	CLA	C2-C1-O2A-CGA
25	B	1215	CLA	C1A-C2A-CAA-CBA
25	B	1215	CLA	C3A-C2A-CAA-CBA
25	B	1216	CLA	CBD-CGD-O2D-CED
25	B	1220	CLA	C1A-C2A-CAA-CBA
25	B	1220	CLA	C3A-C2A-CAA-CBA
25	B	1220	CLA	C2-C3-C5-C6
25	B	1220	CLA	C4-C3-C5-C6
25	B	1221	CLA	CHA-CBD-CGD-O1D
25	B	1221	CLA	CHA-CBD-CGD-O2D
25	B	1222	CLA	C1A-C2A-CAA-CBA
25	B	1222	CLA	C3A-C2A-CAA-CBA
25	B	1223	CLA	C1A-C2A-CAA-CBA
25	B	1224	CLA	C1A-C2A-CAA-CBA
25	B	1224	CLA	C3A-C2A-CAA-CBA
25	B	1225	CLA	C1A-C2A-CAA-CBA
25	B	1225	CLA	C3A-C2A-CAA-CBA
25	B	1228	CLA	C1A-C2A-CAA-CBA
25	B	1228	CLA	C3A-C2A-CAA-CBA
25	B	1228	CLA	C2-C1-O2A-CGA
25	B	1228	CLA	CBD-CGD-O2D-CED
25	B	1230	CLA	C3A-C2A-CAA-CBA
25	B	1230	CLA	CHA-CBD-CGD-O1D
25	B	1230	CLA	CHA-CBD-CGD-O2D
25	B	1231	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	B	1232	CLA	C1A-C2A-CAA-CBA
25	B	1232	CLA	C3A-C2A-CAA-CBA
25	B	1234	CLA	C6-C7-C8-C9
25	B	1235	CLA	CAD-CBD-CGD-O1D
25	B	1235	CLA	CAD-CBD-CGD-O2D
25	B	1235	CLA	C4-C3-C5-C6
25	B	1236	CLA	CHA-CBD-CGD-O1D
25	B	1236	CLA	CHA-CBD-CGD-O2D
25	B	1236	CLA	CBD-CGD-O2D-CED
25	B	1238	CLA	C2-C1-O2A-CGA
25	B	1239	CLA	C3A-C2A-CAA-CBA
25	B	1239	CLA	CBD-CGD-O2D-CED
25	B	1207	CLA	C2-C1-O2A-CGA
25	B	1207	CLA	CBD-CGD-O2D-CED
25	B	1207	CLA	C11-C10-C8-C9
25	F	1301	CLA	CBD-CGD-O2D-CED
25	F	1302	CLA	CBD-CGD-O2D-CED
25	G	1601	CLA	CBD-CGD-O2D-CED
25	G	1602	CLA	CBA-CGA-O2A-C1
25	G	1602	CLA	O1A-CGA-O2A-C1
25	G	1602	CLA	CBD-CGD-O2D-CED
25	G	1603	CLA	C1A-C2A-CAA-CBA
25	G	1603	CLA	C3A-C2A-CAA-CBA
25	G	1603	CLA	CBD-CGD-O2D-CED
25	H	1702	CLA	CHA-CBD-CGD-O1D
25	H	1702	CLA	CHA-CBD-CGD-O2D
25	J	1901	CLA	C1A-C2A-CAA-CBA
25	J	1901	CLA	C3A-C2A-CAA-CBA
25	J	1901	CLA	CBD-CGD-O2D-CED
25	K	1401	CLA	CBD-CGD-O2D-CED
25	K	1403	CLA	CAD-CBD-CGD-O1D
25	K	1403	CLA	CAD-CBD-CGD-O2D
25	K	1404	CLA	CAD-CBD-CGD-O1D
25	K	1404	CLA	CAD-CBD-CGD-O2D
25	L	1503	CLA	C3A-C2A-CAA-CBA
25	O	1802	CLA	CHA-CBD-CGD-O1D
25	O	1802	CLA	CHA-CBD-CGD-O2D
25	1	602	CLA	CBD-CGD-O2D-CED
25	1	605	CLA	C2-C1-O2A-CGA
25	1	606	CLA	C1A-C2A-CAA-CBA
25	1	606	CLA	C3A-C2A-CAA-CBA
25	1	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	612	CLA	C3A-C2A-CAA-CBA
25	1	615	CLA	C1A-C2A-CAA-CBA
25	1	615	CLA	C3A-C2A-CAA-CBA
25	a	601	CLA	CBD-CGD-O2D-CED
25	a	602	CLA	C2-C1-O2A-CGA
25	a	602	CLA	CBD-CGD-O2D-CED
25	a	603	CLA	CBD-CGD-O2D-CED
25	a	605	CLA	CHA-CBD-CGD-O1D
25	a	605	CLA	CHA-CBD-CGD-O2D
25	a	608	CLA	C1A-C2A-CAA-CBA
25	a	608	CLA	C3A-C2A-CAA-CBA
25	a	611	CLA	C1A-C2A-CAA-CBA
25	a	611	CLA	C3A-C2A-CAA-CBA
25	a	611	CLA	C2-C1-O2A-CGA
25	a	611	CLA	CBD-CGD-O2D-CED
25	a	612	CLA	C3A-C2A-CAA-CBA
25	3	601	CLA	C3A-C2A-CAA-CBA
25	3	602	CLA	CHA-CBD-CGD-O1D
25	3	602	CLA	CHA-CBD-CGD-O2D
25	3	605	CLA	CBD-CGD-O2D-CED
25	3	606	CLA	C1A-C2A-CAA-CBA
25	3	606	CLA	C3A-C2A-CAA-CBA
25	3	606	CLA	CBD-CGD-O2D-CED
25	3	607	CLA	C2-C1-O2A-CGA
25	3	612	CLA	C1A-C2A-CAA-CBA
25	3	612	CLA	C3A-C2A-CAA-CBA
25	3	613	CLA	C6-C7-C8-C9
25	3	618	CLA	CBD-CGD-O2D-CED
25	3	616	CLA	C2-C3-C5-C6
25	3	616	CLA	C4-C3-C5-C6
25	4	601	CLA	C2-C3-C5-C6
25	4	601	CLA	C4-C3-C5-C6
25	4	607	CLA	C2-C1-O2A-CGA
25	4	610	CLA	C2-C1-O2A-CGA
25	4	611	CLA	CBD-CGD-O2D-CED
25	4	612	CLA	CHA-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O2D
25	4	615	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	5	606	CLA	C1A-C2A-CAA-CBA
25	5	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	5	608	CLA	CBD-CGD-O2D-CED
25	5	612	CLA	CBD-CGD-O2D-CED
25	5	614	CLA	CBD-CGD-O2D-CED
25	5	615	CLA	C1A-C2A-CAA-CBA
25	6	608	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	6	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	605	CLA	CBD-CGD-O2D-CED
25	6	606	CLA	CHA-CBD-CGD-O1D
25	6	606	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	C1A-C2A-CAA-CBA
25	6	612	CLA	CBD-CGD-O2D-CED
25	6	615	CLA	CAD-CBD-CGD-O2D
25	6	618	CLA	CBD-CGD-O2D-CED
25	7	602	CLA	CBD-CGD-O2D-CED
25	7	603	CLA	CBD-CGD-O2D-CED
25	7	610	CLA	CBD-CGD-O2D-CED
25	8	605	CLA	C3A-C2A-CAA-CBA
25	8	605	CLA	CBD-CGD-O2D-CED
25	8	606	CLA	CBD-CGD-O2D-CED
25	8	607	CLA	CBA-CGA-O2A-C1
25	8	612	CLA	C3A-C2A-CAA-CBA
25	8	618	CLA	C1A-C2A-CAA-CBA
25	8	618	CLA	C3A-C2A-CAA-CBA
25	8	620	CLA	C3A-C2A-CAA-CBA
25	8	620	CLA	CHA-CBD-CGD-O1D
25	8	620	CLA	CHA-CBD-CGD-O2D
25	8	620	CLA	CBD-CGD-O2D-CED
25	2	601	CLA	C2-C1-O2A-CGA
25	2	601	CLA	CBD-CGD-O2D-CED
25	2	602	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	C1A-C2A-CAA-CBA
25	2	604	CLA	C2-C1-O2A-CGA
25	2	605	CLA	C2-C1-O2A-CGA
25	2	605	CLA	CBD-CGD-O2D-CED
25	2	607	CLA	CBD-CGD-O2D-CED
25	2	608	CLA	C1A-C2A-CAA-CBA
25	2	608	CLA	C3A-C2A-CAA-CBA
25	2	612	CLA	CBD-CGD-O2D-CED
25	2	615	CLA	C1A-C2A-CAA-CBA
25	2	615	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	2	621	CLA	C1A-C2A-CAA-CBA
25	2	621	CLA	C3A-C2A-CAA-CBA
25	9	602	CLA	CBD-CGD-O2D-CED
25	9	604	CLA	CHA-CBD-CGD-O2D
25	9	605	CLA	CBD-CGD-O2D-CED
25	9	609	CLA	C1A-C2A-CAA-CBA
25	9	609	CLA	C3A-C2A-CAA-CBA
25	9	609	CLA	CBA-CGA-O2A-C1
25	9	609	CLA	CBD-CGD-O2D-CED
25	9	612	CLA	C1A-C2A-CAA-CBA
26	1	604	CHL	C1A-C2A-CAA-CBA
26	1	604	CHL	C3A-C2A-CAA-CBA
26	1	604	CHL	C11-C10-C8-C9
26	1	604	CHL	C12-C13-C15-C16
26	1	609	CHL	C3A-C2A-CAA-CBA
26	a	604	CHL	C1A-C2A-CAA-CBA
26	a	604	CHL	C3A-C2A-CAA-CBA
26	a	606	CHL	C1A-C2A-CAA-CBA
26	a	606	CHL	C3A-C2A-CAA-CBA
26	3	604	CHL	C2-C1-O2A-CGA
26	4	613	CHL	C1A-C2A-CAA-CBA
26	4	618	CHL	C2-C3-C5-C6
26	4	618	CHL	C4-C3-C5-C6
26	5	610	CHL	C3A-C2A-CAA-CBA
26	6	609	CHL	C14-C13-C15-C16
26	6	611	CHL	C3A-C2A-CAA-CBA
26	7	617	CHL	CAD-CBD-CGD-O1D
26	7	617	CHL	CAD-CBD-CGD-O2D
26	8	601	CHL	C3A-C2A-CAA-CBA
26	8	604	CHL	C1A-C2A-CAA-CBA
26	8	604	CHL	C3A-C2A-CAA-CBA
26	9	601	CHL	C1A-C2A-CAA-CBA
26	9	601	CHL	C3A-C2A-CAA-CBA
26	9	603	CHL	C1A-C2A-CAA-CBA
26	9	603	CHL	C3A-C2A-CAA-CBA
26	9	603	CHL	C4C-C3C-CAC-CBC
26	9	610	CHL	CHA-CBD-CGD-O1D
26	9	610	CHL	CHA-CBD-CGD-O2D
29	A	4001	BCR	C11-C10-C9-C8
29	A	4001	BCR	C11-C10-C9-C34
29	A	4001	BCR	C10-C11-C12-C13
29	A	4001	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	A	4002	BCR	C7-C8-C9-C10
29	A	4002	BCR	C7-C8-C9-C34
29	A	4002	BCR	C11-C10-C9-C8
29	A	4002	BCR	C11-C10-C9-C34
29	A	4002	BCR	C10-C11-C12-C13
29	A	4002	BCR	C13-C14-C15-C16
29	A	4003	BCR	C11-C10-C9-C8
29	A	4003	BCR	C11-C10-C9-C34
29	A	4003	BCR	C9-C10-C11-C12
29	A	4003	BCR	C10-C11-C12-C13
29	A	4003	BCR	C17-C18-C19-C20
29	A	4004	BCR	C7-C8-C9-C10
29	A	4004	BCR	C7-C8-C9-C34
29	A	4004	BCR	C11-C10-C9-C8
29	A	4004	BCR	C11-C10-C9-C34
29	A	4004	BCR	C10-C11-C12-C13
29	A	4005	BCR	C11-C10-C9-C8
29	A	4005	BCR	C11-C10-C9-C34
29	A	4005	BCR	C17-C18-C19-C20
29	A	4005	BCR	C36-C18-C19-C20
29	A	4005	BCR	C21-C22-C23-C24
29	A	4005	BCR	C37-C22-C23-C24
29	B	4001	BCR	C7-C8-C9-C10
29	B	4001	BCR	C7-C8-C9-C34
29	B	4001	BCR	C17-C18-C19-C20
29	B	4001	BCR	C36-C18-C19-C20
29	B	4001	BCR	C21-C22-C23-C24
29	B	4002	BCR	C1-C6-C7-C8
29	B	4002	BCR	C5-C6-C7-C8
29	B	4002	BCR	C7-C8-C9-C10
29	B	4002	BCR	C7-C8-C9-C34
29	B	4002	BCR	C11-C10-C9-C8
29	B	4002	BCR	C11-C10-C9-C34
29	B	4002	BCR	C10-C11-C12-C13
29	B	4002	BCR	C17-C18-C19-C20
29	B	4002	BCR	C36-C18-C19-C20
29	B	4002	BCR	C21-C22-C23-C24
29	B	4005	BCR	C11-C10-C9-C8
29	B	4005	BCR	C11-C10-C9-C34
29	B	4005	BCR	C10-C11-C12-C13
29	B	4005	BCR	C17-C18-C19-C20
29	B	4005	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	B	4007	BCR	C11-C10-C9-C8
29	B	4007	BCR	C11-C10-C9-C34
29	B	4007	BCR	C10-C11-C12-C13
29	B	4006	BCR	C11-C10-C9-C8
29	B	4006	BCR	C11-C10-C9-C34
29	B	4006	BCR	C9-C10-C11-C12
29	B	4006	BCR	C10-C11-C12-C13
29	B	4006	BCR	C17-C18-C19-C20
29	G	4001	BCR	C11-C10-C9-C8
29	G	4001	BCR	C11-C10-C9-C34
29	G	4001	BCR	C10-C11-C12-C13
29	G	4001	BCR	C13-C14-C15-C16
29	G	4001	BCR	C21-C22-C23-C24
29	G	4001	BCR	C37-C22-C23-C24
29	H	4001	BCR	C11-C10-C9-C8
29	H	4001	BCR	C11-C10-C9-C34
29	J	4001	BCR	C11-C10-C9-C8
29	J	4001	BCR	C11-C10-C9-C34
29	J	4001	BCR	C10-C11-C12-C13
29	J	4001	BCR	C17-C18-C19-C20
29	K	4001	BCR	C7-C8-C9-C34
29	K	4001	BCR	C11-C10-C9-C8
29	K	4001	BCR	C11-C10-C9-C34
29	K	4002	BCR	C11-C10-C9-C8
29	K	4002	BCR	C11-C10-C9-C34
29	K	4002	BCR	C10-C11-C12-C13
29	L	4002	BCR	C11-C10-C9-C8
29	L	4002	BCR	C11-C10-C9-C34
29	L	4003	BCR	C11-C10-C9-C8
29	L	4003	BCR	C11-C10-C9-C34
29	L	4003	BCR	C10-C11-C12-C13
29	L	4001	BCR	C11-C10-C9-C8
29	L	4001	BCR	C11-C10-C9-C34
29	L	4001	BCR	C10-C11-C12-C13
29	L	4001	BCR	C21-C22-C23-C24
29	L	4001	BCR	C37-C22-C23-C24
29	L	4001	BCR	C23-C24-C25-C26
29	L	4001	BCR	C23-C24-C25-C30
29	I	4001	BCR	C7-C8-C9-C10
29	I	4001	BCR	C7-C8-C9-C34
29	I	4001	BCR	C11-C10-C9-C8
29	I	4001	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
29	I	4001	BCR	C10-C11-C12-C13
29	I	4001	BCR	C17-C18-C19-C20
29	O	4001	BCR	C11-C10-C9-C8
29	O	4001	BCR	C11-C10-C9-C34
29	O	4001	BCR	C17-C18-C19-C20
29	O	4001	BCR	C36-C18-C19-C20
29	3	503	BCR	C5-C6-C7-C8
29	3	503	BCR	C7-C8-C9-C10
29	3	503	BCR	C7-C8-C9-C34
29	3	503	BCR	C11-C10-C9-C8
29	3	503	BCR	C11-C10-C9-C34
29	3	503	BCR	C10-C11-C12-C13
29	3	504	BCR	C7-C8-C9-C10
29	3	504	BCR	C7-C8-C9-C34
29	3	504	BCR	C11-C10-C9-C8
29	3	504	BCR	C11-C10-C9-C34
29	3	504	BCR	C10-C11-C12-C13
29	3	504	BCR	C17-C18-C19-C20
29	3	504	BCR	C21-C22-C23-C24
29	3	504	BCR	C37-C22-C23-C24
29	3	505	BCR	C11-C10-C9-C8
29	3	505	BCR	C11-C10-C9-C34
29	3	505	BCR	C9-C10-C11-C12
29	3	505	BCR	C10-C11-C12-C13
29	3	505	BCR	C17-C18-C19-C20
29	3	505	BCR	C21-C22-C23-C24
29	3	505	BCR	C37-C22-C23-C24
29	4	503	BCR	C7-C8-C9-C10
29	4	503	BCR	C7-C8-C9-C34
29	4	503	BCR	C11-C10-C9-C8
29	4	503	BCR	C11-C10-C9-C34
29	4	503	BCR	C9-C10-C11-C12
29	4	503	BCR	C10-C11-C12-C13
29	4	503	BCR	C17-C18-C19-C20
29	4	503	BCR	C21-C22-C23-C24
29	4	503	BCR	C37-C22-C23-C24
29	4	503	BCR	C23-C24-C25-C26
29	4	503	BCR	C23-C24-C25-C30
29	5	503	BCR	C5-C6-C7-C8
29	5	503	BCR	C11-C10-C9-C8
29	5	503	BCR	C11-C10-C9-C34
29	5	503	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	5	503	BCR	C17-C18-C19-C20
29	5	503	BCR	C36-C18-C19-C20
29	6	503	BCR	C11-C10-C9-C8
29	6	503	BCR	C11-C10-C9-C34
29	6	503	BCR	C10-C11-C12-C13
29	6	503	BCR	C11-C12-C13-C14
29	6	503	BCR	C21-C22-C23-C24
29	6	503	BCR	C37-C22-C23-C24
29	6	503	BCR	C23-C24-C25-C26
29	6	503	BCR	C23-C24-C25-C30
29	6	504	BCR	C10-C11-C12-C13
29	6	504	BCR	C21-C22-C23-C24
29	7	503	BCR	C7-C8-C9-C10
29	7	503	BCR	C11-C10-C9-C8
29	7	503	BCR	C11-C10-C9-C34
29	7	503	BCR	C10-C11-C12-C13
29	8	503	BCR	C5-C6-C7-C8
29	8	503	BCR	C7-C8-C9-C10
29	8	503	BCR	C7-C8-C9-C34
29	8	503	BCR	C11-C10-C9-C8
29	8	503	BCR	C11-C10-C9-C34
29	8	503	BCR	C10-C11-C12-C13
29	8	503	BCR	C21-C22-C23-C24
29	8	503	BCR	C37-C22-C23-C24
29	8	503	BCR	C23-C24-C25-C26
29	8	503	BCR	C23-C24-C25-C30
30	A	5001	LHG	O1-C1-C2-C3
30	A	5001	LHG	C3-O3-P-O4
30	A	5001	LHG	C3-O3-P-O5
30	A	5001	LHG	C3-O3-P-O6
30	A	5001	LHG	C4-O6-P-O3
30	A	5001	LHG	C4-O6-P-O4
30	A	5001	LHG	C4-O6-P-O5
30	A	5001	LHG	O6-C4-C5-O7
30	A	5001	LHG	O9-C7-O7-C5
30	A	5002	LHG	O1-C1-C2-C3
30	A	5002	LHG	C3-O3-P-O4
30	A	5002	LHG	C3-O3-P-O6
30	A	5002	LHG	C4-O6-P-O3
30	A	5002	LHG	C4-O6-P-O4
30	A	5003	LHG	C4-O6-P-O3
30	A	5003	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
30	A	5003	LHG	C4-O6-P-O5
30	B	5001	LHG	O1-C1-C2-O2
30	B	5001	LHG	O1-C1-C2-C3
30	B	5001	LHG	O2-C2-C3-O3
30	B	5001	LHG	C3-O3-P-O4
30	B	5001	LHG	C3-O3-P-O5
30	B	5001	LHG	C3-O3-P-O6
30	B	5001	LHG	O7-C5-C6-O8
30	B	5002	LHG	C4-O6-P-O4
30	F	5002	LHG	C1-C2-C3-O3
30	F	5001	LHG	O1-C1-C2-C3
30	F	5001	LHG	C3-O3-P-O4
30	F	5001	LHG	C4-O6-P-O3
30	F	5001	LHG	C4-O6-P-O4
30	1	801	LHG	O1-C1-C2-O2
30	1	801	LHG	C1-C2-C3-O3
30	1	801	LHG	O2-C2-C3-O3
30	1	801	LHG	C4-O6-P-O3
30	1	801	LHG	C4-O6-P-O4
30	1	802	LHG	O1-C1-C2-C3
30	1	802	LHG	O2-C2-C3-O3
30	1	802	LHG	C3-O3-P-O5
30	1	802	LHG	C3-O3-P-O6
30	1	802	LHG	C4-O6-P-O5
30	1	802	LHG	O7-C5-C6-O8
30	1	802	LHG	O9-C7-O7-C5
30	a	801	LHG	O1-C1-C2-C3
30	a	801	LHG	C4-O6-P-O3
30	a	801	LHG	C4-O6-P-O4
30	a	801	LHG	C4-O6-P-O5
30	3	801	LHG	O1-C1-C2-C3
30	3	801	LHG	C1-C2-C3-O3
30	3	801	LHG	O2-C2-C3-O3
30	3	801	LHG	C3-O3-P-O6
30	3	801	LHG	C4-O6-P-O3
30	3	801	LHG	C4-O6-P-O5
30	3	801	LHG	O9-C7-O7-C5
30	4	802	LHG	C3-O3-P-O4
30	4	802	LHG	C3-O3-P-O5
30	4	802	LHG	C3-O3-P-O6
30	4	802	LHG	C8-C7-O7-C5
30	4	801	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	4	801	LHG	C4-O6-P-O3
30	4	801	LHG	C4-O6-P-O4
30	5	801	LHG	C3-O3-P-O4
30	5	801	LHG	C3-O3-P-O6
30	6	802	LHG	O1-C1-C2-C3
30	6	802	LHG	C1-C2-C3-O3
30	6	802	LHG	C3-O3-P-O6
30	6	802	LHG	C4-O6-P-O3
30	6	802	LHG	C4-O6-P-O4
30	6	802	LHG	C4-O6-P-O5
30	6	802	LHG	C8-C7-O7-C5
30	6	801	LHG	O1-C1-C2-O2
30	6	801	LHG	C1-C2-C3-O3
30	6	801	LHG	C3-O3-P-O6
30	6	801	LHG	C4-O6-P-O3
30	7	801	LHG	O1-C1-C2-C3
30	7	801	LHG	C4-O6-P-O3
30	7	801	LHG	C4-O6-P-O4
30	7	801	LHG	C4-O6-P-O5
30	7	801	LHG	C8-C7-O7-C5
30	7	802	LHG	C4-O6-P-O3
30	7	802	LHG	C4-O6-P-O4
30	7	803	LHG	C1-C2-C3-O3
30	7	803	LHG	C3-O3-P-O4
30	7	803	LHG	C3-O3-P-O5
30	7	803	LHG	C3-O3-P-O6
30	7	803	LHG	C4-O6-P-O3
30	8	801	LHG	O1-C1-C2-O2
30	8	801	LHG	O1-C1-C2-C3
30	8	801	LHG	C1-C2-C3-O3
30	8	801	LHG	C3-O3-P-O6
30	8	801	LHG	C4-O6-P-O3
30	8	801	LHG	C4-O6-P-O4
30	8	801	LHG	C4-O6-P-O5
30	2	801	LHG	C1-C2-C3-O3
30	2	801	LHG	C8-C7-O7-C5
30	2	802	LHG	O1-C1-C2-C3
30	2	802	LHG	C3-O3-P-O4
30	2	802	LHG	C3-O3-P-O6
30	2	802	LHG	O9-C7-O7-C5
30	9	802	LHG	C1-C2-C3-O3
30	9	802	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	9	802	LHG	C4-O6-P-O3
30	9	801	LHG	O1-C1-C2-C3
32	A	5005	SQD	O5-C1-O6-C44
32	A	5005	SQD	C8-C7-O47-C45
32	A	5005	SQD	O5-C5-C6-S
32	G	5001	SQD	C5-C6-S-O7
32	G	5001	SQD	C5-C6-S-O8
32	G	5001	SQD	C5-C6-S-O9
32	H	5001	SQD	C8-C7-O47-C45
32	I	5001	SQD	C2-C1-O6-C44
32	I	5001	SQD	C8-C7-O47-C45
32	I	5001	SQD	C5-C6-S-O7
32	I	5001	SQD	C5-C6-S-O8
32	I	5001	SQD	C5-C6-S-O9
32	7	805	SQD	O5-C1-O6-C44
32	7	805	SQD	O5-C5-C6-S
33	A	5006	PTY	C11-C8-O7-C6
33	A	5006	PTY	C3-O11-P1-O13
33	A	5006	PTY	C3-O11-P1-O14
33	B	5005	PTY	N1-C2-C3-O11
33	B	5005	PTY	C5-O14-P1-O11
33	B	5005	PTY	C5-O14-P1-O13
33	G	5003	PTY	N1-C2-C3-O11
33	G	5003	PTY	C3-O11-P1-O12
33	G	5003	PTY	C3-O11-P1-O14
33	G	5002	PTY	N1-C2-C3-O11
33	G	5002	PTY	O10-C8-O7-C6
33	G	5002	PTY	C11-C8-O7-C6
33	G	5002	PTY	C3-O11-P1-O12
33	G	5002	PTY	C3-O11-P1-O14
33	J	5001	PTY	O4-C1-C6-O7
33	J	5001	PTY	C3-O11-P1-O12
33	J	5001	PTY	C3-O11-P1-O13
33	J	5001	PTY	C3-O11-P1-O14
33	J	5001	PTY	C5-O14-P1-O11
33	J	5001	PTY	C5-O14-P1-O13
33	a	803	PTY	N1-C2-C3-O11
33	a	802	PTY	C5-O14-P1-O11
33	a	802	PTY	C5-O14-P1-O13
33	3	802	PTY	N1-C2-C3-O11
33	3	802	PTY	O10-C8-O7-C6
33	3	802	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
33	3	802	PTY	C5-O14-P1-O11
33	3	802	PTY	C5-O14-P1-O13
33	5	802	PTY	C11-C8-O7-C6
33	5	802	PTY	C5-O14-P1-O11
33	5	802	PTY	C5-O14-P1-O12
33	5	802	PTY	C5-O14-P1-O13
33	7	804	PTY	C5-C6-O7-C8
33	7	804	PTY	C11-C8-O7-C6
33	9	803	PTY	N1-C2-C3-O11
33	9	803	PTY	C11-C8-O7-C6
33	9	803	PTY	C3-O11-P1-O12
33	9	803	PTY	C3-O11-P1-O14
33	9	803	PTY	C5-O14-P1-O11
33	9	803	PTY	C5-O14-P1-O12
33	9	803	PTY	C5-O14-P1-O13
34	A	5007	3PH	C1-O11-P-O14
34	A	5007	3PH	C1-O11-P-O12
34	A	5007	3PH	C22-C21-O21-C2
35	B	5006	LMT	C2'-C1'-O1'-C1
35	B	5006	LMT	O5'-C1'-O1'-C1
36	7	806	DGD	C2A-C1A-O1G-C1G
36	7	806	DGD	O6E-C1E-O5D-C6D
36	8	802	DGD	O1B-C1B-O2G-C2G
36	8	802	DGD	C2D-C1D-O3G-C3G
36	8	802	DGD	O6D-C1D-O3G-C3G
36	8	803	DGD	O1B-C1B-O2G-C2G
37	B	5004	PCW	C32-C31-O2-C2
37	B	5004	PCW	O31-C31-O2-C2
37	K	5002	PCW	O2-C2-C3-O3
37	K	5002	PCW	O4P-C4-C5-N
37	K	5002	PCW	C1-O3P-P-O1P
37	K	5002	PCW	C1-O3P-P-O4P
37	K	5002	PCW	C4-O4P-P-O2P
37	K	5001	PCW	O2-C2-C3-O3
37	K	5001	PCW	C32-C31-O2-C2
37	6	803	PCW	O2-C2-C3-O3
37	6	803	PCW	O4P-C4-C5-N
37	6	803	PCW	C4-O4P-P-O1P
37	6	803	PCW	C4-O4P-P-O2P
37	6	803	PCW	C4-O4P-P-O3P
38	F	5003	LPX	C3-C4-C5-O6
38	F	5003	LPX	O1-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
38	F	5003	LPX	C1-O2-P1-O1
38	F	5003	LPX	C1-O2-P1-O3
39	F	4001	NEX	C7-C8-C9-C10
39	F	4001	NEX	C7-C8-C9-C19
39	F	4001	NEX	C12-C13-C14-C15
39	F	4001	NEX	C20-C13-C14-C15
39	F	4001	NEX	C14-C15-C35-C34
40	J	4002	RRX	C23-C24-C25-C30
40	J	4002	RRX	C19-C20-C21-C22
40	J	4002	RRX	C36-C18-C19-C20
40	J	4002	RRX	C17-C18-C19-C20
40	J	4002	RRX	C15-C16-C17-C18
40	3	506	RRX	C5-C6-C7-C8
41	J	5002	SPH	O1-C1-C2-N2
41	J	5002	SPH	O1-C1-C2-C3
41	J	5002	SPH	C2-C3-C4-C5
41	J	5002	SPH	O3-C3-C4-C5
41	4	805	SPH	C1-C2-C3-O3
41	4	805	SPH	C1-C2-C3-C4
41	4	805	SPH	N2-C2-C3-O3
41	4	805	SPH	N2-C2-C3-C4
41	6	806	SPH	O1-C1-C2-N2
41	6	806	SPH	O1-C1-C2-C3
41	6	806	SPH	C2-C3-C4-C5
41	6	806	SPH	O3-C3-C4-C5
41	9	804	SPH	O1-C1-C2-N2
41	9	804	SPH	O1-C1-C2-C3
41	9	804	SPH	C1-C2-C3-O3
41	9	804	SPH	C1-C2-C3-C4
41	9	804	SPH	N2-C2-C3-O3
41	9	804	SPH	N2-C2-C3-C4
41	9	804	SPH	C2-C3-C4-C5
41	9	804	SPH	O3-C3-C4-C5
43	1	503	LUT	C13-C14-C15-C35
43	1	503	LUT	C21-C26-C27-C28
43	1	503	LUT	C31-C32-C33-C34
43	a	501	LUT	C5-C6-C7-C8
43	a	503	LUT	C21-C26-C27-C28
43	4	501	LUT	C21-C26-C27-C28
43	4	501	LUT	C27-C28-C29-C30
43	4	501	LUT	C27-C28-C29-C39
43	4	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
43	5	505	LUT	C21-C26-C27-C28
43	5	505	LUT	C31-C32-C33-C34
43	7	501	LUT	C21-C26-C27-C28
43	7	501	LUT	C27-C28-C29-C30
43	7	501	LUT	C27-C28-C29-C39
43	2	502	LUT	C31-C32-C33-C34
43	2	507	LUT	C7-C8-C9-C10
43	2	507	LUT	C7-C8-C9-C19
43	2	507	LUT	C11-C12-C13-C14
43	2	507	LUT	C11-C12-C13-C20
43	2	507	LUT	C25-C26-C27-C28
44	1	502	AXT	C9-C10-C11-C12
44	1	502	AXT	C11-C12-C13-C20
44	1	502	AXT	C31-C32-C33-C34
44	7	504	AXT	C7-C8-C9-C10
44	7	504	AXT	C7-C8-C9-C19
44	7	504	AXT	C25-C26-C27-C28
44	7	504	AXT	C27-C28-C29-C30
46	a	504	QTB	C09-C10-C11-C12
47	4	803	PLM	O2-C1-C2-C3
48	3	803	DGA	CB2-CB1-OG2-CG2
48	3	803	DGA	OG2-CG2-CG3-OXT
48	5	803	DGA	CA2-CA1-OG1-CG1
48	5	803	DGA	CB2-CB1-OG2-CG2
48	5	803	DGA	CG1-CG2-CG3-OXT
48	5	803	DGA	OG2-CG2-CG3-OXT
48	8	804	DGA	OG2-CG2-CG3-OXT
48	2	803	DGA	CG1-CG2-CG3-OXT
48	2	803	DGA	OG2-CG2-CG3-OXT
50	9	504	XAT	C12-C13-C14-C15
50	9	504	XAT	C20-C13-C14-C15
50	9	504	XAT	C14-C15-C35-C34
50	9	504	XAT	C27-C28-C29-C30
50	9	504	XAT	C27-C28-C29-C39
50	9	504	XAT	C32-C33-C34-C35
50	9	504	XAT	C40-C33-C34-C35
50	9	504	XAT	C33-C34-C35-C15
50	9	507	XAT	C7-C8-C9-C10
50	9	507	XAT	C7-C8-C9-C19
50	9	507	XAT	C10-C11-C12-C13
52	8	805	P5S	O-C-CA-N
52	8	805	P5S	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
52	8	805	P5S	OXT-C-CA-CB
52	8	805	P5S	C-CA-CB-OG
52	8	805	P5S	N-CA-CB-OG
53	8	810	LAP	O3-C14-C15-O4
53	8	810	LAP	O6-C16-C17-N8
53	8	810	LAP	C15-O4-P9-O6
53	8	810	LAP	C16-O6-P9-O4
53	8	810	LAP	C16-O6-P9-O5
53	8	810	LAP	C16-O6-P9-O7
25	O	1803	CLA	O1D-CGD-O2D-CED
25	5	615	CLA	O1D-CGD-O2D-CED
25	A	1134	CLA	O1D-CGD-O2D-CED
25	B	1021	CLA	O1D-CGD-O2D-CED
25	L	1504	CLA	O1D-CGD-O2D-CED
25	a	615	CLA	O1D-CGD-O2D-CED
25	4	617	CLA	O1D-CGD-O2D-CED
25	7	606	CLA	O1D-CGD-O2D-CED
25	8	615	CLA	O1D-CGD-O2D-CED
25	A	1012	CLA	CBD-CGD-O2D-CED
25	A	1104	CLA	CBD-CGD-O2D-CED
25	A	1107	CLA	CBD-CGD-O2D-CED
25	A	1110	CLA	CBD-CGD-O2D-CED
25	A	1112	CLA	CBD-CGD-O2D-CED
25	A	1113	CLA	CBD-CGD-O2D-CED
25	A	1117	CLA	CBD-CGD-O2D-CED
25	A	1129	CLA	CBD-CGD-O2D-CED
25	A	1132	CLA	CBD-CGD-O2D-CED
25	A	1134	CLA	CBD-CGD-O2D-CED
25	A	1135	CLA	CBD-CGD-O2D-CED
25	B	1237	CLA	CBD-CGD-O2D-CED
25	B	1206	CLA	CBD-CGD-O2D-CED
25	B	1213	CLA	CBD-CGD-O2D-CED
25	B	1214	CLA	CBD-CGD-O2D-CED
25	B	1215	CLA	CBD-CGD-O2D-CED
25	B	1219	CLA	CBD-CGD-O2D-CED
25	B	1224	CLA	CBD-CGD-O2D-CED
25	B	1226	CLA	CBD-CGD-O2D-CED
25	B	1229	CLA	CBD-CGD-O2D-CED
25	B	1231	CLA	CBD-CGD-O2D-CED
25	B	1232	CLA	CBD-CGD-O2D-CED
25	B	1238	CLA	CBD-CGD-O2D-CED
25	B	1240	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	H	1701	CLA	CBD-CGD-O2D-CED
25	H	1703	CLA	CBD-CGD-O2D-CED
25	K	1402	CLA	CBD-CGD-O2D-CED
25	K	1403	CLA	CBD-CGD-O2D-CED
25	K	1404	CLA	CBD-CGD-O2D-CED
25	L	1501	CLA	CBD-CGD-O2D-CED
25	L	1503	CLA	CBD-CGD-O2D-CED
25	L	1504	CLA	CBD-CGD-O2D-CED
25	O	1802	CLA	CBD-CGD-O2D-CED
25	O	1803	CLA	CBD-CGD-O2D-CED
25	1	601	CLA	CBD-CGD-O2D-CED
25	1	603	CLA	CBD-CGD-O2D-CED
25	1	605	CLA	CBD-CGD-O2D-CED
25	1	612	CLA	CBD-CGD-O2D-CED
25	1	615	CLA	CBD-CGD-O2D-CED
25	a	612	CLA	CBD-CGD-O2D-CED
25	a	615	CLA	CBD-CGD-O2D-CED
25	3	602	CLA	CBD-CGD-O2D-CED
25	3	607	CLA	CBD-CGD-O2D-CED
25	3	612	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBD-CGD-O2D-CED
25	4	602	CLA	CBD-CGD-O2D-CED
25	4	603	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	4	610	CLA	CBD-CGD-O2D-CED
25	4	616	CLA	CBD-CGD-O2D-CED
25	4	617	CLA	CBD-CGD-O2D-CED
25	5	605	CLA	CBD-CGD-O2D-CED
25	5	609	CLA	CBD-CGD-O2D-CED
25	5	615	CLA	CBD-CGD-O2D-CED
25	7	601	CLA	CBD-CGD-O2D-CED
25	7	606	CLA	CBD-CGD-O2D-CED
25	7	612	CLA	CBD-CGD-O2D-CED
25	8	611	CLA	CBD-CGD-O2D-CED
25	8	615	CLA	CBD-CGD-O2D-CED
25	8	618	CLA	CBD-CGD-O2D-CED
25	2	603	CLA	CBD-CGD-O2D-CED
25	2	606	CLA	CBD-CGD-O2D-CED
25	2	608	CLA	CBD-CGD-O2D-CED
25	2	621	CLA	CBD-CGD-O2D-CED
25	9	606	CLA	CBD-CGD-O2D-CED
25	9	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	9	612	CLA	CBD-CGD-O2D-CED
25	A	1101	CLA	O1A-CGA-O2A-C1
25	B	1201	CLA	O1A-CGA-O2A-C1
25	B	1218	CLA	O1A-CGA-O2A-C1
25	H	1703	CLA	O1A-CGA-O2A-C1
25	a	611	CLA	O1A-CGA-O2A-C1
25	3	607	CLA	O1A-CGA-O2A-C1
25	4	607	CLA	O1A-CGA-O2A-C1
25	4	608	CLA	O1A-CGA-O2A-C1
25	4	615	CLA	O1A-CGA-O2A-C1
32	A	5005	SQD	O10-C23-O48-C46
33	5	802	PTY	O30-C30-O4-C1
36	7	806	DGD	O1A-C1A-O1G-C1G
48	5	803	DGA	OA1-CA1-OG1-CG1
51	7	807	4RF	O42-C41-O40-C39
25	1	615	CLA	O1A-CGA-O2A-C1
25	a	615	CLA	O1A-CGA-O2A-C1
25	9	609	CLA	O1A-CGA-O2A-C1
25	B	1023	CLA	O1D-CGD-O2D-CED
25	1	603	CLA	O1D-CGD-O2D-CED
25	1	615	CLA	CBA-CGA-O2A-C1
25	a	615	CLA	CBA-CGA-O2A-C1
25	6	605	CLA	CBA-CGA-O2A-C1
25	2	606	CLA	CBA-CGA-O2A-C1
25	B	1224	CLA	O1D-CGD-O2D-CED
25	B	1232	CLA	O1D-CGD-O2D-CED
25	K	1404	CLA	O1D-CGD-O2D-CED
25	1	612	CLA	O1D-CGD-O2D-CED
25	1	615	CLA	O1D-CGD-O2D-CED
25	a	612	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	O1D-CGD-O2D-CED
25	4	616	CLA	O1D-CGD-O2D-CED
25	8	611	CLA	O1D-CGD-O2D-CED
25	B	1218	CLA	CBA-CGA-O2A-C1
25	1	607	CLA	CBA-CGA-O2A-C1
25	a	611	CLA	CBA-CGA-O2A-C1
25	4	615	CLA	CBA-CGA-O2A-C1
32	A	5005	SQD	C24-C23-O48-C46
33	5	802	PTY	C31-C30-O4-C1
51	7	807	4RF	C43-C41-O40-C39
25	B	1234	CLA	CBD-CGD-O2D-CED
25	3	616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	4	605	CLA	CBD-CGD-O2D-CED
25	4	606	CLA	CBD-CGD-O2D-CED
25	4	612	CLA	CBD-CGD-O2D-CED
25	6	606	CLA	CBD-CGD-O2D-CED
25	7	608	CLA	CBD-CGD-O2D-CED
25	9	604	CLA	CBD-CGD-O2D-CED
25	A	1104	CLA	O1A-CGA-O2A-C1
25	B	1208	CLA	O1A-CGA-O2A-C1
25	B	1209	CLA	O1A-CGA-O2A-C1
25	1	607	CLA	O1A-CGA-O2A-C1
25	3	610	CLA	O1A-CGA-O2A-C1
25	4	611	CLA	O1A-CGA-O2A-C1
25	4	616	CLA	O1A-CGA-O2A-C1
25	5	603	CLA	O1A-CGA-O2A-C1
25	6	607	CLA	O1A-CGA-O2A-C1
25	6	615	CLA	O1A-CGA-O2A-C1
25	8	606	CLA	O1A-CGA-O2A-C1
25	8	609	CLA	O1A-CGA-O2A-C1
25	2	607	CLA	O1A-CGA-O2A-C1
25	2	621	CLA	O1A-CGA-O2A-C1
32	G	5001	SQD	O10-C23-O48-C46
33	a	803	PTY	O30-C30-O4-C1
33	a	802	PTY	O30-C30-O4-C1
33	7	804	PTY	O30-C30-O4-C1
33	9	803	PTY	O30-C30-O4-C1
48	2	803	DGA	OA1-CA1-OG1-CG1
25	8	607	CLA	O1A-CGA-O2A-C1
25	8	615	CLA	O1A-CGA-O2A-C1
25	2	606	CLA	O1A-CGA-O2A-C1
25	A	1012	CLA	O1D-CGD-O2D-CED
25	A	1109	CLA	O1D-CGD-O2D-CED
25	A	1126	CLA	O1D-CGD-O2D-CED
25	A	1140	CLA	O1D-CGD-O2D-CED
25	B	1236	CLA	O1D-CGD-O2D-CED
25	F	1301	CLA	O1D-CGD-O2D-CED
25	G	1601	CLA	O1D-CGD-O2D-CED
25	G	1602	CLA	O1D-CGD-O2D-CED
25	H	1701	CLA	O1D-CGD-O2D-CED
25	a	601	CLA	O1D-CGD-O2D-CED
25	a	602	CLA	O1D-CGD-O2D-CED
25	3	605	CLA	O1D-CGD-O2D-CED
25	3	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	4	610	CLA	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	5	606	CLA	O1D-CGD-O2D-CED
25	5	608	CLA	O1D-CGD-O2D-CED
25	6	618	CLA	O1D-CGD-O2D-CED
25	2	603	CLA	O1D-CGD-O2D-CED
25	2	612	CLA	O1D-CGD-O2D-CED
25	9	602	CLA	O1D-CGD-O2D-CED
25	A	1118	CLA	O1D-CGD-O2D-CED
25	A	1119	CLA	O1D-CGD-O2D-CED
25	B	1022	CLA	O1D-CGD-O2D-CED
25	B	1239	CLA	O1D-CGD-O2D-CED
25	B	1207	CLA	O1D-CGD-O2D-CED
25	G	1603	CLA	O1D-CGD-O2D-CED
25	J	1901	CLA	O1D-CGD-O2D-CED
25	K	1401	CLA	O1D-CGD-O2D-CED
25	1	602	CLA	O1D-CGD-O2D-CED
25	1	606	CLA	O1D-CGD-O2D-CED
25	a	603	CLA	O1D-CGD-O2D-CED
25	a	611	CLA	O1D-CGD-O2D-CED
25	4	615	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	O1D-CGD-O2D-CED
25	6	605	CLA	O1D-CGD-O2D-CED
25	7	603	CLA	O1D-CGD-O2D-CED
25	7	610	CLA	O1D-CGD-O2D-CED
25	8	605	CLA	O1D-CGD-O2D-CED
25	8	606	CLA	O1D-CGD-O2D-CED
25	8	620	CLA	O1D-CGD-O2D-CED
25	2	601	CLA	O1D-CGD-O2D-CED
25	2	605	CLA	O1D-CGD-O2D-CED
25	9	609	CLA	O1D-CGD-O2D-CED
25	A	1101	CLA	CBD-CGD-O2D-CED
25	B	1211	CLA	CBD-CGD-O2D-CED
30	F	5002	LHG	O10-C23-O8-C6
30	4	802	LHG	O9-C7-O7-C5
30	6	802	LHG	O9-C7-O7-C5
30	7	801	LHG	O9-C7-O7-C5
30	2	801	LHG	O9-C7-O7-C5
32	A	5005	SQD	O49-C7-O47-C45
32	H	5001	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
32	I	5001	SQD	O49-C7-O47-C45
33	A	5006	PTY	O10-C8-O7-C6
33	5	802	PTY	O10-C8-O7-C6
33	7	804	PTY	O10-C8-O7-C6
33	9	803	PTY	O10-C8-O7-C6
34	A	5007	3PH	O22-C21-O21-C2
37	K	5001	PCW	O31-C31-O2-C2
48	5	803	DGA	OB1-CB1-OG2-CG2
25	A	1131	CLA	O1D-CGD-O2D-CED
25	B	1216	CLA	O1D-CGD-O2D-CED
25	8	615	CLA	CBA-CGA-O2A-C1
25	K	1401	CLA	O1A-CGA-O2A-C1
25	A	1012	CLA	C3-C5-C6-C7
25	A	1103	CLA	C3-C5-C6-C7
25	A	1106	CLA	C3-C5-C6-C7
25	A	1108	CLA	C3-C5-C6-C7
25	A	1118	CLA	C3-C5-C6-C7
25	A	1130	CLA	C3-C5-C6-C7
25	B	1237	CLA	C3-C5-C6-C7
25	B	1203	CLA	C3-C5-C6-C7
25	B	1204	CLA	C3-C5-C6-C7
25	B	1205	CLA	C3-C5-C6-C7
25	B	1210	CLA	C3-C5-C6-C7
25	B	1218	CLA	C3-C5-C6-C7
25	B	1220	CLA	C3-C5-C6-C7
25	B	1207	CLA	C3-C5-C6-C7
25	H	1701	CLA	C3-C5-C6-C7
25	O	1802	CLA	C3-C5-C6-C7
25	1	606	CLA	C3-C5-C6-C7
25	a	608	CLA	C3-C5-C6-C7
25	3	601	CLA	C3-C5-C6-C7
25	3	605	CLA	C3-C5-C6-C7
25	3	607	CLA	C3-C5-C6-C7
25	3	616	CLA	C3-C5-C6-C7
25	4	612	CLA	C3-C5-C6-C7
25	4	615	CLA	C3-C5-C6-C7
25	6	608	CLA	C3-C5-C6-C7
25	6	601	CLA	C3-C5-C6-C7
25	2	601	CLA	C3-C5-C6-C7
25	2	604	CLA	C3-C5-C6-C7
25	2	607	CLA	C3-C5-C6-C7
30	F	5002	LHG	C5-C6-O8-C23

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Mol	Chain	Res	Type	Atoms
25	B	1203	CLA	O1D-CGD-O2D-CED
25	B	1206	CLA	O1D-CGD-O2D-CED
25	B	1228	CLA	O1D-CGD-O2D-CED
25	F	1302	CLA	O1D-CGD-O2D-CED
25	6	612	CLA	O1D-CGD-O2D-CED
25	A	1118	CLA	CBA-CGA-O2A-C1
25	A	1101	CLA	CBA-CGA-O2A-C1
25	H	1703	CLA	CBA-CGA-O2A-C1
25	3	607	CLA	CBA-CGA-O2A-C1
25	3	610	CLA	CBA-CGA-O2A-C1
25	4	607	CLA	CBA-CGA-O2A-C1
25	4	608	CLA	CBA-CGA-O2A-C1
25	6	607	CLA	CBA-CGA-O2A-C1
25	6	615	CLA	CBA-CGA-O2A-C1
25	7	604	CLA	CBA-CGA-O2A-C1
25	7	607	CLA	CBA-CGA-O2A-C1
25	2	607	CLA	CBA-CGA-O2A-C1
25	2	621	CLA	CBA-CGA-O2A-C1
32	G	5001	SQD	C24-C23-O48-C46
33	a	803	PTY	C31-C30-O4-C1
33	7	804	PTY	C31-C30-O4-C1
33	9	803	PTY	C31-C30-O4-C1
25	A	1013	CLA	CBD-CGD-O2D-CED
25	A	1102	CLA	CBD-CGD-O2D-CED
25	A	1103	CLA	CBD-CGD-O2D-CED
25	A	1106	CLA	CBD-CGD-O2D-CED
25	A	1115	CLA	CBD-CGD-O2D-CED
25	A	1120	CLA	CBD-CGD-O2D-CED
25	A	1124	CLA	CBD-CGD-O2D-CED
25	A	1125	CLA	CBD-CGD-O2D-CED
25	A	1127	CLA	CBD-CGD-O2D-CED
25	A	1130	CLA	CBD-CGD-O2D-CED
25	A	1133	CLA	CBD-CGD-O2D-CED
25	A	1141	CLA	CBD-CGD-O2D-CED
25	B	1202	CLA	CBD-CGD-O2D-CED
25	B	1205	CLA	CBD-CGD-O2D-CED
25	B	1208	CLA	CBD-CGD-O2D-CED
25	B	1210	CLA	CBD-CGD-O2D-CED
25	B	1212	CLA	CBD-CGD-O2D-CED
25	B	1222	CLA	CBD-CGD-O2D-CED
25	B	1223	CLA	CBD-CGD-O2D-CED
25	B	1227	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	1230	CLA	CBD-CGD-O2D-CED
25	H	1702	CLA	CBD-CGD-O2D-CED
25	L	1502	CLA	CBD-CGD-O2D-CED
25	a	605	CLA	CBD-CGD-O2D-CED
25	3	601	CLA	CBD-CGD-O2D-CED
25	4	607	CLA	CBD-CGD-O2D-CED
25	6	601	CLA	CBD-CGD-O2D-CED
25	6	607	CLA	CBD-CGD-O2D-CED
25	6	615	CLA	CBD-CGD-O2D-CED
25	7	604	CLA	CBD-CGD-O2D-CED
25	7	607	CLA	CBD-CGD-O2D-CED
25	8	609	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	615	CLA	CBD-CGD-O2D-CED
30	A	5001	LHG	C8-C7-O7-C5
30	1	802	LHG	C8-C7-O7-C5
30	3	801	LHG	C8-C7-O7-C5
30	2	802	LHG	C8-C7-O7-C5
33	3	802	PTY	C11-C8-O7-C6
36	8	802	DGD	C2B-C1B-O2G-C2G
36	8	803	DGD	C2B-C1B-O2G-C2G
25	A	1116	CLA	O1D-CGD-O2D-CED
25	A	1121	CLA	O1D-CGD-O2D-CED
25	A	1139	CLA	O1D-CGD-O2D-CED
25	B	1231	CLA	O1D-CGD-O2D-CED
25	3	618	CLA	O1D-CGD-O2D-CED
25	4	602	CLA	O1D-CGD-O2D-CED
25	4	611	CLA	O1D-CGD-O2D-CED
25	5	612	CLA	O1D-CGD-O2D-CED
25	5	614	CLA	O1D-CGD-O2D-CED
25	6	608	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	7	602	CLA	O1D-CGD-O2D-CED
25	7	612	CLA	O1D-CGD-O2D-CED
25	2	602	CLA	O1D-CGD-O2D-CED
25	2	607	CLA	O1D-CGD-O2D-CED
25	9	605	CLA	O1D-CGD-O2D-CED
25	9	606	CLA	O1D-CGD-O2D-CED
25	2	605	CLA	O1A-CGA-O2A-C1
25	A	1111	CLA	O1D-CGD-O2D-CED
25	L	1501	CLA	O1D-CGD-O2D-CED
25	A	1111	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	1115	CLA	C4-C3-C5-C6
25	A	1130	CLA	C4-C3-C5-C6
25	B	1208	CLA	C4-C3-C5-C6
25	B	1213	CLA	C4-C3-C5-C6
25	B	1217	CLA	C4-C3-C5-C6
25	B	1218	CLA	C4-C3-C5-C6
25	H	1703	CLA	C4-C3-C5-C6
25	1	606	CLA	C4-C3-C5-C6
25	a	607	CLA	C4-C3-C5-C6
25	3	610	CLA	C4-C3-C5-C6
25	4	612	CLA	C4-C3-C5-C6
25	5	603	CLA	C4-C3-C5-C6
25	6	615	CLA	C4-C3-C5-C6
25	8	606	CLA	C4-C3-C5-C6
26	5	613	CHL	C4-C3-C5-C6
25	A	1108	CLA	C2-C3-C5-C6
25	A	1111	CLA	C2-C3-C5-C6
25	A	1130	CLA	C2-C3-C5-C6
25	A	1136	CLA	C2-C3-C5-C6
25	B	1208	CLA	C2-C3-C5-C6
25	B	1213	CLA	C2-C3-C5-C6
25	B	1217	CLA	C2-C3-C5-C6
25	B	1218	CLA	C2-C3-C5-C6
25	B	1235	CLA	C2-C3-C5-C6
25	H	1703	CLA	C2-C3-C5-C6
25	a	607	CLA	C2-C3-C5-C6
25	4	612	CLA	C2-C3-C5-C6
25	6	615	CLA	C2-C3-C5-C6
25	8	606	CLA	C2-C3-C5-C6
26	5	613	CHL	C2-C3-C5-C6
25	K	1401	CLA	CBA-CGA-O2A-C1
25	A	1128	CLA	CBD-CGD-O2D-CED
25	A	1104	CLA	O1D-CGD-O2D-CED
25	A	1107	CLA	O1D-CGD-O2D-CED
25	A	1112	CLA	O1D-CGD-O2D-CED
25	B	1237	CLA	O1D-CGD-O2D-CED
25	B	1214	CLA	O1D-CGD-O2D-CED
25	B	1229	CLA	O1D-CGD-O2D-CED
25	1	601	CLA	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED
25	2	606	CLA	O1D-CGD-O2D-CED
25	9	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	G	1603	CLA	C2A-CAA-CBA-CGA
25	3	612	CLA	C2A-CAA-CBA-CGA
25	2	602	CLA	C3-C5-C6-C7
26	7	615	CHL	C2A-CAA-CBA-CGA
25	a	603	CLA	O1A-CGA-O2A-C1
25	9	604	CLA	O1A-CGA-O2A-C1
48	8	804	DGA	OA1-CA1-OG1-CG1
25	A	1112	CLA	C3-C5-C6-C7
25	A	1121	CLA	C3-C5-C6-C7
25	A	1122	CLA	C3-C5-C6-C7
25	A	1131	CLA	C3-C5-C6-C7
25	B	1211	CLA	C3-C5-C6-C7
25	B	1212	CLA	C3-C5-C6-C7
25	F	1302	CLA	C3-C5-C6-C7
25	H	1703	CLA	C3-C5-C6-C7
25	a	612	CLA	C3-C5-C6-C7
25	7	610	CLA	C3-C5-C6-C7
25	8	606	CLA	C3-C5-C6-C7
25	2	605	CLA	C3-C5-C6-C7
25	9	606	CLA	C3-C5-C6-C7
25	A	1104	CLA	CBA-CGA-O2A-C1
25	B	1237	CLA	CBA-CGA-O2A-C1
25	B	1204	CLA	CBA-CGA-O2A-C1
25	B	1208	CLA	CBA-CGA-O2A-C1
25	B	1209	CLA	CBA-CGA-O2A-C1
25	B	1213	CLA	CBA-CGA-O2A-C1
25	B	1217	CLA	CBA-CGA-O2A-C1
25	B	1230	CLA	CBA-CGA-O2A-C1
25	B	1231	CLA	CBA-CGA-O2A-C1
25	B	1207	CLA	CBA-CGA-O2A-C1
25	F	1302	CLA	CBA-CGA-O2A-C1
25	a	607	CLA	CBA-CGA-O2A-C1
25	4	606	CLA	CBA-CGA-O2A-C1
25	4	611	CLA	CBA-CGA-O2A-C1
25	4	616	CLA	CBA-CGA-O2A-C1
25	5	603	CLA	CBA-CGA-O2A-C1
25	5	607	CLA	CBA-CGA-O2A-C1
25	7	603	CLA	CBA-CGA-O2A-C1
25	8	606	CLA	CBA-CGA-O2A-C1
25	8	609	CLA	CBA-CGA-O2A-C1
25	8	618	CLA	CBA-CGA-O2A-C1
25	2	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	9	604	CLA	CBA-CGA-O2A-C1
30	A	5001	LHG	C24-C23-O8-C6
30	F	5002	LHG	C24-C23-O8-C6
33	B	5005	PTY	C31-C30-O4-C1
33	a	802	PTY	C31-C30-O4-C1
48	8	804	DGA	CA2-CA1-OG1-CG1
48	2	803	DGA	CA2-CA1-OG1-CG1
30	6	801	LHG	C23-C24-C25-C26
25	6	605	CLA	O1A-CGA-O2A-C1
29	B	4005	BCR	C9-C10-C11-C12
29	B	4007	BCR	C9-C10-C11-C12
29	G	4001	BCR	C9-C10-C11-C12
29	O	4001	BCR	C13-C14-C15-C16
43	7	501	LUT	C29-C30-C31-C32
25	A	1102	CLA	O1A-CGA-O2A-C1
25	A	1118	CLA	O1A-CGA-O2A-C1
25	B	1237	CLA	O1A-CGA-O2A-C1
25	B	1207	CLA	O1A-CGA-O2A-C1
25	7	606	CLA	O1A-CGA-O2A-C1
25	7	607	CLA	O1A-CGA-O2A-C1
25	8	618	CLA	O1A-CGA-O2A-C1
30	A	5001	LHG	O10-C23-O8-C6
33	B	5005	PTY	O30-C30-O4-C1
52	8	805	P5S	O18-C17-O19-C1
30	F	5001	LHG	O9-C7-O7-C5
48	3	803	DGA	OB1-CB1-OG2-CG2
25	K	1402	CLA	O1D-CGD-O2D-CED
25	L	1503	CLA	O1D-CGD-O2D-CED
25	2	608	CLA	O1D-CGD-O2D-CED
36	7	806	DGD	C8A-C9A-CAA-CBA
36	8	802	DGD	C8A-C9A-CAA-CBA
25	9	607	CLA	C2-C1-O2A-CGA
36	B	5003	DGD	C8A-C9A-CAA-CBA
25	B	1213	CLA	O1D-CGD-O2D-CED
25	B	1219	CLA	O1D-CGD-O2D-CED
25	3	602	CLA	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	A	1140	CLA	C3-C5-C6-C7
25	B	1215	CLA	C3-C5-C6-C7
25	5	603	CLA	C3-C5-C6-C7
26	5	613	CHL	C3-C5-C6-C7
26	6	619	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	1201	CLA	CBD-CGD-O2D-CED
25	8	602	CLA	CBD-CGD-O2D-CED
36	B	5003	DGD	CBA-CCA-CDA-CEA
30	A	5003	LHG	O2-C2-C3-O3
30	F	5002	LHG	O2-C2-C3-O3
30	a	801	LHG	O2-C2-C3-O3
30	6	801	LHG	O2-C2-C3-O3
30	7	801	LHG	O2-C2-C3-O3
30	8	801	LHG	O2-C2-C3-O3
30	2	802	LHG	O2-C2-C3-O3
30	9	801	LHG	O2-C2-C3-O3
38	F	5003	LPX	O1-C3-C4-O5
25	A	1117	CLA	O1D-CGD-O2D-CED
25	B	1226	CLA	O1D-CGD-O2D-CED
25	5	609	CLA	O1D-CGD-O2D-CED
25	7	601	CLA	O1D-CGD-O2D-CED
25	A	1111	CLA	CBA-CGA-O2A-C1
25	A	1113	CLA	CBA-CGA-O2A-C1
25	A	1117	CLA	CBA-CGA-O2A-C1
25	A	1120	CLA	CBA-CGA-O2A-C1
25	A	1126	CLA	CBA-CGA-O2A-C1
25	A	1139	CLA	CBA-CGA-O2A-C1
25	B	1215	CLA	CBA-CGA-O2A-C1
25	B	1236	CLA	CBA-CGA-O2A-C1
25	3	616	CLA	CBA-CGA-O2A-C1
25	5	604	CLA	CBA-CGA-O2A-C1
25	5	612	CLA	CBA-CGA-O2A-C1
25	6	608	CLA	CBA-CGA-O2A-C1
25	6	601	CLA	CBA-CGA-O2A-C1
25	6	604	CLA	CBA-CGA-O2A-C1
25	7	606	CLA	CBA-CGA-O2A-C1
25	2	605	CLA	CBA-CGA-O2A-C1
25	9	605	CLA	CBA-CGA-O2A-C1
52	8	805	P5S	C20-C17-O19-C1
35	A	5008	LMT	O5B-C5B-C6B-O6B
25	A	1111	CLA	O1A-CGA-O2A-C1
25	B	1204	CLA	O1A-CGA-O2A-C1
25	B	1213	CLA	O1A-CGA-O2A-C1
25	B	1217	CLA	O1A-CGA-O2A-C1
25	6	601	CLA	O1A-CGA-O2A-C1
25	7	604	CLA	O1A-CGA-O2A-C1
25	9	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	8	802	DGD	O1A-C1A-O1G-C1G
38	F	5003	LPX	O5-C4-C5-O6
25	A	1135	CLA	O1D-CGD-O2D-CED
25	B	1215	CLA	O1D-CGD-O2D-CED
25	1	605	CLA	O1D-CGD-O2D-CED
25	A	1105	CLA	CBD-CGD-O2D-CED
25	1	607	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	CBD-CGD-O2D-CED
25	5	601	CLA	CBD-CGD-O2D-CED
25	5	607	CLA	CBD-CGD-O2D-CED
30	F	5001	LHG	C8-C7-O7-C5
30	8	801	LHG	C8-C7-O7-C5
31	A	5004	LMG	C11-C10-O7-C8
25	5	615	CLA	CBA-CGA-O2A-C1
25	9	602	CLA	CBA-CGA-O2A-C1
25	B	1230	CLA	O1A-CGA-O2A-C1
25	5	607	CLA	O1A-CGA-O2A-C1
25	5	612	CLA	O1A-CGA-O2A-C1
25	7	603	CLA	O1A-CGA-O2A-C1
36	8	803	DGD	O6E-C5E-C6E-O5E
25	A	1110	CLA	O1D-CGD-O2D-CED
25	A	1132	CLA	O1D-CGD-O2D-CED
25	B	1238	CLA	O1D-CGD-O2D-CED
25	H	1703	CLA	O1D-CGD-O2D-CED
25	K	1403	CLA	O1D-CGD-O2D-CED
25	5	605	CLA	O1D-CGD-O2D-CED
25	8	618	CLA	O1D-CGD-O2D-CED
30	5	801	LHG	C7-C8-C9-C10
35	2	804	LMT	O5'-C5'-C6'-O6'
25	A	1113	CLA	O1D-CGD-O2D-CED
25	A	1129	CLA	O1D-CGD-O2D-CED
25	B	1240	CLA	O1D-CGD-O2D-CED
25	3	607	CLA	O1D-CGD-O2D-CED
25	3	612	CLA	O1D-CGD-O2D-CED
25	2	621	CLA	O1D-CGD-O2D-CED
25	A	1102	CLA	CBA-CGA-O2A-C1
25	a	603	CLA	CBA-CGA-O2A-C1
36	8	802	DGD	C2A-C1A-O1G-C1G
25	A	1121	CLA	C4-C3-C5-C6
25	B	1215	CLA	C4-C3-C5-C6
25	O	1802	CLA	C4-C3-C5-C6
26	a	606	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	7	609	CHL	C4-C3-C5-C6
26	2	609	CHL	C4-C3-C5-C6
25	A	1115	CLA	C2-C3-C5-C6
25	A	1121	CLA	C2-C3-C5-C6
25	B	1215	CLA	C2-C3-C5-C6
25	O	1802	CLA	C2-C3-C5-C6
25	3	610	CLA	C2-C3-C5-C6
25	5	603	CLA	C2-C3-C5-C6
26	a	606	CHL	C2-C3-C5-C6
26	7	609	CHL	C2-C3-C5-C6
25	A	1126	CLA	O1A-CGA-O2A-C1
25	B	1231	CLA	O1A-CGA-O2A-C1
25	B	1236	CLA	O1A-CGA-O2A-C1
25	F	1302	CLA	O1A-CGA-O2A-C1
25	3	616	CLA	O1A-CGA-O2A-C1
25	4	606	CLA	O1A-CGA-O2A-C1
25	6	604	CLA	O1A-CGA-O2A-C1
25	2	612	CLA	O1A-CGA-O2A-C1
25	B	1204	CLA	CBD-CGD-O2D-CED
25	5	604	CLA	CBD-CGD-O2D-CED
25	8	612	CLA	CBD-CGD-O2D-CED
25	A	1123	CLA	C8-C10-C11-C12
30	6	802	LHG	C2-C3-O3-P
25	A	1118	CLA	C2A-CAA-CBA-CGA
25	B	1216	CLA	C2A-CAA-CBA-CGA
25	5	609	CLA	C2A-CAA-CBA-CGA
26	4	613	CHL	C2A-CAA-CBA-CGA
26	6	609	CHL	C2A-CAA-CBA-CGA
25	4	605	CLA	O1D-CGD-O2D-CED
25	6	606	CLA	O1D-CGD-O2D-CED
25	7	608	CLA	O1D-CGD-O2D-CED
25	9	612	CLA	O1D-CGD-O2D-CED
25	A	1113	CLA	O1A-CGA-O2A-C1
25	A	1117	CLA	O1A-CGA-O2A-C1
25	A	1120	CLA	O1A-CGA-O2A-C1
25	A	1139	CLA	O1A-CGA-O2A-C1
25	B	1215	CLA	O1A-CGA-O2A-C1
25	a	607	CLA	O1A-CGA-O2A-C1
25	6	608	CLA	O1A-CGA-O2A-C1
35	A	5008	LMT	O5'-C1'-O1'-C1
25	B	1234	CLA	O1D-CGD-O2D-CED
25	O	1802	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	3	616	CLA	O1D-CGD-O2D-CED
25	A	1115	CLA	CBA-CGA-O2A-C1
25	A	1123	CLA	CBA-CGA-O2A-C1
25	B	1219	CLA	CBA-CGA-O2A-C1
25	B	1221	CLA	CBA-CGA-O2A-C1
25	B	1228	CLA	CBA-CGA-O2A-C1
25	9	606	CLA	CBA-CGA-O2A-C1
36	8	803	DGD	C2A-C1A-O1G-C1G
25	4	601	CLA	CBD-CGD-O2D-CED
35	B	5006	LMT	O5'-C5'-C6'-O6'
25	5	604	CLA	O1A-CGA-O2A-C1
25	B	1211	CLA	O1D-CGD-O2D-CED
25	4	606	CLA	O1D-CGD-O2D-CED
25	6	601	CLA	O1D-CGD-O2D-CED
25	9	604	CLA	O1D-CGD-O2D-CED
29	4	503	BCR	C19-C20-C21-C22
40	3	506	RRX	C13-C14-C15-C16
50	9	507	XAT	C13-C14-C15-C35
25	B	1219	CLA	O1A-CGA-O2A-C1
30	A	5003	LHG	C1-C2-C3-O3
30	B	5001	LHG	C1-C2-C3-O3
30	1	802	LHG	C1-C2-C3-O3
30	4	802	LHG	C1-C2-C3-O3
30	5	801	LHG	C1-C2-C3-O3
30	7	801	LHG	C1-C2-C3-O3
30	2	802	LHG	C1-C2-C3-O3
30	9	801	LHG	C1-C2-C3-O3
25	A	1106	CLA	CBA-CGA-O2A-C1
25	A	1108	CLA	CBA-CGA-O2A-C1
25	A	1112	CLA	CBA-CGA-O2A-C1
25	A	1124	CLA	CBA-CGA-O2A-C1
25	A	1125	CLA	CBA-CGA-O2A-C1
25	A	1131	CLA	CBA-CGA-O2A-C1
25	A	1133	CLA	CBA-CGA-O2A-C1
25	A	1134	CLA	CBA-CGA-O2A-C1
25	A	1136	CLA	CBA-CGA-O2A-C1
25	A	1140	CLA	CBA-CGA-O2A-C1
25	B	1023	CLA	CBA-CGA-O2A-C1
25	B	1202	CLA	CBA-CGA-O2A-C1
25	B	1210	CLA	CBA-CGA-O2A-C1
25	B	1220	CLA	CBA-CGA-O2A-C1
25	K	1403	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	L	1501	CLA	CBA-CGA-O2A-C1
25	O	1802	CLA	CBA-CGA-O2A-C1
25	a	605	CLA	CBA-CGA-O2A-C1
25	4	604	CLA	CBA-CGA-O2A-C1
25	4	612	CLA	CBA-CGA-O2A-C1
25	5	609	CLA	CBA-CGA-O2A-C1
25	6	606	CLA	CBA-CGA-O2A-C1
25	7	612	CLA	CBA-CGA-O2A-C1
25	8	602	CLA	CBA-CGA-O2A-C1
25	8	608	CLA	CBA-CGA-O2A-C1
25	9	607	CLA	CBA-CGA-O2A-C1
30	7	802	LHG	C24-C23-O8-C6
48	3	803	DGA	CA2-CA1-OG1-CG1
25	B	1217	CLA	CBD-CGD-O2D-CED
53	8	810	LAP	C16-C17-N8-C18
25	A	1013	CLA	O1D-CGD-O2D-CED
25	A	1127	CLA	O1D-CGD-O2D-CED
25	A	1101	CLA	O1D-CGD-O2D-CED
25	B	1208	CLA	O1D-CGD-O2D-CED
25	B	1223	CLA	O1D-CGD-O2D-CED
25	4	612	CLA	O1D-CGD-O2D-CED
25	6	607	CLA	O1D-CGD-O2D-CED
25	7	604	CLA	O1D-CGD-O2D-CED
25	7	607	CLA	O1D-CGD-O2D-CED
35	A	5008	LMT	C4B-C5B-C6B-O6B
35	B	5006	LMT	C4'-C5'-C6'-O6'
36	8	803	DGD	O1A-C1A-O1G-C1G
25	A	1133	CLA	C4-C3-C5-C6
25	5	602	CLA	C4-C3-C5-C6
25	A	1133	CLA	C2-C3-C5-C6
25	1	606	CLA	C2-C3-C5-C6
25	5	602	CLA	C2-C3-C5-C6
26	2	609	CHL	C2-C3-C5-C6
25	A	1109	CLA	C3-C5-C6-C7
25	B	1022	CLA	C3-C5-C6-C7
25	a	607	CLA	CBD-CGD-O2D-CED
25	A	1013	CLA	C14-C13-C15-C16
25	A	1121	CLA	C6-C7-C8-C9
25	A	1137	CLA	C11-C10-C8-C9
25	B	1201	CLA	C11-C10-C8-C9
25	B	1220	CLA	C11-C10-C8-C9
25	L	1502	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	1	605	CLA	C6-C7-C8-C9
25	3	601	CLA	C14-C13-C15-C16
25	3	605	CLA	C6-C7-C8-C9
25	3	606	CLA	C14-C13-C15-C16
25	3	613	CLA	C11-C12-C13-C14
25	5	612	CLA	C14-C13-C15-C16
25	7	601	CLA	C11-C10-C8-C9
25	2	603	CLA	C11-C10-C8-C9
25	9	605	CLA	C6-C7-C8-C9
26	1	609	CHL	C6-C7-C8-C9
26	3	604	CHL	C6-C7-C8-C9
26	3	611	CHL	C11-C10-C8-C9
26	5	610	CHL	C11-C12-C13-C14
26	5	610	CHL	C14-C13-C15-C16
26	7	609	CHL	C11-C10-C8-C9
26	7	617	CHL	C11-C12-C13-C14
26	8	603	CHL	C11-C12-C13-C14
25	A	1115	CLA	O1D-CGD-O2D-CED
25	A	1130	CLA	O1D-CGD-O2D-CED
25	B	1210	CLA	O1D-CGD-O2D-CED
25	H	1702	CLA	O1D-CGD-O2D-CED
25	8	609	CLA	O1D-CGD-O2D-CED
32	A	5005	SQD	C2-C1-O6-C44
32	7	805	SQD	C2-C1-O6-C44
35	A	5008	LMT	C2'-C1'-O1'-C1
36	7	806	DGD	C2D-C1D-O3G-C3G
32	G	5001	SQD	C7-C8-C9-C10
48	5	803	DGA	CA1-CA2-CA3-CA4
30	B	5002	LHG	O2-C2-C3-O3
30	4	802	LHG	O2-C2-C3-O3
30	5	801	LHG	O2-C2-C3-O3
30	7	803	LHG	O2-C2-C3-O3
30	2	801	LHG	O2-C2-C3-O3
25	A	1129	CLA	CBA-CGA-O2A-C1
25	A	1108	CLA	O1A-CGA-O2A-C1
25	A	1125	CLA	O1A-CGA-O2A-C1
25	A	1136	CLA	O1A-CGA-O2A-C1
25	7	612	CLA	O1A-CGA-O2A-C1
25	8	608	CLA	O1A-CGA-O2A-C1
25	9	606	CLA	O1A-CGA-O2A-C1
35	2	804	LMT	C4'-C5'-C6'-O6'
25	A	1102	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	604	CLA	O1D-CGD-O2D-CED
29	A	4001	BCR	C11-C12-C13-C35
29	A	4002	BCR	C36-C18-C19-C20
29	A	4003	BCR	C36-C18-C19-C20
29	B	4001	BCR	C37-C22-C23-C24
29	B	4002	BCR	C37-C22-C23-C24
29	B	4005	BCR	C7-C8-C9-C34
29	B	4006	BCR	C36-C18-C19-C20
29	G	4001	BCR	C36-C18-C19-C20
29	H	4001	BCR	C37-C22-C23-C24
29	J	4001	BCR	C36-C18-C19-C20
29	K	4001	BCR	C37-C22-C23-C24
29	K	4002	BCR	C36-C18-C19-C20
29	I	4001	BCR	C36-C18-C19-C20
29	3	504	BCR	C36-C18-C19-C20
29	3	505	BCR	C36-C18-C19-C20
29	4	503	BCR	C36-C18-C19-C20
29	5	504	BCR	C36-C18-C19-C20
29	5	504	BCR	C37-C22-C23-C24
29	6	503	BCR	C11-C12-C13-C35
29	6	503	BCR	C36-C18-C19-C20
29	7	503	BCR	C7-C8-C9-C34
39	F	4001	NEX	C27-C28-C29-C39
40	3	506	RRX	C11-C12-C13-C35
40	3	506	RRX	C7-C8-C9-C34
43	1	503	LUT	C31-C32-C33-C40
43	a	503	LUT	C31-C32-C33-C40
43	5	505	LUT	C31-C32-C33-C40
43	2	502	LUT	C31-C32-C33-C40
44	1	502	AXT	C31-C32-C33-C40
44	7	504	AXT	C11-C12-C13-C20
44	7	504	AXT	C27-C28-C29-C39
29	G	4001	BCR	C17-C18-C19-C20
29	K	4001	BCR	C7-C8-C9-C10
29	K	4001	BCR	C21-C22-C23-C24
29	O	4001	BCR	C11-C12-C13-C14
29	5	504	BCR	C21-C22-C23-C24
39	F	4001	NEX	C27-C28-C29-C30
40	3	506	RRX	C11-C12-C13-C14
40	3	506	RRX	C7-C8-C9-C10
44	1	502	AXT	C11-C12-C13-C14
44	7	504	AXT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
50	9	504	XAT	C11-C12-C13-C14
25	A	1127	CLA	C2A-CAA-CBA-CGA
25	B	1206	CLA	C2A-CAA-CBA-CGA
25	B	1239	CLA	C2A-CAA-CBA-CGA
25	7	612	CLA	C2A-CAA-CBA-CGA
25	8	618	CLA	C2A-CAA-CBA-CGA
26	a	613	CHL	C2A-CAA-CBA-CGA
26	8	610	CHL	C2A-CAA-CBA-CGA
33	a	803	PTY	C30-C31-C32-C33
25	A	1103	CLA	O1D-CGD-O2D-CED
25	3	601	CLA	O1D-CGD-O2D-CED
25	A	1131	CLA	O1A-CGA-O2A-C1
25	A	1133	CLA	O1A-CGA-O2A-C1
25	A	1134	CLA	O1A-CGA-O2A-C1
25	A	1140	CLA	O1A-CGA-O2A-C1
25	B	1023	CLA	O1A-CGA-O2A-C1
25	B	1202	CLA	O1A-CGA-O2A-C1
25	a	605	CLA	O1A-CGA-O2A-C1
25	6	606	CLA	O1A-CGA-O2A-C1
25	8	602	CLA	O1A-CGA-O2A-C1
25	9	607	CLA	O1A-CGA-O2A-C1
48	3	803	DGA	OA1-CA1-OG1-CG1
32	G	5001	SQD	C8-C7-O47-C45
51	7	807	4RF	O18-C19-C20-O21
25	A	1124	CLA	O1D-CGD-O2D-CED
25	A	1125	CLA	O1D-CGD-O2D-CED
32	I	5001	SQD	C24-C23-O48-C46
25	1	608	CLA	C5-C6-C7-C8
25	3	613	CLA	C5-C6-C7-C8
32	A	5005	SQD	C23-C24-C25-C26
25	A	1105	CLA	C2-C1-O2A-CGA
25	A	1108	CLA	C2-C1-O2A-CGA
25	A	1133	CLA	C2-C1-O2A-CGA
25	A	1139	CLA	C2-C1-O2A-CGA
25	B	1022	CLA	C2-C1-O2A-CGA
25	B	1203	CLA	C2-C1-O2A-CGA
25	B	1206	CLA	C2-C1-O2A-CGA
25	B	1211	CLA	C2-C1-O2A-CGA
25	B	1212	CLA	C2-C1-O2A-CGA
25	B	1216	CLA	C2-C1-O2A-CGA
25	B	1227	CLA	C2-C1-O2A-CGA
25	B	1229	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	B	1230	CLA	C2-C1-O2A-CGA
25	B	1235	CLA	C2-C1-O2A-CGA
25	B	1236	CLA	C2-C1-O2A-CGA
25	F	1301	CLA	C2-C1-O2A-CGA
25	O	1802	CLA	C2-C1-O2A-CGA
25	4	602	CLA	C2-C1-O2A-CGA
25	4	608	CLA	C2-C1-O2A-CGA
25	4	612	CLA	C2-C1-O2A-CGA
25	4	615	CLA	C2-C1-O2A-CGA
25	5	602	CLA	C2-C1-O2A-CGA
25	5	612	CLA	C2-C1-O2A-CGA
25	6	612	CLA	C2-C1-O2A-CGA
25	7	608	CLA	C2-C1-O2A-CGA
25	7	610	CLA	C2-C1-O2A-CGA
25	7	612	CLA	C2-C1-O2A-CGA
25	8	611	CLA	C2-C1-O2A-CGA
25	2	607	CLA	C2-C1-O2A-CGA
25	2	612	CLA	C2-C1-O2A-CGA
25	2	621	CLA	C2-C1-O2A-CGA
25	9	612	CLA	C2-C1-O2A-CGA
26	6	619	CHL	C2-C1-O2A-CGA
30	B	5002	LHG	C24-C25-C26-C27
25	A	1141	CLA	O1D-CGD-O2D-CED
25	B	1202	CLA	O1D-CGD-O2D-CED
25	B	1205	CLA	O1D-CGD-O2D-CED
25	B	1212	CLA	O1D-CGD-O2D-CED
25	B	1227	CLA	O1D-CGD-O2D-CED
25	B	1230	CLA	O1D-CGD-O2D-CED
25	a	605	CLA	O1D-CGD-O2D-CED
25	6	615	CLA	O1D-CGD-O2D-CED
25	A	1109	CLA	C10-C11-C12-C13
25	B	1202	CLA	C10-C11-C12-C13
25	B	1239	CLA	C15-C16-C17-C18
25	1	605	CLA	C15-C16-C17-C18
25	3	607	CLA	C13-C15-C16-C17
25	4	610	CLA	C5-C6-C7-C8
25	5	604	CLA	C15-C16-C17-C18
25	5	612	CLA	C15-C16-C17-C18
25	A	1106	CLA	O1D-CGD-O2D-CED
30	F	5001	LHG	O1-C1-C2-O2
30	4	801	LHG	O1-C1-C2-O2
30	2	801	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
30	9	802	LHG	O1-C1-C2-O2
25	B	1226	CLA	C3-C5-C6-C7
25	3	610	CLA	C3-C5-C6-C7
35	1	804	LMT	C4B-C5B-C6B-O6B
30	2	802	LHG	C23-C24-C25-C26
37	6	803	PCW	C31-C32-C33-C34
48	2	803	DGA	CB1-CB2-CB3-CB4
25	A	1133	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	C13-C15-C16-C17
25	9	612	CLA	C8-C10-C11-C12
25	B	1021	CLA	C12-C13-C15-C16
25	B	1206	CLA	C12-C13-C15-C16
25	B	1214	CLA	C6-C7-C8-C10
25	2	604	CLA	C6-C7-C8-C10
26	4	609	CHL	C12-C13-C15-C16
26	9	601	CHL	C12-C13-C15-C16
27	B	2002	PQN	C21-C22-C23-C25
25	G	1601	CLA	CBA-CGA-O2A-C1
25	L	1502	CLA	CBA-CGA-O2A-C1
30	2	802	LHG	C24-C23-O8-C6
52	8	805	P5S	OXT-C-CA-N
25	A	1128	CLA	C4-C3-C5-C6
25	6	602	CLA	C4-C3-C5-C6
30	B	5001	LHG	C7-C8-C9-C10
30	9	801	LHG	C23-C24-C25-C26
45	8	808	OLA	C1-C2-C3-C4
48	8	804	DGA	CB1-CB2-CB3-CB4
29	I	4001	BCR	C9-C10-C11-C12
29	I	4001	BCR	C15-C16-C17-C18
29	5	503	BCR	C9-C10-C11-C12
29	5	503	BCR	C13-C14-C15-C16
29	5	503	BCR	C15-C16-C17-C18
40	3	506	RRX	C9-C10-C11-C12
43	2	507	LUT	C9-C10-C11-C12
30	8	801	LHG	O9-C7-O7-C5
31	A	5004	LMG	O9-C10-O7-C8
32	G	5001	SQD	O49-C7-O47-C45
25	B	1222	CLA	O1D-CGD-O2D-CED
25	A	1122	CLA	C8-C10-C11-C12
25	A	1125	CLA	C15-C16-C17-C18
25	B	1226	CLA	C15-C16-C17-C18
25	L	1502	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	1	607	CLA	C5-C6-C7-C8
25	1	612	CLA	C8-C10-C11-C12
25	3	613	CLA	C8-C10-C11-C12
25	2	605	CLA	C10-C11-C12-C13
35	1	804	LMT	O5B-C5B-C6B-O6B
53	8	810	LAP	C16-C17-N8-C19
30	A	5002	LHG	C7-C8-C9-C10
30	B	5001	LHG	C23-C24-C25-C26
30	1	801	LHG	C23-C24-C25-C26
30	7	801	LHG	C7-C8-C9-C10
30	7	803	LHG	C7-C8-C9-C10
33	A	5006	PTY	C30-C31-C32-C33
33	G	5003	PTY	C8-C11-C12-C13
37	K	5001	PCW	C11-C12-C13-C14
45	8	809	OLA	C1-C2-C3-C4
48	3	803	DGA	CA1-CA2-CA3-CA4
48	5	803	DGA	CB1-CB2-CB3-CB4
25	K	1403	CLA	O1A-CGA-O2A-C1
25	L	1501	CLA	O1A-CGA-O2A-C1
25	O	1802	CLA	O1A-CGA-O2A-C1
25	4	612	CLA	O1A-CGA-O2A-C1
30	7	802	LHG	O10-C23-O8-C6
25	5	615	CLA	O1A-CGA-O2A-C1
25	A	1013	CLA	C8-C10-C11-C12
25	A	1125	CLA	C8-C10-C11-C12
25	A	1128	CLA	C10-C11-C12-C13
25	B	1237	CLA	C15-C16-C17-C18
25	B	1206	CLA	C15-C16-C17-C18
25	B	1209	CLA	C13-C15-C16-C17
25	B	1215	CLA	C5-C6-C7-C8
25	B	1216	CLA	C10-C11-C12-C13
25	B	1228	CLA	C13-C15-C16-C17
25	1	601	CLA	C5-C6-C7-C8
25	1	607	CLA	C8-C10-C11-C12
25	1	612	CLA	C5-C6-C7-C8
25	3	607	CLA	C8-C10-C11-C12
25	3	607	CLA	C10-C11-C12-C13
25	9	605	CLA	C10-C11-C12-C13
27	A	2001	PQN	C25-C26-C27-C28
27	B	2002	PQN	C18-C20-C21-C22
35	B	5006	LMT	C3'-C4'-O1B-C1B
25	A	1106	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	A	1111	CLA	C2A-CAA-CBA-CGA
25	A	1113	CLA	C2A-CAA-CBA-CGA
25	A	1119	CLA	C2A-CAA-CBA-CGA
25	A	1125	CLA	C2A-CAA-CBA-CGA
25	A	1135	CLA	C2A-CAA-CBA-CGA
25	A	1140	CLA	C2A-CAA-CBA-CGA
25	B	1237	CLA	C2A-CAA-CBA-CGA
25	B	1204	CLA	C2A-CAA-CBA-CGA
25	B	1209	CLA	C2A-CAA-CBA-CGA
25	B	1225	CLA	C2A-CAA-CBA-CGA
25	B	1227	CLA	C2A-CAA-CBA-CGA
25	F	1302	CLA	C2A-CAA-CBA-CGA
25	a	603	CLA	C2A-CAA-CBA-CGA
25	3	610	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C3-C5-C6-C7
25	7	610	CLA	C2A-CAA-CBA-CGA
25	8	609	CLA	C2A-CAA-CBA-CGA
25	2	612	CLA	C2A-CAA-CBA-CGA
26	1	611	CHL	C2A-CAA-CBA-CGA
26	4	618	CHL	C2A-CAA-CBA-CGA
26	7	611	CHL	C2A-CAA-CBA-CGA
26	7	617	CHL	C2A-CAA-CBA-CGA
25	A	1120	CLA	O1D-CGD-O2D-CED
29	H	4001	BCR	C10-C11-C12-C13
29	K	4001	BCR	C10-C11-C12-C13
50	9	504	XAT	C10-C11-C12-C13
25	A	1106	CLA	C15-C16-C17-C18
25	A	1111	CLA	C15-C16-C17-C18
25	A	1128	CLA	C15-C16-C17-C18
25	A	1133	CLA	C13-C15-C16-C17
25	B	1203	CLA	C8-C10-C11-C12
25	B	1206	CLA	C10-C11-C12-C13
25	B	1216	CLA	C13-C15-C16-C17
25	B	1219	CLA	C8-C10-C11-C12
25	B	1228	CLA	C15-C16-C17-C18
25	K	1402	CLA	C5-C6-C7-C8
25	1	612	CLA	C10-C11-C12-C13
25	a	603	CLA	C15-C16-C17-C18
25	5	601	CLA	C10-C11-C12-C13
25	9	605	CLA	C5-C6-C7-C8
26	2	609	CHL	C10-C11-C12-C13
30	A	5002	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	1	801	LHG	C7-C8-C9-C10
30	1	802	LHG	C23-C24-C25-C26
30	3	801	LHG	C7-C8-C9-C10
30	7	803	LHG	C23-C24-C25-C26
30	2	802	LHG	C7-C8-C9-C10
33	7	804	PTY	C30-C31-C32-C33
36	8	803	DGD	C1A-C2A-C3A-C4A
37	K	5002	PCW	C11-C12-C13-C14
37	6	803	PCW	C11-C12-C13-C14
47	4	804	PLM	C1-C2-C3-C4
51	7	807	4RF	C41-C43-C44-C45
52	8	805	P5S	C38-C39-C40-C41
25	L	1502	CLA	O1D-CGD-O2D-CED
25	4	607	CLA	O1D-CGD-O2D-CED
25	A	1124	CLA	O1A-CGA-O2A-C1
25	B	1220	CLA	O1A-CGA-O2A-C1
25	4	604	CLA	O1A-CGA-O2A-C1
25	A	1111	CLA	C3-C5-C6-C7
25	3	610	CLA	CBD-CGD-O2D-CED
36	8	803	DGD	O6E-C1E-O5D-C6D
30	8	801	LHG	C24-C25-C26-C27
25	2	615	CLA	O1D-CGD-O2D-CED
25	A	1103	CLA	C8-C10-C11-C12
25	A	1104	CLA	C5-C6-C7-C8
25	A	1109	CLA	C13-C15-C16-C17
25	A	1137	CLA	C10-C11-C12-C13
25	B	1202	CLA	C15-C16-C17-C18
25	B	1206	CLA	C8-C10-C11-C12
25	B	1209	CLA	C5-C6-C7-C8
25	B	1226	CLA	C5-C6-C7-C8
25	B	1239	CLA	C13-C15-C16-C17
25	G	1602	CLA	C5-C6-C7-C8
25	a	601	CLA	C10-C11-C12-C13
25	a	603	CLA	C10-C11-C12-C13
25	a	612	CLA	C5-C6-C7-C8
25	3	605	CLA	C13-C15-C16-C17
25	3	606	CLA	C15-C16-C17-C18
25	4	603	CLA	C5-C6-C7-C8
25	4	610	CLA	C8-C10-C11-C12
25	4	612	CLA	C10-C11-C12-C13
25	6	604	CLA	C15-C16-C17-C18
25	7	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	8	609	CLA	C5-C6-C7-C8
32	A	5005	SQD	C27-C28-C29-C30
37	B	5004	PCW	C12-C13-C14-C15
30	A	5001	LHG	O2-C2-C3-O3
30	A	5002	LHG	O2-C2-C3-O3
30	F	5001	LHG	O2-C2-C3-O3
30	6	802	LHG	O2-C2-C3-O3
30	9	802	LHG	O2-C2-C3-O3
25	A	1013	CLA	CBA-CGA-O2A-C1
25	9	612	CLA	CBA-CGA-O2A-C1
25	A	1106	CLA	O1A-CGA-O2A-C1
25	A	1112	CLA	O1A-CGA-O2A-C1
25	A	1115	CLA	O1A-CGA-O2A-C1
25	A	1123	CLA	O1A-CGA-O2A-C1
25	B	1221	CLA	O1A-CGA-O2A-C1
25	B	1228	CLA	O1A-CGA-O2A-C1
25	5	609	CLA	O1A-CGA-O2A-C1
25	3	610	CLA	C8-C10-C11-C12
30	B	5002	LHG	C23-C24-C25-C26
30	7	801	LHG	C23-C24-C25-C26
30	7	802	LHG	C23-C24-C25-C26
32	I	5001	SQD	C23-C24-C25-C26
51	7	807	4RF	C22-C24-C25-C26
25	A	1115	CLA	C10-C11-C12-C13
25	A	1121	CLA	C8-C10-C11-C12
25	B	1201	CLA	C15-C16-C17-C18
25	B	1216	CLA	C8-C10-C11-C12
25	1	605	CLA	C13-C15-C16-C17
25	4	615	CLA	C5-C6-C7-C8
25	7	604	CLA	C13-C15-C16-C17
25	7	612	CLA	C8-C10-C11-C12
25	A	1128	CLA	O1D-CGD-O2D-CED
25	5	601	CLA	O1D-CGD-O2D-CED
25	8	602	CLA	O1D-CGD-O2D-CED
25	A	1113	CLA	C5-C6-C7-C8
25	A	1123	CLA	C15-C16-C17-C18
25	B	1205	CLA	C10-C11-C12-C13
25	B	1206	CLA	C5-C6-C7-C8
25	B	1224	CLA	C8-C10-C11-C12
25	B	1224	CLA	C15-C16-C17-C18
25	B	1234	CLA	C15-C16-C17-C18
25	1	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	B	2002	PQN	C25-C26-C27-C28
25	B	1210	CLA	O1A-CGA-O2A-C1
32	I	5001	SQD	O10-C23-O48-C46
30	6	802	LHG	C23-C24-C25-C26
30	8	801	LHG	C23-C24-C25-C26
30	9	802	LHG	C23-C24-C25-C26
33	B	5005	PTY	C8-C11-C12-C13
25	9	602	CLA	O1A-CGA-O2A-C1
25	A	1012	CLA	C5-C6-C7-C8
25	A	1103	CLA	C5-C6-C7-C8
25	A	1126	CLA	C10-C11-C12-C13
25	B	1021	CLA	C10-C11-C12-C13
25	B	1204	CLA	C15-C16-C17-C18
25	O	1802	CLA	C5-C6-C7-C8
25	3	616	CLA	C5-C6-C7-C8
25	4	610	CLA	C10-C11-C12-C13
25	2	605	CLA	C8-C10-C11-C12
26	A	1114	CHL	C5-C6-C7-C8
25	A	1110	CLA	CBA-CGA-O2A-C1
25	B	1211	CLA	CBA-CGA-O2A-C1
25	B	1226	CLA	CBA-CGA-O2A-C1
30	A	5002	LHG	C8-C7-O7-C5
30	B	5002	LHG	C8-C7-O7-C5
30	1	801	LHG	C8-C7-O7-C5
30	7	803	LHG	C8-C7-O7-C5
48	3	803	DGA	CA2-CA3-CA4-CA5
25	A	1129	CLA	O1A-CGA-O2A-C1
25	3	618	CLA	CBA-CGA-O2A-C1
25	4	605	CLA	CBA-CGA-O2A-C1
25	G	1602	CLA	C8-C10-C11-C12
25	A	1013	CLA	C3-C5-C6-C7
25	a	608	CLA	O1D-CGD-O2D-CED
30	2	802	LHG	C32-C33-C34-C35
29	B	4007	BCR	C13-C14-C15-C16
29	J	4001	BCR	C9-C10-C11-C12
29	L	4001	BCR	C9-C10-C11-C12
29	3	503	BCR	C13-C14-C15-C16
25	A	1012	CLA	C13-C15-C16-C17
25	7	610	CLA	C5-C6-C7-C8
25	G	1601	CLA	O1A-CGA-O2A-C1
30	F	5001	LHG	C23-C24-C25-C26
30	A	5002	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
30	B	5002	LHG	O9-C7-O7-C5
30	7	803	LHG	O9-C7-O7-C5
30	A	5001	LHG	C1-C2-C3-O3
30	F	5001	LHG	C1-C2-C3-O3
30	a	801	LHG	C1-C2-C3-O3
25	F	1301	CLA	C2A-CAA-CBA-CGA
25	5	615	CLA	C2A-CAA-CBA-CGA
26	6	611	CHL	C2A-CAA-CBA-CGA
25	B	1201	CLA	O1D-CGD-O2D-CED
25	A	1116	CLA	CBA-CGA-O2A-C1
25	B	1234	CLA	CBA-CGA-O2A-C1
25	a	602	CLA	CBA-CGA-O2A-C1
25	6	602	CLA	CBA-CGA-O2A-C1
25	2	603	CLA	CBA-CGA-O2A-C1
37	K	5001	PCW	C12-C11-O3-C3
32	H	5001	SQD	C16-C17-C18-C19
25	A	1013	CLA	C13-C15-C16-C17
25	A	1136	CLA	C15-C16-C17-C18
25	B	1203	CLA	C5-C6-C7-C8
25	B	1214	CLA	C5-C6-C7-C8
25	L	1502	CLA	C5-C6-C7-C8
25	3	606	CLA	C5-C6-C7-C8
25	4	610	CLA	C15-C16-C17-C18
25	4	612	CLA	C8-C10-C11-C12
25	5	612	CLA	C5-C6-C7-C8
25	8	609	CLA	C10-C11-C12-C13
25	2	607	CLA	C8-C10-C11-C12
25	9	612	CLA	C13-C15-C16-C17
25	7	608	CLA	C3-C5-C6-C7
35	B	5006	LMT	C5'-C4'-O1B-C1B
25	A	1105	CLA	O1D-CGD-O2D-CED
25	1	607	CLA	O1D-CGD-O2D-CED
25	8	612	CLA	O1D-CGD-O2D-CED
30	6	801	LHG	C7-C8-C9-C10
33	5	802	PTY	C8-C11-C12-C13
25	A	1112	CLA	C5-C6-C7-C8
25	A	1126	CLA	C8-C10-C11-C12
25	1	608	CLA	C10-C11-C12-C13
32	A	5005	SQD	C15-C16-C17-C18
25	B	1231	CLA	C5-C6-C7-C8
25	B	1239	CLA	C5-C6-C7-C8
25	H	1703	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	3	605	CLA	C5-C6-C7-C8
25	7	601	CLA	C10-C11-C12-C13
25	7	612	CLA	C5-C6-C7-C8
25	9	612	CLA	C15-C16-C17-C18
25	A	1128	CLA	CBA-CGA-O2A-C1
30	2	801	LHG	C24-C23-O8-C6
35	A	5008	LMT	O1'-C1-C2-C3
25	B	1201	CLA	C2-C3-C5-C6
25	A	1101	CLA	C15-C16-C17-C18
25	B	1229	CLA	C13-C15-C16-C17
25	B	1235	CLA	C8-C10-C11-C12
25	6	607	CLA	C5-C6-C7-C8
25	4	610	CLA	C3-C5-C6-C7
25	8	605	CLA	C3-C5-C6-C7
30	4	801	LHG	C8-C7-O7-C5
26	8	603	CHL	C11-C10-C8-C9
25	5	604	CLA	O1D-CGD-O2D-CED
25	5	607	CLA	O1D-CGD-O2D-CED
30	1	801	LHG	O9-C7-O7-C5
36	8	802	DGD	C2E-C1E-O5D-C6D
36	8	803	DGD	C2D-C1D-O3G-C3G
36	8	803	DGD	C2E-C1E-O5D-C6D
25	A	1121	CLA	C10-C11-C12-C13
25	B	1201	CLA	C13-C15-C16-C17
30	F	5002	LHG	C23-C24-C25-C26
25	A	1111	CLA	C16-C17-C18-C20
25	B	1234	CLA	C16-C17-C18-C20
25	F	1302	CLA	C6-C7-C8-C10
25	4	607	CLA	C6-C7-C8-C9
25	6	607	CLA	C6-C7-C8-C10
26	5	610	CHL	C5-C6-C7-C8
25	L	1502	CLA	O1A-CGA-O2A-C1
29	B	4004	BCR	C11-C10-C9-C34
29	5	504	BCR	C11-C10-C9-C34
29	6	504	BCR	C11-C10-C9-C34
39	F	4001	NEX	C11-C10-C9-C19
39	F	4001	NEX	C40-C33-C34-C35
30	2	801	LHG	C23-C24-C25-C26
25	B	1201	CLA	C5-C6-C7-C8
25	4	615	CLA	C8-C10-C11-C12
29	A	4001	BCR	C36-C18-C19-C20
29	A	4005	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
29	B	4004	BCR	C7-C8-C9-C34
29	B	4005	BCR	C37-C22-C23-C24
29	B	4006	BCR	C11-C12-C13-C35
29	J	4001	BCR	C37-C22-C23-C24
29	O	4001	BCR	C11-C12-C13-C35
29	6	504	BCR	C37-C22-C23-C24
33	a	803	PTY	C6-C5-O14-P1
33	a	802	PTY	C6-C5-O14-P1
40	J	4002	RRX	C11-C12-C13-C35
43	a	501	LUT	C7-C8-C9-C19
43	2	507	LUT	C31-C32-C33-C40
44	1	502	AXT	C7-C8-C9-C19
44	1	502	AXT	C27-C28-C29-C39
30	2	801	LHG	C25-C26-C27-C28
29	B	4006	BCR	C11-C12-C13-C14
29	6	503	BCR	C17-C18-C19-C20
40	J	4002	RRX	C11-C12-C13-C14
43	a	501	LUT	C7-C8-C9-C10
43	2	507	LUT	C31-C32-C33-C34
44	1	502	AXT	C7-C8-C9-C10
44	1	502	AXT	C27-C28-C29-C30
25	A	1104	CLA	C2A-CAA-CBA-CGA
25	A	1110	CLA	C2A-CAA-CBA-CGA
25	B	1213	CLA	C2A-CAA-CBA-CGA
25	B	1232	CLA	C2A-CAA-CBA-CGA
25	H	1703	CLA	C2A-CAA-CBA-CGA
25	O	1802	CLA	C2A-CAA-CBA-CGA
25	3	616	CLA	C2A-CAA-CBA-CGA
25	5	603	CLA	C2A-CAA-CBA-CGA
25	2	605	CLA	C2A-CAA-CBA-CGA
25	2	615	CLA	C2A-CAA-CBA-CGA
26	a	606	CHL	C2A-CAA-CBA-CGA
26	9	608	CHL	C2A-CAA-CBA-CGA
25	B	1210	CLA	C15-C16-C17-C18
30	A	5003	LHG	O1-C1-C2-C3
30	B	5002	LHG	O1-C1-C2-C3
30	F	5002	LHG	O1-C1-C2-C3
30	1	801	LHG	O1-C1-C2-C3
30	4	802	LHG	O1-C1-C2-C3
30	4	801	LHG	O1-C1-C2-C3
30	6	801	LHG	O1-C1-C2-C3
30	7	802	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	7	803	LHG	O1-C1-C2-C3
30	2	801	LHG	O1-C1-C2-C3
30	9	802	LHG	O1-C1-C2-C3
25	B	1204	CLA	O1D-CGD-O2D-CED
25	A	1122	CLA	CBA-CGA-O2A-C1
36	B	5003	DGD	C6A-C7A-C8A-C9A
24	A	1011	CL0	C16-C17-C18-C19
25	A	1107	CLA	C6-C7-C8-C9
25	B	1234	CLA	C16-C17-C18-C19
25	B	1235	CLA	C16-C17-C18-C19
25	B	1238	CLA	C16-C17-C18-C19
25	1	612	CLA	C16-C17-C18-C19
25	4	615	CLA	C11-C12-C13-C15
25	5	601	CLA	C11-C12-C13-C15
25	4	601	CLA	O1D-CGD-O2D-CED
25	B	1211	CLA	O1A-CGA-O2A-C1
25	B	1234	CLA	O1A-CGA-O2A-C1
25	6	602	CLA	O1A-CGA-O2A-C1
30	2	802	LHG	O10-C23-O8-C6
25	A	1132	CLA	C3-C5-C6-C7
29	B	4004	BCR	C11-C10-C9-C8
29	6	504	BCR	C11-C10-C9-C8
39	F	4001	NEX	C11-C10-C9-C8
39	F	4001	NEX	C32-C33-C34-C35
48	2	803	DGA	CA5-CA6-CA7-CA8
35	1	804	LMT	O5'-C1'-O1'-C1
36	8	802	DGD	O6E-C1E-O5D-C6D
36	8	803	DGD	O6D-C1D-O3G-C3G
36	B	5003	DGD	C2G-C1G-O1G-C1A
30	9	802	LHG	C8-C7-O7-C5
33	G	5003	PTY	C11-C8-O7-C6
25	B	1214	CLA	C8-C10-C11-C12
30	4	802	LHG	C12-C13-C14-C15
25	A	1121	CLA	CBA-CGA-O2A-C1
25	A	1103	CLA	C10-C11-C12-C13
25	A	1132	CLA	C15-C16-C17-C18
25	a	605	CLA	C5-C6-C7-C8
53	8	810	LAP	C16-C17-N8-C20
48	3	803	DGA	CA4-CA5-CA6-CA7
25	A	1103	CLA	C2-C1-O2A-CGA
25	A	1112	CLA	C2-C1-O2A-CGA
25	A	1118	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	A	1119	CLA	C2-C1-O2A-CGA
25	A	1124	CLA	C2-C1-O2A-CGA
25	A	1140	CLA	C2-C1-O2A-CGA
25	A	1101	CLA	C2-C1-O2A-CGA
25	B	1201	CLA	C2-C1-O2A-CGA
25	B	1208	CLA	C2-C1-O2A-CGA
25	B	1219	CLA	C2-C1-O2A-CGA
25	B	1220	CLA	C2-C1-O2A-CGA
25	G	1601	CLA	C2-C1-O2A-CGA
25	H	1701	CLA	C2-C1-O2A-CGA
25	K	1403	CLA	C2-C1-O2A-CGA
25	L	1501	CLA	C2-C1-O2A-CGA
25	L	1504	CLA	C2-C1-O2A-CGA
25	1	612	CLA	C2-C1-O2A-CGA
25	3	613	CLA	C2-C1-O2A-CGA
25	4	611	CLA	C2-C1-O2A-CGA
25	4	616	CLA	C2-C1-O2A-CGA
25	5	609	CLA	C2-C1-O2A-CGA
25	6	602	CLA	C2-C1-O2A-CGA
25	8	609	CLA	C2-C1-O2A-CGA
25	2	615	CLA	C2-C1-O2A-CGA
25	A	1107	CLA	C6-C7-C8-C10
25	A	1117	CLA	C16-C17-C18-C20
25	A	1128	CLA	C16-C17-C18-C20
25	4	607	CLA	C6-C7-C8-C10
25	4	615	CLA	C11-C12-C13-C14
25	5	601	CLA	C11-C12-C13-C14
25	8	605	CLA	C6-C7-C8-C9
25	8	605	CLA	C6-C7-C8-C10
25	2	605	CLA	C11-C12-C13-C15
27	A	2001	PQN	C26-C27-C28-C30
25	A	1013	CLA	O1A-CGA-O2A-C1
25	A	1110	CLA	O1A-CGA-O2A-C1
25	B	1226	CLA	O1A-CGA-O2A-C1
30	5	801	LHG	C13-C14-C15-C16
30	F	5002	LHG	C11-C12-C13-C14
30	1	802	LHG	C25-C26-C27-C28
30	1	802	LHG	C34-C35-C36-C37
30	3	801	LHG	C9-C10-C11-C12
30	5	801	LHG	C31-C32-C33-C34
30	2	801	LHG	C11-C12-C13-C14
30	9	802	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	B	5003	DGD	C3A-C4A-C5A-C6A
48	8	804	DGA	CBB-CCB-CDB-CEB
53	8	810	LAP	C3-C4-C5-C6
30	B	5002	LHG	C7-C8-C9-C10
30	4	801	LHG	C23-C24-C25-C26
25	6	615	CLA	C8-C10-C11-C12
25	8	606	CLA	C5-C6-C7-C8
30	B	5001	LHG	C13-C14-C15-C16
30	1	802	LHG	C11-C12-C13-C14
30	6	802	LHG	C24-C25-C26-C27
36	8	802	DGD	C7A-C8A-C9A-CAA
36	8	802	DGD	C9A-CAA-CBA-CCA
48	8	804	DGA	CA3-CA4-CA5-CA6
25	a	602	CLA	O1A-CGA-O2A-C1
25	2	603	CLA	O1A-CGA-O2A-C1
25	F	1301	CLA	CBA-CGA-O2A-C1
30	A	5001	LHG	C33-C34-C35-C36
30	A	5002	LHG	C34-C35-C36-C37
30	1	801	LHG	C30-C31-C32-C33
30	1	802	LHG	C10-C11-C12-C13
45	1	803	OLA	C3-C4-C5-C6
47	6	804	PLM	C4-C5-C6-C7
30	4	801	LHG	O9-C7-O7-C5
30	A	5001	LHG	O1-C1-C2-O2
30	B	5002	LHG	O1-C1-C2-O2
30	F	5002	LHG	O1-C1-C2-O2
30	a	801	LHG	O1-C1-C2-O2
30	4	802	LHG	O1-C1-C2-O2
30	7	801	LHG	O1-C1-C2-O2
30	7	802	LHG	O1-C1-C2-O2
30	7	803	LHG	O1-C1-C2-O2
30	F	5001	LHG	C11-C12-C13-C14
30	2	802	LHG	C13-C14-C15-C16
30	9	802	LHG	C34-C35-C36-C37
37	K	5002	PCW	C14-C15-C16-C17
26	7	613	CHL	C2C-C3C-CAC-CBC
25	A	1122	CLA	C4B-C3B-CAB-CBB
25	B	1224	CLA	C4B-C3B-CAB-CBB
25	H	1703	CLA	C4B-C3B-CAB-CBB
25	2	621	CLA	C4B-C3B-CAB-CBB
30	B	5001	LHG	C11-C12-C13-C14
30	B	5001	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
30	1	801	LHG	C26-C27-C28-C29
41	4	805	SPH	C10-C11-C12-C13
25	B	1211	CLA	C6-C7-C8-C10
25	B	1213	CLA	C6-C7-C8-C10
25	B	1235	CLA	C16-C17-C18-C20
25	F	1302	CLA	C6-C7-C8-C9
25	a	608	CLA	C6-C7-C8-C9
25	7	606	CLA	C6-C7-C8-C9
25	7	606	CLA	C6-C7-C8-C10
36	8	803	DGD	C4E-C5E-C6E-O5E
25	G	1602	CLA	C2A-CAA-CBA-CGA
25	7	604	CLA	C2A-CAA-CBA-CGA
25	7	608	CLA	C2A-CAA-CBA-CGA
26	9	601	CHL	C2A-CAA-CBA-CGA
30	A	5003	LHG	C14-C15-C16-C17
30	6	801	LHG	C12-C13-C14-C15
45	a	805	OLA	C14-C15-C16-C17
25	3	606	CLA	C13-C15-C16-C17
26	6	619	CHL	C5-C6-C7-C8
30	a	801	LHG	C8-C7-O7-C5
30	6	801	LHG	C8-C7-O7-C5
37	6	803	PCW	C32-C31-O2-C2
30	3	801	LHG	C31-C32-C33-C34
25	A	1125	CLA	C6-C7-C8-C10
25	A	1101	CLA	C11-C10-C8-C7
25	B	1231	CLA	C12-C13-C15-C16
25	B	1239	CLA	C12-C13-C15-C16
25	a	607	CLA	C6-C7-C8-C10
25	2	607	CLA	C12-C13-C15-C16
30	A	5002	LHG	C9-C10-C11-C12
30	A	5002	LHG	C30-C31-C32-C33
30	A	5003	LHG	C17-C18-C19-C20
30	4	801	LHG	C17-C18-C19-C20
30	7	802	LHG	C25-C26-C27-C28
30	2	801	LHG	C28-C29-C30-C31
48	2	803	DGA	CB7-CB8-CB9-CAB
30	A	5001	LHG	C7-C8-C9-C10
36	8	803	DGD	C1B-C2B-C3B-C4B
25	6	603	CLA	CBA-CGA-O2A-C1
30	A	5001	LHG	C11-C12-C13-C14
30	B	5001	LHG	C34-C35-C36-C37
30	6	802	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	6	801	LHG	C30-C31-C32-C33
33	9	803	PTY	C34-C35-C36-C37
45	a	805	OLA	C12-C13-C14-C15
25	A	1116	CLA	O1A-CGA-O2A-C1
37	K	5001	PCW	O11-C11-O3-C3
26	A	1114	CHL	C3-C5-C6-C7
25	A	1104	CLA	C3A-C2A-CAA-CBA
25	A	1109	CLA	C3A-C2A-CAA-CBA
25	A	1126	CLA	C3A-C2A-CAA-CBA
25	A	1130	CLA	C3A-C2A-CAA-CBA
25	A	1133	CLA	C3A-C2A-CAA-CBA
25	A	1135	CLA	C3A-C2A-CAA-CBA
25	A	1101	CLA	C3A-C2A-CAA-CBA
25	B	1223	CLA	C3A-C2A-CAA-CBA
25	B	1207	CLA	C3A-C2A-CAA-CBA
25	H	1701	CLA	C3A-C2A-CAA-CBA
25	L	1504	CLA	C3A-C2A-CAA-CBA
25	1	602	CLA	C3A-C2A-CAA-CBA
25	a	602	CLA	C3A-C2A-CAA-CBA
25	4	610	CLA	C3A-C2A-CAA-CBA
25	5	606	CLA	C3A-C2A-CAA-CBA
25	5	615	CLA	C3A-C2A-CAA-CBA
25	8	615	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	9	612	CLA	C3A-C2A-CAA-CBA
26	4	613	CHL	C3A-C2A-CAA-CBA
26	6	619	CHL	C3A-C2A-CAA-CBA
30	F	5001	LHG	C26-C27-C28-C29
45	1	803	OLA	C13-C14-C15-C16
25	A	1128	CLA	C2-C3-C5-C6
37	K	5001	PCW	C32-C33-C34-C35
47	8	807	PLM	C6-C7-C8-C9
25	B	1213	CLA	C5-C6-C7-C8
25	a	603	CLA	C5-C6-C7-C8
25	5	612	CLA	C10-C11-C12-C13
30	4	802	LHG	C23-C24-C25-C26
30	F	5001	LHG	C7-C8-C9-C10
29	A	4004	BCR	C13-C14-C15-C16
29	B	4003	BCR	C19-C20-C21-C22
29	B	4006	BCR	C19-C20-C21-C22
29	I	4001	BCR	C13-C14-C15-C16
43	6	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	A	1128	CLA	C16-C17-C18-C19
25	B	1211	CLA	C6-C7-C8-C9
25	B	1213	CLA	C6-C7-C8-C9
25	1	612	CLA	C16-C17-C18-C20
25	a	608	CLA	C6-C7-C8-C10
25	5	612	CLA	C16-C17-C18-C19
25	A	1128	CLA	O1A-CGA-O2A-C1
25	9	612	CLA	O1A-CGA-O2A-C1
30	B	5001	LHG	C30-C31-C32-C33
33	a	802	PTY	C33-C34-C35-C36
36	B	5003	DGD	C9A-CAA-CBA-CCA
30	8	801	LHG	C11-C12-C13-C14
45	8	809	OLA	C12-C13-C14-C15
25	A	1137	CLA	CBA-CGA-O2A-C1
25	1	605	CLA	CBA-CGA-O2A-C1
33	5	802	PTY	O4-C1-C6-C5
30	A	5003	LHG	C28-C29-C30-C31
30	a	801	LHG	C26-C27-C28-C29
30	3	801	LHG	C13-C14-C15-C16
37	K	5002	PCW	C12-C13-C14-C15
37	K	5001	PCW	C33-C34-C35-C36
30	A	5001	LHG	C23-C24-C25-C26
25	A	1101	CLA	C13-C15-C16-C17
30	B	5001	LHG	C14-C15-C16-C17
30	a	801	LHG	C11-C10-C9-C8
30	8	801	LHG	C26-C27-C28-C29
33	a	803	PTY	C35-C36-C37-C38
36	8	803	DGD	C2B-C3B-C4B-C5B
41	6	806	SPH	C11-C12-C13-C14
45	8	809	OLA	C14-C15-C16-C17
48	2	803	DGA	CB9-CAB-CBB-CCB
30	2	801	LHG	O10-C23-O8-C6
30	A	5001	LHG	C30-C31-C32-C33
32	A	5005	SQD	C30-C31-C32-C33
33	J	5001	PTY	C32-C33-C34-C35
37	6	803	PCW	C13-C14-C15-C16
38	F	5003	LPX	C7-C8-C9-C10
25	1	605	CLA	C16-C17-C18-C19
25	A	1121	CLA	O1A-CGA-O2A-C1
25	A	1122	CLA	C2B-C3B-CAB-CBB
25	H	1703	CLA	C2B-C3B-CAB-CBB
29	A	4001	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	A	4004	BCR	C1-C6-C7-C8
29	B	4004	BCR	C1-C6-C7-C8
29	B	4004	BCR	C5-C6-C7-C8
29	B	4005	BCR	C1-C6-C7-C8
29	B	4005	BCR	C5-C6-C7-C8
29	H	4001	BCR	C23-C24-C25-C26
29	H	4001	BCR	C23-C24-C25-C30
29	J	4001	BCR	C23-C24-C25-C30
29	K	4002	BCR	C23-C24-C25-C26
29	K	4002	BCR	C23-C24-C25-C30
29	L	4002	BCR	C1-C6-C7-C8
29	L	4002	BCR	C5-C6-C7-C8
29	I	4001	BCR	C1-C6-C7-C8
29	O	4001	BCR	C1-C6-C7-C8
29	O	4001	BCR	C5-C6-C7-C8
29	O	4001	BCR	C23-C24-C25-C26
29	O	4001	BCR	C23-C24-C25-C30
29	3	503	BCR	C1-C6-C7-C8
29	3	505	BCR	C23-C24-C25-C26
29	3	505	BCR	C23-C24-C25-C30
29	4	503	BCR	C1-C6-C7-C8
29	5	503	BCR	C1-C6-C7-C8
29	5	504	BCR	C1-C6-C7-C8
29	5	504	BCR	C5-C6-C7-C8
29	5	504	BCR	C23-C24-C25-C26
29	5	504	BCR	C23-C24-C25-C30
29	6	503	BCR	C1-C6-C7-C8
29	6	503	BCR	C5-C6-C7-C8
29	6	504	BCR	C23-C24-C25-C30
29	7	503	BCR	C1-C6-C7-C8
29	7	503	BCR	C5-C6-C7-C8
29	8	503	BCR	C1-C6-C7-C8
40	J	4002	RRX	C23-C24-C25-C26
42	M	4001	ECH	C23-C24-C25-C26
43	a	501	LUT	C1-C6-C7-C8
43	2	507	LUT	C1-C6-C7-C8
43	2	507	LUT	C5-C6-C7-C8
44	7	504	AXT	C21-C26-C27-C28
30	F	5002	LHG	C26-C27-C28-C29
32	A	5005	SQD	C26-C27-C28-C29
41	J	5002	SPH	C11-C12-C13-C14
52	8	805	P5S	C39-C38-O37-C2

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Mol	Chain	Res	Type	Atoms
41	9	804	SPH	C5-C6-C7-C8
25	1	603	CLA	CBA-CGA-O2A-C1
25	A	1125	CLA	C13-C15-C16-C17
25	B	1216	CLA	C3-C5-C6-C7
41	9	804	SPH	C10-C11-C12-C13
47	a	804	PLM	C4-C5-C6-C7
47	8	806	PLM	C2-C3-C4-C5
25	A	1139	CLA	C2A-CAA-CBA-CGA
25	B	1208	CLA	C2A-CAA-CBA-CGA
25	B	1214	CLA	C2A-CAA-CBA-CGA
25	6	618	CLA	C2A-CAA-CBA-CGA
25	9	604	CLA	C2A-CAA-CBA-CGA
25	A	1119	CLA	C13-C15-C16-C17
30	A	5001	LHG	C13-C14-C15-C16
30	A	5001	LHG	C31-C32-C33-C34
33	B	5005	PTY	C18-C19-C20-C21
25	A	1122	CLA	O1A-CGA-O2A-C1
25	A	1137	CLA	O1A-CGA-O2A-C1
25	F	1301	CLA	O1A-CGA-O2A-C1
25	6	603	CLA	O1A-CGA-O2A-C1
30	F	5001	LHG	C13-C14-C15-C16
30	4	801	LHG	C28-C29-C30-C31
48	2	803	DGA	CAB-CBB-CCB-CDB
30	a	801	LHG	O9-C7-O7-C5
30	6	801	LHG	O9-C7-O7-C5
33	G	5003	PTY	O10-C8-O7-C6
37	6	803	PCW	O31-C31-O2-C2
25	5	603	CLA	C11-C10-C8-C7
33	G	5003	PTY	C13-C14-C15-C16
29	A	4005	BCR	C10-C11-C12-C13
29	O	4001	BCR	C10-C11-C12-C13
25	B	1207	CLA	C10-C11-C12-C13
25	a	601	CLA	C5-C6-C7-C8
25	6	602	CLA	C2-C3-C5-C6
25	B	1221	CLA	C16-C17-C18-C19
30	4	802	LHG	C11-C12-C13-C14
30	7	802	LHG	C26-C27-C28-C29
30	7	802	LHG	C28-C29-C30-C31
25	A	1119	CLA	CBA-CGA-O2A-C1
25	B	1224	CLA	CBA-CGA-O2A-C1
25	5	606	CLA	CBA-CGA-O2A-C1
37	K	5002	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
25	A	1125	CLA	C3-C5-C6-C7
25	A	1115	CLA	C11-C10-C8-C9
25	3	607	CLA	C14-C13-C15-C16
30	2	801	LHG	C31-C32-C33-C34
30	2	801	LHG	C33-C34-C35-C36
30	2	802	LHG	C30-C31-C32-C33
36	B	5003	DGD	C2B-C3B-C4B-C5B
48	8	804	DGA	CB6-CB7-CB8-CB9
30	A	5003	LHG	C13-C14-C15-C16
30	A	5003	LHG	C16-C17-C18-C19
30	2	802	LHG	C27-C28-C29-C30
32	H	5001	SQD	O5-C1-O6-C44
30	2	802	LHG	C11-C12-C13-C14
33	B	5005	PTY	C13-C14-C15-C16
33	3	802	PTY	C16-C17-C18-C19
48	8	804	DGA	CA2-CA3-CA4-CA5
25	A	1126	CLA	C15-C16-C17-C18
25	B	1231	CLA	C13-C15-C16-C17
25	B	1235	CLA	C5-C6-C7-C8
25	2	607	CLA	C10-C11-C12-C13
30	1	802	LHG	C28-C29-C30-C31
30	3	801	LHG	C17-C18-C19-C20
30	2	802	LHG	C12-C13-C14-C15
47	8	807	PLM	CB-CC-CD-CE
52	8	805	P5S	C42-C43-C44-C45
35	1	804	LMT	C1-C2-C3-C4
30	B	5002	LHG	C13-C14-C15-C16
30	F	5001	LHG	C28-C29-C30-C31
30	6	801	LHG	C28-C29-C30-C31
51	7	807	4RF	C12-C13-C14-C15
25	A	1108	CLA	C8-C10-C11-C12
29	A	4003	BCR	C15-C16-C17-C18
29	6	503	BCR	C15-C16-C17-C18
29	6	504	BCR	C9-C10-C11-C12
43	a	503	LUT	C29-C30-C31-C32
43	6	502	LUT	C29-C30-C31-C32
50	9	507	XAT	C29-C30-C31-C32
25	A	1109	CLA	C16-C17-C18-C20
25	7	601	CLA	C11-C12-C13-C15
25	2	605	CLA	C11-C12-C13-C14
30	9	801	LHG	C8-C7-O7-C5
32	7	805	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
33	B	5005	PTY	C11-C8-O7-C6
33	a	802	PTY	C11-C8-O7-C6
48	2	803	DGA	CB2-CB1-OG2-CG2
51	7	807	4RF	C24-C22-O21-C20
30	F	5002	LHG	C7-C8-C9-C10
32	H	5001	SQD	C7-C8-C9-C10
51	7	807	4RF	C13-C14-C15-C16
30	1	802	LHG	C16-C17-C18-C19
30	9	801	LHG	C11-C10-C9-C8
30	9	802	LHG	O9-C7-O7-C5
30	9	801	LHG	O9-C7-O7-C5
33	B	5005	PTY	O10-C8-O7-C6
52	8	805	P5S	O47-C38-O37-C2
33	5	802	PTY	C32-C33-C34-C35
37	B	5004	PCW	C40-C41-C42-C43
45	8	809	OLA	C6-C7-C8-C9
25	A	1110	CLA	C5-C6-C7-C8
30	3	801	LHG	C11-C12-C13-C14
41	J	5002	SPH	C10-C11-C12-C13
25	B	1209	CLA	CBD-CGD-O2D-CED
25	A	1127	CLA	C13-C15-C16-C17
25	B	1216	CLA	C15-C16-C17-C18
29	A	4003	BCR	C37-C22-C23-C24
29	A	4004	BCR	C36-C18-C19-C20
43	5	505	LUT	C27-C28-C29-C39
50	9	504	XAT	C11-C12-C13-C20
30	7	801	LHG	C11-C12-C13-C14
48	3	803	DGA	CB1-CB2-CB3-CB4
48	2	803	DGA	CA9-CAA-CBA-CCA
52	8	805	P5S	C40-C41-C42-C43
29	A	4002	BCR	C17-C18-C19-C20
29	A	4003	BCR	C21-C22-C23-C24
29	B	4005	BCR	C7-C8-C9-C10
29	K	4002	BCR	C17-C18-C19-C20
29	5	504	BCR	C17-C18-C19-C20
43	a	503	LUT	C31-C32-C33-C34
36	8	802	DGD	C5D-C6D-O5D-C1E
36	8	803	DGD	C5D-C6D-O5D-C1E
47	4	804	PLM	C4-C5-C6-C7
25	7	603	CLA	C13-C15-C16-C17
25	A	1129	CLA	C2A-CAA-CBA-CGA
25	A	1130	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	1023	CLA	C2A-CAA-CBA-CGA
25	B	1217	CLA	C2A-CAA-CBA-CGA
24	A	1011	CL0	C16-C17-C18-C20
25	A	1117	CLA	C16-C17-C18-C19
25	A	1137	CLA	C11-C12-C13-C14
25	A	1137	CLA	C11-C12-C13-C15
25	B	1221	CLA	C16-C17-C18-C20
25	B	1238	CLA	C16-C17-C18-C20
25	1	605	CLA	C16-C17-C18-C20
25	6	607	CLA	C6-C7-C8-C9
25	7	601	CLA	C11-C12-C13-C14
26	3	611	CHL	C11-C12-C13-C15
27	A	2001	PQN	C26-C27-C28-C29
30	1	802	LHG	C12-C13-C14-C15
30	5	801	LHG	C24-C25-C26-C27
35	1	804	LMT	C5-C6-C7-C8
25	B	1201	CLA	C4-C3-C5-C6
25	B	1216	CLA	C4-C3-C5-C6
25	B	1225	CLA	C4-C3-C5-C6
25	B	1229	CLA	C4-C3-C5-C6
30	B	5001	LHG	C28-C29-C30-C31
33	a	803	PTY	C15-C16-C17-C18
25	A	1126	CLA	C5-C6-C7-C8
25	A	1130	CLA	C5-C6-C7-C8
25	B	1205	CLA	C13-C15-C16-C17
51	7	807	4RF	C43-C44-C45-C46
33	a	803	PTY	C11-C12-C13-C14
33	9	803	PTY	C11-C12-C13-C14
25	1	603	CLA	O1A-CGA-O2A-C1
25	B	1206	CLA	C3-C5-C6-C7
25	L	1502	CLA	C3-C5-C6-C7
25	A	1108	CLA	C10-C11-C12-C13
25	A	1133	CLA	C8-C10-C11-C12
30	B	5002	LHG	C11-C12-C13-C14
37	6	803	PCW	C32-C33-C34-C35
33	a	802	PTY	O10-C8-O7-C6
37	B	5004	PCW	O3P-C1-C2-O2
30	2	801	LHG	C9-C10-C11-C12
30	9	802	LHG	C13-C14-C15-C16
32	G	5001	SQD	C29-C30-C31-C32
30	5	801	LHG	C8-C7-O7-C5
25	A	1013	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	a	607	CLA	C5-C6-C7-C8
25	4	601	CLA	C5-C6-C7-C8
25	A	1111	CLA	C16-C17-C18-C19
25	A	1122	CLA	C11-C12-C13-C15
30	4	802	LHG	C13-C14-C15-C16
35	1	804	LMT	C6-C7-C8-C9
25	1	605	CLA	O1A-CGA-O2A-C1
25	B	1217	CLA	O1D-CGD-O2D-CED
30	A	5001	LHG	C28-C29-C30-C31
30	F	5002	LHG	C28-C29-C30-C31
30	6	801	LHG	C13-C14-C15-C16
34	A	5007	3PH	C27-C28-C29-C2A
30	2	801	LHG	C7-C8-C9-C10
25	A	1104	CLA	C8-C10-C11-C12
25	A	1117	CLA	C13-C15-C16-C17
25	A	1131	CLA	C15-C16-C17-C18
25	A	1136	CLA	C8-C10-C11-C12
25	B	1203	CLA	C13-C15-C16-C17
33	B	5005	PTY	C23-C24-C25-C26
25	B	1236	CLA	C3-C5-C6-C7
25	4	601	CLA	C3-C5-C6-C7
25	7	603	CLA	C3-C5-C6-C7
33	5	802	PTY	O4-C1-C6-O7
45	1	803	OLA	C6-C7-C8-C9
30	1	801	LHG	C11-C10-C9-C8
48	5	803	DGA	CA4-CA5-CA6-CA7
48	8	804	DGA	CB3-CB4-CB5-CB6
30	2	802	LHG	C9-C10-C11-C12
30	9	802	LHG	C16-C17-C18-C19
47	4	804	PLM	C9-CA-CB-CC
25	A	1133	CLA	C5-C6-C7-C8
25	2	601	CLA	C5-C6-C7-C8
30	B	5002	LHG	C26-C27-C28-C29
30	4	802	LHG	C11-C10-C9-C8
30	5	801	LHG	C29-C30-C31-C32
32	A	5005	SQD	C28-C29-C30-C31
51	7	807	4RF	C29-C30-C31-C32
30	9	802	LHG	C28-C29-C30-C31
41	6	806	SPH	C10-C11-C12-C13
48	8	804	DGA	CB5-CB6-CB7-CB8
48	2	803	DGA	CB5-CB6-CB7-CB8
25	6	607	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	8	612	CLA	C2-C1-O2A-CGA
25	2	602	CLA	C2-C1-O2A-CGA
25	a	607	CLA	O1D-CGD-O2D-CED
25	B	1207	CLA	C11-C12-C13-C15
25	a	605	CLA	C6-C7-C8-C9
25	B	1209	CLA	C10-C11-C12-C13
25	4	611	CLA	C5-C6-C7-C8
30	6	801	LHG	C11-C12-C13-C14
30	2	802	LHG	C31-C32-C33-C34
33	a	802	PTY	C11-C12-C13-C14
48	2	803	DGA	CB2-CB3-CB4-CB5
30	9	802	LHG	C33-C34-C35-C36
33	a	803	PTY	C14-C15-C16-C17
25	5	612	CLA	C4-C3-C5-C6
26	3	611	CHL	C4-C3-C5-C6
25	A	1119	CLA	C3-C5-C6-C7
25	B	1225	CLA	C2-C3-C5-C6
25	B	1229	CLA	C2-C3-C5-C6
26	3	611	CHL	C2-C3-C5-C6
48	2	803	DGA	OB1-CB1-OG2-CG2
30	B	5001	LHG	C33-C34-C35-C36
30	7	801	LHG	C28-C29-C30-C31
30	9	802	LHG	C24-C25-C26-C27
33	a	803	PTY	C31-C32-C33-C34
33	3	802	PTY	C12-C13-C14-C15
25	B	1235	CLA	C2A-CAA-CBA-CGA
25	1	612	CLA	C2A-CAA-CBA-CGA
25	a	612	CLA	C2A-CAA-CBA-CGA
25	4	604	CLA	C2A-CAA-CBA-CGA
25	5	604	CLA	C2A-CAA-CBA-CGA
25	7	603	CLA	C2A-CAA-CBA-CGA
25	8	612	CLA	C2A-CAA-CBA-CGA
26	1	604	CHL	C2A-CAA-CBA-CGA
26	3	603	CHL	C2A-CAA-CBA-CGA
26	8	604	CHL	C2A-CAA-CBA-CGA
34	A	5007	3PH	C24-C25-C26-C27
37	6	803	PCW	C33-C34-C35-C36
45	a	805	OLA	C11-C12-C13-C14
25	B	1223	CLA	C8-C10-C11-C12
25	1	607	CLA	C13-C15-C16-C17
25	6	615	CLA	C10-C11-C12-C13
30	8	801	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
41	9	804	SPH	C7-C8-C9-C10
48	8	804	DGA	CA8-CA9-CAA-CBA
33	a	803	PTY	C36-C37-C38-C39
41	J	5002	SPH	C7-C8-C9-C10
30	A	5002	LHG	O1-C1-C2-O2
30	1	802	LHG	O1-C1-C2-O2
30	3	801	LHG	O1-C1-C2-O2
30	6	802	LHG	O1-C1-C2-O2
30	2	802	LHG	O1-C1-C2-O2
30	9	801	LHG	O1-C1-C2-O2
25	5	606	CLA	O1A-CGA-O2A-C1
37	K	5002	PCW	O11-C11-O3-C3
25	6	607	CLA	C3-C5-C6-C7
33	a	802	PTY	C36-C37-C38-C39
25	A	1103	CLA	C1A-C2A-CAA-CBA
25	A	1104	CLA	C1A-C2A-CAA-CBA
25	A	1106	CLA	C1A-C2A-CAA-CBA
25	A	1107	CLA	C1A-C2A-CAA-CBA
25	A	1108	CLA	C1A-C2A-CAA-CBA
25	A	1113	CLA	C1A-C2A-CAA-CBA
25	A	1118	CLA	C1A-C2A-CAA-CBA
25	A	1121	CLA	C1A-C2A-CAA-CBA
25	A	1122	CLA	C1A-C2A-CAA-CBA
25	A	1124	CLA	C1A-C2A-CAA-CBA
25	A	1132	CLA	C1A-C2A-CAA-CBA
25	A	1134	CLA	C1A-C2A-CAA-CBA
25	A	1135	CLA	C1A-C2A-CAA-CBA
25	B	1021	CLA	C1A-C2A-CAA-CBA
25	B	1202	CLA	C1A-C2A-CAA-CBA
25	B	1214	CLA	C1A-C2A-CAA-CBA
25	B	1216	CLA	C1A-C2A-CAA-CBA
25	B	1217	CLA	C1A-C2A-CAA-CBA
25	B	1227	CLA	C1A-C2A-CAA-CBA
25	B	1229	CLA	C1A-C2A-CAA-CBA
25	B	1230	CLA	C1A-C2A-CAA-CBA
25	B	1235	CLA	C1A-C2A-CAA-CBA
25	B	1239	CLA	C1A-C2A-CAA-CBA
25	B	1240	CLA	C1A-C2A-CAA-CBA
25	B	1207	CLA	C1A-C2A-CAA-CBA
25	F	1301	CLA	C1A-C2A-CAA-CBA
25	F	1302	CLA	C1A-C2A-CAA-CBA
25	H	1701	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	K	1402	CLA	C1A-C2A-CAA-CBA
25	L	1502	CLA	C1A-C2A-CAA-CBA
25	L	1503	CLA	C1A-C2A-CAA-CBA
25	L	1504	CLA	C1A-C2A-CAA-CBA
25	1	601	CLA	C1A-C2A-CAA-CBA
25	1	602	CLA	C1A-C2A-CAA-CBA
25	1	607	CLA	C1A-C2A-CAA-CBA
25	1	608	CLA	C1A-C2A-CAA-CBA
25	1	612	CLA	C1A-C2A-CAA-CBA
25	a	601	CLA	C1A-C2A-CAA-CBA
25	a	602	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C1A-C2A-CAA-CBA
25	a	612	CLA	C1A-C2A-CAA-CBA
25	3	601	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	601	CLA	C1A-C2A-CAA-CBA
25	4	606	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	C1A-C2A-CAA-CBA
25	4	611	CLA	C1A-C2A-CAA-CBA
25	4	616	CLA	C1A-C2A-CAA-CBA
25	4	617	CLA	C1A-C2A-CAA-CBA
25	5	601	CLA	C1A-C2A-CAA-CBA
25	5	607	CLA	C1A-C2A-CAA-CBA
25	6	601	CLA	C1A-C2A-CAA-CBA
25	7	606	CLA	C1A-C2A-CAA-CBA
25	7	608	CLA	C1A-C2A-CAA-CBA
25	7	610	CLA	C1A-C2A-CAA-CBA
25	7	612	CLA	C1A-C2A-CAA-CBA
25	8	605	CLA	C1A-C2A-CAA-CBA
25	8	612	CLA	C1A-C2A-CAA-CBA
25	8	615	CLA	C1A-C2A-CAA-CBA
25	8	620	CLA	C1A-C2A-CAA-CBA
25	2	601	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA
25	B	1021	CLA	C15-C16-C17-C18
25	B	1210	CLA	C10-C11-C12-C13
25	4	610	CLA	C13-C15-C16-C17
30	B	5001	LHG	C26-C27-C28-C29
37	K	5002	PCW	C32-C33-C34-C35
34	A	5007	3PH	C34-C35-C36-C37
45	8	808	OLA	C11-C12-C13-C14
30	1	802	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	6	802	LHG	O6-C4-C5-C6
30	7	802	LHG	O6-C4-C5-C6
30	8	801	LHG	O6-C4-C5-C6
37	K	5001	PCW	O3P-C1-C2-C3
30	7	801	LHG	C10-C11-C12-C13
25	A	1013	CLA	C11-C12-C13-C15
25	A	1104	CLA	C11-C10-C8-C7
25	A	1104	CLA	C12-C13-C15-C16
25	A	1106	CLA	C11-C12-C13-C15
25	A	1109	CLA	C11-C12-C13-C15
25	A	1119	CLA	C6-C7-C8-C10
25	A	1121	CLA	C6-C7-C8-C10
25	A	1122	CLA	C6-C7-C8-C10
25	A	1123	CLA	C11-C10-C8-C7
25	A	1126	CLA	C12-C13-C15-C16
25	A	1128	CLA	C11-C10-C8-C7
25	A	1131	CLA	C6-C7-C8-C10
25	A	1101	CLA	C6-C7-C8-C10
25	B	1022	CLA	C11-C10-C8-C7
25	B	1023	CLA	C11-C10-C8-C7
25	B	1204	CLA	C12-C13-C15-C16
25	B	1210	CLA	C11-C10-C8-C7
25	B	1212	CLA	C6-C7-C8-C10
25	B	1221	CLA	C6-C7-C8-C10
25	B	1235	CLA	C12-C13-C15-C16
25	K	1402	CLA	C6-C7-C8-C10
25	3	601	CLA	C11-C12-C13-C15
25	3	605	CLA	C6-C7-C8-C10
25	3	605	CLA	C12-C13-C15-C16
25	3	613	CLA	C6-C7-C8-C10
25	7	601	CLA	C11-C10-C8-C7
25	7	603	CLA	C11-C10-C8-C7
25	7	604	CLA	C11-C10-C8-C7
25	8	606	CLA	C6-C7-C8-C10
25	8	606	CLA	C11-C10-C8-C7
26	3	604	CHL	C11-C12-C13-C15
26	4	609	CHL	C11-C12-C13-C15
26	5	610	CHL	C12-C13-C15-C16
26	2	609	CHL	C12-C13-C15-C16
27	A	2001	PQN	C21-C22-C23-C25
27	B	2002	PQN	C17-C18-C20-C21
30	3	801	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	2	801	LHG	C16-C17-C18-C19
37	B	5004	PCW	C32-C33-C34-C35
53	8	810	LAP	C7-C8-C9-C10
25	A	1125	CLA	C16-C17-C18-C20
25	9	605	CLA	C11-C12-C13-C15
25	A	1104	CLA	C13-C15-C16-C17
35	2	804	LMT	O5B-C5B-C6B-O6B
30	9	802	LHG	C29-C30-C31-C32
36	8	803	DGD	O6D-C5D-C6D-O5D
25	B	1231	CLA	C8-C10-C11-C12
30	4	802	LHG	C7-C8-C9-C10
30	6	802	LHG	C7-C8-C9-C10
36	7	806	DGD	C1B-C2B-C3B-C4B
25	A	1109	CLA	C4-C3-C5-C6
25	A	1109	CLA	C2-C3-C5-C6
25	2	605	CLA	C2-C3-C5-C6
25	A	1119	CLA	O1A-CGA-O2A-C1
30	7	802	LHG	C29-C30-C31-C32
30	a	801	LHG	C29-C30-C31-C32
37	B	5004	PCW	C33-C34-C35-C36
47	a	804	PLM	CC-CD-CE-CF
25	A	1106	CLA	C5-C6-C7-C8
25	A	1136	CLA	C13-C15-C16-C17
25	4	601	CLA	C10-C11-C12-C13
30	B	5001	LHG	C8-C7-O7-C5
25	A	1116	CLA	C2A-CAA-CBA-CGA
25	A	1122	CLA	C2A-CAA-CBA-CGA
25	a	611	CLA	C2A-CAA-CBA-CGA
26	a	604	CHL	C2A-CAA-CBA-CGA
25	A	1104	CLA	C14-C13-C15-C16
25	A	1109	CLA	C11-C12-C13-C14
25	A	1111	CLA	C6-C7-C8-C9
25	A	1119	CLA	C6-C7-C8-C9
25	A	1125	CLA	C11-C10-C8-C9
25	A	1126	CLA	C11-C10-C8-C9
25	A	1131	CLA	C6-C7-C8-C9
25	A	1133	CLA	C11-C10-C8-C9
25	A	1101	CLA	C6-C7-C8-C9
25	B	1237	CLA	C6-C7-C8-C9
25	B	1023	CLA	C11-C10-C8-C9
25	B	1212	CLA	C6-C7-C8-C9
25	B	1215	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	1223	CLA	C11-C10-C8-C9
25	B	1230	CLA	C6-C7-C8-C9
25	B	1231	CLA	C11-C10-C8-C9
25	1	603	CLA	C11-C12-C13-C14
25	1	607	CLA	C11-C12-C13-C14
25	1	612	CLA	C11-C10-C8-C9
25	3	601	CLA	C11-C12-C13-C14
25	3	605	CLA	C14-C13-C15-C16
25	5	604	CLA	C14-C13-C15-C16
25	6	604	CLA	C11-C10-C8-C9
25	7	603	CLA	C11-C10-C8-C9
25	7	603	CLA	C11-C12-C13-C14
25	7	604	CLA	C11-C10-C8-C9
25	8	606	CLA	C6-C7-C8-C9
26	1	609	CHL	C14-C13-C15-C16
26	4	609	CHL	C11-C12-C13-C14
26	6	609	CHL	C11-C12-C13-C14
26	8	604	CHL	C11-C10-C8-C9
30	1	802	LHG	C13-C14-C15-C16
30	4	801	LHG	C11-C12-C13-C14
36	B	5003	DGD	O6E-C5E-C6E-O5E
33	B	5005	PTY	C30-C31-C32-C33
43	3	502	LUT	C29-C30-C31-C32
30	a	801	LHG	C24-C25-C26-C27
30	7	801	LHG	C29-C30-C31-C32
25	B	1227	CLA	CBA-CGA-O2A-C1
25	7	601	CLA	CBA-CGA-O2A-C1
34	A	5007	3PH	C32-C31-O31-C3
36	B	5003	DGD	C2A-C1A-O1G-C1G
25	6	608	CLA	C5-C6-C7-C8
30	2	802	LHG	C35-C36-C37-C38
25	3	610	CLA	O1D-CGD-O2D-CED
32	A	5005	SQD	C29-C30-C31-C32
48	2	803	DGA	CA7-CA8-CA9-CAA
32	7	805	SQD	O49-C7-O47-C45
35	1	804	LMT	C2'-C1'-O1'-C1
36	7	806	DGD	C2E-C1E-O5D-C6D
30	B	5001	LHG	C4-C5-C6-O8
30	F	5001	LHG	C4-C5-C6-O8
30	6	801	LHG	C4-C5-C6-O8
30	8	801	LHG	C4-C5-C6-O8
30	2	801	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
32	G	5001	SQD	O6-C44-C45-C46
33	9	803	PTY	O4-C1-C6-C5
36	B	5003	DGD	O1G-C1G-C2G-C3G
37	K	5002	PCW	C1-C2-C3-O3
48	5	803	DGA	OG1-CG1-CG2-CG3
48	8	804	DGA	CA4-CA5-CA6-CA7
25	B	1224	CLA	O1A-CGA-O2A-C1
25	6	606	CLA	C3-C5-C6-C7
45	a	805	OLA	C10-C11-C12-C13
45	8	808	OLA	C10-C11-C12-C13
30	7	801	LHG	C9-C10-C11-C12
25	A	1127	CLA	C8-C10-C11-C12
25	A	1132	CLA	C13-C15-C16-C17
25	A	1101	CLA	C8-C10-C11-C12
25	B	1022	CLA	C10-C11-C12-C13
25	a	603	CLA	C8-C10-C11-C12
30	F	5001	LHG	C25-C26-C27-C28
25	B	1235	CLA	CBA-CGA-O2A-C1
36	7	806	DGD	O6E-C5E-C6E-O5E
25	A	1109	CLA	C16-C17-C18-C19
25	a	605	CLA	C6-C7-C8-C10
25	3	601	CLA	C16-C17-C18-C20
25	8	618	CLA	C11-C12-C13-C15
30	7	802	LHG	C27-C28-C29-C30
36	8	803	DGD	C2G-C1G-O1G-C1A
30	A	5002	LHG	C25-C26-C27-C28
30	7	801	LHG	C25-C26-C27-C28
32	I	5001	SQD	C14-C15-C16-C17
25	4	605	CLA	O1A-CGA-O2A-C1
48	8	804	DGA	CB7-CB8-CB9-CAB
26	4	613	CHL	CHA-CBD-CGD-O1D
26	4	613	CHL	CHA-CBD-CGD-O2D
26	5	613	CHL	CHA-CBD-CGD-O2D
26	9	613	CHL	CHA-CBD-CGD-O1D
26	9	613	CHL	CHA-CBD-CGD-O2D
25	B	1228	CLA	C5-C6-C7-C8
25	1	605	CLA	C10-C11-C12-C13
25	6	604	CLA	C8-C10-C11-C12
25	7	603	CLA	C10-C11-C12-C13
32	I	5001	SQD	C28-C29-C30-C31
33	3	802	PTY	C33-C34-C35-C36
36	B	5003	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
25	A	1119	CLA	C2-C3-C5-C6
25	B	1204	CLA	C2-C3-C5-C6
25	4	603	CLA	C2-C3-C5-C6
25	5	612	CLA	C2-C3-C5-C6
25	3	618	CLA	O1A-CGA-O2A-C1
30	A	5002	LHG	C11-C12-C13-C14
25	1	607	CLA	C10-C11-C12-C13
29	L	4002	BCR	C37-C22-C23-C24
42	M	4001	ECH	C37-C22-C23-C24
43	5	505	LUT	C7-C8-C9-C19
32	A	5005	SQD	C13-C14-C15-C16
25	B	1207	CLA	C11-C12-C13-C14
30	3	801	LHG	C10-C11-C12-C13
30	5	801	LHG	C11-C12-C13-C14
47	4	803	PLM	C4-C5-C6-C7
29	B	4004	BCR	C7-C8-C9-C10
29	L	4002	BCR	C21-C22-C23-C24
25	A	1115	CLA	C8-C10-C11-C12
25	8	618	CLA	C10-C11-C12-C13
30	B	5001	LHG	C9-C10-C11-C12
25	4	602	CLA	C3-C5-C6-C7
25	5	607	CLA	C2A-CAA-CBA-CGA
30	5	801	LHG	C23-C24-C25-C26
48	3	803	DGA	CB3-CB4-CB5-CB6
24	A	1011	CL0	CBA-CGA-O2A-C1
33	3	802	PTY	C5-C6-O7-C8
33	5	802	PTY	C5-C6-O7-C8
30	B	5002	LHG	C31-C32-C33-C34
30	6	801	LHG	C9-C10-C11-C12
30	3	801	LHG	C32-C33-C34-C35
29	A	4003	BCR	C13-C14-C15-C16
29	L	4003	BCR	C9-C10-C11-C12
29	O	4001	BCR	C19-C20-C21-C22
43	3	501	LUT	C29-C30-C31-C32
50	9	507	XAT	C33-C34-C35-C15
25	9	605	CLA	C11-C12-C13-C14
30	A	5002	LHG	C26-C27-C28-C29
35	A	5008	LMT	C4-C5-C6-C7
29	5	504	BCR	C11-C10-C9-C8
30	3	801	LHG	C25-C26-C27-C28
30	1	801	LHG	O6-C4-C5-O7
33	J	5001	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
25	2	621	CLA	C5-C6-C7-C8
30	A	5001	LHG	C25-C26-C27-C28
30	A	5003	LHG	C30-C31-C32-C33
32	7	805	SQD	C11-C12-C13-C14
25	B	1203	CLA	CBA-CGA-O2A-C1
25	H	1701	CLA	CBA-CGA-O2A-C1
25	2	602	CLA	CBA-CGA-O2A-C1
33	5	802	PTY	C37-C38-C39-C40
33	9	803	PTY	C38-C39-C40-C41
48	8	804	DGA	CA6-CA7-CA8-CA9
48	8	804	DGA	CCB-CDB-CEB-CFB
30	3	801	LHG	C35-C36-C37-C38
25	A	1119	CLA	C4-C3-C5-C6
25	2	602	CLA	C4-C3-C5-C6
26	8	603	CHL	C4-C3-C5-C6
25	B	1234	CLA	C2-C3-C5-C6
25	7	603	CLA	C2-C3-C5-C6
30	7	803	LHG	C11-C12-C13-C14
30	4	801	LHG	C13-C14-C15-C16
32	G	5001	SQD	C12-C13-C14-C15
32	I	5001	SQD	C11-C10-C9-C8
25	1	601	CLA	C11-C12-C13-C15
37	6	803	PCW	C14-C15-C16-C17
52	8	805	P5S	C39-C40-C41-C42
36	B	5003	DGD	O1A-C1A-O1G-C1G
30	3	801	LHG	C27-C28-C29-C30
30	4	801	LHG	C25-C26-C27-C28
33	A	5006	PTY	C31-C32-C33-C34
30	1	801	LHG	O7-C5-C6-O8
30	8	801	LHG	O7-C5-C6-O8
32	7	805	SQD	O47-C45-C46-O48
48	5	803	DGA	CB3-CB4-CB5-CB6
48	2	803	DGA	CBB-CAB-CB9-CB8
30	B	5001	LHG	C35-C36-C37-C38
30	2	802	LHG	C19-C20-C21-C22
48	2	803	DGA	CBB-CCB-CDB-CEB
25	B	1227	CLA	CAA-CBA-CGA-O2A
26	6	610	CHL	CAA-CBA-CGA-O2A
30	1	802	LHG	O8-C23-C24-C25
52	8	805	P5S	C45-C46-C48-C49
25	A	1013	CLA	C2A-CAA-CBA-CGA
25	A	1141	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	5	602	CLA	C2A-CAA-CBA-CGA
26	1	609	CHL	C2A-CAA-CBA-CGA
25	A	1127	CLA	C3-C5-C6-C7
30	F	5001	LHG	C11-C10-C9-C8
30	6	802	LHG	C9-C10-C11-C12
30	2	802	LHG	C11-C10-C9-C8
33	B	5005	PTY	C26-C27-C28-C29
48	3	803	DGA	CA6-CA7-CA8-CA9
25	a	612	CLA	C2-C1-O2A-CGA
30	9	801	LHG	C11-C12-C13-C14
25	B	1227	CLA	O1A-CGA-O2A-C1
30	B	5002	LHG	C35-C36-C37-C38
37	B	5004	PCW	C42-C43-C44-C45
25	B	1237	CLA	C10-C11-C12-C13
25	5	612	CLA	C13-C15-C16-C17
25	4	610	CLA	CBA-CGA-O2A-C1
25	8	611	CLA	CBA-CGA-O2A-C1
30	A	5002	LHG	C16-C17-C18-C19
30	3	801	LHG	C28-C29-C30-C31
48	5	803	DGA	CA6-CA7-CA8-CA9
48	2	803	DGA	CA6-CA7-CA8-CA9
25	B	1224	CLA	C13-C15-C16-C17
30	7	802	LHG	C11-C12-C13-C14
33	a	802	PTY	C31-C32-C33-C34
51	7	807	4RF	C26-C27-C28-C29
25	B	1224	CLA	C10-C11-C12-C13
29	5	504	BCR	C13-C14-C15-C16
25	A	1125	CLA	C16-C17-C18-C19
25	7	604	CLA	C16-C17-C18-C20
25	A	1125	CLA	C4-C3-C5-C6
25	B	1204	CLA	C4-C3-C5-C6
25	B	1214	CLA	C4-C3-C5-C6
25	4	603	CLA	C4-C3-C5-C6
25	7	603	CLA	C4-C3-C5-C6
25	7	610	CLA	C4-C3-C5-C6
30	2	801	LHG	C35-C36-C37-C38
30	2	801	LHG	C34-C35-C36-C37
48	2	803	DGA	CA8-CA9-CAA-CBA
25	B	1023	CLA	C13-C15-C16-C17
25	2	607	CLA	C13-C15-C16-C17
30	8	801	LHG	C27-C28-C29-C30
26	1	611	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	B	5002	LHG	C29-C30-C31-C32
33	B	5005	PTY	C25-C26-C27-C28
45	8	808	OLA	C13-C14-C15-C16
51	7	807	4RF	O23-C22-O21-C20
35	A	5008	LMT	C2-C1-O1'-C1'
35	1	804	LMT	C2-C1-O1'-C1'
25	A	1104	CLA	C11-C10-C8-C9
25	A	1106	CLA	C11-C10-C8-C9
25	A	1106	CLA	C11-C12-C13-C14
25	A	1117	CLA	C11-C12-C13-C14
25	A	1122	CLA	C6-C7-C8-C9
25	A	1123	CLA	C11-C10-C8-C9
25	A	1126	CLA	C14-C13-C15-C16
25	A	1128	CLA	C11-C10-C8-C9
25	A	1132	CLA	C6-C7-C8-C9
25	A	1137	CLA	C6-C7-C8-C9
25	B	1021	CLA	C11-C10-C8-C9
25	B	1021	CLA	C14-C13-C15-C16
25	B	1022	CLA	C11-C10-C8-C9
25	B	1204	CLA	C6-C7-C8-C9
25	B	1204	CLA	C14-C13-C15-C16
25	B	1210	CLA	C11-C10-C8-C9
25	B	1216	CLA	C11-C12-C13-C14
25	B	1221	CLA	C6-C7-C8-C9
25	B	1223	CLA	C11-C12-C13-C14
25	B	1224	CLA	C11-C10-C8-C9
25	B	1234	CLA	C11-C10-C8-C9
25	B	1235	CLA	C14-C13-C15-C16
25	B	1240	CLA	C14-C13-C15-C16
25	K	1402	CLA	C6-C7-C8-C9
25	L	1502	CLA	C6-C7-C8-C9
25	1	607	CLA	C14-C13-C15-C16
25	3	605	CLA	C11-C12-C13-C14
25	4	610	CLA	C11-C12-C13-C14
25	5	603	CLA	C6-C7-C8-C9
26	1	604	CHL	C14-C13-C15-C16
26	3	604	CHL	C11-C12-C13-C14
26	3	611	CHL	C6-C7-C8-C9
26	5	610	CHL	C11-C10-C8-C9
26	6	619	CHL	C11-C10-C8-C9
26	8	604	CHL	C11-C12-C13-C14
27	A	2001	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
32	G	5001	SQD	C27-C28-C29-C30
25	A	1106	CLA	C8-C10-C11-C12
25	A	1117	CLA	C8-C10-C11-C12
25	B	1222	CLA	C8-C10-C11-C12
25	1	608	CLA	C8-C10-C11-C12
25	3	601	CLA	C15-C16-C17-C18
26	1	609	CHL	C5-C6-C7-C8
30	a	801	LHG	C2-C3-O3-P
24	A	1011	CL0	O1A-CGA-O2A-C1
25	A	1012	CLA	C4B-C3B-CAB-CBB
25	A	1126	CLA	C4B-C3B-CAB-CBB
25	A	1131	CLA	C4B-C3B-CAB-CBB
25	A	1132	CLA	C4B-C3B-CAB-CBB
25	B	1022	CLA	C4B-C3B-CAB-CBB
25	B	1205	CLA	C4B-C3B-CAB-CBB
25	2	608	CLA	C4B-C3B-CAB-CBB
25	2	615	CLA	C4B-C3B-CAB-CBB
25	9	612	CLA	C4B-C3B-CAB-CBB
48	3	803	DGA	OG1-CA1-CA2-CA3
25	A	1112	CLA	C6-C7-C8-C9
37	6	803	PCW	C12-C11-O3-C3
25	B	1224	CLA	C2A-CAA-CBA-CGA
25	6	604	CLA	C2A-CAA-CBA-CGA
30	A	5002	LHG	C13-C14-C15-C16
30	A	5003	LHG	C26-C27-C28-C29
32	7	805	SQD	C13-C14-C15-C16
36	B	5003	DGD	C4B-C5B-C6B-C7B
25	A	1101	CLA	C3-C5-C6-C7
47	a	804	PLM	CD-CE-CF-CG
30	A	5001	LHG	O6-C4-C5-C6
30	F	5001	LHG	O6-C4-C5-C6
30	1	801	LHG	O6-C4-C5-C6
30	4	801	LHG	O6-C4-C5-C6
33	J	5001	PTY	O14-C5-C6-C1
33	5	802	PTY	O14-C5-C6-C1
34	A	5007	3PH	O11-C1-C2-C3
37	B	5004	PCW	O3P-C1-C2-C3
30	6	802	LHG	C11-C12-C13-C14
30	1	801	LHG	C31-C32-C33-C34
30	4	801	LHG	C35-C36-C37-C38
25	A	1106	CLA	C11-C10-C8-C7
25	A	1111	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	A	1125	CLA	C11-C10-C8-C7
25	A	1126	CLA	C11-C10-C8-C7
25	A	1128	CLA	C6-C7-C8-C10
25	A	1134	CLA	C6-C7-C8-C10
25	A	1137	CLA	C6-C7-C8-C10
25	B	1237	CLA	C6-C7-C8-C10
25	B	1021	CLA	C11-C10-C8-C7
25	B	1203	CLA	C6-C7-C8-C10
25	B	1204	CLA	C6-C7-C8-C10
25	B	1206	CLA	C6-C7-C8-C10
25	B	1215	CLA	C11-C10-C8-C7
25	B	1216	CLA	C11-C12-C13-C15
25	B	1223	CLA	C11-C10-C8-C7
25	B	1223	CLA	C11-C12-C13-C15
25	B	1230	CLA	C6-C7-C8-C10
25	B	1231	CLA	C11-C10-C8-C7
25	B	1234	CLA	C11-C10-C8-C7
25	B	1235	CLA	C11-C10-C8-C7
25	B	1240	CLA	C12-C13-C15-C16
25	L	1502	CLA	C11-C10-C8-C7
25	1	607	CLA	C11-C12-C13-C15
25	a	603	CLA	C6-C7-C8-C10
25	3	605	CLA	C11-C12-C13-C15
25	3	606	CLA	C11-C10-C8-C7
25	5	603	CLA	C6-C7-C8-C10
25	5	604	CLA	C12-C13-C15-C16
25	6	604	CLA	C11-C10-C8-C7
25	7	601	CLA	C6-C7-C8-C10
25	7	603	CLA	C11-C12-C13-C15
25	2	621	CLA	C6-C7-C8-C10
26	1	604	CHL	C11-C10-C8-C7
26	1	609	CHL	C12-C13-C15-C16
26	3	603	CHL	C12-C13-C15-C16
26	3	604	CHL	C6-C7-C8-C10
26	5	610	CHL	C11-C10-C8-C7
26	6	609	CHL	C11-C12-C13-C15
26	6	609	CHL	C12-C13-C15-C16
26	8	604	CHL	C11-C10-C8-C7
26	2	609	CHL	C11-C12-C13-C15
33	9	803	PTY	C24-C25-C26-C27
36	8	802	DGD	CDA-CEA-CFA-CGA
51	7	807	4RF	C45-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
25	5	614	CLA	CBA-CGA-O2A-C1
30	2	802	LHG	C33-C34-C35-C36
30	3	801	LHG	C29-C30-C31-C32
41	9	804	SPH	C6-C7-C8-C9
47	4	804	PLM	C2-C3-C4-C5
48	8	804	DGA	CA9-CAA-CBA-CCA
25	1	608	CLA	CBA-CGA-O2A-C1
25	B	1201	CLA	C16-C17-C18-C19
25	1	601	CLA	C11-C12-C13-C14
33	B	5005	PTY	C11-C12-C13-C14
25	7	601	CLA	O1A-CGA-O2A-C1
34	A	5007	3PH	O32-C31-O31-C3
25	A	1124	CLA	C3A-C2A-CAA-CBA
25	A	1101	CLA	C4-C3-C5-C6
25	B	1021	CLA	C3A-C2A-CAA-CBA
25	B	1227	CLA	C3A-C2A-CAA-CBA
25	B	1235	CLA	C3A-C2A-CAA-CBA
25	1	603	CLA	C4-C3-C5-C6
25	1	608	CLA	C4-C3-C5-C6
25	2	604	CLA	C3A-C2A-CAA-CBA
25	2	605	CLA	C4-C3-C5-C6
26	7	611	CHL	C3A-C2A-CAA-CBA
25	A	1103	CLA	C2-C3-C5-C6
26	8	603	CHL	C2-C3-C5-C6
47	8	806	PLM	CA-CB-CC-CD
25	4	612	CLA	C13-C15-C16-C17
25	B	1235	CLA	O1A-CGA-O2A-C1
25	8	605	CLA	C5-C6-C7-C8
27	B	2002	PQN	C23-C25-C26-C27
25	4	602	CLA	CBA-CGA-O2A-C1
25	7	608	CLA	CBA-CGA-O2A-C1
29	B	4002	BCR	C9-C10-C11-C12
29	B	4004	BCR	C19-C20-C21-C22
29	B	4005	BCR	C19-C20-C21-C22
29	B	4006	BCR	C15-C16-C17-C18
29	L	4002	BCR	C13-C14-C15-C16
29	L	4001	BCR	C13-C14-C15-C16
29	I	4001	BCR	C19-C20-C21-C22
29	3	503	BCR	C19-C20-C21-C22
29	3	504	BCR	C9-C10-C11-C12
29	5	504	BCR	C19-C20-C21-C22
43	a	501	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
43	a	502	LUT	C29-C30-C31-C32
43	4	502	LUT	C29-C30-C31-C32
43	5	501	LUT	C29-C30-C31-C32
43	5	502	LUT	C29-C30-C31-C32
43	2	507	LUT	C29-C30-C31-C32
43	2	507	LUT	C33-C34-C35-C15
43	9	502	LUT	C29-C30-C31-C32
44	7	504	AXT	C33-C34-C35-C15
25	8	618	CLA	C3-C5-C6-C7
25	A	1121	CLA	C5-C6-C7-C8
29	L	4002	BCR	C36-C18-C19-C20
31	A	5004	LMG	C13-C14-C15-C16
33	G	5002	PTY	C11-C12-C13-C14
25	H	1701	CLA	O1A-CGA-O2A-C1
30	5	801	LHG	C19-C20-C21-C22
42	M	4001	ECH	C21-C22-C23-C24
30	5	801	LHG	C28-C29-C30-C31
52	8	805	P5S	C43-C44-C45-C46
30	5	801	LHG	C35-C36-C37-C38
35	A	5008	LMT	C5-C6-C7-C8
30	B	5002	LHG	C1-C2-C3-O3
25	3	606	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C3-C5-C6-C7
30	F	5001	LHG	C29-C30-C31-C32
25	B	1209	CLA	O1D-CGD-O2D-CED
25	1	601	CLA	CBA-CGA-O2A-C1
30	A	5003	LHG	C15-C16-C17-C18
37	K	5002	PCW	C13-C14-C15-C16
30	7	803	LHG	C4-C5-C6-O8
32	7	805	SQD	C44-C45-C46-O48
33	J	5001	PTY	O4-C1-C6-C5
37	B	5004	PCW	C1-C2-C3-O3
37	6	803	PCW	C1-C2-C3-O3
51	7	807	4RF	O18-C19-C20-C39
52	8	805	P5S	O19-C1-C2-C3
30	a	801	LHG	C9-C10-C11-C12
33	J	5001	PTY	C11-C12-C13-C14
30	A	5002	LHG	C12-C13-C14-C15
25	A	1121	CLA	C11-C12-C13-C15
25	A	1122	CLA	C11-C12-C13-C14
25	3	601	CLA	C16-C17-C18-C19
30	7	802	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	2	801	LHG	C13-C14-C15-C16
41	J	5002	SPH	C11-C10-C9-C8
26	6	619	CHL	C1A-C2A-CAA-CBA
48	8	804	DGA	CG1-CG2-CG3-OXT
33	A	5006	PTY	C11-C12-C13-C14
25	A	1103	CLA	C4-C3-C5-C6
25	A	1112	CLA	C4-C3-C5-C6
25	B	1234	CLA	C4-C3-C5-C6
25	B	1219	CLA	C10-C11-C12-C13
47	8	806	PLM	C6-C7-C8-C9
48	2	803	DGA	CA2-CA3-CA4-CA5
25	5	614	CLA	CAA-CBA-CGA-O2A
25	A	1112	CLA	C2-C3-C5-C6
25	B	1214	CLA	C2-C3-C5-C6
25	1	603	CLA	C2-C3-C5-C6
25	7	610	CLA	C2-C3-C5-C6
25	A	1104	CLA	C3-C5-C6-C7
25	5	612	CLA	C16-C17-C18-C20
25	7	604	CLA	C16-C17-C18-C19
30	B	5001	LHG	O6-C4-C5-O7
30	B	5002	LHG	O6-C4-C5-O7
30	F	5002	LHG	O6-C4-C5-O7
30	F	5001	LHG	O6-C4-C5-O7
30	a	801	LHG	O6-C4-C5-O7
30	4	802	LHG	O6-C4-C5-O7
30	7	802	LHG	O6-C4-C5-O7
52	8	805	P5S	O37-C2-C3-O16
37	B	5004	PCW	C41-C42-C43-C44
25	B	1205	CLA	C2B-C3B-CAB-CBB
29	A	4003	BCR	C23-C24-C25-C30
29	B	4001	BCR	C1-C6-C7-C8
29	B	4002	BCR	C23-C24-C25-C30
29	B	4004	BCR	C23-C24-C25-C30
29	H	4001	BCR	C1-C6-C7-C8
29	L	4003	BCR	C1-C6-C7-C8
29	L	4003	BCR	C23-C24-C25-C30
29	L	4001	BCR	C1-C6-C7-C8
29	I	4001	BCR	C5-C6-C7-C8
29	3	503	BCR	C23-C24-C25-C30
44	1	502	AXT	C21-C26-C27-C28
33	J	5001	PTY	C11-C8-O7-C6
30	4	801	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
25	5	603	CLA	C11-C10-C8-C9
37	K	5001	PCW	C42-C43-C44-C45
30	B	5001	LHG	C25-C26-C27-C28
30	8	801	LHG	C28-C29-C30-C31
41	4	805	SPH	C11-C12-C13-C14
25	4	604	CLA	C8-C10-C11-C12
25	2	621	CLA	C15-C16-C17-C18
33	3	802	PTY	C34-C35-C36-C37
30	F	5001	LHG	C16-C17-C18-C19
30	3	801	LHG	C34-C35-C36-C37
36	B	5003	DGD	C5A-C6A-C7A-C8A
25	6	618	CLA	CAA-CBA-CGA-O2A
25	A	1134	CLA	C2A-CAA-CBA-CGA
25	1	606	CLA	C2A-CAA-CBA-CGA
30	B	5002	LHG	O7-C5-C6-O8
30	4	801	LHG	O7-C5-C6-O8
30	2	801	LHG	O7-C5-C6-O8
32	G	5001	SQD	O47-C45-C46-O48
33	9	803	PTY	O4-C1-C6-O7
37	B	5004	PCW	O2-C2-C3-O3
41	J	5002	SPH	C13-C14-C15-C16
30	a	801	LHG	C23-C24-C25-C26
25	B	1203	CLA	O1A-CGA-O2A-C1
37	K	5001	PCW	C12-C13-C14-C15
51	7	807	4RF	C28-C29-C30-C31
25	8	618	CLA	C5-C6-C7-C8
25	A	1125	CLA	C2-C3-C5-C6
25	A	1101	CLA	C2-C3-C5-C6
25	1	608	CLA	C2-C3-C5-C6
53	8	810	LAP	C6-C7-C8-C9
30	A	5003	LHG	C25-C26-C27-C28
30	4	801	LHG	C31-C32-C33-C34
34	A	5007	3PH	C22-C23-C24-C25
25	K	1402	CLA	C3-C5-C6-C7
25	B	1239	CLA	C6-C7-C8-C9
25	1	601	CLA	C6-C7-C8-C9
25	a	603	CLA	C11-C12-C13-C14
25	4	612	CLA	C11-C12-C13-C14
25	8	606	CLA	C11-C10-C8-C9
25	2	621	CLA	C6-C7-C8-C9
26	6	609	CHL	C11-C10-C8-C9
27	B	2002	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
30	7	803	LHG	C25-C26-C27-C28
51	7	807	4RF	C44-C45-C46-C47
30	1	802	LHG	C35-C36-C37-C38
25	2	604	CLA	CAA-CBA-CGA-O2A
30	A	5002	LHG	C11-C10-C9-C8
30	1	802	LHG	C33-C34-C35-C36
30	2	801	LHG	C26-C27-C28-C29
30	A	5001	LHG	C35-C36-C37-C38
48	8	804	DGA	CAA-CBA-CCA-CDA
25	6	601	CLA	C5-C6-C7-C8
30	a	801	LHG	C28-C29-C30-C31
33	7	804	PTY	C15-C16-C17-C18
26	9	610	CHL	C2A-CAA-CBA-CGA
30	B	5001	LHG	C24-C25-C26-C27
30	4	801	LHG	C9-C10-C11-C12
45	a	805	OLA	C13-C14-C15-C16
47	4	804	PLM	CD-CE-CF-CG
30	5	801	LHG	O1-C1-C2-O2
25	B	1234	CLA	C3-C5-C6-C7
29	A	4002	BCR	C15-C16-C17-C18
29	A	4005	BCR	C19-C20-C21-C22
29	B	4006	BCR	C13-C14-C15-C16
29	6	503	BCR	C9-C10-C11-C12
25	a	603	CLA	C16-C17-C18-C20
26	3	611	CHL	C11-C12-C13-C14
25	B	1206	CLA	C2C-C3C-CAC-CBC
30	1	802	LHG	C26-C27-C28-C29
30	5	801	LHG	C17-C18-C19-C20
30	4	801	LHG	C34-C35-C36-C37
25	A	1125	CLA	C10-C11-C12-C13
25	B	1234	CLA	C10-C11-C12-C13
25	3	610	CLA	C5-C6-C7-C8
53	8	810	LAP	C13-C14-C15-O4
25	2	602	CLA	O1A-CGA-O2A-C1
25	A	1138	CLA	C5-C6-C7-C8
30	1	801	LHG	C9-C10-C11-C12
33	A	5006	PTY	C13-C14-C15-C16
30	A	5003	LHG	O6-C4-C5-C6
30	2	802	LHG	O6-C4-C5-C6
33	3	802	PTY	O14-C5-C6-C1
33	9	803	PTY	O14-C5-C6-C1
25	B	1209	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	4	610	CLA	C16-C17-C18-C20
25	8	618	CLA	C11-C12-C13-C14
26	8	601	CHL	C11-C12-C13-C15
30	a	801	LHG	C31-C32-C33-C34
30	9	801	LHG	C25-C26-C27-C28
25	A	1012	CLA	C10-C11-C12-C13
25	6	603	CLA	C8-C10-C11-C12
29	B	4006	BCR	C37-C22-C23-C24
29	7	503	BCR	C11-C12-C13-C35
40	J	4002	RRX	C37-C22-C23-C24
38	F	5003	LPX	C11-C10-C9-C8
25	A	1117	CLA	C11-C12-C13-C15
25	A	1125	CLA	C11-C12-C13-C15
25	A	1132	CLA	C6-C7-C8-C10
25	A	1137	CLA	C11-C10-C8-C7
25	B	1237	CLA	C11-C10-C8-C7
25	B	1022	CLA	C6-C7-C8-C10
25	B	1023	CLA	C12-C13-C15-C16
25	B	1201	CLA	C11-C10-C8-C7
25	B	1201	CLA	C12-C13-C15-C16
25	B	1202	CLA	C11-C12-C13-C15
25	B	1206	CLA	C11-C12-C13-C15
25	B	1217	CLA	C6-C7-C8-C10
25	B	1226	CLA	C11-C10-C8-C7
25	B	1239	CLA	C6-C7-C8-C10
25	B	1207	CLA	C6-C7-C8-C10
25	B	1207	CLA	C11-C10-C8-C7
25	1	607	CLA	C12-C13-C15-C16
25	1	612	CLA	C12-C13-C15-C16
25	a	603	CLA	C11-C12-C13-C15
25	3	607	CLA	C6-C7-C8-C10
25	3	607	CLA	C11-C10-C8-C7
25	3	610	CLA	C6-C7-C8-C10
25	4	612	CLA	C11-C12-C13-C15
25	5	601	CLA	C11-C10-C8-C7
25	5	612	CLA	C6-C7-C8-C10
26	3	611	CHL	C6-C7-C8-C10
26	3	611	CHL	C11-C10-C8-C7
26	6	609	CHL	C11-C10-C8-C7
26	7	609	CHL	C11-C10-C8-C7
26	9	603	CHL	C11-C10-C8-C7
30	A	5002	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	2	609	CHL	CAA-CBA-CGA-O2A
30	1	801	LHG	C28-C29-C30-C31
30	7	802	LHG	C11-C10-C9-C8
33	A	5006	PTY	C34-C35-C36-C37
25	a	607	CLA	C3-C5-C6-C7
29	A	4001	BCR	C17-C18-C19-C20
29	A	4005	BCR	C7-C8-C9-C10
29	B	4005	BCR	C21-C22-C23-C24
29	J	4001	BCR	C21-C22-C23-C24
40	J	4002	RRX	C21-C22-C23-C24
30	3	801	LHG	C24-C23-O8-C6
33	J	5001	PTY	C31-C30-O4-C1
41	4	805	SPH	C14-C15-C16-C17
25	1	608	CLA	O1A-CGA-O2A-C1
25	8	611	CLA	O1A-CGA-O2A-C1
34	A	5007	3PH	C1-O11-P-O13
25	7	604	CLA	C8-C10-C11-C12
30	B	5001	LHG	O9-C7-O7-C5
30	5	801	LHG	O9-C7-O7-C5
25	1	601	CLA	O1A-CGA-O2A-C1
25	4	610	CLA	O1A-CGA-O2A-C1
25	A	1123	CLA	C2-C3-C5-C6
30	5	801	LHG	O1-C1-C2-C3
30	B	5002	LHG	C30-C31-C32-C33
47	8	806	PLM	C9-CA-CB-CC
25	B	1021	CLA	C13-C15-C16-C17
30	2	801	LHG	C4-C5-O7-C7
32	G	5001	SQD	C46-C45-O47-C7
37	6	803	PCW	O11-C11-O3-C3
35	1	804	LMT	C5'-C4'-O1B-C1B
45	8	809	OLA	C2-C3-C4-C5
25	5	612	CLA	C8-C10-C11-C12
29	G	4001	BCR	C15-C16-C17-C18
43	5	505	LUT	C29-C30-C31-C32
43	8	502	LUT	C29-C30-C31-C32
35	A	5008	LMT	C1-C2-C3-C4
25	4	602	CLA	O1A-CGA-O2A-C1
25	7	608	CLA	O1A-CGA-O2A-C1
25	A	1128	CLA	C3-C5-C6-C7
25	B	1204	CLA	C13-C15-C16-C17
25	3	607	CLA	C5-C6-C7-C8
32	I	5001	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	A	1107	CLA	C5-C6-C7-C8
25	B	1234	CLA	C5-C6-C7-C8
30	4	801	LHG	O6-C4-C5-O7
30	2	801	LHG	O6-C4-C5-O7
33	3	802	PTY	O14-C5-C6-O7
33	9	803	PTY	O14-C5-C6-O7
34	A	5007	3PH	O11-C1-C2-O21
37	6	803	PCW	O3P-C1-C2-O2
30	2	802	LHG	C24-C25-C26-C27
30	A	5003	LHG	C4-C5-C6-O8
30	1	801	LHG	C4-C5-C6-O8
30	1	802	LHG	C4-C5-C6-O8
30	4	801	LHG	C4-C5-C6-O8
32	G	5001	SQD	C44-C45-C46-O48
36	7	806	DGD	C1G-C2G-C3G-O3G
37	K	5001	PCW	C1-C2-C3-O3
48	2	803	DGA	OG1-CG1-CG2-CG3
25	A	1104	CLA	C10-C11-C12-C13
25	A	1139	CLA	C5-C6-C7-C8
25	B	1228	CLA	C10-C11-C12-C13
25	A	1112	CLA	C6-C7-C8-C10
25	A	1121	CLA	C11-C12-C13-C14
25	B	1201	CLA	C16-C17-C18-C20
25	B	1220	CLA	C5-C6-C7-C8
25	A	1123	CLA	C4-C3-C5-C6
25	5	607	CLA	C4-C3-C5-C6
25	A	1132	CLA	C2A-CAA-CBA-CGA
26	4	609	CHL	CAA-CBA-CGA-O2A
25	B	1216	CLA	C2-C3-C5-C6
30	5	801	LHG	C34-C35-C36-C37
32	I	5001	SQD	C12-C13-C14-C15
33	a	802	PTY	C35-C36-C37-C38
37	K	5001	PCW	C5-C4-O4P-P
37	6	803	PCW	C5-C4-O4P-P
38	F	5003	LPX	C2-C1-O2-P1
30	9	802	LHG	C7-C8-C9-C10
32	A	5005	SQD	C34-C35-C36-C37
30	7	803	LHG	O7-C5-C6-O8
32	I	5001	SQD	O47-C45-C46-O48
36	B	5003	DGD	O1G-C1G-C2G-O2G
36	7	806	DGD	O2G-C2G-C3G-O3G
48	2	803	DGA	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
25	5	601	CLA	C5-C6-C7-C8
26	6	609	CHL	C8-C10-C11-C12
25	A	1013	CLA	C6-C7-C8-C9
25	A	1103	CLA	C11-C10-C8-C9
25	A	1134	CLA	C6-C7-C8-C9
25	B	1237	CLA	C11-C10-C8-C9
25	B	1023	CLA	C11-C12-C13-C14
25	B	1210	CLA	C6-C7-C8-C9
25	B	1217	CLA	C6-C7-C8-C9
25	B	1239	CLA	C11-C10-C8-C9
25	G	1602	CLA	C11-C10-C8-C9
25	3	610	CLA	C6-C7-C8-C9
25	5	612	CLA	C6-C7-C8-C9
25	6	604	CLA	C14-C13-C15-C16
26	1	604	CHL	C11-C12-C13-C14
26	3	603	CHL	C14-C13-C15-C16
26	2	609	CHL	C11-C12-C13-C14
33	a	803	PTY	C32-C33-C34-C35
33	9	803	PTY	C36-C37-C38-C39
48	8	804	DGA	CBB-CAB-CB9-CB8
25	8	605	CLA	CBA-CGA-O2A-C1
36	7	806	DGD	C9A-CAA-CBA-CCA
30	F	5002	LHG	C10-C11-C12-C13
25	2	601	CLA	O1A-CGA-O2A-C1
41	J	5002	SPH	C6-C7-C8-C9
48	8	804	DGA	CAB-CBB-CCB-CDB
25	A	1119	CLA	C5-C6-C7-C8
25	7	601	CLA	C8-C10-C11-C12
25	9	605	CLA	C8-C10-C11-C12
48	8	804	DGA	CB9-CAB-CBB-CCB
25	A	1127	CLA	C2-C1-O2A-CGA
25	8	618	CLA	C2-C1-O2A-CGA
25	1	612	CLA	C13-C15-C16-C17
30	7	803	LHG	C2-C3-O3-P
30	6	801	LHG	C19-C20-C21-C22
31	A	5004	LMG	C32-C33-C34-C35
37	B	5004	PCW	O4P-C4-C5-N
37	K	5001	PCW	O4P-C4-C5-N
25	A	1012	CLA	C4-C3-C5-C6
25	A	1116	CLA	C4-C3-C5-C6
25	A	1126	CLA	C4-C3-C5-C6
36	B	5003	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
25	B	1201	CLA	C10-C11-C12-C13
25	A	1012	CLA	CBA-CGA-O2A-C1
25	A	1136	CLA	C16-C17-C18-C19
25	B	1240	CLA	C16-C17-C18-C20
25	5	604	CLA	C16-C17-C18-C20
25	7	603	CLA	C16-C17-C18-C20
25	4	604	CLA	C10-C11-C12-C13
30	7	803	LHG	C11-C10-C9-C8
30	8	801	LHG	C7-C8-C9-C10
30	B	5001	LHG	C19-C20-C21-C22
25	1	605	CLA	C5-C6-C7-C8
25	A	1115	CLA	C3-C5-C6-C7
25	5	612	CLA	C3-C5-C6-C7
47	a	804	PLM	C1-C2-C3-C4
33	J	5001	PTY	O30-C30-O4-C1
25	2	601	CLA	CBA-CGA-O2A-C1
33	J	5001	PTY	O10-C8-O7-C6
25	A	1012	CLA	O1A-CGA-O2A-C1
25	B	1021	CLA	O1A-CGA-O2A-C1
24	A	1011	CL0	CBD-CGD-O2D-CED
30	8	801	LHG	C11-C10-C9-C8
25	A	1125	CLA	C4B-C3B-CAB-CBB
25	A	1133	CLA	C4B-C3B-CAB-CBB
25	A	1134	CLA	C4B-C3B-CAB-CBB
25	A	1136	CLA	C4B-C3B-CAB-CBB
25	B	1237	CLA	C4B-C3B-CAB-CBB
25	B	1209	CLA	C1A-C2A-CAA-CBA
25	B	1211	CLA	C1A-C2A-CAA-CBA
25	B	1214	CLA	C4B-C3B-CAB-CBB
25	1	605	CLA	C1A-C2A-CAA-CBA
25	a	608	CLA	C4B-C3B-CAB-CBB
25	4	610	CLA	C4B-C3B-CAB-CBB
25	4	612	CLA	C1A-C2A-CAA-CBA
25	4	616	CLA	C4B-C3B-CAB-CBB
25	6	607	CLA	C1A-C2A-CAA-CBA
25	6	618	CLA	C4B-C3B-CAB-CBB
25	7	607	CLA	C1A-C2A-CAA-CBA
25	8	607	CLA	C4B-C3B-CAB-CBB
25	8	615	CLA	C4B-C3B-CAB-CBB
25	2	612	CLA	C4B-C3B-CAB-CBB
25	9	606	CLA	C1A-C2A-CAA-CBA
25	L	1504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	B	5003	DGD	CFB-CGB-CHB-CIB
25	A	1122	CLA	C4-C3-C5-C6
30	B	5002	LHG	C9-C10-C11-C12
38	F	5003	LPX	C14-C15-C16-C17
29	A	4004	BCR	C17-C18-C19-C20
29	7	503	BCR	C11-C12-C13-C14
43	5	505	LUT	C7-C8-C9-C10
43	5	505	LUT	C27-C28-C29-C30
30	9	802	LHG	C30-C31-C32-C33
30	3	801	LHG	C11-C10-C9-C8
30	3	801	LHG	O10-C23-O8-C6
25	A	1109	CLA	C2A-CAA-CBA-CGA
25	5	612	CLA	C2A-CAA-CBA-CGA
25	6	601	CLA	C2A-CAA-CBA-CGA
25	B	1207	CLA	C5-C6-C7-C8
30	A	5002	LHG	O6-C4-C5-C6
30	B	5001	LHG	O6-C4-C5-C6
30	B	5002	LHG	O6-C4-C5-C6
30	F	5002	LHG	O6-C4-C5-C6
30	a	801	LHG	O6-C4-C5-C6
30	4	802	LHG	O6-C4-C5-C6
30	9	802	LHG	O6-C4-C5-C6
33	a	803	PTY	O14-C5-C6-C1
37	6	803	PCW	O3P-C1-C2-C3
52	8	805	P5S	C1-C2-C3-O16
30	4	802	LHG	C9-C10-C11-C12
30	9	801	LHG	C26-C27-C28-C29
24	A	1011	CL0	C3-C5-C6-C7
25	A	1013	CLA	C12-C13-C15-C16
25	A	1122	CLA	C11-C10-C8-C7
25	B	1209	CLA	C11-C10-C8-C7
25	B	1229	CLA	C11-C10-C8-C7
25	B	1240	CLA	C6-C7-C8-C10
25	1	601	CLA	C11-C10-C8-C7
25	1	605	CLA	C6-C7-C8-C10
25	1	608	CLA	C6-C7-C8-C10
25	3	606	CLA	C6-C7-C8-C10
25	3	613	CLA	C11-C12-C13-C15
25	4	610	CLA	C12-C13-C15-C16
25	4	611	CLA	C6-C7-C8-C10
25	6	615	CLA	C11-C10-C8-C7
26	3	603	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	A	1126	CLA	C16-C17-C18-C19
25	B	1021	CLA	C16-C17-C18-C20
25	6	604	CLA	C16-C17-C18-C19
25	B	1021	CLA	CBA-CGA-O2A-C1
25	a	601	CLA	CBA-CGA-O2A-C1
30	2	802	LHG	C10-C11-C12-C13
25	6	601	CLA	C8-C10-C11-C12
25	8	609	CLA	C8-C10-C11-C12
45	8	809	OLA	C13-C14-C15-C16
26	a	613	CHL	C2C-C3C-CAC-CBC
33	a	802	PTY	C30-C31-C32-C33
30	1	802	LHG	C2-C3-O3-P
30	7	802	LHG	C2-C3-O3-P
48	5	803	DGA	CA5-CA6-CA7-CA8
25	B	1202	CLA	C16-C17-C18-C20
25	2	621	CLA	C16-C17-C18-C19
47	6	804	PLM	C3-C4-C5-C6
25	9	607	CLA	CAA-CBA-CGA-O2A
32	A	5005	SQD	C31-C32-C33-C34
26	2	609	CHL	C2C-C3C-CAC-CBC
30	A	5002	LHG	O6-C4-C5-O7
30	A	5003	LHG	O6-C4-C5-O7
30	1	802	LHG	O6-C4-C5-O7
30	6	802	LHG	O6-C4-C5-O7
30	2	802	LHG	O6-C4-C5-O7
30	9	802	LHG	O6-C4-C5-O7
33	a	803	PTY	O14-C5-C6-O7
33	5	802	PTY	O14-C5-C6-O7
37	K	5001	PCW	O3P-C1-C2-O2
30	2	801	LHG	C24-C25-C26-C27
30	2	802	LHG	C25-C26-C27-C28
25	A	1108	CLA	C11-C10-C8-C9
25	B	1022	CLA	C6-C7-C8-C9
25	B	1023	CLA	C14-C13-C15-C16
25	B	1201	CLA	C14-C13-C15-C16
25	B	1202	CLA	C11-C12-C13-C14
25	B	1206	CLA	C11-C12-C13-C14
25	B	1226	CLA	C11-C10-C8-C9
25	B	1235	CLA	C11-C10-C8-C9
25	3	606	CLA	C11-C10-C8-C9
25	3	607	CLA	C6-C7-C8-C9
25	3	607	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	5	601	CLA	C11-C10-C8-C9
25	2	604	CLA	C6-C7-C8-C9
26	9	603	CHL	C11-C10-C8-C9
25	8	605	CLA	O1A-CGA-O2A-C1
29	B	4002	BCR	C13-C14-C15-C16
29	H	4001	BCR	C9-C10-C11-C12
29	7	503	BCR	C9-C10-C11-C12
29	7	503	BCR	C19-C20-C21-C22
43	1	503	LUT	C29-C30-C31-C32
43	8	501	LUT	C29-C30-C31-C32
24	A	1011	CL0	O1D-CGD-O2D-CED
26	8	603	CHL	C10-C11-C12-C13
25	A	1120	CLA	C1-C2-C3-C4
43	2	507	LUT	C21-C26-C27-C28
30	a	801	LHG	C30-C31-C32-C33
25	B	1214	CLA	O1A-CGA-O2A-C1
30	A	5002	LHG	O7-C5-C6-O8
30	A	5003	LHG	O7-C5-C6-O8
30	6	801	LHG	O7-C5-C6-O8
30	7	801	LHG	O7-C5-C6-O8
30	2	802	LHG	O7-C5-C6-O8
32	G	5001	SQD	O6-C44-C45-O47
36	8	802	DGD	O2G-C2G-C3G-O3G
48	5	803	DGA	OG1-CG1-CG2-OG2
52	8	805	P5S	O19-C1-C2-O37
35	B	5006	LMT	C4-C5-C6-C7
25	6	604	CLA	C16-C17-C18-C20
30	B	5002	LHG	C4-C5-C6-O8
30	9	801	LHG	C4-C5-C6-O8
32	I	5001	SQD	C44-C45-C46-O48
32	H	5001	SQD	C15-C16-C17-C18
51	7	807	4RF	C11-C12-C13-C14
25	6	615	CLA	C5-C6-C7-C8
25	A	1103	CLA	CAA-CBA-CGA-O2A
45	8	809	OLA	C10-C11-C12-C13
25	A	1112	CLA	CAD-CBD-CGD-O2D
25	A	1129	CLA	CAD-CBD-CGD-O2D
25	A	1136	CLA	CAD-CBD-CGD-O2D
25	B	1223	CLA	CAD-CBD-CGD-O2D
25	B	1227	CLA	CAD-CBD-CGD-O2D
25	4	606	CLA	CAD-CBD-CGD-O2D
25	6	605	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	8	609	CLA	CAD-CBD-CGD-O2D
26	a	609	CHL	CAD-CBD-CGD-O2D
26	7	609	CHL	CAD-CBD-CGD-O2D
25	A	1108	CLA	C15-C16-C17-C18
25	B	1206	CLA	C4C-C3C-CAC-CBC
34	A	5007	3PH	C26-C27-C28-C29
41	9	804	SPH	C4-C5-C6-C7
32	I	5001	SQD	O5-C1-O6-C44
25	A	1116	CLA	C8-C10-C11-C12
25	2	601	CLA	C8-C10-C11-C12
48	2	803	DGA	CB4-CB5-CB6-CB7
25	A	1131	CLA	C16-C17-C18-C19
25	A	1111	CLA	C13-C15-C16-C17
25	A	1138	CLA	C8-C10-C11-C12
25	L	1504	CLA	O1A-CGA-O2A-C1
25	a	601	CLA	O1A-CGA-O2A-C1
30	9	802	LHG	C19-C20-C21-C22
45	1	803	OLA	C4-C5-C6-C7
25	B	1229	CLA	CAA-CBA-CGA-O2A
25	B	1214	CLA	CBA-CGA-O2A-C1
24	A	1011	CL0	CHA-CBD-CGD-O1D
24	A	1011	CL0	CHA-CBD-CGD-O2D
25	A	1112	CLA	CAD-CBD-CGD-O1D
25	A	1123	CLA	CHA-CBD-CGD-O1D
25	A	1123	CLA	CHA-CBD-CGD-O2D
25	A	1125	CLA	CAD-CBD-CGD-O1D
25	A	1129	CLA	CAD-CBD-CGD-O1D
25	A	1133	CLA	CHA-CBD-CGD-O1D
25	A	1133	CLA	CHA-CBD-CGD-O2D
25	A	1135	CLA	CHA-CBD-CGD-O1D
25	A	1135	CLA	CHA-CBD-CGD-O2D
25	A	1136	CLA	CAD-CBD-CGD-O1D
25	B	1208	CLA	CHA-CBD-CGD-O2D
25	B	1210	CLA	CAD-CBD-CGD-O1D
25	B	1223	CLA	CAD-CBD-CGD-O1D
25	B	1227	CLA	CAD-CBD-CGD-O1D
25	L	1503	CLA	CHA-CBD-CGD-O1D
25	L	1503	CLA	CHA-CBD-CGD-O2D
25	1	605	CLA	CAD-CBD-CGD-O1D
25	4	606	CLA	CAD-CBD-CGD-O1D
25	6	605	CLA	CAD-CBD-CGD-O1D
25	6	615	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	7	604	CLA	CHA-CBD-CGD-O1D
25	7	604	CLA	CHA-CBD-CGD-O2D
25	8	609	CLA	CAD-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O2D
25	9	604	CLA	CHA-CBD-CGD-O1D
26	a	609	CHL	CAD-CBD-CGD-O1D
26	a	610	CHL	CHA-CBD-CGD-O1D
26	a	610	CHL	CHA-CBD-CGD-O2D
26	3	604	CHL	CHA-CBD-CGD-O2D
26	3	611	CHL	CHA-CBD-CGD-O1D
26	3	611	CHL	CHA-CBD-CGD-O2D
26	5	611	CHL	CHA-CBD-CGD-O2D
26	5	613	CHL	CHA-CBD-CGD-O1D
26	6	609	CHL	CAD-CBD-CGD-O1D
26	7	609	CHL	CAD-CBD-CGD-O1D
26	7	615	CHL	CHA-CBD-CGD-O1D
26	7	615	CHL	CHA-CBD-CGD-O2D
26	8	601	CHL	CHA-CBD-CGD-O2D
26	2	610	CHL	CHA-CBD-CGD-O1D
26	2	610	CHL	CHA-CBD-CGD-O2D
26	9	601	CHL	CHA-CBD-CGD-O2D
29	B	4001	BCR	C19-C20-C21-C22
29	B	4007	BCR	C19-C20-C21-C22
29	K	4002	BCR	C9-C10-C11-C12
29	L	4003	BCR	C13-C14-C15-C16
29	L	4003	BCR	C19-C20-C21-C22
29	5	503	BCR	C19-C20-C21-C22
29	6	503	BCR	C19-C20-C21-C22
29	8	503	BCR	C9-C10-C11-C12
29	8	503	BCR	C19-C20-C21-C22
30	A	5003	LHG	C3-O3-P-O5
30	B	5002	LHG	C4-O6-P-O3
30	F	5002	LHG	C3-O3-P-O5
30	F	5001	LHG	C3-O3-P-O6
30	1	801	LHG	C4-O6-P-O5
30	a	801	LHG	C3-O3-P-O5
30	3	801	LHG	C3-O3-P-O5
30	3	801	LHG	C4-O6-P-O4
30	4	801	LHG	C3-O3-P-O4
30	4	801	LHG	C3-O3-P-O6
30	6	802	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
30	6	801	LHG	C3-O3-P-O5
30	6	801	LHG	C4-O6-P-O5
30	7	803	LHG	C4-O6-P-O5
30	8	801	LHG	C3-O3-P-O5
30	2	802	LHG	C3-O3-P-O5
30	9	802	LHG	C3-O3-P-O6
30	9	802	LHG	C4-O6-P-O5
30	9	801	LHG	C4-O6-P-O5
33	B	5005	PTY	C5-O14-P1-O12
33	G	5003	PTY	C3-O11-P1-O13
33	G	5002	PTY	C3-O11-P1-O13
33	J	5001	PTY	C5-O14-P1-O12
33	a	803	PTY	C3-O11-P1-O13
33	a	803	PTY	C3-O11-P1-O14
33	a	803	PTY	C5-O14-P1-O11
33	a	803	PTY	C5-O14-P1-O12
33	a	803	PTY	C5-O14-P1-O13
33	a	802	PTY	N1-C2-C3-O11
33	a	802	PTY	C5-O14-P1-O12
33	3	802	PTY	C3-O11-P1-O13
33	5	802	PTY	N1-C2-C3-O11
33	5	802	PTY	C3-O11-P1-O13
33	5	802	PTY	C3-O11-P1-O14
33	7	804	PTY	C3-O11-P1-O12
33	7	804	PTY	C3-O11-P1-O13
33	7	804	PTY	C3-O11-P1-O14
37	B	5004	PCW	C1-O3P-P-O1P
37	B	5004	PCW	C1-O3P-P-O2P
37	B	5004	PCW	C1-O3P-P-O4P
37	B	5004	PCW	C4-O4P-P-O2P
37	K	5002	PCW	C4-O4P-P-O3P
37	K	5001	PCW	C4-O4P-P-O2P
37	6	803	PCW	C1-O3P-P-O1P
43	9	501	LUT	C29-C30-C31-C32
44	7	504	AXT	C9-C10-C11-C12
44	7	504	AXT	C29-C30-C31-C32
50	9	504	XAT	C9-C10-C11-C12
52	8	805	P5S	C3-O16-P12-O15
53	8	810	LAP	C15-O4-P9-O5
30	4	801	LHG	C19-C20-C21-C22
25	A	1115	CLA	C11-C12-C13-C15
25	A	1133	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	1136	CLA	C2B-C3B-CAB-CBB
25	B	1237	CLA	C2B-C3B-CAB-CBB
25	8	607	CLA	C2B-C3B-CAB-CBB
25	8	615	CLA	C2B-C3B-CAB-CBB
25	2	621	CLA	C2B-C3B-CAB-CBB
43	1	501	LUT	C1-C6-C7-C8
43	6	501	LUT	C1-C6-C7-C8
35	B	5006	LMT	C7-C8-C9-C10
29	6	504	BCR	C36-C18-C19-C20
30	B	5002	LHG	C5-C4-O6-P
30	F	5002	LHG	C2-C3-O3-P
30	6	801	LHG	C2-C3-O3-P
30	2	802	LHG	C2-C3-O3-P
43	8	502	LUT	C7-C8-C9-C19
30	9	801	LHG	C10-C11-C12-C13
25	A	1012	CLA	C2A-CAA-CBA-CGA
25	A	1107	CLA	C2A-CAA-CBA-CGA
30	2	802	LHG	C28-C29-C30-C31
25	A	1101	CLA	C16-C17-C18-C20
30	6	801	LHG	C11-C10-C9-C8
26	7	609	CHL	C12-C13-C15-C16
26	8	604	CHL	C12-C13-C15-C16
25	1	607	CLA	C3-C5-C6-C7
29	H	4001	BCR	C18-C19-C20-C21
43	2	507	LUT	C10-C11-C12-C13
43	2	507	LUT	C30-C31-C32-C33
44	7	504	AXT	C30-C31-C32-C33
25	A	1126	CLA	C2-C3-C5-C6
36	B	5003	DGD	C1B-C2B-C3B-C4B
33	9	803	PTY	C32-C33-C34-C35
37	K	5002	PCW	C15-C16-C17-C18
30	6	801	LHG	C31-C32-C33-C34
29	A	4004	BCR	C19-C20-C21-C22
25	a	603	CLA	C16-C17-C18-C19
25	2	621	CLA	C16-C17-C18-C20
30	2	801	LHG	O6-C4-C5-C6
30	A	5001	LHG	C9-C10-C11-C12
25	B	1206	CLA	C6-C7-C8-C9
25	B	1214	CLA	C6-C7-C8-C9
25	B	1207	CLA	C6-C7-C8-C9
25	1	608	CLA	C6-C7-C8-C9
25	1	612	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	1	612	CLA	C14-C13-C15-C16
25	3	606	CLA	C6-C7-C8-C9
25	7	601	CLA	C6-C7-C8-C9
26	A	1114	CHL	C11-C10-C8-C9
26	1	609	CHL	C11-C12-C13-C14
26	3	603	CHL	C6-C7-C8-C9
26	9	601	CHL	C14-C13-C15-C16
26	9	603	CHL	C14-C13-C15-C16
30	7	801	LHG	C30-C31-C32-C33
25	B	1228	CLA	C11-C12-C13-C15
25	1	607	CLA	C11-C10-C8-C7
25	7	610	CLA	C6-C7-C8-C10
25	9	605	CLA	C6-C7-C8-C10
26	A	1114	CHL	C11-C10-C8-C7
25	B	1210	CLA	C8-C10-C11-C12
30	4	801	LHG	C7-C8-C9-C10
30	7	801	LHG	O6-C4-C5-O7
30	8	801	LHG	O6-C4-C5-O7
25	5	604	CLA	C16-C17-C18-C19
25	7	603	CLA	C16-C17-C18-C19
30	B	5002	LHG	O8-C23-C24-C25
30	5	801	LHG	C30-C31-C32-C33
33	a	803	PTY	C33-C34-C35-C36
25	B	1215	CLA	C8-C10-C11-C12
25	1	606	CLA	C5-C6-C7-C8
25	2	602	CLA	C2-C3-C5-C6
37	6	803	PCW	C12-C13-C14-C15
25	A	1136	CLA	C16-C17-C18-C20
25	B	1240	CLA	C16-C17-C18-C19
25	4	610	CLA	C16-C17-C18-C19
25	8	608	CLA	O1D-CGD-O2D-CED
30	7	803	LHG	C28-C29-C30-C31
33	J	5001	PTY	C8-C11-C12-C13
30	A	5003	LHG	C2-C3-O3-P
30	B	5002	LHG	C2-C3-O3-P
30	3	801	LHG	C2-C3-O3-P
30	F	5001	LHG	O7-C5-C6-O8
26	1	610	CHL	CAA-CBA-CGA-O2A
25	B	1221	CLA	C15-C16-C17-C18
26	3	603	CHL	C10-C11-C12-C13
36	8	802	DGD	CAA-CBA-CCA-CDA
29	3	505	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
39	F	4001	NEX	C33-C34-C35-C15
25	O	1802	CLA	CAA-CBA-CGA-O2A
30	4	801	LHG	C30-C31-C32-C33
25	H	1702	CLA	C2A-CAA-CBA-CGA
25	8	611	CLA	C2A-CAA-CBA-CGA
25	7	603	CLA	C15-C16-C17-C18
27	B	2002	PQN	C15-C16-C17-C18
35	B	5006	LMT	C4B-C5B-C6B-O6B
25	A	1115	CLA	C2-C1-O2A-CGA
25	B	1215	CLA	C2-C1-O2A-CGA
25	5	607	CLA	C2-C1-O2A-CGA
25	5	614	CLA	O1A-CGA-O2A-C1
25	A	1102	CLA	C4-C3-C5-C6
25	A	1107	CLA	C4-C3-C5-C6
25	A	1134	CLA	C4-C3-C5-C6
47	6	804	PLM	CC-CD-CE-CF
25	A	1127	CLA	CAA-CBA-CGA-O2A
33	3	802	PTY	C12-C11-C8-O7
33	G	5003	PTY	C11-C12-C13-C14
47	6	804	PLM	C6-C7-C8-C9
25	1	603	CLA	C3-C5-C6-C7
26	3	603	CHL	C3-C5-C6-C7
25	B	1224	CLA	CAA-CBA-CGA-O2A
34	A	5007	3PH	O21-C21-C22-C23
29	8	503	BCR	C11-C12-C13-C35
29	L	4002	BCR	C17-C18-C19-C20
26	3	611	CHL	CAA-CBA-CGA-O2A
36	7	806	DGD	C2G-C3G-O3G-C1D
32	G	5001	SQD	C9-C10-C11-C12
24	A	1011	CL0	C5-C6-C7-C8
25	B	1219	CLA	C5-C6-C7-C8
25	F	1302	CLA	C5-C6-C7-C8
30	5	801	LHG	C18-C19-C20-C21
25	2	604	CLA	C2A-CAA-CBA-CGA
26	4	609	CHL	C2A-CAA-CBA-CGA
29	A	4001	BCR	C15-C16-C17-C18
29	A	4004	BCR	C9-C10-C11-C12
29	J	4001	BCR	C19-C20-C21-C22
29	3	503	BCR	C9-C10-C11-C12
29	8	503	BCR	C13-C14-C15-C16
39	F	4001	NEX	C29-C30-C31-C32
40	J	4002	RRX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
50	9	504	XAT	C13-C14-C15-C35
25	B	1210	CLA	C16-C17-C18-C20
25	6	615	CLA	C16-C17-C18-C19
47	4	803	PLM	C9-CA-CB-CC
25	B	1205	CLA	C4-C3-C5-C6
25	B	1224	CLA	C4-C3-C5-C6
25	A	1123	CLA	C13-C15-C16-C17
33	5	802	PTY	C38-C39-C40-C41
25	B	1227	CLA	CAA-CBA-CGA-O1A
25	B	1237	CLA	C16-C17-C18-C20
35	2	804	LMT	C11-C10-C9-C8
38	F	5003	LPX	C6-C7-C8-C9
25	A	1136	CLA	C11-C10-C8-C9
25	B	1229	CLA	C11-C10-C8-C9
25	B	1240	CLA	C6-C7-C8-C9
25	1	601	CLA	C11-C10-C8-C9
25	4	611	CLA	C6-C7-C8-C9
25	7	603	CLA	C14-C13-C15-C16
25	7	604	CLA	C14-C13-C15-C16
30	4	802	LHG	C24-C23-O8-C6
25	B	1236	CLA	C5-C6-C7-C8
25	A	1104	CLA	C4B-C3B-CAB-CBB
25	B	1204	CLA	C4B-C3B-CAB-CBB
25	1	612	CLA	C4B-C3B-CAB-CBB
25	a	612	CLA	C4B-C3B-CAB-CBB
25	4	607	CLA	C4B-C3B-CAB-CBB
25	4	615	CLA	C4B-C3B-CAB-CBB
25	5	615	CLA	C4B-C3B-CAB-CBB
25	8	609	CLA	C4B-C3B-CAB-CBB
25	3	605	CLA	C8-C10-C11-C12
35	A	5008	LMT	C3-C4-C5-C6
52	8	805	P5S	C41-C42-C43-C44
36	B	5003	DGD	O6D-C5D-C6D-O5D
33	B	5005	PTY	C24-C25-C26-C27
25	2	607	CLA	C16-C17-C18-C19
26	7	613	CHL	C11-C12-C13-C15
25	B	1238	CLA	CBA-CGA-O2A-C1
47	4	804	PLM	O1-C1-C2-C3
26	7	613	CHL	C4-C3-C5-C6
25	A	1012	CLA	C2-C3-C5-C6
25	A	1107	CLA	C2-C3-C5-C6
25	A	1134	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	1	802	LHG	C30-C31-C32-C33
33	a	802	PTY	C37-C38-C39-C40
43	1	501	LUT	C29-C30-C31-C32
25	A	1115	CLA	C11-C12-C13-C14
25	B	1219	CLA	C11-C12-C13-C14
25	A	1128	CLA	C12-C13-C15-C16
25	B	1220	CLA	C11-C10-C8-C7
25	7	604	CLA	C12-C13-C15-C16
25	2	621	CLA	C11-C12-C13-C15
26	7	617	CHL	C11-C12-C13-C15
33	7	804	PTY	C13-C14-C15-C16
25	B	1202	CLA	C16-C17-C18-C19
37	B	5004	PCW	C37-C38-C39-C40
37	K	5001	PCW	C39-C40-C41-C42
25	A	1140	CLA	C3A-C2A-CAA-CBA
25	B	1212	CLA	C3A-C2A-CAA-CBA
25	L	1501	CLA	C3A-C2A-CAA-CBA
25	1	605	CLA	C3A-C2A-CAA-CBA
25	3	613	CLA	C3A-C2A-CAA-CBA
25	4	610	CLA	C4-C3-C5-C6
26	A	1114	CHL	C4-C3-C5-C6
26	5	618	CHL	C3A-C2A-CAA-CBA
26	6	610	CHL	C4-C3-C5-C6
26	7	615	CHL	C3A-C2A-CAA-CBA
25	3	602	CLA	CAA-CBA-CGA-O2A
25	A	1102	CLA	C2-C3-C5-C6
33	A	5006	PTY	C35-C36-C37-C38
30	4	801	LHG	C16-C17-C18-C19
25	1	602	CLA	CAA-CBA-CGA-O2A
29	A	4005	BCR	C16-C17-C18-C36
29	B	4003	BCR	C11-C10-C9-C34
29	B	4003	BCR	C20-C21-C22-C37
29	H	4001	BCR	C20-C21-C22-C37
40	3	506	RRX	C16-C17-C18-C36
43	1	503	LUT	C39-C29-C30-C31
43	2	507	LUT	C11-C10-C9-C19
43	2	507	LUT	C40-C33-C34-C35
44	7	504	AXT	C40-C33-C34-C35
30	6	801	LHG	C35-C36-C37-C38
35	1	804	LMT	O1'-C1-C2-C3
25	A	1136	CLA	C10-C11-C12-C13
30	B	5001	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	A	1127	CLA	C5-C6-C7-C8
30	A	5001	LHG	C34-C35-C36-C37
30	5	801	LHG	C26-C27-C28-C29
32	I	5001	SQD	C15-C16-C17-C18
25	A	1109	CLA	C2-C1-O2A-CGA
25	B	1226	CLA	C2-C1-O2A-CGA
25	7	601	CLA	C2-C1-O2A-CGA
25	7	607	CLA	C2-C1-O2A-CGA
29	A	4001	BCR	C9-C10-C11-C12
29	B	4002	BCR	C15-C16-C17-C18
29	3	504	BCR	C13-C14-C15-C16
25	B	1209	CLA	C16-C17-C18-C19
25	6	606	CLA	C16-C17-C18-C19
29	6	504	BCR	C7-C8-C9-C34
30	5	801	LHG	C2-C3-O3-P
30	5	801	LHG	C5-C4-O6-P
30	2	802	LHG	C5-C4-O6-P
33	3	802	PTY	C6-C5-O14-P1
47	4	804	PLM	O2-C1-C2-C3
30	1	802	LHG	C18-C19-C20-C21
25	3	605	CLA	C15-C16-C17-C18
26	A	1114	CHL	C10-C11-C12-C13
37	6	803	PCW	C16-C17-C18-C19
25	A	1117	CLA	C4-C3-C5-C6
25	B	1231	CLA	C4-C3-C5-C6
25	7	606	CLA	C4-C3-C5-C6
26	7	617	CHL	C4-C3-C5-C6
25	A	1122	CLA	C2-C3-C5-C6
25	1	602	CLA	CAA-CBA-CGA-O1A
25	A	1133	CLA	C10-C11-C12-C13
25	B	1223	CLA	C10-C11-C12-C13
30	1	802	LHG	O10-C23-C24-C25
30	5	801	LHG	C9-C10-C11-C12
25	2	605	CLA	C5-C6-C7-C8
25	A	1116	CLA	C11-C10-C8-C9
25	A	1119	CLA	C11-C10-C8-C9
25	A	1122	CLA	C11-C10-C8-C9
25	A	1132	CLA	C11-C10-C8-C9
25	A	1101	CLA	C11-C10-C8-C9
25	B	1231	CLA	C6-C7-C8-C9
25	6	615	CLA	C6-C7-C8-C9
25	2	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	8	604	CHL	C6-C7-C8-C9
26	6	610	CHL	CAA-CBA-CGA-O1A
25	B	1240	CLA	C13-C15-C16-C17
25	3	613	CLA	CAA-CBA-CGA-O2A
33	9	803	PTY	C5-C6-O7-C8
36	8	803	DGD	C1G-C2G-O2G-C1B
25	A	1101	CLA	C10-C11-C12-C13
26	3	604	CHL	C1A-C2A-CAA-CBA
26	8	610	CHL	C1A-C2A-CAA-CBA
48	3	803	DGA	CG1-CG2-CG3-OXT
25	A	1109	CLA	C15-C16-C17-C18
29	K	4001	BCR	C9-C10-C11-C12
29	L	4001	BCR	C19-C20-C21-C22
25	B	1214	CLA	C10-C11-C12-C13
25	B	1021	CLA	CAA-CBA-CGA-O2A
25	4	607	CLA	CAA-CBA-CGA-O2A
25	B	1224	CLA	C2-C3-C5-C6
26	7	613	CHL	C2-C3-C5-C6
25	B	1212	CLA	C8-C10-C11-C12
30	3	801	LHG	C30-C31-C32-C33
32	I	5001	SQD	C24-C25-C26-C27
30	A	5003	LHG	O1-C1-C2-O2
30	4	802	LHG	O10-C23-O8-C6
25	A	1126	CLA	C13-C15-C16-C17
25	B	1022	CLA	C2A-CAA-CBA-CGA
25	B	1202	CLA	C2A-CAA-CBA-CGA
25	1	603	CLA	C2A-CAA-CBA-CGA
25	6	603	CLA	C2A-CAA-CBA-CGA
25	B	1210	CLA	C13-C15-C16-C17
48	2	803	DGA	CA4-CA5-CA6-CA7
25	A	1105	CLA	C1A-C2A-CAA-CBA
25	A	1140	CLA	C1A-C2A-CAA-CBA
25	3	613	CLA	C1A-C2A-CAA-CBA
25	6	606	CLA	C1A-C2A-CAA-CBA
25	6	618	CLA	C1A-C2A-CAA-CBA
25	8	608	CLA	C1A-C2A-CAA-CBA
29	A	4005	BCR	C16-C17-C18-C19
29	B	4003	BCR	C11-C10-C9-C8
29	B	4003	BCR	C20-C21-C22-C23
40	3	506	RRX	C16-C17-C18-C19
43	1	503	LUT	C28-C29-C30-C31
43	2	507	LUT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
43	2	507	LUT	C32-C33-C34-C35
44	7	504	AXT	C32-C33-C34-C35
25	8	620	CLA	C2C-C3C-CAC-CBC
51	7	807	4RF	C15-C16-O18-C19
41	4	805	SPH	C6-C7-C8-C9
25	A	1110	CLA	C6-C7-C8-C9
25	A	1116	CLA	C11-C12-C13-C15
25	A	1132	CLA	C16-C17-C18-C20
37	B	5004	PCW	C35-C36-C37-C38
41	6	806	SPH	C7-C8-C9-C10
26	4	609	CHL	C15-C16-C17-C18
25	A	1104	CLA	C2B-C3B-CAB-CBB
25	A	1125	CLA	C2B-C3B-CAB-CBB
25	A	1134	CLA	C2B-C3B-CAB-CBB
25	B	1022	CLA	C2B-C3B-CAB-CBB
25	B	1204	CLA	C2B-C3B-CAB-CBB
25	B	1214	CLA	C2B-C3B-CAB-CBB
25	B	1220	CLA	C2B-C3B-CAB-CBB
25	B	1224	CLA	C2B-C3B-CAB-CBB
25	K	1404	CLA	C2B-C3B-CAB-CBB
25	1	612	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C2B-C3B-CAB-CBB
25	a	612	CLA	C2B-C3B-CAB-CBB
25	4	607	CLA	C2B-C3B-CAB-CBB
25	4	610	CLA	C2B-C3B-CAB-CBB
25	4	615	CLA	C2B-C3B-CAB-CBB
25	4	616	CLA	C2B-C3B-CAB-CBB
25	5	607	CLA	C2B-C3B-CAB-CBB
25	5	615	CLA	C2B-C3B-CAB-CBB
25	6	618	CLA	C2B-C3B-CAB-CBB
25	8	609	CLA	C2B-C3B-CAB-CBB
25	2	608	CLA	C2B-C3B-CAB-CBB
25	2	612	CLA	C2B-C3B-CAB-CBB
25	2	615	CLA	C2B-C3B-CAB-CBB
29	A	4001	BCR	C23-C24-C25-C26
29	A	4004	BCR	C5-C6-C7-C8
29	B	4001	BCR	C5-C6-C7-C8
29	B	4001	BCR	C23-C24-C25-C30
29	B	4002	BCR	C23-C24-C25-C26
29	B	4004	BCR	C23-C24-C25-C26
29	B	4005	BCR	C23-C24-C25-C30
29	B	4006	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	G	4001	BCR	C1-C6-C7-C8
29	H	4001	BCR	C5-C6-C7-C8
29	J	4001	BCR	C23-C24-C25-C26
29	K	4001	BCR	C1-C6-C7-C8
29	L	4003	BCR	C5-C6-C7-C8
29	L	4003	BCR	C23-C24-C25-C26
29	L	4001	BCR	C5-C6-C7-C8
29	3	503	BCR	C23-C24-C25-C26
29	4	503	BCR	C5-C6-C7-C8
29	5	503	BCR	C23-C24-C25-C30
29	6	504	BCR	C23-C24-C25-C26
40	J	4002	RRX	C1-C6-C7-C8
42	M	4001	ECH	C23-C24-C25-C30
43	5	505	LUT	C1-C6-C7-C8
43	7	501	LUT	C1-C6-C7-C8
43	9	502	LUT	C1-C6-C7-C8
30	B	5001	LHG	C29-C30-C31-C32
41	6	806	SPH	C6-C7-C8-C9
26	7	609	CHL	C14-C13-C15-C16
26	8	604	CHL	C14-C13-C15-C16
25	A	1101	CLA	C16-C17-C18-C19
41	4	805	SPH	O1-C1-C2-N2
45	1	803	OLA	O1-C1-C2-C3
25	A	1113	CLA	C4-C3-C5-C6
25	B	1239	CLA	C4-C3-C5-C6
25	B	1207	CLA	C4-C3-C5-C6
25	4	602	CLA	C4-C3-C5-C6
26	a	609	CHL	C4-C3-C5-C6
26	9	601	CHL	C4-C3-C5-C6
30	A	5002	LHG	C33-C34-C35-C36
30	5	801	LHG	O6-C4-C5-C6
25	A	1117	CLA	C2-C3-C5-C6
26	6	610	CHL	C2-C3-C5-C6
30	9	802	LHG	C10-C11-C12-C13
25	B	1237	CLA	C5-C6-C7-C8
25	B	1202	CLA	C5-C6-C7-C8
25	7	610	CLA	C10-C11-C12-C13
25	A	1013	CLA	C11-C10-C8-C7
25	A	1113	CLA	C6-C7-C8-C10
25	A	1121	CLA	C11-C10-C8-C7
25	A	1133	CLA	C6-C7-C8-C10
25	A	1133	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	A	1136	CLA	C11-C10-C8-C7
25	A	1138	CLA	C11-C12-C13-C15
25	1	605	CLA	C12-C13-C15-C16
25	4	604	CLA	C6-C7-C8-C10
25	4	612	CLA	C11-C10-C8-C7
25	6	606	CLA	C11-C12-C13-C15
25	7	603	CLA	C12-C13-C15-C16
26	5	610	CHL	C11-C12-C13-C15
26	8	603	CHL	C11-C12-C13-C15
25	A	1119	CLA	C16-C17-C18-C20
25	B	1215	CLA	C11-C12-C13-C15
25	2	607	CLA	C16-C17-C18-C20
25	B	1201	CLA	C2A-CAA-CBA-CGA
25	9	612	CLA	C2A-CAA-CBA-CGA
26	1	609	CHL	C2C-C3C-CAC-CBC
30	1	801	LHG	C25-C26-C27-C28
30	6	801	LHG	C26-C27-C28-C29
47	4	804	PLM	C8-C9-CA-CB
25	B	1209	CLA	C3-C5-C6-C7
25	8	608	CLA	CBD-CGD-O2D-CED
32	G	5001	SQD	C15-C16-C17-C18
30	A	5002	LHG	C1-C2-C3-O3
25	G	1602	CLA	C4-C3-C5-C6
25	A	1116	CLA	C2-C3-C5-C6
25	B	1205	CLA	C2-C3-C5-C6
25	4	610	CLA	C2-C3-C5-C6
25	5	607	CLA	C2-C3-C5-C6
26	7	617	CHL	C2-C3-C5-C6
25	7	604	CLA	C2-C1-O2A-CGA
26	8	610	CHL	C2-C1-O2A-CGA
43	8	502	LUT	C7-C8-C9-C10
32	I	5001	SQD	C30-C31-C32-C33
33	9	803	PTY	C31-C32-C33-C34
48	3	803	DGA	OA1-CA1-CA2-CA3
30	1	802	LHG	C11-C10-C9-C8
34	A	5007	3PH	C25-C26-C27-C28
25	A	1109	CLA	CBA-CGA-O2A-C1
47	4	803	PLM	CC-CD-CE-CF
25	B	1234	CLA	C2A-CAA-CBA-CGA
25	B	1229	CLA	C6-C7-C8-C9
25	a	607	CLA	C6-C7-C8-C9
25	7	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
53	8	810	LAP	O1-C13-C14-C15
47	6	804	PLM	CA-CB-CC-CD
47	8	807	PLM	C4-C5-C6-C7
29	B	4007	BCR	C15-C16-C17-C18
29	H	4001	BCR	C13-C14-C15-C16
30	A	5002	LHG	C29-C30-C31-C32
37	K	5002	PCW	C16-C17-C18-C19
30	2	802	LHG	C29-C30-C31-C32
25	B	1206	CLA	C4-C3-C5-C6
30	A	5002	LHG	C2-C3-O3-P
25	2	603	CLA	CAA-CBA-CGA-O2A
25	B	1231	CLA	C2-C3-C5-C6
25	B	1207	CLA	C2-C3-C5-C6
25	7	606	CLA	C2-C3-C5-C6
25	B	1222	CLA	CBA-CGA-O2A-C1
33	9	803	PTY	C39-C40-C41-C42
25	7	602	CLA	CAA-CBA-CGA-O2A
32	H	5001	SQD	C2-C1-O6-C44
30	A	5002	LHG	C4-C5-C6-O8
30	7	801	LHG	C4-C5-C6-O8
36	8	802	DGD	C1G-C2G-C3G-O3G
45	1	803	OLA	O2-C1-C2-C3
47	8	806	PLM	C7-C8-C9-CA
25	B	1238	CLA	O1A-CGA-O2A-C1
51	7	807	4RF	O17-C16-O18-C19
25	B	1203	CLA	C16-C17-C18-C19
25	A	1113	CLA	CAA-CBA-CGA-O2A
41	J	5002	SPH	C15-C16-C17-C18
30	6	801	LHG	O6-C4-C5-O7
33	a	802	PTY	O14-C5-C6-O7
25	A	1127	CLA	C4-C3-C5-C6
25	B	1210	CLA	C4-C3-C5-C6
25	L	1502	CLA	C4-C3-C5-C6
25	B	1232	CLA	CAA-CBA-CGA-O2A
47	6	804	PLM	O2-C1-C2-C3
25	5	614	CLA	CAA-CBA-CGA-O1A
25	2	604	CLA	CAA-CBA-CGA-O1A
30	1	802	LHG	C17-C18-C19-C20
30	2	801	LHG	C30-C31-C32-C33
25	A	1129	CLA	C4B-C3B-CAB-CBB
25	B	1220	CLA	C4B-C3B-CAB-CBB
25	K	1404	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	5	607	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	C4B-C3B-CAB-CBB
25	8	612	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	O1A-CGA-O2A-C1
32	I	5001	SQD	C16-C17-C18-C19
47	6	804	PLM	O1-C1-C2-C3
25	B	1214	CLA	C11-C12-C13-C14
25	3	612	CLA	CAA-CBA-CGA-O2A
25	5	601	CLA	C8-C10-C11-C12
25	L	1503	CLA	CAA-CBA-CGA-O2A
26	a	613	CHL	CHA-CBD-CGD-O1D
26	a	613	CHL	CHA-CBD-CGD-O2D
26	3	603	CHL	CHA-CBD-CGD-O1D
26	3	603	CHL	CHA-CBD-CGD-O2D
26	3	604	CHL	CHA-CBD-CGD-O1D
26	5	610	CHL	CHA-CBD-CGD-O1D
26	5	610	CHL	CHA-CBD-CGD-O2D
26	5	611	CHL	CHA-CBD-CGD-O1D
26	5	618	CHL	CHA-CBD-CGD-O1D
26	5	618	CHL	CHA-CBD-CGD-O2D
26	6	611	CHL	CHA-CBD-CGD-O1D
26	6	611	CHL	CHA-CBD-CGD-O2D
26	8	601	CHL	CHA-CBD-CGD-O1D
26	8	603	CHL	CHA-CBD-CGD-O1D
26	8	603	CHL	CHA-CBD-CGD-O2D
26	8	610	CHL	CHA-CBD-CGD-O1D
26	8	610	CHL	CHA-CBD-CGD-O2D
26	9	601	CHL	CHA-CBD-CGD-O1D
26	9	603	CHL	CHA-CBD-CGD-O1D
26	9	603	CHL	CHA-CBD-CGD-O2D
26	9	608	CHL	CHA-CBD-CGD-O1D
26	9	608	CHL	CHA-CBD-CGD-O2D
50	9	507	XAT	C40-C33-C34-C35
25	B	1226	CLA	C13-C15-C16-C17
25	a	602	CLA	C2A-CAA-CBA-CGA
33	J	5001	PTY	C33-C34-C35-C36
25	K	1404	CLA	CAA-CBA-CGA-O2A
25	4	617	CLA	CAA-CBA-CGA-O2A
25	7	605	CLA	CAA-CBA-CGA-O1A
47	5	804	PLM	O2-C1-C2-C3
37	B	5004	PCW	C13-C14-C15-C16
30	7	802	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	4	802	LHG	C5-C6-O8-C23
30	7	801	LHG	O6-C4-C5-C6
37	K	5002	PCW	O3P-C1-C2-C3
25	a	608	CLA	CAA-CBA-CGA-O2A
33	9	803	PTY	C37-C38-C39-C40
47	6	804	PLM	C7-C8-C9-CA
25	7	607	CLA	C2-C3-C5-C6
45	8	809	OLA	C7-C8-C9-C10
30	A	5001	LHG	C17-C18-C19-C20
30	4	802	LHG	C2-C3-O3-P
25	L	1503	CLA	CAA-CBA-CGA-O1A
36	8	802	DGD	CCA-CDA-CEA-CFA
29	A	4005	BCR	C9-C10-C11-C12
25	6	603	CLA	C16-C17-C18-C20
33	3	802	PTY	C13-C14-C15-C16
47	5	804	PLM	O1-C1-C2-C3
25	A	1103	CLA	C6-C7-C8-C9
25	A	1138	CLA	C11-C10-C8-C9
25	B	1216	CLA	C11-C10-C8-C9
25	B	1235	CLA	C11-C12-C13-C14
25	7	610	CLA	C11-C10-C8-C9
26	4	609	CHL	C14-C13-C15-C16
27	A	2001	PQN	C19-C18-C20-C21
30	F	5001	LHG	C17-C18-C19-C20
32	A	5005	SQD	C45-C44-O6-C1
30	A	5003	LHG	C9-C10-C11-C12
25	6	618	CLA	CAA-CBA-CGA-O1A
25	7	605	CLA	CAA-CBA-CGA-O2A
25	a	605	CLA	C2A-CAA-CBA-CGA
26	5	610	CHL	C2A-CAA-CBA-CGA
25	A	1102	CLA	C2-C1-O2A-CGA
25	B	1239	CLA	C2-C1-O2A-CGA
25	5	601	CLA	C2-C1-O2A-CGA
25	6	603	CLA	C2-C1-O2A-CGA
25	6	604	CLA	C2-C1-O2A-CGA
25	8	605	CLA	C2-C1-O2A-CGA
26	a	606	CHL	C2-C1-O2A-CGA
25	B	1204	CLA	C16-C17-C18-C20
47	4	803	PLM	CD-CE-CF-CG
25	A	1127	CLA	C3A-C2A-CAA-CBA
25	B	1201	CLA	C3A-C2A-CAA-CBA
25	B	1231	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	a	613	CHL	C3A-C2A-CAA-CBA
26	7	617	CHL	C3A-C2A-CAA-CBA
26	8	610	CHL	C4-C3-C5-C6
25	B	1232	CLA	CAA-CBA-CGA-O1A
35	1	804	LMT	C3'-C4'-O1B-C1B
25	B	1206	CLA	O1A-CGA-O2A-C1
30	A	5002	LHG	C10-C11-C12-C13
32	I	5001	SQD	C17-C18-C19-C20
25	7	602	CLA	CAA-CBA-CGA-O1A
25	6	612	CLA	CBA-CGA-O2A-C1
25	A	1126	CLA	CAA-CBA-CGA-O2A
33	9	803	PTY	C1-C6-O7-C8
36	8	803	DGD	C3G-C2G-O2G-C1B
45	a	805	OLA	C7-C8-C9-C10
45	8	809	OLA	C9-C10-C11-C12
41	J	5002	SPH	C9-C10-C11-C12
30	7	803	LHG	C10-C11-C12-C13
30	2	802	LHG	O8-C23-C24-C25
25	6	615	CLA	C16-C17-C18-C20
37	K	5001	PCW	C14-C15-C16-C17
25	B	1206	CLA	CBA-CGA-O2A-C1
37	B	5004	PCW	C39-C40-C41-C42
25	H	1702	CLA	CBA-CGA-O2A-C1
30	9	801	LHG	C2-C3-O3-P
25	B	1225	CLA	C3-C5-C6-C7
30	5	801	LHG	O6-C4-C5-O7
25	4	608	CLA	O1D-CGD-O2D-CED
33	G	5002	PTY	C15-C16-C17-C18
45	8	809	OLA	O2-C1-C2-C3
25	A	1109	CLA	O1A-CGA-O2A-C1
25	B	1222	CLA	O1A-CGA-O2A-C1
25	1	603	CLA	C8-C10-C11-C12
25	K	1404	CLA	CAA-CBA-CGA-O1A
30	2	801	LHG	C32-C33-C34-C35
41	6	806	SPH	C4-C5-C6-C7
25	B	1219	CLA	C2A-CAA-CBA-CGA
33	G	5003	PTY	C6-C1-O4-C30
36	B	5003	DGD	CCA-CDA-CEA-CFA
25	B	1213	CLA	CAA-CBA-CGA-O2A
25	3	616	CLA	CAA-CBA-CGA-O2A
25	2	602	CLA	CAA-CBA-CGA-O2A
30	5	801	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	8	618	CLA	C8-C10-C11-C12
30	6	802	LHG	C26-C27-C28-C29
30	6	801	LHG	C29-C30-C31-C32
30	9	801	LHG	O7-C5-C6-O8
25	5	608	CLA	CAA-CBA-CGA-O1A
25	5	607	CLA	C8-C10-C11-C12
25	B	1021	CLA	C11-C12-C13-C14
25	B	1209	CLA	C11-C10-C8-C9
25	B	1224	CLA	C6-C7-C8-C9
25	B	1239	CLA	C14-C13-C15-C16
25	6	615	CLA	C11-C10-C8-C9
25	2	605	CLA	C6-C7-C8-C9
26	A	1114	CHL	C11-C12-C13-C14
25	A	1119	CLA	C16-C17-C18-C19
25	B	1210	CLA	C16-C17-C18-C19
25	A	1121	CLA	CAA-CBA-CGA-O2A
25	7	612	CLA	CAA-CBA-CGA-O2A
37	K	5001	PCW	O2-C31-C32-C33
48	8	804	DGA	OG2-CB1-CB2-CB3
25	5	608	CLA	CAA-CBA-CGA-O2A
29	8	503	BCR	C11-C12-C13-C14
25	1	606	CLA	O1A-CGA-O2A-C1
33	G	5002	PTY	C18-C19-C20-C21
30	8	801	LHG	O8-C23-C24-C25
37	B	5004	PCW	O2-C31-C32-C33
26	9	608	CHL	C2-C1-O2A-CGA
25	4	617	CLA	CAA-CBA-CGA-O1A
25	1	601	CLA	C2A-CAA-CBA-CGA
25	8	615	CLA	C2A-CAA-CBA-CGA
32	H	5001	SQD	C17-C18-C19-C20
25	A	1103	CLA	C6-C7-C8-C10
25	A	1111	CLA	C11-C10-C8-C7
25	A	1138	CLA	C11-C10-C8-C7
25	B	1203	CLA	C11-C10-C8-C7
25	B	1224	CLA	C11-C12-C13-C15
25	B	1229	CLA	C6-C7-C8-C10
25	B	1234	CLA	C6-C7-C8-C10
25	7	612	CLA	C6-C7-C8-C10
25	2	603	CLA	C11-C10-C8-C7
25	2	605	CLA	C11-C10-C8-C7
26	1	609	CHL	C11-C12-C13-C15
26	9	603	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
47	4	803	PLM	C8-C9-CA-CB
25	5	602	CLA	O1A-CGA-O2A-C1
30	1	802	LHG	C19-C20-C21-C22
45	8	809	OLA	O1-C1-C2-C3
25	A	1012	CLA	C2B-C3B-CAB-CBB
25	A	1126	CLA	C2B-C3B-CAB-CBB
25	A	1131	CLA	C2B-C3B-CAB-CBB
25	A	1132	CLA	C2B-C3B-CAB-CBB
25	5	603	CLA	C2B-C3B-CAB-CBB
25	5	614	CLA	C2B-C3B-CAB-CBB
25	6	608	CLA	C2B-C3B-CAB-CBB
25	8	612	CLA	C2B-C3B-CAB-CBB
25	8	618	CLA	C2B-C3B-CAB-CBB
25	9	607	CLA	C2B-C3B-CAB-CBB
25	9	612	CLA	C2B-C3B-CAB-CBB
29	A	4001	BCR	C1-C6-C7-C8
29	A	4001	BCR	C5-C6-C7-C8
29	A	4003	BCR	C23-C24-C25-C26
29	B	4001	BCR	C23-C24-C25-C26
29	B	4003	BCR	C23-C24-C25-C26
29	B	4003	BCR	C23-C24-C25-C30
29	B	4005	BCR	C23-C24-C25-C26
29	B	4006	BCR	C23-C24-C25-C26
29	K	4001	BCR	C5-C6-C7-C8
29	K	4002	BCR	C1-C6-C7-C8
29	K	4002	BCR	C5-C6-C7-C8
29	5	503	BCR	C23-C24-C25-C26
40	3	506	RRX	C23-C24-C25-C26
42	M	4001	ECH	C5-C6-C7-C8
43	1	501	LUT	C5-C6-C7-C8
43	4	501	LUT	C1-C6-C7-C8
43	4	501	LUT	C5-C6-C7-C8
43	5	502	LUT	C1-C6-C7-C8
43	5	502	LUT	C5-C6-C7-C8
43	6	501	LUT	C5-C6-C7-C8
43	6	502	LUT	C1-C6-C7-C8
43	6	502	LUT	C5-C6-C7-C8
43	7	501	LUT	C5-C6-C7-C8
43	8	502	LUT	C1-C6-C7-C8
43	8	502	LUT	C5-C6-C7-C8
43	9	501	LUT	C1-C6-C7-C8
43	9	502	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	1110	CLA	CAA-CBA-CGA-O2A
25	B	1240	CLA	CAA-CBA-CGA-O2A
25	2	605	CLA	CAA-CBA-CGA-O2A
26	9	608	CHL	CAA-CBA-CGA-O2A
30	A	5002	LHG	O7-C7-C8-C9
30	B	5001	LHG	O8-C23-C24-C25
33	A	5006	PTY	C12-C11-C8-O7
33	5	802	PTY	O4-C30-C31-C32
47	8	806	PLM	C3-C4-C5-C6
25	A	1127	CLA	O1A-CGA-O2A-C1
36	B	5003	DGD	CAA-CBA-CCA-CDA
30	6	802	LHG	O8-C23-C24-C25
25	A	1113	CLA	C10-C11-C12-C13
25	5	602	CLA	CBA-CGA-O2A-C1
25	B	1237	CLA	C16-C17-C18-C19
30	6	801	LHG	C15-C16-C17-C18
25	B	1204	CLA	CAA-CBA-CGA-O2A
25	6	601	CLA	CAA-CBA-CGA-O2A
25	7	608	CLA	CAA-CBA-CGA-O2A
26	9	601	CHL	CAA-CBA-CGA-O2A
25	B	1023	CLA	C2C-C3C-CAC-CBC
47	8	807	PLM	O1-C1-C2-C3
45	8	808	OLA	C9-C10-C11-C12
25	B	1222	CLA	C2A-CAA-CBA-CGA
25	7	601	CLA	C2A-CAA-CBA-CGA
30	6	802	LHG	C29-C30-C31-C32
33	a	802	PTY	C34-C35-C36-C37
25	A	1109	CLA	C5-C6-C7-C8
35	2	804	LMT	C5'-C4'-O1B-C1B
25	A	1112	CLA	CAA-CBA-CGA-O2A
26	7	611	CHL	CAA-CBA-CGA-O2A
30	6	801	LHG	O8-C23-C24-C25
33	a	803	PTY	O4-C30-C31-C32
33	9	803	PTY	C41-C42-C43-C44
36	B	5003	DGD	CFA-CGA-CHA-CIA
25	A	1122	CLA	CAA-CBA-CGA-O2A
25	B	1211	CLA	CAA-CBA-CGA-O2A
25	B	1238	CLA	CAA-CBA-CGA-O2A
25	a	603	CLA	CAA-CBA-CGA-O2A
26	6	619	CHL	CAA-CBA-CGA-O2A
26	7	615	CHL	CAA-CBA-CGA-O2A
30	A	5002	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	G	5003	PTY	C12-C11-C8-O7
33	J	5001	PTY	C12-C11-C8-O7
30	A	5002	LHG	C19-C20-C21-C22
32	7	805	SQD	C4-C5-C6-S
25	6	606	CLA	C4-C3-C5-C6
25	B	1210	CLA	CAA-CBA-CGA-O2A
25	L	1504	CLA	CAA-CBA-CGA-O2A
25	6	603	CLA	CAA-CBA-CGA-O2A
25	8	609	CLA	CAA-CBA-CGA-O2A
25	B	1239	CLA	C2-C3-C5-C6
26	4	609	CHL	C16-C17-C18-C20
34	A	5007	3PH	C33-C34-C35-C36
25	4	607	CLA	C5-C6-C7-C8
33	7	804	PTY	O4-C30-C31-C32
26	2	609	CHL	CAA-CBA-CGA-O1A
25	A	1131	CLA	C13-C15-C16-C17
25	A	1013	CLA	C11-C10-C8-C9
25	A	1013	CLA	C11-C12-C13-C14
25	A	1132	CLA	C14-C13-C15-C16
25	B	1205	CLA	C14-C13-C15-C16
25	B	1220	CLA	C6-C7-C8-C9
25	B	1228	CLA	C11-C12-C13-C14
25	4	604	CLA	C6-C7-C8-C9
25	4	610	CLA	C14-C13-C15-C16
25	6	606	CLA	C11-C12-C13-C14
25	A	1134	CLA	C5-C6-C7-C8
29	I	4001	BCR	C11-C12-C13-C35
24	A	1011	CL0	CAA-CBA-CGA-O2A
25	5	606	CLA	CAA-CBA-CGA-O2A
25	7	603	CLA	CAA-CBA-CGA-O2A
26	1	613	CHL	CAA-CBA-CGA-O2A
26	a	604	CHL	CAA-CBA-CGA-O2A
32	A	5005	SQD	O48-C23-C24-C25
25	3	601	CLA	O1A-CGA-O2A-C1
30	A	5001	LHG	C4-C5-C6-O8
30	2	802	LHG	C4-C5-C6-O8
32	A	5005	SQD	O6-C44-C45-C46
47	4	804	PLM	C3-C4-C5-C6
25	A	1115	CLA	C4B-C3B-CAB-CBB
25	A	1139	CLA	C4B-C3B-CAB-CBB
25	B	1023	CLA	C4B-C3B-CAB-CBB
25	B	1218	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	1232	CLA	C4B-C3B-CAB-CBB
25	B	1238	CLA	C4B-C3B-CAB-CBB
25	G	1601	CLA	C1A-C2A-CAA-CBA
25	G	1601	CLA	C4B-C3B-CAB-CBB
25	K	1403	CLA	C4B-C3B-CAB-CBB
25	4	617	CLA	C4B-C3B-CAB-CBB
25	5	603	CLA	C4B-C3B-CAB-CBB
25	5	609	CLA	C1A-C2A-CAA-CBA
25	5	614	CLA	C4B-C3B-CAB-CBB
25	6	608	CLA	C4B-C3B-CAB-CBB
25	6	602	CLA	C4B-C3B-CAB-CBB
25	6	603	CLA	C4B-C3B-CAB-CBB
25	6	606	CLA	C4B-C3B-CAB-CBB
25	7	602	CLA	C4B-C3B-CAB-CBB
25	8	602	CLA	C4B-C3B-CAB-CBB
25	8	606	CLA	C1A-C2A-CAA-CBA
25	8	607	CLA	C1A-C2A-CAA-CBA
25	8	618	CLA	C4B-C3B-CAB-CBB
25	2	602	CLA	C4B-C3B-CAB-CBB
25	2	612	CLA	C1A-C2A-CAA-CBA
25	9	607	CLA	C4B-C3B-CAB-CBB
30	7	803	LHG	C29-C30-C31-C32
25	A	1127	CLA	CBA-CGA-O2A-C1
25	8	609	CLA	C3-C5-C6-C7
25	A	1106	CLA	C4-C3-C5-C6
26	4	609	CHL	C4-C3-C5-C6
25	B	1023	CLA	C10-C11-C12-C13
25	A	1108	CLA	CAA-CBA-CGA-O2A
25	A	1130	CLA	CAA-CBA-CGA-O2A
25	1	603	CLA	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
30	4	801	LHG	O8-C23-C24-C25
30	7	801	LHG	O8-C23-C24-C25
26	A	1114	CHL	C2-C3-C5-C6
29	B	4006	BCR	C21-C22-C23-C24
29	I	4001	BCR	C11-C12-C13-C14
29	6	504	BCR	C7-C8-C9-C10
29	6	504	BCR	C17-C18-C19-C20
29	L	4002	BCR	C15-C16-C17-C18
29	L	4002	BCR	C19-C20-C21-C22
30	A	5002	LHG	C17-C18-C19-C20
26	4	609	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	B	1209	CLA	CAA-CBA-CGA-O2A
25	1	605	CLA	CAA-CBA-CGA-O2A
25	5	603	CLA	CAA-CBA-CGA-O2A
25	2	601	CLA	CAA-CBA-CGA-O2A
25	9	605	CLA	C2A-CAA-CBA-CGA
36	7	806	DGD	C7A-C8A-C9A-CAA
33	a	802	PTY	O14-C5-C6-C1
25	B	1208	CLA	CAA-CBA-CGA-O2A
25	a	607	CLA	CAA-CBA-CGA-O2A
25	6	612	CLA	CAA-CBA-CGA-O2A
26	1	611	CHL	CAA-CBA-CGA-O2A
25	B	1215	CLA	C10-C11-C12-C13
25	A	1135	CLA	C2-C3-C5-C6
25	5	609	CLA	C2-C3-C5-C6
33	G	5003	PTY	C15-C16-C17-C18
25	B	1217	CLA	C2-C1-O2A-CGA
25	5	604	CLA	C2-C1-O2A-CGA
25	7	603	CLA	C2-C1-O2A-CGA
26	7	611	CHL	C2-C1-O2A-CGA
26	9	610	CHL	C2-C1-O2A-CGA
30	8	801	LHG	O7-C7-C8-C9
30	5	801	LHG	C25-C26-C27-C28
25	A	1108	CLA	C11-C12-C13-C15
25	B	1205	CLA	C11-C12-C13-C15
25	B	1234	CLA	C12-C13-C15-C16
25	5	612	CLA	C12-C13-C15-C16
25	6	606	CLA	C11-C10-C8-C7
25	7	610	CLA	C11-C10-C8-C7
26	1	609	CHL	C6-C7-C8-C10
26	7	617	CHL	C11-C10-C8-C7
27	A	2001	PQN	C17-C18-C20-C21
25	1	606	CLA	CBA-CGA-O2A-C1
25	1	607	CLA	C16-C17-C18-C20
36	8	802	DGD	C6A-C7A-C8A-C9A
33	a	802	PTY	O4-C30-C31-C32
30	5	801	LHG	C16-C17-C18-C19
26	8	603	CHL	C2A-CAA-CBA-CGA
26	8	601	CHL	C11-C12-C13-C14
25	A	1133	CLA	C15-C16-C17-C18
25	6	606	CLA	C5-C6-C7-C8
25	2	603	CLA	C10-C11-C12-C13
26	1	604	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	3	601	CLA	CBA-CGA-O2A-C1
25	B	1206	CLA	C3A-C2A-CAA-CBA
25	G	1601	CLA	C3A-C2A-CAA-CBA
25	6	612	CLA	C3A-C2A-CAA-CBA
25	7	605	CLA	CHA-CBD-CGD-O1D
26	4	618	CHL	C3A-C2A-CAA-CBA
25	A	1121	CLA	CAA-CBA-CGA-O1A
25	3	616	CLA	CAA-CBA-CGA-O1A
26	9	608	CHL	CAA-CBA-CGA-O1A
25	A	1113	CLA	C8-C10-C11-C12
25	A	1113	CLA	C2-C3-C5-C6
25	G	1602	CLA	C2-C3-C5-C6
25	4	602	CLA	C2-C3-C5-C6
47	8	807	PLM	O2-C1-C2-C3
30	A	5001	LHG	C5-C6-O8-C23
30	7	801	LHG	C24-C25-C26-C27
33	5	802	PTY	C16-C17-C18-C19
25	A	1112	CLA	CAA-CBA-CGA-O1A
25	B	1213	CLA	CAA-CBA-CGA-O1A
33	A	5006	PTY	C12-C11-C8-O10
30	A	5003	LHG	C18-C19-C20-C21
30	6	802	LHG	C30-C31-C32-C33
25	6	604	CLA	C5-C6-C7-C8
30	B	5002	LHG	C27-C28-C29-C30
25	F	1301	CLA	CAA-CBA-CGA-O2A
25	H	1702	CLA	CAA-CBA-CGA-O2A
25	K	1402	CLA	CAA-CBA-CGA-O2A
26	8	604	CHL	CAA-CBA-CGA-O2A
48	2	803	DGA	OG2-CB1-CB2-CB3
33	a	803	PTY	C13-C14-C15-C16
25	A	1130	CLA	CAA-CBA-CGA-O1A
26	6	619	CHL	CAA-CBA-CGA-O1A
26	7	611	CHL	CAA-CBA-CGA-O1A
25	2	608	CLA	CAA-CBA-CGA-O2A
25	A	1125	CLA	C6-C7-C8-C9
25	A	1133	CLA	C6-C7-C8-C9
25	A	1138	CLA	C11-C12-C13-C14
25	B	1234	CLA	C14-C13-C15-C16
25	1	605	CLA	C14-C13-C15-C16
25	G	1602	CLA	CAA-CBA-CGA-O2A
25	B	1211	CLA	CAA-CBA-CGA-O1A
25	2	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	7	615	CHL	CAA-CBA-CGA-O1A
30	A	5002	LHG	O10-C23-C24-C25
30	8	801	LHG	O9-C7-C8-C9
30	F	5001	LHG	C27-C28-C29-C30
25	3	605	CLA	C4-C3-C5-C6
25	A	1108	CLA	CAA-CBA-CGA-O1A
25	A	1122	CLA	CAA-CBA-CGA-O1A
25	L	1504	CLA	CAA-CBA-CGA-O1A
25	a	603	CLA	CAA-CBA-CGA-O1A
25	6	603	CLA	CAA-CBA-CGA-O1A
26	1	611	CHL	CAA-CBA-CGA-O1A
30	8	801	LHG	O10-C23-C24-C25
47	5	804	PLM	C9-CA-CB-CC
30	5	801	LHG	O8-C23-C24-C25
25	3	605	CLA	C2-C3-C5-C6
32	G	5001	SQD	O5-C5-C6-S
32	I	5001	SQD	O5-C5-C6-S
43	a	502	LUT	C21-C26-C27-C28
43	3	501	LUT	C21-C26-C27-C28
43	3	502	LUT	C21-C26-C27-C28
43	6	502	LUT	C21-C26-C27-C28
46	a	504	QTB	C09-C10-C11-C17
26	a	613	CHL	CAA-CBA-CGA-O2A
25	B	1210	CLA	CAA-CBA-CGA-O1A
25	5	606	CLA	CAA-CBA-CGA-O1A
25	7	608	CLA	CAA-CBA-CGA-O1A
30	A	5002	LHG	O9-C7-C8-C9
30	5	801	LHG	O9-C7-C8-C9
33	J	5001	PTY	C12-C11-C8-O10
33	a	803	PTY	O30-C30-C31-C32
25	7	606	CLA	C5-C6-C7-C8
30	A	5003	LHG	C31-C32-C33-C34
30	6	801	LHG	C18-C19-C20-C21
35	1	804	LMT	C3-C4-C5-C6
25	B	1237	CLA	CAA-CBA-CGA-O2A
25	B	1023	CLA	C16-C17-C18-C20
25	A	1132	CLA	C5-C6-C7-C8
25	3	605	CLA	C10-C11-C12-C13
33	B	5005	PTY	C22-C23-C24-C25
25	A	1110	CLA	CAA-CBA-CGA-O1A
25	7	603	CLA	CAA-CBA-CGA-O1A
32	A	5005	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
37	K	5001	PCW	O31-C31-C32-C33
25	5	601	CLA	O1A-CGA-O2A-C1
30	F	5002	LHG	O7-C5-C6-O8
25	B	1224	CLA	C3-C5-C6-C7
25	B	1208	CLA	CAA-CBA-CGA-O1A
25	5	603	CLA	CAA-CBA-CGA-O1A
25	6	601	CLA	CAA-CBA-CGA-O1A
25	7	612	CLA	CAA-CBA-CGA-O1A
26	9	601	CHL	CAA-CBA-CGA-O1A
30	B	5001	LHG	O10-C23-C24-C25
30	4	801	LHG	O10-C23-C24-C25
30	6	802	LHG	O10-C23-C24-C25
30	6	801	LHG	O10-C23-C24-C25
33	5	802	PTY	O30-C30-C31-C32
48	8	804	DGA	OB1-CB1-CB2-CB3
25	A	1116	CLA	CAA-CBA-CGA-O2A
30	1	801	LHG	O8-C23-C24-C25
25	L	1501	CLA	C2A-CAA-CBA-CGA
26	2	613	CHL	C2A-CAA-CBA-CGA
30	B	5002	LHG	C34-C35-C36-C37
30	F	5002	LHG	C4-C5-C6-O8
25	B	1238	CLA	CAA-CBA-CGA-O1A
25	1	603	CLA	CAA-CBA-CGA-O1A
25	6	612	CLA	CAA-CBA-CGA-O1A
25	8	609	CLA	CAA-CBA-CGA-O1A
33	7	804	PTY	O30-C30-C31-C32
25	A	1108	CLA	C5-C6-C7-C8
25	B	1228	CLA	CAA-CBA-CGA-O2A
25	B	1204	CLA	CAA-CBA-CGA-O1A
30	7	801	LHG	O10-C23-C24-C25
33	G	5003	PTY	C12-C11-C8-O10
37	B	5004	PCW	O31-C31-C32-C33
25	A	1123	CLA	CAD-CBD-CGD-O2D
25	A	1133	CLA	CAD-CBD-CGD-O2D
25	A	1135	CLA	CAD-CBD-CGD-O2D
25	B	1217	CLA	CAD-CBD-CGD-O2D
25	L	1503	CLA	CAD-CBD-CGD-O2D
25	2	602	CLA	CAD-CBD-CGD-O2D
26	A	1114	CHL	CAD-CBD-CGD-O2D
26	8	613	CHL	CAD-CBD-CGD-O2D
25	A	1128	CLA	CAA-CBA-CGA-O2A
25	K	1403	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	1	608	CLA	CAA-CBA-CGA-O2A
33	7	804	PTY	C12-C11-C8-O7
48	2	803	DGA	OG1-CA1-CA2-CA3
26	8	604	CHL	CAA-CBA-CGA-O1A
30	A	5001	LHG	C19-C20-C21-C22
25	B	1224	CLA	C2-C1-O2A-CGA
25	1	608	CLA	C2-C1-O2A-CGA
25	4	601	CLA	C2-C1-O2A-CGA
25	6	608	CLA	C2-C1-O2A-CGA
25	9	604	CLA	C2-C1-O2A-CGA
26	5	611	CHL	C2-C1-O2A-CGA
30	6	801	LHG	C25-C26-C27-C28
25	A	1139	CLA	CAA-CBA-CGA-O2A
25	7	607	CLA	CAA-CBA-CGA-O2A
26	4	613	CHL	CAA-CBA-CGA-O2A
30	3	801	LHG	O8-C23-C24-C25
30	9	802	LHG	O8-C23-C24-C25
25	A	1111	CLA	CAA-CBA-CGA-O1A
25	B	1228	CLA	CAA-CBA-CGA-O1A
25	1	605	CLA	CAA-CBA-CGA-O1A
25	2	601	CLA	CAA-CBA-CGA-O1A
25	A	1118	CLA	CAA-CBA-CGA-O2A
25	G	1601	CLA	CAA-CBA-CGA-O2A
25	1	615	CLA	CAA-CBA-CGA-O2A
25	5	602	CLA	CAA-CBA-CGA-O2A
25	8	605	CLA	CAA-CBA-CGA-O2A
25	8	618	CLA	CAA-CBA-CGA-O2A
30	F	5001	LHG	O8-C23-C24-C25
52	8	805	P5S	O19-C17-C20-C21
33	9	803	PTY	C17-C18-C19-C20
25	8	620	CLA	CAA-CBA-CGA-O2A
26	a	613	CHL	CAA-CBA-CGA-O1A
36	8	802	DGD	O6D-C5D-C6D-O5D
25	H	1702	CLA	CAA-CBA-CGA-O1A
25	a	607	CLA	CAA-CBA-CGA-O1A
25	A	1140	CLA	C5-C6-C7-C8
41	4	805	SPH	C4-C5-C6-C7
25	A	1120	CLA	CAA-CBA-CGA-O2A
25	A	1134	CLA	CAA-CBA-CGA-O2A
25	B	1218	CLA	CAA-CBA-CGA-O2A
25	5	609	CLA	CAA-CBA-CGA-O2A
25	5	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	B	5005	PTY	C12-C11-C8-O7
25	B	1237	CLA	CAA-CBA-CGA-O1A
26	a	604	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

372 monomers are involved in 1151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1113	CLA	8	0
25	1	608	CLA	6	0
25	K	1401	CLA	5	0
33	G	5002	PTY	1	0
25	A	1111	CLA	7	0
45	1	803	OLA	2	0
29	I	4001	BCR	2	0
25	B	1231	CLA	7	0
25	2	615	CLA	3	0
29	A	4004	BCR	3	0
30	4	801	LHG	4	0
43	8	501	LUT	6	0
43	3	502	LUT	4	0
26	8	610	CHL	2	0
26	1	611	CHL	4	0
25	8	607	CLA	2	0
25	3	602	CLA	2	0
35	1	804	LMT	2	0
29	3	503	BCR	2	0
25	5	606	CLA	3	0
40	J	4002	RRX	3	0
25	A	1101	CLA	5	0
43	a	501	LUT	5	0
25	B	1204	CLA	6	0
26	a	610	CHL	2	0
25	B	1238	CLA	2	0
43	6	501	LUT	5	0
25	A	1106	CLA	6	0
25	4	610	CLA	5	0
25	A	1138	CLA	8	0
25	H	1703	CLA	5	0
37	K	5002	PCW	1	0
25	5	609	CLA	1	0
25	O	1802	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	G	5003	PTY	1	0
25	2	604	CLA	12	0
26	6	610	CHL	2	0
45	a	805	OLA	2	0
25	5	605	CLA	2	0
29	K	4001	BCR	4	0
25	9	605	CLA	4	0
29	6	504	BCR	4	0
33	a	802	PTY	2	0
25	a	607	CLA	2	0
43	2	507	LUT	7	0
36	8	802	DGD	3	0
30	8	801	LHG	1	0
25	B	1225	CLA	4	0
25	A	1107	CLA	1	0
25	A	1102	CLA	2	0
25	5	603	CLA	2	0
26	8	613	CHL	4	0
25	A	1103	CLA	8	0
25	A	1121	CLA	1	0
32	A	5005	SQD	8	0
25	A	1115	CLA	8	0
25	A	1120	CLA	3	0
30	F	5002	LHG	2	0
26	6	611	CHL	3	0
25	G	1601	CLA	2	0
29	L	4002	BCR	2	0
25	1	606	CLA	2	0
25	a	608	CLA	1	0
43	5	502	LUT	4	0
25	9	607	CLA	2	0
25	L	1502	CLA	5	0
47	8	806	PLM	1	0
25	2	605	CLA	3	0
43	9	502	LUT	8	0
25	3	613	CLA	6	0
47	8	807	PLM	5	0
32	I	5001	SQD	4	0
32	G	5001	SQD	4	0
25	5	614	CLA	1	0
25	8	620	CLA	2	0
29	G	4001	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	2002	PQN	5	0
29	5	503	BCR	4	0
30	2	802	LHG	6	0
25	A	1118	CLA	2	0
25	6	603	CLA	5	0
25	B	1229	CLA	6	0
25	8	615	CLA	2	0
25	5	608	CLA	1	0
26	a	606	CHL	8	0
26	1	613	CHL	6	0
26	8	603	CHL	5	0
26	4	618	CHL	4	0
29	B	4006	BCR	5	0
26	6	613	CHL	3	0
25	4	611	CLA	2	0
26	5	611	CHL	1	0
25	A	1110	CLA	4	0
25	7	610	CLA	7	0
25	B	1205	CLA	6	0
25	8	618	CLA	4	0
43	1	503	LUT	2	0
25	A	1137	CLA	4	0
26	6	609	CHL	7	0
50	9	507	XAT	5	0
25	B	1232	CLA	1	0
25	2	621	CLA	2	0
29	B	4005	BCR	6	0
25	1	615	CLA	2	0
43	9	501	LUT	9	0
25	2	608	CLA	1	0
43	7	501	LUT	5	0
43	2	502	LUT	4	0
25	B	1207	CLA	4	0
25	3	601	CLA	7	0
43	a	503	LUT	4	0
25	7	607	CLA	2	0
25	A	1119	CLA	8	0
25	B	1209	CLA	5	0
25	A	1117	CLA	7	0
25	6	604	CLA	3	0
48	8	804	DGA	5	0
25	4	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	601	CLA	7	0
25	4	603	CLA	2	0
26	1	604	CHL	6	0
26	2	613	CHL	1	0
25	B	1234	CLA	8	0
25	A	1104	CLA	2	0
25	L	1504	CLA	2	0
30	A	5002	LHG	3	0
43	6	502	LUT	5	0
25	a	615	CLA	2	0
25	A	1128	CLA	5	0
25	J	1901	CLA	2	0
25	a	605	CLA	3	0
41	J	5002	SPH	1	0
37	6	803	PCW	3	0
26	2	609	CHL	4	0
25	A	1108	CLA	8	0
25	B	1022	CLA	4	0
25	B	1203	CLA	1	0
36	8	803	DGD	4	0
26	6	617	CHL	1	0
43	8	502	LUT	5	0
25	1	601	CLA	7	0
24	A	1011	CL0	6	0
25	B	1208	CLA	2	0
30	3	801	LHG	1	0
25	A	1116	CLA	8	0
25	L	1503	CLA	5	0
29	B	4003	BCR	2	0
35	A	5008	LMT	1	0
25	1	607	CLA	4	0
25	B	1236	CLA	6	0
33	B	5005	PTY	2	0
30	1	801	LHG	2	0
30	6	801	LHG	5	0
29	B	4001	BCR	5	0
26	7	613	CHL	10	0
34	A	5007	3PH	3	0
29	5	504	BCR	4	0
50	9	504	XAT	3	0
50	2	501	XAT	3	0
25	4	612	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	1201	CLA	6	0
25	5	615	CLA	1	0
25	A	1013	CLA	8	0
26	1	610	CHL	3	0
25	K	1404	CLA	1	0
26	5	617	CHL	2	0
43	3	501	LUT	3	0
43	a	502	LUT	4	0
25	4	604	CLA	6	0
33	3	802	PTY	3	0
25	3	607	CLA	1	0
25	A	1130	CLA	7	0
25	A	1133	CLA	8	0
26	a	604	CHL	9	0
29	A	4003	BCR	4	0
25	5	601	CLA	4	0
25	G	1603	CLA	4	0
43	1	501	LUT	4	0
25	B	1023	CLA	8	0
47	6	804	PLM	1	0
29	A	4001	BCR	4	0
25	8	606	CLA	4	0
43	4	502	LUT	6	0
25	4	616	CLA	2	0
25	7	612	CLA	7	0
30	9	801	LHG	3	0
26	a	613	CHL	7	0
25	A	1129	CLA	4	0
29	L	4001	BCR	3	0
25	4	605	CLA	3	0
29	B	4007	BCR	4	0
25	9	612	CLA	7	0
38	F	5003	LPX	2	0
25	F	1301	CLA	3	0
40	3	506	RRX	1	0
25	B	1230	CLA	8	0
33	J	5001	PTY	2	0
25	8	605	CLA	2	0
25	9	604	CLA	4	0
25	B	1220	CLA	12	0
25	B	1227	CLA	4	0
25	7	604	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	1226	CLA	5	0
25	2	601	CLA	6	0
26	3	608	CHL	1	0
43	4	501	LUT	4	0
25	B	1219	CLA	5	0
43	5	505	LUT	4	0
48	3	803	DGA	3	0
41	6	806	SPH	1	0
36	B	5003	DGD	4	0
30	B	5001	LHG	5	0
44	1	502	AXT	3	0
37	K	5001	PCW	2	0
25	4	608	CLA	4	0
26	3	611	CHL	6	0
47	4	804	PLM	3	0
25	7	608	CLA	1	0
50	7	502	XAT	3	0
26	5	610	CHL	5	0
25	B	1221	CLA	5	0
25	B	1224	CLA	10	0
25	1	602	CLA	1	0
30	B	5002	LHG	1	0
25	9	609	CLA	3	0
25	B	1216	CLA	6	0
25	2	612	CLA	4	0
43	5	501	LUT	4	0
25	1	605	CLA	6	0
25	B	1206	CLA	5	0
25	A	1012	CLA	10	0
28	C	3003	SF4	1	0
25	A	1131	CLA	6	0
25	8	611	CLA	4	0
29	L	4003	BCR	1	0
25	A	1127	CLA	8	0
25	B	1218	CLA	3	0
25	B	1235	CLA	4	0
29	J	4001	BCR	5	0
26	9	608	CHL	2	0
25	6	612	CLA	2	0
25	a	602	CLA	3	0
26	4	613	CHL	5	0
25	9	606	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	803	PTY	2	0
25	B	1217	CLA	4	0
33	5	802	PTY	3	0
36	7	806	DGD	3	0
25	B	1237	CLA	2	0
25	B	1239	CLA	2	0
25	H	1701	CLA	2	0
30	9	802	LHG	4	0
25	K	1403	CLA	3	0
26	A	1114	CHL	8	0
25	B	1215	CLA	4	0
51	7	807	4RF	6	0
44	7	504	AXT	10	0
29	A	4002	BCR	4	0
25	B	1202	CLA	4	0
25	F	1302	CLA	4	0
25	1	612	CLA	11	0
26	a	609	CHL	5	0
26	3	604	CHL	6	0
29	H	4001	BCR	4	0
25	A	1125	CLA	10	0
25	4	615	CLA	3	0
53	8	810	LAP	4	0
29	6	503	BCR	4	0
26	5	613	CHL	3	0
26	4	609	CHL	6	0
32	H	5001	SQD	3	0
25	A	1112	CLA	3	0
25	B	1212	CLA	3	0
25	5	602	CLA	4	0
25	6	602	CLA	3	0
25	3	610	CLA	2	0
25	3	616	CLA	3	0
25	B	1228	CLA	4	0
42	M	4001	ECH	5	0
30	5	801	LHG	2	0
25	a	603	CLA	2	0
25	6	608	CLA	4	0
25	7	606	CLA	2	0
25	2	602	CLA	2	0
25	A	1136	CLA	4	0
25	8	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	612	CLA	5	0
37	B	5004	PCW	1	0
25	a	601	CLA	5	0
25	B	1214	CLA	5	0
26	7	609	CHL	4	0
35	2	804	LMT	5	0
30	2	801	LHG	5	0
30	7	803	LHG	3	0
29	8	503	BCR	3	0
30	1	802	LHG	3	0
25	K	1402	CLA	3	0
25	7	605	CLA	3	0
45	8	809	OLA	1	0
26	9	613	CHL	3	0
25	B	1240	CLA	4	0
25	4	601	CLA	6	0
29	3	504	BCR	5	0
29	B	4004	BCR	8	0
25	A	1140	CLA	5	0
26	3	603	CHL	5	0
27	A	2001	PQN	7	0
29	A	4005	BCR	9	0
29	B	4002	BCR	4	0
33	9	803	PTY	4	0
26	9	610	CHL	6	0
26	8	604	CHL	3	0
25	G	1602	CLA	2	0
25	5	612	CLA	9	0
26	2	610	CHL	2	0
25	A	1124	CLA	4	0
25	8	602	CLA	5	0
25	B	1021	CLA	7	0
25	A	1132	CLA	3	0
25	O	1801	CLA	1	0
26	6	619	CHL	7	0
29	3	505	BCR	4	0
32	7	805	SQD	1	0
25	5	604	CLA	3	0
25	A	1109	CLA	7	0
33	A	5006	PTY	4	0
35	B	5006	LMT	2	0
26	9	601	CHL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	1223	CLA	3	0
30	A	5003	LHG	2	0
25	7	601	CLA	3	0
25	8	612	CLA	5	0
47	5	804	PLM	3	0
25	A	1134	CLA	2	0
25	3	606	CLA	6	0
25	6	615	CLA	6	0
25	7	603	CLA	4	0
52	8	805	P5S	2	0
25	B	1213	CLA	2	0
26	5	618	CHL	4	0
25	2	607	CLA	4	0
29	7	503	BCR	9	0
25	A	1126	CLA	12	0
26	8	601	CHL	5	0
29	O	4001	BCR	1	0
30	A	5001	LHG	3	0
25	A	1139	CLA	4	0
25	4	606	CLA	3	0
25	6	606	CLA	1	0
48	5	803	DGA	3	0
25	5	607	CLA	2	0
29	K	4002	BCR	3	0
25	3	605	CLA	5	0
25	3	612	CLA	2	0
29	4	503	BCR	8	0
26	9	603	CHL	6	0
26	1	609	CHL	8	0
48	2	803	DGA	6	0
26	7	611	CHL	1	0
26	7	617	CHL	5	0
25	B	1211	CLA	1	0
25	A	1135	CLA	3	0
25	A	1105	CLA	5	0
26	7	615	CHL	1	0
39	F	4001	NEX	4	0
25	A	1122	CLA	5	0
25	2	603	CLA	5	0
25	A	1123	CLA	4	0
25	B	1222	CLA	5	0
25	1	603	CLA	4	0

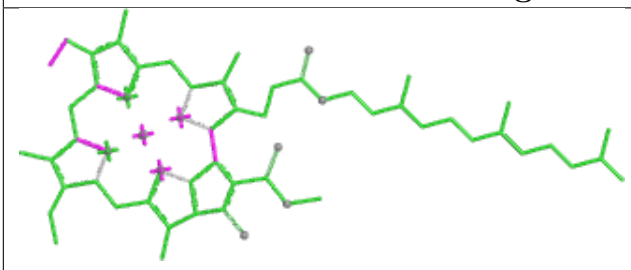
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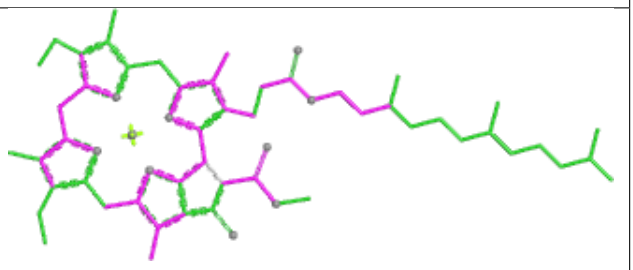
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	801	LHG	2	0
41	9	804	SPH	2	0

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

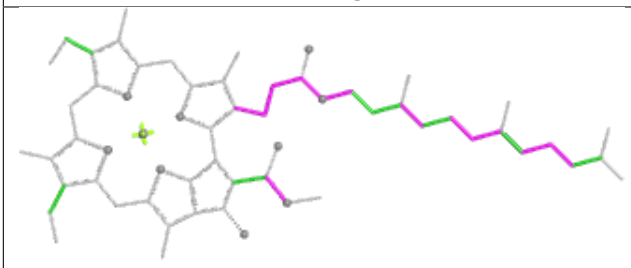
Ligand CLA A 1113



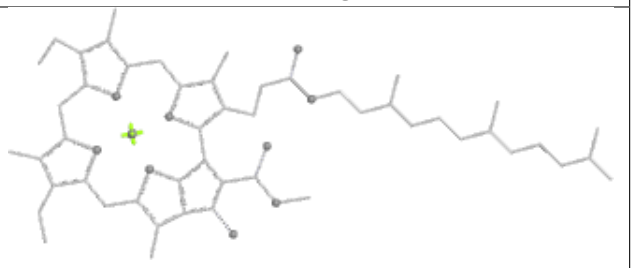
Bond lengths



Bond angles

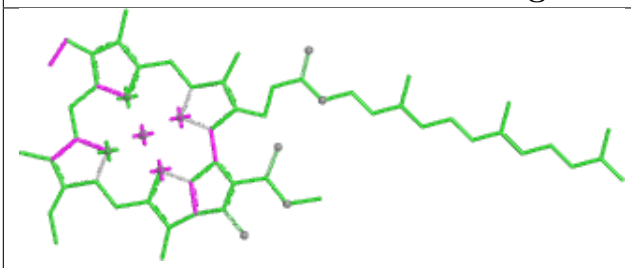


Torsions

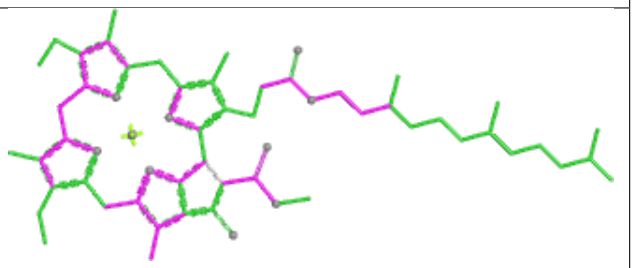


Rings

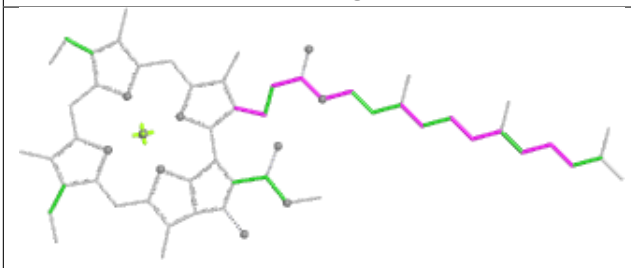
Ligand CLA 1 608



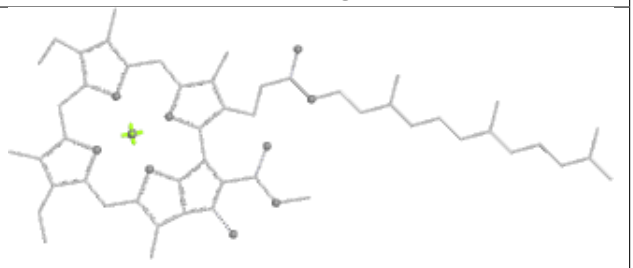
Bond lengths



Bond angles

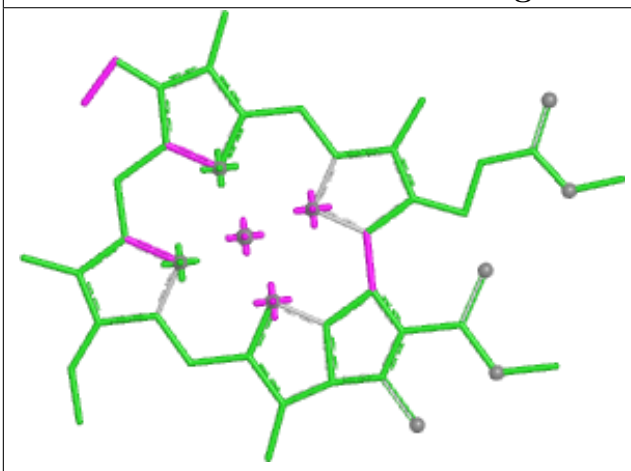


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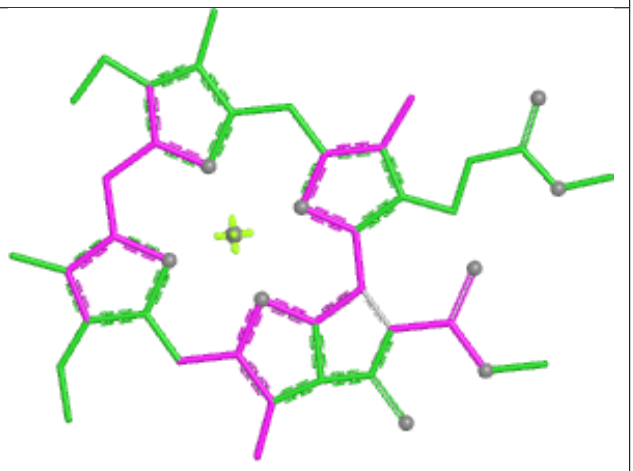


Rings

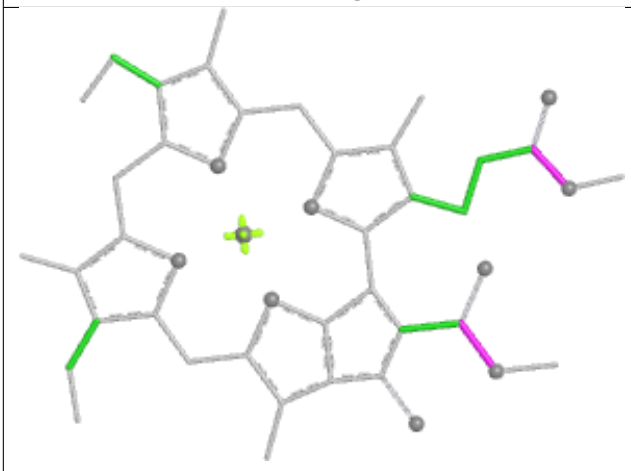
Ligand CLA K 1401



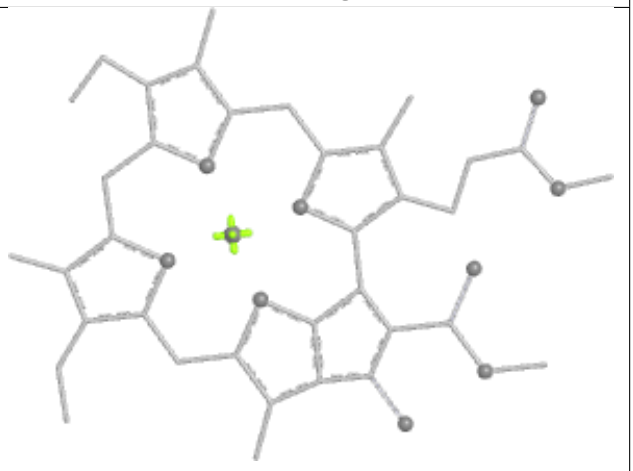
Bond lengths



Bond angles

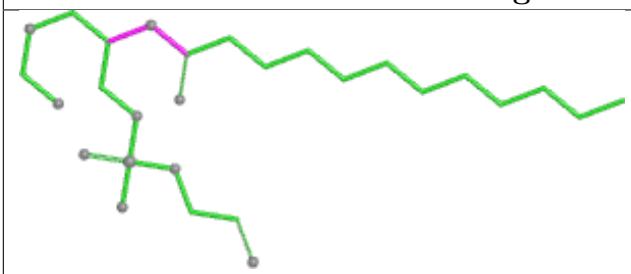


Torsions

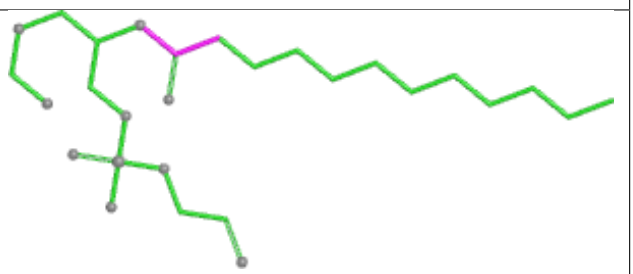


Rings

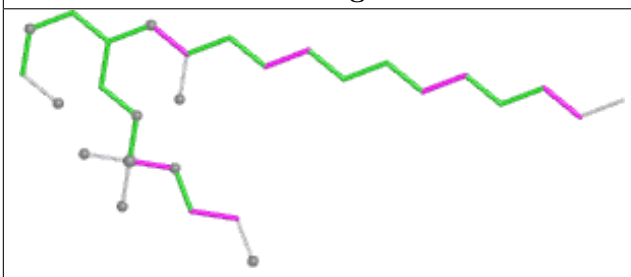
Ligand PTY G 5002



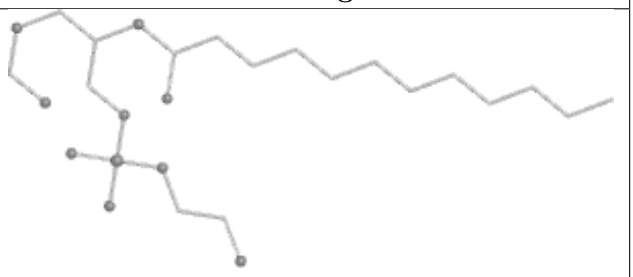
Bond lengths



Bond angles

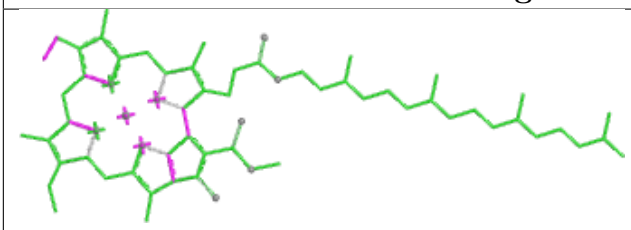


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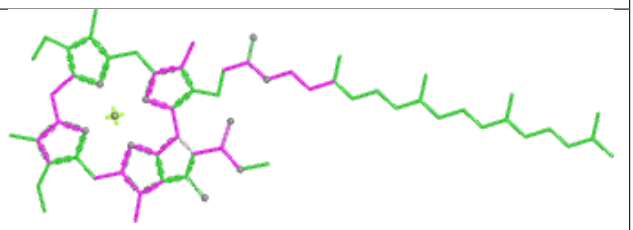


Rings

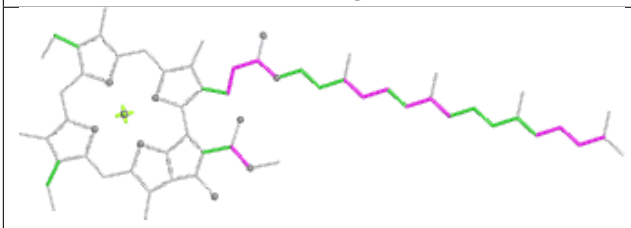
Ligand CLA A 1111



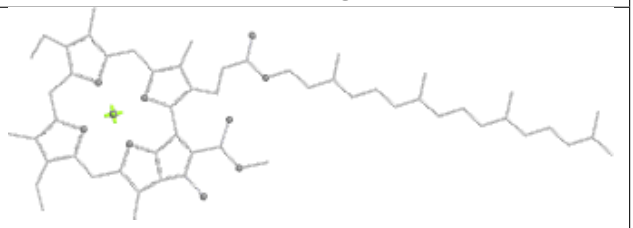
Bond lengths



Bond angles

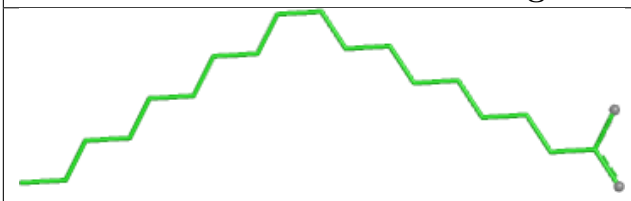


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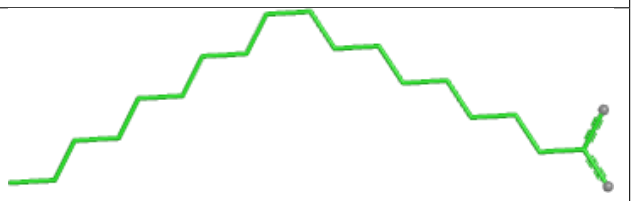


Rings

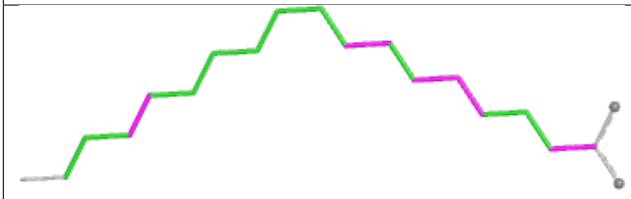
Ligand OLA 1 803



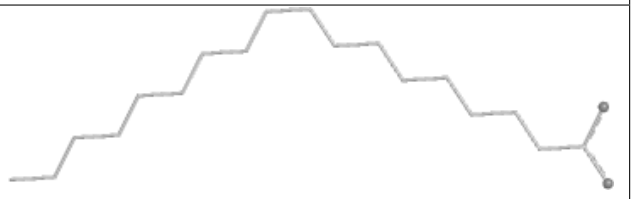
Bond lengths



Bond angles

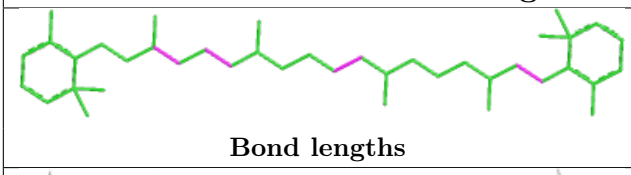


Torsions

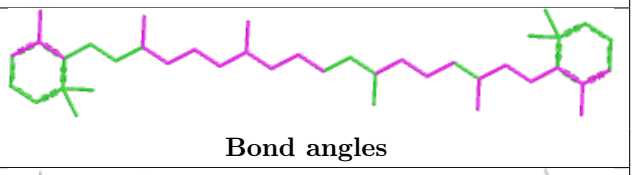


Rings

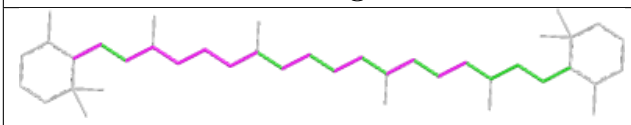
Ligand BCR I 4001



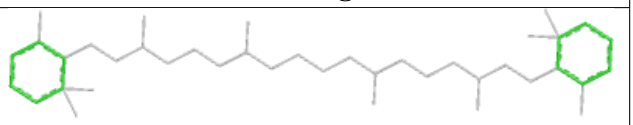
Bond lengths



Bond angles

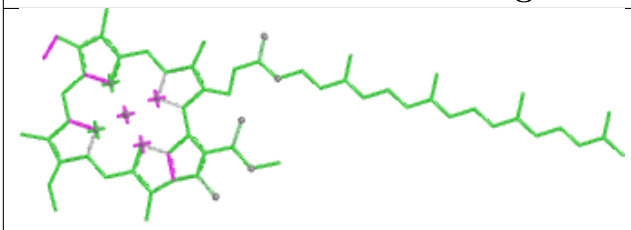


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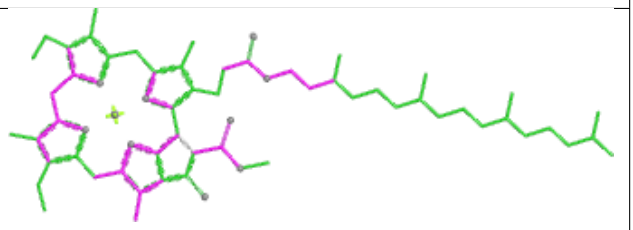


Rings

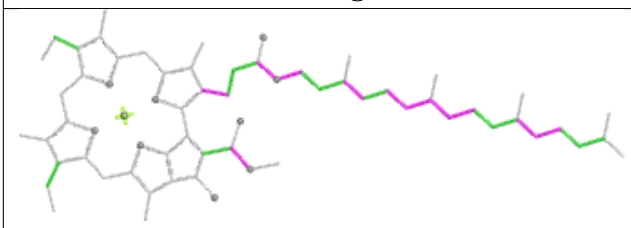
Ligand CLA B 1231



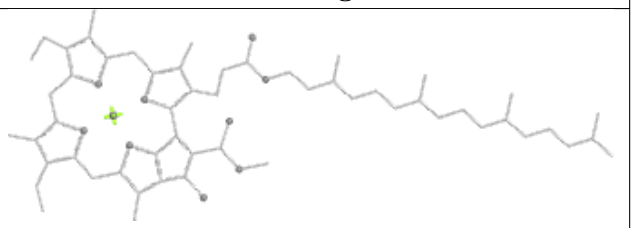
Bond lengths



Bond angles

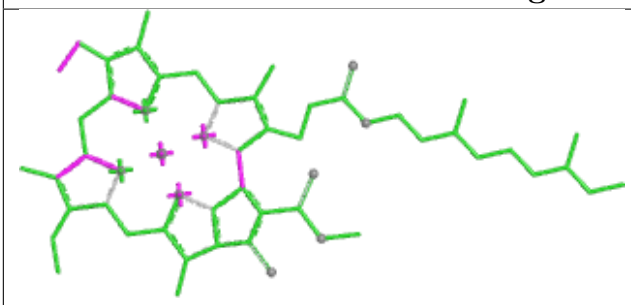


Torsions

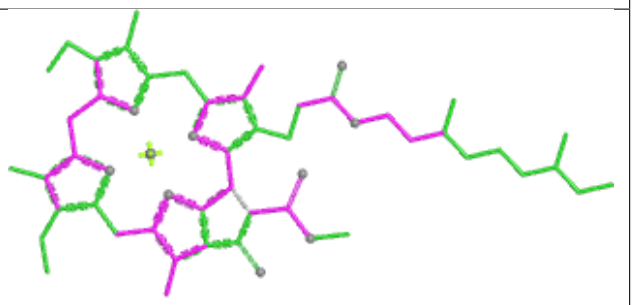


Rings

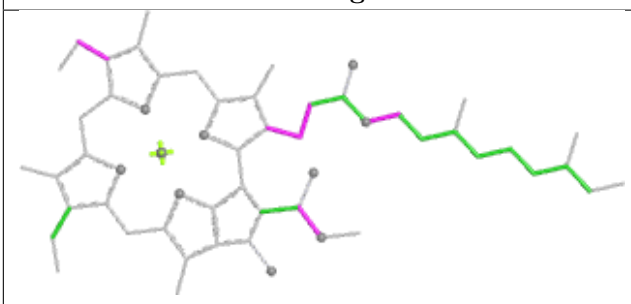
Ligand CLA 2 615



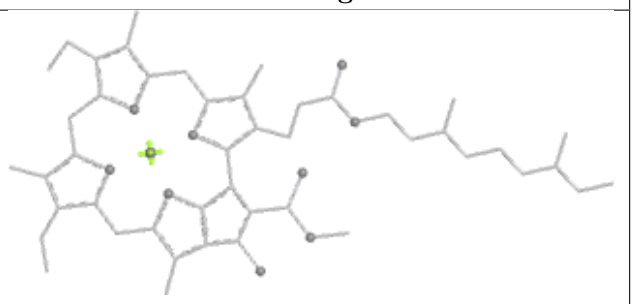
Bond lengths



Bond angles

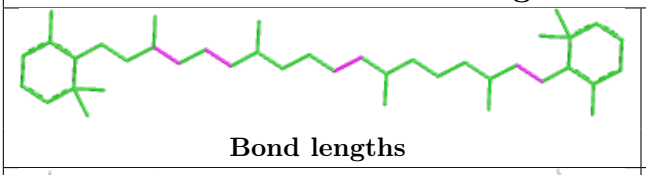


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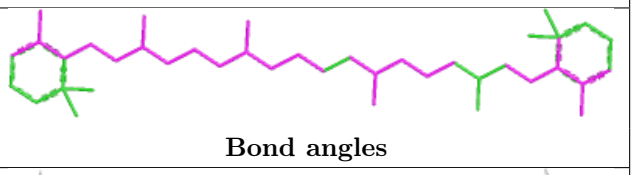


Rings

Ligand BCR A 4004



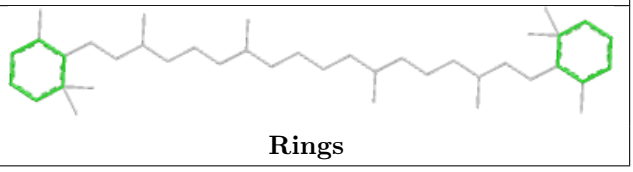
Bond lengths



Bond angles

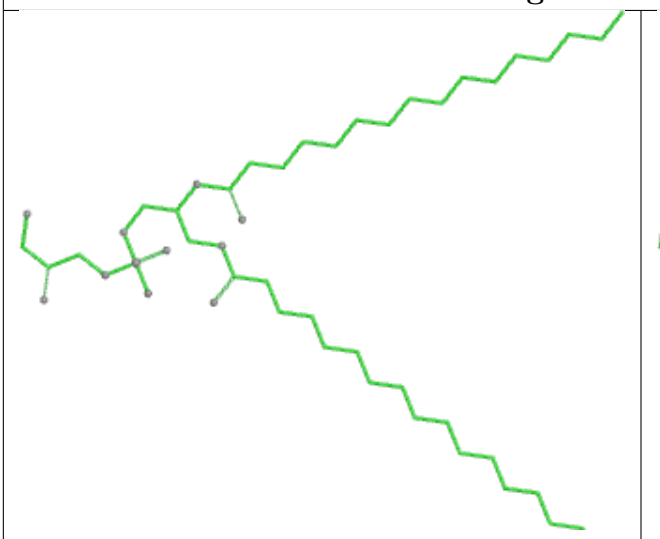


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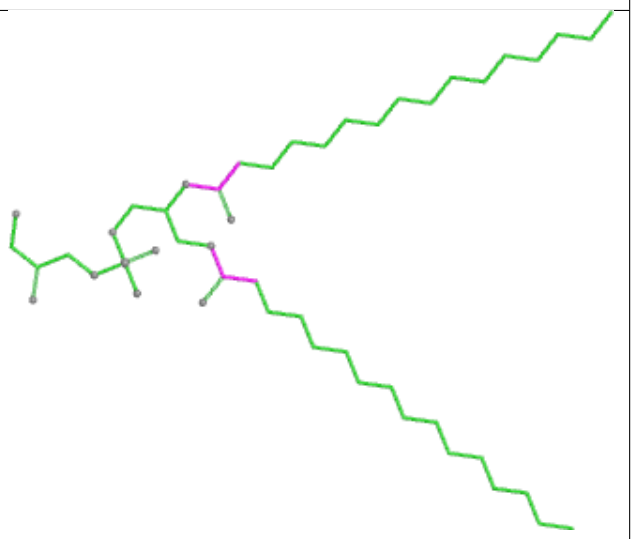


Rings

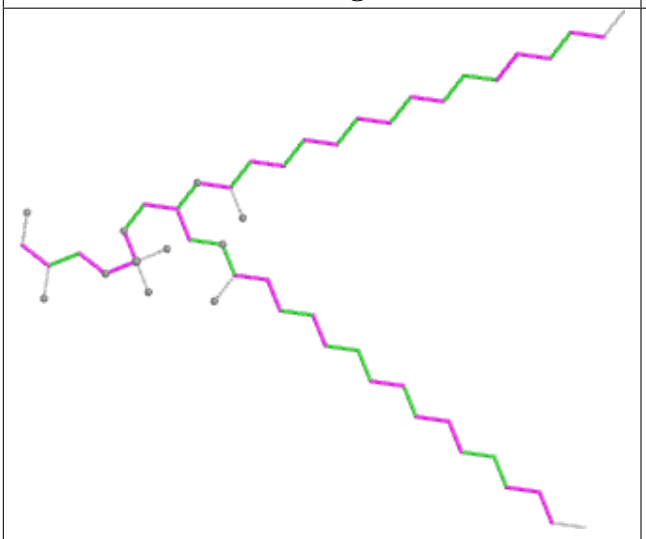
Ligand LHG 4 801



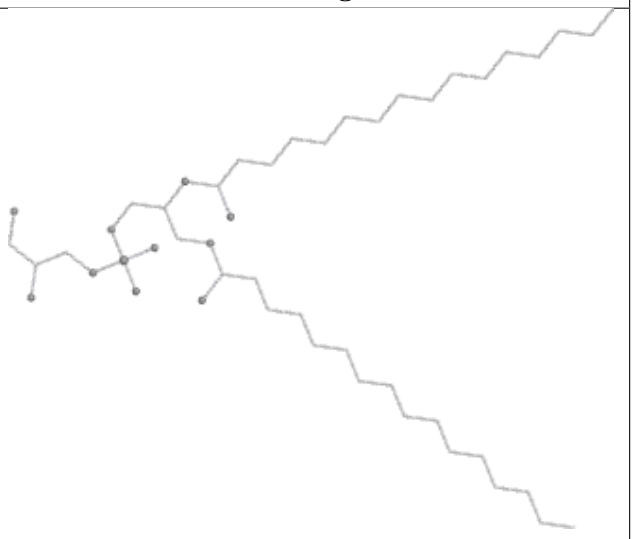
Bond lengths



Bond angles

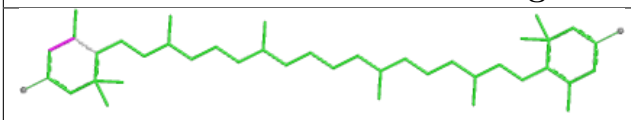


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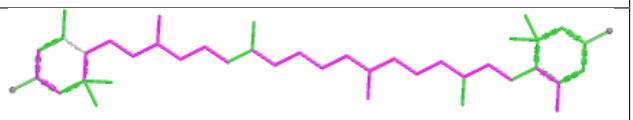


Rings

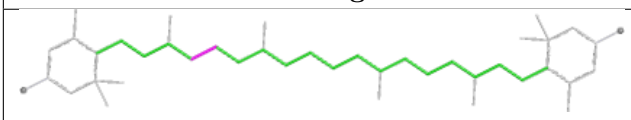
Ligand LUT 8 501



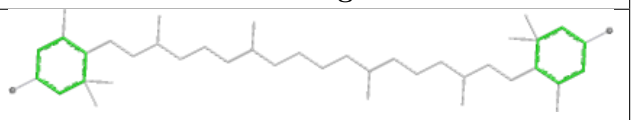
Bond lengths



Bond angles



Torsions

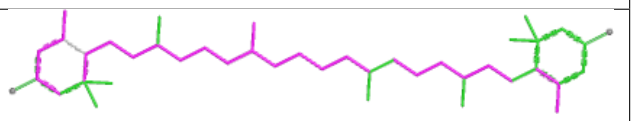


Rings

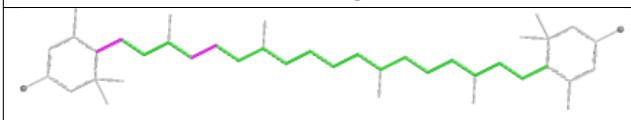
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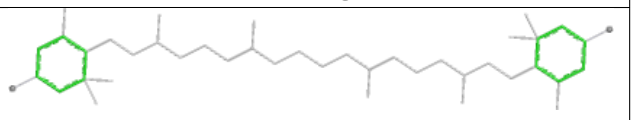
Bond lengths



Bond angles

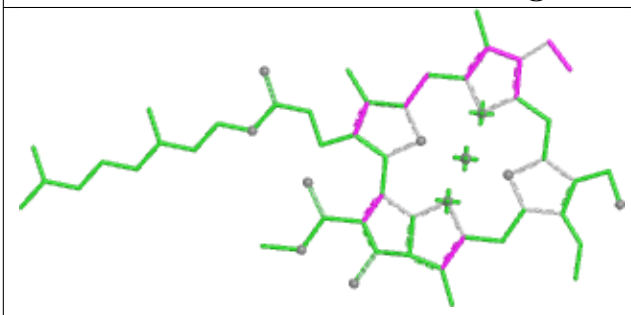


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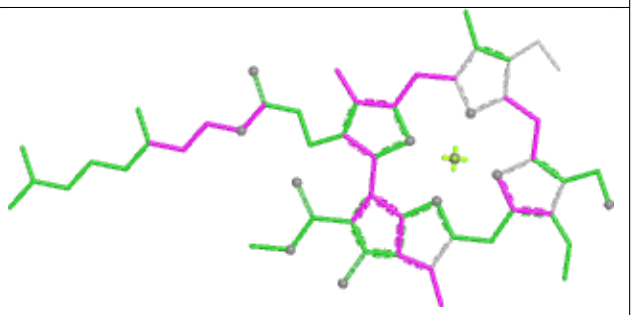


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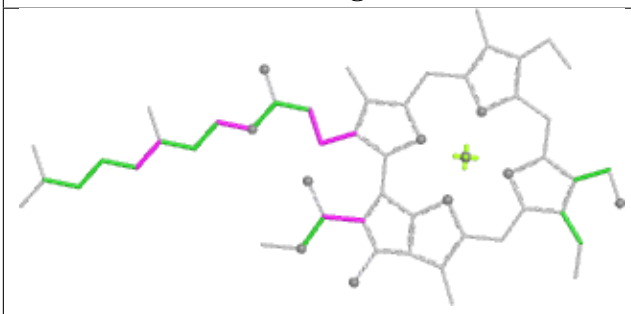
Ligand CHL 8 610



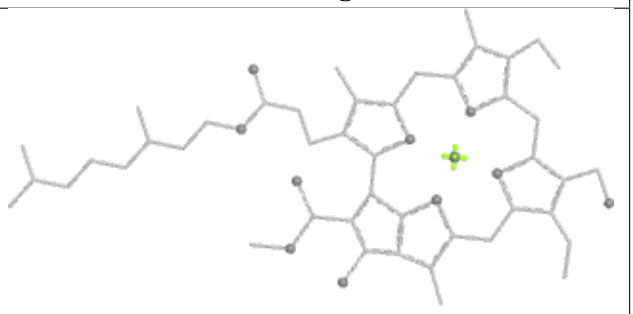
Bond lengths



Bond angles

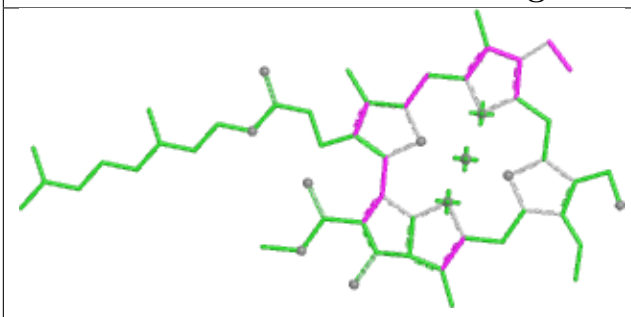


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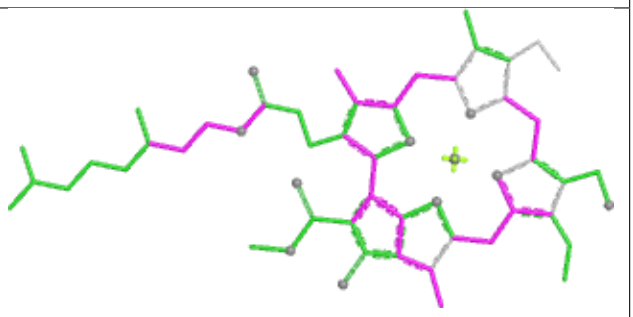


Rings

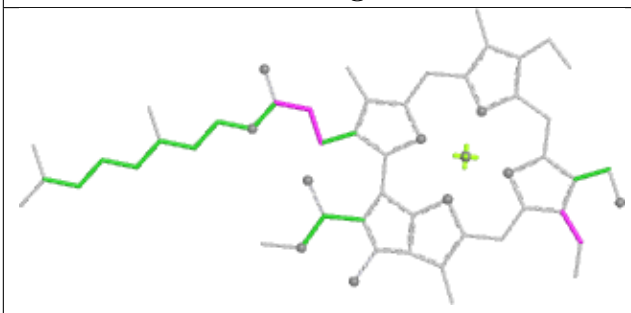
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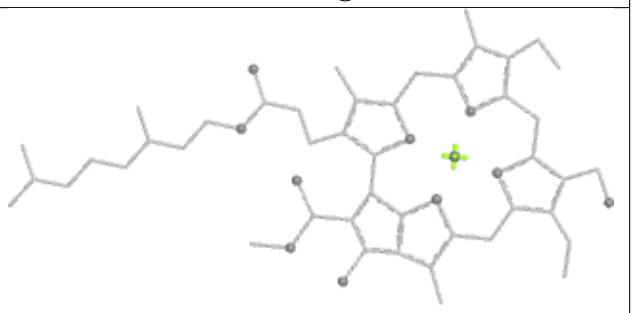
Bond lengths



Bond angles

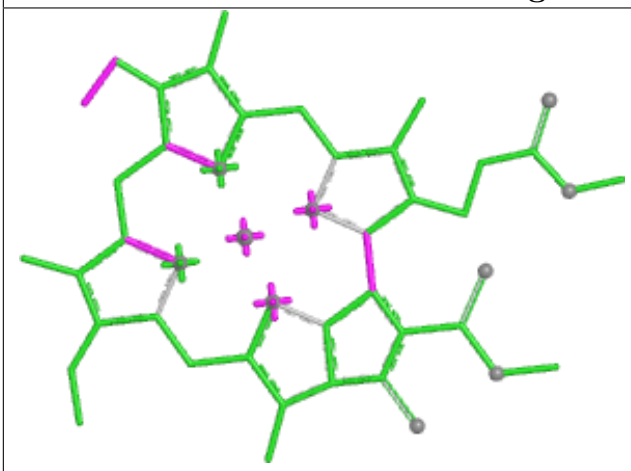


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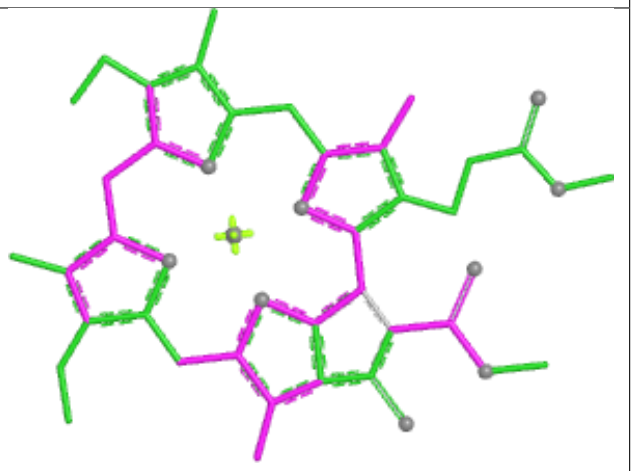


Rings

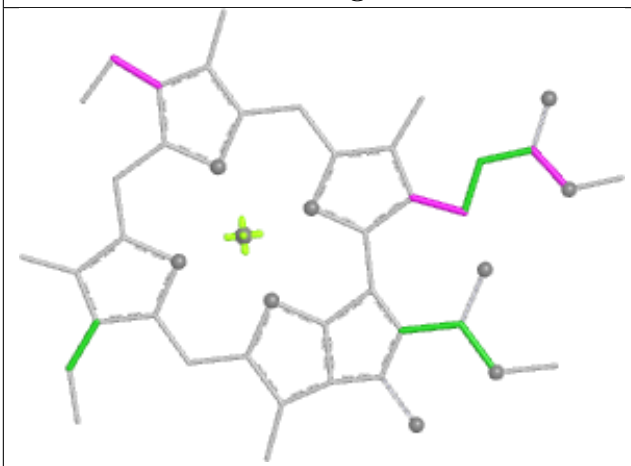
Ligand CLA 8 607



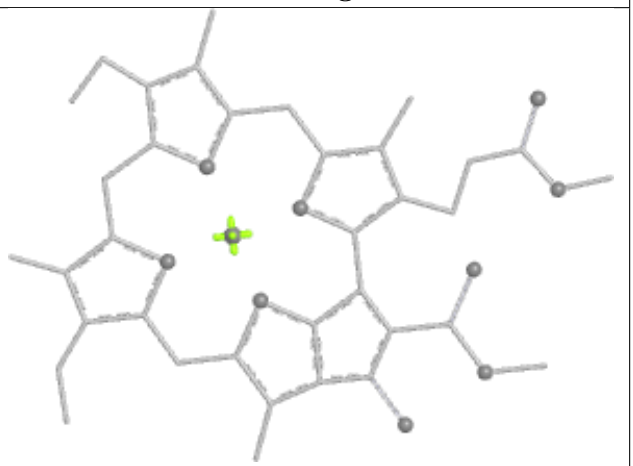
Bond lengths



Bond angles

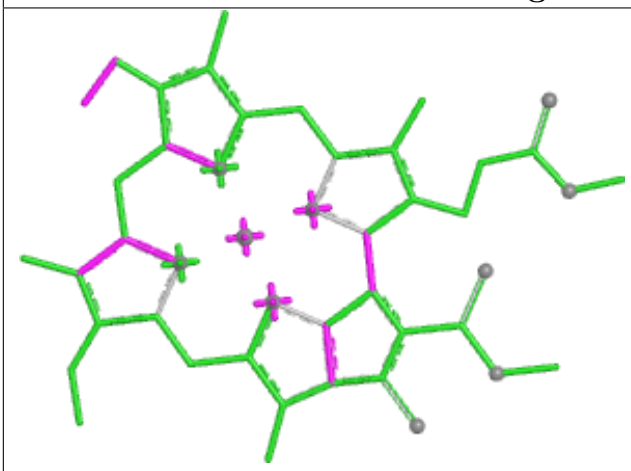


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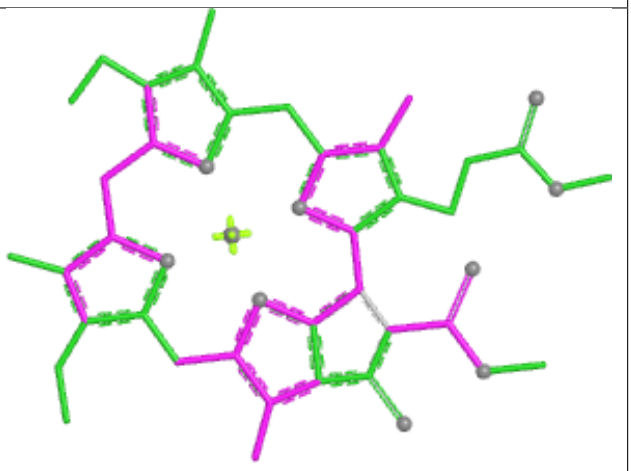


Rings

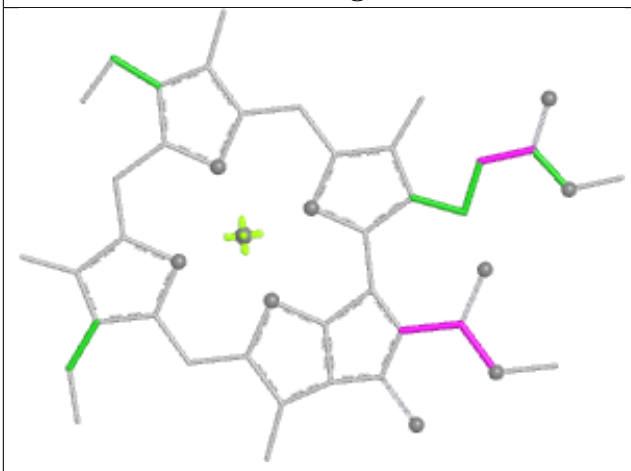
Ligand CLA 3 602



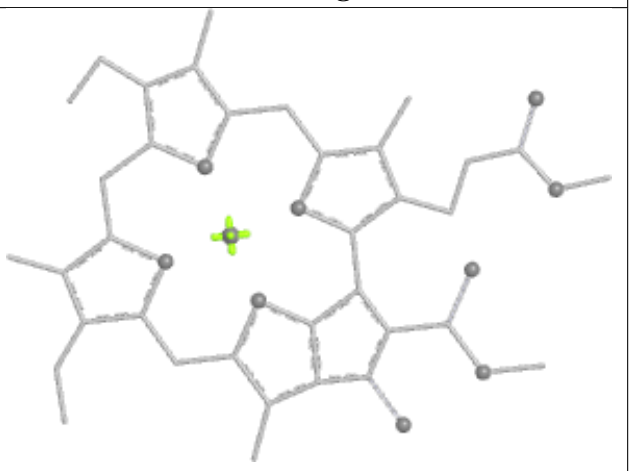
Bond lengths



Bond angles

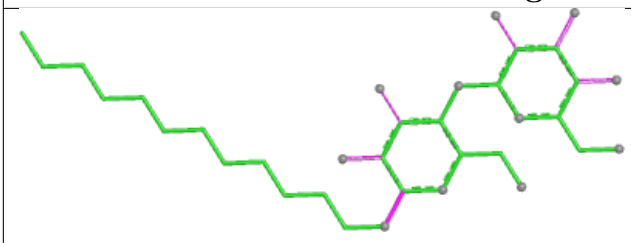


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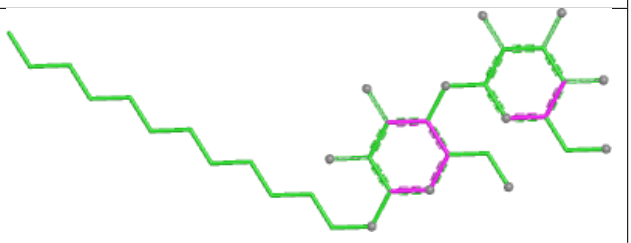


Rings

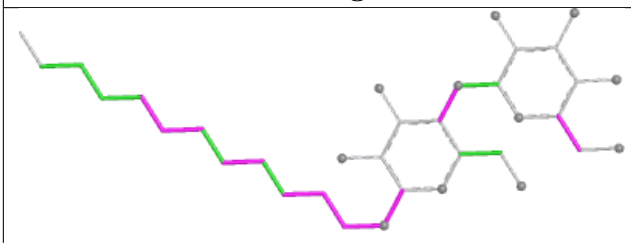
Ligand LMT 1 804



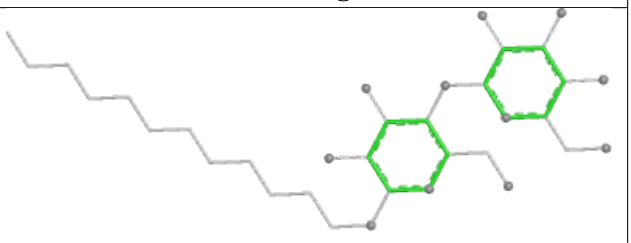
Bond lengths



Bond angles

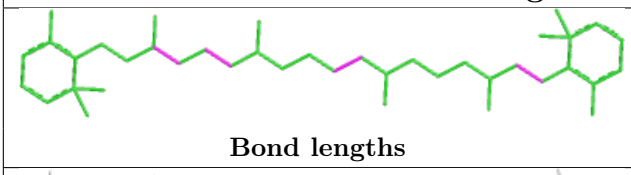


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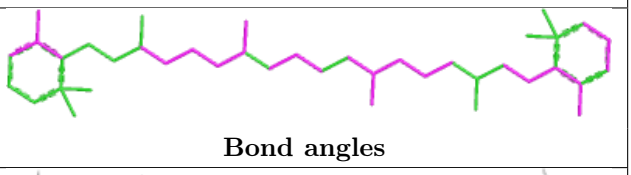


Rings

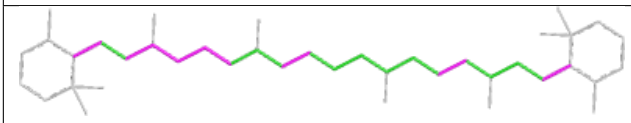
Ligand BCR 3 503



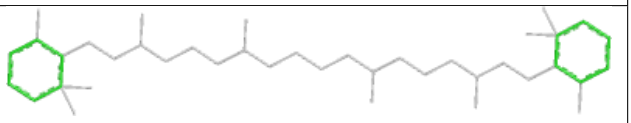
Bond lengths



Bond angles

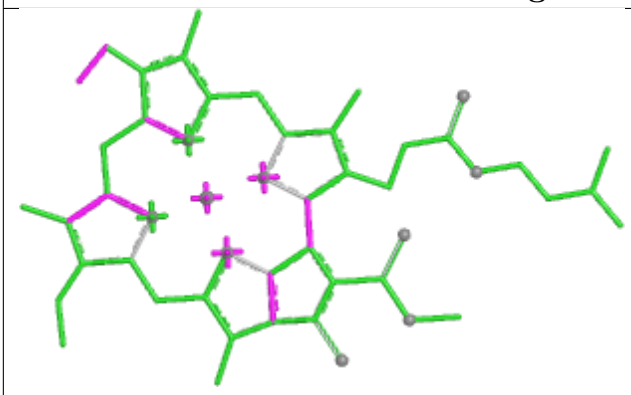


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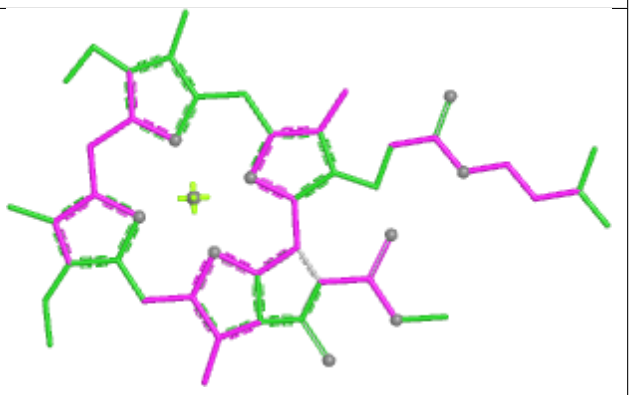


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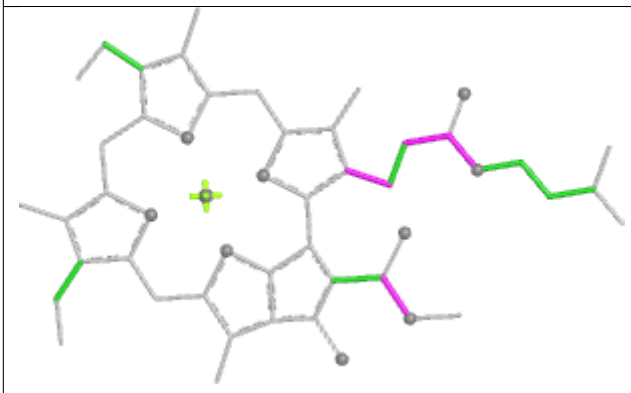
Ligand CLA 5 606



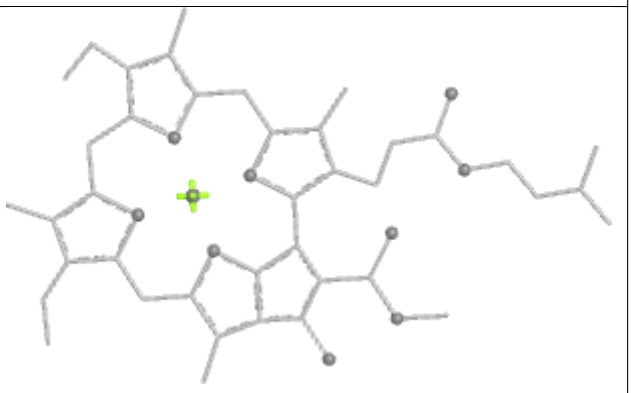
Bond lengths



Bond angles

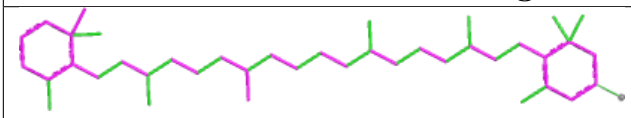


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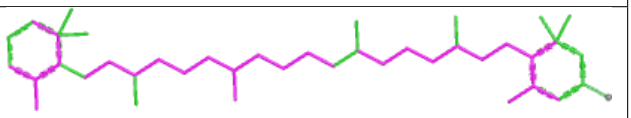


Rings

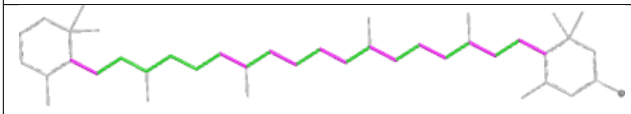
Ligand RRX J 4002



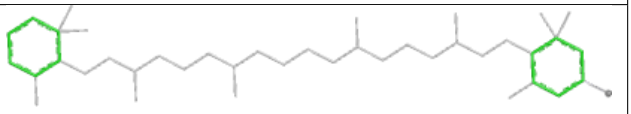
Bond lengths



Bond angles

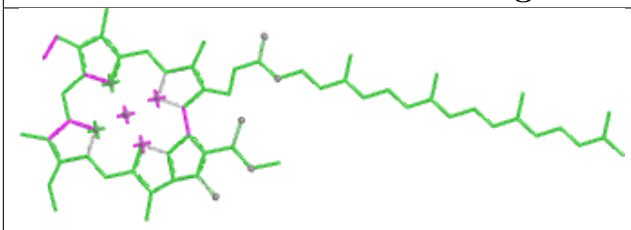


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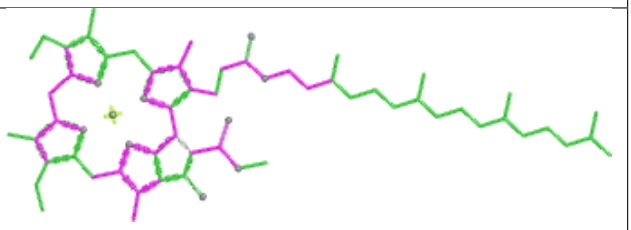


Rings

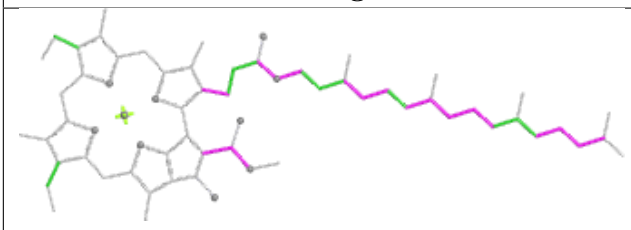
Ligand CLA A 1101



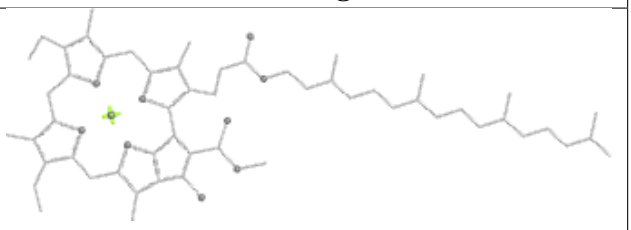
Bond lengths



Bond angles

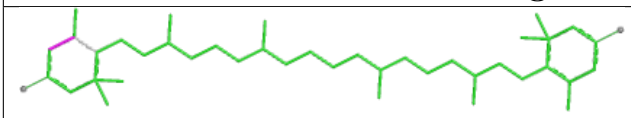


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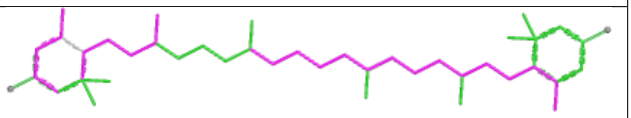


Rings

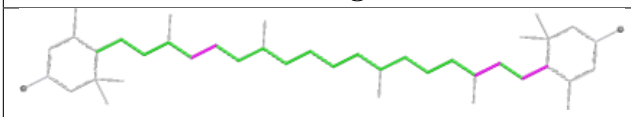
Ligand LUT a 501



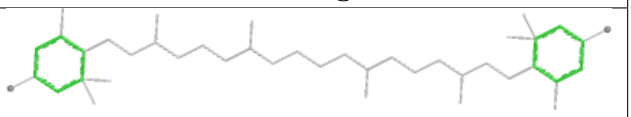
Bond lengths



Bond angles

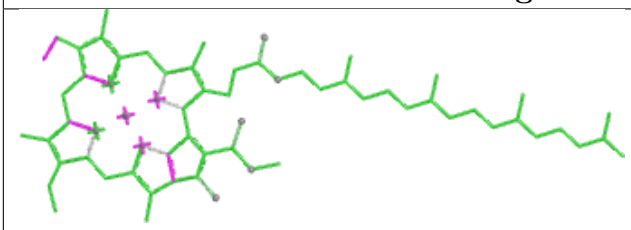


Torsions

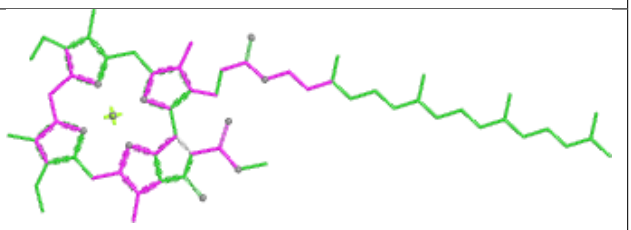


Rings

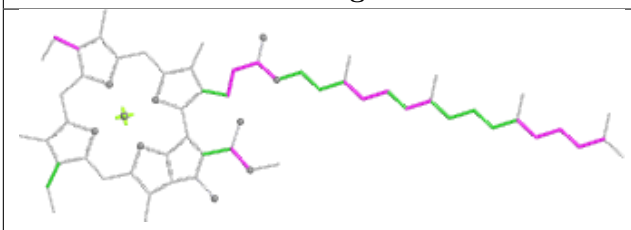
Ligand CLA B 1204



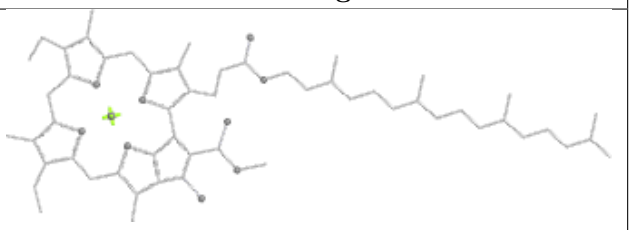
Bond lengths



Bond angles

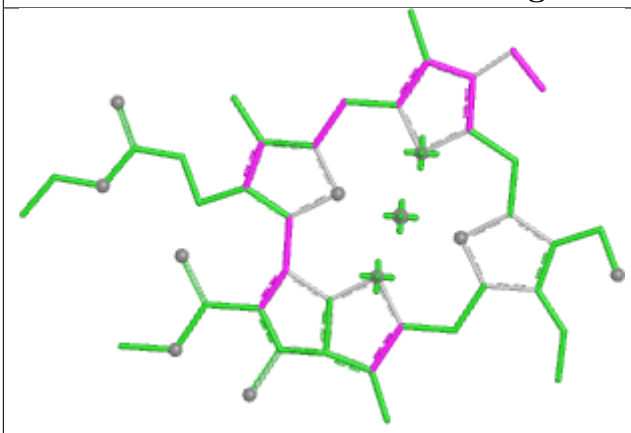


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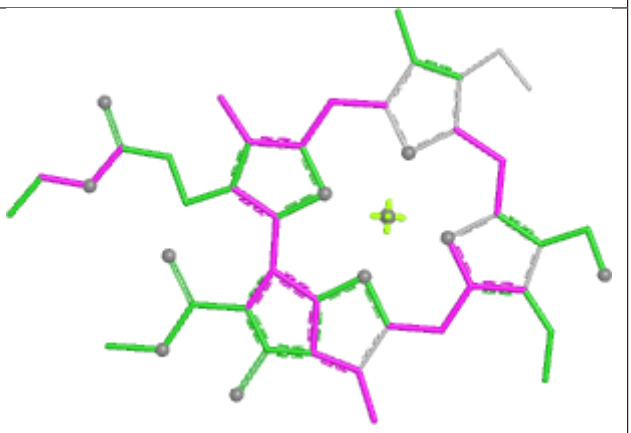


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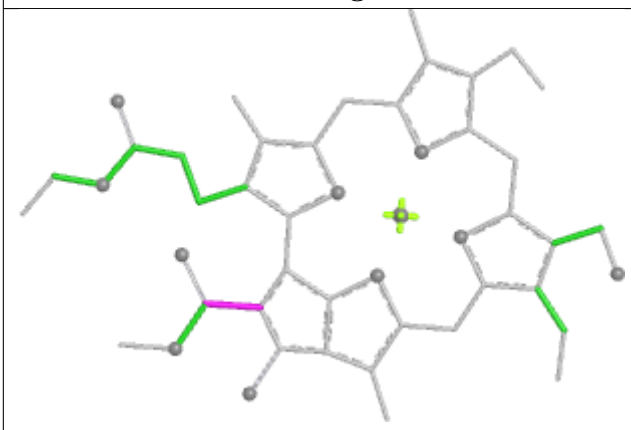
Ligand CHL a 610



Bond lengths



Bond angles

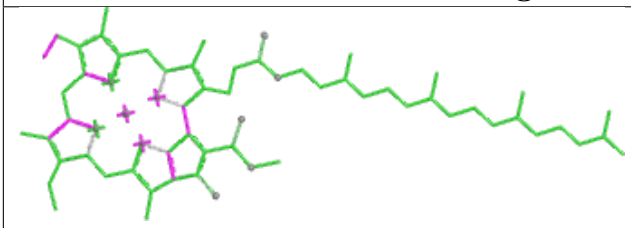


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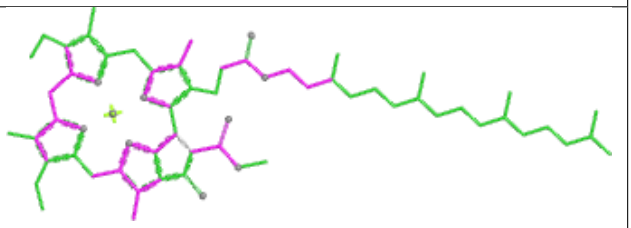


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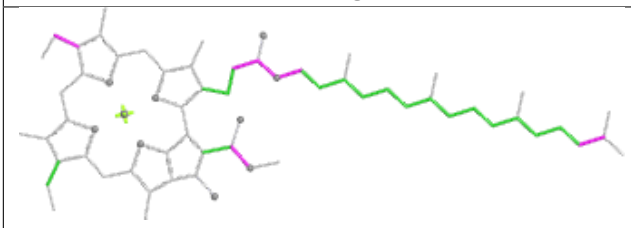
Ligand CLA B 1238



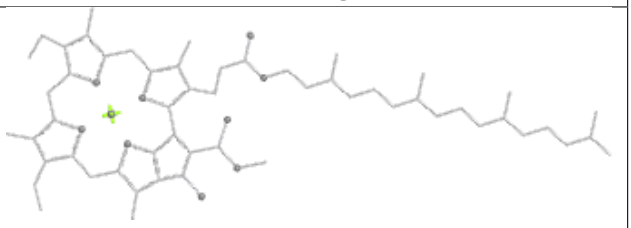
Bond lengths



Bond angles

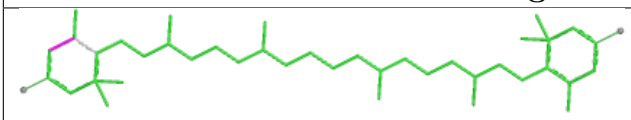


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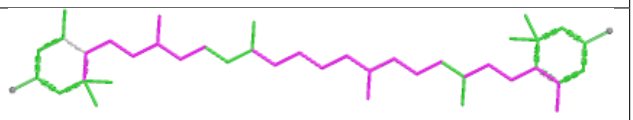


Rings

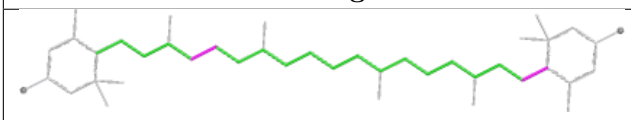
Ligand LUT 6 501



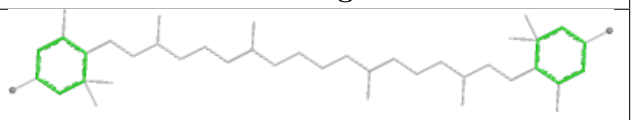
Bond lengths



Bond angles

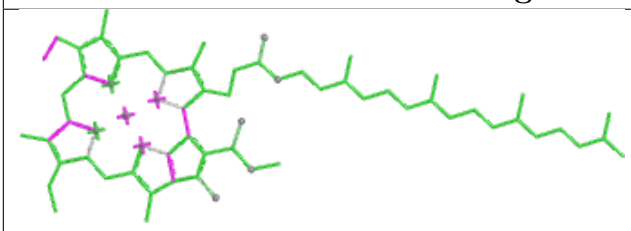


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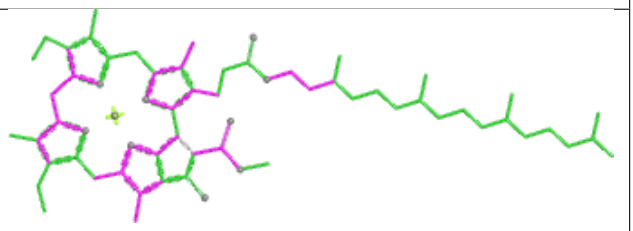


Rings

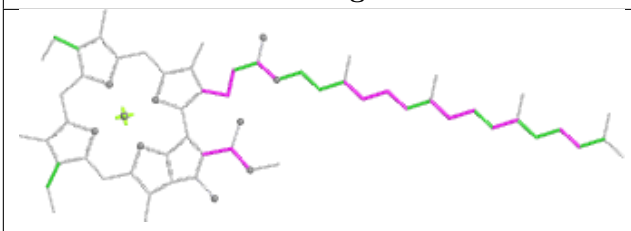
Ligand CLA A 1106



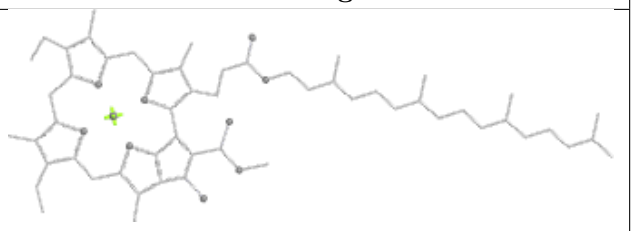
Bond lengths



Bond angles

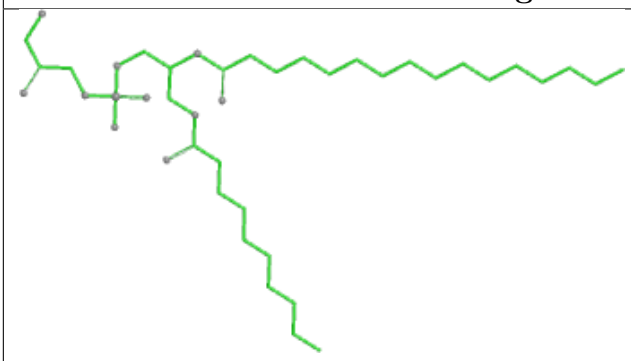


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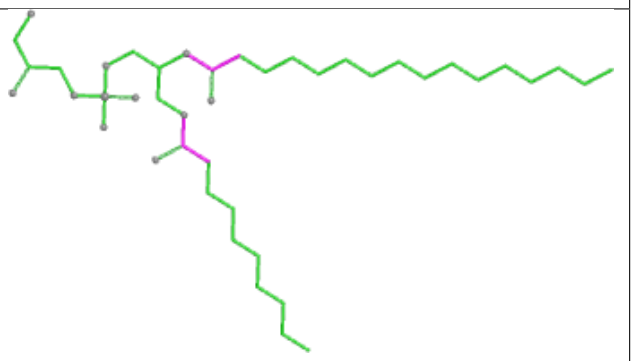


Rings

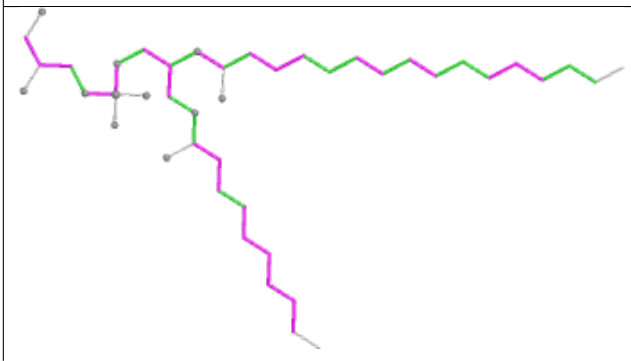
Ligand LHG F 5001



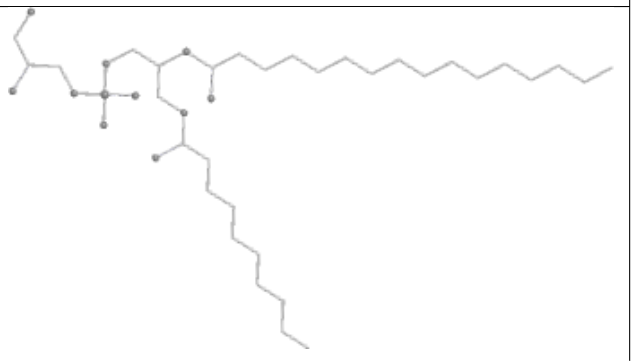
Bond lengths



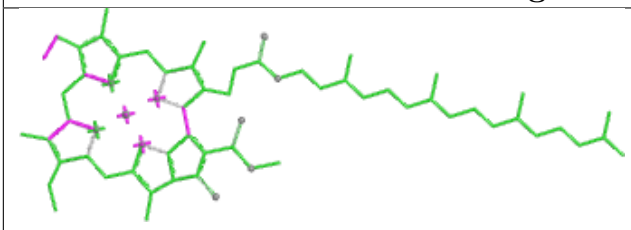
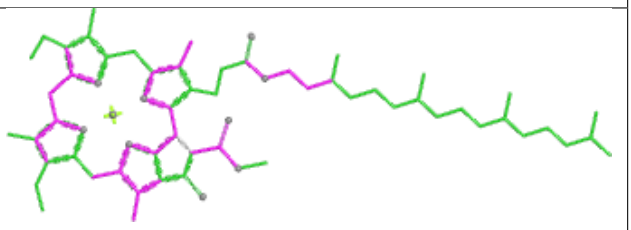
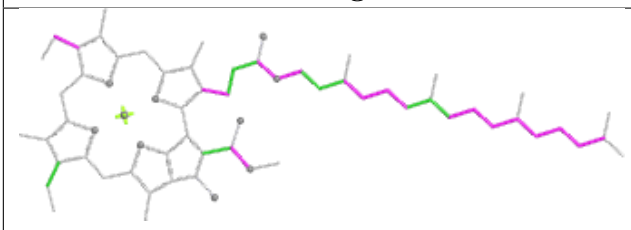
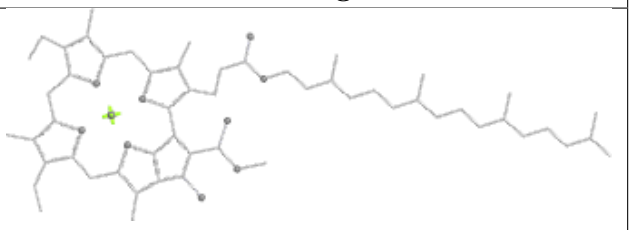
Bond angles

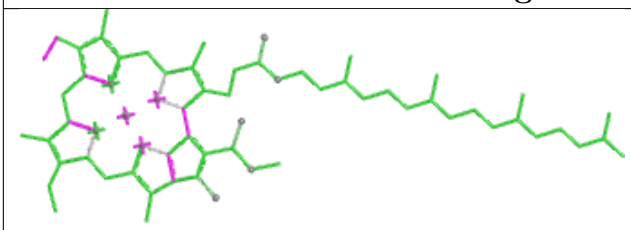
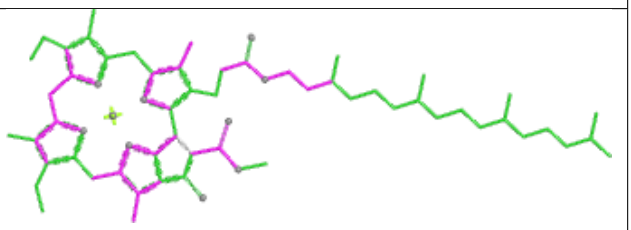
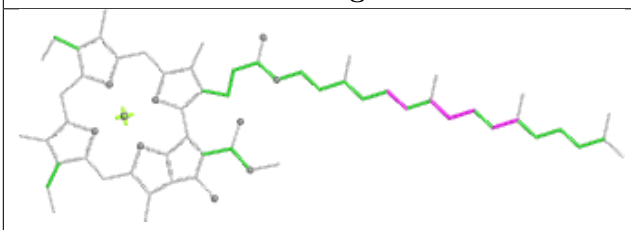
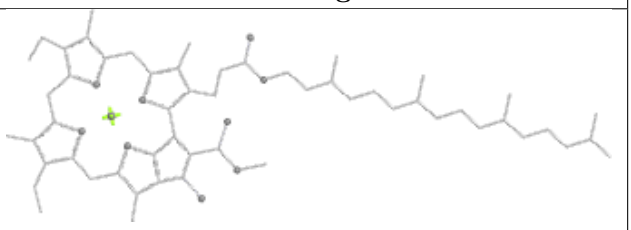


Torsions

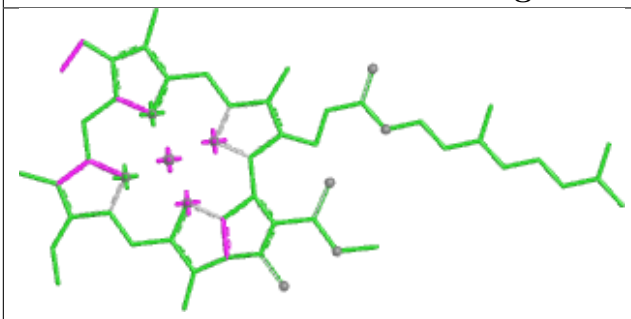


Rings

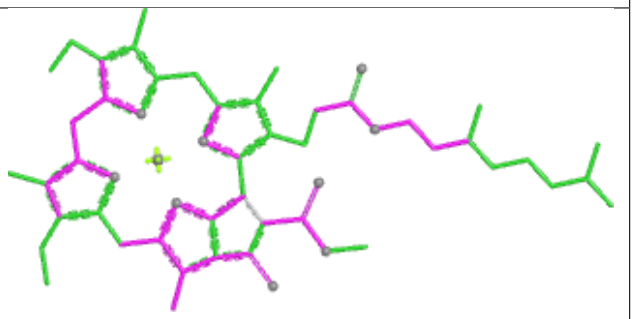
Ligand CLA 4 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1138	
	
Bond lengths	Bond angles
	
Torsions	Rings

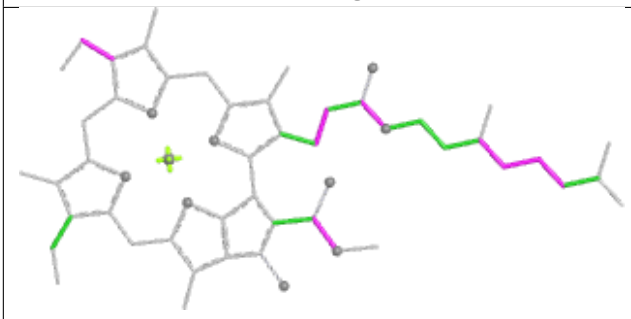
Ligand CLA H 1703



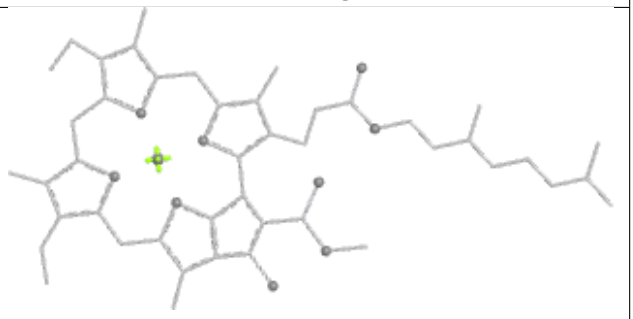
Bond lengths



Bond angles

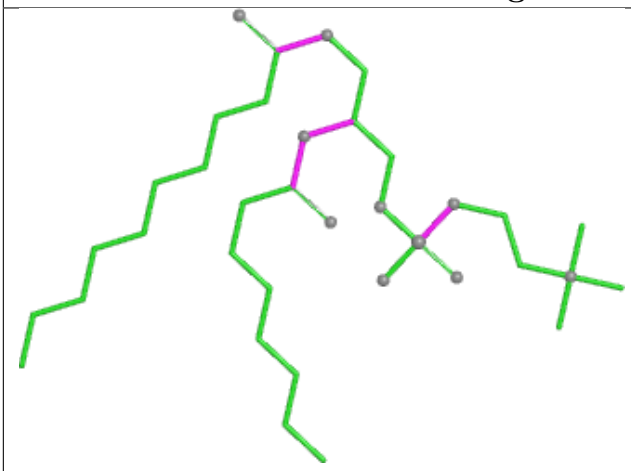


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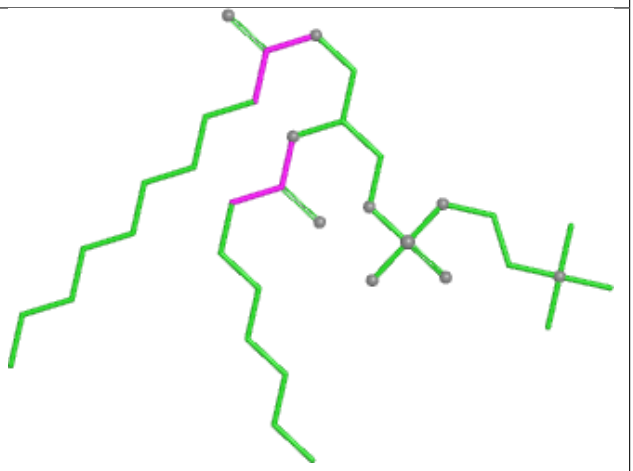


Rings

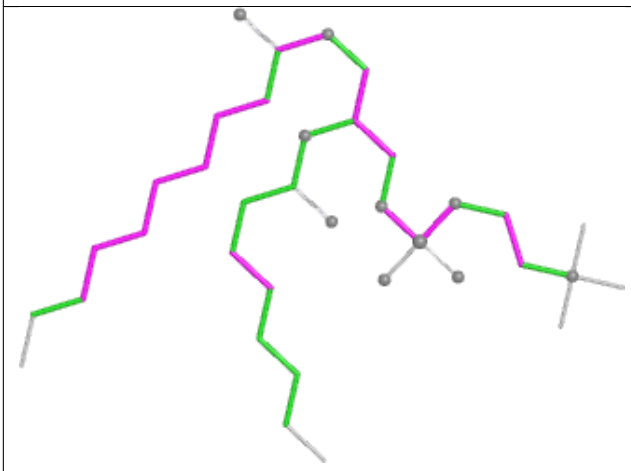
Ligand PCW K 5002



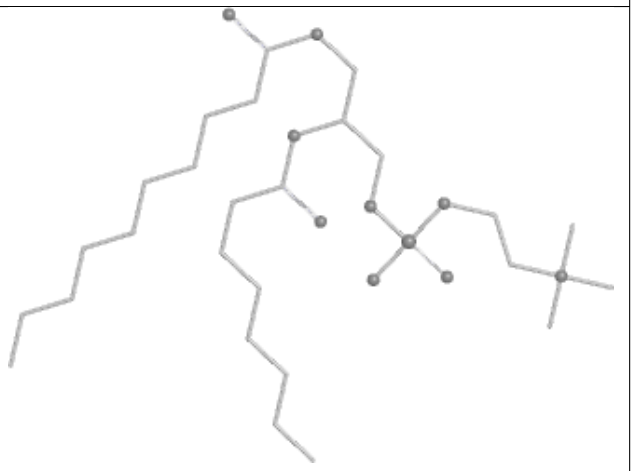
Bond lengths



Bond angles

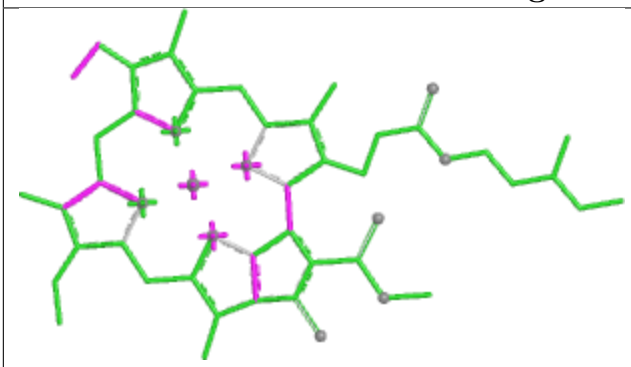


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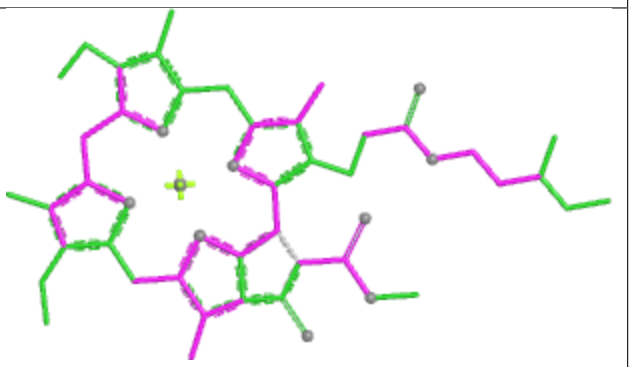


Rings

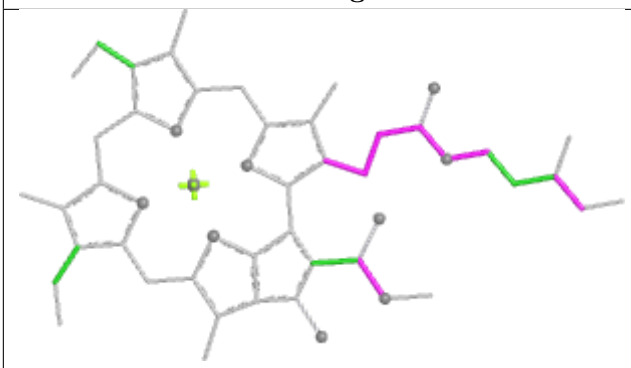
Ligand CLA 5 609



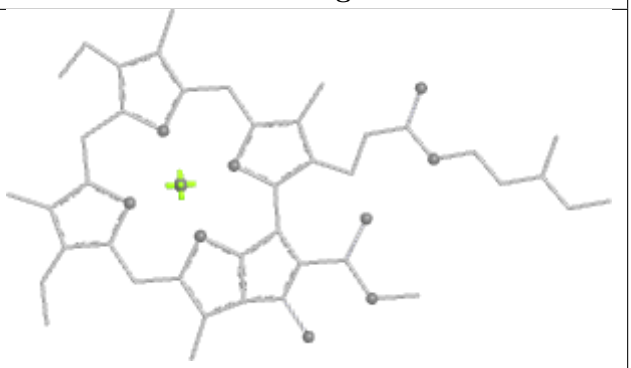
Bond lengths



Bond angles

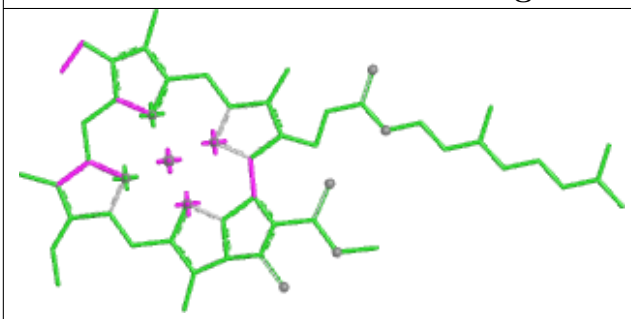


Torsions

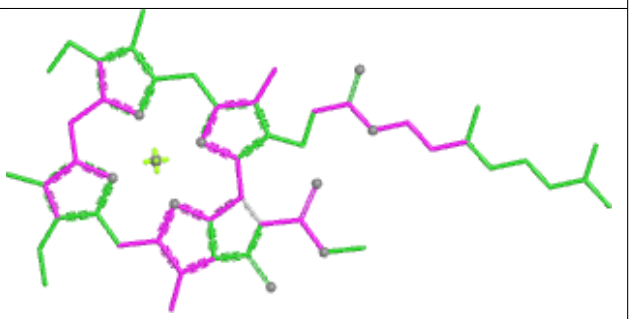


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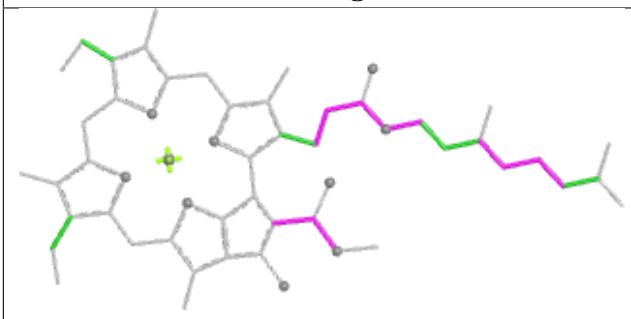
Ligand CLA O 1802



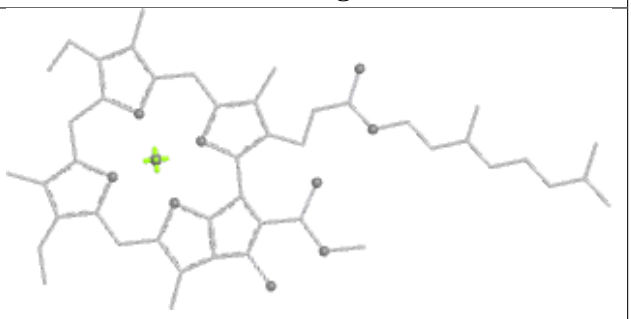
Bond lengths



Bond angles

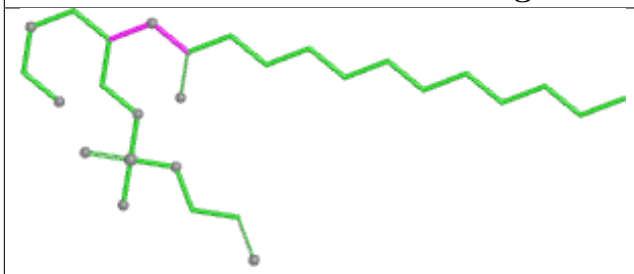


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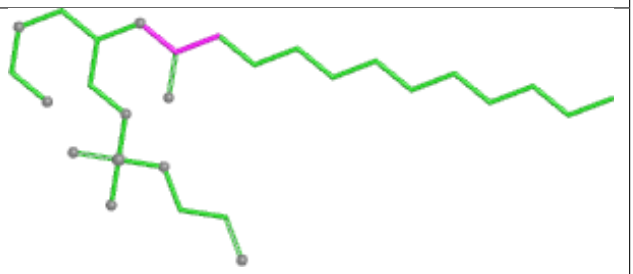


Rings

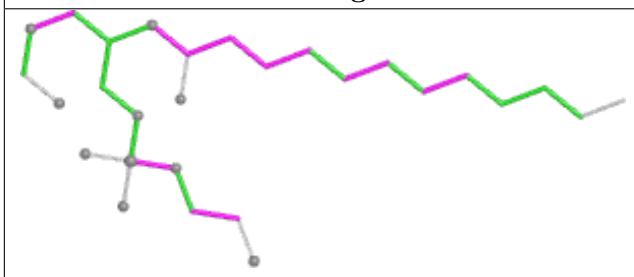
Ligand PTY G 5003



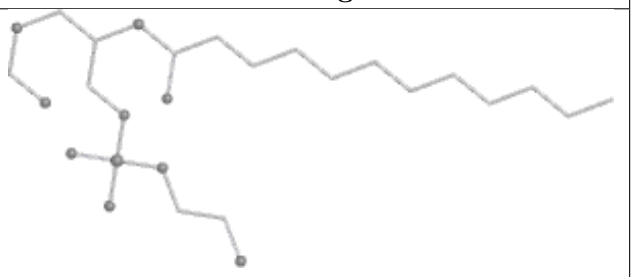
Bond lengths



Bond angles

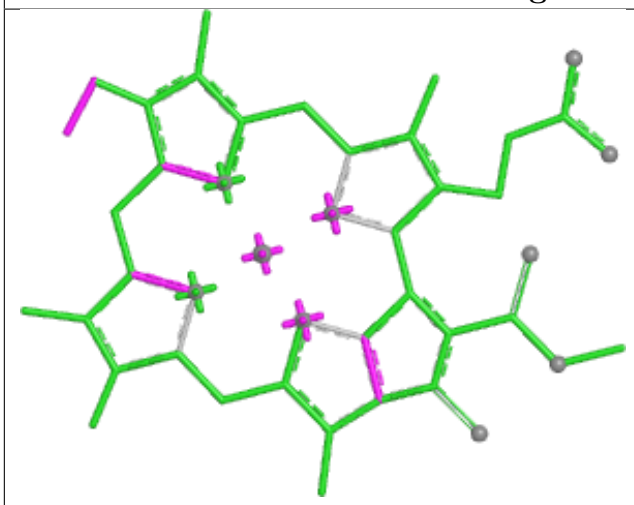


Torsions

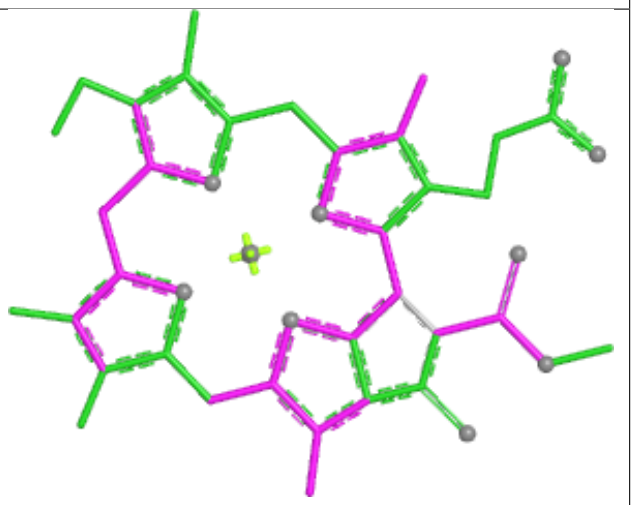


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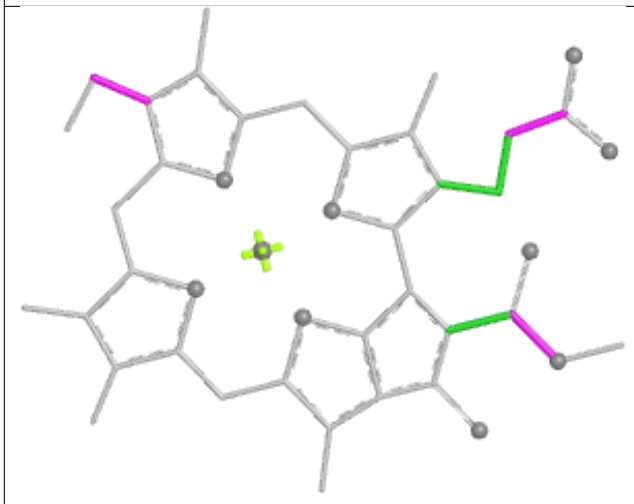
Ligand CLA 7 602



Bond lengths



Bond angles

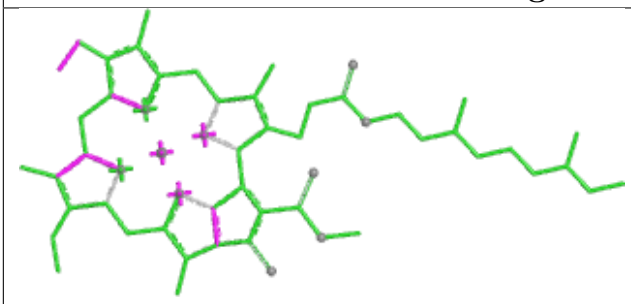


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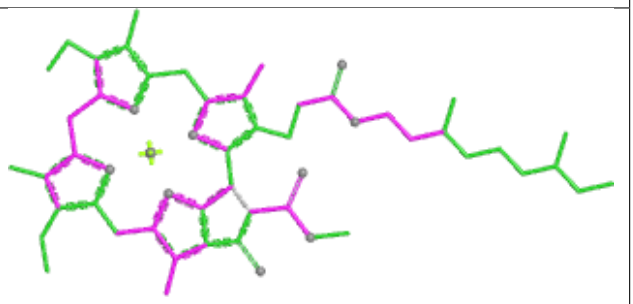


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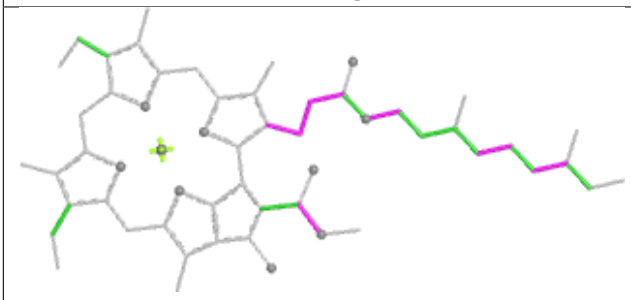
Ligand CLA 2 604



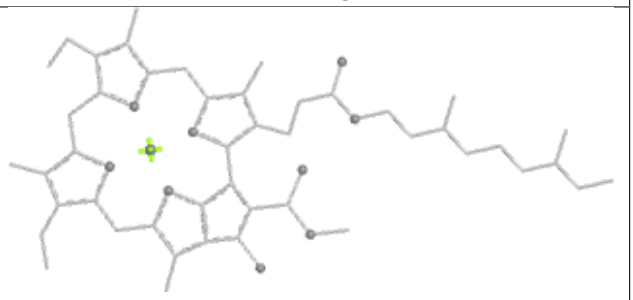
Bond lengths



Bond angles

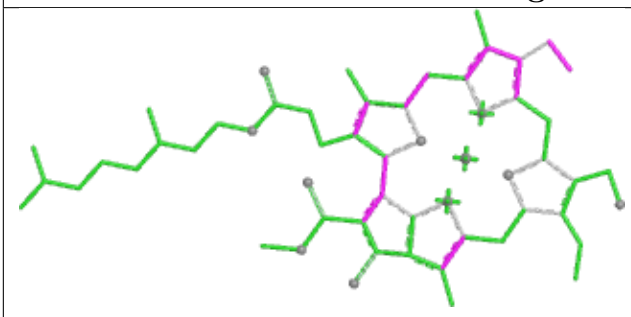


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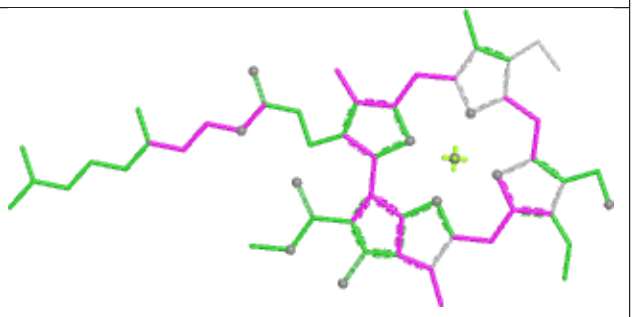


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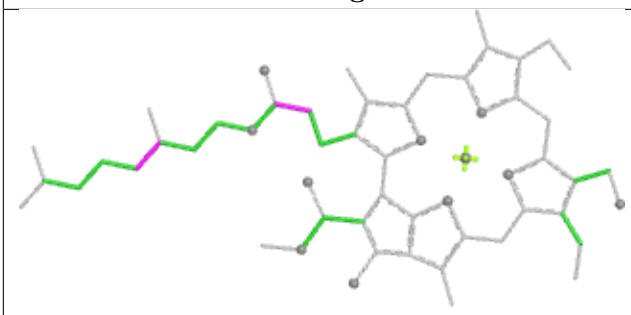
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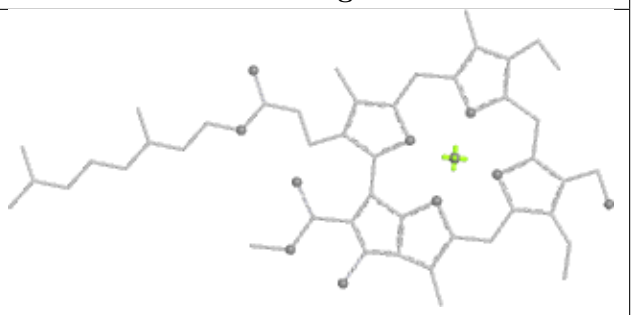
Bond lengths



Bond angles

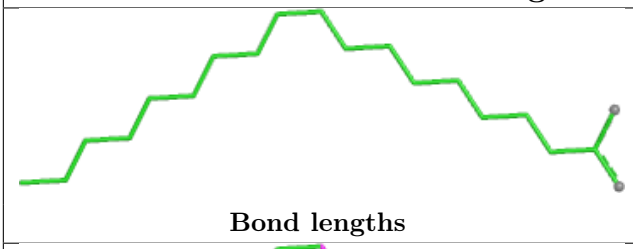


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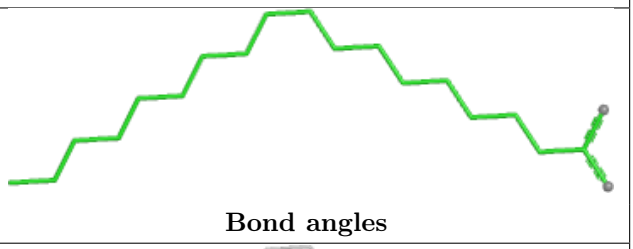


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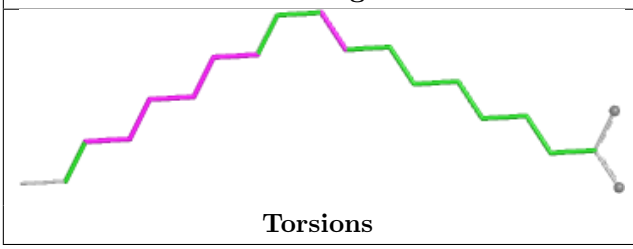
Ligand OLA a 805



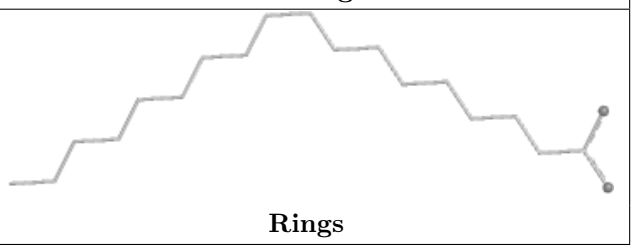
Bond lengths



Bond angles

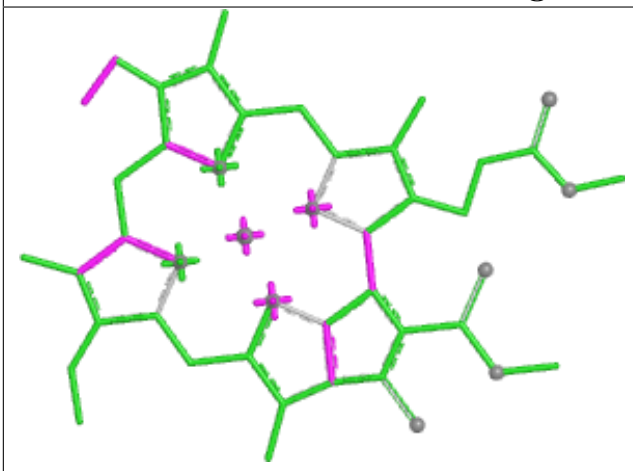


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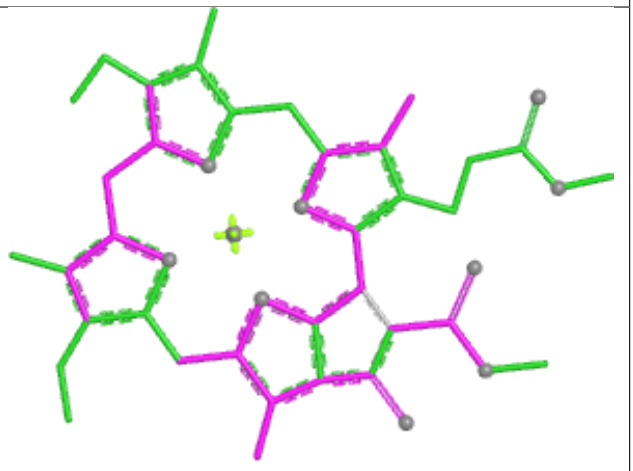


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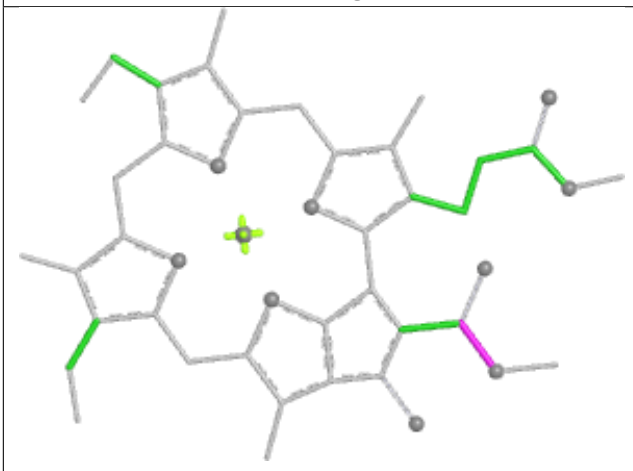
Ligand CLA 5 605



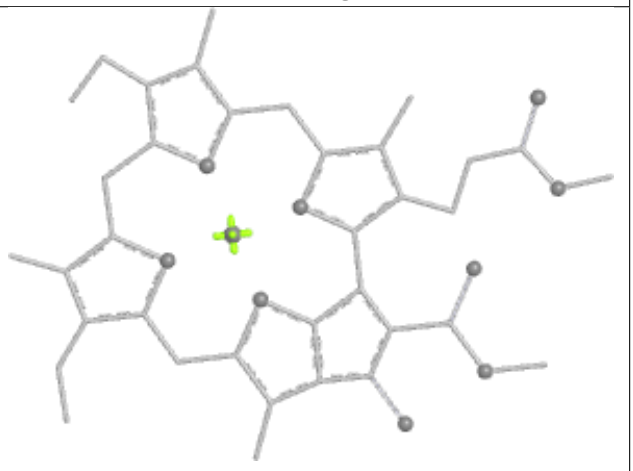
Bond lengths



Bond angles

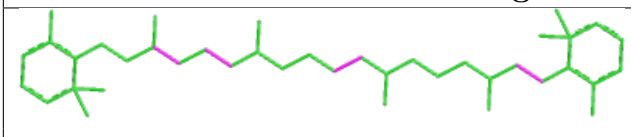


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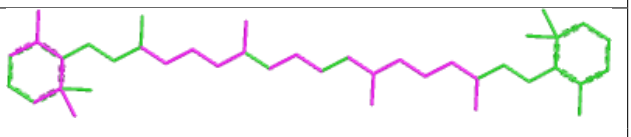


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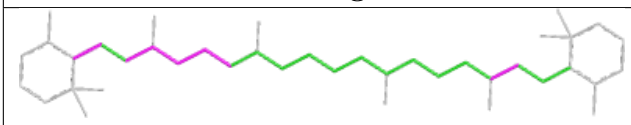
Ligand BCR K 4001



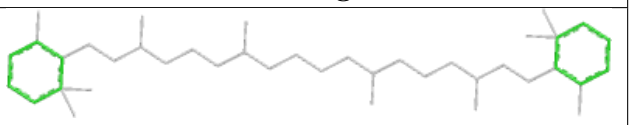
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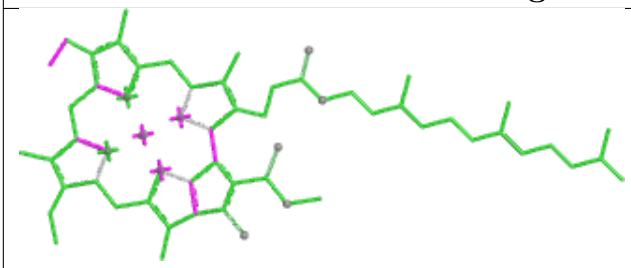


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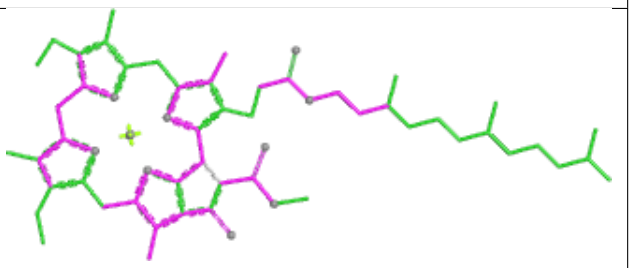


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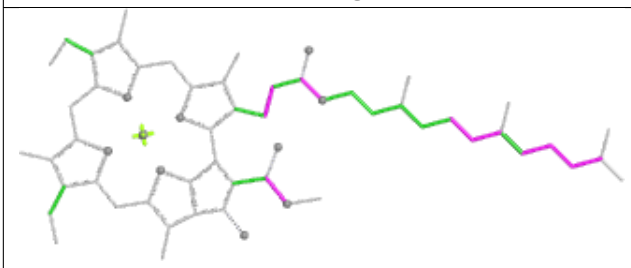
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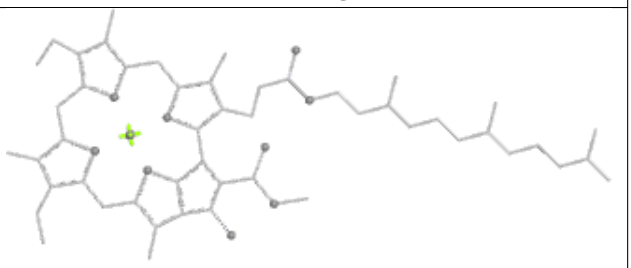
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Bond angles

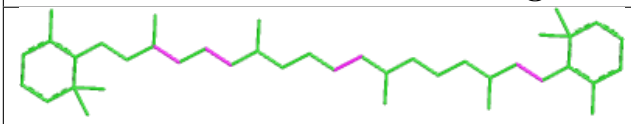


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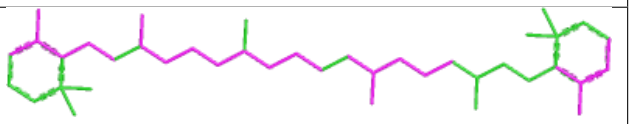


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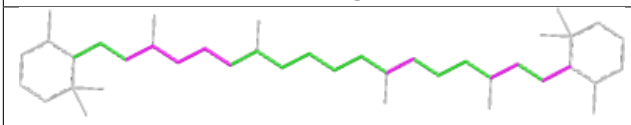
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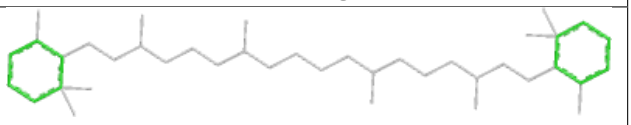
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Bond angles

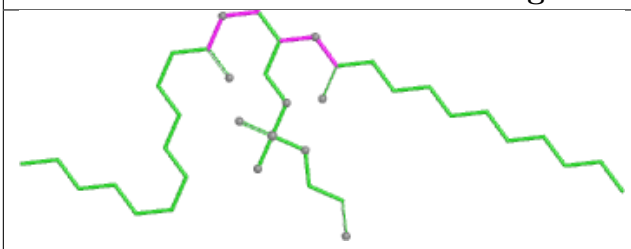


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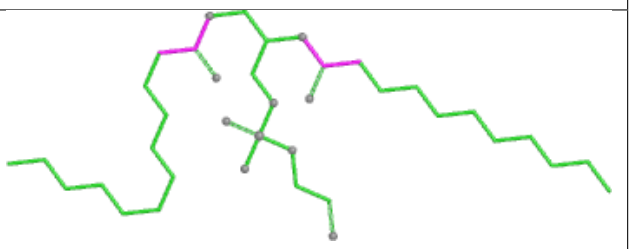


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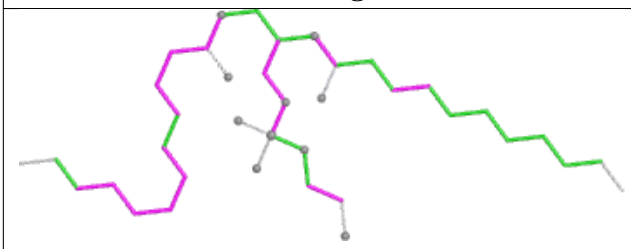
Ligand PTY a 802



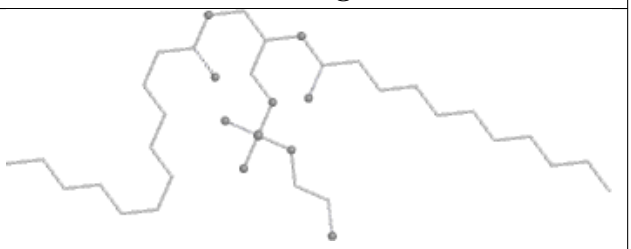
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Bond angles

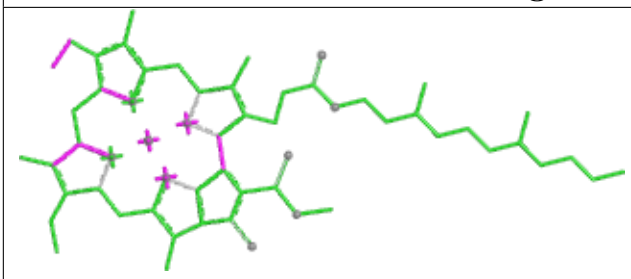


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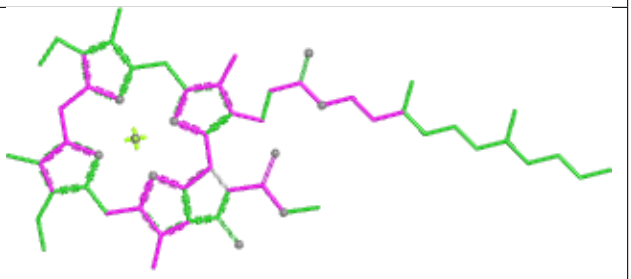


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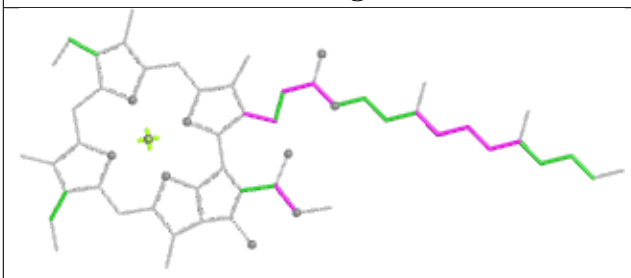
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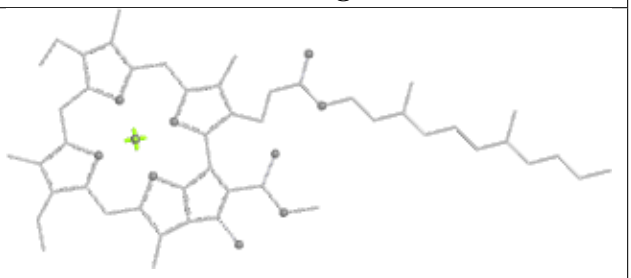
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Bond angles

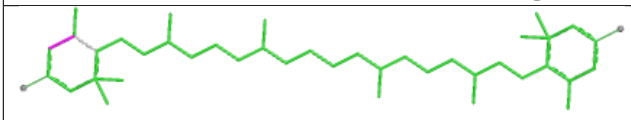


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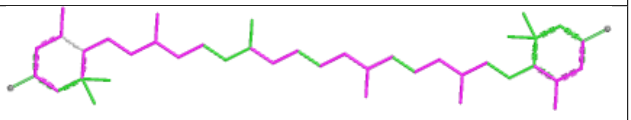


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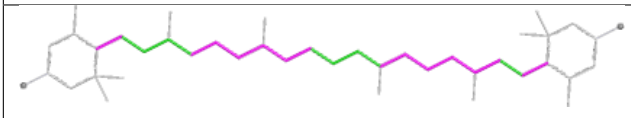
Ligand LUT 2 507



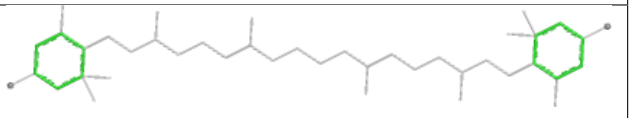
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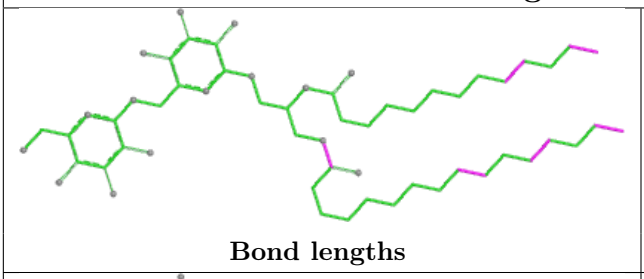


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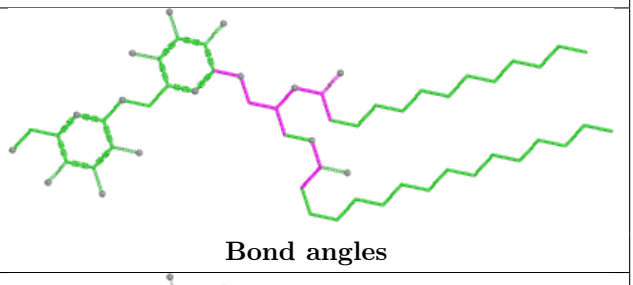


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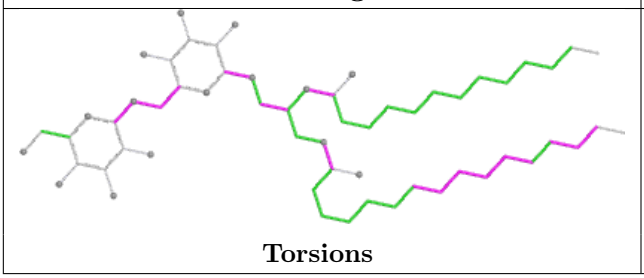
Ligand DGD 8 802



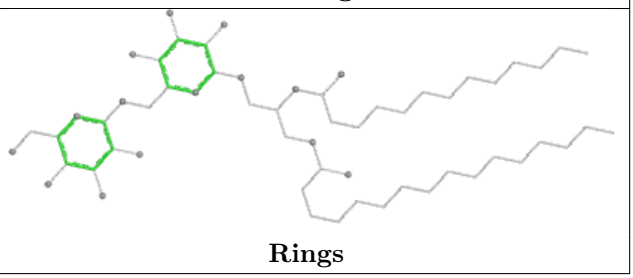
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Bond angles

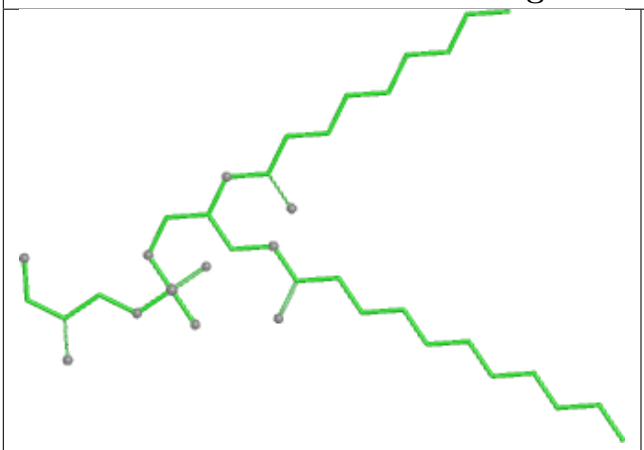


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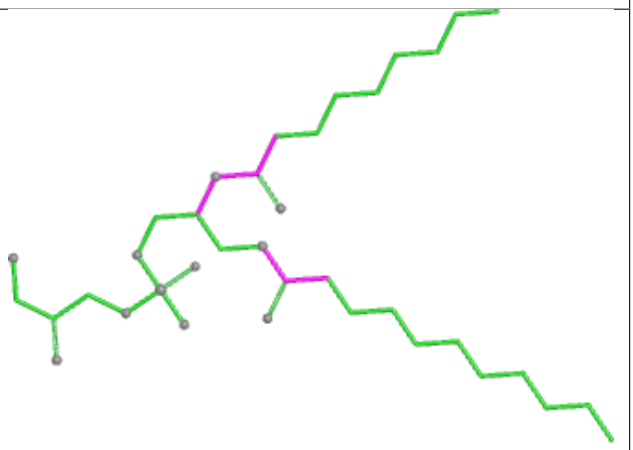


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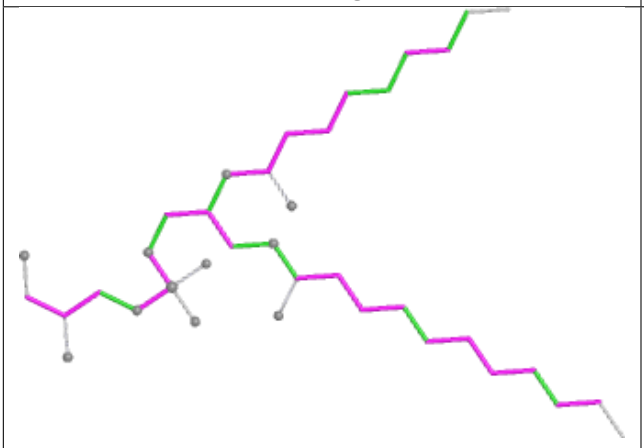
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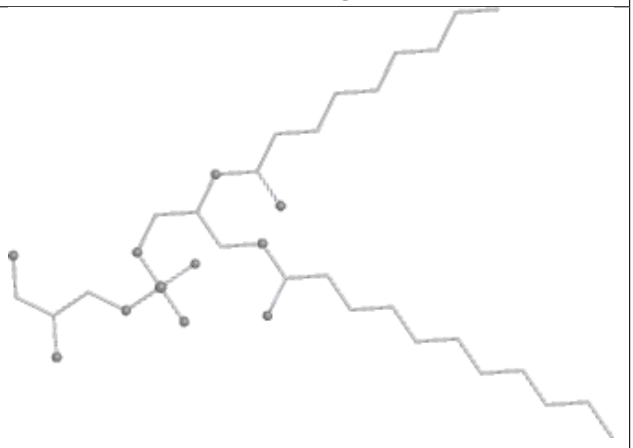
Bond lengths



Bond angles

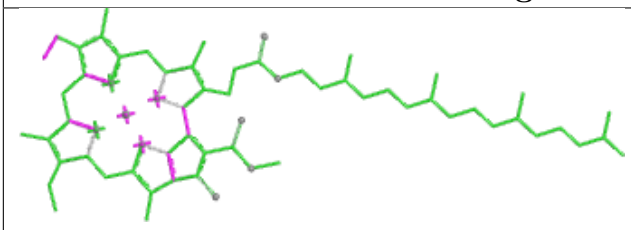


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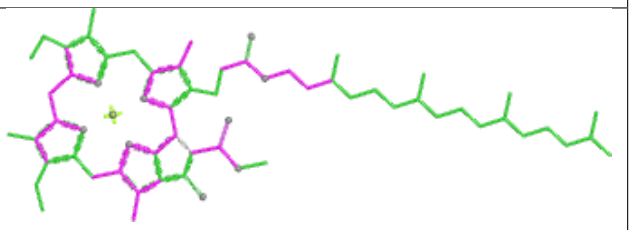


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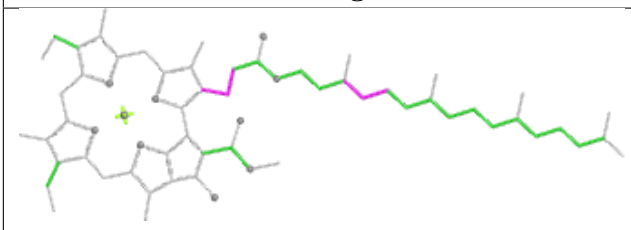
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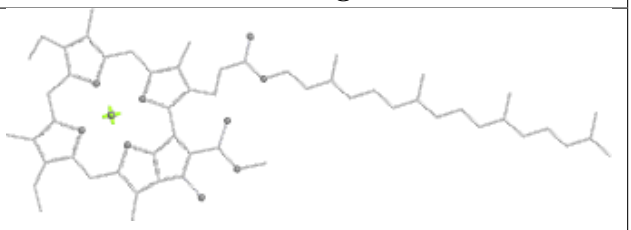
Bond lengths



Bond angles

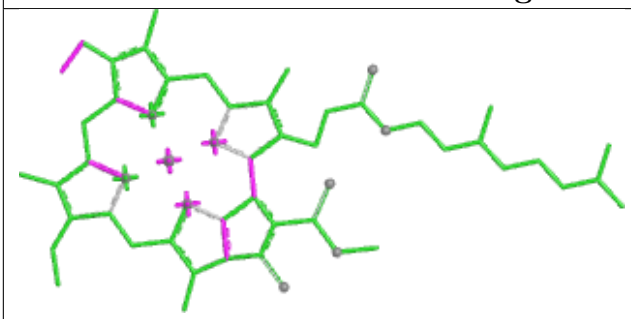


Torsions

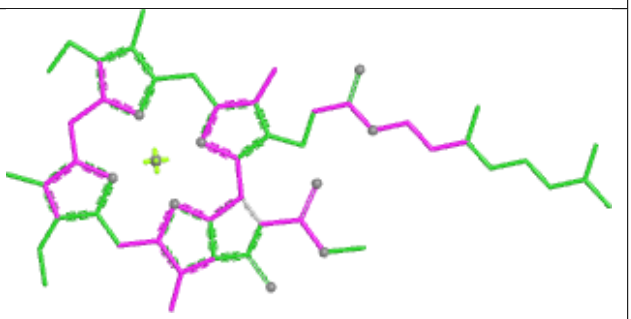


Rings

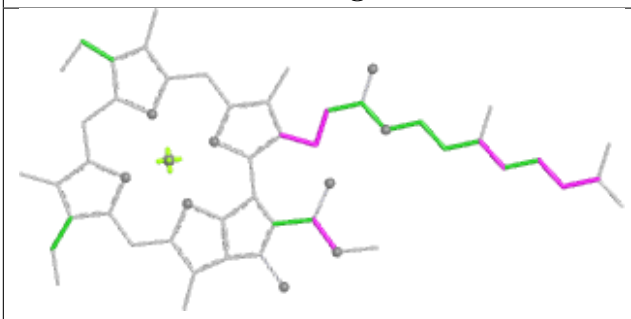
Ligand CLA A 1107



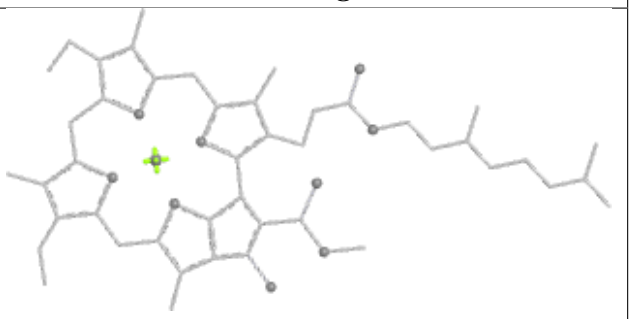
Bond lengths



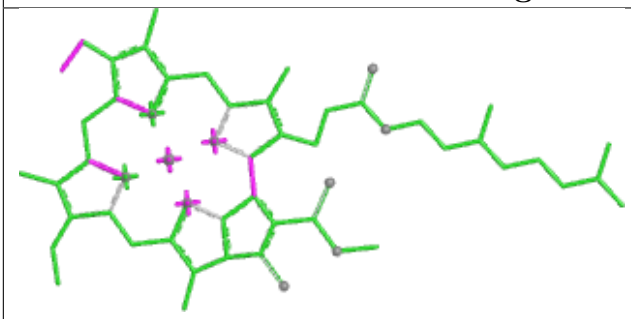
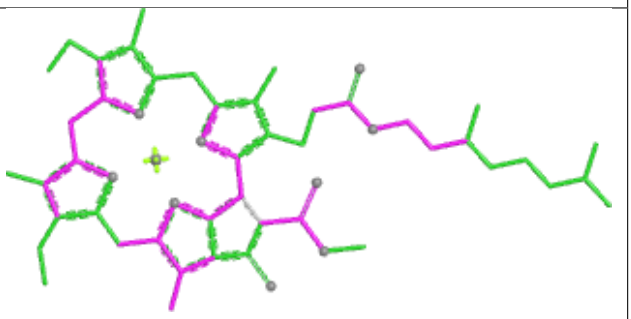
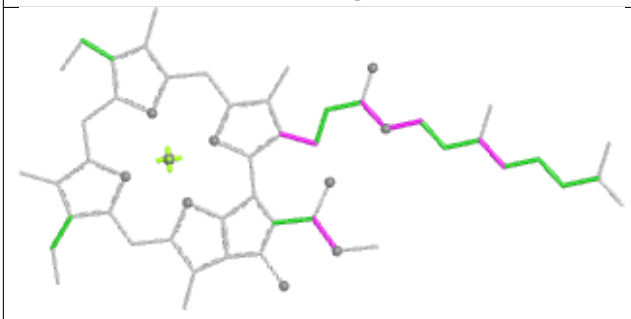
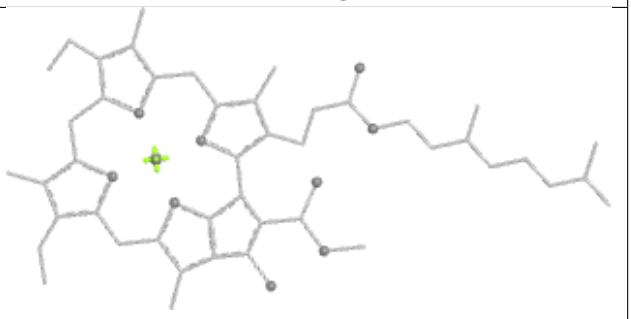
Bond angles

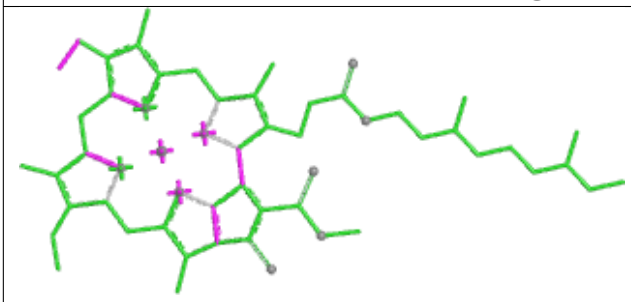
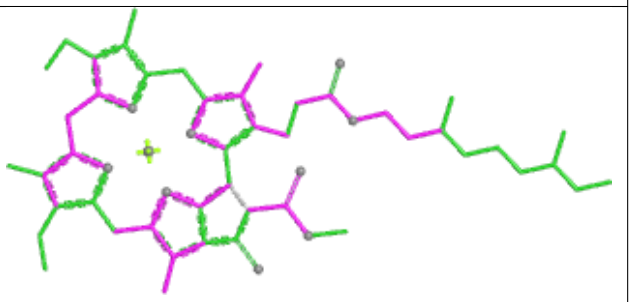
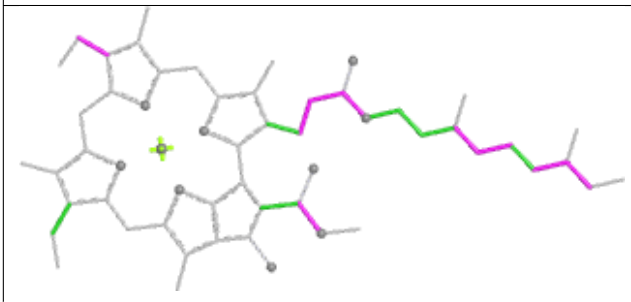
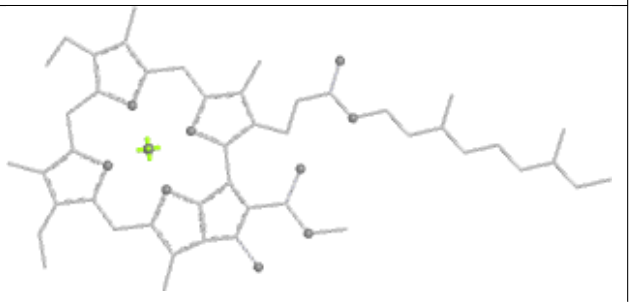


Torsions

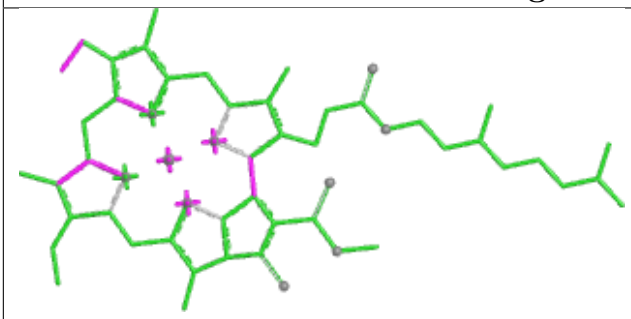


Rings

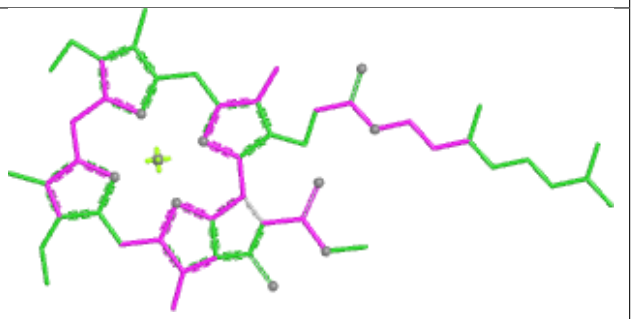
Ligand CLA A 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

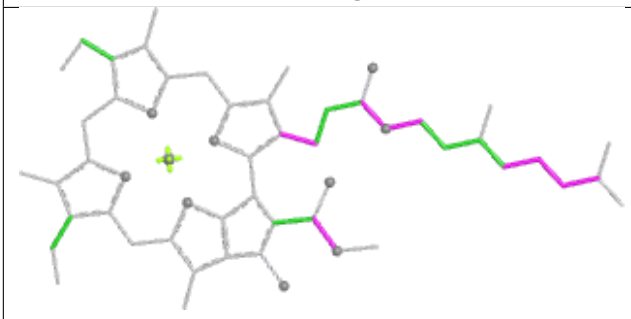
Ligand CLA 6 607



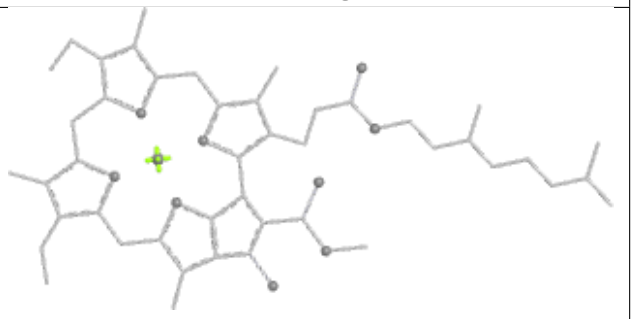
Bond lengths



Bond angles

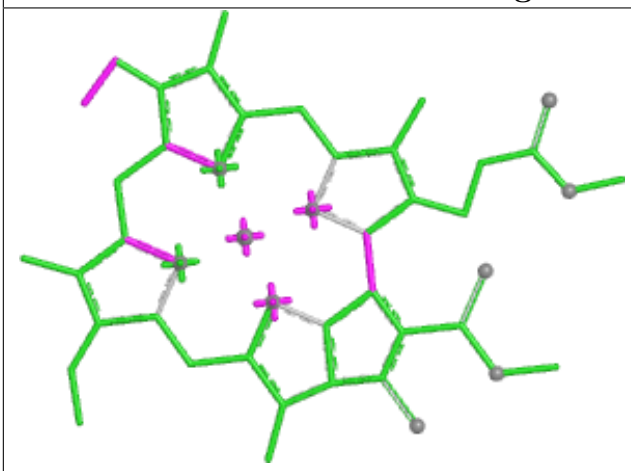


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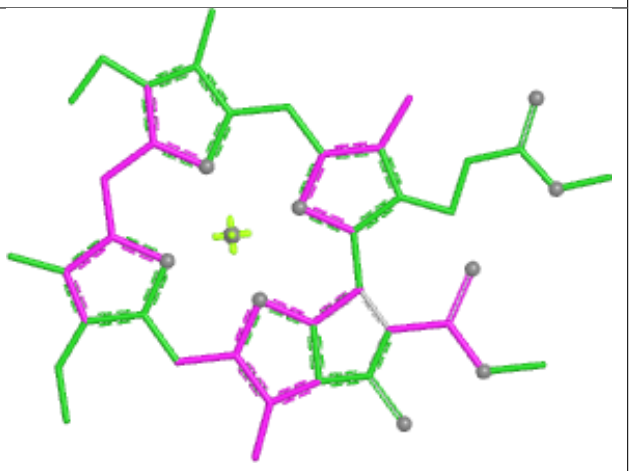


Rings

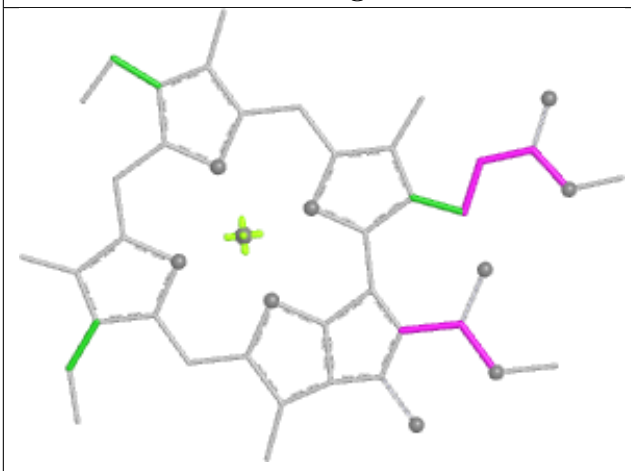
Ligand CLA H 1702



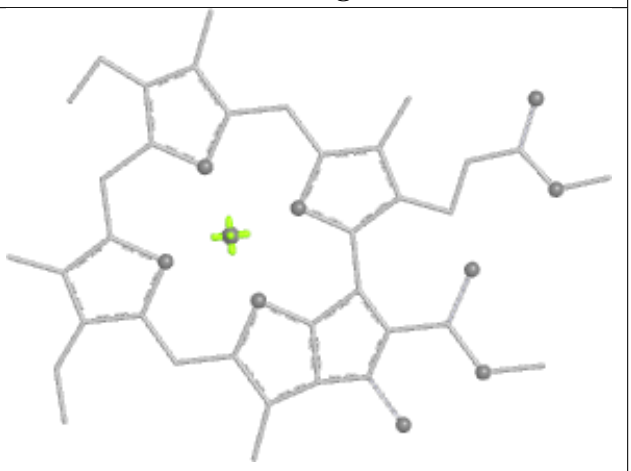
Bond lengths



Bond angles

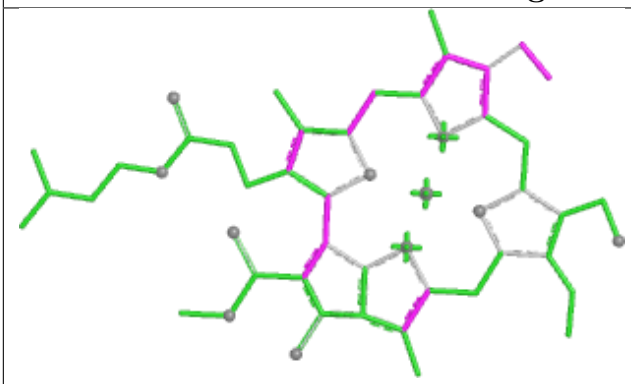


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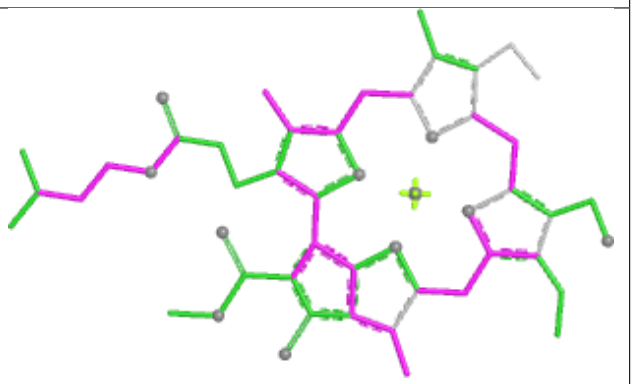


Rings

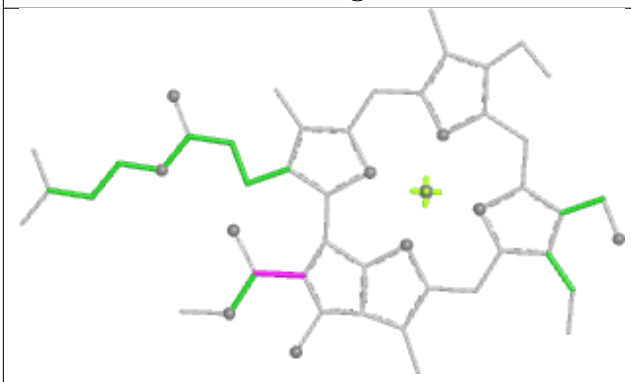
Ligand CHL 8 613



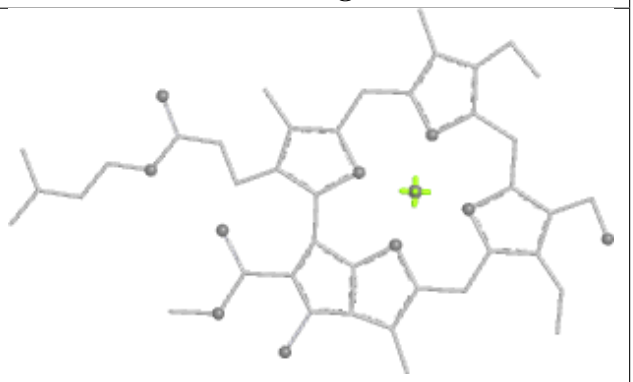
Bond lengths



Bond angles

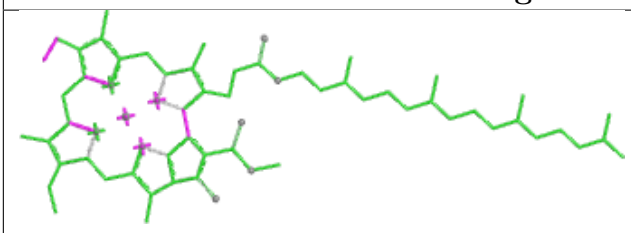


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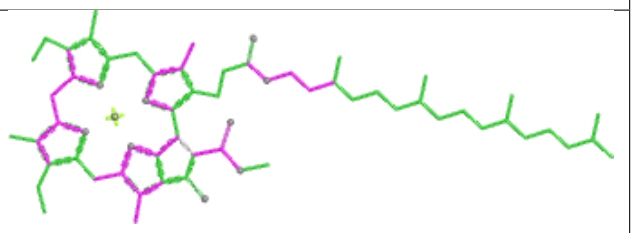


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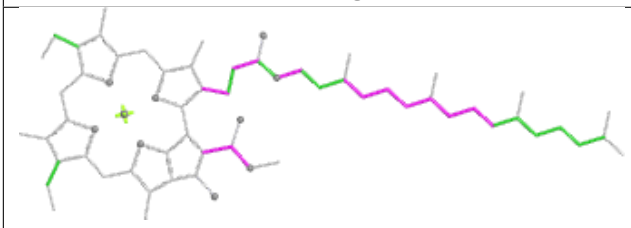
Ligand CLA A 1103



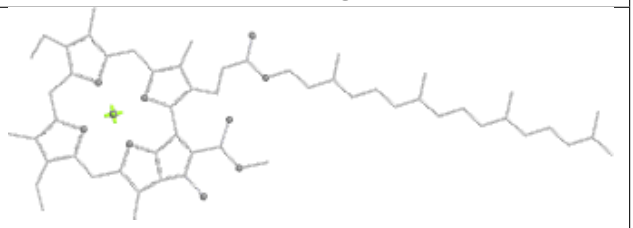
Bond lengths



Bond angles

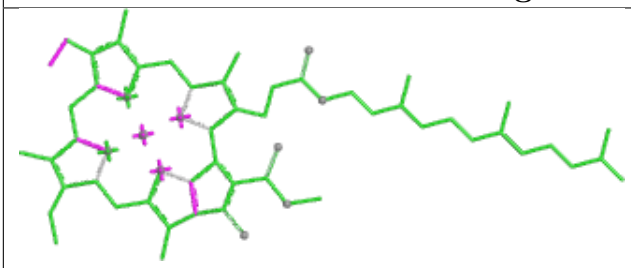


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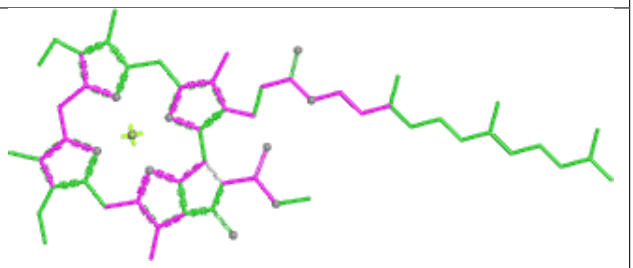


Rings

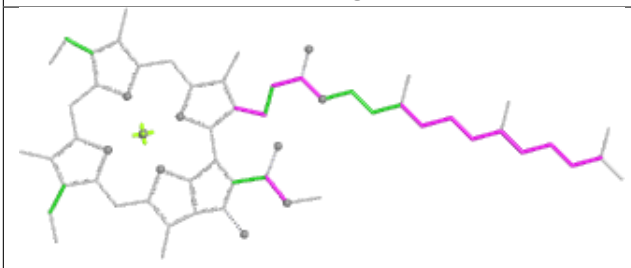
Ligand CLA A 1121



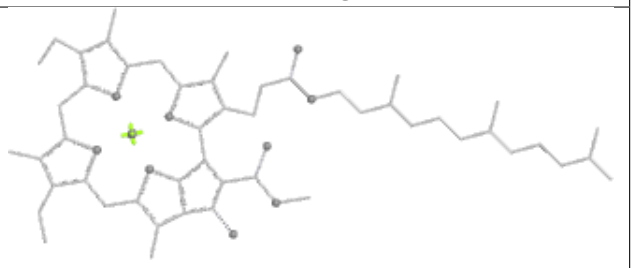
Bond lengths



Bond angles

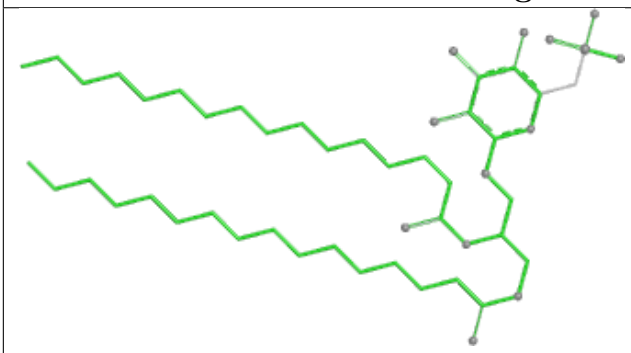


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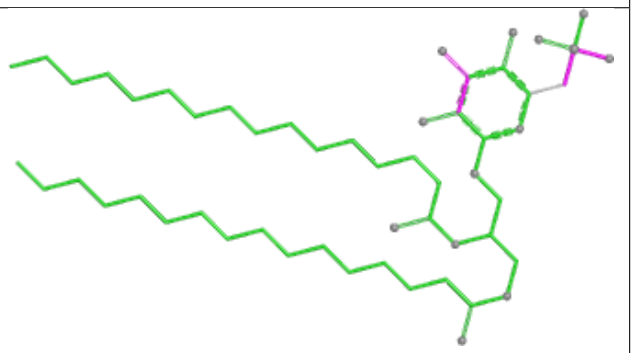


Rings

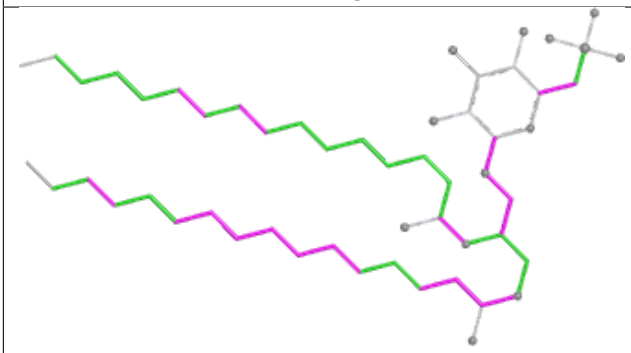
Ligand SQD A 5005



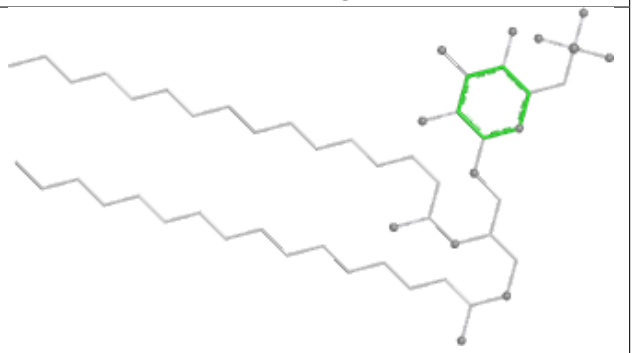
Bond lengths



Bond angles

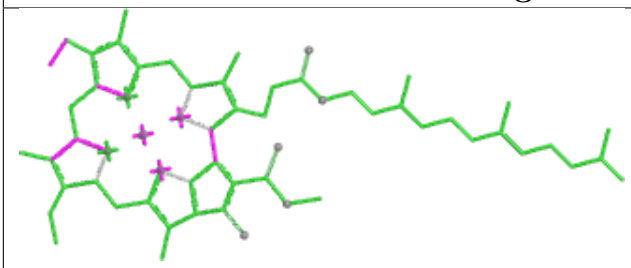


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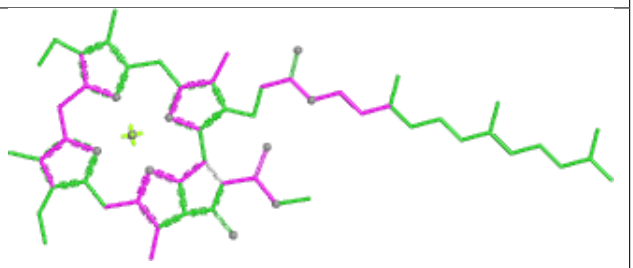


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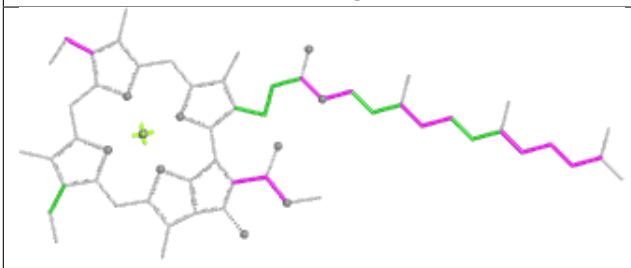
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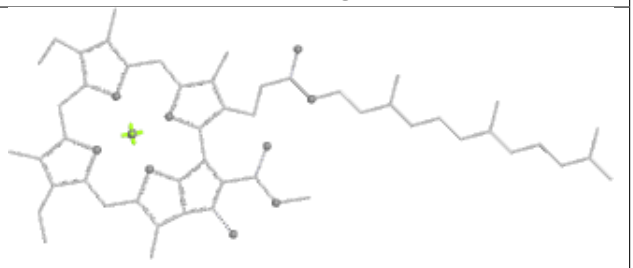
Bond lengths



Bond angles

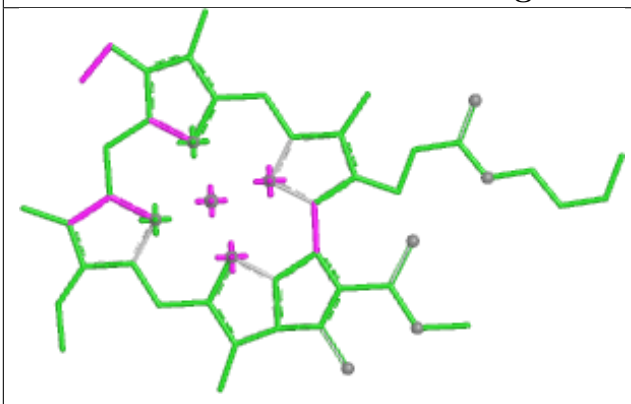


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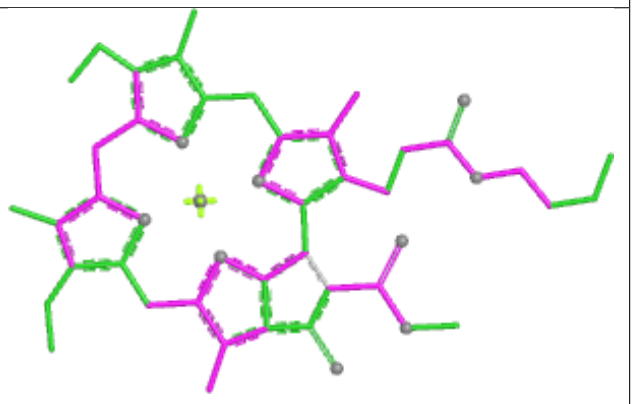


Rings

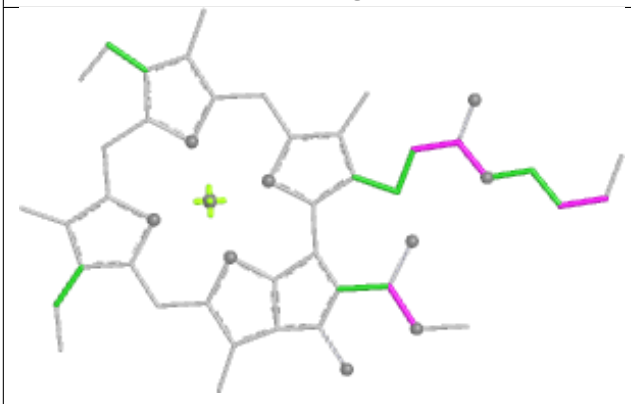
Ligand CLA A 1120



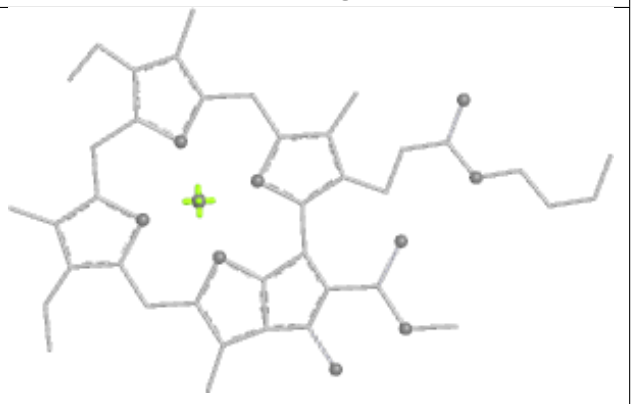
Bond lengths



Bond angles

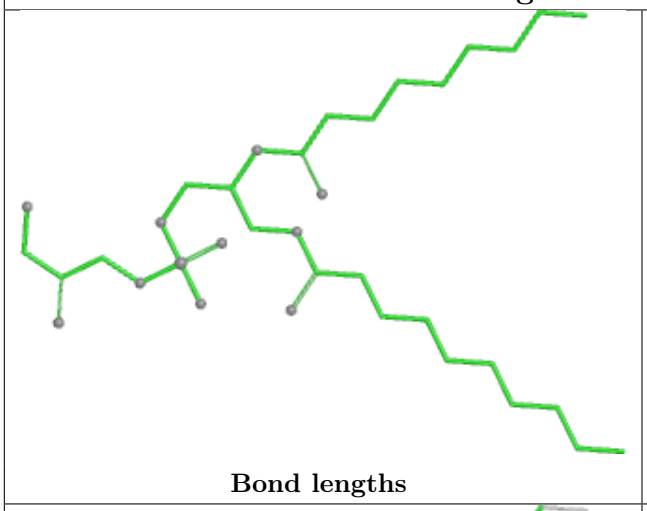


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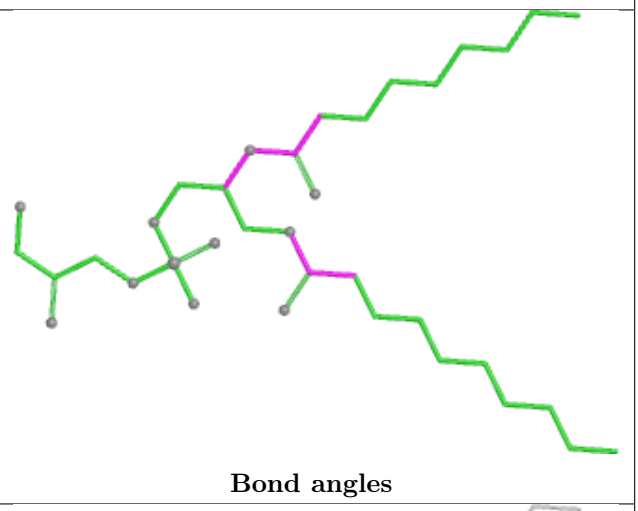


Rings

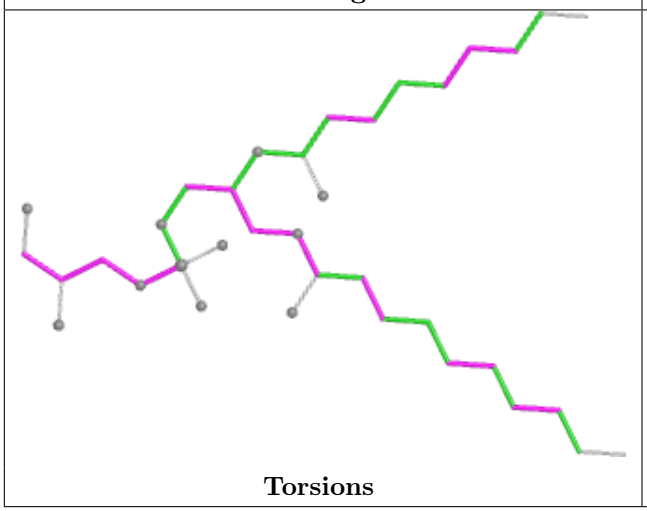
Ligand LHG F 5002



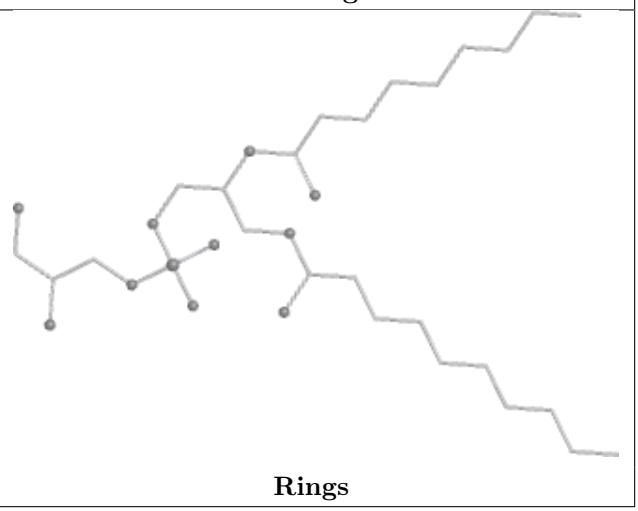
Bond lengths



Bond angles

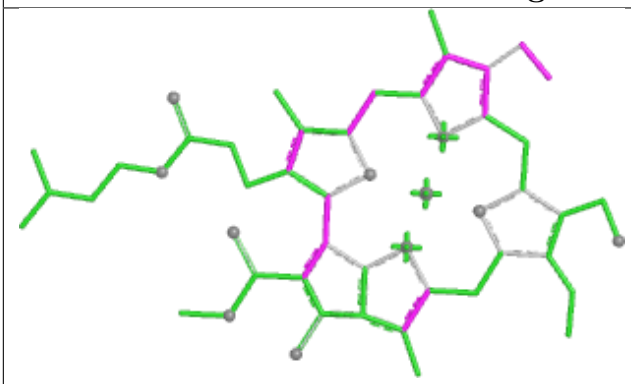


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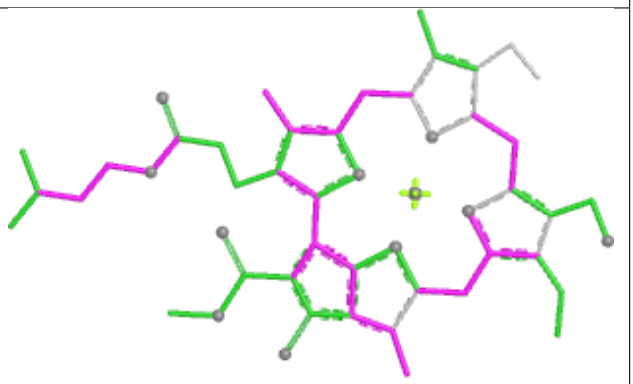


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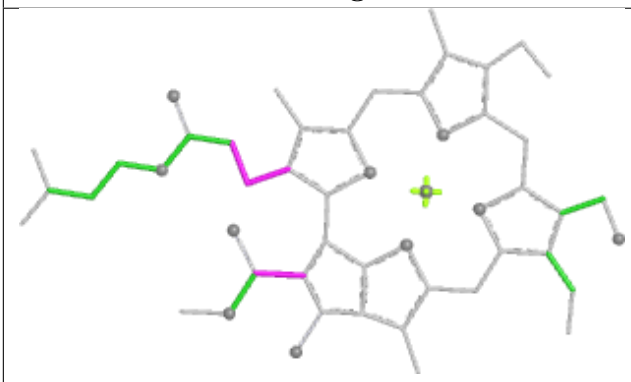
Ligand CHL 6 611



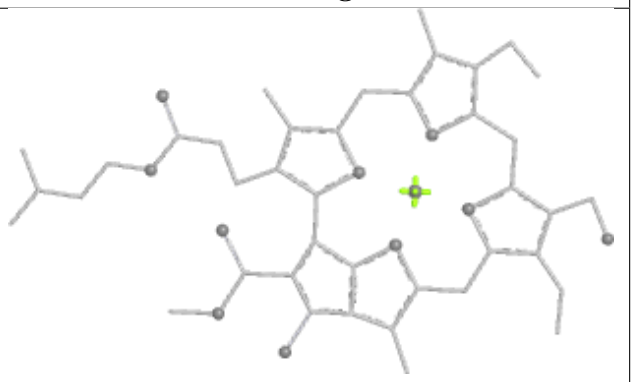
Bond lengths



Bond angles

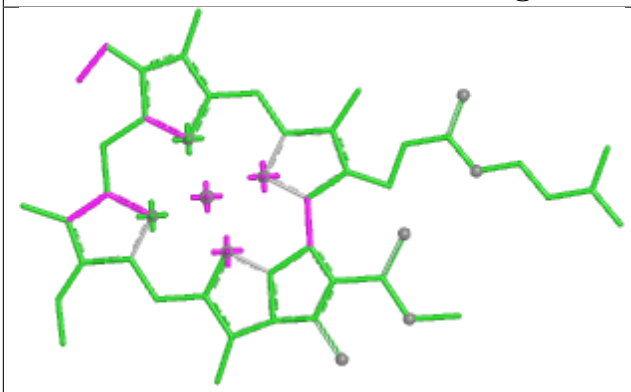


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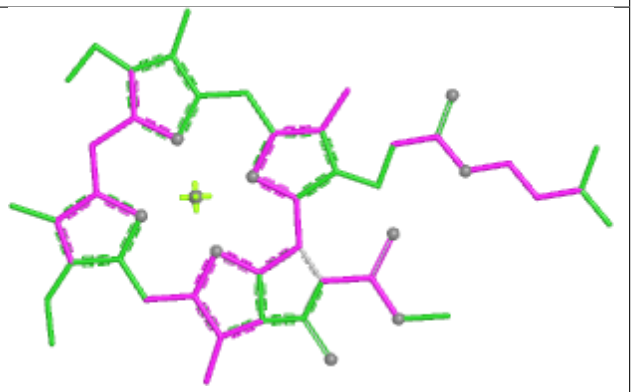


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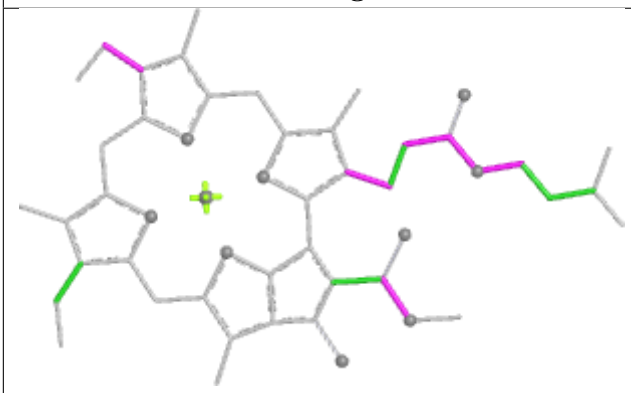
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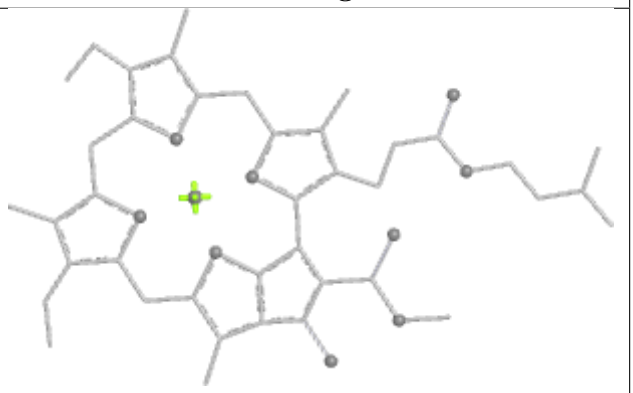
Bond lengths



Bond angles

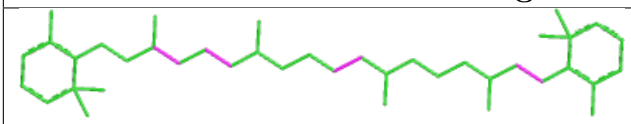


Torsions

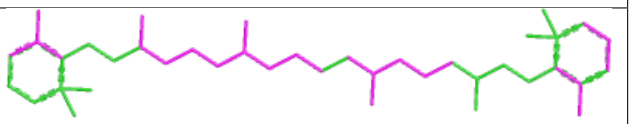


Rings

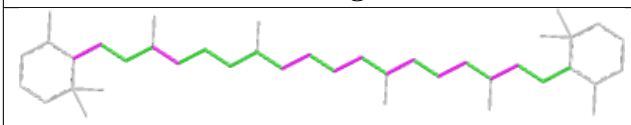
Ligand BCR L 4002



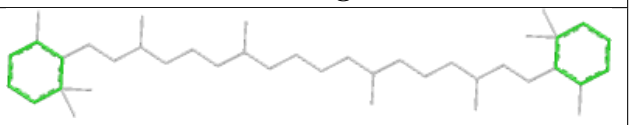
Bond lengths



Bond angles

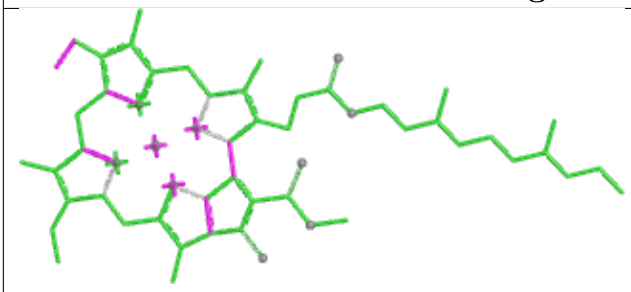


Torsions

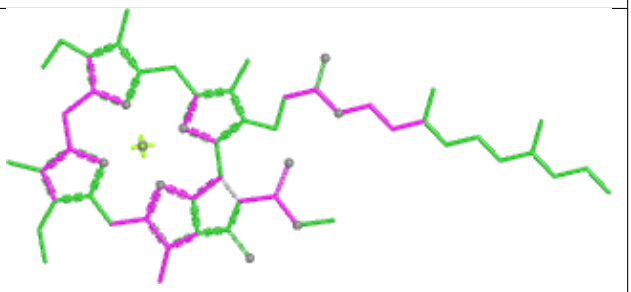


Rings

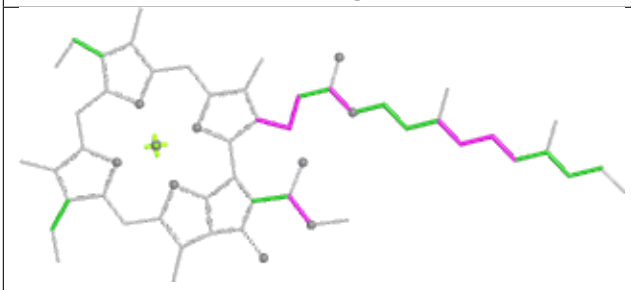
Ligand CLA 1 606



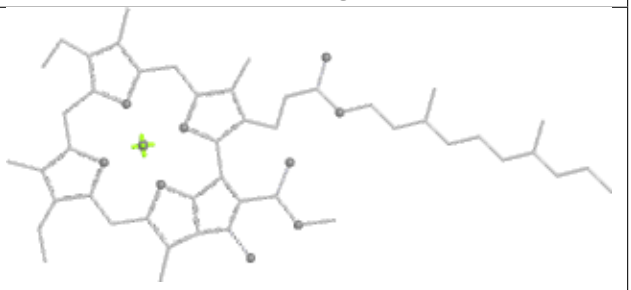
Bond lengths



Bond angles

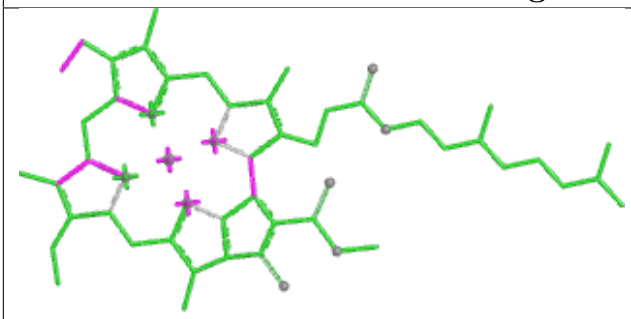


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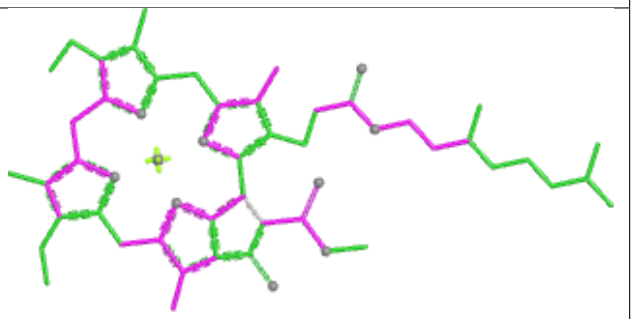


Rings

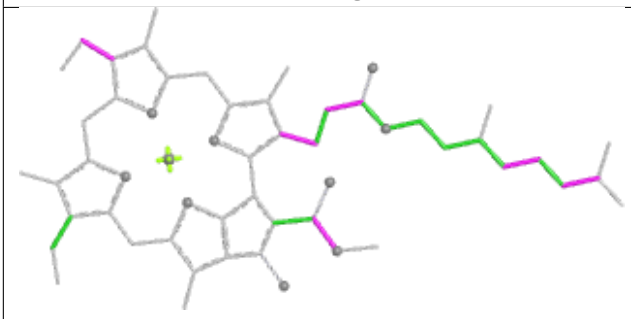
Ligand CLA a 608



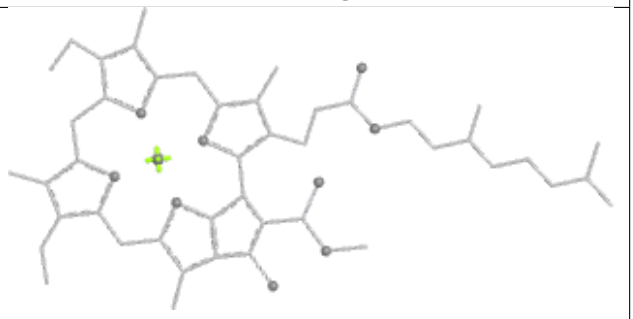
Bond lengths



Bond angles

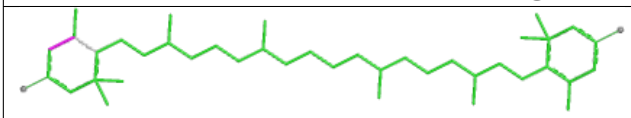


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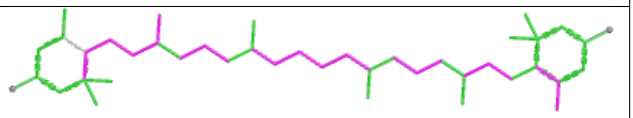


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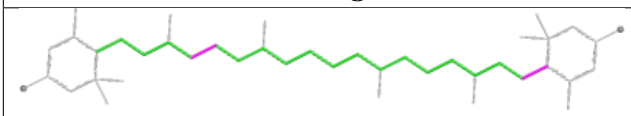
Ligand LUT 5 502



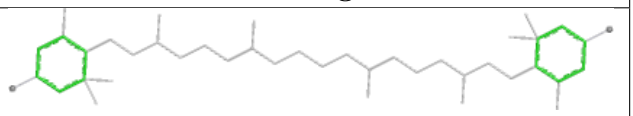
Bond lengths



Bond angles

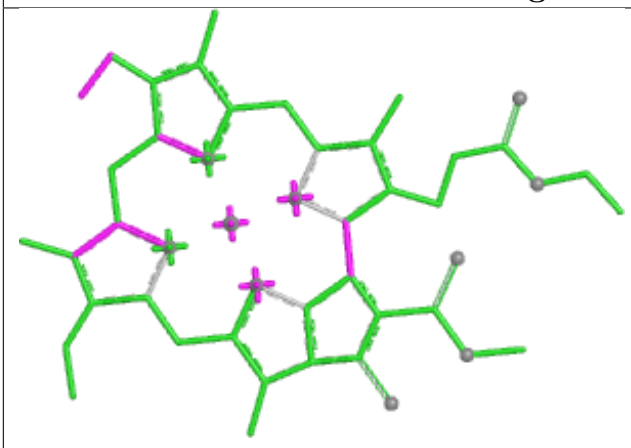


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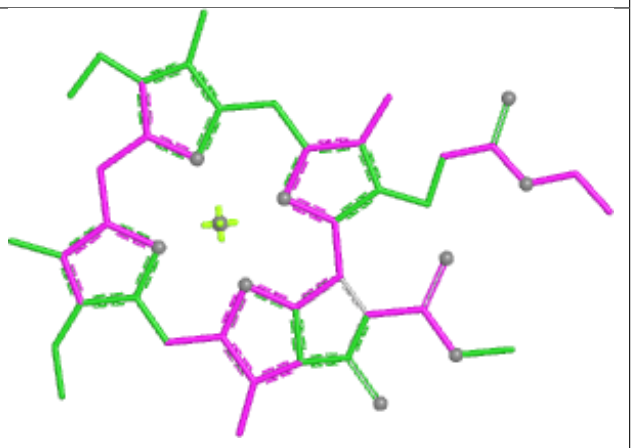


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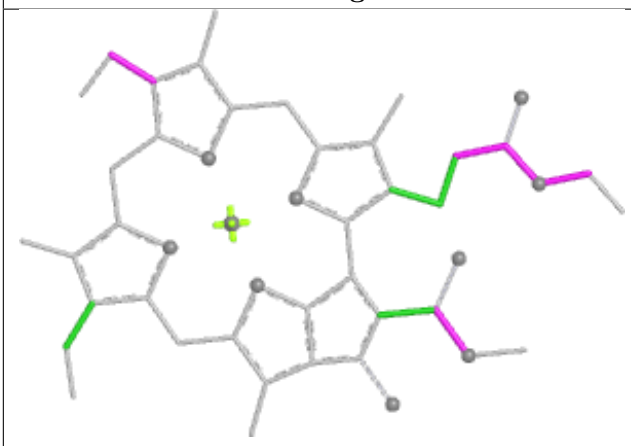
Ligand CLA 9 607



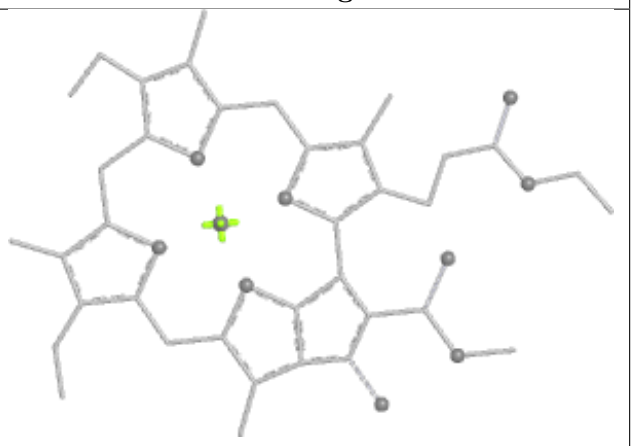
Bond lengths



Bond angles

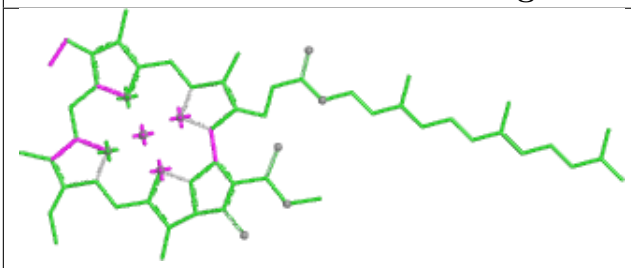


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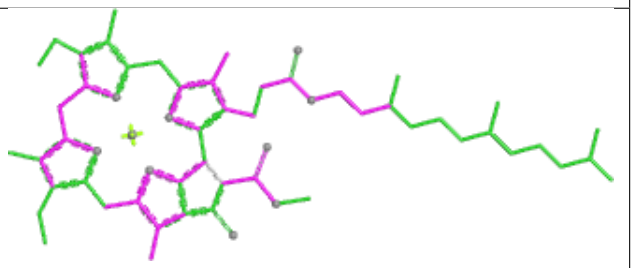


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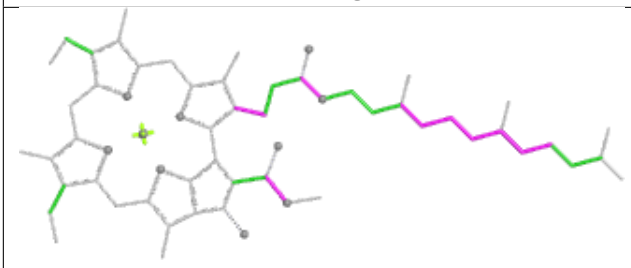
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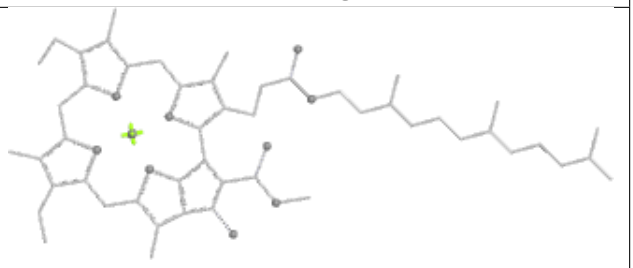
Bond lengths



Bond angles

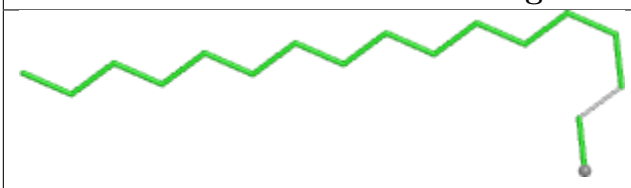


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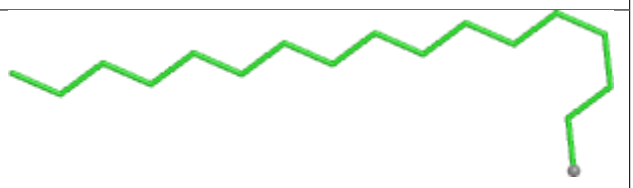


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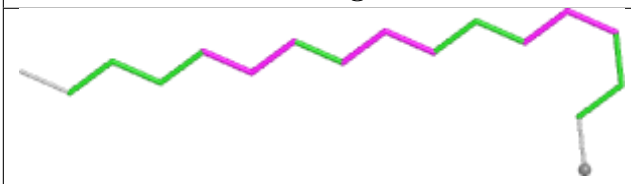
Ligand PLM 8 806



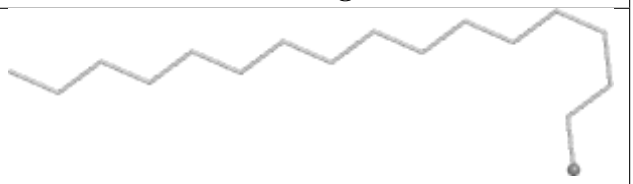
Bond lengths



Bond angles

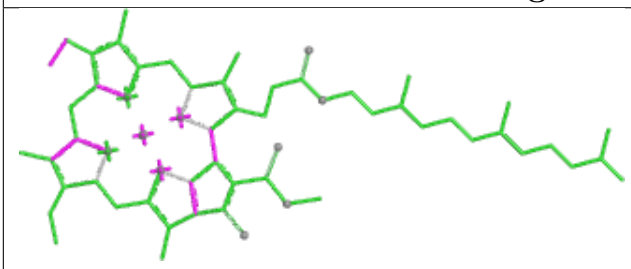


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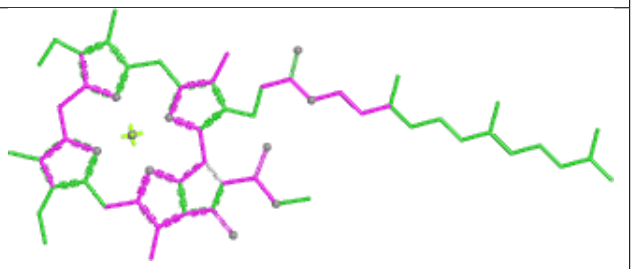


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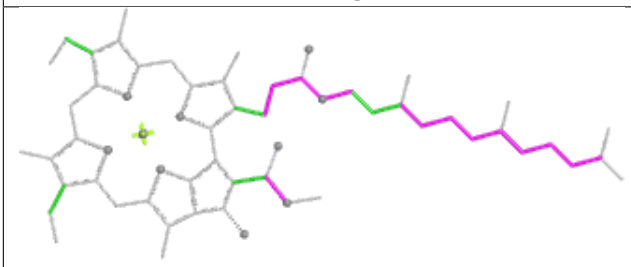
Ligand CLA 2 605



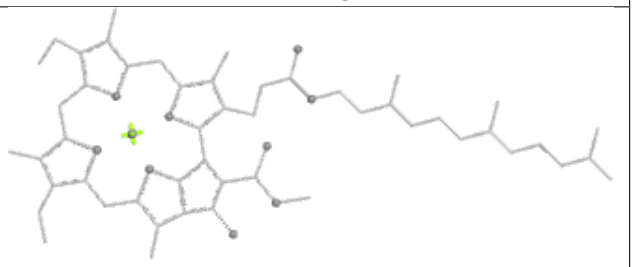
Bond lengths



Bond angles

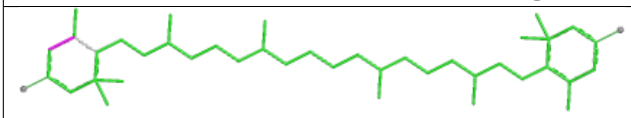


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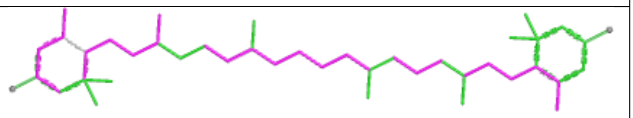


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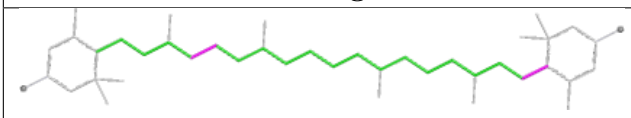
Ligand LUT 9 502



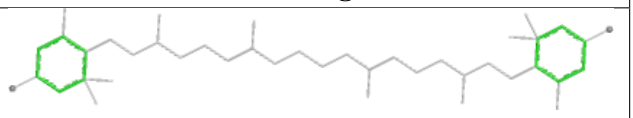
Bond lengths



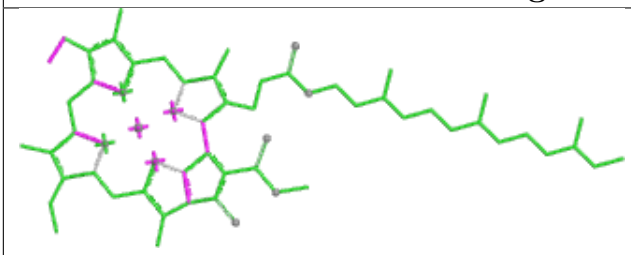
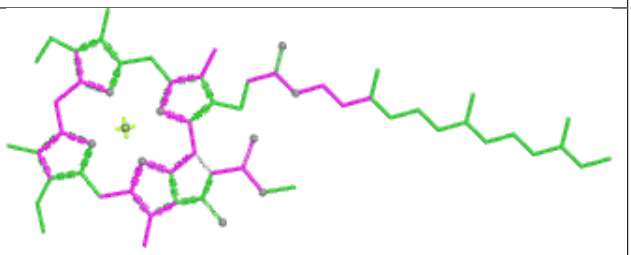
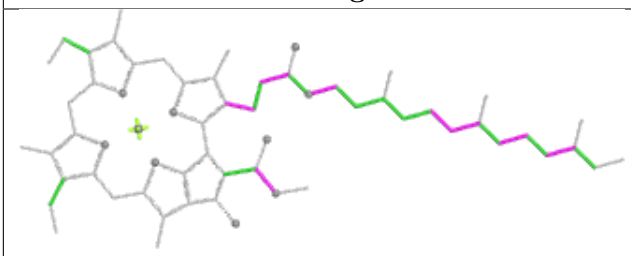
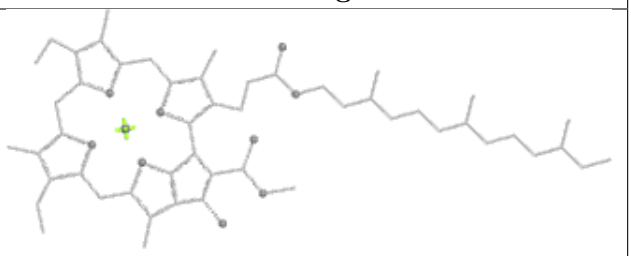
Bond angles

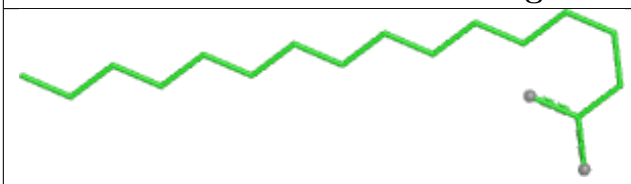
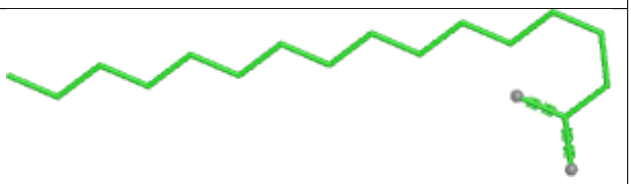
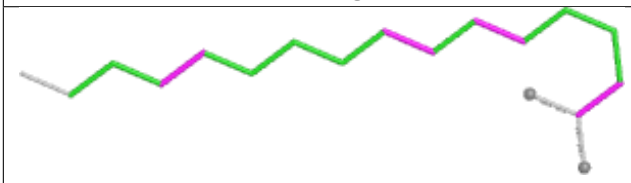
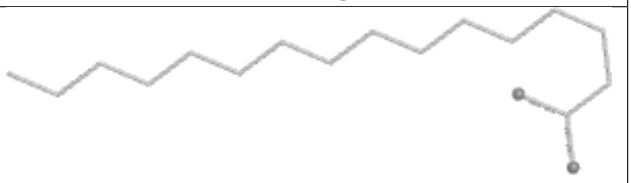


Torsions

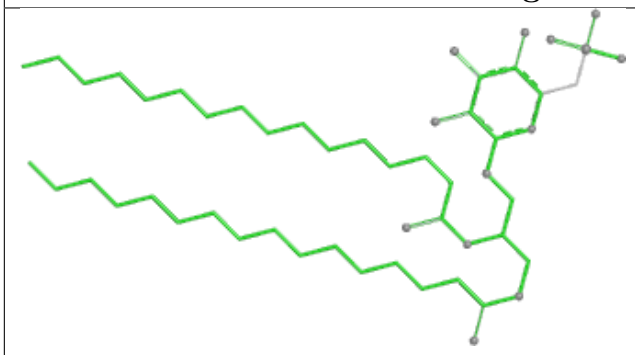


Rings

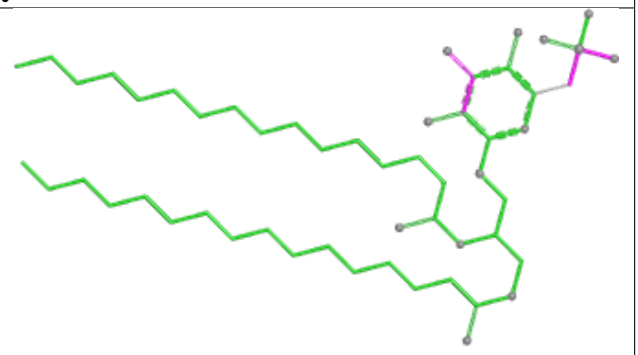
Ligand CLA 3 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM 8 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

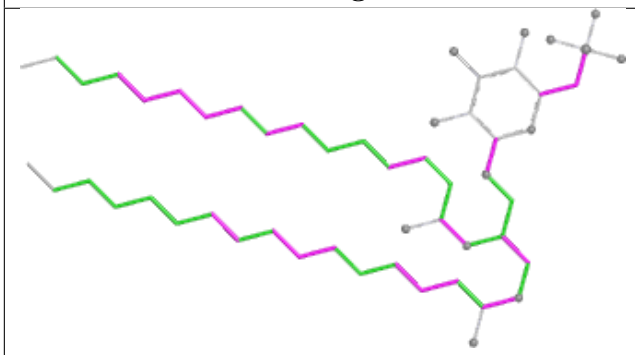
Ligand SQD I 5001



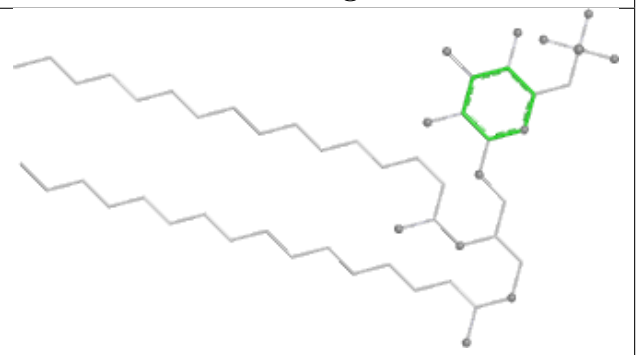
Bond lengths



Bond angles

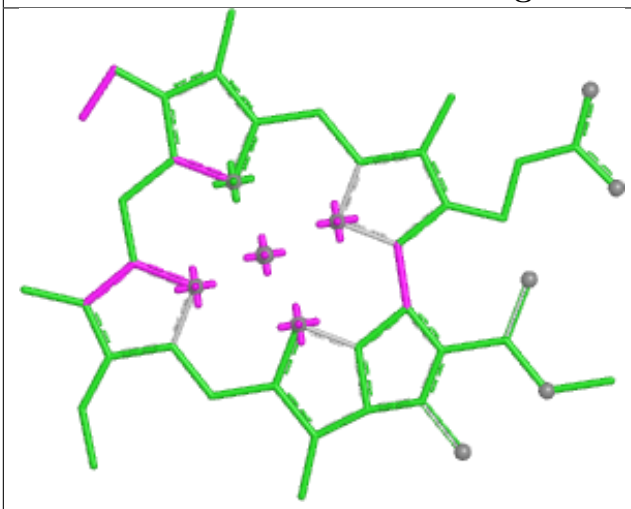


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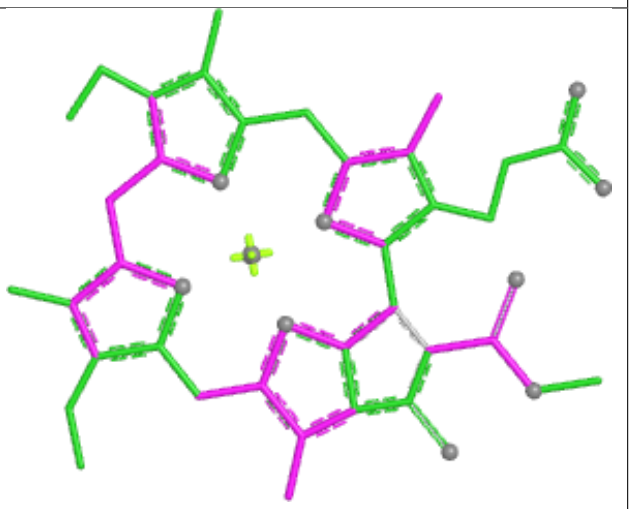


Rings

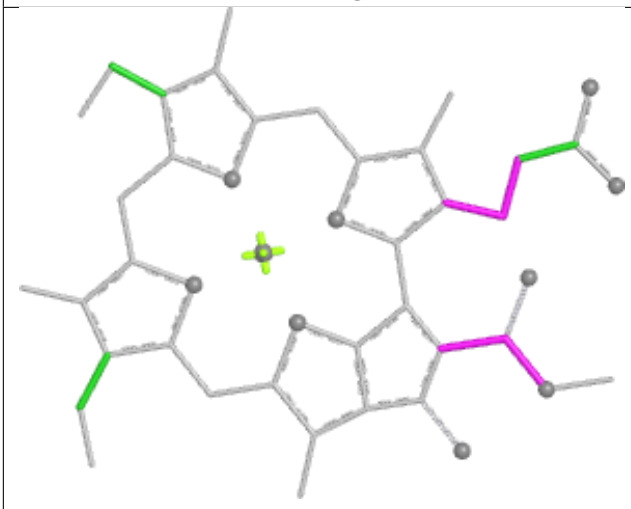
Ligand CLA A 1141



Bond lengths



Bond angles

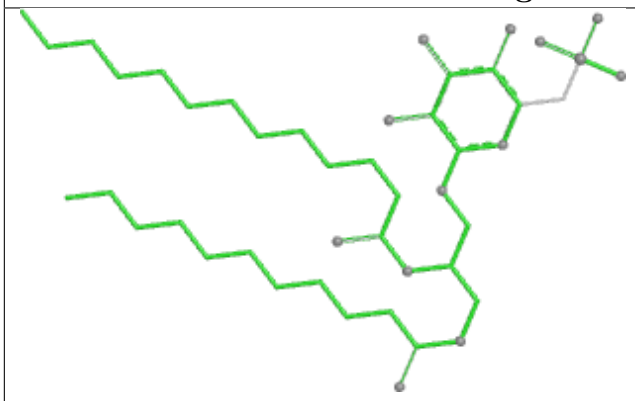


Torsions

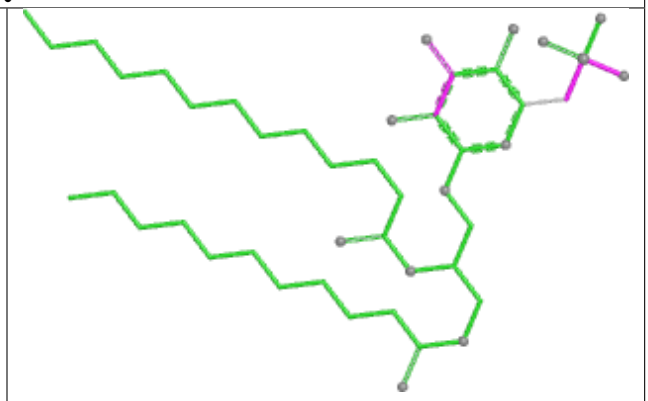


Rings

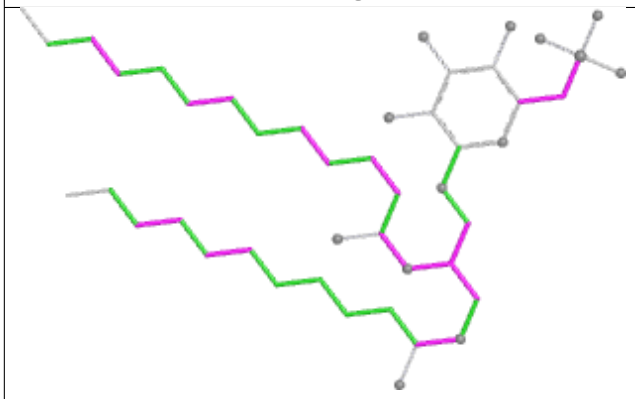
Ligand SQD G 5001



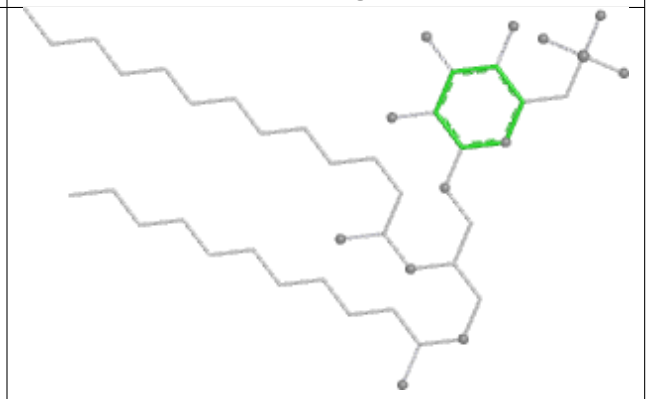
Bond lengths



Bond angles

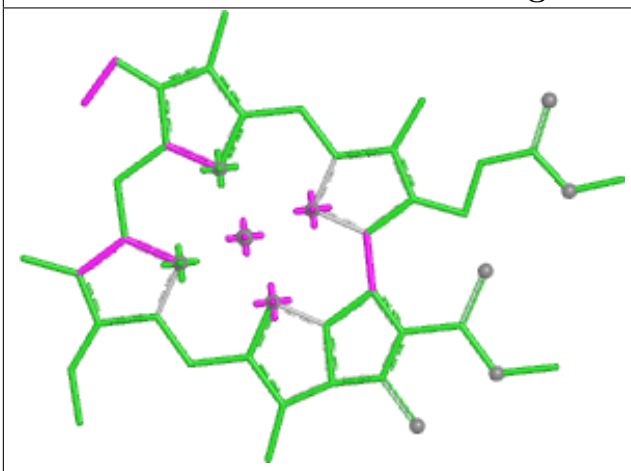


Torsions

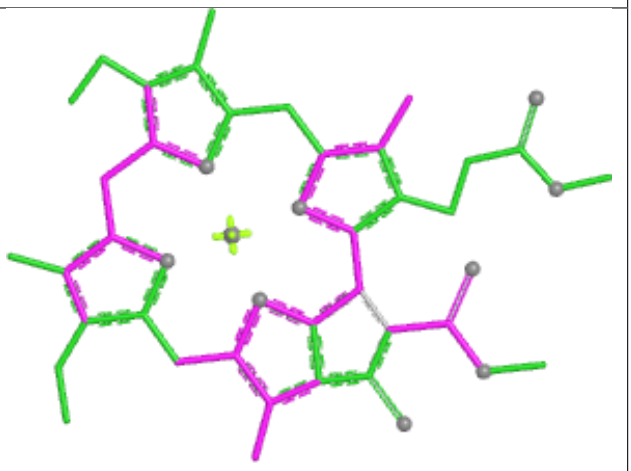


Rings

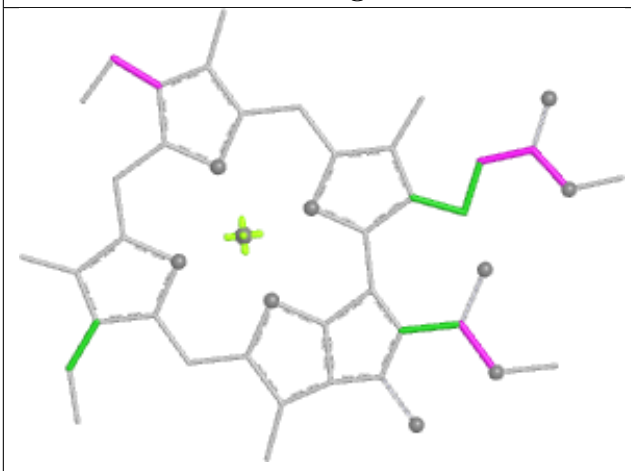
Ligand CLA 5 614



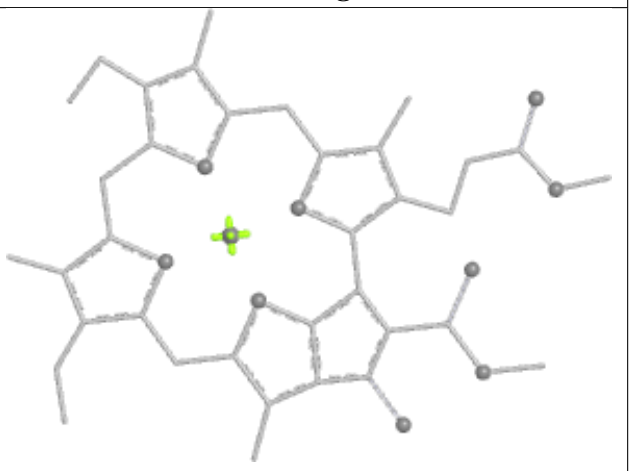
Bond lengths



Bond angles

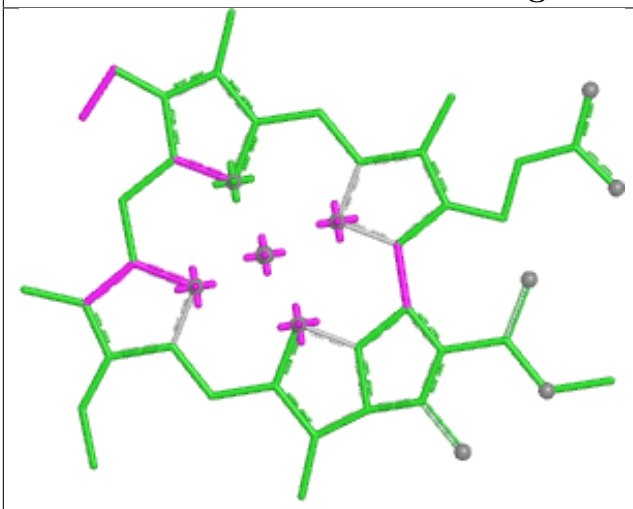


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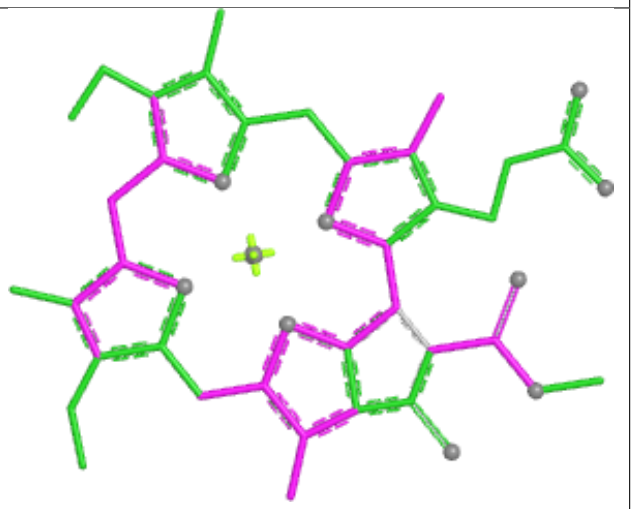


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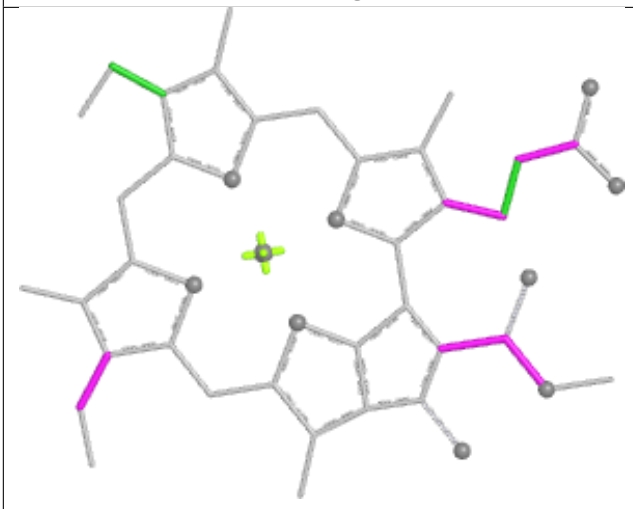
Ligand CLA 8 620



Bond lengths



Bond angles

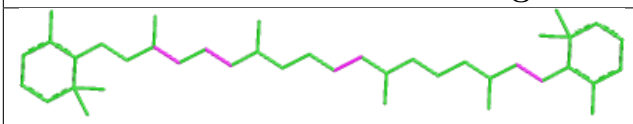


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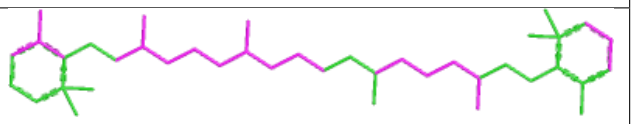


Rings

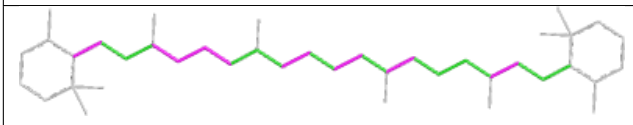
Ligand BCR G 4001



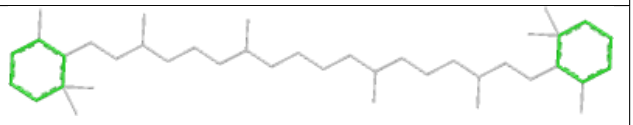
Bond lengths



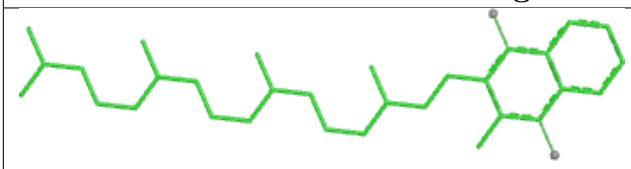
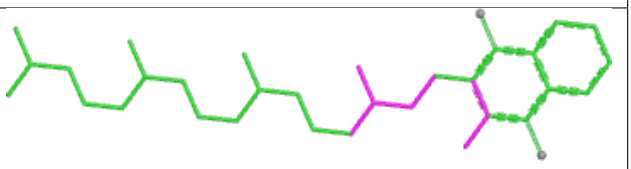
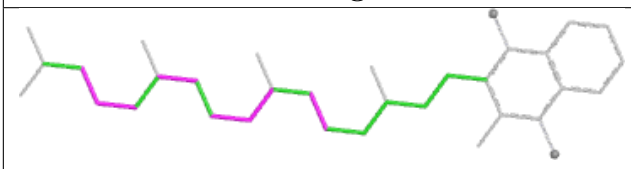
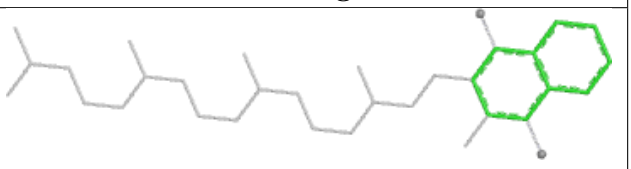
Bond angles

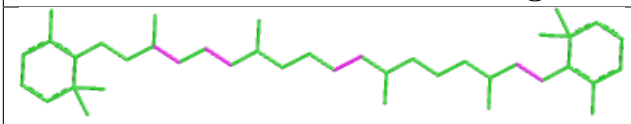
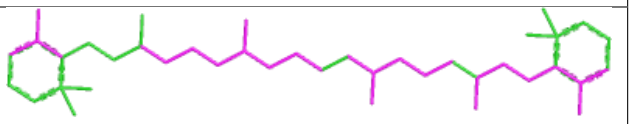
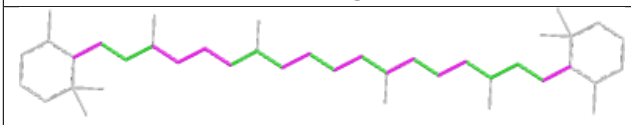
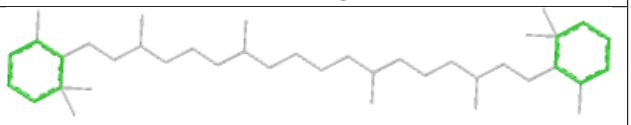


Torsions

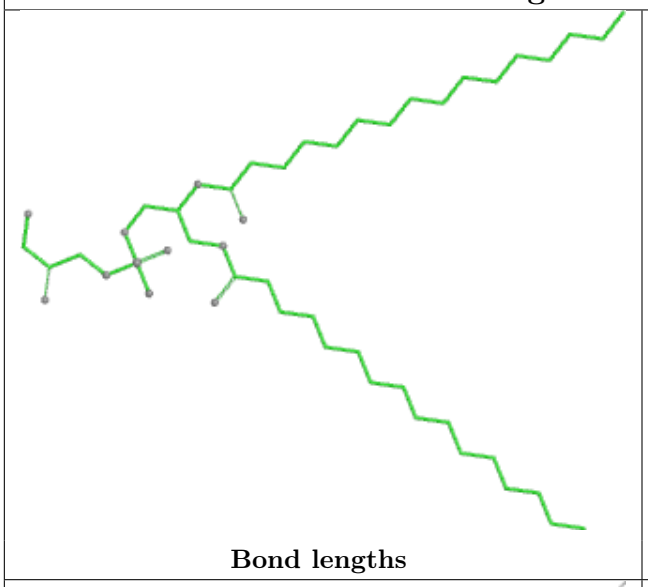


Rings

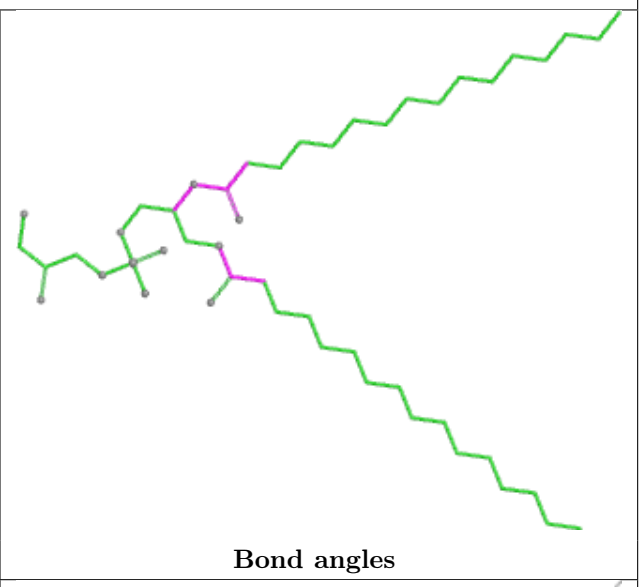
Ligand PQN B 2002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 5 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

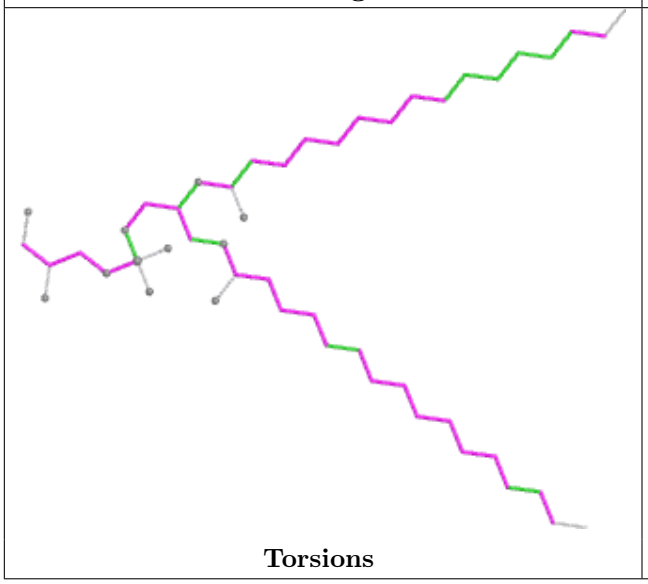
Ligand LHG 2 802



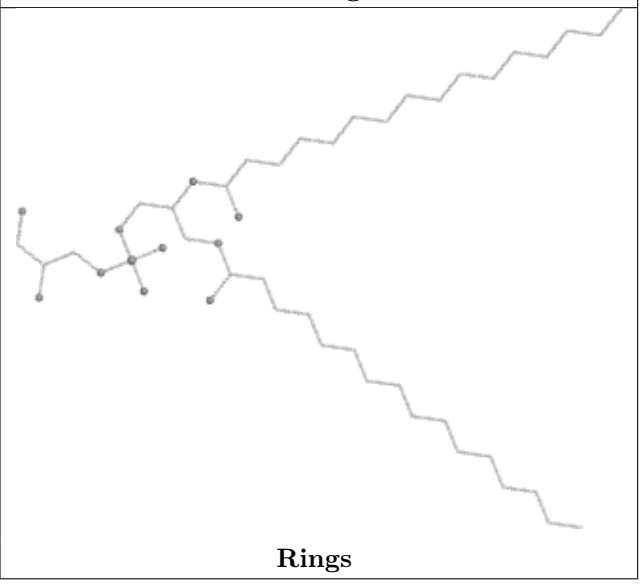
Bond lengths



Bond angles

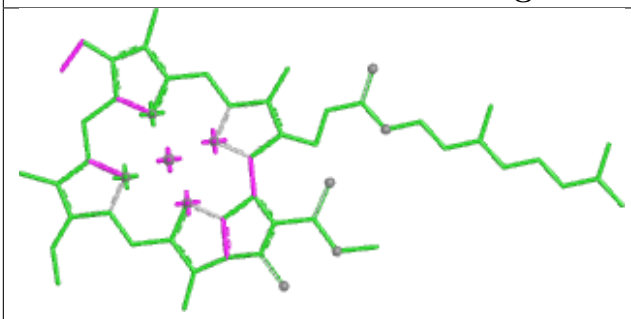


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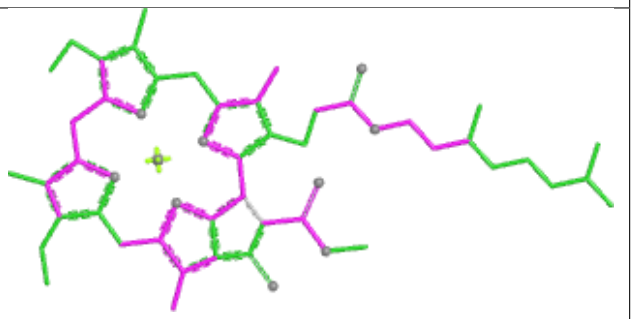


Rings

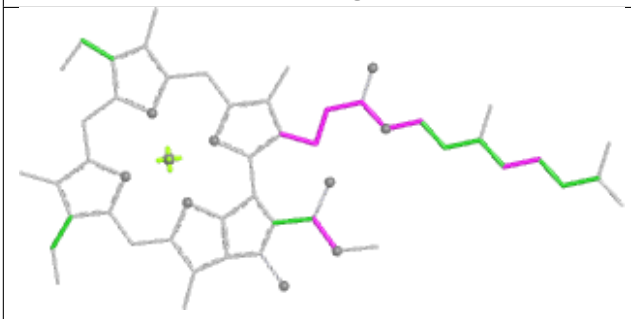
Ligand CLA A 1118



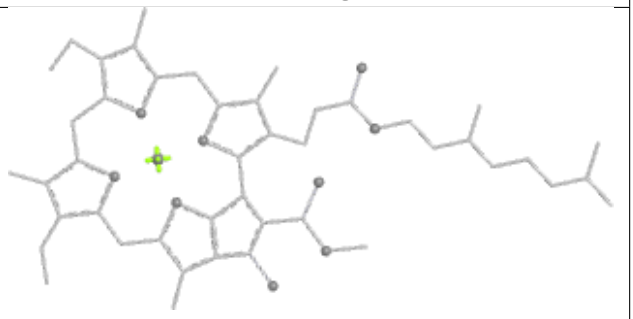
Bond lengths



Bond angles

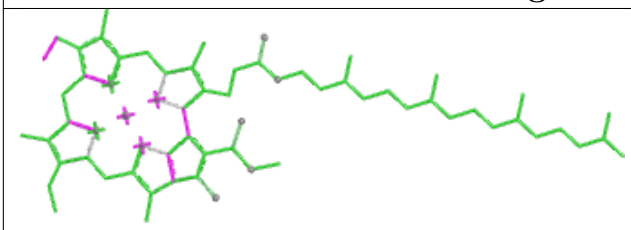


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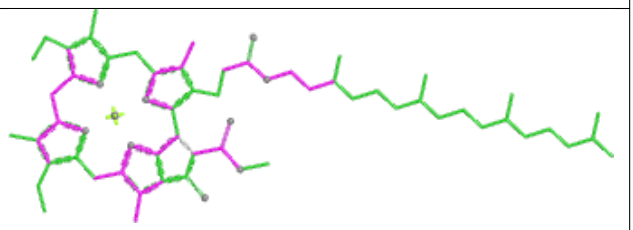


Rings

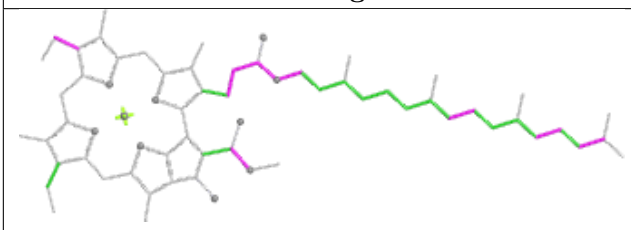
Ligand CLA 6 603



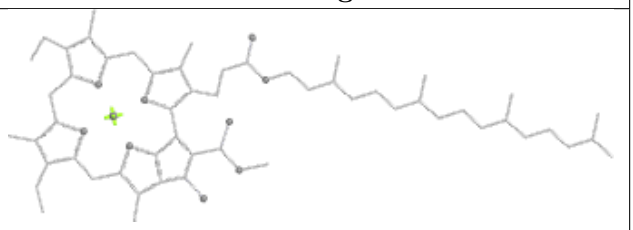
Bond lengths



Bond angles

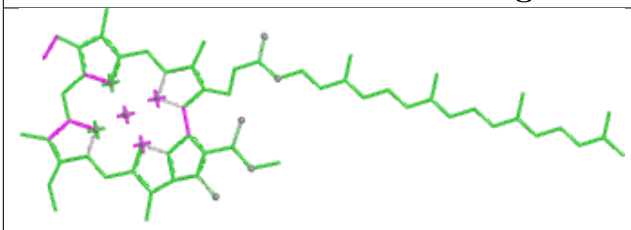


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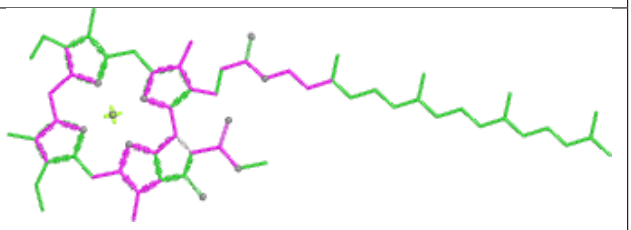


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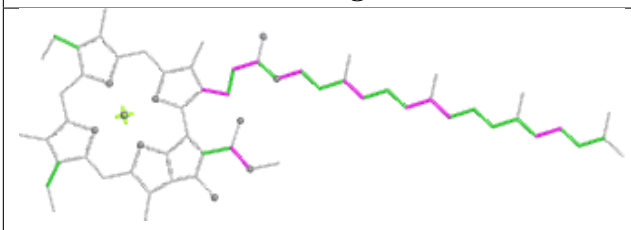
Ligand CLA B 1229



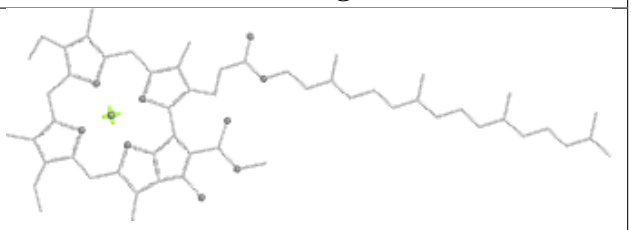
Bond lengths



Bond angles

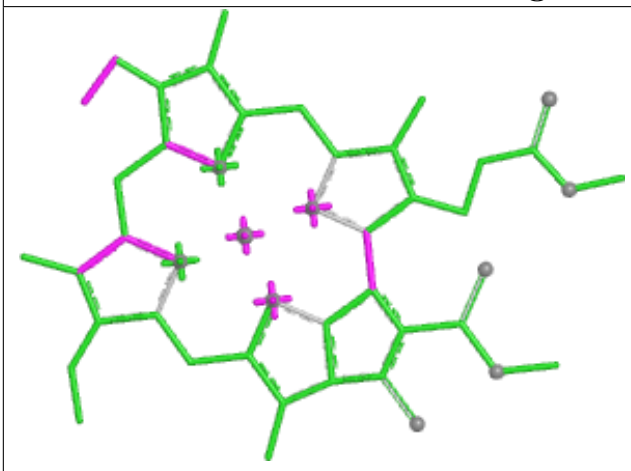


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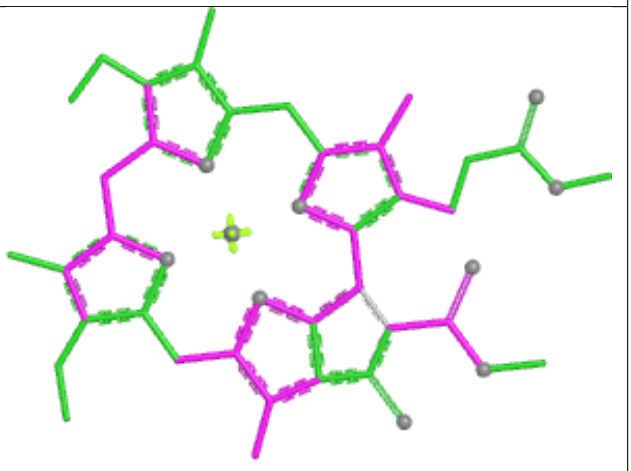


Rings

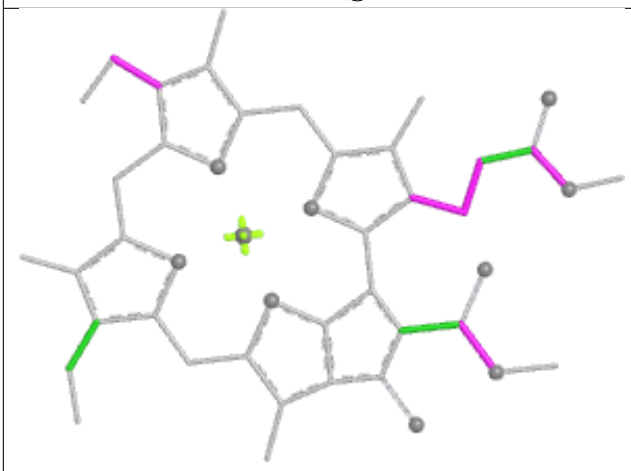
Ligand CLA 8 615



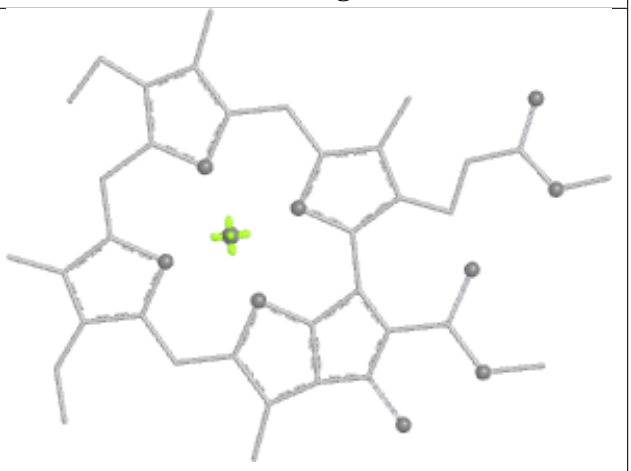
Bond lengths



Bond angles

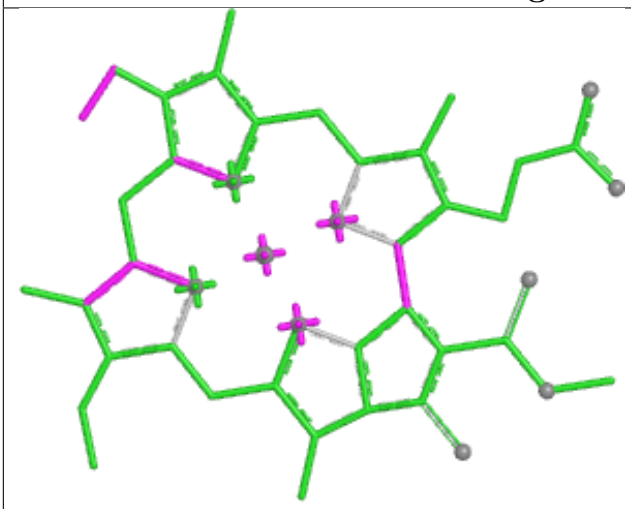


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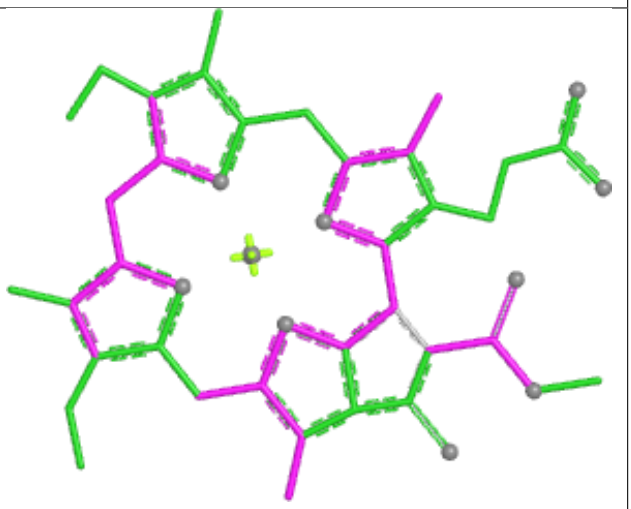


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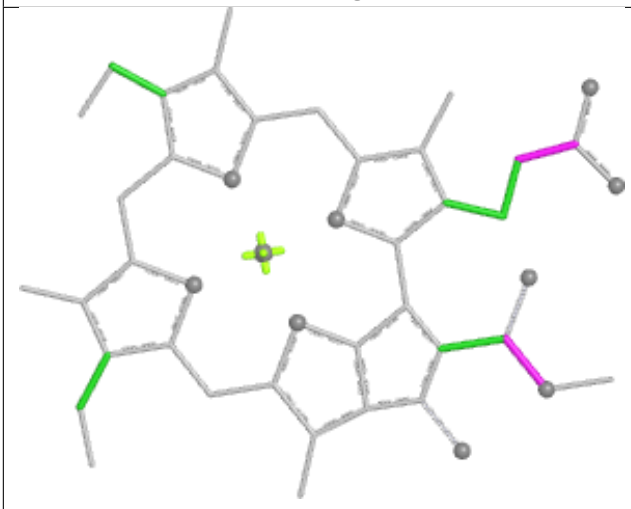
Ligand CLA 5 608



Bond lengths



Bond angles

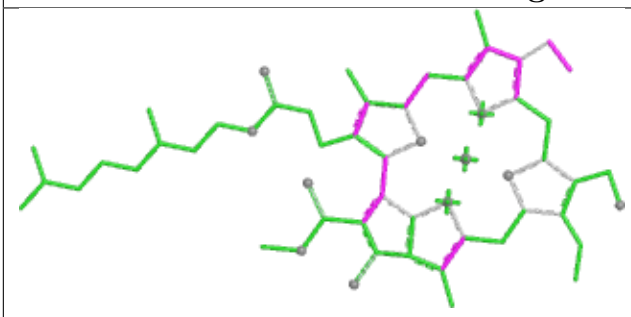


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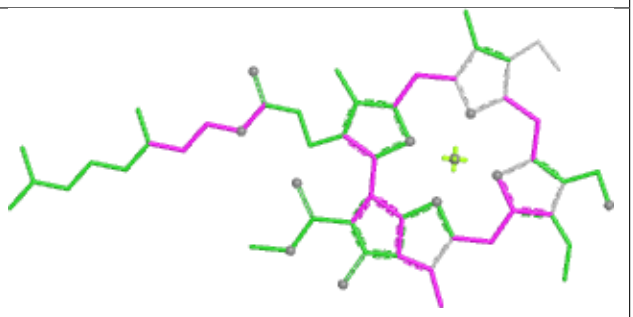


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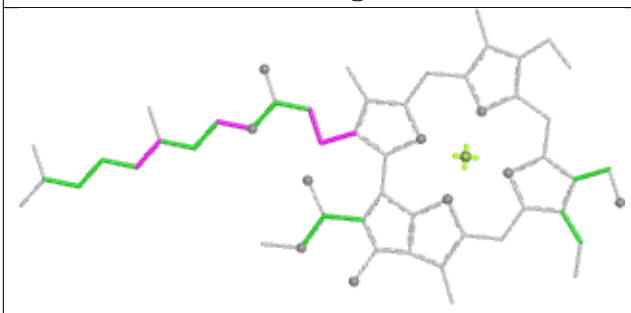
Ligand CHL a 606



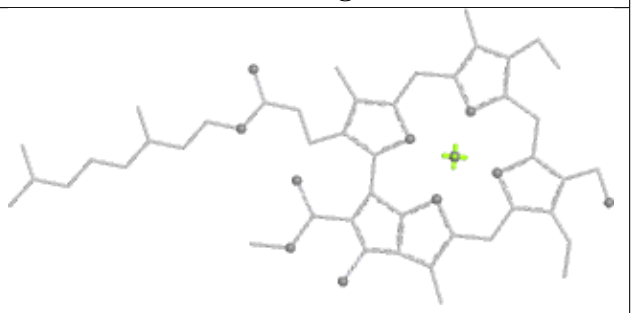
Bond lengths



Bond angles

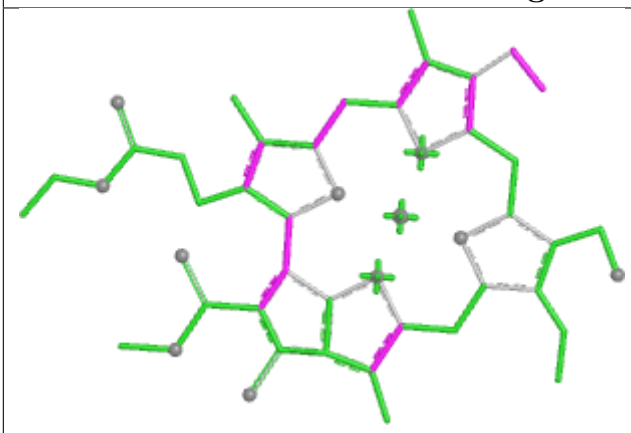


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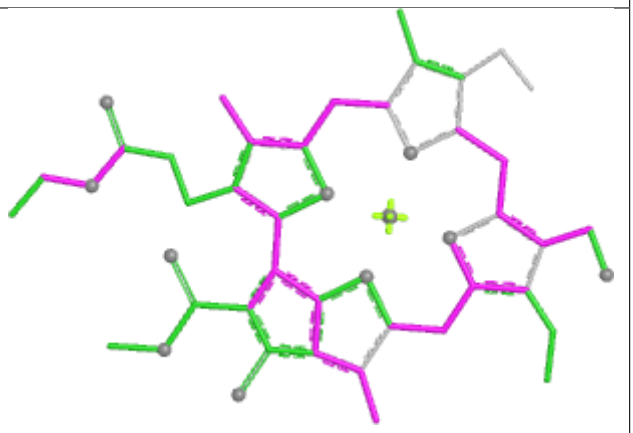


Rings

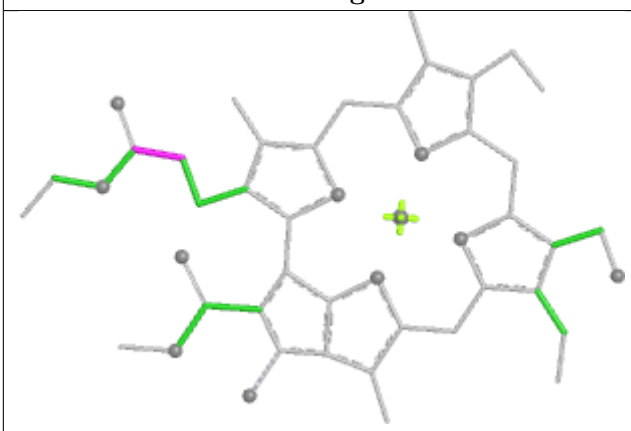
Ligand CHL 1 613



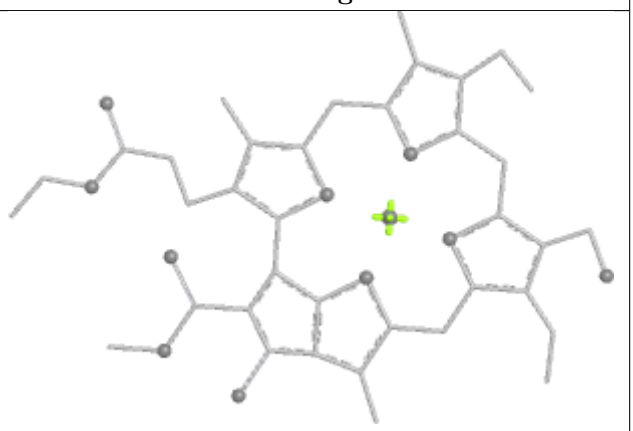
Bond lengths



Bond angles

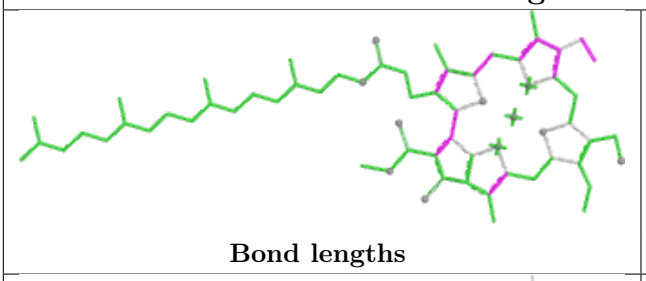


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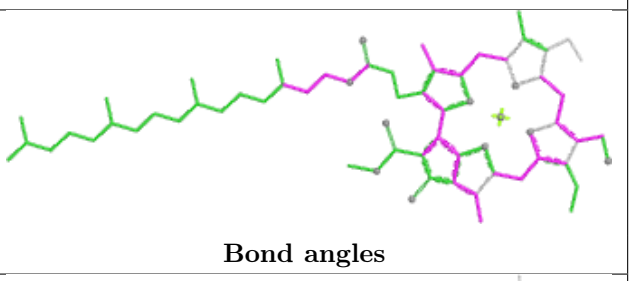


Rings

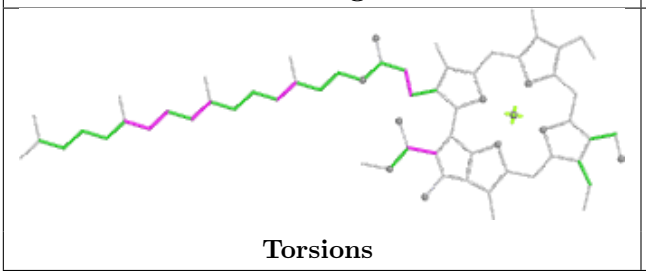
Ligand CHL 8 603



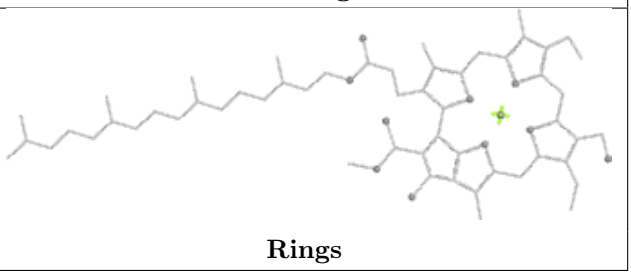
Bond lengths



Bond angles

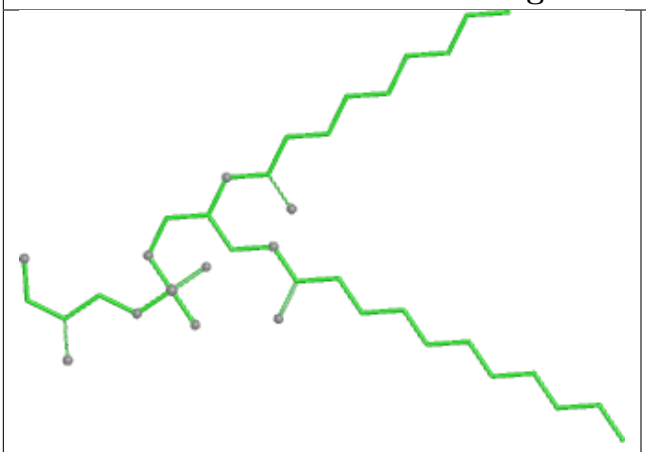


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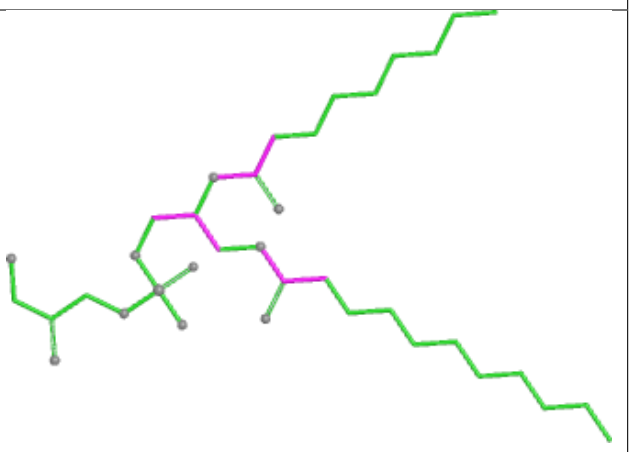


Rings

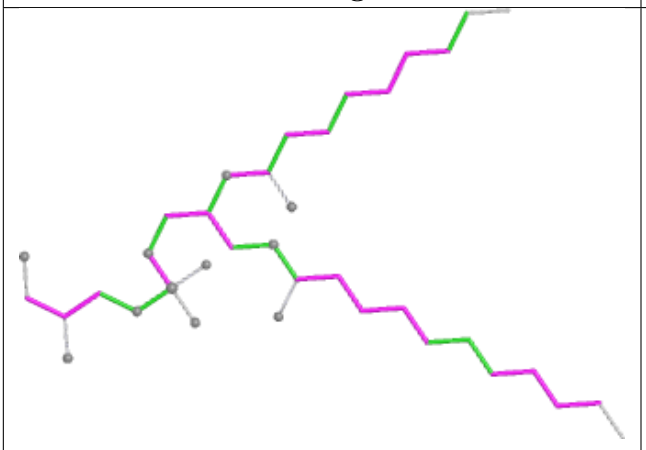
Ligand LHG 7 801



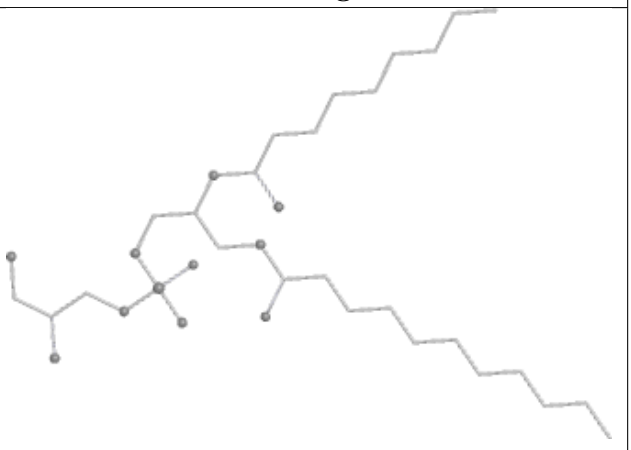
Bond lengths



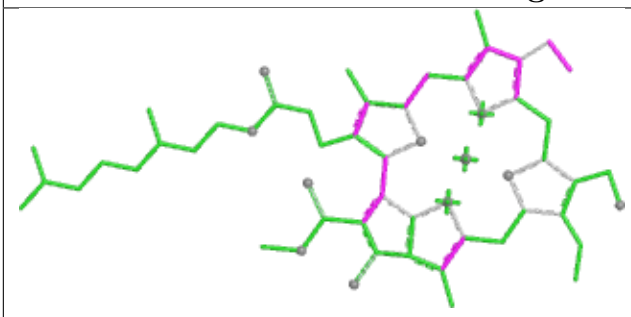
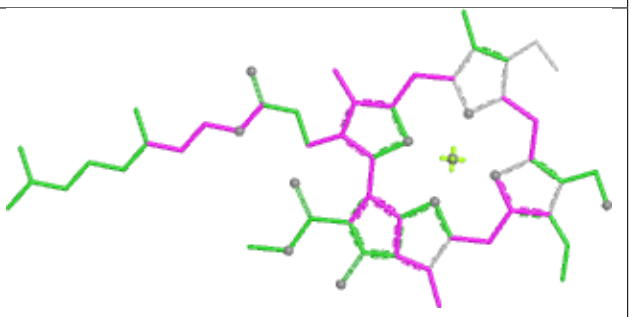
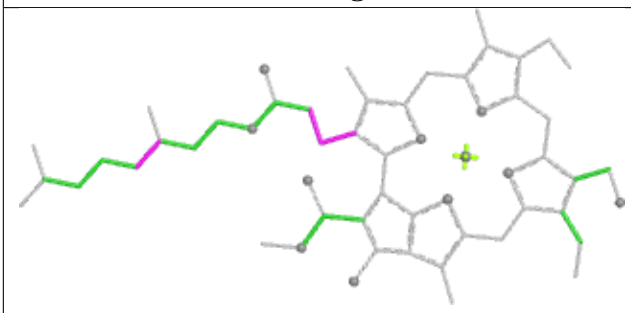
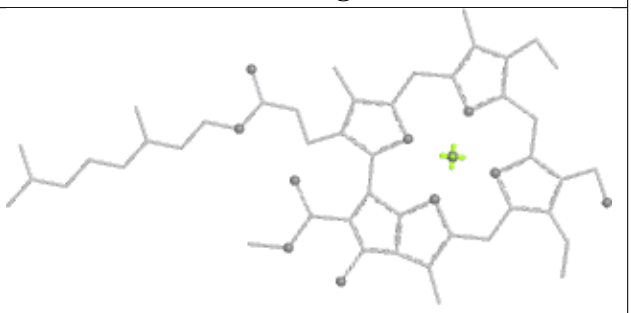
Bond angles

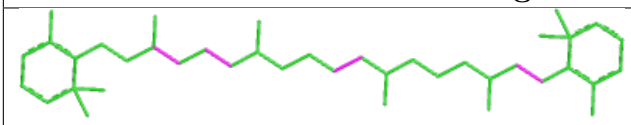
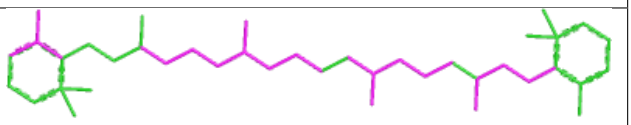
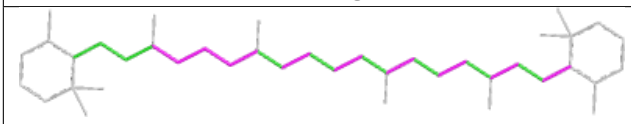
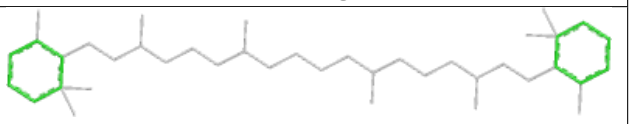


Torsions

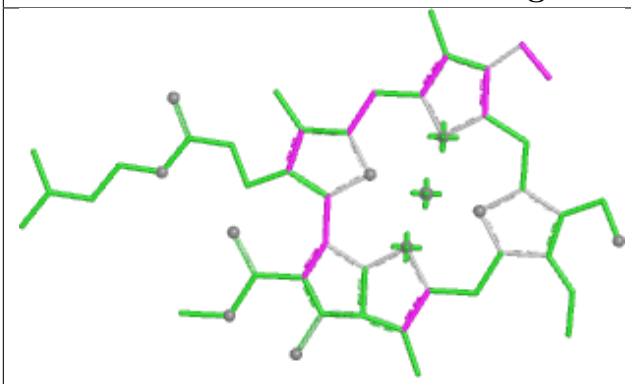


Rings

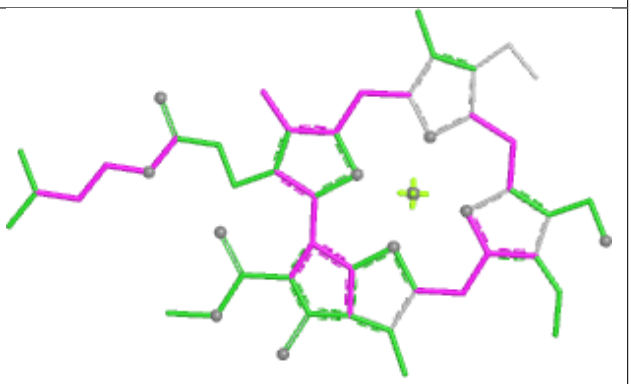
Ligand CHL 4 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4006	
	
Bond lengths	Bond angles
	
Torsions	Rings

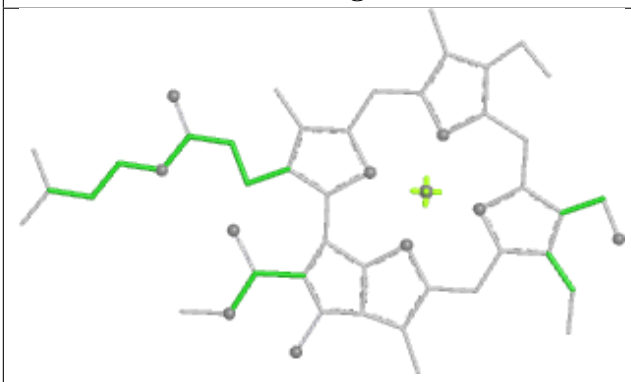
Ligand CHL 6 613



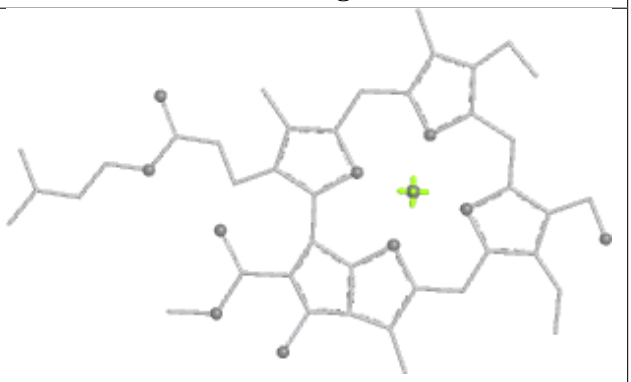
Bond lengths



Bond angles

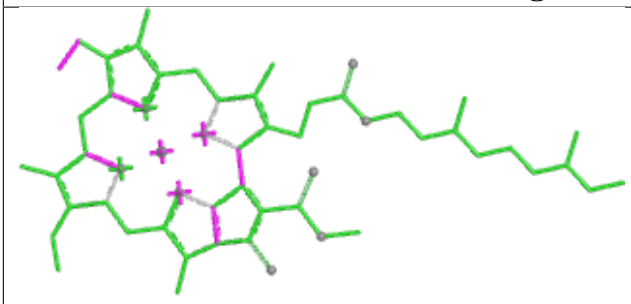


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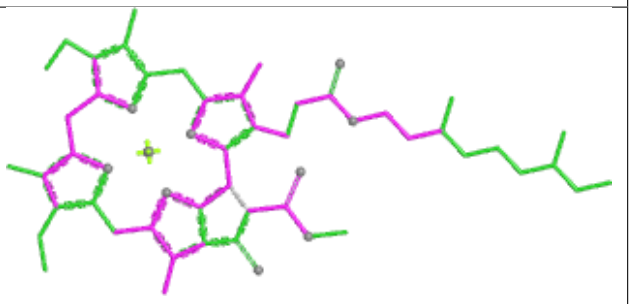


Rings

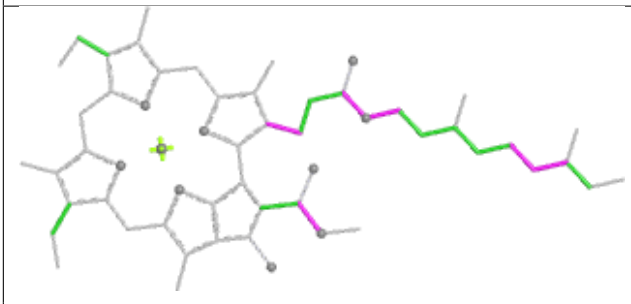
Ligand CLA 4 611



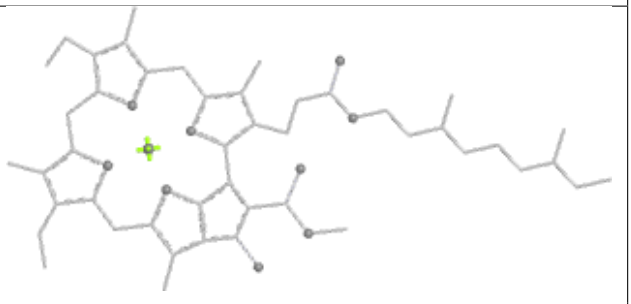
Bond lengths



Bond angles

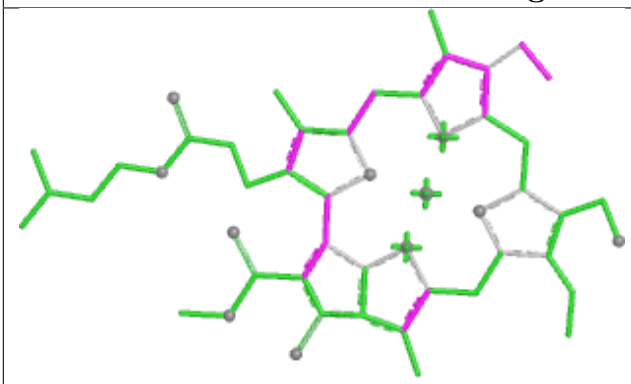


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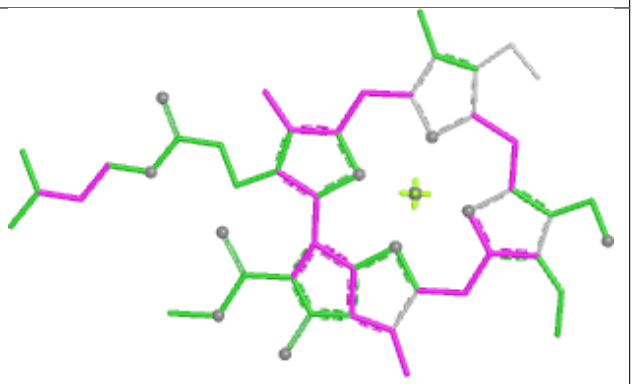


Rings

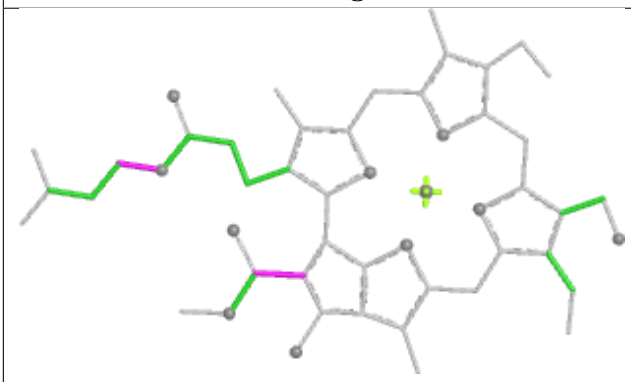
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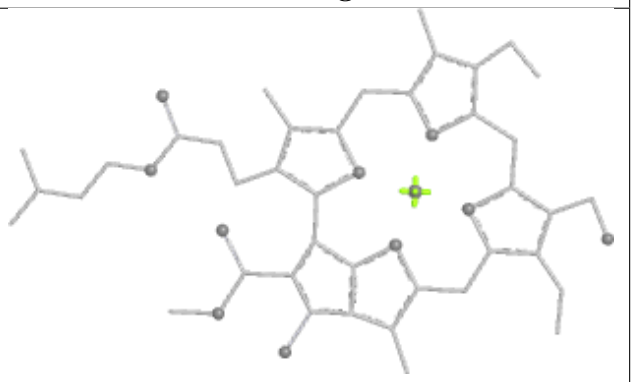
Bond lengths



Bond angles

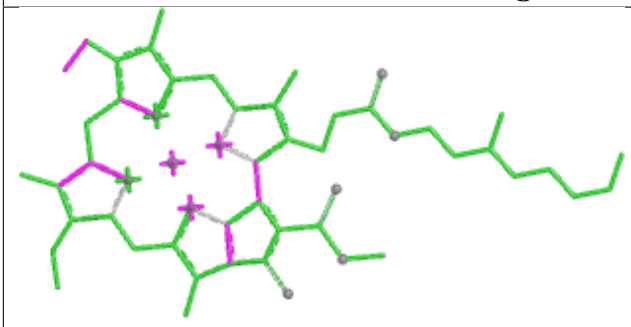


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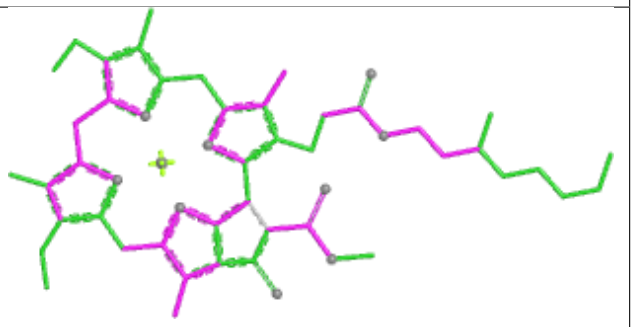


Rings

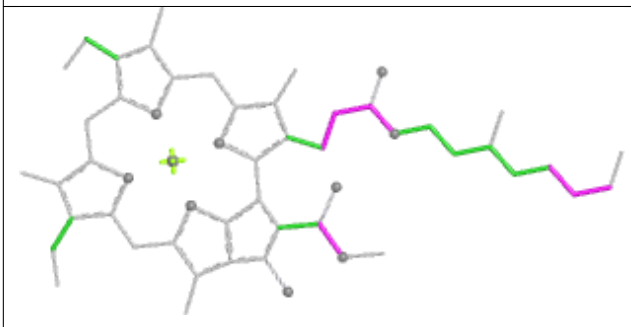
Ligand CLA A 1110



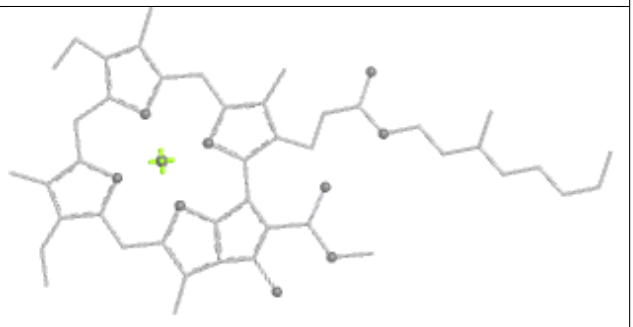
Bond lengths



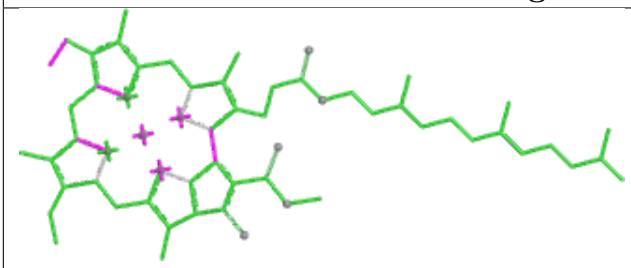
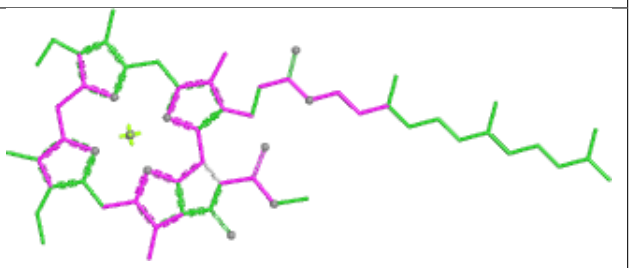
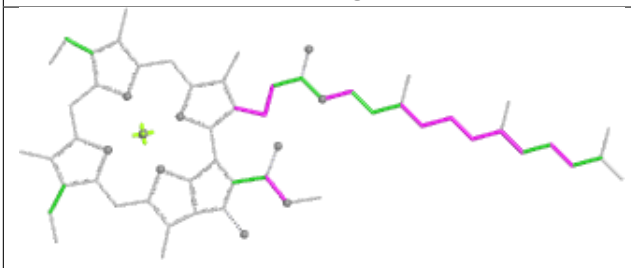
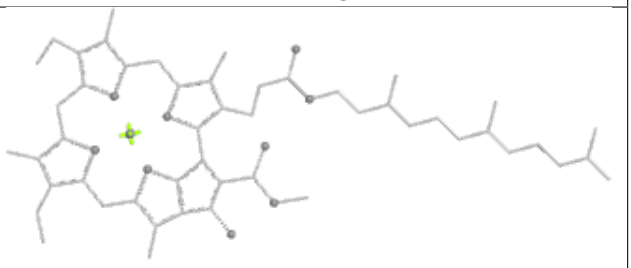
Bond angles

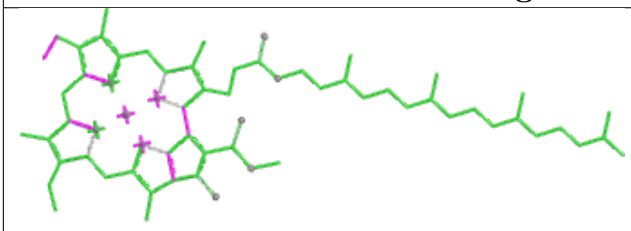
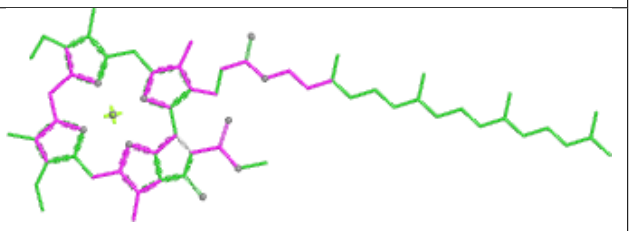
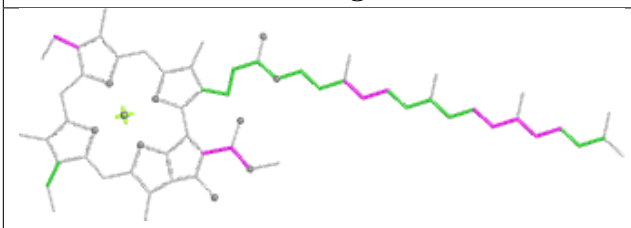
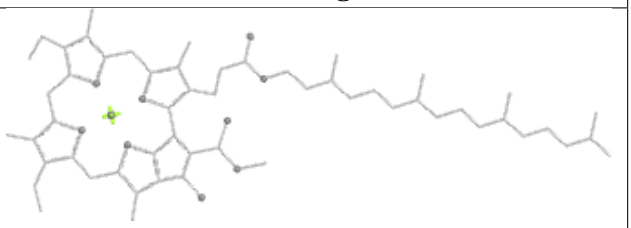


Torsions

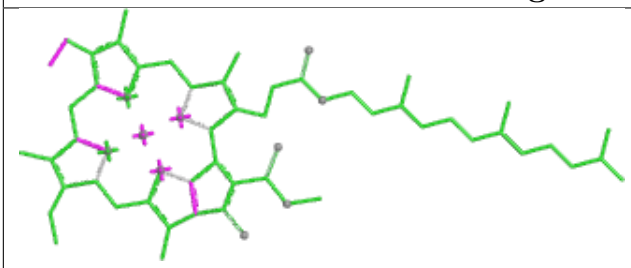


Rings

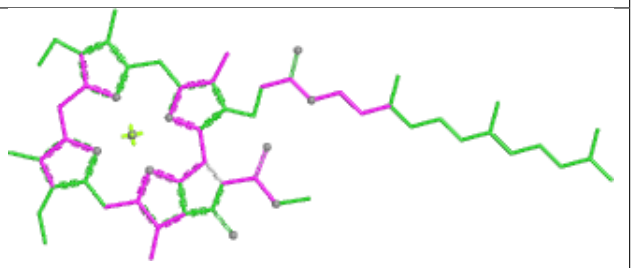
Ligand CLA 7 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

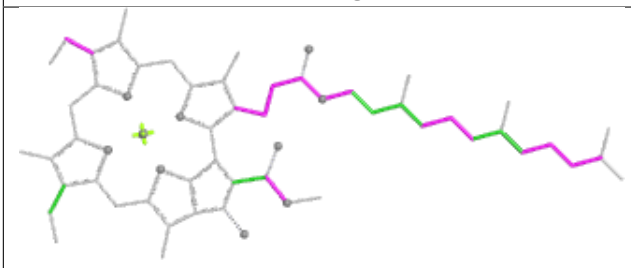
Ligand CLA 8 618



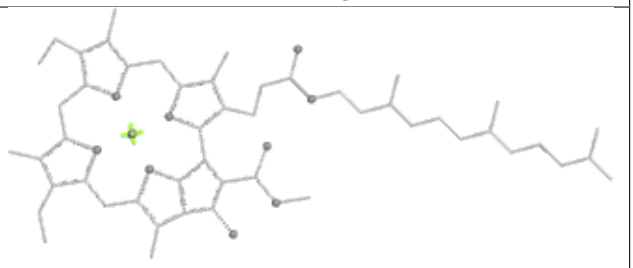
Bond lengths



Bond angles

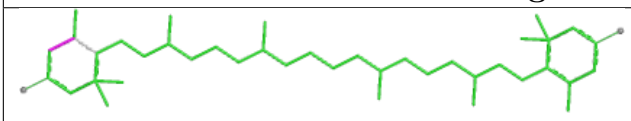


Torsions

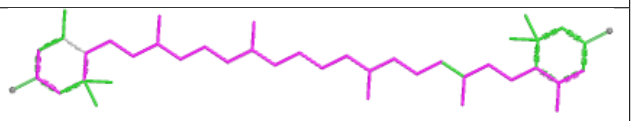


Rings

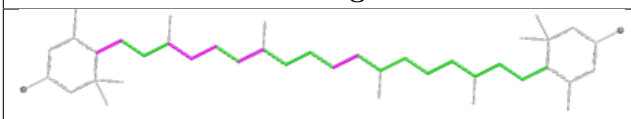
Ligand LUT 1 503



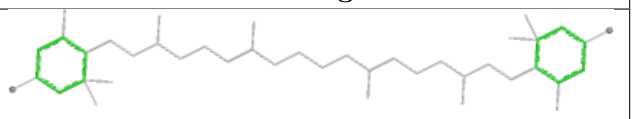
Bond lengths



Bond angles

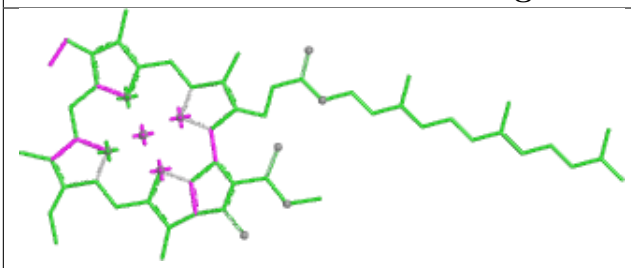


Torsions

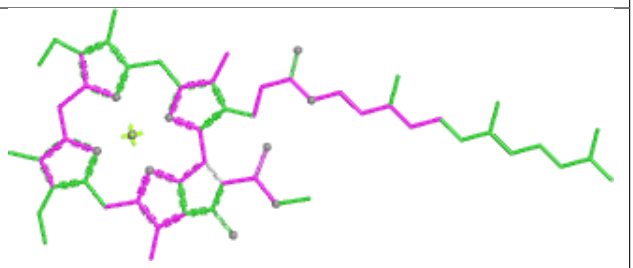


Rings

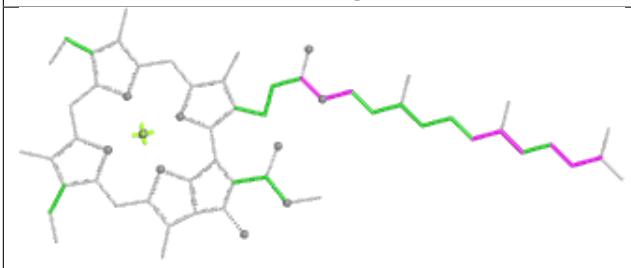
Ligand CLA A 1137



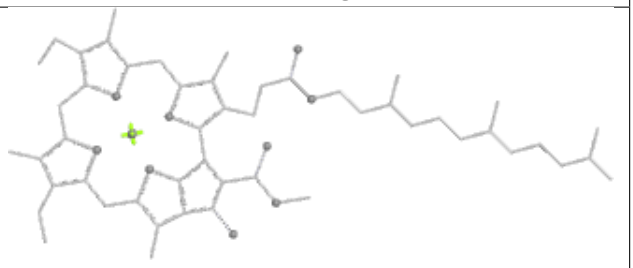
Bond lengths



Bond angles

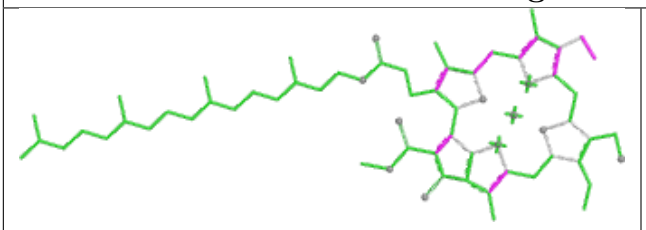


Torsions

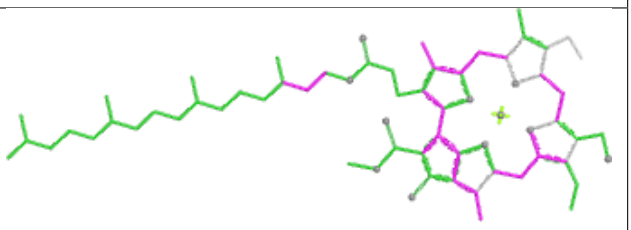


Rings

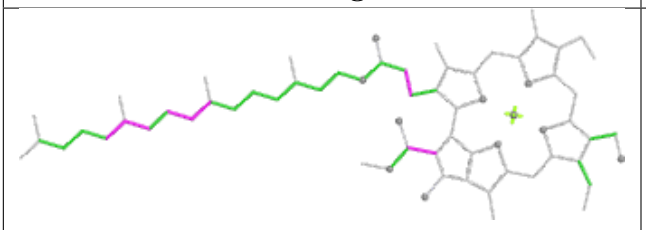
Ligand CHL 6 609



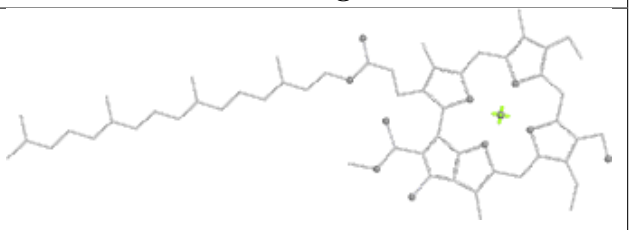
Bond lengths



Bond angles

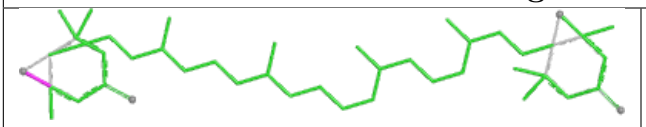


Torsions

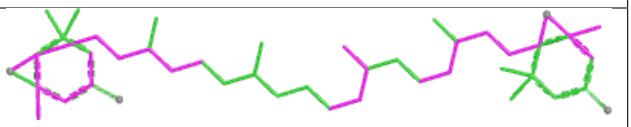


Rings

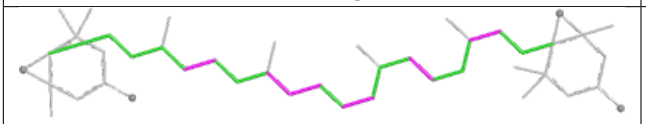
Ligand XAT 9 507



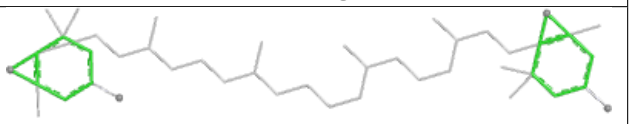
Bond lengths



Bond angles

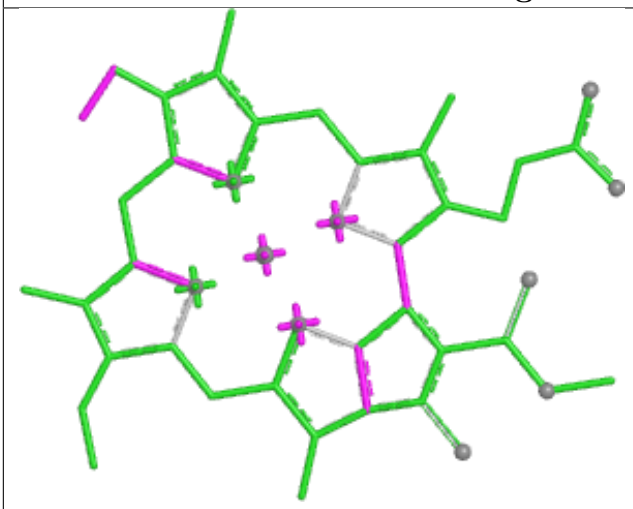


Torsions

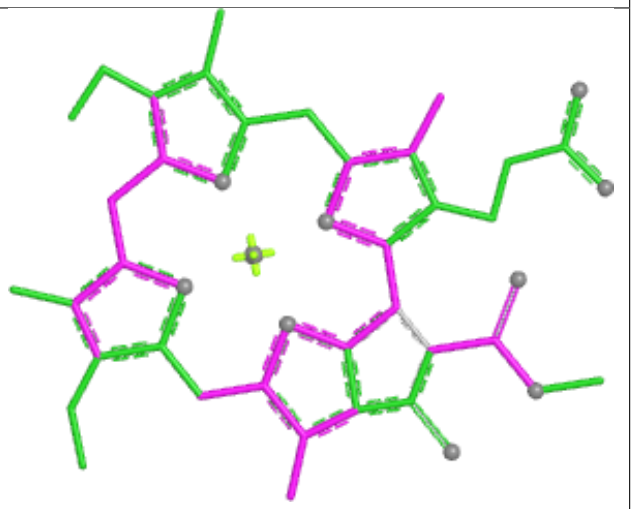


Rings

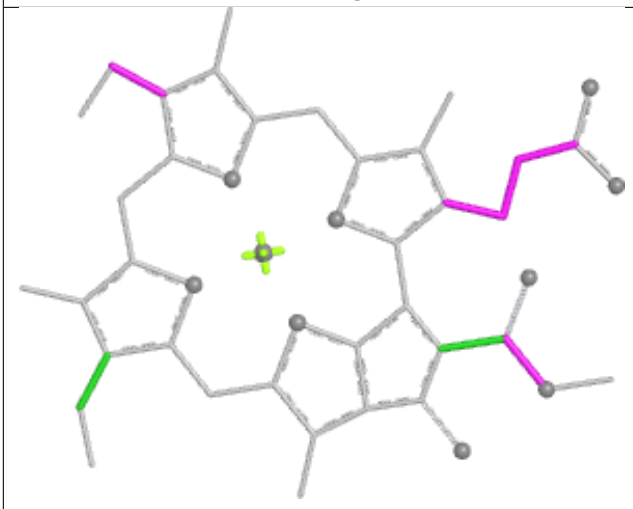
Ligand CLA B 1232



Bond lengths



Bond angles

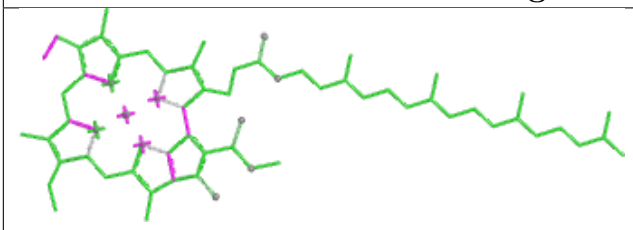


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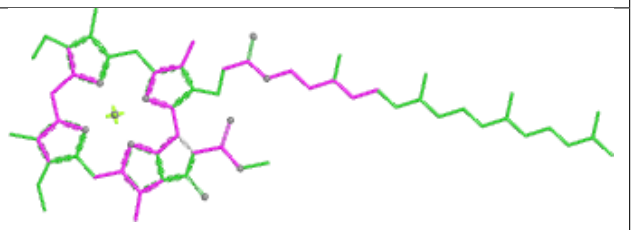


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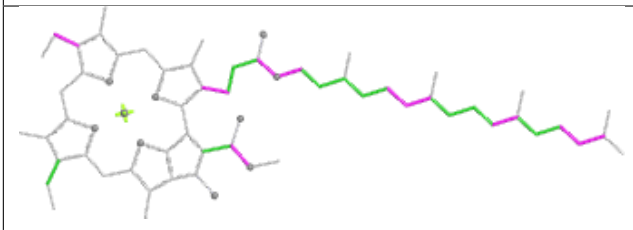
Ligand CLA 2 621



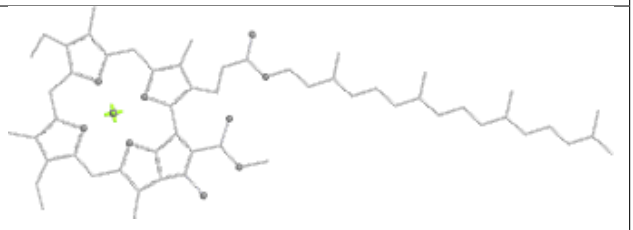
Bond lengths



Bond angles

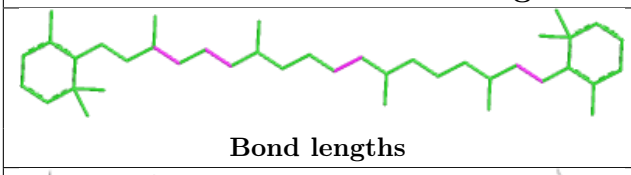


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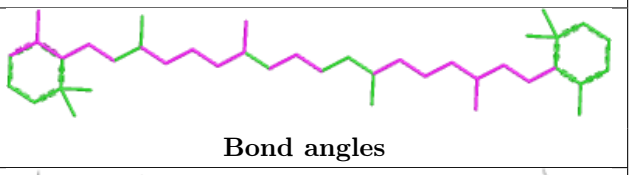


Rings

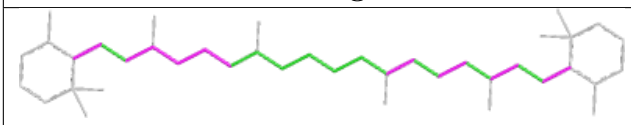
Ligand BCR B 4005



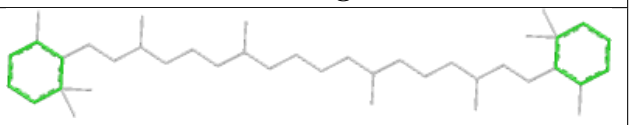
Bond lengths



Bond angles

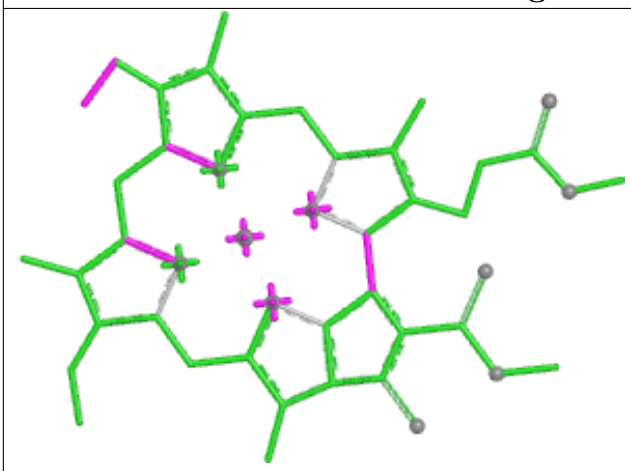


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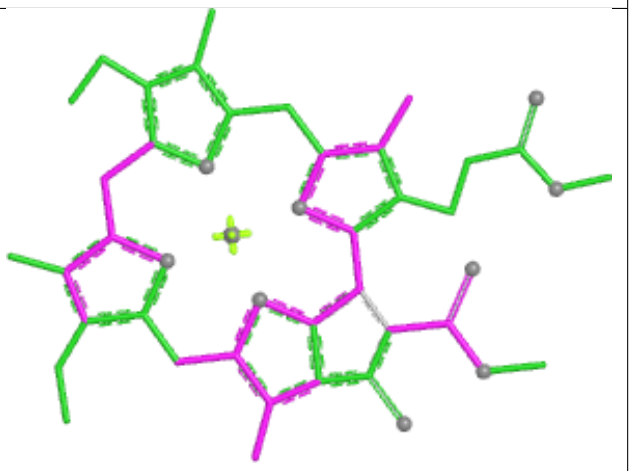


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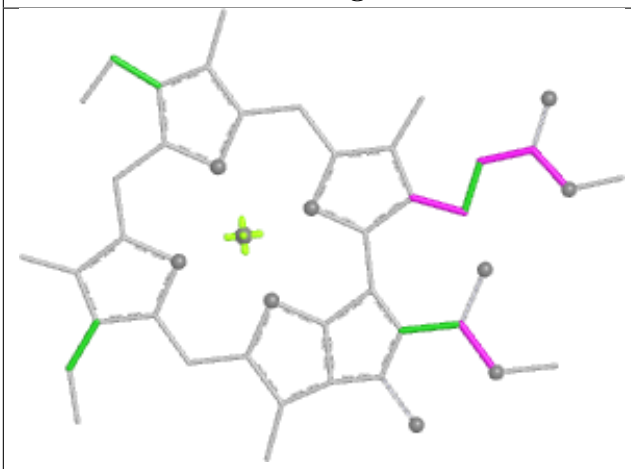
Ligand CLA 1 615



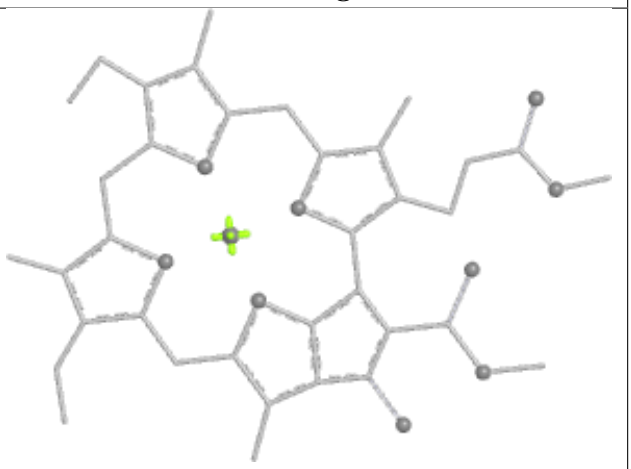
Bond lengths



Bond angles

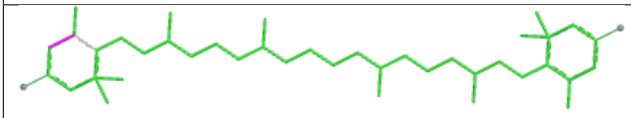


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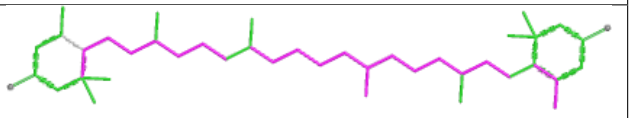


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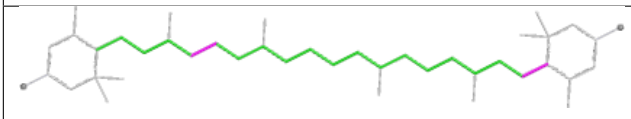
Ligand LUT 9 501



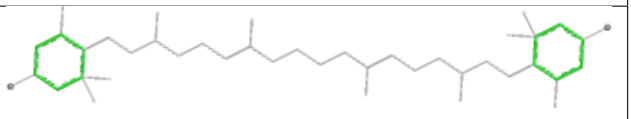
Bond lengths



Bond angles

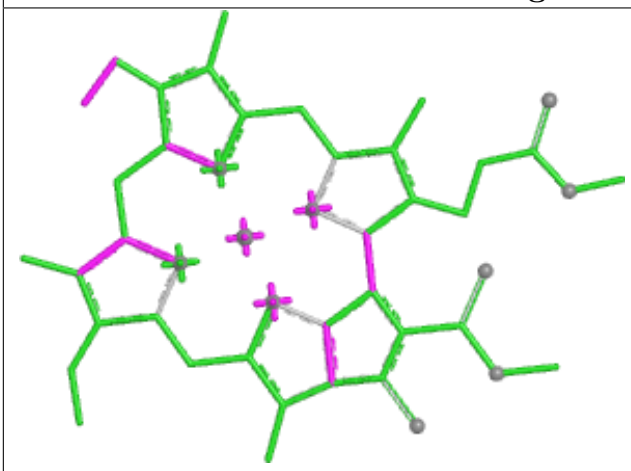


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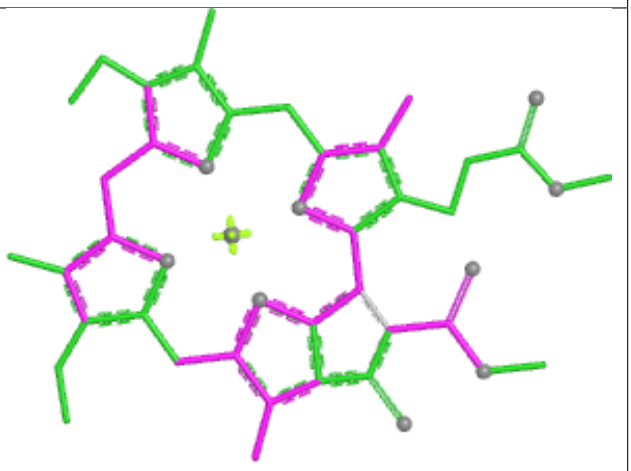


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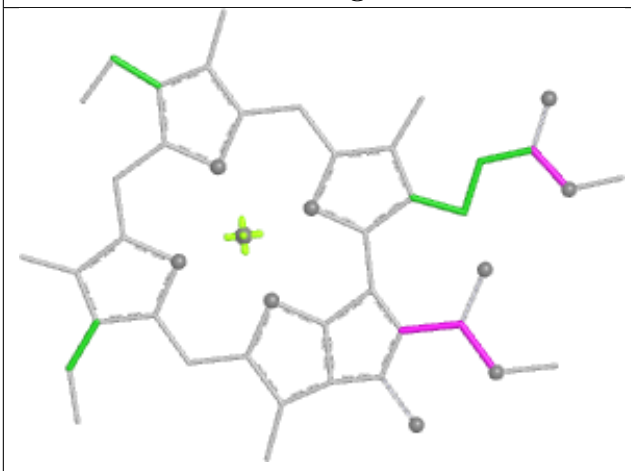
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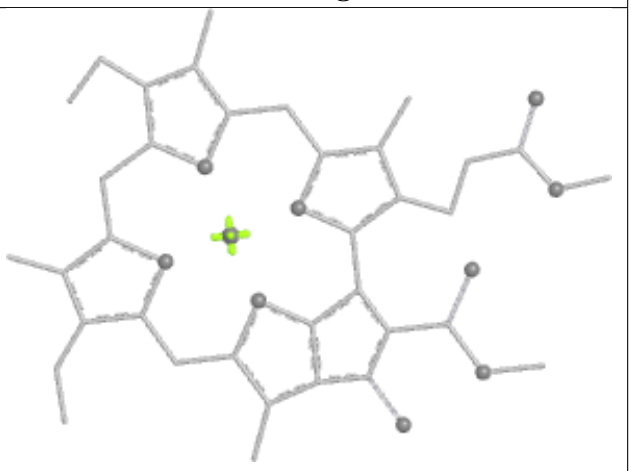
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Bond angles

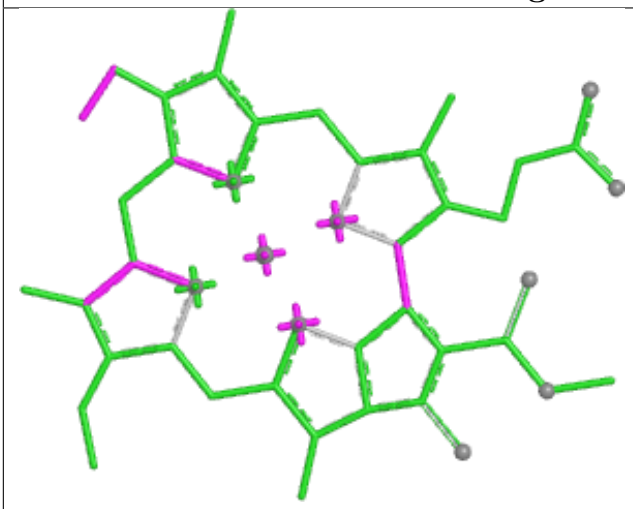


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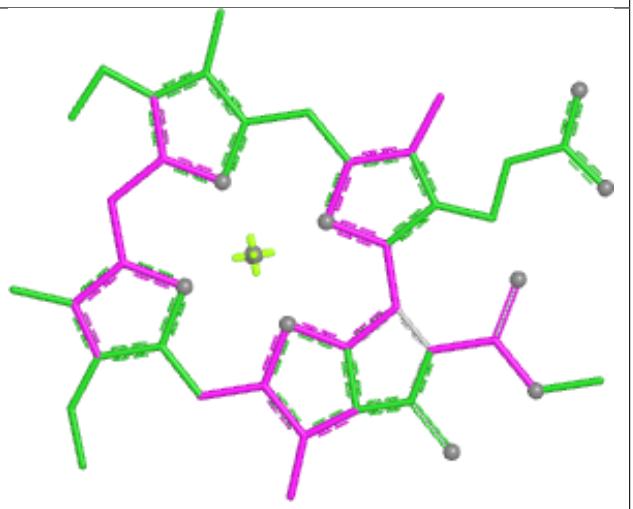


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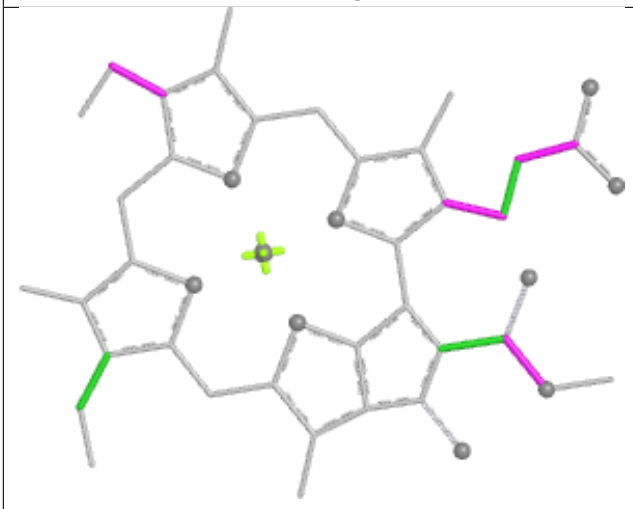
Ligand CLA 2 608



Bond lengths



Bond angles

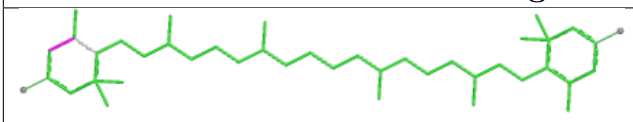


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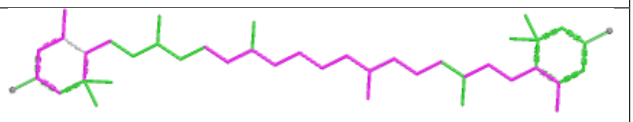


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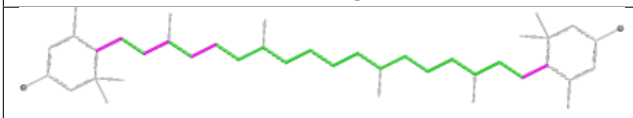
Ligand LUT 7 501



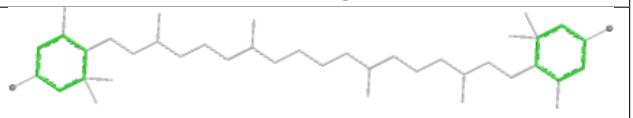
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Bond angles

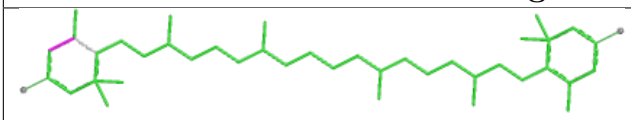


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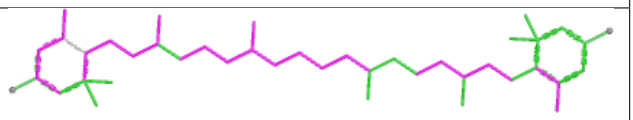


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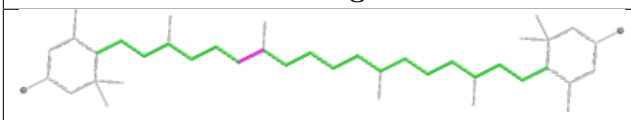
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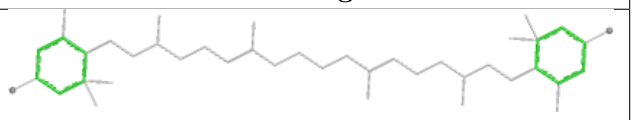
Bond lengths



Bond angles

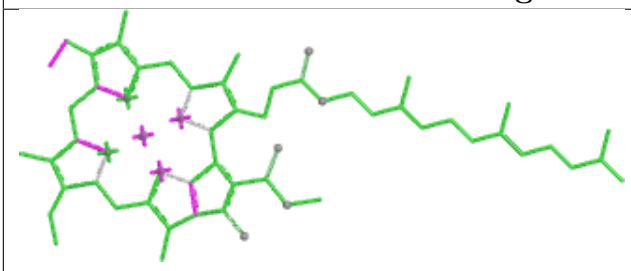


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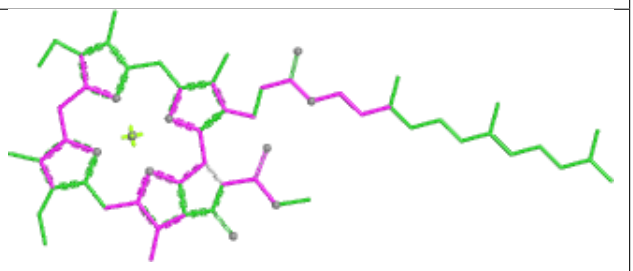


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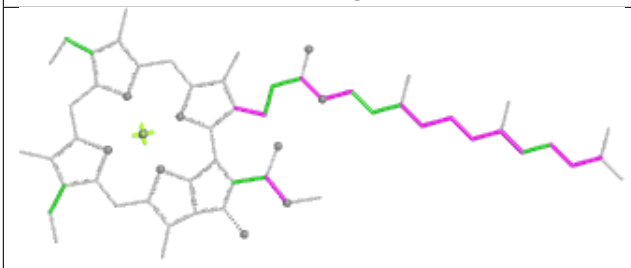
Ligand CLA B 1207



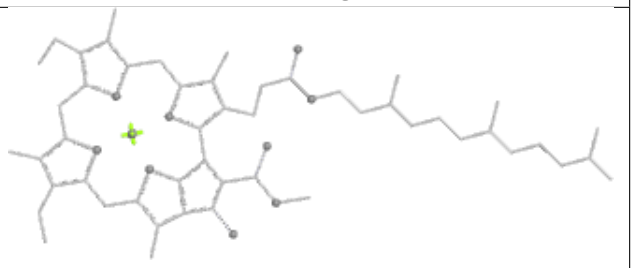
Bond lengths



Bond angles

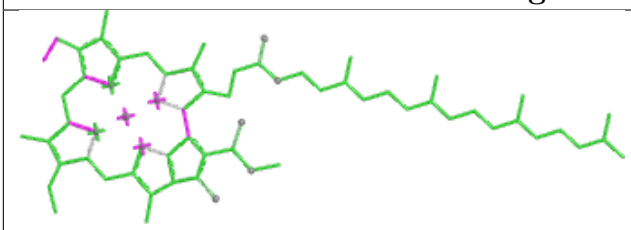


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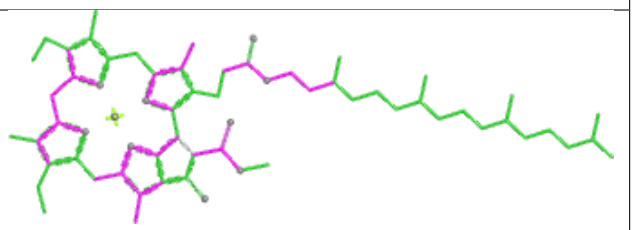


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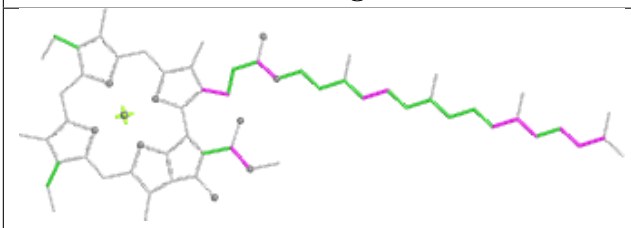
Ligand CLA 3 601



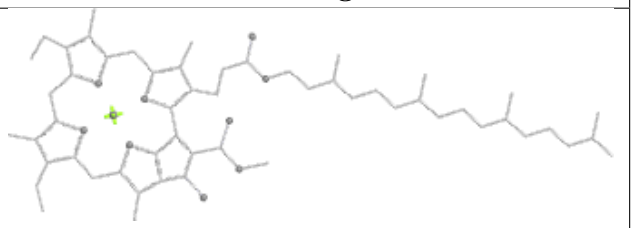
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Bond angles

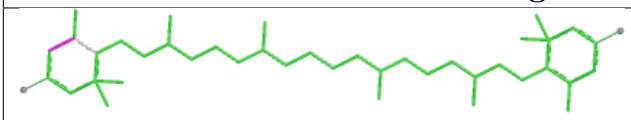


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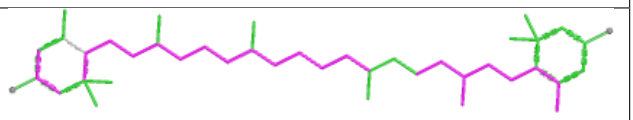


Rings

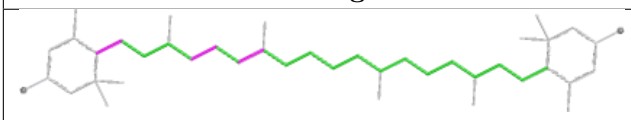
Ligand LUT a 503



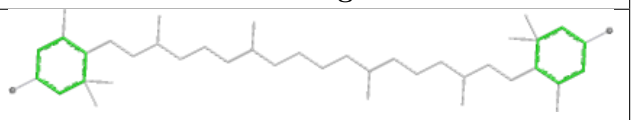
Bond lengths



Bond angles

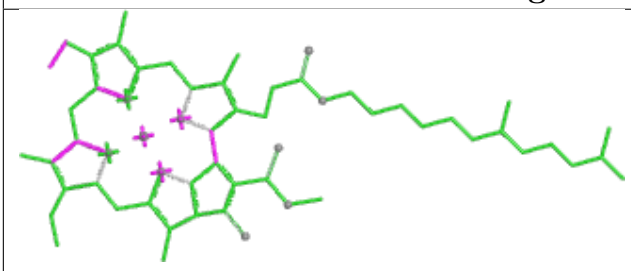


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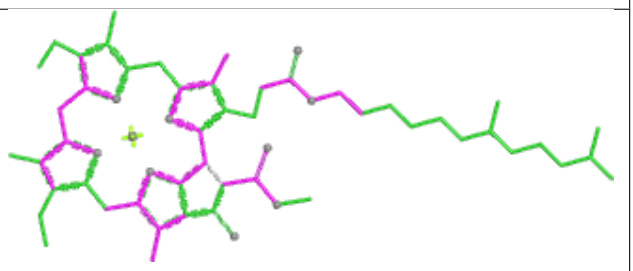


Rings

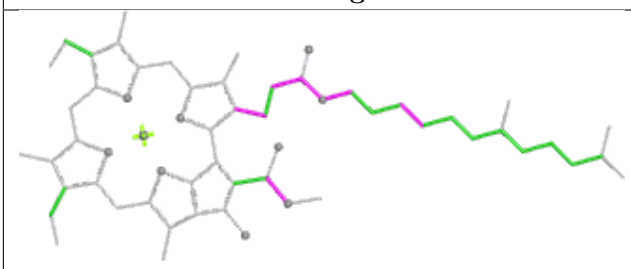
Ligand CLA 7 607



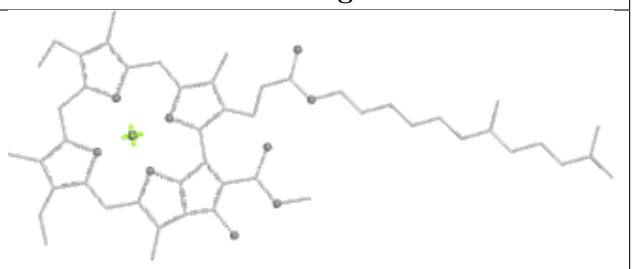
Bond lengths



Bond angles

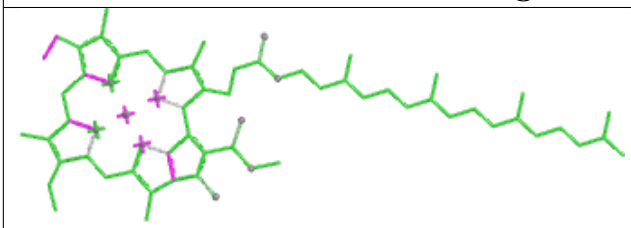


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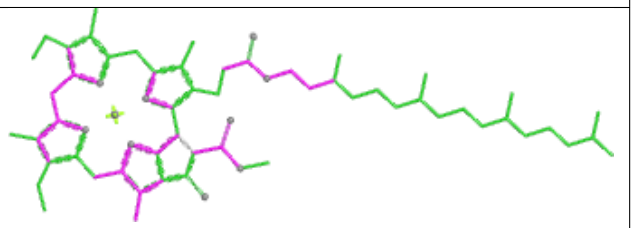


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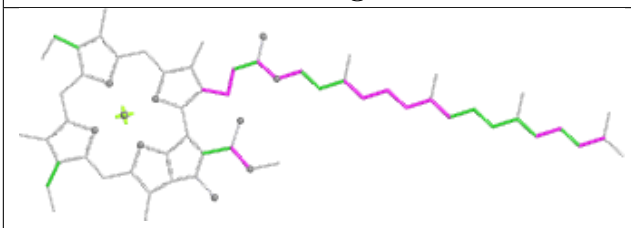
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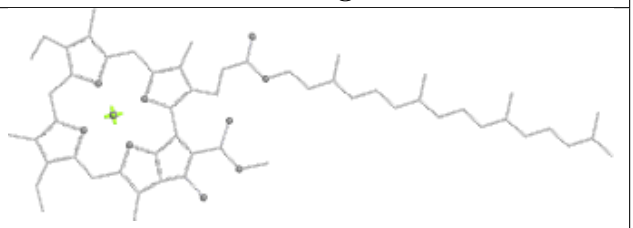
Bond lengths



Bond angles

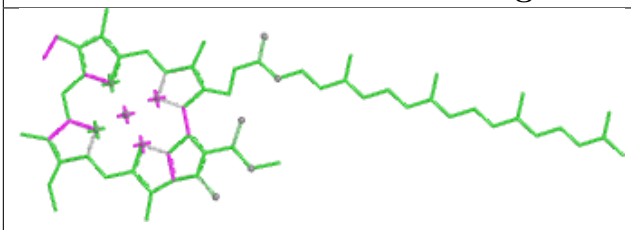


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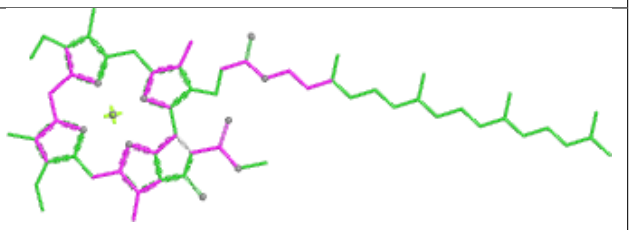


Rings

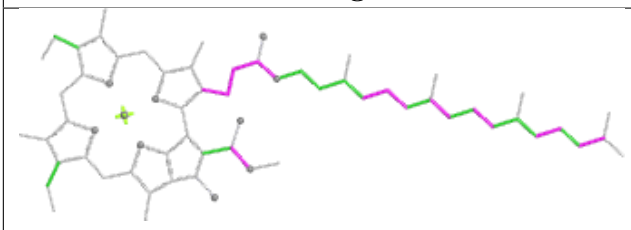
Ligand CLA B 1209



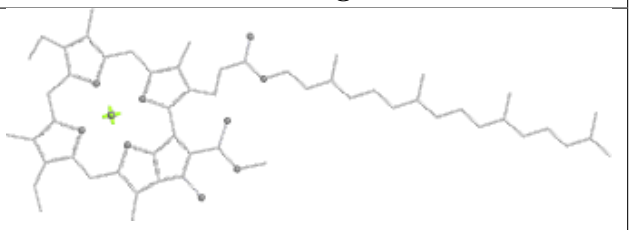
Bond lengths



Bond angles

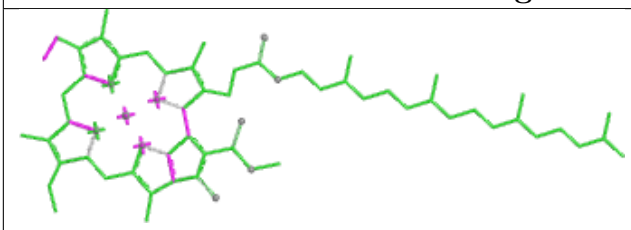


Torsions

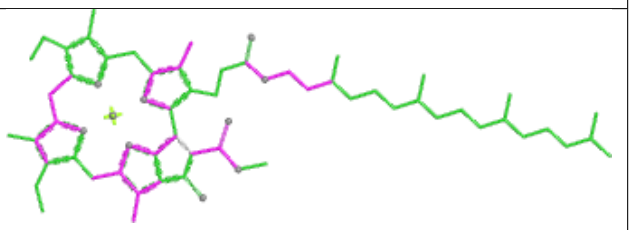


Rings

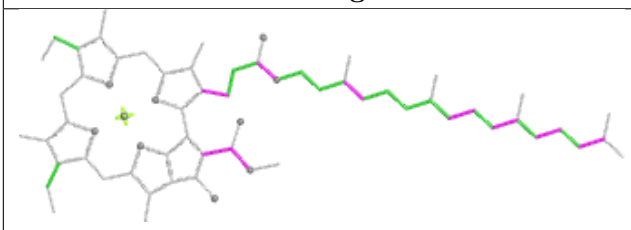
Ligand CLA A 1117



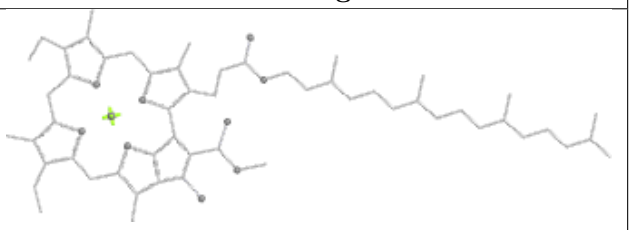
Bond lengths



Bond angles

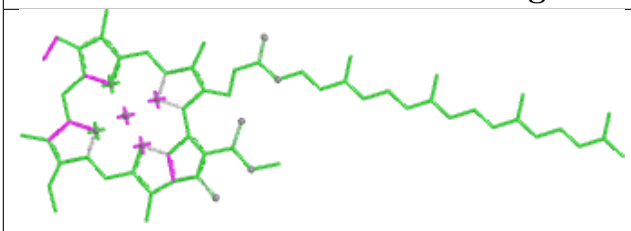


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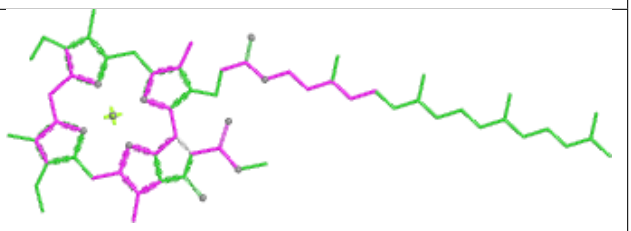


Rings

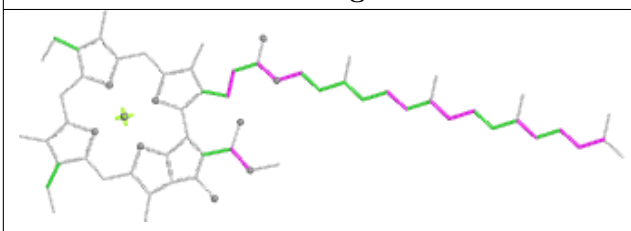
Ligand CLA 6 604



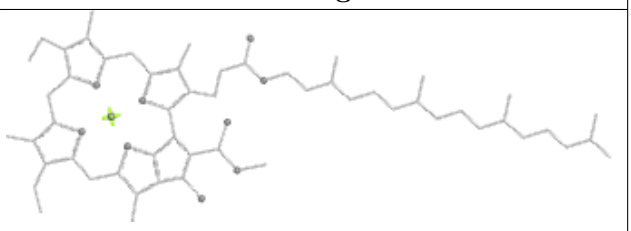
Bond lengths



Bond angles

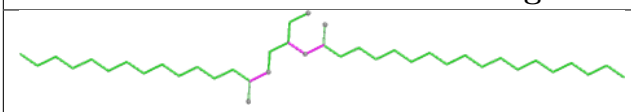


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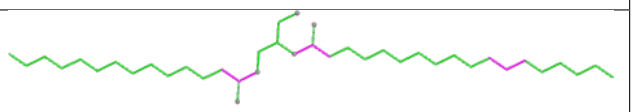


Rings

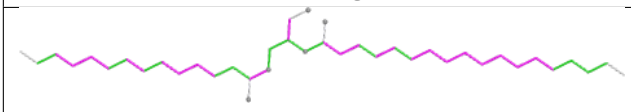
Ligand DGA 8 804



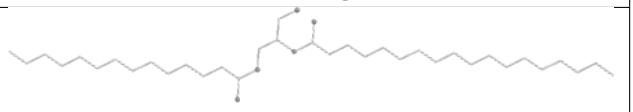
Bond lengths



Bond angles

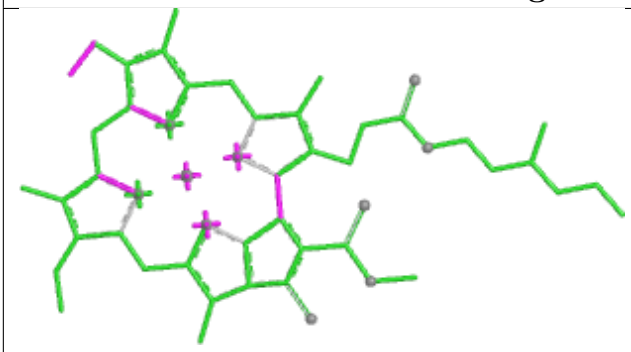


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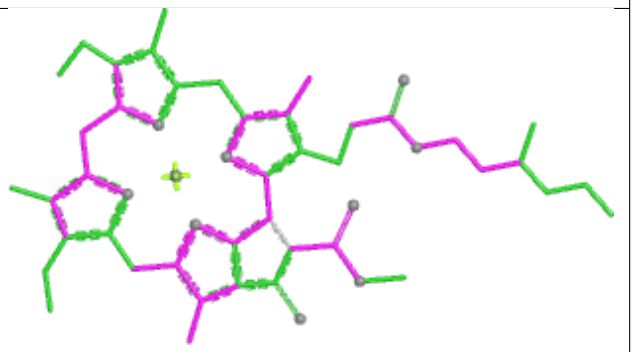


Rings

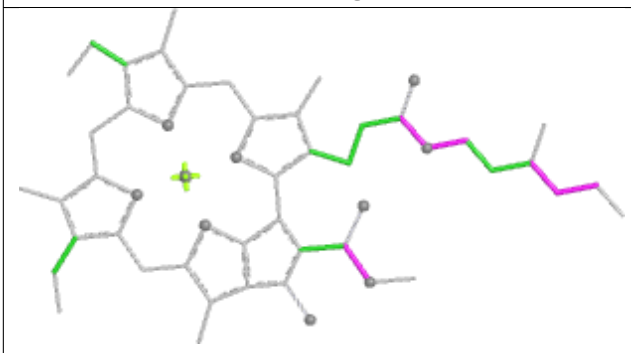
Ligand CLA 4 602



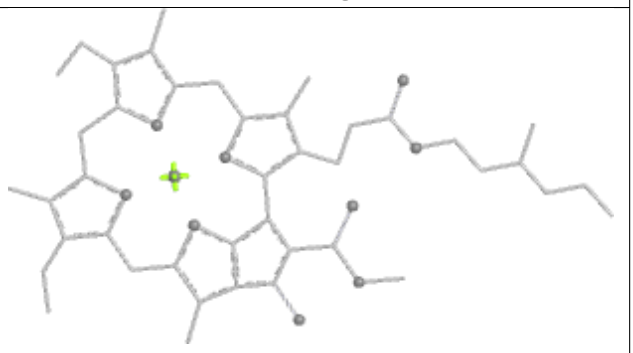
Bond lengths



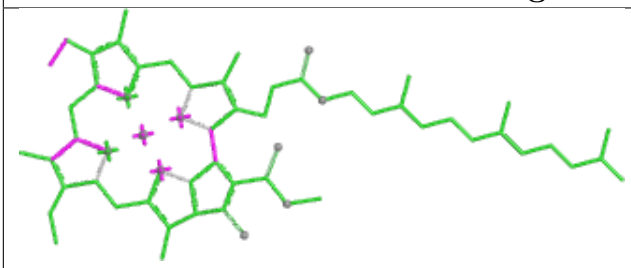
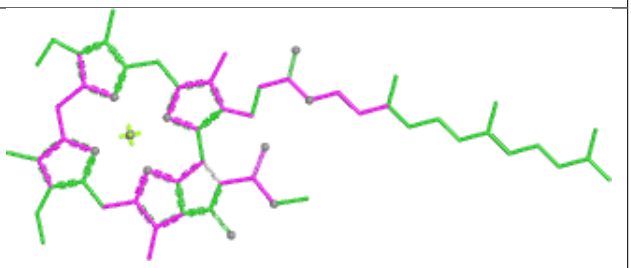
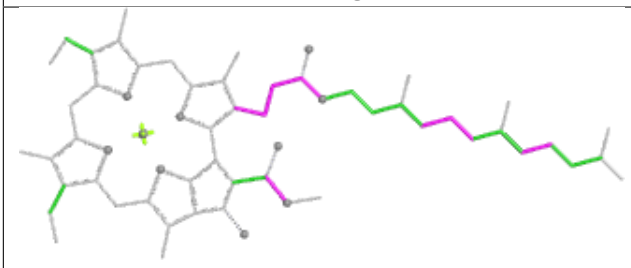
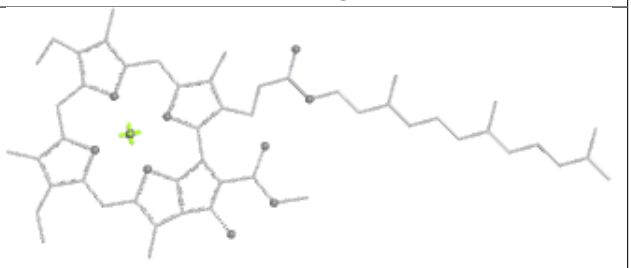
Bond angles

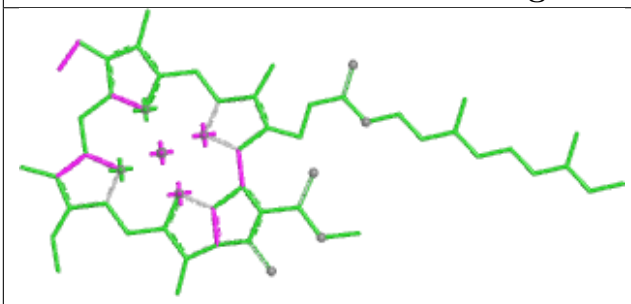
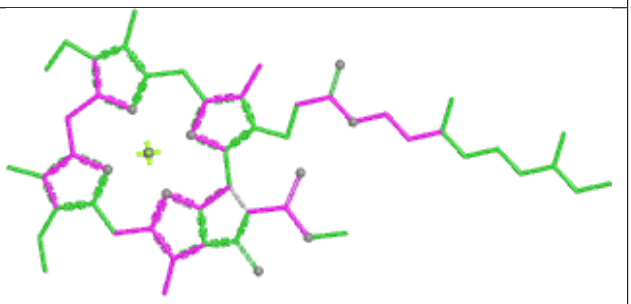
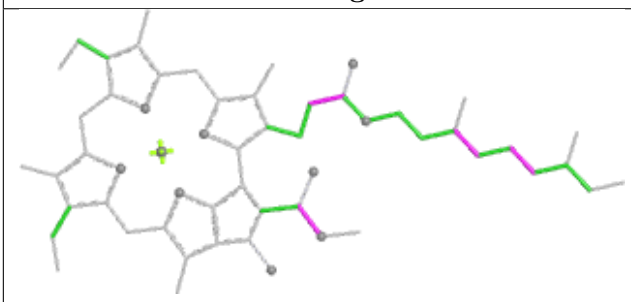
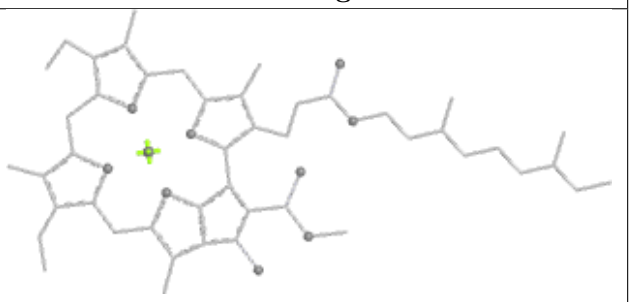


Torsions

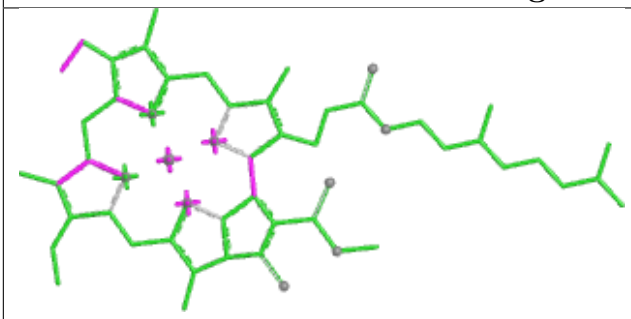


Rings

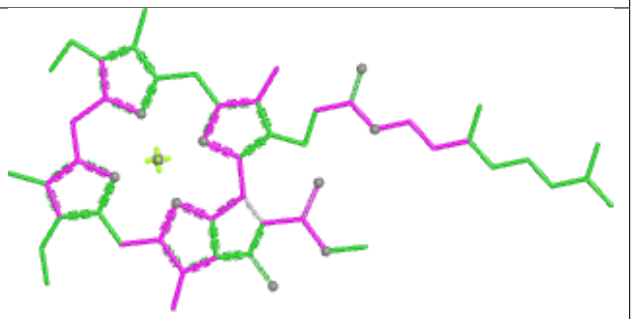
Ligand CLA 6 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

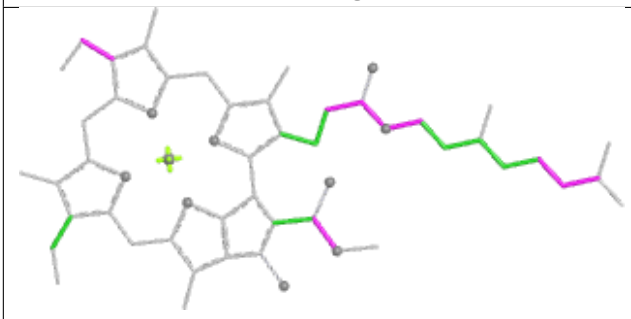
Ligand CLA 4 607



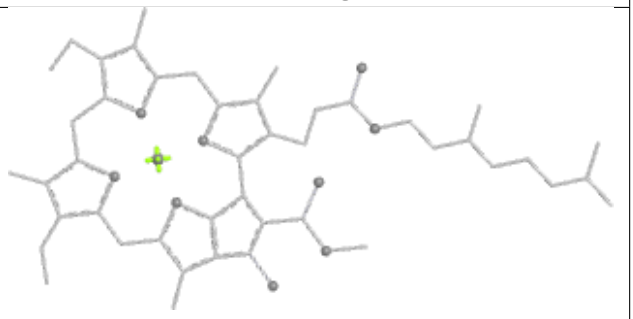
Bond lengths



Bond angles

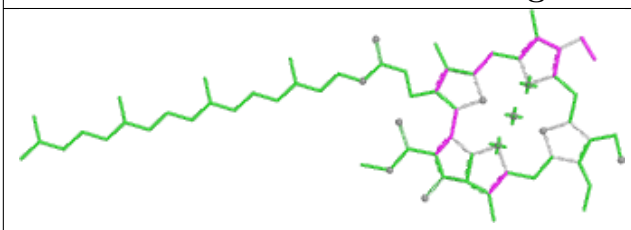


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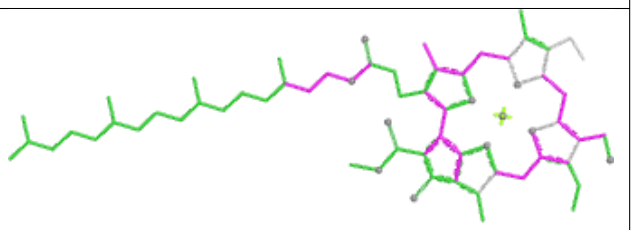


Rings

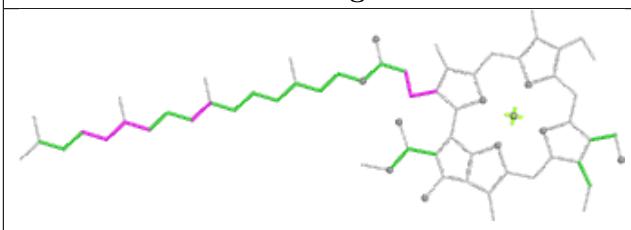
Ligand CHL 1 604



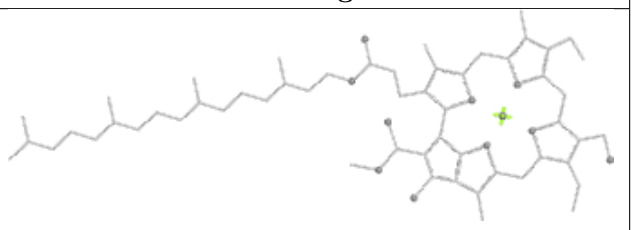
Bond lengths



Bond angles

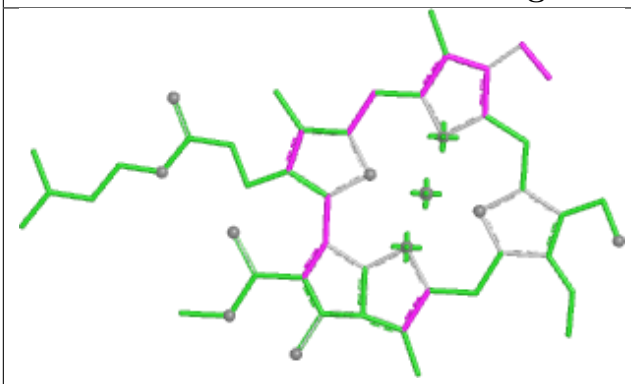


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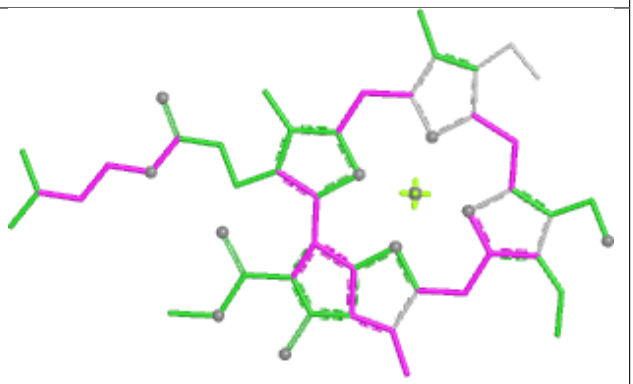


Rings

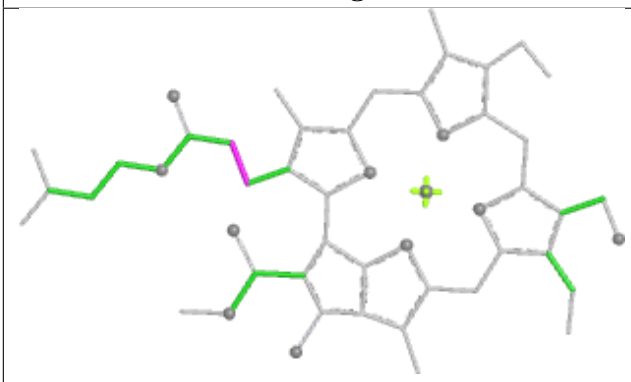
Ligand CHL 2 613



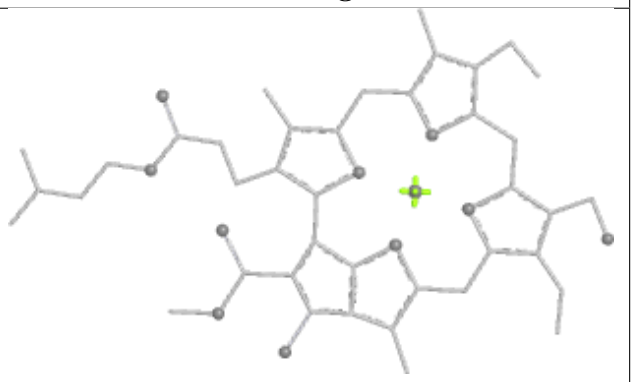
Bond lengths



Bond angles

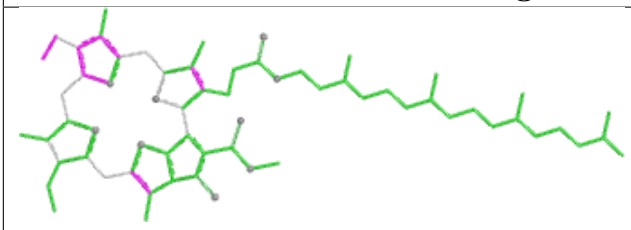


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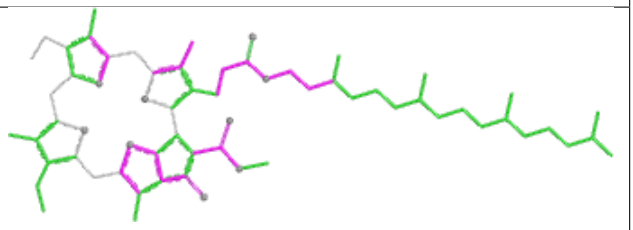


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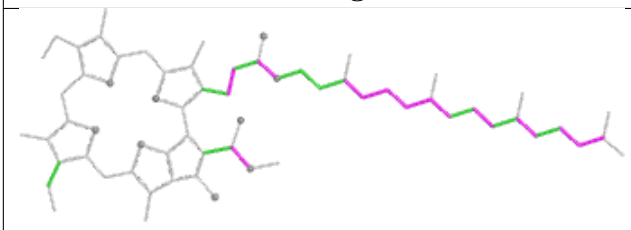
Ligand CLA B 1234



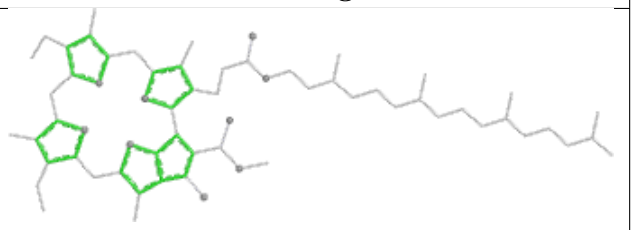
Bond lengths



Bond angles

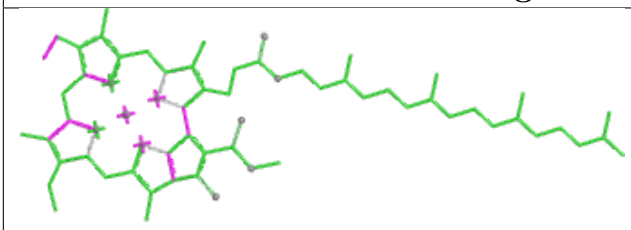


Torsions

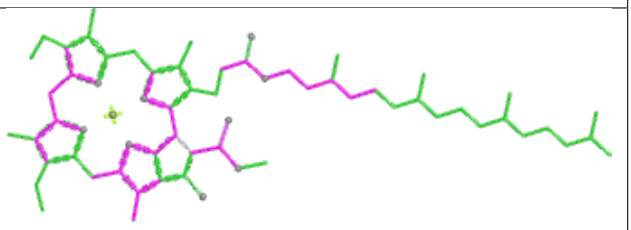


Rings

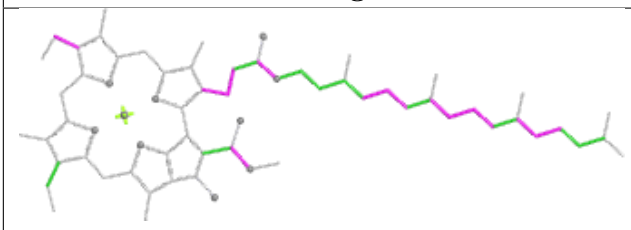
Ligand CLA A 1104



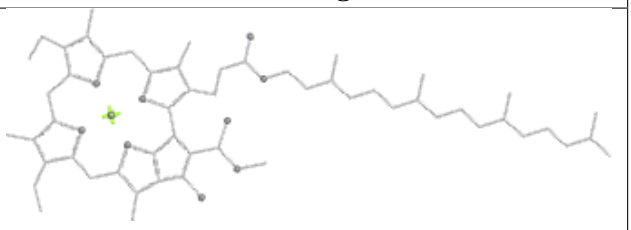
Bond lengths



Bond angles

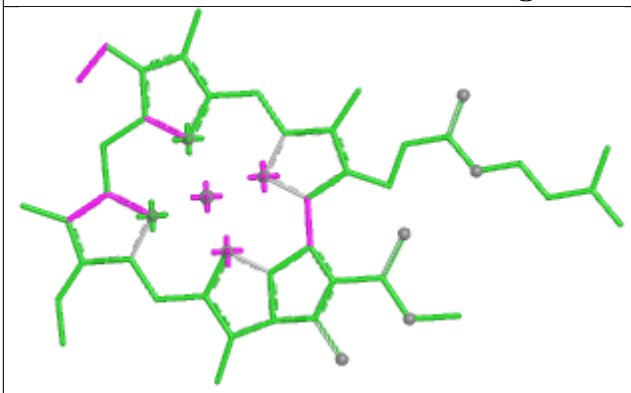


Torsions

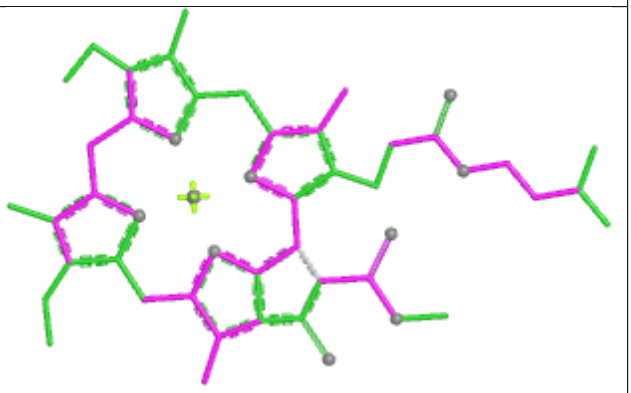


Rings

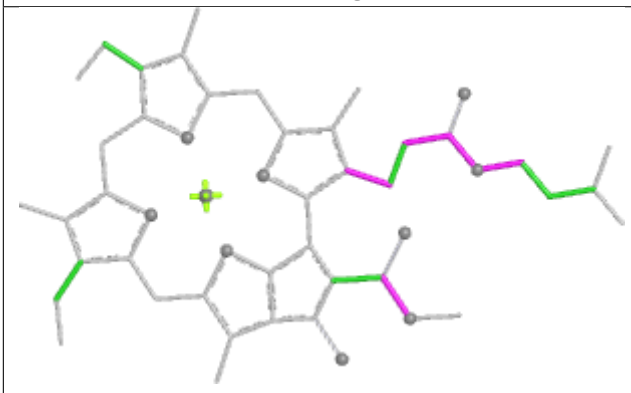
Ligand CLA L 1504



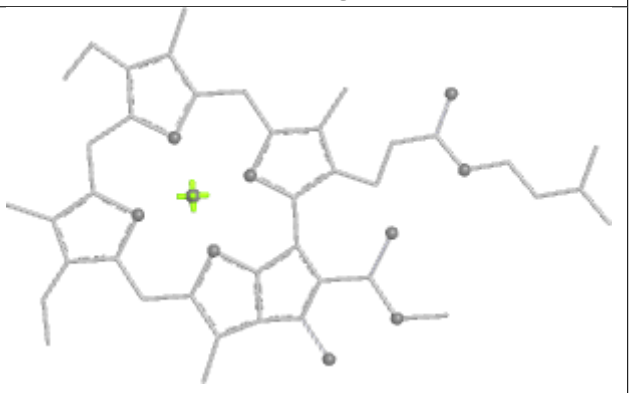
Bond lengths



Bond angles

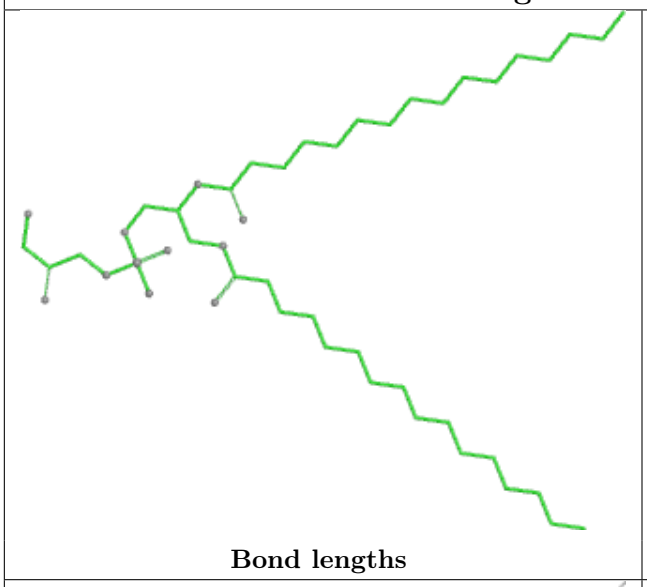


Torsions

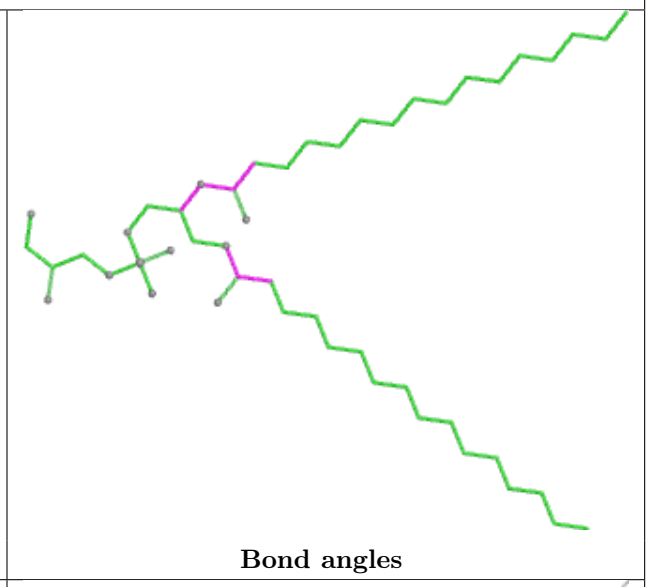


Rings

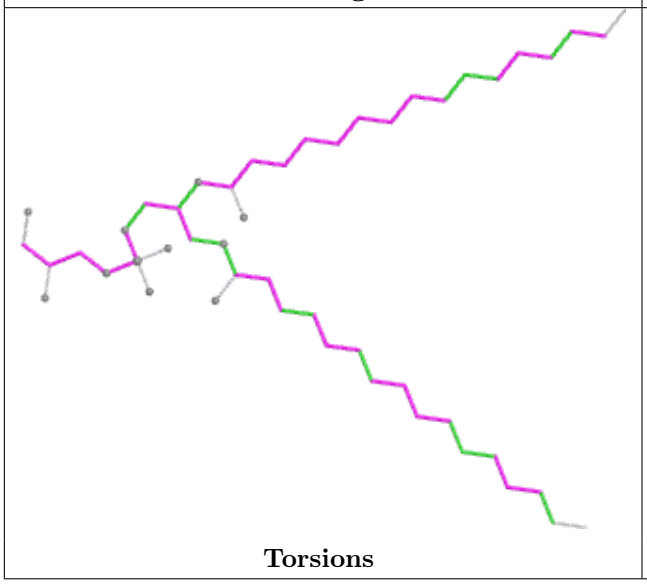
Ligand LHG A 5002



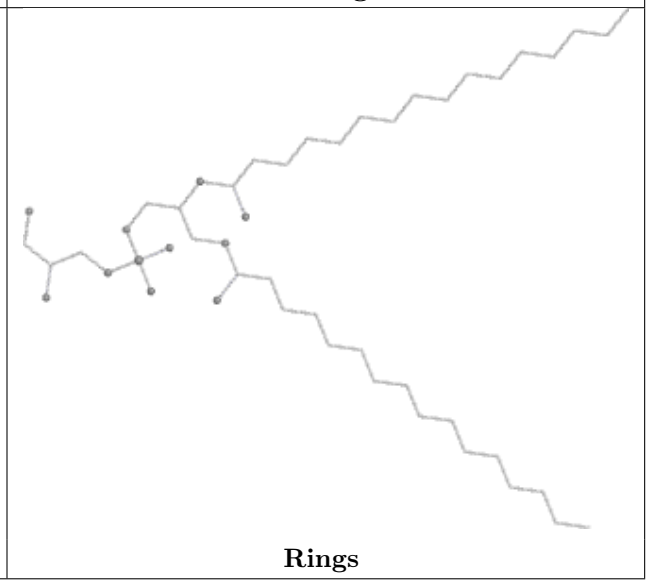
Bond lengths



Bond angles

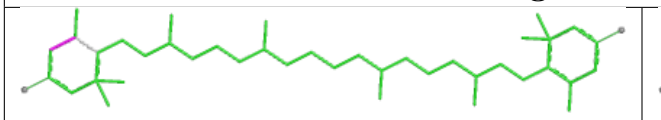


Torsions

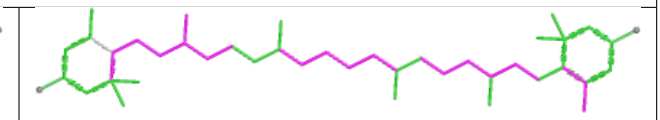


Rings

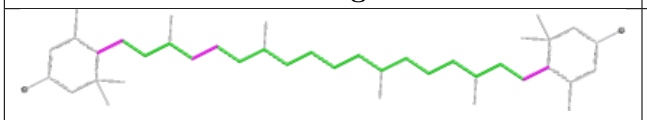
Ligand LUT 6 502



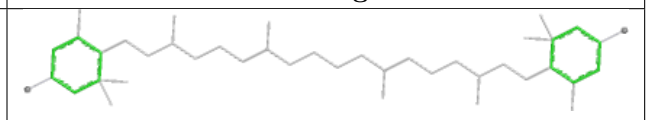
Bond lengths



Bond angles

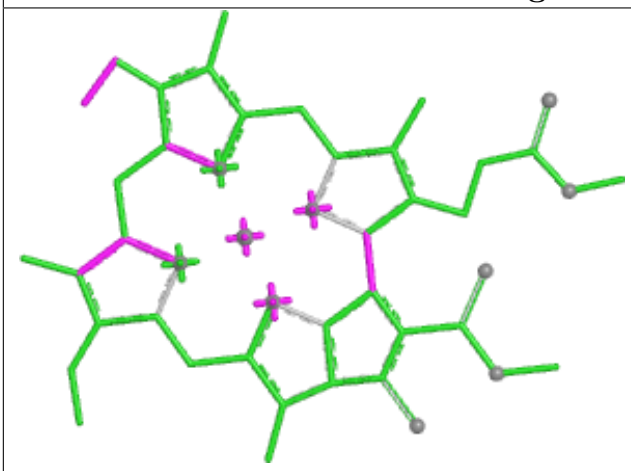


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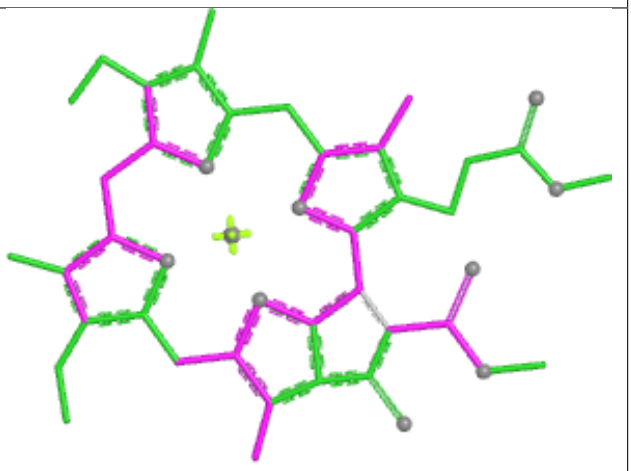


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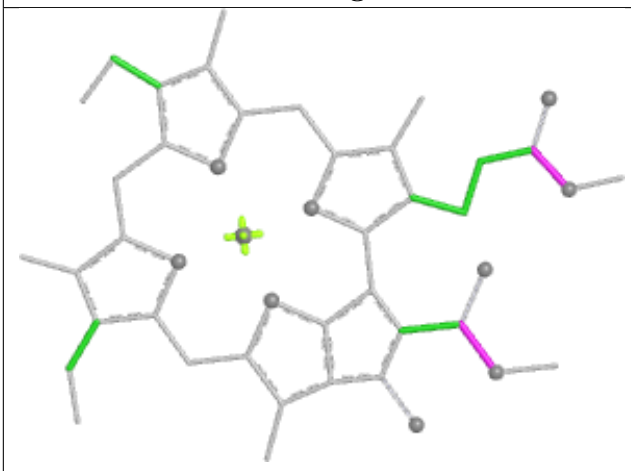
Ligand CLA a 615



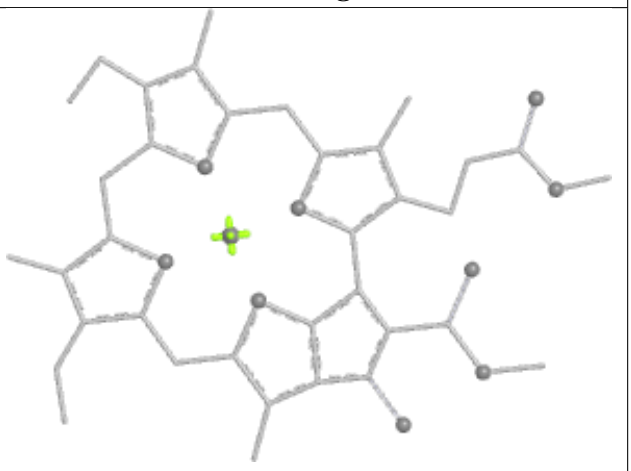
Bond lengths



Bond angles

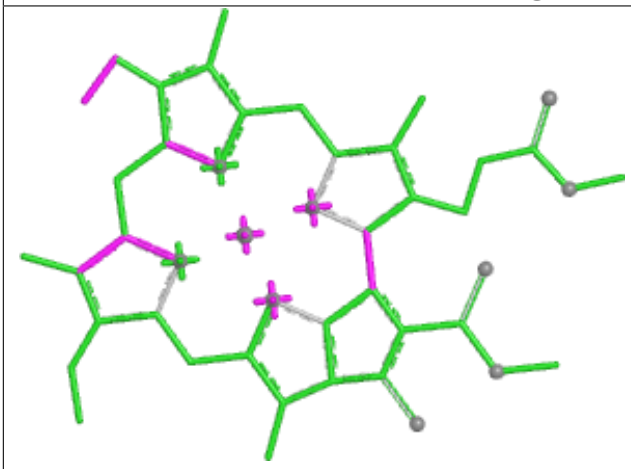


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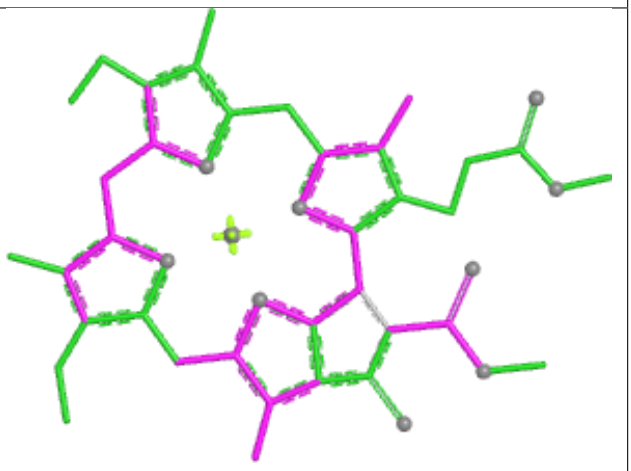


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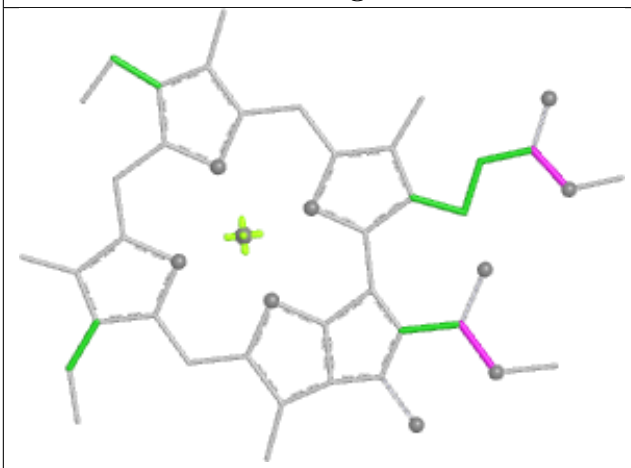
Ligand CLA 2 606



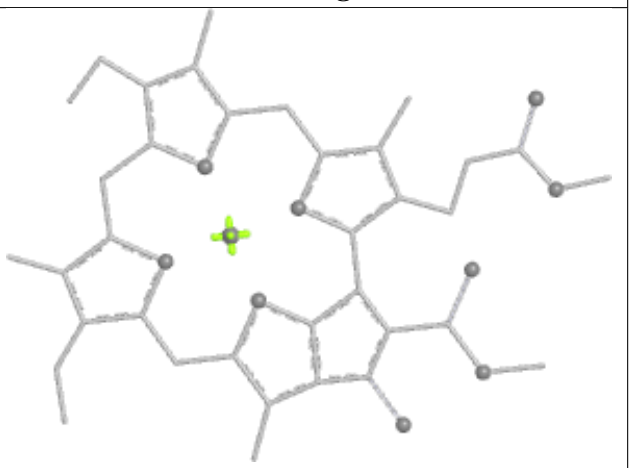
Bond lengths



Bond angles

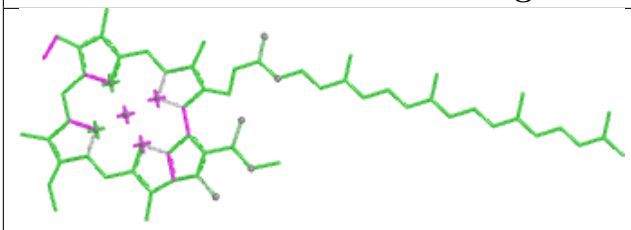


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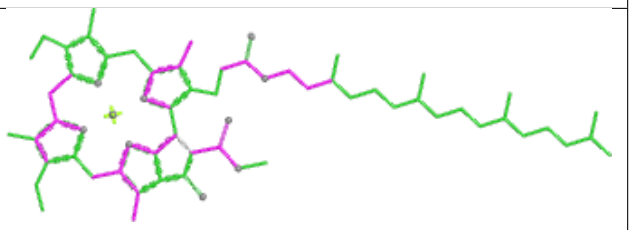


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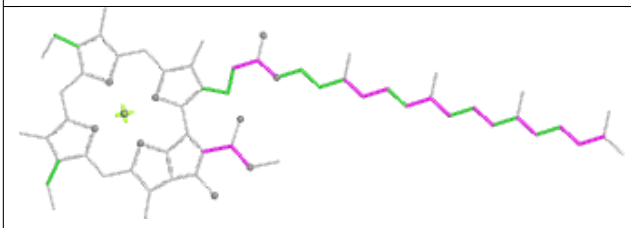
Ligand CLA A 1128



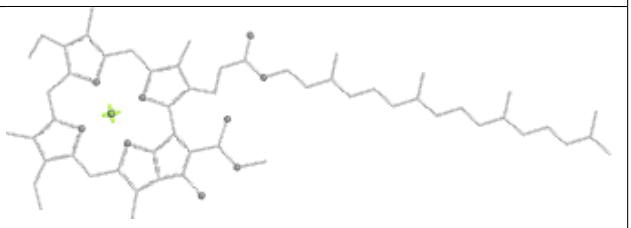
Bond lengths



Bond angles

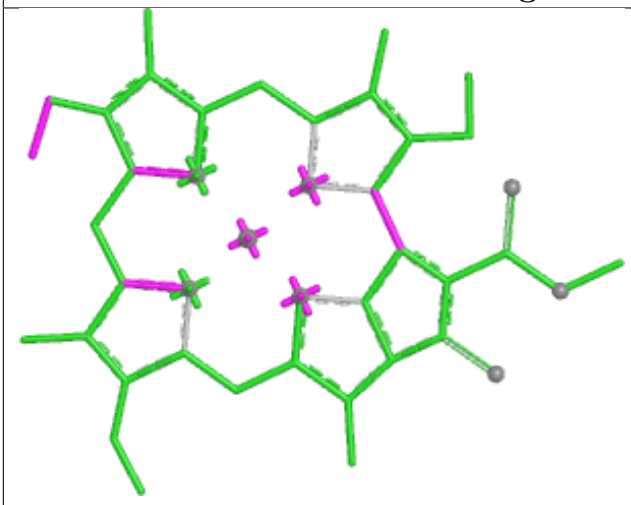


Torsions



Rings

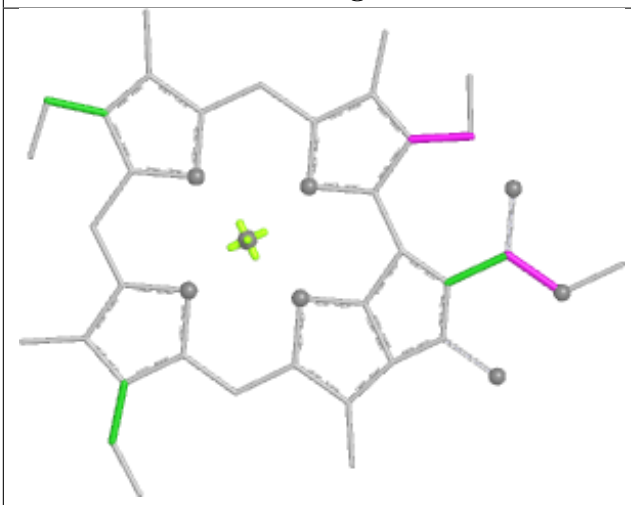
Ligand CLA J 1901



Bond lengths



Bond angles

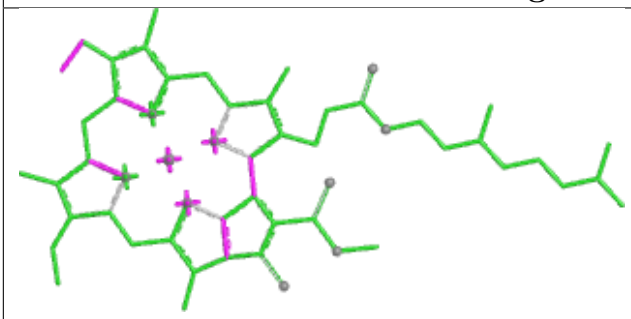


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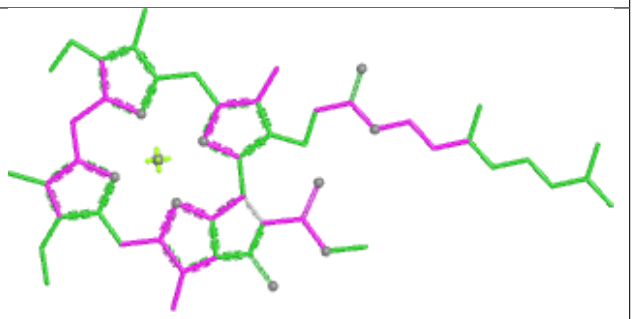


Rings

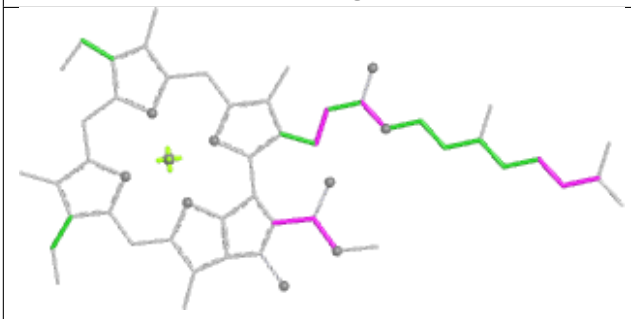
Ligand CLA a 605



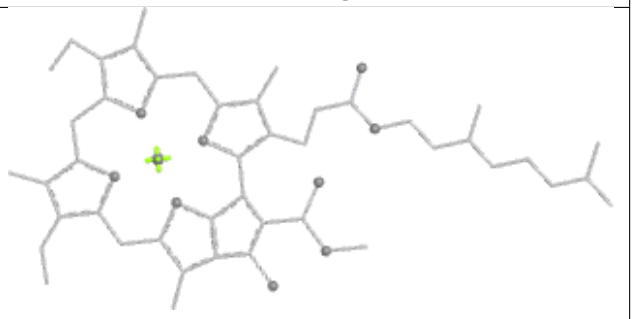
Bond lengths



Bond angles

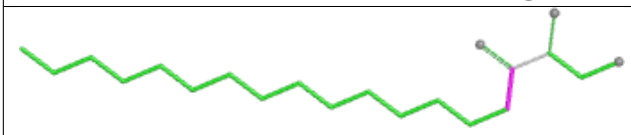


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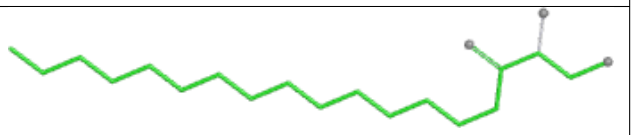


Rings

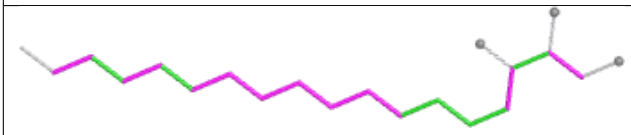
Ligand SPH J 5002



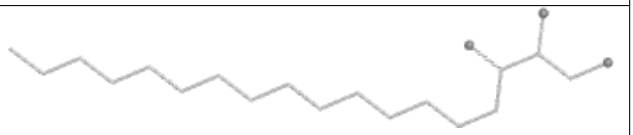
Bond lengths



Bond angles



Torsions

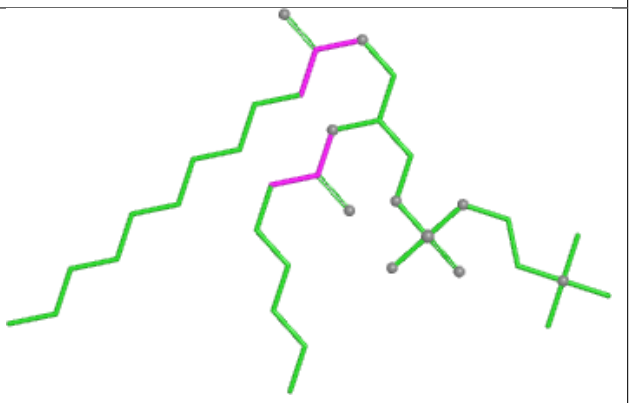


Rings

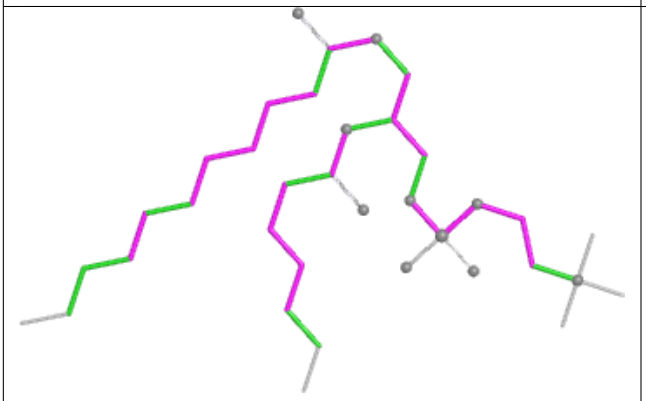
Ligand PCW 6 803



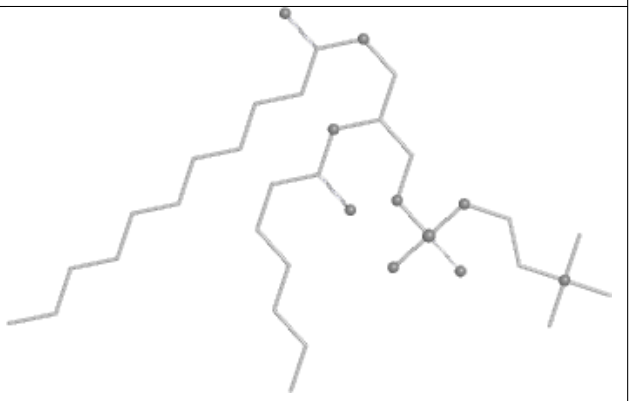
Bond lengths



Bond angles

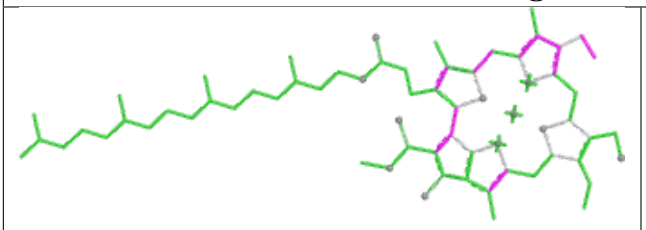


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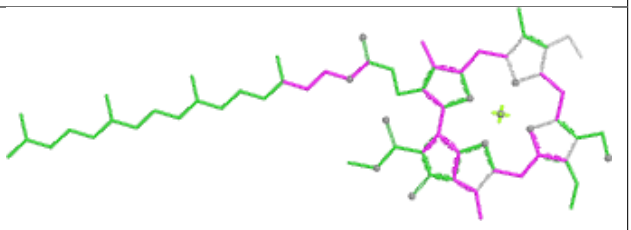


Rings

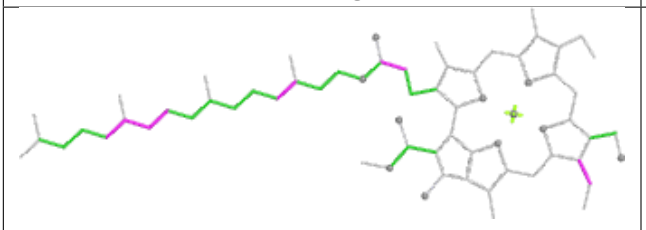
Ligand CHL 2 609



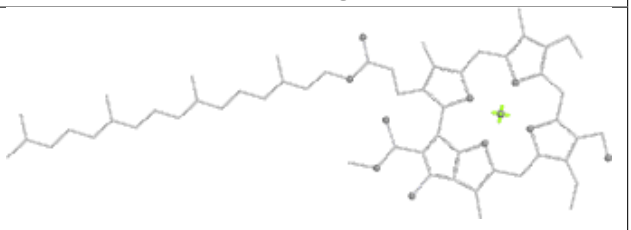
Bond lengths



Bond angles

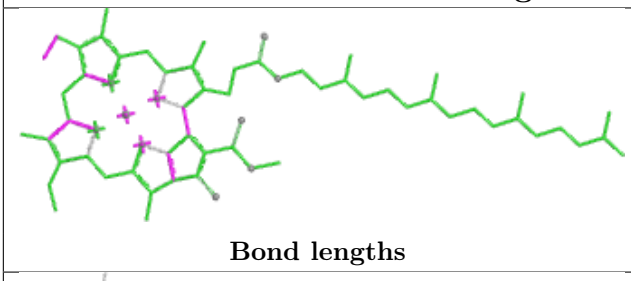


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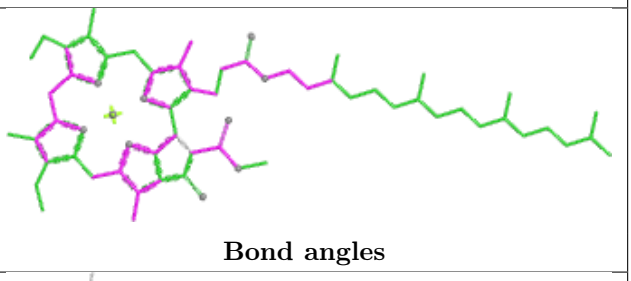


Rings

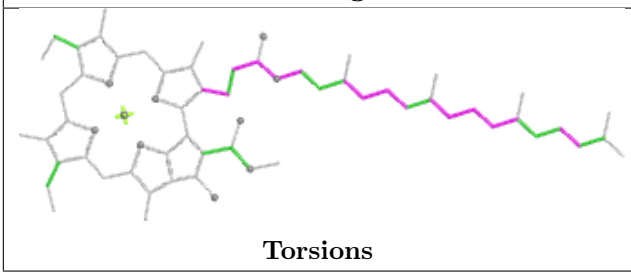
Ligand CLA A 1108



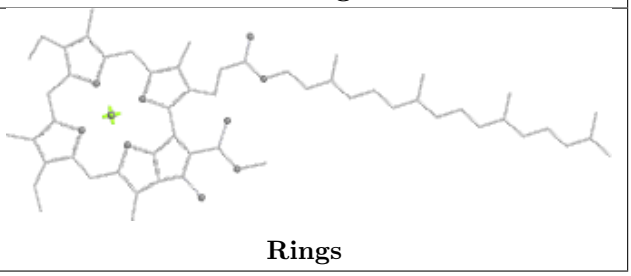
Bond lengths



Bond angles

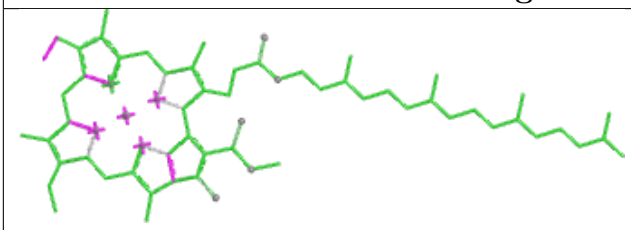


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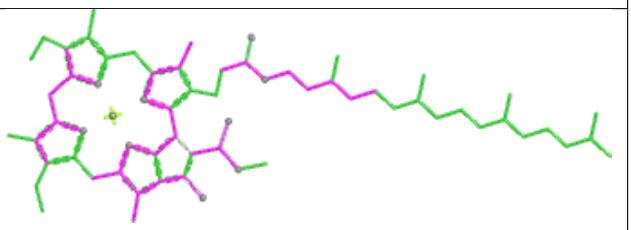


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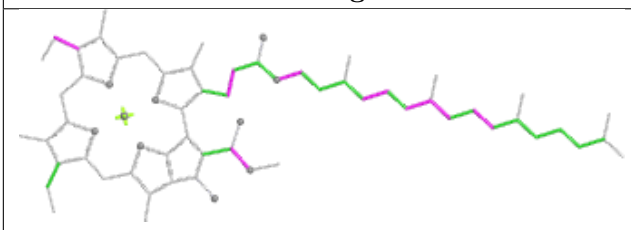
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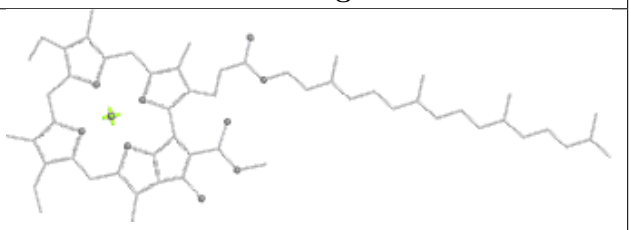
Bond lengths



Bond angles

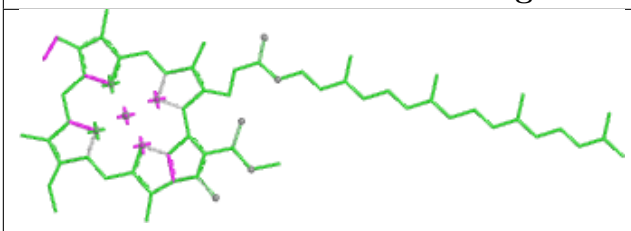


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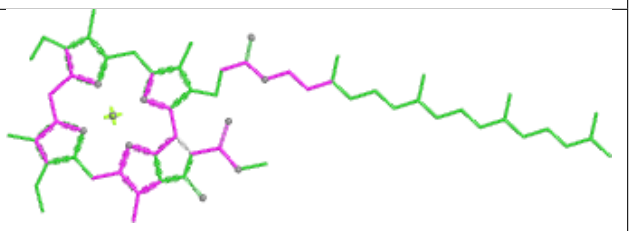


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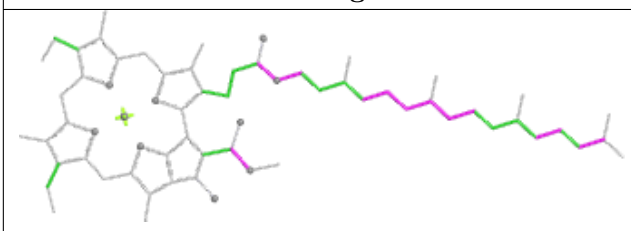
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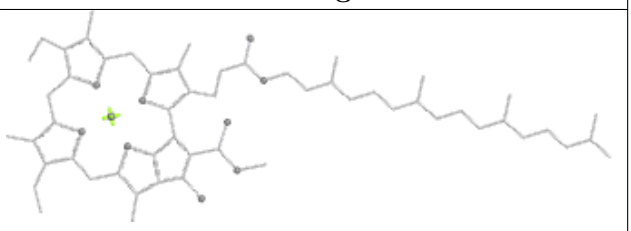
Bond lengths



Bond angles

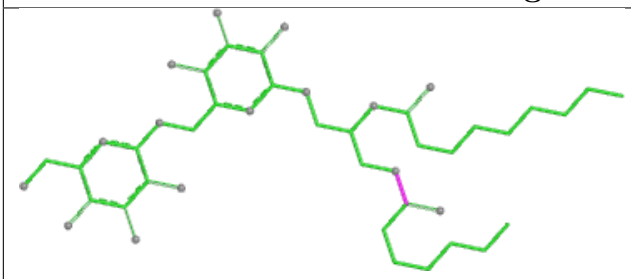


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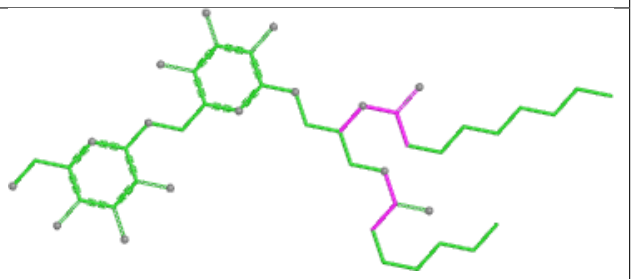


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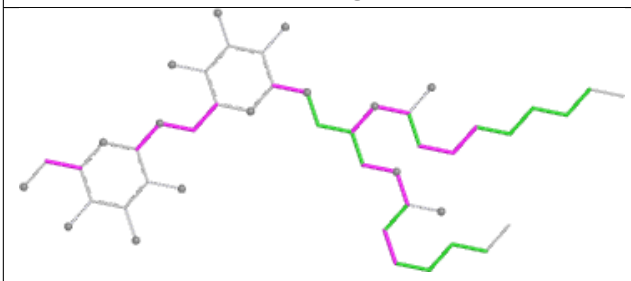
Ligand DGD 8 803



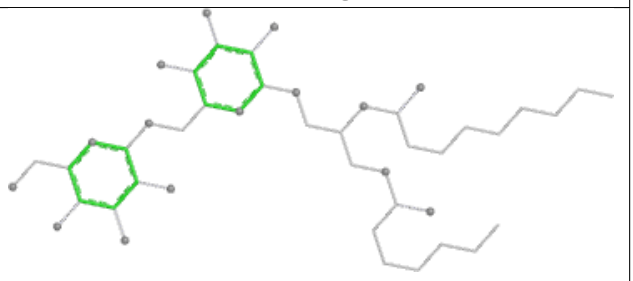
Bond lengths



Bond angles

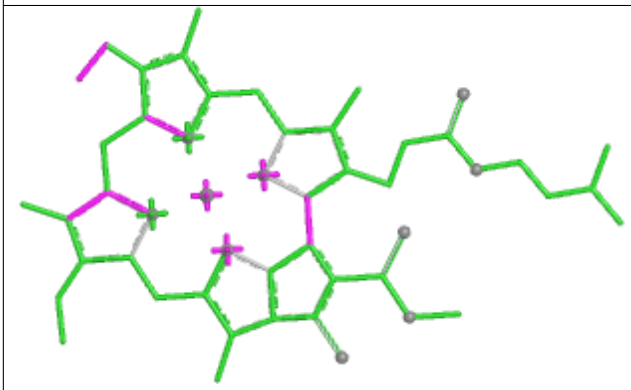


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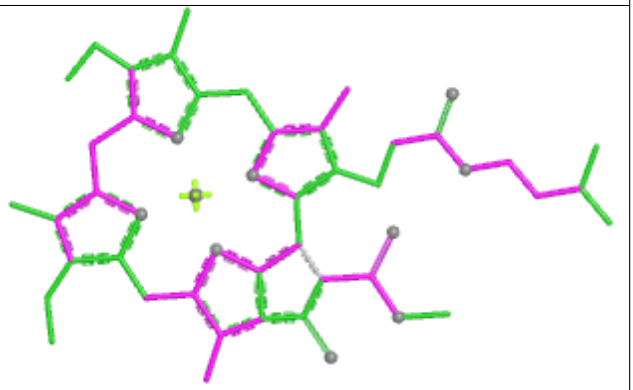


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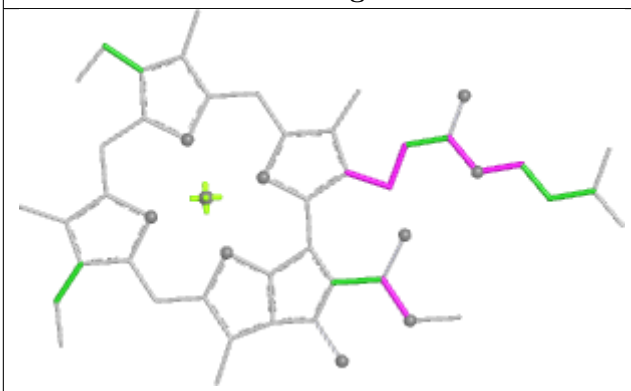
Ligand CLA L 1501



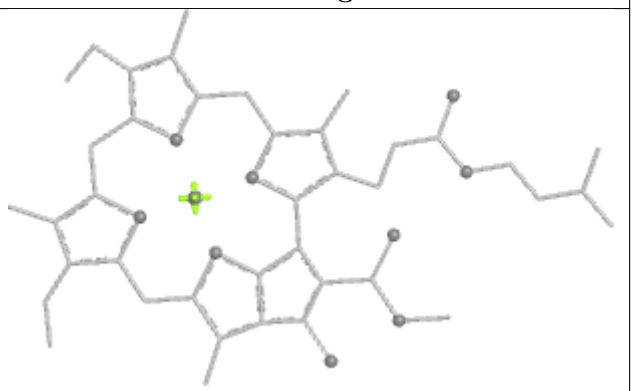
Bond lengths



Bond angles

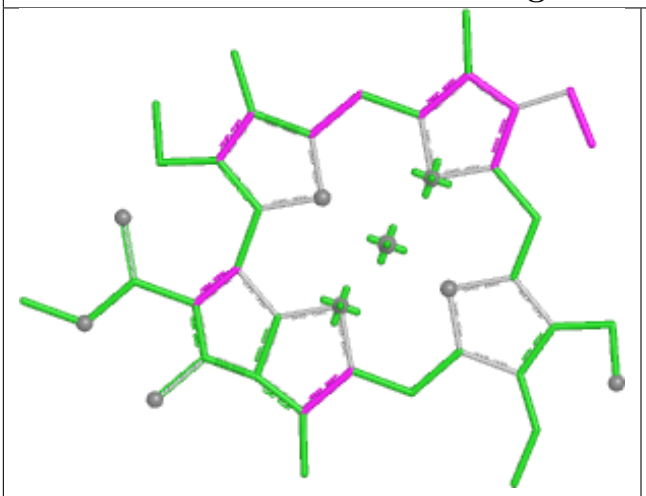


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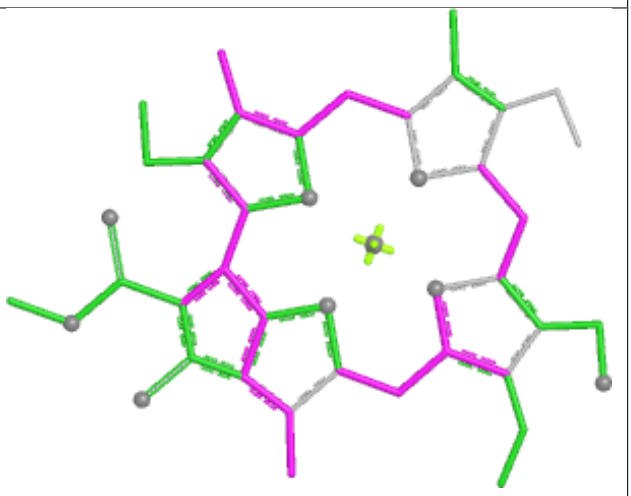


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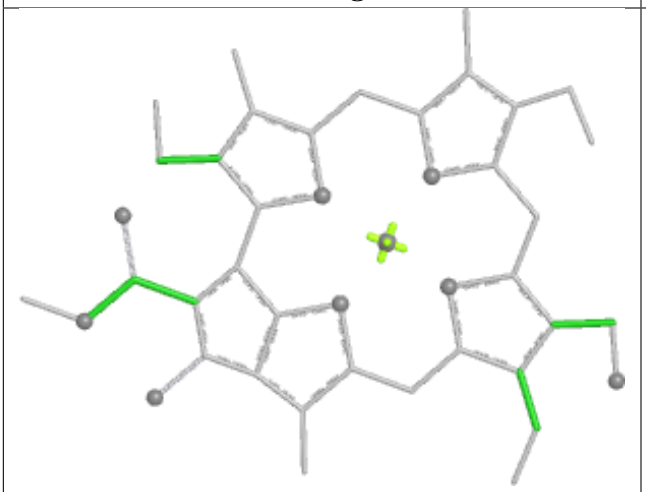
Ligand CHL 6 617



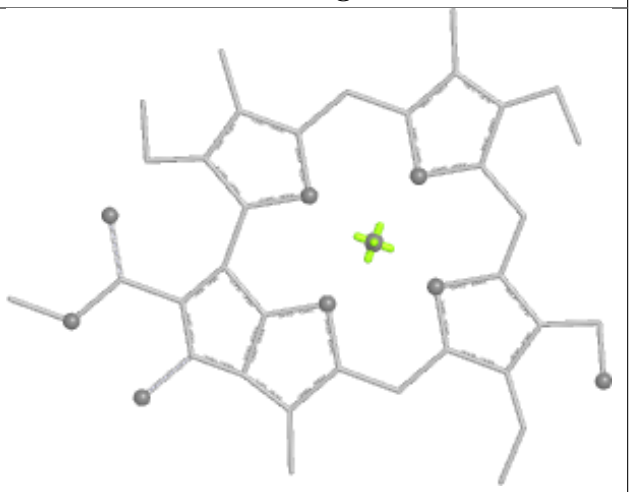
Bond lengths



Bond angles

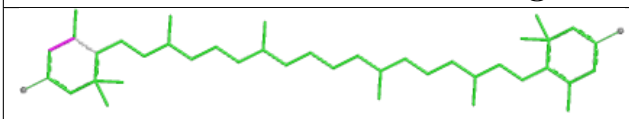


Torsions

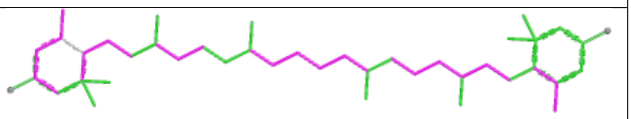


Rings

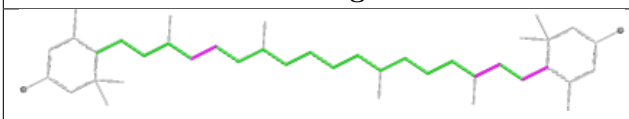
Ligand LUT 8 502



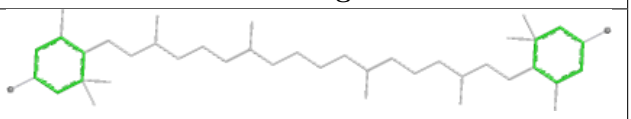
Bond lengths



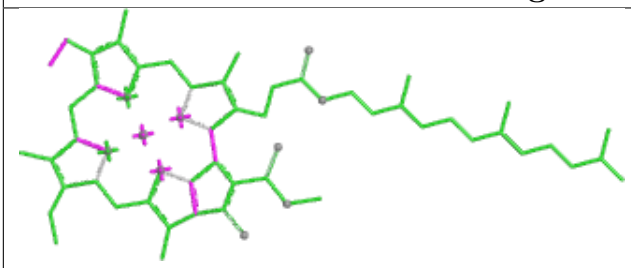
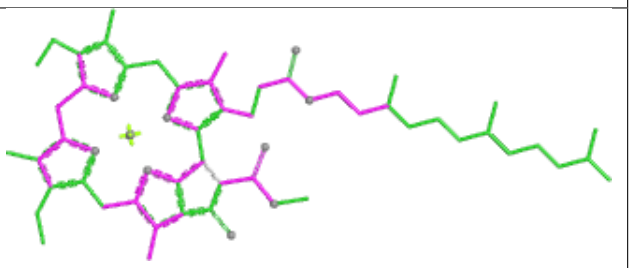
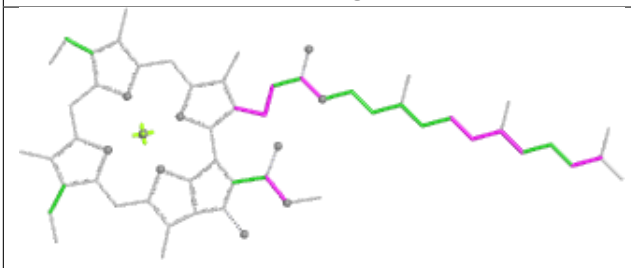
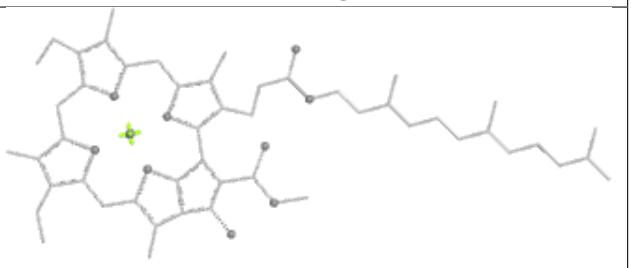
Bond angles

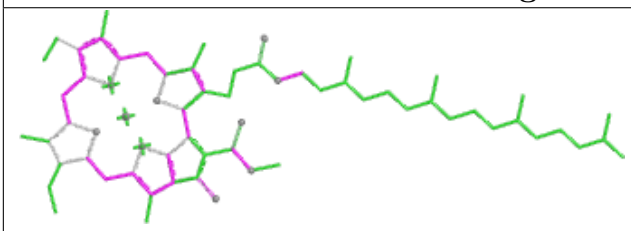
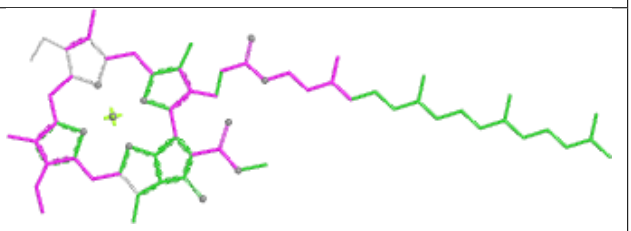
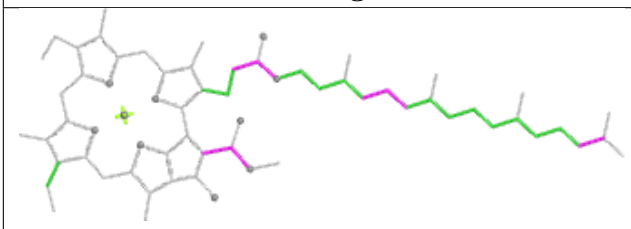
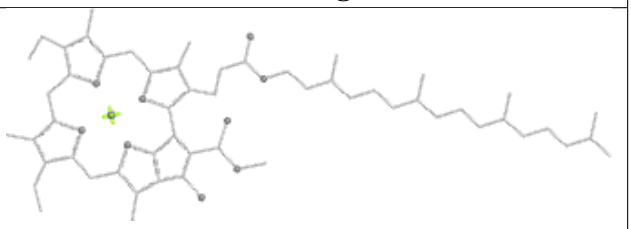


Torsions

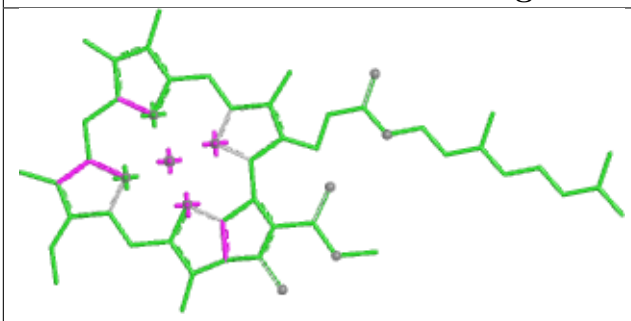


Rings

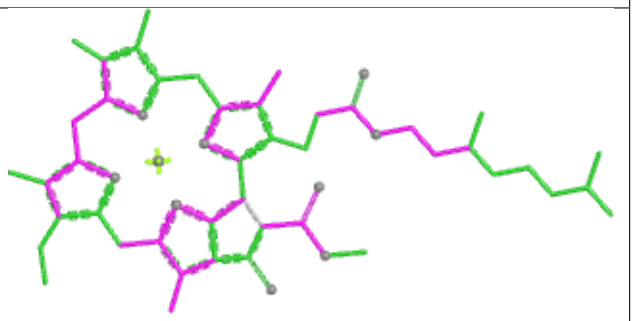
Ligand CLA 1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 A 1011	
	
Bond lengths	Bond angles
	
Torsions	Rings

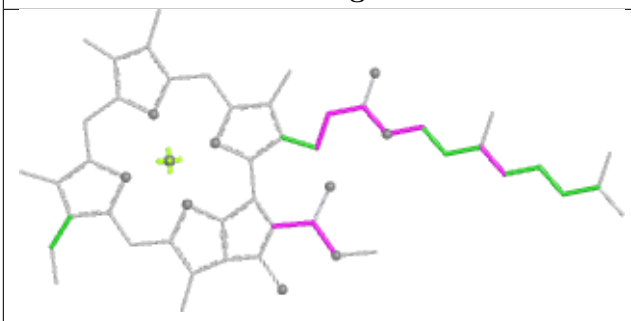
Ligand CLA B 1208



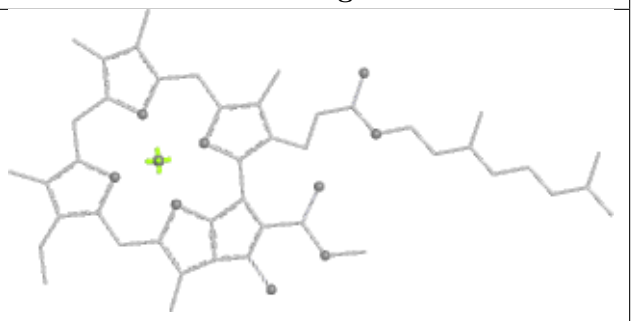
Bond lengths



Bond angles

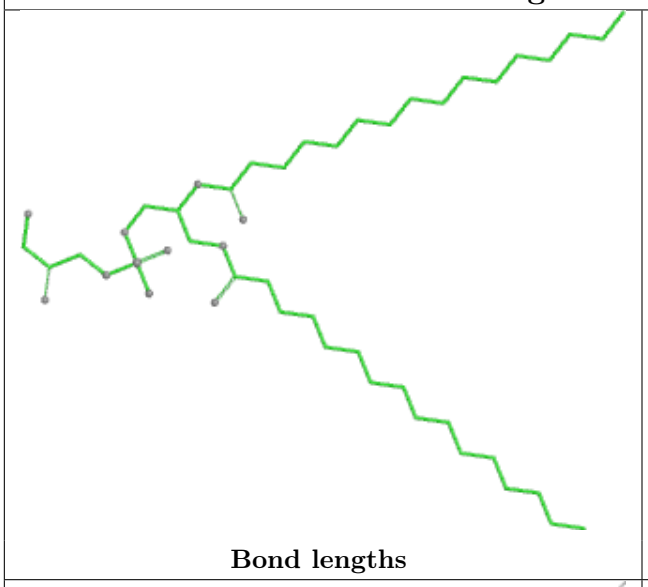


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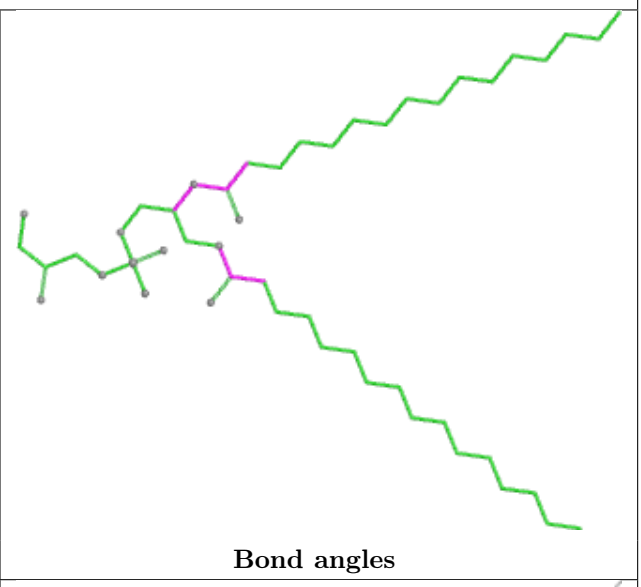


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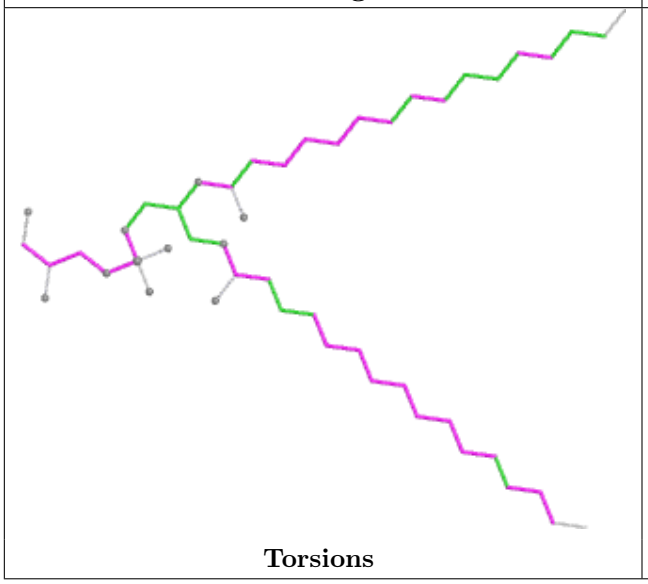
Ligand LHG 3 801



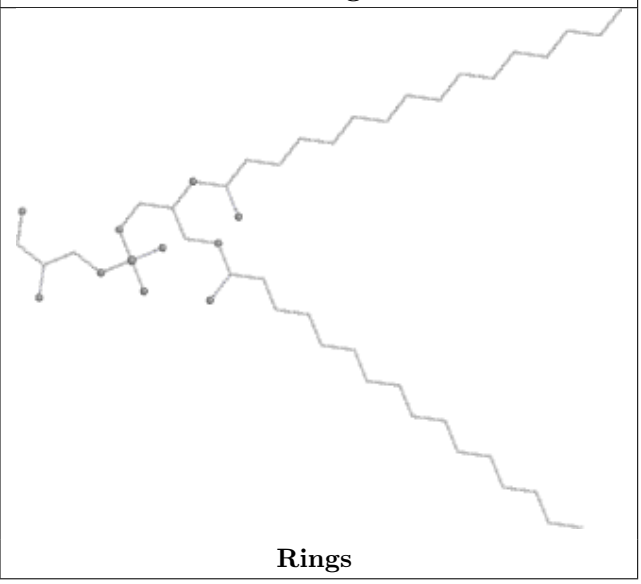
Bond lengths



Bond angles

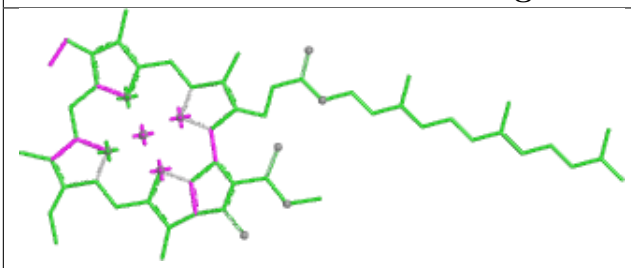


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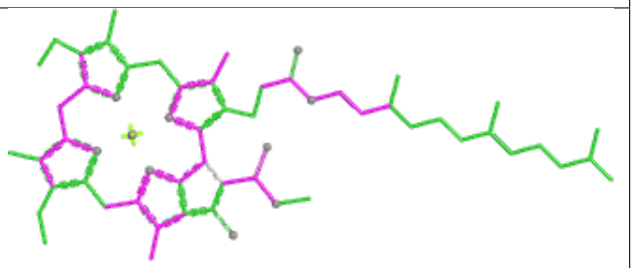


Rings

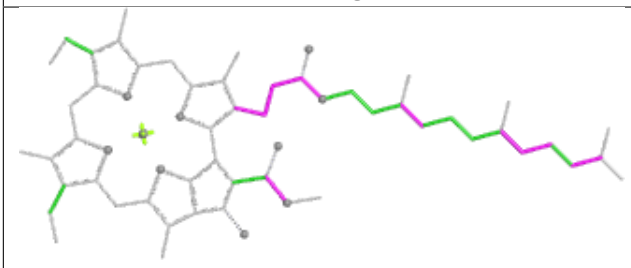
Ligand CLA A 1116



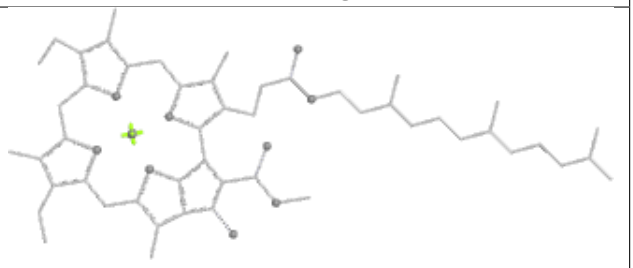
Bond lengths



Bond angles

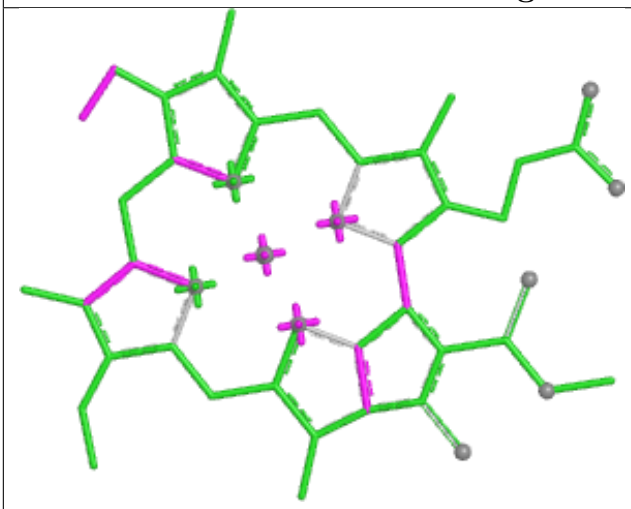


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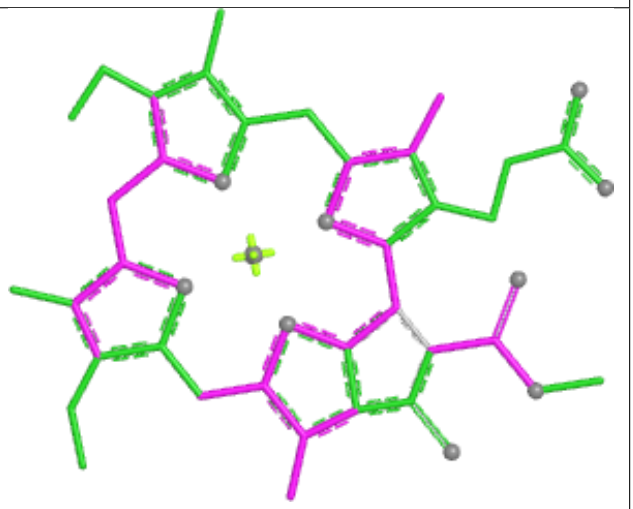


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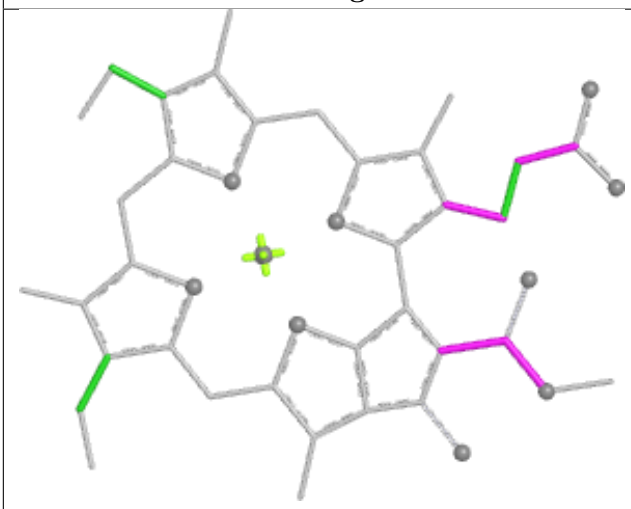
Ligand CLA L 1503



Bond lengths



Bond angles

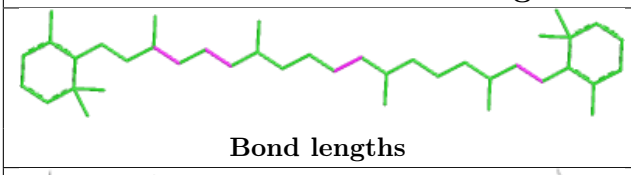


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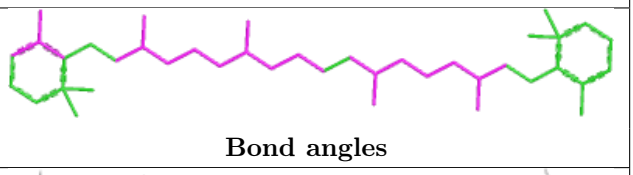


Rings

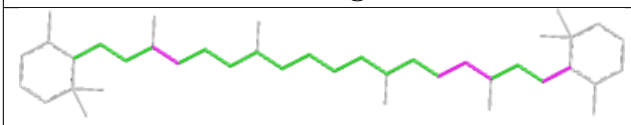
Ligand BCR B 4003



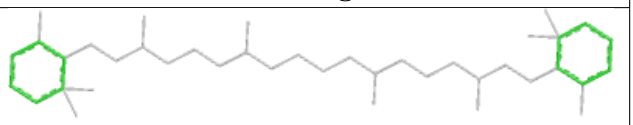
Bond lengths



Bond angles

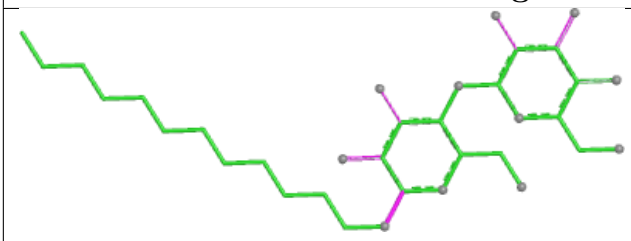


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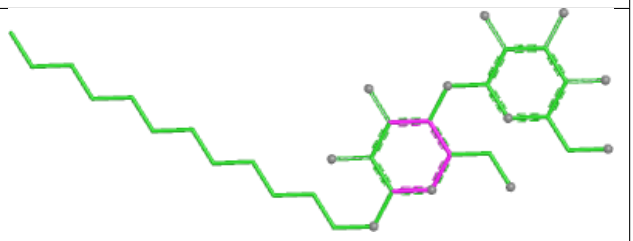


Rings

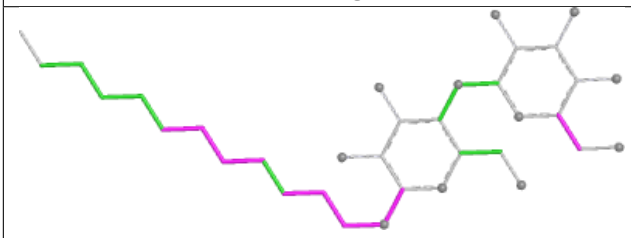
Ligand LMT A 5008



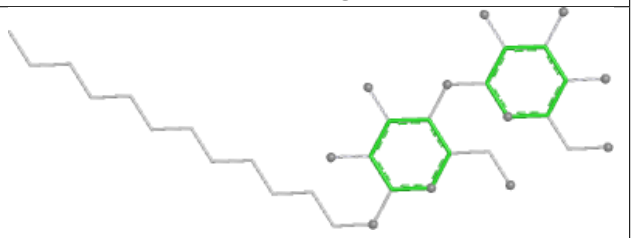
Bond lengths



Bond angles

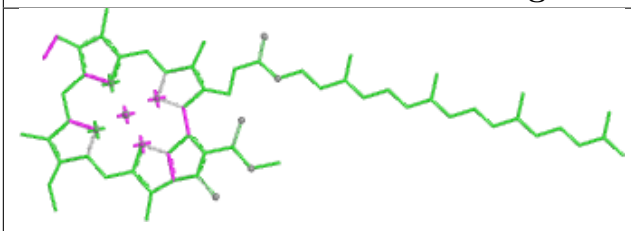


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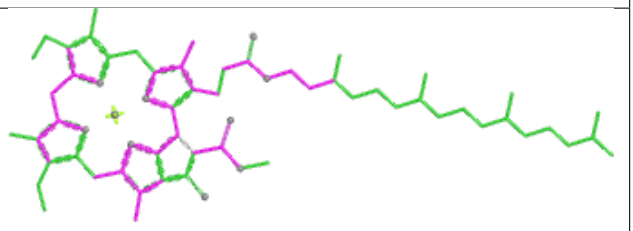


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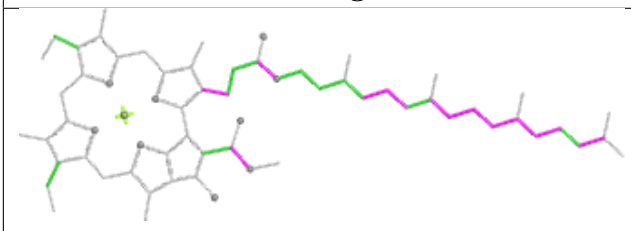
Ligand CLA 1 607



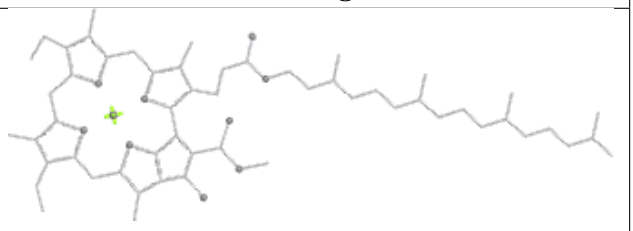
Bond lengths



Bond angles

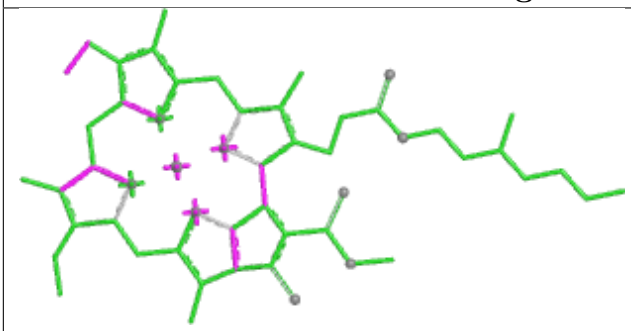


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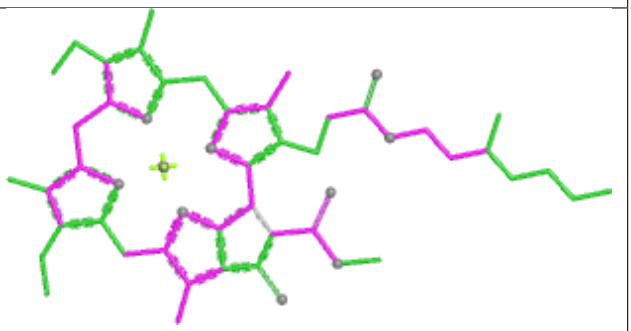


Rings

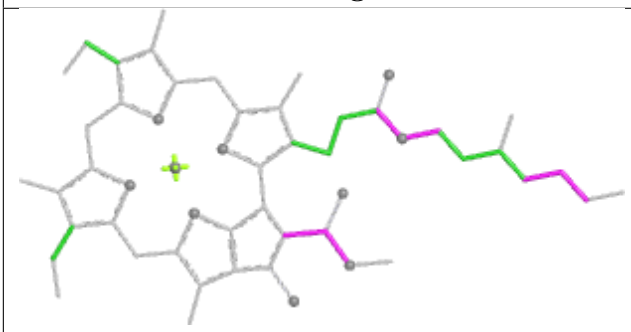
Ligand CLA B 1236



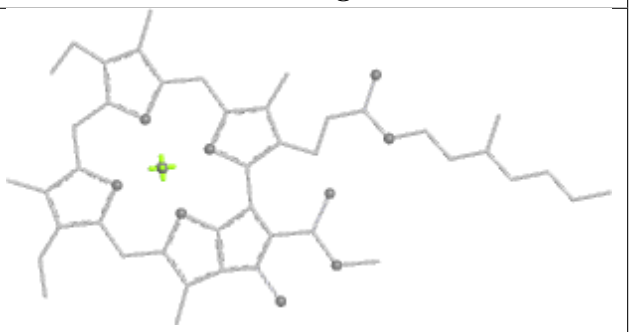
Bond lengths



Bond angles

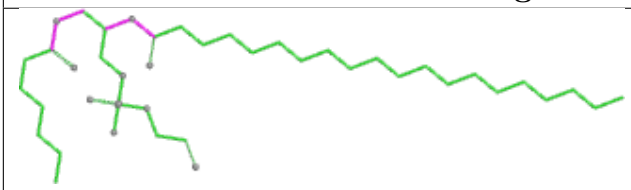


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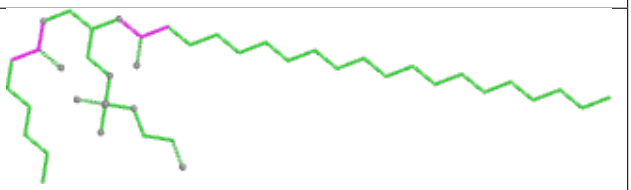


Rings

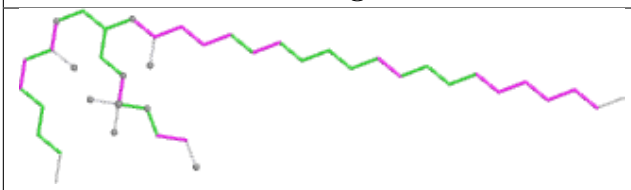
Ligand PTY B 5005



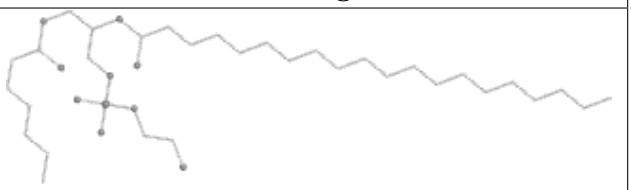
Bond lengths



Bond angles

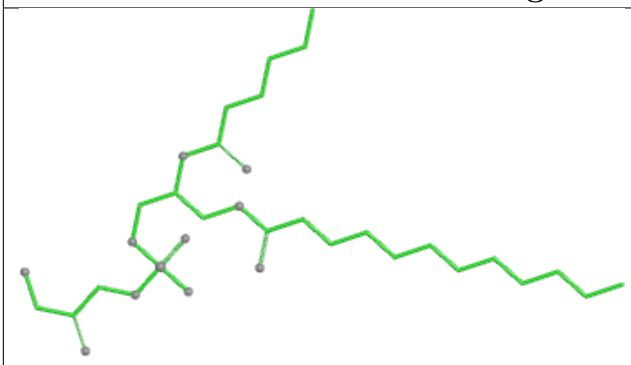


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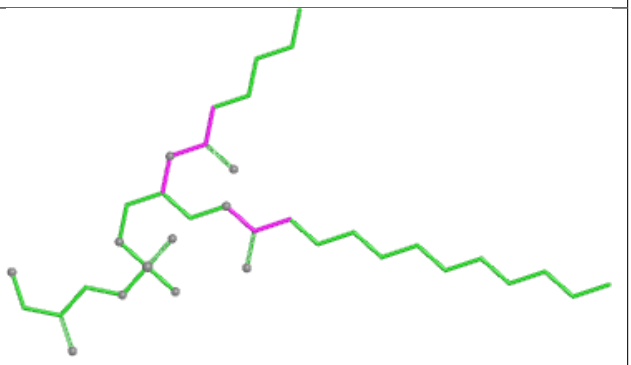


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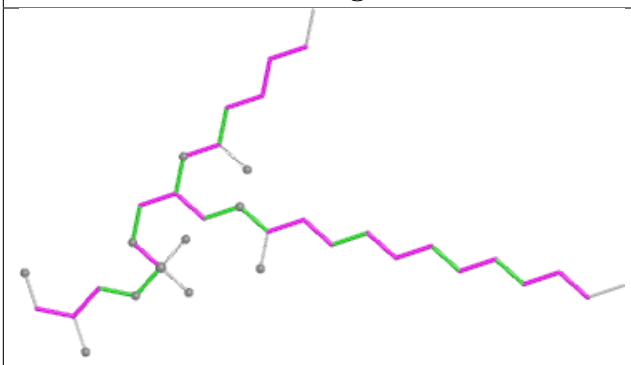
Ligand LHG 1 801



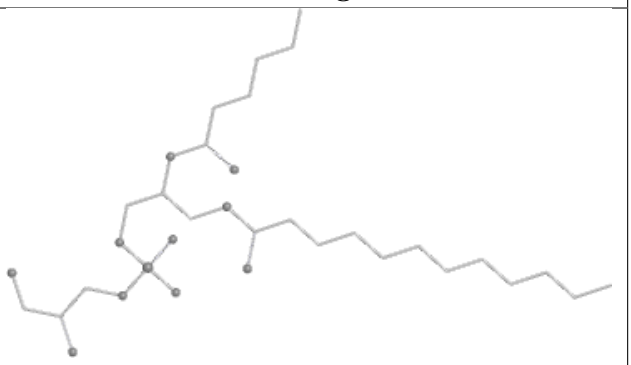
Bond lengths



Bond angles

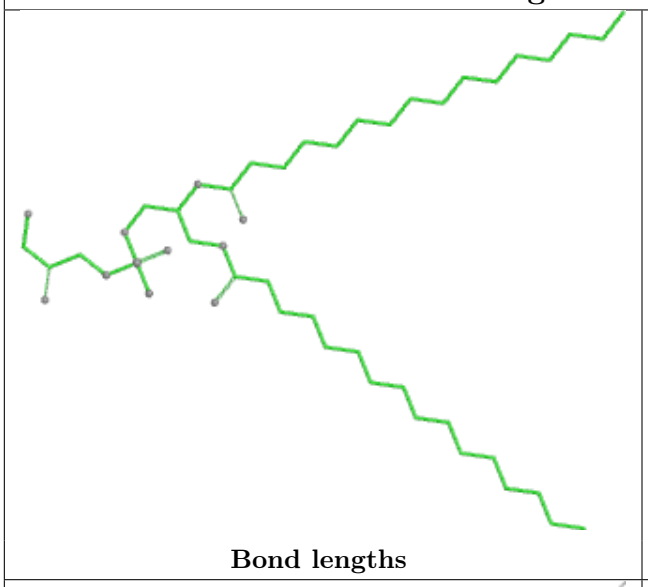


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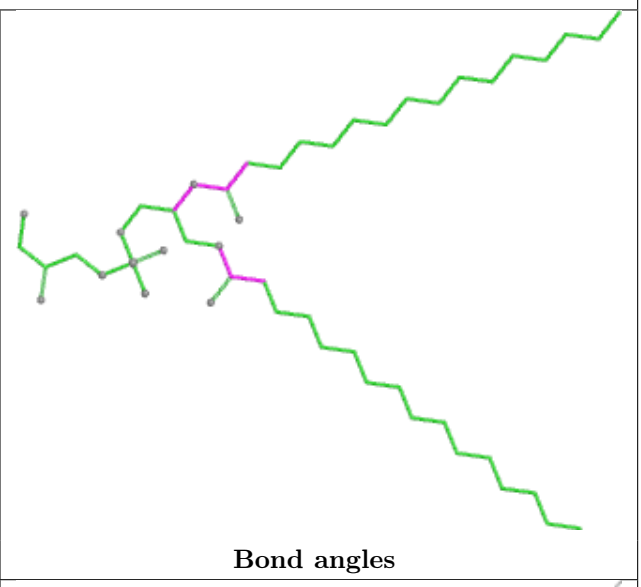


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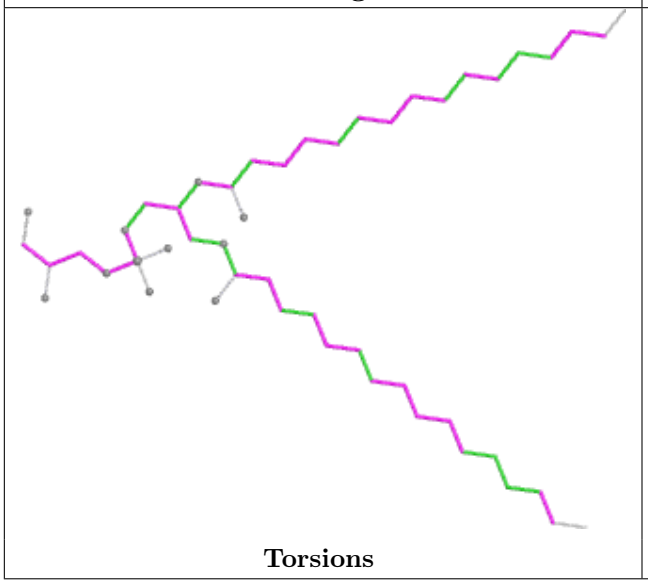
Ligand LHG 6 801



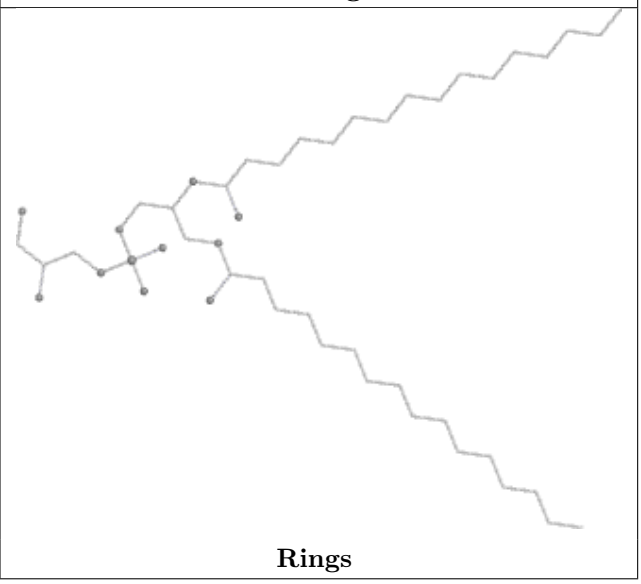
Bond lengths



Bond angles

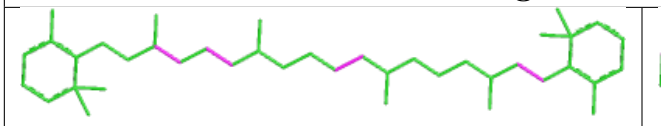


Torsions



Rings

Ligand BCR B 4001



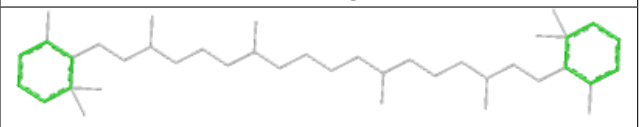
Bond lengths



Bond angles

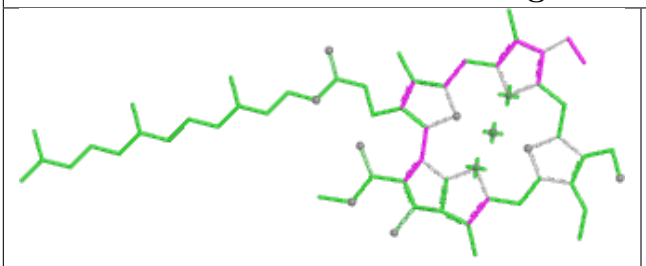


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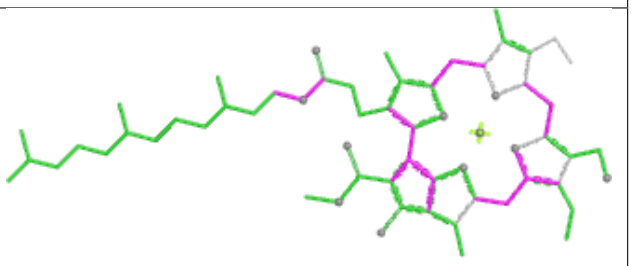


Rings

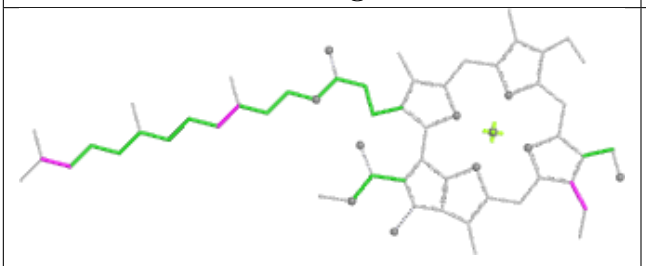
Ligand CHL 7 613



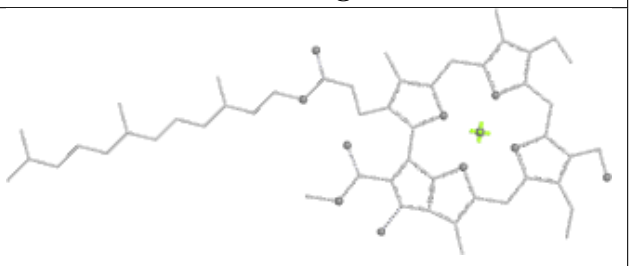
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Bond angles

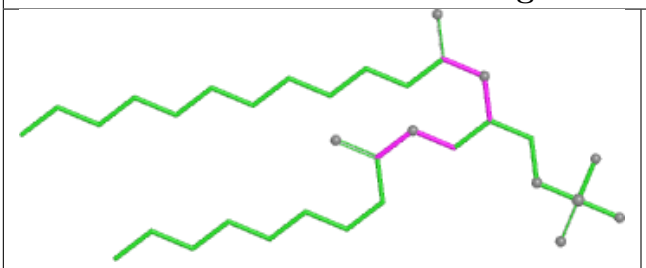


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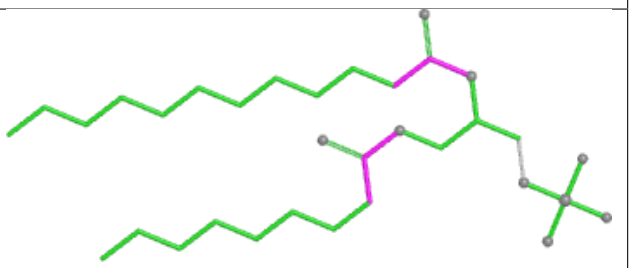


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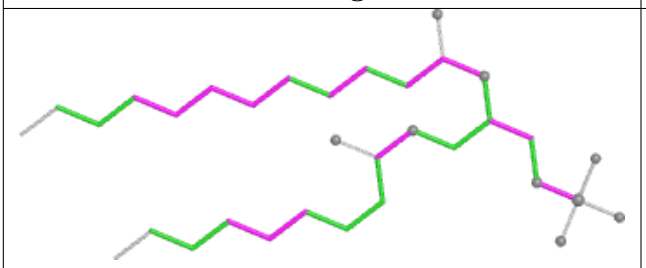
Ligand 3PH A 5007



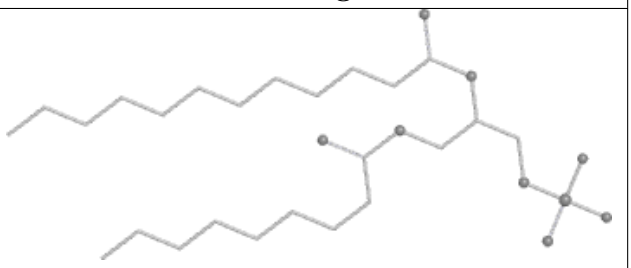
Bond lengths



Bond angles

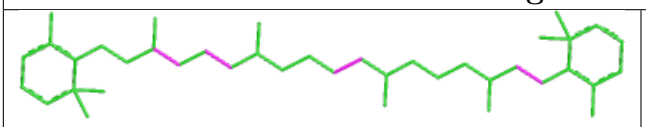


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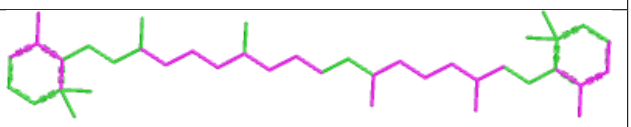


Rings

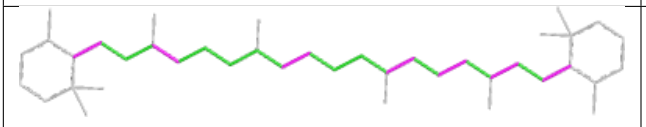
Ligand BCR 5 504



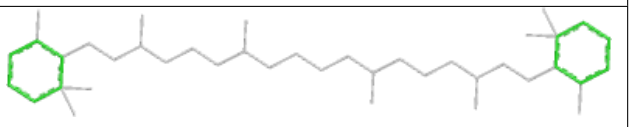
Bond lengths



Bond angles

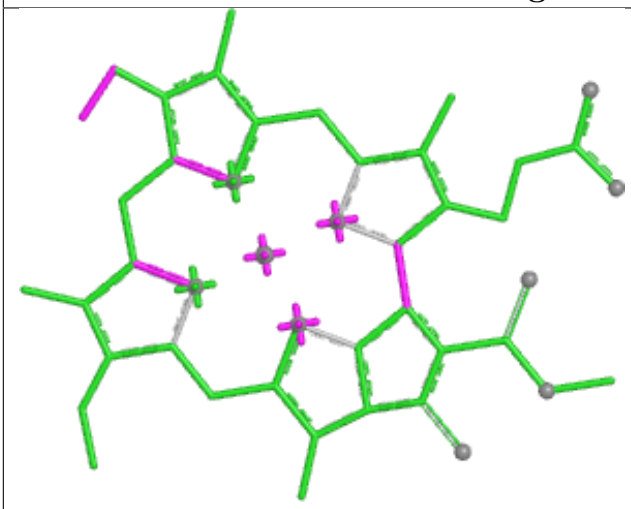


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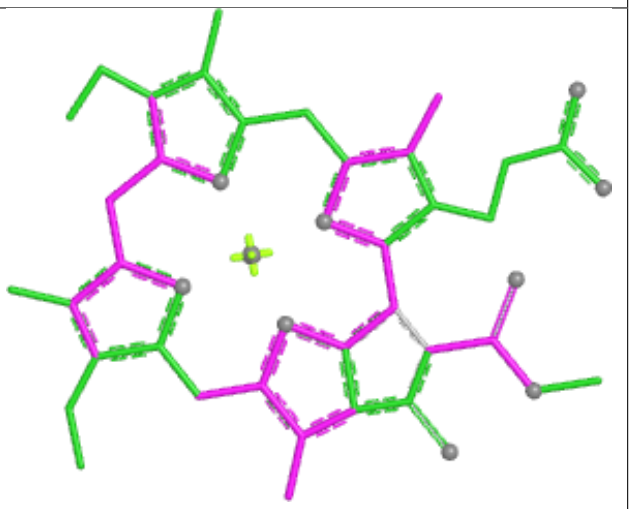


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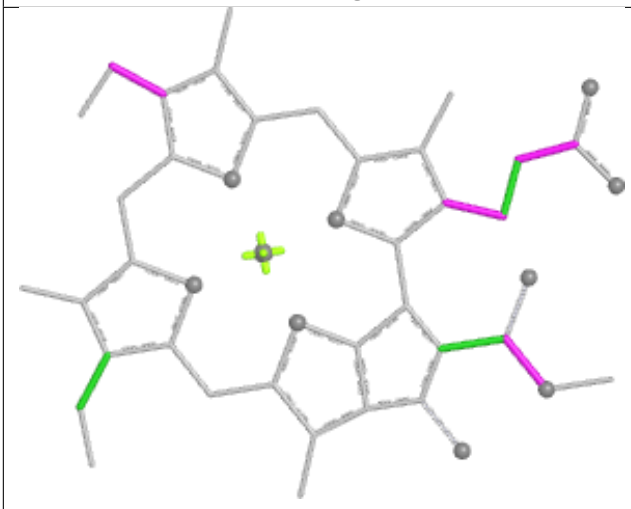
Ligand CLA 4 617



Bond lengths



Bond angles

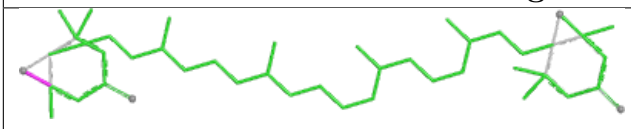


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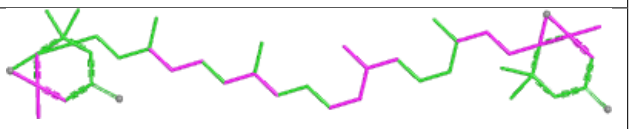


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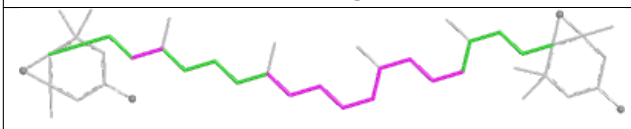
Ligand XAT 9 504



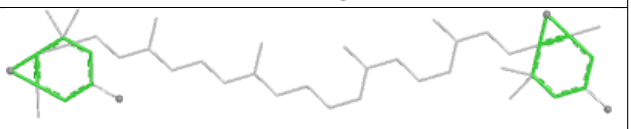
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Bond angles

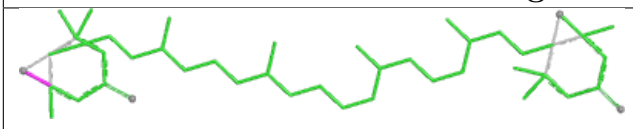


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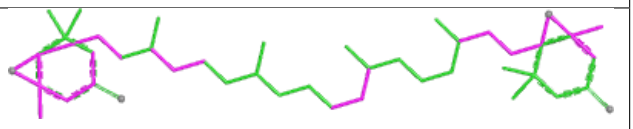


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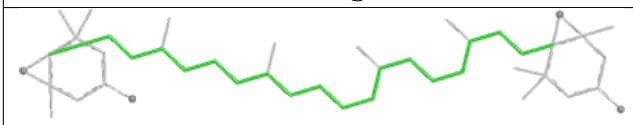
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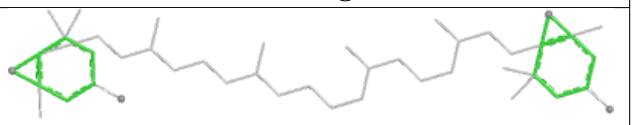
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Bond angles

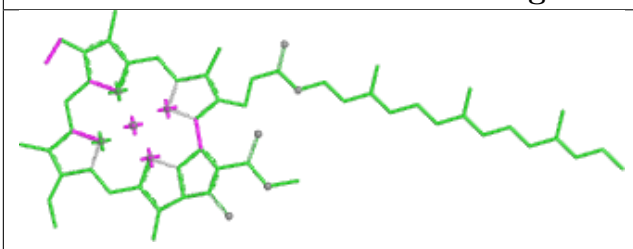


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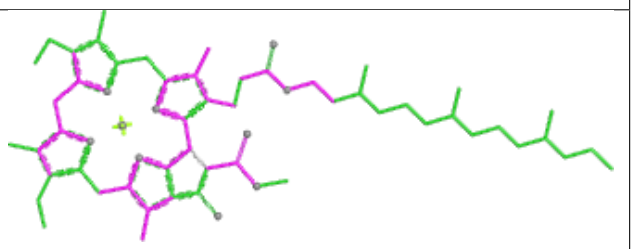


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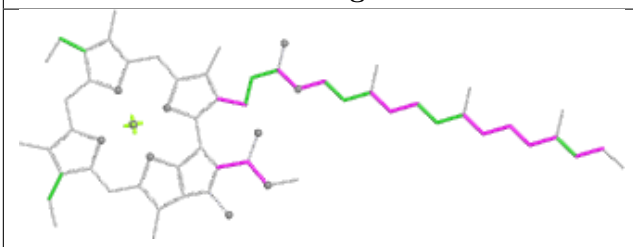
Ligand CLA 4 612



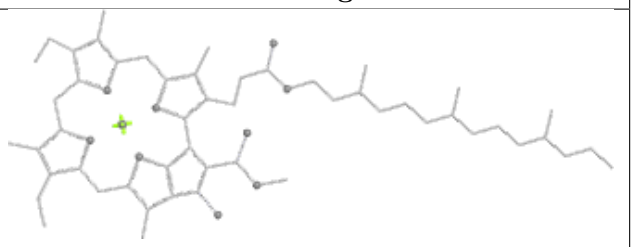
Bond lengths



Bond angles

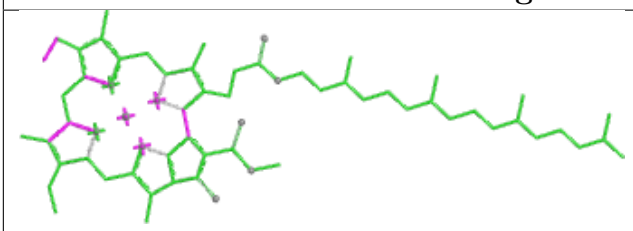


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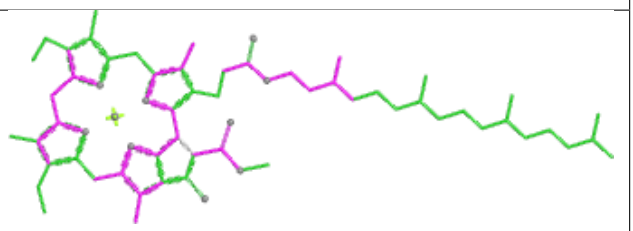


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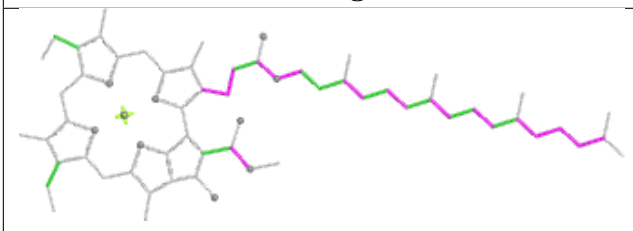
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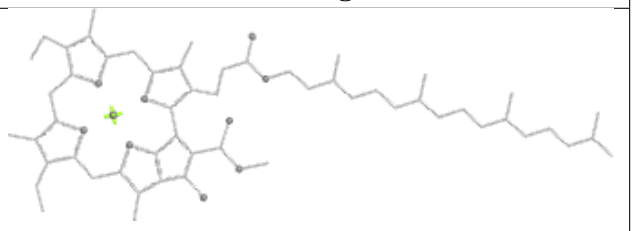
Bond lengths



Bond angles

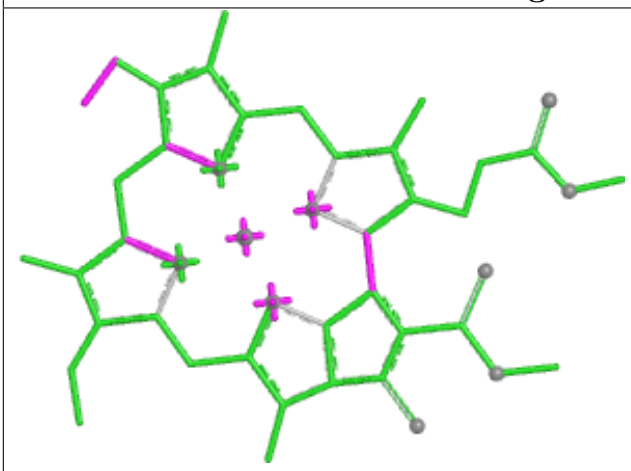


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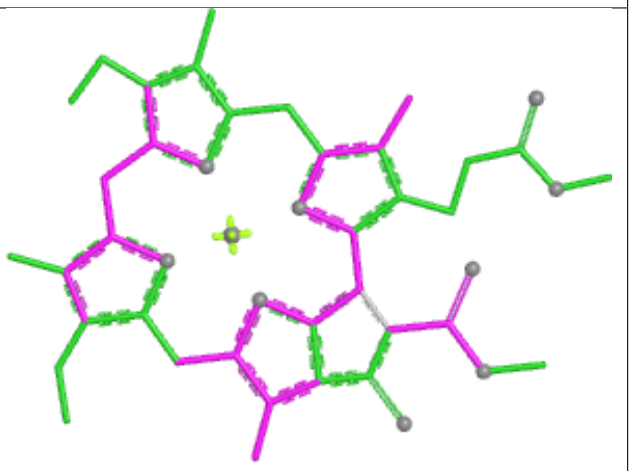


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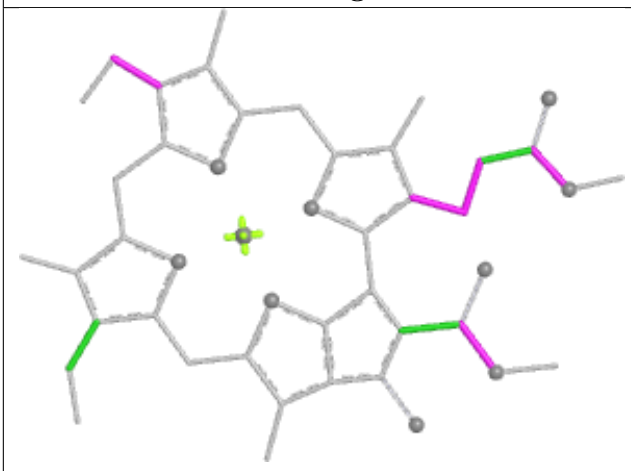
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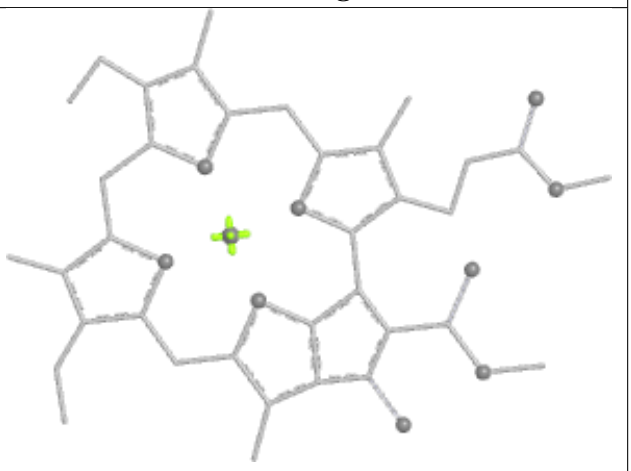
Bond lengths



Bond angles

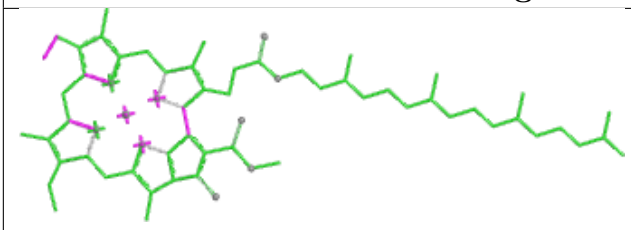


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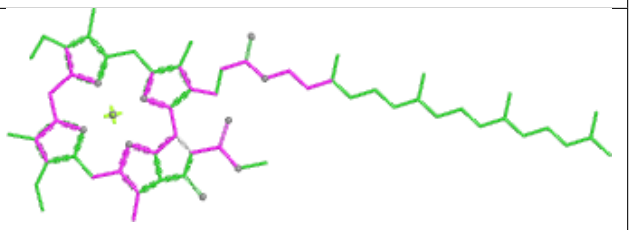


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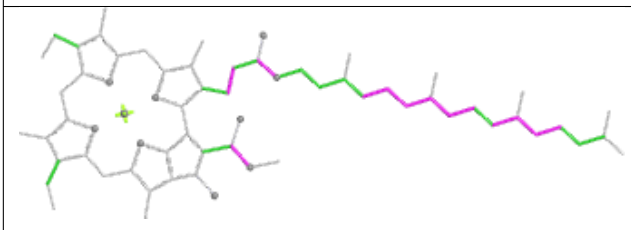
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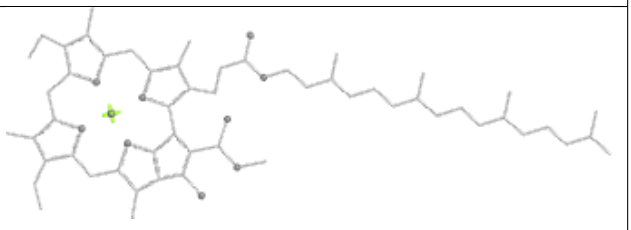
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Bond angles

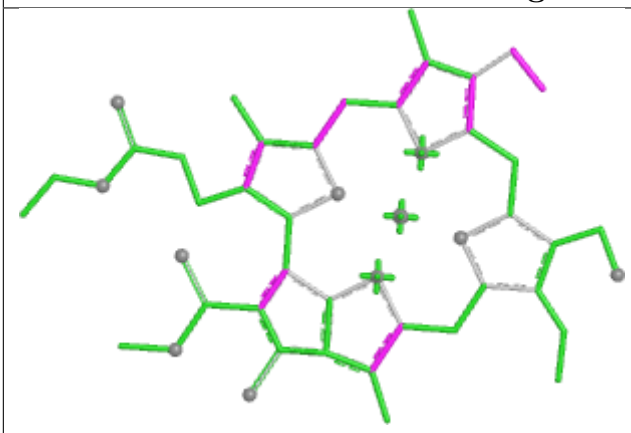


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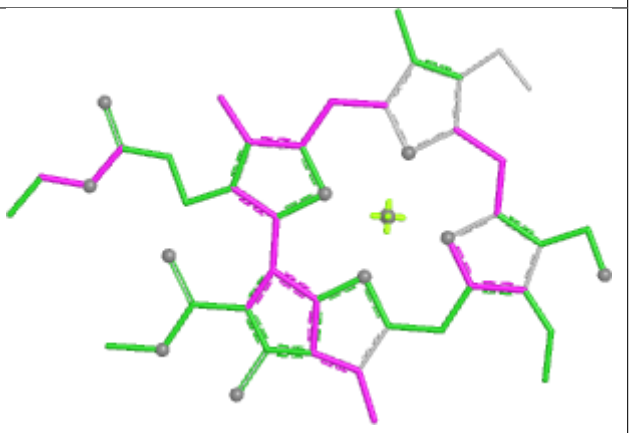


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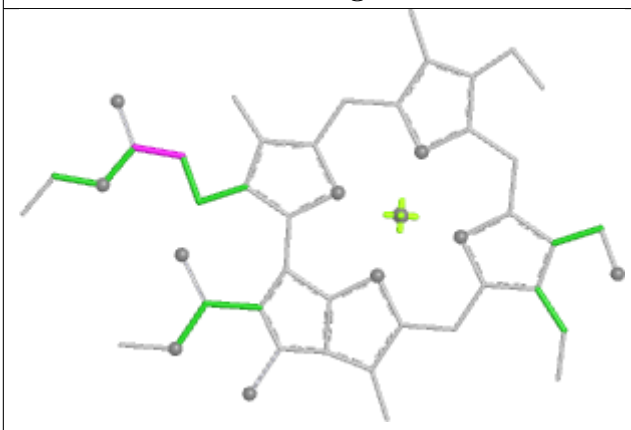
Ligand CHL 1 610



Bond lengths



Bond angles

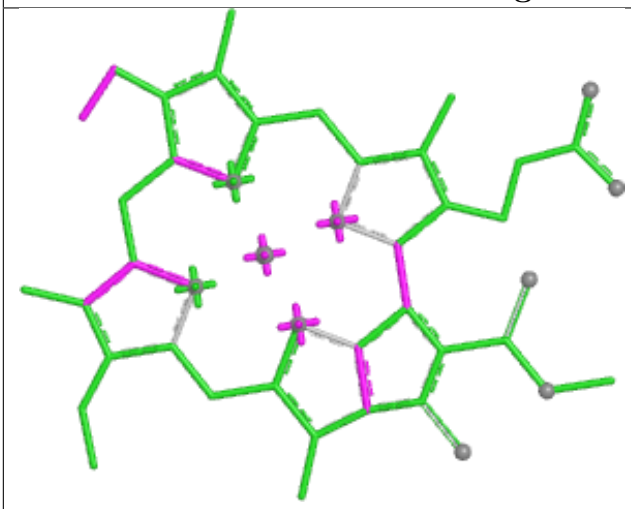


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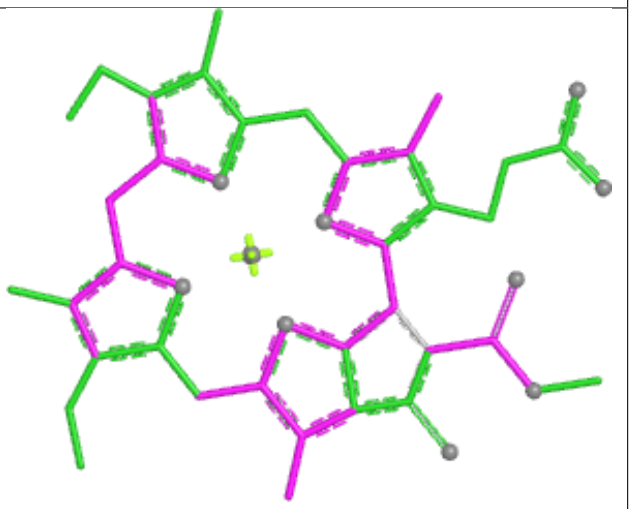


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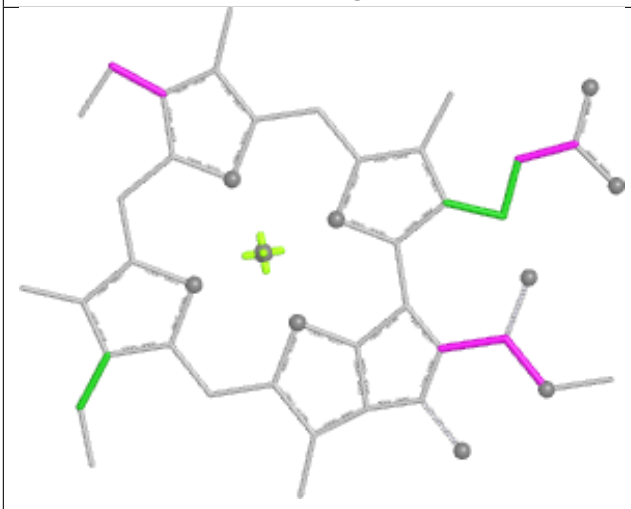
Ligand CLA K 1404



Bond lengths



Bond angles

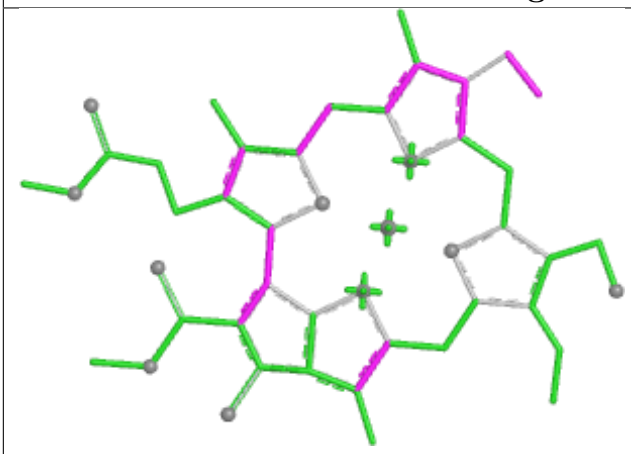


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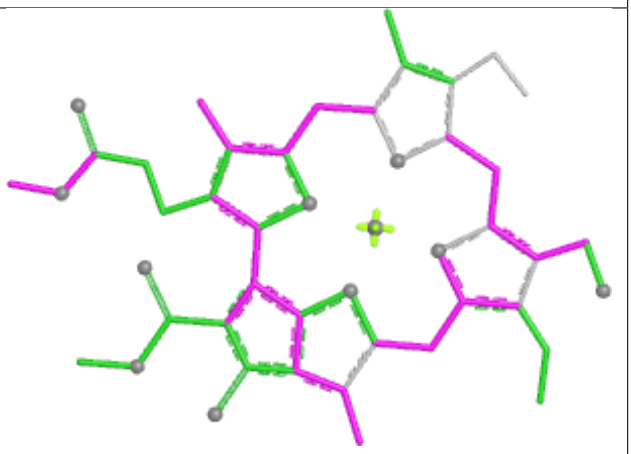


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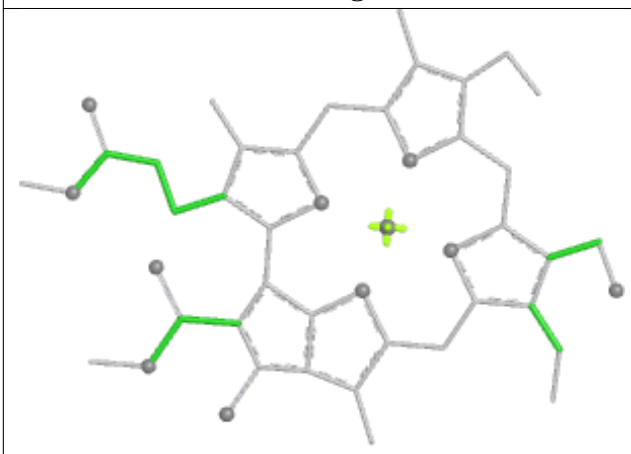
Ligand CHL 5 617



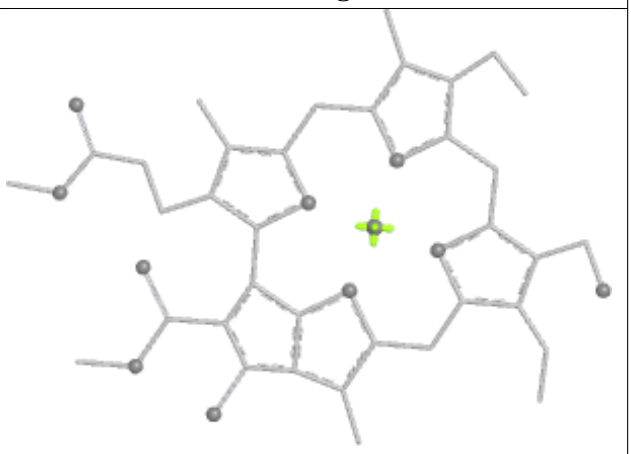
Bond lengths



Bond angles



Torsions

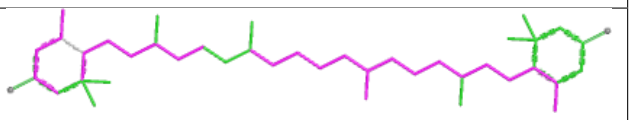


Rings

Ligand LUT 3 501



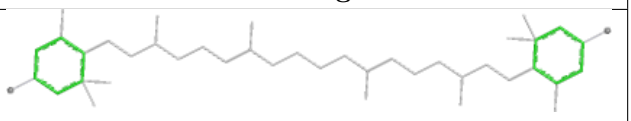
Bond lengths



Bond angles



Torsions



Rings

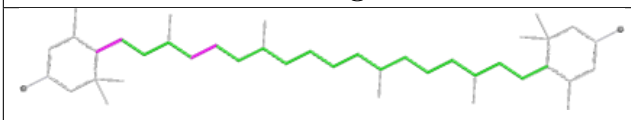
Ligand LUT a 502



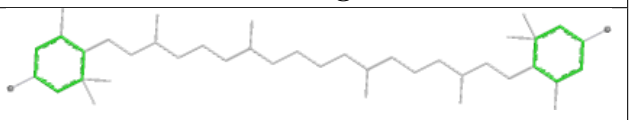
Bond lengths



Bond angles

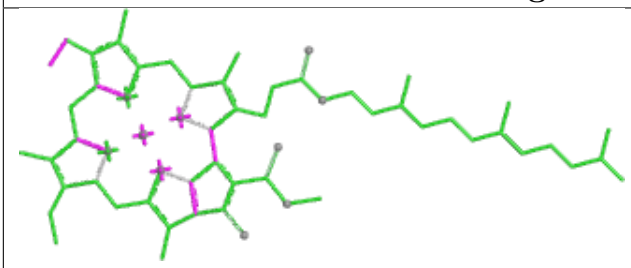


Torsions

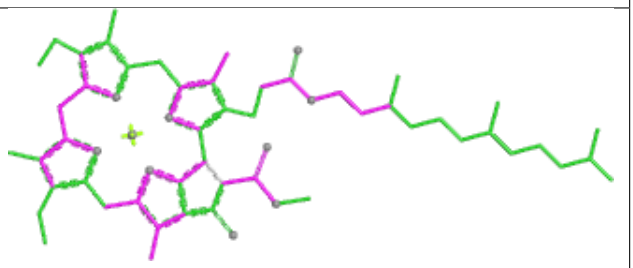


Rings

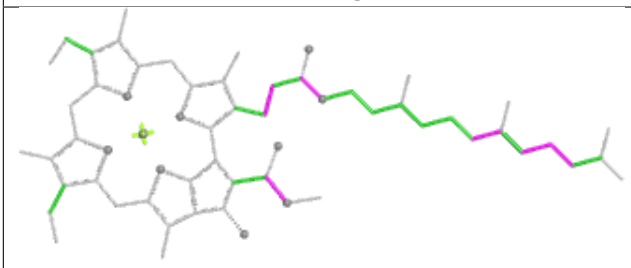
Ligand CLA 4 604



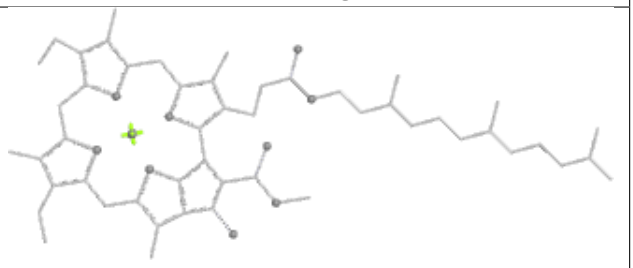
Bond lengths



Bond angles

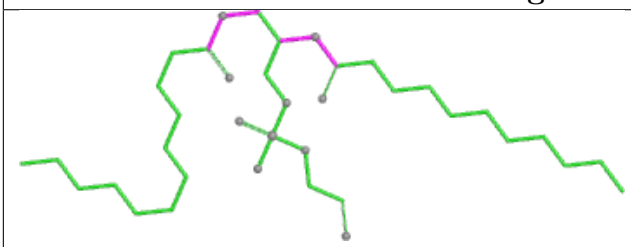


Torsions

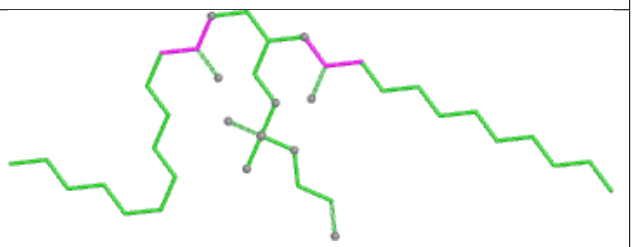


Rings

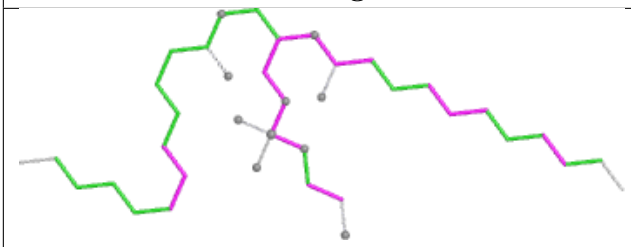
Ligand PTY 3 802



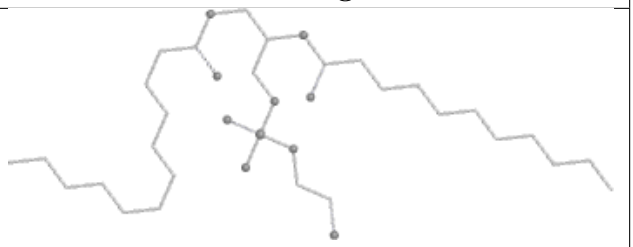
Bond lengths



Bond angles

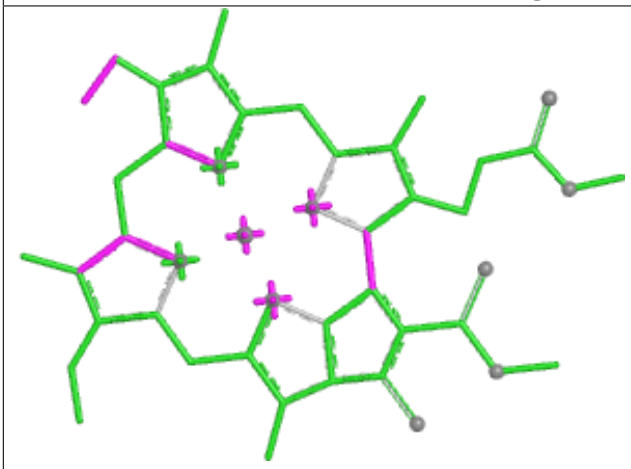


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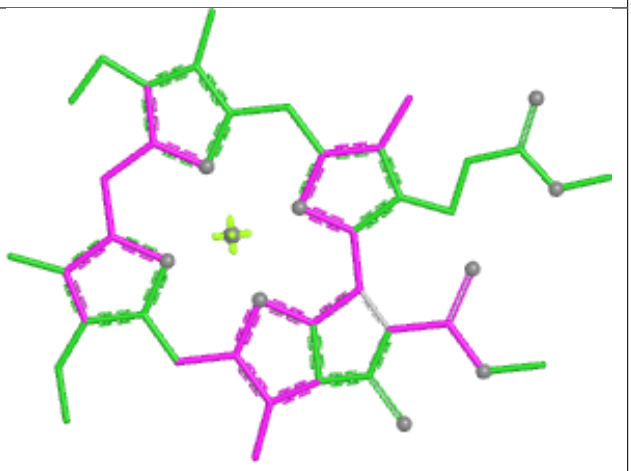


Rings

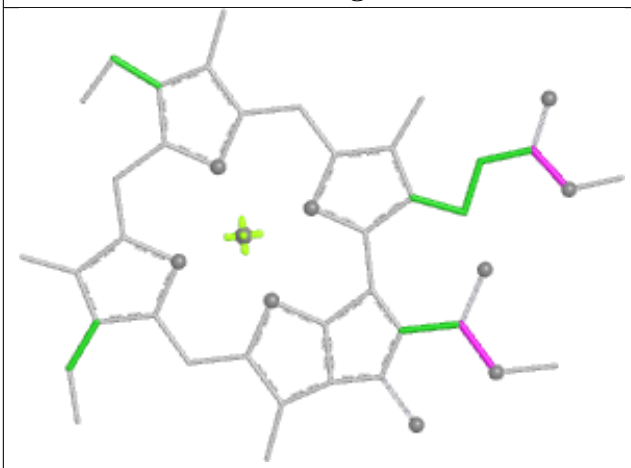
Ligand CLA 9 602



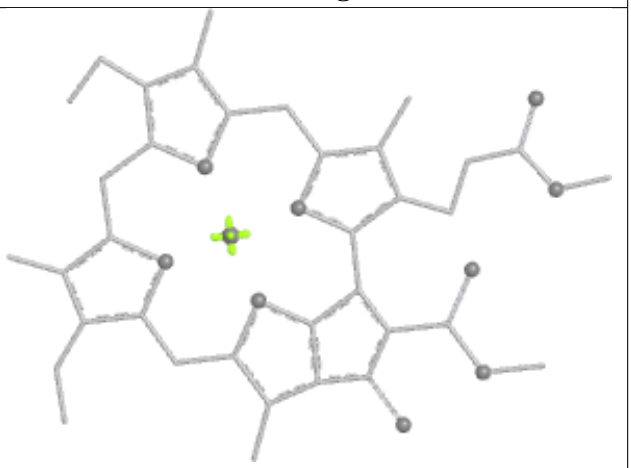
Bond lengths



Bond angles

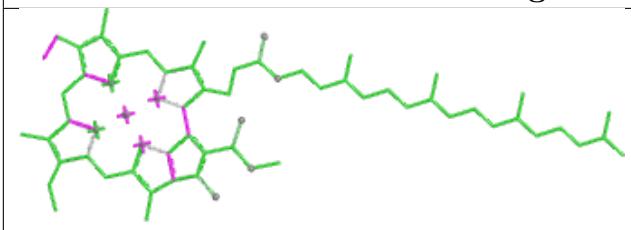


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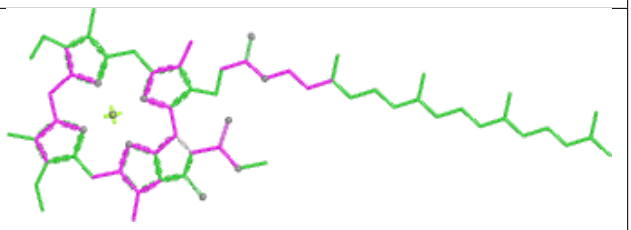


Rings

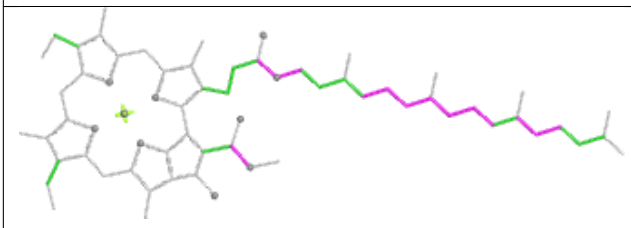
Ligand CLA 3 607



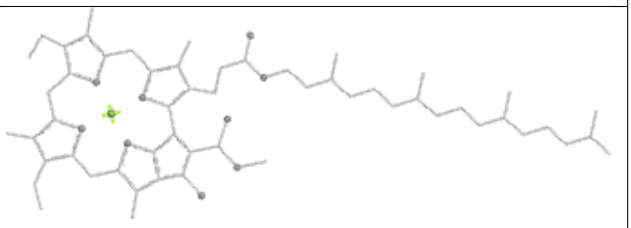
Bond lengths



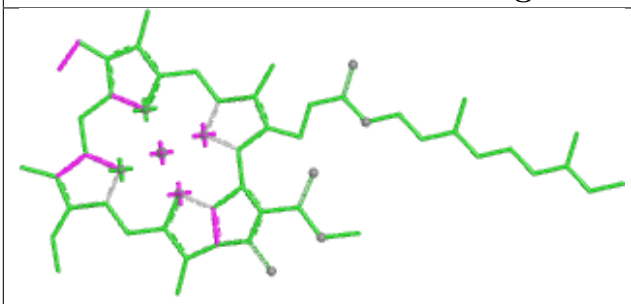
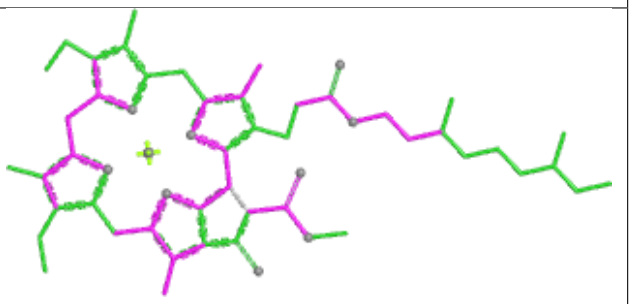
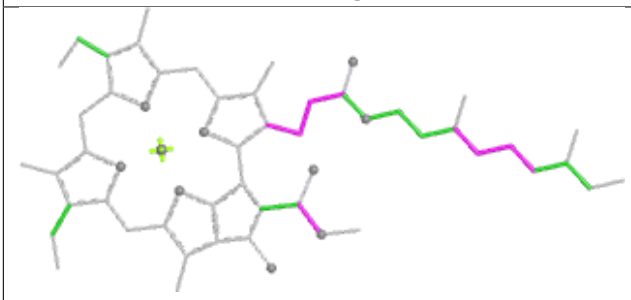
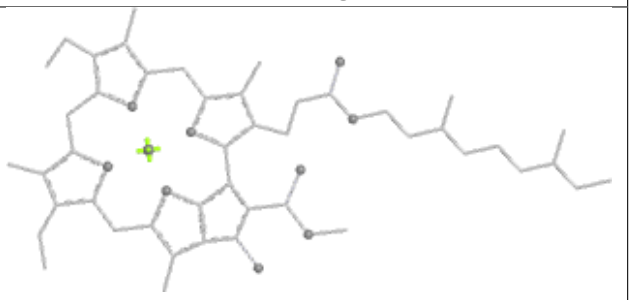
Bond angles

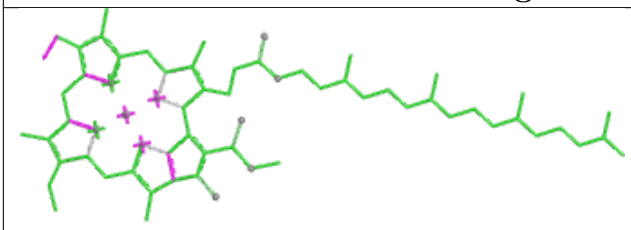
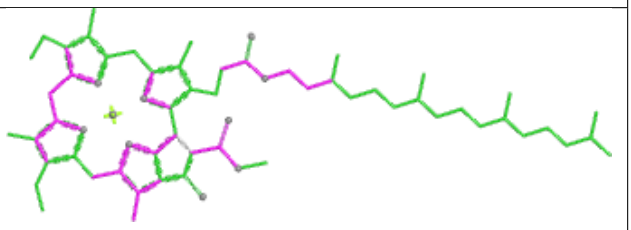
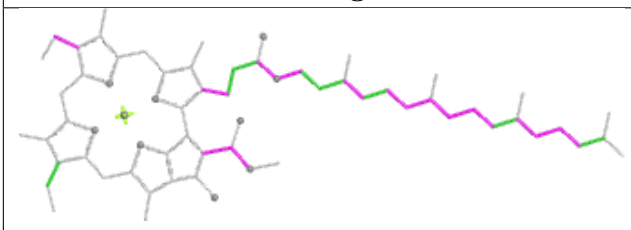
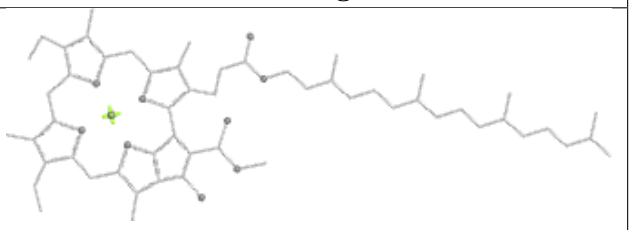


Torsions

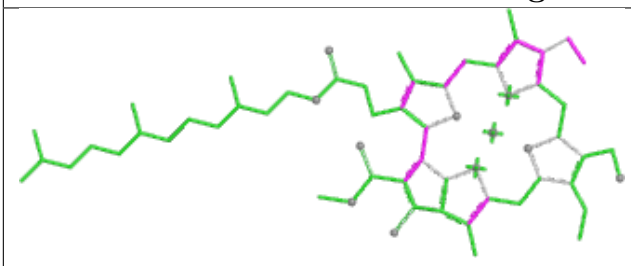


Rings

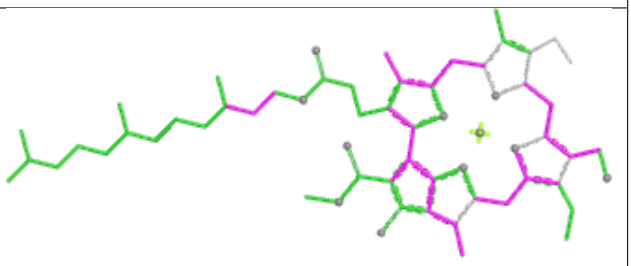
Ligand CLA A 1130	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1133	
	
Bond lengths	Bond angles
	
Torsions	Rings

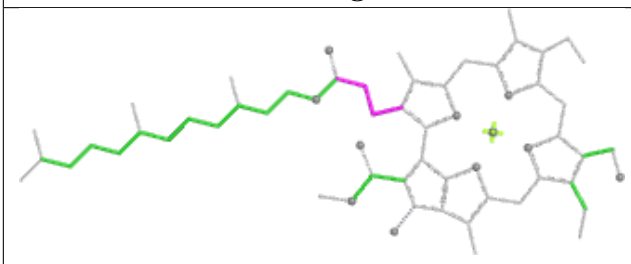
Ligand CHL a 604



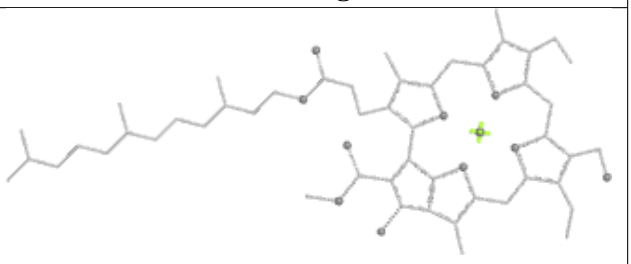
Bond lengths



Bond angles

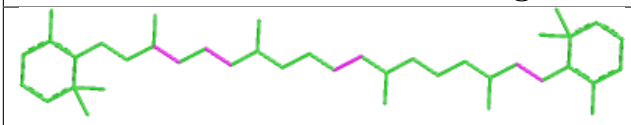


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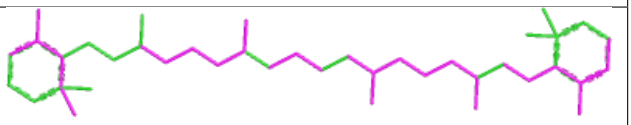


Rings

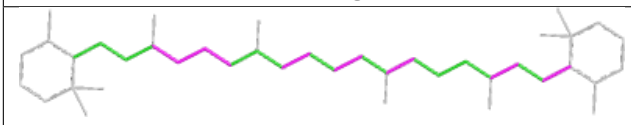
Ligand BCR A 4003



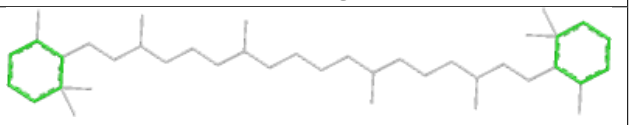
Bond lengths



Bond angles

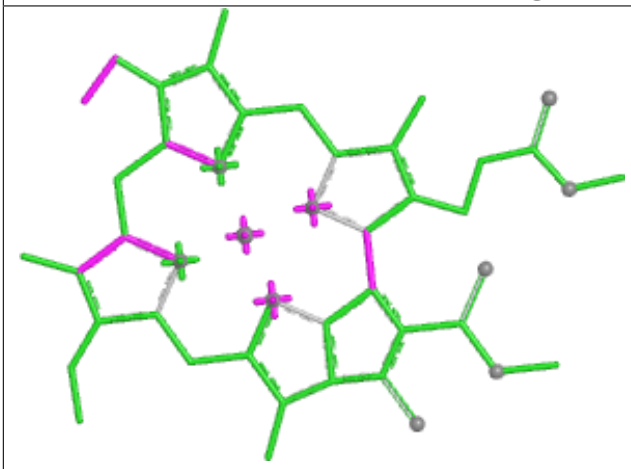


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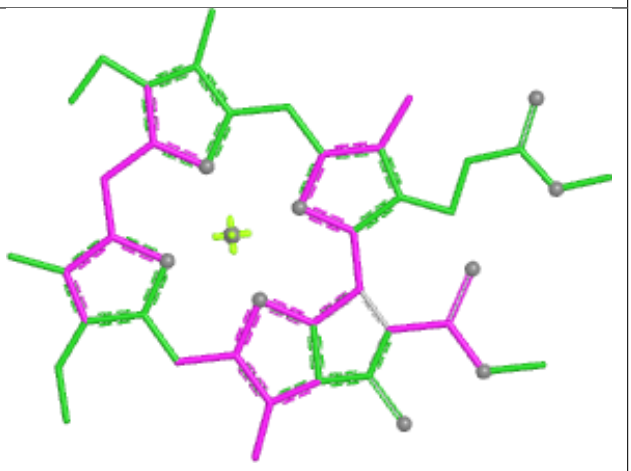


Rings

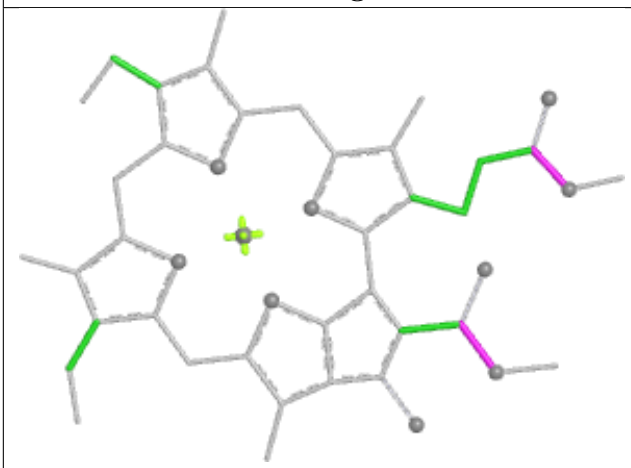
Ligand CLA 3 618



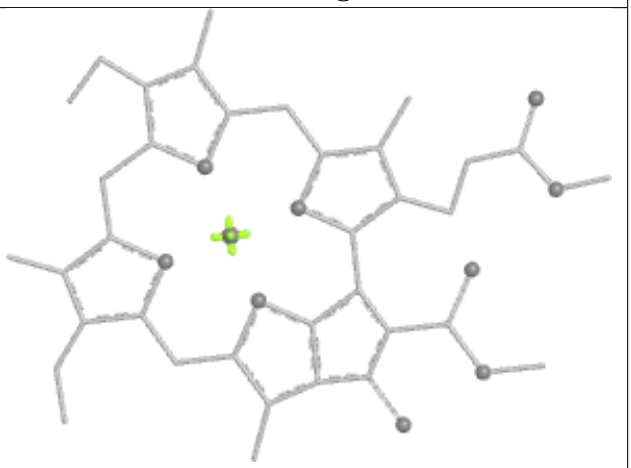
Bond lengths



Bond angles

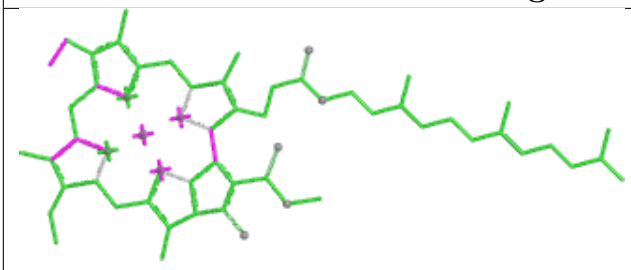


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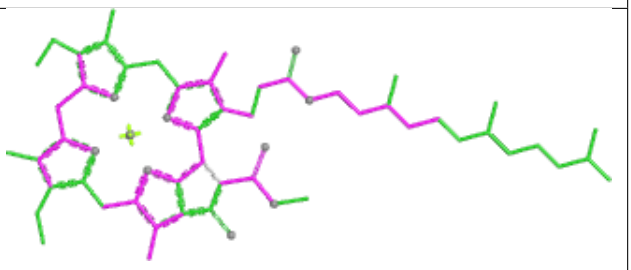


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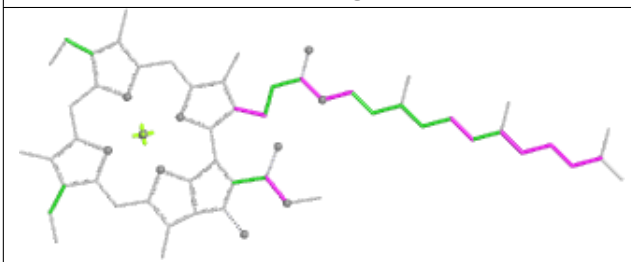
Ligand CLA 5 601



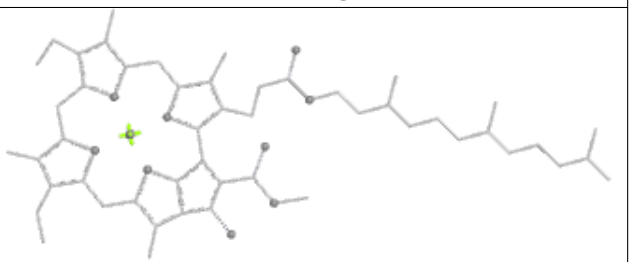
Bond lengths



Bond angles

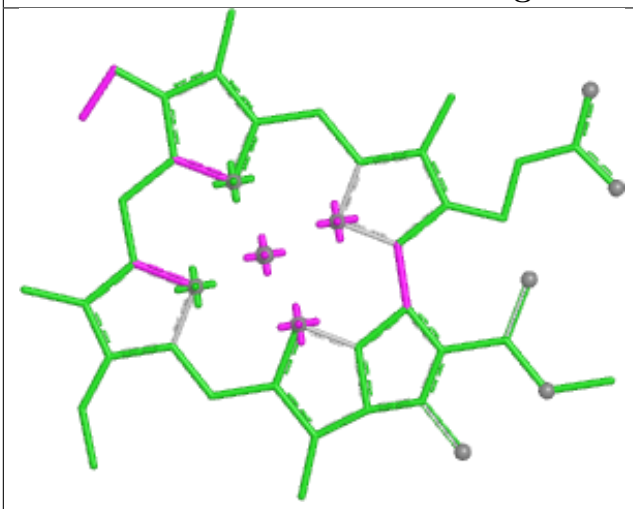


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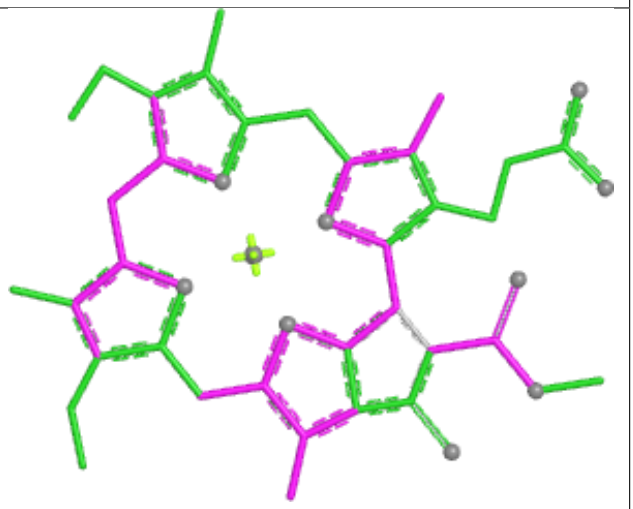


Rings

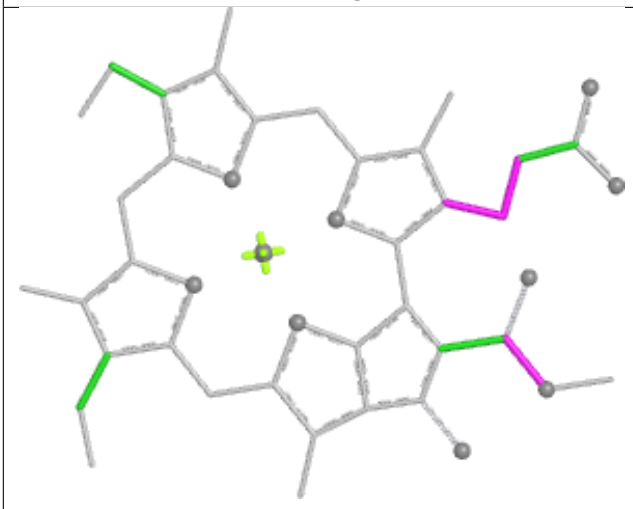
Ligand CLA G 1603



Bond lengths



Bond angles

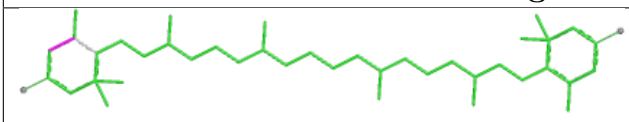


Torsions

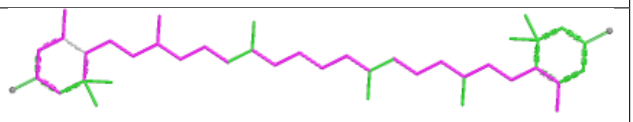


Rings

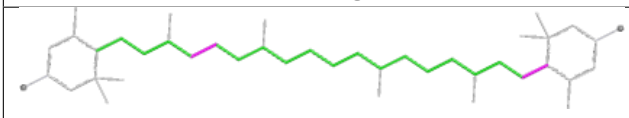
Ligand LUT 1 501



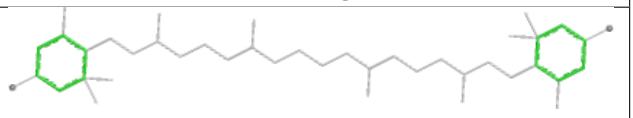
Bond lengths



Bond angles

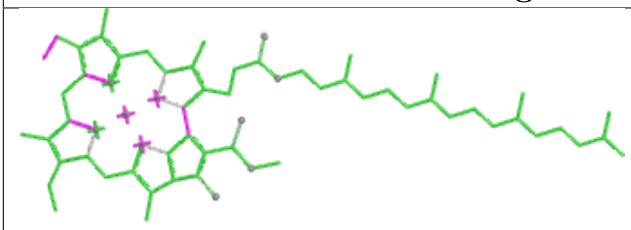


Torsions

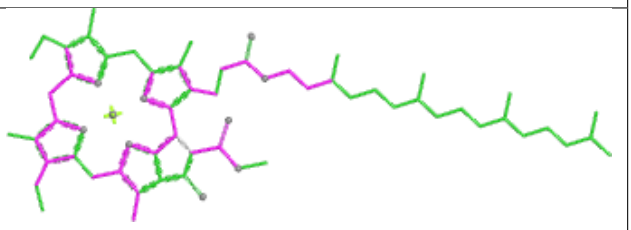


Rings

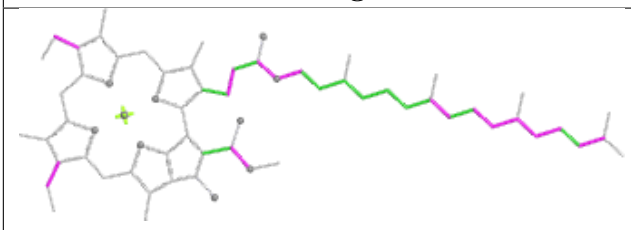
Ligand CLA B 1023



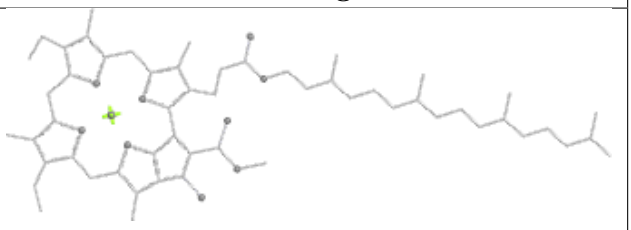
Bond lengths



Bond angles

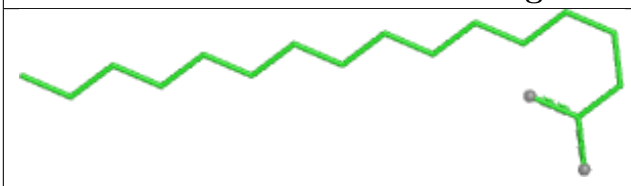


Torsions

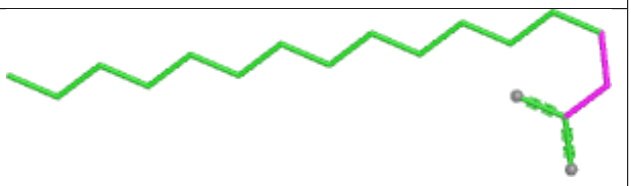


Rings

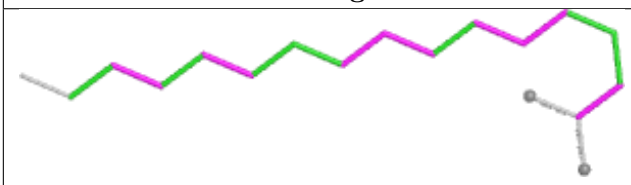
Ligand PLM 6 804



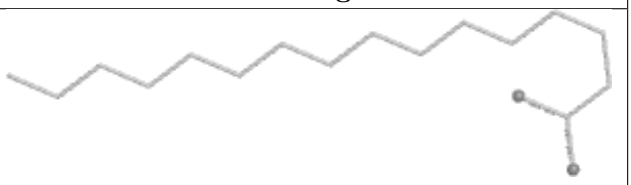
Bond lengths



Bond angles

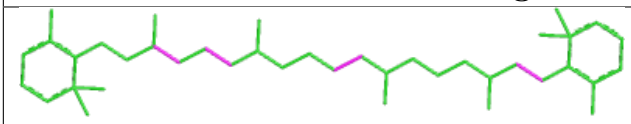


Torsions

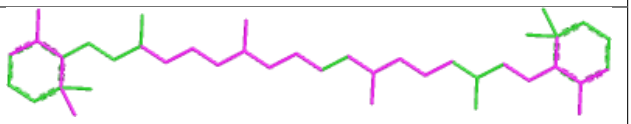


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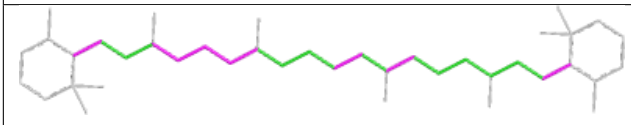
Ligand BCR A 4001



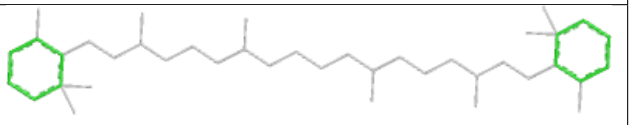
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Bond angles

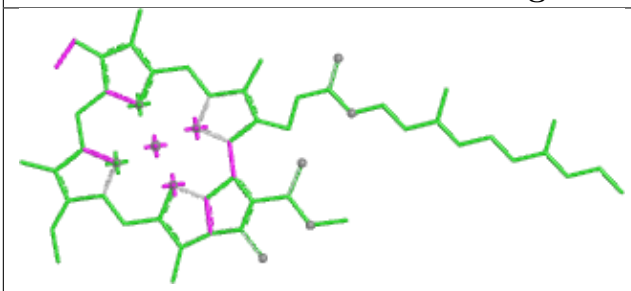


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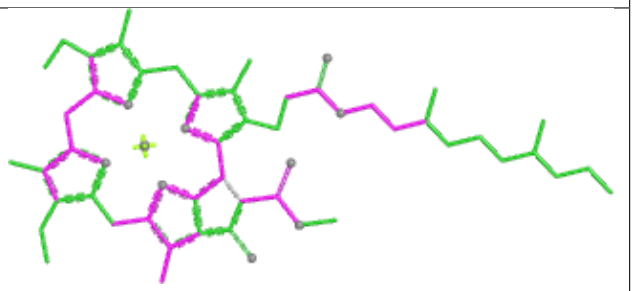


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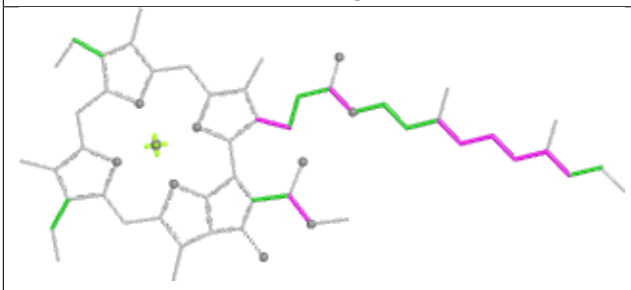
Ligand CLA 8 606



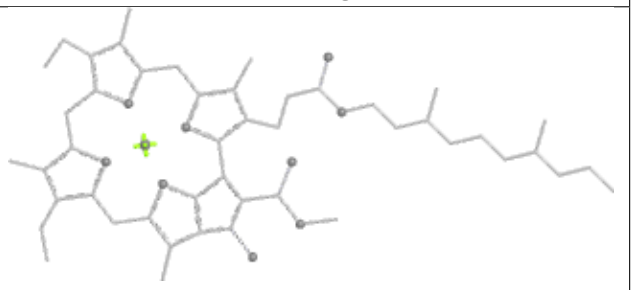
Bond lengths



Bond angles



Torsions

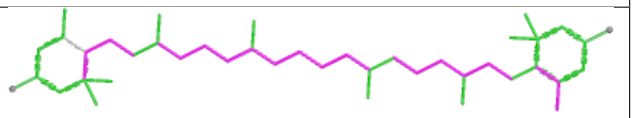


Rings

Ligand LUT 4 502



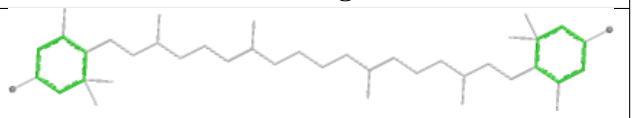
Bond lengths



Bond angles

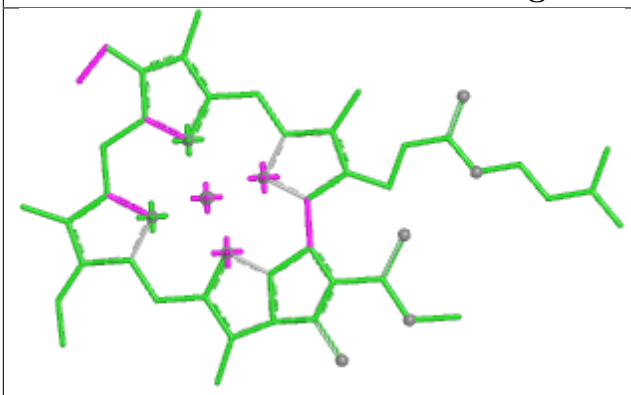


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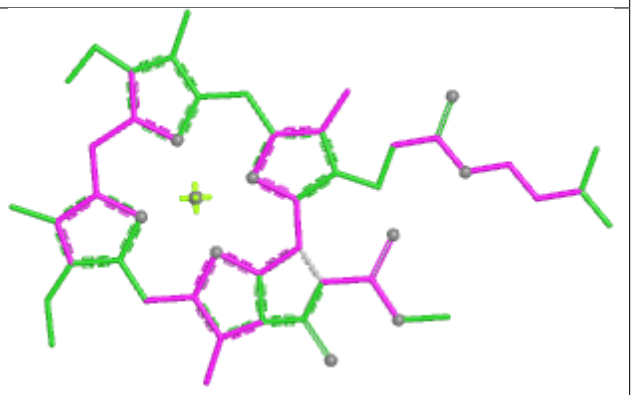


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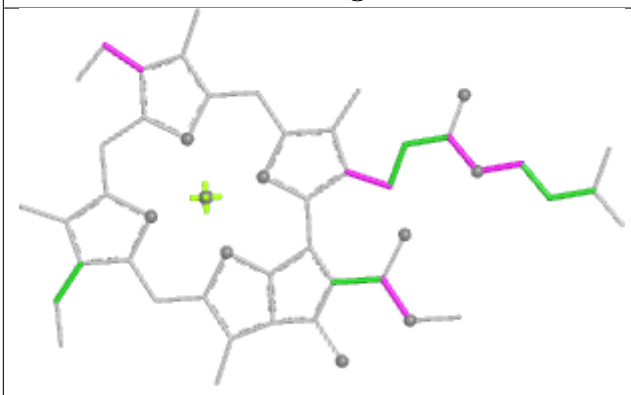
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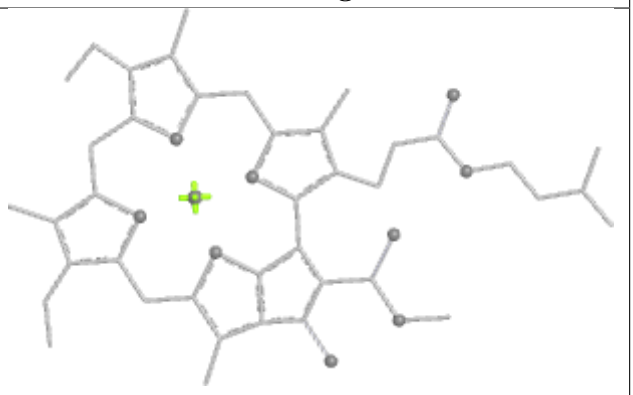
Bond lengths



Bond angles

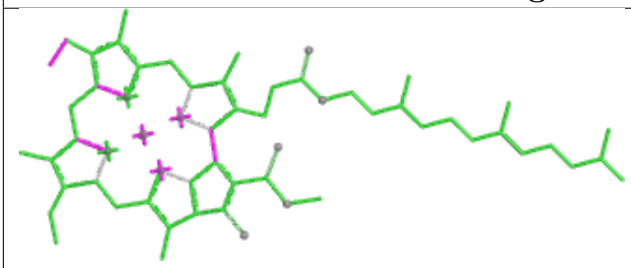


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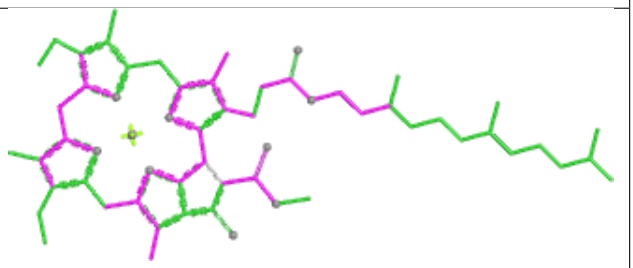


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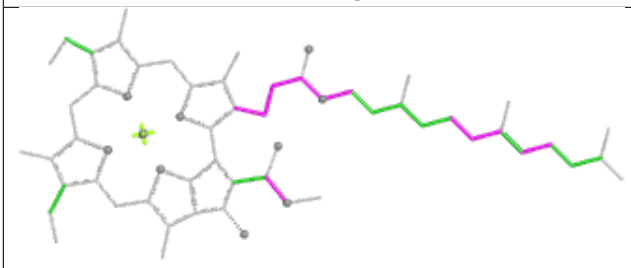
Ligand CLA 7 612



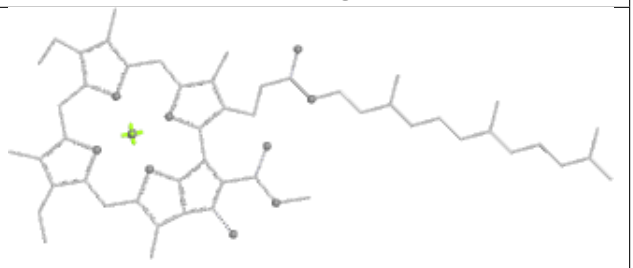
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Bond angles

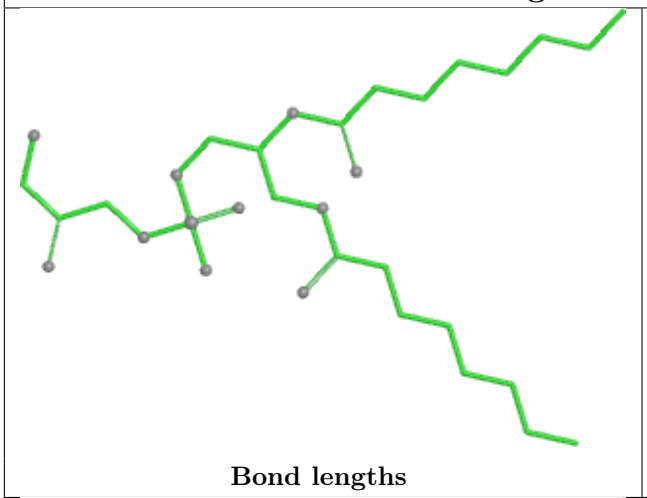


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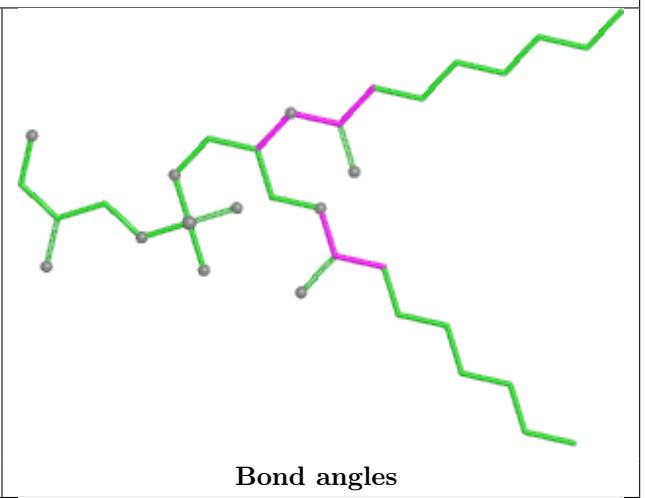


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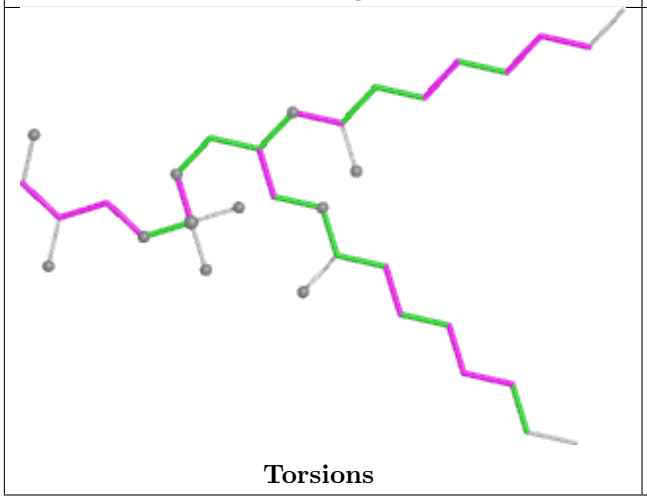
Ligand LHG 9 801



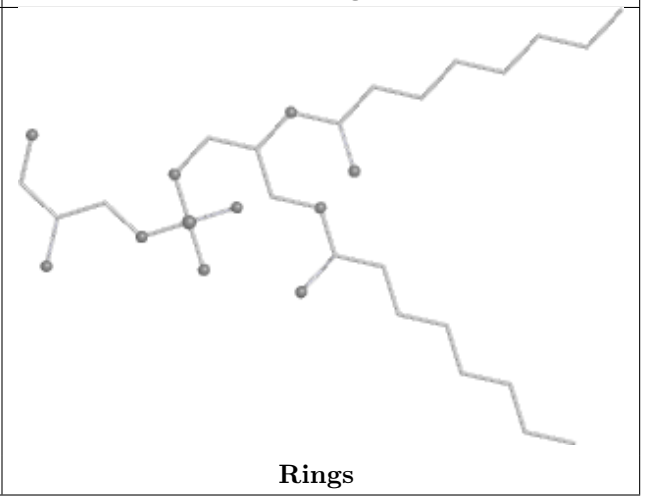
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Bond angles

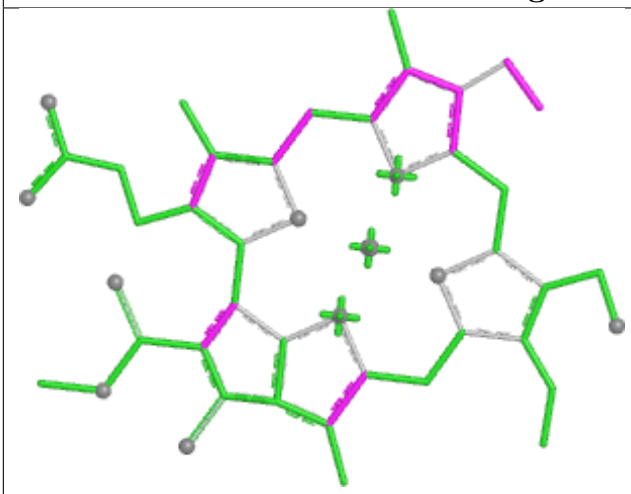


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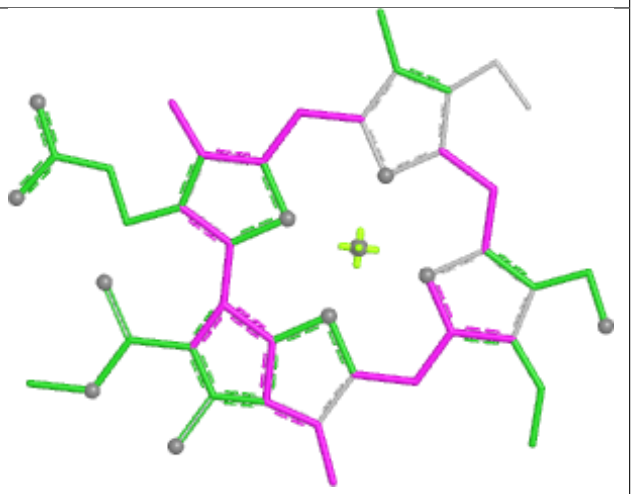


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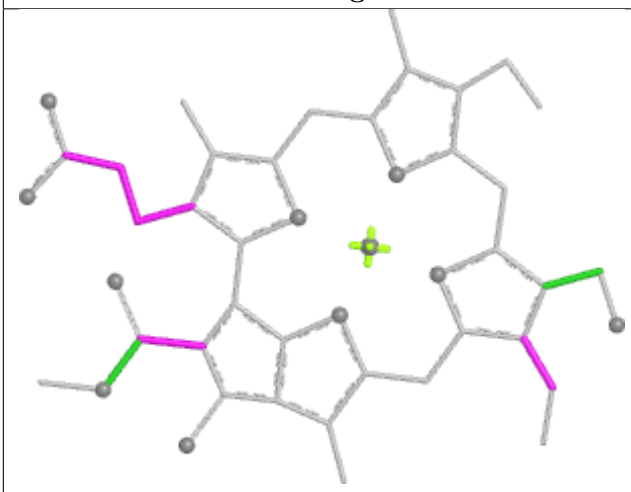
Ligand CHL a 613



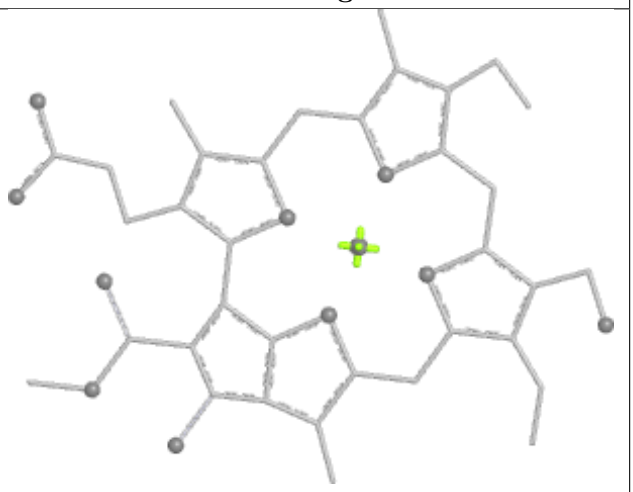
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Bond angles

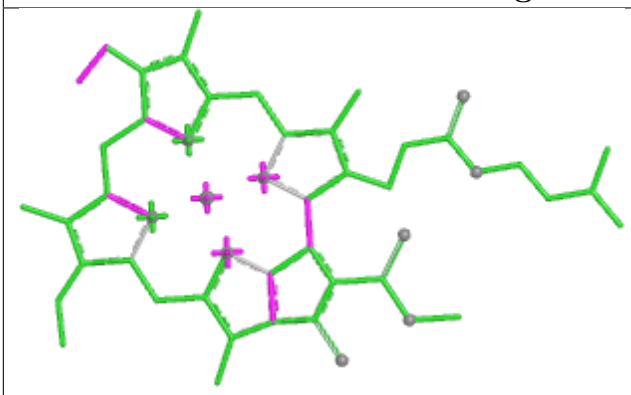


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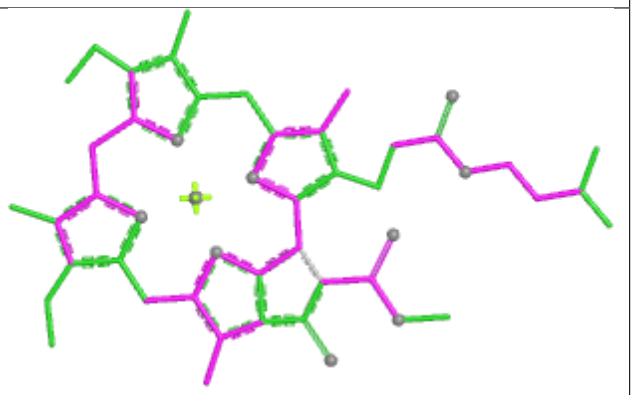


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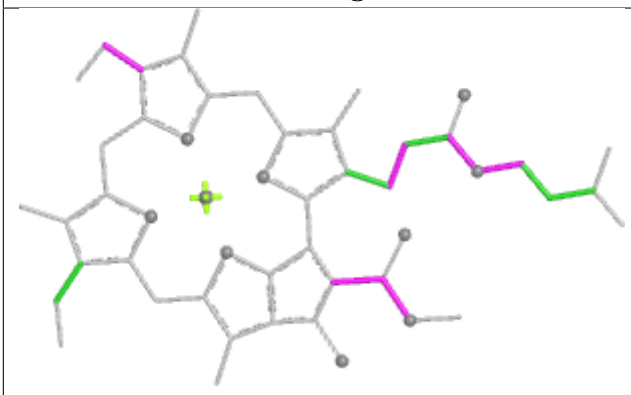
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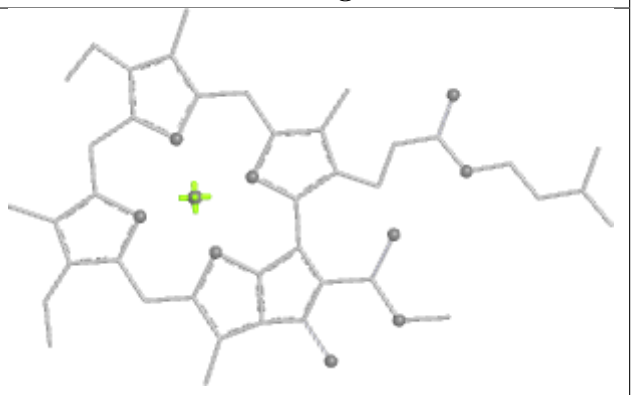
Bond lengths



Bond angles

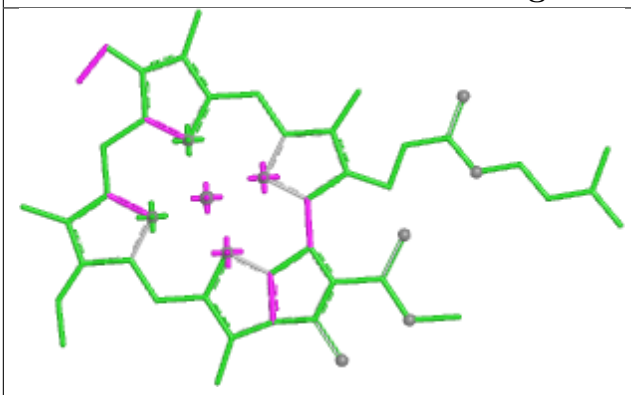


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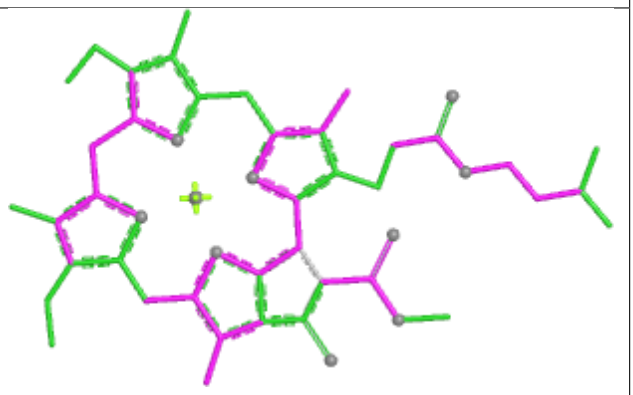


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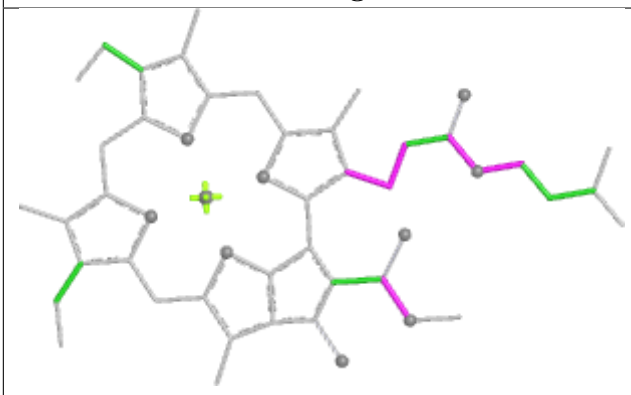
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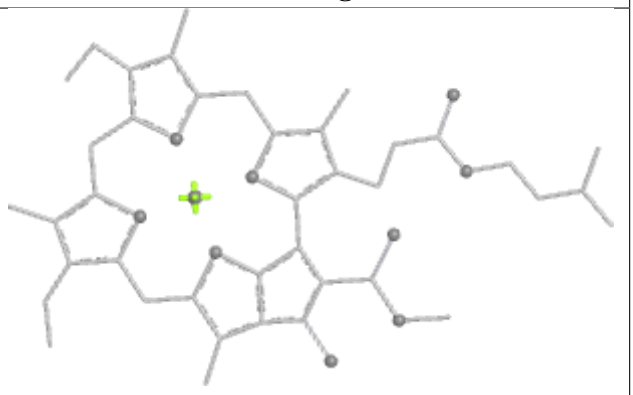
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Bond angles

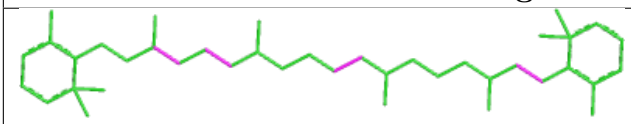


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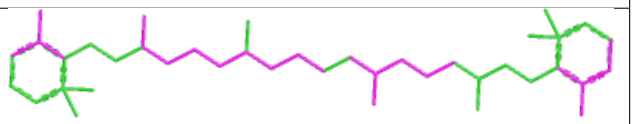


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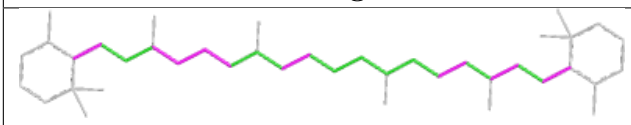
Ligand BCR L 4001



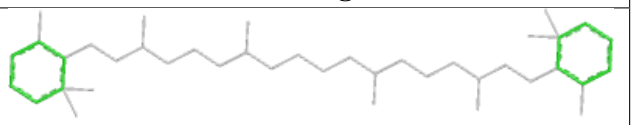
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Bond angles

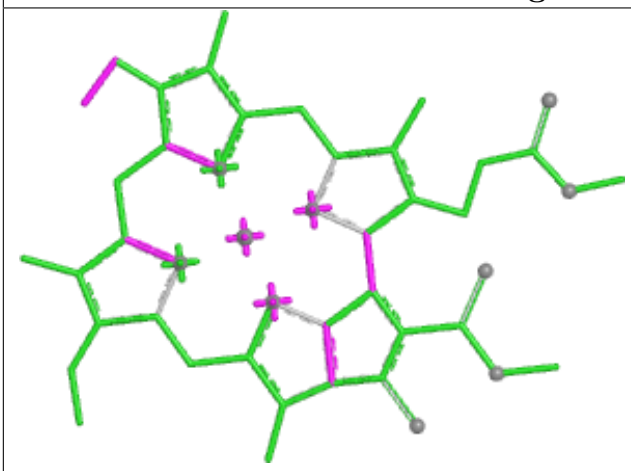


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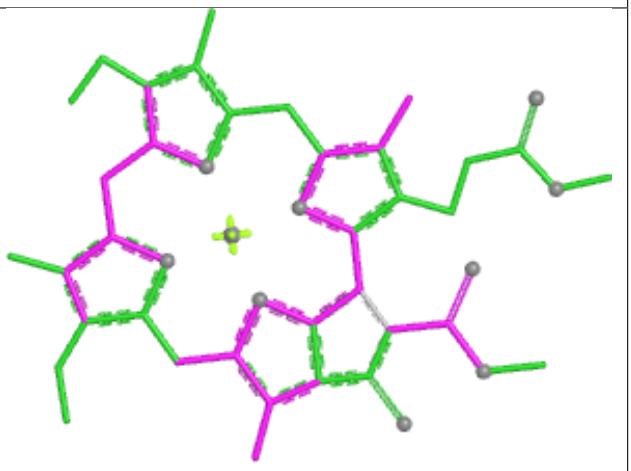


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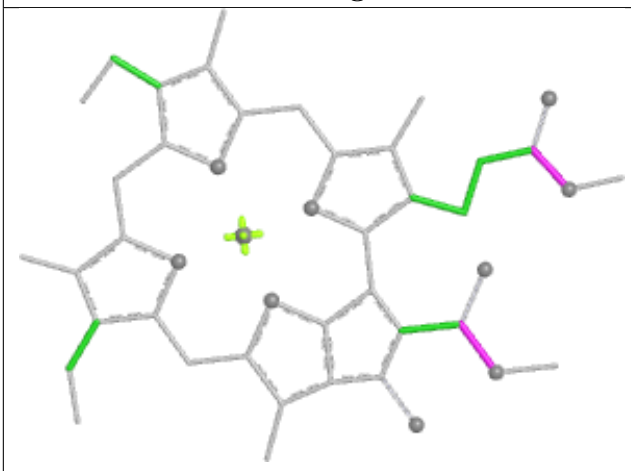
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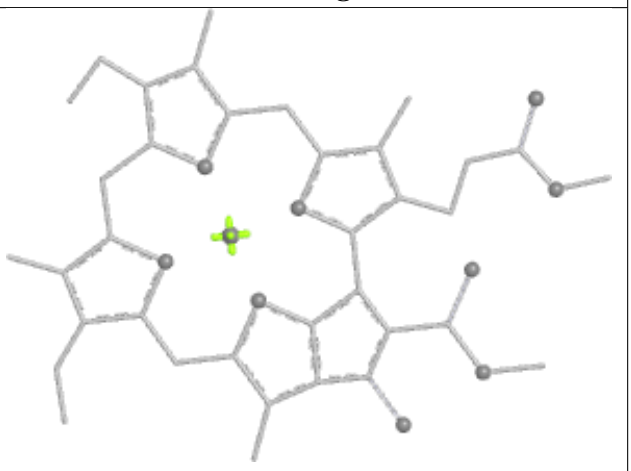
Bond lengths



Bond angles

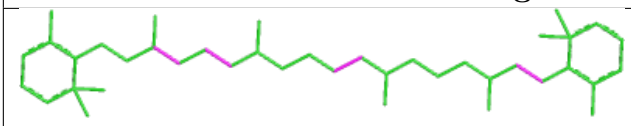


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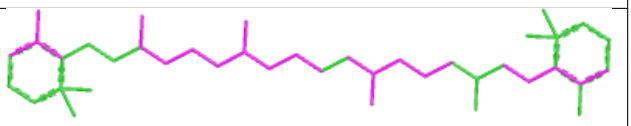


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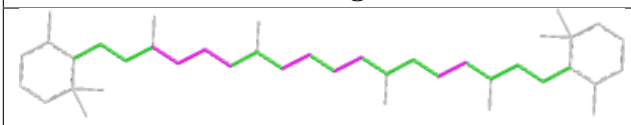
Ligand BCR B 4007



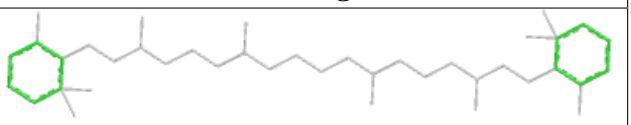
Bond lengths



Bond angles

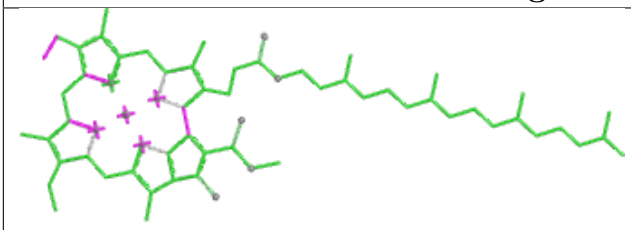


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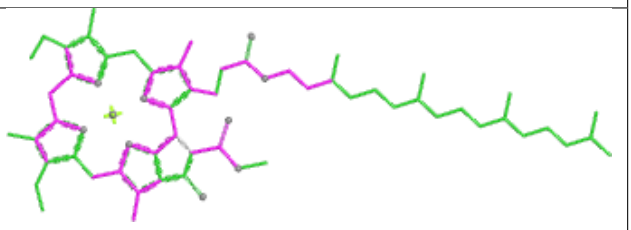


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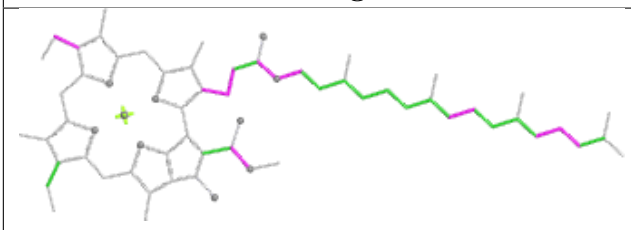
Ligand CLA 9 612



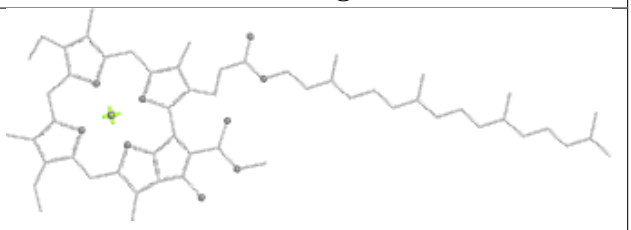
Bond lengths



Bond angles

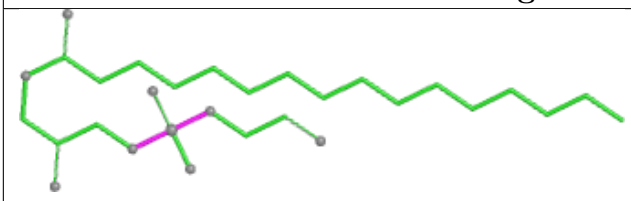


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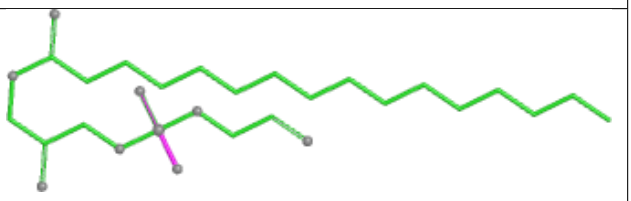


Rings

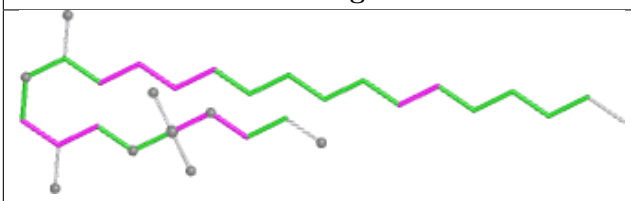
Ligand LPX F 5003



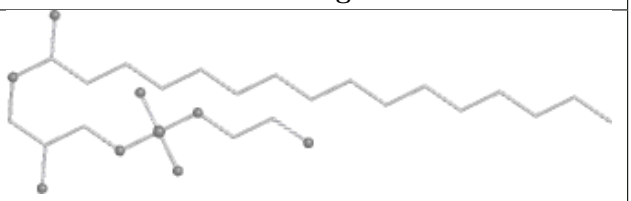
Bond lengths



Bond angles

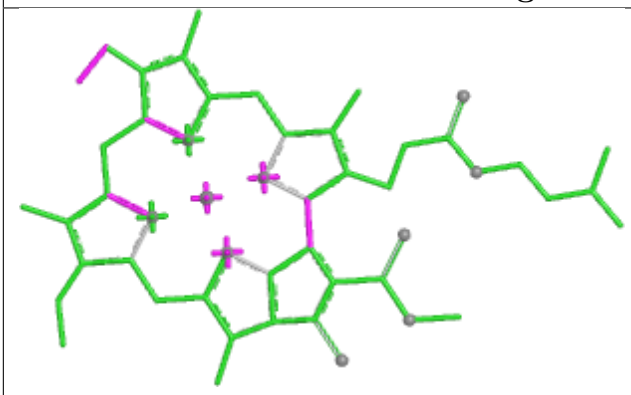


Torsions

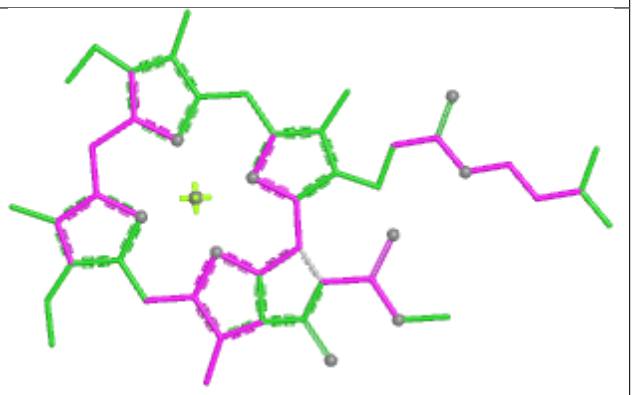


Rings

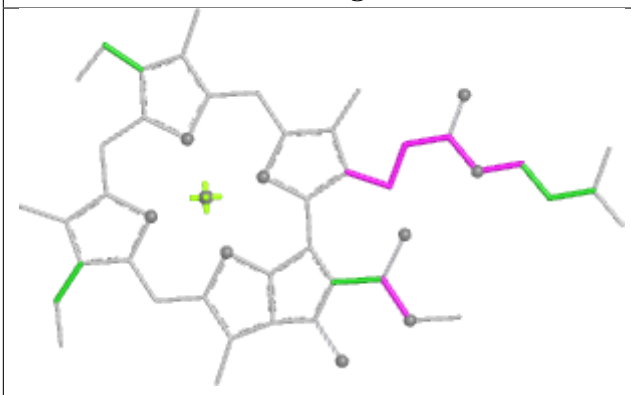
Ligand CLA F 1301



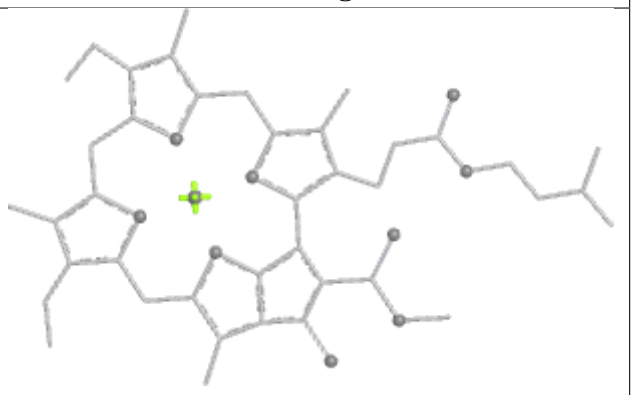
Bond lengths



Bond angles

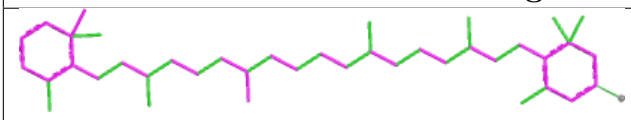


Torsions

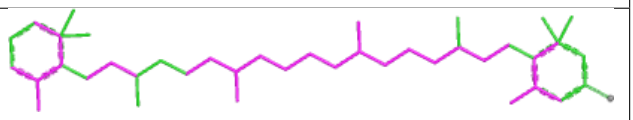


Rings

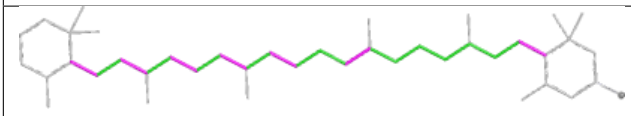
Ligand RRX 3 506



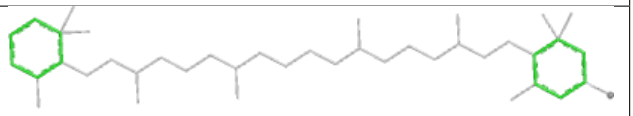
Bond lengths



Bond angles

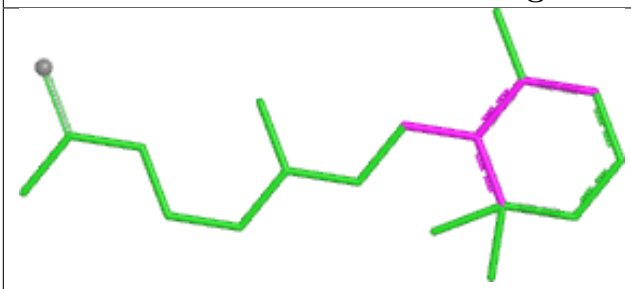


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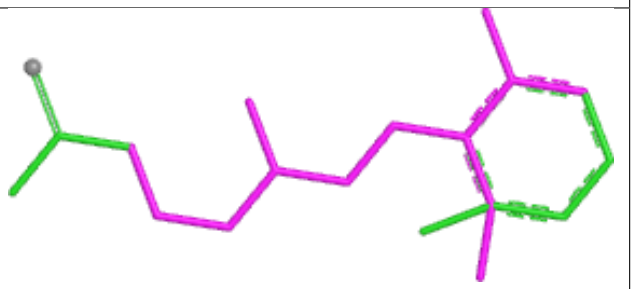


Rings

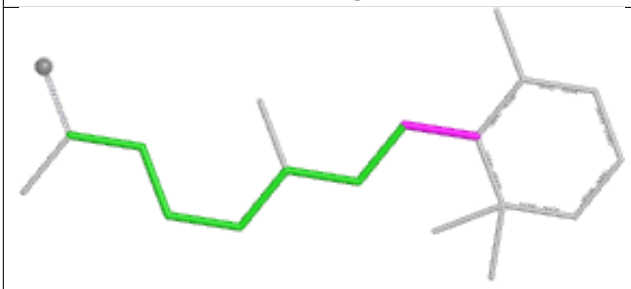
Ligand QTB a 504



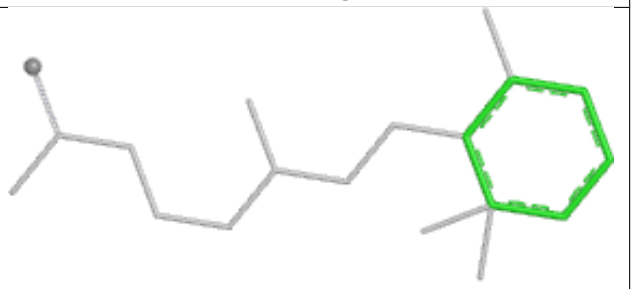
Bond lengths



Bond angles

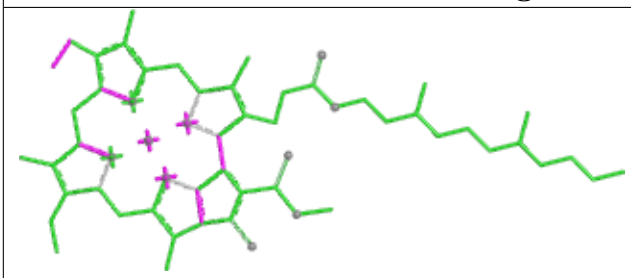


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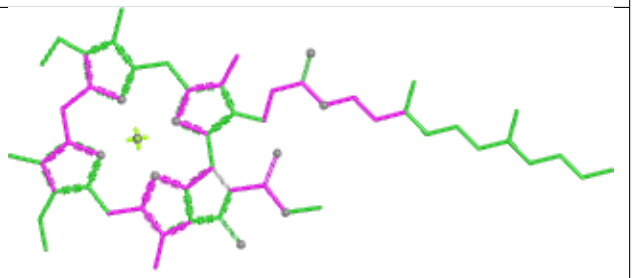


Rings

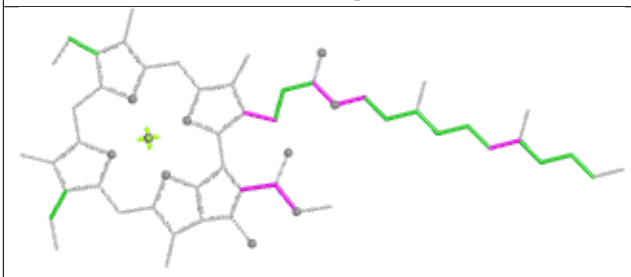
Ligand CLA B 1230



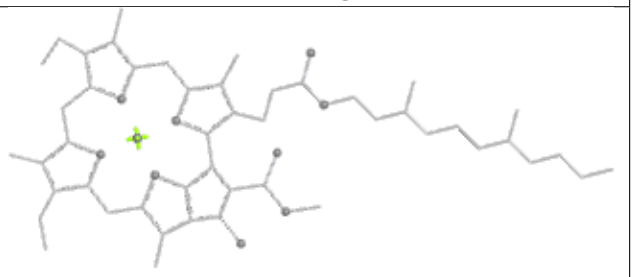
Bond lengths



Bond angles

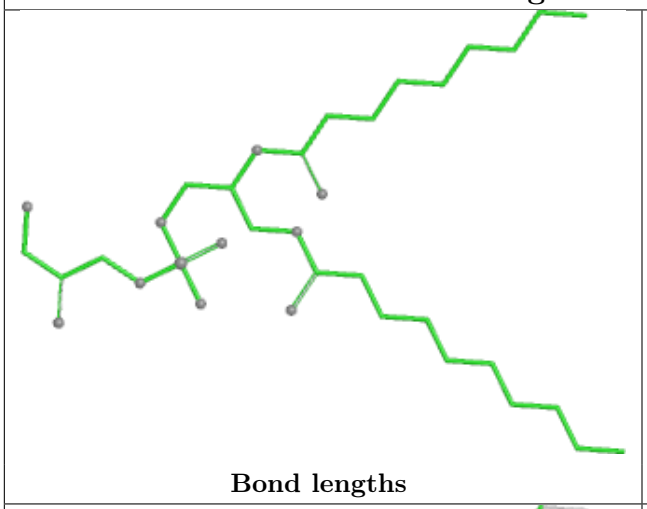


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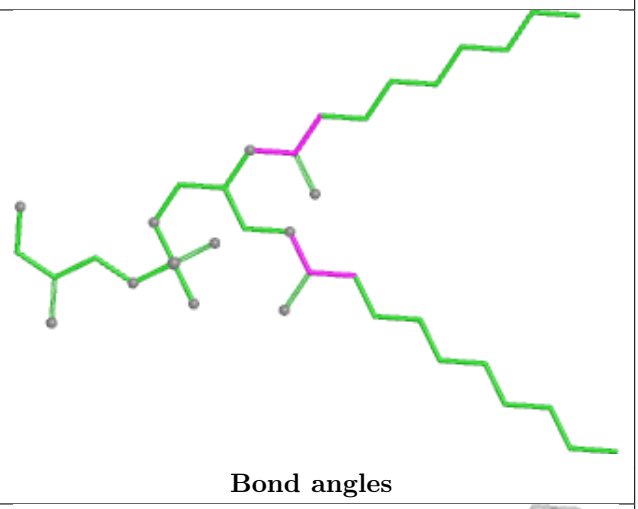


Rings

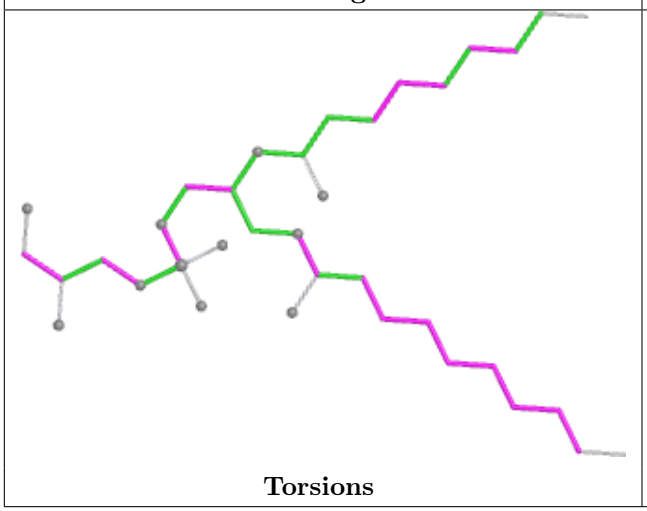
Ligand LHG 7 802



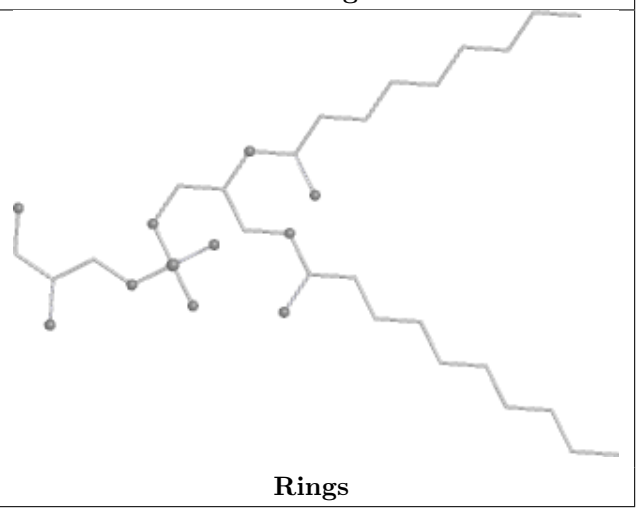
Bond lengths



Bond angles

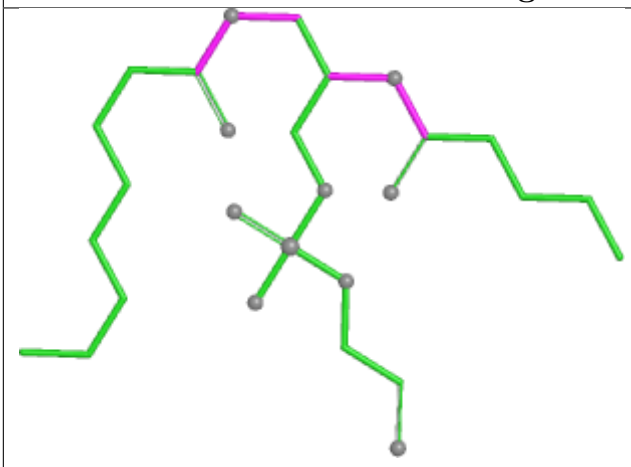


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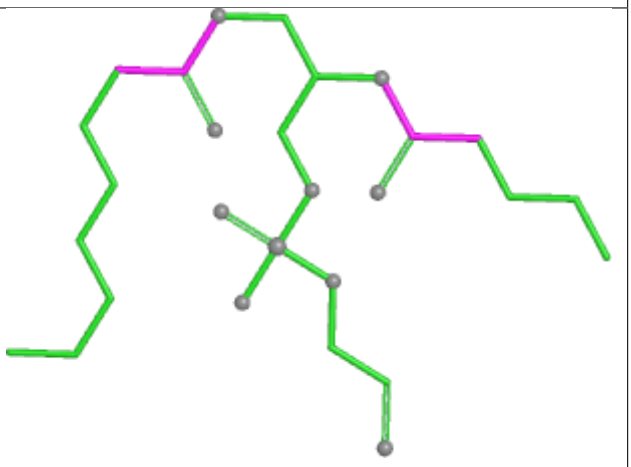


Rings

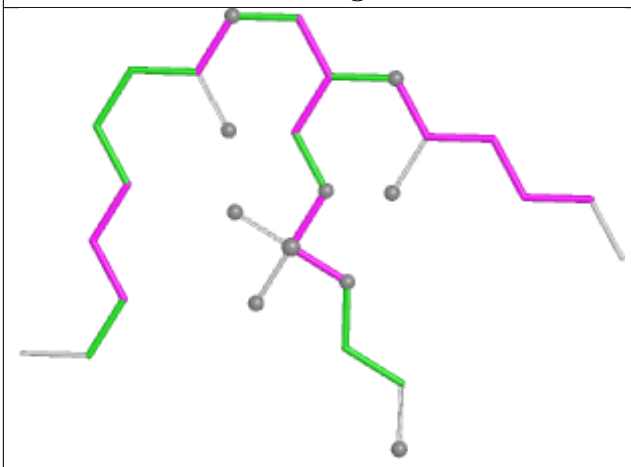
Ligand PTY J 5001



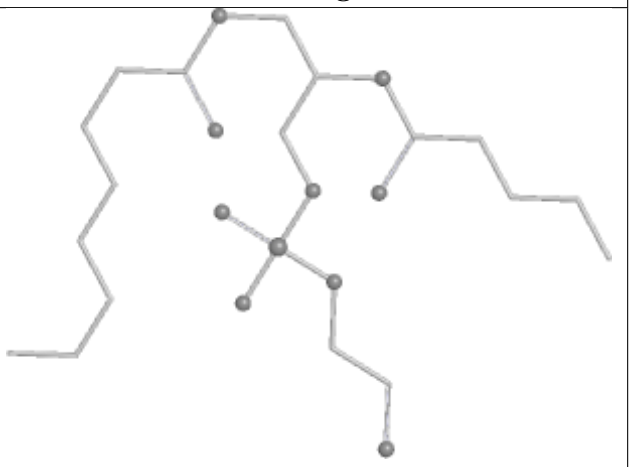
Bond lengths



Bond angles

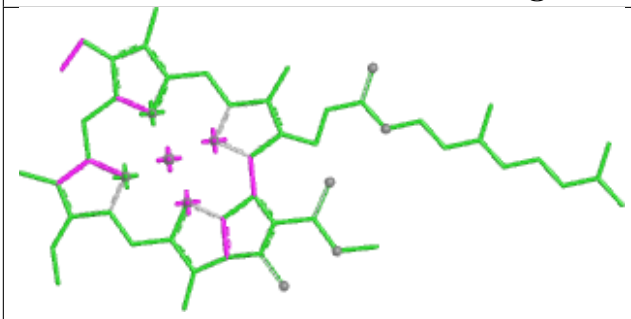


Torsions

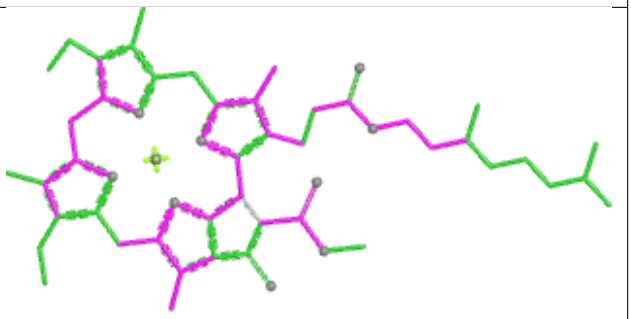


Rings

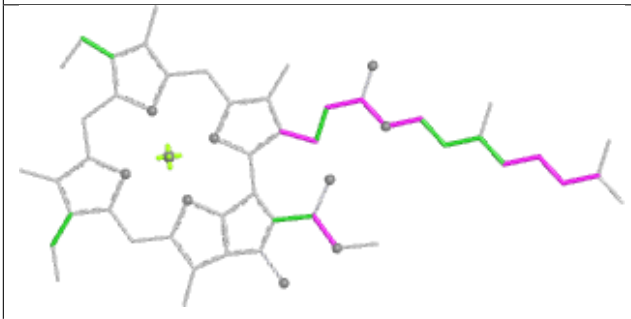
Ligand CLA 8 605



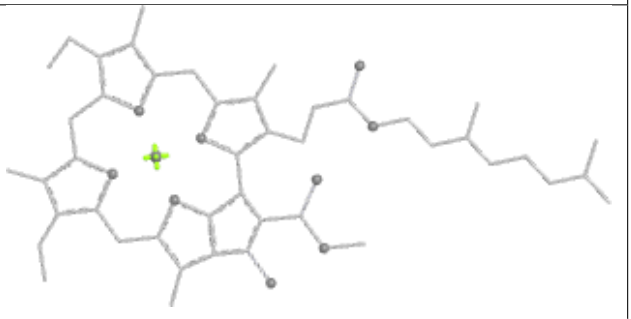
Bond lengths



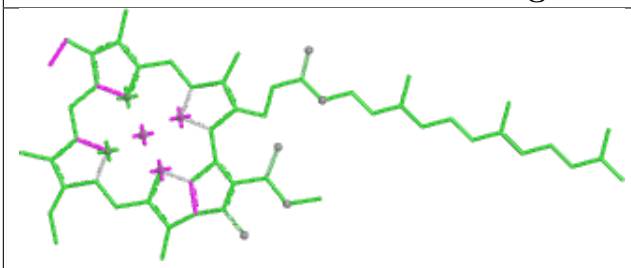
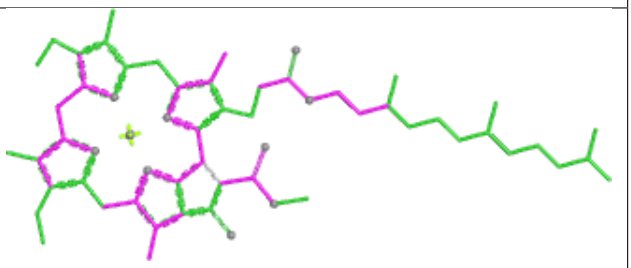
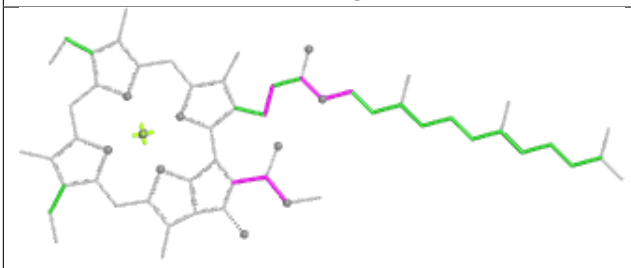
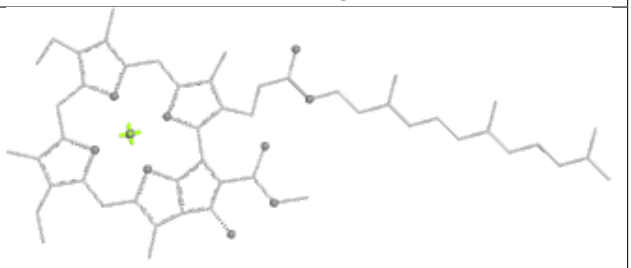
Bond angles

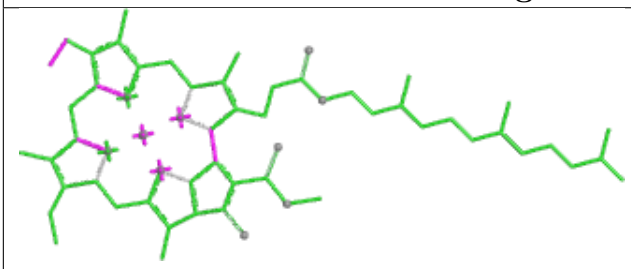
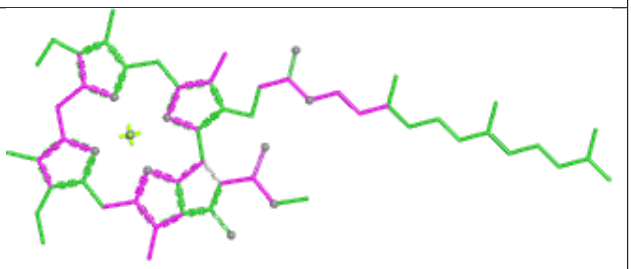
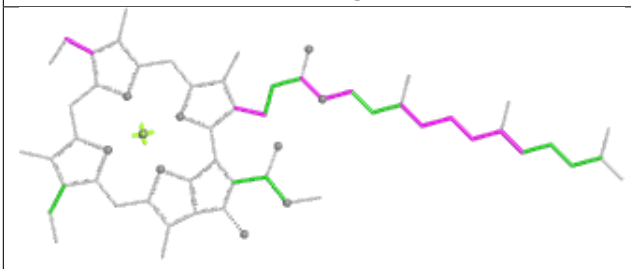
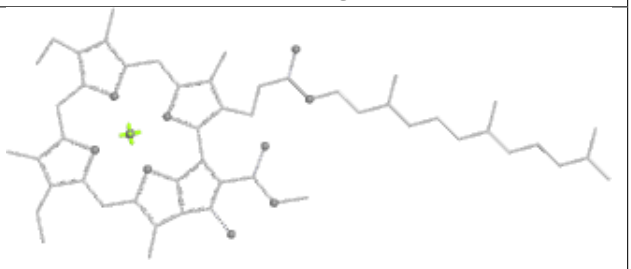


Torsions

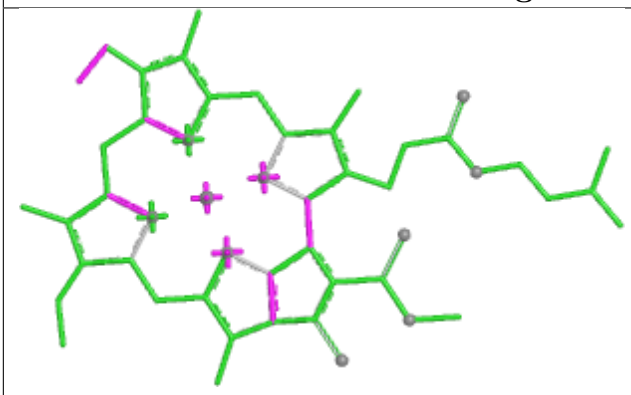


Rings

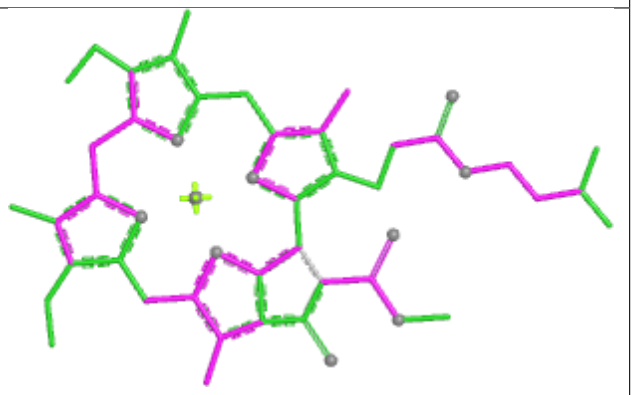
Ligand CLA 9 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1220	
	
Bond lengths	Bond angles
	
Torsions	Rings

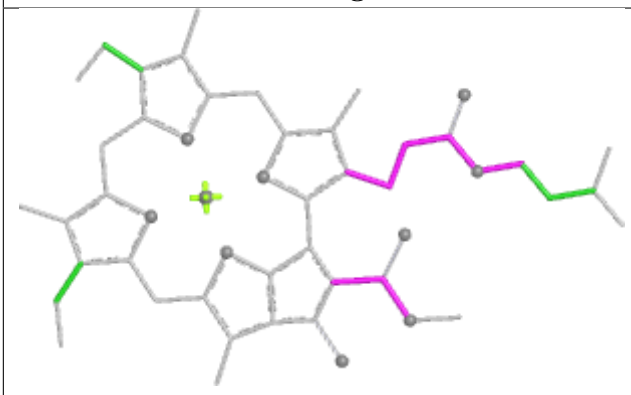
Ligand CLA B 1227



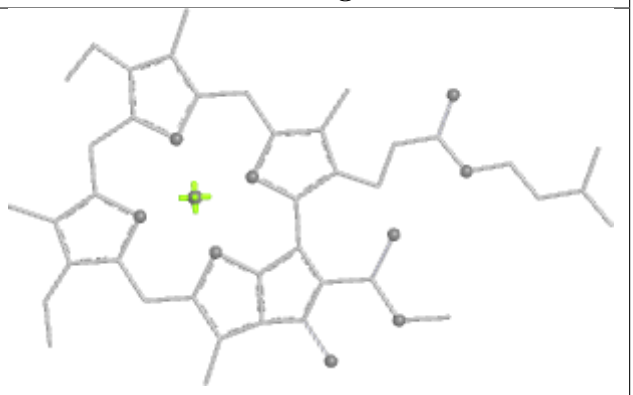
Bond lengths



Bond angles

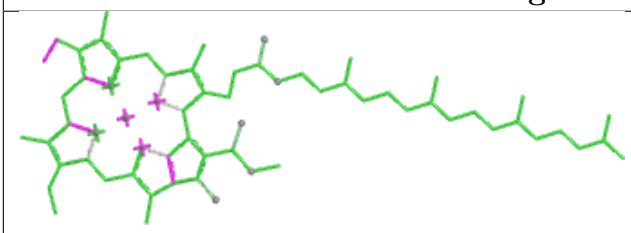


Torsions

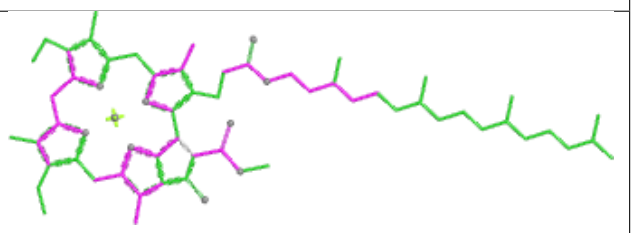


Rings

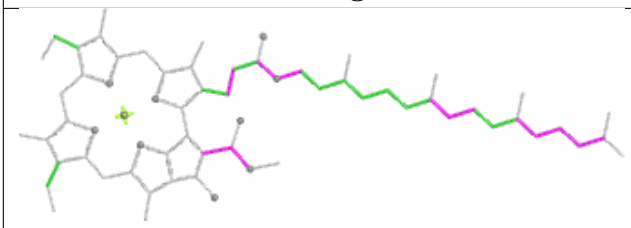
Ligand CLA 7 604



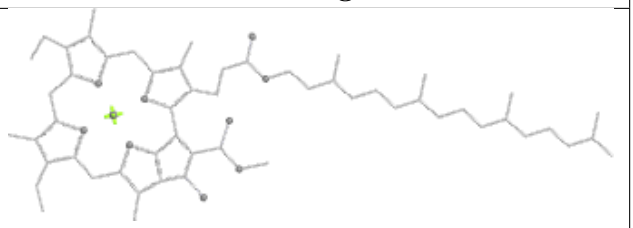
Bond lengths



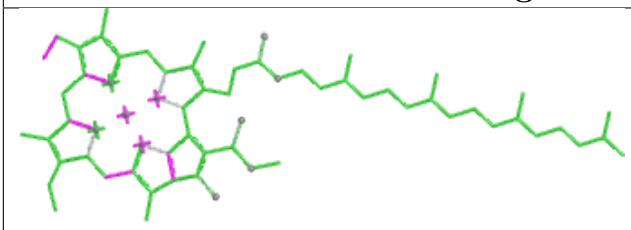
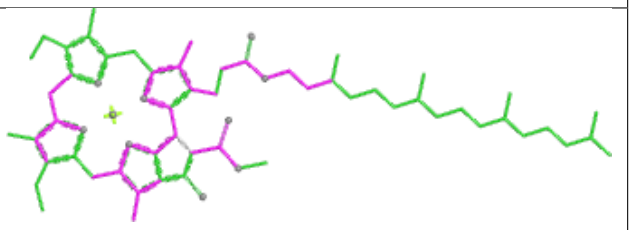
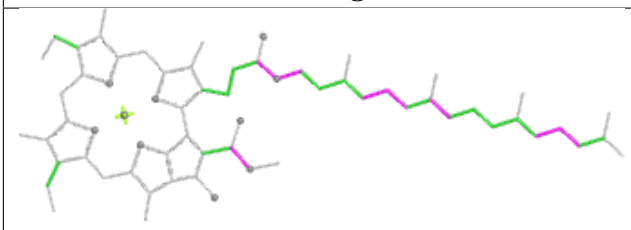
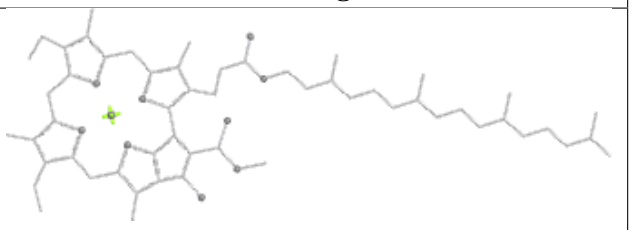
Bond angles

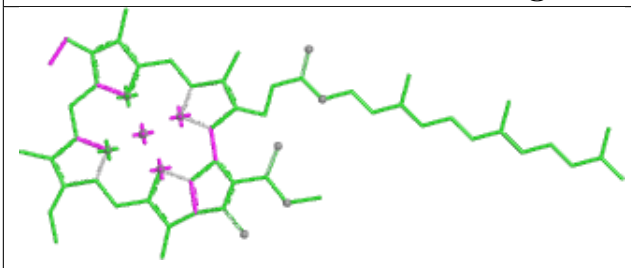
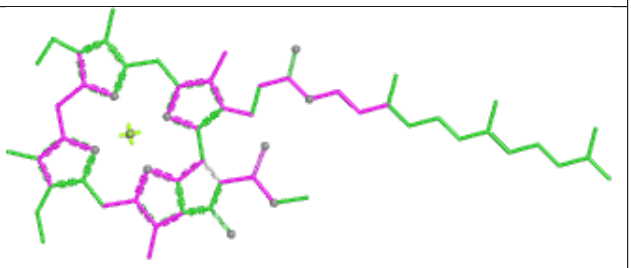
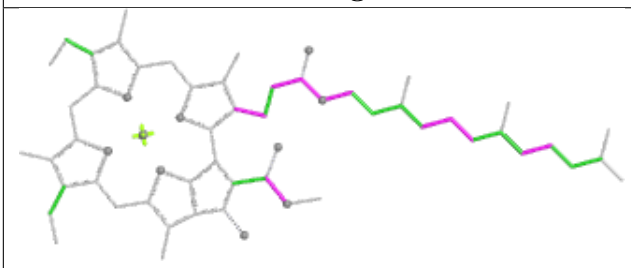
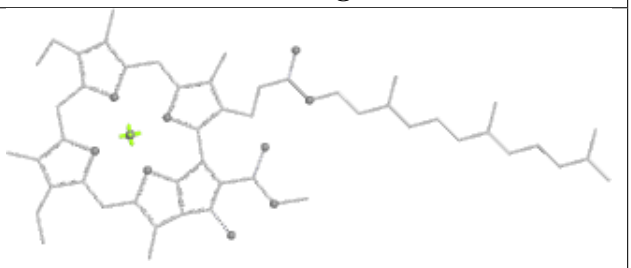


Torsions

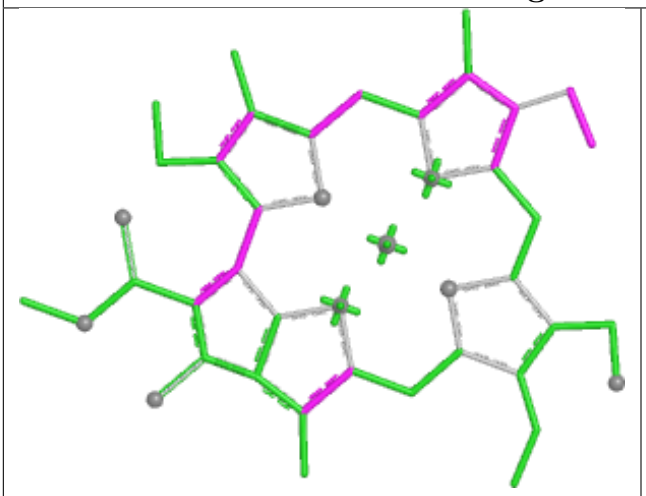


Rings

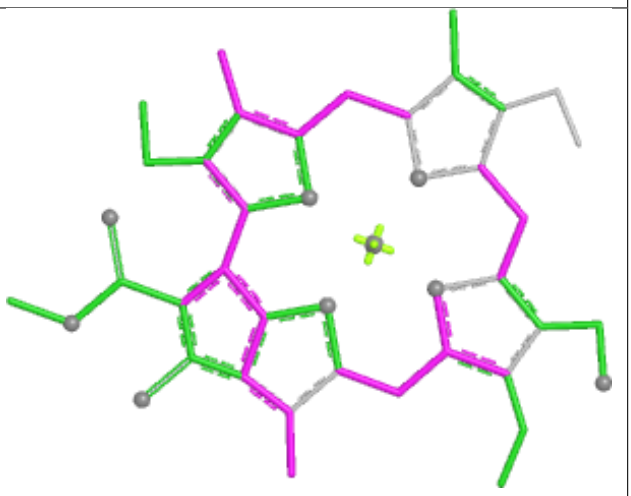
Ligand CLA B 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

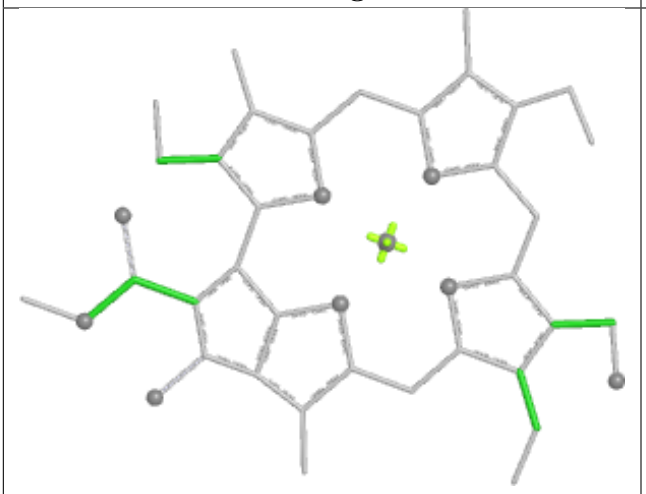
Ligand CHL 3 608



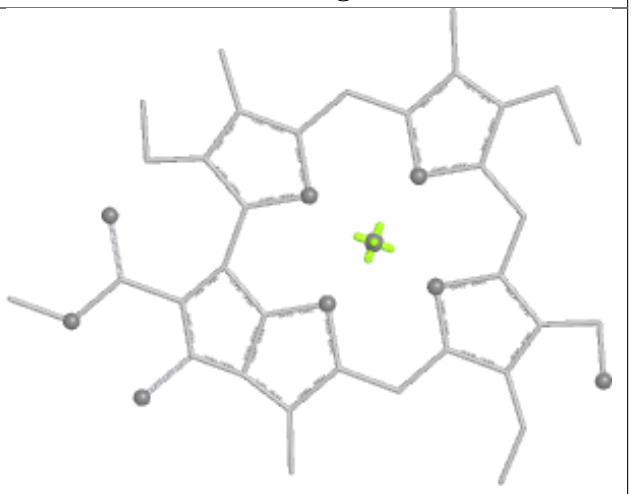
Bond lengths



Bond angles

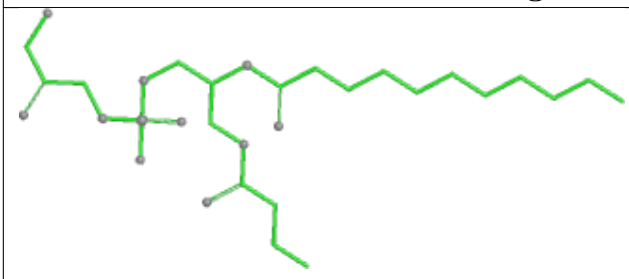


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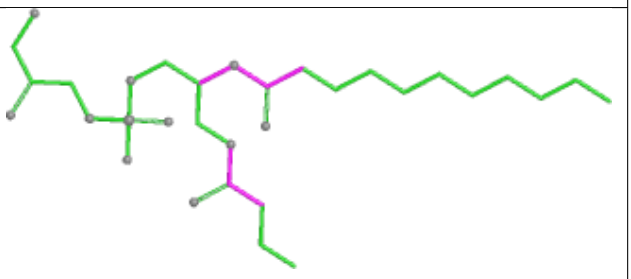


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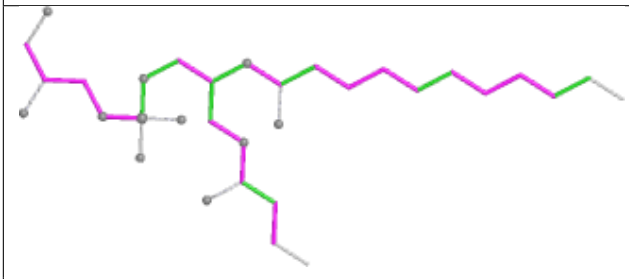
Ligand LHG 4 802



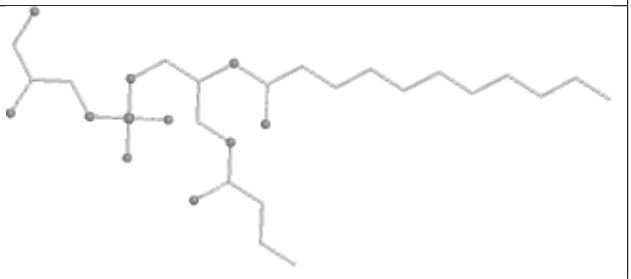
Bond lengths



Bond angles

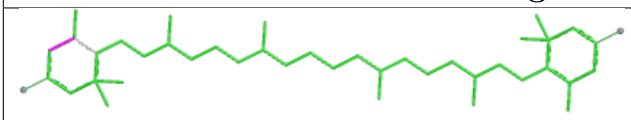


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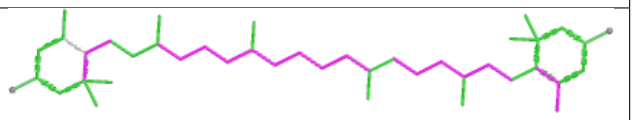


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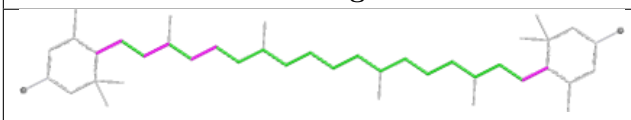
Ligand LUT 4 501



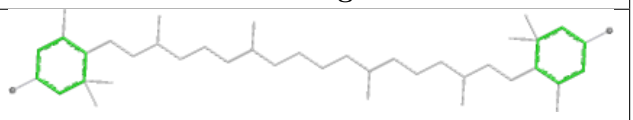
Bond lengths



Bond angles

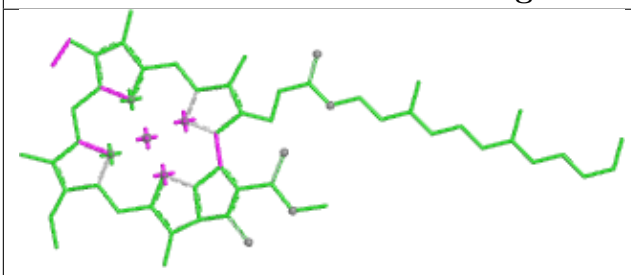


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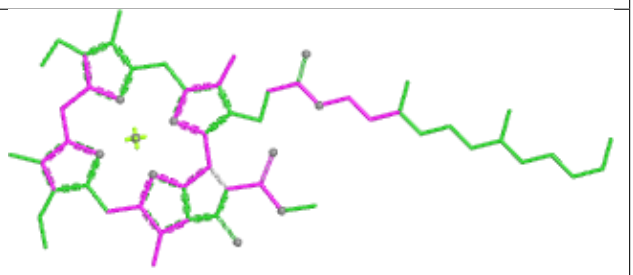


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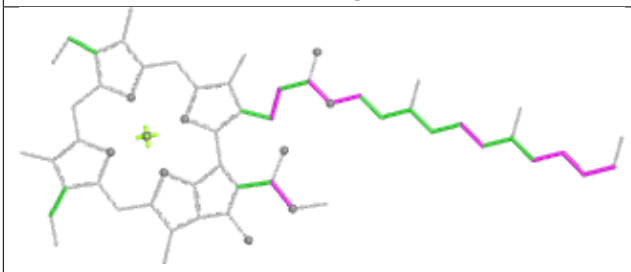
Ligand CLA B 1219



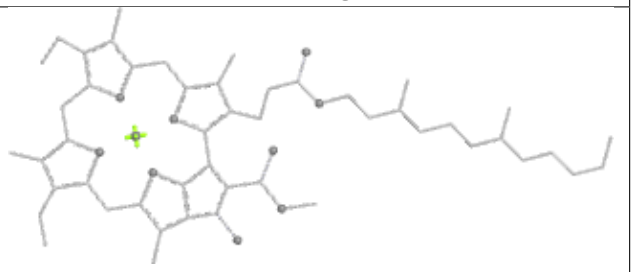
Bond lengths



Bond angles



Torsions

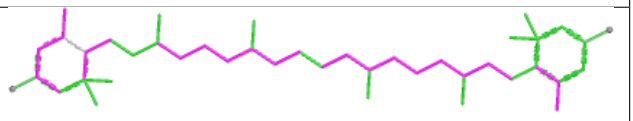


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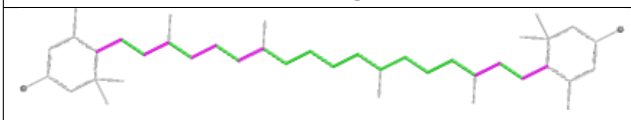
Ligand LUT 5 505



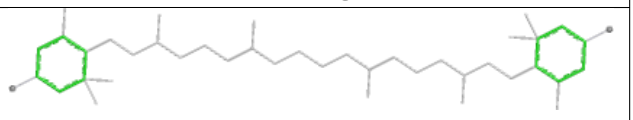
Bond lengths



Bond angles

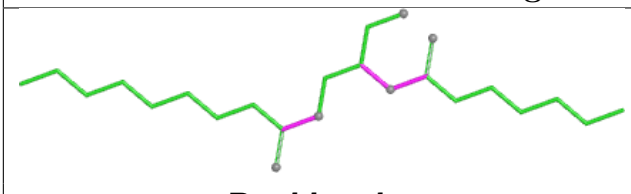


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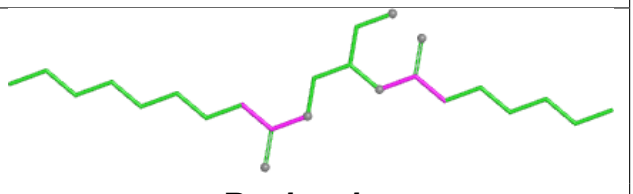


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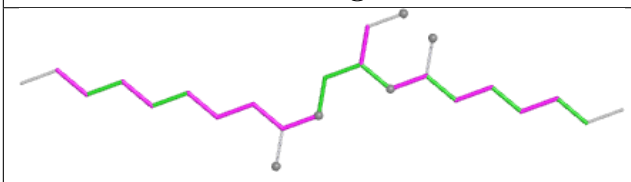
Ligand DGA 3 803



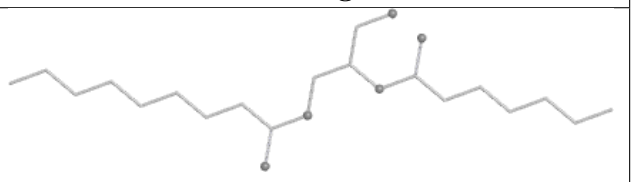
Bond lengths



Bond angles

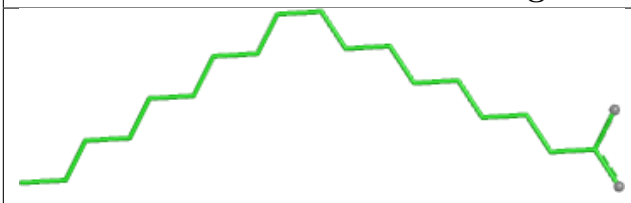


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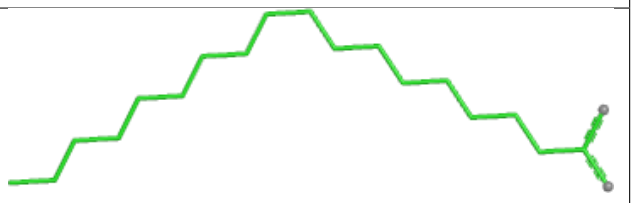


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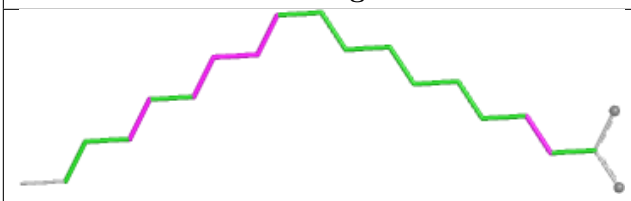
Ligand OLA 8 808



Bond lengths



Bond angles

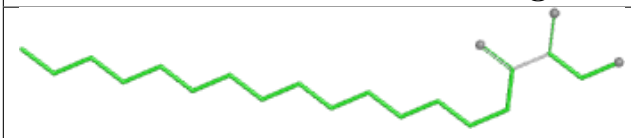


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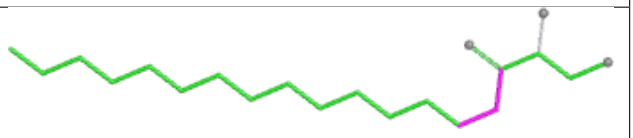


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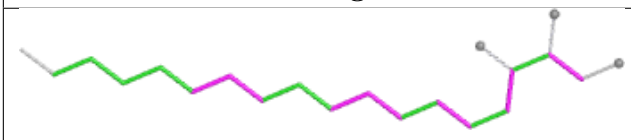
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Bond lengths



Bond angles

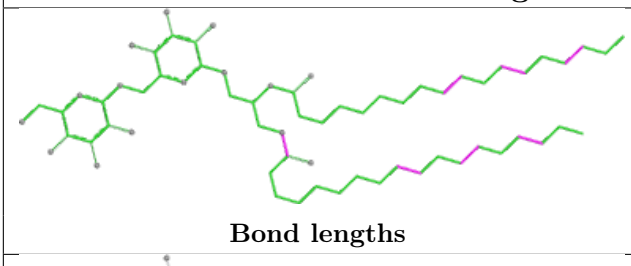


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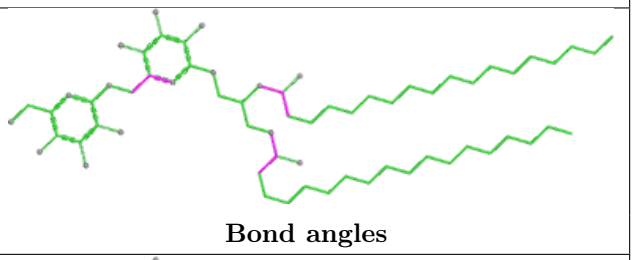


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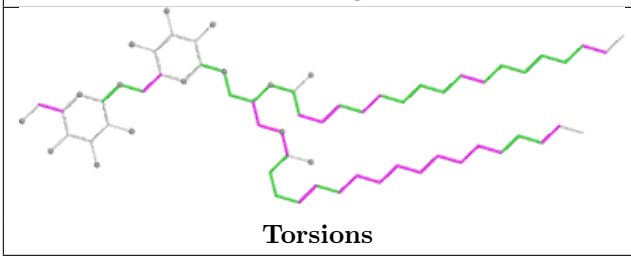
Ligand DGD B 5003



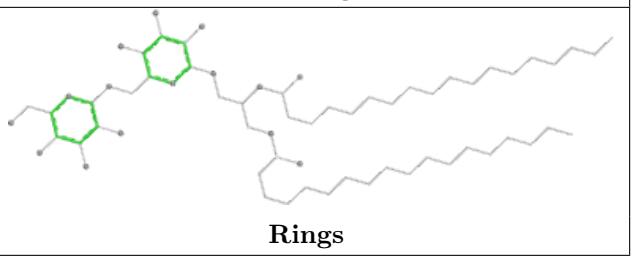
Bond lengths



Bond angles

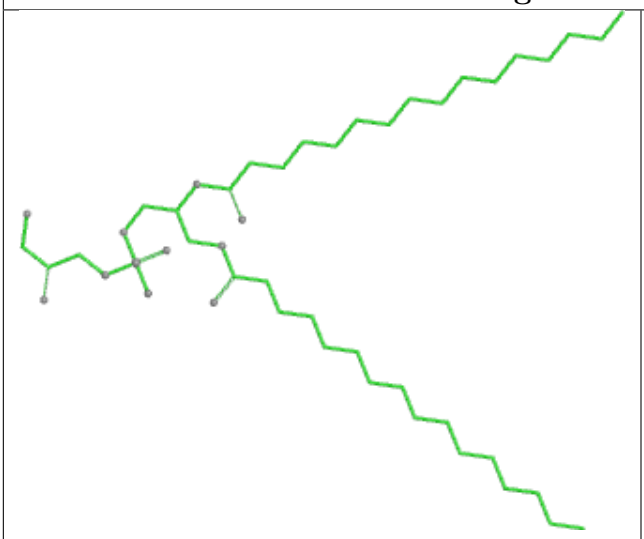


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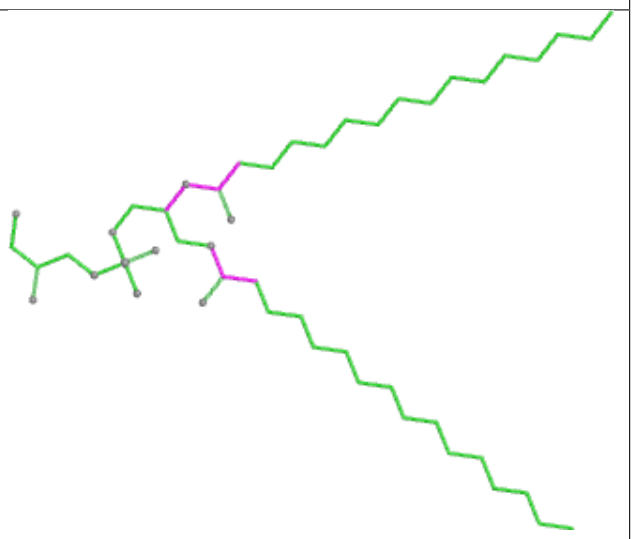


Rings

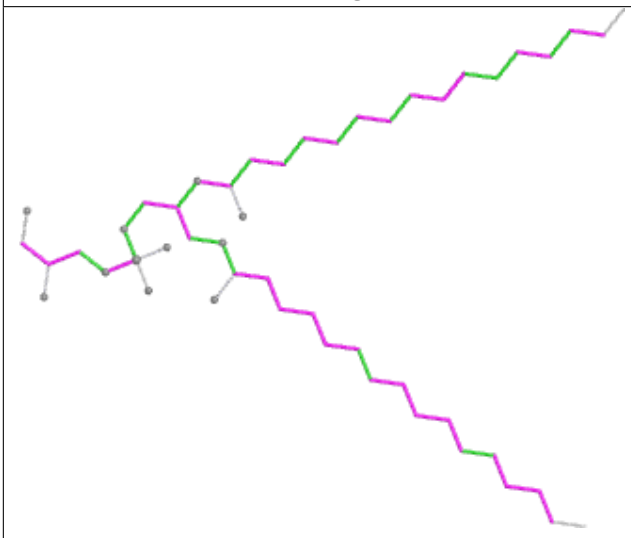
Ligand LHG B 5001



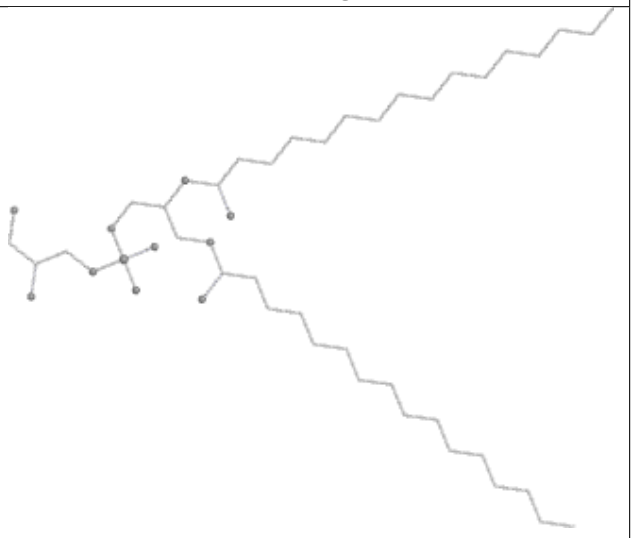
Bond lengths



Bond angles

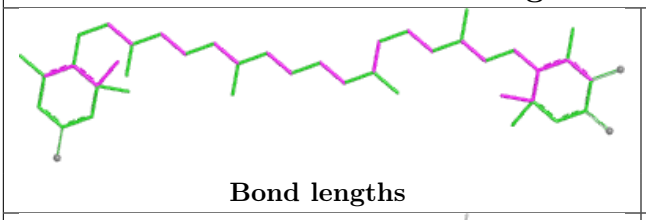


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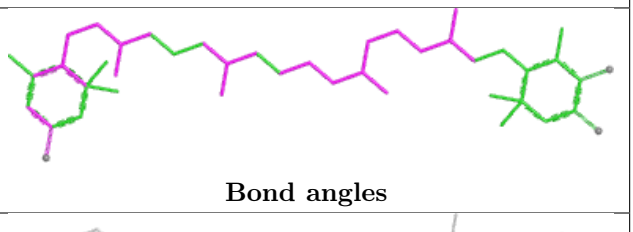


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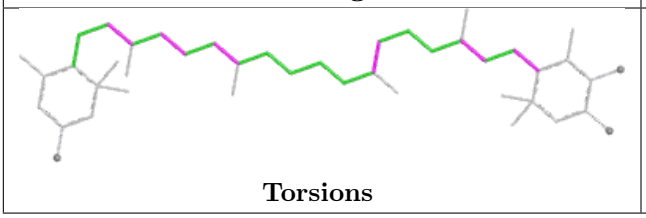
Ligand AXT 1 502



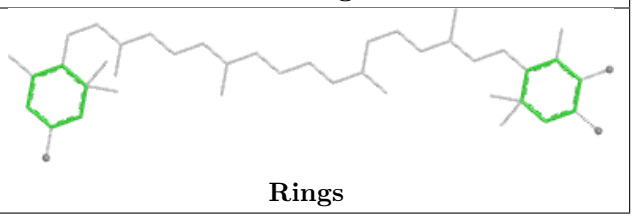
Bond lengths



Bond angles

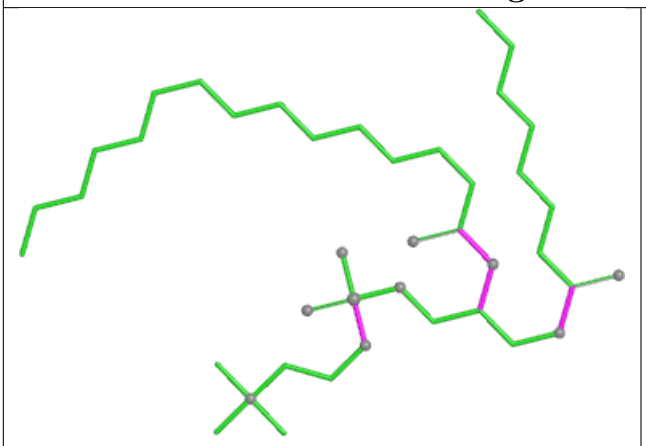


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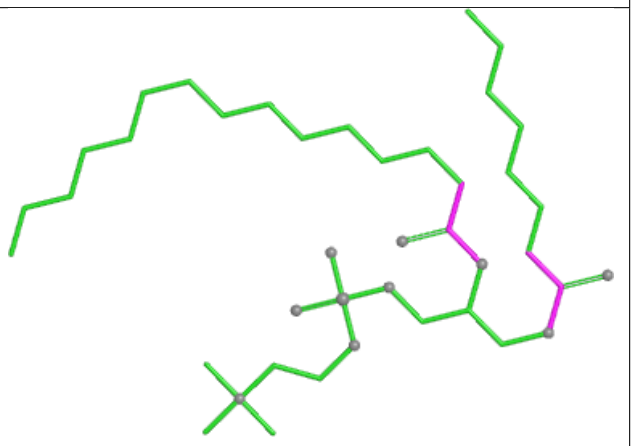


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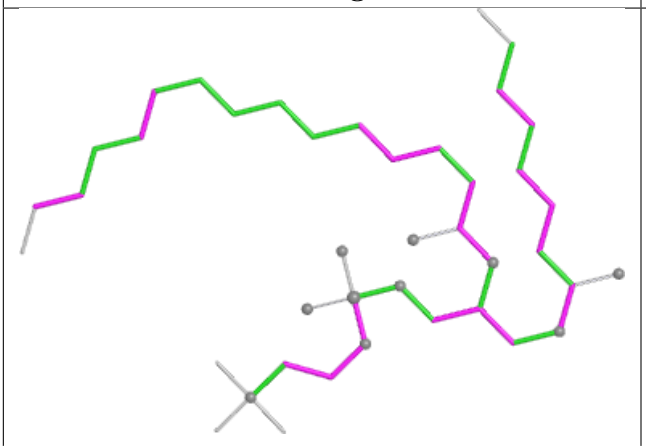
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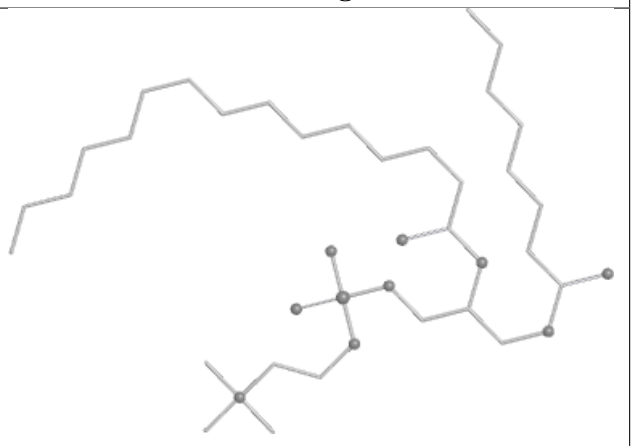
Bond lengths



Bond angles

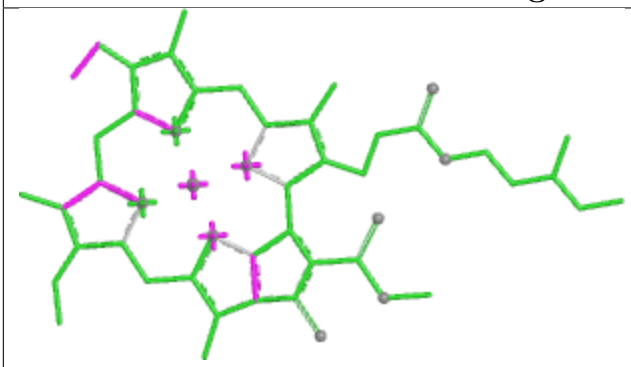


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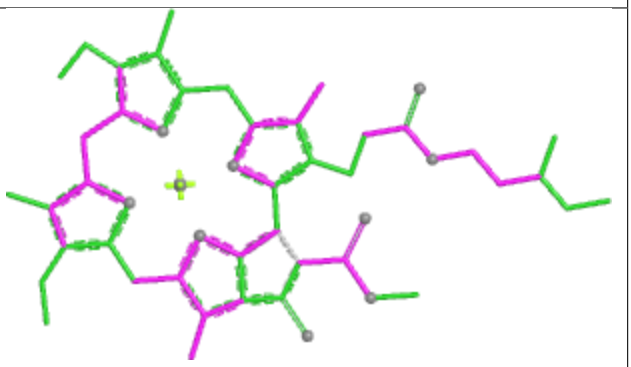


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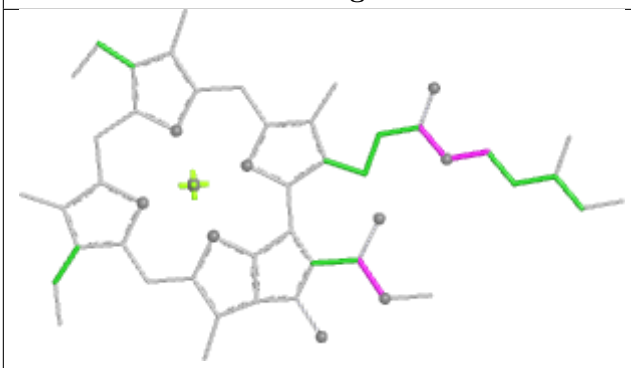
Ligand CLA 4 608



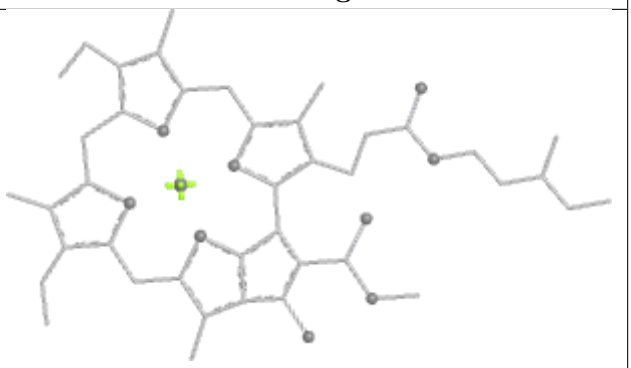
Bond lengths



Bond angles

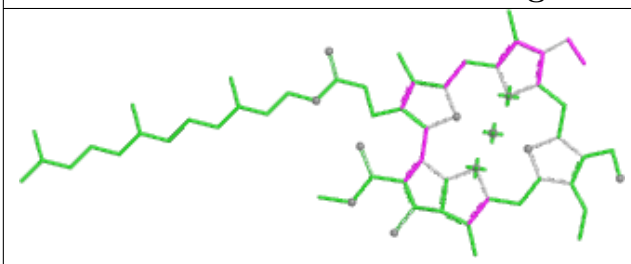


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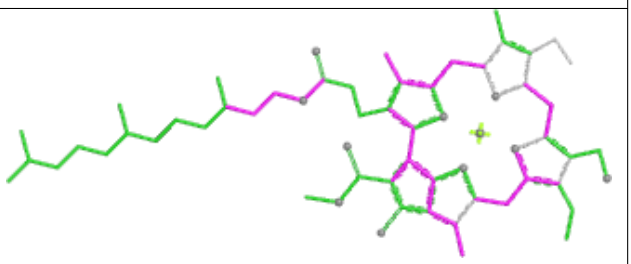


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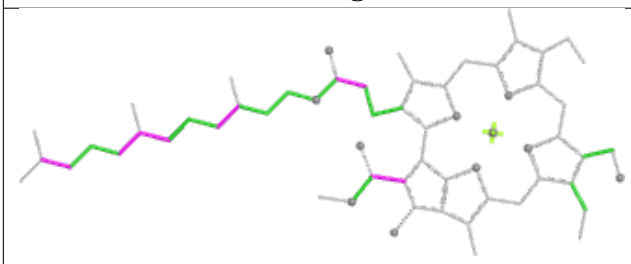
Ligand CHL 3 611



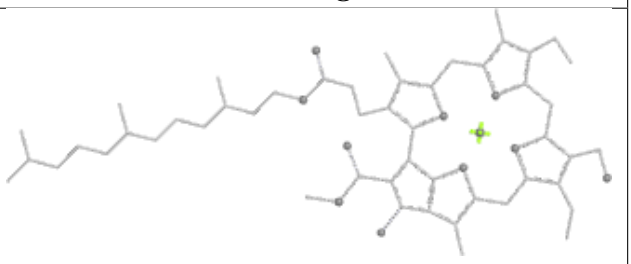
Bond lengths



Bond angles

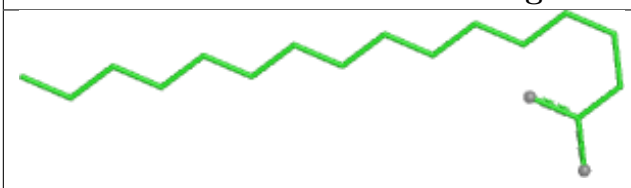


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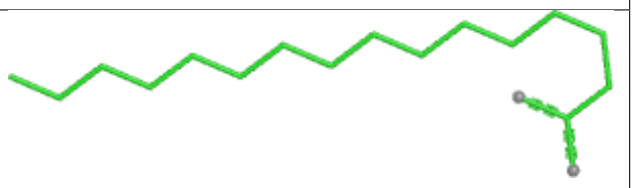


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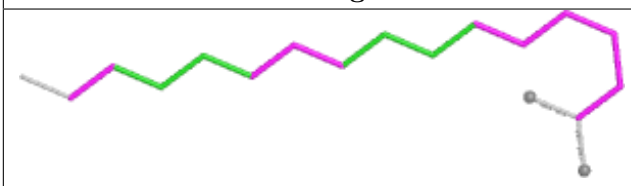
Ligand PLM 4 804



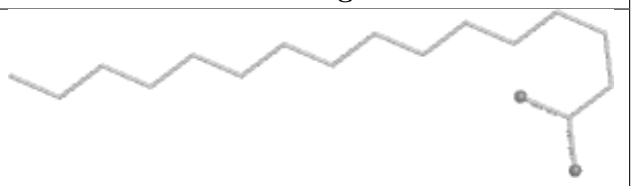
Bond lengths



Bond angles

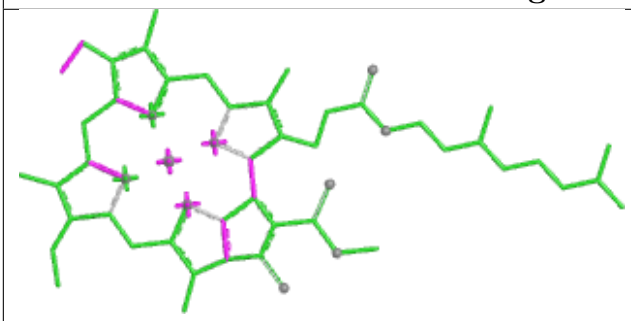


Torsions

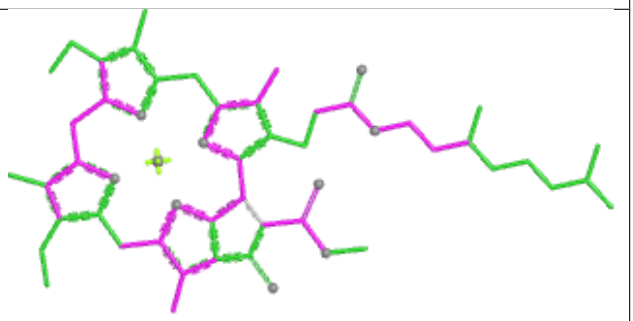


Rings

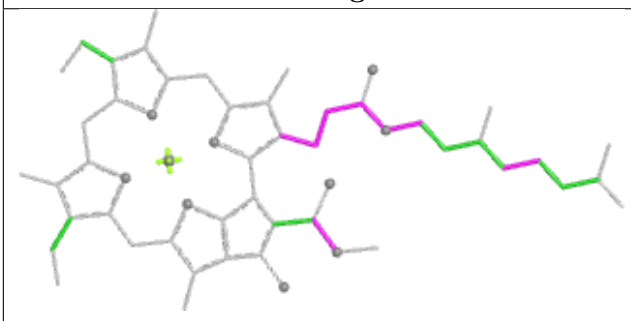
Ligand CLA 7 608



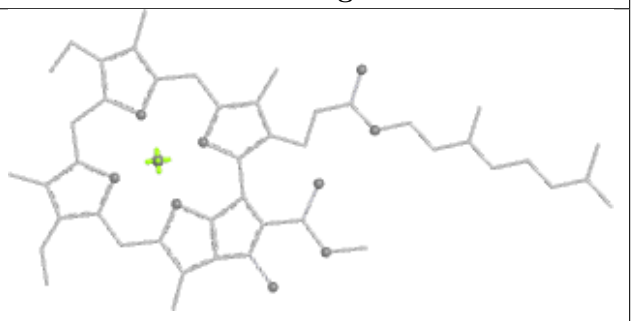
Bond lengths



Bond angles

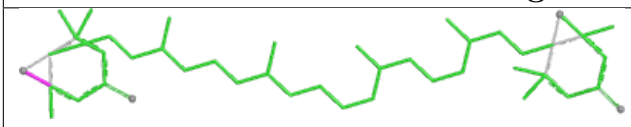


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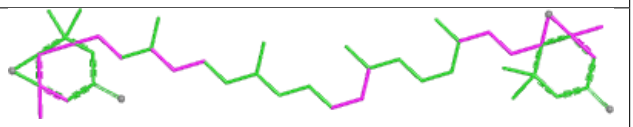


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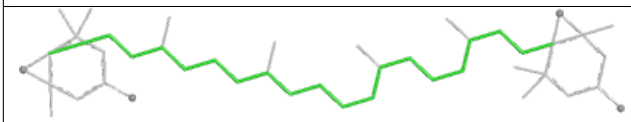
Ligand XAT 7 502



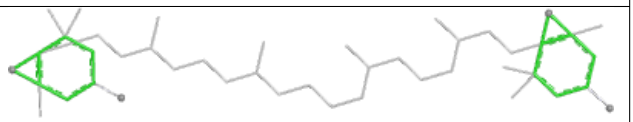
Bond lengths



Bond angles

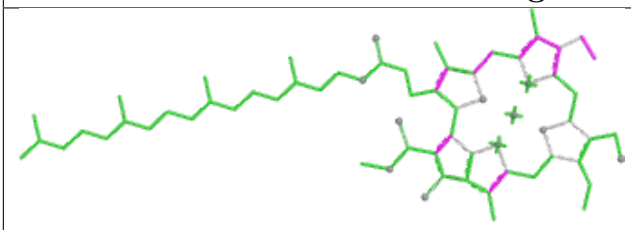


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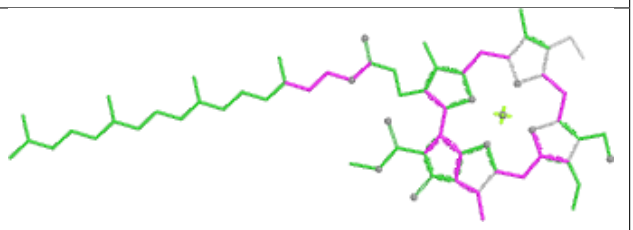


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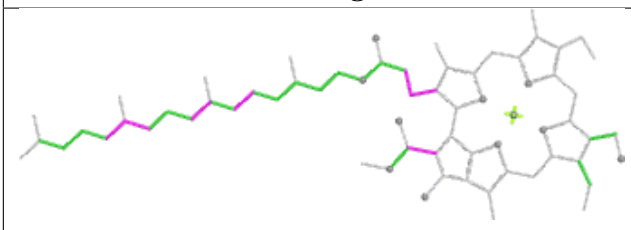
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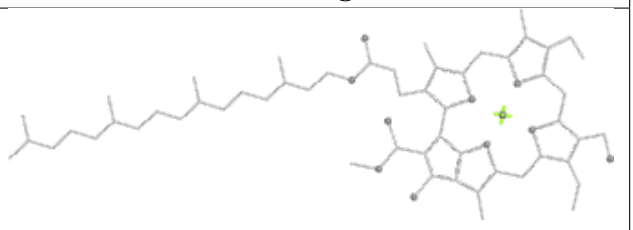
Bond lengths



Bond angles

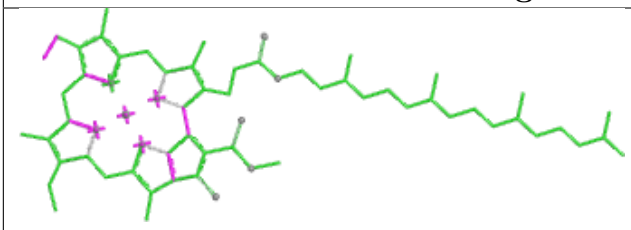


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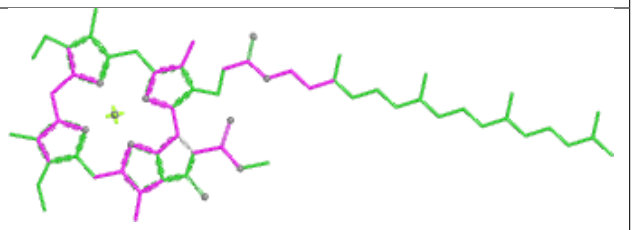


Rings

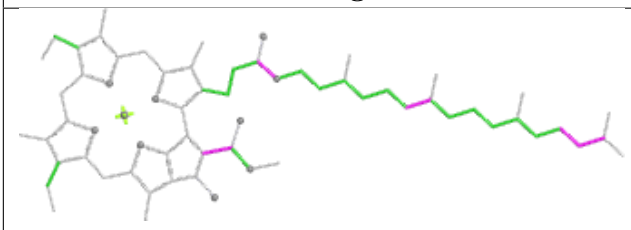
Ligand CLA B 1221



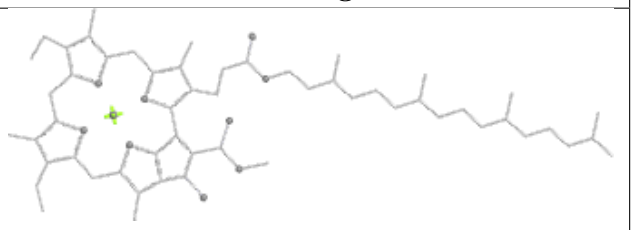
Bond lengths



Bond angles

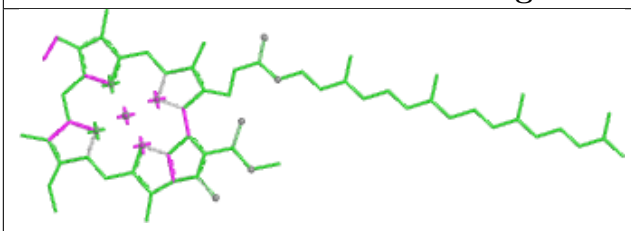


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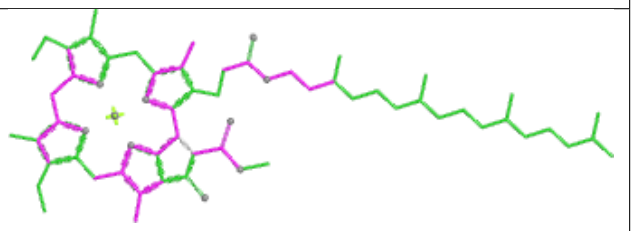


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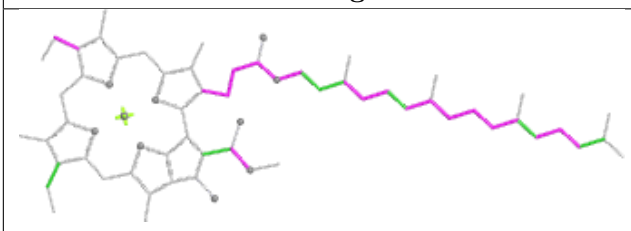
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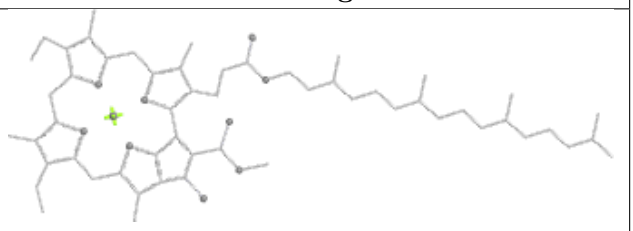
Bond lengths



Bond angles

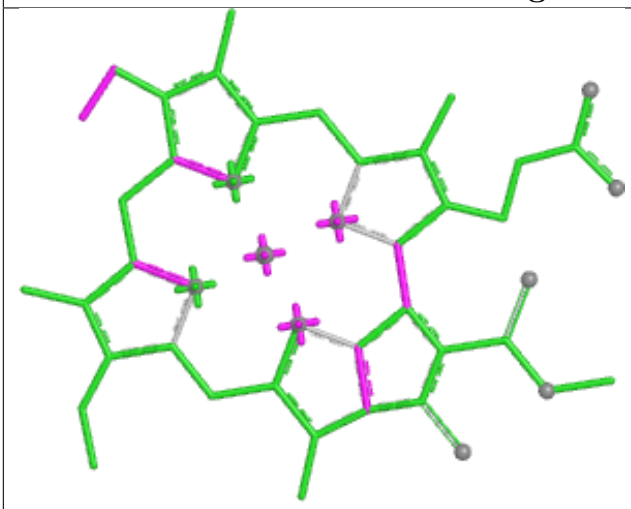


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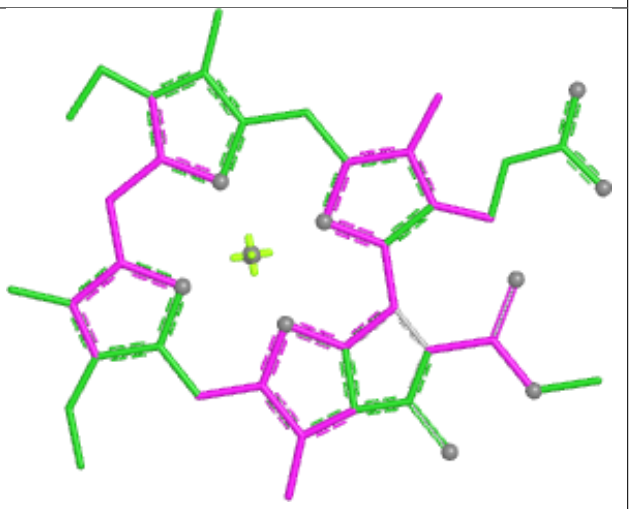


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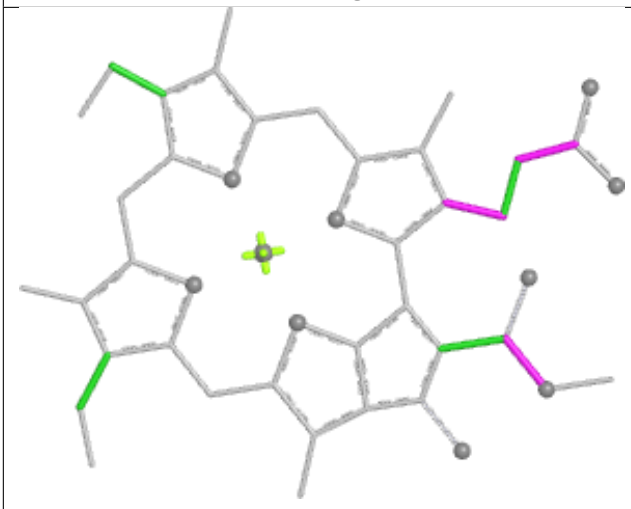
Ligand CLA 1 602



Bond lengths



Bond angles

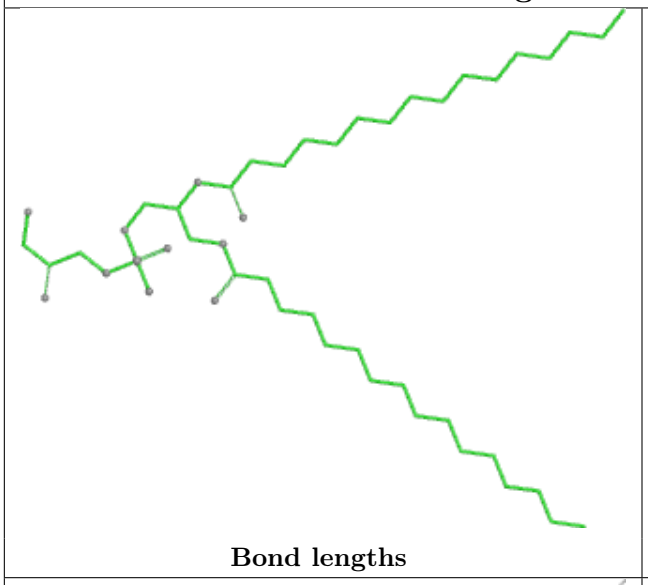


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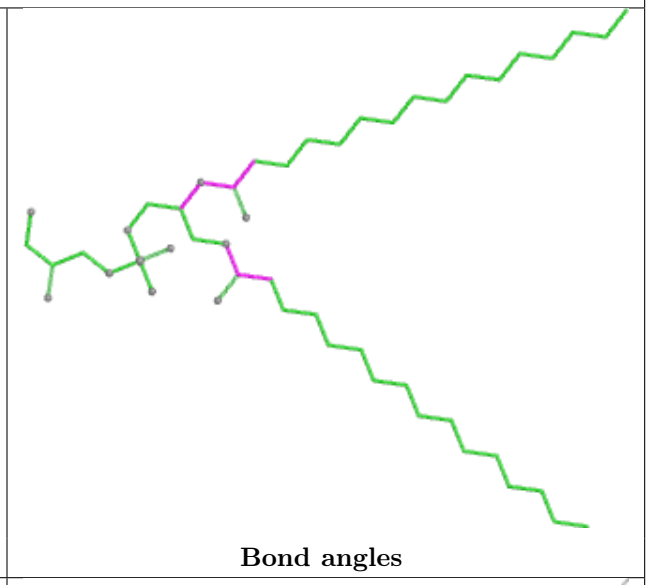


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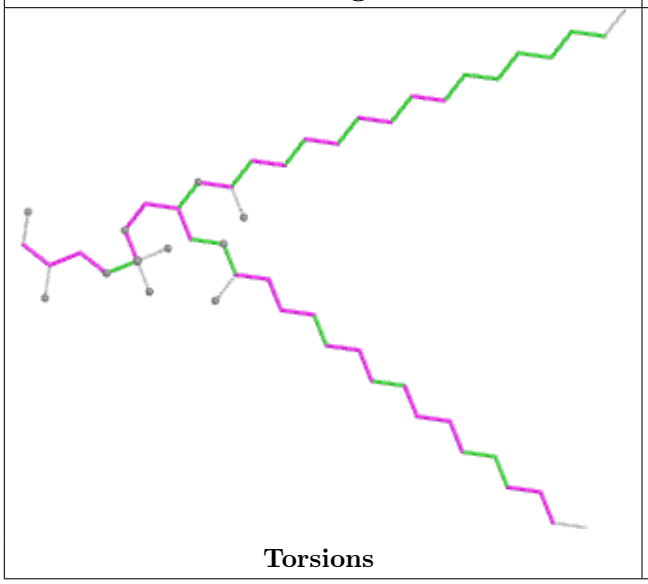
Ligand LHG B 5002



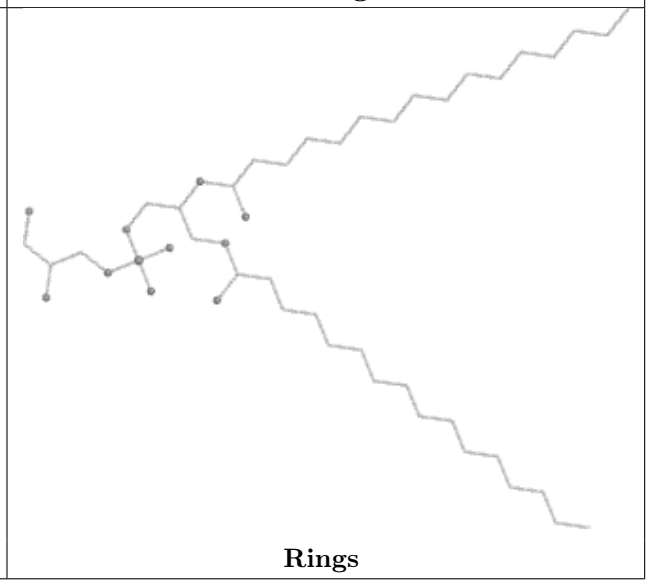
Bond lengths



Bond angles

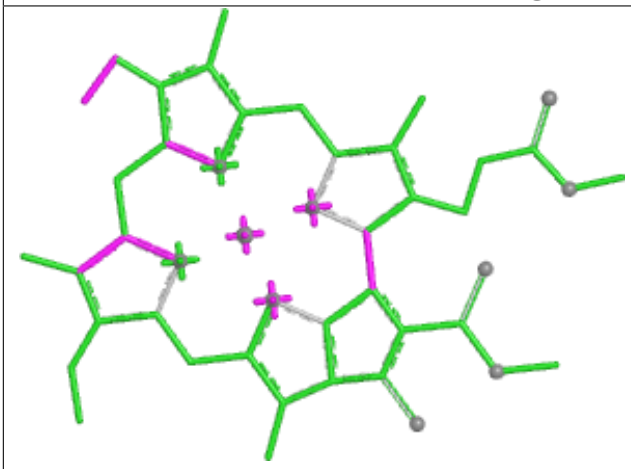


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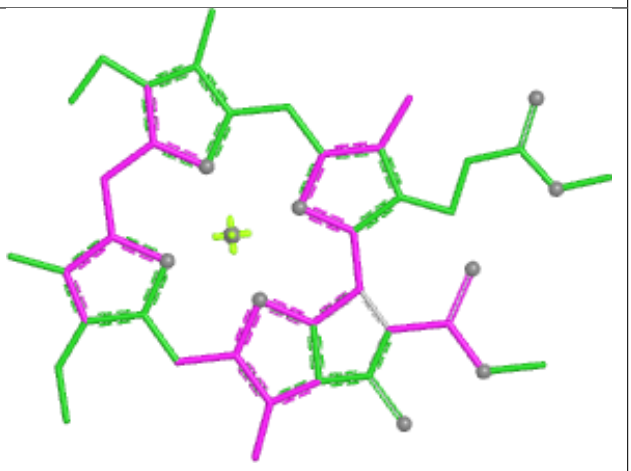


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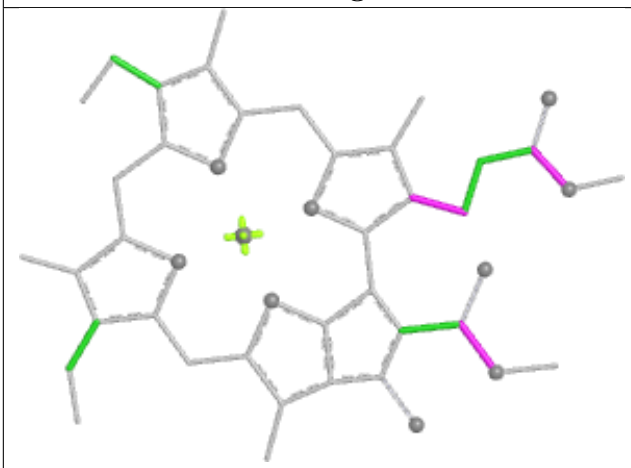
Ligand CLA 9 609



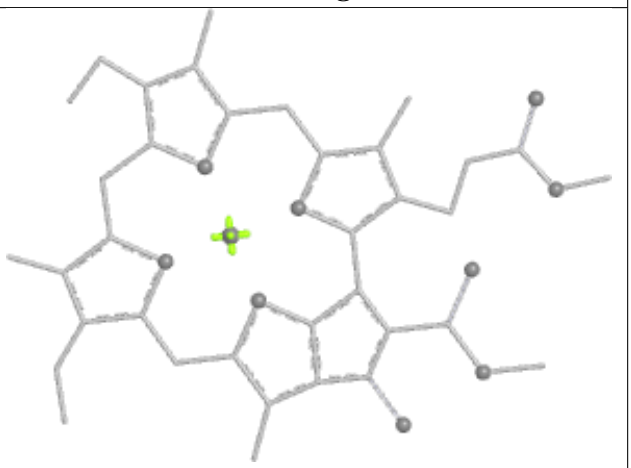
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Bond angles

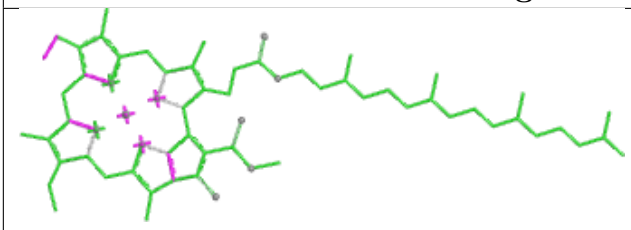


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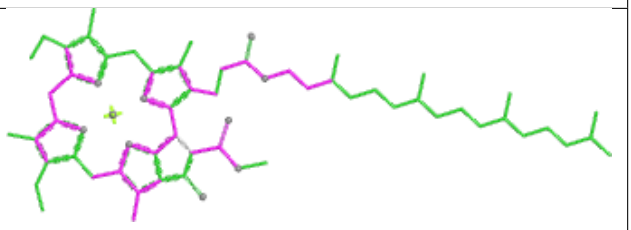


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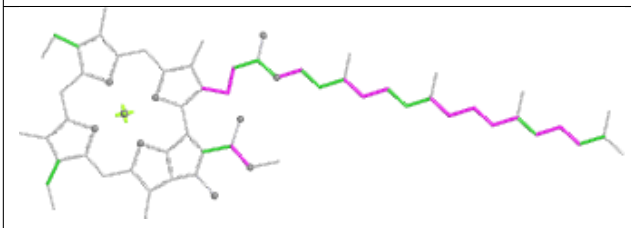
Ligand CLA B 1216



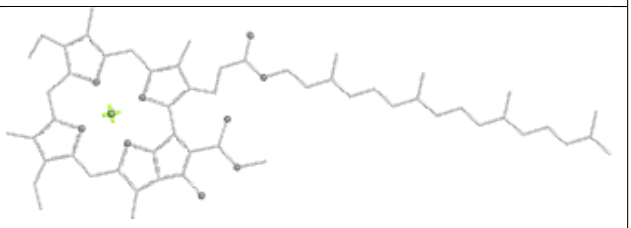
Bond lengths



Bond angles

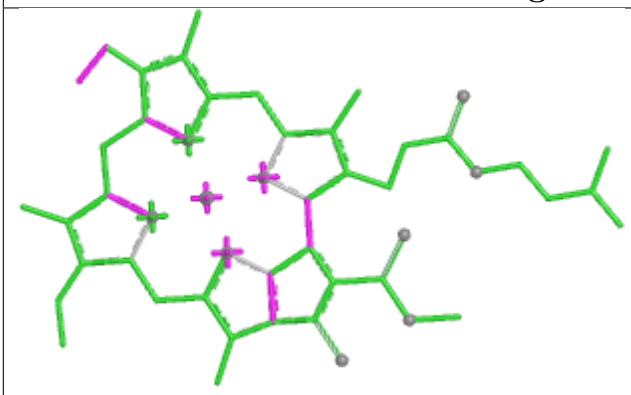


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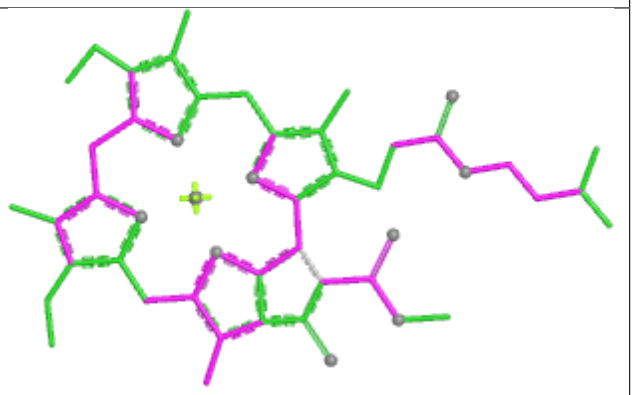


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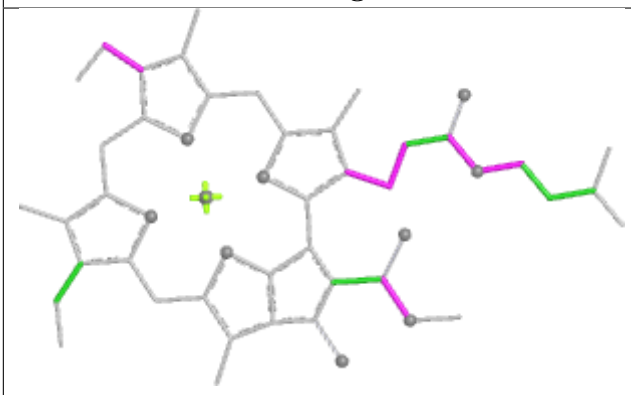
Ligand CLA 2 612



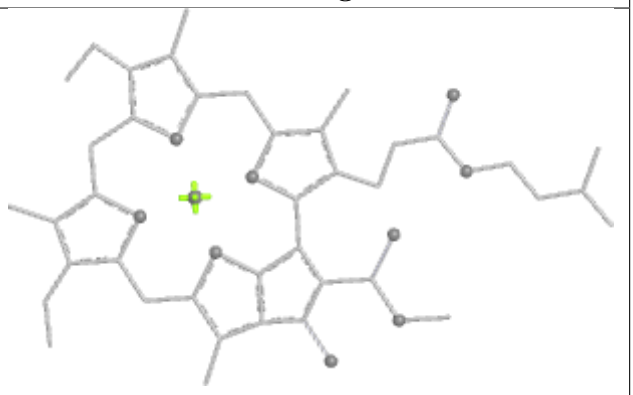
Bond lengths



Bond angles



Torsions

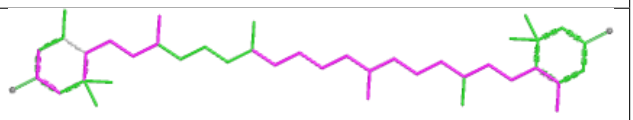


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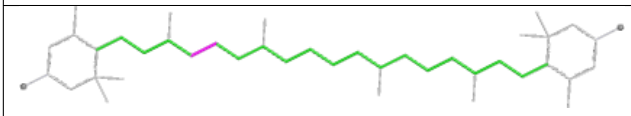
Ligand LUT 5 501



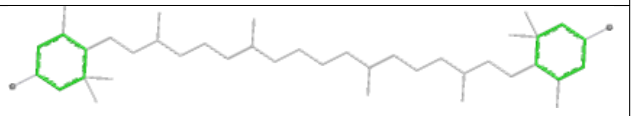
Bond lengths



Bond angles

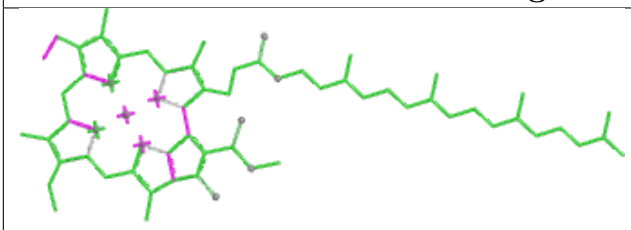


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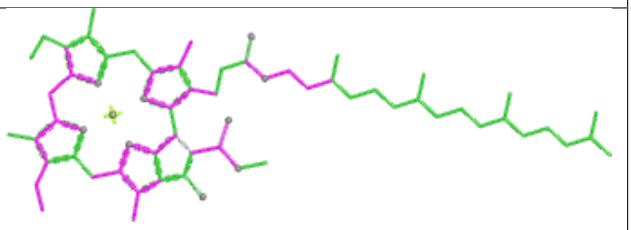


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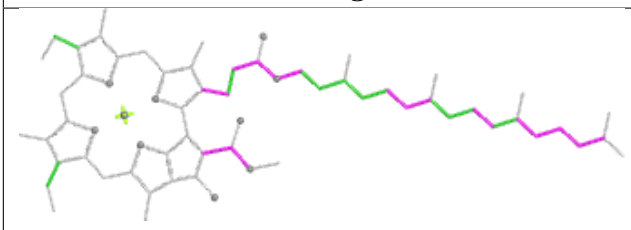
Ligand CLA 1 605



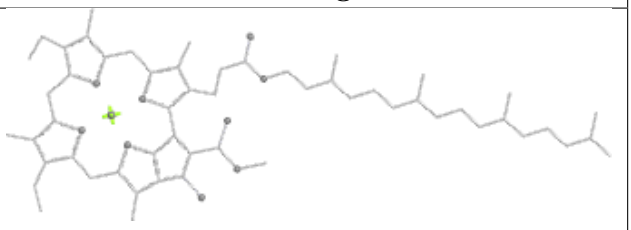
Bond lengths



Bond angles

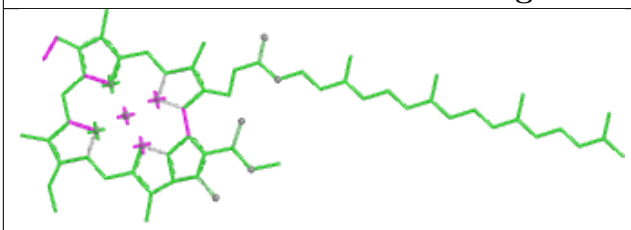


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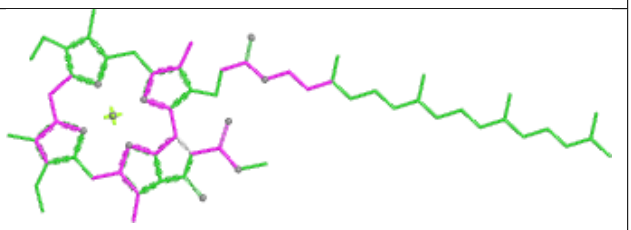


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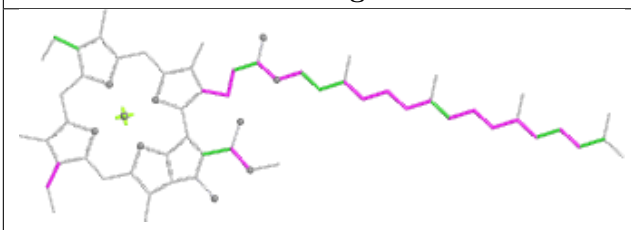
Ligand CLA B 1206



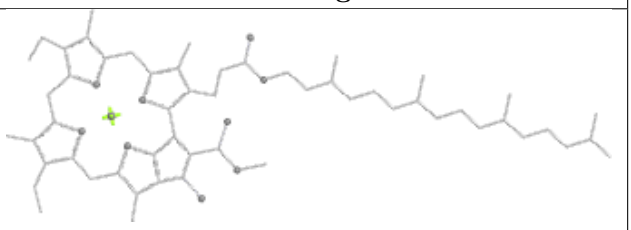
Bond lengths



Bond angles



Torsions



Rings

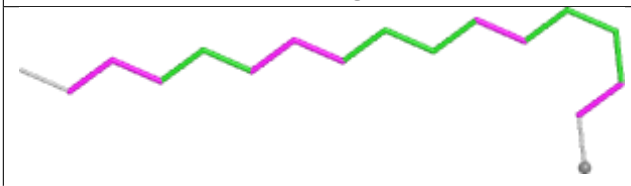
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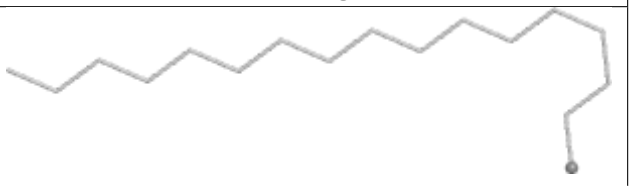
Bond lengths



Bond angles

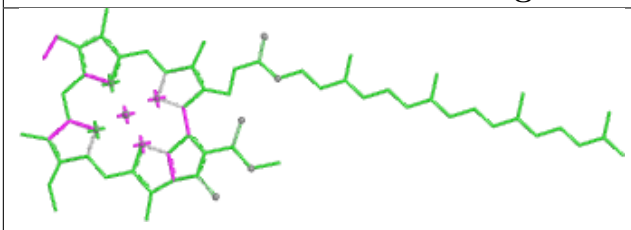


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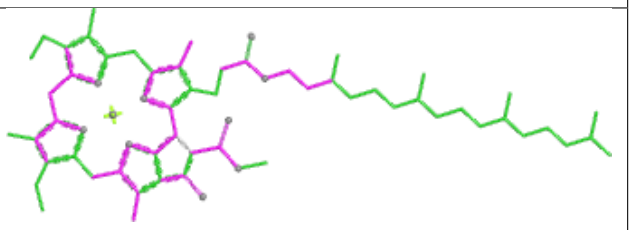


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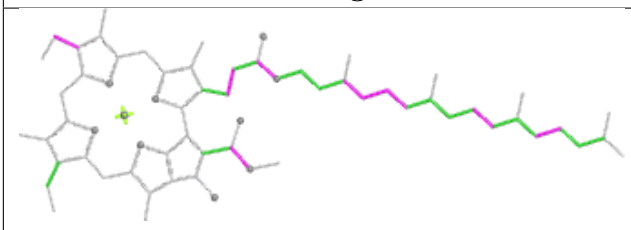
Ligand CLA A 1012



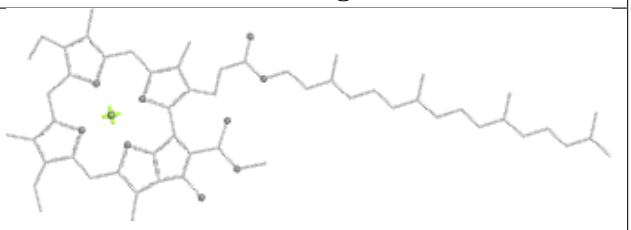
Bond lengths



Bond angles

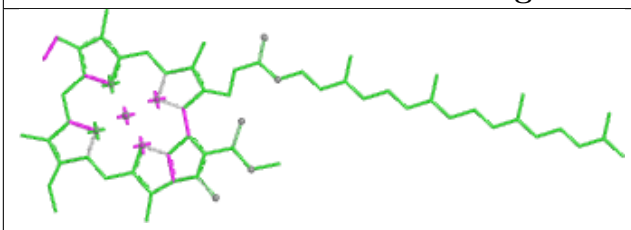


Torsions

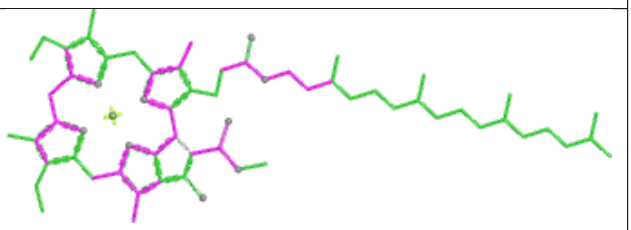


Rings

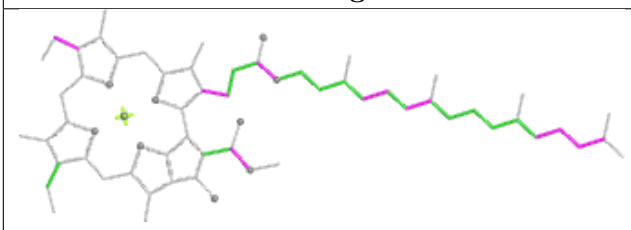
Ligand CLA A 1131



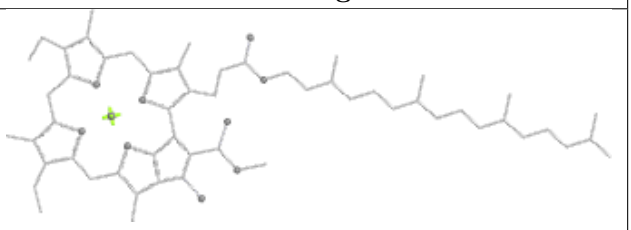
Bond lengths



Bond angles

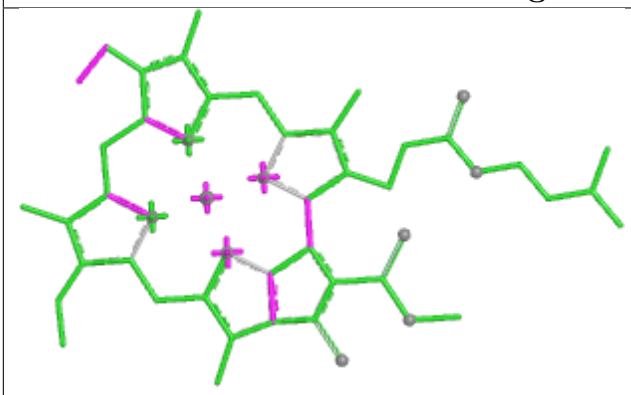


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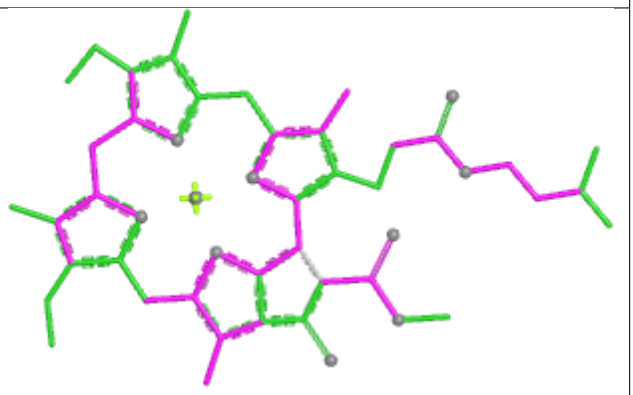


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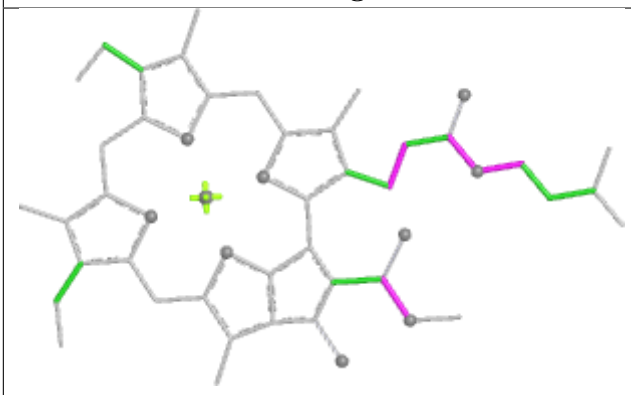
Ligand CLA 8 611



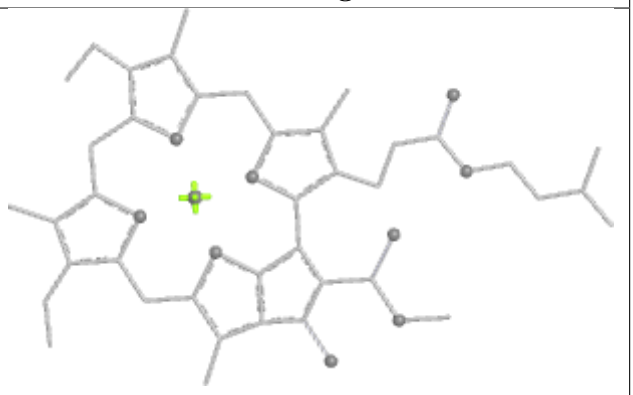
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Bond angles

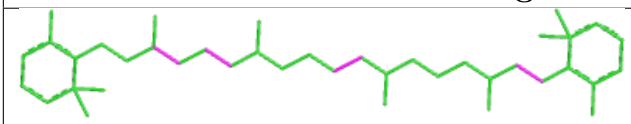


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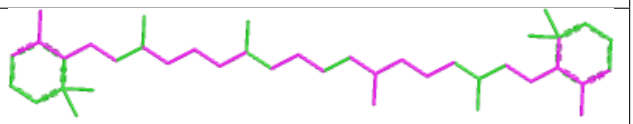


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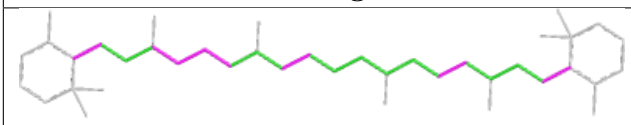
Ligand BCR L 4003



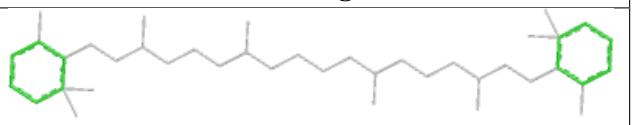
Bond lengths



Bond angles

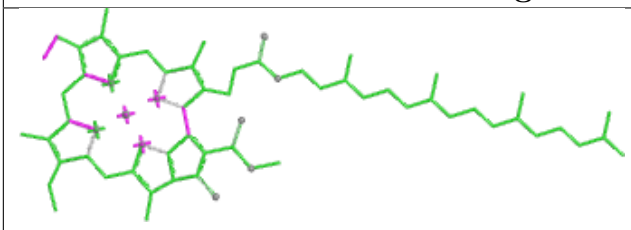


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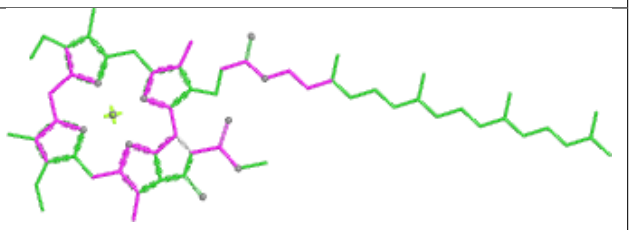


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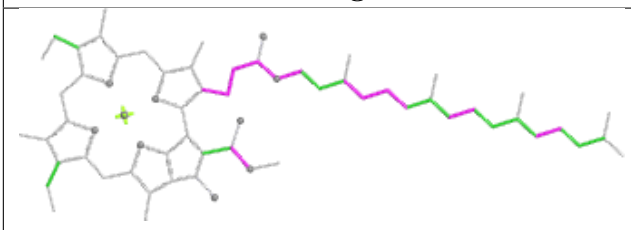
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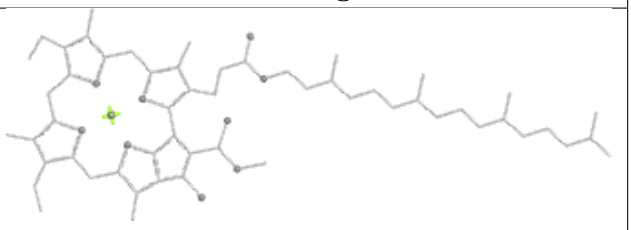
Bond lengths



Bond angles

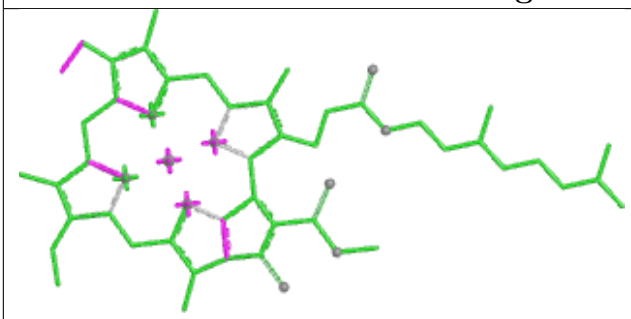


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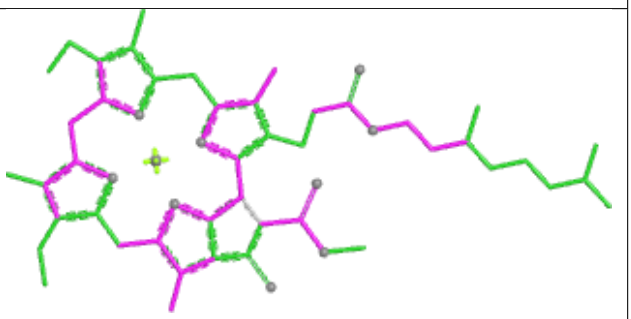


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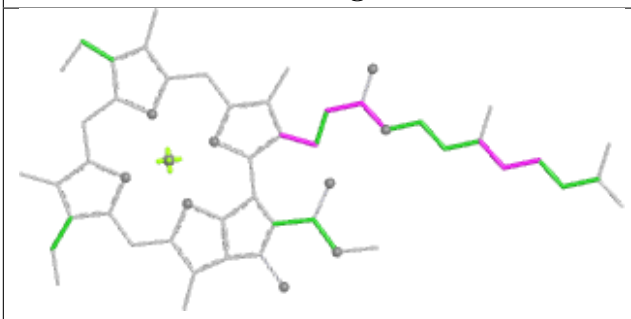
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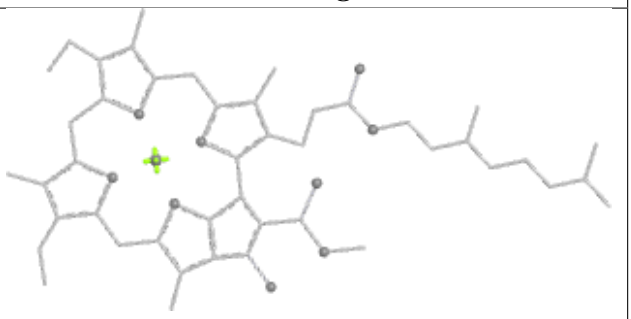
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Bond angles

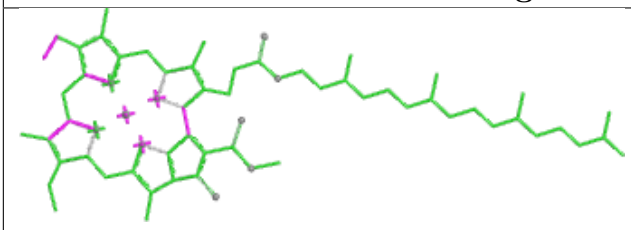


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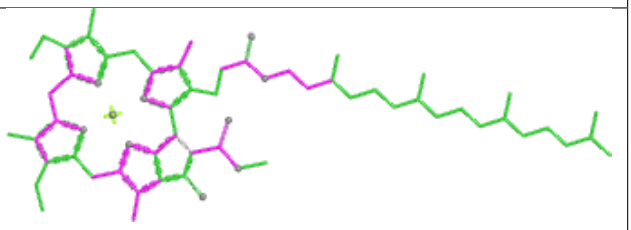


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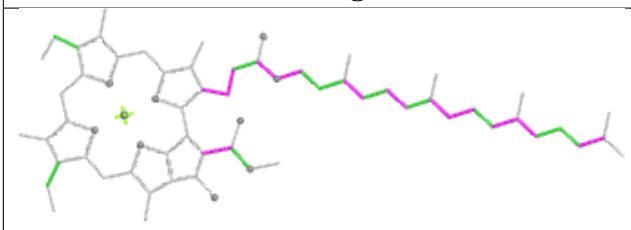
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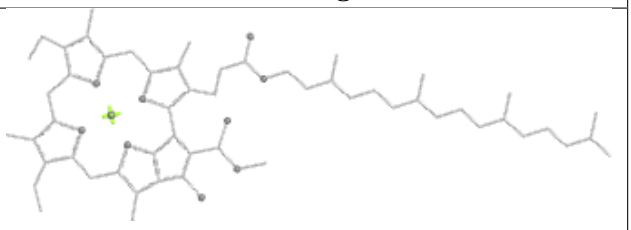
Bond lengths



Bond angles

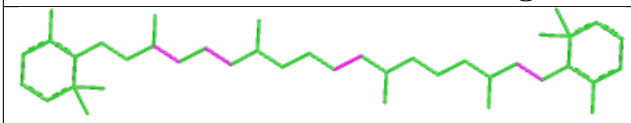


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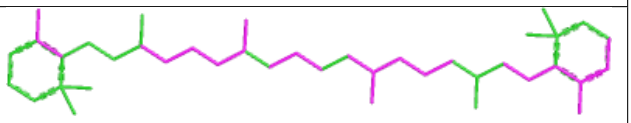


Rings

Ligand BCR J 4001



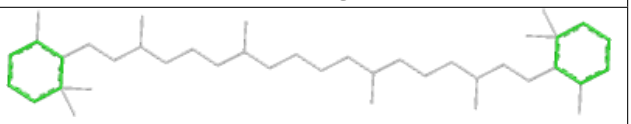
Bond lengths



Bond angles

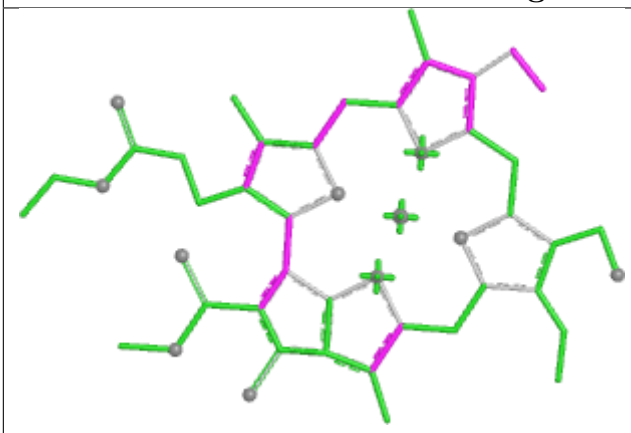


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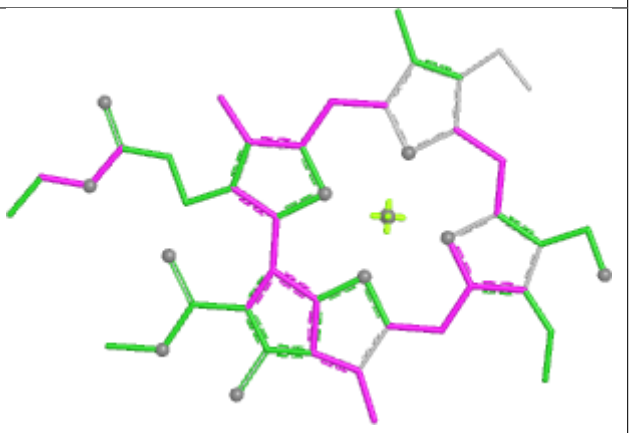


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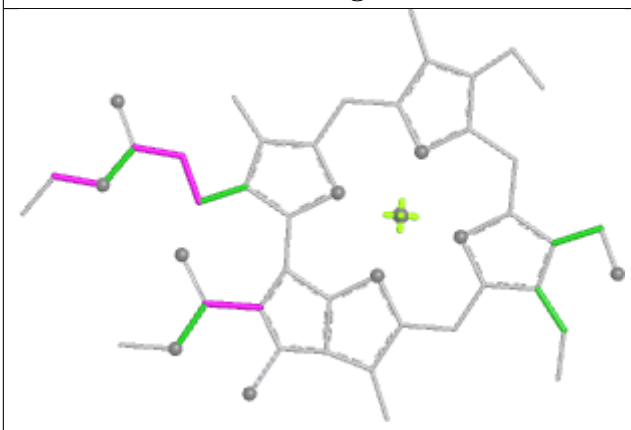
Ligand CHL 9 608



Bond lengths



Bond angles

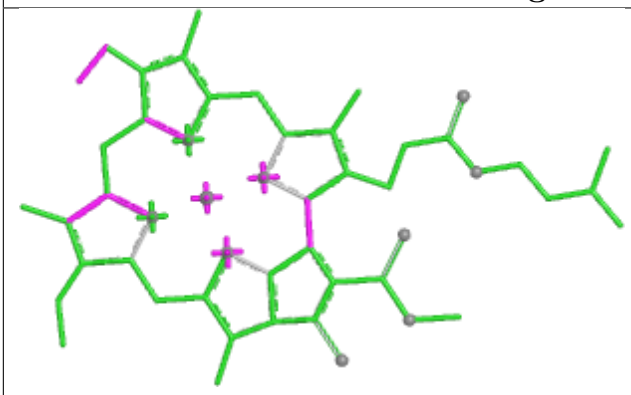


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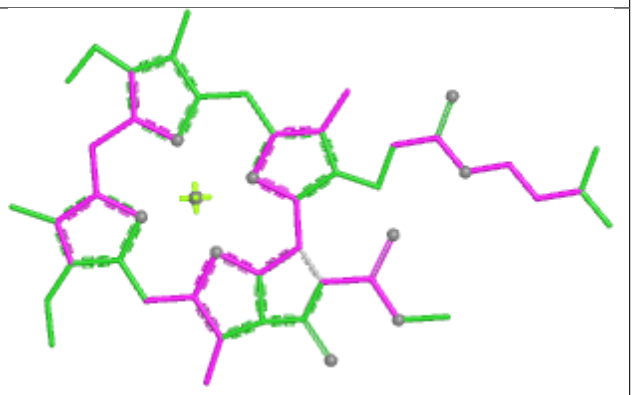


Rings

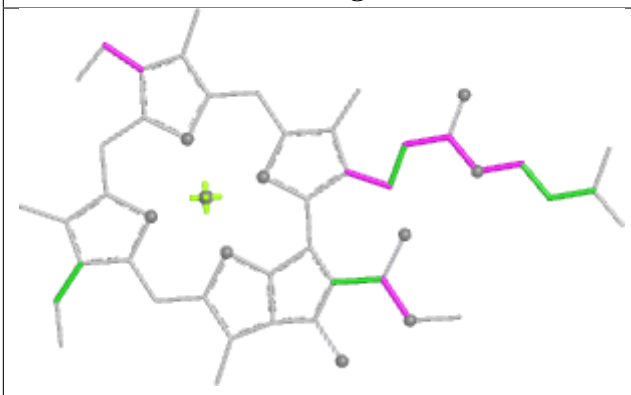
Ligand CLA 6 612



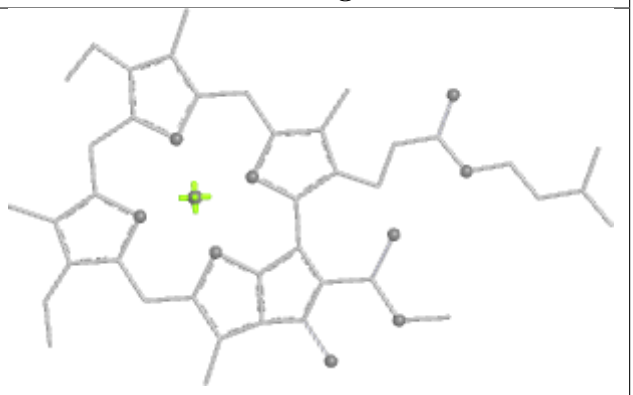
Bond lengths



Bond angles

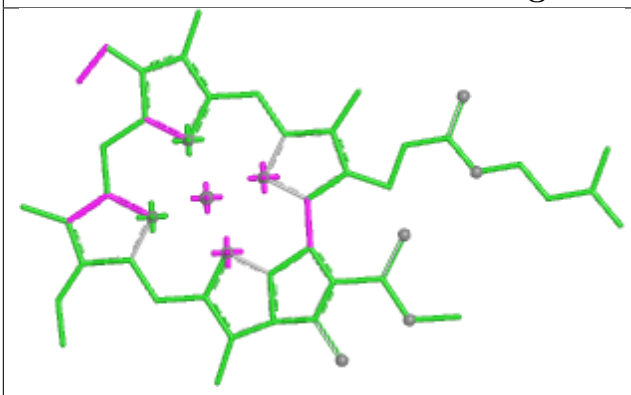


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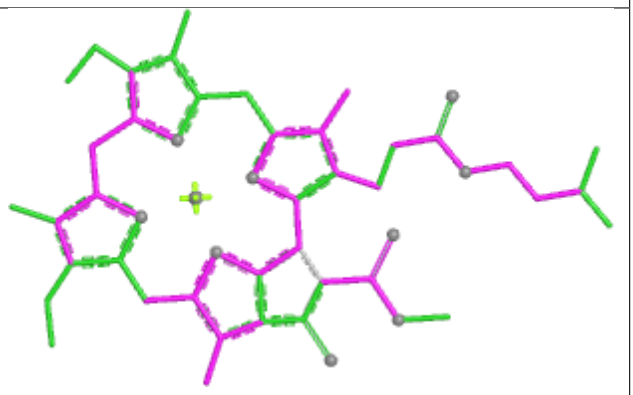


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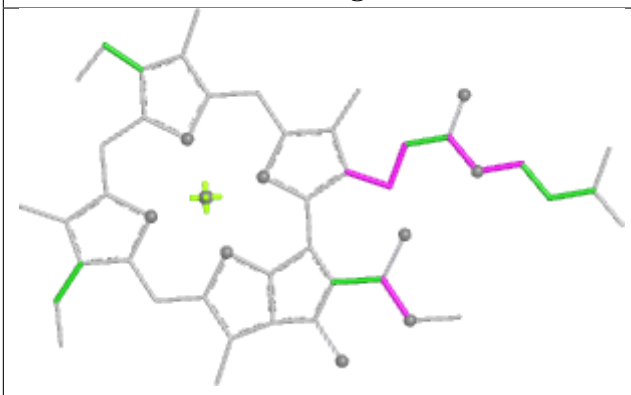
Ligand CLA a 602



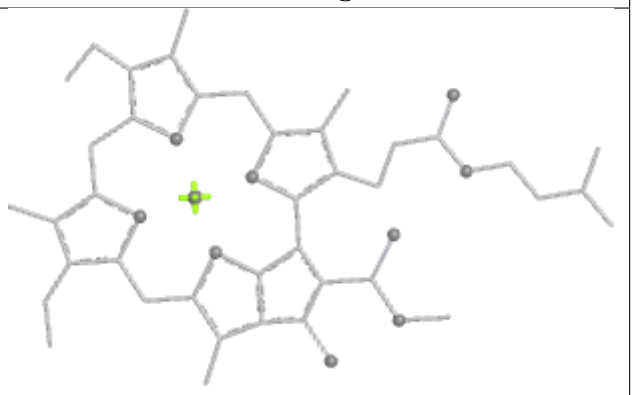
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Bond angles

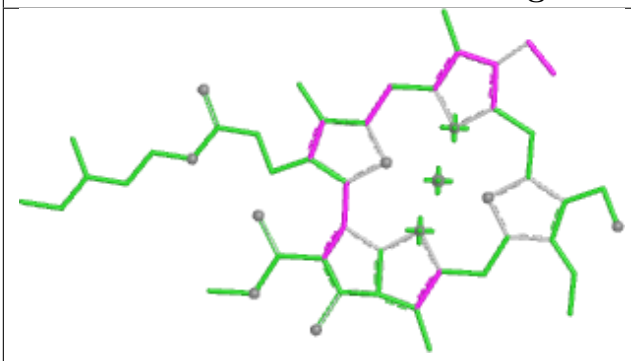


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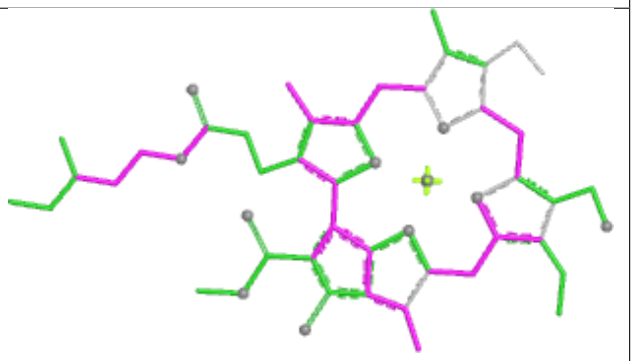


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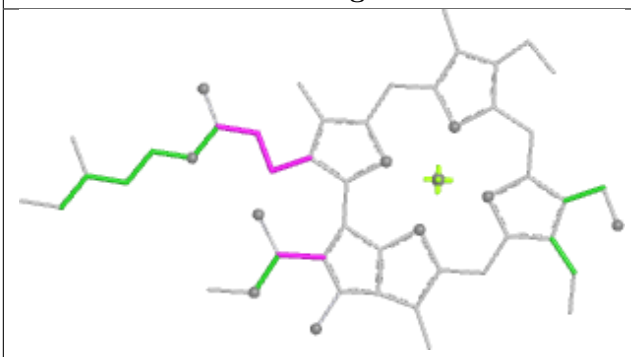
Ligand CHL 4 613



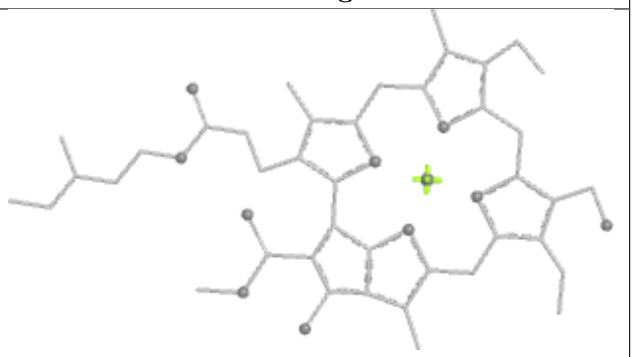
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Bond angles

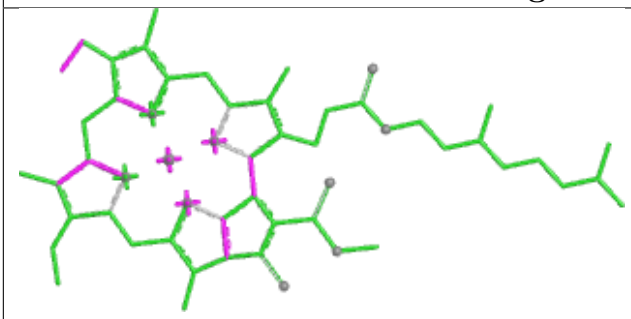


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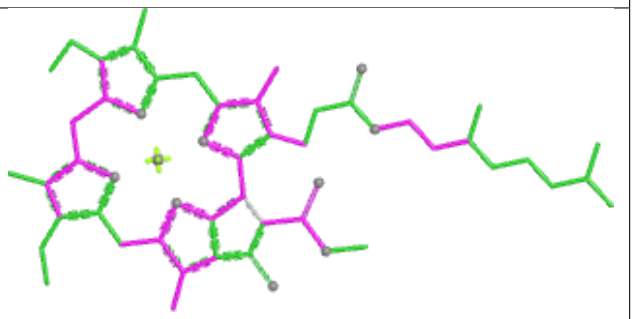


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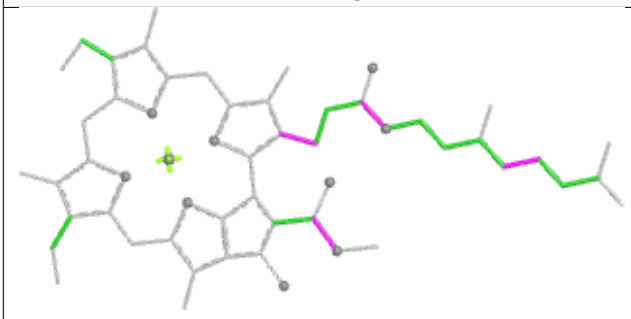
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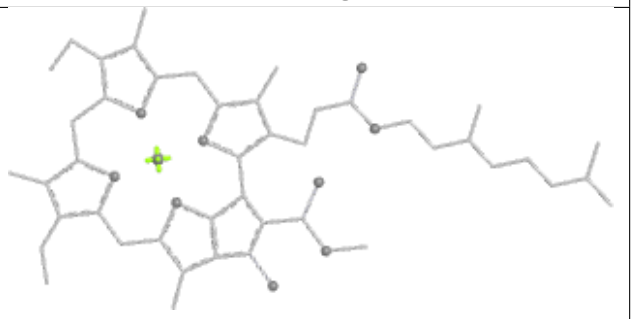
Bond lengths



Bond angles

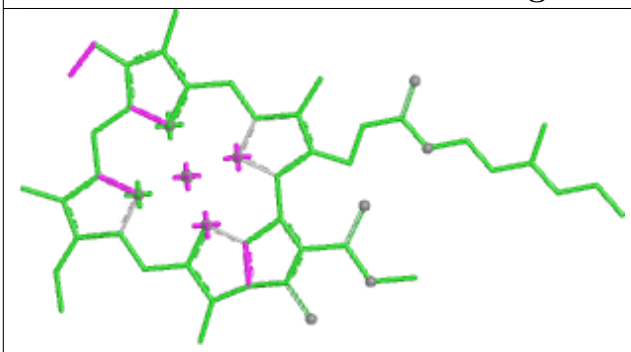


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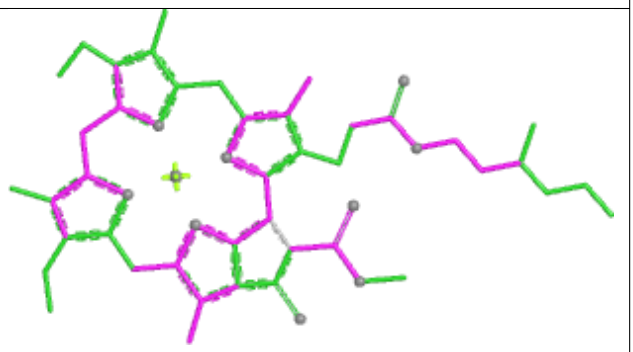


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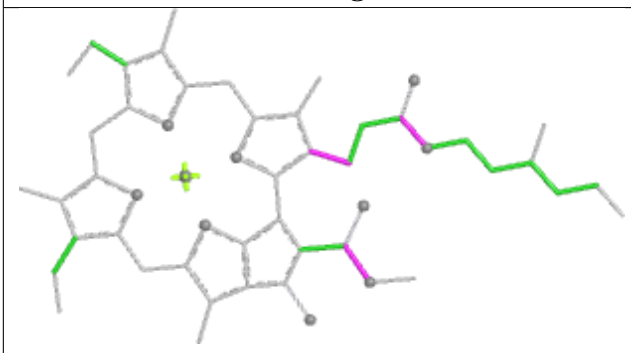
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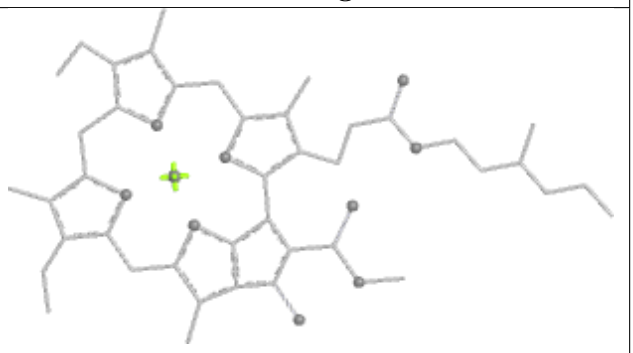
Bond lengths



Bond angles

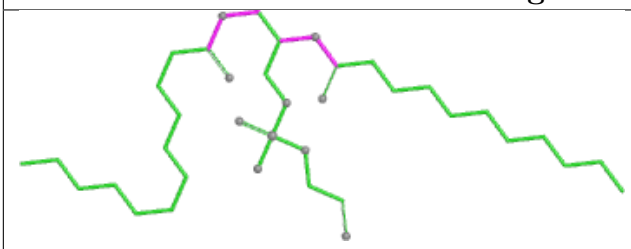


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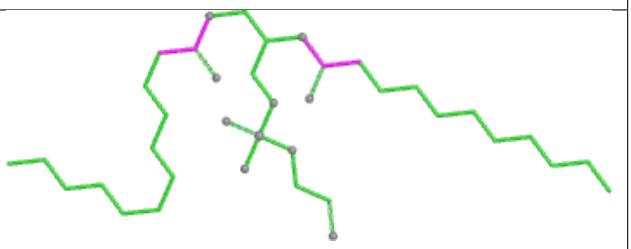


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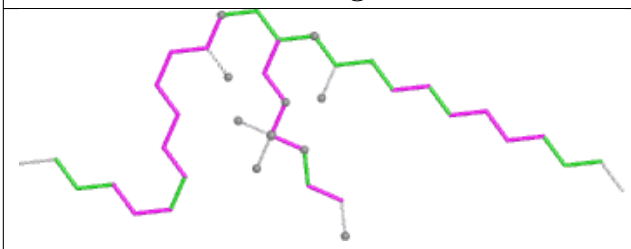
Ligand PTY a 803



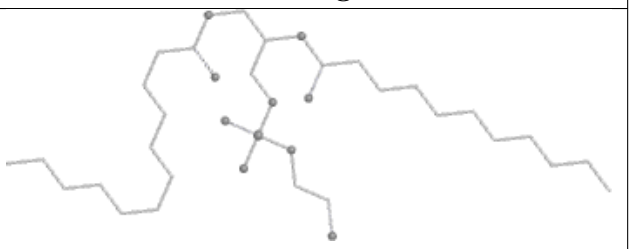
Bond lengths



Bond angles

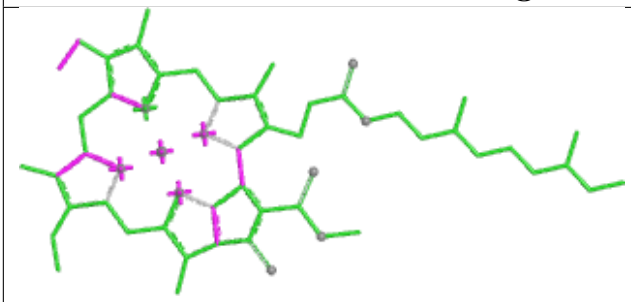


Torsions

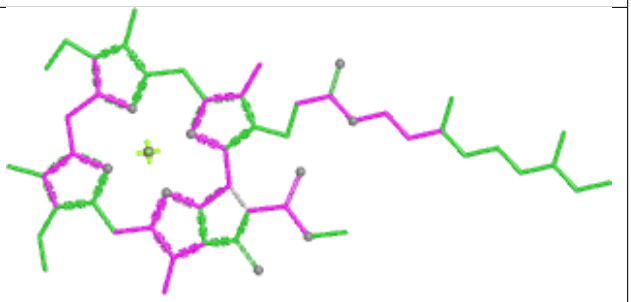


Rings

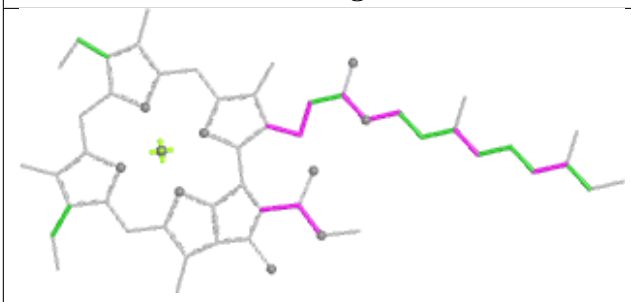
Ligand CLA B 1217



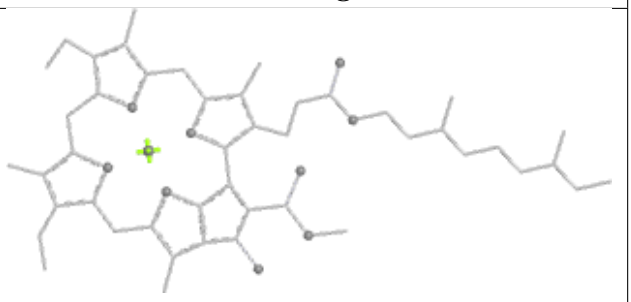
Bond lengths



Bond angles

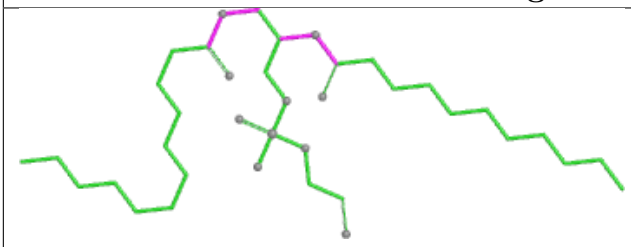


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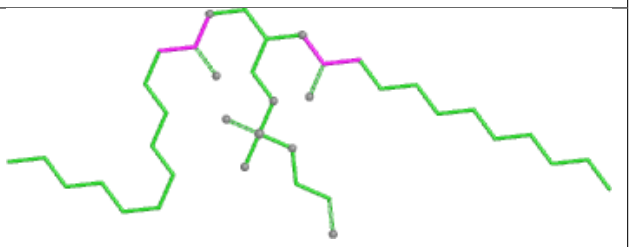


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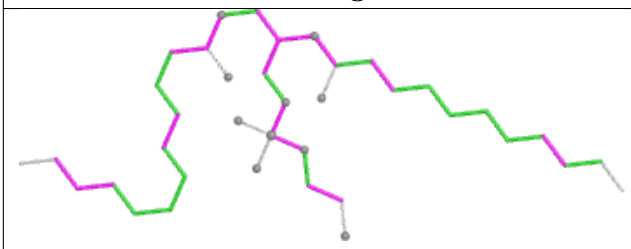
Ligand PTY 5 802



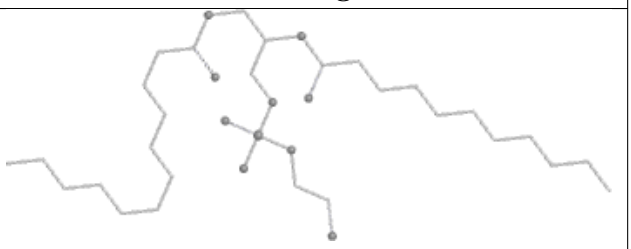
Bond lengths



Bond angles

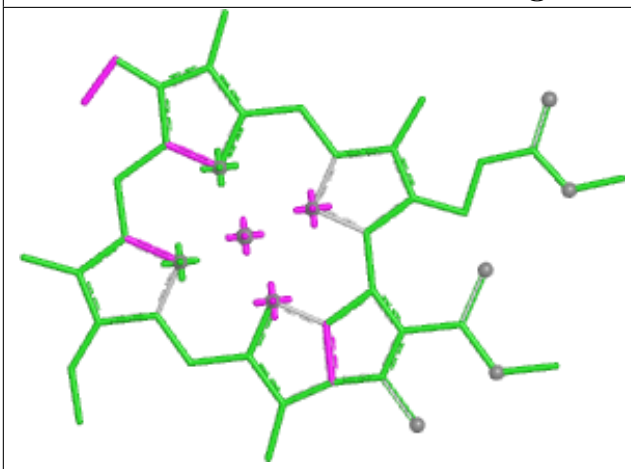


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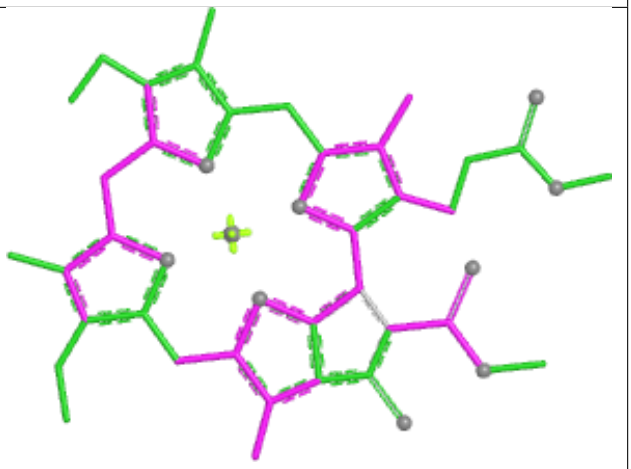


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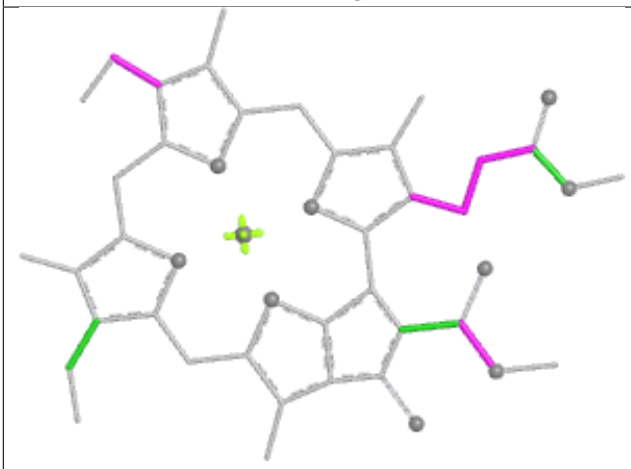
Ligand CLA 6 618



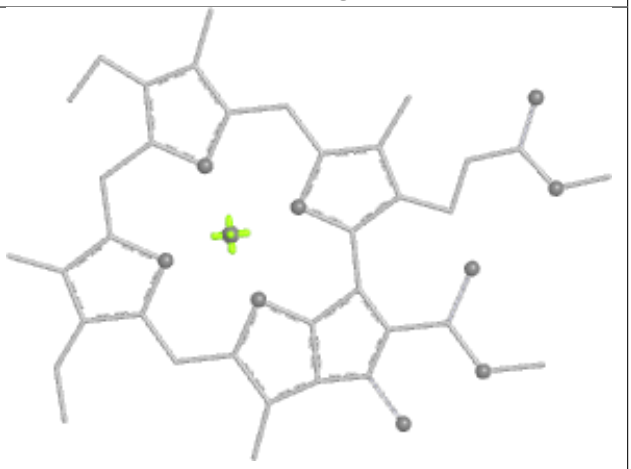
Bond lengths



Bond angles

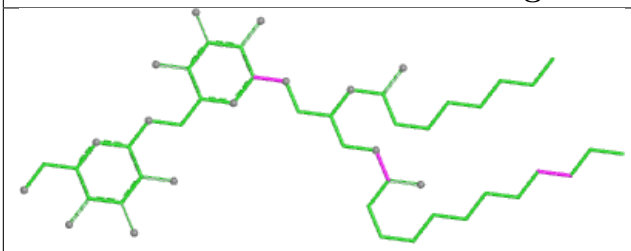


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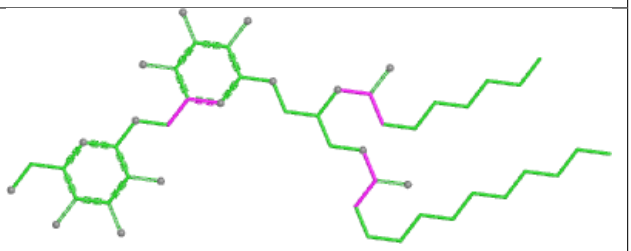


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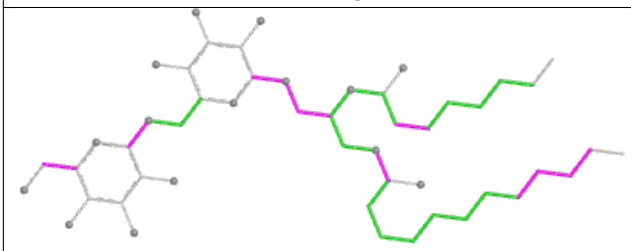
Ligand DGD 7 806



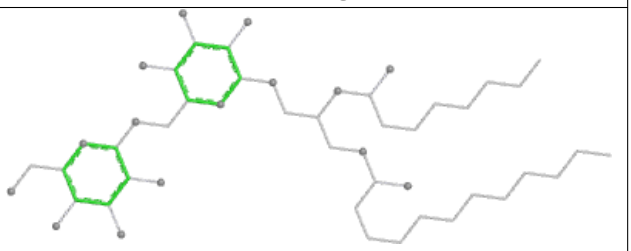
Bond lengths



Bond angles

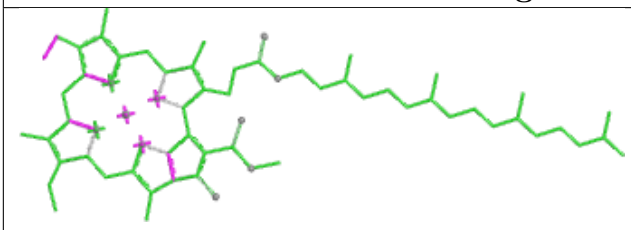


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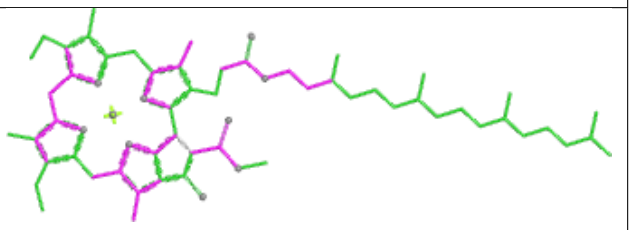


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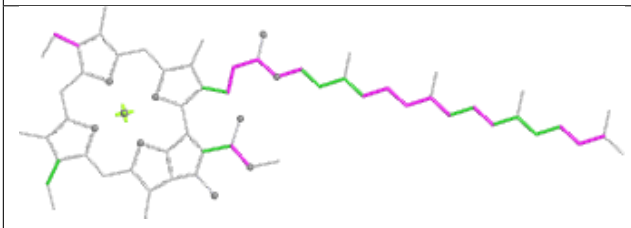
Ligand CLA B 1237



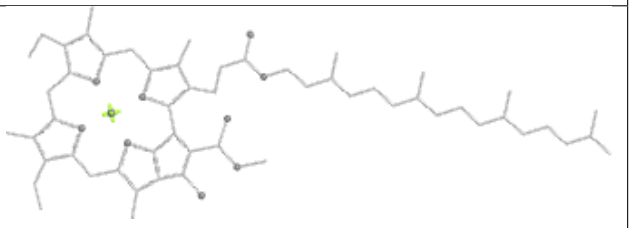
Bond lengths



Bond angles

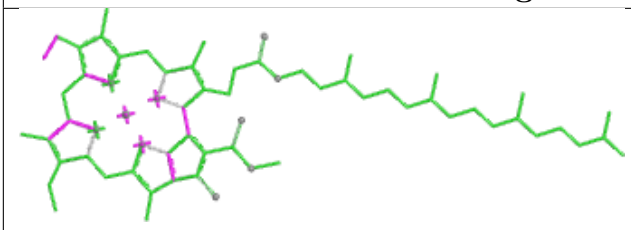


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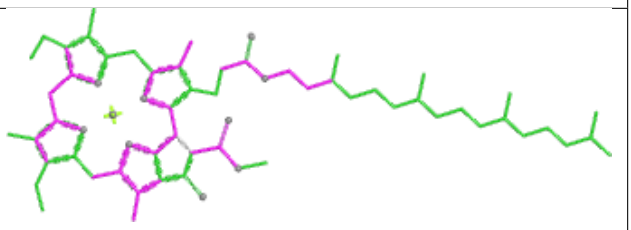


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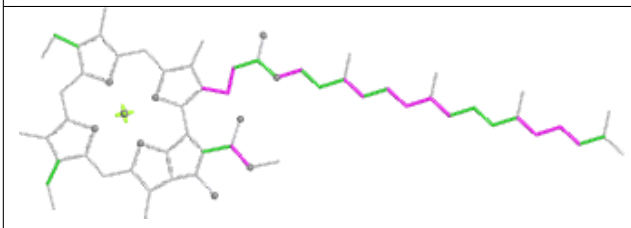
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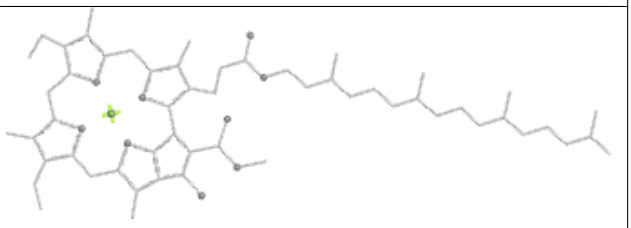
Bond lengths



Bond angles

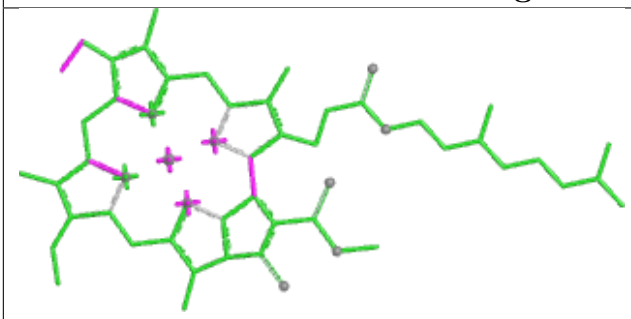


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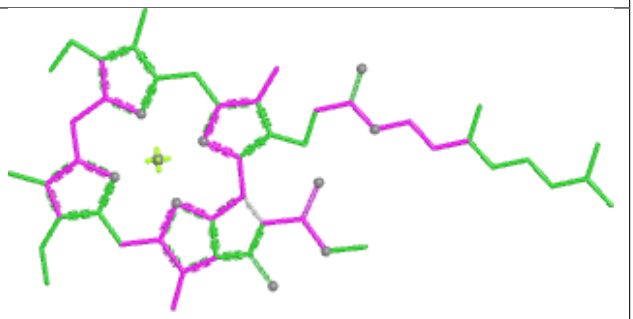


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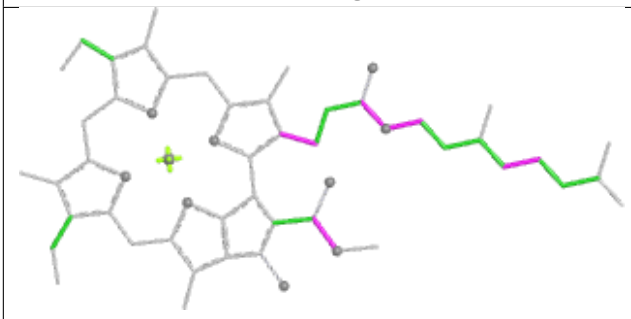
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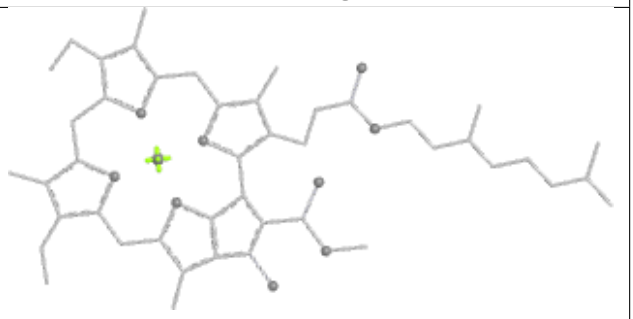
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Bond angles

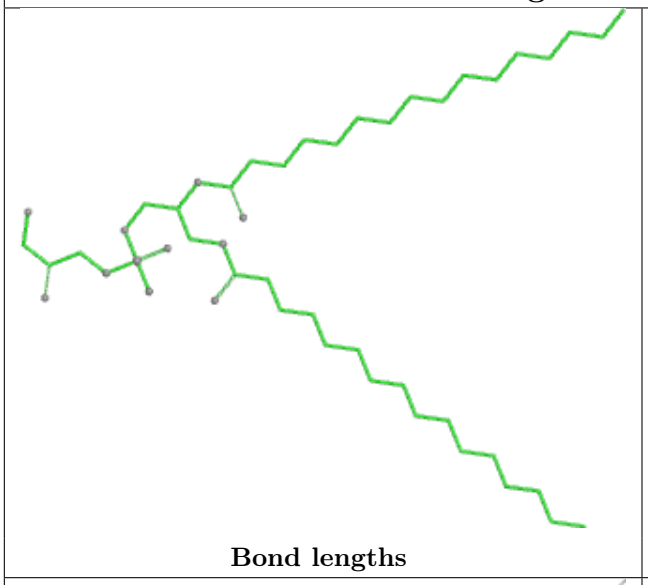


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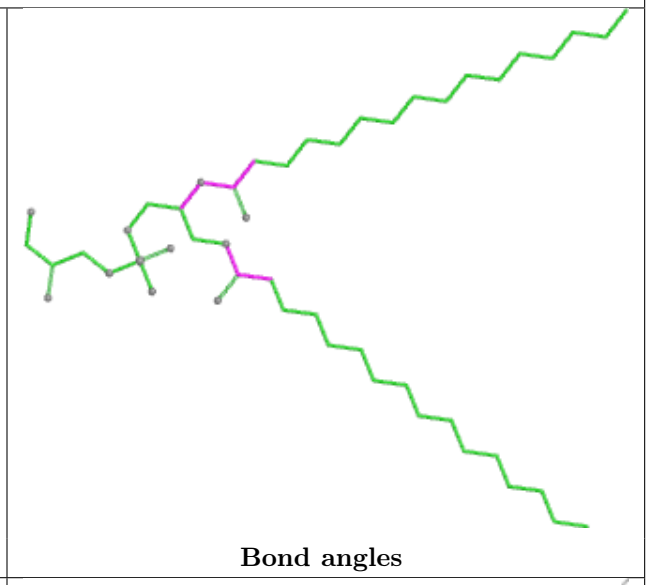


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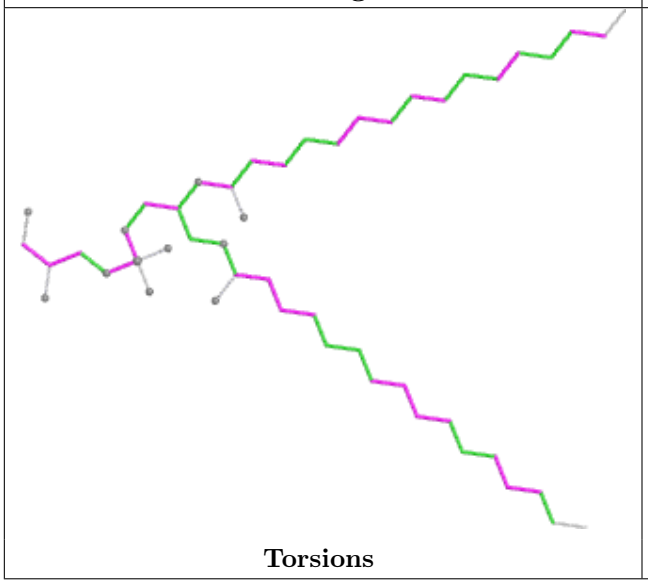
Ligand LHG 9 802



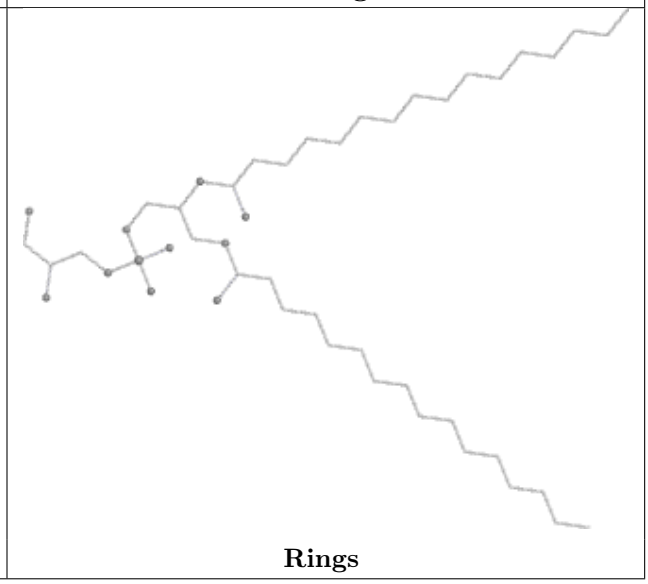
Bond lengths



Bond angles

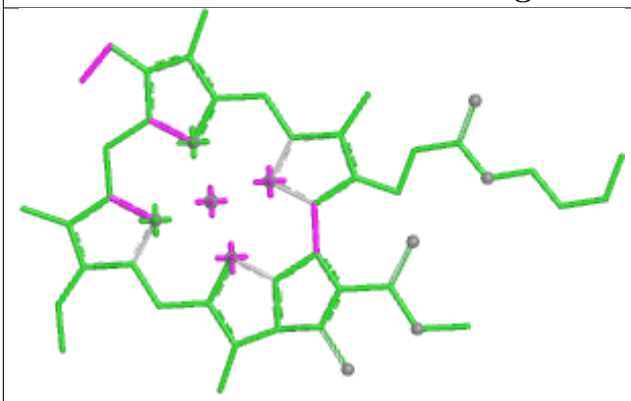


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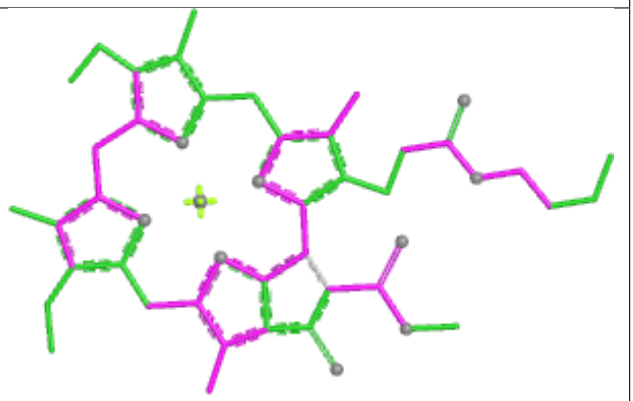


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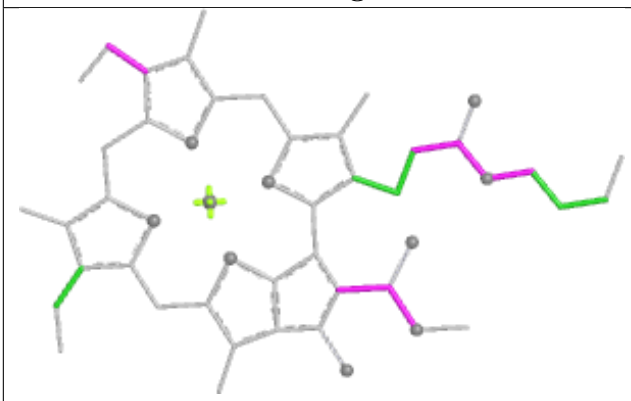
Ligand CLA K 1403



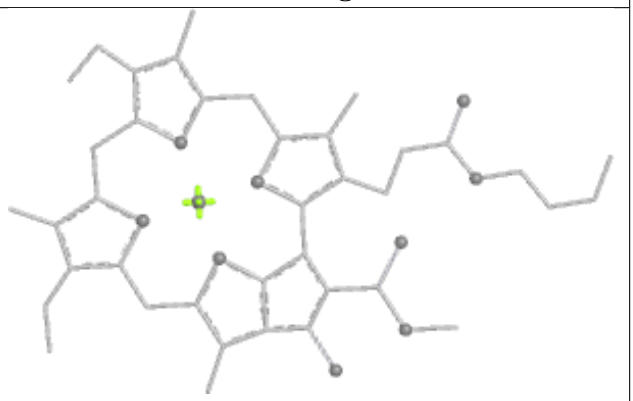
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Bond angles

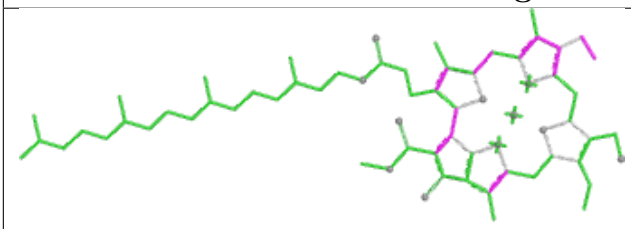


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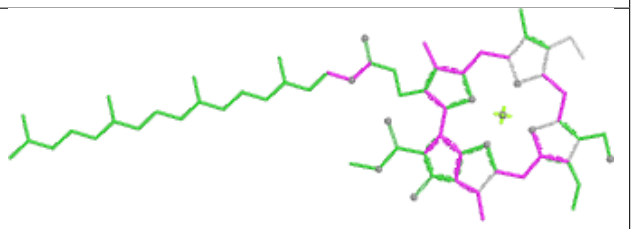


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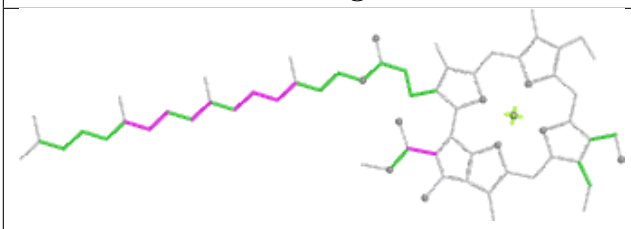
Ligand CHL A 1114



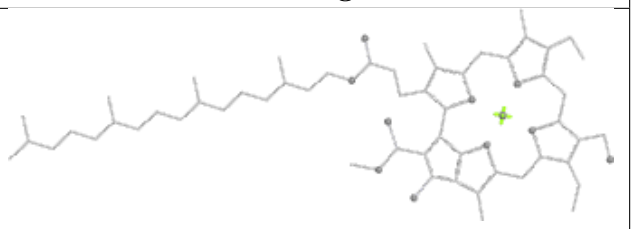
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Bond angles

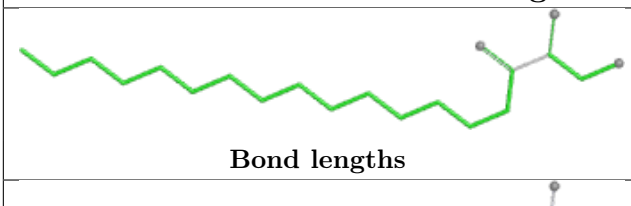


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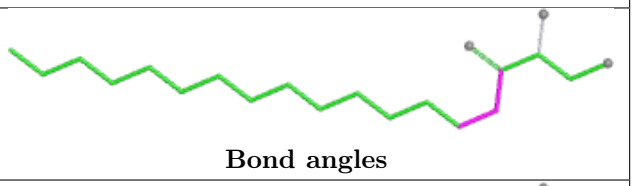


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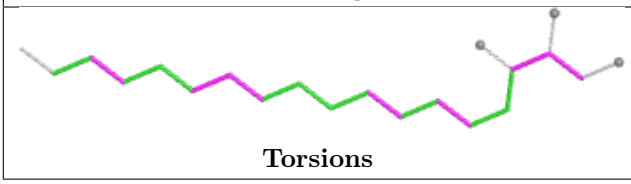
Ligand SPH 4 805



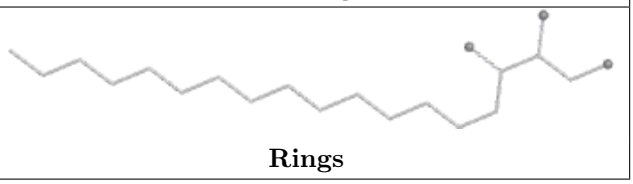
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Bond angles

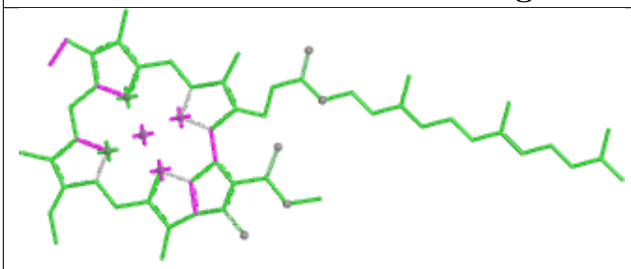


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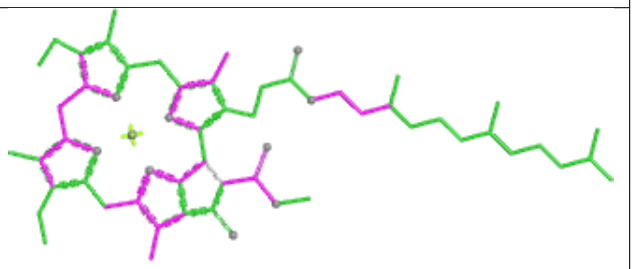


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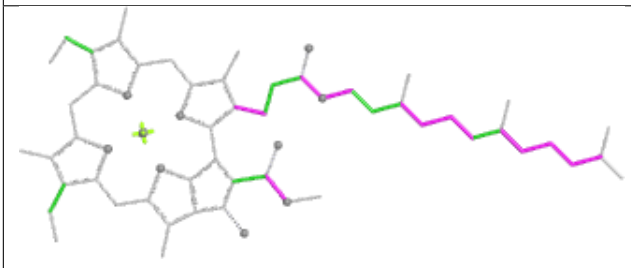
Ligand CLA B 1215



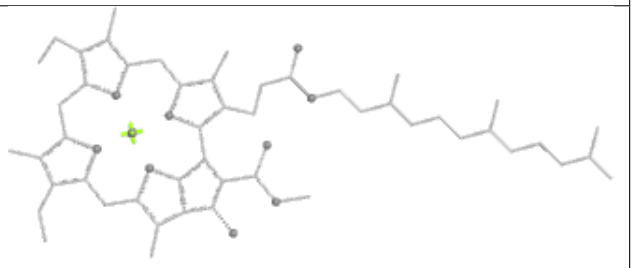
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Bond angles

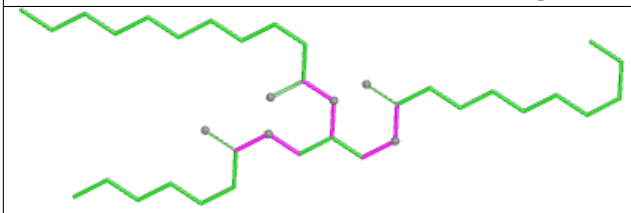


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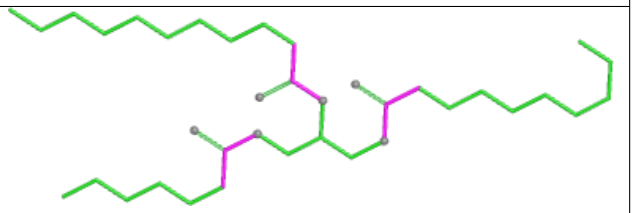


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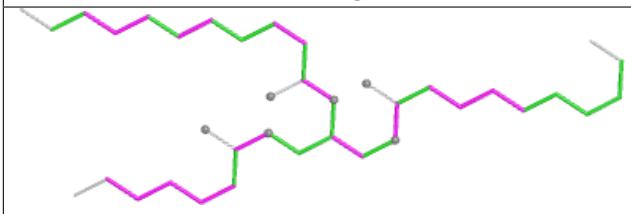
Ligand 4RF 7 807



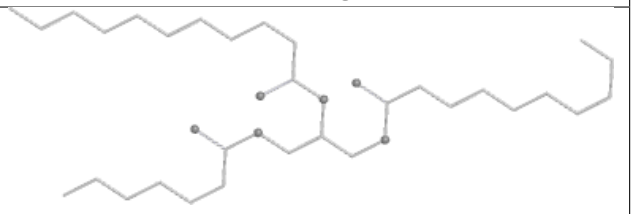
Bond lengths



Bond angles

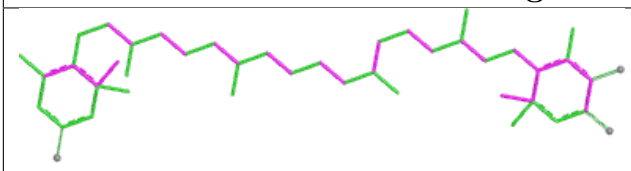


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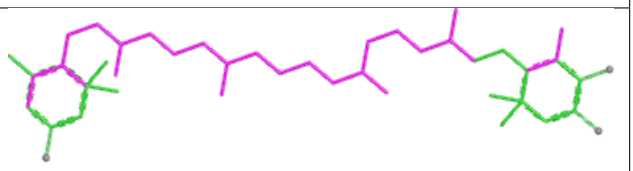


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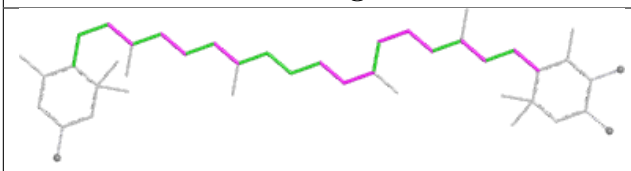
Ligand AXT 7 504



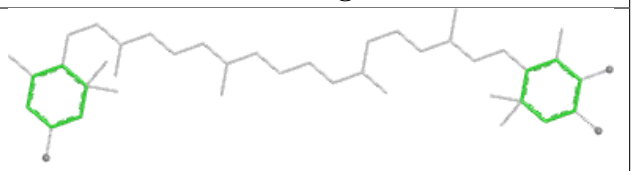
Bond lengths



Bond angles

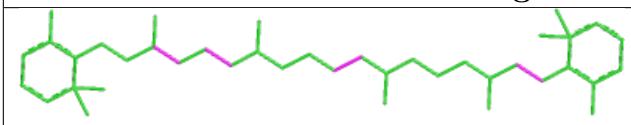


Torsions

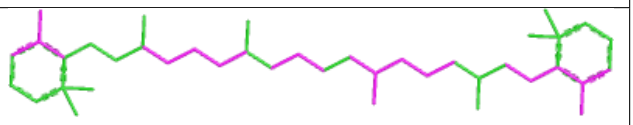


Rings

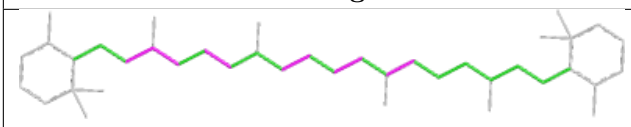
Ligand BCR A 4002



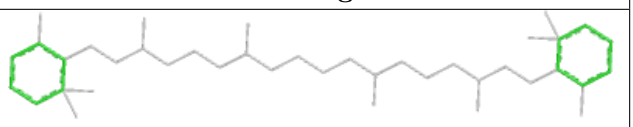
Bond lengths



Bond angles

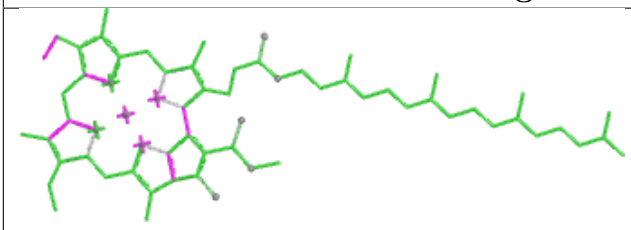


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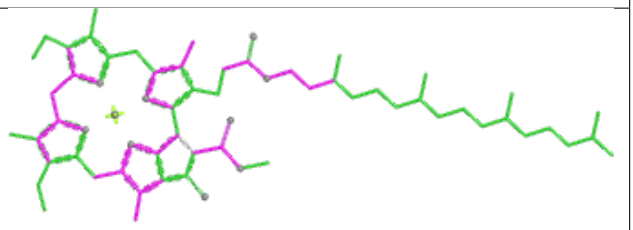


Rings

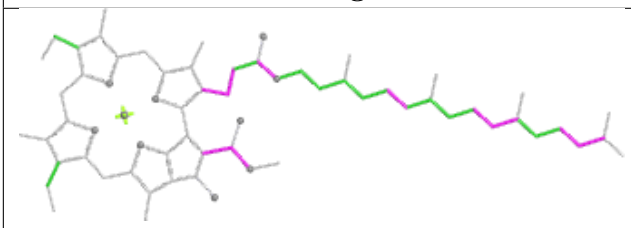
Ligand CLA B 1202



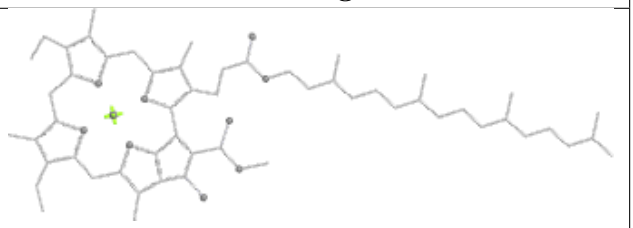
Bond lengths



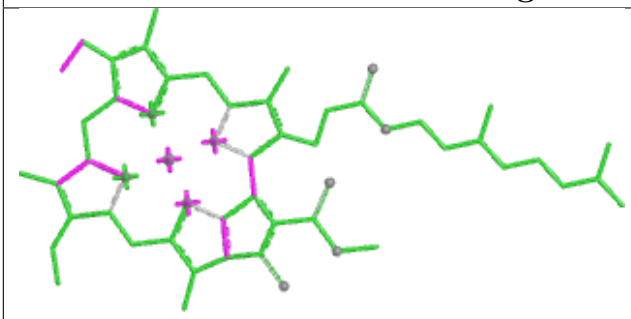
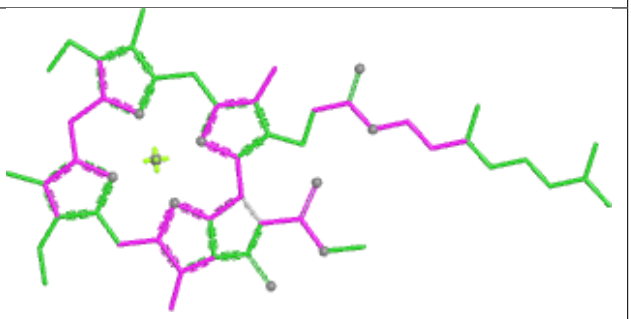
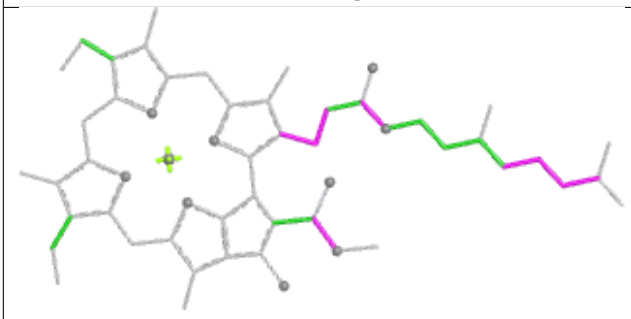
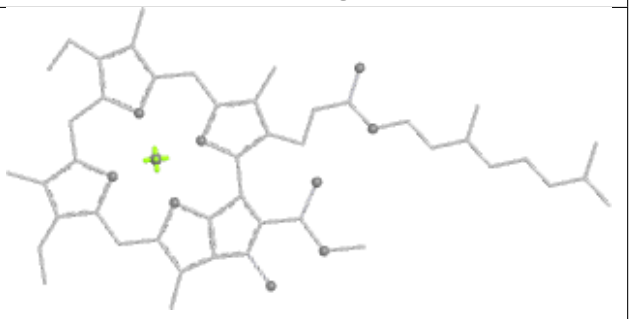
Bond angles

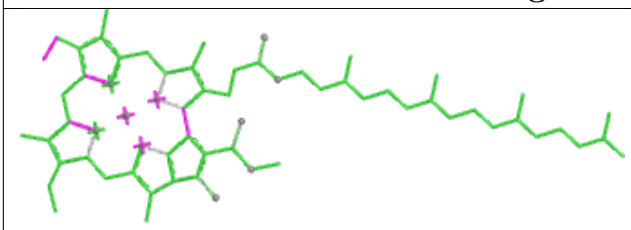
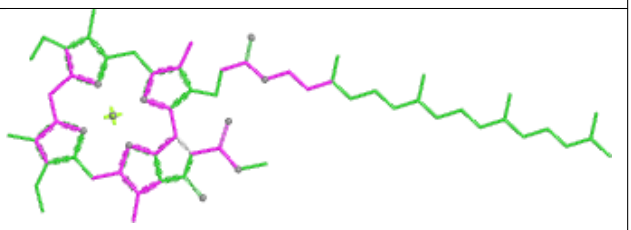
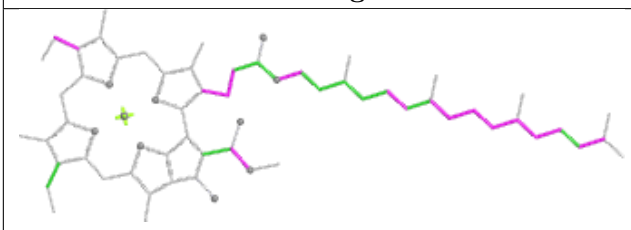
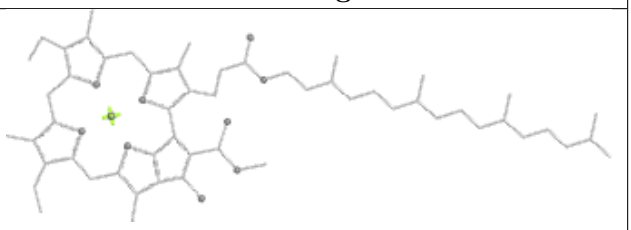


Torsions

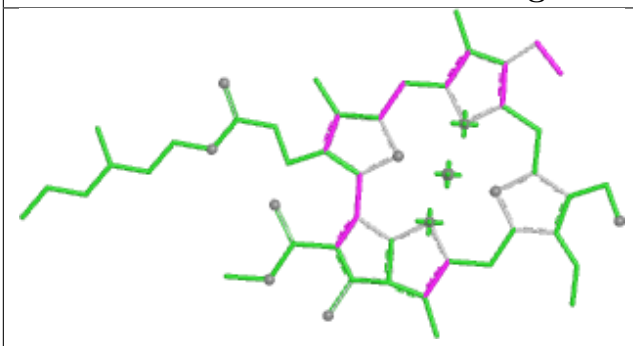


Rings

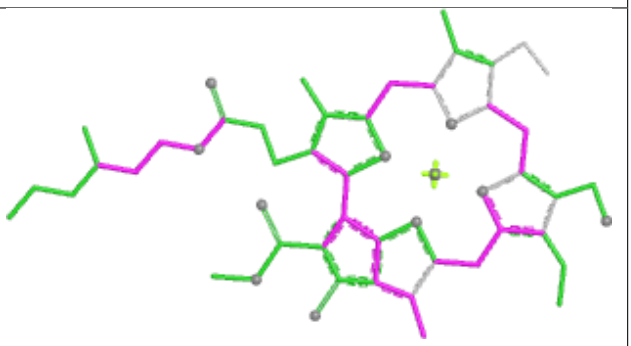
Ligand CLA F 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

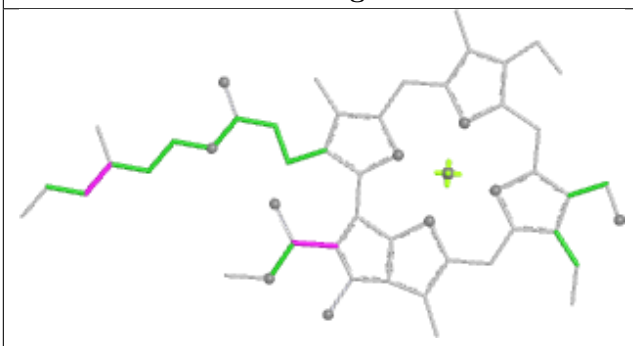
Ligand CHL a 609



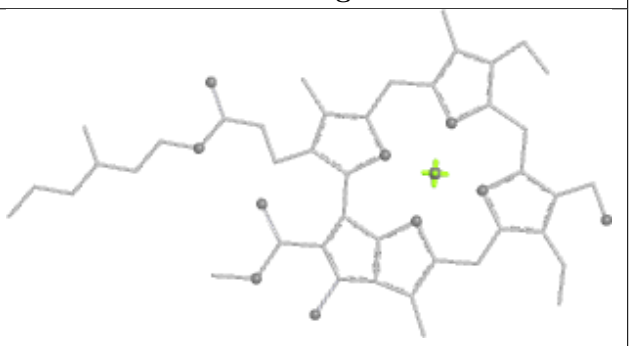
Bond lengths



Bond angles

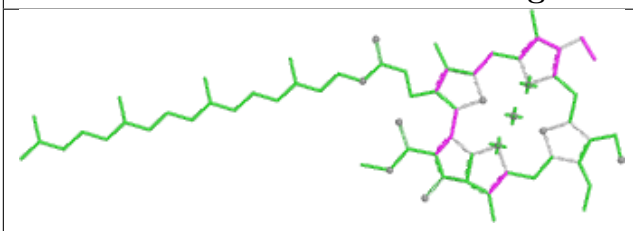


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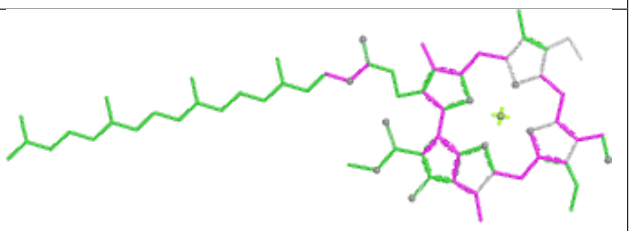


Rings

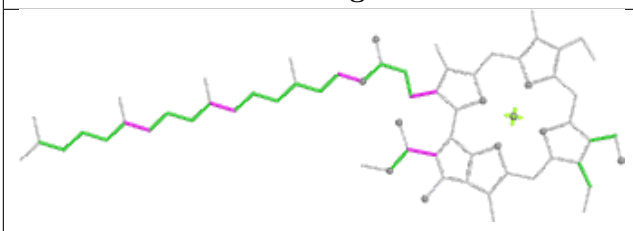
Ligand CHL 3 604



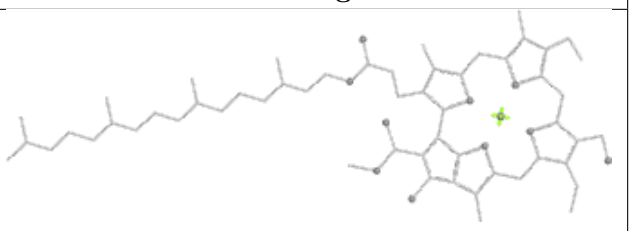
Bond lengths



Bond angles

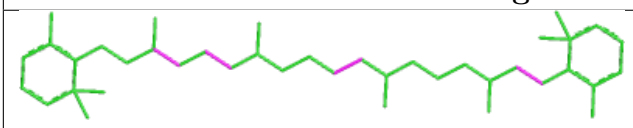


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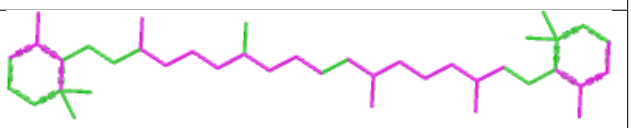


Rings

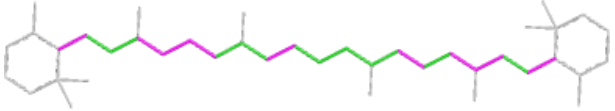
Ligand BCR H 4001



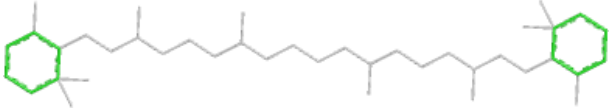
Bond lengths



Bond angles

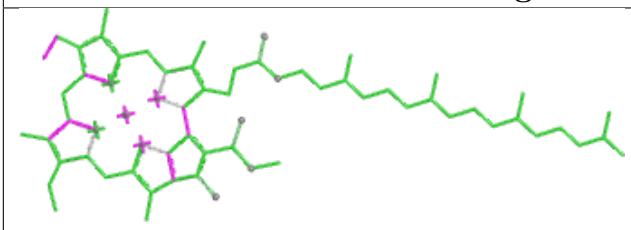


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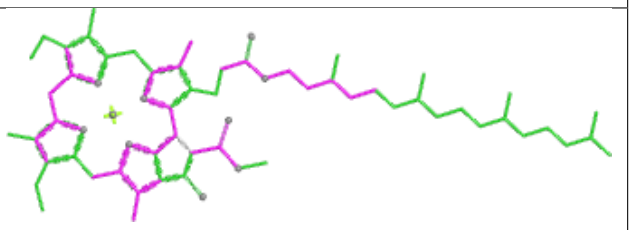


Rings

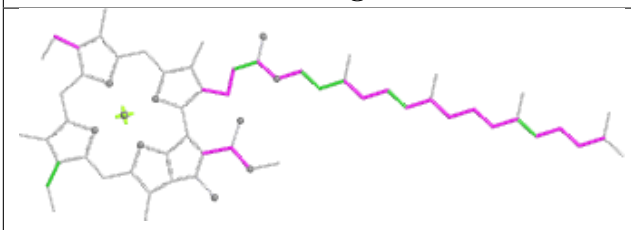
Ligand CLA A 1125



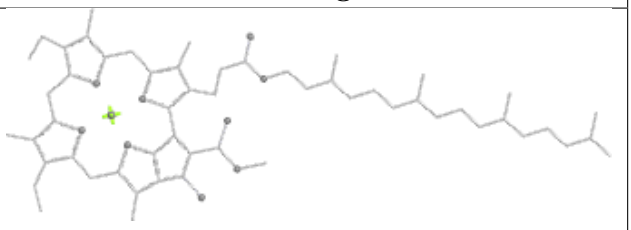
Bond lengths



Bond angles

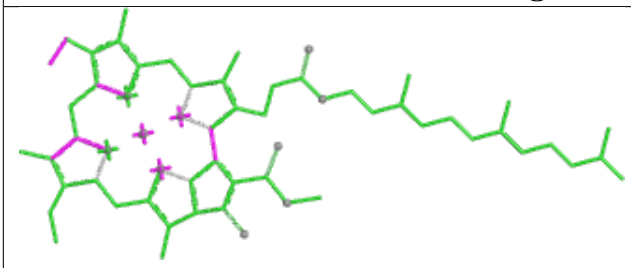


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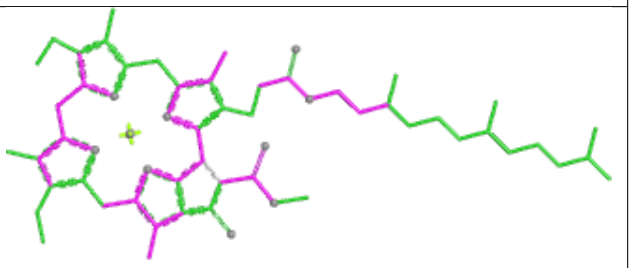


Rings

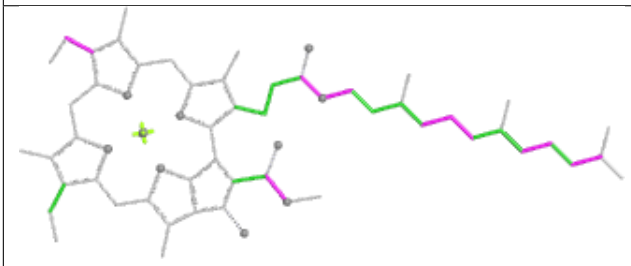
Ligand CLA 4 615



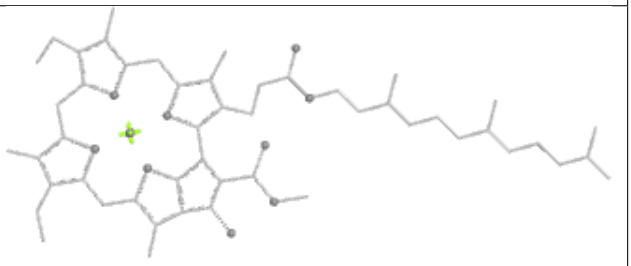
Bond lengths



Bond angles

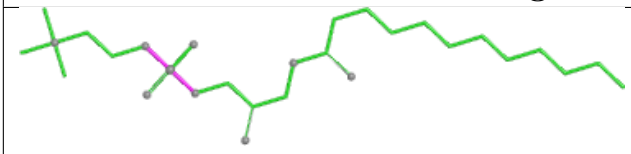


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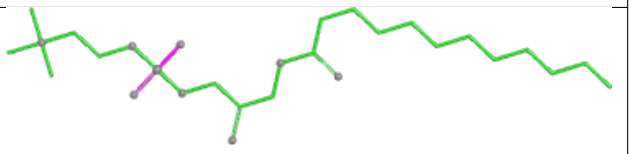


Rings

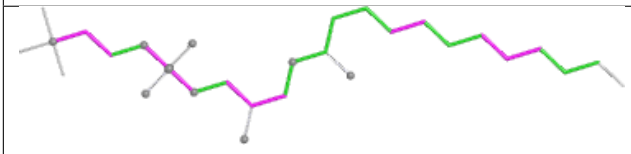
Ligand LAP 8 810



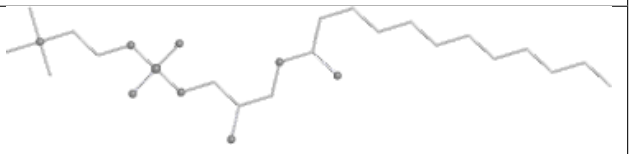
Bond lengths



Bond angles

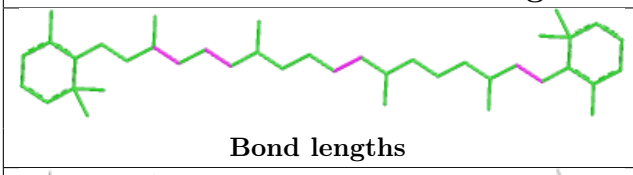


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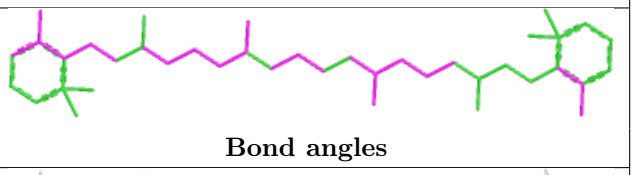


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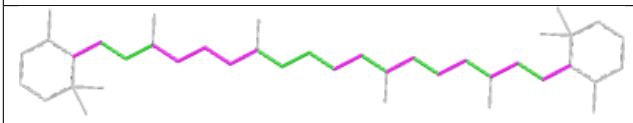
Ligand BCR 6 503



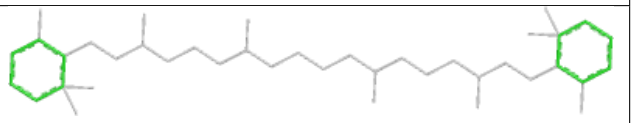
Bond lengths



Bond angles



Torsions

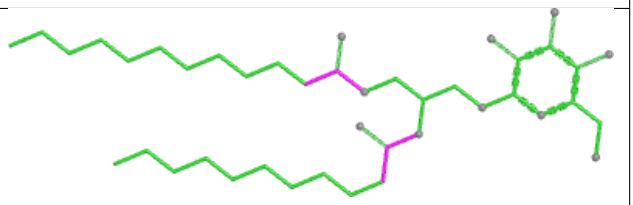


Rings

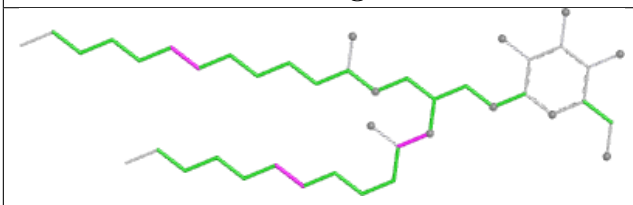
Ligand LMG A 5004



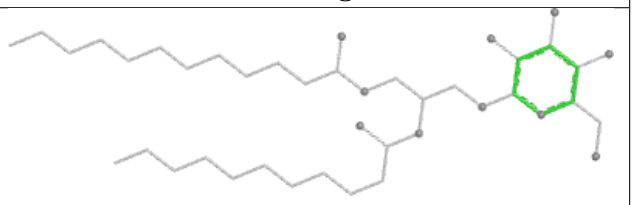
Bond lengths



Bond angles

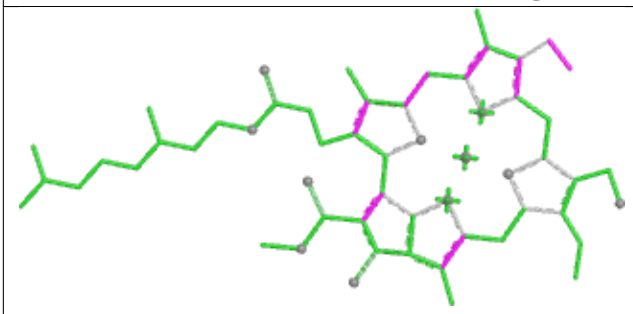


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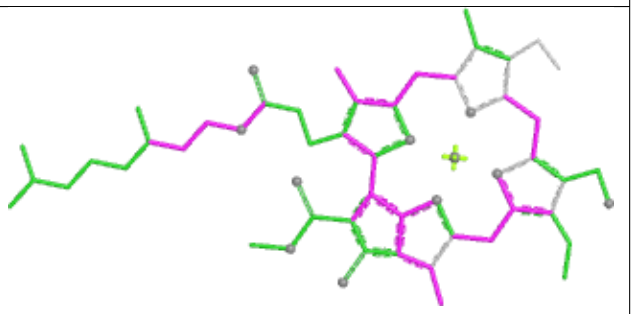


Rings

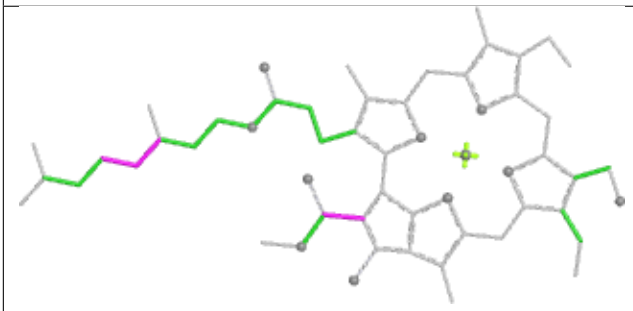
Ligand CHL 5 613



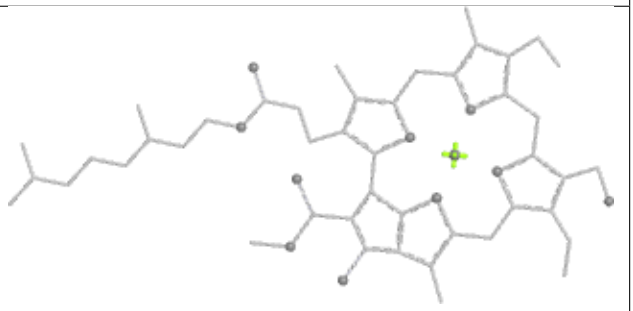
Bond lengths



Bond angles

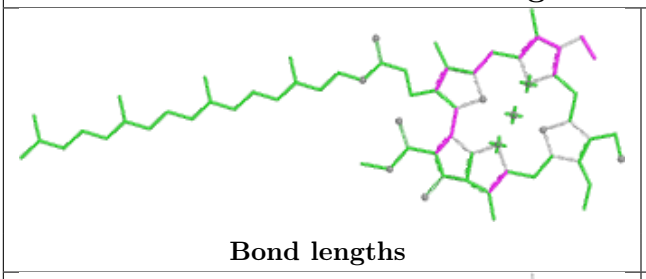


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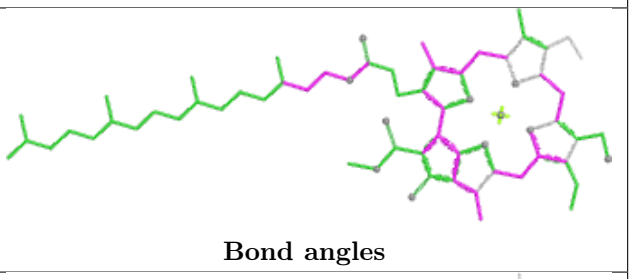


Rings

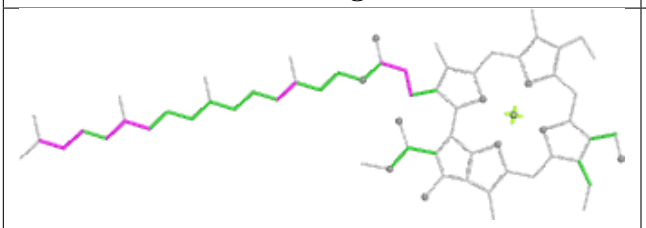
Ligand CHL 4 609



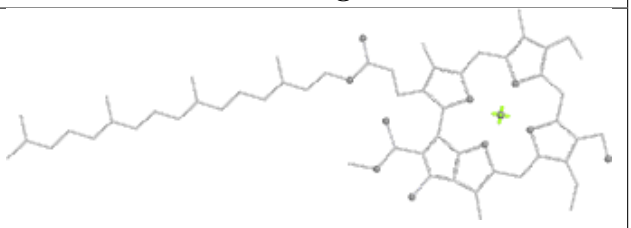
Bond lengths



Bond angles

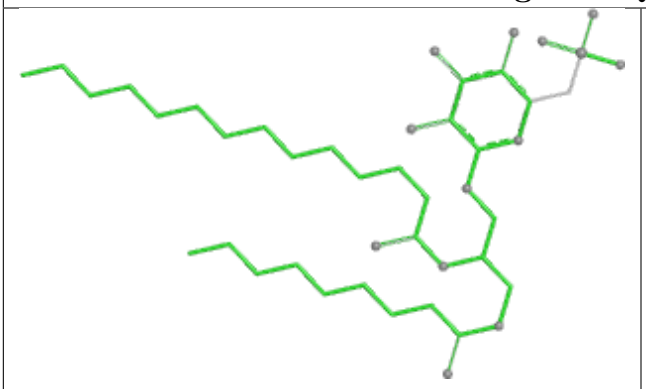


Torsions

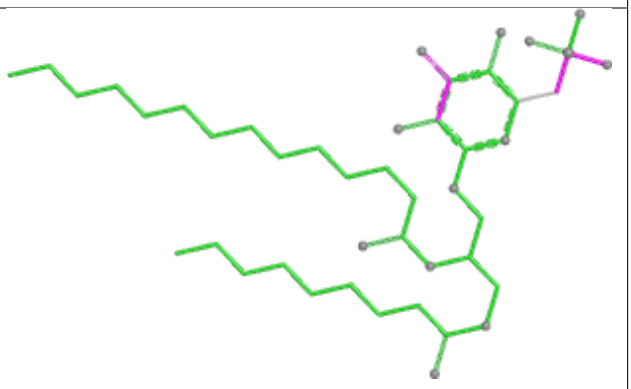


Rings

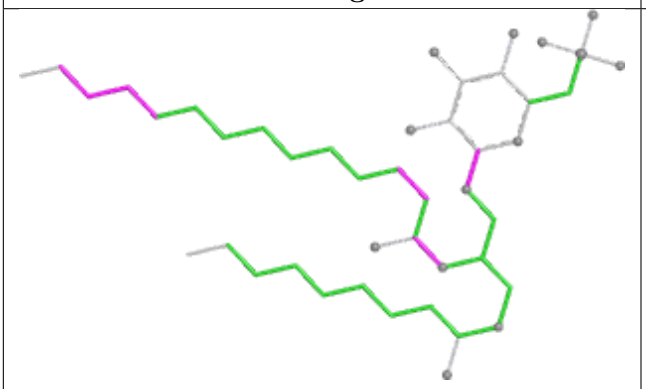
Ligand SQD H 5001



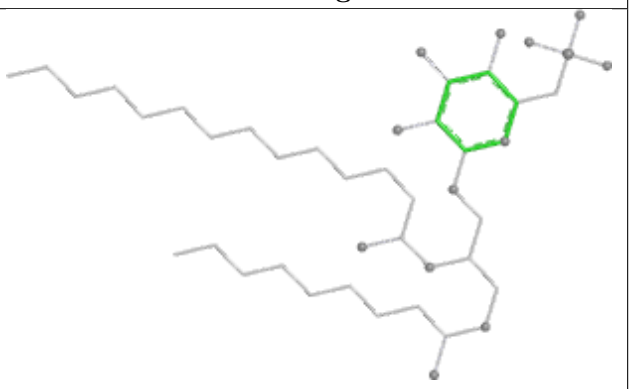
Bond lengths



Bond angles

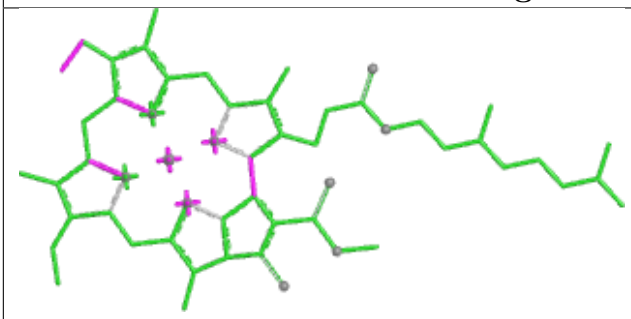


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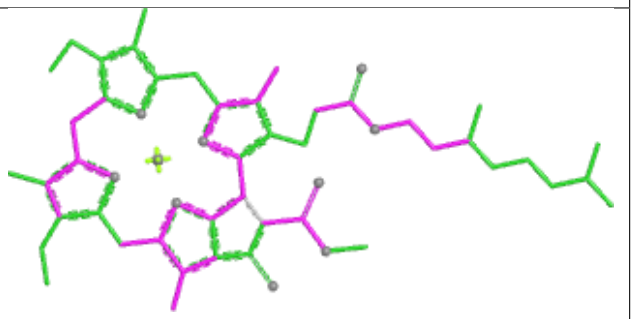


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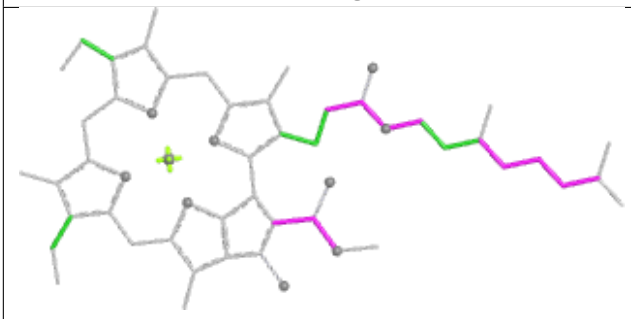
Ligand CLA A 1112



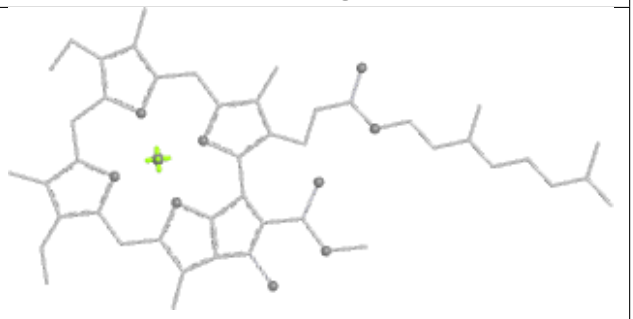
Bond lengths



Bond angles

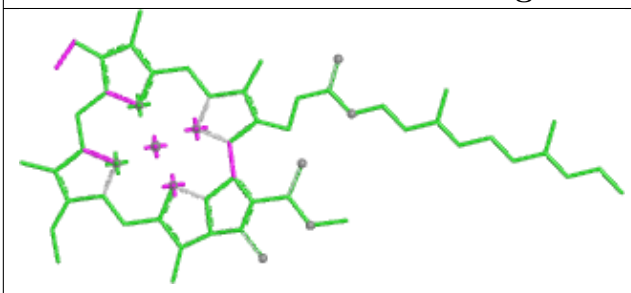


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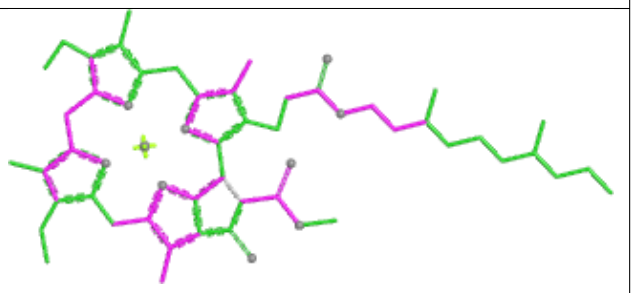


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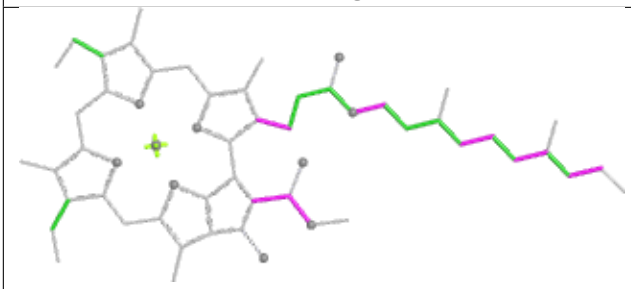
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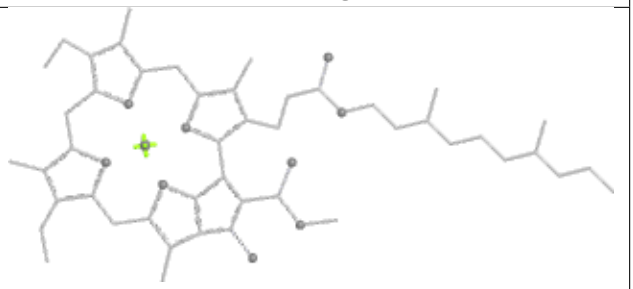
Bond lengths



Bond angles

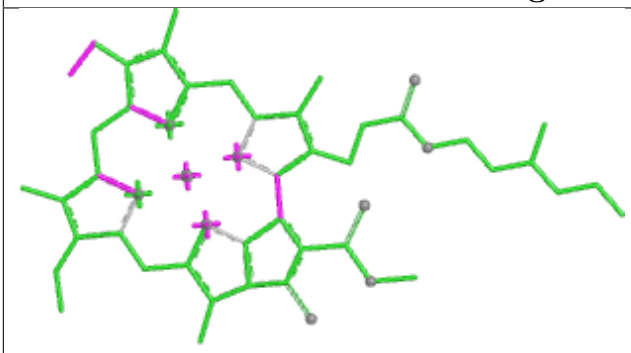


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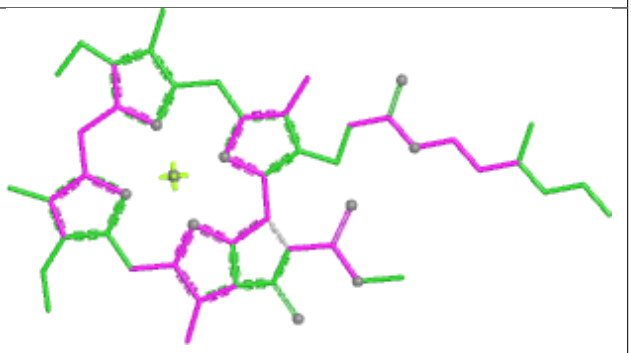


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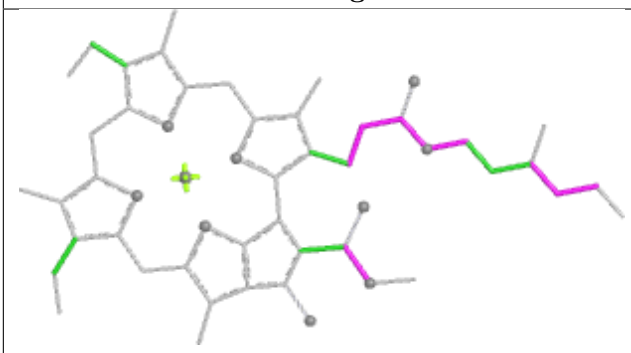
Ligand CLA 5 602



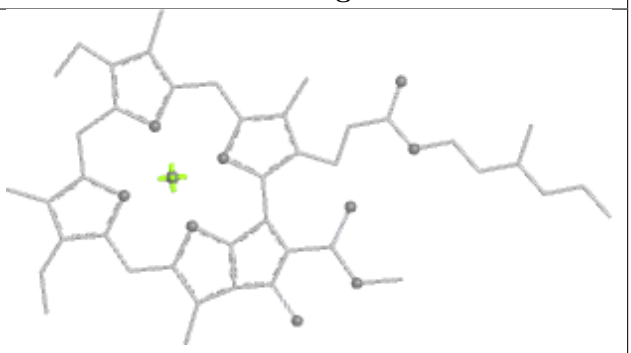
Bond lengths



Bond angles

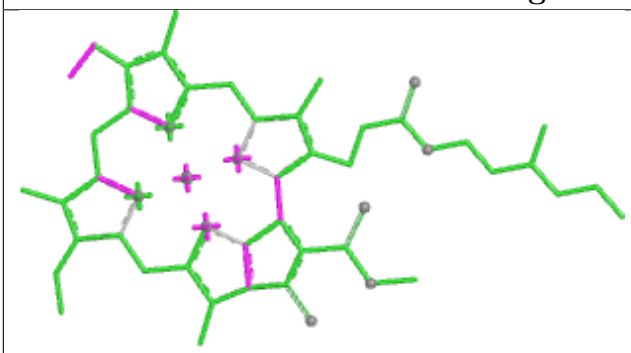


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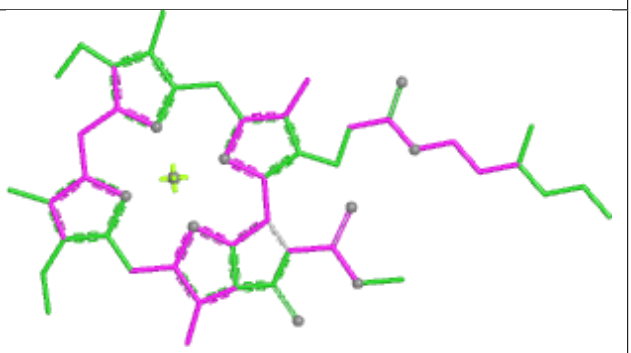


Rings

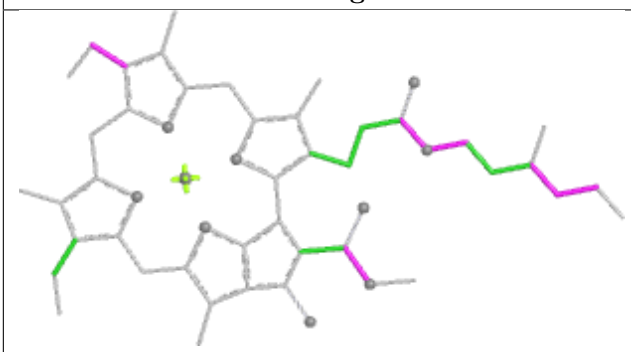
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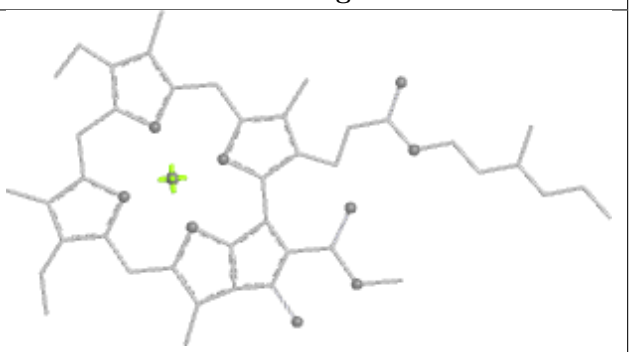
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Bond angles

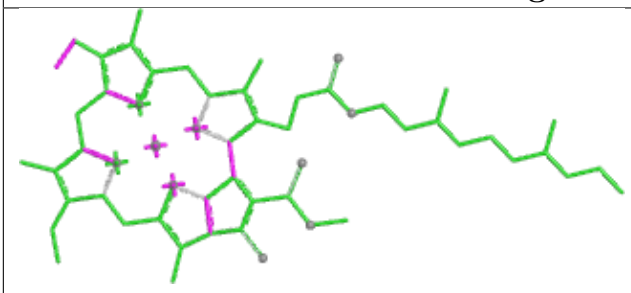


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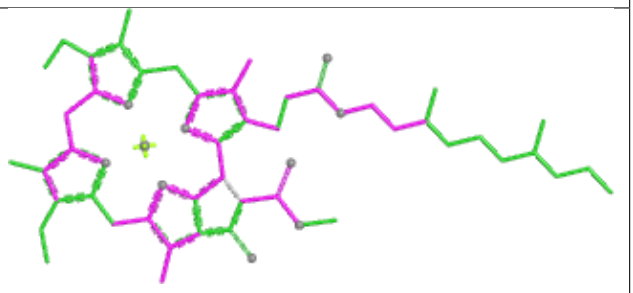


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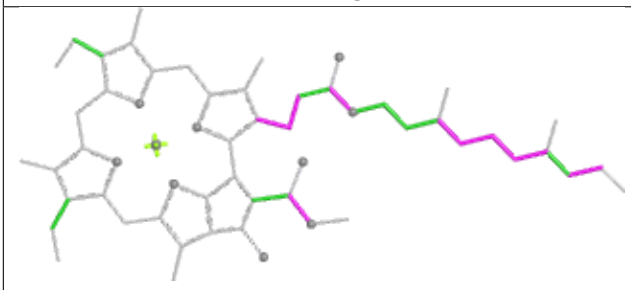
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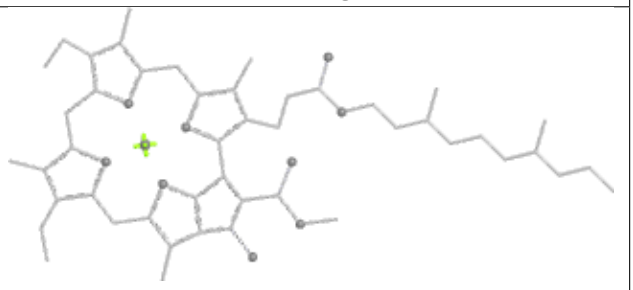
Bond lengths



Bond angles

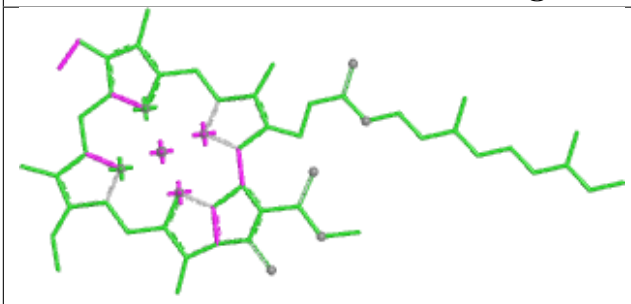


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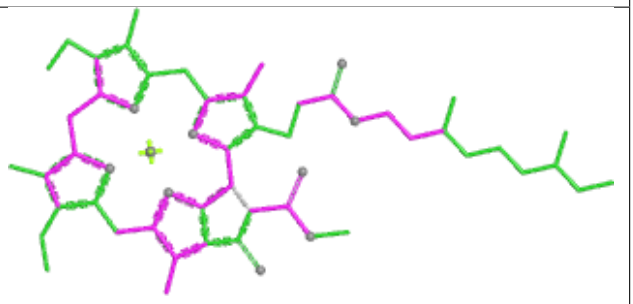


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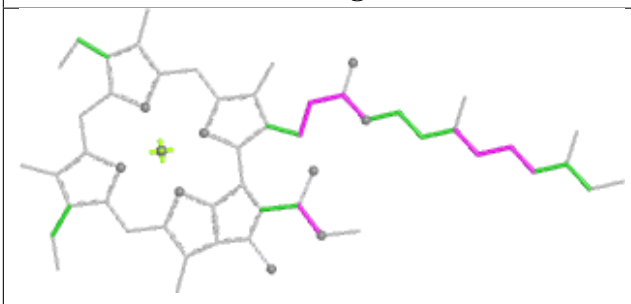
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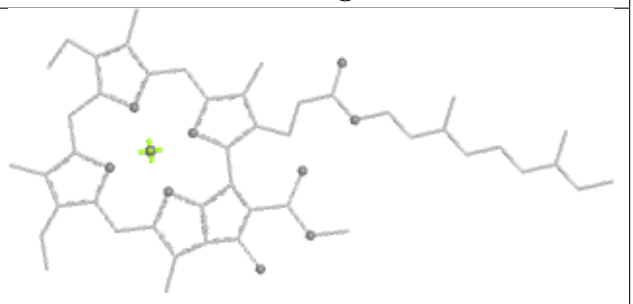
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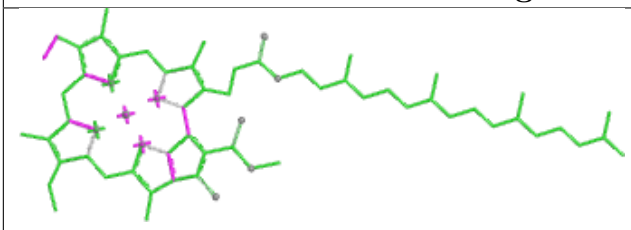
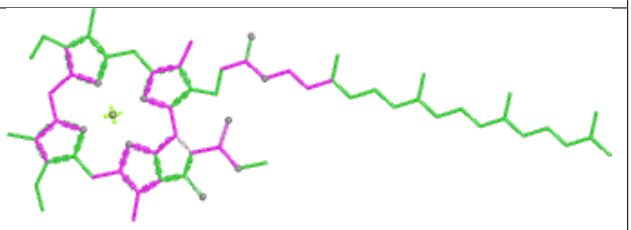
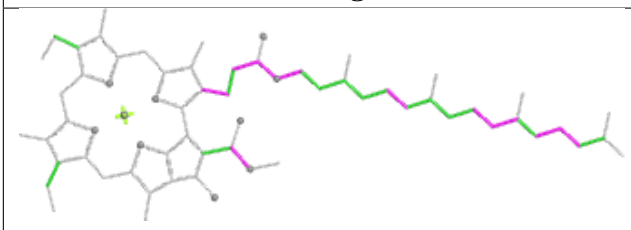
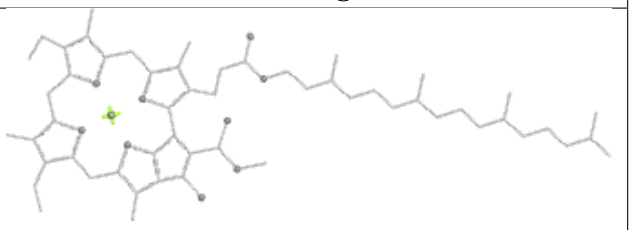
Bond angles

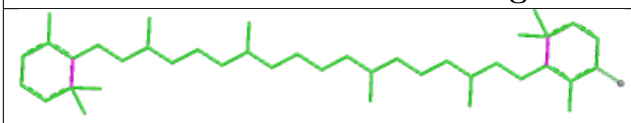
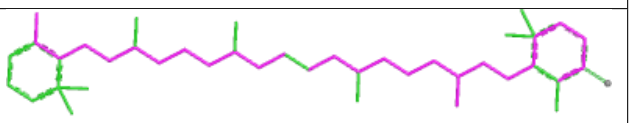
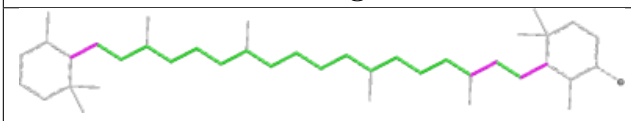
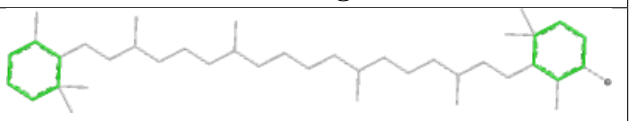


Torsions

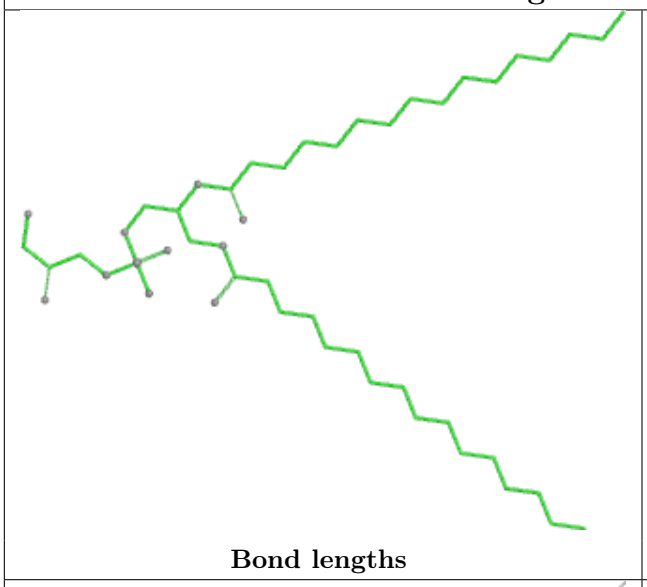


Rings

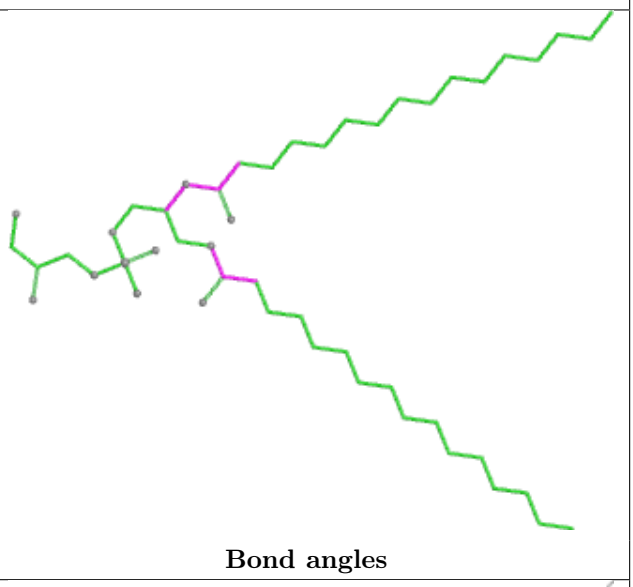
Ligand CLA B 1228	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH M 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

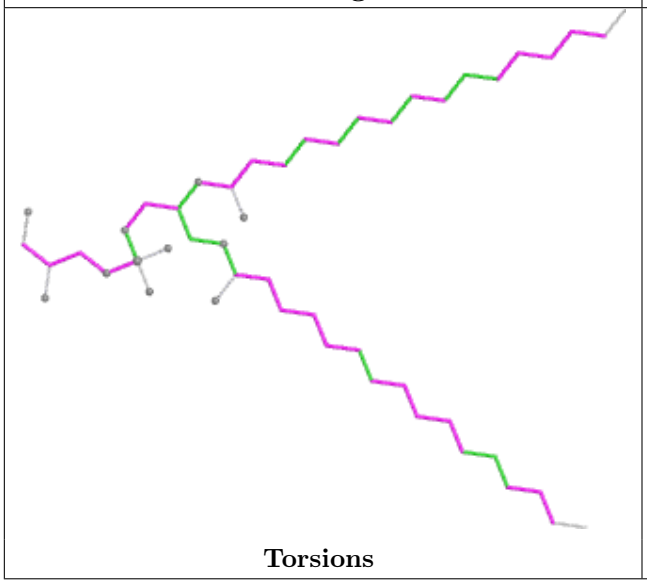
Ligand LHG 5 801



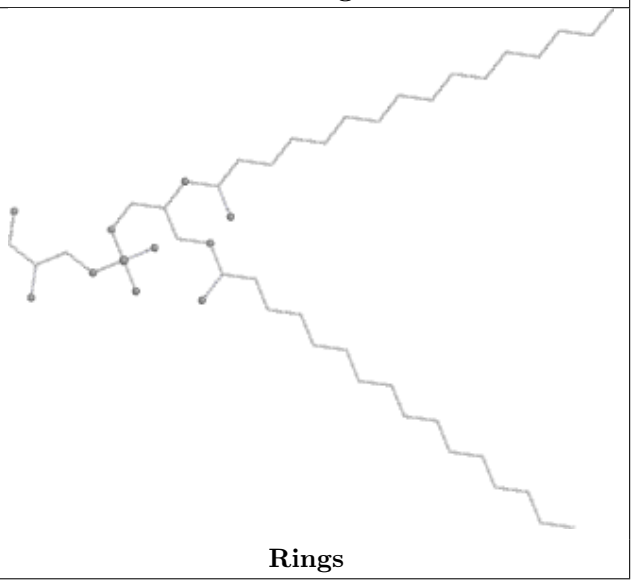
Bond lengths



Bond angles

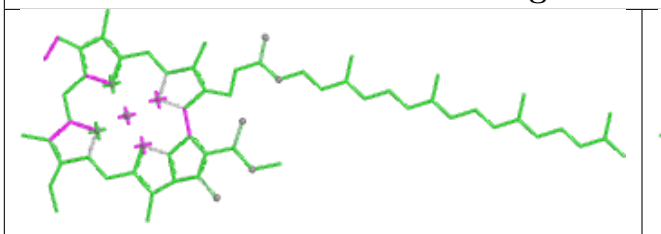


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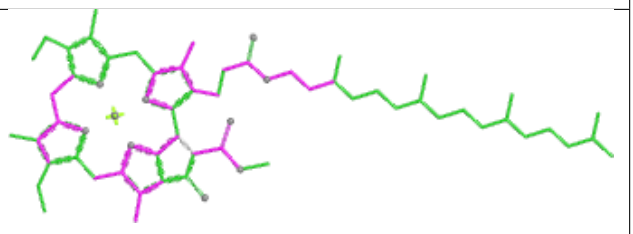


Rings

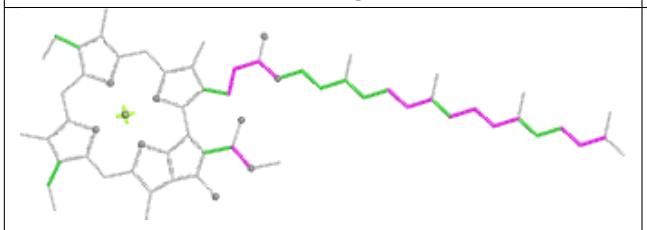
Ligand CLA a 603



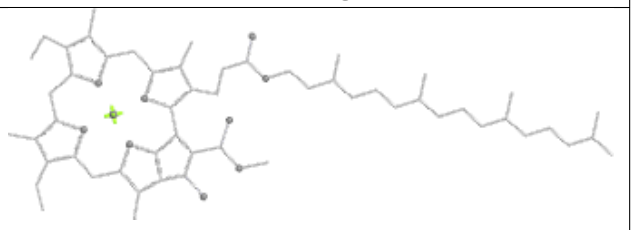
Bond lengths



Bond angles

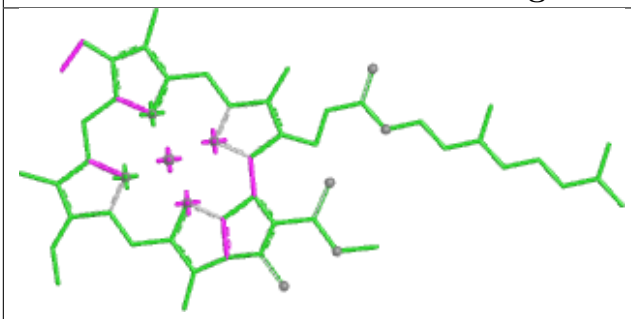


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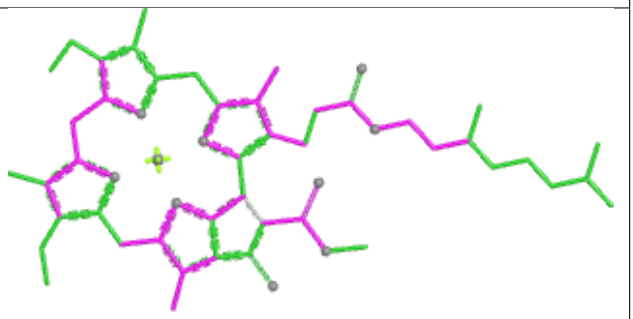


Rings

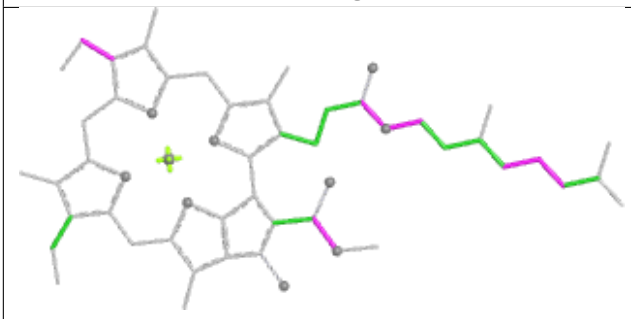
Ligand CLA 6 608



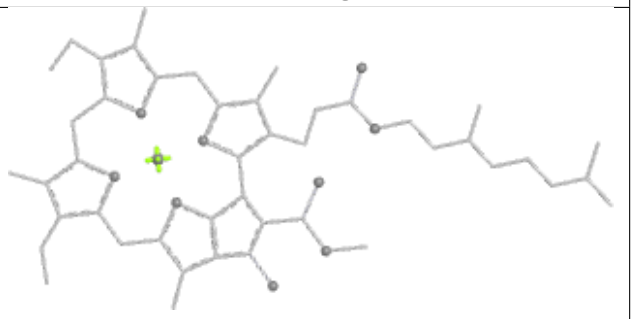
Bond lengths



Bond angles

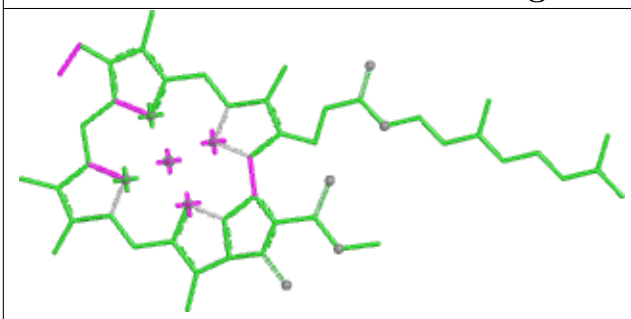


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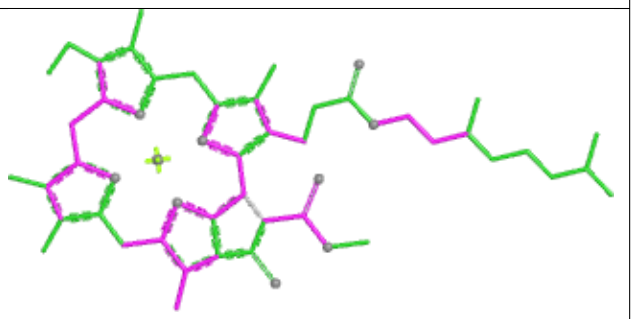


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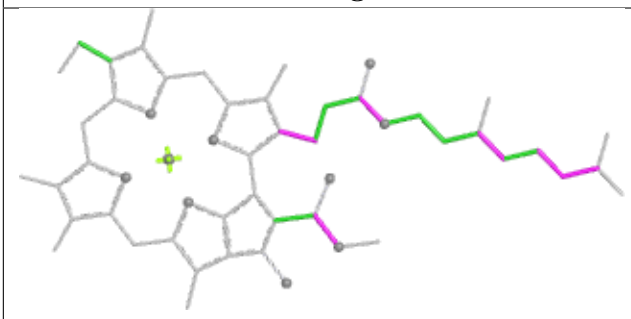
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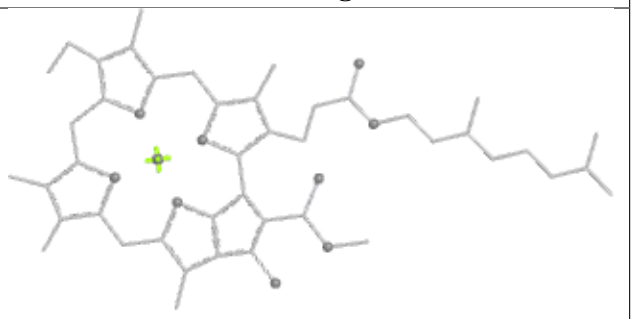
Bond lengths



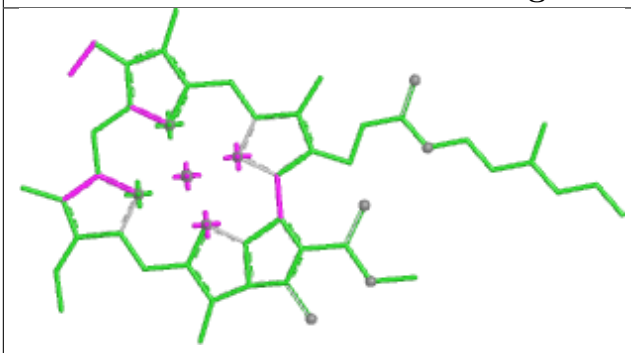
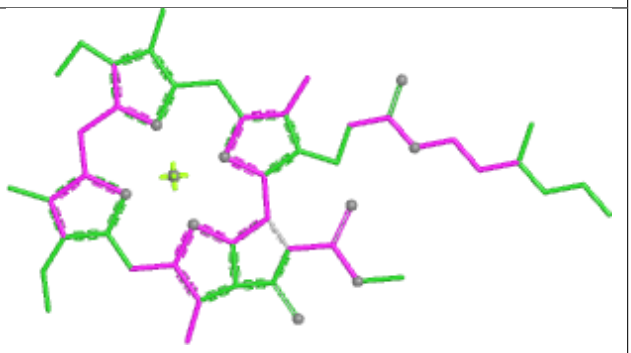
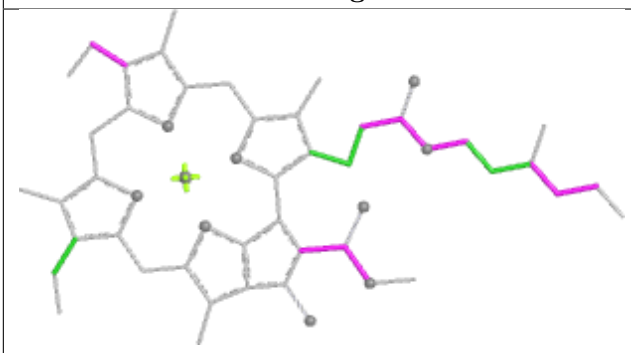
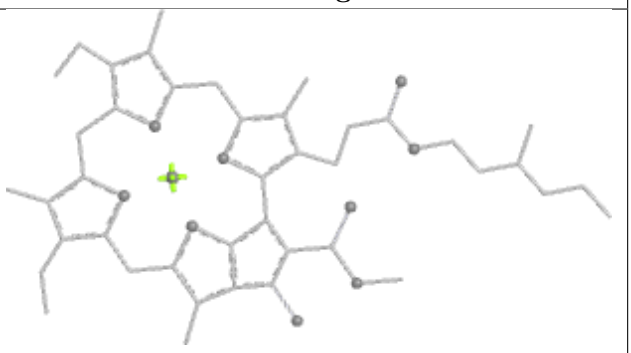
Bond angles

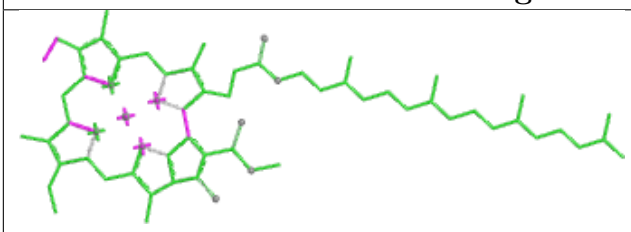
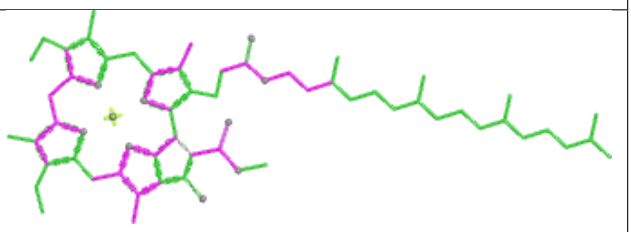
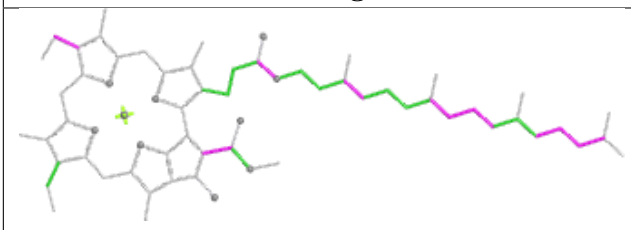
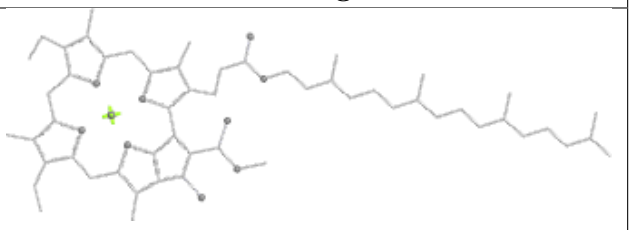


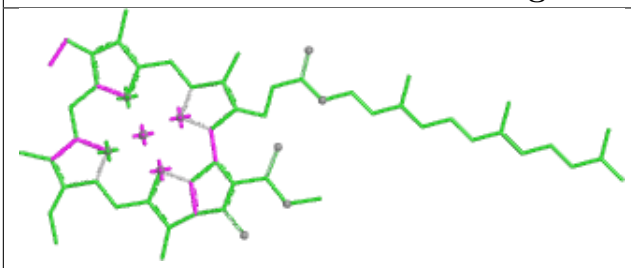
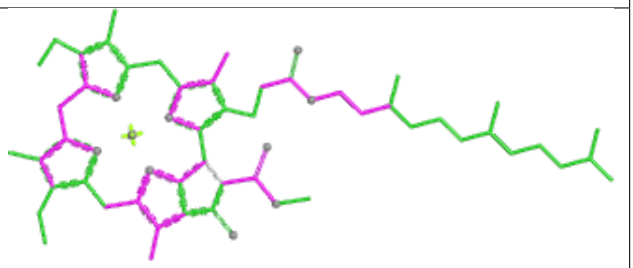
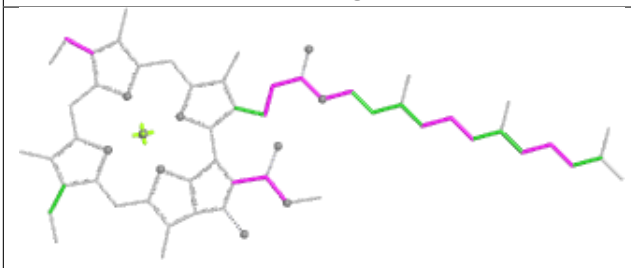
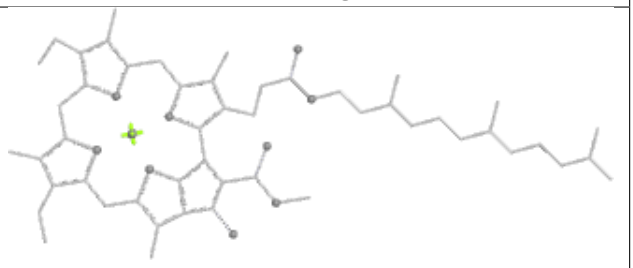
Torsions

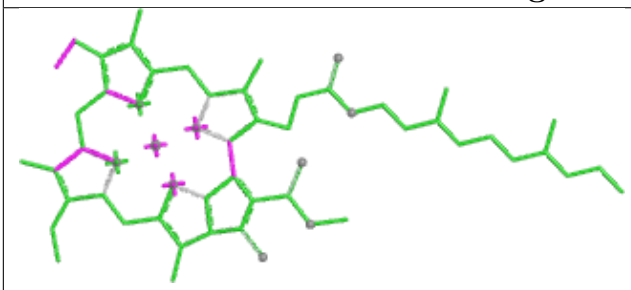
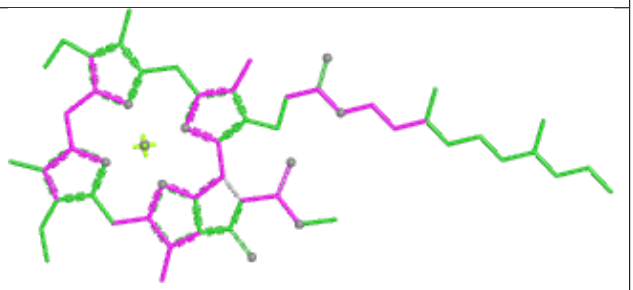
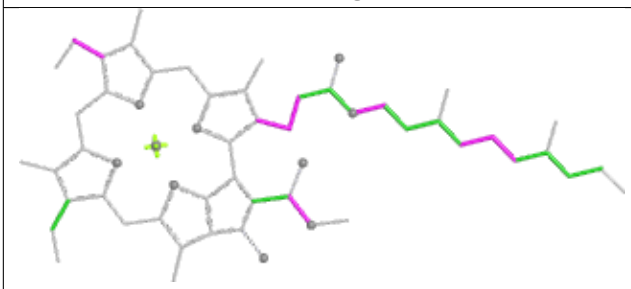
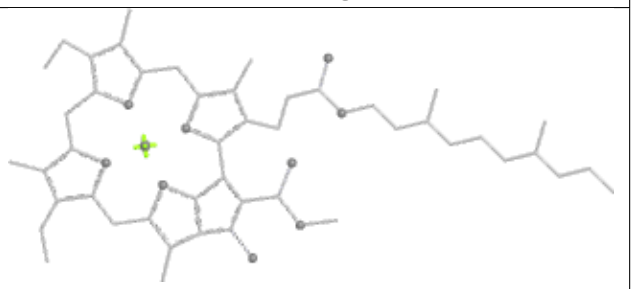


Rings

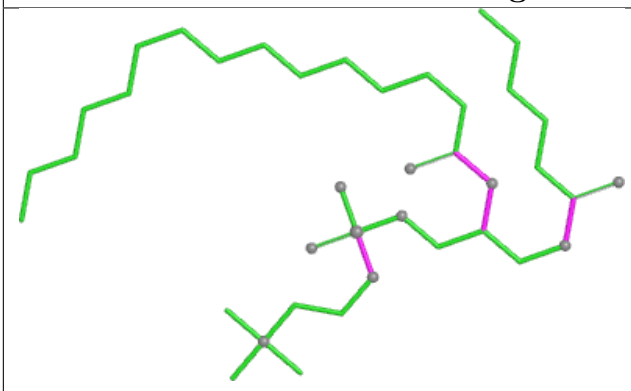
Ligand CLA 2 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

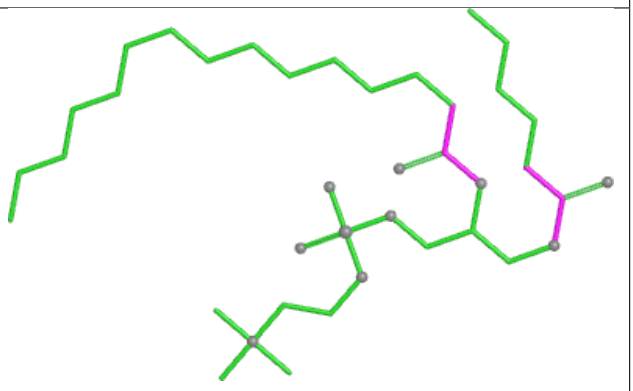
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

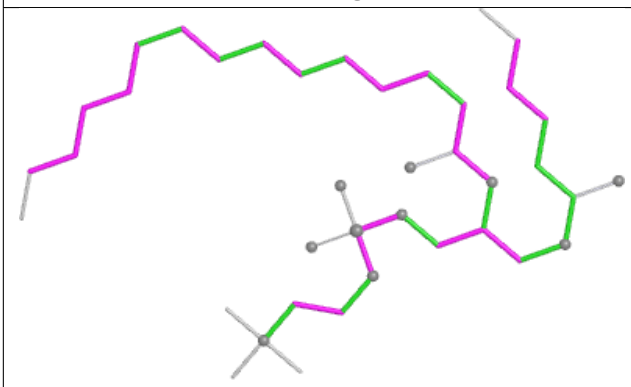
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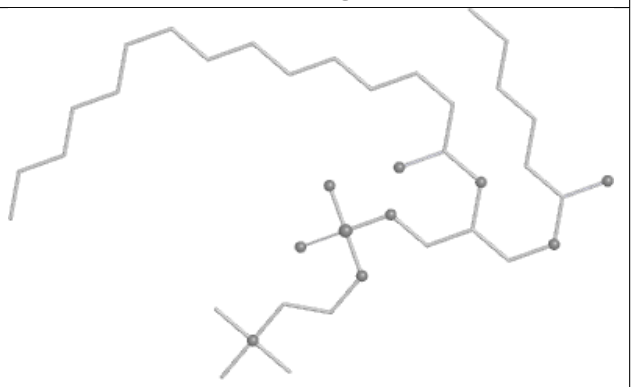
Bond lengths



Bond angles

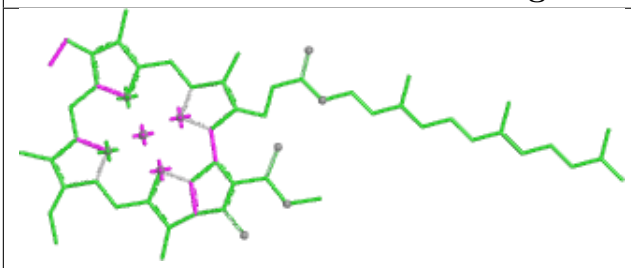


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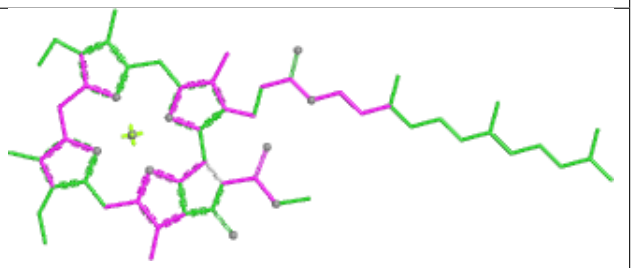


Rings

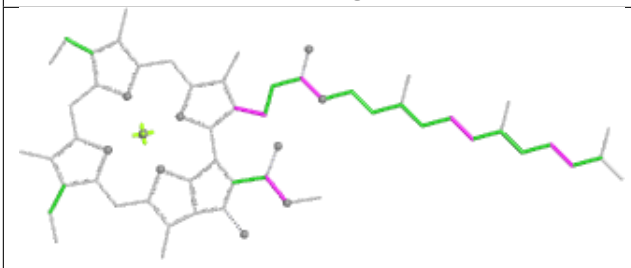
Ligand CLA a 601



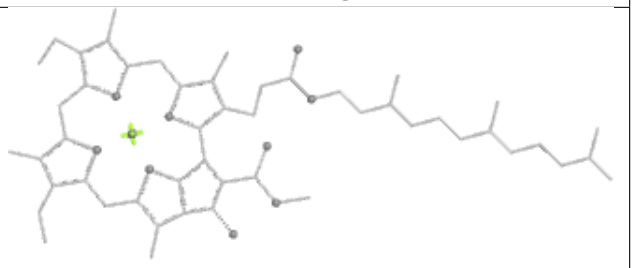
Bond lengths



Bond angles

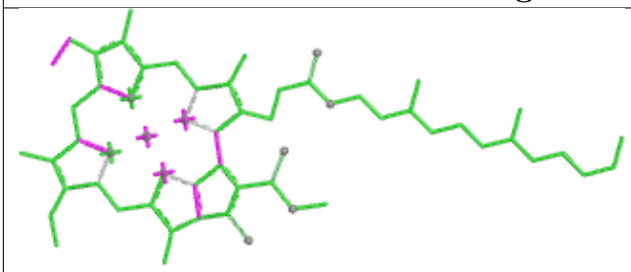


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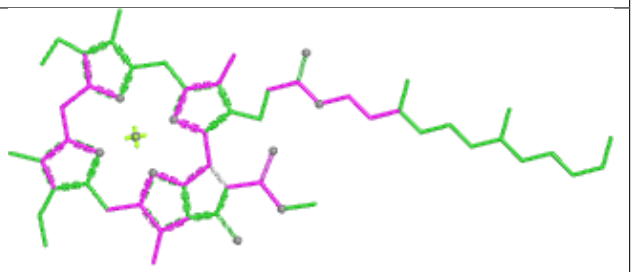


Rings

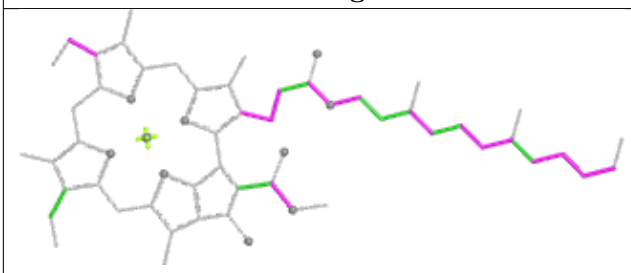
Ligand CLA B 1214



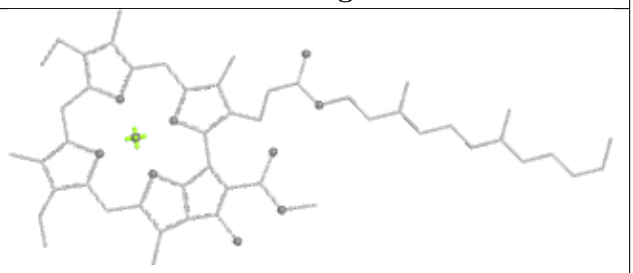
Bond lengths



Bond angles

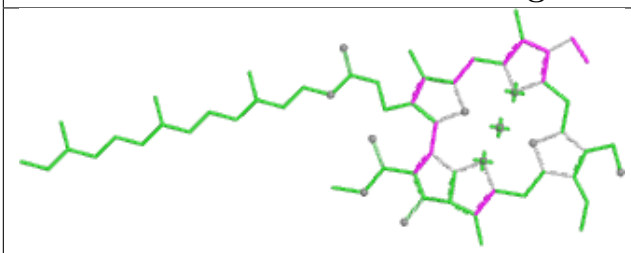


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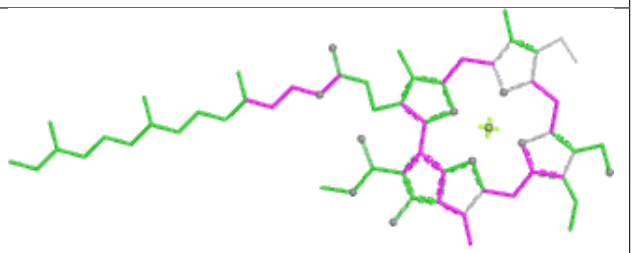


Rings

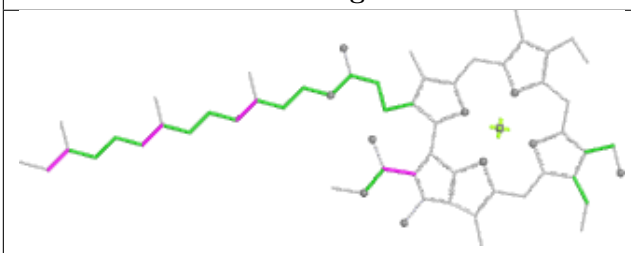
Ligand CHL 7 609



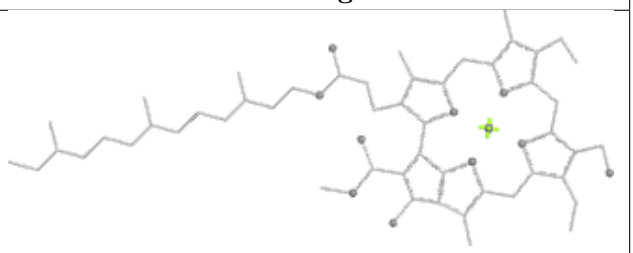
Bond lengths



Bond angles

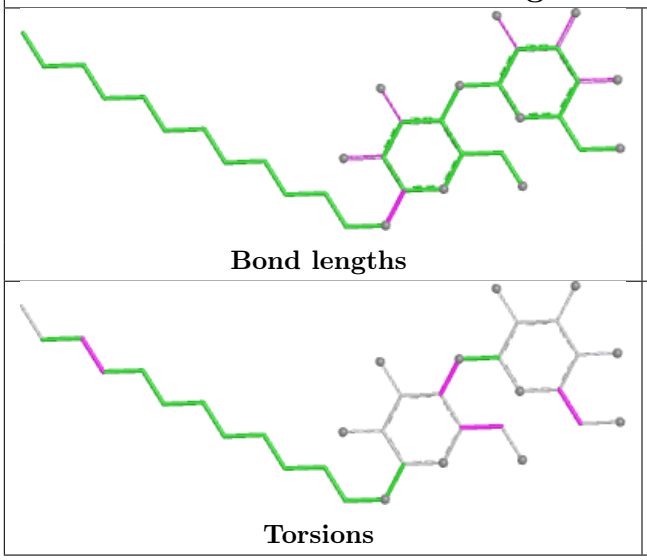


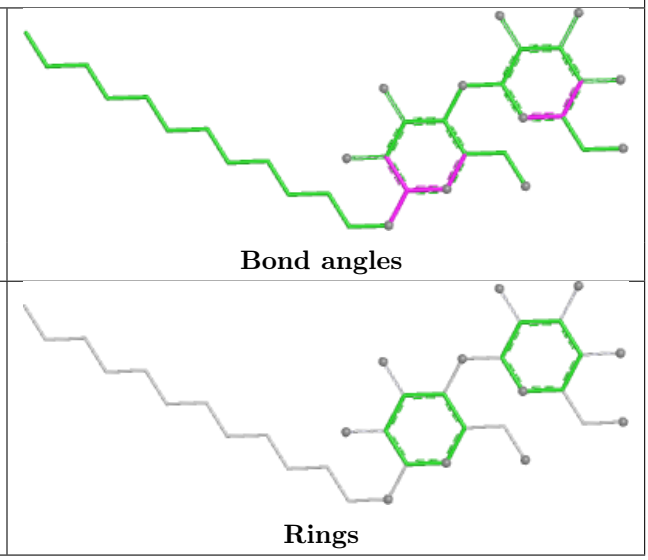
Torsions



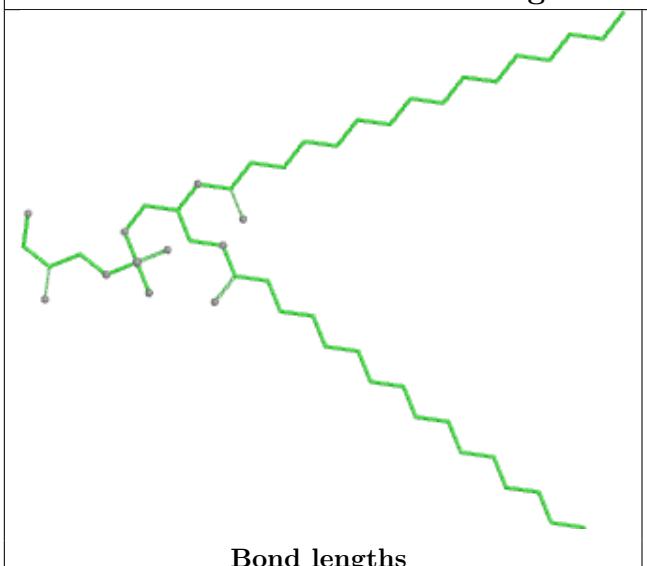
Rings

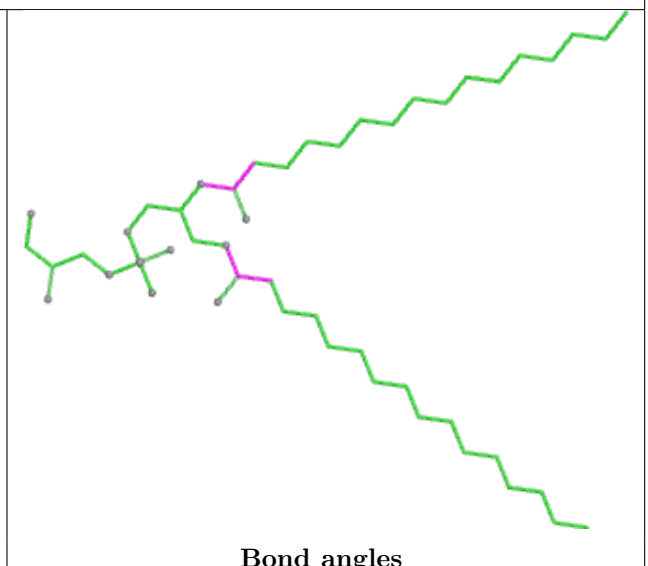
Ligand LMT 2 804

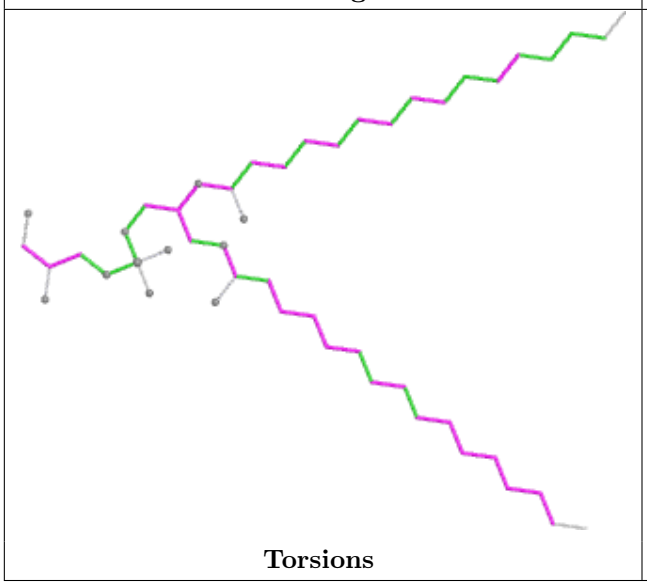


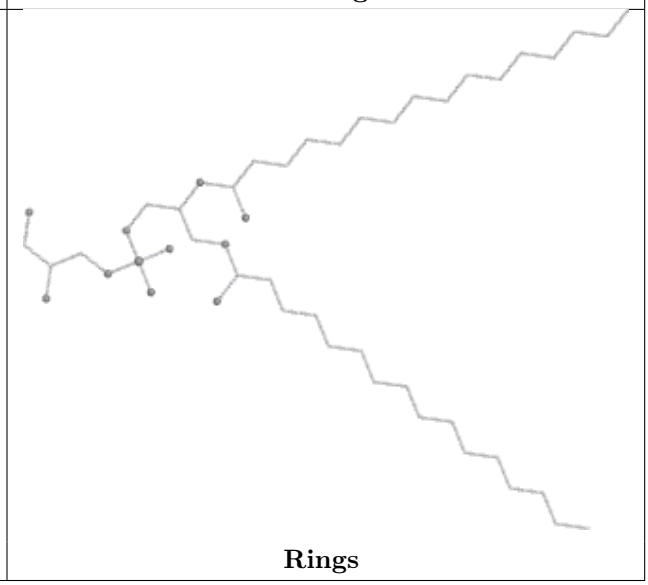


Ligand LHG 2 801

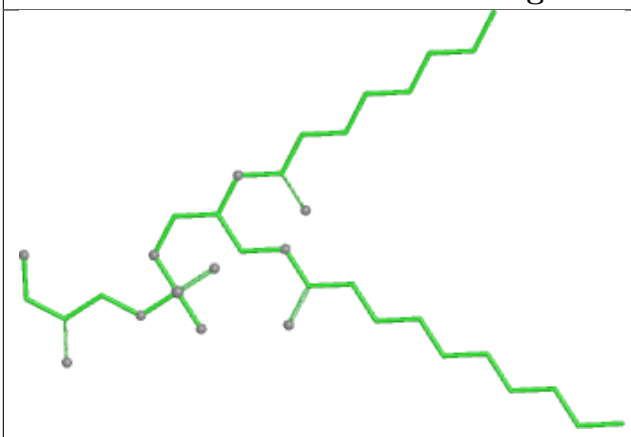




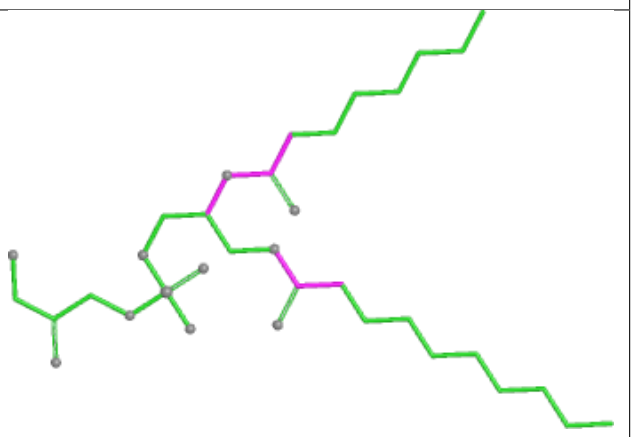




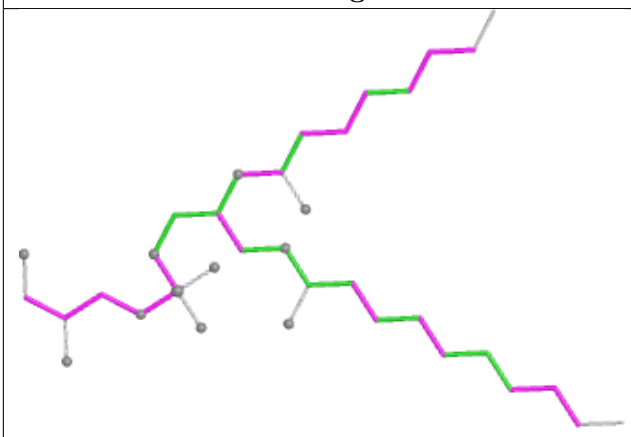
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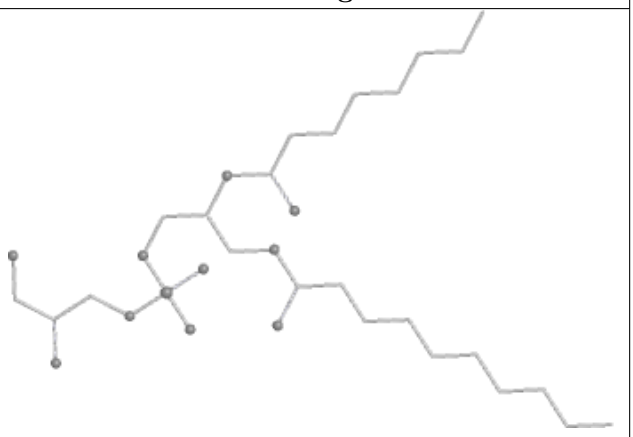
Bond lengths



Bond angles

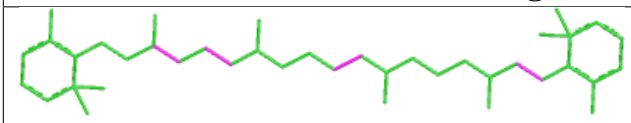


Torsions

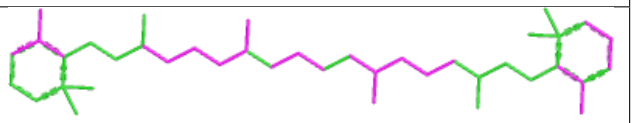


Rings

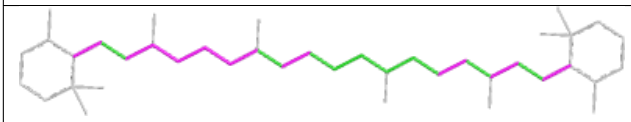
Ligand BCR 8 503



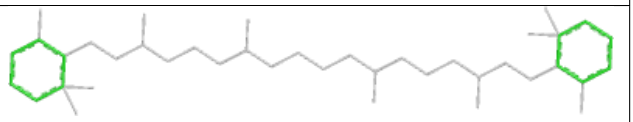
Bond lengths



Bond angles

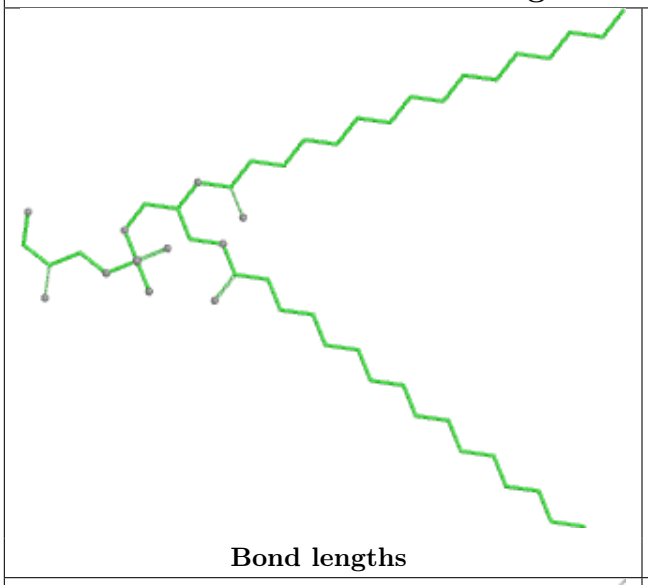


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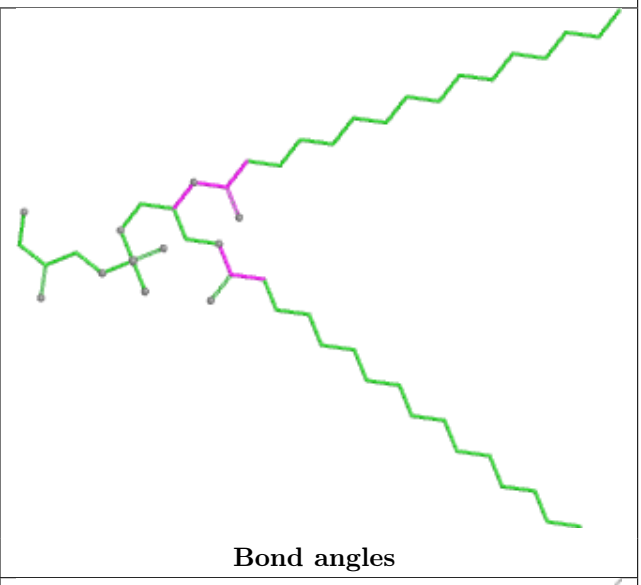


Rings

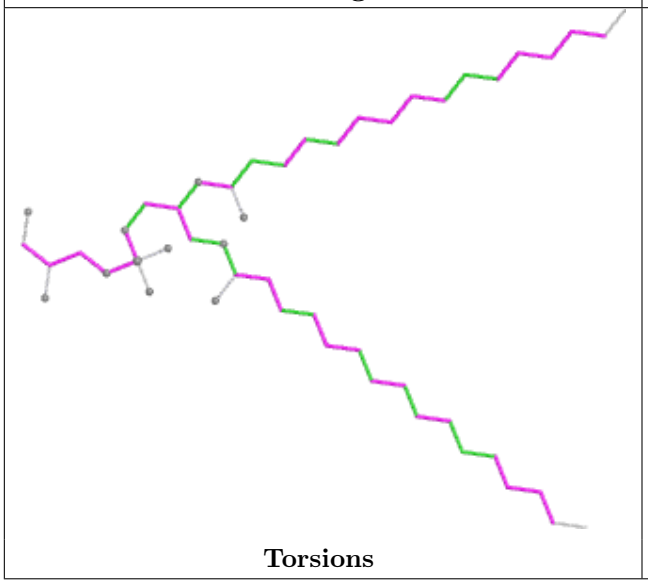
Ligand LHG 1 802



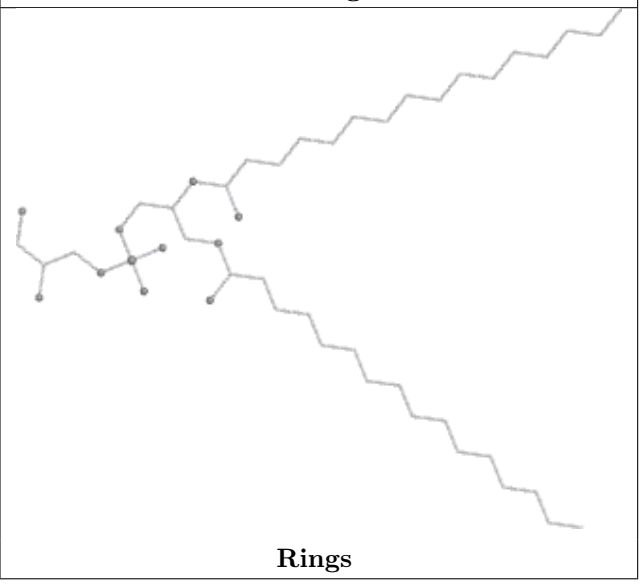
Bond lengths



Bond angles

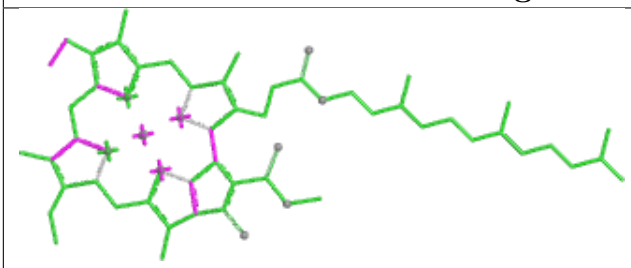


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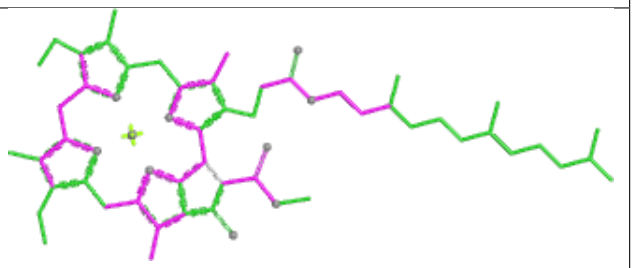


Rings

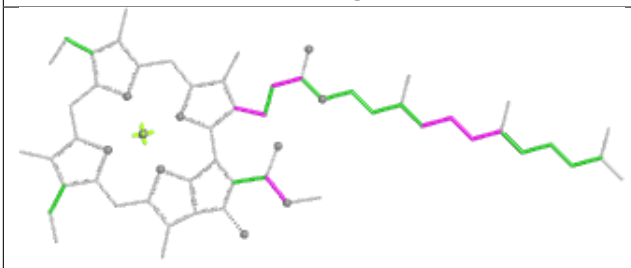
Ligand CLA K 1402



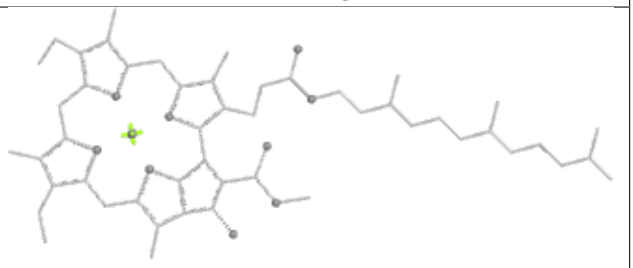
Bond lengths



Bond angles

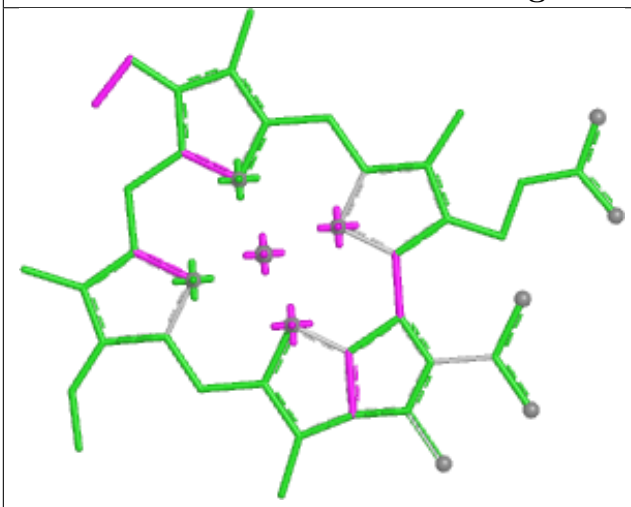


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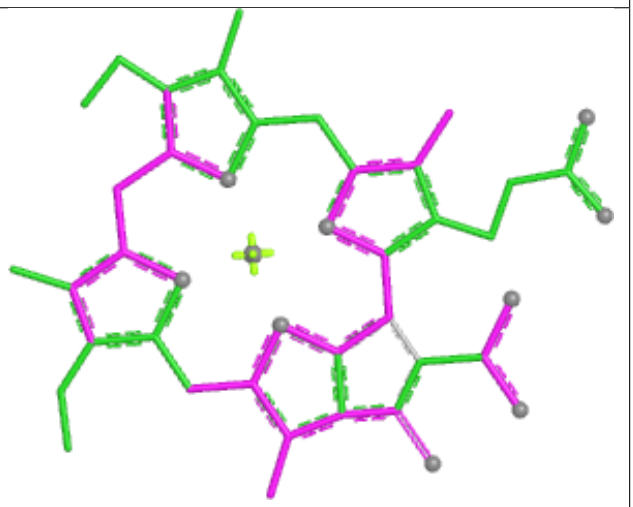


Rings

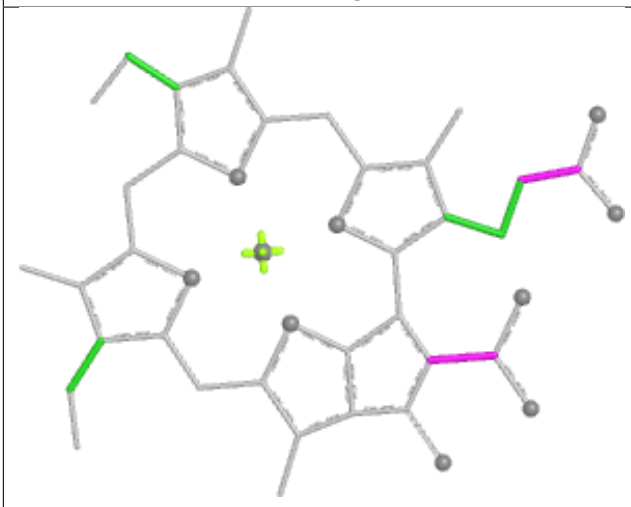
Ligand CLA 7 605



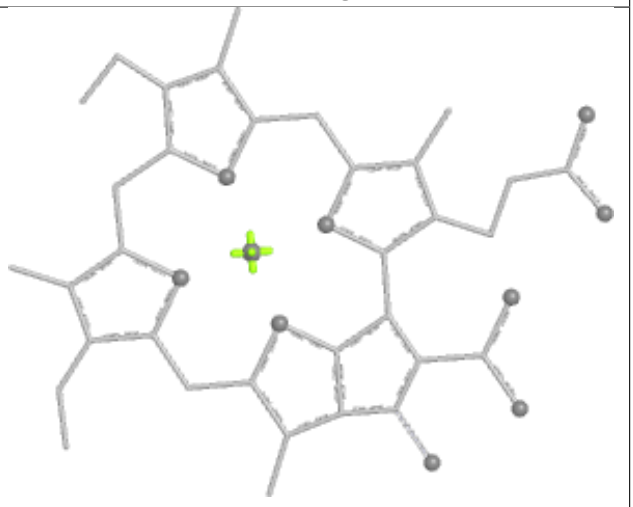
Bond lengths



Bond angles

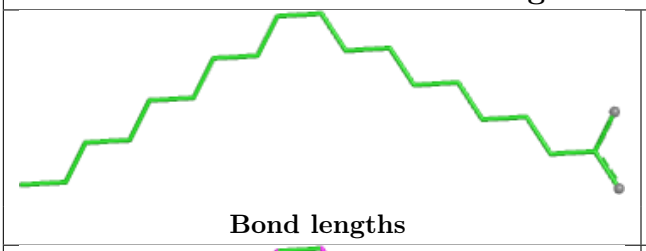


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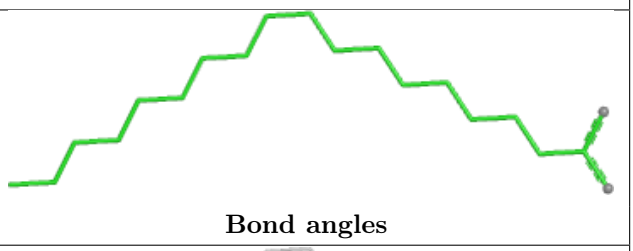


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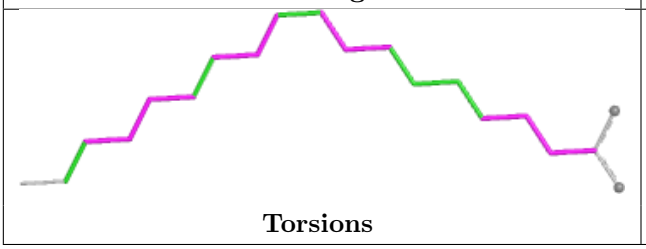
Ligand OLA 8 809



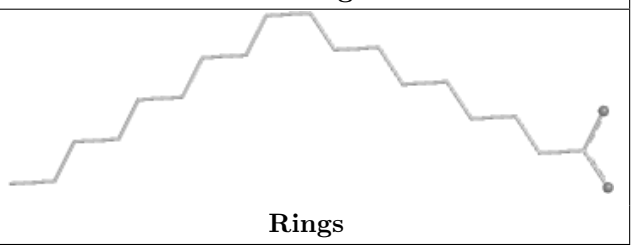
Bond lengths



Bond angles

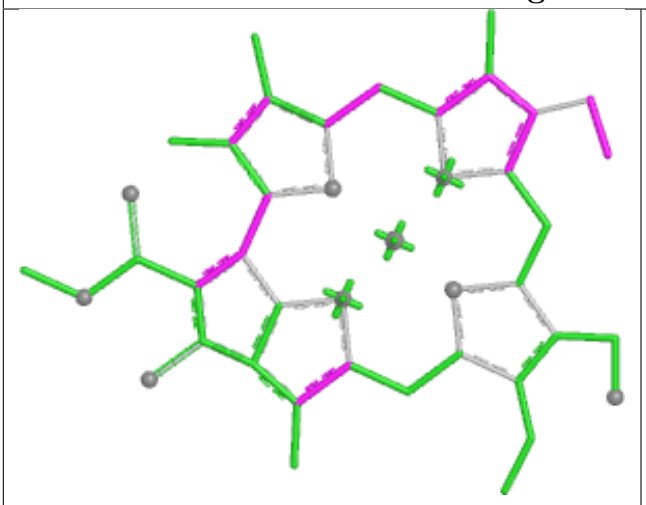


Torsions



Rings

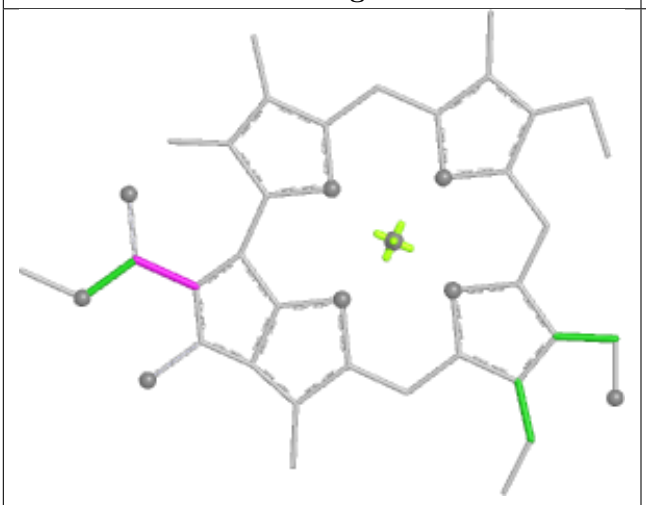
Ligand CHL 9 613



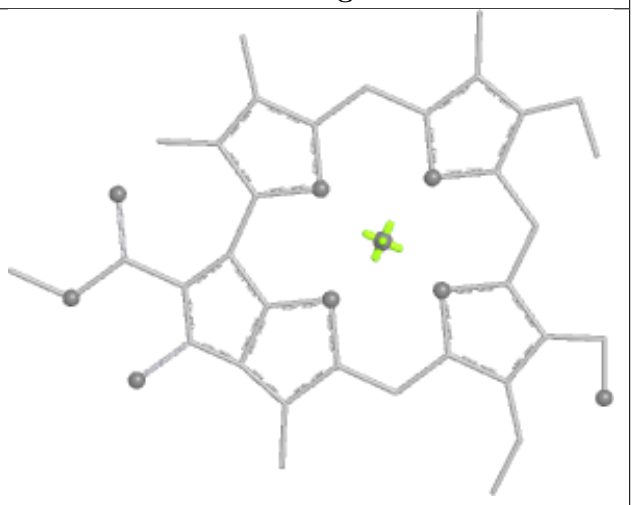
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Bond angles

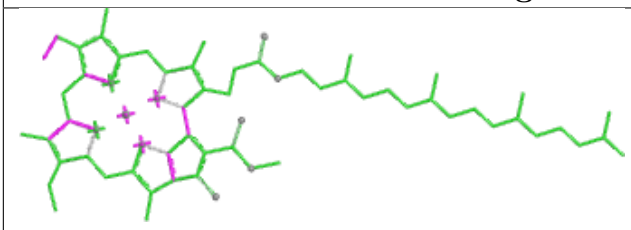


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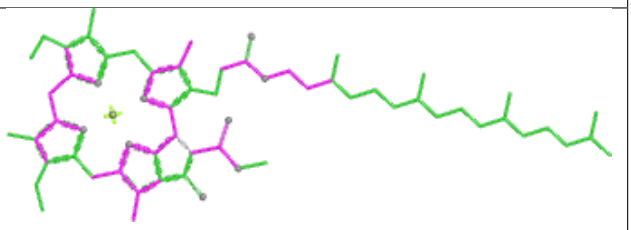


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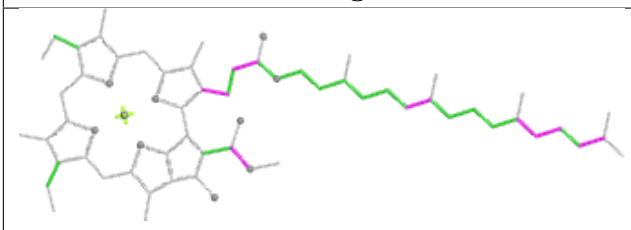
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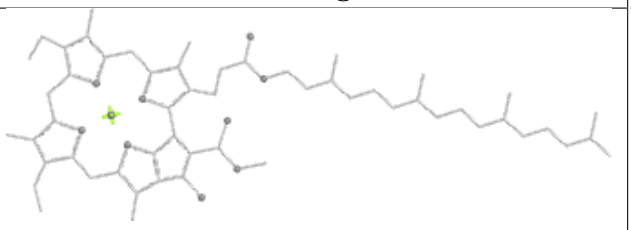
Bond lengths



Bond angles

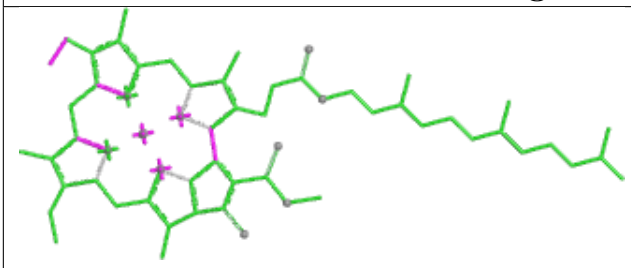


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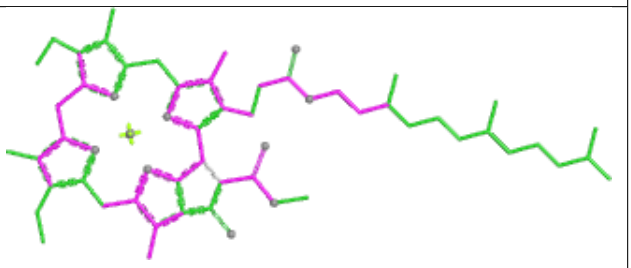


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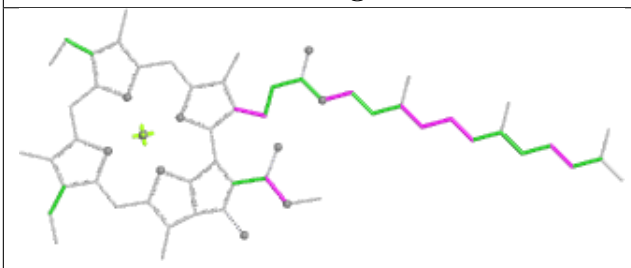
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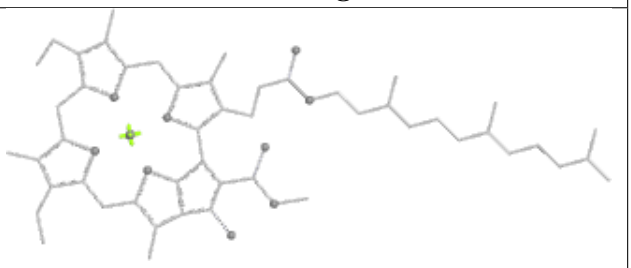
Bond lengths



Bond angles

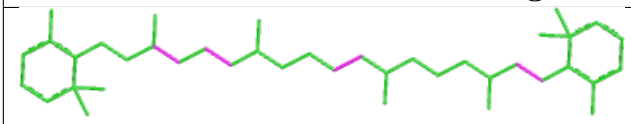


Torsions



Rings

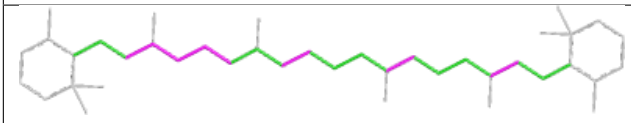
Ligand BCR 3 504



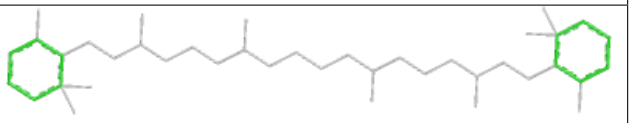
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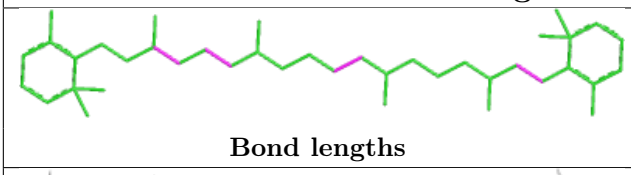


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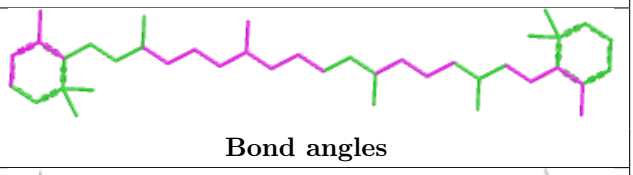


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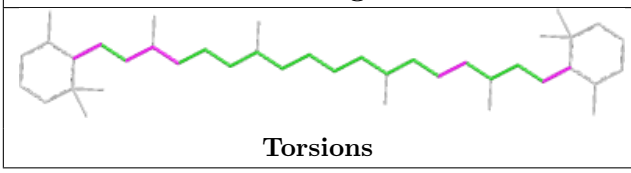
Ligand BCR B 4004



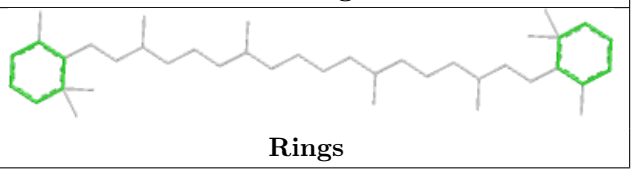
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Bond angles

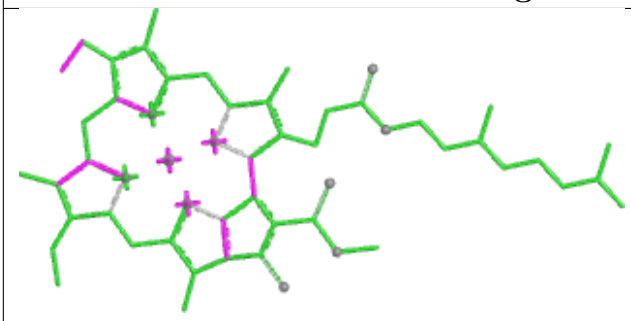


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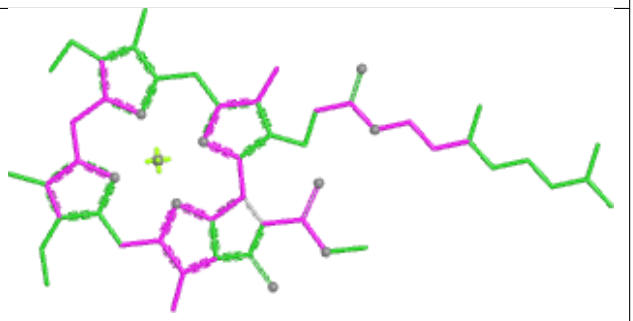


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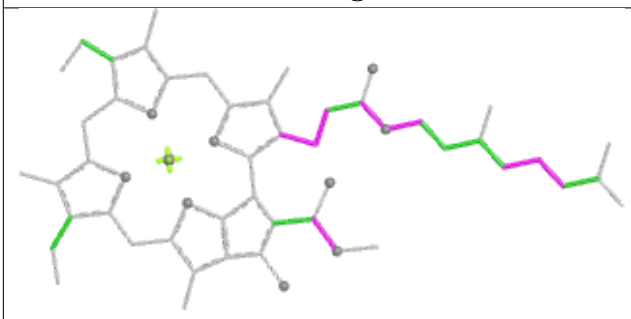
Ligand CLA A 1140



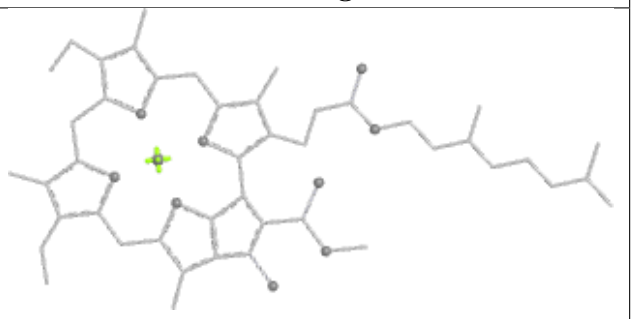
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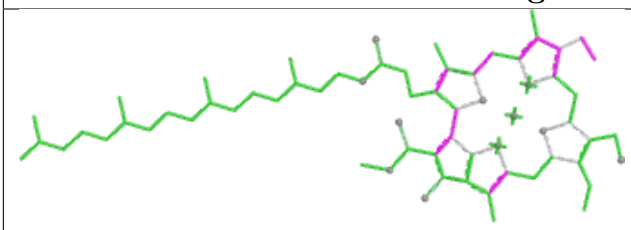


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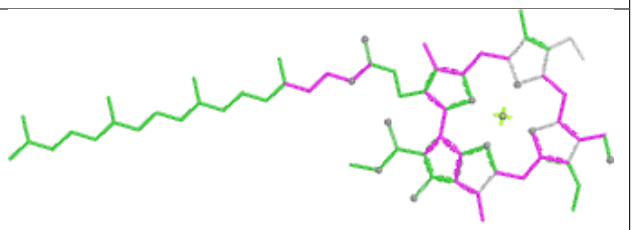


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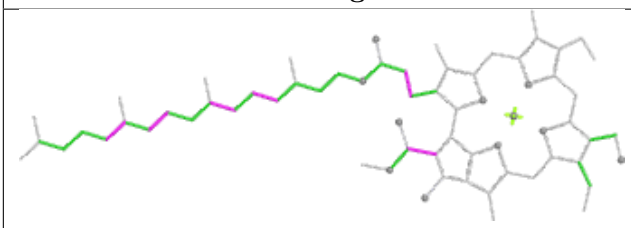
Ligand CHL 3 603



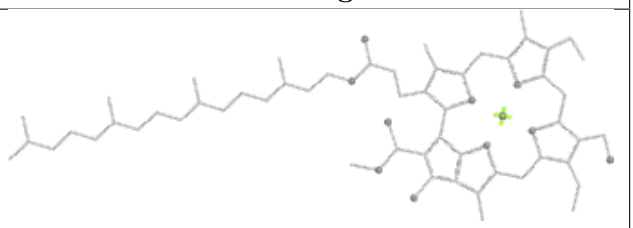
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Bond angles

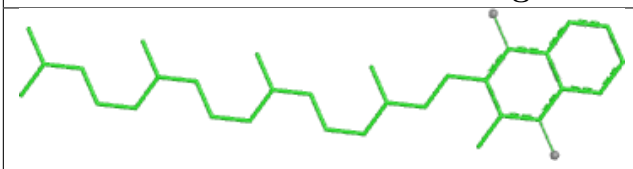


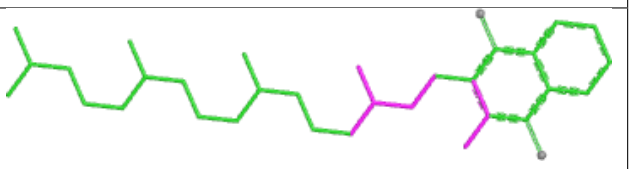
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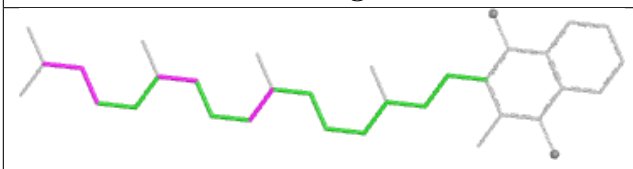


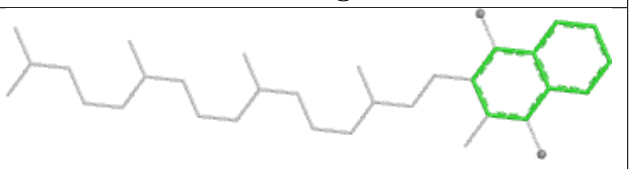
Rings

Ligand PQN A 2001

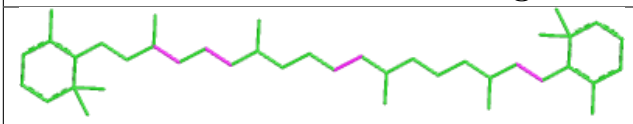

Bond lengths

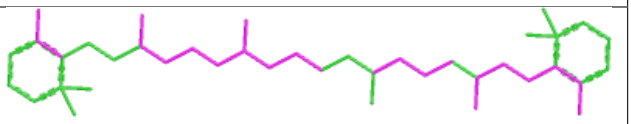

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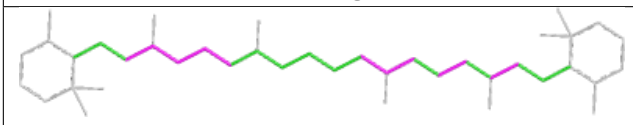

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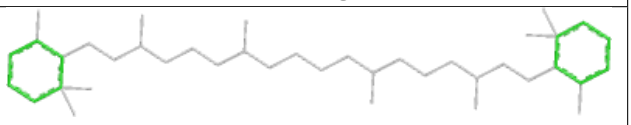

Rings

Ligand BCR A 4005

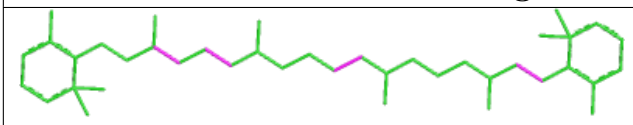

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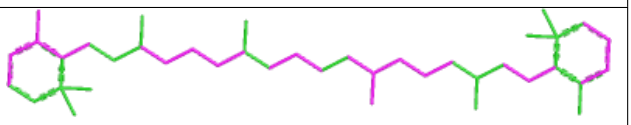

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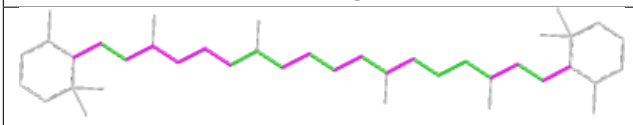

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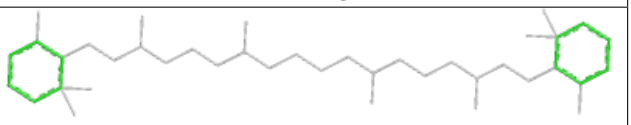

Rings

Ligand BCR B 4002

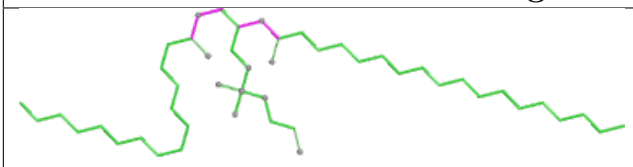

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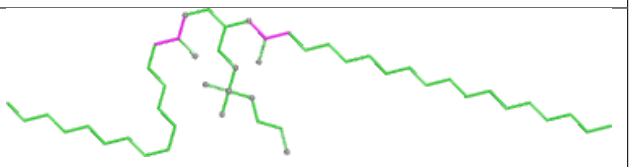

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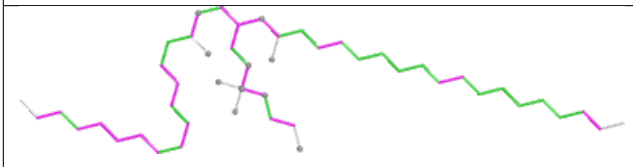

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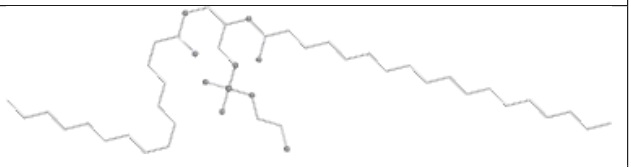

Rings

Ligand PTY 9 803

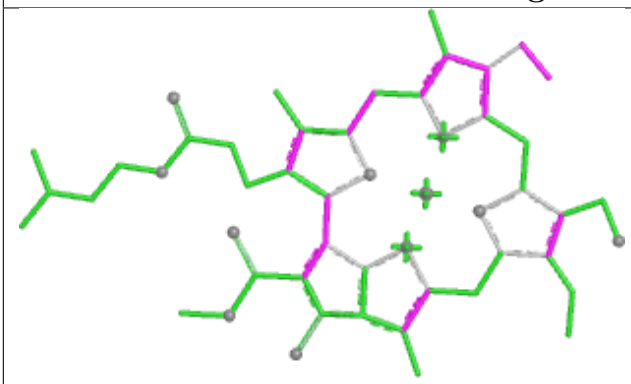

Bond lengths


Bond angles

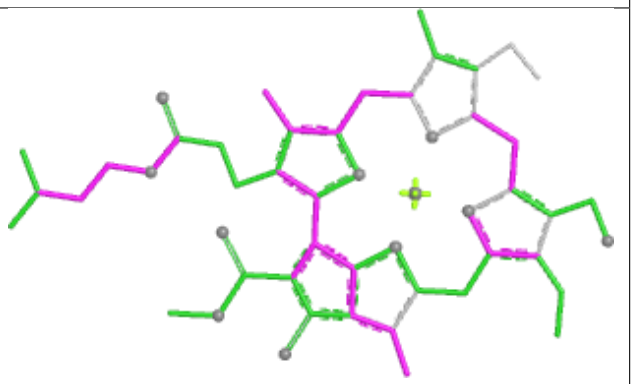

Torsions


Rings

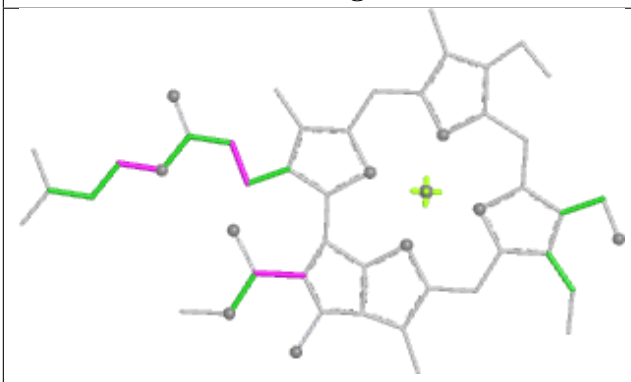
Ligand CHL 9 610



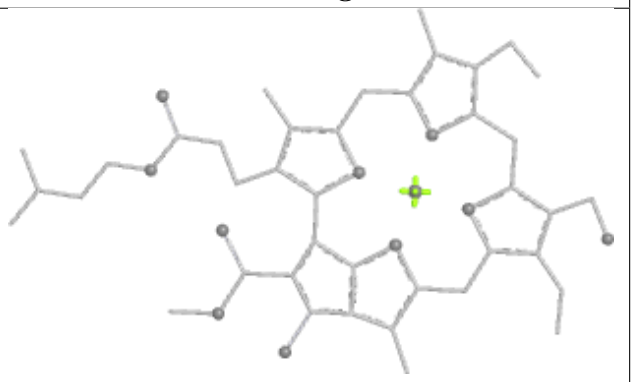
Bond lengths



Bond angles

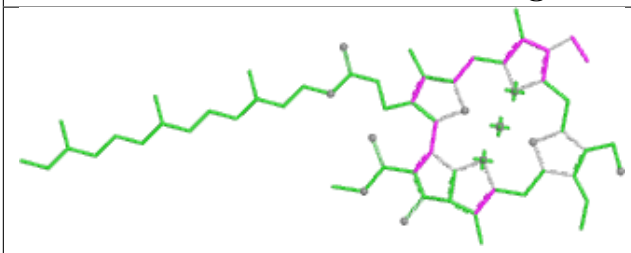


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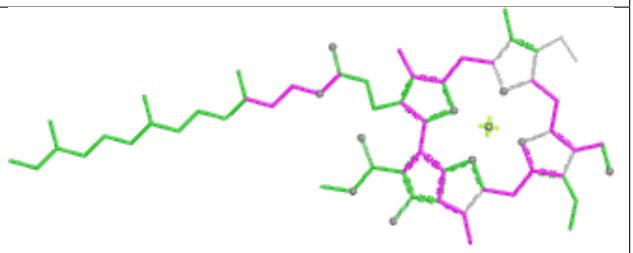


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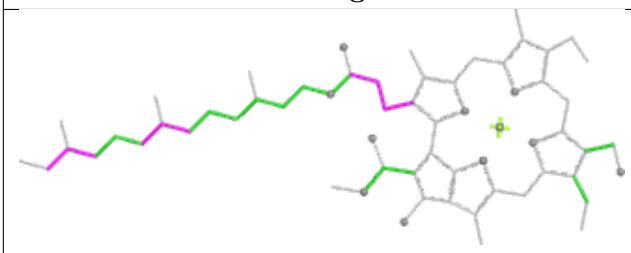
Ligand CHL 8 604



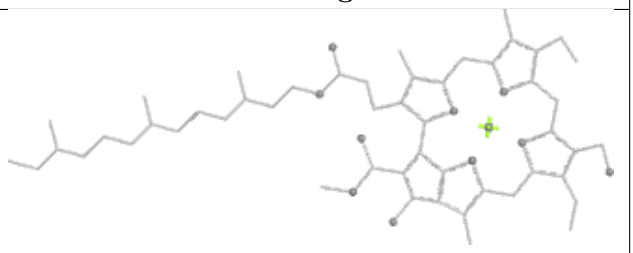
Bond lengths



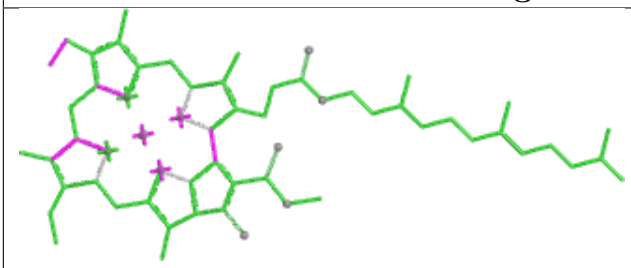
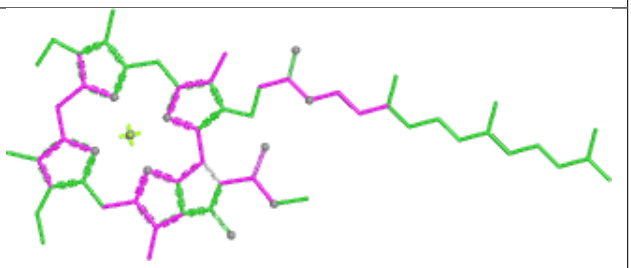
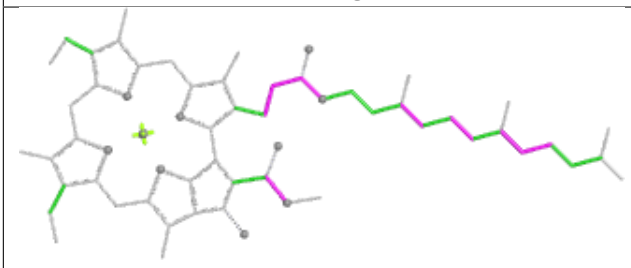
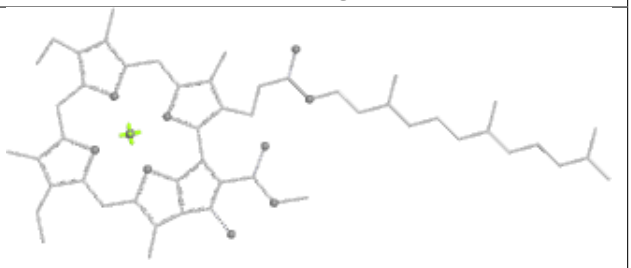
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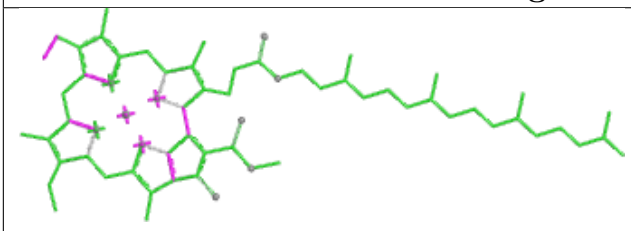
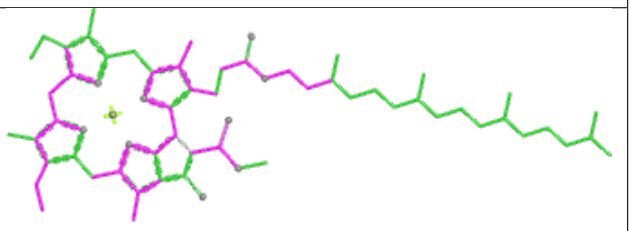
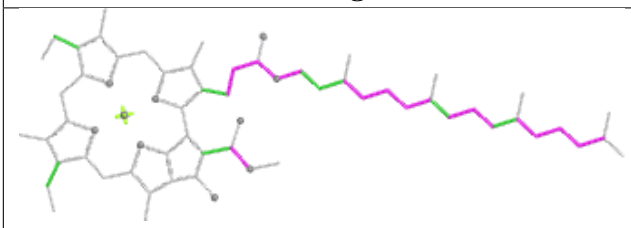
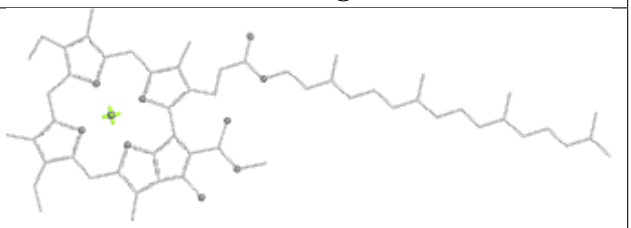


Torsions

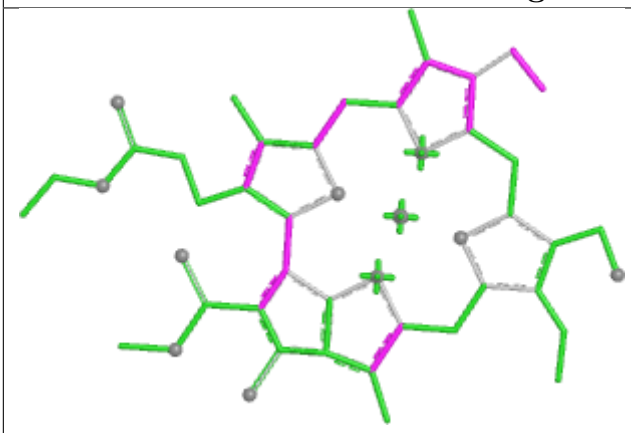


Rings

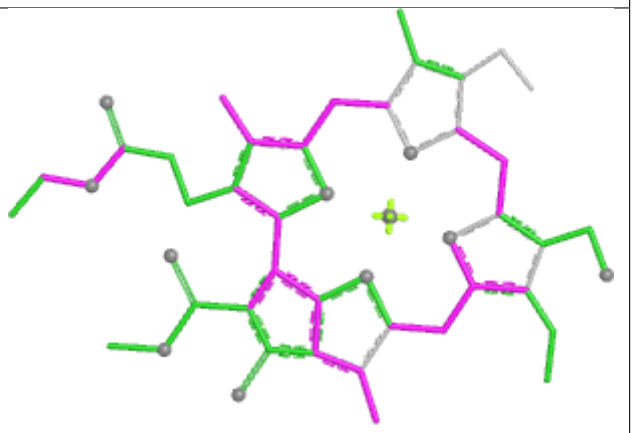
Ligand CLA G 1602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

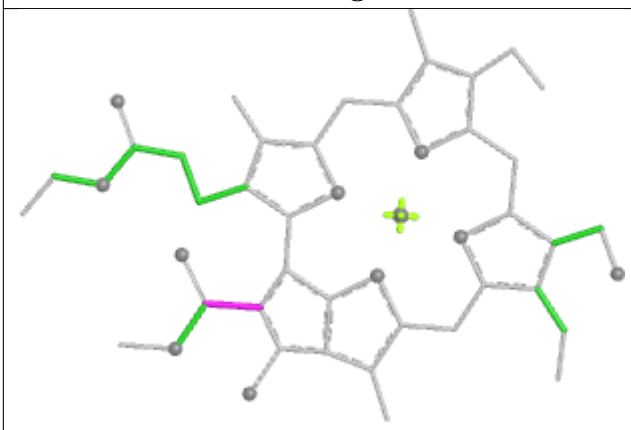
Ligand CHL 2 610



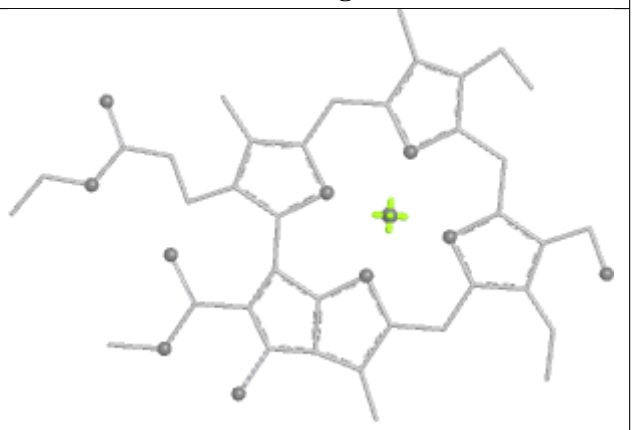
Bond lengths



Bond angles

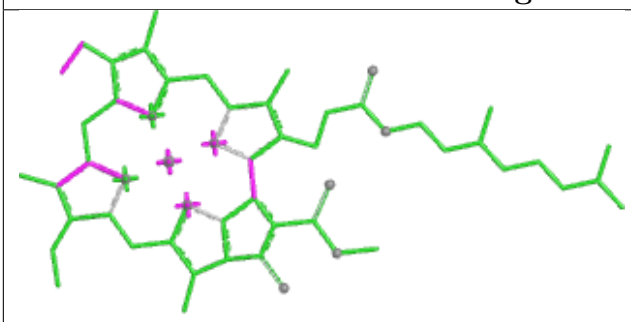


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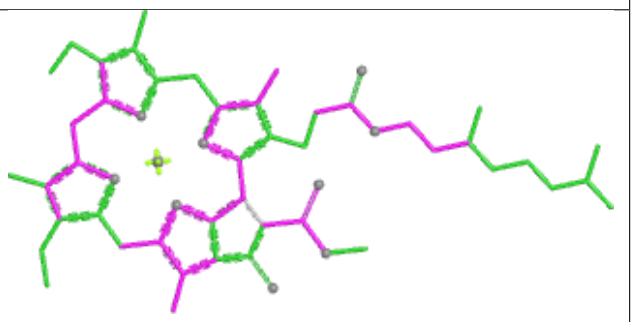


Rings

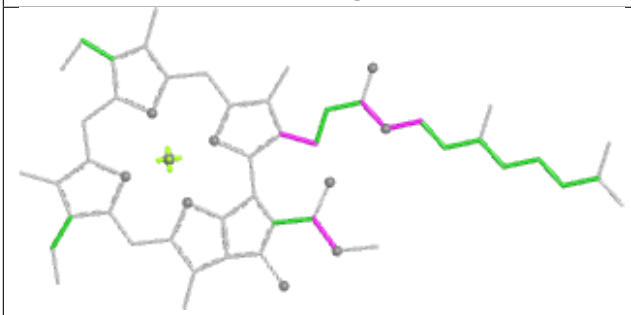
Ligand CLA A 1124



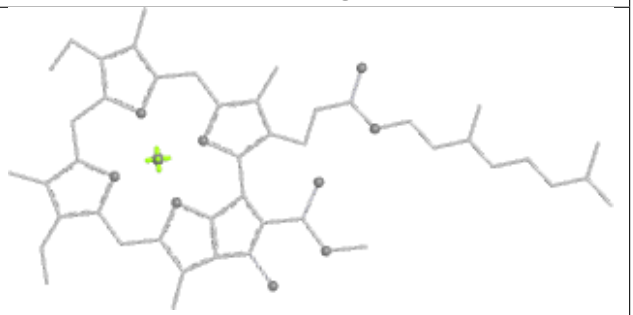
Bond lengths



Bond angles

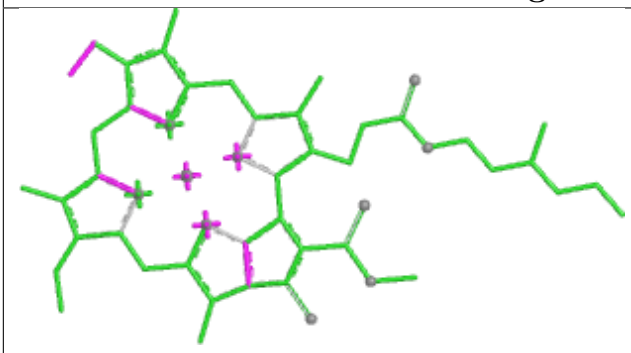


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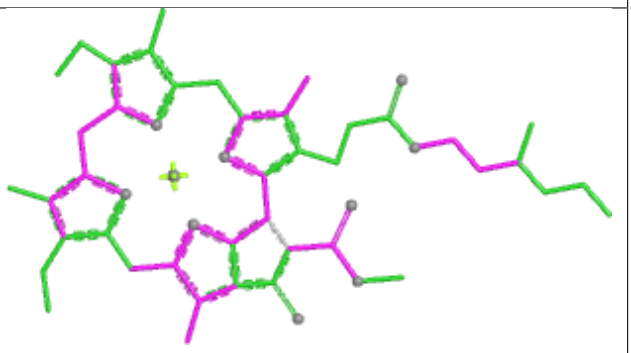


Rings

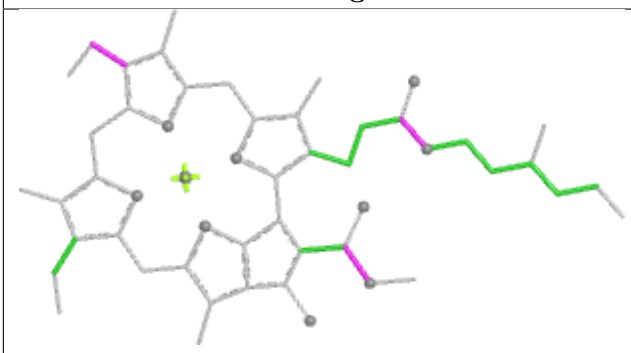
Ligand CLA 8 602



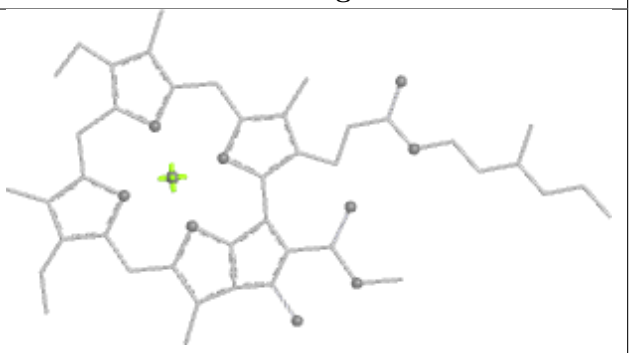
Bond lengths



Bond angles

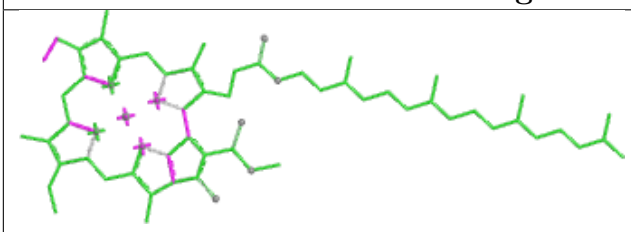


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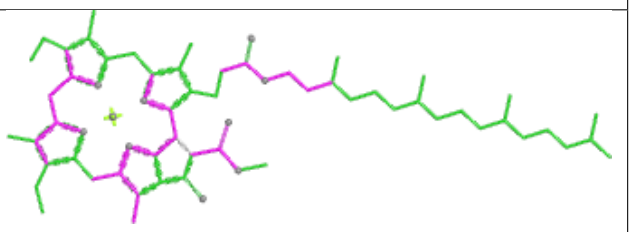


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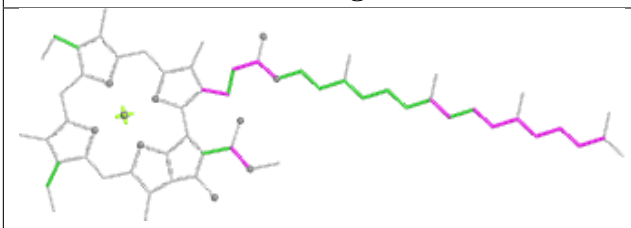
Ligand CLA B 1021



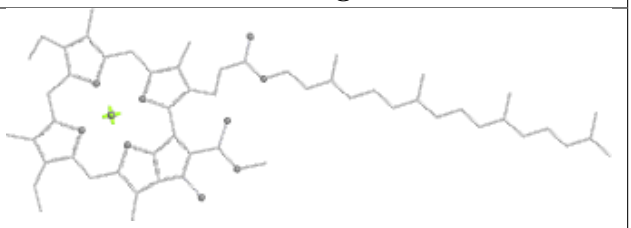
Bond lengths



Bond angles

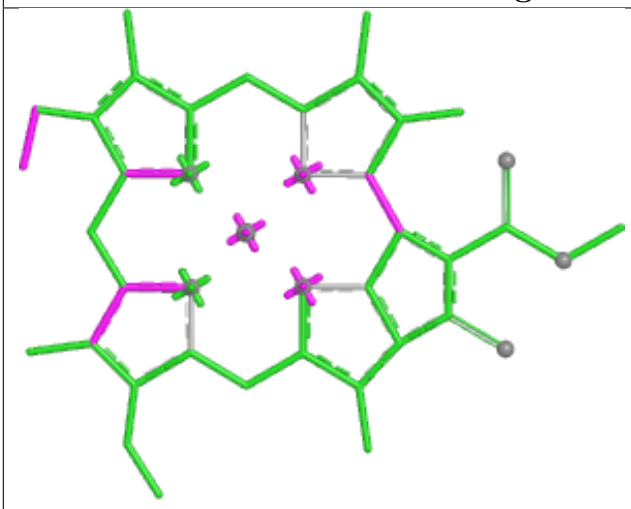


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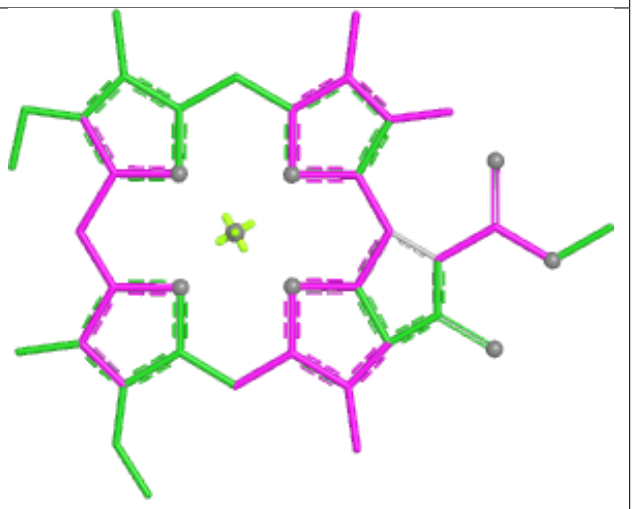


Rings

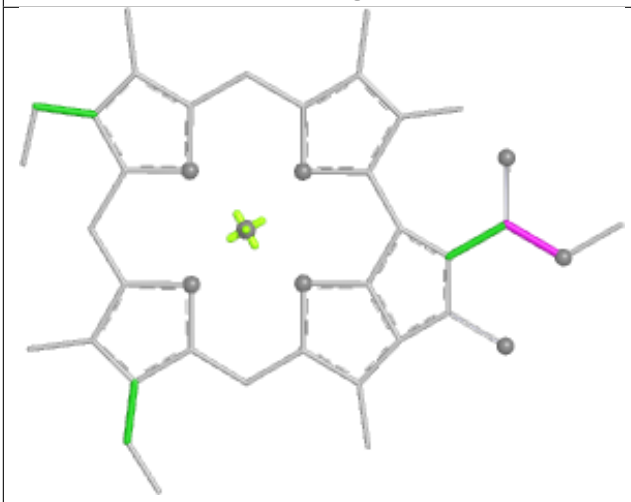
Ligand CLA O 1803



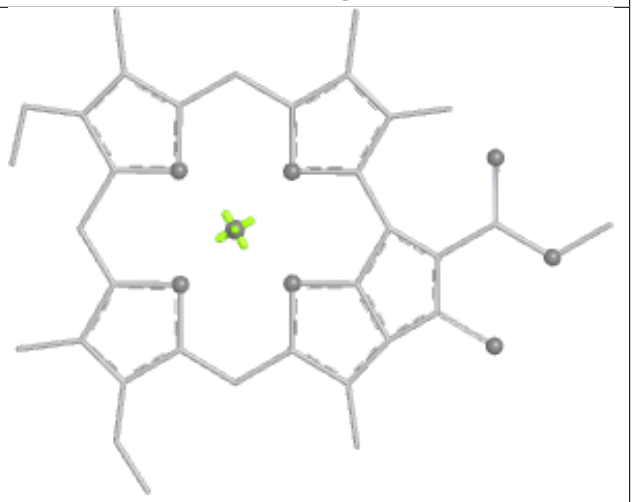
Bond lengths



Bond angles

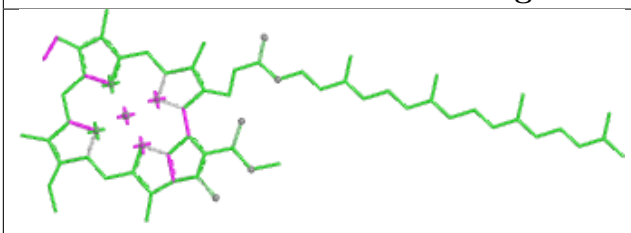


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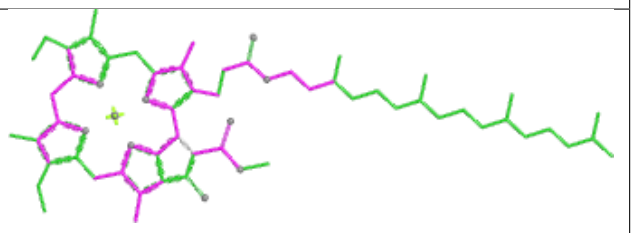


Rings

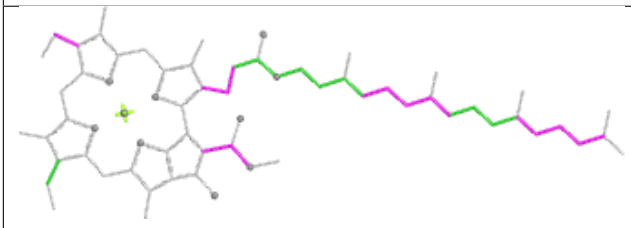
Ligand CLA A 1132



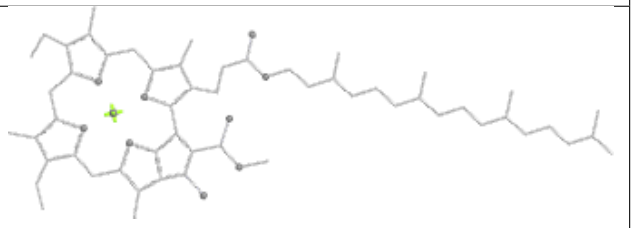
Bond lengths



Bond angles

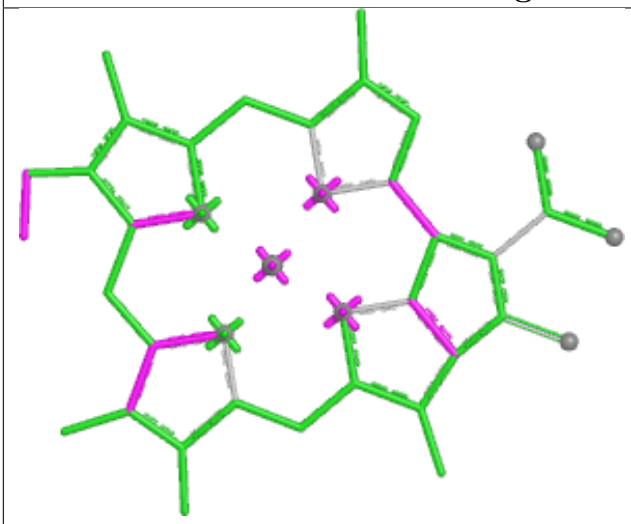


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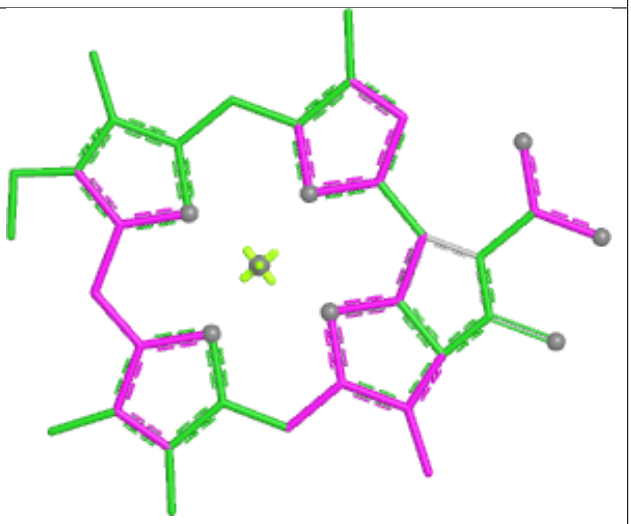


Rings

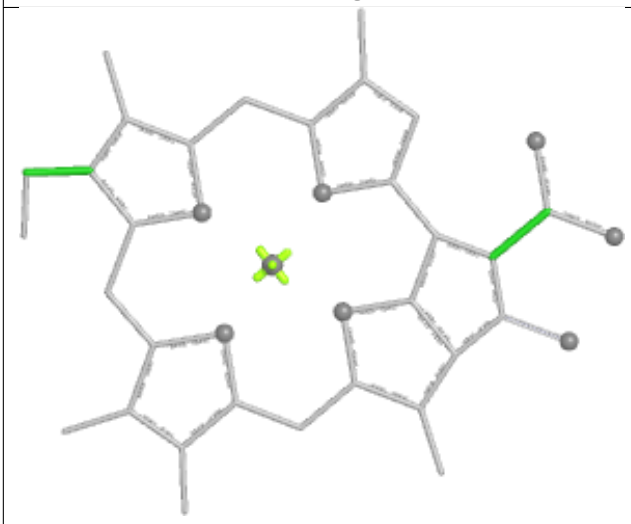
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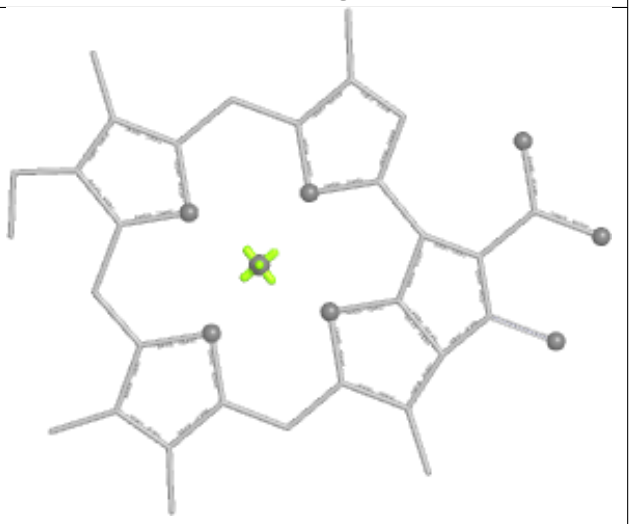
Bond lengths



Bond angles

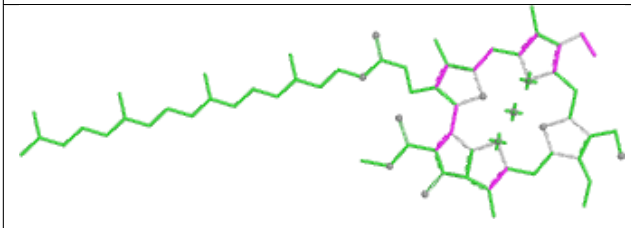


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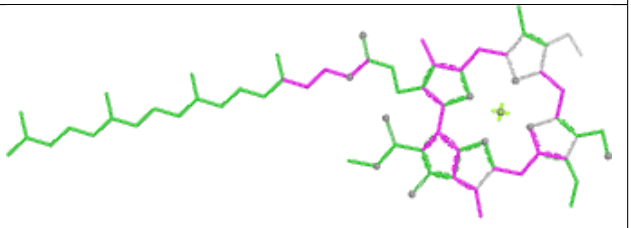


Rings

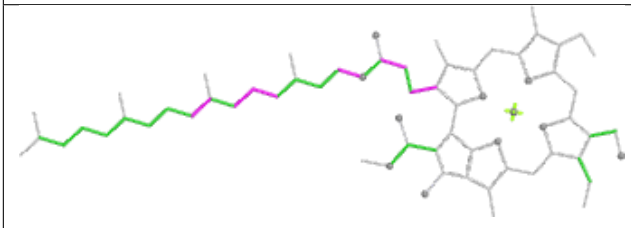
Ligand CHL 6 619



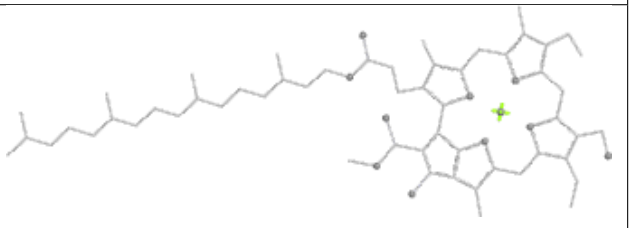
Bond lengths



Bond angles

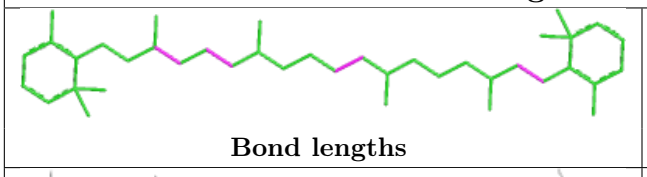


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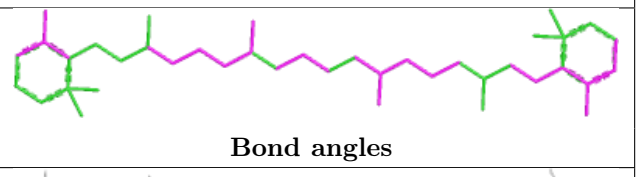


Rings

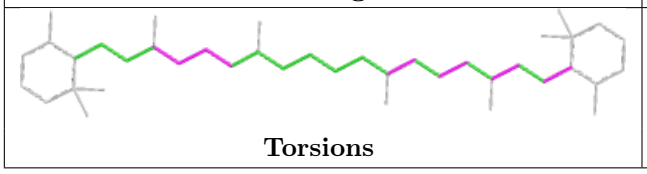
Ligand BCR 3 505



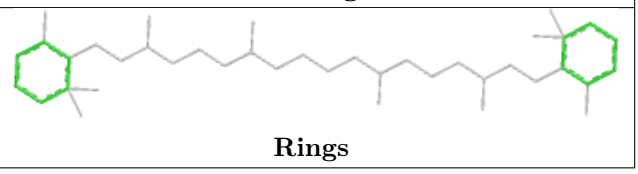
Bond lengths



Bond angles

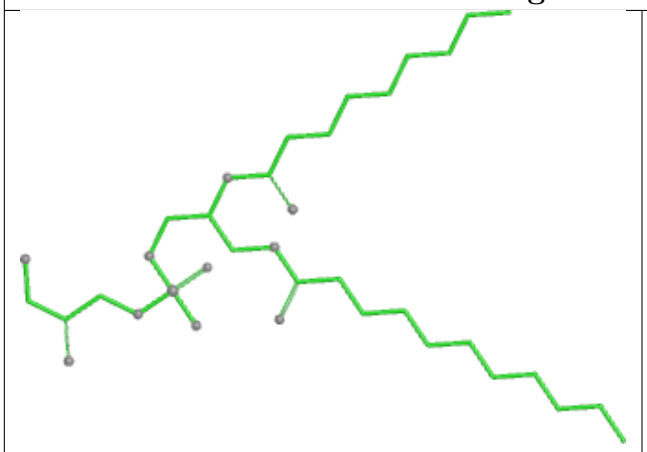


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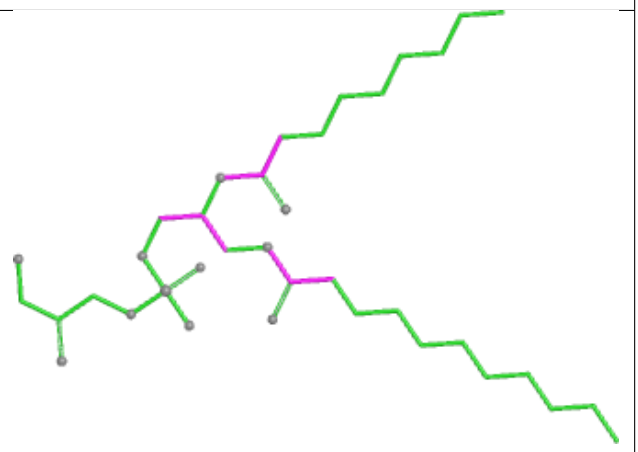


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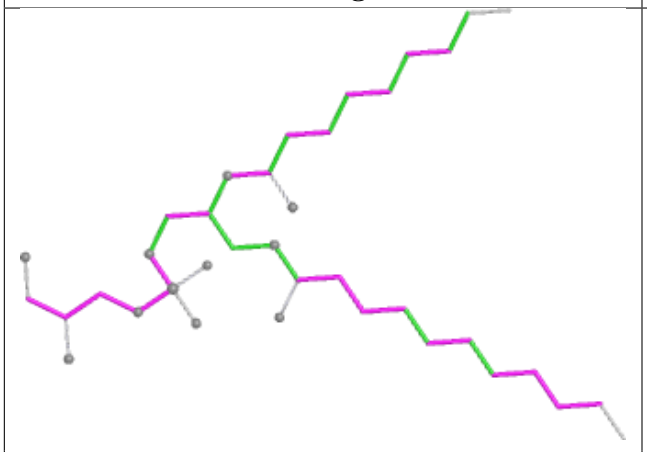
Ligand LHG 6 802



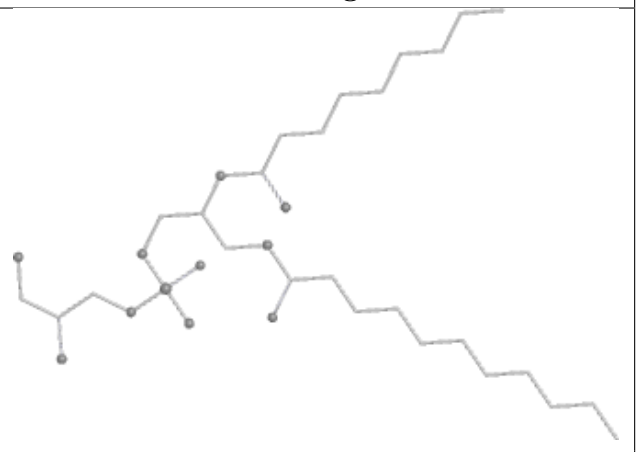
Bond lengths



Bond angles

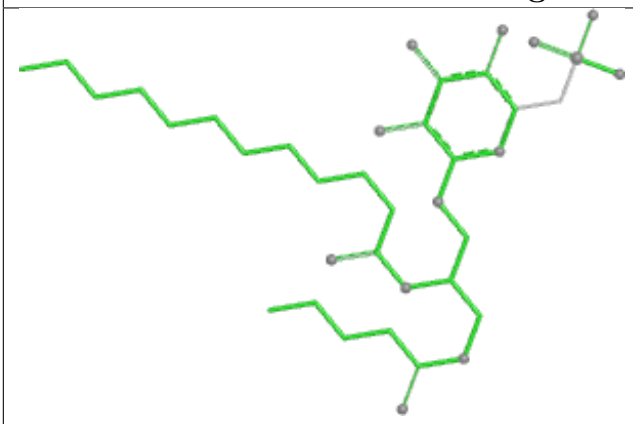


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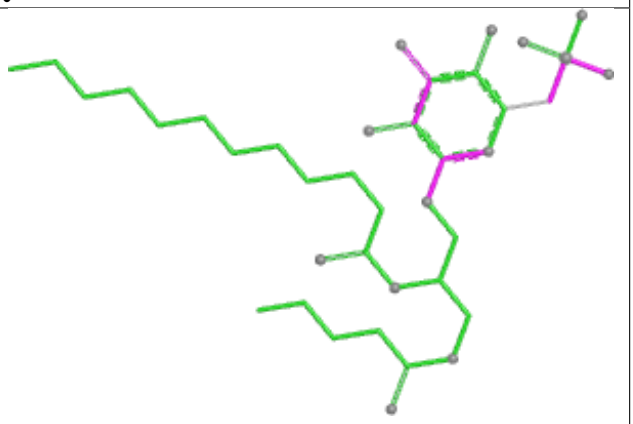


Rings

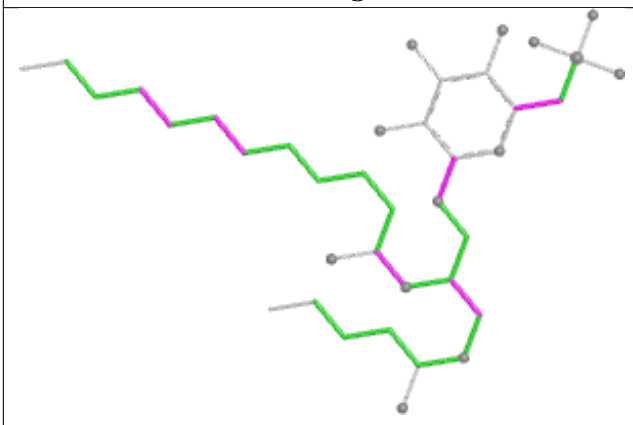
Ligand SQD 7 805



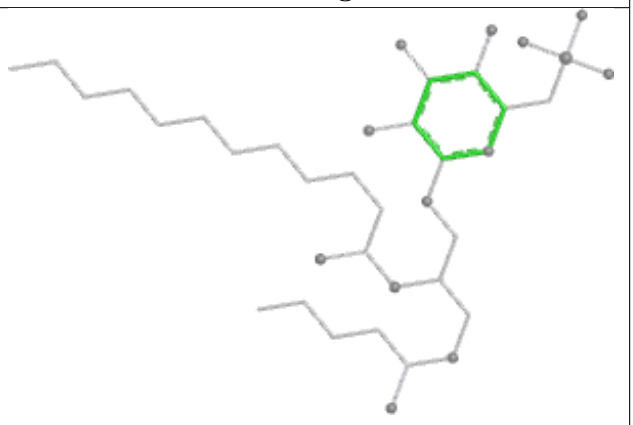
Bond lengths



Bond angles

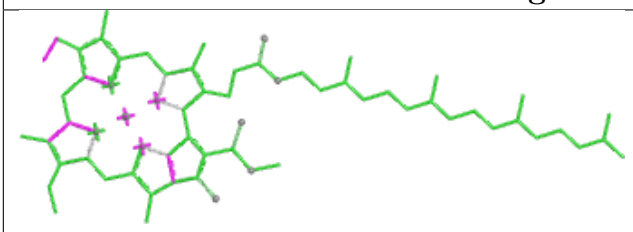


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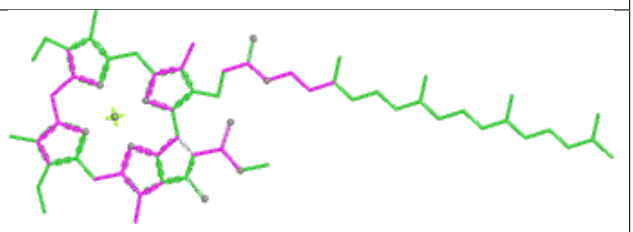


Rings

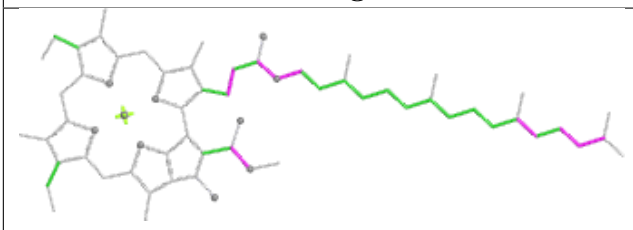
Ligand CLA 5 604



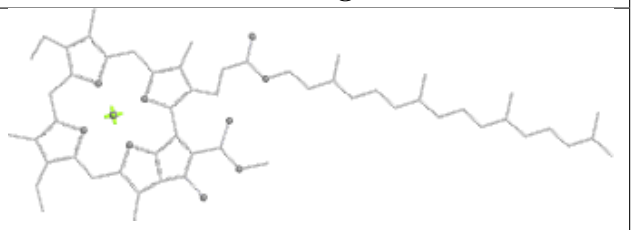
Bond lengths



Bond angles

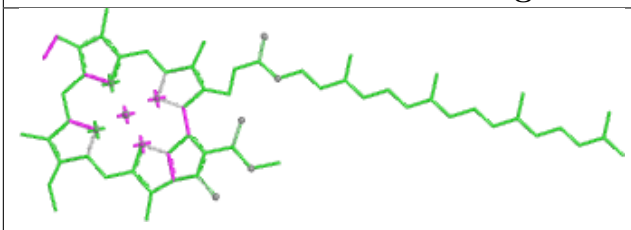


Torsions

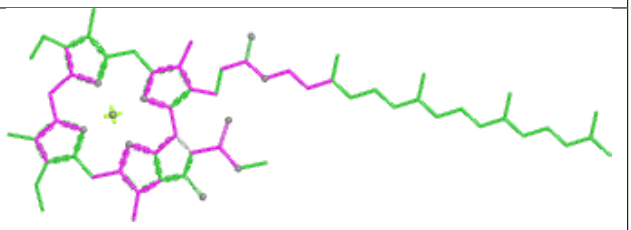


Rings

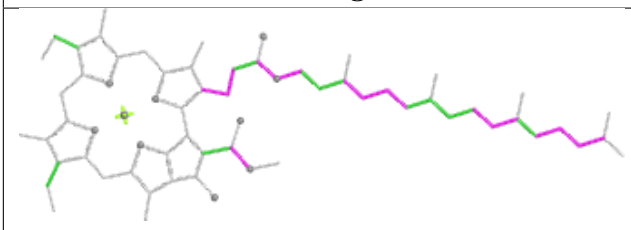
Ligand CLA A 1109



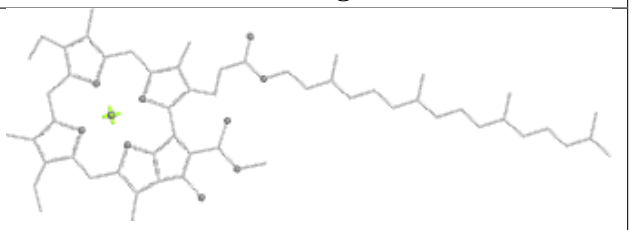
Bond lengths



Bond angles

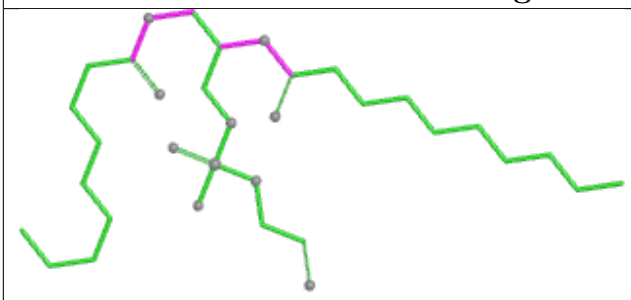


Torsions

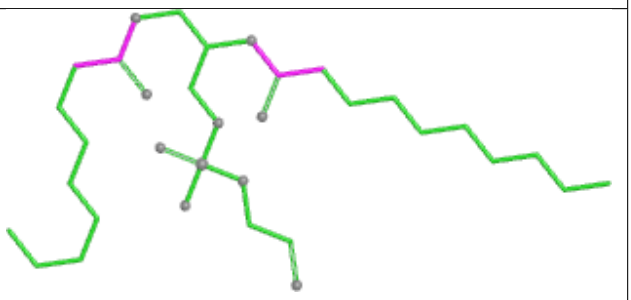


Rings

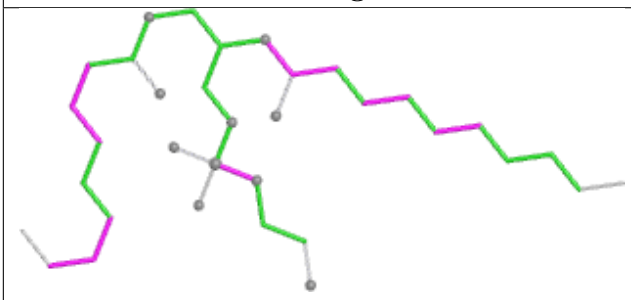
Ligand PTY A 5006



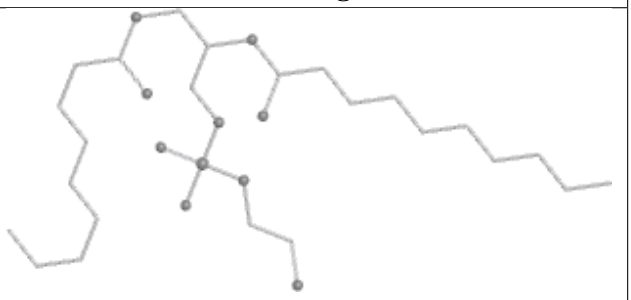
Bond lengths



Bond angles

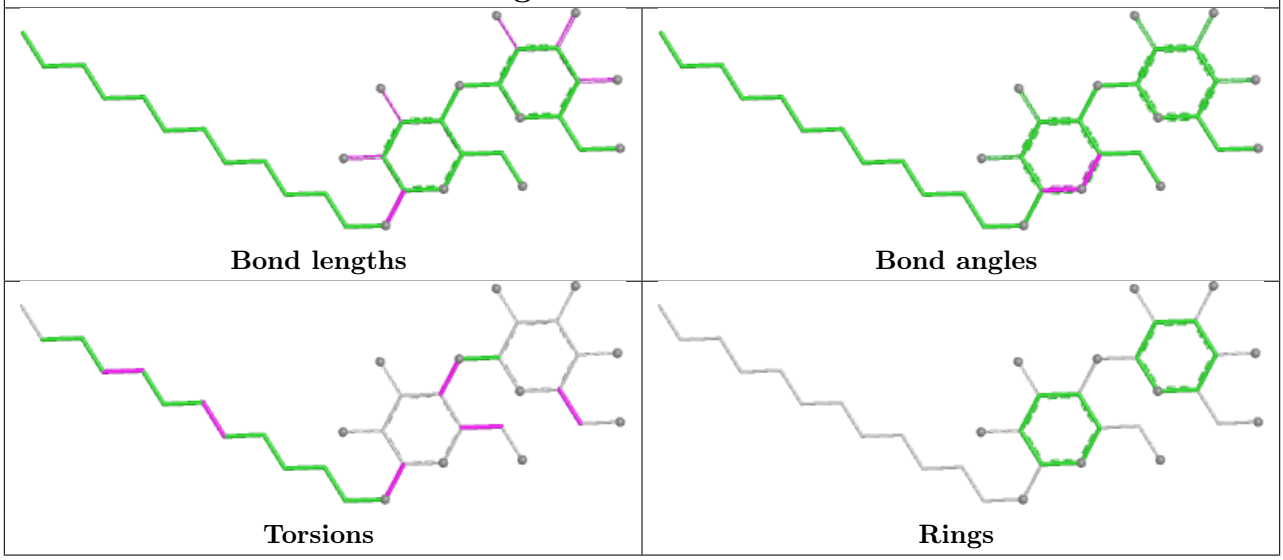


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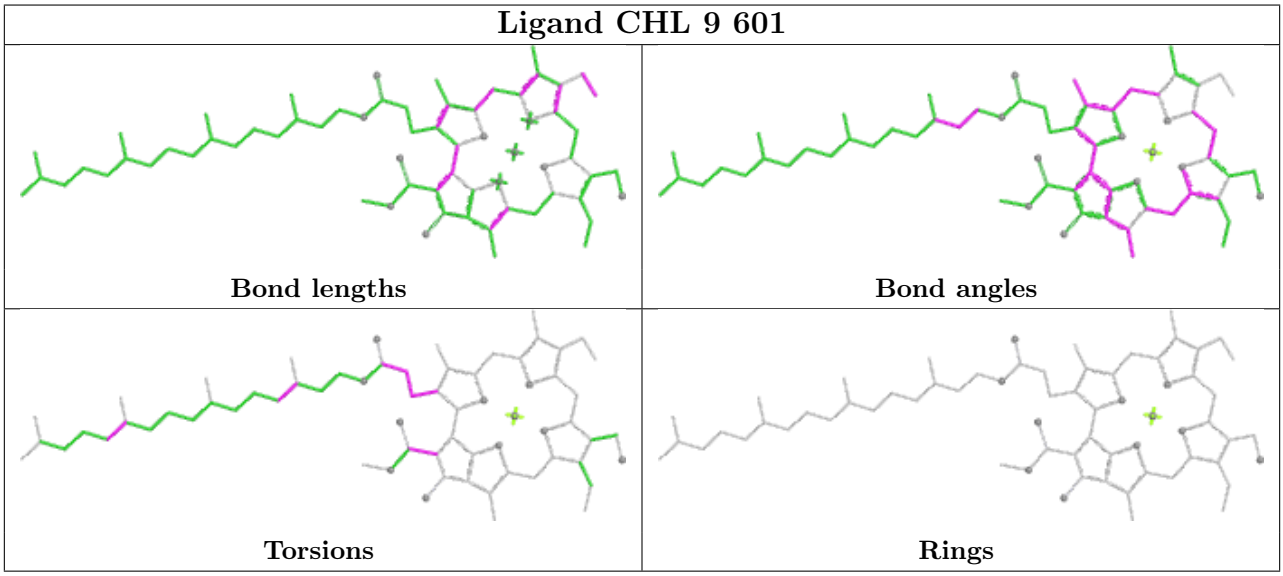


Rings

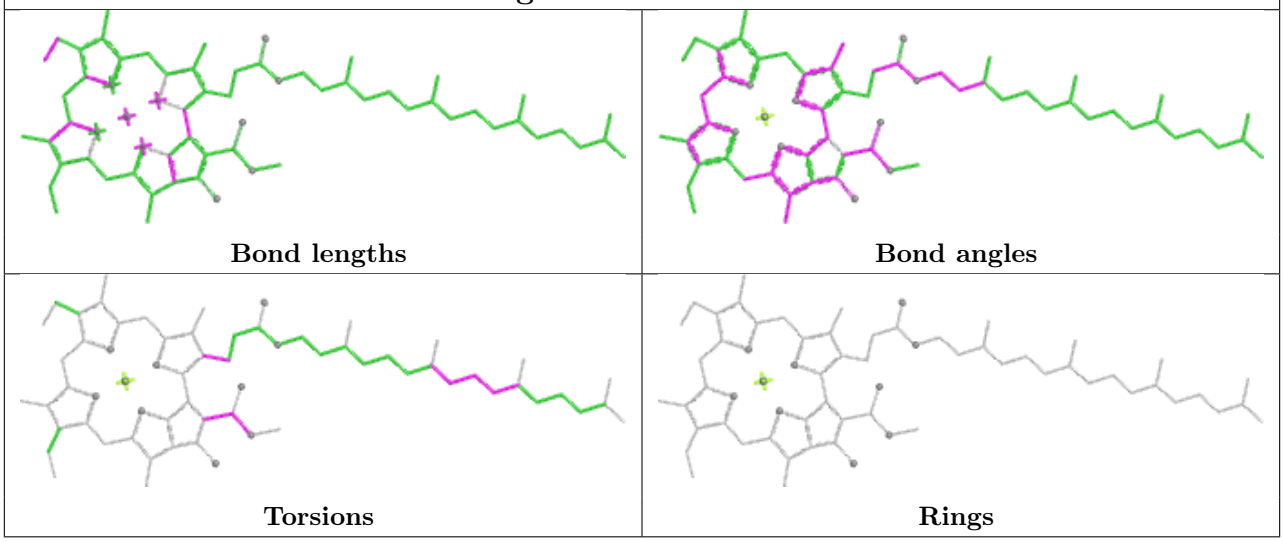
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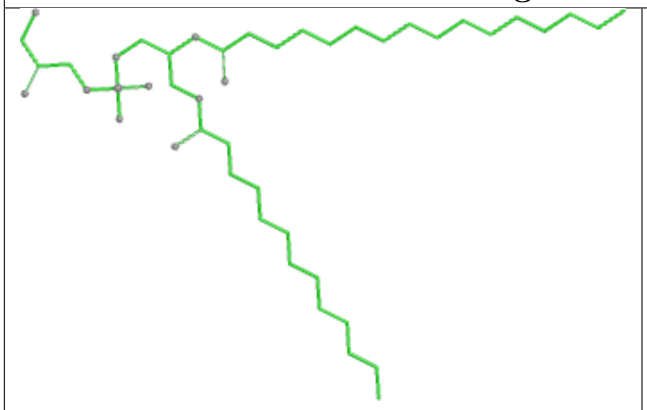
Ligand CHL 9 601



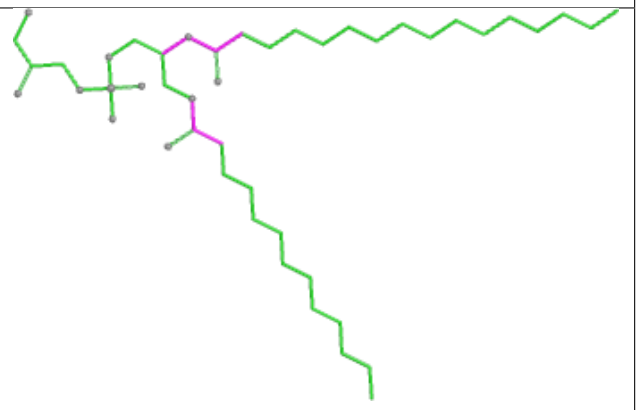
Ligand CLA B 1223



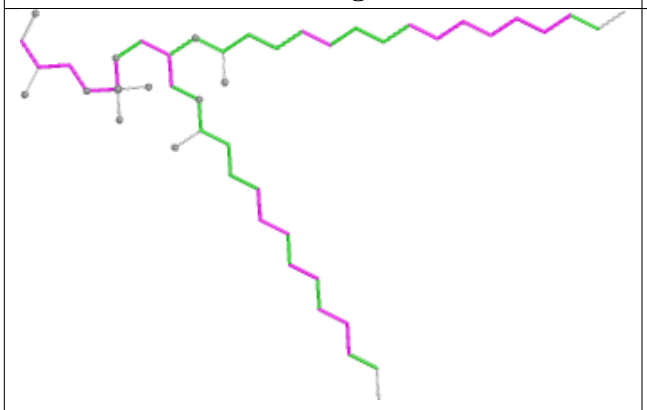
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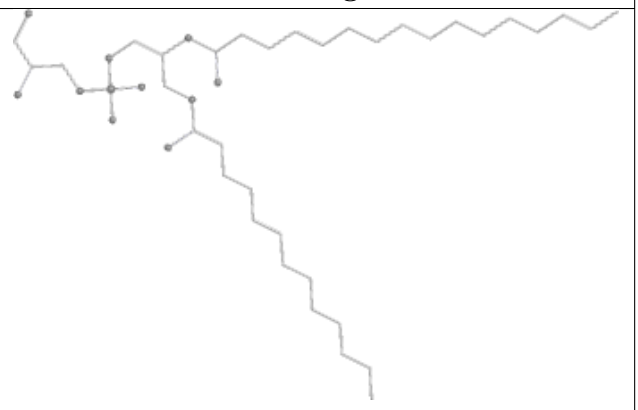
Bond lengths



Bond angles

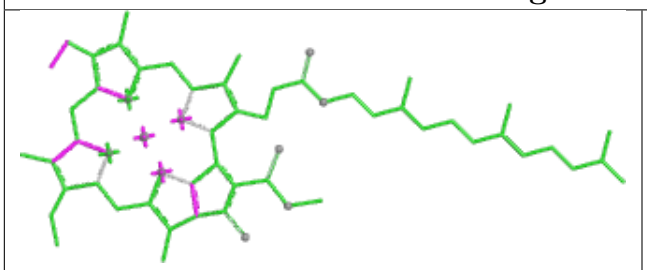


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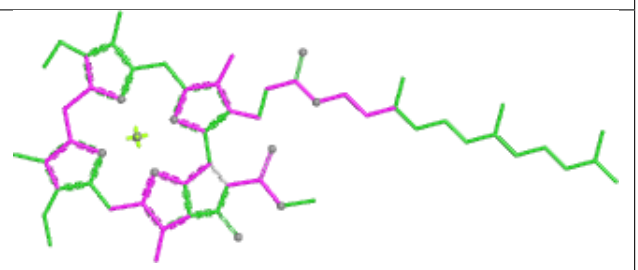


Rings

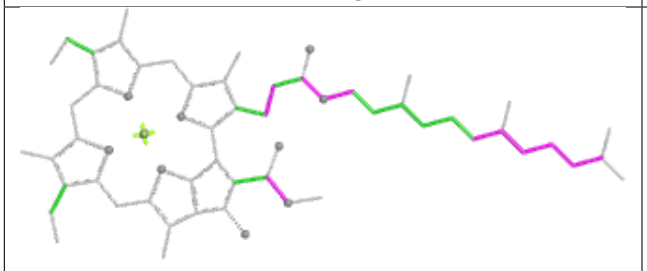
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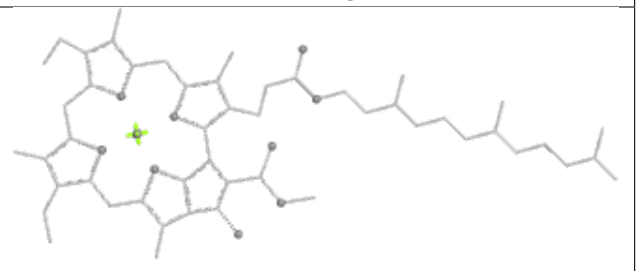
Bond lengths



Bond angles

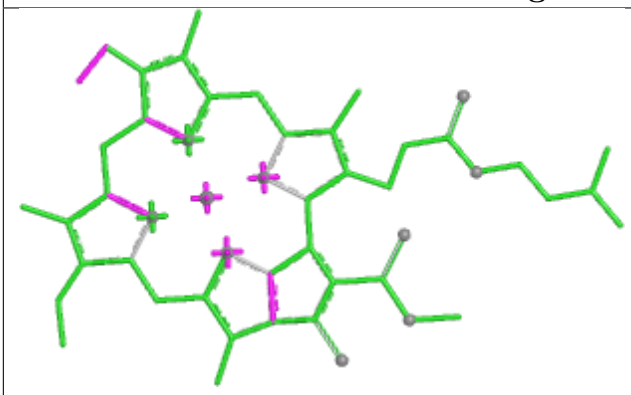


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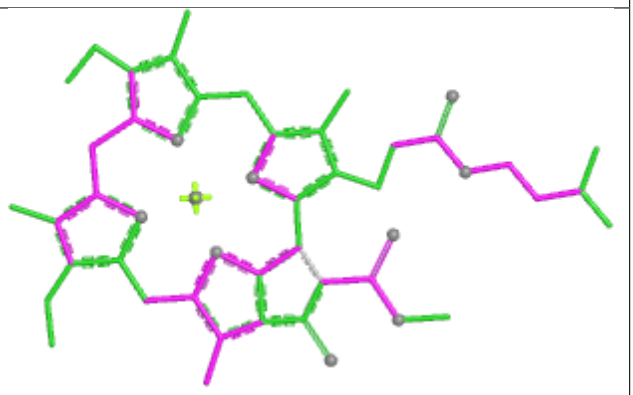


Rings

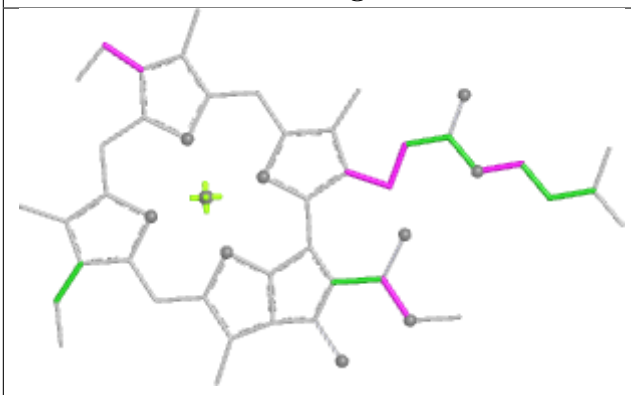
Ligand CLA 8 612



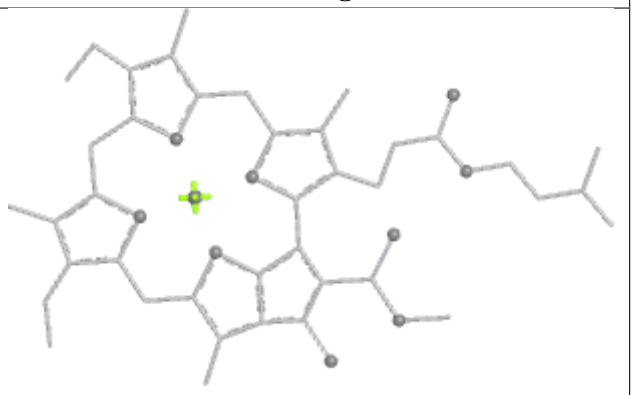
Bond lengths



Bond angles



Torsions

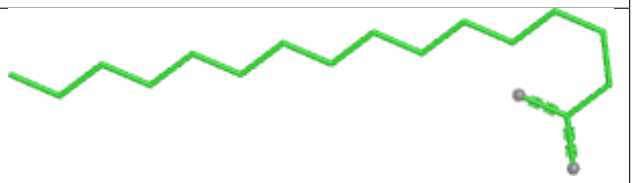


Rings

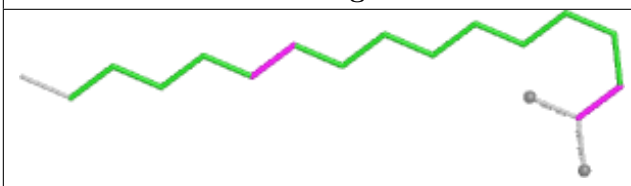
Ligand PLM 5 804



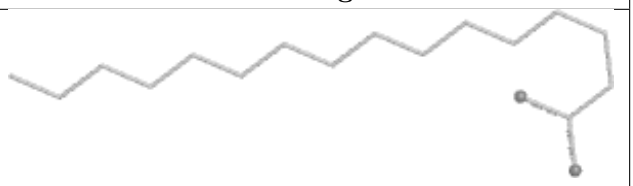
Bond lengths



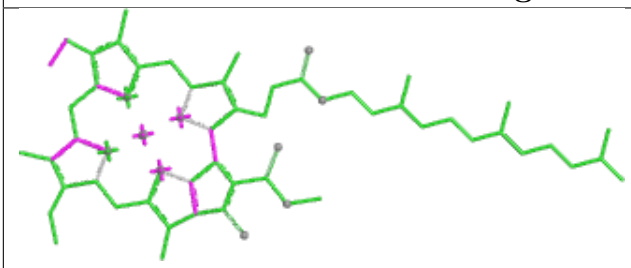
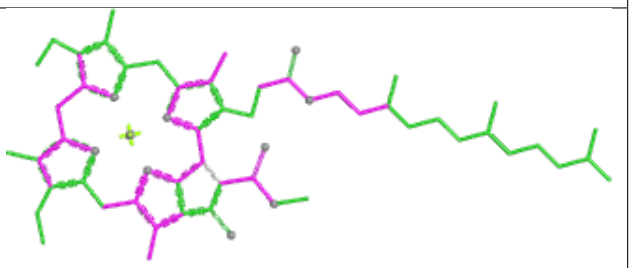
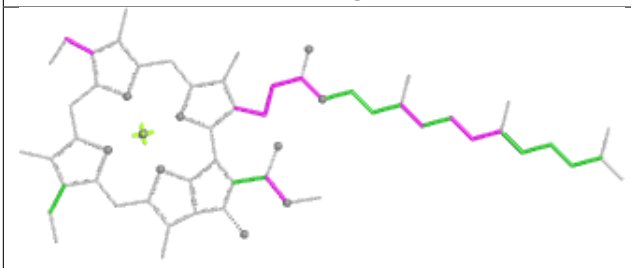
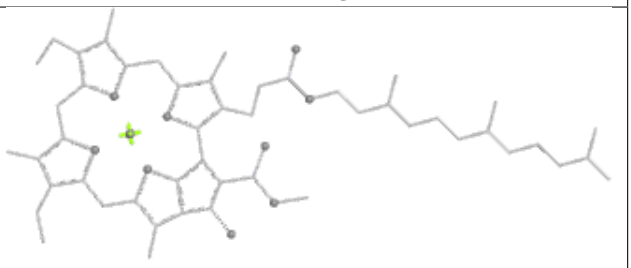
Bond angles

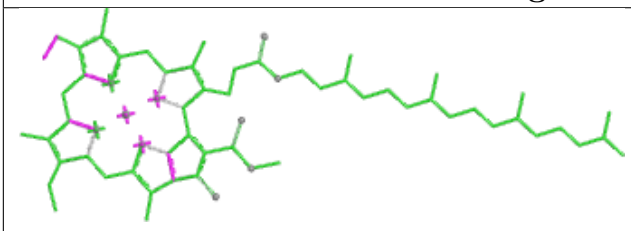
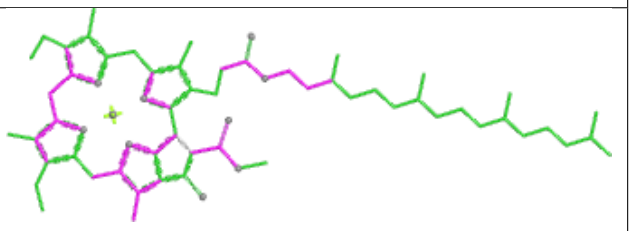
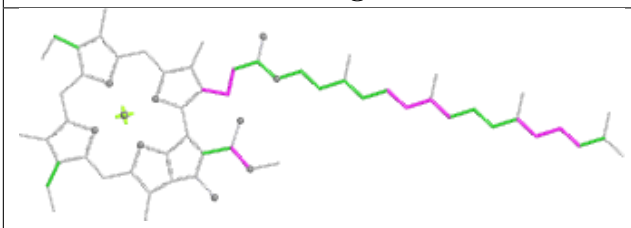
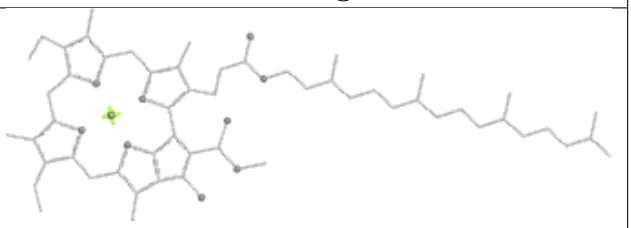


Torsions

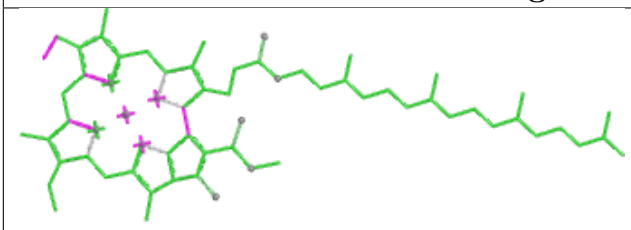


Rings

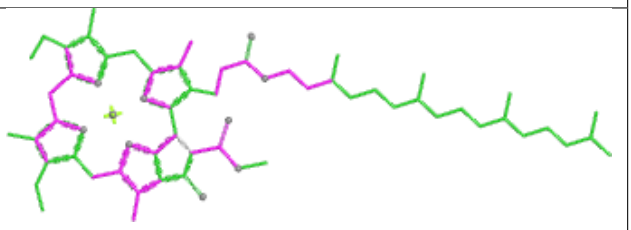
Ligand CLA A 1134	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

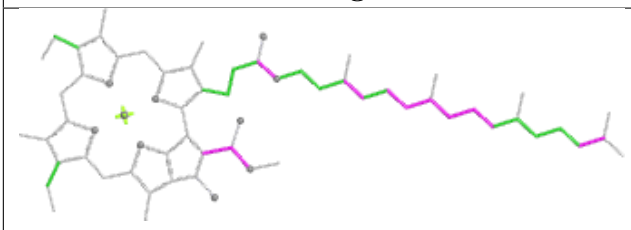
Ligand CLA 6 615



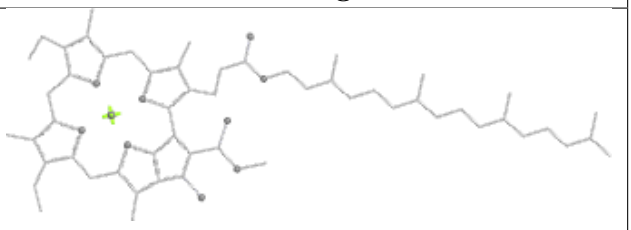
Bond lengths



Bond angles

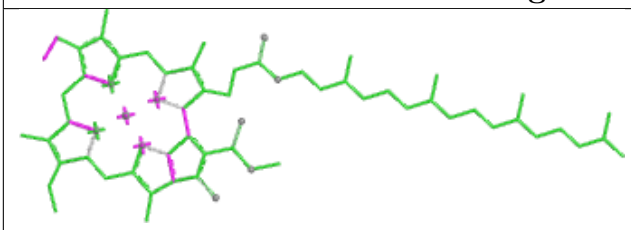


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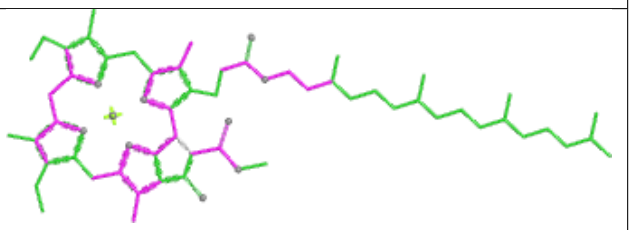


Rings

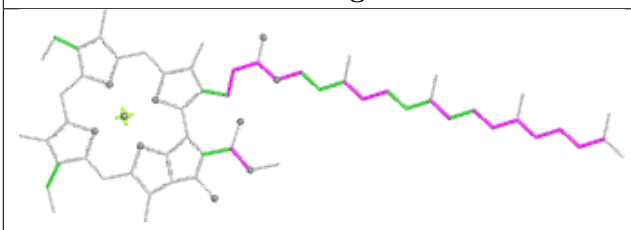
Ligand CLA 7 603



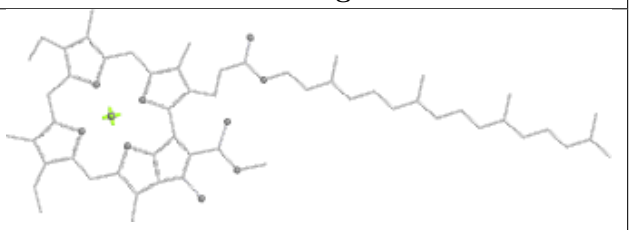
Bond lengths



Bond angles

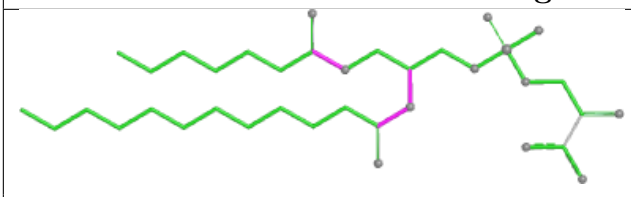


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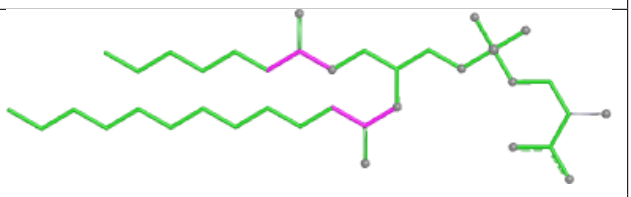


Rings

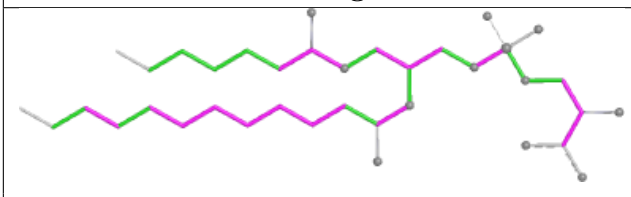
Ligand P5S 8 805



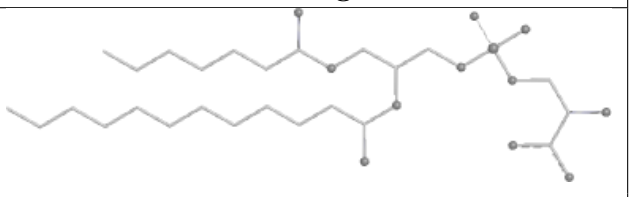
Bond lengths



Bond angles

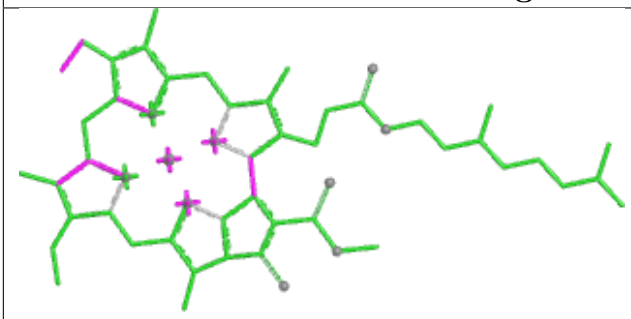


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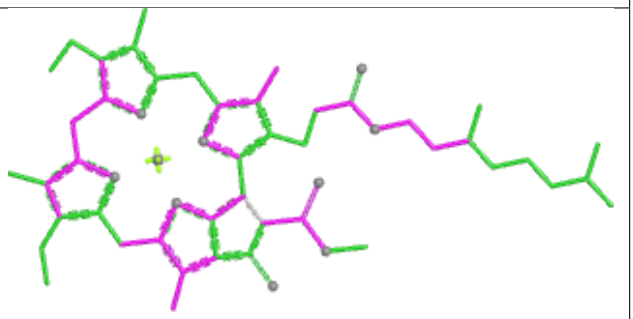


Rings

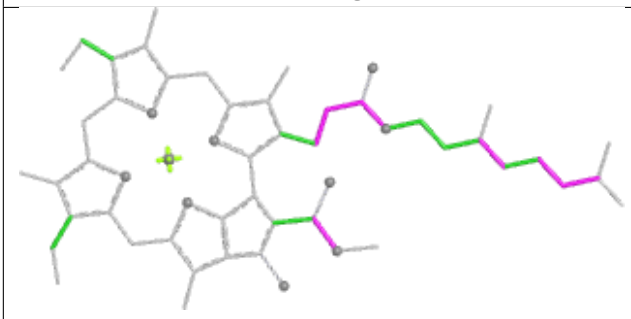
Ligand CLA B 1213



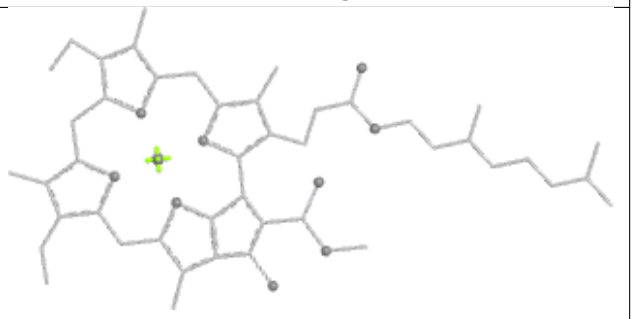
Bond lengths



Bond angles

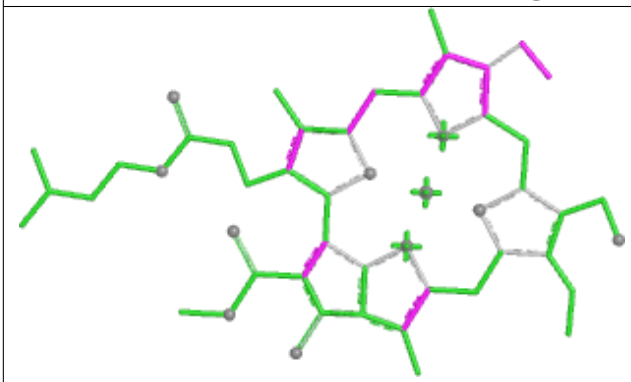


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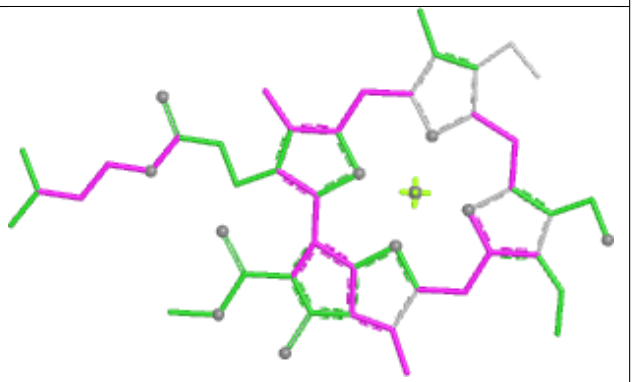


Rings

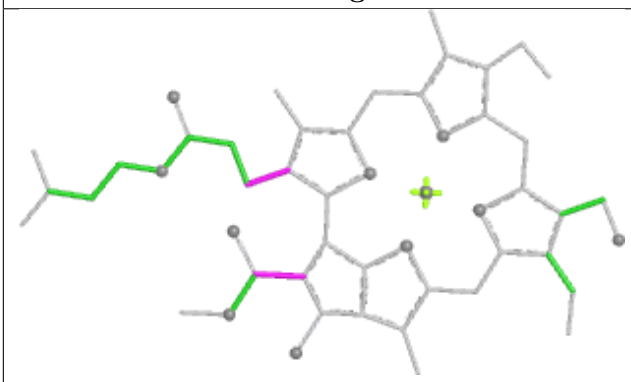
Ligand CHL 5 618



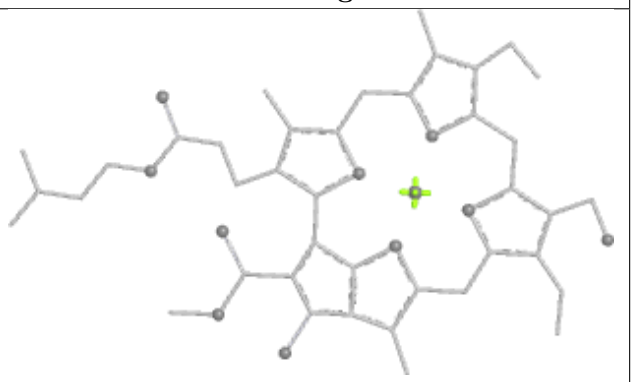
Bond lengths



Bond angles

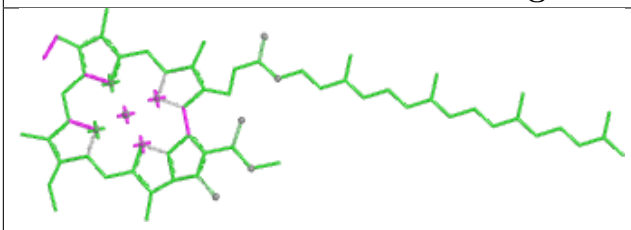


Torsions

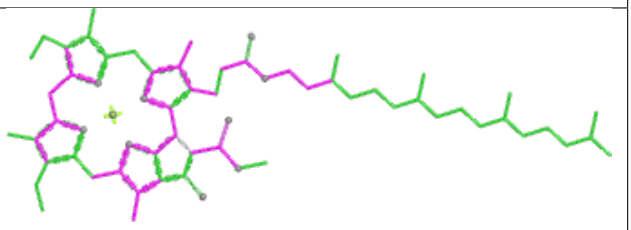


Rings

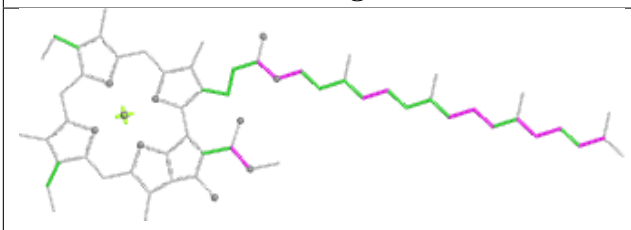
Ligand CLA 2 607



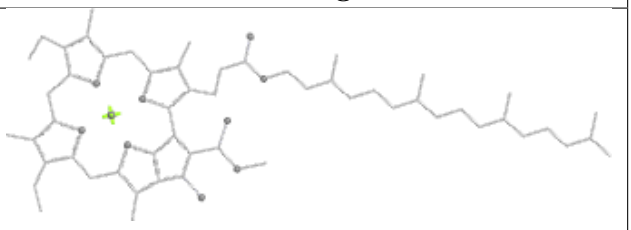
Bond lengths



Bond angles

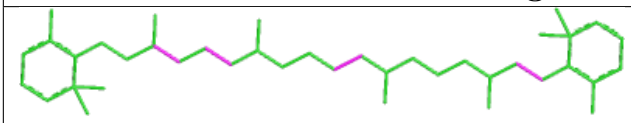


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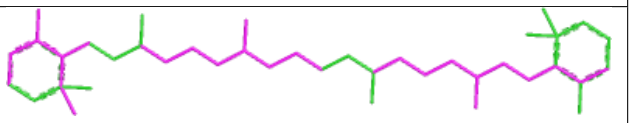


Rings

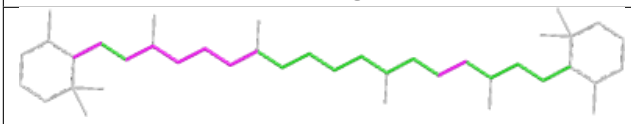
Ligand BCR 7 503



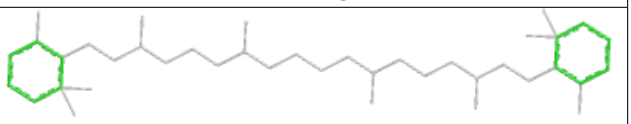
Bond lengths



Bond angles

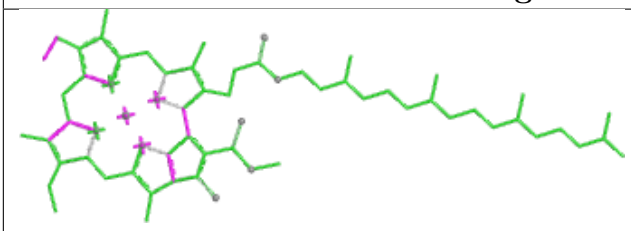


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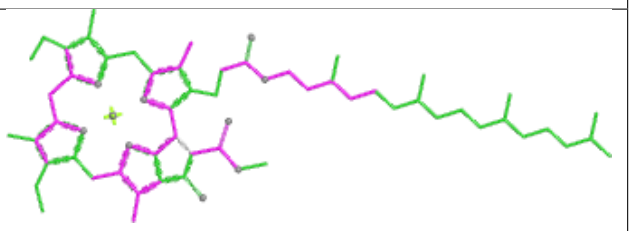


Rings

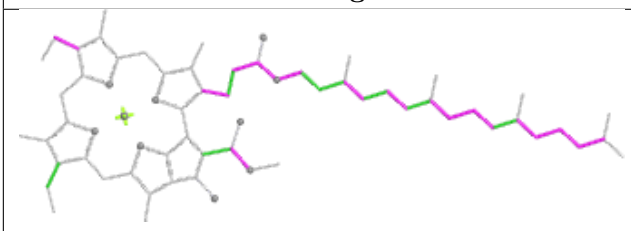
Ligand CLA A 1126



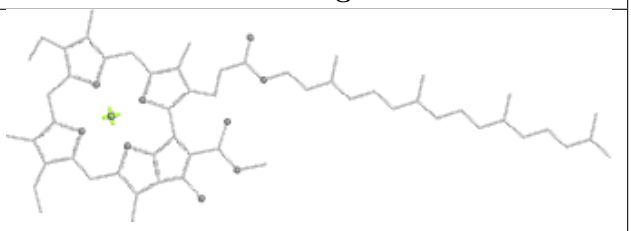
Bond lengths



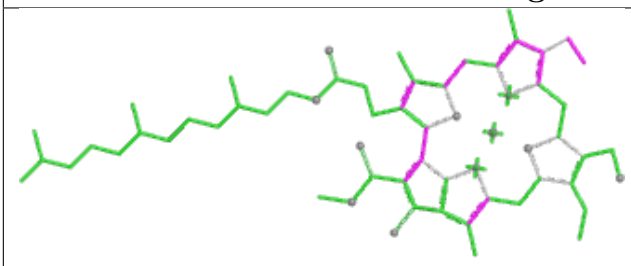
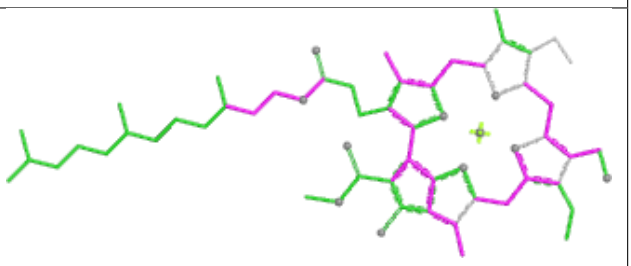
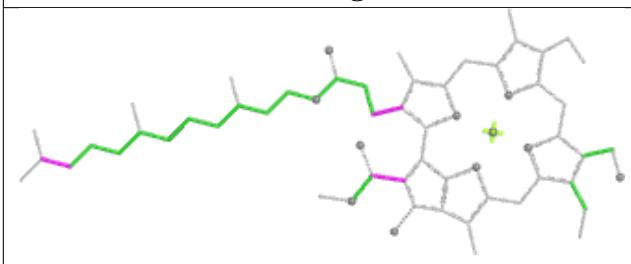
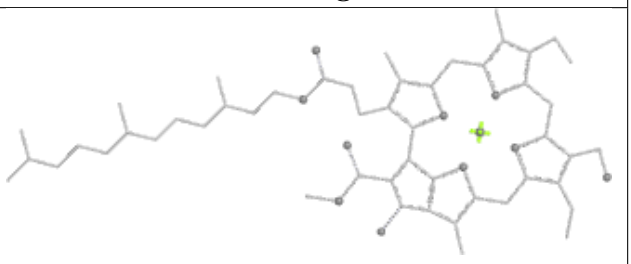
Bond angles

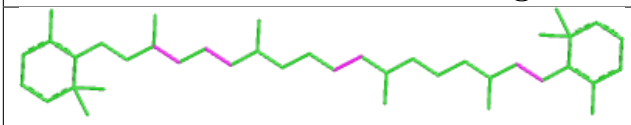
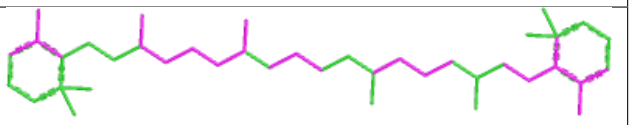
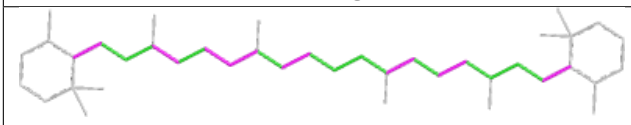
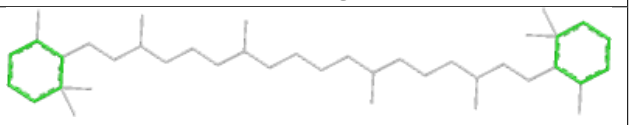


Torsions

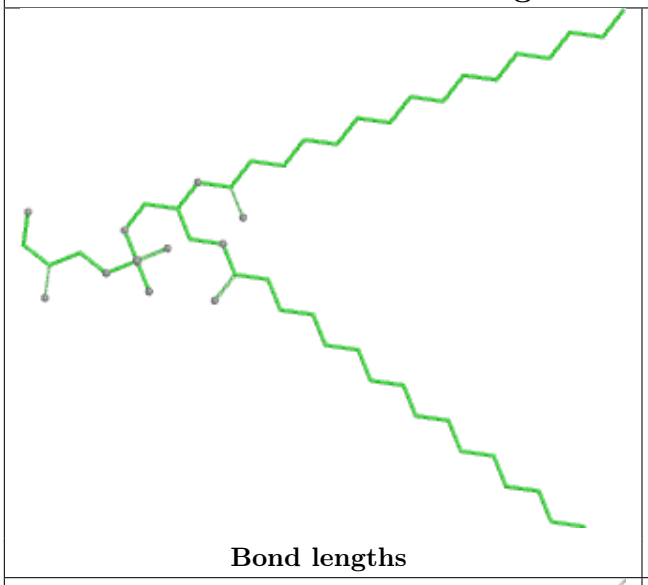


Rings

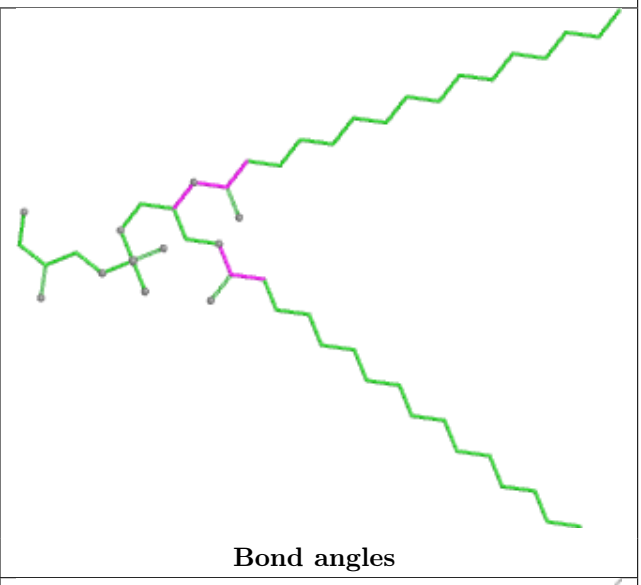
Ligand CHL 8 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR O 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

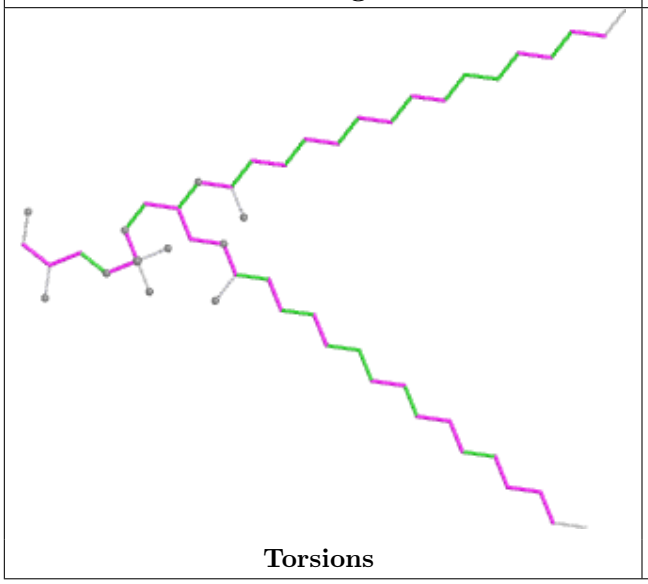
Ligand LHG A 5001



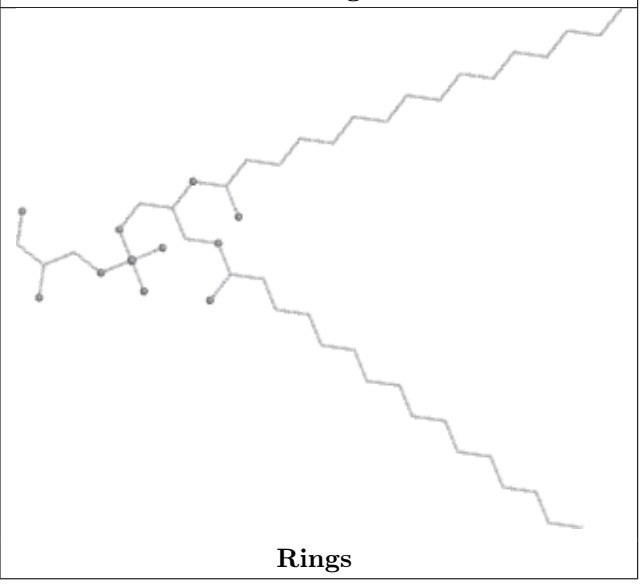
Bond lengths



Bond angles

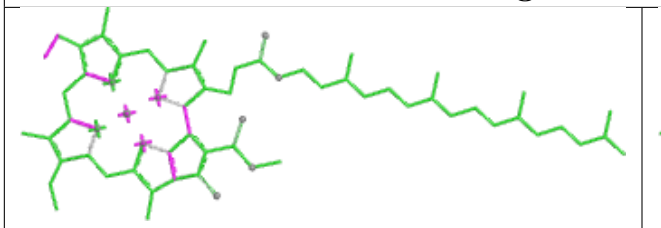


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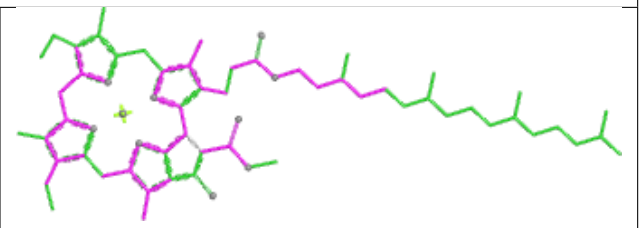


Rings

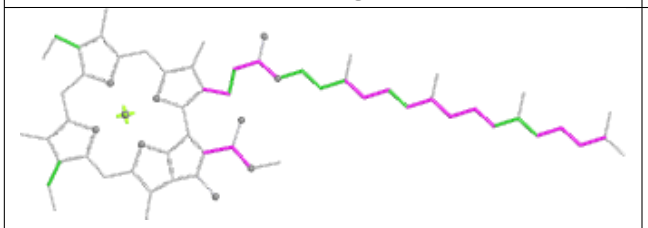
Ligand CLA B 1210



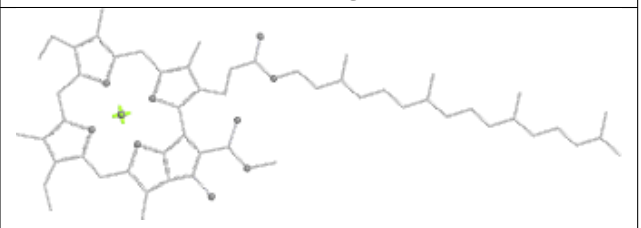
Bond lengths



Bond angles

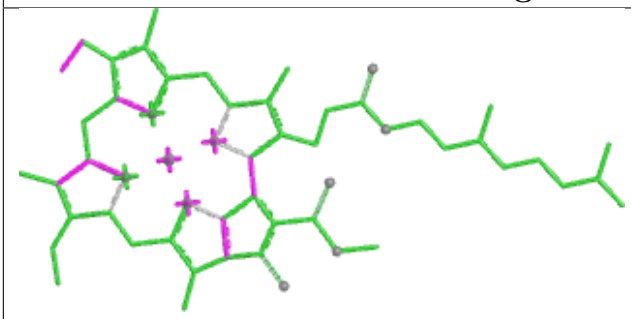


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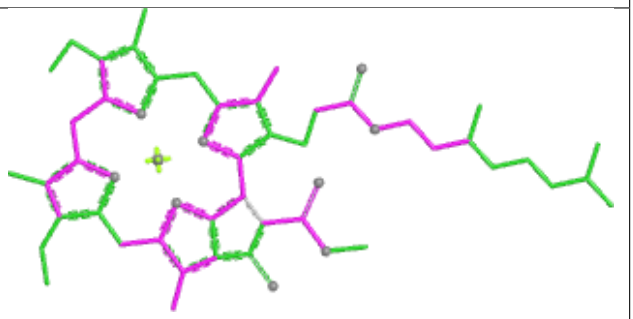


Rings

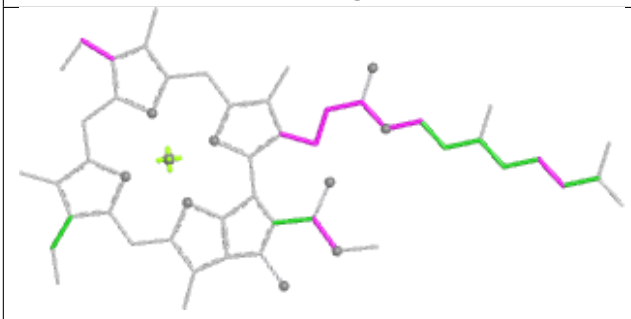
Ligand CLA A 1139



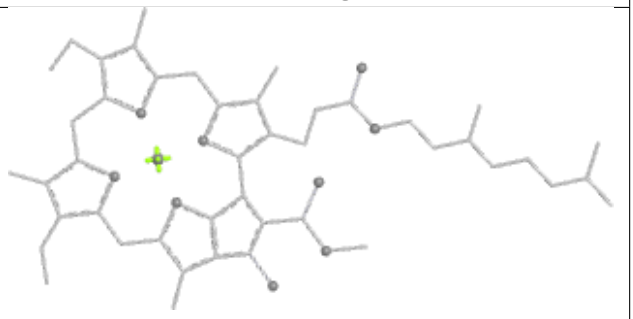
Bond lengths



Bond angles

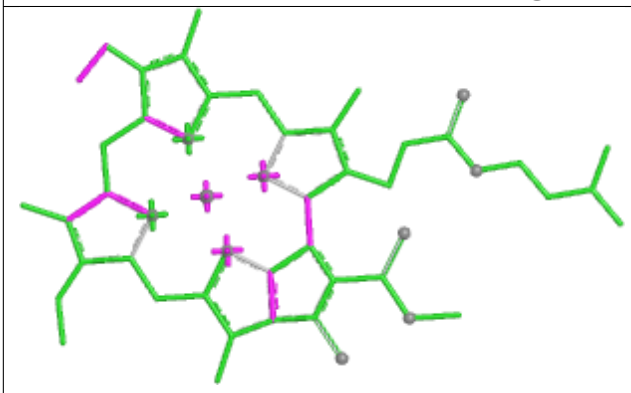


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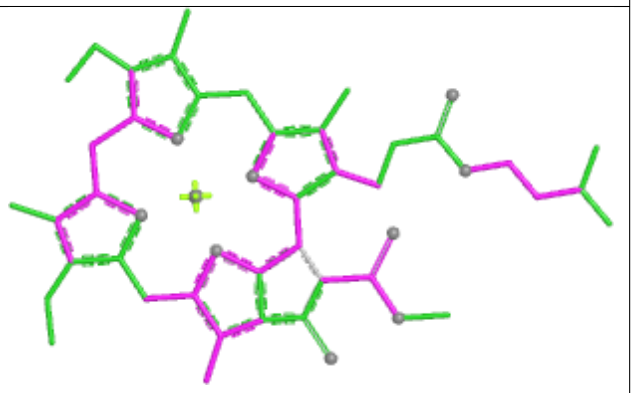


Rings

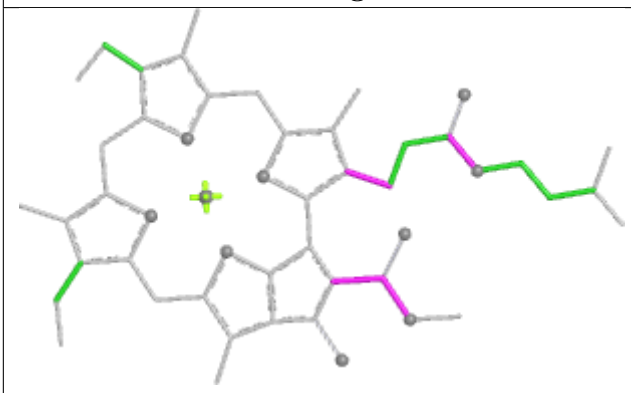
Ligand CLA 4 606



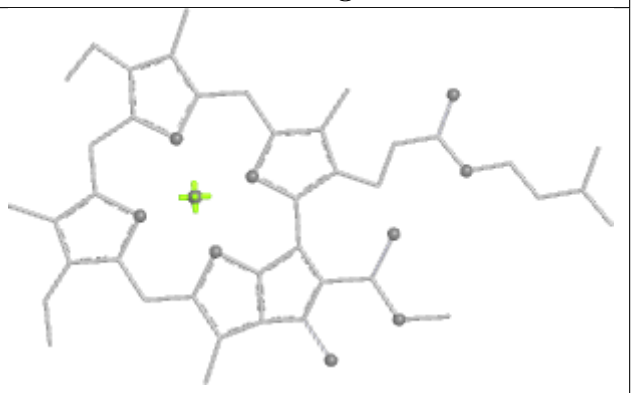
Bond lengths



Bond angles

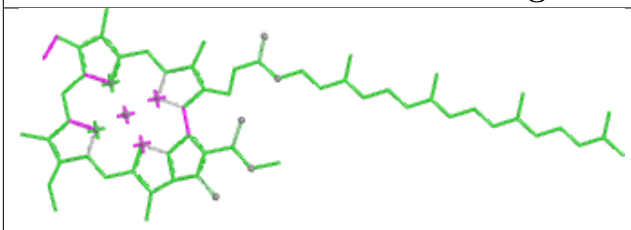


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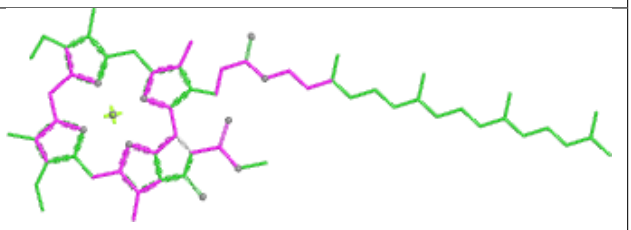


Rings

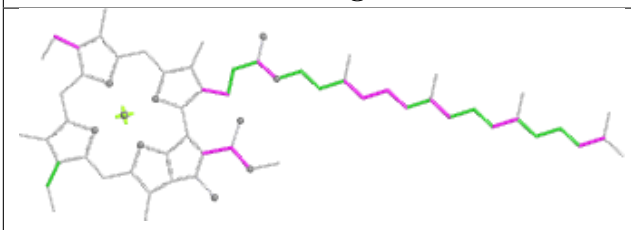
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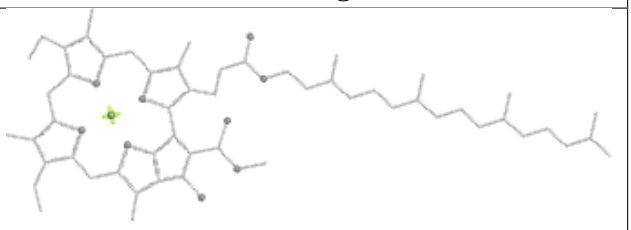
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Bond angles

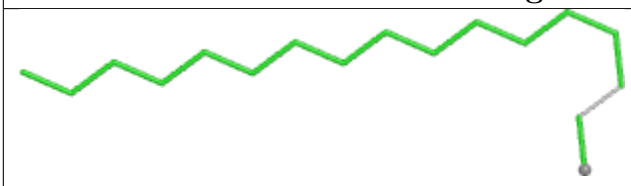


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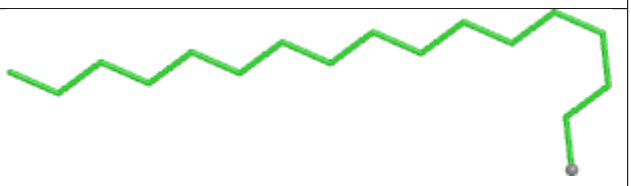


Rings

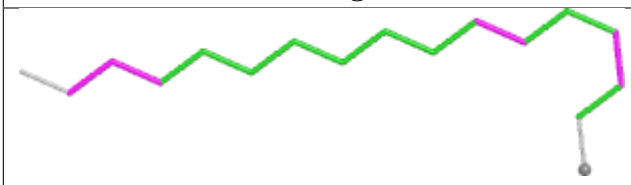
Ligand PLM a 804



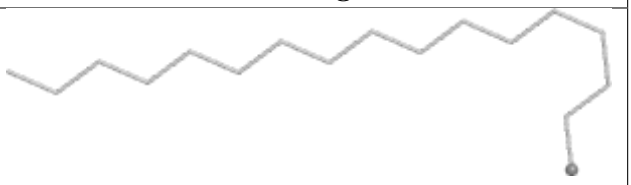
Bond lengths



Bond angles

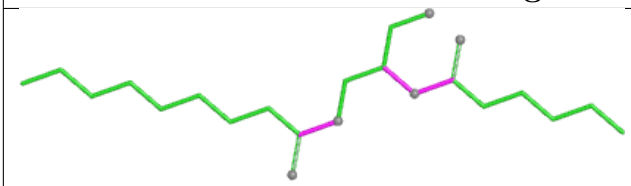


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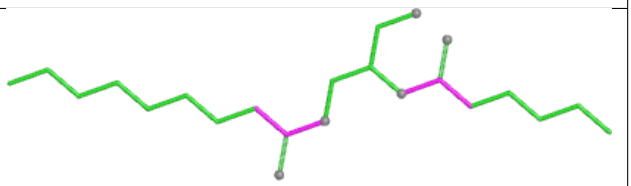


Rings

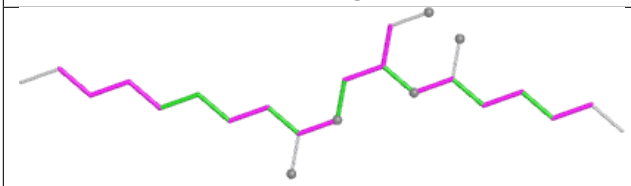
Ligand DGA 5 803



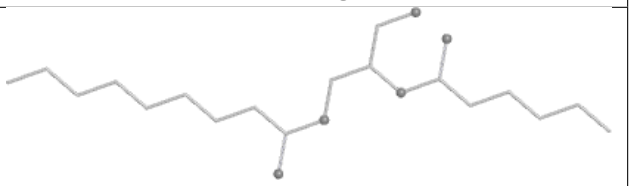
Bond lengths



Bond angles

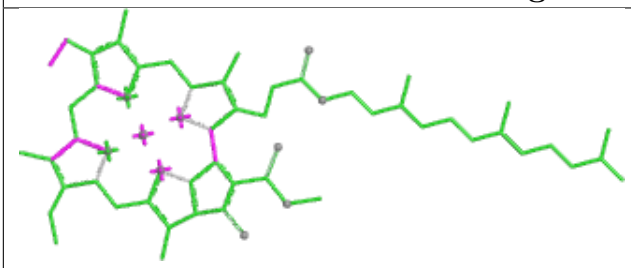


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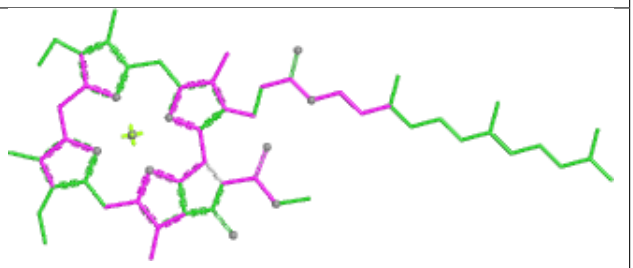


Rings

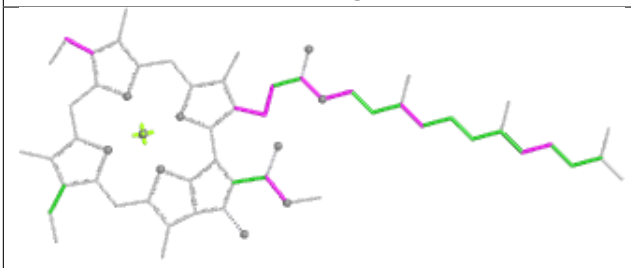
Ligand CLA 5 607



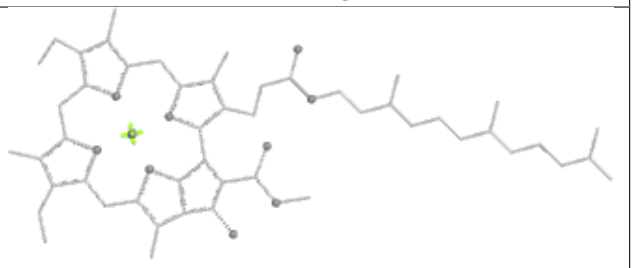
Bond lengths



Bond angles

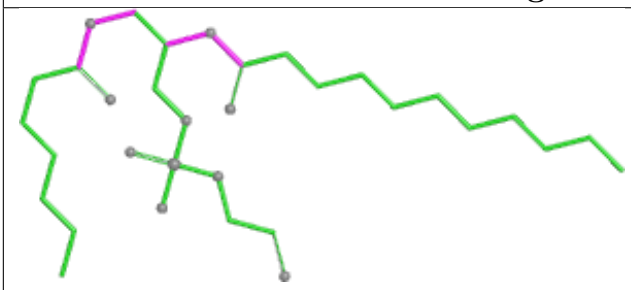


Torsions

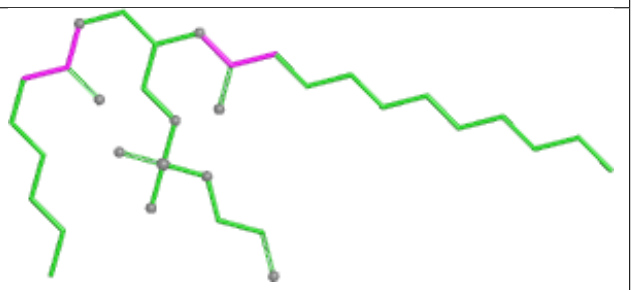


Rings

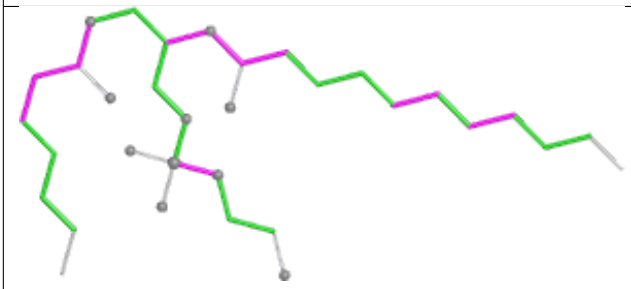
Ligand PTY 7 804



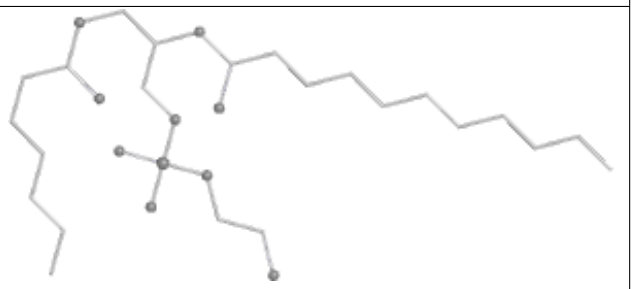
Bond lengths



Bond angles

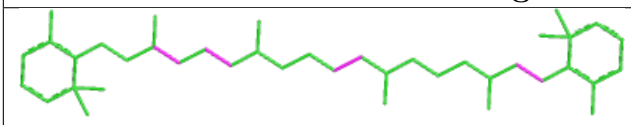


Torsions

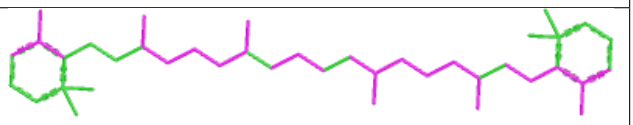


Rings

Ligand BCR K 4002



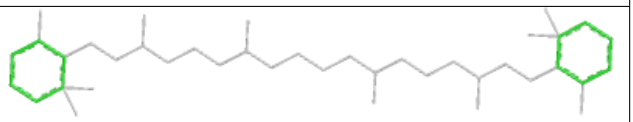
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Bond angles

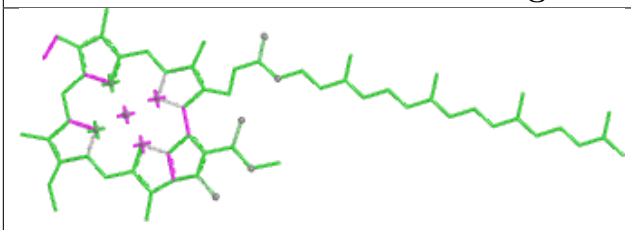


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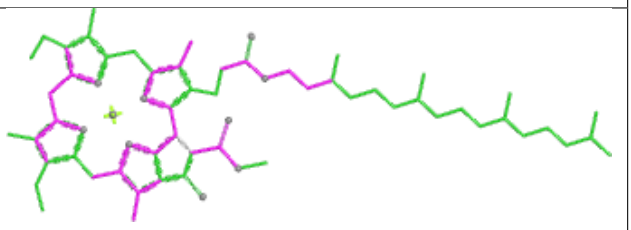


Rings

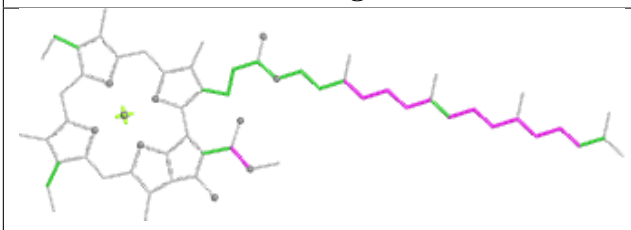
Ligand CLA 3 605



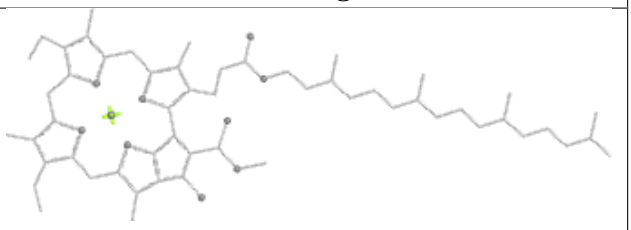
Bond lengths



Bond angles

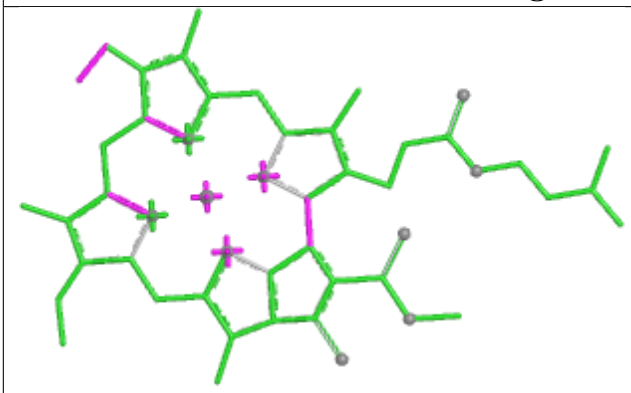


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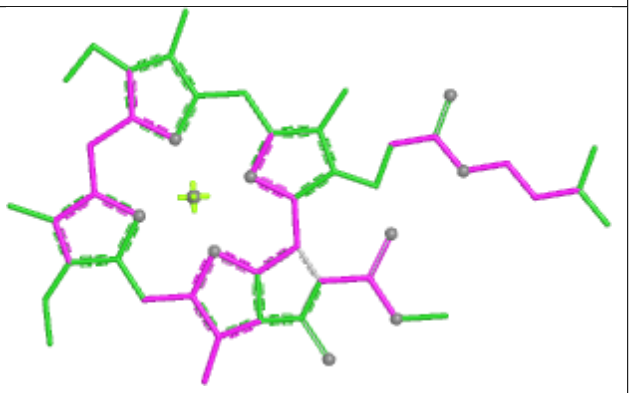


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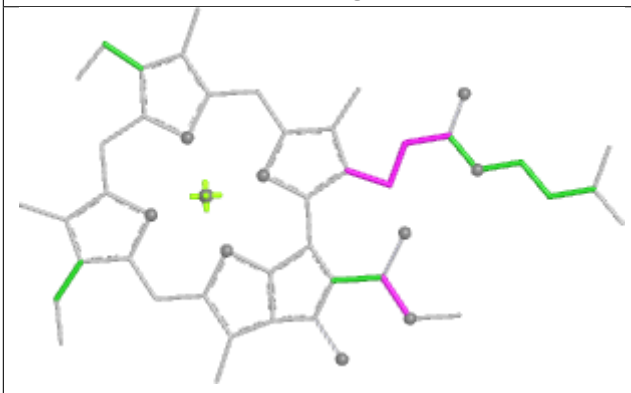
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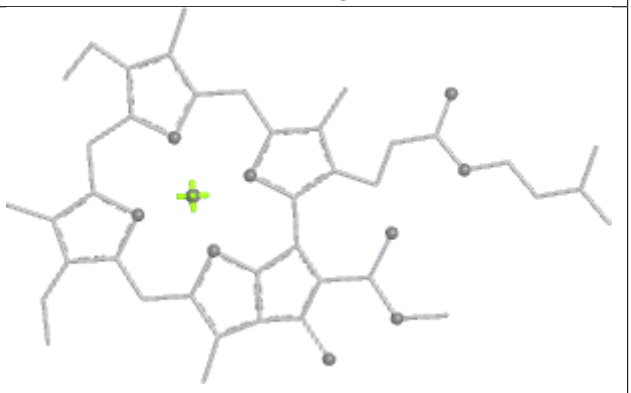
Bond lengths



Bond angles

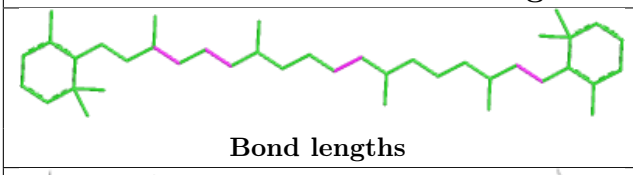


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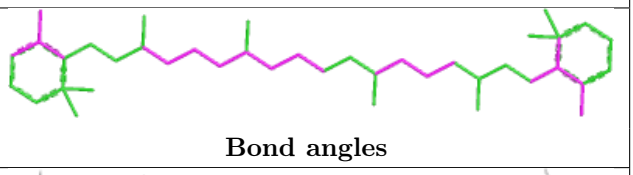


Rings

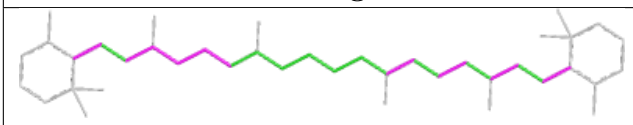
Ligand BCR 4 503



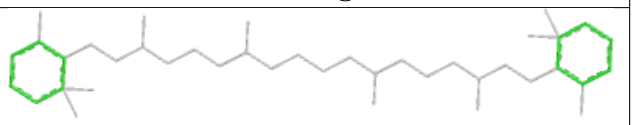
Bond lengths



Bond angles

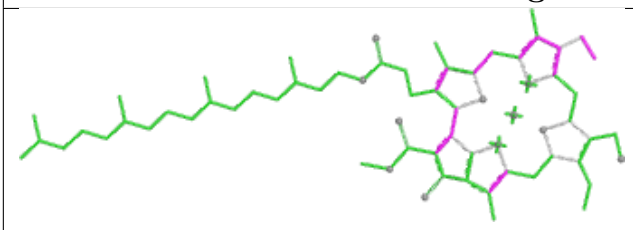


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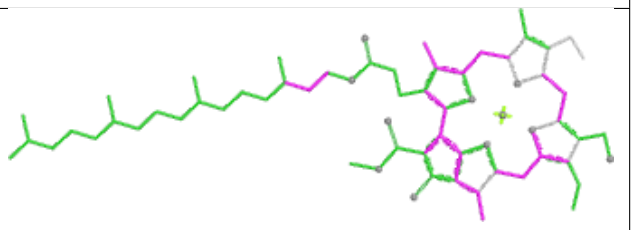


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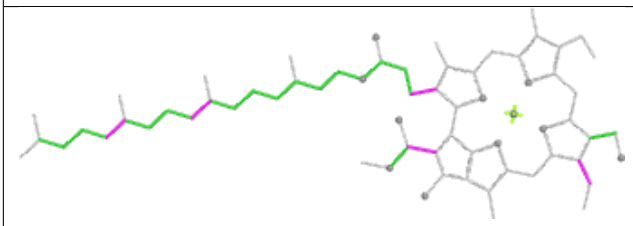
Ligand CHL 9 603



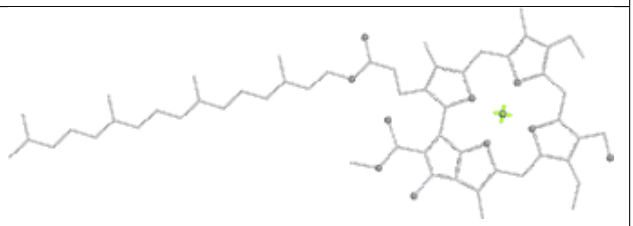
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Bond angles

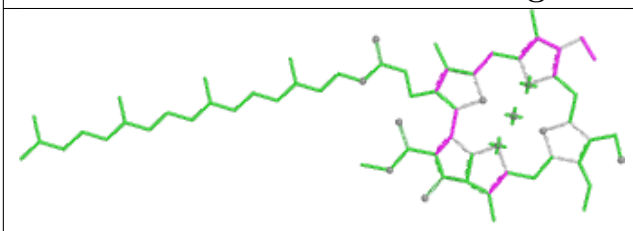


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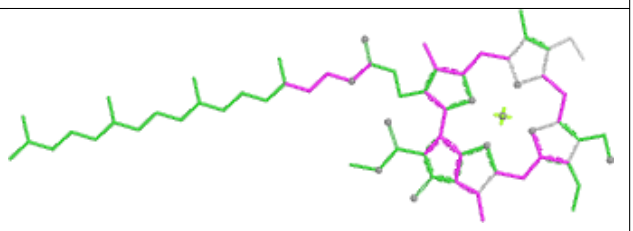


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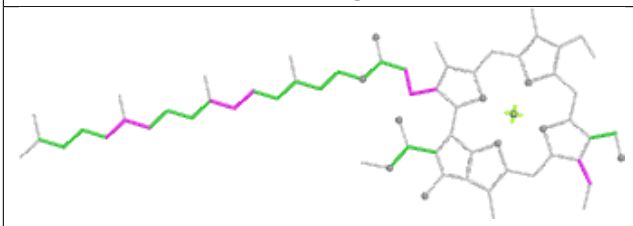
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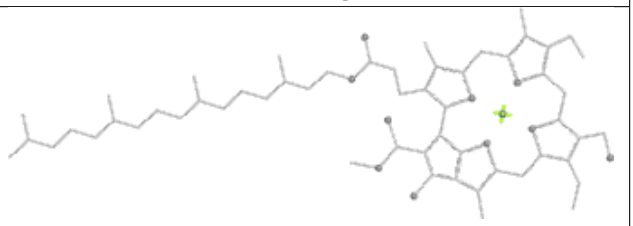
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Bond angles

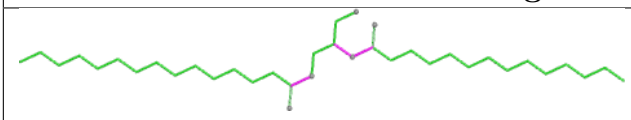


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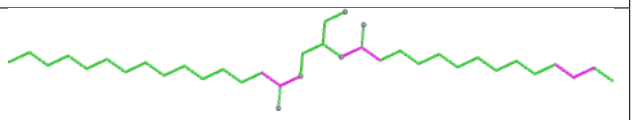


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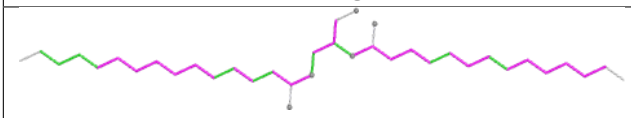
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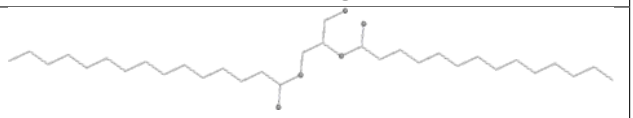
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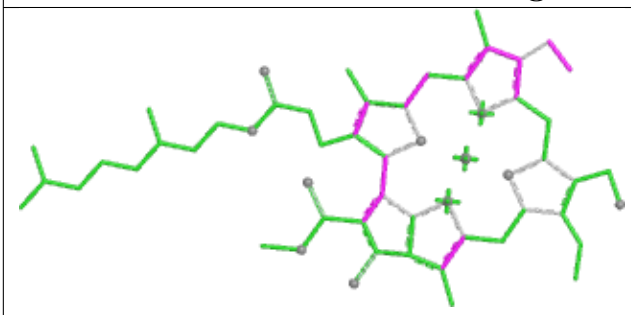


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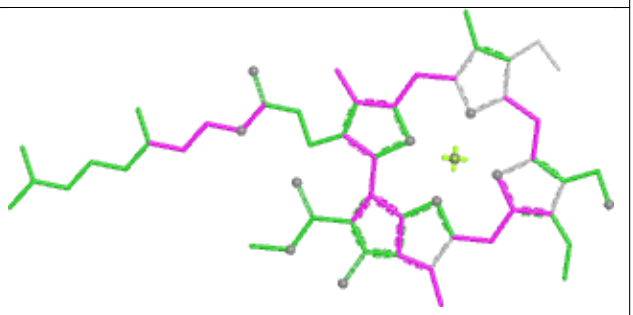


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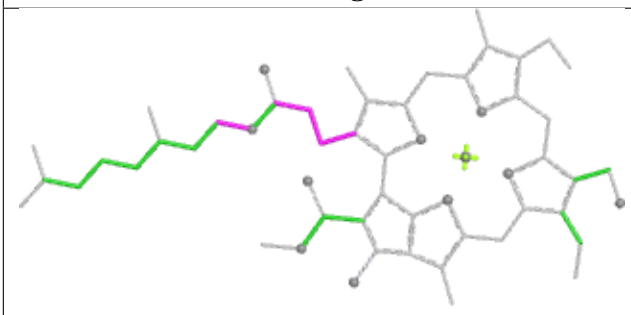
Ligand CHL 7 611



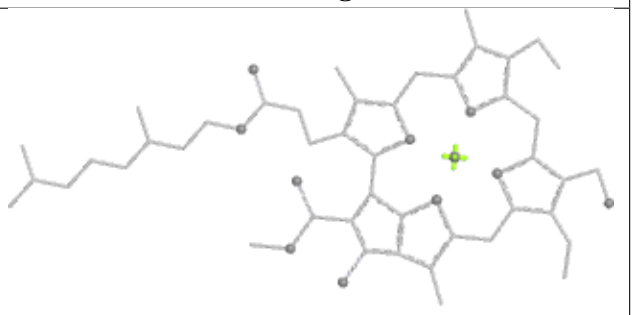
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Bond angles

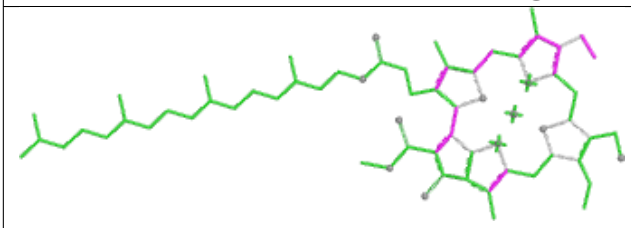


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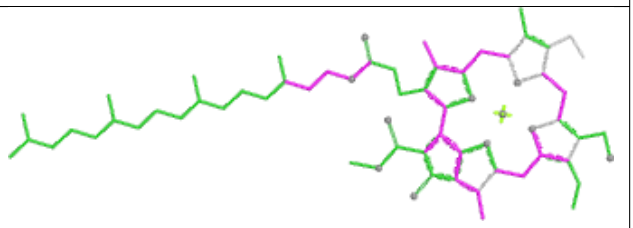


Rings

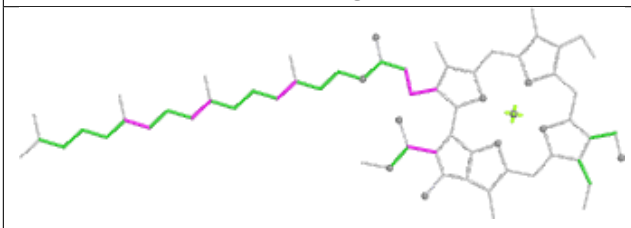
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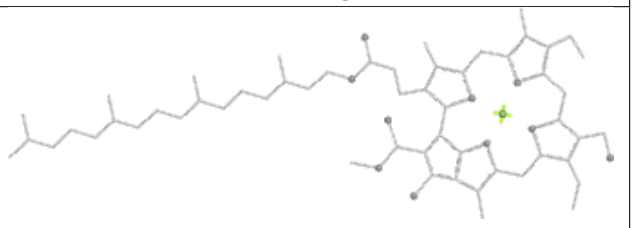
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Bond angles

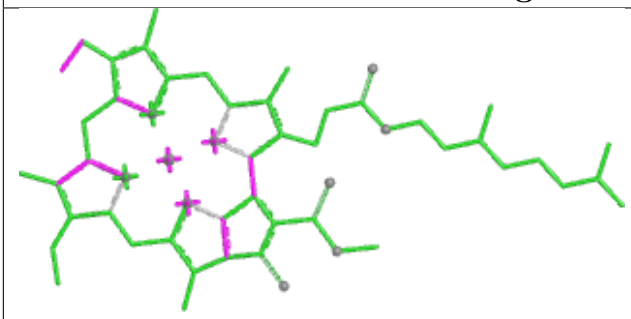


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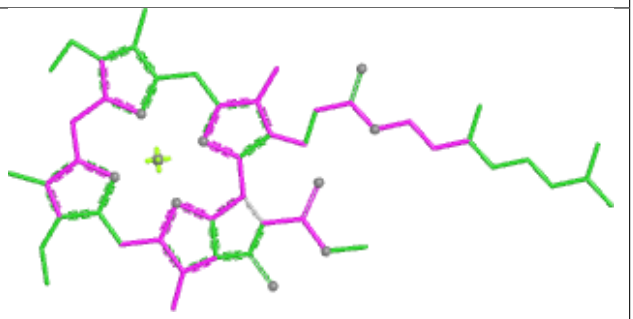


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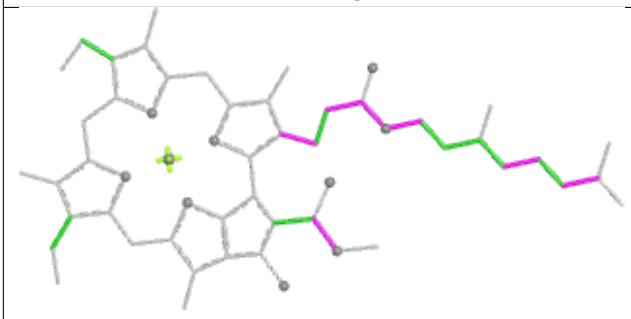
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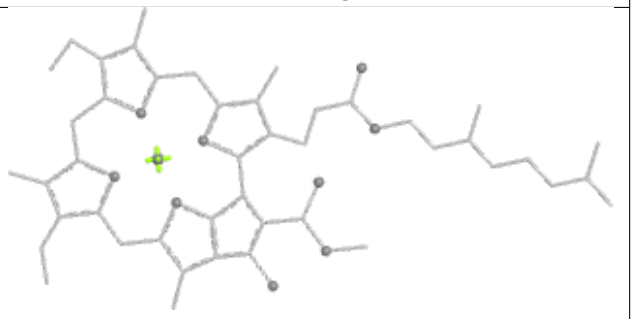
Bond lengths



Bond angles

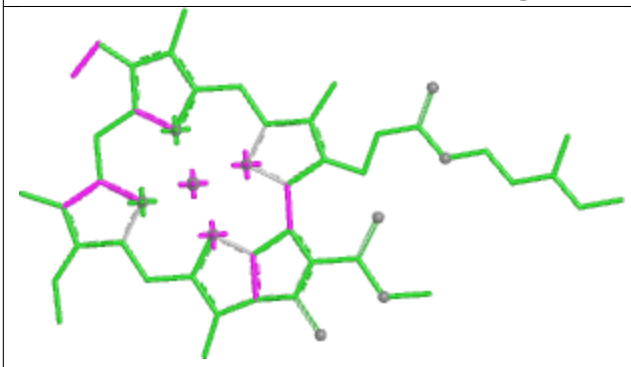


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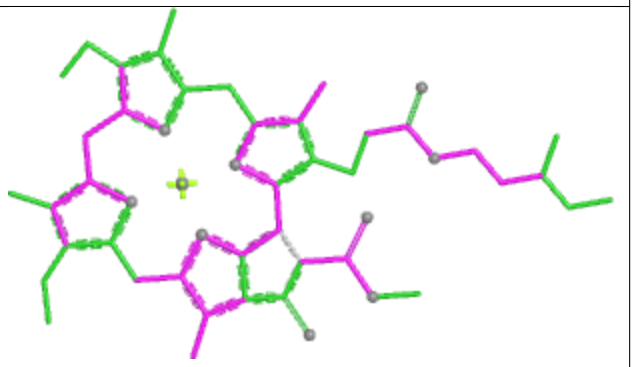


Rings

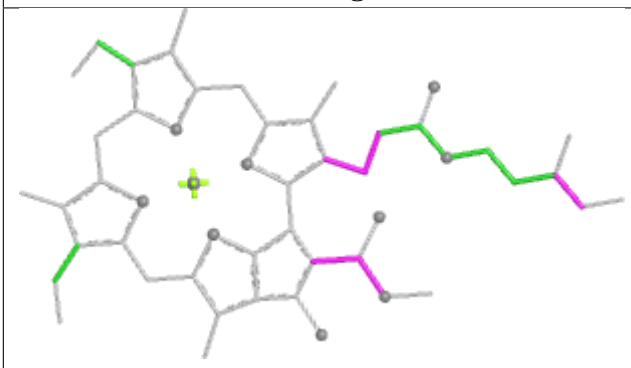
Ligand CLA A 1135



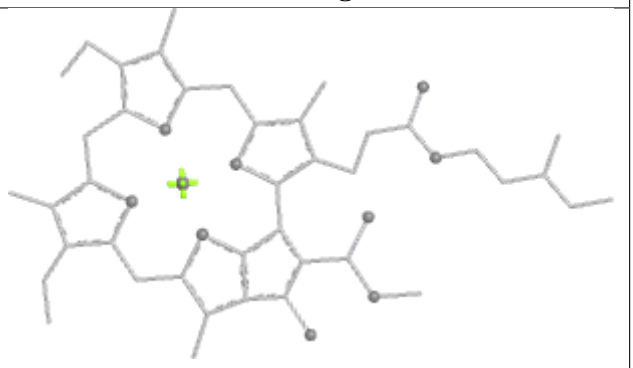
Bond lengths



Bond angles

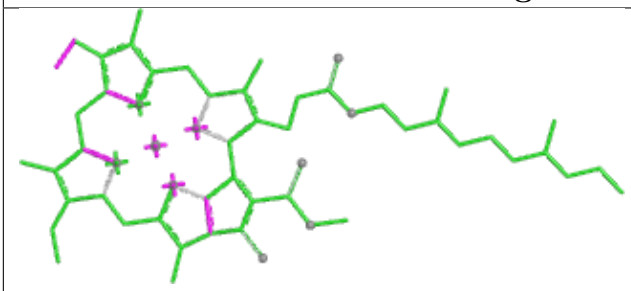


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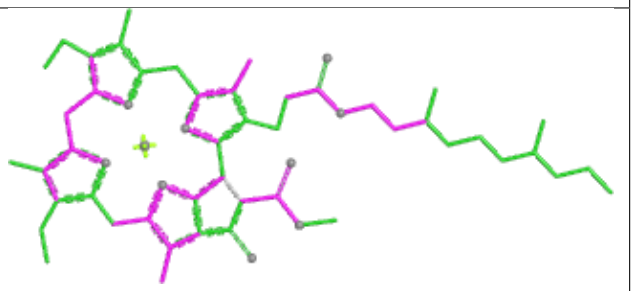


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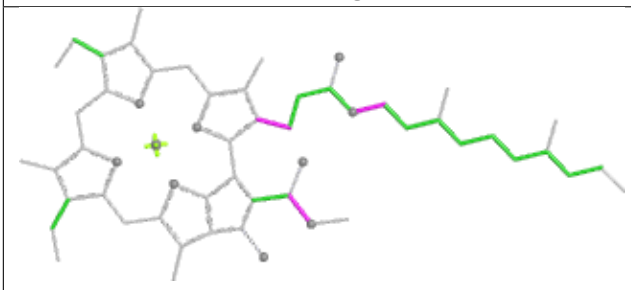
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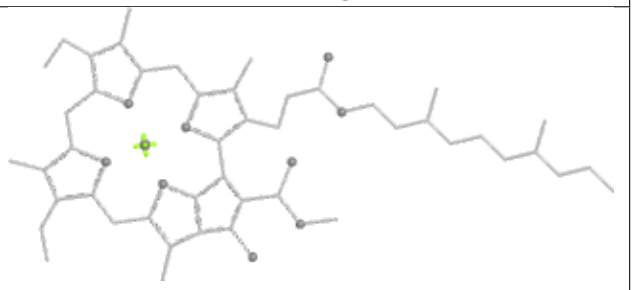
Bond lengths



Bond angles

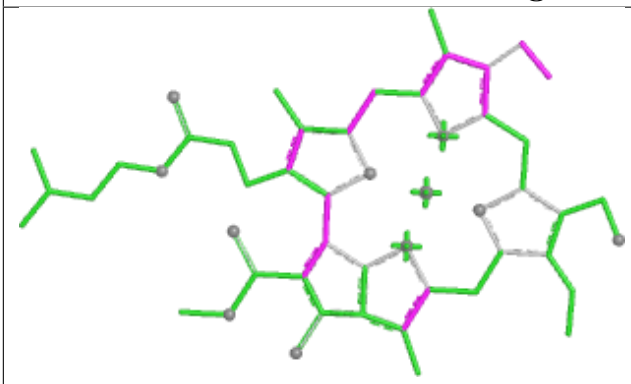


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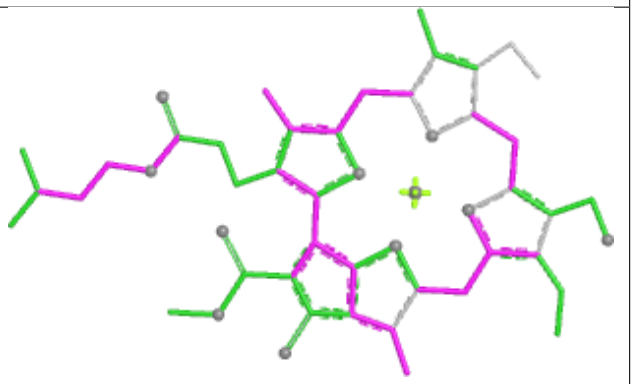


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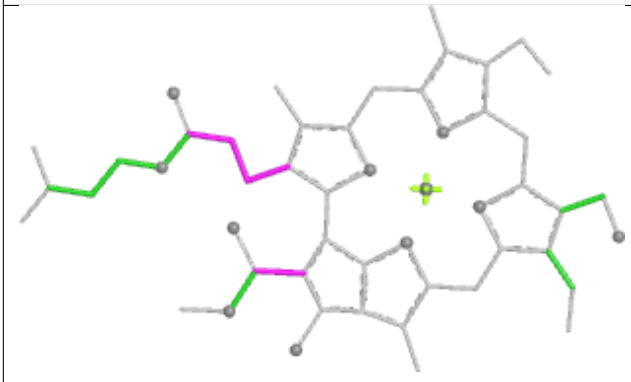
Ligand CHL 7 615



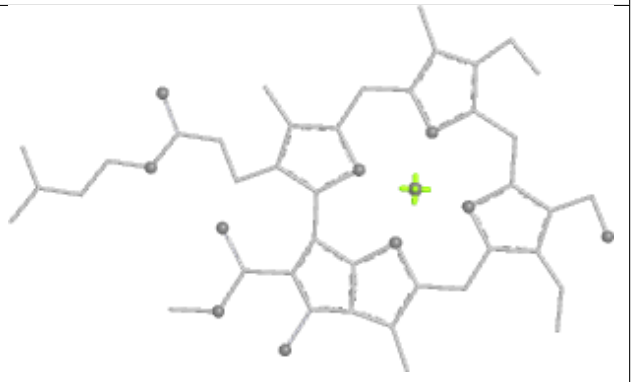
Bond lengths



Bond angles

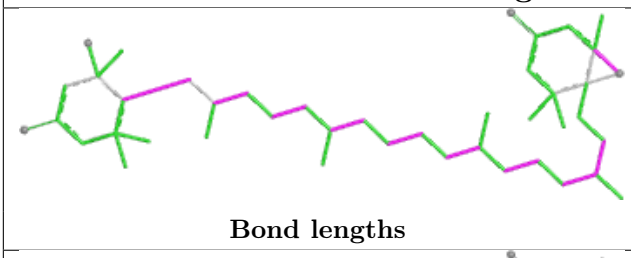


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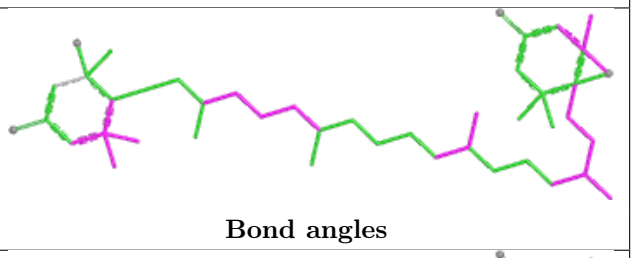


Rings

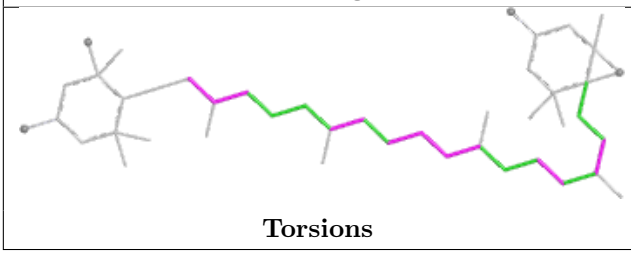
Ligand NEX F 4001



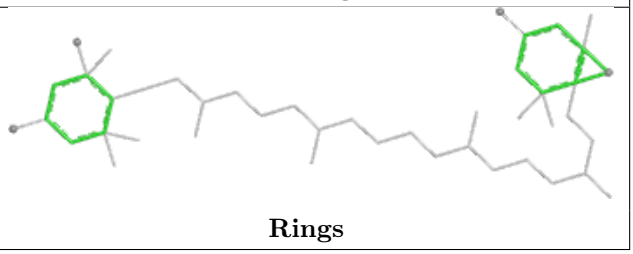
Bond lengths



Bond angles

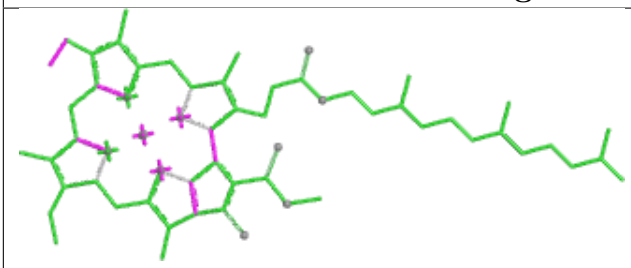


Torsions

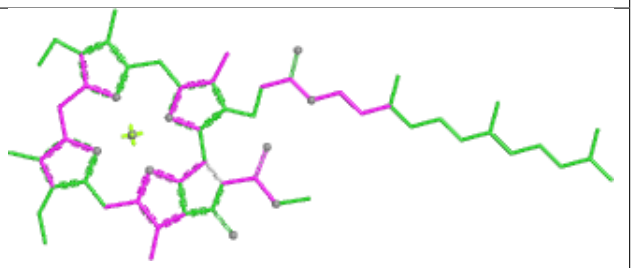


Rings

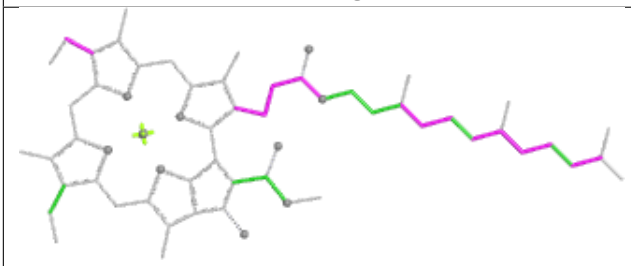
Ligand CLA A 1122



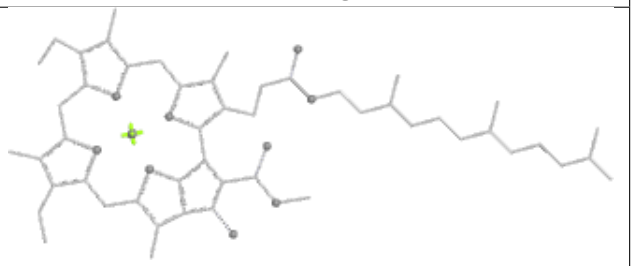
Bond lengths



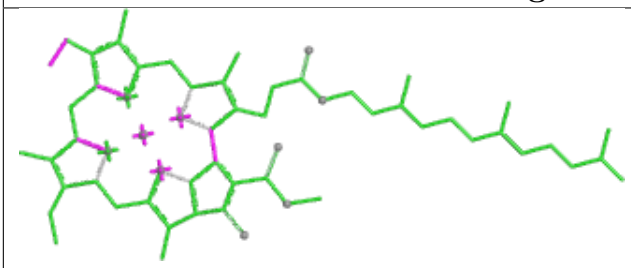
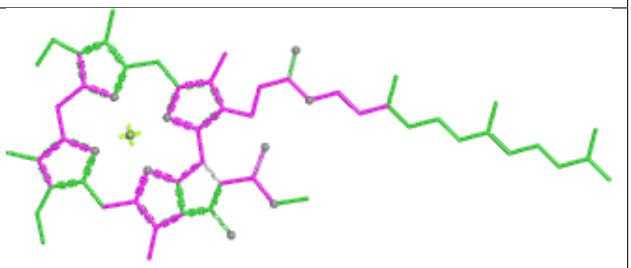
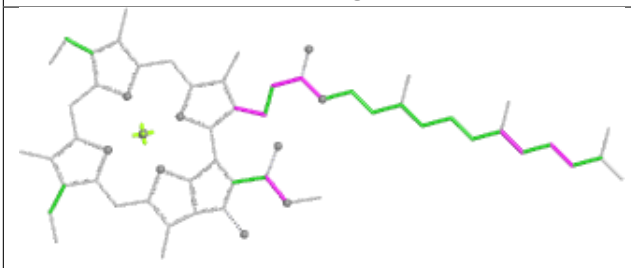
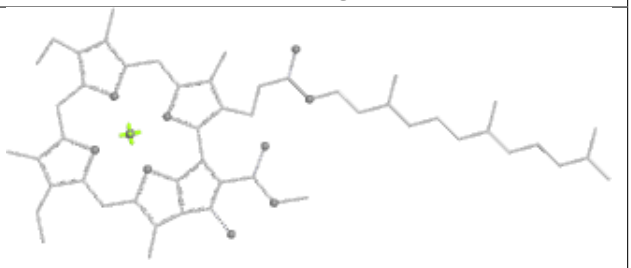
Bond angles

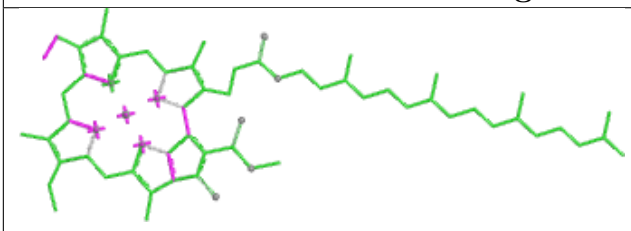
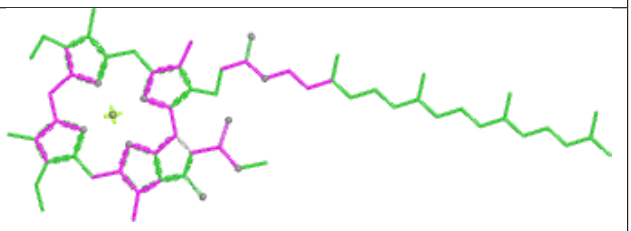
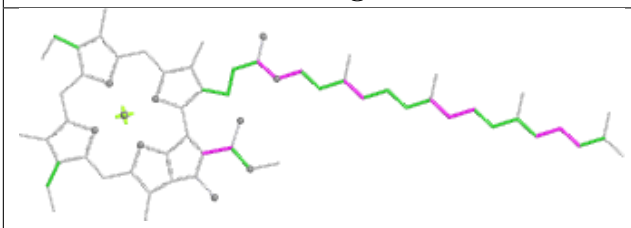
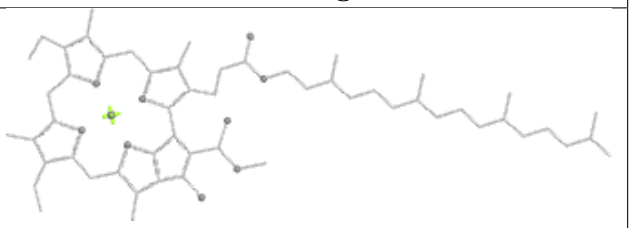


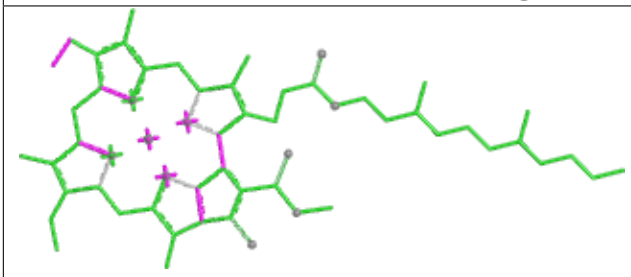
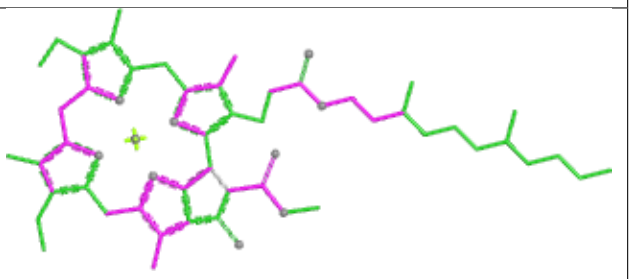
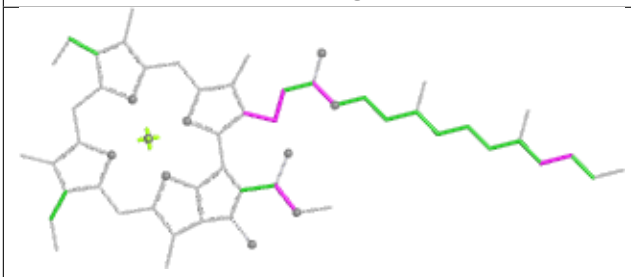
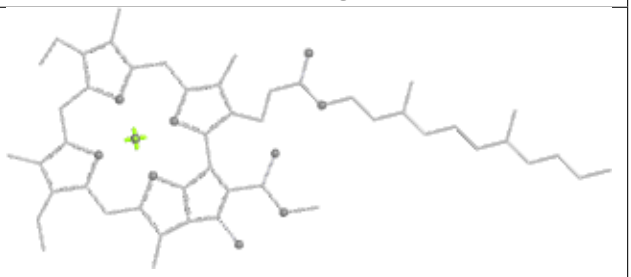
Torsions

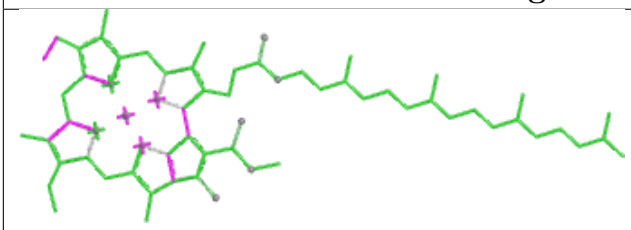
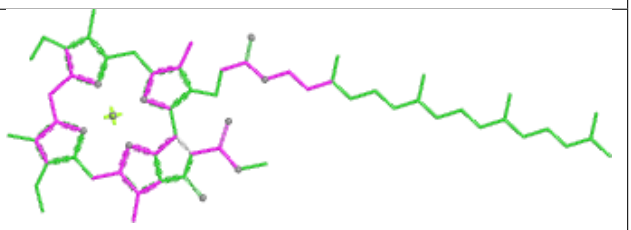
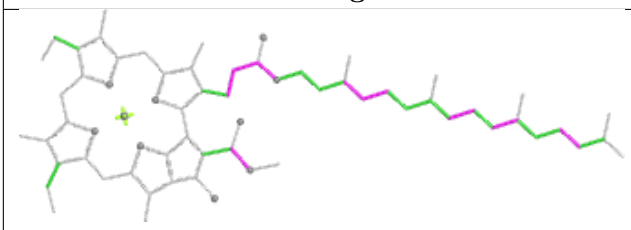
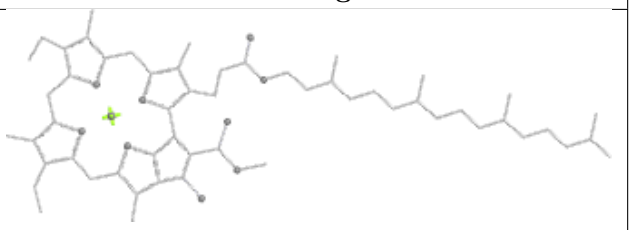


Rings

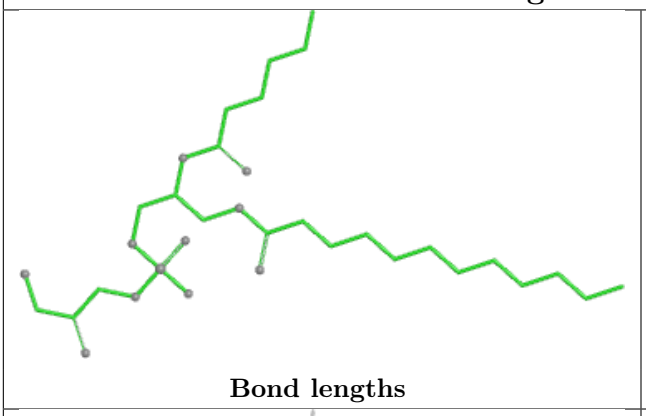
Ligand CLA 2 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

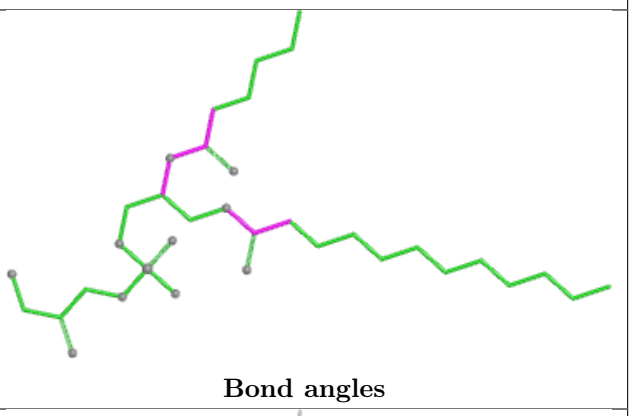
Ligand CLA B 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

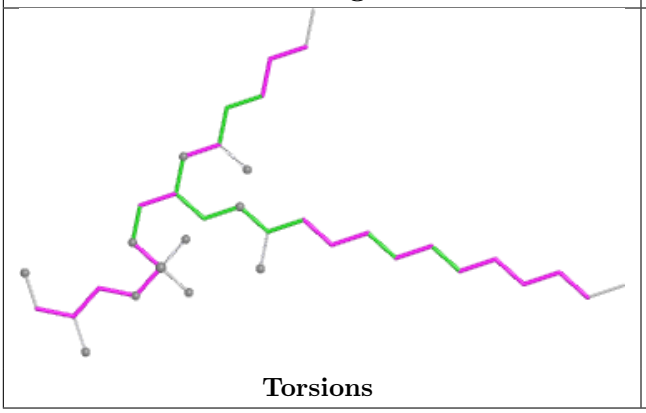
Ligand LHG a 801



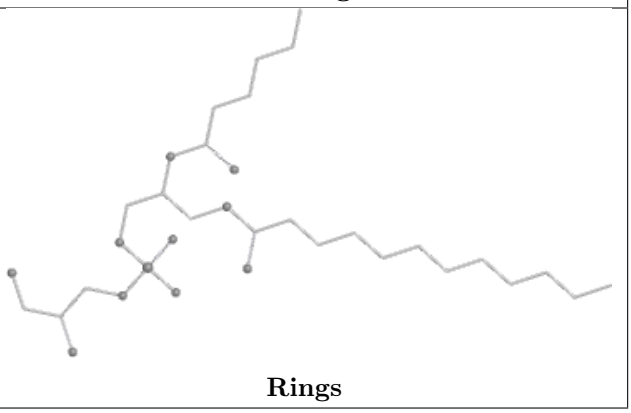
Bond lengths



Bond angles

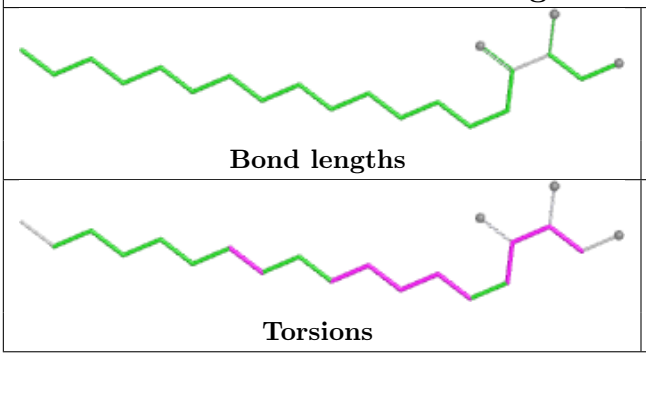


Torsions

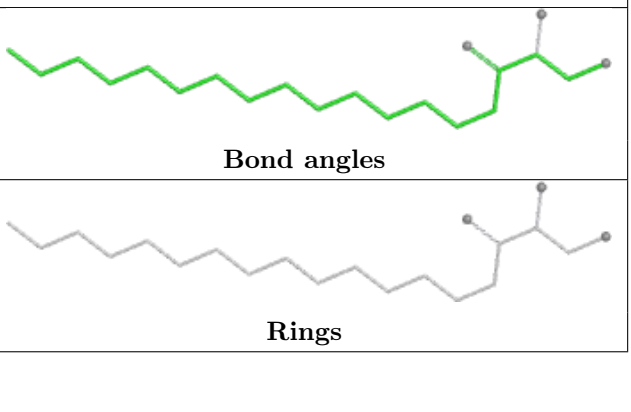


Rings

Ligand SPH 9 804



Bond lengths



Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

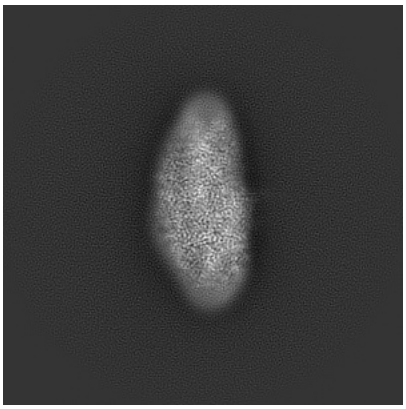
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11588. These allow visual inspection of the internal detail of the map and identification of artifacts.

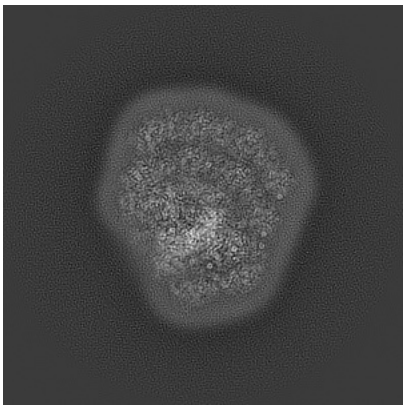
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

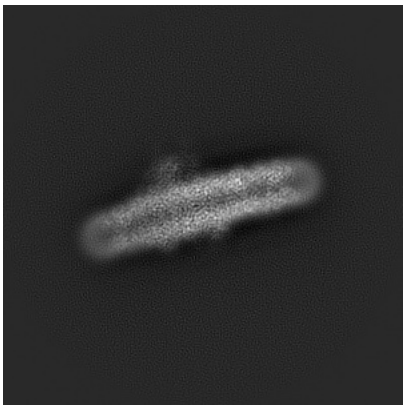
6.1.1 Primary map



X

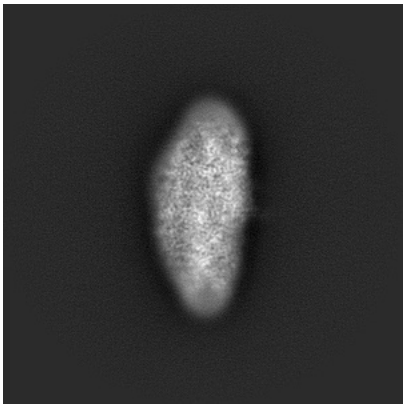


Y

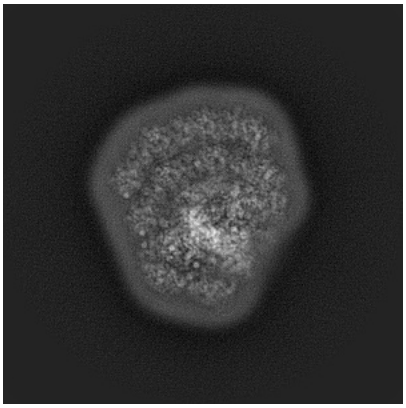


Z

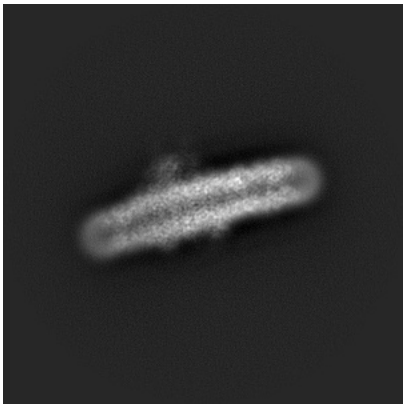
6.1.2 Raw map



X



Y

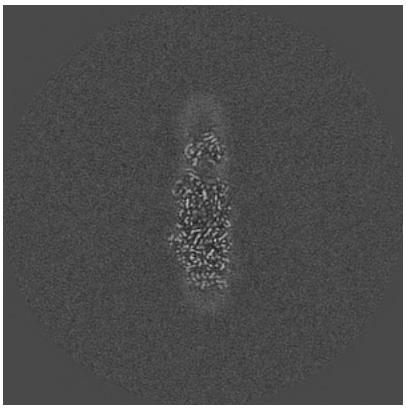


Z

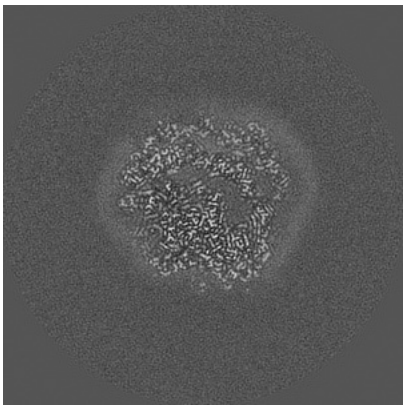
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

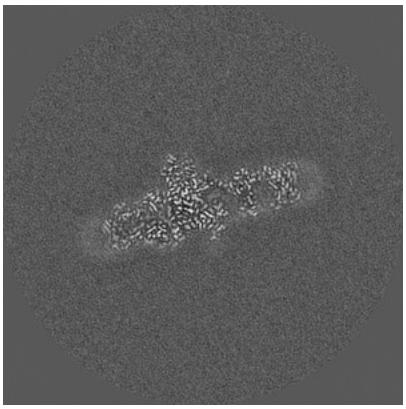
6.2.1 Primary map



X Index: 240

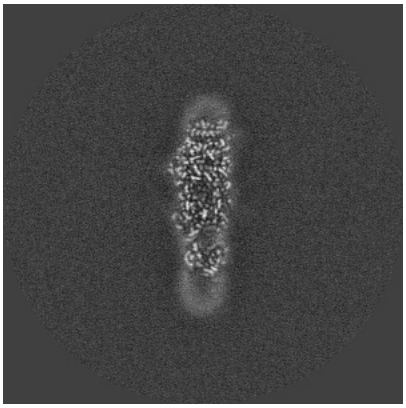


Y Index: 240

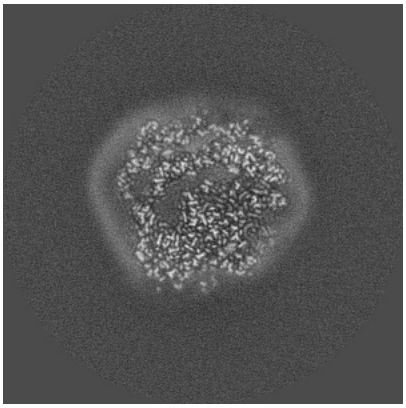


Z Index: 240

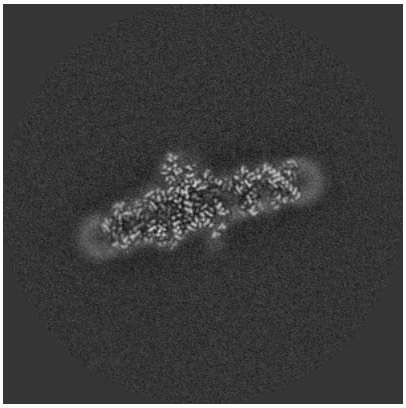
6.2.2 Raw map



X Index: 240



Y Index: 240

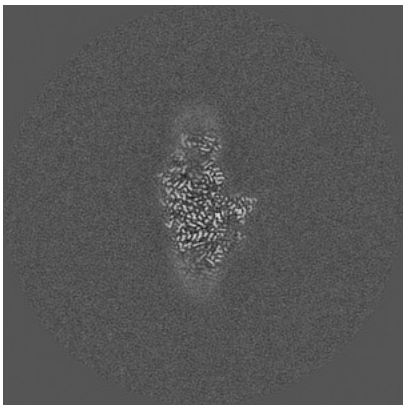


Z Index: 240

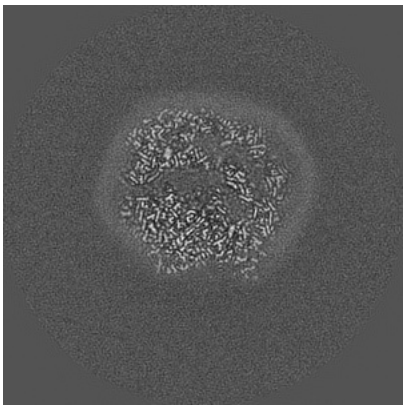
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

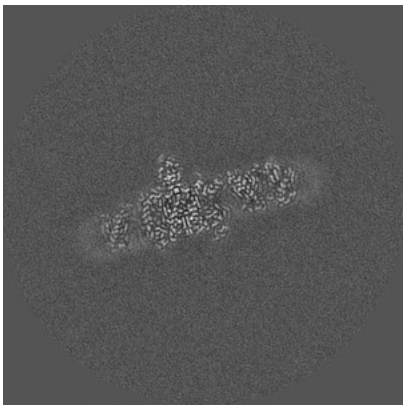
6.3.1 Primary map



X Index: 208

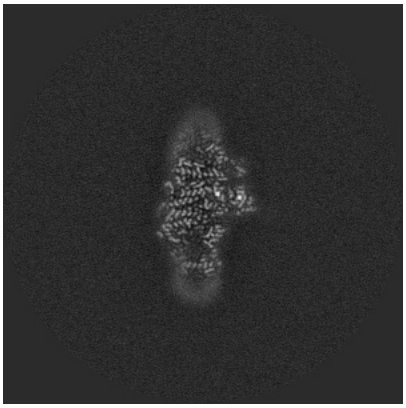


Y Index: 248

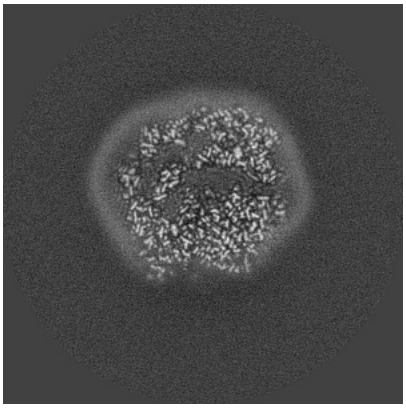


Z Index: 227

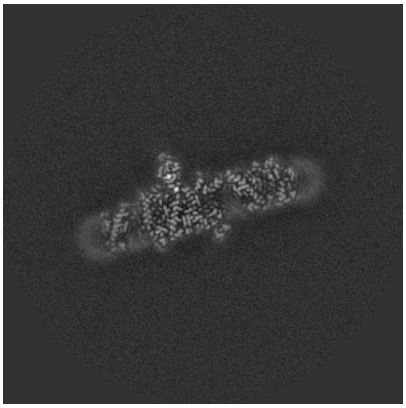
6.3.2 Raw map



X Index: 207



Y Index: 248

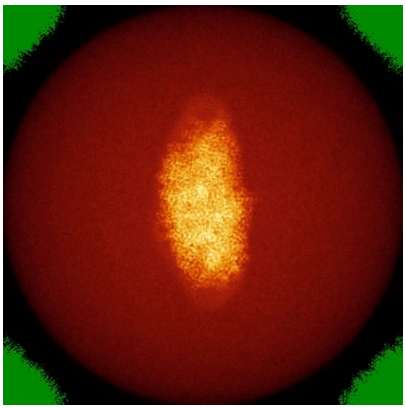


Z Index: 253

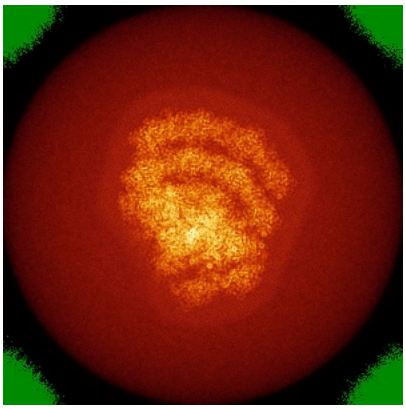
The images above show the largest variance slices of the map in three orthogonal directions.

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

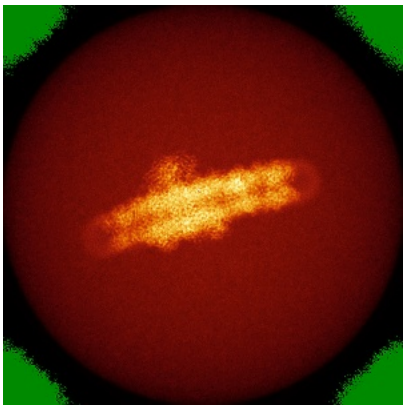
6.4.1 Primary map



X

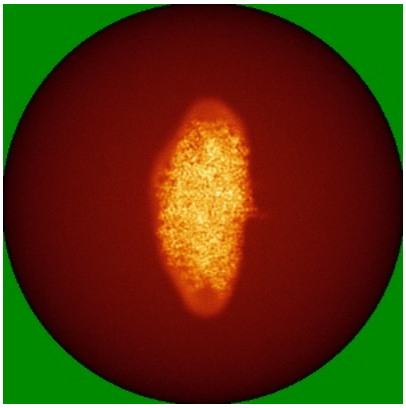


Y

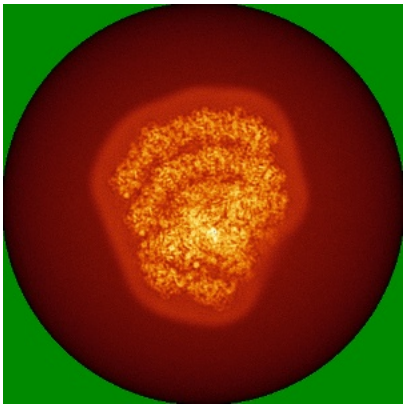


Z

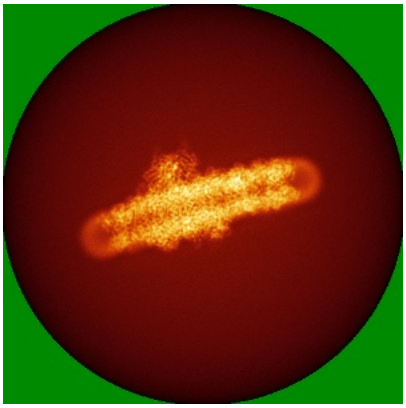
6.4.2 Raw map



X



Y

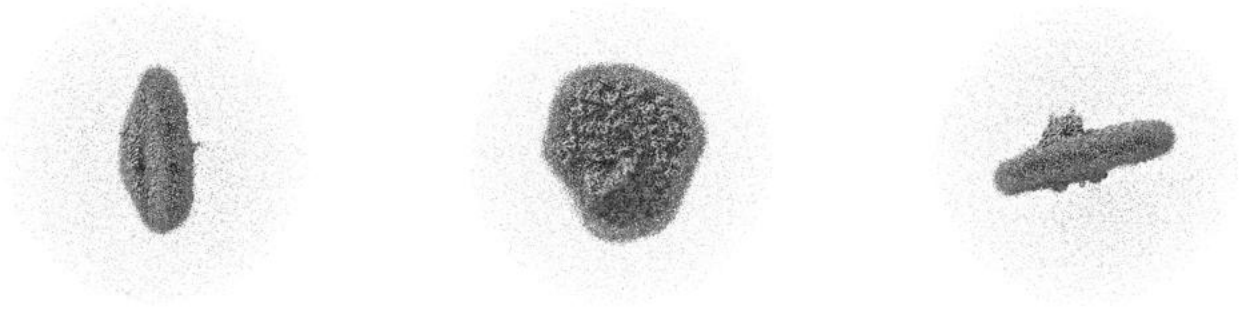


Z

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

6.5 Orthogonal surface views (i)

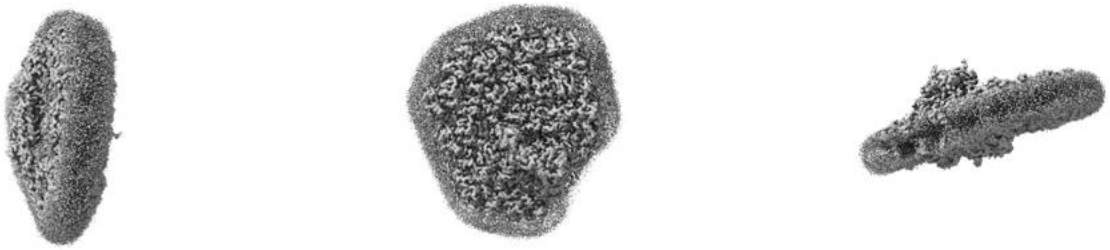
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

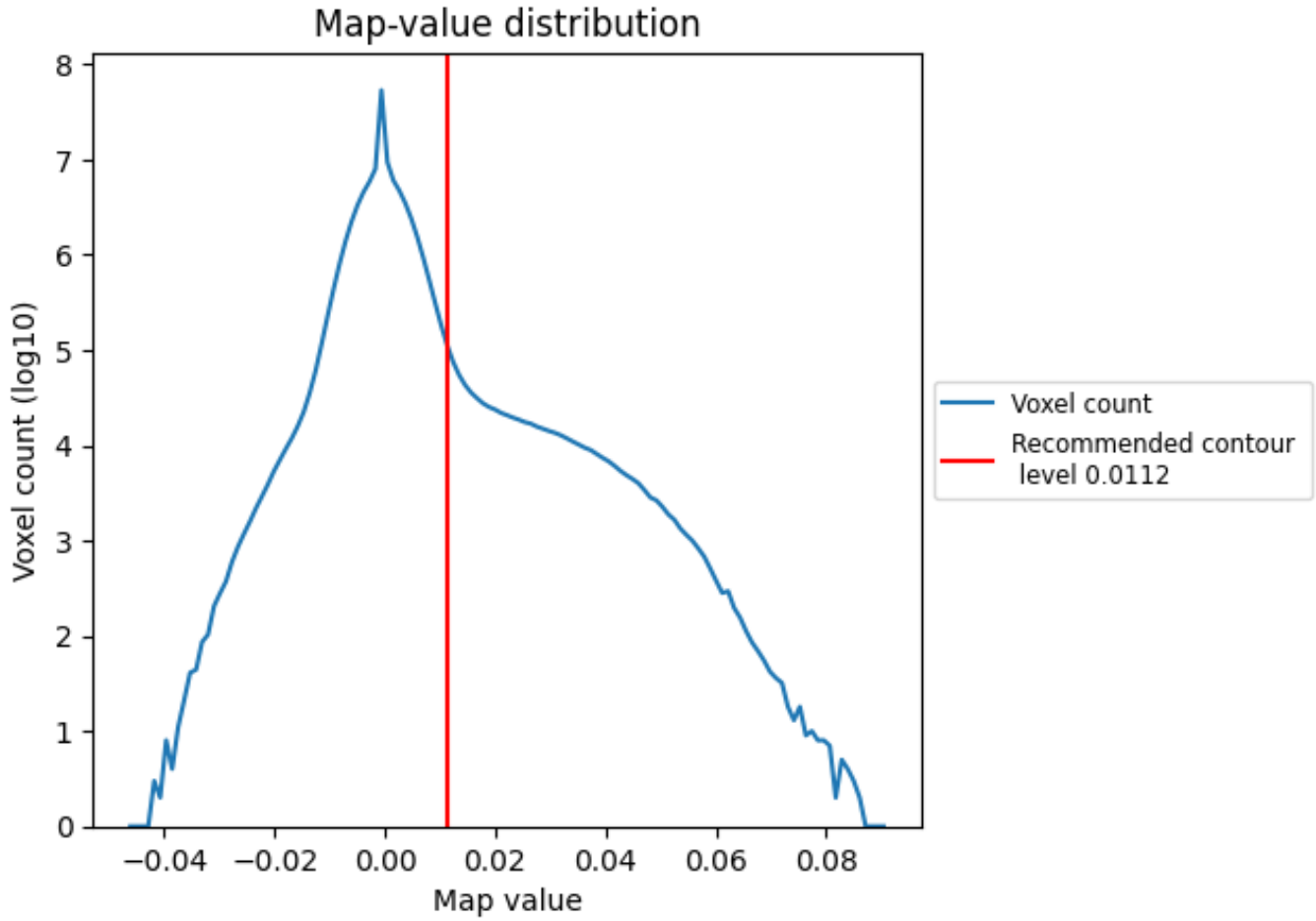
6.6 Mask visualisation (i)

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

7 Map analysis

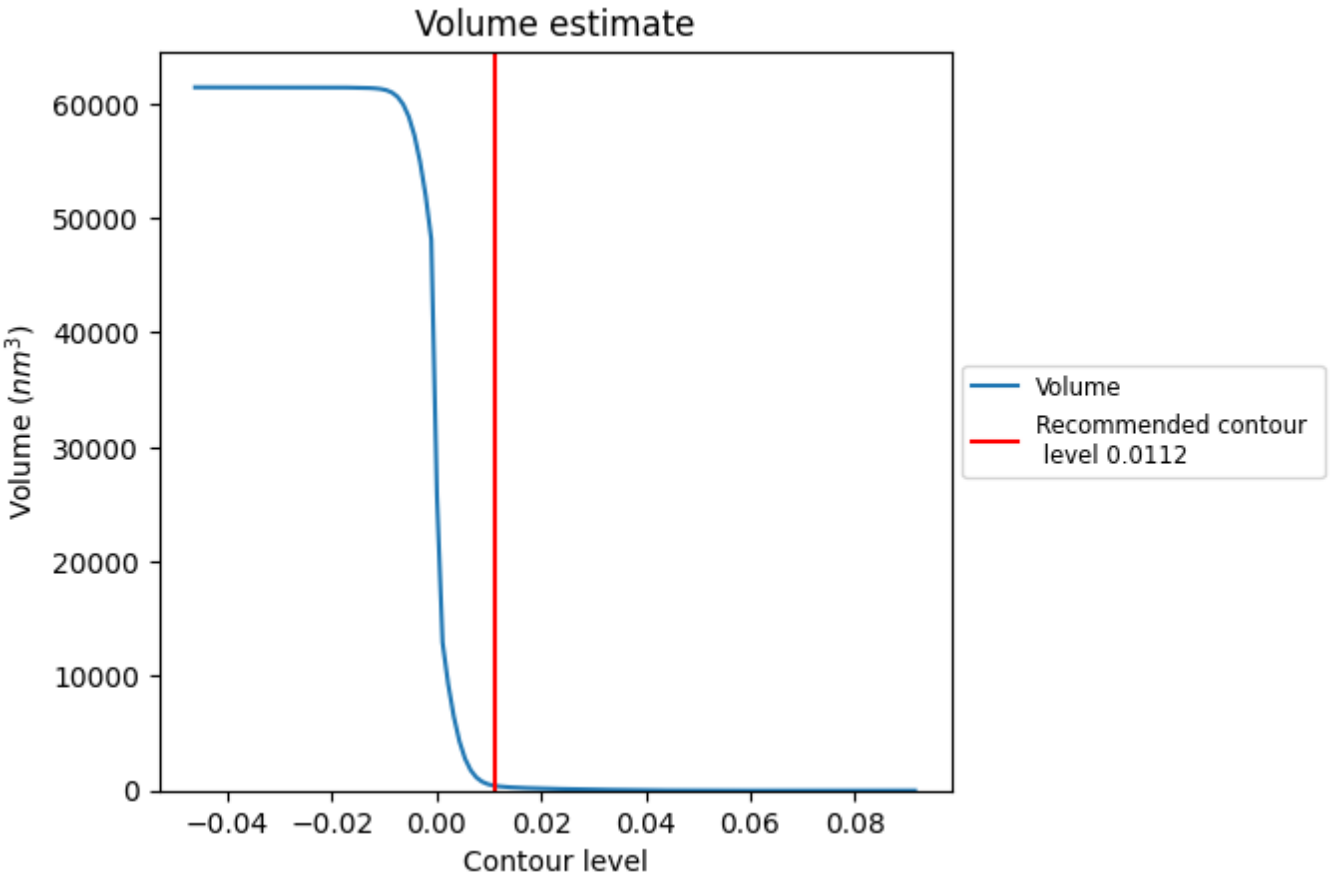
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

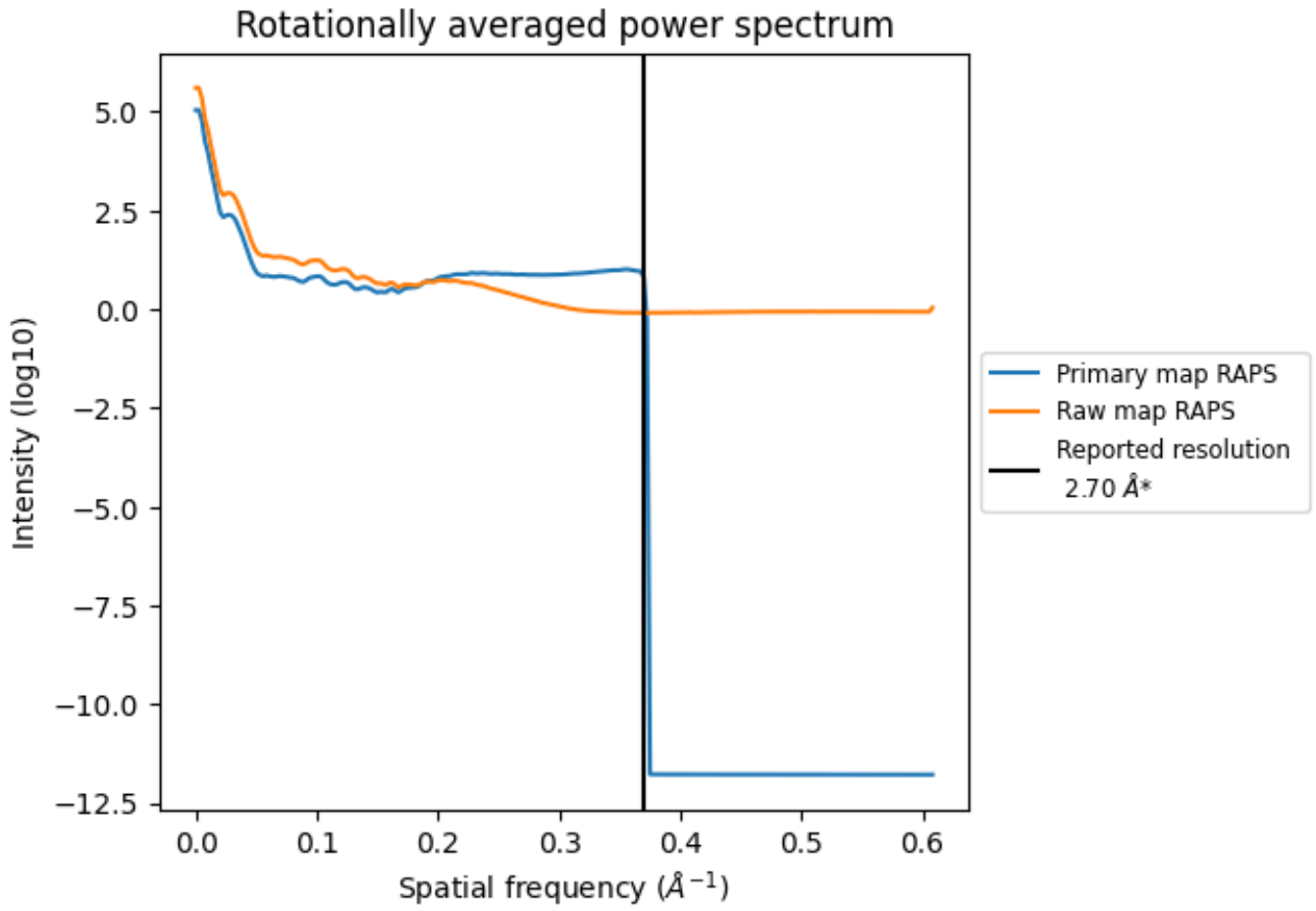
7.2 Volume estimate



The volume at the recommended contour level is 418 nm^3; this corresponds to an approximate mass of 378 kDa.

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

7.3 Rotationally averaged power spectrum (i)

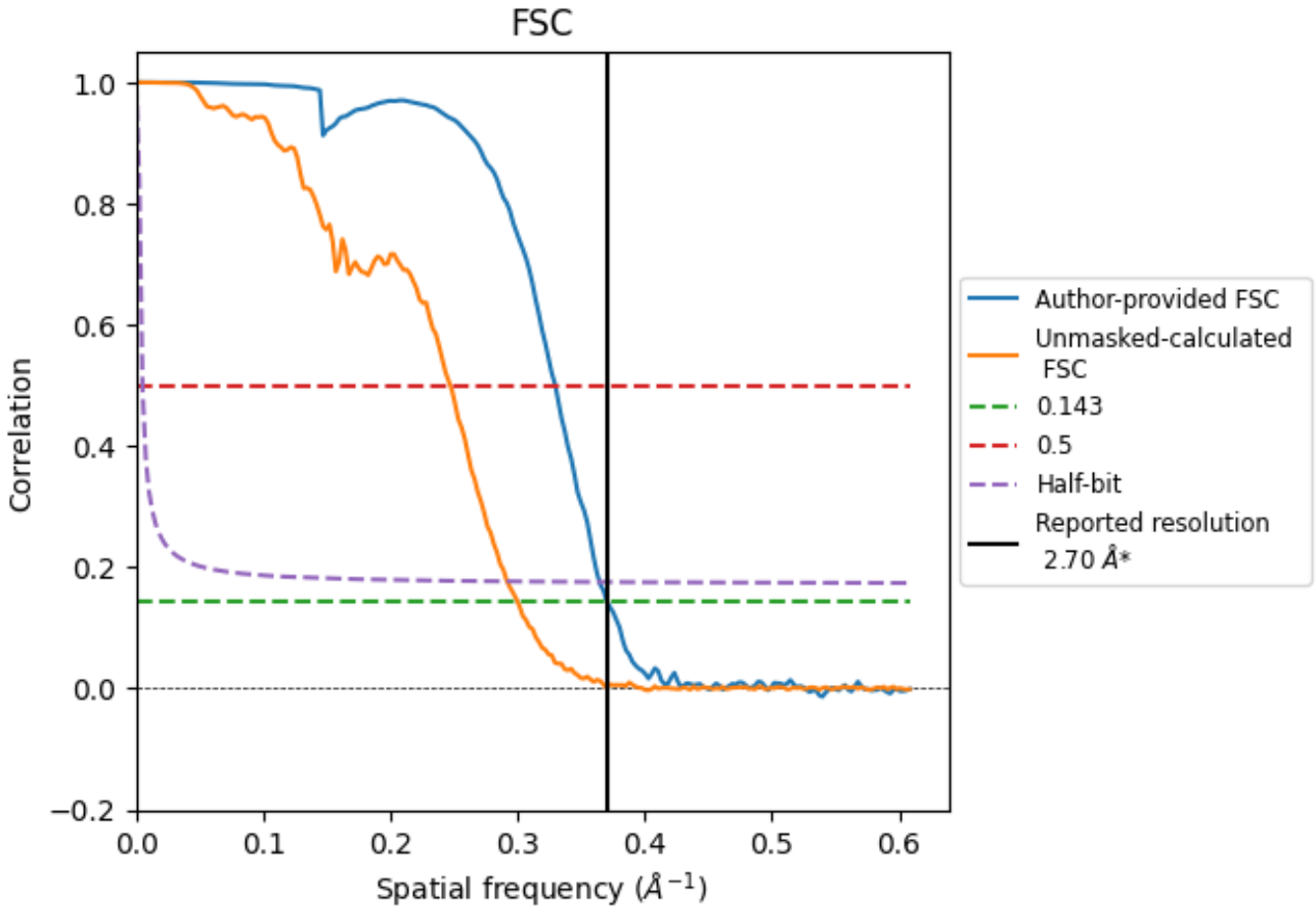


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

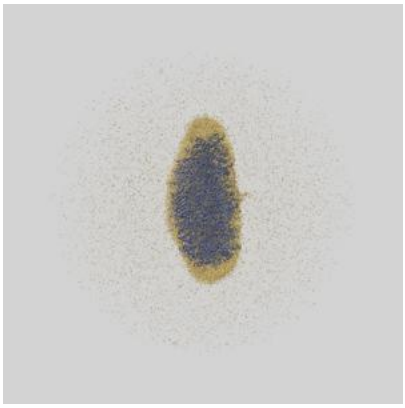
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.03	2.74
Unmasked-calculated*	3.33	4.05	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 2.7 by more than 10 %

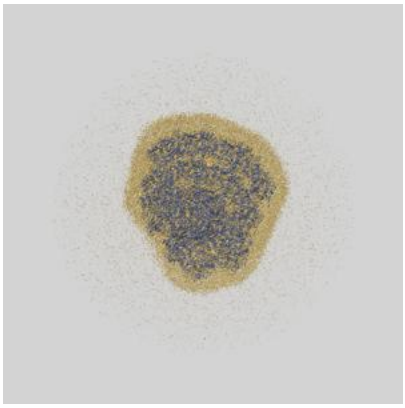
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11588 and PDB model 6ZZX. Per-residue inclusion information can be found in section 3 on page 55.

9.1 Map-model overlay



X



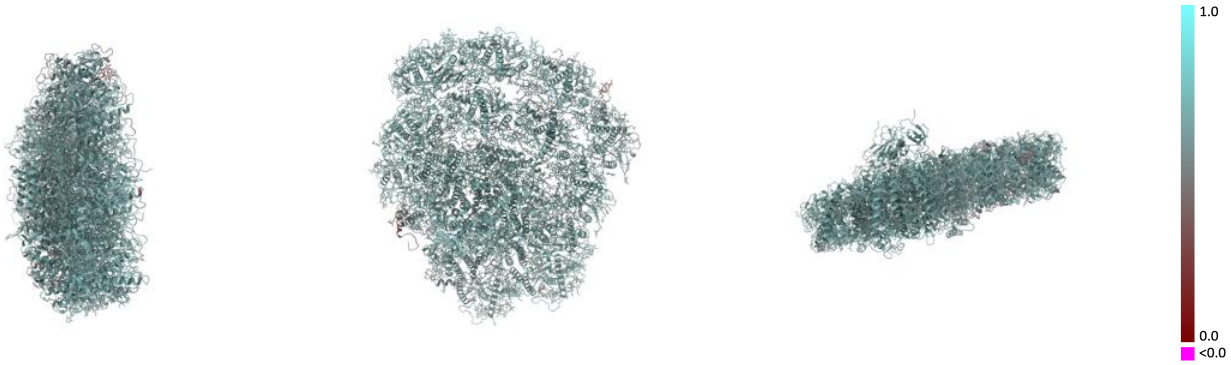
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

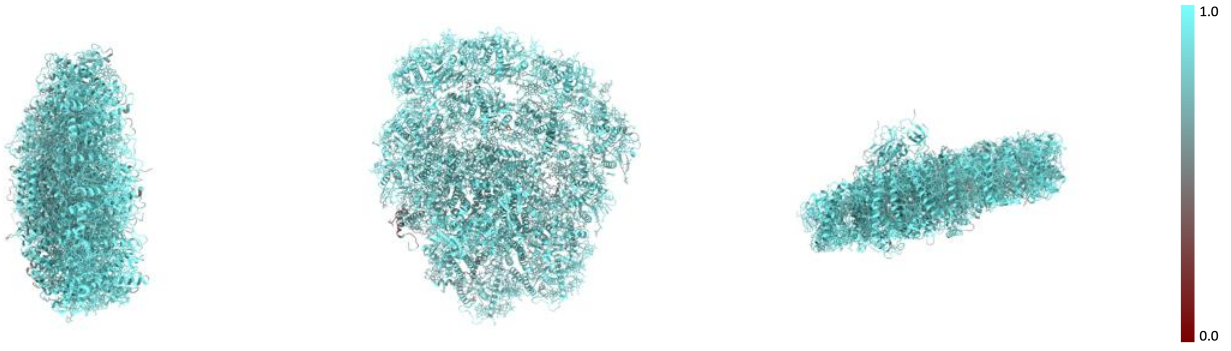
9.2 Q-score mapped to coordinate model



X Y Z

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

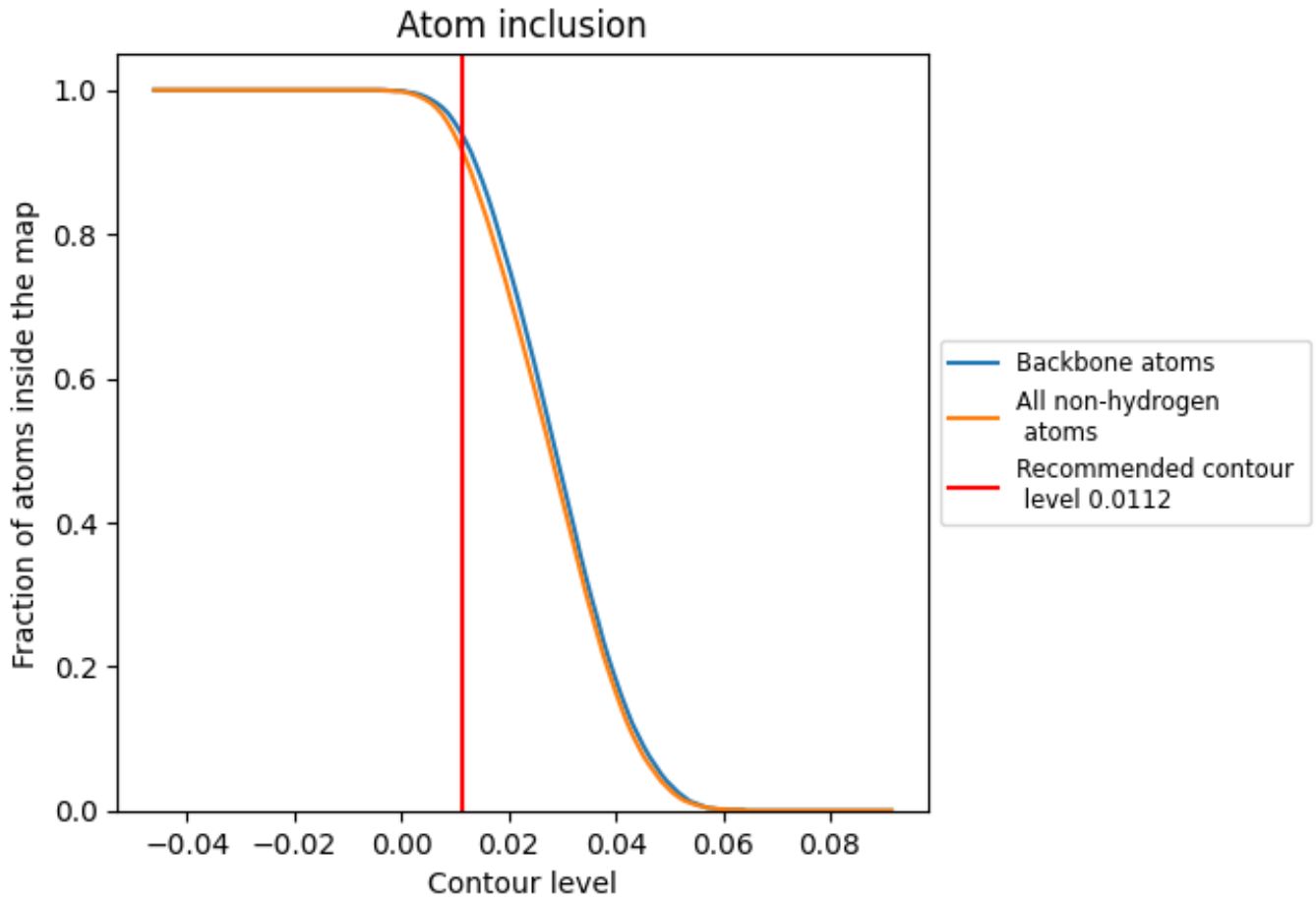
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.6210
1	0.9060	0.6130
2	0.8860	0.6000
3	0.9370	0.6350
4	0.8970	0.5980
5	0.9340	0.6190
6	0.9200	0.6190
7	0.9090	0.6200
8	0.9050	0.6190
9	0.9160	0.6190
A	0.9560	0.6480
B	0.9600	0.6500
C	0.9780	0.6530
D	0.9320	0.6250
E	0.9310	0.6160
F	0.9120	0.6210
G	0.8990	0.6170
H	0.7480	0.5440
I	0.9010	0.6100
J	0.9020	0.6260
K	0.8960	0.6010
L	0.8820	0.5930
M	0.9640	0.6330
O	0.5450	0.4140
a	0.8550	0.5770

