Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 08:10 AM UTC

PDB ID	:	6TCL / pdb_00006tcl
EMDB ID	:	EMD-10461
Title	:	Photosystem I tetramer
Authors	:	Chen, M.; Perez-Boerema, A.; Li, S.; Amunts, A.
Deposited on	:	2019-11-06
Resolution	:	3.20 Å(reported)

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

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

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

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

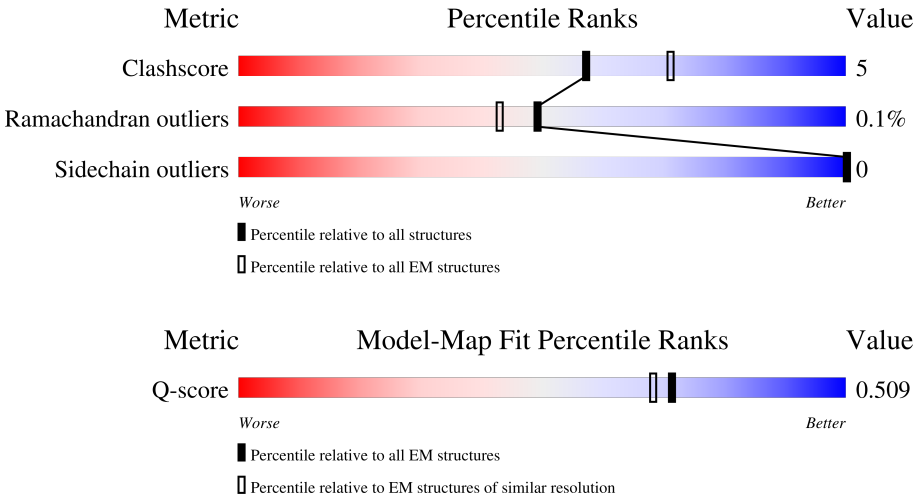
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	740	90% 10%
1	A1	740	90% 10%
1	A2	740	86% 14%
1	AA	740	90% 10%

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Mol	Chain	Length	Quality of chain
2	B	739	88% 12%
2	B1	739	86% 14%
2	B2	739	87% 13%
2	BB	739	85% 15%
3	C	80	6% 86% 14%
3	C1	80	5% 84% 16%
3	C2	80	6% 90% 10%
3	CC	80	6% 86% 14%
4	D	134	91% 9%
4	D1	134	92% 8%
4	D2	134	91% 9%
4	DD	134	93% 7%
5	E1	60	5% 92% 8%
5	E2	60	92% 8%
6	F	139	93% 7%
6	F1	139	88% 12%
6	FF	139	88% 12%
7	I	31	90% 10%
7	I1	31	97%
7	II	31	97%
8	J	48	83% 6% 10%
8	J1	48	81% 8% 10%
8	J2	48	79% 10% 10%
8	JJ	48	77% 12% 10%
9	K	74	68% 14% 19%

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Mol	Chain	Length	Quality of chain
9	K1	74	91% 9%
9	KK	74	73% 8% 19%
10	L1	166	89% 11%
11	M	31	84% 16%
11	M1	31	10% 94% 6%
11	M2	31	10% 100%
11	MM	31	90% 10%
12	X	39	8% 95% 5%
12	X1	39	10% 92% 8%
12	X2	39	8% 90% 10%
12	XX	39	8% 97%
13	F2	137	86% 12%
14	I2	33	94% 6%
15	K2	73	88% 12%
16	L2	167	89% 11%
17	E	63	90% 10%
17	EE	63	87% 13%
18	L	154	95% 5%
18	LL	154	94% 6%

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
19	CLA	A	801	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A1	801	X	-	-	-
19	CLA	A1	803	X	-	-	-
19	CLA	A1	804	X	-	-	-
19	CLA	A1	806	X	-	-	-
19	CLA	A1	807	X	-	-	-
19	CLA	A1	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A1	809	X	-	-	-
19	CLA	A1	810	X	-	-	-
19	CLA	A1	811	X	-	-	-
19	CLA	A1	812	X	-	-	-
19	CLA	A1	813	X	-	-	-
19	CLA	A1	814	X	-	-	-
19	CLA	A1	815	X	-	-	-
19	CLA	A1	816	X	-	-	-
19	CLA	A1	817	X	-	-	-
19	CLA	A1	818	X	-	-	-
19	CLA	A1	820	X	-	-	-
19	CLA	A1	821	X	-	-	-
19	CLA	A1	822	X	-	-	-
19	CLA	A1	823	X	-	-	-
19	CLA	A1	824	X	-	-	-
19	CLA	A1	825	X	-	-	-
19	CLA	A1	826	X	-	-	-
19	CLA	A1	827	X	-	-	-
19	CLA	A1	828	X	-	-	-
19	CLA	A1	829	X	-	-	-
19	CLA	A1	830	X	-	-	-
19	CLA	A1	831	X	-	-	-
19	CLA	A1	832	X	-	-	-
19	CLA	A1	833	X	-	-	-
19	CLA	A1	834	X	-	-	-
19	CLA	A1	835	X	-	-	-
19	CLA	A1	836	X	-	-	-
19	CLA	A1	837	X	-	-	-
19	CLA	A1	838	X	-	-	-
19	CLA	A1	839	X	-	-	-
19	CLA	A1	840	X	-	-	-
19	CLA	A1	841	X	-	-	-
19	CLA	A1	842	X	-	-	-
19	CLA	A1	844	X	-	-	-
19	CLA	A1	852	X	-	-	-
19	CLA	A2	801	X	-	-	-
19	CLA	A2	802	X	-	-	-
19	CLA	A2	804	X	-	-	-
19	CLA	A2	805	X	-	-	-
19	CLA	A2	806	X	-	-	-
19	CLA	A2	807	X	-	-	-
19	CLA	A2	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A2	809	X	-	-	-
19	CLA	A2	810	X	-	-	-
19	CLA	A2	811	X	-	-	-
19	CLA	A2	812	X	-	-	-
19	CLA	A2	813	X	-	-	-
19	CLA	A2	814	X	-	-	-
19	CLA	A2	815	X	-	-	-
19	CLA	A2	816	X	-	-	-
19	CLA	A2	817	X	-	-	-
19	CLA	A2	818	X	-	-	-
19	CLA	A2	819	X	-	-	-
19	CLA	A2	820	X	-	-	-
19	CLA	A2	821	X	-	-	-
19	CLA	A2	822	X	-	-	-
19	CLA	A2	823	X	-	-	-
19	CLA	A2	824	X	-	-	-
19	CLA	A2	825	X	-	-	-
19	CLA	A2	826	X	-	-	-
19	CLA	A2	827	X	-	-	-
19	CLA	A2	828	X	-	-	-
19	CLA	A2	829	X	-	-	-
19	CLA	A2	830	X	-	-	-
19	CLA	A2	831	X	-	-	-
19	CLA	A2	832	X	-	-	-
19	CLA	A2	833	X	-	-	-
19	CLA	A2	834	X	-	-	-
19	CLA	A2	835	X	-	-	-
19	CLA	A2	837	X	-	-	-
19	CLA	A2	838	X	-	-	-
19	CLA	A2	839	X	-	-	-
19	CLA	A2	840	X	-	-	-
19	CLA	A2	841	X	-	-	-
19	CLA	A2	842	X	-	-	-
19	CLA	A2	844	X	-	-	-
19	CLA	A2	852	X	-	-	-
19	CLA	AA	801	X	-	-	-
19	CLA	AA	804	X	-	-	-
19	CLA	AA	805	X	-	-	-
19	CLA	AA	806	X	-	-	-
19	CLA	AA	807	X	-	-	-
19	CLA	AA	808	X	-	-	-
19	CLA	AA	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	AA	810	X	-	-	-
19	CLA	AA	811	X	-	-	-
19	CLA	AA	812	X	-	-	-
19	CLA	AA	813	X	-	-	-
19	CLA	AA	814	X	-	-	-
19	CLA	AA	815	X	-	-	-
19	CLA	AA	816	X	-	-	-
19	CLA	AA	817	X	-	-	-
19	CLA	AA	818	X	-	-	-
19	CLA	AA	819	X	-	-	-
19	CLA	AA	820	X	-	-	-
19	CLA	AA	821	X	-	-	-
19	CLA	AA	823	X	-	-	-
19	CLA	AA	824	X	-	-	-
19	CLA	AA	825	X	-	-	-
19	CLA	AA	826	X	-	-	-
19	CLA	AA	827	X	-	-	-
19	CLA	AA	828	X	-	-	-
19	CLA	AA	829	X	-	-	-
19	CLA	AA	830	X	-	-	-
19	CLA	AA	831	X	-	-	-
19	CLA	AA	832	X	-	-	-
19	CLA	AA	833	X	-	-	-
19	CLA	AA	834	X	-	-	-
19	CLA	AA	835	X	-	-	-
19	CLA	AA	836	X	-	-	-
19	CLA	AA	837	X	-	-	-
19	CLA	AA	838	X	-	-	-
19	CLA	AA	839	X	-	-	-
19	CLA	AA	840	X	-	-	-
19	CLA	AA	841	X	-	-	-
19	CLA	AA	842	X	-	-	-
19	CLA	AA	843	X	-	-	-
19	CLA	AA	845	X	-	-	-
19	CLA	AA	853	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	B	854	X	-	-	-
19	CLA	B	858	X	-	-	-
19	CLA	B	859	X	-	-	-
19	CLA	B	860	X	-	-	-
19	CLA	B1	801	X	-	-	-
19	CLA	B1	802	X	-	-	-
19	CLA	B1	803	X	-	-	-
19	CLA	B1	804	X	-	-	-
19	CLA	B1	805	X	-	-	-
19	CLA	B1	806	X	-	-	-
19	CLA	B1	807	X	-	-	-
19	CLA	B1	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B1	809	X	-	-	-
19	CLA	B1	810	X	-	-	-
19	CLA	B1	811	X	-	-	-
19	CLA	B1	812	X	-	-	-
19	CLA	B1	813	X	-	-	-
19	CLA	B1	814	X	-	-	-
19	CLA	B1	815	X	-	-	-
19	CLA	B1	816	X	-	-	-
19	CLA	B1	817	X	-	-	-
19	CLA	B1	818	X	-	-	-
19	CLA	B1	819	X	-	-	-
19	CLA	B1	820	X	-	-	-
19	CLA	B1	821	X	-	-	-
19	CLA	B1	822	X	-	-	-
19	CLA	B1	823	X	-	-	-
19	CLA	B1	824	X	-	-	-
19	CLA	B1	825	X	-	-	-
19	CLA	B1	826	X	-	-	-
19	CLA	B1	827	X	-	-	-
19	CLA	B1	828	X	-	-	-
19	CLA	B1	829	X	-	-	-
19	CLA	B1	830	X	-	-	-
19	CLA	B1	831	X	-	-	-
19	CLA	B1	832	X	-	-	-
19	CLA	B1	833	X	-	-	-
19	CLA	B1	834	X	-	-	-
19	CLA	B1	835	X	-	-	-
19	CLA	B1	836	X	-	-	-
19	CLA	B1	845	X	-	-	-
19	CLA	B1	848	X	-	-	-
19	CLA	B1	849	X	-	-	-
19	CLA	B1	850	X	-	-	-
19	CLA	B2	801	X	-	-	-
19	CLA	B2	802	X	-	-	-
19	CLA	B2	803	X	-	-	-
19	CLA	B2	804	X	-	-	-
19	CLA	B2	805	X	-	-	-
19	CLA	B2	806	X	-	-	-
19	CLA	B2	807	X	-	-	-
19	CLA	B2	808	X	-	-	-
19	CLA	B2	809	X	-	-	-
19	CLA	B2	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B2	811	X	-	-	-
19	CLA	B2	812	X	-	-	-
19	CLA	B2	813	X	-	-	-
19	CLA	B2	814	X	-	-	-
19	CLA	B2	815	X	-	-	-
19	CLA	B2	816	X	-	-	-
19	CLA	B2	817	X	-	-	-
19	CLA	B2	818	X	-	-	-
19	CLA	B2	819	X	-	-	-
19	CLA	B2	820	X	-	-	-
19	CLA	B2	821	X	-	-	-
19	CLA	B2	822	X	-	-	-
19	CLA	B2	823	X	-	-	-
19	CLA	B2	824	X	-	-	-
19	CLA	B2	825	X	-	-	-
19	CLA	B2	826	X	-	-	-
19	CLA	B2	827	X	-	-	-
19	CLA	B2	828	X	-	-	-
19	CLA	B2	829	X	-	-	-
19	CLA	B2	830	X	-	-	-
19	CLA	B2	831	X	-	-	-
19	CLA	B2	832	X	-	-	-
19	CLA	B2	834	X	-	-	-
19	CLA	B2	835	X	-	-	-
19	CLA	B2	836	X	-	-	-
19	CLA	B2	837	X	-	-	-
19	CLA	B2	846	X	-	-	-
19	CLA	B2	849	X	-	-	-
19	CLA	B2	850	X	-	-	-
19	CLA	B2	851	X	-	-	-
19	CLA	B2	852	X	-	-	-
19	CLA	BB	801	X	-	-	-
19	CLA	BB	802	X	-	-	-
19	CLA	BB	803	X	-	-	-
19	CLA	BB	804	X	-	-	-
19	CLA	BB	805	X	-	-	-
19	CLA	BB	806	X	-	-	-
19	CLA	BB	807	X	-	-	-
19	CLA	BB	808	X	-	-	-
19	CLA	BB	809	X	-	-	-
19	CLA	BB	810	X	-	-	-
19	CLA	BB	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	BB	812	X	-	-	-
19	CLA	BB	813	X	-	-	-
19	CLA	BB	814	X	-	-	-
19	CLA	BB	815	X	-	-	-
19	CLA	BB	816	X	-	-	-
19	CLA	BB	817	X	-	-	-
19	CLA	BB	818	X	-	-	-
19	CLA	BB	819	X	-	-	-
19	CLA	BB	820	X	-	-	-
19	CLA	BB	821	X	-	-	-
19	CLA	BB	822	X	-	-	-
19	CLA	BB	823	X	-	-	-
19	CLA	BB	824	X	-	-	-
19	CLA	BB	825	X	-	-	-
19	CLA	BB	826	X	-	-	-
19	CLA	BB	827	X	-	-	-
19	CLA	BB	828	X	-	-	-
19	CLA	BB	829	X	-	-	-
19	CLA	BB	830	X	-	-	-
19	CLA	BB	831	X	-	-	-
19	CLA	BB	833	X	-	-	-
19	CLA	BB	834	X	-	-	-
19	CLA	BB	835	X	-	-	-
19	CLA	BB	836	X	-	-	-
19	CLA	BB	845	X	-	-	-
19	CLA	BB	852	X	-	-	-
19	CLA	BB	855	X	-	-	-
19	CLA	BB	856	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F1	301	X	-	-	-
19	CLA	F1	302	X	-	-	-
19	CLA	F1	305	X	-	-	-
19	CLA	F2	301	X	-	-	-
19	CLA	F2	302	X	-	-	-
19	CLA	FF	301	X	-	-	-
19	CLA	FF	302	X	-	-	-
19	CLA	FF	305	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	J1	101	X	-	-	-
19	CLA	J1	103	X	-	-	-
19	CLA	J2	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J2	103	X	-	-	-
19	CLA	JJ	101	X	-	-	-
19	CLA	JJ	103	X	-	-	-
19	CLA	K	101	X	-	-	-
19	CLA	K	102	X	-	-	-
19	CLA	K1	102	X	-	-	-
19	CLA	K1	103	X	-	-	-
19	CLA	K1	105	X	-	-	-
19	CLA	K2	102	X	-	-	-
19	CLA	K2	104	X	-	-	-
19	CLA	KK	101	X	-	-	-
19	CLA	KK	102	X	-	-	-
19	CLA	L	202	X	-	-	-
19	CLA	L	203	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L1	205	X	-	-	-
19	CLA	L1	206	X	-	-	-
19	CLA	L1	207	X	-	-	-
19	CLA	L2	204	X	-	-	-
19	CLA	L2	205	X	-	-	-
19	CLA	L2	206	X	-	-	-
19	CLA	LL	201	X	-	-	-
19	CLA	LL	202	X	-	-	-
19	CLA	LL	203	X	-	-	-
19	CLA	X	101	X	-	-	-
19	CLA	X1	101	X	-	-	-
19	CLA	X2	101	X	-	-	-
19	CLA	XX	101	X	-	-	-
20	CL0	A	803	X	-	-	-
20	CL0	A1	802	X	-	-	-
20	CL0	A2	803	X	-	-	-
20	CL0	AA	803	X	-	-	-
24	AJP	A	802	X	-	-	-
24	AJP	A	855	X	-	-	-
24	AJP	A1	854	X	-	-	-
24	AJP	A1	855	X	-	-	-
24	AJP	A2	854	X	-	-	-
24	AJP	AA	802	X	-	-	-
24	AJP	AA	856	X	-	-	-
24	AJP	B	849	X	-	-	-
24	AJP	B	850	X	-	-	-
24	AJP	B	857	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	BB	848	X	-	-	-
24	AJP	BB	849	X	-	-	-
24	AJP	I2	104	X	-	-	-
24	AJP	K	104	X	-	-	-
24	AJP	KK	104	X	-	-	-
24	AJP	L	208	X	-	-	-
24	AJP	L	209	X	-	-	-
24	AJP	L1	203	X	-	-	-
24	AJP	L1	204	X	-	-	-
24	AJP	L2	202	X	-	-	-
24	AJP	L2	203	X	-	-	-
24	AJP	M2	101	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 199181 atoms, of which 99577 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	740	Total	C	H	N	O	S	0	0
			11478	3809	5672	1000	976	21		
1	A2	740	Total	C	H	N	O	S	0	0
			11486	3809	5680	1000	976	21		
1	A	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		
1	AA	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B1	739	Total	C	H	N	O	S	0	0
			11579	3905	5660	990	1006	18		
2	B2	739	Total	C	H	N	O	S	0	0
			11581	3905	5662	990	1006	18		
2	B	739	Total	C	H	N	O	S	0	0
			11586	3905	5667	990	1006	18		
2	BB	739	Total	C	H	N	O	S	0	0
			11595	3905	5676	990	1006	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	80	Total	C	H	N	O	S	0	0
			1183	367	584	103	118	11		
3	C2	80	Total	C	H	N	O	S	0	0
			1179	367	580	103	118	11		
3	C	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		
3	CC	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	134	Total	C	H	N	O	S	0	0
			2073	664	1037	178	193	1		
4	D2	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	D	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	DD	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	60	Total	C	H	N	O	0	0
			958	308	477	83	90		
5	E2	60	Total	C	H	N	O	0	0
			958	308	477	83	90		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F1	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		
6	F	139	Total	C	H	N	O	S	0	0
			2111	678	1051	179	201	2		
6	FF	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I1	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	I	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	II	31	Total	C	H	N	O	0	0
			508	177	255	35	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J1	43	Total	C	H	N	O	0	0
			701	237	355	52	57		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J2	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	J	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	JJ	43	Total	C	H	N	O	0	0
			700	237	354	52	57		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K1	74	Total	C	H	N	O	S	0	0
			1091	356	555	87	92	1		
9	K	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		
9	KK	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L1	166	Total	C	H	N	O	S	0	0
			2483	810	1239	213	220	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M2	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	MM	31	Total	C	H	N	O	0	0
			496	160	256	37	43		

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X1	39	Total	C	H	N	O	0	0
			627	212	318	49	48		
12	X2	39	Total	C	H	N	O	0	0
			627	212	318	49	48		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	39	Total	C	H	N	O	0	0
			628	212	319	49	48		
12	XX	39	Total	C	H	N	O	0	0
			628	212	319	49	48		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	F2	137	Total	C	H	N	O	S	0	0
			2087	670	1040	177	198	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I2	33	Total	C	H	N	O	0	0
			536	186	268	37	45		

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K2	73	Total	C	H	N	O	S	0	0
			1081	353	550	86	91	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L2	167	Total	C	H	N	O	S	0	0
			2498	815	1245	215	222	1		

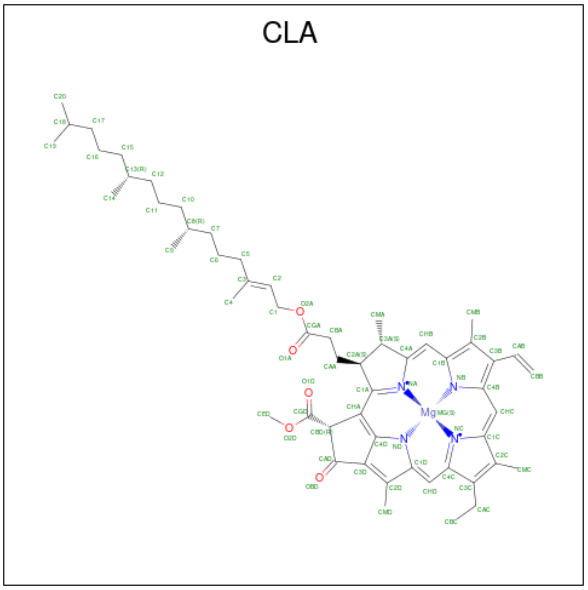
- Molecule 17 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	63	Total	C	H	N	O	0	0
			994	321	492	86	95		
17	EE	63	Total	C	H	N	O	0	0
			994	321	492	86	95		

- Molecule 18 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	154	Total	C	H	N	O	S	0	0
			2309	758	1153	196	201	1		
18	LL	154	Total	C	H	N	O	S	0	0
			2310	758	1154	196	201	1		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			104	46	48	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			133	55	68	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A1	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			135	55	70	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			105	46	49	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F1	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	F1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	J1	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	J1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K1	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	K1	1	Total	C	H	Mg	N	O	0
			67	32	27	1	4	3	
19	L1	1	Total	C	H	Mg	N	O	0
			120	51	59	1	4	5	
19	L1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	L1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	X1	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A2	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			135	55	70	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			105	46	49	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	F2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F2	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	J2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	J2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K2	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	L2	1	Total	C	H	Mg	N	O	0
			119	51	58	1	4	5	
19	L2	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	L2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	X2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	F	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	J	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	J	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			116	51	55	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	X	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	AA	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	

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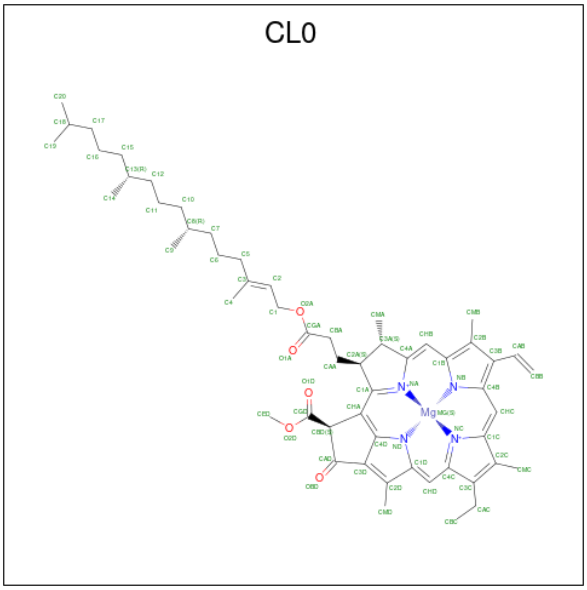
Mol	Chain	Residues	Atoms						AltConf
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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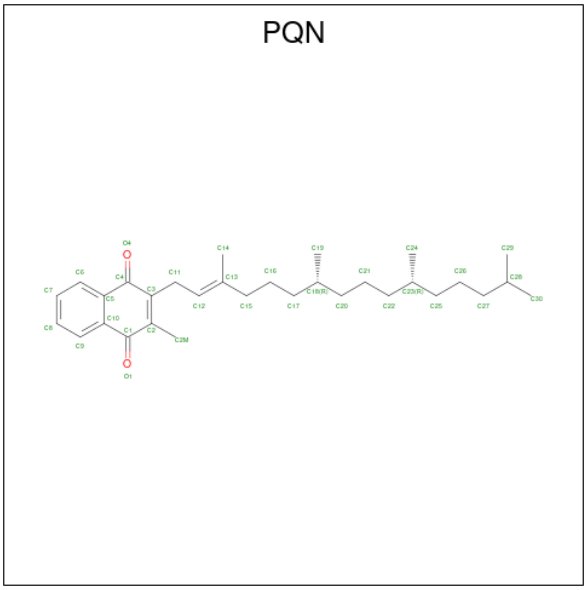
Mol	Chain	Residues	Atoms						AltConf
19	FF	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	FF	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	FF	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	JJ	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	JJ	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	KK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	KK	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			116	51	55	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			70	34	28	1	4	3	
19	XX	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



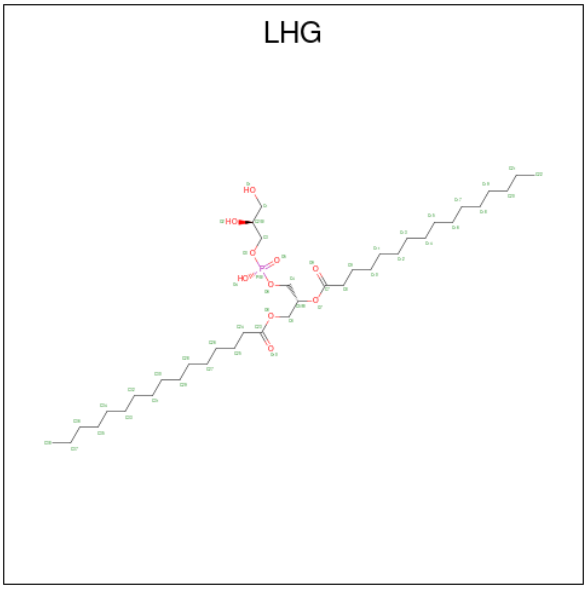
Mol	Chain	Residues	Atoms						AltConf
20	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
21	A1	1	Total	C	H	O	0
			79	31	46	2	
21	B1	1	Total	C	H	O	0
			79	31	46	2	
21	A2	1	Total	C	H	O	0
			79	31	46	2	
21	B2	1	Total	C	H	O	0
			79	31	46	2	
21	A	1	Total	C	H	O	0
			79	31	46	2	
21	B	1	Total	C	H	O	0
			79	31	46	2	
21	AA	1	Total	C	H	O	0
			79	31	46	2	
21	BB	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



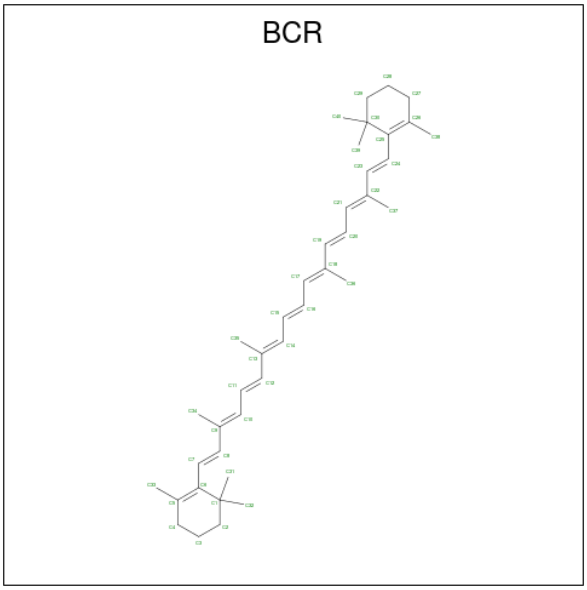
Mol	Chain	Residues	Atoms					AltConf
22	A1	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A1	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B1	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L1	1	Total	C	H	O	P	0
			68	22	35	10	1	
22	X1	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	X1	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A2	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A2	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B2	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L2	1	Total	C	H	O	P	0
			74	24	39	10	1	
22	X2	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	X2	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	B	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	L	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	X	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	AA	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	AA	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	BB	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	BB	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	LL	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	XX	1	Total	C	H	O	P	0
			89	29	49	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
23	A1	1	Total C H 92 39 53	0
23	A1	1	Total C H 96 40 56	0
23	A1	1	Total C H 96 40 56	0
23	A1	1	Total C H 96 40 56	0
23	A1	1	Total C H 96 40 56	0
23	A1	1	Total C H 96 40 56	0
23	B1	1	Total C H 96 40 56	0
23	B1	1	Total C H 96 40 56	0
23	B1	1	Total C H 96 40 56	0
23	B1	1	Total C H 96 40 56	0
23	B1	1	Total C H 96 40 56	0
23	F1	1	Total C H 96 40 56	0
23	F1	1	Total C H 96 40 56	0
23	F1	1	Total C H 91 40 51	0
23	I1	1	Total C H 96 40 56	0
23	J1	1	Total C H 96 40 56	0
23	J1	1	Total C H 96 40 56	0
23	K1	1	Total C H 96 40 56	0
23	K1	1	Total C H 96 40 56	0
23	L1	1	Total C H 96 40 56	0
23	L1	1	Total C H 96 40 56	0
23	L1	1	Total C H 96 40 56	0

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Mol	Chain	Residues	Atoms	AltConf
23	M1	1	Total C H 96 40 56	0
23	A2	1	Total C H 92 39 53	0
23	A2	1	Total C H 96 40 56	0
23	A2	1	Total C H 96 40 56	0
23	A2	1	Total C H 96 40 56	0
23	A2	1	Total C H 96 40 56	0
23	A2	1	Total C H 96 40 56	0
23	B2	1	Total C H 96 40 56	0
23	B2	1	Total C H 96 40 56	0
23	B2	1	Total C H 91 40 51	0
23	B2	1	Total C H 96 40 56	0
23	B2	1	Total C H 96 40 56	0
23	F2	1	Total C H 96 40 56	0
23	F2	1	Total C H 96 40 56	0
23	F2	1	Total C H 91 40 51	0
23	I2	1	Total C H 96 40 56	0
23	I2	1	Total C H 96 40 56	0
23	I2	1	Total C H 96 40 56	0
23	J2	1	Total C H 96 40 56	0
23	J2	1	Total C H 96 40 56	0
23	K2	1	Total C H 96 40 56	0

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Mol	Chain	Residues	Atoms	AltConf
23	K2	1	Total C H 96 40 56	0
23	L2	1	Total C H 96 40 56	0
23	M2	1	Total C H 96 40 56	0
23	A	1	Total C H 92 39 53	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	A	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	B	1	Total C H 96 40 56	0
23	F	1	Total C H 96 40 56	0
23	F	1	Total C H 96 40 56	0
23	F	1	Total C H 91 40 51	0
23	I	1	Total C H 96 40 56	0
23	I	1	Total C H 96 40 56	0

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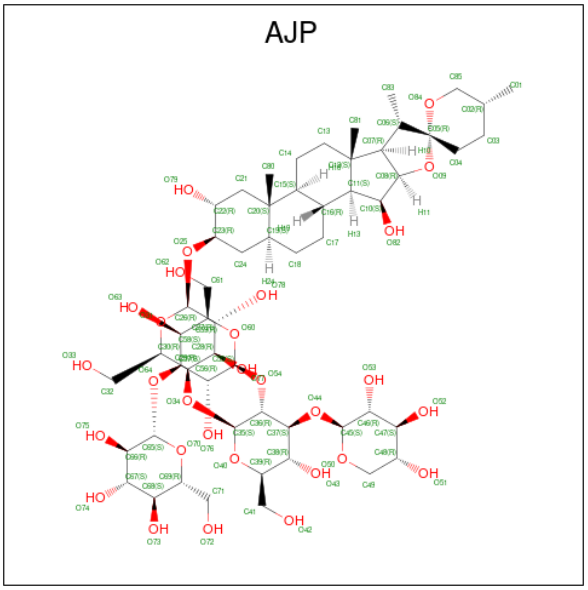
Mol	Chain	Residues	Atoms	AltConf
23	J	1	Total C H 96 40 56	0
23	J	1	Total C H 96 40 56	0
23	K	1	Total C H 96 40 56	0
23	L	1	Total C H 96 40 56	0
23	L	1	Total C H 96 40 56	0
23	M	1	Total C H 91 40 51	0
23	AA	1	Total C H 92 39 53	0
23	AA	1	Total C H 96 40 56	0
23	AA	1	Total C H 96 40 56	0
23	AA	1	Total C H 96 40 56	0
23	AA	1	Total C H 96 40 56	0
23	AA	1	Total C H 96 40 56	0
23	AA	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	BB	1	Total C H 96 40 56	0
23	FF	1	Total C H 96 40 56	0
23	FF	1	Total C H 96 40 56	0

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Mol	Chain	Residues	Atoms	AltConf
23	FF	1	Total C H 91 40 51	0
23	II	1	Total C H 96 40 56	0
23	II	1	Total C H 96 40 56	0
23	II	1	Total C H 96 40 56	0
23	JJ	1	Total C H 96 40 56	0
23	JJ	1	Total C H 96 40 56	0
23	KK	1	Total C H 96 40 56	0
23	LL	1	Total C H 96 40 56	0
23	MM	1	Total C H 93 40 53	0

- Molecule 24 is Digitonin (CCD ID: AJP) (formula: $C_{56}H_{92}O_{29}$).



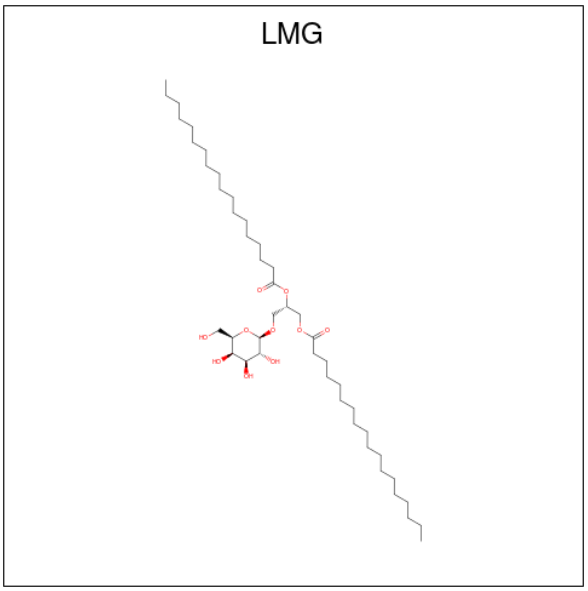
Mol	Chain	Residues	Atoms	AltConf
24	A1	1	Total C H O 96 33 53 10	0
24	A1	1	Total C H O 75 27 43 5	0

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Mol	Chain	Residues	Atoms				AltConf
24	L1	1	Total	C	H	O	0
			96	33	53	10	
24	L1	1	Total	C	H	O	0
			96	33	53	10	
24	A2	1	Total	C	H	O	0
			75	27	43	5	
24	I2	1	Total	C	H	O	0
			73	27	42	4	
24	L2	1	Total	C	H	O	0
			96	33	53	10	
24	L2	1	Total	C	H	O	0
			96	33	53	10	
24	M2	1	Total	C	H	O	0
			74	27	43	4	
24	A	1	Total	C	H	O	0
			72	27	42	3	
24	A	1	Total	C	H	O	0
			81	29	46	6	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	K	1	Total	C	H	O	0
			91	32	50	9	
24	L	1	Total	C	H	O	0
			73	27	42	4	
24	L	1	Total	C	H	O	0
			74	27	43	4	
24	AA	1	Total	C	H	O	0
			72	27	42	3	
24	AA	1	Total	C	H	O	0
			81	29	46	6	
24	BB	1	Total	C	H	O	0
			96	33	53	10	
24	BB	1	Total	C	H	O	0
			96	33	53	10	
24	KK	1	Total	C	H	O	0
			91	32	50	9	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



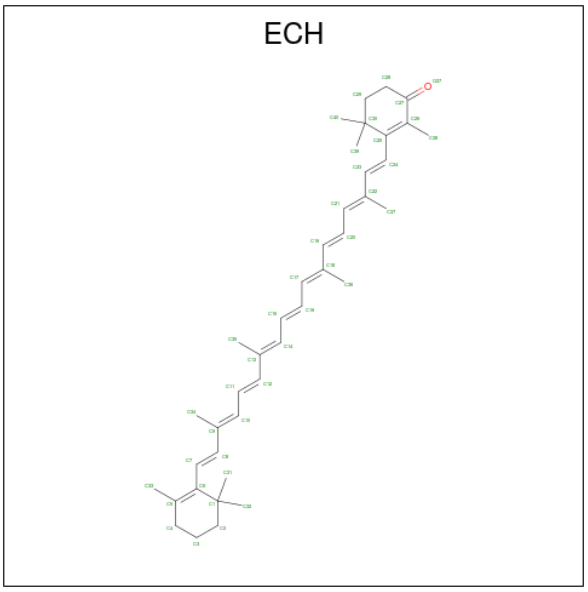
Mol	Chain	Residues	Atoms				AltConf
25	A1	1	Total	C	H	O	1
			88	28	50	10	
25	A1	1	Total	C	H	O	1
			64	20	34	10	
25	B1	1	Total	C	H	O	0
			140	45	85	10	
25	B1	1	Total	C	H	O	0
			65	22	33	10	
25	B1	1	Total	C	H	O	0
			60	20	30	10	
25	I1	1	Total	C	H	O	0
			75	25	40	10	
25	K1	1	Total	C	H	O	1
			68	22	36	10	
25	K1	1	Total	C	H	O	1
			52	16	26	10	
25	L1	1	Total	C	H	O	1
			82	26	46	10	
25	L1	1	Total	C	H	O	0
			141	45	86	10	
25	A2	1	Total	C	H	O	1
			107	34	63	10	
25	A2	1	Total	C	H	O	1
			64	20	34	10	
25	B2	1	Total	C	H	O	0
			140	45	85	10	
25	B2	1	Total	C	H	O	0
			65	22	33	10	

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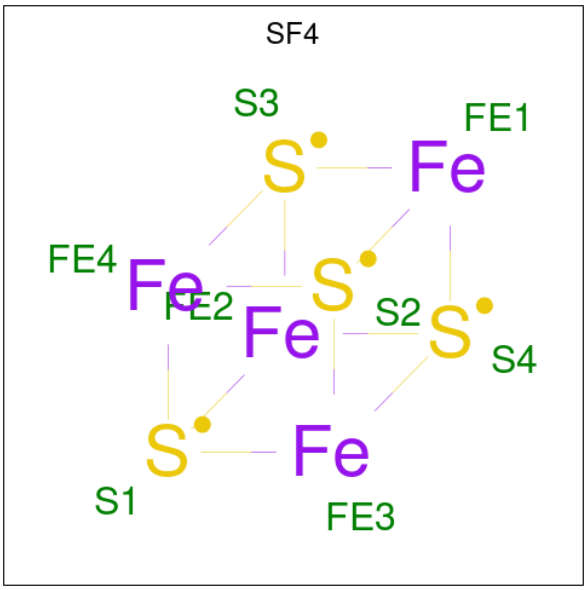
Mol	Chain	Residues	Atoms				AltConf
25	B2	1	Total	C	H	O	0
			60	20	30	10	
25	I2	1	Total	C	H	O	0
			75	25	40	10	
25	K2	1	Total	C	H	O	1
			62	20	32	10	
25	K2	1	Total	C	H	O	1
			52	16	26	10	
25	L2	1	Total	C	H	O	1
			82	26	46	10	
25	B	1	Total	C	H	O	0
			140	45	85	10	
25	B	1	Total	C	H	O	1
			79	25	44	10	
25	B	1	Total	C	H	O	0
			141	45	86	10	
25	B	1	Total	C	H	O	1
			67	21	36	10	
25	L	1	Total	C	H	O	1
			85	27	48	10	
25	M	1	Total	C	H	O	0
			105	36	59	10	
25	BB	1	Total	C	H	O	0
			140	45	85	10	
25	BB	1	Total	C	H	O	1
			82	26	46	10	
25	BB	1	Total	C	H	O	1
			67	21	36	10	
25	II	1	Total	C	H	O	1
			85	27	48	10	
25	II	1	Total	C	H	O	0
			96	32	54	10	

- Molecule 26 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



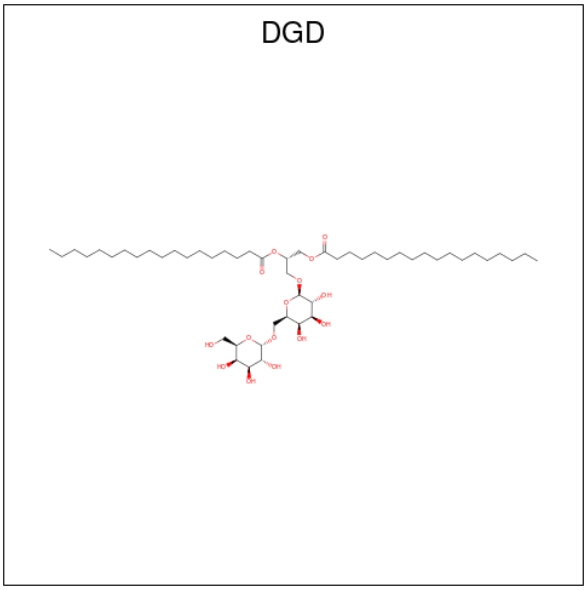
Mol	Chain	Residues	Atoms				AltConf
26	B1	1	Total	C	H	O	0
			95	40	54	1	
26	B2	1	Total	C	H	O	0
			95	40	54	1	
26	B	1	Total	C	H	O	0
			95	40	54	1	
26	BB	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
27	B1	1	Total Fe S 8 4 4	0
27	C1	1	Total Fe S 8 4 4	0
27	C1	1	Total Fe S 8 4 4	0
27	B2	1	Total Fe S 8 4 4	0
27	C2	1	Total Fe S 8 4 4	0
27	C2	1	Total Fe S 8 4 4	0
27	B	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0
27	BB	1	Total Fe S 8 4 4	0
27	CC	1	Total Fe S 8 4 4	0
27	CC	1	Total Fe S 8 4 4	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	H	O	0
			88	27	46	15	
28	BB	1	Total	C	H	O	0
			88	27	46	15	

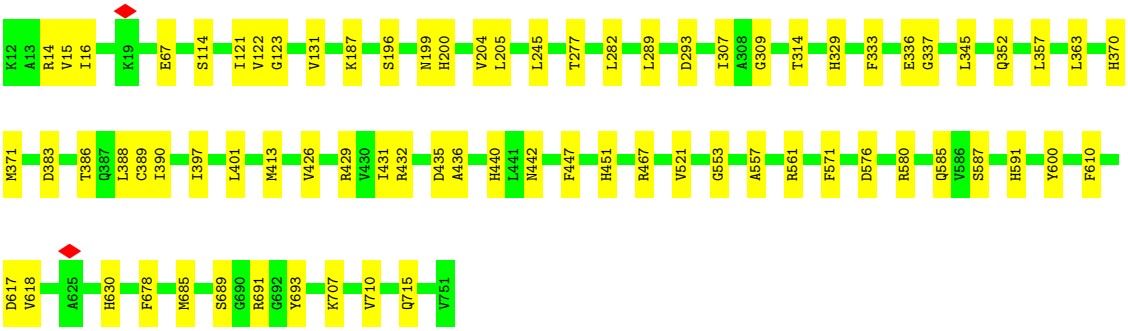
3 Residue-property plots (i)

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 A1:

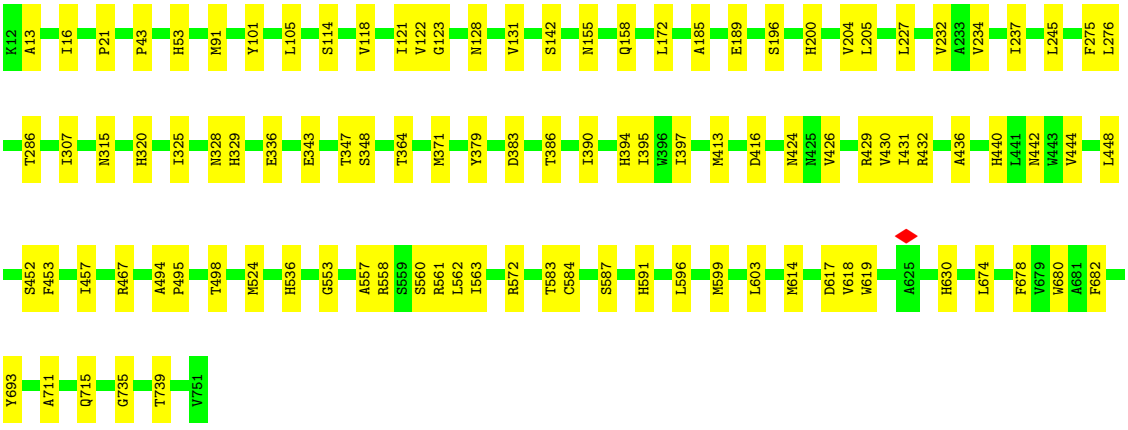




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A2:

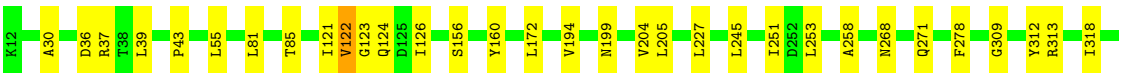


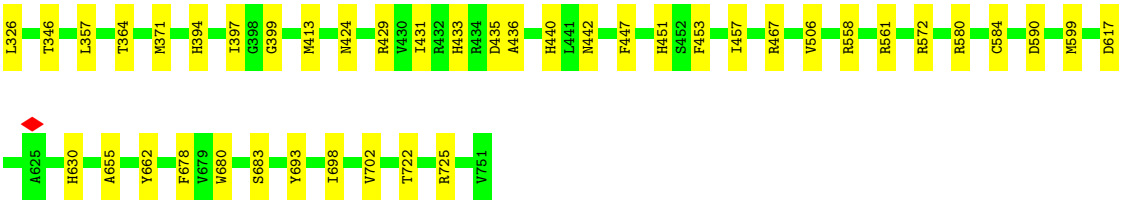


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:







• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA:





• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B1:

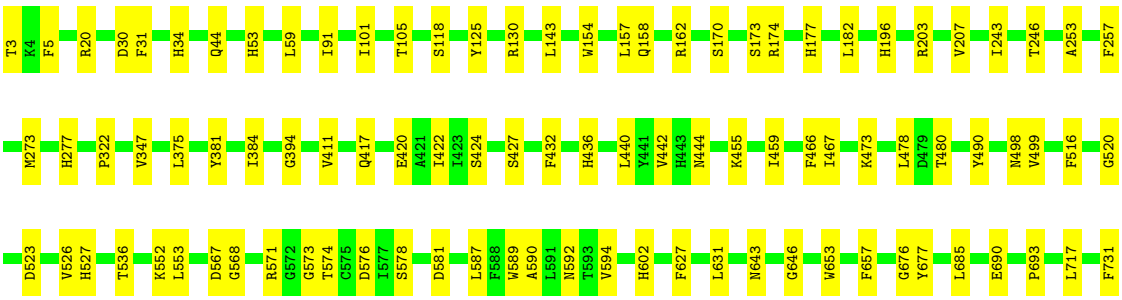




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B2:

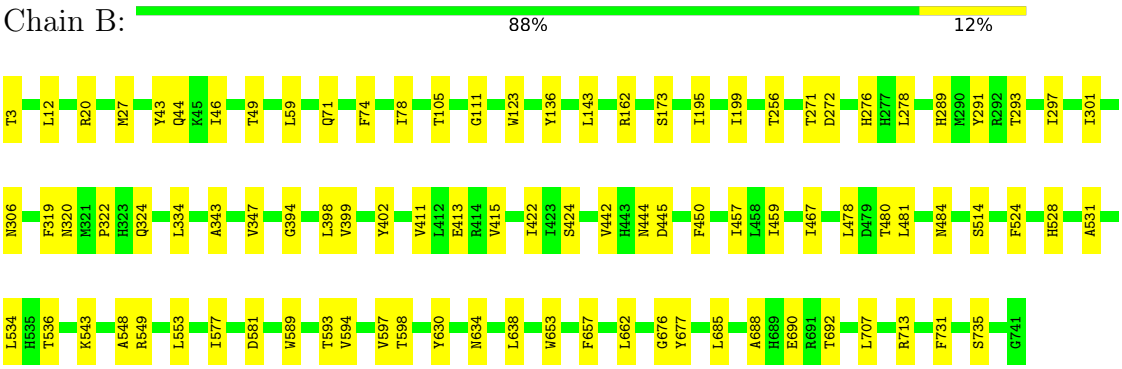






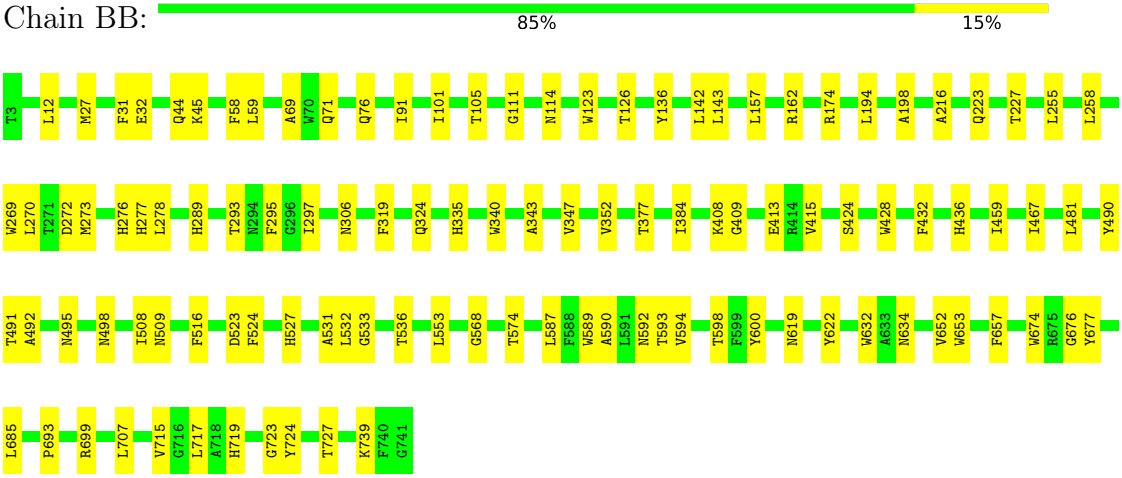
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B:



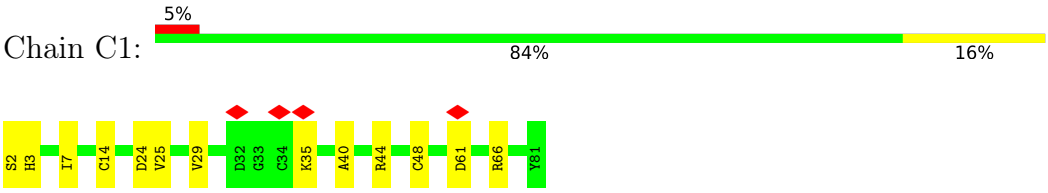
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain BB:



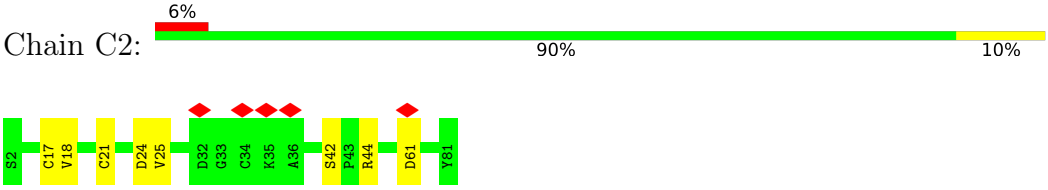
• Molecule 3: Photosystem I iron-sulfur center

Chain C1:



• Molecule 3: Photosystem I iron-sulfur center

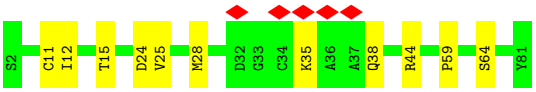
Chain C2:



• Molecule 3: Photosystem I iron-sulfur center

Chain C:

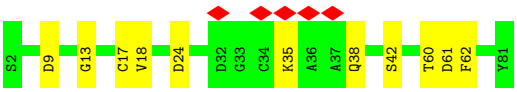




• Molecule 3: Photosystem I iron-sulfur center

Chain CC:

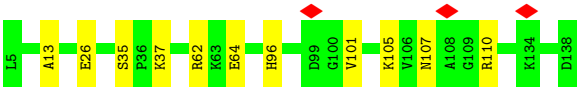




• Molecule 4: Photosystem I reaction center subunit II

Chain D1:





• Molecule 4: Photosystem I reaction center subunit II

Chain D2:





• Molecule 4: Photosystem I reaction center subunit II

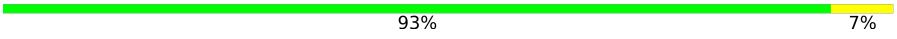
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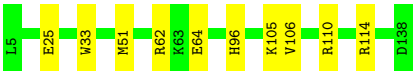




• Molecule 4: Photosystem I reaction center subunit II

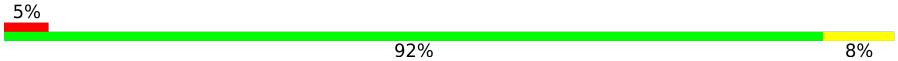
Chain DD:

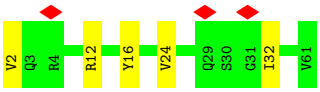




• Molecule 5: Photosystem I reaction center subunit IV

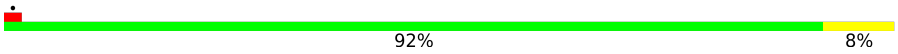
Chain E1:

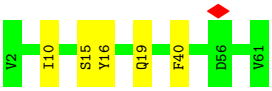




• Molecule 5: Photosystem I reaction center subunit IV

Chain E2:

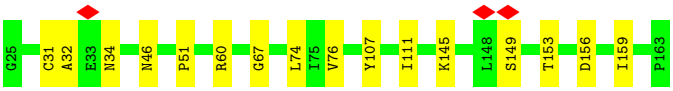




• Molecule 6: Photosystem I reaction center subunit III

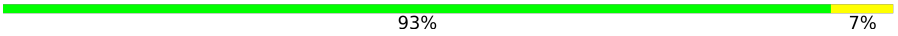
Chain F1:





• Molecule 6: Photosystem I reaction center subunit III

Chain F:

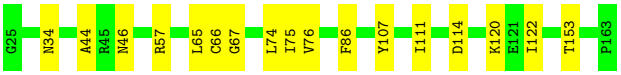




• Molecule 6: Photosystem I reaction center subunit III

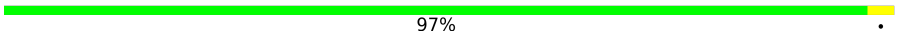
Chain FF:





• Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:

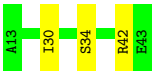




• Molecule 7: Photosystem I reaction center subunit VIII

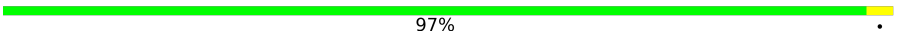
Chain I:





• Molecule 7: Photosystem I reaction center subunit VIII

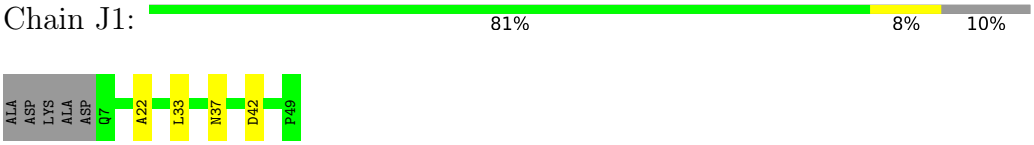
Chain II:





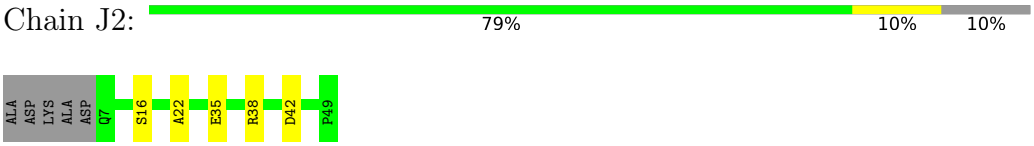
• Molecule 8: Photosystem I reaction center subunit IX

Chain J1:



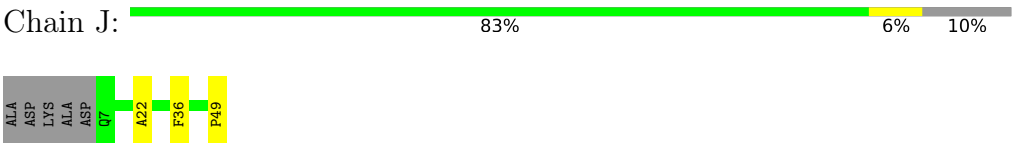
• Molecule 8: Photosystem I reaction center subunit IX

Chain J2:



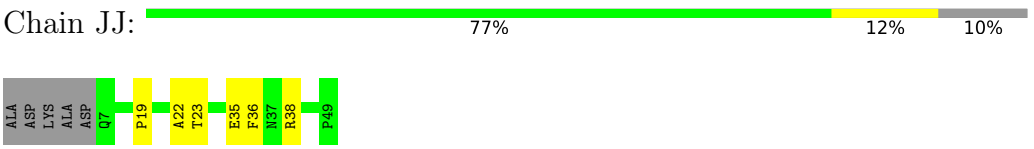
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



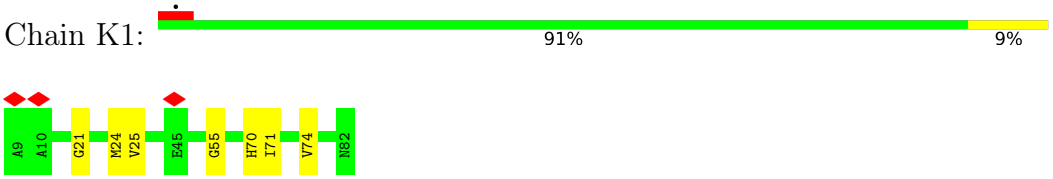
• Molecule 8: Photosystem I reaction center subunit IX

Chain JJ:



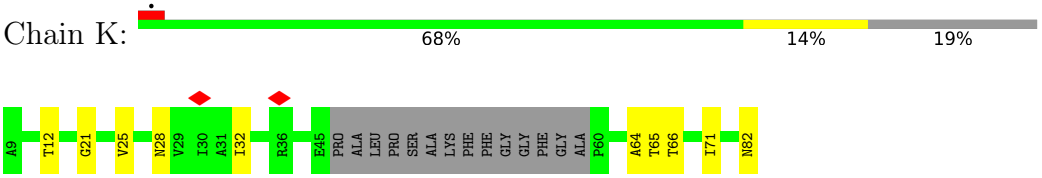
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K1:



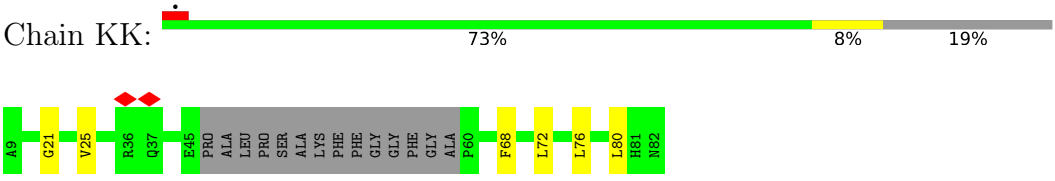
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:



• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain KK:



• Molecule 10: Photosystem I reaction center subunit XI

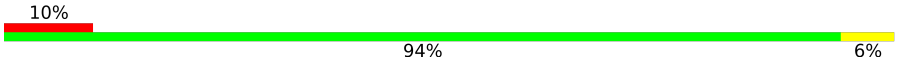
Chain L1:

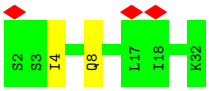




• Molecule 11: Photosystem I reaction center subunit XII

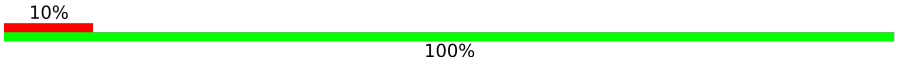
Chain M1:

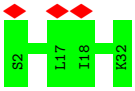




• Molecule 11: Photosystem I reaction center subunit XII

Chain M2:

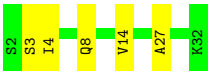




• Molecule 11: Photosystem I reaction center subunit XII

Chain M:

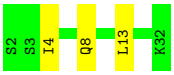




• Molecule 11: Photosystem I reaction center subunit XII

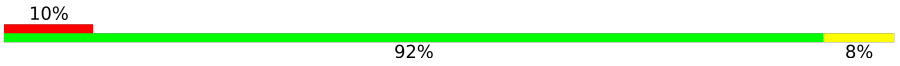
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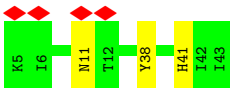




• Molecule 12: Photosystem I 4.8 kDa protein

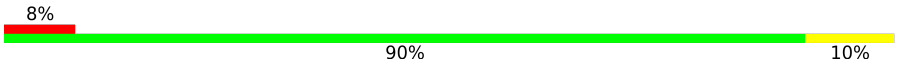
Chain X1:

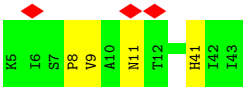




• Molecule 12: Photosystem I 4.8 kDa protein

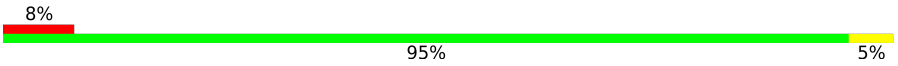
Chain X2:

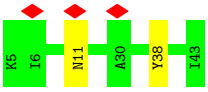




• Molecule 12: Photosystem I 4.8 kDa protein

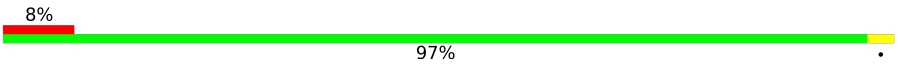
Chain X:

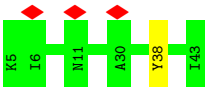




• Molecule 12: Photosystem I 4.8 kDa protein

Chain XX:

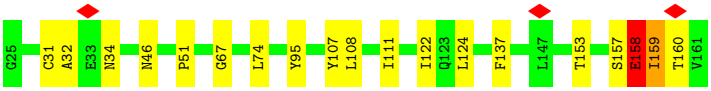




• Molecule 13: Photosystem I reaction center subunit III

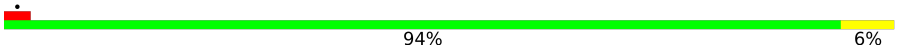
Chain F2:

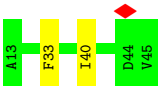




• Molecule 14: Photosystem I reaction center subunit VIII

Chain I2:

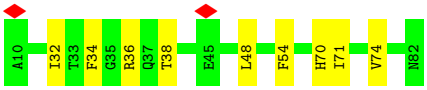




• Molecule 15: Photosystem I reaction center subunit PsaK 1

Chain K2:





• Molecule 16: Photosystem I reaction center subunit XI

Chain L2:

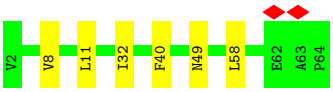




• Molecule 17: Photosystem I reaction center subunit IV

Chain E:

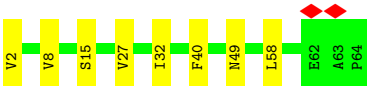




• Molecule 17: Photosystem I reaction center subunit IV

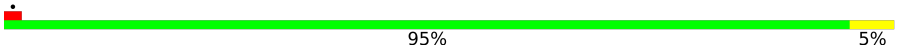
Chain EE:





• Molecule 18: Photosystem I reaction center subunit XI

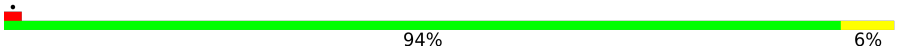
Chain L:





• Molecule 18: Photosystem I reaction center subunit XI

Chain LL:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.390	Depositor
Minimum map value	-1.168	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.434	Depositor
Map size (Å)	392.19998, 392.19998, 392.19998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/6004	0.35	0/8193
1	A1	0.20	0/6004	0.36	0/8193
1	A2	0.20	0/6004	0.39	2/8193 (0.0%)
1	AA	0.20	0/6004	0.36	0/8193
2	B	0.23	0/6143	0.40	0/8396
2	B1	0.20	0/6143	0.37	0/8396
2	B2	0.20	0/6143	0.38	0/8396
2	BB	0.23	0/6143	0.39	0/8396
3	C	0.19	0/609	0.40	0/826
3	C1	0.21	0/609	0.41	0/826
3	C2	0.21	0/609	0.39	0/826
3	CC	0.20	0/609	0.38	0/826
4	D	0.19	0/1060	0.41	0/1431
4	D1	0.17	0/1060	0.39	0/1431
4	D2	0.18	0/1060	0.41	0/1431
4	DD	0.18	0/1060	0.42	0/1431
5	E1	0.17	0/490	0.41	0/665
5	E2	0.19	0/490	0.42	0/665
6	F	0.18	0/1084	0.38	0/1475
6	F1	0.15	0/1084	0.36	0/1475
6	FF	0.17	0/1084	0.34	0/1475
7	I	0.20	0/262	0.37	0/358
7	I1	0.21	0/262	0.31	0/358
7	II	0.19	0/262	0.37	0/358
8	J	0.18	0/358	0.35	0/491
8	J1	0.17	0/358	0.35	0/491
8	J2	0.16	0/358	0.32	0/491
8	JJ	0.18	0/358	0.35	0/491
9	K	0.14	0/448	0.33	0/613
9	K1	0.18	0/551	0.44	0/755
9	KK	0.16	0/448	0.36	0/613
10	L1	0.20	0/1281	0.39	0/1756

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	M	0.16	0/244	0.27	0/334
11	M1	0.16	0/244	0.32	0/334
11	M2	0.15	0/244	0.36	0/334
11	MM	0.17	0/244	0.30	0/334
12	X	0.22	0/320	0.41	0/439
12	X1	0.18	0/320	0.36	0/439
12	X2	0.18	0/320	0.38	0/439
12	XX	0.19	0/320	0.37	0/439
13	F2	0.19	0/1070	0.50	2/1455 (0.1%)
14	I2	0.20	0/277	0.36	0/379
15	K2	0.16	0/546	0.34	0/748
16	L2	0.21	0/1290	0.39	0/1768
17	E	0.18	0/512	0.43	0/696
17	EE	0.17	0/512	0.41	0/696
18	L	0.20	0/1191	0.39	0/1632
18	LL	0.21	0/1191	0.38	0/1632
All	All	0.20	0/73287	0.38	4/100012 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	F2	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	536	HIS	CA-C-N	8.62	133.41	120.31
1	A2	536	HIS	C-N-CA	8.62	133.41	120.31
13	F2	158	GLU	CA-C-N	5.78	132.37	121.97
13	F2	158	GLU	C-N-CA	5.78	132.37	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F2	158	GLU	Peptide
13	F2	159	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5806	5677	5682	53	0
1	A1	5806	5672	5682	63	0
1	A2	5806	5680	5682	72	0
1	AA	5806	5677	5682	54	0
2	B	5919	5667	5677	67	0
2	B1	5919	5660	5677	80	0
2	B2	5919	5662	5677	77	0
2	BB	5919	5676	5677	88	0
3	C	599	582	585	8	0
3	C1	599	584	585	10	0
3	C2	599	580	585	5	0
3	CC	599	582	585	9	0
4	D	1036	1042	1042	10	0
4	D1	1036	1037	1042	9	0
4	D2	1036	1042	1042	10	0
4	DD	1036	1042	1042	8	0
5	E1	481	477	478	4	0
5	E2	481	477	478	7	0
6	F	1060	1051	1054	7	0
6	F1	1060	1052	1054	12	0
6	FF	1060	1052	1054	11	0
7	I	253	255	255	2	0
7	I1	253	255	255	1	0
7	II	253	255	255	1	0
8	J	346	355	355	3	0
8	J1	346	355	355	4	0
8	J2	346	355	355	5	0
8	JJ	346	354	355	5	0
9	K	439	461	461	6	0
9	K1	536	555	555	5	0
9	KK	439	461	461	3	0
10	L1	1244	1239	1242	16	0
11	M	240	256	256	5	0
11	M1	240	256	256	3	0
11	M2	240	256	256	0	0
11	MM	240	256	256	5	0
12	X	309	319	319	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X1	309	318	319	4	0
12	X2	309	318	319	5	0
12	XX	309	319	319	1	0
13	F2	1047	1040	1042	14	0
14	I2	268	268	268	2	0
15	K2	531	550	550	7	0
16	L2	1253	1245	1250	12	0
17	E	502	492	496	5	0
17	EE	502	492	496	6	0
18	L	1156	1153	1157	5	0
18	LL	1156	1154	1157	7	0
19	A	2339	2207	2215	35	0
19	A1	2394	2261	2275	39	0
19	A2	2375	2227	2236	35	0
19	AA	2404	2279	2287	31	0
19	B	2401	2357	2375	54	0
19	B1	2291	2253	2270	44	0
19	B2	2401	2358	2375	36	0
19	BB	2271	2219	2231	55	0
19	F	102	89	90	2	0
19	F1	147	122	123	5	0
19	F2	102	89	90	2	0
19	FF	167	161	162	4	0
19	J	82	58	58	2	0
19	J1	82	57	58	1	0
19	J2	82	58	58	1	0
19	JJ	82	57	58	1	0
19	K	91	65	66	0	0
19	K1	131	92	94	2	0
19	K2	86	61	62	1	0
19	KK	91	65	66	0	0
19	L	191	198	205	4	0
19	L1	191	202	205	5	0
19	L2	186	187	191	0	0
19	LL	168	155	164	4	0
19	X	45	32	33	0	0
19	X1	45	32	33	0	0
19	X2	45	32	33	1	0
19	XX	45	32	33	0	0
20	A	65	72	72	2	0
20	A1	65	72	71	4	0
20	A2	65	72	70	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AA	65	72	71	1	0
21	A	33	46	46	1	0
21	A1	33	46	46	2	0
21	A2	33	46	46	1	0
21	AA	33	46	46	1	0
21	B	33	46	46	2	0
21	B1	33	46	46	0	0
21	B2	33	46	46	0	0
21	BB	33	46	46	2	0
22	A	87	122	123	2	0
22	A1	87	122	123	1	0
22	A2	87	122	123	2	0
22	AA	87	122	123	3	0
22	B	82	110	110	1	0
22	B1	33	36	36	1	0
22	B2	33	36	36	0	0
22	BB	82	110	110	0	0
22	L	34	42	38	0	0
22	L1	33	35	36	2	0
22	L2	35	39	40	1	0
22	LL	34	42	38	0	0
22	X	40	49	50	0	0
22	X1	89	123	124	0	0
22	X2	89	123	124	0	0
22	XX	40	49	50	0	0
23	A	279	389	389	7	0
23	A1	239	333	333	6	0
23	A2	239	333	333	7	0
23	AA	279	389	389	8	0
23	B	240	336	336	12	0
23	B1	200	280	280	7	0
23	B2	200	275	280	9	0
23	BB	240	336	336	11	0
23	F	120	163	168	6	0
23	F1	120	163	168	6	0
23	F2	120	163	168	6	0
23	FF	120	163	168	6	0
23	I	80	112	112	0	0
23	I1	40	56	56	1	0
23	I2	120	168	168	1	0
23	II	120	168	168	0	0
23	J	80	112	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J1	80	112	112	2	0
23	J2	80	112	112	3	0
23	JJ	80	112	112	2	0
23	K	40	56	56	0	0
23	K1	80	112	112	3	0
23	K2	80	112	112	3	0
23	KK	40	56	56	0	0
23	L	80	112	112	1	0
23	L1	120	168	168	0	0
23	L2	40	56	56	0	0
23	LL	40	56	56	1	0
23	M	40	51	56	2	0
23	M1	40	56	56	0	0
23	M2	40	56	56	0	0
23	MM	40	53	56	1	0
24	A	65	88	0	0	0
24	A1	75	96	0	0	0
24	A2	32	43	0	0	0
24	AA	65	88	0	0	0
24	B	129	159	0	1	0
24	BB	86	106	0	1	0
24	I2	31	42	0	0	0
24	K	41	50	0	0	0
24	KK	41	50	0	0	0
24	L	62	85	0	0	0
24	L1	86	106	0	1	0
24	L2	86	106	0	1	0
24	M2	31	43	0	0	0
25	A1	68	84	0	0	0
25	A2	74	97	0	0	0
25	B	176	251	172	0	0
25	B1	117	148	150	0	0
25	B2	117	148	150	0	0
25	BB	122	167	86	0	0
25	I1	35	40	40	0	0
25	I2	35	40	40	1	0
25	II	79	102	54	0	0
25	K1	58	62	0	0	0
25	K2	56	58	0	0	0
25	L	37	48	0	0	0
25	L1	91	132	86	1	0
25	L2	36	46	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	M	46	59	62	1	0
26	B	41	54	54	2	0
26	B1	41	54	54	1	0
26	B2	41	54	54	1	0
26	BB	41	54	54	2	0
27	B	8	0	0	0	0
27	B1	8	0	0	0	0
27	B2	8	0	0	0	0
27	BB	8	0	0	0	0
27	C	16	0	0	1	0
27	C1	16	0	0	1	0
27	C2	16	0	0	0	0
27	CC	16	0	0	0	0
28	B	42	46	42	1	0
28	BB	42	46	42	0	0
All	All	99604	99577	98156	943	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 5.

All (943) 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)
2:B2:587:LEU:HD23	2:B2:717:LEU:HD21	1.55	0.88
2:B:553:LEU:HD23	2:B:577:ILE:HD11	1.56	0.86
19:B2:822:CLA:H93	23:B2:843:BCR:H333	1.57	0.84
19:B1:822:CLA:H93	23:B1:842:BCR:H333	1.58	0.83
2:B1:534:LEU:HD12	19:B1:834:CLA:HED3	1.63	0.81
2:B:415:VAL:HG11	23:B:842:BCR:H401	1.62	0.81
19:B:834:CLA:H93	19:B:835:CLA:HBC1	1.63	0.79
19:BB:833:CLA:H93	19:BB:834:CLA:HBC1	1.64	0.79
1:A:199:ASN:ND2	1:A:309:GLY:O	2.16	0.79
19:B:822:CLA:H93	23:B:843:BCR:H333	1.66	0.78
19:B1:833:CLA:H93	19:B1:834:CLA:HBC1	1.66	0.77
1:A1:199:ASN:ND2	1:A1:309:GLY:O	2.18	0.77
1:AA:413:MET:HE1	1:AA:431:ILE:HD11	1.67	0.76
1:A2:572:ARG:NH1	22:A2:845:LHG:O10	2.20	0.75
6:F1:31:CYS:SG	6:F1:32:ALA:N	2.59	0.75
19:BB:822:CLA:H93	23:BB:842:BCR:H333	1.68	0.75
2:B1:587:LEU:HD12	2:B1:717:LEU:HD21	1.69	0.75
2:B2:490:TYR:O	2:B2:498:ASN:ND2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:473:LYS:NZ	2:B1:516:PHE:O	2.20	0.74
1:A:693:TYR:O	2:B:543:LYS:NZ	2.20	0.74
2:B1:490:TYR:O	2:B1:498:ASN:ND2	2.21	0.74
4:D:105:LYS:O	4:D:110:ARG:NH2	2.22	0.73
2:B2:44:GLN:OE1	2:B2:162:ARG:NH2	2.22	0.73
2:B2:473:LYS:NZ	2:B2:516:PHE:O	2.20	0.72
2:BB:44:GLN:OE1	2:BB:162:ARG:NH2	2.23	0.72
1:A1:693:TYR:O	2:B1:543:LYS:NZ	2.21	0.71
2:B:402:TYR:OH	2:B:413:GLU:OE2	2.08	0.71
6:F1:46:ASN:ND2	6:F1:51:PRO:O	2.23	0.70
13:F2:31:CYS:SG	13:F2:32:ALA:N	2.64	0.70
1:A1:576:ASP:OD2	1:A1:580:ARG:NH2	2.24	0.70
1:A2:715:GLN:NE2	5:E2:16:TYR:OH	2.25	0.69
1:A2:413:MET:HE1	1:A2:431:ILE:HD11	1.74	0.69
2:B2:567:ASP:OD2	2:B2:571:ARG:NH2	2.25	0.69
4:D1:62:ARG:NH2	4:D1:64:GLU:OE1	2.26	0.69
2:BB:377:THR:HG23	2:BB:598:THR:HG21	1.73	0.69
18:LL:61:ARG:NH2	18:LL:65:GLU:OE1	2.26	0.69
1:A1:333:PHE:O	1:A1:429:ARG:NH1	2.25	0.68
1:A2:735:GLY:O	1:A2:739:THR:OG1	2.10	0.68
2:BB:306:ASN:ND2	2:BB:324:GLN:O	2.27	0.68
1:A1:435:ASP:OD2	1:A1:561:ARG:NH2	2.26	0.68
19:B1:833:CLA:HBC2	19:B1:834:CLA:HBC3	1.76	0.68
3:C1:61:ASP:OD1	5:E1:12:ARG:NH1	2.26	0.68
1:AA:722:THR:OG1	22:AA:846:LHG:O5	2.12	0.68
16:L2:114:ASN:ND2	22:L2:208:LHG:O9	2.28	0.67
23:A1:851:BCR:H362	19:A1:852:CLA:H43	1.77	0.67
1:A:722:THR:OG1	22:A:845:LHG:O5	2.13	0.67
19:B1:832:CLA:O2D	19:B1:833:CLA:HMB1	1.94	0.67
23:A:851:BCR:H362	19:A:852:CLA:H43	1.76	0.67
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.27	0.67
16:L2:11:LEU:O	16:L2:17:ASN:ND2	2.27	0.67
5:E2:19:GLN:NE2	13:F2:153:THR:O	2.28	0.67
19:A1:844:CLA:OBD	10:L1:18:ARG:NH2	2.28	0.67
2:B1:409:GLY:N	2:B1:413:GLU:OE1	2.28	0.66
19:B:821:CLA:HMA2	19:B:821:CLA:O2A	1.95	0.66
2:B1:693:PRO:O	10:L1:53:TYR:OH	2.13	0.66
19:B:834:CLA:HBB2	19:B:835:CLA:HED2	1.78	0.66
4:D2:62:ARG:NH2	4:D2:64:GLU:OE1	2.29	0.66
19:B:806:CLA:H18	25:M:102:LMG:H392	1.78	0.66
2:B2:384:ILE:CG2	2:B2:590:ALA:HB1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:804:CLA:O1A	2:BB:532:LEU:HD11	1.96	0.65
1:A1:571:PHE:O	1:A1:587:SER:OG	2.14	0.65
1:A2:329:HIS:O	22:A2:846:LHG:O2	2.10	0.65
2:B2:432:PHE:O	2:B2:436:HIS:ND1	2.29	0.65
19:BB:821:CLA:O2A	19:BB:821:CLA:HMA2	1.95	0.65
1:AA:580:ARG:NH1	4:DD:64:GLU:OE2	2.30	0.65
3:C:64:SER:OG	27:C:102:SF4:S2	2.50	0.65
19:BB:833:CLA:HBC2	19:BB:834:CLA:HBC3	1.78	0.65
2:B1:236:ASN:ND2	2:B1:252:THR:OG1	2.22	0.65
3:C2:61:ASP:OD2	5:E2:15:SER:OG	2.09	0.65
2:B1:432:PHE:O	2:B1:436:HIS:ND1	2.29	0.64
2:BB:490:TYR:O	2:BB:498:ASN:ND2	2.31	0.64
2:BB:12:LEU:HD11	2:BB:27:MET:HE3	1.77	0.64
23:A2:851:BCR:H362	19:A2:852:CLA:H43	1.78	0.64
2:B:690:GLU:OE2	4:D:21:THR:OG1	2.16	0.64
3:CC:9:ASP:OD1	3:CC:35:LYS:NZ	2.31	0.64
15:K2:34:PHE:O	15:K2:38:THR:OG1	2.15	0.64
2:B2:693:PRO:O	16:L2:53:TYR:OH	2.14	0.64
1:AA:621:THR:OG1	1:AA:629:SER:OG	2.15	0.64
19:B:833:CLA:O2D	19:B:834:CLA:HMB1	1.97	0.63
3:C:25:VAL:HG23	3:C:44:ARG:O	1.99	0.63
3:C2:25:VAL:HG23	3:C2:44:ARG:O	1.99	0.63
2:B2:552:LYS:NZ	5:E2:15:SER:O	2.32	0.63
1:AA:371:MET:HE1	19:AA:831:CLA:O1D	1.99	0.63
1:A1:691:ARG:N	2:B1:575:CYS:SG	2.70	0.63
1:A2:205:LEU:HD11	19:A2:815:CLA:H42	1.80	0.63
19:AA:843:CLA:H202	19:BB:835:CLA:H192	1.81	0.63
1:A1:467:ARG:NH2	19:A1:835:CLA:O1D	2.32	0.63
13:F2:124:LEU:O	8:J2:16:SER:OG	2.16	0.63
1:AA:277:THR:HG1	1:AA:292:THR:HG1	1.47	0.63
1:AA:397:ILE:HD13	19:AA:830:CLA:HBC3	1.79	0.63
1:A1:371:MET:HE1	19:A1:830:CLA:O1D	1.99	0.62
1:A1:585:GLN:OE1	2:B1:674:TRP:N	2.32	0.62
1:AA:205:LEU:HD11	19:AA:815:CLA:H42	1.81	0.62
1:A1:277:THR:OG1	1:A1:293:ASP:OD1	2.17	0.62
1:A2:680:TRP:NE1	20:A2:803:CL0:O1A	2.32	0.62
2:BB:467:ILE:HD11	19:BB:832:CLA:H43	1.81	0.62
2:B2:440:LEU:O	2:B2:444:ASN:ND2	2.32	0.62
4:D2:101:VAL:HG11	4:D2:107:ASN:HB2	1.81	0.62
23:F2:305:BCR:H311	23:F2:305:BCR:HC8	1.82	0.62
2:B:480:THR:O	2:B:484:ASN:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:834:CLA:HBC2	19:B:835:CLA:HBC3	1.81	0.62
19:B:833:CLA:HED2	19:B:834:CLA:HBB1	1.81	0.62
2:BB:324:GLN:NE2	2:BB:408:LYS:O	2.33	0.62
3:C1:25:VAL:HG23	3:C1:44:ARG:O	1.99	0.61
2:B1:384:ILE:HG23	2:B1:590:ALA:HB1	1.83	0.61
2:B:306:ASN:ND2	2:B:324:GLN:O	2.33	0.61
4:D1:105:LYS:O	4:D1:110:ARG:NH1	2.33	0.61
1:A:371:MET:HE1	19:A:831:CLA:O1D	2.00	0.61
1:A:580:ARG:NH2	4:D:64:GLU:OE2	2.33	0.61
9:K:12:THR:OG1	9:K:82:ASN:O	2.16	0.61
2:BB:273:MET:O	2:BB:277:HIS:ND1	2.26	0.61
3:C2:21:CYS:SG	3:C2:24:ASP:N	2.73	0.61
4:D:21:THR:HG21	18:L:121:LEU:HD11	1.83	0.61
1:AA:348:SER:OG	1:AA:416:ASP:OD2	2.15	0.61
1:A1:329:HIS:O	22:A1:846:LHG:O2	2.10	0.60
2:B:593:THR:O	2:B:597:VAL:HG23	2.00	0.60
1:AA:575:CYS:O	1:AA:583:THR:OG1	2.08	0.60
1:A1:205:LEU:HD11	19:A1:814:CLA:H42	1.82	0.60
2:B1:723:GLY:O	2:B1:727:THR:HG22	2.01	0.60
1:A2:155:ASN:ND2	1:A2:158:GLN:OE1	2.34	0.60
19:B:801:CLA:H12	11:M:27:ALA:HB1	1.82	0.60
2:BB:634:ASN:OD1	2:BB:739:LYS:NZ	2.35	0.60
1:A1:707:LYS:NZ	6:F1:156:ASP:OD1	2.30	0.60
1:A:436:ALA:O	1:A:440:HIS:ND1	2.34	0.60
19:B1:832:CLA:HED2	19:B1:833:CLA:CBB	2.32	0.60
2:B1:44:GLN:OE1	2:B1:162:ARG:NH2	2.35	0.60
2:B2:568:GLY:O	2:B2:574:THR:OG1	2.19	0.60
23:BB:841:BCR:H311	23:BB:841:BCR:H343	1.84	0.60
19:B:834:CLA:HAB	19:B:835:CLA:CGD	2.32	0.59
23:B:842:BCR:H311	23:B:842:BCR:H343	1.84	0.59
1:AA:91:MET:HE1	19:AA:810:CLA:H2A	1.83	0.59
2:B2:203:ARG:NH2	2:B2:253:ALA:O	2.34	0.59
1:A:205:LEU:HD11	19:A:815:CLA:H42	1.83	0.59
1:AA:318:ILE:HG23	19:AA:822:CLA:HED1	1.84	0.59
6:FF:107:TYR:CZ	6:FF:111:ILE:HD11	2.37	0.59
19:B2:829:CLA:H142	23:F2:303:BCR:H333	1.83	0.59
13:F2:107:TYR:CZ	13:F2:111:ILE:HD11	2.38	0.59
1:A2:674:LEU:HD11	2:B2:627:PHE:CZ	2.38	0.59
5:E2:19:GLN:NE2	13:F2:157:SER:OG	2.36	0.59
2:BB:432:PHE:O	2:BB:436:HIS:ND1	2.35	0.59
2:B1:440:LEU:O	2:B1:444:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D2:105:LYS:O	4:D2:110:ARG:NH2	2.34	0.59
1:A1:363:LEU:HD21	19:A1:828:CLA:H43	1.85	0.59
2:BB:619:ASN:OD1	2:BB:622:TYR:OH	2.12	0.59
23:F1:306:BCR:HC8	23:F1:306:BCR:H311	1.84	0.59
16:L2:110:SER:O	16:L2:114:ASN:ND2	2.35	0.59
1:A1:345:LEU:HD23	1:A1:352:GLN:OE1	2.03	0.58
1:A1:442:ASN:ND2	2:B1:685:LEU:HD21	2.18	0.58
8:JJ:35:GLU:OE1	8:JJ:38:ARG:NE	2.35	0.58
6:F1:60:ARG:NH2	8:J1:42:ASP:O	2.36	0.58
19:B:833:CLA:HED2	19:B:834:CLA:CBB	2.34	0.58
1:AA:245:LEU:HD21	19:AA:818:CLA:HBC1	1.85	0.58
1:A:413:MET:HE1	1:A:431:ILE:HD11	1.85	0.58
2:B:459:ILE:HD11	2:B:524:PHE:CE1	2.38	0.58
19:BB:832:CLA:CGD	19:BB:833:CLA:HMB3	2.34	0.58
1:A2:371:MET:HE1	19:A2:831:CLA:O1D	2.04	0.58
19:B:810:CLA:H143	19:B:815:CLA:H42	1.85	0.58
19:B2:833:CLA:O2D	19:B2:834:CLA:HMB1	2.04	0.58
2:B:467:ILE:HD11	19:B:833:CLA:H43	1.85	0.58
1:AA:572:ARG:NH1	22:AA:846:LHG:O10	2.36	0.58
19:BB:833:CLA:HAB	19:BB:834:CLA:CGD	2.33	0.58
19:B1:828:CLA:H142	23:F1:303:BCR:H333	1.86	0.58
19:B1:833:CLA:O1D	6:F1:76:VAL:HG13	2.03	0.58
8:J2:35:GLU:OE2	8:J2:38:ARG:NH2	2.36	0.58
16:L2:53:TYR:CD2	16:L2:126:VAL:HG21	2.38	0.57
2:BB:459:ILE:HG22	6:FF:74:LEU:HB2	1.87	0.57
2:B1:243:ILE:O	2:B1:246:THR:OG1	2.17	0.57
2:BB:293:THR:HG21	19:BB:817:CLA:OBD	2.05	0.57
23:FF:306:BCR:HC8	23:FF:306:BCR:H311	1.85	0.57
2:B1:467:ILE:HD11	19:B1:832:CLA:H43	1.86	0.57
2:B1:469:ALA:O	2:B1:483:SER:OG	2.21	0.57
2:B:3:THR:OG1	2:B:20:ARG:NH2	2.38	0.57
2:B:594:VAL:O	2:B:598:THR:OG1	2.17	0.57
13:F2:34:ASN:ND2	13:F2:67:GLY:O	2.36	0.57
1:A2:121:ILE:O	1:A2:123:GLY:N	2.37	0.57
1:AA:424:ASN:OD1	1:AA:429:ARG:NH2	2.37	0.57
1:AA:436:ALA:O	1:AA:440:HIS:ND1	2.37	0.57
2:B2:527:HIS:HB3	19:B2:833:CLA:HED1	1.84	0.57
23:F:305:BCR:HC8	23:F:305:BCR:H311	1.85	0.57
4:DD:62:ARG:NH2	4:DD:64:GLU:OE1	2.37	0.57
17:EE:8:VAL:CG1	17:EE:58:LEU:HD22	2.34	0.57
2:B2:467:ILE:HD11	19:B2:833:CLA:H43	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B2:836:CLA:H192	19:B2:852:CLA:H202	1.85	0.57
1:A:442:ASN:ND2	2:B:685:LEU:HD21	2.20	0.57
2:B:195:ILE:HA	2:B:199:ILE:HD12	1.87	0.57
19:BB:810:CLA:H143	19:BB:815:CLA:H42	1.84	0.57
1:A:572:ARG:NH1	22:A:845:LHG:O10	2.37	0.56
1:A2:383:ASP:OD2	1:A2:386:THR:OG1	2.12	0.56
20:A2:803:CL0:CBB	2:B2:631:LEU:HD13	2.35	0.56
2:BB:723:GLY:O	2:BB:727:THR:HG22	2.05	0.56
1:A1:600:TYR:OH	20:A1:802:CL0:O1A	2.17	0.56
2:B1:69:ALA:HB1	11:M1:4:ILE:HD11	1.86	0.56
19:B1:833:CLA:HBB2	19:B1:834:CLA:HED2	1.87	0.56
1:A2:424:ASN:OD1	1:A2:429:ARG:NH2	2.38	0.56
1:A2:599:MET:O	1:A2:603:LEU:HD23	2.05	0.56
3:C:38:GLN:HB3	4:D:106:VAL:HG21	1.86	0.56
1:A1:14:ARG:NH2	1:A1:16:ILE:HD11	2.21	0.56
6:F1:107:TYR:CZ	6:F1:111:ILE:HD11	2.41	0.56
1:A1:401:LEU:HD21	19:A1:807:CLA:H142	1.88	0.56
2:B2:573:GLY:O	2:B2:574:THR:OG1	2.23	0.56
19:B:836:CLA:H192	19:B:860:CLA:H202	1.85	0.56
1:AA:442:ASN:ND2	2:BB:685:LEU:HD21	2.21	0.56
19:BB:832:CLA:HED2	19:BB:833:CLA:CBB	2.35	0.56
2:B1:727:THR:HG23	19:B1:848:CLA:O1D	2.06	0.56
1:A2:307:ILE:HG12	23:K2:105:BCR:H362	1.87	0.56
23:AA:852:BCR:H362	19:AA:853:CLA:H43	1.87	0.56
2:BB:424:SER:OG	19:BB:856:CLA:HED3	2.06	0.56
4:D:33:TRP:HE1	4:D:51:MET:HE3	1.70	0.56
1:A1:617:ASP:O	1:A1:630:HIS:NE2	2.39	0.56
10:L1:118:PRO:O	10:L1:119:THR:HG23	2.06	0.56
1:A2:142:SER:O	1:A2:390:ILE:HD11	2.05	0.56
19:B:812:CLA:HMA2	26:B:841:ECH:H34B	1.88	0.56
19:A2:820:CLA:CMD	19:A2:821:CLA:H202	2.36	0.56
2:B2:455:LYS:NZ	8:J2:42:ASP:OD2	2.23	0.56
2:B:424:SER:OG	19:B:859:CLA:HED3	2.06	0.56
1:A2:328:ASN:OD1	19:A2:825:CLA:HED3	2.06	0.56
2:B2:381:TYR:CE1	2:B2:594:VAL:HG11	2.41	0.56
1:A:318:ILE:HG23	19:A:822:CLA:HED1	1.88	0.56
1:A:43:PRO:HG3	6:F:122:ILE:HD12	1.87	0.55
1:A:245:LEU:HD21	19:A:818:CLA:HBC1	1.89	0.55
1:A:617:ASP:O	1:A:630:HIS:NE2	2.39	0.55
2:BB:459:ILE:HD11	2:BB:524:PHE:CE1	2.41	0.55
19:F1:301:CLA:H43	19:F1:302:CLA:CBC	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:227:LEU:O	1:A2:232:VAL:HG22	2.05	0.55
19:B2:811:CLA:H43	26:B2:841:ECH:H36A	1.88	0.55
2:B:322:PRO:O	2:B:411:VAL:HG23	2.07	0.55
2:B:123:TRP:CZ2	19:B:810:CLA:H191	2.41	0.55
19:B:811:CLA:H43	26:B:841:ECH:H36A	1.89	0.55
16:L2:61:ARG:NH2	16:L2:65:GLU:OE1	2.39	0.55
1:A:397:ILE:HD13	19:A:830:CLA:HBC3	1.88	0.55
1:A:467:ARG:NH2	19:A:836:CLA:O1D	2.40	0.55
19:B:810:CLA:HMA3	23:B:840:BCR:H362	1.89	0.55
2:BB:693:PRO:O	18:LL:53:TYR:OH	2.19	0.55
8:JJ:19:PRO:O	8:JJ:23:THR:HG23	2.05	0.55
2:B:320:ASN:ND2	22:B:852:LHG:O4	2.39	0.55
2:B1:5:PHE:CD1	7:I1:40:ILE:HG22	2.42	0.55
19:B1:833:CLA:HAB	19:B1:834:CLA:CGD	2.37	0.55
1:A1:363:LEU:CD2	19:A1:828:CLA:H43	2.35	0.55
19:A1:842:CLA:H202	19:B1:835:CLA:H192	1.88	0.55
19:AA:801:CLA:OBD	2:BB:677:TYR:OH	2.15	0.55
2:B1:320:ASN:ND2	22:B1:847:LHG:O4	2.39	0.55
5:E2:10:ILE:HD11	5:E2:40:PHE:HZ	1.72	0.55
19:BB:833:CLA:HBB2	19:BB:834:CLA:HED2	1.88	0.55
19:A:804:CLA:H193	19:A:852:CLA:H192	1.88	0.55
1:AA:617:ASP:O	1:AA:630:HIS:NE2	2.40	0.55
19:B1:833:CLA:H42	23:F1:303:BCR:H392	1.89	0.54
2:B2:417:GLN:OE1	12:X2:11:ASN:ND2	2.40	0.54
2:BB:508:ILE:HG23	2:BB:509:ASN:OD1	2.07	0.54
2:B1:520:GLY:N	2:B1:523:ASP:OD2	2.41	0.54
19:B2:826:CLA:H41	19:B2:826:CLA:C7	2.37	0.54
1:A1:715:GLN:NE2	5:E1:16:TYR:OH	2.40	0.54
2:B2:173:SER:O	2:B2:177:HIS:ND1	2.40	0.54
9:K:32:ILE:HA	9:K:65:THR:HG21	1.88	0.54
11:MM:13:LEU:HB3	23:MM:101:BCR:H371	1.89	0.54
2:B1:322:PRO:O	2:B1:411:VAL:HG13	2.08	0.54
2:B:291:TYR:HE1	2:B:301:ILE:HD11	1.72	0.54
2:BB:69:ALA:CB	11:MM:4:ILE:HD11	2.38	0.54
19:B1:826:CLA:H41	19:B1:826:CLA:C7	2.37	0.54
23:A2:851:BCR:H362	19:A2:852:CLA:C4	2.38	0.54
19:F2:301:CLA:H43	19:F2:302:CLA:CBC	2.37	0.54
19:F:301:CLA:H42	8:J:22:ALA:HA	1.90	0.54
19:B1:811:CLA:H43	26:B1:840:ECH:H36A	1.87	0.54
25:L1:210:LMG:H161	2:BB:297:ILE:HD12	1.88	0.54
23:A2:851:BCR:H403	23:A2:851:BCR:H23C	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:478:LEU:O	12:X1:41:HIS:NE2	2.41	0.54
2:B2:322:PRO:O	2:B2:411:VAL:HG13	2.08	0.54
2:B2:553:LEU:HD21	2:B2:574:THR:HG22	1.89	0.54
1:AA:345:LEU:HD22	1:AA:352:GLN:OE1	2.07	0.54
1:A1:386:THR:HG22	1:A1:390:ILE:HD12	1.90	0.54
22:L1:211:LHG:HC61	19:L:202:CLA:HBC1	1.90	0.54
2:B2:417:GLN:NE2	12:X2:8:PRO:O	2.41	0.54
23:B2:842:BCR:H382	23:B2:843:BCR:H21C	1.90	0.54
19:BB:826:CLA:H41	19:BB:826:CLA:C7	2.38	0.54
1:A1:383:ASP:OD2	1:A1:386:THR:OG1	2.11	0.54
19:BB:810:CLA:HMA3	23:BB:839:BCR:H362	1.90	0.54
1:A1:691:ARG:NH1	2:B1:573:GLY:O	2.41	0.53
2:B1:459:ILE:HD11	2:B1:524:PHE:CE1	2.43	0.53
1:AA:397:ILE:CD1	19:AA:830:CLA:HBC3	2.38	0.53
6:FF:44:ALA:O	6:FF:57:ARG:NH2	2.41	0.53
1:A2:275:PHE:O	1:A2:276:LEU:HD12	2.09	0.53
15:K2:32:ILE:HG12	19:K2:104:CLA:HBA2	1.91	0.53
19:A:805:CLA:C15	23:J:102:BCR:H353	2.38	0.53
3:CC:24:ASP:OD2	4:DD:96:HIS:ND1	2.41	0.53
1:AA:467:ARG:NH2	19:AA:836:CLA:O1D	2.41	0.53
17:EE:8:VAL:HG11	17:EE:58:LEU:HD22	1.90	0.53
19:B:837:CLA:HBC2	19:B:837:CLA:HHD	1.91	0.53
2:BB:289:HIS:CE1	23:BB:838:BCR:H363	2.43	0.53
19:LL:201:CLA:H92	19:LL:201:CLA:C4	2.38	0.53
1:A2:678:PHE:CD2	23:A2:851:BCR:H363	2.43	0.53
2:B2:578:SER:N	2:B2:581:ASP:OD2	2.41	0.53
2:B:581:ASP:OD1	2:B:713:ARG:NH1	2.41	0.53
2:B:731:PHE:O	2:B:735:SER:OG	2.10	0.53
1:A1:121:ILE:O	1:A1:123:GLY:N	2.42	0.53
2:B2:347:VAL:HB	19:B2:823:CLA:H43	1.89	0.53
1:A:678:PHE:CD2	23:A:851:BCR:H363	2.44	0.53
20:A:803:CL0:H13	19:A:852:CLA:OBD	2.08	0.53
2:B:688:ALA:O	2:B:692:THR:HG23	2.09	0.53
10:L1:8:SER:OG	10:L1:14:ASP:OD1	2.27	0.53
1:A2:413:MET:HE1	1:A2:431:ILE:CD1	2.38	0.53
19:AA:804:CLA:H193	19:AA:853:CLA:H192	1.91	0.53
19:BB:832:CLA:HED2	19:BB:833:CLA:HBB1	1.91	0.53
2:B1:136:TYR:OH	11:M1:8:GLN:O	2.25	0.53
5:E1:2:VAL:HG21	5:E1:24:VAL:HG21	1.91	0.53
2:B1:123:TRP:CZ2	19:B1:810:CLA:H191	2.44	0.53
25:I2:105:LMG:O5	25:I2:105:LMG:O4	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:546:THR:HG21	19:AA:828:CLA:HBC3	1.91	0.53
1:A1:245:LEU:HD21	19:A1:817:CLA:HBC1	1.91	0.52
2:B2:424:SER:OG	19:B2:851:CLA:HED3	2.09	0.52
13:F2:95:TYR:OH	13:F2:137:PHE:O	2.17	0.52
9:K1:71:ILE:HD11	23:K1:106:BCR:C36	2.39	0.52
1:A2:442:ASN:HD22	2:B2:685:LEU:HD21	1.74	0.52
2:B2:170:SER:OG	19:B2:810:CLA:HBC1	2.10	0.52
17:E:8:VAL:CG2	17:E:58:LEU:HD22	2.38	0.52
2:BB:553:LEU:HD21	2:BB:574:THR:HG22	1.91	0.52
6:FF:76:VAL:HG12	6:FF:86:PHE:HB2	1.90	0.52
1:A1:337:GLY:C	1:A1:426:VAL:HG23	2.34	0.52
2:B1:248:GLN:N	2:B1:248:GLN:OE1	2.43	0.52
9:K1:24:MET:HE3	9:K1:70:HIS:HA	1.90	0.52
2:B:459:ILE:HG22	6:F:74:LEU:HB2	1.91	0.52
19:B:834:CLA:H42	23:F:303:BCR:H392	1.91	0.52
19:LL:201:CLA:H92	19:LL:201:CLA:C3	2.40	0.52
1:A:172:LEU:HD11	19:A:812:CLA:HBC1	1.90	0.52
1:A1:14:ARG:HH21	1:A1:16:ILE:HD11	1.75	0.52
23:B1:841:BCR:H343	23:B1:841:BCR:H311	1.90	0.52
2:B:347:VAL:HB	19:B:823:CLA:H43	1.91	0.52
19:A2:805:CLA:C15	23:J2:102:BCR:H353	2.39	0.52
2:B2:384:ILE:HG21	2:B2:590:ALA:HB1	1.91	0.52
13:F2:157:SER:HB3	12:X2:9:VAL:HG11	1.90	0.52
1:A1:587:SER:O	1:A1:591:HIS:ND1	2.42	0.52
23:A1:851:BCR:H403	23:A1:851:BCR:H23C	1.91	0.52
3:CC:38:GLN:HB3	4:DD:106:VAL:HG21	1.91	0.52
1:A1:67:GLU:N	1:A1:67:GLU:OE1	2.43	0.52
1:AA:193:ASN:OD1	19:AA:815:CLA:HBC1	2.09	0.52
1:A:251:ILE:HD11	1:A:258:ALA:HB2	1.91	0.51
19:BB:828:CLA:O1A	6:FF:153:THR:HG21	2.10	0.51
2:B1:455:LYS:NZ	8:J1:42:ASP:OD1	2.29	0.51
19:A2:852:CLA:H42	2:B2:442:VAL:HG22	1.91	0.51
19:F:301:CLA:H43	19:F:302:CLA:CBC	2.41	0.51
2:BB:340:TRP:CH2	23:BB:841:BCR:H372	2.46	0.51
23:F1:306:BCR:H382	23:F1:306:BCR:H371	1.92	0.51
19:A2:816:CLA:CHC	23:A2:847:BCR:H352	2.40	0.51
4:D2:5:LEU:CD1	4:D2:86:ILE:HD11	2.40	0.51
18:LL:74:LEU:HD13	18:LL:101:LEU:HD22	1.91	0.51
1:A1:357:LEU:HD11	1:A1:401:LEU:HD22	1.92	0.51
1:A1:561:ARG:O	4:D1:62:ARG:NH1	2.43	0.51
19:A1:801:CLA:OBD	2:B1:677:TYR:OH	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:682:PHE:HZ	19:A2:842:CLA:HBC2	1.76	0.51
1:AA:678:PHE:CD2	23:AA:852:BCR:H363	2.45	0.51
2:B2:478:LEU:HB3	2:B2:480:THR:HG23	1.93	0.51
2:B2:520:GLY:N	2:B2:523:ASP:OD2	2.42	0.51
4:DD:33:TRP:HE1	4:DD:51:MET:HE3	1.74	0.51
1:A:194:VAL:HG21	1:A:346:THR:HG22	1.92	0.51
19:BB:826:CLA:H41	19:BB:826:CLA:H72	1.93	0.51
1:A2:114:SER:HB3	1:A2:131:VAL:HG21	1.91	0.51
1:A2:286:THR:HG22	1:A2:379:TYR:CE2	2.45	0.51
19:A:852:CLA:H41	19:A:852:CLA:H71	1.93	0.51
19:B:828:CLA:HBC3	23:F:303:BCR:H362	1.91	0.51
19:AA:805:CLA:C15	23:JJ:102:BCR:H353	2.40	0.51
2:BB:727:THR:HG23	19:BB:852:CLA:O1D	2.10	0.51
2:B2:466:PHE:HD1	2:B2:480:THR:HG21	1.76	0.51
2:B2:552:LYS:NZ	13:F2:158:GLU:OE1	2.42	0.51
2:BB:653:TRP:O	2:BB:657:PHE:N	2.43	0.51
2:B1:236:ASN:HD21	2:B1:252:THR:HG1	1.54	0.51
1:A2:467:ARG:NH2	19:A2:836:CLA:O1D	2.43	0.51
4:D:32:THR:HG22	4:D:57:LEU:HD13	1.92	0.51
1:AA:453:PHE:CZ	1:AA:457:ILE:HD11	2.46	0.51
17:EE:40:PHE:O	17:EE:49:ASN:ND2	2.41	0.51
1:A2:587:SER:O	1:A2:591:HIS:ND1	2.44	0.51
2:B2:422:ILE:HG23	19:B2:835:CLA:CBB	2.41	0.51
2:B2:478:LEU:O	12:X2:41:HIS:NE2	2.44	0.51
2:B:44:GLN:OE1	2:B:162:ARG:NH2	2.44	0.51
19:A1:804:CLA:C15	23:J1:102:BCR:H353	2.40	0.50
2:B1:352:VAL:HG22	19:B1:815:CLA:C2	2.41	0.50
19:B:830:CLA:H42	8:J:36:PHE:CE2	2.45	0.50
1:AA:448:LEU:O	1:AA:452:SER:OG	2.13	0.50
2:B1:461:PRO:HG2	2:B1:519:ILE:HD12	1.93	0.50
19:A:816:CLA:CHC	23:A:847:BCR:H352	2.41	0.50
2:BB:126:THR:CG2	2:BB:270:LEU:HD21	2.41	0.50
6:FF:34:ASN:ND2	6:FF:67:GLY:O	2.45	0.50
1:A2:693:TYR:N	2:B2:576:ASP:O	2.45	0.50
23:A:854:BCR:H361	23:A:854:BCR:H21C	1.92	0.50
1:AA:571:PHE:O	1:AA:587:SER:OG	2.29	0.50
2:B1:420:GLU:N	2:B1:420:GLU:OE1	2.45	0.50
1:A2:245:LEU:HD21	19:A2:818:CLA:HBC1	1.93	0.50
19:B2:821:CLA:O2A	19:B2:821:CLA:HMA2	2.12	0.50
15:K2:71:ILE:HD11	23:K2:105:BCR:C36	2.41	0.50
1:A:680:TRP:O	1:A:683:SER:OG	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:204:VAL:HG11	19:AA:815:CLA:CBB	2.42	0.50
19:B2:820:CLA:HBC2	19:B2:820:CLA:HHD	1.93	0.50
3:CC:35:LYS:HA	17:EE:32:ILE:HG22	1.94	0.50
1:A1:204:VAL:HG11	19:A1:814:CLA:CBB	2.42	0.50
1:A2:524:MET:HE3	1:A2:618:VAL:O	2.11	0.50
19:A2:833:CLA:HMA1	19:A2:834:CLA:O1D	2.12	0.50
18:L:17:ASN:OD1	18:L:18:ARG:N	2.44	0.50
19:BB:828:CLA:HBC3	23:FF:303:BCR:H362	1.93	0.50
2:BB:592:ASN:OD1	19:BB:852:CLA:H42	2.11	0.50
19:A1:832:CLA:HMA1	19:A1:833:CLA:O1D	2.12	0.49
1:A2:614:MET:O	1:A2:619:TRP:N	2.41	0.49
2:B2:157:LEU:O	2:B2:162:ARG:NE	2.43	0.49
23:F2:305:BCR:H382	23:F2:305:BCR:H371	1.94	0.49
2:B1:736:THR:O	2:B1:740:PHE:N	2.45	0.49
2:B2:455:LYS:NZ	19:B2:830:CLA:OBD	2.39	0.49
19:B:828:CLA:O1A	6:F:153:THR:HG21	2.13	0.49
2:B1:556:ASP:OD1	3:C1:66:ARG:NH2	2.45	0.49
1:A2:320:HIS:CB	1:A2:325:ILE:HD11	2.43	0.49
23:AA:852:BCR:H403	23:AA:852:BCR:H23C	1.93	0.49
2:BB:523:ASP:O	2:BB:527:HIS:ND1	2.44	0.49
3:CC:61:ASP:OD2	17:EE:15:SER:OG	2.15	0.49
1:A1:436:ALA:O	1:A1:440:HIS:ND1	2.45	0.49
2:B1:445:ASP:OD1	2:B1:623:LEU:N	2.44	0.49
2:B2:154:TRP:O	2:B2:158:GLN:NE2	2.43	0.49
19:A2:802:CLA:H3A	23:K2:103:BCR:H362	1.94	0.49
2:B2:257:PHE:HD2	2:B2:499:VAL:HG23	1.76	0.49
2:B2:422:ILE:HG23	19:B2:835:CLA:HBB2	1.94	0.49
1:A:364:THR:HG22	1:A:394:HIS:HB3	1.93	0.49
19:BB:833:CLA:H42	23:FF:303:BCR:H392	1.94	0.49
3:CC:42:SER:O	4:DD:114:ARG:NH1	2.46	0.49
1:A2:711:ALA:O	13:F2:108:LEU:HD21	2.13	0.49
2:B:662:LEU:HD12	19:B:858:CLA:O1A	2.13	0.49
6:F:34:ASN:ND2	6:F:67:GLY:O	2.44	0.49
19:L:202:CLA:H92	19:L:202:CLA:C4	2.43	0.49
2:B1:347:VAL:HB	19:B1:823:CLA:H43	1.95	0.49
2:B1:480:THR:OG1	2:B1:481:LEU:N	2.46	0.49
3:C1:29:VAL:HG12	4:D1:110:ARG:HB3	1.94	0.49
2:B2:690:GLU:OE1	4:D2:20:LEU:HD22	2.13	0.49
19:AA:816:CLA:CHC	23:AA:848:BCR:H352	2.42	0.49
1:A:121:ILE:O	1:A:123:GLY:N	2.45	0.49
19:B:826:CLA:H41	19:B:826:CLA:C7	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LEU:HD22	19:B:802:CLA:H201	1.94	0.49
1:AA:364:THR:HG22	1:AA:394:HIS:HB3	1.95	0.49
1:A2:245:LEU:CD2	19:A2:818:CLA:HBC1	2.43	0.49
1:A2:617:ASP:O	1:A2:630:HIS:NE2	2.46	0.49
1:A:30:ALA:O	6:F:123:GLN:NE2	2.45	0.49
23:A:851:BCR:H23C	23:A:851:BCR:H403	1.93	0.49
19:B:820:CLA:HBC3	19:B:820:CLA:HHD	1.94	0.49
19:BB:828:CLA:CBB	19:FF:305:CLA:H202	2.43	0.49
1:A1:307:ILE:HG12	23:K1:106:BCR:H362	1.95	0.48
19:B1:827:CLA:O1D	12:X1:11:ASN:ND2	2.46	0.48
2:BB:136:TYR:OH	11:MM:8:GLN:O	2.31	0.48
1:A1:245:LEU:CD2	19:A1:817:CLA:HBC1	2.44	0.48
1:A1:710:VAL:HG12	1:A1:710:VAL:O	2.13	0.48
19:A1:815:CLA:CHC	23:A1:847:BCR:H352	2.43	0.48
13:F2:46:ASN:ND2	13:F2:51:PRO:O	2.46	0.48
9:K:28:ASN:HD21	9:K:66:THR:HG22	1.79	0.48
1:AA:18:ASP:OD2	1:AA:71:ARG:NH2	2.43	0.48
2:BB:32:GLU:OE1	2:BB:335:HIS:NE2	2.43	0.48
2:BB:384:ILE:HG23	2:BB:590:ALA:HB1	1.94	0.48
19:F1:301:CLA:H42	8:J1:22:ALA:HA	1.95	0.48
1:A2:204:VAL:HG11	19:A2:815:CLA:CBB	2.44	0.48
16:L2:152:GLY:O	16:L2:156:VAL:HG23	2.13	0.48
19:B:828:CLA:CBB	19:B:829:CLA:H202	2.43	0.48
19:AA:820:CLA:CMD	19:AA:821:CLA:H202	2.43	0.48
19:BB:833:CLA:C9	19:BB:834:CLA:HBC1	2.40	0.48
19:B2:828:CLA:CBB	19:B2:829:CLA:H202	2.43	0.48
19:F2:301:CLA:H42	8:J2:22:ALA:HA	1.96	0.48
19:A:820:CLA:CMD	19:A:821:CLA:H202	2.43	0.48
1:AA:326:LEU:HD23	19:AA:826:CLA:O1D	2.14	0.48
23:B1:841:BCR:H343	23:B1:841:BCR:C31	2.43	0.48
1:AA:24:THR:HG21	1:AA:178:TRP:HE1	1.77	0.48
1:AA:710:VAL:HG12	1:AA:710:VAL:O	2.13	0.48
3:CC:60:THR:OG1	3:CC:62:PHE:O	2.27	0.48
2:B:272:ASP:O	2:B:276:HIS:N	2.47	0.48
2:BB:568:GLY:O	2:BB:574:THR:OG1	2.29	0.48
2:BB:216:ALA:HA	19:BB:812:CLA:HED1	1.95	0.48
6:FF:66:CYS:SG	6:FF:67:GLY:N	2.86	0.48
20:A1:802:CL0:CAB	19:A1:852:CLA:HED1	2.43	0.48
19:K1:103:CLA:H3A	23:K1:104:BCR:H362	1.95	0.48
1:A2:562:LEU:HD21	1:A2:583:THR:HG22	1.95	0.48
19:A2:806:CLA:HBC2	19:A2:832:CLA:H43	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:524:MET:CE	1:AA:628:VAL:HG11	2.44	0.48
19:AA:828:CLA:HED2	19:AA:828:CLA:OBD	2.14	0.48
18:LL:61:ARG:NH1	19:LL:201:CLA:O2D	2.47	0.48
2:B1:459:ILE:HG22	6:F1:74:LEU:HB2	1.95	0.48
2:B1:460:GLU:OE2	2:B1:465:GLN:NE2	2.45	0.48
3:C1:2:SER:OG	3:C1:3:HIS:N	2.46	0.48
19:B2:834:CLA:H42	23:F2:303:BCR:H392	1.96	0.48
9:KK:21:GLY:O	9:KK:25:VAL:HG23	2.14	0.48
1:A1:447:PHE:O	1:A1:451:HIS:ND1	2.45	0.47
20:A1:802:CL0:H13	19:A1:852:CLA:OBD	2.14	0.47
19:A1:839:CLA:H91	19:L1:206:CLA:H192	1.96	0.47
2:B1:356:MET:HE1	19:B1:825:CLA:O2D	2.14	0.47
1:A:326:LEU:HD23	19:A:826:CLA:O1D	2.14	0.47
21:A:843:PQN:H211	19:B:859:CLA:HBC1	1.96	0.47
6:F:76:VAL:HG12	6:F:86:PHE:HB2	1.96	0.47
2:B1:124:TRP:HA	2:B1:127:ILE:HD12	1.95	0.47
2:B1:531:ALA:HB2	19:B1:833:CLA:HBB1	1.96	0.47
10:L1:68:MET:CE	19:L1:205:CLA:HED2	2.43	0.47
3:C1:14:CYS:N	27:C1:102:SF4:S1	2.87	0.47
2:B2:394:GLY:HA2	23:B2:843:BCR:H393	1.95	0.47
19:A:801:CLA:OBD	2:B:677:TYR:OH	2.22	0.47
2:B:481:LEU:HD21	12:X:38:TYR:CD1	2.49	0.47
1:AA:585:GLN:OE1	2:BB:674:TRP:N	2.41	0.47
2:BB:105:THR:HG22	2:BB:111:GLY:C	2.39	0.47
1:A1:114:SER:HB3	1:A1:131:VAL:HG21	1.94	0.47
2:B1:123:TRP:NE1	2:B1:127:ILE:HD11	2.29	0.47
1:A2:561:ARG:O	4:D2:62:ARG:NH1	2.47	0.47
9:K:21:GLY:O	9:K:25:VAL:HG23	2.14	0.47
2:BB:123:TRP:CZ2	19:BB:810:CLA:H191	2.49	0.47
19:A1:852:CLA:H42	2:B1:442:VAL:HG22	1.96	0.47
2:B1:343:ALA:HB2	23:B1:842:BCR:H372	1.96	0.47
1:A2:101:TYR:O	1:A2:105:LEU:HD23	2.13	0.47
1:A:156:SER:O	1:A:160:TYR:N	2.47	0.47
1:A:435:ASP:OD2	1:A:561:ARG:NH2	2.47	0.47
4:DD:105:LYS:O	4:DD:110:ARG:NH2	2.47	0.47
19:A1:834:CLA:H93	19:B1:836:CLA:H142	1.96	0.47
2:B1:126:THR:CG2	2:B1:270:LEU:HD21	2.45	0.47
23:F1:306:BCR:H381	19:J1:103:CLA:HBC3	1.96	0.47
2:B2:3:THR:OG1	2:B2:20:ARG:NH2	2.47	0.47
19:BB:804:CLA:HAA2	19:BB:806:CLA:HED1	1.96	0.47
19:BB:811:CLA:H43	26:BB:840:ECH:H36A	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:EE:2:VAL:O	17:EE:27:VAL:HG21	2.13	0.47
1:A1:114:SER:CB	1:A1:131:VAL:HG21	2.45	0.47
19:A1:841:CLA:H41	19:A1:841:CLA:H71	1.97	0.47
2:B1:157:LEU:O	2:B1:162:ARG:NE	2.43	0.47
2:B1:394:GLY:HA2	23:B1:842:BCR:H393	1.97	0.47
19:B1:828:CLA:H202	19:F1:305:CLA:CBB	2.44	0.47
2:B2:273:MET:O	2:B2:277:HIS:ND1	2.46	0.47
3:C2:17:CYS:SG	3:C2:18:VAL:N	2.87	0.47
2:B:692:THR:HG21	19:B:860:CLA:HMA1	1.97	0.47
2:BB:126:THR:HG23	2:BB:270:LEU:HD21	1.97	0.47
1:A2:596:LEU:HD21	19:A2:832:CLA:HBC1	1.97	0.47
2:B2:91:ILE:HG22	19:B2:806:CLA:OBD	2.14	0.47
3:C:24:ASP:OD2	4:D:96:HIS:ND1	2.48	0.47
2:B1:59:LEU:HD23	2:B1:143:LEU:HD23	1.95	0.47
2:B1:123:TRP:CE2	2:B1:127:ILE:HD11	2.50	0.47
3:C1:7:ILE:HD13	3:C1:40:ALA:C	2.39	0.47
10:L1:148:ILE:HD11	18:L:64:LEU:HD21	1.96	0.47
19:A:828:CLA:OBD	19:A:828:CLA:HED2	2.15	0.47
2:BB:59:LEU:HD23	2:BB:143:LEU:HD23	1.97	0.47
2:BB:69:ALA:HB3	11:MM:4:ILE:HD11	1.97	0.47
2:B:71:GLN:NE2	19:B:804:CLA:O1D	2.47	0.47
1:AA:680:TRP:O	1:AA:683:SER:OG	2.30	0.47
23:AA:855:BCR:H21C	23:AA:855:BCR:H361	1.97	0.47
1:A1:685:MET:HE2	21:A1:843:PQN:H2M3	1.97	0.46
1:A2:432:ARG:NH1	4:D2:14:GLY:O	2.46	0.46
19:A2:842:CLA:H71	19:A2:842:CLA:H41	1.97	0.46
1:A:121:ILE:HG22	1:A:124:GLN:HE21	1.80	0.46
1:A2:16:ILE:HD11	1:A2:189:GLU:HB2	1.97	0.46
15:K2:70:HIS:O	15:K2:74:VAL:HG23	2.16	0.46
3:C:35:LYS:HA	17:E:32:ILE:HG22	1.97	0.46
19:BB:829:CLA:H42	8:JJ:36:PHE:CE2	2.50	0.46
1:A1:337:GLY:O	1:A1:426:VAL:HG23	2.15	0.46
2:B2:59:LEU:HD23	2:B2:143:LEU:HD23	1.97	0.46
2:BB:319:PHE:CD2	19:BB:820:CLA:HMA1	2.51	0.46
2:BB:523:ASP:OD1	2:BB:600:TYR:OH	2.20	0.46
19:B1:804:CLA:HAA2	19:B1:806:CLA:HED1	1.97	0.46
19:B1:807:CLA:H141	19:B1:807:CLA:H162	1.72	0.46
15:K2:48:LEU:HD23	15:K2:54:PHE:CG	2.50	0.46
19:B:826:CLA:H41	19:B:826:CLA:H72	1.96	0.46
8:J:49:PRO:HB3	19:J:103:CLA:HED1	1.96	0.46
1:AA:119:TRP:HE1	23:AA:854:BCR:H332	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:125:TYR:O	2:B2:130:ARG:NH1	2.48	0.46
2:B2:420:GLU:OE1	2:B2:420:GLU:N	2.49	0.46
2:B2:526:VAL:HG23	19:B2:849:CLA:H141	1.97	0.46
2:B:256:THR:HG1	2:B:271:THR:HG1	1.55	0.46
19:B:836:CLA:HAB	21:B:838:PQN:H192	1.98	0.46
19:BB:820:CLA:HBC3	19:BB:820:CLA:HHD	1.96	0.46
2:B1:170:SER:OG	19:B1:810:CLA:HBC1	2.14	0.46
2:B2:118:SER:O	2:B2:375:LEU:HD21	2.16	0.46
19:A:822:CLA:HMA1	9:K:64:ALA:HB2	1.97	0.46
19:BB:820:CLA:O1A	23:BB:841:BCR:H352	2.15	0.46
2:B1:526:VAL:HG23	19:B1:848:CLA:H141	1.96	0.46
2:B2:174:ARG:HB2	19:B2:810:CLA:HBC2	1.96	0.46
2:B:278:LEU:HD21	19:B:812:CLA:HMC2	1.97	0.46
19:BB:832:CLA:O1D	19:BB:833:CLA:HMB3	2.16	0.46
1:A2:114:SER:CB	1:A2:131:VAL:HG21	2.46	0.46
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.51	0.46
1:AA:155:ASN:N	1:AA:155:ASN:OD1	2.49	0.46
1:A1:15:VAL:HG11	19:A1:811:CLA:CBA	2.46	0.46
19:B1:833:CLA:C9	19:B1:834:CLA:HBC1	2.43	0.46
6:F1:153:THR:HG21	19:F1:305:CLA:O1A	2.16	0.46
19:A2:801:CLA:OBD	2:B2:677:TYR:OH	2.27	0.46
19:A:806:CLA:HBC2	19:A:832:CLA:H43	1.96	0.46
2:B:524:PHE:O	2:B:528:HIS:ND1	2.48	0.46
19:AA:834:CLA:HBC2	19:AA:841:CLA:HMC3	1.98	0.46
2:BB:533:GLY:HA3	2:BB:593:THR:HG22	1.96	0.46
1:A1:678:PHE:CD2	23:A1:851:BCR:H363	2.51	0.45
1:A2:678:PHE:CG	23:A2:851:BCR:H363	2.51	0.45
5:E2:10:ILE:HD11	5:E2:40:PHE:CZ	2.51	0.45
1:AA:426:VAL:O	1:AA:430:VAL:HG23	2.16	0.45
2:BB:352:VAL:CG2	19:BB:815:CLA:H43	2.46	0.45
6:FF:65:LEU:HD12	6:FF:75:ILE:HD12	1.98	0.45
19:A1:803:CLA:H193	19:A1:852:CLA:H192	1.99	0.45
2:B1:174:ARG:HB2	19:B1:810:CLA:HBC2	1.98	0.45
8:J1:33:LEU:O	8:J1:37:ASN:ND2	2.48	0.45
9:K1:55:GLY:HA3	19:K1:105:CLA:HMD2	1.98	0.45
1:A2:43:PRO:HG3	13:F2:122:ILE:HD12	1.98	0.45
19:B:827:CLA:O1D	12:X:11:ASN:ND2	2.49	0.45
19:A2:828:CLA:HAB	23:A2:850:BCR:H311	1.99	0.45
2:B2:101:ILE:O	2:B2:105:THR:HG23	2.16	0.45
16:L2:27:ASP:OD1	16:L2:29:GLN:NE2	2.49	0.45
19:AA:806:CLA:HBC2	19:AA:832:CLA:H43	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:343:ALA:HB2	23:BB:842:BCR:H372	1.97	0.45
23:F2:305:BCR:H15C	23:F2:305:BCR:H351	1.79	0.45
1:A:227:LEU:HD21	1:A:253:LEU:HD11	1.99	0.45
17:E:40:PHE:O	17:E:49:ASN:ND2	2.49	0.45
1:A1:389:CYS:HB3	19:A1:829:CLA:HMA1	1.99	0.45
10:L1:126:VAL:HG13	10:L1:126:VAL:O	2.16	0.45
1:A2:172:LEU:HD11	19:A2:812:CLA:HBC1	1.98	0.45
1:A2:584:CYS:O	2:B2:676:GLY:N	2.49	0.45
11:M:14:VAL:HG23	23:M:101:BCR:H391	1.98	0.45
21:AA:844:PQN:H211	19:BB:856:CLA:HBC1	1.98	0.45
19:BB:835:CLA:HAB	21:BB:837:PQN:H192	1.99	0.45
23:B2:842:BCR:H331	23:B2:842:BCR:HC8	1.99	0.45
23:B:842:BCR:H343	23:B:842:BCR:C31	2.46	0.45
2:BB:58:PHE:HD1	2:BB:142:LEU:HD22	1.81	0.45
23:BB:841:BCR:H343	23:BB:841:BCR:C31	2.45	0.45
1:A2:560:SER:N	1:A2:563:ILE:O	2.49	0.45
1:A:268:ASN:ND2	1:A:271:GLN:OE1	2.50	0.45
1:A:655:ALA:HB2	20:A:803:CL0:H25	1.99	0.45
19:A:852:CLA:H42	2:B:442:VAL:HG22	1.99	0.45
6:F:87:LEU:O	6:F:90:SER:OG	2.13	0.45
18:LL:118:PRO:O	18:LL:119:THR:HG23	2.17	0.45
3:C1:25:VAL:HG21	3:C1:48:CYS:HB2	1.98	0.45
10:L1:114:ASN:ND2	22:L1:211:LHG:O9	2.50	0.45
19:A2:852:CLA:H41	19:A2:852:CLA:H71	1.99	0.45
16:L2:118:PRO:O	16:L2:119:THR:HG23	2.17	0.45
19:AA:805:CLA:CGA	19:AA:842:CLA:H43	2.47	0.45
23:AA:852:BCR:H362	19:AA:853:CLA:C4	2.46	0.45
9:K1:21:GLY:O	9:K1:25:VAL:HG23	2.17	0.45
19:A2:844:CLA:OBD	16:L2:18:ARG:NH2	2.50	0.45
1:A:204:VAL:HG11	19:A:815:CLA:CBB	2.47	0.45
19:B:833:CLA:CGD	19:B:834:CLA:HMB1	2.47	0.45
17:E:8:VAL:HG21	17:E:58:LEU:HD22	1.98	0.45
2:BB:69:ALA:HB1	11:MM:4:ILE:HD11	1.99	0.45
2:BB:384:ILE:HD11	2:BB:594:VAL:HB	1.98	0.45
19:BB:833:CLA:HBC3	19:BB:833:CLA:HMC1	1.99	0.45
1:A1:336:GLU:OE1	1:A1:336:GLU:N	2.49	0.44
1:A1:553:GLY:O	1:A1:557:ALA:HB2	2.17	0.44
2:B2:5:PHE:CD1	14:I2:40:ILE:HG22	2.52	0.44
2:BB:101:ILE:O	2:BB:105:THR:HG23	2.17	0.44
2:BB:347:VAL:HB	19:BB:823:CLA:H43	1.99	0.44
2:BB:707:LEU:N	21:BB:837:PQN:O4	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:59:LEU:CD2	2:B2:143:LEU:HD23	2.47	0.44
17:E:11:LEU:HD12	17:E:11:LEU:O	2.17	0.44
1:AA:43:PRO:HG3	6:FF:122:ILE:HD12	1.97	0.44
1:AA:658:VAL:HG22	1:AA:746:ALA:HB3	1.99	0.44
2:BB:76:GLN:N	2:BB:76:GLN:OE1	2.50	0.44
2:B1:424:SER:OG	19:B1:850:CLA:HED3	2.17	0.44
10:L1:68:MET:HE1	19:L1:205:CLA:HED2	1.98	0.44
23:B2:842:BCR:H331	23:B2:842:BCR:C8	2.46	0.44
13:F2:107:TYR:CE2	13:F2:111:ILE:HD11	2.53	0.44
1:A:429:ARG:O	1:A:433:HIS:ND1	2.51	0.44
19:A:842:CLA:H41	19:A:842:CLA:H71	2.00	0.44
23:A:851:BCR:H362	19:A:852:CLA:C4	2.45	0.44
2:B:173:SER:HA	2:B:293:THR:HG22	1.99	0.44
19:B:804:CLA:HAA2	19:B:806:CLA:HED1	1.98	0.44
2:BB:492:ALA:HB3	2:BB:495:ASN:O	2.17	0.44
2:B2:243:ILE:O	2:B2:246:THR:OG1	2.33	0.44
2:BB:428:TRP:HZ3	19:BB:834:CLA:HBC2	1.82	0.44
2:BB:481:LEU:HD21	12:XX:38:TYR:CD1	2.52	0.44
19:B1:821:CLA:HMA1	19:B1:821:CLA:O2A	2.18	0.44
6:F1:145:LYS:O	6:F1:149:SER:OG	2.29	0.44
1:A2:453:PHE:CZ	1:A2:457:ILE:HD11	2.53	0.44
8:J2:38:ARG:HH11	23:J2:104:BCR:H311	1.82	0.44
2:B:398:LEU:O	2:B:549:ARG:NH1	2.50	0.44
23:B:839:BCR:HC8	23:B:839:BCR:H311	1.98	0.44
23:F:305:BCR:H381	19:J:103:CLA:HBC3	1.98	0.44
19:A2:842:CLA:H93	21:A2:843:PQN:H293	2.00	0.44
2:B2:587:LEU:HD23	2:B2:717:LEU:CD2	2.38	0.44
4:D2:5:LEU:HD11	4:D2:86:ILE:HD11	1.99	0.44
1:AA:577:GLY:O	1:AA:583:THR:OG1	2.35	0.44
19:A1:827:CLA:HAB	23:A1:850:BCR:H311	1.98	0.44
19:A1:852:CLA:H41	19:A1:852:CLA:H71	2.00	0.44
1:A2:397:ILE:HD13	19:A2:830:CLA:HBC3	1.99	0.44
19:B:806:CLA:H203	23:L:205:BCR:C31	2.47	0.44
19:B:822:CLA:H143	19:B:832:CLA:HBB2	2.00	0.44
2:BB:715:VAL:O	2:BB:719:HIS:ND1	2.50	0.44
23:BB:838:BCR:HC8	23:BB:838:BCR:H311	1.98	0.44
15:K2:48:LEU:HD23	15:K2:54:PHE:CD2	2.53	0.44
2:B:289:HIS:CE1	23:B:839:BCR:H363	2.53	0.44
1:A1:16:ILE:HG21	1:A1:187:LYS:HD3	2.00	0.44
1:A1:432:ARG:NH1	4:D1:13:ALA:HB3	2.33	0.44
2:B1:69:ALA:CB	11:M1:4:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:675:ARG:O	2:B1:678:TRP:N	2.46	0.44
19:B1:850:CLA:C14	19:F1:301:CLA:HED2	2.48	0.44
6:F1:76:VAL:O	6:F1:76:VAL:HG22	2.17	0.44
1:A2:101:TYR:CZ	1:A2:105:LEU:HD21	2.53	0.44
2:BB:157:LEU:O	2:BB:162:ARG:NE	2.45	0.44
19:A1:804:CLA:CGA	19:A1:841:CLA:H43	2.48	0.43
1:A2:118:VAL:O	1:A2:128:ASN:ND2	2.50	0.43
1:A:506:VAL:HG23	19:A:837:CLA:HED3	2.00	0.43
1:A:590:ASP:OD1	1:A:725:ARG:NH1	2.51	0.43
2:B:59:LEU:HD23	2:B:143:LEU:HD23	2.00	0.43
2:B1:481:LEU:HD21	12:X1:38:TYR:CD1	2.53	0.43
1:A:584:CYS:O	2:B:676:GLY:N	2.51	0.43
23:F:305:BCR:H382	23:F:305:BCR:H371	2.00	0.43
9:K1:24:MET:HE1	9:K1:74:VAL:HG23	1.99	0.43
1:A:447:PHE:O	1:A:451:HIS:ND1	2.45	0.43
2:BB:258:LEU:HD23	2:BB:269:TRP:CE2	2.53	0.43
2:BB:516:PHE:CE1	19:BB:823:CLA:HBC2	2.54	0.43
23:FF:303:BCR:H333	19:FF:305:CLA:H142	2.00	0.43
2:B1:531:ALA:HB2	19:B1:833:CLA:CBB	2.48	0.43
2:B:297:ILE:HG22	19:B:818:CLA:HMD1	1.99	0.43
2:B:653:TRP:O	2:B:657:PHE:N	2.46	0.43
11:M:14:VAL:CG2	23:M:101:BCR:H391	2.48	0.43
2:BB:31:PHE:CD2	19:BB:802:CLA:HMC2	2.53	0.43
19:B1:820:CLA:HBC2	19:B1:820:CLA:HHD	2.01	0.43
19:B1:832:CLA:CGD	19:B1:833:CLA:HMB1	2.48	0.43
1:A2:436:ALA:O	1:A2:440:HIS:ND1	2.52	0.43
23:J2:104:BCR:H23C	23:J2:104:BCR:H392	2.01	0.43
24:L2:203:AJP:O33	24:L2:203:AJP:O34	2.36	0.43
1:A1:282:LEU:HD23	1:A1:289:LEU:HD23	2.00	0.43
2:B:531:ALA:HB2	19:B:834:CLA:CBB	2.49	0.43
19:AA:842:CLA:H41	19:AA:842:CLA:H71	2.01	0.43
2:BB:531:ALA:HB2	19:BB:833:CLA:CBB	2.48	0.43
24:L1:204:AJP:O33	24:L1:204:AJP:O34	2.36	0.43
1:A2:91:MET:HE1	19:A2:810:CLA:H2A	2.01	0.43
2:B2:30:ASP:O	2:B2:34:HIS:ND1	2.52	0.43
2:B2:257:PHE:CD2	2:B2:499:VAL:HG23	2.53	0.43
2:B2:731:PHE:O	2:B2:735:SER:OG	2.29	0.43
19:B2:834:CLA:H43	19:X2:101:CLA:C4D	2.49	0.43
1:A:39:LEU:HD11	1:A:55:LEU:HD12	2.01	0.43
1:A:313:ARG:O	19:A:822:CLA:HED2	2.18	0.43
2:B:43:TYR:CZ	2:B:334:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:477:ILE:O	1:AA:477:ILE:HG22	2.19	0.43
2:BB:123:TRP:CH2	19:BB:810:CLA:H191	2.54	0.43
1:A1:196:SER:O	1:A1:200:HIS:ND1	2.45	0.43
19:A1:805:CLA:HBC2	19:A1:831:CLA:H43	2.00	0.43
19:A1:841:CLA:H93	21:A1:843:PQN:H293	2.00	0.43
2:B1:273:MET:SD	19:B1:815:CLA:HED1	2.59	0.43
23:B1:838:BCR:HC8	23:B1:838:BCR:H311	2.01	0.43
3:C1:24:ASP:OD2	4:D1:96:HIS:ND1	2.51	0.43
4:D1:101:VAL:HG11	4:D1:107:ASN:HB2	2.00	0.43
19:A2:805:CLA:CGA	19:A2:842:CLA:H43	2.49	0.43
19:A2:840:CLA:CBB	19:A2:841:CLA:HBC3	2.49	0.43
19:B2:809:CLA:CMC	23:B2:840:BCR:H343	2.49	0.43
1:A1:114:SER:OG	1:A1:131:VAL:HG21	2.19	0.43
19:A1:815:CLA:HHB	23:A1:847:BCR:H331	2.00	0.43
19:A1:839:CLA:CBB	19:A1:840:CLA:HBC3	2.49	0.43
2:B:105:THR:HG22	2:B:111:GLY:C	2.44	0.43
19:B:820:CLA:O1A	23:B:842:BCR:H352	2.19	0.43
1:AA:245:LEU:CD2	19:AA:818:CLA:HBC1	2.48	0.43
2:B1:118:SER:O	2:B1:375:LEU:HD21	2.19	0.42
2:B1:257:PHE:CD2	2:B1:499:VAL:HG23	2.53	0.42
2:B1:428:TRP:HZ3	19:B1:834:CLA:HBC2	1.84	0.42
19:B1:809:CLA:CMC	23:B1:839:BCR:H343	2.49	0.42
1:A2:13:ALA:HB3	1:A2:315:ASN:OD1	2.18	0.42
16:L2:147:LEU:HD21	19:LL:201:CLA:O1A	2.18	0.42
1:A:424:ASN:OD1	1:A:429:ARG:NH1	2.52	0.42
19:A:833:CLA:HMA1	19:A:834:CLA:O1D	2.18	0.42
1:A1:521:VAL:HG11	1:A1:618:VAL:O	2.19	0.42
2:B1:703:LYS:NZ	4:D1:26:GLU:OE1	2.48	0.42
19:B1:827:CLA:HED3	12:X1:11:ASN:CB	2.49	0.42
1:A2:336:GLU:N	1:A2:336:GLU:OE1	2.52	0.42
2:B2:643:ASN:OD1	2:B2:646:GLY:N	2.48	0.42
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.54	0.42
2:B:478:LEU:HB3	2:B:480:THR:HG23	2.01	0.42
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.92	0.42
2:BB:415:VAL:HG11	23:BB:841:BCR:H401	2.01	0.42
23:FF:306:BCR:H382	23:FF:306:BCR:H371	2.01	0.42
2:B2:466:PHE:CD1	2:B2:480:THR:HG21	2.54	0.42
19:A:820:CLA:H92	19:A:837:CLA:O1A	2.19	0.42
19:BB:829:CLA:HBC2	19:BB:829:CLA:HMC3	2.01	0.42
2:B1:125:TYR:O	2:B1:130:ARG:NH1	2.52	0.42
19:A2:815:CLA:HBA2	19:A2:815:CLA:H3A	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:835:CLA:H93	19:B2:837:CLA:H142	2.02	0.42
18:L:73:PHE:CZ	19:L:203:CLA:HMB1	2.54	0.42
20:AA:803:CL0:H22	2:BB:632:TRP:HD1	1.84	0.42
1:A2:553:GLY:O	1:A2:557:ALA:HB2	2.19	0.42
19:A2:805:CLA:H41	19:A2:805:CLA:H71	2.01	0.42
19:B2:806:CLA:H41	19:B2:806:CLA:H72	2.01	0.42
23:B2:839:BCR:HC8	23:B2:839:BCR:H311	2.01	0.42
19:B:834:CLA:C9	19:B:835:CLA:HBC1	2.40	0.42
2:BB:223:GLN:NE2	2:BB:227:THR:OG1	2.53	0.42
9:KK:76:LEU:O	9:KK:80:LEU:HD23	2.20	0.42
1:A1:370:HIS:ND1	19:A1:819:CLA:OBD	2.53	0.42
1:A2:395:ILE:HG22	1:A2:603:LEU:HD12	2.01	0.42
2:B2:459:ILE:HG22	13:F2:74:LEU:HB2	2.00	0.42
2:B:46:ILE:O	2:B:49:THR:OG1	2.35	0.42
2:B:343:ALA:HB2	23:B:843:BCR:H372	2.01	0.42
11:M:3:SER:OG	11:M:4:ILE:N	2.53	0.42
1:AA:334:THR:HG21	22:AA:847:LHG:HC12	2.01	0.42
1:AA:532:ASP:O	1:AA:536:HIS:ND1	2.46	0.42
2:BB:594:VAL:HG22	2:BB:598:THR:HG23	2.01	0.42
23:BB:841:BCR:C8	23:BB:841:BCR:H331	2.50	0.42
2:B1:105:THR:HG23	2:B1:105:THR:O	2.19	0.42
1:A2:21:PRO:HG3	1:A2:185:ALA:HB2	2.01	0.42
1:A2:343:GLU:OE2	1:A2:343:GLU:N	2.53	0.42
20:A2:803:CL0:H48	19:B2:850:CLA:HMA3	2.01	0.42
3:C:15:THR:HG22	3:C:28:MET:HE3	2.02	0.42
2:BB:491:THR:O	2:BB:491:THR:HG23	2.20	0.42
23:J1:104:BCR:H392	23:J1:104:BCR:H23C	2.02	0.42
1:A2:196:SER:O	1:A2:200:HIS:ND1	2.43	0.42
1:A2:364:THR:HG22	1:A2:394:HIS:HB3	2.00	0.42
1:A2:448:LEU:O	1:A2:452:SER:N	2.53	0.42
23:B2:842:BCR:H24C	23:B2:842:BCR:H371	1.90	0.42
1:A:278:PHE:CD2	19:A:820:CLA:HMB3	2.55	0.42
1:A:357:LEU:HD21	19:A:832:CLA:CBB	2.50	0.42
23:FF:306:BCR:H381	19:JJ:103:CLA:HBC3	2.02	0.42
2:B1:593:THR:O	2:B1:597:VAL:HG23	2.19	0.42
1:A2:426:VAL:O	1:A2:430:VAL:HG23	2.20	0.42
2:B2:182:LEU:HD21	19:B2:810:CLA:C2	2.50	0.42
2:B:514:SER:O	2:B:514:SER:OG	2.34	0.42
2:B:707:LEU:N	21:B:838:PQN:O4	2.48	0.42
19:L:202:CLA:H91	19:L:202:CLA:H143	2.01	0.42
2:BB:174:ARG:HB2	19:BB:810:CLA:HBC2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:JJ:23:THR:HG21	23:JJ:104:BCR:H403	2.02	0.42
9:KK:68:PHE:CE2	9:KK:72:LEU:HD11	2.55	0.42
18:LL:101:LEU:HD21	18:LL:105:PHE:CZ	2.55	0.42
1:A1:600:TYR:CE2	20:A1:802:CL0:H36	2.54	0.42
2:B1:268:LEU:HB2	2:B1:273:MET:HE3	2.02	0.42
2:B1:440:LEU:HD11	23:F1:306:BCR:H311	2.01	0.42
6:F1:34:ASN:ND2	6:F1:67:GLY:O	2.50	0.42
20:A2:803:CL0:H16	2:B2:631:LEU:HD22	2.02	0.42
19:A2:804:CLA:H193	19:A2:852:CLA:H192	2.00	0.42
19:B2:810:CLA:HMA2	23:B2:840:BCR:H362	2.02	0.42
19:B2:834:CLA:HBB2	19:B2:835:CLA:O2D	2.20	0.42
1:A:698:ILE:O	1:A:702:VAL:HG23	2.20	0.42
2:B:534:LEU:HD12	19:B:835:CLA:CED	2.50	0.42
3:C:12:ILE:HD11	3:C:59:PRO:HG2	2.02	0.42
2:BB:71:GLN:NE2	19:BB:804:CLA:O1D	2.49	0.42
19:BB:812:CLA:HMA2	26:BB:840:ECH:H34B	2.01	0.42
18:LL:126:VAL:O	18:LL:126:VAL:HG13	2.20	0.42
19:A:805:CLA:H41	19:A:805:CLA:H71	2.02	0.41
23:F:305:BCR:H15C	23:F:305:BCR:H351	1.78	0.41
23:J:104:BCR:H392	23:J:104:BCR:H23C	2.02	0.41
23:LL:204:BCR:H15C	23:LL:204:BCR:H351	1.95	0.41
1:A1:707:LYS:HA	6:F1:159:ILE:HD11	2.01	0.41
10:L1:11:LEU:O	10:L1:17:ASN:ND2	2.53	0.41
1:A2:558:ARG:NH2	4:D2:42:GLU:OE2	2.52	0.41
2:B2:592:ASN:OD1	19:B2:849:CLA:H42	2.20	0.41
19:A:805:CLA:CGA	19:A:842:CLA:H43	2.49	0.41
19:A:815:CLA:HBA2	19:A:815:CLA:H3A	1.90	0.41
1:AA:81:LEU:O	1:AA:85:THR:HG23	2.19	0.41
1:AA:112:ARG:HB2	1:AA:131:VAL:HG22	2.02	0.41
2:BB:724:TYR:CD1	19:BB:852:CLA:HED1	2.56	0.41
4:D1:35:SER:OG	4:D1:37:LYS:O	2.37	0.41
1:A:558:ARG:NH2	4:D:42:GLU:OE2	2.46	0.41
2:B:536:THR:HG21	2:B:589:TRP:CZ2	2.55	0.41
2:B:630:TYR:O	2:B:634:ASN:ND2	2.53	0.41
19:B:833:CLA:C3D	19:B:833:CLA:HED3	2.51	0.41
1:AA:575:CYS:SG	1:AA:577:GLY:N	2.87	0.41
2:BB:45:LYS:NZ	19:BB:801:CLA:HED1	2.36	0.41
2:BB:293:THR:O	2:BB:295:PHE:N	2.53	0.41
19:FF:301:CLA:H42	8:JJ:22:ALA:HA	2.02	0.41
1:A1:199:ASN:OD1	1:A1:314:THR:HG21	2.20	0.41
2:B1:31:PHE:CD2	19:B1:802:CLA:HMC2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:491:THR:O	2:B1:491:THR:HG23	2.21	0.41
19:B2:826:CLA:H41	19:B2:826:CLA:H72	2.02	0.41
14:I2:33:PHE:CE1	23:I2:103:BCR:H342	2.56	0.41
16:L2:62:ARG:NH1	16:L2:131:ASP:OD1	2.53	0.41
10:L1:152:GLY:O	10:L1:156:VAL:HG23	2.20	0.41
2:B2:653:TRP:O	2:B2:657:PHE:N	2.50	0.41
1:A:81:LEU:O	1:A:85:THR:HG23	2.21	0.41
1:A:121:ILE:HG23	1:A:122:VAL:N	2.35	0.41
1:A:399:GLY:C	1:A:599:MET:HE2	2.46	0.41
2:B:422:ILE:HG23	19:B:835:CLA:HBB2	2.01	0.41
7:I:30:ILE:O	7:I:34:SER:OG	2.25	0.41
1:AA:115:ALA:HB3	1:AA:140:ILE:CD1	2.51	0.41
6:FF:46:ASN:OD1	6:FF:46:ASN:N	2.53	0.41
1:A1:413:MET:CE	1:A1:431:ILE:HD11	2.51	0.41
19:A1:824:CLA:HMC1	19:A1:828:CLA:H202	2.03	0.41
2:B2:196:HIS:O	2:B2:207:VAL:HG11	2.21	0.41
19:B:818:CLA:HBB1	19:B:818:CLA:HHC	2.02	0.41
3:C:11:CYS:SG	3:C:12:ILE:N	2.92	0.41
1:AA:320:HIS:HB3	1:AA:325:ILE:HD11	2.02	0.41
19:AA:820:CLA:HMD1	19:AA:821:CLA:H202	2.03	0.41
2:BB:536:THR:HG21	2:BB:589:TRP:CZ2	2.56	0.41
19:A1:833:CLA:HED1	10:L1:32:ASN:OD1	2.21	0.41
10:L1:61:ARG:NH2	19:L1:205:CLA:HED1	2.35	0.41
1:A2:494:ALA:HB3	1:A2:495:PRO:HD3	2.02	0.41
2:B2:53:HIS:CE1	19:B2:802:CLA:HMA2	2.56	0.41
1:A:36:ASP:OD1	1:A:37:ARG:N	2.54	0.41
2:BB:255:LEU:HD21	2:BB:278:LEU:HD23	2.03	0.41
2:BB:652:VAL:HG11	19:BB:805:CLA:CBC	2.51	0.41
2:B2:31:PHE:CD2	19:B2:802:CLA:HMC2	2.56	0.41
18:L:131:ASP:OD1	18:L:131:ASP:N	2.54	0.41
1:AA:91:MET:HE2	19:AA:830:CLA:HED2	2.03	0.41
2:BB:724:TYR:CE1	19:BB:852:CLA:HED1	2.55	0.41
1:A1:397:ILE:HD13	19:A1:829:CLA:HBC3	2.03	0.41
1:A1:685:MET:O	1:A1:689:SER:OG	2.32	0.41
2:B1:15:ASP:O	2:B1:20:ARG:NH1	2.53	0.41
2:B1:429:VAL:HG11	2:B1:535:HIS:CD2	2.56	0.41
2:B2:536:THR:HG21	2:B2:589:TRP:CZ2	2.56	0.41
3:C2:42:SER:O	4:D2:114:ARG:NH1	2.54	0.41
23:F2:305:BCR:H381	19:J2:103:CLA:HBC3	2.03	0.41
1:A:126:ILE:HG21	2:B:450:PHE:HA	2.03	0.41
1:A:199:ASN:HD21	1:A:312:TYR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:834:CLA:HBC2	19:A:841:CLA:HMC2	2.02	0.41
2:B:12:LEU:HD11	2:B:27:MET:HE3	2.03	0.41
2:B:136:TYR:OH	11:M:8:GLN:O	2.38	0.41
19:B:834:CLA:HBC3	19:B:834:CLA:HMC1	2.03	0.41
23:B:842:BCR:C8	23:B:842:BCR:H331	2.50	0.41
1:AA:584:CYS:O	2:BB:676:GLY:N	2.53	0.41
2:BB:272:ASP:O	2:BB:276:HIS:N	2.53	0.41
19:A1:834:CLA:HMA1	23:I1:101:BCR:H282	2.02	0.41
2:B2:427:SER:OG	19:B2:851:CLA:OBD	2.31	0.41
2:B2:602:HIS:CD2	2:B2:732:LEU:HD12	2.56	0.41
19:B2:827:CLA:HED3	12:X2:11:ASN:CB	2.51	0.41
23:A:854:BCR:H362	9:K:71:ILE:HD11	2.03	0.41
2:B:444:ASN:OD1	2:B:457:ILE:N	2.47	0.41
2:BB:91:ILE:HD11	2:BB:114:ASN:OD1	2.21	0.41
2:BB:587:LEU:HD12	2:BB:717:LEU:HD21	2.03	0.41
19:BB:806:CLA:H41	19:BB:806:CLA:H72	2.01	0.41
3:CC:13:GLY:O	3:CC:38:GLN:NE2	2.54	0.41
19:A1:814:CLA:HBA2	19:A1:814:CLA:H3A	1.89	0.40
2:B1:584:TYR:OH	2:B1:671:LEU:HD22	2.21	0.40
10:L1:57:LEU:HD13	10:L1:61:ARG:HD3	2.03	0.40
1:A2:234:VAL:HA	1:A2:237:ILE:HD12	2.03	0.40
2:B:319:PHE:CD2	19:B:820:CLA:HMA1	2.56	0.40
1:AA:194:VAL:HG13	19:AA:827:CLA:HMD3	2.02	0.40
2:BB:58:PHE:CD1	2:BB:142:LEU:HD22	2.54	0.40
2:BB:270:LEU:HD23	2:BB:273:MET:SD	2.61	0.40
2:BB:699:ARG:NH2	4:DD:25:GLU:OE2	2.54	0.40
19:A1:819:CLA:H92	19:A1:836:CLA:O1A	2.21	0.40
10:L1:72:TYR:OH	19:L1:207:CLA:OBD	2.29	0.40
1:A2:53:HIS:HD2	19:A2:806:CLA:HBC1	1.86	0.40
1:A2:343:GLU:O	1:A2:347:THR:OG1	2.12	0.40
19:A:840:CLA:CBB	19:A:841:CLA:HBC3	2.51	0.40
2:B:534:LEU:HD12	19:B:835:CLA:HED3	2.03	0.40
2:BB:319:PHE:HD2	19:BB:820:CLA:HMA1	1.86	0.40
6:FF:114:ASP:OD1	6:FF:120:LYS:NZ	2.34	0.40
10:L1:61:ARG:NH2	10:L1:65:GLU:OE1	2.54	0.40
1:A2:444:VAL:HG12	1:A2:448:LEU:HD12	2.04	0.40
1:A2:498:THR:OG1	19:A2:837:CLA:OBD	2.39	0.40
2:B:394:GLY:HA2	23:B:843:BCR:H393	2.03	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CG	2.57	0.40
19:B:854:CLA:H62	19:B:854:CLA:H41	1.96	0.40
28:B:856:DGD:HO2D	28:B:856:DGD:C1A	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:194:LEU:HA	2:BB:198:ALA:HB3	2.03	0.40
3:CC:17:CYS:SG	3:CC:18:VAL:N	2.95	0.40
19:FF:301:CLA:H43	19:FF:302:CLA:CBC	2.52	0.40
19:B1:833:CLA:HBC3	19:B1:833:CLA:HMC1	2.02	0.40
3:C1:35:LYS:HA	5:E1:32:ILE:HG22	2.02	0.40
1:A2:348:SER:OG	1:A2:416:ASP:OD2	2.34	0.40
19:B2:852:CLA:HHD	19:B2:852:CLA:HBC2	2.02	0.40
1:A:599:MET:HE1	19:A:828:CLA:HAC2	2.03	0.40
1:A:662:TYR:OH	2:B:445:ASP:OD2	2.39	0.40
2:B:399:VAL:CG2	2:B:548:ALA:HB1	2.51	0.40
19:BB:822:CLA:H143	19:BB:831:CLA:HBB2	2.04	0.40
1:A1:388:LEU:HD23	1:A1:610:PHE:CD1	2.57	0.40
2:B1:422:ILE:HG23	19:B1:834:CLA:CBB	2.52	0.40
2:B1:534:LEU:HD12	19:B1:834:CLA:CED	2.42	0.40
2:B:467:ILE:CD1	19:B:831:CLA:HMC2	2.52	0.40
19:AA:828:CLA:HAB	23:AA:851:BCR:H311	2.03	0.40
2:BB:409:GLY:N	2:BB:413:GLU:OE1	2.50	0.40
19:BB:832:CLA:HED3	19:BB:832:CLA:C3D	2.52	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	738/740 (100%)	713 (97%)	24 (3%)	1 (0%)	48 79
1	A1	738/740 (100%)	710 (96%)	27 (4%)	1 (0%)	48 79
1	A2	738/740 (100%)	714 (97%)	23 (3%)	1 (0%)	48 79
1	AA	738/740 (100%)	709 (96%)	28 (4%)	1 (0%)	48 79
2	B	737/739 (100%)	712 (97%)	25 (3%)	0	100 100
2	B1	737/739 (100%)	715 (97%)	22 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	737/739 (100%)	713 (97%)	24 (3%)	0	100	100
2	BB	737/739 (100%)	710 (96%)	27 (4%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	C1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	CC	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
4	D1	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
4	D2	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
4	DD	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
5	E1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
5	E2	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
6	F	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
6	F1	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	FF	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
7	I	29/31 (94%)	29 (100%)	0	0	100	100
7	I1	29/31 (94%)	29 (100%)	0	0	100	100
7	II	29/31 (94%)	29 (100%)	0	0	100	100
8	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
8	J1	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
8	J2	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
8	JJ	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
9	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
9	K1	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	KK	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
10	L1	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	MM	29/31 (94%)	29 (100%)	0	0	100	100
12	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	X1	37/39 (95%)	35 (95%)	2 (5%)	0	100 100
12	X2	37/39 (95%)	35 (95%)	2 (5%)	0	100 100
12	XX	37/39 (95%)	35 (95%)	2 (5%)	0	100 100
13	F2	135/137 (98%)	125 (93%)	7 (5%)	3 (2%)	5 29
14	I2	31/33 (94%)	31 (100%)	0	0	100 100
15	K2	71/73 (97%)	70 (99%)	1 (1%)	0	100 100
16	L2	165/167 (99%)	160 (97%)	5 (3%)	0	100 100
17	E	61/63 (97%)	61 (100%)	0	0	100 100
17	EE	61/63 (97%)	60 (98%)	1 (2%)	0	100 100
18	L	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	18 52
18	LL	152/154 (99%)	148 (97%)	4 (3%)	0	100 100
All	All	8958/9106 (98%)	8634 (96%)	316 (4%)	8 (0%)	49 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	122	VAL
13	F2	159	ILE
1	A1	122	VAL
1	A	122	VAL
1	AA	477	ILE
13	F2	158	GLU
13	F2	160	THR
18	L	118	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	594/594 (100%)	594 (100%)	0	100 100
1	A1	594/594 (100%)	594 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A2	594/594 (100%)	594 (100%)	0	100	100
1	AA	594/594 (100%)	594 (100%)	0	100	100
2	B	601/601 (100%)	601 (100%)	0	100	100
2	B1	601/601 (100%)	601 (100%)	0	100	100
2	B2	601/601 (100%)	601 (100%)	0	100	100
2	BB	601/601 (100%)	601 (100%)	0	100	100
3	C	68/68 (100%)	68 (100%)	0	100	100
3	C1	68/68 (100%)	68 (100%)	0	100	100
3	C2	68/68 (100%)	68 (100%)	0	100	100
3	CC	68/68 (100%)	68 (100%)	0	100	100
4	D	107/107 (100%)	107 (100%)	0	100	100
4	D1	107/107 (100%)	107 (100%)	0	100	100
4	D2	107/107 (100%)	107 (100%)	0	100	100
4	DD	107/107 (100%)	107 (100%)	0	100	100
5	E1	53/53 (100%)	53 (100%)	0	100	100
5	E2	53/53 (100%)	53 (100%)	0	100	100
6	F	108/108 (100%)	108 (100%)	0	100	100
6	F1	108/108 (100%)	108 (100%)	0	100	100
6	FF	108/108 (100%)	108 (100%)	0	100	100
7	I	28/28 (100%)	28 (100%)	0	100	100
7	I1	28/28 (100%)	28 (100%)	0	100	100
7	II	28/28 (100%)	28 (100%)	0	100	100
8	J	38/41 (93%)	38 (100%)	0	100	100
8	J1	38/41 (93%)	38 (100%)	0	100	100
8	J2	38/41 (93%)	38 (100%)	0	100	100
8	JJ	38/41 (93%)	38 (100%)	0	100	100
9	K	46/54 (85%)	46 (100%)	0	100	100
9	K1	54/54 (100%)	54 (100%)	0	100	100
9	KK	46/54 (85%)	46 (100%)	0	100	100
10	L1	127/127 (100%)	127 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	MM	26/26 (100%)	26 (100%)	0	100	100
12	X	31/31 (100%)	31 (100%)	0	100	100
12	X1	31/31 (100%)	31 (100%)	0	100	100
12	X2	31/31 (100%)	31 (100%)	0	100	100
12	XX	31/31 (100%)	31 (100%)	0	100	100
13	F2	106/106 (100%)	106 (100%)	0	100	100
14	I2	30/30 (100%)	30 (100%)	0	100	100
15	K2	54/54 (100%)	54 (100%)	0	100	100
16	L2	128/128 (100%)	128 (100%)	0	100	100
17	E	55/55 (100%)	55 (100%)	0	100	100
17	EE	55/55 (100%)	55 (100%)	0	100	100
18	L	117/117 (100%)	117 (100%)	0	100	100
18	LL	117/117 (100%)	117 (100%)	0	100	100
All	All	7309/7337 (100%)	7309 (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	A1	158	GLN
1	A1	180	HIS
1	A1	539	HIS
1	A1	715	GLN
2	B1	29	ASN
2	B1	205	GLN
2	B1	206	HIS
2	B1	275	HIS
2	B1	323	HIS
3	C1	38	GLN
5	E1	51	ASN
10	L1	114	ASN
1	A2	356	ASN
1	A2	715	GLN

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Mol	Chain	Res	Type
2	B2	114	ASN
2	B2	323	HIS
2	B2	711	GLN
5	E2	19	GLN
16	L2	3	GLN
16	L2	114	ASN
1	A	356	ASN
1	A	394	HIS
1	A	501	ASN
2	B	41	ASN
2	B	289	HIS
2	B	306	ASN
2	B	406	GLN
6	F	43	ASN
1	AA	182	HIS
1	AA	344	ASN
1	AA	422	ASN
1	AA	501	ASN
1	AA	654	GLN
2	BB	176	ASN
2	BB	196	HIS
2	BB	223	GLN
2	BB	236	ASN
2	BB	294	ASN
3	CC	38	GLN
17	EE	51	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

594 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	$\#\|Z\| > 2$
19	CLA	AA	841	-	50,54,73	1.33	7 (14%)	59,90,113	1.40	5 (8%)
19	CLA	A2	840	-	60,64,73	1.23	9 (15%)	71,102,113	1.30	4 (5%)
19	CLA	X2	101	-	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
23	BCR	K1	106	-	41,41,41	1.17	3 (7%)	56,56,56	1.37	9 (16%)
19	CLA	B1	821	2	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
19	CLA	A1	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	6 (7%)
19	CLA	A1	842	-	69,73,73	1.17	9 (13%)	82,113,113	1.48	8 (9%)
20	CL0	A	803	-	58,73,73	3.23	17 (29%)	60,113,113	2.72	20 (33%)
19	CLA	F1	302	-	46,50,73	1.41	8 (17%)	53,85,113	1.50	5 (9%)
24	AJP	AA	802	-	35,35,95	4.63	22 (62%)	54,58,149	4.56	29 (53%)
19	CLA	BB	824	-	59,63,73	1.25	9 (15%)	70,101,113	1.27	5 (7%)
27	SF4	C	101	-	0,12,12	-	-	-		
24	AJP	B	850	-	49,49,95	4.05	25 (51%)	75,80,149	4.50	46 (61%)
23	BCR	M1	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	9 (16%)
22	LHG	X2	102	-	39,39,48	0.82	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	B1	813	-	46,50,73	1.40	8 (17%)	53,85,113	1.39	5 (9%)
19	CLA	A1	836	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
23	BCR	F	305	-	41,41,41	1.17	3 (7%)	56,56,56	1.49	11 (19%)
19	CLA	A	833	-	54,58,73	1.31	9 (16%)	64,95,113	1.34	5 (7%)
19	CLA	KK	102	-	50,54,73	1.35	7 (14%)	59,90,113	1.38	4 (6%)
19	CLA	B	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	4 (4%)
19	CLA	LL	201	18	65,69,73	1.20	8 (12%)	77,108,113	1.53	8 (10%)
19	CLA	B	812	-	45,49,73	1.39	8 (17%)	54,84,113	1.53	6 (11%)
25	LMG	BB	844	-	55,55,55	0.69	0	63,63,63	1.27	4 (6%)
22	LHG	X1	102	-	39,39,48	0.83	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	AA	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	A2	853	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	7 (12%)
19	CLA	JJ	103	-	45,49,73	1.41	8 (17%)	54,84,113	1.41	5 (9%)
23	BCR	A1	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	6 (10%)
19	CLA	K	101	-	49,53,73	1.38	8 (16%)	58,89,113	1.50	7 (12%)
19	CLA	B	824	-	59,63,73	1.25	9 (15%)	70,101,113	1.25	5 (7%)
19	CLA	B1	817	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
19	CLA	AA	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
23	BCR	II	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.25	8 (14%)
19	CLA	B	859	-	64,68,73	1.20	8 (12%)	76,107,113	1.60	13 (17%)
19	CLA	BB	823	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	4 (4%)
19	CLA	A2	819	-	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
23	BCR	AA	852	-	41,41,41	1.11	1 (2%)	56,56,56	1.46	9 (16%)
23	BCR	F2	304	-	41,41,41	1.23	4 (9%)	56,56,56	1.28	8 (14%)
19	CLA	B1	830	-	60,64,73	1.25	8 (13%)	71,102,113	1.28	4 (5%)
23	BCR	AA	855	-	41,41,41	1.17	3 (7%)	56,56,56	1.30	8 (14%)
19	CLA	B	858	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
23	BCR	A1	851	-	41,41,41	1.08	1 (2%)	56,56,56	1.49	9 (16%)
19	CLA	A	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.41	7 (10%)
21	PQN	A2	843	-	34,34,34	0.65	0	43,45,45	1.10	4 (9%)
19	CLA	K1	102	-	49,53,73	1.37	9 (18%)	58,89,113	1.50	7 (12%)
19	CLA	BB	809	-	49,53,73	1.38	8 (16%)	58,89,113	1.45	5 (8%)
23	BCR	K	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	7 (12%)
19	CLA	B1	806	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
19	CLA	JJ	101	8	45,49,73	1.42	8 (17%)	54,84,113	1.43	4 (7%)
19	CLA	A	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
22	LHG	B2	848	-	32,32,48	0.91	2 (6%)	35,38,54	1.00	2 (5%)
23	BCR	J2	104	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	B	814	-	63,67,73	1.23	9 (14%)	74,105,113	1.36	7 (9%)
19	CLA	A	817	-	47,52,73	1.39	7 (14%)	55,87,113	1.41	4 (7%)
23	BCR	K2	105	-	41,41,41	1.16	3 (7%)	56,56,56	1.34	8 (14%)
19	CLA	X	101	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
23	BCR	AA	848	-	40,40,41	1.12	2 (5%)	54,54,56	1.30	10 (18%)
23	BCR	F2	303	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	8 (14%)
19	CLA	A1	839	-	60,64,73	1.23	9 (15%)	71,102,113	1.28	4 (5%)
19	CLA	B	809	-	49,53,73	1.37	8 (16%)	58,89,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	J	103	-	45,49,73	1.41	6 (13%)	54,84,113	1.39	5 (9%)
19	CLA	B2	821	-	69,73,73	1.15	7 (10%)	82,113,113	1.31	9 (10%)
19	CLA	A	838	-	47,52,73	1.37	9 (19%)	55,87,113	1.45	5 (9%)
19	CLA	J1	101	-	45,49,73	1.42	8 (17%)	54,84,113	1.41	5 (9%)
22	LHG	BB	850	-	32,32,48	0.90	1 (3%)	35,38,54	1.04	3 (8%)
19	CLA	B1	815	-	69,73,73	1.17	8 (11%)	82,113,113	1.38	10 (12%)
19	CLA	B2	833	-	69,73,73	1.18	5 (7%)	82,113,113	1.45	10 (12%)
19	CLA	B2	807	-	69,73,73	1.19	8 (11%)	82,113,113	1.46	10 (12%)
19	CLA	A1	820	-	69,73,73	1.13	8 (11%)	82,113,113	1.34	8 (9%)
19	CLA	BB	804	-	66,70,73	1.19	9 (13%)	78,109,113	1.30	7 (8%)
23	BCR	A	851	-	41,41,41	1.08	1 (2%)	56,56,56	1.48	8 (14%)
19	CLA	BB	834	-	49,53,73	1.37	9 (18%)	58,89,113	1.39	4 (6%)
19	CLA	A2	824	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	5 (8%)
19	CLA	B2	834	-	69,73,73	1.20	7 (10%)	82,113,113	1.53	16 (19%)
19	CLA	A1	811	-	50,54,73	1.34	8 (16%)	59,90,113	1.41	5 (8%)
23	BCR	J2	102	-	41,41,41	1.22	2 (4%)	56,56,56	1.37	9 (16%)
24	AJP	L	208	-	36,36,95	4.64	25 (69%)	56,60,149	4.95	36 (64%)
19	CLA	J2	103	-	45,49,73	1.42	6 (13%)	54,84,113	1.40	6 (11%)
19	CLA	A	828	-	60,64,73	1.23	8 (13%)	71,102,113	1.32	6 (8%)
19	CLA	A	837	-	49,53,73	1.39	9 (18%)	58,89,113	1.39	4 (6%)
19	CLA	AA	811	1	55,59,73	1.31	9 (16%)	64,96,113	1.47	7 (10%)
19	CLA	BB	816	-	61,65,73	1.25	8 (13%)	72,103,113	1.32	5 (6%)
19	CLA	A1	852	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
19	CLA	B2	804	-	66,70,73	1.20	9 (13%)	78,109,113	1.32	6 (7%)
19	CLA	B2	813	-	46,50,73	1.40	8 (17%)	53,85,113	1.37	5 (9%)
19	CLA	A1	810	-	55,59,73	1.30	9 (16%)	64,96,113	1.45	6 (9%)
19	CLA	F2	302	-	46,50,73	1.42	8 (17%)	53,85,113	1.51	5 (9%)
19	CLA	A2	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
23	BCR	M2	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	9 (16%)
19	CLA	F2	301	-	64,68,73	1.22	8 (12%)	76,107,113	1.36	9 (11%)
19	CLA	AA	814	-	46,50,73	1.40	8 (17%)	53,85,113	1.39	4 (7%)
19	CLA	BB	830	-	60,64,73	1.24	8 (13%)	71,102,113	1.27	5 (7%)
19	CLA	B2	824	-	59,63,73	1.24	9 (15%)	70,101,113	1.29	6 (8%)
19	CLA	K2	104	-	45,49,73	1.43	8 (17%)	54,83,113	1.45	4 (7%)
22	LHG	L1	211	-	32,32,48	0.97	3 (9%)	35,38,54	1.04	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	AJP	BB	848	-	49,49,95	4.03	25 (51%)	75,80,149	4.47	45 (60%)
19	CLA	B	833	-	69,73,73	1.19	7 (10%)	82,113,113	1.38	9 (10%)
20	CL0	AA	803	-	58,73,73	3.22	18 (31%)	60,113,113	2.95	21 (35%)
19	CLA	A	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	7 (8%)
19	CLA	B2	849	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	4 (4%)
19	CLA	B	807	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	6 (7%)
19	CLA	A1	824	-	46,50,73	1.40	9 (19%)	53,85,113	1.39	4 (7%)
19	CLA	A	818	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	BB	808	-	64,68,73	1.21	8 (12%)	76,107,113	1.25	4 (5%)
19	CLA	BB	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
21	PQN	B	838	-	34,34,34	0.65	0	43,45,45	0.90	1 (2%)
19	CLA	B2	808	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	4 (5%)
19	CLA	BB	856	-	64,68,73	1.19	8 (12%)	76,107,113	1.59	13 (17%)
19	CLA	B2	806	2	69,73,73	1.15	7 (10%)	82,113,113	1.32	8 (9%)
19	CLA	A	811	1	55,59,73	1.31	9 (16%)	64,96,113	1.46	7 (10%)
19	CLA	B	846	-	43,47,73	1.43	9 (20%)	51,80,113	1.43	5 (9%)
19	CLA	B	817	-	46,50,73	1.40	8 (17%)	53,85,113	1.49	5 (9%)
19	CLA	AA	840	-	60,64,73	1.23	9 (15%)	71,102,113	1.28	4 (5%)
19	CLA	B1	845	-	43,47,73	1.44	9 (20%)	51,80,113	1.40	4 (7%)
23	BCR	BB	842	-	41,41,41	1.21	3 (7%)	56,56,56	1.20	5 (8%)
25	LMG	I2	105	-	35,35,55	0.92	1 (2%)	43,43,63	1.22	4 (9%)
27	SF4	C	102	3	0,12,12	-	-	-		
19	CLA	B	825	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	B2	823	-	69,73,73	1.18	9 (13%)	82,113,113	1.29	5 (6%)
19	CLA	BB	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
19	CLA	B1	811	-	65,69,73	1.20	7 (10%)	77,108,113	1.18	3 (3%)
19	CLA	B1	834	-	49,53,73	1.36	9 (18%)	58,89,113	1.39	6 (10%)
23	BCR	F	304	-	41,41,41	1.24	3 (7%)	56,56,56	1.31	8 (14%)
19	CLA	A	815	-	59,63,73	1.24	8 (13%)	70,101,113	1.32	4 (5%)
19	CLA	A2	833	-	54,58,73	1.31	9 (16%)	64,95,113	1.30	6 (9%)
19	CLA	B2	805	-	68,72,73	1.15	9 (13%)	80,111,113	1.34	7 (8%)
20	CL0	A2	803	-	58,73,73	3.17	18 (31%)	60,113,113	2.80	21 (35%)
23	BCR	I2	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	6 (10%)
22	LHG	B	852	-	32,32,48	0.91	1 (3%)	35,38,54	1.04	3 (8%)
22	LHG	B	853	-	48,48,48	0.76	1 (2%)	51,54,54	0.99	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B1	814	-	63,67,73	1.23	8 (12%)	74,105,113	1.28	5 (6%)
23	BCR	B2	844	-	41,41,41	1.24	4 (9%)	56,56,56	1.21	6 (10%)
19	CLA	B2	810	-	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
19	CLA	BB	817	-	46,50,73	1.39	8 (17%)	53,85,113	1.45	4 (7%)
19	CLA	B1	807	-	69,73,73	1.19	8 (11%)	82,113,113	1.46	10 (12%)
19	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
19	CLA	B2	817	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
27	SF4	C1	101	-	0,12,12	-	-	-		
23	BCR	I2	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	A1	804	-	64,68,73	1.20	7 (10%)	76,107,113	1.25	6 (7%)
19	CLA	B1	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
23	BCR	B	843	-	41,41,41	1.21	2 (4%)	56,56,56	1.20	6 (10%)
19	CLA	B2	837	-	64,68,73	1.21	8 (12%)	76,107,113	1.35	6 (7%)
19	CLA	A1	817	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
22	LHG	A1	845	-	48,48,48	0.79	2 (4%)	51,54,54	0.97	3 (5%)
22	LHG	BB	851	-	48,48,48	0.77	2 (4%)	51,54,54	0.99	4 (7%)
23	BCR	J1	104	-	41,41,41	1.16	2 (4%)	56,56,56	1.36	6 (10%)
23	BCR	B	844	-	41,41,41	1.27	4 (9%)	56,56,56	1.24	7 (12%)
22	LHG	X	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.96	2 (4%)
19	CLA	A1	828	-	69,73,73	1.15	10 (14%)	82,113,113	1.28	6 (7%)
25	LMG	B1	852	-	30,30,55	0.99	1 (3%)	38,38,63	1.22	4 (10%)
24	AJP	M2	101	-	36,36,95	4.66	24 (66%)	56,60,149	4.79	30 (53%)
19	CLA	A1	825	-	49,53,73	1.36	9 (18%)	58,89,113	1.43	5 (8%)
19	CLA	A2	817	-	47,52,73	1.39	9 (19%)	55,87,113	1.40	4 (7%)
22	LHG	L2	208	-	34,34,48	0.88	3 (8%)	37,40,54	1.07	3 (8%)
27	SF4	C1	102	-	0,12,12	-	-	-		
19	CLA	L2	205	-	63,67,73	1.20	9 (14%)	74,105,113	1.40	5 (6%)
19	CLA	A	824	-	49,53,73	1.37	8 (16%)	58,89,113	1.45	5 (8%)
19	CLA	B1	802	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	6 (7%)
19	CLA	A	844	-	45,49,73	1.40	9 (20%)	54,84,113	1.47	5 (9%)
19	CLA	BB	822	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	5 (6%)
19	CLA	A2	838	-	47,52,73	1.37	8 (17%)	55,87,113	1.48	5 (9%)
19	CLA	A1	823	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	5 (8%)
19	CLA	A2	807	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
19	CLA	BB	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	819	-	45,49,73	1.40	8 (17%)	54,84,113	1.44	5 (9%)
19	CLA	AA	812	-	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
19	CLA	B2	815	-	69,73,73	1.17	8 (11%)	82,113,113	1.33	9 (10%)
19	CLA	AA	853	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	6 (7%)
19	CLA	B2	836	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	5 (6%)
19	CLA	A	830	-	66,70,73	1.16	7 (10%)	78,109,113	1.27	6 (7%)
25	LMG	B	845	-	55,55,55	0.68	0	63,63,63	1.27	4 (6%)
23	BCR	B2	840	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
19	CLA	A2	828	-	60,64,73	1.25	8 (13%)	71,102,113	1.35	5 (7%)
19	CLA	BB	814	-	63,67,73	1.22	10 (15%)	74,105,113	1.35	5 (6%)
23	BCR	J	102	-	41,41,41	1.27	2 (4%)	56,56,56	1.40	11 (19%)
19	CLA	A	825	-	56,60,73	1.28	9 (16%)	65,97,113	1.37	5 (7%)
19	CLA	A2	816	-	54,58,73	1.30	8 (14%)	64,95,113	1.36	5 (7%)
23	BCR	L2	207	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	9 (16%)
19	CLA	B2	852	-	69,73,73	1.17	7 (10%)	82,113,113	1.45	8 (9%)
19	CLA	B	837	-	64,68,73	1.21	6 (9%)	76,107,113	1.30	7 (9%)
19	CLA	AA	843	-	69,73,73	1.17	8 (11%)	82,113,113	1.46	8 (9%)
19	CLA	B1	836	-	64,68,73	1.22	8 (12%)	76,107,113	1.37	6 (7%)
19	CLA	L1	207	-	69,73,73	1.18	9 (13%)	82,113,113	1.25	4 (4%)
19	CLA	A2	836	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
19	CLA	B2	825	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
19	CLA	A1	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
19	CLA	B1	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
23	BCR	A2	847	-	40,40,41	1.13	2 (5%)	54,54,56	1.27	7 (12%)
19	CLA	BB	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
19	CLA	A2	802	-	50,54,73	1.35	7 (14%)	59,90,113	1.38	4 (6%)
19	CLA	A	823	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	7 (9%)
23	BCR	B2	839	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	10 (17%)
24	AJP	I2	104	-	36,36,95	4.55	22 (61%)	56,60,149	4.71	34 (60%)
19	CLA	A2	818	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	AA	809	-	54,58,73	1.29	8 (14%)	64,95,113	1.40	6 (9%)
19	CLA	F	301	-	64,68,73	1.21	8 (12%)	76,107,113	1.41	8 (10%)
19	CLA	XX	101	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	A1	819	-	62,66,73	1.22	10 (16%)	73,104,113	1.34	7 (9%)
23	BCR	I1	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	B	842	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	AA	837	-	49,53,73	1.39	9 (18%)	58,89,113	1.40	4 (6%)
23	BCR	MM	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.37	11 (19%)
19	CLA	A1	809	-	69,73,73	1.14	7 (10%)	82,113,113	1.29	8 (9%)
19	CLA	A1	838	-	56,60,73	1.29	9 (16%)	65,97,113	1.37	5 (7%)
24	AJP	KK	104	-	47,47,95	4.10	24 (51%)	72,77,149	4.55	39 (54%)
19	CLA	AA	819	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
19	CLA	A2	835	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
19	CLA	A2	826	-	49,53,73	1.37	8 (16%)	58,89,113	1.44	6 (10%)
24	AJP	B	857	-	49,49,95	4.03	25 (51%)	75,80,149	3.56	21 (28%)
19	CLA	A2	815	-	59,63,73	1.25	7 (11%)	70,101,113	1.27	4 (5%)
19	CLA	A1	837	1	47,52,73	1.37	8 (17%)	55,87,113	1.47	5 (9%)
19	CLA	A	834	-	45,49,73	1.40	9 (20%)	54,84,113	1.42	6 (11%)
23	BCR	BB	839	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	A1	815	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	5 (7%)
19	CLA	AA	821	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	7 (8%)
19	CLA	B1	801	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	8 (9%)
19	CLA	L1	206	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	6 (7%)
19	CLA	A2	837	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
23	BCR	AA	851	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	5 (8%)
26	ECH	B2	841	-	42,42,42	0.78	1 (2%)	55,58,58	2.42	18 (32%)
19	CLA	A1	808	-	54,58,73	1.30	8 (14%)	64,95,113	1.41	5 (7%)
23	BCR	J1	102	-	41,41,41	1.22	2 (4%)	56,56,56	1.38	8 (14%)
19	CLA	A1	840	-	50,54,73	1.34	8 (16%)	59,90,113	1.41	5 (8%)
19	CLA	L	202	18	65,69,73	1.19	8 (12%)	77,108,113	1.50	7 (9%)
23	BCR	F1	306	-	41,41,41	1.14	3 (7%)	56,56,56	1.48	9 (16%)
27	SF4	BB	857	-	0,12,12	-	-	-		
22	LHG	XX	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.95	2 (4%)
19	CLA	B1	833	-	69,73,73	1.18	7 (10%)	82,113,113	1.53	19 (23%)
22	LHG	L	207	-	33,33,48	0.95	3 (9%)	36,39,54	1.07	4 (11%)
24	AJP	L1	203	-	49,49,95	4.03	24 (48%)	75,80,149	4.01	37 (49%)
25	LMG	B1	846	-	32,32,55	0.93	1 (3%)	40,40,63	1.22	5 (12%)
19	CLA	B1	827	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	6 (10%)
25	LMG	B1	844	-	55,55,55	0.68	0	63,63,63	1.28	4 (6%)
19	CLA	A1	812	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	A	848	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	9 (16%)
19	CLA	A	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
23	BCR	J	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.38	8 (14%)
19	CLA	L	204	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	7 (8%)
23	BCR	FF	304	-	41,41,41	1.25	4 (9%)	56,56,56	1.31	8 (14%)
19	CLA	B	827	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	6 (10%)
19	CLA	A2	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
19	CLA	A2	813	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	5 (6%)
19	CLA	K1	105	9	44,48,73	1.44	7 (15%)	51,82,113	1.46	6 (11%)
19	CLA	BB	811	-	65,69,73	1.19	8 (12%)	77,108,113	1.20	3 (3%)
23	BCR	I	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	7 (12%)
19	CLA	B	831	-	60,64,73	1.24	8 (13%)	71,102,113	1.28	5 (7%)
24	AJP	L2	202	-	49,49,95	4.04	23 (46%)	75,80,149	4.65	47 (62%)
24	AJP	BB	849	-	49,49,95	4.08	25 (51%)	75,80,149	4.48	48 (64%)
19	CLA	A	804	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
23	BCR	A	854	-	41,41,41	1.15	3 (7%)	56,56,56	1.30	9 (16%)
19	CLA	A	805	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	7 (9%)
19	CLA	A	807	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
25	LMG	B2	854	-	30,30,55	0.99	1 (3%)	38,38,63	1.22	4 (10%)
19	CLA	B1	829	-	60,64,73	1.23	9 (15%)	71,102,113	1.33	7 (9%)
19	CLA	BB	807	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	6 (7%)
19	CLA	A2	830	-	66,70,73	1.16	7 (10%)	78,109,113	1.25	6 (7%)
23	BCR	I	101	-	41,41,41	1.21	2 (4%)	56,56,56	1.23	7 (12%)
22	LHG	A	846	-	37,37,48	0.82	1 (2%)	40,43,54	1.03	3 (7%)
22	LHG	A1	846	-	37,37,48	0.82	1 (2%)	40,43,54	1.03	3 (7%)
19	CLA	AA	820	-	62,66,73	1.23	9 (14%)	73,104,113	1.39	7 (9%)
19	CLA	J	101	8	45,49,73	1.41	8 (17%)	54,84,113	1.43	4 (7%)
19	CLA	J2	101	8	45,49,73	1.42	8 (17%)	54,84,113	1.40	4 (7%)
19	CLA	B2	851	-	64,68,73	1.20	9 (14%)	76,107,113	1.55	13 (17%)
19	CLA	A	806	-	60,64,73	1.24	9 (15%)	71,102,113	1.44	7 (9%)
24	AJP	A2	854	-	37,37,95	4.54	24 (64%)	58,62,149	3.71	22 (37%)
19	CLA	B1	812	-	45,49,73	1.40	9 (20%)	54,84,113	1.48	4 (7%)
27	SF4	C2	102	-	0,12,12	-	-	-		
25	LMG	B2	847	-	32,32,55	0.93	1 (3%)	40,40,63	1.22	2 (5%)
19	CLA	A	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.35	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A1	822	-	64,68,73	1.20	9 (14%)	76,107,113	1.35	7 (9%)
19	CLA	AA	810	-	69,73,73	1.15	7 (10%)	82,113,113	1.36	9 (10%)
19	CLA	BB	845	-	43,47,73	1.43	9 (20%)	51,80,113	1.44	5 (9%)
19	CLA	B	835	-	49,53,73	1.36	8 (16%)	58,89,113	1.41	6 (10%)
19	CLA	A2	832	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)
19	CLA	BB	833	-	69,73,73	1.17	5 (7%)	82,113,113	1.50	19 (23%)
19	CLA	B	804	-	66,70,73	1.19	9 (13%)	78,109,113	1.29	8 (10%)
23	BCR	M	101	-	41,41,41	1.23	3 (7%)	56,56,56	1.35	10 (17%)
23	BCR	K2	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	6 (10%)
19	CLA	BB	855	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	3 (3%)
25	LMG	L1	210	-	55,55,55	0.67	0	63,63,63	1.29	6 (9%)
20	CL0	A1	802	-	58,73,73	3.26	18 (31%)	60,113,113	2.60	22 (36%)
19	CLA	B	832	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
19	CLA	A2	821	-	69,73,73	1.14	8 (11%)	82,113,113	1.29	7 (8%)
23	BCR	B1	841	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	6 (10%)
21	PQN	A1	843	-	34,34,34	0.65	0	43,45,45	1.10	4 (9%)
19	CLA	B2	811	-	65,69,73	1.20	7 (10%)	77,108,113	1.18	3 (3%)
19	CLA	L1	205	10	65,69,73	1.20	9 (13%)	77,108,113	1.34	8 (10%)
22	LHG	A	845	-	48,48,48	0.81	2 (4%)	51,54,54	0.99	3 (5%)
19	CLA	F1	301	-	64,68,73	1.22	8 (12%)	76,107,113	1.41	8 (10%)
19	CLA	A1	833	-	45,49,73	1.39	9 (20%)	54,84,113	1.43	6 (11%)
19	CLA	BB	805	-	68,72,73	1.16	9 (13%)	80,111,113	1.34	7 (8%)
19	CLA	A1	807	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	6 (7%)
19	CLA	A	822	-	55,59,73	1.31	8 (14%)	64,96,113	1.35	4 (6%)
19	CLA	A2	834	-	45,49,73	1.39	9 (20%)	54,84,113	1.44	6 (11%)
19	CLA	A2	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
27	SF4	CC	101	-	0,12,12	-	-	-		
19	CLA	BB	829	-	60,64,73	1.24	8 (13%)	71,102,113	1.31	7 (9%)
19	CLA	BB	801	-	69,73,73	1.17	7 (10%)	82,113,113	1.50	9 (10%)
19	CLA	L2	204	16	65,69,73	1.20	9 (13%)	77,108,113	1.33	8 (10%)
19	CLA	AA	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
19	CLA	BB	821	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	6 (7%)
19	CLA	B2	816	-	61,65,73	1.25	8 (13%)	72,103,113	1.29	4 (5%)
19	CLA	B2	801	-	69,73,73	1.15	9 (13%)	82,113,113	1.42	7 (8%)
19	CLA	B2	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	BB	825	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
21	PQN	A	843	-	34,34,34	0.62	0	43,45,45	1.10	4 (9%)
23	BCR	B1	842	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	6 (10%)
23	BCR	AA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	8 (14%)
19	CLA	A	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
19	CLA	B1	805	-	68,72,73	1.16	9 (13%)	80,111,113	1.33	7 (8%)
23	BCR	A	850	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	6 (10%)
19	CLA	B	829	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	4 (4%)
19	CLA	LL	203	-	46,50,73	1.44	8 (17%)	53,85,113	1.58	9 (16%)
23	BCR	F2	305	-	41,41,41	1.14	3 (7%)	56,56,56	1.48	9 (16%)
19	CLA	BB	819	-	45,49,73	1.40	8 (17%)	54,84,113	1.43	5 (9%)
23	BCR	A1	853	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
19	CLA	BB	812	-	45,49,73	1.40	8 (17%)	54,84,113	1.44	5 (9%)
19	CLA	AA	825	-	56,60,73	1.28	9 (16%)	65,97,113	1.35	5 (7%)
19	CLA	A	814	-	46,50,73	1.40	8 (17%)	53,85,113	1.36	4 (7%)
19	CLA	BB	820	-	49,53,73	1.39	8 (16%)	58,89,113	1.68	10 (17%)
19	CLA	B	813	-	46,50,73	1.39	8 (17%)	53,85,113	1.38	5 (9%)
23	BCR	FF	303	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
19	CLA	B1	820	-	49,53,73	1.39	8 (16%)	58,89,113	1.35	5 (8%)
19	CLA	B2	820	-	49,53,73	1.39	8 (16%)	58,89,113	1.56	8 (13%)
25	LMG	II	105	-	42,42,55	0.82	0	50,50,63	1.25	6 (12%)
23	BCR	A2	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
19	CLA	A2	801	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	5 (6%)
19	CLA	A2	820	-	62,66,73	1.22	10 (16%)	73,104,113	1.38	8 (10%)
19	CLA	B1	816	-	61,65,73	1.25	8 (13%)	72,103,113	1.28	5 (6%)
22	LHG	B1	847	-	32,32,48	0.89	1 (3%)	35,38,54	1.05	3 (8%)
23	BCR	L1	201	-	41,41,41	1.19	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	B	828	-	49,53,73	1.37	8 (16%)	58,89,113	1.37	4 (6%)
19	CLA	A2	811	-	55,59,73	1.30	9 (16%)	64,96,113	1.46	7 (10%)
19	CLA	AA	833	-	54,58,73	1.31	9 (16%)	64,95,113	1.30	4 (6%)
24	AJP	AA	856	-	40,40,95	4.42	24 (60%)	61,65,149	3.79	22 (36%)
24	AJP	B	849	-	49,49,95	4.04	25 (51%)	75,80,149	4.55	44 (58%)
19	CLA	BB	810	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
28	DGD	BB	854	-	43,43,67	1.04	0	57,57,81	1.40	8 (14%)
19	CLA	FF	305	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B1	810	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
19	CLA	F1	305	-	49,53,73	1.37	7 (14%)	58,89,113	1.36	4 (6%)
19	CLA	B	830	-	60,64,73	1.22	7 (11%)	71,102,113	1.36	7 (9%)
23	BCR	II	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	8 (14%)
23	BCR	BB	841	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	6 (10%)
19	CLA	A2	805	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
19	CLA	AA	839	-	56,60,73	1.29	8 (14%)	65,97,113	1.35	5 (7%)
19	CLA	BB	836	-	64,68,73	1.22	8 (12%)	76,107,113	1.62	10 (13%)
23	BCR	A2	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	9 (16%)
23	BCR	A	853	-	41,41,41	1.16	2 (4%)	56,56,56	1.37	10 (17%)
19	CLA	A1	829	-	66,70,73	1.19	7 (10%)	78,109,113	1.26	6 (7%)
19	CLA	AA	805	-	64,68,73	1.20	9 (14%)	76,107,113	1.31	8 (10%)
22	LHG	A2	846	-	37,37,48	0.83	1 (2%)	40,43,54	1.03	3 (7%)
19	CLA	A1	821	-	55,59,73	1.31	8 (14%)	64,96,113	1.37	6 (9%)
19	CLA	B2	814	-	63,67,73	1.23	9 (14%)	74,105,113	1.28	4 (5%)
19	CLA	B1	832	-	69,73,73	1.18	6 (8%)	82,113,113	1.34	9 (10%)
19	CLA	AA	824	-	49,53,73	1.37	8 (16%)	58,89,113	1.44	5 (8%)
19	CLA	A	826	-	49,53,73	1.36	9 (18%)	58,89,113	1.40	5 (8%)
23	BCR	B	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	7 (12%)
19	CLA	AA	830	-	66,70,73	1.16	7 (10%)	78,109,113	1.25	6 (7%)
19	CLA	A2	806	-	60,64,73	1.24	9 (15%)	71,102,113	1.45	7 (9%)
27	SF4	B2	853	-	0,12,12	-	-	-		
19	CLA	AA	817	-	47,52,73	1.39	8 (17%)	55,87,113	1.41	4 (7%)
19	CLA	A	827	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	6 (7%)
19	CLA	B	808	-	64,68,73	1.20	8 (12%)	76,107,113	1.22	4 (5%)
23	BCR	A1	847	-	40,40,41	1.14	3 (7%)	54,54,56	1.28	8 (14%)
19	CLA	A2	841	-	50,54,73	1.33	7 (14%)	59,90,113	1.40	4 (6%)
23	BCR	B	840	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	11 (13%)
19	CLA	AA	806	-	60,64,73	1.24	9 (15%)	71,102,113	1.44	7 (9%)
19	CLA	B1	850	-	64,68,73	1.20	8 (12%)	76,107,113	1.55	13 (17%)
25	LMG	M	102	-	46,46,55	0.82	1 (2%)	54,54,63	1.28	7 (12%)
19	CLA	B2	850	-	69,73,73	1.17	9 (13%)	82,113,113	1.19	4 (4%)
22	LHG	X2	103	-	48,48,48	0.77	2 (4%)	51,54,54	0.97	4 (7%)
19	CLA	AA	838	-	47,52,73	1.37	9 (19%)	55,87,113	1.45	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	832	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
19	CLA	AA	823	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	7 (9%)
19	CLA	FF	302	-	46,50,73	1.41	8 (17%)	53,85,113	1.48	5 (9%)
19	CLA	A2	810	1	69,73,73	1.15	7 (10%)	82,113,113	1.35	8 (9%)
19	CLA	A	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
24	AJP	A1	854	-	49,49,95	4.04	25 (51%)	75,80,149	3.56	21 (28%)
19	CLA	B	834	-	69,73,73	1.17	7 (10%)	82,113,113	1.50	17 (20%)
19	CLA	B2	829	-	69,73,73	1.18	8 (11%)	82,113,113	1.17	4 (4%)
19	CLA	B1	824	-	59,63,73	1.26	9 (15%)	70,101,113	1.27	5 (7%)
19	CLA	BB	852	-	69,73,73	1.16	6 (8%)	82,113,113	1.31	5 (6%)
24	AJP	A	802	-	35,35,95	4.64	22 (62%)	54,58,149	4.56	29 (53%)
22	LHG	AA	847	-	37,37,48	0.82	1 (2%)	40,43,54	1.03	3 (7%)
22	LHG	A2	845	-	48,48,48	0.77	2 (4%)	51,54,54	0.97	3 (5%)
24	AJP	L	209	-	36,36,95	4.67	24 (66%)	56,60,149	4.89	33 (58%)
19	CLA	B1	822	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
19	CLA	A2	822	-	55,59,73	1.31	8 (14%)	64,96,113	1.38	6 (9%)
19	CLA	AA	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
19	CLA	A2	825	-	46,50,73	1.40	9 (19%)	53,85,113	1.43	4 (7%)
19	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
19	CLA	AA	807	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
19	CLA	AA	828	-	60,64,73	1.24	8 (13%)	71,102,113	1.35	6 (8%)
19	CLA	A1	814	-	59,63,73	1.25	7 (11%)	70,101,113	1.30	4 (5%)
19	CLA	L2	206	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
19	CLA	AA	845	-	45,49,73	1.40	9 (20%)	54,84,113	1.48	4 (7%)
23	BCR	L1	208	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	9 (16%)
19	CLA	B2	809	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	6 (10%)
19	CLA	AA	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
19	CLA	L	203	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
24	AJP	A	855	-	40,40,95	4.42	24 (60%)	61,65,149	3.79	22 (36%)
19	CLA	B	820	-	49,53,73	1.39	8 (16%)	58,89,113	1.66	10 (17%)
19	CLA	K	102	-	50,54,73	1.35	7 (14%)	59,90,113	1.38	4 (6%)
19	CLA	A	813	-	69,73,73	1.14	8 (11%)	82,113,113	1.25	5 (6%)
19	CLA	A2	812	-	50,54,73	1.33	8 (16%)	59,90,113	1.42	6 (10%)
19	CLA	AA	818	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
19	CLA	A2	823	-	64,68,73	1.21	8 (12%)	76,107,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	LMG	B2	845	-	55,55,55	0.68	0	63,63,63	1.27	5 (7%)
19	CLA	B	811	-	65,69,73	1.20	8 (12%)	77,108,113	1.19	3 (3%)
26	ECH	BB	840	-	42,42,42	0.87	1 (2%)	55,58,58	2.45	18 (32%)
19	CLA	B2	827	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	6 (10%)
23	BCR	B1	839	-	41,41,41	1.14	2 (4%)	56,56,56	1.18	3 (5%)
23	BCR	B	839	-	41,41,41	1.17	3 (7%)	56,56,56	1.28	8 (14%)
23	BCR	FF	306	-	41,41,41	1.17	3 (7%)	56,56,56	1.48	11 (19%)
26	ECH	B	841	-	42,42,42	0.89	1 (2%)	55,58,58	2.50	21 (38%)
24	AJP	L2	203	-	49,49,95	4.01	24 (48%)	75,80,149	4.25	45 (60%)
22	LHG	X1	103	-	48,48,48	0.77	1 (2%)	51,54,54	0.97	3 (5%)
19	CLA	B1	809	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)
19	CLA	B1	804	-	66,70,73	1.19	9 (13%)	78,109,113	1.31	6 (7%)
19	CLA	B1	818	-	45,49,73	1.42	7 (15%)	54,84,113	1.39	4 (7%)
19	CLA	A	820	-	62,66,73	1.22	9 (14%)	73,104,113	1.36	7 (9%)
23	BCR	JJ	102	-	41,41,41	1.26	2 (4%)	56,56,56	1.39	9 (16%)
19	CLA	B	810	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
25	LMG	I1	102	-	35,35,55	1.03	1 (2%)	43,43,63	1.28	3 (6%)
23	BCR	A1	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	9 (16%)
19	CLA	AA	815	-	59,63,73	1.24	8 (13%)	70,101,113	1.32	4 (5%)
19	CLA	B	816	-	61,65,73	1.24	8 (13%)	72,103,113	1.34	5 (6%)
19	CLA	B	822	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	4 (4%)
19	CLA	B	860	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	9 (10%)
27	SF4	B1	851	-	0,12,12	-	-	-		
23	BCR	B2	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	7 (12%)
19	CLA	B1	848	-	69,73,73	1.18	7 (10%)	82,113,113	1.33	5 (6%)
27	SF4	B	861	-	0,12,12	-	-	-		
21	PQN	AA	844	-	34,34,34	0.67	0	43,45,45	1.06	4 (9%)
19	CLA	B1	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.17	4 (4%)
19	CLA	A2	814	-	46,50,73	1.39	9 (19%)	53,85,113	1.38	4 (7%)
19	CLA	A2	852	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	6 (7%)
19	CLA	K1	103	-	50,54,73	1.35	7 (14%)	59,90,113	1.37	4 (6%)
19	CLA	A1	806	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
23	BCR	A2	850	-	41,41,41	1.18	3 (7%)	56,56,56	1.26	6 (10%)
19	CLA	B1	819	-	45,49,73	1.40	7 (15%)	54,84,113	1.43	5 (9%)
23	BCR	A	849	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
23	BCR	AA	854	-	41,41,41	1.16	2 (4%)	56,56,56	1.37	10 (17%)
19	CLA	A1	827	-	60,64,73	1.25	8 (13%)	71,102,113	1.33	5 (7%)
19	CLA	A2	839	-	56,60,73	1.29	9 (16%)	65,97,113	1.36	5 (7%)
19	CLA	A	821	-	69,73,73	1.14	8 (11%)	82,113,113	1.33	7 (8%)
21	PQN	B2	838	-	34,34,34	0.63	0	43,45,45	0.90	0
19	CLA	BB	832	-	69,73,73	1.19	7 (10%)	82,113,113	1.35	8 (9%)
19	CLA	B2	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	7 (8%)
19	CLA	AA	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
19	CLA	B2	832	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	4 (6%)
19	CLA	A2	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	6 (7%)
28	DGD	B	856	-	43,43,67	1.05	0	57,57,81	1.39	6 (10%)
19	CLA	B2	846	-	43,47,73	1.44	8 (18%)	51,80,113	1.40	4 (7%)
19	CLA	A1	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
22	LHG	AA	846	-	48,48,48	0.81	2 (4%)	51,54,54	0.98	3 (5%)
26	ECH	B1	840	-	42,42,42	0.80	1 (2%)	55,58,58	2.45	18 (32%)
19	CLA	A1	832	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	6 (9%)
23	BCR	B1	843	-	41,41,41	1.24	4 (9%)	56,56,56	1.21	7 (12%)
19	CLA	B2	828	-	49,53,73	1.38	7 (14%)	58,89,113	1.37	4 (6%)
19	CLA	A	840	-	60,64,73	1.24	9 (15%)	71,102,113	1.30	4 (5%)
23	BCR	LL	204	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	8 (14%)
23	BCR	A	847	-	40,40,41	1.12	2 (5%)	54,54,56	1.30	10 (18%)
24	AJP	A1	855	-	37,37,95	4.54	24 (64%)	58,62,149	3.69	22 (37%)
19	CLA	FF	301	-	64,68,73	1.21	8 (12%)	76,107,113	1.28	7 (9%)
23	BCR	F	303	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	A1	816	-	47,52,73	1.39	9 (19%)	55,87,113	1.39	4 (7%)
23	BCR	I2	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.39	10 (17%)
19	CLA	A	841	-	50,54,73	1.33	7 (14%)	59,90,113	1.40	5 (8%)
19	CLA	AA	816	-	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
21	PQN	BB	837	-	34,34,34	0.67	0	43,45,45	0.89	0
23	BCR	A2	851	-	41,41,41	1.08	1 (2%)	56,56,56	1.50	9 (16%)
19	CLA	B2	802	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
19	CLA	KK	101	-	49,53,73	1.38	8 (16%)	58,89,113	1.50	7 (12%)
19	CLA	B1	808	-	64,68,73	1.21	9 (14%)	76,107,113	1.23	4 (5%)
19	CLA	A2	829	-	69,73,73	1.17	10 (14%)	82,113,113	1.23	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	BB	818	-	45,49,73	1.42	8 (17%)	54,84,113	1.37	5 (9%)
23	BCR	KK	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.35	10 (17%)
24	AJP	K	104	-	47,47,95	4.11	24 (51%)	72,77,149	4.51	39 (54%)
19	CLA	A2	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	5 (6%)
19	CLA	A	810	1	69,73,73	1.15	7 (10%)	82,113,113	1.35	8 (9%)
19	CLA	B2	818	-	45,49,73	1.42	7 (15%)	54,84,113	1.38	4 (7%)
19	CLA	A1	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
23	BCR	BB	843	-	41,41,41	1.25	4 (9%)	56,56,56	1.21	6 (10%)
19	CLA	BB	835	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	6 (7%)
23	BCR	B2	843	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	6 (10%)
19	CLA	B	826	-	69,73,73	1.20	8 (11%)	82,113,113	1.36	8 (9%)
19	CLA	BB	826	-	69,73,73	1.23	9 (13%)	82,113,113	1.42	12 (14%)
19	CLA	BB	828	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	4 (6%)
22	LHG	LL	205	-	33,33,48	0.95	3 (9%)	36,39,54	1.07	4 (11%)
19	CLA	B2	835	-	49,53,73	1.37	9 (18%)	58,89,113	1.39	5 (8%)
19	CLA	AA	834	-	45,49,73	1.39	9 (20%)	54,84,113	1.42	6 (11%)
19	CLA	B1	826	-	69,73,73	1.20	8 (11%)	82,113,113	1.37	9 (10%)
19	CLA	B2	826	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	10 (12%)
19	CLA	A1	835	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
19	CLA	B	818	-	45,49,73	1.43	6 (13%)	54,84,113	1.39	5 (9%)
19	CLA	B	801	-	69,73,73	1.15	9 (13%)	82,113,113	1.53	10 (12%)
19	CLA	LL	202	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
19	CLA	B1	831	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
19	CLA	A2	809	-	54,58,73	1.29	8 (14%)	64,95,113	1.40	5 (7%)
19	CLA	AA	835	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	5 (6%)
23	BCR	BB	847	-	41,41,41	1.20	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	B1	823	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	4 (4%)
19	CLA	B	823	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	4 (4%)
19	CLA	AA	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
19	CLA	K2	102	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	7 (12%)
19	CLA	AA	822	-	55,59,73	1.31	8 (14%)	64,96,113	1.36	4 (6%)
23	BCR	L	206	-	41,41,41	1.20	3 (7%)	56,56,56	1.27	9 (16%)
19	CLA	AA	832	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
23	BCR	L	205	-	41,41,41	1.16	3 (7%)	56,56,56	1.34	9 (16%)
23	BCR	BB	838	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B2	819	-	45,49,73	1.40	8 (17%)	54,84,113	1.46	5 (9%)
19	CLA	B	805	-	68,72,73	1.15	9 (13%)	80,111,113	1.35	7 (8%)
19	CLA	B1	849	-	69,73,73	1.17	9 (13%)	82,113,113	1.15	4 (4%)
27	SF4	C2	101	-	0,12,12	-	-	-		
19	CLA	J1	103	-	45,49,73	1.42	6 (13%)	54,84,113	1.41	4 (7%)
21	PQN	B1	837	-	34,34,34	0.72	0	43,45,45	0.92	1 (2%)
25	LMG	B	851	-	55,55,55	0.67	0	63,63,63	1.29	7 (11%)
19	CLA	A	812	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
23	BCR	AA	850	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	10 (17%)
19	CLA	A	835	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
27	SF4	CC	102	-	0,12,12	-	-	-		
23	BCR	A1	850	-	41,41,41	1.19	3 (7%)	56,56,56	1.28	6 (10%)
19	CLA	F	302	-	46,50,73	1.41	8 (17%)	53,85,113	1.49	5 (9%)
19	CLA	A1	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
23	BCR	F1	304	-	41,41,41	1.24	4 (9%)	56,56,56	1.30	8 (14%)
23	BCR	B1	838	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	10 (17%)
19	CLA	A1	818	-	64,68,73	1.21	9 (14%)	76,107,113	1.30	5 (6%)
19	CLA	AA	826	-	49,53,73	1.36	9 (18%)	58,89,113	1.42	6 (10%)
19	CLA	B	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	9 (10%)
19	CLA	B1	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
19	CLA	BB	813	-	46,50,73	1.39	8 (17%)	53,85,113	1.43	5 (9%)
23	BCR	F1	303	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	7 (12%)
19	CLA	A1	813	-	46,50,73	1.39	9 (19%)	53,85,113	1.38	4 (7%)
19	CLA	A	852	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	7 (8%)
19	CLA	B	836	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
19	CLA	X1	101	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
19	CLA	AA	813	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	5 (6%)
19	CLA	BB	827	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	6 (10%)
19	CLA	A1	844	-	45,49,73	1.40	9 (20%)	54,84,113	1.46	4 (7%)
19	CLA	A	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	4 (4%)
23	BCR	K1	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.20	6 (10%)
19	CLA	A1	805	-	60,64,73	1.25	9 (15%)	71,102,113	1.30	5 (7%)
19	CLA	A2	844	-	45,49,73	1.40	9 (20%)	54,84,113	1.45	4 (7%)
19	CLA	BB	831	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	5 (8%)
23	BCR	L1	209	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	AJP	L1	204	-	49,49,95	4.01	25 (51%)	75,80,149	4.25	49 (65%)
19	CLA	A	839	-	56,60,73	1.29	8 (14%)	65,97,113	1.36	6 (9%)
19	CLA	A1	841	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
19	CLA	B2	831	-	60,64,73	1.24	7 (11%)	71,102,113	1.29	5 (7%)
23	BCR	II	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	5 (8%)
19	CLA	B2	812	-	45,49,73	1.40	9 (20%)	54,84,113	1.48	5 (9%)
19	CLA	B2	830	-	60,64,73	1.23	9 (15%)	71,102,113	1.35	6 (8%)
19	CLA	AA	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	6 (7%)
23	BCR	JJ	104	-	41,41,41	1.20	3 (7%)	56,56,56	1.27	8 (14%)
19	CLA	A1	830	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
19	CLA	B	821	2	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)

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
19	CLA	AA	841	-	1/1/15/20	2/17/93/115	-
19	CLA	A2	840	-	1/1/18/20	3/29/105/115	-
19	CLA	X2	101	-	1/1/15/20	4/15/91/115	-
23	BCR	K1	106	-	-	17/29/63/63	0/2/2/2
19	CLA	B1	821	2	1/1/20/20	13/39/115/115	-
19	CLA	A1	834	-	1/1/20/20	9/39/115/115	-
19	CLA	A1	842	-	1/1/20/20	15/39/115/115	-
20	CL0	A	803	-	4/4/25/25	18/37/135/135	-
19	CLA	F1	302	-	1/1/14/20	5/12/88/115	-
24	AJP	AA	802	-	11/11/14/38	-	0/6/6/11
19	CLA	BB	824	-	1/1/18/20	11/27/103/115	-
27	SF4	C	101	-	-	-	0/6/5/5
24	AJP	B	850	-	17/17/19/38	2/6/121/220	0/7/7/11
23	BCR	M1	101	-	-	18/29/63/63	0/2/2/2
22	LHG	X2	102	-	-	14/44/44/53	-
19	CLA	B1	813	-	1/1/14/20	8/12/88/115	-
19	CLA	A1	836	-	1/1/15/20	5/15/91/115	-
23	BCR	F	305	-	-	23/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	833	-	1/1/17/20	4/21/97/115	-
19	CLA	KK	102	-	1/1/15/20	9/17/93/115	-
19	CLA	B	854	-	1/1/20/20	11/39/115/115	-
19	CLA	LL	201	18	1/1/19/20	12/35/111/115	-
19	CLA	B	812	-	1/1/14/20	4/10/86/115	-
25	LMG	BB	844	-	-	18/50/70/70	0/1/1/1
22	LHG	X1	102	-	-	16/44/44/53	-
19	CLA	AA	829	-	1/1/20/20	11/39/115/115	-
23	BCR	A2	853	-	-	16/29/63/63	0/2/2/2
19	CLA	JJ	103	-	1/1/14/20	2/10/86/115	-
23	BCR	A1	848	-	-	13/29/63/63	0/2/2/2
19	CLA	K	101	-	1/1/15/20	1/15/91/115	-
19	CLA	B	824	-	1/1/18/20	11/27/103/115	-
19	CLA	B1	817	-	1/1/14/20	4/12/88/115	-
19	CLA	AA	808	-	1/1/20/20	14/39/115/115	-
23	BCR	II	101	-	-	17/29/63/63	0/2/2/2
19	CLA	B	859	-	1/1/19/20	13/33/109/115	-
19	CLA	BB	823	-	1/1/20/20	13/39/115/115	-
19	CLA	A2	819	-	1/1/19/20	9/33/109/115	-
23	BCR	AA	852	-	-	19/29/63/63	0/2/2/2
23	BCR	F2	304	-	-	15/29/63/63	0/2/2/2
19	CLA	B1	830	-	1/1/18/20	6/29/105/115	-
23	BCR	AA	855	-	-	17/29/63/63	0/2/2/2
19	CLA	B	858	-	1/1/20/20	5/39/115/115	-
23	BCR	A1	851	-	-	19/29/63/63	0/2/2/2
19	CLA	A	809	-	1/1/17/20	4/21/97/115	-
21	PQN	A2	843	-	-	8/23/43/43	0/2/2/2
19	CLA	K1	102	-	1/1/15/20	0/15/91/115	-
19	CLA	BB	809	-	1/1/15/20	5/15/91/115	-
23	BCR	K	103	-	-	18/29/63/63	0/2/2/2
19	CLA	B1	806	-	1/1/20/20	13/39/115/115	-
19	CLA	JJ	101	8	1/1/14/20	4/10/86/115	-
19	CLA	A	836	-	1/1/20/20	14/39/115/115	-
22	LHG	B2	848	-	-	8/37/37/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	J2	104	-	-	16/29/63/63	0/2/2/2
19	CLA	B	814	-	1/1/18/20	10/32/108/115	-
19	CLA	A	817	-	1/1/14/20	4/14/90/115	-
23	BCR	K2	105	-	-	16/29/63/63	0/2/2/2
19	CLA	X	101	-	1/1/15/20	4/15/91/115	-
23	BCR	AA	848	-	-	11/27/61/63	0/2/2/2
23	BCR	F2	303	-	-	21/29/63/63	0/2/2/2
19	CLA	A1	839	-	1/1/18/20	6/29/105/115	-
19	CLA	B	809	-	1/1/15/20	4/15/91/115	-
19	CLA	J	103	-	-	6/10/86/115	-
19	CLA	B2	821	-	1/1/20/20	14/39/115/115	-
19	CLA	A	838	-	1/1/14/20	4/14/90/115	-
19	CLA	J1	101	-	1/1/13/20	4/10/86/115	-
22	LHG	BB	850	-	-	12/37/37/53	-
19	CLA	B1	815	-	1/1/20/20	17/39/115/115	-
19	CLA	B2	833	-	-	14/39/115/115	-
19	CLA	B2	807	-	1/1/20/20	14/39/115/115	-
19	CLA	A1	820	-	1/1/20/20	17/39/115/115	-
19	CLA	BB	804	-	1/1/19/20	7/36/112/115	-
23	BCR	A	851	-	-	19/29/63/63	0/2/2/2
19	CLA	BB	834	-	1/1/15/20	1/15/91/115	-
19	CLA	A2	824	-	1/1/15/20	3/15/91/115	-
19	CLA	B2	834	-	1/1/19/20	20/39/115/115	-
19	CLA	A1	811	-	1/1/15/20	7/17/93/115	-
24	AJP	L	208	-	13/13/14/38	-	0/6/6/11
23	BCR	J2	102	-	-	17/29/63/63	0/2/2/2
19	CLA	J2	103	-	1/1/14/20	2/10/86/115	-
19	CLA	A	828	-	1/1/18/20	11/29/105/115	-
19	CLA	A	837	-	1/1/15/20	5/15/91/115	-
19	CLA	AA	811	1	1/1/17/20	8/23/99/115	-
19	CLA	BB	816	-	1/1/18/20	9/30/106/115	-
19	CLA	A1	852	-	1/1/20/20	16/39/115/115	-
19	CLA	B2	804	-	1/1/19/20	9/36/112/115	-
19	CLA	B2	813	-	1/1/14/20	8/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A1	810	-	1/1/17/20	9/23/99/115	-
19	CLA	F2	302	-	1/1/14/20	6/12/88/115	-
19	CLA	A2	831	-	1/1/20/20	11/39/115/115	-
23	BCR	M2	102	-	-	18/29/63/63	0/2/2/2
19	CLA	F2	301	-	1/1/19/20	8/33/109/115	-
19	CLA	AA	814	-	1/1/14/20	4/12/88/115	-
19	CLA	BB	830	-	1/1/18/20	6/29/105/115	-
19	CLA	B2	824	-	1/1/18/20	10/27/103/115	-
19	CLA	K2	104	-	1/1/13/20	6/9/81/115	-
22	LHG	L1	211	-	-	14/37/37/53	-
24	AJP	BB	848	-	17/17/19/38	3/6/121/220	0/7/7/11
19	CLA	B	833	-	-	13/39/115/115	-
20	CL0	AA	803	-	4/4/25/25	14/37/135/135	-
19	CLA	A	808	-	1/1/20/20	13/39/115/115	-
19	CLA	B2	849	-	1/1/20/20	11/39/115/115	-
19	CLA	B	807	-	1/1/20/20	11/39/115/115	-
19	CLA	A1	824	-	1/1/14/20	3/12/88/115	-
19	CLA	A	818	-	1/1/15/20	5/15/91/115	-
19	CLA	BB	808	-	1/1/19/20	13/33/109/115	-
19	CLA	BB	806	-	1/1/20/20	13/39/115/115	-
21	PQN	B	838	-	-	7/23/43/43	0/2/2/2
19	CLA	B2	808	-	1/1/19/20	12/33/109/115	-
19	CLA	BB	856	-	1/1/19/20	13/33/109/115	-
19	CLA	B2	806	2	1/1/20/20	13/39/115/115	-
19	CLA	A	811	1	1/1/17/20	8/23/99/115	-
19	CLA	B	846	-	1/1/12/20	1/7/79/115	-
19	CLA	B	817	-	1/1/14/20	5/12/88/115	-
19	CLA	AA	840	-	1/1/18/20	7/29/105/115	-
19	CLA	B1	845	-	1/1/12/20	0/7/79/115	-
23	BCR	BB	842	-	-	16/29/63/63	0/2/2/2
25	LMG	I2	105	-	-	11/29/49/70	0/1/1/1
27	SF4	C	102	3	-	-	0/6/5/5
19	CLA	B	825	-	1/1/20/20	16/39/115/115	-
19	CLA	B2	823	-	1/1/20/20	16/39/115/115	-
19	CLA	BB	802	-	1/1/20/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	811	-	1/1/19/20	14/35/111/115	-
19	CLA	B1	834	-	1/1/15/20	1/15/91/115	-
23	BCR	F	304	-	-	15/29/63/63	0/2/2/2
19	CLA	A	815	-	1/1/18/20	7/27/103/115	-
19	CLA	A2	833	-	1/1/17/20	3/21/97/115	-
19	CLA	B2	805	-	1/1/19/20	10/38/114/115	-
20	CL0	A2	803	-	4/4/25/25	17/37/135/135	-
23	BCR	I2	102	-	-	11/29/63/63	0/2/2/2
22	LHG	B	852	-	-	11/37/37/53	-
22	LHG	B	853	-	-	21/53/53/53	-
19	CLA	B1	814	-	1/1/18/20	12/32/108/115	-
23	BCR	B2	844	-	-	13/29/63/63	0/2/2/2
19	CLA	B2	810	-	1/1/20/20	16/39/115/115	-
19	CLA	BB	817	-	1/1/14/20	2/12/88/115	-
19	CLA	B1	807	-	1/1/20/20	11/39/115/115	-
19	CLA	B	802	-	1/1/20/20	10/39/115/115	-
19	CLA	B2	817	-	1/1/14/20	4/12/88/115	-
27	SF4	C1	101	-	-	-	0/6/5/5
23	BCR	I2	101	-	-	16/29/63/63	0/2/2/2
19	CLA	A1	804	-	1/1/19/20	11/33/109/115	-
19	CLA	B1	803	-	1/1/20/20	12/39/115/115	-
23	BCR	B	843	-	-	16/29/63/63	0/2/2/2
19	CLA	B2	837	-	1/1/19/20	11/33/109/115	-
19	CLA	A1	817	-	1/1/15/20	5/15/91/115	-
22	LHG	A1	845	-	-	19/53/53/53	-
22	LHG	BB	851	-	-	20/53/53/53	-
23	BCR	J1	104	-	-	18/29/63/63	0/2/2/2
23	BCR	B	844	-	-	14/29/63/63	0/2/2/2
22	LHG	X	102	-	-	17/44/44/53	-
19	CLA	A1	828	-	1/1/20/20	16/39/115/115	-
25	LMG	B1	852	-	-	5/25/45/70	0/1/1/1
24	AJP	M2	101	-	12/12/14/38	-	0/6/6/11
19	CLA	A1	825	-	1/1/15/20	7/15/91/115	-
19	CLA	A2	817	-	1/1/14/20	2/14/90/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	L2	208	-	-	16/39/39/53	-
27	SF4	C1	102	-	-	-	0/6/5/5
19	CLA	L2	205	-	1/1/18/20	8/32/108/115	-
19	CLA	A	824	-	1/1/15/20	7/15/91/115	-
19	CLA	B1	802	-	1/1/20/20	12/39/115/115	-
19	CLA	A	844	-	1/1/14/20	4/10/86/115	-
19	CLA	BB	822	-	1/1/20/20	7/39/115/115	-
19	CLA	A2	838	-	1/1/14/20	4/14/90/115	-
19	CLA	A1	823	-	1/1/15/20	5/15/91/115	-
19	CLA	A2	807	-	1/1/20/20	16/39/115/115	-
19	CLA	BB	815	-	1/1/20/20	14/39/115/115	-
19	CLA	B	819	-	1/1/14/20	3/10/86/115	-
19	CLA	AA	812	-	1/1/15/20	9/17/93/115	-
19	CLA	B2	815	-	1/1/20/20	13/39/115/115	-
19	CLA	AA	853	-	1/1/20/20	14/39/115/115	-
19	CLA	B2	836	-	1/1/20/20	13/39/115/115	-
19	CLA	A	830	-	1/1/19/20	13/36/112/115	-
25	LMG	B	845	-	-	19/50/70/70	0/1/1/1
23	BCR	B2	840	-	-	7/29/63/63	0/2/2/2
19	CLA	A2	828	-	1/1/18/20	11/29/105/115	-
19	CLA	BB	814	-	1/1/18/20	10/32/108/115	-
23	BCR	J	102	-	-	19/29/63/63	0/2/2/2
19	CLA	A	825	-	1/1/17/20	5/24/100/115	-
19	CLA	A2	816	-	1/1/17/20	6/21/97/115	-
23	BCR	L2	207	-	-	19/29/63/63	0/2/2/2
19	CLA	B2	852	-	1/1/20/20	15/39/115/115	-
19	CLA	B	837	-	1/1/19/20	10/33/109/115	-
19	CLA	AA	843	-	1/1/20/20	15/39/115/115	-
19	CLA	B1	836	-	1/1/19/20	10/33/109/115	-
19	CLA	L1	207	-	1/1/20/20	10/39/115/115	-
19	CLA	B2	825	-	1/1/20/20	16/39/115/115	-
19	CLA	A2	836	-	-	15/39/115/115	-
19	CLA	A1	801	-	1/1/20/20	13/39/115/115	-
19	CLA	B1	825	-	1/1/20/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A2	847	-	-	11/27/61/63	0/2/2/2
19	CLA	BB	803	-	1/1/20/20	11/39/115/115	-
19	CLA	A2	802	-	1/1/15/20	7/17/93/115	-
19	CLA	A	823	-	1/1/19/20	15/33/109/115	-
23	BCR	B2	839	-	-	19/29/63/63	0/2/2/2
24	AJP	I2	104	-	12/12/14/38	-	0/6/6/11
19	CLA	A2	818	-	1/1/15/20	5/15/91/115	-
19	CLA	AA	809	-	1/1/17/20	5/21/97/115	-
19	CLA	F	301	-	1/1/19/20	10/33/109/115	-
19	CLA	XX	101	-	1/1/15/20	7/15/91/115	-
19	CLA	A1	819	-	-	11/31/107/115	-
23	BCR	I1	101	-	-	17/29/63/63	0/2/2/2
23	BCR	B	842	-	-	18/29/63/63	0/2/2/2
19	CLA	AA	837	-	1/1/15/20	1/15/91/115	-
23	BCR	MM	101	-	-	23/29/63/63	0/2/2/2
19	CLA	A1	809	-	1/1/20/20	9/39/115/115	-
19	CLA	A1	838	-	1/1/17/20	8/24/100/115	-
24	AJP	KK	104	-	16/16/19/38	2/4/116/220	0/7/7/11
19	CLA	AA	819	-	1/1/19/20	11/33/109/115	-
19	CLA	A2	835	-	1/1/20/20	10/39/115/115	-
19	CLA	A2	826	-	1/1/15/20	7/15/91/115	-
24	AJP	B	857	-	16/16/19/38	0/6/121/220	0/7/7/11
19	CLA	A2	815	-	1/1/18/20	7/27/103/115	-
19	CLA	A1	837	1	1/1/14/20	4/14/90/115	-
19	CLA	A	834	-	1/1/14/20	2/10/86/115	-
23	BCR	BB	839	-	-	8/29/63/63	0/2/2/2
19	CLA	A1	815	-	1/1/17/20	8/21/97/115	-
19	CLA	AA	821	-	1/1/20/20	12/39/115/115	-
19	CLA	B1	801	-	1/1/20/20	21/39/115/115	-
19	CLA	L1	206	-	1/1/20/20	5/39/115/115	-
19	CLA	A2	837	-	1/1/15/20	5/15/91/115	-
23	BCR	AA	851	-	-	15/29/63/63	0/2/2/2
26	ECH	B2	841	-	-	16/29/66/66	0/2/2/2
19	CLA	A1	808	-	1/1/17/20	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	J1	102	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	840	-	1/1/15/20	2/17/93/115	-
19	CLA	L	202	18	1/1/19/20	12/35/111/115	-
23	BCR	F1	306	-	-	24/29/63/63	0/2/2/2
27	SF4	BB	857	-	-	-	0/6/5/5
22	LHG	XX	102	-	-	17/44/44/53	-
19	CLA	B1	833	-	1/1/19/20	20/39/115/115	-
22	LHG	L	207	-	-	12/38/38/53	-
24	AJP	L1	203	-	16/16/19/38	4/6/121/220	0/7/7/11
25	LMG	B1	846	-	-	10/27/47/70	0/1/1/1
19	CLA	B1	827	-	1/1/15/20	6/15/91/115	-
25	LMG	B1	844	-	-	19/50/70/70	0/1/1/1
19	CLA	A1	812	-	1/1/20/20	11/39/115/115	-
23	BCR	A	848	-	-	16/29/63/63	0/2/2/2
19	CLA	A	801	-	1/1/20/20	11/39/115/115	-
23	BCR	J	104	-	-	16/29/63/63	0/2/2/2
19	CLA	L	204	-	1/1/20/20	14/39/115/115	-
23	BCR	FF	304	-	-	14/29/63/63	0/2/2/2
19	CLA	B	827	-	1/1/15/20	8/15/91/115	-
19	CLA	A2	804	-	1/1/20/20	18/39/115/115	-
19	CLA	A2	813	-	1/1/20/20	13/39/115/115	-
19	CLA	K1	105	9	1/1/13/20	4/10/82/115	-
19	CLA	BB	811	-	1/1/19/20	15/35/111/115	-
23	BCR	I	102	-	-	10/29/63/63	0/2/2/2
19	CLA	B	831	-	1/1/18/20	4/29/105/115	-
24	AJP	L2	202	-	17/17/19/38	3/6/121/220	0/7/7/11
24	AJP	BB	849	-	17/17/19/38	3/6/121/220	0/7/7/11
19	CLA	A	804	-	1/1/20/20	18/39/115/115	-
23	BCR	A	854	-	-	17/29/63/63	0/2/2/2
19	CLA	A	805	-	1/1/19/20	8/33/109/115	-
19	CLA	A	807	-	1/1/20/20	18/39/115/115	-
25	LMG	B2	854	-	-	5/25/45/70	0/1/1/1
19	CLA	B1	829	-	1/1/18/20	5/29/105/115	-
19	CLA	BB	807	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A2	830	-	1/1/19/20	15/36/112/115	-
23	BCR	I	101	-	-	21/29/63/63	0/2/2/2
22	LHG	A	846	-	-	11/42/42/53	-
22	LHG	A1	846	-	-	11/42/42/53	-
19	CLA	AA	820	-	1/1/18/20	10/31/107/115	-
19	CLA	J	101	8	1/1/14/20	4/10/86/115	-
19	CLA	J2	101	8	1/1/14/20	4/10/86/115	-
19	CLA	B2	851	-	1/1/19/20	11/33/109/115	-
19	CLA	A	806	-	1/1/18/20	9/29/105/115	-
24	AJP	A2	854	-	12/12/14/38	-	0/6/6/11
19	CLA	B1	812	-	1/1/14/20	4/10/86/115	-
27	SF4	C2	102	-	-	-	0/6/5/5
25	LMG	B2	847	-	-	9/27/47/70	0/1/1/1
19	CLA	A	816	-	1/1/17/20	6/21/97/115	-
19	CLA	A1	822	-	1/1/19/20	12/33/109/115	-
19	CLA	AA	810	-	1/1/20/20	8/39/115/115	-
19	CLA	BB	845	-	1/1/12/20	1/7/79/115	-
19	CLA	B	835	-	1/1/15/20	1/15/91/115	-
19	CLA	A2	832	-	1/1/20/20	8/39/115/115	-
19	CLA	BB	833	-	1/1/19/20	20/39/115/115	-
19	CLA	B	804	-	1/1/19/20	6/36/112/115	-
23	BCR	M	101	-	-	21/29/63/63	0/2/2/2
23	BCR	K2	103	-	-	10/29/63/63	0/2/2/2
19	CLA	BB	855	-	1/1/20/20	4/39/115/115	-
25	LMG	L1	210	-	-	16/50/70/70	0/1/1/1
20	CL0	A1	802	-	4/4/25/25	11/37/135/135	-
19	CLA	B	832	-	1/1/15/20	7/15/91/115	-
19	CLA	A2	821	-	1/1/20/20	11/39/115/115	-
23	BCR	B1	841	-	-	20/29/63/63	0/2/2/2
21	PQN	A1	843	-	-	8/23/43/43	0/2/2/2
19	CLA	B2	811	-	1/1/19/20	14/35/111/115	-
19	CLA	L1	205	10	1/1/19/20	10/35/111/115	-
22	LHG	A	845	-	-	18/53/53/53	-
19	CLA	F1	301	-	1/1/19/20	8/33/109/115	-
19	CLA	A1	833	-	1/1/14/20	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	805	-	1/1/19/20	9/38/114/115	-
19	CLA	A1	807	-	1/1/20/20	14/39/115/115	-
19	CLA	A	822	-	1/1/17/20	7/23/99/115	-
19	CLA	A2	834	-	1/1/14/20	2/10/86/115	-
19	CLA	A2	842	-	1/1/20/20	11/39/115/115	-
27	SF4	CC	101	-	-	-	0/6/5/5
19	CLA	BB	829	-	1/1/18/20	6/29/105/115	-
19	CLA	BB	801	-	1/1/20/20	20/39/115/115	-
19	CLA	L2	204	16	1/1/19/20	14/35/111/115	-
19	CLA	AA	831	-	1/1/20/20	12/39/115/115	-
19	CLA	BB	821	-	1/1/20/20	16/39/115/115	-
19	CLA	B2	816	-	1/1/18/20	10/30/106/115	-
19	CLA	B2	801	-	1/1/20/20	19/39/115/115	-
19	CLA	B2	822	-	1/1/20/20	8/39/115/115	-
19	CLA	BB	825	-	1/1/20/20	16/39/115/115	-
21	PQN	A	843	-	-	8/23/43/43	0/2/2/2
23	BCR	B1	842	-	-	15/29/63/63	0/2/2/2
23	BCR	AA	849	-	-	16/29/63/63	0/2/2/2
19	CLA	A	819	-	1/1/19/20	10/33/109/115	-
19	CLA	B1	805	-	1/1/19/20	9/38/114/115	-
23	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	B	829	-	1/1/20/20	13/39/115/115	-
19	CLA	LL	203	-	1/1/14/20	6/12/88/115	-
23	BCR	F2	305	-	-	26/29/63/63	0/2/2/2
19	CLA	BB	819	-	1/1/14/20	2/10/86/115	-
23	BCR	A1	853	-	-	16/29/63/63	0/2/2/2
19	CLA	BB	812	-	1/1/14/20	4/10/86/115	-
19	CLA	AA	825	-	1/1/17/20	4/24/100/115	-
19	CLA	A	814	-	1/1/14/20	5/12/88/115	-
19	CLA	BB	820	-	1/1/15/20	11/15/91/115	-
19	CLA	B	813	-	1/1/14/20	8/12/88/115	-
23	BCR	FF	303	-	-	20/29/63/63	0/2/2/2
19	CLA	B1	820	-	1/1/15/20	11/15/91/115	-
19	CLA	B2	820	-	1/1/15/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	II	105	-	-	20/37/57/70	0/1/1/1
23	BCR	A2	848	-	-	14/29/63/63	0/2/2/2
19	CLA	A2	801	-	1/1/20/20	13/39/115/115	-
19	CLA	A2	820	-	1/1/18/20	10/31/107/115	-
19	CLA	B1	816	-	1/1/18/20	9/30/106/115	-
22	LHG	B1	847	-	-	13/37/37/53	-
23	BCR	L1	201	-	-	12/29/63/63	0/2/2/2
19	CLA	B	828	-	1/1/15/20	4/15/91/115	-
19	CLA	A2	811	-	1/1/17/20	8/23/99/115	-
19	CLA	AA	833	-	1/1/17/20	4/21/97/115	-
24	AJP	AA	856	-	12/12/16/38	2/4/99/220	0/6/6/11
24	AJP	B	849	-	18/18/19/38	3/6/121/220	0/7/7/11
19	CLA	BB	810	-	1/1/20/20	15/39/115/115	-
28	DGD	BB	854	-	-	23/31/71/95	0/2/2/2
19	CLA	FF	305	-	1/1/20/20	11/39/115/115	-
19	CLA	B1	810	-	1/1/20/20	13/39/115/115	-
19	CLA	F1	305	-	1/1/15/20	3/15/91/115	-
19	CLA	B	830	-	1/1/18/20	4/29/105/115	-
23	BCR	II	104	-	-	17/29/63/63	0/2/2/2
23	BCR	BB	841	-	-	20/29/63/63	0/2/2/2
19	CLA	A2	805	-	1/1/19/20	8/33/109/115	-
19	CLA	AA	839	-	1/1/17/20	8/24/100/115	-
19	CLA	BB	836	-	1/1/19/20	11/33/109/115	-
23	BCR	A2	849	-	-	13/29/63/63	0/2/2/2
23	BCR	A	853	-	-	16/29/63/63	0/2/2/2
19	CLA	A1	829	-	1/1/19/20	14/36/112/115	-
19	CLA	AA	805	-	1/1/19/20	8/33/109/115	-
22	LHG	A2	846	-	-	11/42/42/53	-
19	CLA	A1	821	-	1/1/17/20	6/23/99/115	-
19	CLA	B2	814	-	1/1/18/20	12/32/108/115	-
19	CLA	B1	832	-	1/1/20/20	13/39/115/115	-
19	CLA	AA	824	-	1/1/15/20	7/15/91/115	-
19	CLA	A	826	-	1/1/15/20	7/15/91/115	-
23	BCR	B	848	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	830	-	1/1/19/20	12/36/112/115	-
19	CLA	A2	806	-	1/1/18/20	9/29/105/115	-
27	SF4	B2	853	-	-	-	0/6/5/5
19	CLA	AA	817	-	1/1/14/20	4/14/90/115	-
19	CLA	A	827	-	1/1/20/20	15/39/115/115	-
19	CLA	B	808	-	1/1/19/20	11/33/109/115	-
23	BCR	A1	847	-	-	11/27/61/63	0/2/2/2
19	CLA	A2	841	-	1/1/15/20	3/17/93/115	-
23	BCR	B	840	-	-	9/29/63/63	0/2/2/2
19	CLA	B	815	-	1/1/20/20	15/39/115/115	-
19	CLA	AA	806	-	1/1/18/20	9/29/105/115	-
19	CLA	B1	850	-	1/1/19/20	12/33/109/115	-
25	LMG	M	102	-	-	15/41/61/70	0/1/1/1
19	CLA	B2	850	-	1/1/20/20	4/39/115/115	-
22	LHG	X2	103	-	-	22/53/53/53	-
19	CLA	AA	838	-	1/1/14/20	4/14/90/115	-
19	CLA	A	832	-	1/1/20/20	9/39/115/115	-
19	CLA	AA	823	-	1/1/19/20	14/33/109/115	-
19	CLA	FF	302	-	1/1/14/20	4/12/88/115	-
19	CLA	A2	810	1	1/1/20/20	8/39/115/115	-
19	CLA	A	829	-	1/1/20/20	12/39/115/115	-
24	AJP	A1	854	-	16/16/19/38	2/6/121/220	0/7/7/11
19	CLA	B	834	-	1/1/19/20	20/39/115/115	-
19	CLA	B2	829	-	1/1/20/20	13/39/115/115	-
19	CLA	B1	824	-	1/1/18/20	13/27/103/115	-
19	CLA	BB	852	-	1/1/20/20	11/39/115/115	-
24	AJP	A	802	-	11/11/14/38	-	0/6/6/11
22	LHG	AA	847	-	-	11/42/42/53	-
22	LHG	A2	845	-	-	15/53/53/53	-
24	AJP	L	209	-	13/13/14/38	-	0/6/6/11
19	CLA	B1	822	-	1/1/20/20	4/39/115/115	-
19	CLA	A2	822	-	1/1/17/20	6/23/99/115	-
19	CLA	AA	836	-	1/1/20/20	18/39/115/115	-
19	CLA	A2	825	-	1/1/14/20	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	842	-	1/1/20/20	10/39/115/115	-
19	CLA	AA	807	-	1/1/20/20	17/39/115/115	-
19	CLA	AA	828	-	1/1/18/20	11/29/105/115	-
19	CLA	A1	814	-	1/1/18/20	7/27/103/115	-
19	CLA	L2	206	-	1/1/20/20	12/39/115/115	-
19	CLA	AA	845	-	1/1/14/20	4/10/86/115	-
23	BCR	L1	208	-	-	15/29/63/63	0/2/2/2
19	CLA	B2	809	-	1/1/15/20	5/15/91/115	-
19	CLA	AA	842	-	1/1/20/20	10/39/115/115	-
19	CLA	L	203	-	1/1/20/20	10/39/115/115	-
24	AJP	A	855	-	12/12/16/38	2/4/99/220	1/6/6/11
19	CLA	B	820	-	1/1/15/20	11/15/91/115	-
19	CLA	K	102	-	1/1/15/20	9/17/93/115	-
19	CLA	A	813	-	1/1/20/20	11/39/115/115	-
19	CLA	A2	812	-	1/1/15/20	7/17/93/115	-
19	CLA	AA	818	-	1/1/15/20	5/15/91/115	-
19	CLA	A2	823	-	1/1/19/20	14/33/109/115	-
25	LMG	B2	845	-	-	21/50/70/70	0/1/1/1
19	CLA	B	811	-	1/1/19/20	13/35/111/115	-
26	ECH	BB	840	-	-	16/29/66/66	0/2/2/2
19	CLA	B2	827	-	1/1/15/20	6/15/91/115	-
23	BCR	B1	839	-	-	8/29/63/63	0/2/2/2
23	BCR	B	839	-	-	16/29/63/63	0/2/2/2
23	BCR	FF	306	-	-	21/29/63/63	0/2/2/2
26	ECH	B	841	-	-	16/29/66/66	0/2/2/2
24	AJP	L2	203	-	16/16/19/38	4/6/121/220	0/7/7/11
22	LHG	X1	103	-	-	18/53/53/53	-
19	CLA	B1	809	-	1/1/15/20	5/15/91/115	-
19	CLA	B1	804	-	1/1/19/20	9/36/112/115	-
19	CLA	B1	818	-	1/1/14/20	0/10/86/115	-
19	CLA	A	820	-	-	12/31/107/115	-
23	BCR	JJ	102	-	-	20/29/63/63	0/2/2/2
19	CLA	B	810	-	1/1/20/20	15/39/115/115	-
25	LMG	I1	102	-	-	17/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A1	849	-	-	12/29/63/63	0/2/2/2
19	CLA	AA	815	-	1/1/18/20	7/27/103/115	-
19	CLA	B	816	-	1/1/18/20	9/30/106/115	-
19	CLA	B	822	-	1/1/20/20	4/39/115/115	-
19	CLA	B	860	-	1/1/20/20	15/39/115/115	-
27	SF4	B1	851	-	-	-	0/6/5/5
23	BCR	B2	842	-	-	21/29/63/63	0/2/2/2
19	CLA	B1	848	-	1/1/20/20	12/39/115/115	-
27	SF4	B	861	-	-	-	0/6/5/5
21	PQN	AA	844	-	-	4/23/43/43	0/2/2/2
19	CLA	B1	828	-	1/1/20/20	11/39/115/115	-
19	CLA	A2	814	-	1/1/14/20	5/12/88/115	-
19	CLA	A2	852	-	1/1/20/20	12/39/115/115	-
19	CLA	K1	103	-	1/1/15/20	7/17/93/115	-
19	CLA	A1	806	-	1/1/20/20	16/39/115/115	-
23	BCR	A2	850	-	-	14/29/63/63	0/2/2/2
19	CLA	B1	819	-	1/1/14/20	2/10/86/115	-
23	BCR	A	849	-	-	17/29/63/63	0/2/2/2
19	CLA	B	803	-	1/1/20/20	10/39/115/115	-
23	BCR	AA	854	-	-	16/29/63/63	0/2/2/2
19	CLA	A1	827	-	1/1/18/20	11/29/105/115	-
19	CLA	A2	839	-	1/1/17/20	8/24/100/115	-
19	CLA	A	821	-	1/1/20/20	13/39/115/115	-
21	PQN	B2	838	-	-	7/23/43/43	0/2/2/2
19	CLA	BB	832	-	-	12/39/115/115	-
19	CLA	B2	803	-	1/1/20/20	10/39/115/115	-
19	CLA	AA	827	-	1/1/20/20	15/39/115/115	-
19	CLA	B2	832	-	1/1/15/20	8/15/91/115	-
19	CLA	A2	827	-	1/1/20/20	15/39/115/115	-
28	DGD	B	856	-	-	23/31/71/95	0/2/2/2
19	CLA	B2	846	-	1/1/12/20	0/7/79/115	-
19	CLA	A1	831	-	1/1/20/20	8/39/115/115	-
22	LHG	AA	846	-	-	19/53/53/53	-
26	ECH	B1	840	-	-	16/29/66/66	0/2/2/2
19	CLA	A1	832	-	1/1/17/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B1	843	-	-	13/29/63/63	0/2/2/2
19	CLA	B2	828	-	1/1/15/20	0/15/91/115	-
19	CLA	A	840	-	1/1/18/20	5/29/105/115	-
24	AJP	A1	855	-	12/12/14/38	-	0/6/6/11
23	BCR	A	847	-	-	12/27/61/63	0/2/2/2
23	BCR	LL	204	-	-	17/29/63/63	0/2/2/2
19	CLA	FF	301	-	1/1/19/20	12/33/109/115	-
23	BCR	F	303	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	816	-	1/1/14/20	0/14/90/115	-
23	BCR	I2	103	-	-	16/29/63/63	0/2/2/2
19	CLA	A	841	-	1/1/15/20	2/17/93/115	-
19	CLA	AA	816	-	1/1/17/20	8/21/97/115	-
21	PQN	BB	837	-	-	7/23/43/43	0/2/2/2
23	BCR	A2	851	-	-	17/29/63/63	0/2/2/2
19	CLA	B2	802	-	1/1/20/20	7/39/115/115	-
19	CLA	KK	101	-	1/1/15/20	0/15/91/115	-
19	CLA	B1	808	-	1/1/19/20	12/33/109/115	-
19	CLA	A2	829	-	1/1/20/20	13/39/115/115	-
19	CLA	BB	818	-	1/1/14/20	2/10/86/115	-
23	BCR	KK	103	-	-	18/29/63/63	0/2/2/2
24	AJP	K	104	-	16/16/19/38	2/4/116/220	0/7/7/11
19	CLA	A2	808	-	1/1/20/20	15/39/115/115	-
19	CLA	A	810	1	1/1/20/20	9/39/115/115	-
19	CLA	B2	818	-	1/1/14/20	0/10/86/115	-
19	CLA	A1	803	-	1/1/20/20	17/39/115/115	-
23	BCR	BB	843	-	-	13/29/63/63	0/2/2/2
19	CLA	BB	835	-	1/1/20/20	11/39/115/115	-
23	BCR	B2	843	-	-	18/29/63/63	0/2/2/2
19	CLA	B	826	-	1/1/20/20	14/39/115/115	-
19	CLA	BB	826	-	1/1/20/20	16/39/115/115	-
19	CLA	BB	828	-	1/1/15/20	1/15/91/115	-
22	LHG	LL	205	-	-	12/38/38/53	-
19	CLA	B2	835	-	1/1/15/20	1/15/91/115	-
19	CLA	AA	834	-	1/1/14/20	2/10/86/115	-
19	CLA	B1	826	-	1/1/20/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	826	-	1/1/20/20	14/39/115/115	-
19	CLA	A1	835	-	1/1/20/20	13/39/115/115	-
19	CLA	B	818	-	1/1/14/20	2/10/86/115	-
19	CLA	B	801	-	1/1/20/20	16/39/115/115	-
19	CLA	LL	202	-	1/1/20/20	6/39/115/115	-
19	CLA	B1	831	-	1/1/15/20	8/15/91/115	-
19	CLA	A2	809	-	1/1/17/20	5/21/97/115	-
19	CLA	AA	835	-	1/1/20/20	10/39/115/115	-
23	BCR	BB	847	-	-	16/29/63/63	0/2/2/2
19	CLA	B1	823	-	1/1/20/20	16/39/115/115	-
19	CLA	B	823	-	1/1/20/20	12/39/115/115	-
19	CLA	AA	804	-	1/1/20/20	16/39/115/115	-
19	CLA	K2	102	-	1/1/15/20	0/15/91/115	-
19	CLA	AA	822	-	-	8/23/99/115	-
23	BCR	L	206	-	-	17/29/63/63	0/2/2/2
19	CLA	AA	832	-	1/1/20/20	6/39/115/115	-
23	BCR	L	205	-	-	17/29/63/63	0/2/2/2
23	BCR	BB	838	-	-	15/29/63/63	0/2/2/2
19	CLA	B2	819	-	1/1/14/20	2/10/86/115	-
19	CLA	B	805	-	1/1/19/20	10/38/114/115	-
19	CLA	B1	849	-	1/1/20/20	4/39/115/115	-
27	SF4	C2	101	-	-	-	0/6/5/5
19	CLA	J1	103	-	1/1/14/20	2/10/86/115	-
21	PQN	B1	837	-	-	7/23/43/43	0/2/2/2
25	LMG	B	851	-	-	17/50/70/70	0/1/1/1
19	CLA	A	812	-	1/1/15/20	9/17/93/115	-
23	BCR	AA	850	-	-	15/29/63/63	0/2/2/2
19	CLA	A	835	-	1/1/20/20	10/39/115/115	-
27	SF4	CC	102	-	-	-	0/6/5/5
23	BCR	A1	850	-	-	13/29/63/63	0/2/2/2
19	CLA	F	302	-	1/1/14/20	4/12/88/115	-
19	CLA	A1	826	-	1/1/20/20	17/39/115/115	-
23	BCR	F1	304	-	-	15/29/63/63	0/2/2/2
23	BCR	B1	838	-	-	19/29/63/63	0/2/2/2
19	CLA	A1	818	-	1/1/19/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	826	-	1/1/15/20	7/15/91/115	-
19	CLA	B	806	-	1/1/20/20	13/39/115/115	-
19	CLA	B1	835	-	1/1/20/20	12/39/115/115	-
19	CLA	BB	813	-	1/1/14/20	6/12/88/115	-
23	BCR	F1	303	-	-	16/29/63/63	0/2/2/2
19	CLA	A1	813	-	1/1/14/20	5/12/88/115	-
19	CLA	A	852	-	1/1/20/20	13/39/115/115	-
19	CLA	B	836	-	1/1/20/20	11/39/115/115	-
19	CLA	X1	101	-	1/1/15/20	6/15/91/115	-
19	CLA	AA	813	-	1/1/20/20	10/39/115/115	-
19	CLA	BB	827	-	1/1/15/20	4/15/91/115	-
19	CLA	A1	844	-	1/1/14/20	4/10/86/115	-
19	CLA	A	831	-	1/1/20/20	10/39/115/115	-
23	BCR	K1	104	-	-	17/29/63/63	0/2/2/2
19	CLA	A2	844	-	1/1/14/20	4/10/86/115	-
19	CLA	A1	805	-	-	8/29/105/115	-
19	CLA	BB	831	-	1/1/15/20	6/15/91/115	-
24	AJP	L1	204	-	16/16/19/38	3/6/121/220	0/7/7/11
23	BCR	L1	209	-	-	18/29/63/63	0/2/2/2
19	CLA	A	839	-	1/1/17/20	8/24/100/115	-
19	CLA	A1	841	-	1/1/20/20	9/39/115/115	-
19	CLA	B2	831	-	1/1/18/20	6/29/105/115	-
23	BCR	II	102	-	-	9/29/63/63	0/2/2/2
19	CLA	B2	812	-	1/1/14/20	4/10/86/115	-
19	CLA	B2	830	-	1/1/18/20	4/29/105/115	-
19	CLA	AA	801	-	1/1/20/20	13/39/115/115	-
23	BCR	JJ	104	-	-	16/29/63/63	0/2/2/2
19	CLA	A1	830	-	1/1/20/20	12/39/115/115	-
19	CLA	B	821	2	1/1/20/20	12/39/115/115	-

All (3996) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	AJP	C14-C15	-11.31	1.35	1.53
24	AA	802	AJP	C14-C15	-11.24	1.35	1.53
24	L	208	AJP	C14-C15	-11.10	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	849	AJP	C14-C15	-11.05	1.35	1.53
24	L2	202	AJP	C14-C15	-10.79	1.36	1.53
24	B	850	AJP	C14-C15	-10.69	1.36	1.53
24	AA	856	AJP	C16-C11	-10.68	1.39	1.54
24	L2	202	AJP	C16-C11	-10.66	1.39	1.54
24	A	855	AJP	C16-C11	-10.66	1.39	1.54
24	M2	101	AJP	C14-C15	-10.64	1.36	1.53
24	L1	203	AJP	C14-C15	-10.64	1.36	1.53
24	L1	203	AJP	C16-C11	-10.64	1.39	1.54
24	L2	203	AJP	C14-C15	-10.62	1.36	1.53
24	L	209	AJP	C14-C15	-10.61	1.36	1.53
24	BB	848	AJP	C16-C11	-10.59	1.39	1.54
24	L1	204	AJP	C14-C15	-10.57	1.36	1.53
24	AA	802	AJP	C16-C11	-10.54	1.39	1.54
24	L1	204	AJP	C16-C11	-10.53	1.39	1.54
24	A	802	AJP	C16-C11	-10.52	1.39	1.54
24	B	849	AJP	C14-C15	-10.51	1.36	1.53
24	KK	104	AJP	C14-C15	-10.50	1.36	1.53
24	B	849	AJP	C16-C11	-10.48	1.40	1.54
24	A1	854	AJP	C16-C11	-10.45	1.40	1.54
24	K	104	AJP	C14-C15	-10.44	1.36	1.53
24	BB	848	AJP	C14-C15	-10.43	1.36	1.53
24	B	850	AJP	C16-C11	-10.39	1.40	1.54
24	B	857	AJP	C14-C15	-10.38	1.36	1.53
24	K	104	AJP	C16-C11	-10.38	1.40	1.54
24	A1	854	AJP	C14-C15	-10.29	1.36	1.53
24	M2	101	AJP	C16-C11	-10.29	1.40	1.54
24	B	857	AJP	C16-C11	-10.28	1.40	1.54
24	L	209	AJP	C16-C11	-10.28	1.40	1.54
24	A1	855	AJP	C14-C15	-10.27	1.36	1.53
24	A2	854	AJP	C14-C15	-10.26	1.36	1.53
24	I2	104	AJP	C14-C15	-10.24	1.36	1.53
24	I2	104	AJP	C16-C11	-10.24	1.40	1.54
24	L2	203	AJP	C16-C11	-10.24	1.40	1.54
20	AA	803	CL0	C3B-C4B	10.22	1.51	1.41
20	A1	802	CL0	C3B-C4B	10.20	1.51	1.41
24	BB	849	AJP	C16-C11	-10.14	1.40	1.54
24	KK	104	AJP	C16-C11	-10.03	1.40	1.54
24	A1	855	AJP	C16-C11	-10.02	1.40	1.54
24	A2	854	AJP	C16-C11	-10.01	1.40	1.54
24	A	855	AJP	C14-C15	-9.93	1.37	1.53
24	AA	856	AJP	C14-C15	-9.92	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	803	CL0	C3B-C4B	9.88	1.51	1.41
20	A	803	CL0	C1D-C2D	9.68	1.50	1.39
24	BB	848	AJP	C18-C17	-9.61	1.29	1.52
20	A2	803	CL0	C3B-C4B	9.55	1.50	1.41
24	B	849	AJP	C18-C17	-9.53	1.29	1.52
20	A2	803	CL0	C1D-C2D	9.51	1.50	1.39
24	L1	203	AJP	C18-C17	-9.51	1.29	1.52
24	L2	202	AJP	C18-C17	-9.50	1.29	1.52
20	A1	802	CL0	C1D-C2D	9.45	1.50	1.39
24	L	208	AJP	C16-C11	-9.41	1.41	1.54
24	BB	849	AJP	C13-C12	-9.37	1.37	1.54
24	A	855	AJP	C13-C12	-9.36	1.37	1.54
24	AA	856	AJP	C13-C12	-9.35	1.37	1.54
24	A1	854	AJP	C13-C12	-9.35	1.37	1.54
24	B	857	AJP	C13-C12	-9.35	1.37	1.54
24	L	209	AJP	C13-C12	-9.30	1.37	1.54
24	L	208	AJP	C13-C12	-9.28	1.38	1.54
24	I2	104	AJP	C18-C17	-9.27	1.30	1.52
24	L1	204	AJP	C18-C17	-9.27	1.30	1.52
24	A1	855	AJP	C18-C17	-9.26	1.30	1.52
24	A2	854	AJP	C18-C17	-9.26	1.30	1.52
24	AA	802	AJP	C18-C17	-9.25	1.30	1.52
24	L	208	AJP	C18-C17	-9.25	1.30	1.52
24	A	802	AJP	C18-C17	-9.24	1.30	1.52
24	KK	104	AJP	C18-C17	-9.24	1.30	1.52
24	K	104	AJP	C18-C17	-9.23	1.30	1.52
20	AA	803	CL0	C1D-C2D	9.21	1.50	1.39
24	M2	101	AJP	C13-C12	-9.18	1.38	1.54
24	BB	849	AJP	C18-C17	-9.18	1.30	1.52
24	B	850	AJP	C18-C17	-9.16	1.30	1.52
24	A1	855	AJP	C13-C12	-9.14	1.38	1.54
24	L2	202	AJP	C13-C12	-9.13	1.38	1.54
24	L1	203	AJP	C13-C12	-9.12	1.38	1.54
24	B	850	AJP	C13-C12	-9.11	1.38	1.54
24	K	104	AJP	C13-C12	-9.10	1.38	1.54
24	L2	203	AJP	C18-C17	-9.09	1.30	1.52
24	A1	854	AJP	C18-C17	-9.09	1.30	1.52
24	A	855	AJP	C18-C17	-9.08	1.30	1.52
24	AA	856	AJP	C18-C17	-9.07	1.30	1.52
24	L2	203	AJP	C13-C12	-9.07	1.38	1.54
24	B	857	AJP	C18-C17	-9.05	1.31	1.52
24	A2	854	AJP	C13-C12	-9.05	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M2	101	AJP	C18-C17	-9.04	1.31	1.52
24	L	209	AJP	C18-C17	-9.03	1.31	1.52
20	A2	803	CL0	C1A-CHA	9.03	1.50	1.40
24	L1	204	AJP	C13-C12	-8.98	1.38	1.54
24	KK	104	AJP	C13-C12	-8.96	1.38	1.54
24	B	849	AJP	C13-C12	-8.96	1.38	1.54
24	A	802	AJP	C13-C12	-8.86	1.38	1.54
24	AA	802	AJP	C13-C12	-8.86	1.38	1.54
24	I2	104	AJP	C13-C12	-8.69	1.39	1.54
24	BB	848	AJP	C13-C12	-8.60	1.39	1.54
20	AA	803	CL0	C1A-CHA	8.50	1.49	1.40
20	A1	802	CL0	C1A-CHA	8.45	1.49	1.40
24	L2	203	AJP	O09-C05	8.23	1.59	1.42
24	BB	849	AJP	O09-C05	8.23	1.59	1.42
24	A1	855	AJP	O09-C05	8.22	1.59	1.42
24	A	802	AJP	O09-C05	8.20	1.59	1.42
24	KK	104	AJP	O09-C05	8.19	1.59	1.42
24	A2	854	AJP	O09-C05	8.19	1.59	1.42
24	AA	802	AJP	O09-C05	8.19	1.59	1.42
24	L	208	AJP	O09-C05	8.13	1.59	1.42
24	B	850	AJP	O09-C05	8.10	1.59	1.42
24	B	849	AJP	O09-C05	8.10	1.59	1.42
24	K	104	AJP	O09-C05	8.09	1.59	1.42
24	A	855	AJP	O09-C05	8.09	1.59	1.42
24	AA	856	AJP	O09-C05	8.09	1.59	1.42
24	L	209	AJP	O09-C05	8.08	1.59	1.42
24	M2	101	AJP	O09-C05	8.08	1.59	1.42
24	B	857	AJP	O09-C05	8.07	1.59	1.42
24	A1	854	AJP	O09-C05	8.07	1.59	1.42
24	L2	202	AJP	O09-C05	8.04	1.59	1.42
20	A	803	CL0	C1A-CHA	8.04	1.49	1.40
24	I2	104	AJP	O09-C05	8.01	1.59	1.42
24	L1	204	AJP	O09-C05	7.97	1.59	1.42
24	BB	848	AJP	O09-C05	7.97	1.59	1.42
24	L1	203	AJP	O09-C05	7.80	1.59	1.42
20	AA	803	CL0	C1B-C2B	7.63	1.48	1.39
20	A1	802	CL0	C1B-C2B	7.61	1.48	1.39
20	A2	803	CL0	C1B-C2B	7.60	1.48	1.39
20	A	803	CL0	C1B-C2B	7.57	1.48	1.39
24	L	209	AJP	C13-C14	-7.50	1.38	1.53
24	L	208	AJP	C13-C14	-7.50	1.38	1.53
24	B	857	AJP	C13-C14	-7.32	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	AJP	C13-C14	-7.28	1.38	1.53
24	AA	802	AJP	C13-C14	-7.26	1.38	1.53
24	AA	856	AJP	C13-C14	-7.25	1.39	1.53
24	A	855	AJP	C13-C14	-7.24	1.39	1.53
24	M2	101	AJP	C13-C14	-7.24	1.39	1.53
24	A1	854	AJP	C13-C14	-7.21	1.39	1.53
24	A2	854	AJP	C13-C14	-7.14	1.39	1.53
24	KK	104	AJP	C13-C14	-7.06	1.39	1.53
24	A1	855	AJP	C13-C14	-7.04	1.39	1.53
24	BB	849	AJP	C13-C14	-6.95	1.39	1.53
24	L2	202	AJP	C13-C14	-6.95	1.39	1.53
24	B	849	AJP	C13-C14	-6.94	1.39	1.53
24	L1	203	AJP	C13-C14	-6.92	1.39	1.53
24	K	104	AJP	C13-C14	-6.91	1.39	1.53
24	BB	848	AJP	C13-C14	-6.89	1.39	1.53
24	B	850	AJP	C13-C14	-6.80	1.39	1.53
24	L2	203	AJP	C13-C14	-6.63	1.40	1.53
24	I2	104	AJP	C12-C07	6.56	1.68	1.56
24	L1	204	AJP	C13-C14	-6.44	1.40	1.53
24	B	850	AJP	C12-C07	6.39	1.67	1.56
24	I2	104	AJP	C13-C14	-6.35	1.40	1.53
24	B	849	AJP	C12-C07	6.30	1.67	1.56
24	I2	104	AJP	C80-C20	6.26	1.64	1.54
24	K	104	AJP	C12-C07	6.23	1.67	1.56
24	BB	848	AJP	C12-C07	6.23	1.67	1.56
24	M2	101	AJP	C12-C07	6.22	1.67	1.56
24	L2	202	AJP	C12-C07	6.14	1.67	1.56
24	KK	104	AJP	C12-C07	6.14	1.67	1.56
24	L	209	AJP	C12-C07	6.11	1.67	1.56
24	B	850	AJP	C80-C20	6.09	1.64	1.54
24	L	208	AJP	C12-C07	6.03	1.67	1.56
24	L1	204	AJP	C80-C20	6.02	1.64	1.54
24	AA	802	AJP	C12-C07	6.00	1.67	1.56
24	A	802	AJP	C12-C07	5.97	1.66	1.56
24	L2	203	AJP	C80-C20	5.95	1.64	1.54
24	I2	104	AJP	C21-C22	5.90	1.60	1.52
24	BB	849	AJP	C80-C20	5.86	1.64	1.54
24	K	104	AJP	C80-C20	5.84	1.64	1.54
24	BB	849	AJP	C12-C07	5.83	1.66	1.56
24	L1	203	AJP	C21-C22	5.83	1.61	1.53
24	L	208	AJP	C21-C22	5.82	1.60	1.52
24	KK	104	AJP	C80-C20	5.82	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L1	204	AJP	C12-C07	5.82	1.66	1.56
24	M2	101	AJP	C21-C22	5.77	1.60	1.52
24	A1	854	AJP	C21-C22	5.75	1.61	1.53
24	BB	848	AJP	C21-C22	5.75	1.61	1.53
20	A	803	CL0	CHB-C4A	-5.67	1.31	1.38
24	L1	203	AJP	C12-C07	5.67	1.66	1.56
24	L	209	AJP	C21-C22	5.65	1.60	1.52
24	BB	848	AJP	C80-C20	5.64	1.63	1.54
24	L2	202	AJP	C21-C22	5.64	1.61	1.53
24	B	849	AJP	C21-C22	5.62	1.61	1.53
24	B	857	AJP	C21-C22	5.62	1.61	1.53
24	B	849	AJP	C80-C20	5.61	1.63	1.54
24	M2	101	AJP	C80-C20	5.59	1.63	1.54
24	A	855	AJP	C12-C07	5.59	1.66	1.56
24	AA	856	AJP	C12-C07	5.59	1.66	1.56
24	A2	854	AJP	C12-C07	5.58	1.66	1.56
24	A1	855	AJP	C12-C07	5.55	1.66	1.56
24	A1	854	AJP	C12-C07	5.54	1.66	1.56
24	B	857	AJP	C12-C07	5.54	1.66	1.56
24	L2	203	AJP	C12-C07	5.50	1.66	1.56
24	L	209	AJP	C80-C20	5.44	1.63	1.54
24	L2	202	AJP	C80-C20	5.44	1.63	1.54
24	L1	203	AJP	C80-C20	5.43	1.63	1.54
20	A	803	CL0	C3D-C4D	-5.43	1.33	1.41
24	AA	856	AJP	C21-C22	5.37	1.61	1.53
24	A	855	AJP	C21-C22	5.36	1.61	1.53
24	L	208	AJP	C80-C20	5.32	1.63	1.54
24	L1	204	AJP	C21-C22	5.31	1.61	1.53
20	A1	802	CL0	CHB-C4A	-5.29	1.32	1.38
20	A1	802	CL0	C3D-C4D	-5.26	1.33	1.41
24	BB	849	AJP	C21-C22	5.24	1.61	1.53
20	AA	803	CL0	CHB-C4A	-5.18	1.32	1.38
24	L2	203	AJP	C21-C22	5.15	1.60	1.53
20	AA	803	CL0	C3D-C4D	-5.12	1.33	1.41
24	AA	802	AJP	C80-C20	5.09	1.62	1.54
24	B	850	AJP	C21-C22	5.08	1.60	1.53
24	A	802	AJP	C80-C20	5.07	1.62	1.54
20	A2	803	CL0	C3D-C4D	-5.04	1.33	1.41
20	A1	802	CL0	CHC-C4B	4.98	1.47	1.39
20	A	803	CL0	O2D-CGD	4.97	1.45	1.33
20	A	803	CL0	OBD-CAD	4.95	1.28	1.22
24	A1	854	AJP	C12-C11	-4.93	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AA	803	CL0	OBD-CAD	4.92	1.28	1.22
20	A	803	CL0	CHC-C4B	4.91	1.47	1.39
24	A1	855	AJP	C21-C22	4.91	1.60	1.53
24	B	857	AJP	C12-C11	-4.90	1.47	1.56
20	A1	802	CL0	C3A-C2A	-4.90	1.50	1.54
20	A1	802	CL0	C3B-C2B	4.90	1.47	1.40
20	AA	803	CL0	CHC-C4B	4.90	1.47	1.39
20	AA	803	CL0	C3B-C2B	4.89	1.47	1.40
20	A2	803	CL0	OBD-CAD	4.88	1.28	1.22
20	A1	802	CL0	OBD-CAD	4.88	1.28	1.22
24	A2	854	AJP	C80-C20	4.86	1.62	1.54
24	A1	854	AJP	C80-C20	4.85	1.62	1.54
24	A2	854	AJP	C12-C11	-4.85	1.47	1.56
24	A1	855	AJP	C80-C20	4.85	1.62	1.54
24	A1	855	AJP	C12-C11	-4.84	1.47	1.56
24	AA	856	AJP	C80-C20	4.84	1.62	1.54
24	A	855	AJP	C80-C20	4.83	1.62	1.54
24	A	855	AJP	C12-C11	-4.83	1.47	1.56
24	AA	856	AJP	C12-C11	-4.83	1.47	1.56
24	B	857	AJP	C80-C20	4.82	1.62	1.54
24	M2	101	AJP	C20-C15	-4.81	1.47	1.56
24	A2	854	AJP	C21-C22	4.81	1.60	1.53
24	L1	203	AJP	C12-C11	-4.80	1.47	1.56
20	A2	803	CL0	CHB-C4A	-4.74	1.32	1.38
20	A1	802	CL0	O2D-CGD	4.71	1.44	1.33
20	AA	803	CL0	O2D-CGD	4.68	1.44	1.33
24	L	209	AJP	C20-C15	-4.67	1.47	1.56
24	AA	856	AJP	C16-C15	4.66	1.62	1.53
20	A	803	CL0	C3B-C2B	4.66	1.46	1.40
24	A	855	AJP	C16-C15	4.66	1.62	1.53
20	A	803	CL0	C3A-C2A	-4.64	1.50	1.54
24	A1	855	AJP	C16-C15	4.61	1.62	1.53
24	A2	854	AJP	C16-C15	4.61	1.62	1.53
24	KK	104	AJP	C21-C22	4.59	1.60	1.53
24	A1	854	AJP	C16-C15	4.58	1.62	1.53
24	BB	849	AJP	C20-C15	-4.58	1.48	1.56
20	AA	803	CL0	C3A-C2A	-4.58	1.50	1.54
24	L2	203	AJP	C20-C15	-4.57	1.48	1.56
24	K	104	AJP	C21-C22	4.57	1.60	1.53
24	L2	203	AJP	C12-C11	-4.54	1.47	1.56
24	L1	204	AJP	C12-C11	-4.54	1.47	1.56
20	A2	803	CL0	CHC-C4B	4.52	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	857	AJP	C16-C15	4.51	1.62	1.53
20	A2	803	CL0	O2D-CGD	4.50	1.44	1.33
20	A1	802	CL0	C3D-C2D	4.46	1.47	1.39
24	B	850	AJP	C20-C15	-4.45	1.48	1.56
20	AA	803	CL0	C3D-C2D	4.41	1.47	1.39
20	A2	803	CL0	C3D-C2D	4.40	1.47	1.39
24	L1	203	AJP	O82-C10	-4.40	1.32	1.43
20	A2	803	CL0	C3B-C2B	4.39	1.46	1.40
23	AA	855	BCR	C1-C6	-4.37	1.48	1.53
20	A2	803	CL0	CHD-C4C	4.35	1.47	1.39
23	A	854	BCR	C1-C6	-4.35	1.48	1.53
20	A	803	CL0	C3D-C2D	4.35	1.47	1.39
23	BB	839	BCR	C1-C6	-4.33	1.48	1.53
20	A1	802	CL0	CHC-C1C	4.32	1.47	1.39
23	K2	105	BCR	C1-C6	-4.32	1.48	1.53
20	AA	803	CL0	CHD-C4C	4.31	1.47	1.39
20	A2	803	CL0	C3A-C2A	-4.30	1.51	1.54
23	K1	106	BCR	C1-C6	-4.30	1.48	1.53
24	L1	204	AJP	C20-C15	-4.29	1.48	1.56
24	BB	849	AJP	C11-C10	4.28	1.61	1.53
23	B	844	BCR	C30-C25	-4.27	1.48	1.53
24	L	208	AJP	C11-C10	4.27	1.61	1.53
23	B1	839	BCR	C1-C6	-4.26	1.48	1.53
23	B	840	BCR	C1-C6	-4.25	1.48	1.53
24	L2	202	AJP	C12-C11	-4.25	1.48	1.56
23	JJ	104	BCR	C1-C6	-4.25	1.48	1.53
20	AA	803	CL0	CHC-C1C	4.25	1.47	1.39
23	B2	840	BCR	C1-C6	-4.24	1.48	1.53
20	A	803	CL0	CHC-C1C	4.23	1.47	1.39
24	B	850	AJP	C12-C11	-4.22	1.48	1.56
24	L	208	AJP	C20-C15	-4.21	1.48	1.56
24	BB	848	AJP	C12-C11	-4.20	1.48	1.56
24	K	104	AJP	C12-C11	-4.20	1.48	1.56
24	AA	856	AJP	C20-C15	-4.19	1.48	1.56
24	A	855	AJP	C20-C15	-4.18	1.48	1.56
24	I2	104	AJP	C12-C11	-4.18	1.48	1.56
24	BB	849	AJP	C12-C11	-4.18	1.48	1.56
23	B2	844	BCR	C30-C25	-4.18	1.48	1.53
20	A	803	CL0	CHD-C4C	4.17	1.47	1.39
20	A1	802	CL0	CHD-C4C	4.16	1.47	1.39
24	B	857	AJP	O82-C10	-4.16	1.32	1.43
23	M	101	BCR	C1-C6	-4.16	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A1	855	AJP	O82-C10	-4.15	1.32	1.43
23	B1	843	BCR	C30-C25	-4.14	1.48	1.53
24	A2	854	AJP	O82-C10	-4.14	1.32	1.43
23	J	102	BCR	C1-C6	-4.14	1.48	1.53
24	A1	854	AJP	O82-C10	-4.14	1.32	1.43
24	L2	203	AJP	C07-C06	-4.13	1.42	1.54
23	MM	101	BCR	C1-C6	-4.13	1.48	1.53
20	A1	802	CL0	O2A-CGA	4.13	1.45	1.33
24	A	855	AJP	O82-C10	-4.11	1.32	1.43
24	AA	856	AJP	O82-C10	-4.11	1.32	1.43
24	BB	849	AJP	C07-C06	-4.11	1.42	1.54
24	L	209	AJP	C11-C10	4.10	1.61	1.53
23	BB	847	BCR	C1-C6	-4.09	1.48	1.53
24	A	802	AJP	C07-C06	-4.09	1.42	1.54
23	J2	104	BCR	C1-C6	-4.08	1.48	1.53
24	B	849	AJP	C12-C11	-4.08	1.48	1.56
23	F1	304	BCR	C30-C25	-4.08	1.48	1.53
24	AA	802	AJP	C07-C06	-4.08	1.42	1.54
24	A	802	AJP	C11-C10	4.08	1.61	1.53
24	M2	101	AJP	C12-C11	-4.07	1.48	1.56
23	B	848	BCR	C1-C6	-4.07	1.48	1.53
20	A2	803	CL0	CHC-C1C	4.07	1.47	1.39
24	AA	802	AJP	C11-C10	4.07	1.61	1.53
23	BB	842	BCR	C1-C6	-4.05	1.48	1.53
23	J2	102	BCR	C1-C6	-4.05	1.48	1.53
23	JJ	102	BCR	C1-C6	-4.05	1.48	1.53
24	L	209	AJP	C12-C11	-4.05	1.48	1.56
23	JJ	102	BCR	C30-C25	-4.03	1.48	1.53
23	B	843	BCR	C1-C6	-4.03	1.48	1.53
24	KK	104	AJP	C11-C10	4.02	1.61	1.53
24	L	209	AJP	C16-C15	4.01	1.61	1.53
24	A2	854	AJP	C11-C10	4.01	1.61	1.53
24	AA	856	AJP	C07-C06	-4.01	1.43	1.54
23	BB	843	BCR	C30-C25	-4.00	1.48	1.53
24	A	855	AJP	C07-C06	-4.00	1.43	1.54
24	A2	854	AJP	C20-C15	-3.99	1.49	1.56
23	I1	101	BCR	C30-C25	-3.99	1.48	1.53
23	B1	842	BCR	C1-C6	-3.98	1.48	1.53
23	FF	304	BCR	C30-C25	-3.98	1.48	1.53
23	J1	102	BCR	C1-C6	-3.98	1.48	1.53
23	BB	838	BCR	C1-C6	-3.98	1.48	1.53
23	B2	843	BCR	C1-C6	-3.97	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A1	854	AJP	C11-C10	3.97	1.61	1.53
23	B	839	BCR	C1-C6	-3.96	1.48	1.53
24	B	857	AJP	C11-C10	3.96	1.61	1.53
23	F2	304	BCR	C30-C25	-3.96	1.48	1.53
24	L	209	AJP	C07-C06	-3.96	1.43	1.54
23	J1	102	BCR	C30-C25	-3.96	1.48	1.53
24	K	104	AJP	C20-C15	-3.96	1.49	1.56
24	L2	202	AJP	C07-C06	-3.96	1.43	1.54
23	F	304	BCR	C1-C6	-3.95	1.48	1.53
24	A1	855	AJP	C11-C10	3.95	1.61	1.53
24	A1	855	AJP	C07-C06	-3.95	1.43	1.54
23	J	102	BCR	C30-C25	-3.94	1.48	1.53
24	KK	104	AJP	C16-C15	3.94	1.61	1.53
24	KK	104	AJP	C20-C15	-3.94	1.49	1.56
24	KK	104	AJP	C07-C06	-3.93	1.43	1.54
23	F	305	BCR	C1-C6	-3.93	1.48	1.53
24	I2	104	AJP	C11-C10	3.93	1.61	1.53
24	A2	854	AJP	C07-C06	-3.93	1.43	1.54
23	FF	306	BCR	C1-C6	-3.92	1.48	1.53
24	L1	204	AJP	C07-C06	-3.92	1.43	1.54
24	M2	101	AJP	C11-C10	3.92	1.61	1.53
23	I2	101	BCR	C30-C25	-3.92	1.48	1.53
23	F2	304	BCR	C1-C6	-3.91	1.48	1.53
24	BB	848	AJP	O82-C10	-3.91	1.33	1.43
23	AA	852	BCR	C1-C6	-3.91	1.48	1.53
23	KK	103	BCR	C1-C6	-3.91	1.48	1.53
24	KK	104	AJP	C12-C11	-3.91	1.48	1.56
23	BB	843	BCR	C1-C6	-3.90	1.48	1.53
24	L	208	AJP	C07-C06	-3.90	1.43	1.54
23	F1	304	BCR	C1-C6	-3.90	1.48	1.53
23	B	844	BCR	C1-C6	-3.90	1.48	1.53
24	A1	855	AJP	C20-C15	-3.90	1.49	1.56
23	K2	103	BCR	C1-C6	-3.90	1.48	1.53
23	FF	304	BCR	C1-C6	-3.90	1.48	1.53
24	B	857	AJP	C20-C15	-3.89	1.49	1.56
24	AA	856	AJP	C11-C10	3.89	1.61	1.53
24	A	855	AJP	C11-C10	3.89	1.61	1.53
24	M2	101	AJP	C16-C15	3.89	1.60	1.53
23	M1	101	BCR	C1-C6	-3.89	1.48	1.53
23	K1	104	BCR	C1-C6	-3.88	1.48	1.53
24	AA	856	AJP	C24-C19	3.88	1.60	1.53
24	A	855	AJP	C24-C19	3.88	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K	103	BCR	C1-C6	-3.87	1.48	1.53
24	K	104	AJP	C11-C10	3.86	1.61	1.53
23	L	206	BCR	C1-C6	-3.86	1.48	1.53
23	B1	838	BCR	C1-C6	-3.86	1.48	1.53
20	AA	803	CL0	O2A-CGA	3.86	1.44	1.33
24	B	849	AJP	C07-C06	-3.85	1.43	1.54
23	B2	839	BCR	C1-C6	-3.85	1.48	1.53
24	K	104	AJP	C16-C15	3.85	1.60	1.53
24	M2	101	AJP	C07-C06	-3.84	1.43	1.54
24	B	850	AJP	C11-C10	3.84	1.61	1.53
24	AA	802	AJP	C12-C11	-3.84	1.48	1.56
23	I2	101	BCR	C1-C6	-3.84	1.48	1.53
24	A	802	AJP	C20-C15	-3.83	1.49	1.56
24	L2	203	AJP	C11-C10	3.83	1.61	1.53
24	B	849	AJP	C16-C15	3.83	1.60	1.53
23	I1	101	BCR	C1-C6	-3.83	1.48	1.53
23	A1	850	BCR	C1-C6	-3.83	1.48	1.53
23	F	304	BCR	C30-C25	-3.82	1.48	1.53
24	L2	203	AJP	C16-C15	3.82	1.60	1.53
23	A2	848	BCR	C1-C6	-3.82	1.48	1.53
23	J2	102	BCR	C30-C25	-3.82	1.48	1.53
24	A	802	AJP	C12-C11	-3.82	1.49	1.56
23	A1	848	BCR	C1-C6	-3.81	1.48	1.53
23	AA	854	BCR	C30-C25	-3.81	1.48	1.53
23	A2	850	BCR	C1-C6	-3.81	1.48	1.53
23	II	101	BCR	C1-C6	-3.81	1.48	1.53
24	BB	848	AJP	C16-C15	3.80	1.60	1.53
23	A1	847	BCR	C1-C6	-3.80	1.48	1.53
24	K	104	AJP	C07-C06	-3.80	1.43	1.54
24	A1	854	AJP	C07-C06	-3.80	1.43	1.54
24	K	104	AJP	C24-C19	3.80	1.59	1.53
23	A	853	BCR	C30-C25	-3.80	1.48	1.53
20	A	803	CL0	O2A-CGA	3.79	1.44	1.33
23	B1	843	BCR	C1-C6	-3.79	1.48	1.53
23	M2	102	BCR	C1-C6	-3.79	1.48	1.53
23	A2	847	BCR	C1-C6	-3.78	1.48	1.53
23	II	104	BCR	C1-C6	-3.78	1.48	1.53
23	I	101	BCR	C1-C6	-3.78	1.48	1.53
24	B	850	AJP	C07-C06	-3.78	1.43	1.54
24	AA	802	AJP	C20-C15	-3.78	1.49	1.56
24	B	857	AJP	C07-C06	-3.78	1.43	1.54
24	L2	202	AJP	O82-C10	-3.78	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	I2	104	AJP	C16-C15	3.78	1.60	1.53
23	B2	844	BCR	C1-C6	-3.77	1.49	1.53
23	L1	209	BCR	C1-C6	-3.77	1.49	1.53
24	L2	202	AJP	C20-C15	-3.77	1.49	1.56
23	II	102	BCR	C1-C6	-3.76	1.49	1.53
23	A1	853	BCR	C30-C25	-3.76	1.49	1.53
23	L2	207	BCR	C1-C6	-3.76	1.49	1.53
24	L	208	AJP	C16-C15	3.76	1.60	1.53
23	A2	853	BCR	C30-C25	-3.76	1.49	1.53
24	BB	848	AJP	C20-C15	-3.75	1.49	1.56
23	I2	103	BCR	C1-C6	-3.75	1.49	1.53
23	AA	849	BCR	C1-C6	-3.75	1.49	1.53
23	A	847	BCR	C1-C6	-3.75	1.49	1.53
24	L1	203	AJP	C07-C06	-3.75	1.43	1.54
23	A	848	BCR	C1-C6	-3.75	1.49	1.53
24	L	209	AJP	O82-C10	-3.75	1.33	1.43
24	A1	854	AJP	C20-C15	-3.75	1.49	1.56
23	L	205	BCR	C1-C6	-3.74	1.49	1.53
19	B2	833	CLA	C1D-ND	3.74	1.42	1.37
23	L	206	BCR	C30-C25	-3.74	1.49	1.53
24	B	849	AJP	C20-C15	-3.74	1.49	1.56
24	BB	849	AJP	C16-C15	3.74	1.60	1.53
20	A2	803	CL0	O2A-CGA	3.74	1.44	1.33
23	J1	104	BCR	C1-C6	-3.74	1.49	1.53
19	LL	203	CLA	C1D-ND	3.74	1.42	1.37
24	L	208	AJP	O82-C10	-3.74	1.33	1.43
23	AA	848	BCR	C1-C6	-3.74	1.49	1.53
23	L1	201	BCR	C1-C6	-3.73	1.49	1.53
24	KK	104	AJP	O82-C10	-3.73	1.33	1.43
20	A	803	CL0	CHD-C1D	3.73	1.45	1.39
24	K	104	AJP	O82-C10	-3.73	1.33	1.43
24	A1	855	AJP	C24-C19	3.73	1.59	1.53
24	A2	854	AJP	C24-C19	3.73	1.59	1.53
24	L2	202	AJP	C11-C10	3.73	1.60	1.53
24	I2	104	AJP	O82-C10	-3.72	1.33	1.43
24	BB	848	AJP	C07-C06	-3.72	1.43	1.54
23	F1	306	BCR	C1-C6	-3.71	1.49	1.53
24	B	850	AJP	C16-C15	3.71	1.60	1.53
24	L1	204	AJP	O82-C10	-3.71	1.33	1.43
24	B	850	AJP	O82-C10	-3.71	1.33	1.43
24	KK	104	AJP	C24-C19	3.70	1.59	1.53
23	B	848	BCR	C30-C25	-3.69	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F2	305	BCR	C1-C6	-3.69	1.49	1.53
19	B	818	CLA	C4B-NB	3.69	1.42	1.37
23	I2	102	BCR	C1-C6	-3.68	1.49	1.53
23	BB	847	BCR	C30-C25	-3.68	1.49	1.53
23	II	101	BCR	C30-C25	-3.68	1.49	1.53
23	F1	303	BCR	C1-C6	-3.67	1.49	1.53
23	LL	204	BCR	C30-C25	-3.67	1.49	1.53
23	AA	854	BCR	C1-C6	-3.67	1.49	1.53
24	B	850	AJP	C24-C19	3.66	1.59	1.53
24	L1	204	AJP	C16-C15	3.66	1.60	1.53
24	B	849	AJP	O82-C10	-3.66	1.33	1.43
23	I	101	BCR	C30-C25	-3.66	1.49	1.53
24	L1	204	AJP	C11-C10	3.66	1.60	1.53
23	I	102	BCR	C1-C6	-3.65	1.49	1.53
24	BB	848	AJP	C11-C10	3.65	1.60	1.53
24	L1	203	AJP	C16-C15	3.65	1.60	1.53
23	A	853	BCR	C1-C6	-3.65	1.49	1.53
24	M2	101	AJP	O82-C10	-3.65	1.33	1.43
23	AA	851	BCR	C1-C6	-3.63	1.49	1.53
23	A	851	BCR	C1-C6	-3.63	1.49	1.53
24	B	849	AJP	C11-C10	3.62	1.60	1.53
23	B1	842	BCR	C30-C25	-3.62	1.49	1.53
23	LL	204	BCR	C1-C6	-3.62	1.49	1.53
23	M	101	BCR	C30-C25	-3.62	1.49	1.53
24	BB	849	AJP	O82-C10	-3.61	1.34	1.43
23	A	850	BCR	C1-C6	-3.61	1.49	1.53
24	L	208	AJP	C12-C11	-3.61	1.49	1.56
23	B2	843	BCR	C30-C25	-3.61	1.49	1.53
23	L2	207	BCR	C30-C25	-3.61	1.49	1.53
23	L1	208	BCR	C1-C6	-3.61	1.49	1.53
23	A2	851	BCR	C1-C6	-3.61	1.49	1.53
23	K2	103	BCR	C30-C25	-3.61	1.49	1.53
23	B	842	BCR	C1-C6	-3.61	1.49	1.53
24	AA	802	AJP	O82-C10	-3.61	1.34	1.43
24	A	802	AJP	O82-C10	-3.61	1.34	1.43
24	L2	202	AJP	C16-C15	3.61	1.60	1.53
23	BB	841	BCR	C1-C6	-3.60	1.49	1.53
20	A1	802	CL0	CHD-C1D	3.60	1.45	1.39
23	K1	104	BCR	C30-C25	-3.60	1.49	1.53
23	A1	853	BCR	C1-C6	-3.59	1.49	1.53
23	FF	303	BCR	C1-C6	-3.59	1.49	1.53
23	A1	851	BCR	C1-C6	-3.59	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	803	CL0	CHB-C1B	3.58	1.45	1.39
19	B2	832	CLA	C1D-ND	3.58	1.42	1.37
23	B1	841	BCR	C1-C6	-3.58	1.49	1.53
23	F	303	BCR	C1-C6	-3.58	1.49	1.53
24	AA	802	AJP	C16-C15	3.57	1.60	1.53
19	B1	831	CLA	C1D-ND	3.57	1.42	1.37
23	L1	209	BCR	C30-C25	-3.57	1.49	1.53
23	A2	853	BCR	C1-C6	-3.57	1.49	1.53
24	BB	849	AJP	C24-C19	3.57	1.59	1.53
24	L2	203	AJP	C24-C19	3.56	1.59	1.53
24	A	802	AJP	C16-C15	3.55	1.60	1.53
24	AA	802	AJP	C21-C22	3.55	1.61	1.52
24	L1	204	AJP	C24-C19	3.55	1.59	1.53
19	BB	832	CLA	C1D-ND	3.55	1.42	1.37
23	J	104	BCR	C30-C25	-3.54	1.49	1.53
24	A	802	AJP	C21-C22	3.54	1.61	1.52
23	B	843	BCR	C30-C25	-3.54	1.49	1.53
24	L2	203	AJP	O82-C10	-3.53	1.34	1.43
23	F2	303	BCR	C1-C6	-3.52	1.49	1.53
20	AA	803	CL0	CHD-C1D	3.52	1.45	1.39
23	J	104	BCR	C1-C6	-3.51	1.49	1.53
23	BB	842	BCR	C30-C25	-3.50	1.49	1.53
24	B	857	AJP	C24-C19	3.50	1.59	1.53
24	I2	104	AJP	C20-C15	-3.50	1.50	1.56
24	I2	104	AJP	C07-C06	-3.50	1.44	1.54
23	I	102	BCR	C30-C25	-3.49	1.49	1.53
20	A2	803	CL0	CHD-C1D	3.49	1.45	1.39
23	B2	839	BCR	C30-C25	-3.48	1.49	1.53
19	BB	826	CLA	C4B-NB	3.48	1.42	1.37
23	B1	838	BCR	C30-C25	-3.48	1.49	1.53
19	B1	830	CLA	C1D-ND	3.48	1.42	1.37
19	J2	103	CLA	C1D-ND	3.48	1.42	1.37
19	B	818	CLA	C1D-ND	3.48	1.42	1.37
23	J2	104	BCR	C30-C25	-3.47	1.49	1.53
19	B	833	CLA	C1D-ND	3.47	1.42	1.37
19	J1	103	CLA	C1D-ND	3.47	1.42	1.37
24	L1	203	AJP	C11-C10	3.47	1.60	1.53
19	F1	302	CLA	C1D-ND	3.47	1.42	1.37
23	AA	849	BCR	C30-C25	-3.46	1.49	1.53
19	B2	831	CLA	C1D-ND	3.46	1.42	1.37
19	A	822	CLA	C1D-ND	3.46	1.42	1.37
19	B1	845	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	846	CLA	C1D-ND	3.46	1.42	1.37
23	A1	850	BCR	C30-C25	-3.46	1.49	1.53
23	B2	842	BCR	C1-C6	-3.46	1.49	1.53
19	BB	833	CLA	C1D-ND	3.46	1.42	1.37
19	F2	302	CLA	C1D-ND	3.46	1.42	1.37
19	J	103	CLA	C1D-ND	3.46	1.42	1.37
19	B1	812	CLA	C1D-ND	3.45	1.42	1.37
19	B2	812	CLA	C1D-ND	3.45	1.42	1.37
23	J1	104	BCR	C30-C25	-3.45	1.49	1.53
19	X2	101	CLA	C1D-ND	3.45	1.42	1.37
23	A	848	BCR	C30-C25	-3.44	1.49	1.53
19	K2	104	CLA	C1D-ND	3.44	1.42	1.37
19	J2	101	CLA	C1D-ND	3.44	1.42	1.37
24	BB	848	AJP	C24-C19	3.44	1.59	1.53
24	L1	203	AJP	C20-C15	-3.44	1.50	1.56
24	A1	854	AJP	C24-C19	3.43	1.59	1.53
19	AA	838	CLA	C1D-ND	3.43	1.42	1.37
19	A	838	CLA	C1D-ND	3.43	1.42	1.37
23	II	102	BCR	C30-C25	-3.43	1.49	1.53
23	A2	850	BCR	C30-C25	-3.42	1.49	1.53
19	B1	833	CLA	C1D-ND	3.42	1.42	1.37
23	I2	102	BCR	C30-C25	-3.42	1.49	1.53
19	B1	817	CLA	C1D-ND	3.42	1.42	1.37
23	L1	201	BCR	C30-C25	-3.41	1.49	1.53
19	F	302	CLA	C1D-ND	3.41	1.42	1.37
19	B2	826	CLA	C4B-NB	3.41	1.42	1.37
19	B1	815	CLA	C1D-ND	3.41	1.42	1.37
19	B2	822	CLA	C1D-ND	3.41	1.42	1.37
19	B	825	CLA	C1D-ND	3.41	1.42	1.37
23	BB	838	BCR	C30-C25	-3.41	1.49	1.53
19	K1	103	CLA	C1D-ND	3.41	1.42	1.37
19	B2	809	CLA	C1D-ND	3.40	1.42	1.37
19	B1	809	CLA	C1D-ND	3.40	1.42	1.37
19	A	852	CLA	C1D-ND	3.40	1.42	1.37
19	A2	802	CLA	C1D-ND	3.40	1.42	1.37
19	BB	830	CLA	C1D-ND	3.40	1.42	1.37
19	A	839	CLA	C1D-ND	3.40	1.42	1.37
19	B2	817	CLA	C1D-ND	3.40	1.42	1.37
19	JJ	101	CLA	C1D-ND	3.40	1.42	1.37
19	A	817	CLA	C1D-ND	3.39	1.42	1.37
23	B	839	BCR	C30-C25	-3.39	1.49	1.53
19	AA	811	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	XX	101	CLA	C1D-ND	3.38	1.42	1.37
19	AA	817	CLA	C1D-ND	3.38	1.42	1.37
19	B	823	CLA	C1D-ND	3.38	1.42	1.37
19	BB	801	CLA	C1D-ND	3.38	1.42	1.37
19	KK	102	CLA	C1D-ND	3.38	1.42	1.37
19	X	101	CLA	C1D-ND	3.38	1.42	1.37
19	FF	302	CLA	C1D-ND	3.38	1.42	1.37
19	X1	101	CLA	C1D-ND	3.38	1.42	1.37
19	L1	205	CLA	C1D-ND	3.38	1.42	1.37
19	BB	845	CLA	C1D-ND	3.38	1.42	1.37
19	J	101	CLA	C1D-ND	3.38	1.42	1.37
19	B1	825	CLA	C1D-ND	3.38	1.42	1.37
19	KK	101	CLA	C1D-ND	3.38	1.42	1.37
23	MM	101	BCR	C30-C25	-3.37	1.49	1.53
19	K1	102	CLA	C1D-ND	3.37	1.42	1.37
19	K	102	CLA	C1D-ND	3.37	1.42	1.37
19	J1	101	CLA	C1D-ND	3.37	1.42	1.37
19	K2	102	CLA	C1D-ND	3.37	1.42	1.37
19	A	833	CLA	C1D-ND	3.37	1.42	1.37
19	L2	204	CLA	C1D-ND	3.37	1.42	1.37
19	JJ	103	CLA	C1D-ND	3.37	1.42	1.37
19	F2	301	CLA	C1D-ND	3.37	1.42	1.37
19	A	832	CLA	C1D-ND	3.37	1.42	1.37
19	A1	829	CLA	C1D-ND	3.36	1.42	1.37
19	K1	105	CLA	C1D-ND	3.36	1.42	1.37
19	A1	831	CLA	C1D-ND	3.36	1.42	1.37
19	B1	832	CLA	C1D-ND	3.36	1.42	1.37
19	B2	823	CLA	C1D-ND	3.36	1.42	1.37
19	AA	822	CLA	C1D-ND	3.36	1.42	1.37
19	K	101	CLA	C1D-ND	3.36	1.42	1.37
19	B	834	CLA	C1D-ND	3.36	1.42	1.37
19	B1	823	CLA	C1D-ND	3.36	1.42	1.37
19	A	824	CLA	C1D-ND	3.36	1.42	1.37
19	A1	817	CLA	C1D-ND	3.36	1.42	1.37
19	B2	828	CLA	C1D-ND	3.36	1.42	1.37
19	AA	827	CLA	C1D-ND	3.36	1.42	1.37
19	AA	853	CLA	C1D-ND	3.36	1.42	1.37
19	B	846	CLA	C1D-ND	3.35	1.42	1.37
19	A1	835	CLA	C1D-ND	3.35	1.42	1.37
19	AA	836	CLA	C1D-ND	3.35	1.42	1.37
19	BB	812	CLA	C1D-ND	3.35	1.42	1.37
23	AA	851	BCR	C30-C25	-3.35	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	818	CLA	C1D-ND	3.35	1.42	1.37
19	B1	813	CLA	C1D-ND	3.35	1.42	1.37
19	B1	850	CLA	C1D-ND	3.35	1.42	1.37
19	AA	807	CLA	C1D-ND	3.35	1.42	1.37
19	A	818	CLA	C1D-ND	3.35	1.42	1.37
19	B	809	CLA	C1D-ND	3.35	1.42	1.37
19	A2	826	CLA	C1D-ND	3.34	1.42	1.37
19	B	831	CLA	C1D-ND	3.34	1.42	1.37
19	AA	818	CLA	C1D-ND	3.34	1.42	1.37
19	B1	822	CLA	C1D-ND	3.34	1.42	1.37
19	B1	826	CLA	C4B-NB	3.34	1.42	1.37
24	BB	848	AJP	C83-C06	3.34	1.60	1.53
23	A	850	BCR	C30-C25	-3.34	1.49	1.53
19	F1	301	CLA	C1D-ND	3.34	1.42	1.37
19	BB	823	CLA	C1D-ND	3.34	1.42	1.37
19	BB	835	CLA	C1D-ND	3.34	1.42	1.37
23	JJ	104	BCR	C30-C25	-3.34	1.49	1.53
19	A2	832	CLA	C1D-ND	3.34	1.42	1.37
19	B2	825	CLA	C1D-ND	3.34	1.42	1.37
19	BB	809	CLA	C1D-ND	3.34	1.42	1.37
19	BB	825	CLA	C1D-ND	3.34	1.42	1.37
19	A	816	CLA	C1D-ND	3.34	1.42	1.37
19	B2	811	CLA	C1D-ND	3.33	1.42	1.37
19	B2	813	CLA	C1D-ND	3.33	1.42	1.37
19	B2	834	CLA	C1D-ND	3.33	1.42	1.37
19	B	815	CLA	C1D-ND	3.33	1.42	1.37
19	B	826	CLA	C1D-ND	3.33	1.42	1.37
19	AA	845	CLA	C1D-ND	3.33	1.42	1.37
19	A	811	CLA	C1D-ND	3.33	1.42	1.37
19	AA	816	CLA	C1D-ND	3.33	1.42	1.37
19	B	832	CLA	C1D-ND	3.33	1.42	1.37
19	A	807	CLA	C1D-ND	3.33	1.42	1.37
19	B2	814	CLA	C1D-ND	3.33	1.42	1.37
20	AA	803	CL0	CHB-C1B	3.33	1.45	1.39
19	AA	832	CLA	C1D-ND	3.32	1.42	1.37
19	A	823	CLA	C1D-ND	3.32	1.42	1.37
19	B1	818	CLA	C1D-ND	3.32	1.42	1.37
19	B2	819	CLA	C1D-ND	3.32	1.42	1.37
19	B2	804	CLA	C1D-ND	3.32	1.42	1.37
19	B1	849	CLA	C1D-ND	3.32	1.42	1.37
19	B	817	CLA	C1D-ND	3.32	1.42	1.37
19	L2	206	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	814	CLA	C1D-ND	3.32	1.42	1.37
19	B2	836	CLA	C1D-ND	3.32	1.42	1.37
23	M1	101	BCR	C30-C25	-3.32	1.49	1.53
23	A1	848	BCR	C30-C25	-3.32	1.49	1.53
19	B1	806	CLA	C1D-ND	3.31	1.42	1.37
19	AA	826	CLA	C1D-ND	3.31	1.42	1.37
19	BB	819	CLA	C1D-ND	3.31	1.42	1.37
19	A2	822	CLA	C1D-ND	3.31	1.42	1.37
19	AA	839	CLA	C1D-ND	3.31	1.42	1.37
19	A2	841	CLA	C1D-ND	3.31	1.42	1.37
19	B1	804	CLA	C1D-ND	3.31	1.42	1.37
19	A2	852	CLA	C1D-ND	3.31	1.42	1.37
19	BB	817	CLA	C1D-ND	3.31	1.42	1.37
19	BB	815	CLA	C1D-ND	3.31	1.42	1.37
19	B2	835	CLA	C1D-ND	3.31	1.42	1.37
19	BB	831	CLA	C1D-ND	3.31	1.42	1.37
19	A	836	CLA	C1D-ND	3.31	1.42	1.37
19	A2	842	CLA	C1D-ND	3.30	1.42	1.37
19	B2	818	CLA	C1D-ND	3.30	1.42	1.37
19	A1	815	CLA	C1D-ND	3.30	1.42	1.37
19	B1	801	CLA	C1D-ND	3.30	1.42	1.37
19	A2	808	CLA	C1D-ND	3.30	1.42	1.37
23	A2	848	BCR	C30-C25	-3.30	1.49	1.53
19	A1	840	CLA	C1D-ND	3.30	1.42	1.37
19	B1	811	CLA	C1D-ND	3.30	1.42	1.37
19	A1	805	CLA	C1D-ND	3.30	1.42	1.37
19	B2	851	CLA	C1D-ND	3.30	1.42	1.37
19	A	814	CLA	C1D-ND	3.30	1.42	1.37
19	AA	815	CLA	C1D-ND	3.30	1.42	1.37
19	F	301	CLA	C1D-ND	3.30	1.42	1.37
19	B1	836	CLA	C1D-ND	3.30	1.42	1.37
23	F	303	BCR	C30-C25	-3.30	1.49	1.53
19	L1	207	CLA	C1D-ND	3.29	1.42	1.37
19	A	827	CLA	C1D-ND	3.29	1.42	1.37
19	AA	823	CLA	C1D-ND	3.29	1.42	1.37
19	A2	807	CLA	C1D-ND	3.29	1.42	1.37
19	A2	823	CLA	C1D-ND	3.29	1.42	1.37
19	LL	201	CLA	C1D-ND	3.29	1.42	1.37
19	AA	808	CLA	C1D-ND	3.29	1.42	1.37
19	A1	808	CLA	C1D-ND	3.29	1.42	1.37
19	AA	833	CLA	C1D-ND	3.29	1.42	1.37
19	A2	813	CLA	C1D-ND	3.29	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	208	AJP	C18-C19	-3.29	1.45	1.53
19	B1	820	CLA	C1D-ND	3.29	1.42	1.37
19	F1	305	CLA	C1D-ND	3.29	1.42	1.37
19	A	815	CLA	C1D-ND	3.29	1.42	1.37
19	A1	822	CLA	C1D-ND	3.28	1.42	1.37
19	A1	844	CLA	C1D-ND	3.28	1.42	1.37
19	BB	828	CLA	C1D-ND	3.28	1.42	1.37
19	A	809	CLA	C1D-ND	3.28	1.42	1.37
19	A1	806	CLA	C1D-ND	3.28	1.42	1.37
19	B2	808	CLA	C1D-ND	3.28	1.42	1.37
19	B1	819	CLA	C1D-ND	3.28	1.42	1.37
19	B2	815	CLA	C1D-ND	3.28	1.42	1.37
19	B	812	CLA	C1D-ND	3.28	1.42	1.37
19	B1	808	CLA	C1D-ND	3.28	1.42	1.37
19	BB	804	CLA	C1D-ND	3.28	1.42	1.37
19	A2	815	CLA	C1D-ND	3.28	1.42	1.37
19	A2	817	CLA	C1D-ND	3.28	1.42	1.37
19	A1	812	CLA	C1D-ND	3.28	1.42	1.37
19	A2	816	CLA	C1D-ND	3.28	1.42	1.37
19	B	836	CLA	C1D-ND	3.28	1.42	1.37
19	B	807	CLA	C1D-ND	3.28	1.42	1.37
19	A1	841	CLA	C1D-ND	3.27	1.42	1.37
19	A2	839	CLA	C1D-ND	3.27	1.42	1.37
19	A2	844	CLA	C1D-ND	3.27	1.42	1.37
19	A	844	CLA	C1D-ND	3.27	1.42	1.37
19	A1	810	CLA	C1D-ND	3.27	1.42	1.37
19	A1	813	CLA	C1D-ND	3.27	1.42	1.37
19	B	803	CLA	C1D-ND	3.27	1.42	1.37
19	BB	807	CLA	C1D-ND	3.27	1.42	1.37
19	A2	812	CLA	C1D-ND	3.27	1.42	1.37
23	M2	102	BCR	C30-C25	-3.27	1.49	1.53
19	BB	811	CLA	C1D-ND	3.27	1.42	1.37
19	B1	835	CLA	C1D-ND	3.27	1.42	1.37
19	B2	802	CLA	C1D-ND	3.27	1.42	1.37
19	AA	841	CLA	C1D-ND	3.27	1.42	1.37
19	BB	808	CLA	C1D-ND	3.27	1.42	1.37
24	BB	848	AJP	O79-C22	-3.26	1.36	1.43
24	B	849	AJP	C24-C19	3.26	1.59	1.53
19	A	841	CLA	C1D-ND	3.26	1.42	1.37
19	A	837	CLA	C1D-ND	3.26	1.42	1.37
19	B1	802	CLA	C1D-ND	3.26	1.42	1.37
19	A	812	CLA	C1D-ND	3.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	812	CLA	C1D-ND	3.26	1.42	1.37
23	A1	849	BCR	C30-C25	-3.26	1.49	1.53
19	A1	811	CLA	C1D-ND	3.26	1.42	1.37
19	A1	823	CLA	C1D-ND	3.26	1.42	1.37
19	B2	816	CLA	C1D-ND	3.26	1.42	1.37
19	A1	821	CLA	C1D-ND	3.26	1.42	1.37
19	B2	837	CLA	C1D-ND	3.26	1.42	1.37
19	B2	850	CLA	C1D-ND	3.26	1.42	1.37
19	A1	816	CLA	C1D-ND	3.26	1.42	1.37
19	AA	814	CLA	C1D-ND	3.25	1.42	1.37
19	A1	814	CLA	C1D-ND	3.25	1.42	1.37
19	AA	837	CLA	C1D-ND	3.25	1.42	1.37
19	A1	824	CLA	C1D-ND	3.25	1.42	1.37
23	KK	103	BCR	C30-C25	-3.25	1.49	1.53
19	A2	833	CLA	C1D-ND	3.25	1.42	1.37
19	B	828	CLA	C1D-ND	3.25	1.42	1.37
19	A1	827	CLA	C1D-ND	3.25	1.42	1.37
19	AA	824	CLA	C1D-ND	3.25	1.42	1.37
19	B	804	CLA	C1D-ND	3.25	1.42	1.37
19	BB	813	CLA	C1D-ND	3.25	1.42	1.37
23	K	103	BCR	C30-C25	-3.25	1.49	1.53
19	A2	814	CLA	C1D-ND	3.25	1.42	1.37
19	A2	838	CLA	C1D-ND	3.25	1.42	1.37
19	B	811	CLA	C1D-ND	3.25	1.42	1.37
19	B	858	CLA	C1D-ND	3.25	1.42	1.37
19	A2	809	CLA	C1D-ND	3.24	1.42	1.37
19	A2	810	CLA	C1D-ND	3.24	1.42	1.37
19	B1	816	CLA	C1D-ND	3.24	1.42	1.37
19	AA	840	CLA	C1D-ND	3.24	1.42	1.37
19	B2	807	CLA	C1D-ND	3.24	1.42	1.37
19	AA	809	CLA	C1D-ND	3.24	1.42	1.37
19	B1	807	CLA	C1D-ND	3.24	1.42	1.37
19	A2	828	CLA	C1D-ND	3.24	1.42	1.37
19	AA	821	CLA	C1D-ND	3.24	1.42	1.37
19	B	837	CLA	C1D-ND	3.24	1.42	1.37
19	B2	801	CLA	C1D-ND	3.24	1.42	1.37
19	AA	825	CLA	C1D-ND	3.23	1.42	1.37
23	A1	849	BCR	C1-C6	-3.23	1.49	1.53
23	II	104	BCR	C30-C25	-3.23	1.49	1.53
19	A2	811	CLA	C1D-ND	3.23	1.42	1.37
19	AA	813	CLA	C1D-ND	3.23	1.42	1.37
19	AA	830	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F2	305	BCR	C30-C25	-3.23	1.49	1.53
19	A2	836	CLA	C1D-ND	3.23	1.42	1.37
19	B1	803	CLA	C1D-ND	3.23	1.42	1.37
19	B	808	CLA	C1D-ND	3.23	1.42	1.37
19	A	813	CLA	C1D-ND	3.23	1.42	1.37
19	A2	824	CLA	C1D-ND	3.23	1.42	1.37
19	L	202	CLA	C1D-ND	3.23	1.42	1.37
19	A1	838	CLA	C1D-ND	3.23	1.42	1.37
19	BB	803	CLA	C1D-ND	3.23	1.42	1.37
23	A2	849	BCR	C30-C25	-3.23	1.49	1.53
24	L1	204	AJP	O79-C22	-3.23	1.36	1.43
23	A	849	BCR	C30-C25	-3.23	1.49	1.53
19	BB	855	CLA	C1D-ND	3.22	1.42	1.37
23	AA	850	BCR	C30-C25	-3.22	1.49	1.53
19	AA	842	CLA	C1D-ND	3.22	1.42	1.37
19	BB	822	CLA	C4B-NB	3.22	1.42	1.37
19	B	801	CLA	C1D-ND	3.22	1.42	1.37
19	A1	839	CLA	C1D-ND	3.22	1.42	1.37
19	A	821	CLA	C1D-ND	3.22	1.42	1.37
24	L2	203	AJP	O79-C22	-3.22	1.36	1.43
19	B1	810	CLA	C1D-ND	3.22	1.42	1.37
19	A2	827	CLA	C1D-ND	3.22	1.42	1.37
20	A1	802	CL0	CHB-C1B	3.22	1.44	1.39
23	FF	303	BCR	C30-C25	-3.22	1.49	1.53
19	A1	818	CLA	C1D-ND	3.22	1.42	1.37
19	A	840	CLA	C1D-ND	3.22	1.42	1.37
19	BB	856	CLA	C1D-ND	3.22	1.42	1.37
23	F1	306	BCR	C30-C25	-3.22	1.49	1.53
19	A2	820	CLA	C1D-ND	3.22	1.42	1.37
19	A	819	CLA	C1D-ND	3.22	1.42	1.37
19	A2	840	CLA	C1D-ND	3.22	1.42	1.37
19	A1	832	CLA	C1D-ND	3.21	1.42	1.37
19	B2	810	CLA	C1D-ND	3.21	1.42	1.37
19	A1	826	CLA	C1D-ND	3.21	1.42	1.37
19	B2	803	CLA	C1D-ND	3.21	1.42	1.37
19	B	859	CLA	C1D-ND	3.21	1.42	1.37
19	A1	852	CLA	C1D-ND	3.21	1.42	1.37
19	A2	825	CLA	C1D-ND	3.21	1.42	1.37
19	B2	829	CLA	C1D-ND	3.21	1.42	1.37
19	A	835	CLA	C1D-ND	3.21	1.42	1.37
19	AA	810	CLA	C1D-ND	3.21	1.42	1.37
19	B	826	CLA	C4B-NB	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	842	CLA	C1D-ND	3.21	1.42	1.37
19	A1	837	CLA	C1D-ND	3.21	1.42	1.37
19	A1	804	CLA	C1D-ND	3.20	1.42	1.37
19	B1	826	CLA	C1D-ND	3.20	1.42	1.37
19	A	830	CLA	C1D-ND	3.20	1.42	1.37
19	B	814	CLA	C1D-ND	3.20	1.42	1.37
19	A	828	CLA	C1D-ND	3.20	1.42	1.37
19	A1	801	CLA	C1D-ND	3.20	1.42	1.37
19	AA	819	CLA	C1D-ND	3.20	1.42	1.37
24	B	850	AJP	O79-C22	-3.20	1.36	1.43
19	A1	825	CLA	C1D-ND	3.20	1.42	1.37
19	A1	833	CLA	C1D-ND	3.20	1.42	1.37
19	A2	819	CLA	C1D-ND	3.20	1.42	1.37
19	A2	837	CLA	C1D-ND	3.20	1.42	1.37
19	A1	836	CLA	C1D-ND	3.19	1.42	1.37
19	B	813	CLA	C1D-ND	3.19	1.42	1.37
24	BB	849	AJP	O79-C22	-3.19	1.36	1.43
23	A	849	BCR	C1-C6	-3.19	1.49	1.53
19	A	826	CLA	C1D-ND	3.19	1.42	1.37
24	M2	101	AJP	C83-C06	3.19	1.59	1.53
19	A2	806	CLA	C1D-ND	3.19	1.42	1.37
19	A	806	CLA	C1D-ND	3.19	1.42	1.37
19	A	808	CLA	C1D-ND	3.19	1.42	1.37
19	BB	826	CLA	CMB-C2B	-3.19	1.44	1.50
19	A1	807	CLA	C1D-ND	3.19	1.42	1.37
19	BB	816	CLA	C1D-ND	3.19	1.42	1.37
25	I1	102	LMG	C4-C5	3.19	1.59	1.53
19	B2	824	CLA	C1D-ND	3.19	1.42	1.37
19	A1	834	CLA	C1D-ND	3.18	1.42	1.37
19	A1	809	CLA	C1D-ND	3.18	1.42	1.37
19	A	825	CLA	C1D-ND	3.18	1.42	1.37
23	L	205	BCR	C30-C25	-3.18	1.49	1.53
19	A	810	CLA	C1D-ND	3.18	1.42	1.37
23	AA	848	BCR	C30-C25	-3.18	1.49	1.53
19	AA	806	CLA	C1D-ND	3.18	1.42	1.37
19	AA	828	CLA	C1D-ND	3.18	1.42	1.37
19	B	819	CLA	C1D-ND	3.18	1.42	1.37
19	BB	834	CLA	C1D-ND	3.17	1.42	1.37
19	A1	829	CLA	C1B-C2B	3.17	1.50	1.43
23	A	847	BCR	C30-C25	-3.17	1.49	1.53
19	A2	830	CLA	C1D-ND	3.17	1.42	1.37
19	B	824	CLA	C1D-ND	3.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	820	CLA	C1D-ND	3.17	1.42	1.37
19	A2	821	CLA	C1D-ND	3.17	1.42	1.37
19	A	834	CLA	C1D-ND	3.17	1.42	1.37
24	L2	202	AJP	O79-C22	-3.16	1.36	1.43
19	B1	821	CLA	C1D-ND	3.16	1.42	1.37
19	BB	802	CLA	C1D-ND	3.16	1.42	1.37
24	B	849	AJP	O79-C22	-3.16	1.36	1.43
19	A1	819	CLA	C1D-ND	3.16	1.42	1.37
19	AA	835	CLA	C1D-ND	3.16	1.42	1.37
24	A2	854	AJP	O79-C22	-3.16	1.36	1.43
19	B1	834	CLA	C1D-ND	3.16	1.42	1.37
19	A2	835	CLA	C1D-ND	3.16	1.42	1.37
23	F2	303	BCR	C30-C25	-3.15	1.49	1.53
20	A2	803	CL0	CHB-C1B	3.15	1.44	1.39
19	B1	827	CLA	C1D-ND	3.15	1.42	1.37
19	F2	301	CLA	C4B-NB	3.15	1.42	1.37
19	BB	824	CLA	C1D-ND	3.15	1.42	1.37
19	A2	834	CLA	C1D-ND	3.15	1.42	1.37
24	A1	854	AJP	O79-C22	-3.15	1.36	1.43
23	B	842	BCR	C30-C25	-3.15	1.49	1.53
19	A1	805	CLA	C4B-NB	3.15	1.42	1.37
19	A1	820	CLA	C1D-ND	3.15	1.42	1.37
19	B	821	CLA	C1D-ND	3.15	1.42	1.37
19	FF	301	CLA	C1D-ND	3.15	1.42	1.37
24	B	857	AJP	O79-C22	-3.14	1.36	1.43
19	B	802	CLA	C1D-ND	3.14	1.42	1.37
24	B	849	AJP	C83-C06	3.14	1.59	1.53
19	F1	301	CLA	C4B-NB	3.14	1.42	1.37
19	B	829	CLA	C1D-ND	3.14	1.42	1.37
19	B2	826	CLA	C1D-ND	3.14	1.42	1.37
24	A1	855	AJP	O79-C22	-3.14	1.36	1.43
19	AA	820	CLA	C1D-ND	3.14	1.42	1.37
19	J2	103	CLA	C4B-NB	3.14	1.42	1.37
19	B1	818	CLA	C4B-NB	3.14	1.42	1.37
19	BB	806	CLA	C1D-ND	3.13	1.42	1.37
19	B2	827	CLA	C1D-ND	3.13	1.42	1.37
19	FF	305	CLA	C1D-ND	3.13	1.42	1.37
23	BB	841	BCR	C30-C25	-3.13	1.49	1.53
19	AA	801	CLA	C1D-ND	3.13	1.42	1.37
19	J1	103	CLA	C4B-NB	3.13	1.42	1.37
19	A2	831	CLA	C1D-ND	3.13	1.42	1.37
24	L	209	AJP	C83-C06	3.12	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	814	CLA	C1D-ND	3.12	1.42	1.37
19	BB	805	CLA	C1D-ND	3.12	1.42	1.37
19	X2	101	CLA	C4B-NB	3.12	1.42	1.37
19	A1	830	CLA	C1D-ND	3.12	1.42	1.37
24	L1	203	AJP	O79-C22	-3.12	1.36	1.43
24	KK	104	AJP	O79-C22	-3.11	1.36	1.43
24	L2	202	AJP	C24-C19	3.11	1.58	1.53
19	B2	806	CLA	C1D-ND	3.11	1.41	1.37
19	B2	818	CLA	C4B-NB	3.11	1.41	1.37
19	BB	810	CLA	C1D-ND	3.11	1.41	1.37
19	BB	820	CLA	C1D-ND	3.11	1.41	1.37
24	BB	849	AJP	C07-C08	-3.11	1.48	1.53
19	B2	821	CLA	C1D-ND	3.11	1.41	1.37
19	B	854	CLA	C1D-ND	3.11	1.41	1.37
19	A2	805	CLA	C1D-ND	3.11	1.41	1.37
24	BB	848	AJP	C18-C19	-3.11	1.45	1.53
19	B1	805	CLA	C1D-ND	3.11	1.41	1.37
19	AA	831	CLA	C1D-ND	3.10	1.41	1.37
19	B1	828	CLA	C1D-ND	3.10	1.41	1.37
19	F2	302	CLA	C4B-NB	3.10	1.41	1.37
19	BB	818	CLA	C1D-ND	3.10	1.41	1.37
19	AA	829	CLA	C1D-ND	3.10	1.41	1.37
19	AA	804	CLA	C1D-ND	3.10	1.41	1.37
23	A1	847	BCR	C30-C25	-3.10	1.49	1.53
19	B	829	CLA	C4B-NB	3.10	1.41	1.37
19	AA	834	CLA	C1D-ND	3.10	1.41	1.37
23	I2	103	BCR	C30-C25	-3.09	1.49	1.53
24	AA	856	AJP	O79-C22	-3.09	1.36	1.43
19	B	816	CLA	C1D-ND	3.09	1.41	1.37
24	K	104	AJP	O79-C22	-3.09	1.36	1.43
24	L2	202	AJP	C18-C19	-3.09	1.45	1.53
19	FF	302	CLA	C4B-NB	3.09	1.41	1.37
19	B1	824	CLA	C1D-ND	3.09	1.41	1.37
19	B	810	CLA	C1D-ND	3.09	1.41	1.37
19	A	831	CLA	C1D-ND	3.09	1.41	1.37
24	A	855	AJP	O79-C22	-3.09	1.36	1.43
19	B	835	CLA	C1D-ND	3.08	1.41	1.37
19	B1	828	CLA	C4B-NB	3.08	1.41	1.37
19	B2	829	CLA	C4B-NB	3.08	1.41	1.37
19	B	827	CLA	C1D-ND	3.08	1.41	1.37
19	F	302	CLA	C4B-NB	3.08	1.41	1.37
19	A	801	CLA	C1D-ND	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	847	BCR	C30-C25	-3.08	1.49	1.53
19	B2	805	CLA	C1D-ND	3.07	1.41	1.37
24	L1	204	AJP	C83-C06	3.07	1.59	1.53
23	B1	841	BCR	C30-C25	-3.07	1.49	1.53
24	B	849	AJP	C18-C19	-3.07	1.45	1.53
19	B	822	CLA	C1D-ND	3.07	1.41	1.37
19	BB	826	CLA	CMD-C2D	-3.07	1.44	1.50
19	J	103	CLA	C4B-NB	3.07	1.41	1.37
19	AA	822	CLA	C4B-NB	3.07	1.41	1.37
19	L2	206	CLA	C4B-NB	3.06	1.41	1.37
19	A2	801	CLA	C1D-ND	3.06	1.41	1.37
19	B2	823	CLA	C4B-NB	3.06	1.41	1.37
19	A2	806	CLA	C4B-NB	3.06	1.41	1.37
19	A2	814	CLA	C4B-NB	3.06	1.41	1.37
19	A	814	CLA	C4B-NB	3.06	1.41	1.37
23	FF	306	BCR	C30-C25	-3.06	1.49	1.53
24	L1	203	AJP	C24-C19	3.06	1.58	1.53
19	F	301	CLA	C4B-NB	3.06	1.41	1.37
24	L2	203	AJP	C83-C06	3.06	1.59	1.53
19	A1	813	CLA	C4B-NB	3.06	1.41	1.37
19	BB	832	CLA	C4B-NB	3.05	1.41	1.37
19	A	829	CLA	C1D-ND	3.05	1.41	1.37
24	AA	802	AJP	C18-C19	-3.05	1.45	1.53
24	L1	203	AJP	C18-C19	-3.05	1.45	1.53
19	B	806	CLA	C1D-ND	3.05	1.41	1.37
24	K	104	AJP	C83-C06	3.04	1.59	1.53
23	L1	208	BCR	C30-C25	-3.04	1.49	1.53
19	BB	804	CLA	C4B-NB	3.04	1.41	1.37
24	A	802	AJP	C18-C19	-3.04	1.45	1.53
19	AA	805	CLA	C1D-ND	3.04	1.41	1.37
19	L	204	CLA	C1D-ND	3.04	1.41	1.37
24	L	209	AJP	C18-C19	-3.04	1.45	1.53
19	FF	305	CLA	C4B-NB	3.03	1.41	1.37
19	A1	836	CLA	C4B-NB	3.03	1.41	1.37
24	L	208	AJP	C83-C06	3.03	1.59	1.53
19	A	805	CLA	C1D-ND	3.03	1.41	1.37
19	B	837	CLA	C4B-NB	3.03	1.41	1.37
23	F	305	BCR	C30-C25	-3.03	1.49	1.53
19	F1	302	CLA	C4B-NB	3.03	1.41	1.37
19	LL	202	CLA	C1D-ND	3.02	1.41	1.37
19	AA	806	CLA	C4B-NB	3.02	1.41	1.37
19	X1	101	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	820	CLA	C1D-ND	3.02	1.41	1.37
19	BB	836	CLA	C1D-ND	3.02	1.41	1.37
19	B2	820	CLA	C1D-ND	3.02	1.41	1.37
19	A	827	CLA	C4B-NB	3.02	1.41	1.37
19	AA	817	CLA	C4B-NB	3.02	1.41	1.37
19	BB	821	CLA	C1D-ND	3.02	1.41	1.37
19	JJ	103	CLA	C4B-NB	3.01	1.41	1.37
19	B	818	CLA	C3B-C4B	3.01	1.51	1.42
23	F1	303	BCR	C30-C25	-3.01	1.49	1.53
19	B	854	CLA	C1B-C2B	3.00	1.50	1.43
19	B2	816	CLA	C4B-NB	3.00	1.41	1.37
19	B1	848	CLA	C1D-ND	3.00	1.41	1.37
19	A	817	CLA	C4B-NB	3.00	1.41	1.37
19	A2	829	CLA	C1D-ND	3.00	1.41	1.37
19	A	837	CLA	C4B-NB	3.00	1.41	1.37
19	AA	837	CLA	C4B-NB	3.00	1.41	1.37
19	JJ	101	CLA	C4B-NB	3.00	1.41	1.37
19	A	806	CLA	C4B-NB	3.00	1.41	1.37
19	BB	827	CLA	C1D-ND	3.00	1.41	1.37
19	A	810	CLA	C4B-NB	3.00	1.41	1.37
19	A1	816	CLA	C4B-NB	2.99	1.41	1.37
19	AA	810	CLA	C4B-NB	2.99	1.41	1.37
19	L	203	CLA	C1D-ND	2.99	1.41	1.37
19	B1	823	CLA	C4B-NB	2.99	1.41	1.37
19	B2	849	CLA	C1D-ND	2.99	1.41	1.37
19	B1	816	CLA	C4B-NB	2.99	1.41	1.37
19	A2	817	CLA	C4B-NB	2.99	1.41	1.37
19	J1	101	CLA	C4B-NB	2.99	1.41	1.37
19	B	804	CLA	C4B-NB	2.99	1.41	1.37
23	AA	850	BCR	C1-C6	-2.98	1.50	1.53
19	B2	833	CLA	C4B-NB	2.98	1.41	1.37
19	B	805	CLA	C1D-ND	2.98	1.41	1.37
19	J2	101	CLA	C4B-NB	2.98	1.41	1.37
19	A	822	CLA	C4B-NB	2.97	1.41	1.37
19	X	101	CLA	C4B-NB	2.97	1.41	1.37
19	AA	814	CLA	C4B-NB	2.97	1.41	1.37
24	KK	104	AJP	C83-C06	2.97	1.59	1.53
19	B1	820	CLA	C4B-NB	2.97	1.41	1.37
19	B1	809	CLA	C4B-NB	2.97	1.41	1.37
19	A2	818	CLA	C4B-NB	2.97	1.41	1.37
19	A	824	CLA	C4B-NB	2.97	1.41	1.37
19	BB	822	CLA	C1D-ND	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M2	101	AJP	C18-C19	-2.97	1.46	1.53
19	A2	837	CLA	C4B-NB	2.97	1.41	1.37
19	B1	831	CLA	C4B-NB	2.97	1.41	1.37
19	B2	817	CLA	C4B-NB	2.97	1.41	1.37
19	B2	811	CLA	C4B-NB	2.96	1.41	1.37
19	J	101	CLA	C4B-NB	2.96	1.41	1.37
19	B1	807	CLA	C4B-NB	2.96	1.41	1.37
19	B1	822	CLA	C4B-NB	2.96	1.41	1.37
19	B2	809	CLA	C4B-NB	2.96	1.41	1.37
24	I2	104	AJP	C83-C06	2.96	1.59	1.53
24	B	857	AJP	C83-C06	2.96	1.59	1.53
19	A1	828	CLA	C1D-ND	2.96	1.41	1.37
19	AA	825	CLA	C4B-NB	2.96	1.41	1.37
19	L1	206	CLA	C1D-ND	2.95	1.41	1.37
19	B1	848	CLA	C1B-C2B	2.95	1.50	1.43
19	B1	817	CLA	C4B-NB	2.95	1.41	1.37
19	B2	852	CLA	C1D-ND	2.95	1.41	1.37
19	A	825	CLA	C4B-NB	2.95	1.41	1.37
24	A1	854	AJP	C83-C06	2.95	1.59	1.53
24	AA	802	AJP	C83-C06	2.95	1.59	1.53
19	AA	838	CLA	C4B-NB	2.95	1.41	1.37
19	B	860	CLA	C1D-ND	2.95	1.41	1.37
19	B2	832	CLA	C1B-C2B	2.95	1.50	1.43
19	J2	103	CLA	C1B-C2B	2.95	1.50	1.43
19	B	807	CLA	C4B-NB	2.95	1.41	1.37
19	K1	105	CLA	C4B-NB	2.94	1.41	1.37
19	B2	827	CLA	C4B-NB	2.94	1.41	1.37
19	B2	804	CLA	C4B-NB	2.94	1.41	1.37
19	AA	824	CLA	C4B-NB	2.94	1.41	1.37
19	B2	846	CLA	C4B-NB	2.94	1.41	1.37
19	A2	825	CLA	C4B-NB	2.94	1.41	1.37
19	AA	827	CLA	C4B-NB	2.94	1.41	1.37
19	A1	835	CLA	C1B-C2B	2.94	1.50	1.43
19	BB	852	CLA	C1D-ND	2.94	1.41	1.37
24	L2	202	AJP	C83-C06	2.94	1.59	1.53
19	A	818	CLA	C4B-NB	2.94	1.41	1.37
19	B1	831	CLA	C1B-C2B	2.94	1.50	1.43
19	B1	832	CLA	C1B-C2B	2.94	1.50	1.43
19	A1	817	CLA	C4B-NB	2.94	1.41	1.37
24	A2	854	AJP	C83-C06	2.94	1.59	1.53
19	BB	823	CLA	C4B-NB	2.94	1.41	1.37
19	A1	837	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	822	CLA	C4B-NB	2.93	1.41	1.37
19	A1	812	CLA	C4B-NB	2.93	1.41	1.37
19	B1	845	CLA	C4B-NB	2.93	1.41	1.37
24	A	802	AJP	C83-C06	2.93	1.59	1.53
19	B1	827	CLA	C4B-NB	2.93	1.41	1.37
19	B1	804	CLA	C4B-NB	2.93	1.41	1.37
19	AA	842	CLA	C4B-NB	2.93	1.41	1.37
24	L1	204	AJP	C18-C19	-2.93	1.46	1.53
19	L1	207	CLA	C4B-NB	2.93	1.41	1.37
19	A2	802	CLA	C4B-NB	2.93	1.41	1.37
19	AA	818	CLA	C4B-NB	2.93	1.41	1.37
19	L2	206	CLA	C1B-C2B	2.93	1.50	1.43
19	A	838	CLA	C4B-NB	2.93	1.41	1.37
19	K	101	CLA	C4B-NB	2.93	1.41	1.37
19	LL	203	CLA	C4B-NB	2.93	1.41	1.37
19	XX	101	CLA	C4B-NB	2.93	1.41	1.37
19	A2	838	CLA	C4B-NB	2.93	1.41	1.37
19	A1	834	CLA	C4B-NB	2.92	1.41	1.37
19	KK	101	CLA	C4B-NB	2.92	1.41	1.37
19	B2	814	CLA	C4B-NB	2.92	1.41	1.37
19	BB	807	CLA	C4B-NB	2.92	1.41	1.37
19	B1	819	CLA	C4B-NB	2.92	1.41	1.37
19	AA	843	CLA	C1D-ND	2.92	1.41	1.37
19	B	823	CLA	C4B-NB	2.92	1.41	1.37
23	B1	839	BCR	C30-C25	-2.92	1.50	1.53
19	BB	813	CLA	C4B-NB	2.92	1.41	1.37
19	A	832	CLA	C1B-C2B	2.92	1.50	1.43
19	A1	821	CLA	C4B-NB	2.92	1.41	1.37
19	K1	103	CLA	C4B-NB	2.92	1.41	1.37
19	A1	809	CLA	C4B-NB	2.92	1.41	1.37
19	BB	811	CLA	C4B-NB	2.92	1.41	1.37
19	F1	305	CLA	C4B-NB	2.91	1.41	1.37
24	BB	849	AJP	C18-C19	-2.91	1.46	1.53
19	B1	811	CLA	C4B-NB	2.91	1.41	1.37
19	AA	833	CLA	C4B-NB	2.91	1.41	1.37
19	A2	835	CLA	C4B-NB	2.91	1.41	1.37
19	A1	835	CLA	C4B-NB	2.91	1.41	1.37
19	AA	819	CLA	C4B-NB	2.91	1.41	1.37
24	KK	104	AJP	C81-C12	2.91	1.59	1.54
19	J	103	CLA	C1B-C2B	2.91	1.50	1.43
19	A1	832	CLA	C4B-NB	2.91	1.41	1.37
19	K2	104	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	FF	301	CLA	C4B-NB	2.91	1.41	1.37
19	A1	818	CLA	C4B-NB	2.91	1.41	1.37
19	K	102	CLA	C4B-NB	2.91	1.41	1.37
19	B2	801	CLA	C4B-NB	2.91	1.41	1.37
19	A	804	CLA	C1D-ND	2.91	1.41	1.37
19	B2	813	CLA	C4B-NB	2.91	1.41	1.37
19	A2	804	CLA	C1D-ND	2.90	1.41	1.37
19	A1	831	CLA	C4B-NB	2.90	1.41	1.37
19	A2	819	CLA	C4B-NB	2.90	1.41	1.37
19	A2	833	CLA	C4B-NB	2.90	1.41	1.37
19	AA	808	CLA	C4B-NB	2.90	1.41	1.37
19	BB	827	CLA	C4B-NB	2.90	1.41	1.37
19	A1	824	CLA	C4B-NB	2.90	1.41	1.37
19	A1	804	CLA	C1B-C2B	2.90	1.49	1.43
19	BB	821	CLA	C1B-C2B	2.90	1.49	1.43
19	B	826	CLA	CMB-C2B	-2.90	1.44	1.50
19	A1	842	CLA	C1D-ND	2.90	1.41	1.37
19	B2	807	CLA	C4B-NB	2.90	1.41	1.37
19	BB	845	CLA	C4B-NB	2.90	1.41	1.37
19	A2	813	CLA	C4B-NB	2.90	1.41	1.37
19	B2	832	CLA	C4B-NB	2.90	1.41	1.37
19	A	833	CLA	C4B-NB	2.90	1.41	1.37
24	B	850	AJP	C18-C19	-2.90	1.46	1.53
24	L2	203	AJP	C18-C19	-2.89	1.46	1.53
19	B1	814	CLA	C4B-NB	2.89	1.41	1.37
19	B2	837	CLA	C4B-NB	2.89	1.41	1.37
19	B	817	CLA	C4B-NB	2.89	1.41	1.37
19	B1	836	CLA	C4B-NB	2.89	1.41	1.37
19	B	811	CLA	C4B-NB	2.89	1.41	1.37
19	B	846	CLA	C4B-NB	2.89	1.41	1.37
19	B	818	CLA	C1B-C2B	2.89	1.49	1.43
23	A2	849	BCR	C1-C6	-2.89	1.50	1.53
19	AA	835	CLA	C4B-NB	2.89	1.41	1.37
19	A	819	CLA	C4B-NB	2.89	1.41	1.37
19	B2	851	CLA	C4B-NB	2.89	1.41	1.37
19	B	816	CLA	C4B-NB	2.89	1.41	1.37
19	BB	805	CLA	C4B-NB	2.89	1.41	1.37
19	A	818	CLA	C1B-C2B	2.89	1.49	1.43
19	B2	808	CLA	C4B-NB	2.88	1.41	1.37
19	J1	103	CLA	C1B-C2B	2.88	1.49	1.43
19	B	832	CLA	C4B-NB	2.88	1.41	1.37
19	B1	813	CLA	C4B-NB	2.88	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	KK	102	CLA	C4B-NB	2.88	1.41	1.37
19	B1	812	CLA	C4B-NB	2.88	1.41	1.37
19	BB	816	CLA	C4B-NB	2.88	1.41	1.37
23	K1	106	BCR	C30-C25	-2.88	1.50	1.53
19	B1	832	CLA	C4B-NB	2.88	1.41	1.37
19	B1	850	CLA	C4B-NB	2.88	1.41	1.37
19	A	832	CLA	C4B-NB	2.88	1.41	1.37
19	AA	832	CLA	C4B-NB	2.88	1.41	1.37
19	BB	855	CLA	C4B-NB	2.88	1.41	1.37
19	A1	826	CLA	C4B-NB	2.88	1.41	1.37
19	A2	810	CLA	C4B-NB	2.87	1.41	1.37
19	K	102	CLA	C1B-C2B	2.87	1.49	1.43
19	B1	830	CLA	C4B-NB	2.87	1.41	1.37
19	B2	822	CLA	C4B-NB	2.87	1.41	1.37
19	B2	828	CLA	C4B-NB	2.87	1.41	1.37
19	BB	831	CLA	C1B-C2B	2.87	1.49	1.43
19	B1	824	CLA	C4B-NB	2.87	1.41	1.37
19	A1	803	CLA	C1D-ND	2.87	1.41	1.37
19	AA	821	CLA	C1B-C2B	2.87	1.49	1.43
19	B1	801	CLA	C4B-NB	2.87	1.41	1.37
24	L2	202	AJP	C07-C08	-2.87	1.49	1.53
19	L2	205	CLA	C1D-ND	2.87	1.41	1.37
19	AA	823	CLA	C4B-NB	2.87	1.41	1.37
23	BB	839	BCR	C30-C25	-2.87	1.50	1.53
24	BB	849	AJP	C83-C06	2.87	1.59	1.53
24	L1	203	AJP	C07-C08	-2.87	1.49	1.53
19	AA	818	CLA	C1B-C2B	2.87	1.49	1.43
19	BB	801	CLA	C1B-C2B	2.87	1.49	1.43
19	B	830	CLA	C1D-ND	2.87	1.41	1.37
19	BB	817	CLA	C4B-NB	2.86	1.41	1.37
19	A1	841	CLA	C4B-NB	2.86	1.41	1.37
19	B1	835	CLA	C1B-C2B	2.86	1.49	1.43
24	L	209	AJP	C17-C16	2.86	1.58	1.53
19	B2	831	CLA	C4B-NB	2.86	1.41	1.37
19	A	823	CLA	C4B-NB	2.86	1.41	1.37
23	B	840	BCR	C30-C25	-2.86	1.50	1.53
19	B1	808	CLA	C4B-NB	2.86	1.41	1.37
24	L1	203	AJP	C05-C06	2.86	1.59	1.53
19	K2	102	CLA	C4B-NB	2.86	1.41	1.37
19	B2	833	CLA	C1B-C2B	2.86	1.49	1.43
19	A2	810	CLA	C3B-C4B	2.86	1.51	1.42
19	B1	827	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	821	CLA	C1B-C2B	2.85	1.49	1.43
19	A2	823	CLA	C4B-NB	2.85	1.41	1.37
19	A2	832	CLA	C4B-NB	2.85	1.41	1.37
19	B2	812	CLA	C4B-NB	2.85	1.41	1.37
19	L	203	CLA	C4B-NB	2.85	1.41	1.37
24	K	104	AJP	C18-C19	-2.85	1.46	1.53
24	B	850	AJP	C07-C08	-2.85	1.49	1.53
19	A	808	CLA	C4B-NB	2.85	1.41	1.37
19	B	822	CLA	C4B-NB	2.85	1.41	1.37
24	A1	855	AJP	C83-C06	2.85	1.59	1.53
19	B	813	CLA	C4B-NB	2.85	1.41	1.37
24	L	208	AJP	C07-C08	-2.85	1.49	1.53
24	I2	104	AJP	C24-C19	2.85	1.59	1.53
19	B	827	CLA	C1B-C2B	2.85	1.49	1.43
19	B1	849	CLA	C4B-NB	2.85	1.41	1.37
19	A2	827	CLA	C4B-NB	2.85	1.41	1.37
19	JJ	103	CLA	C1B-C2B	2.84	1.49	1.43
19	A2	824	CLA	C4B-NB	2.84	1.41	1.37
19	B2	805	CLA	C4B-NB	2.84	1.41	1.37
19	B	827	CLA	C4B-NB	2.84	1.41	1.37
19	L1	207	CLA	C1B-C2B	2.84	1.49	1.43
19	B2	821	CLA	C1B-C2B	2.84	1.49	1.43
19	B2	819	CLA	C4B-NB	2.84	1.41	1.37
19	B2	834	CLA	C4B-NB	2.84	1.41	1.37
19	B	819	CLA	C4B-NB	2.84	1.41	1.37
19	B	833	CLA	C4B-NB	2.84	1.41	1.37
19	A	816	CLA	C1B-C2B	2.84	1.49	1.43
19	A1	823	CLA	C4B-NB	2.84	1.41	1.37
19	B2	849	CLA	C4B-NB	2.84	1.41	1.37
19	AA	843	CLA	C1B-C2B	2.84	1.49	1.43
19	AA	827	CLA	C1B-C2B	2.84	1.49	1.43
19	A	812	CLA	C4B-NB	2.83	1.41	1.37
19	AA	813	CLA	C4B-NB	2.83	1.41	1.37
19	A1	811	CLA	C4B-NB	2.83	1.41	1.37
19	BB	818	CLA	C4B-NB	2.83	1.41	1.37
19	AA	840	CLA	C1B-C2B	2.83	1.49	1.43
19	B	805	CLA	C4B-NB	2.83	1.41	1.37
19	BB	852	CLA	C4B-NB	2.83	1.41	1.37
19	AA	825	CLA	C1B-C2B	2.83	1.49	1.43
19	BB	828	CLA	C4B-NB	2.83	1.41	1.37
19	B	801	CLA	C1B-C2B	2.83	1.49	1.43
19	BB	835	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	815	CLA	C4B-NB	2.83	1.41	1.37
19	B1	835	CLA	C4B-NB	2.83	1.41	1.37
19	B2	806	CLA	C4B-NB	2.83	1.41	1.37
19	A	825	CLA	C1B-C2B	2.83	1.49	1.43
24	M2	101	AJP	C07-C08	-2.83	1.49	1.53
19	BB	826	CLA	C1D-ND	2.83	1.41	1.37
24	KK	104	AJP	C18-C19	-2.82	1.46	1.53
19	L2	205	CLA	C4B-NB	2.82	1.41	1.37
24	L	209	AJP	C07-C08	-2.82	1.49	1.53
19	AA	828	CLA	C4B-NB	2.82	1.41	1.37
19	BB	812	CLA	C4B-NB	2.82	1.41	1.37
19	B	821	CLA	C1B-C2B	2.82	1.49	1.43
19	A	835	CLA	C4B-NB	2.82	1.41	1.37
19	B	809	CLA	C4B-NB	2.82	1.41	1.37
19	B	836	CLA	C4B-NB	2.82	1.41	1.37
19	K1	102	CLA	C4B-NB	2.82	1.41	1.37
19	AA	822	CLA	C1B-C2B	2.82	1.49	1.43
19	B	832	CLA	C1B-C2B	2.82	1.49	1.43
19	B1	805	CLA	C4B-NB	2.82	1.41	1.37
19	L1	205	CLA	C4B-NB	2.82	1.41	1.37
19	B	814	CLA	C4B-NB	2.82	1.41	1.37
19	AA	812	CLA	C4B-NB	2.82	1.41	1.37
19	AA	830	CLA	C1B-C2B	2.81	1.49	1.43
24	AA	856	AJP	C81-C12	2.81	1.59	1.54
19	A1	807	CLA	C4B-NB	2.81	1.41	1.37
19	BB	801	CLA	C4B-NB	2.81	1.41	1.37
19	B2	815	CLA	C4B-NB	2.81	1.41	1.37
19	AA	826	CLA	C4B-NB	2.81	1.41	1.37
19	A2	812	CLA	C4B-NB	2.81	1.41	1.37
19	B	828	CLA	C4B-NB	2.81	1.41	1.37
19	A1	820	CLA	C1B-C2B	2.81	1.49	1.43
19	B	830	CLA	C1B-C2B	2.81	1.49	1.43
19	BB	827	CLA	C1B-C2B	2.81	1.49	1.43
19	BB	822	CLA	C3B-C4B	2.81	1.50	1.42
19	B2	849	CLA	C1B-C2B	2.81	1.49	1.43
19	A1	808	CLA	C4B-NB	2.81	1.41	1.37
19	B2	836	CLA	C1B-C2B	2.81	1.49	1.43
19	A1	844	CLA	C4B-NB	2.81	1.41	1.37
19	A2	844	CLA	C4B-NB	2.81	1.41	1.37
24	I2	104	AJP	C18-C19	-2.81	1.46	1.53
19	B1	826	CLA	CMB-C2B	-2.80	1.45	1.50
19	A	817	CLA	C1B-C2B	2.80	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	836	CLA	C4B-NB	2.80	1.41	1.37
19	A	830	CLA	C1B-C2B	2.80	1.49	1.43
19	B	837	CLA	C1B-C2B	2.80	1.49	1.43
19	A	816	CLA	C4B-NB	2.80	1.41	1.37
24	A	855	AJP	C81-C12	2.80	1.58	1.54
19	A2	808	CLA	C4B-NB	2.80	1.41	1.37
19	B2	828	CLA	C1B-C2B	2.80	1.49	1.43
19	A	836	CLA	C4B-NB	2.80	1.41	1.37
19	A2	816	CLA	C1B-C2B	2.80	1.49	1.43
19	A1	831	CLA	C1B-C2B	2.80	1.49	1.43
19	B2	836	CLA	C4B-NB	2.80	1.41	1.37
19	A1	827	CLA	C4B-NB	2.80	1.41	1.37
19	B1	810	CLA	C4B-NB	2.80	1.41	1.37
19	A2	809	CLA	C4B-NB	2.80	1.41	1.37
19	AA	841	CLA	C1B-C2B	2.80	1.49	1.43
19	A	844	CLA	C4B-NB	2.80	1.41	1.37
19	KK	102	CLA	C1B-C2B	2.80	1.49	1.43
19	A	842	CLA	C4B-NB	2.79	1.41	1.37
24	A1	855	AJP	C18-C19	-2.79	1.46	1.53
19	A1	833	CLA	C4B-NB	2.79	1.41	1.37
23	AA	855	BCR	C30-C25	-2.79	1.50	1.53
19	A	808	CLA	C1B-C2B	2.79	1.49	1.43
24	A	802	AJP	C24-C19	2.79	1.59	1.53
19	A	813	CLA	C4B-NB	2.79	1.41	1.37
19	AA	845	CLA	C4B-NB	2.79	1.41	1.37
19	A	810	CLA	C3B-C4B	2.79	1.50	1.42
19	B2	808	CLA	C1B-C2B	2.79	1.49	1.43
24	AA	802	AJP	C24-C19	2.79	1.59	1.53
19	B2	812	CLA	C1B-C2B	2.79	1.49	1.43
19	BB	809	CLA	C4B-NB	2.79	1.41	1.37
19	A2	841	CLA	C1B-C2B	2.79	1.49	1.43
19	AA	836	CLA	C1B-C2B	2.79	1.49	1.43
19	A	841	CLA	C1B-C2B	2.79	1.49	1.43
19	B1	829	CLA	C1D-ND	2.79	1.41	1.37
19	A2	816	CLA	C4B-NB	2.79	1.41	1.37
19	A2	826	CLA	C4B-NB	2.79	1.41	1.37
19	K1	105	CLA	C1B-C2B	2.79	1.49	1.43
19	L1	206	CLA	C4B-NB	2.79	1.41	1.37
19	A	826	CLA	C4B-NB	2.79	1.41	1.37
19	L2	204	CLA	C4B-NB	2.79	1.41	1.37
19	BB	821	CLA	C4B-NB	2.79	1.41	1.37
19	B	808	CLA	C1B-C2B	2.79	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	819	CLA	C1B-C2B	2.79	1.49	1.43
19	AA	808	CLA	C1B-C2B	2.79	1.49	1.43
19	A2	805	CLA	C4B-NB	2.78	1.41	1.37
23	B2	840	BCR	C30-C25	-2.78	1.50	1.53
19	B1	812	CLA	C1B-C2B	2.78	1.49	1.43
23	B2	842	BCR	C30-C25	-2.78	1.50	1.53
19	AA	810	CLA	C3B-C4B	2.78	1.50	1.42
19	AA	817	CLA	C1B-C2B	2.78	1.49	1.43
19	B	858	CLA	C4B-NB	2.78	1.41	1.37
19	BB	829	CLA	C1D-ND	2.78	1.41	1.37
19	F1	305	CLA	C1B-C2B	2.78	1.49	1.43
19	A2	844	CLA	C1B-C2B	2.78	1.49	1.43
19	B2	817	CLA	C1B-C2B	2.78	1.49	1.43
19	BB	818	CLA	C1B-C2B	2.78	1.49	1.43
19	B	819	CLA	C1B-C2B	2.78	1.49	1.43
19	A	809	CLA	C4B-NB	2.78	1.41	1.37
19	L	202	CLA	C4B-NB	2.78	1.41	1.37
24	B	849	AJP	C07-C08	-2.78	1.49	1.53
19	B	801	CLA	C4B-NB	2.78	1.41	1.37
19	A2	801	CLA	C1B-C2B	2.78	1.49	1.43
19	B2	830	CLA	C1D-ND	2.77	1.41	1.37
19	B2	849	CLA	CMB-C2B	-2.77	1.45	1.50
19	A2	834	CLA	C4B-NB	2.77	1.41	1.37
19	A2	842	CLA	C4B-NB	2.77	1.41	1.37
19	BB	824	CLA	C4B-NB	2.77	1.41	1.37
19	A	836	CLA	C1B-C2B	2.77	1.49	1.43
24	A	855	AJP	C07-C08	-2.77	1.49	1.53
23	K2	105	BCR	C30-C25	-2.77	1.50	1.53
24	AA	856	AJP	C07-C08	-2.77	1.49	1.53
19	A	834	CLA	C4B-NB	2.77	1.41	1.37
19	AA	845	CLA	C1B-C2B	2.77	1.49	1.43
19	A1	840	CLA	C1B-C2B	2.77	1.49	1.43
19	J	101	CLA	C1B-C2B	2.77	1.49	1.43
19	B1	808	CLA	C1B-C2B	2.77	1.49	1.43
24	A2	854	AJP	C18-C19	-2.77	1.46	1.53
19	A1	844	CLA	C1B-C2B	2.77	1.49	1.43
19	A1	852	CLA	C1B-C2B	2.77	1.49	1.43
19	JJ	101	CLA	C1B-C2B	2.77	1.49	1.43
19	B1	817	CLA	C1B-C2B	2.77	1.49	1.43
19	B1	819	CLA	C1B-C2B	2.77	1.49	1.43
19	B2	820	CLA	C4B-NB	2.77	1.41	1.37
19	A1	815	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	827	CLA	C1B-C2B	2.76	1.49	1.43
19	BB	831	CLA	C4B-NB	2.76	1.41	1.37
19	AA	833	CLA	C1B-C2B	2.76	1.49	1.43
19	A2	802	CLA	C1B-C2B	2.76	1.49	1.43
19	A1	809	CLA	C3B-C4B	2.76	1.50	1.42
19	X1	101	CLA	C1B-C2B	2.76	1.49	1.43
19	LL	201	CLA	C4B-NB	2.76	1.41	1.37
19	BB	819	CLA	C4B-NB	2.76	1.41	1.37
19	A1	825	CLA	C4B-NB	2.76	1.41	1.37
19	B	824	CLA	C4B-NB	2.75	1.41	1.37
19	A2	828	CLA	C4B-NB	2.75	1.41	1.37
19	B	859	CLA	C4B-NB	2.75	1.41	1.37
19	A1	817	CLA	C1B-C2B	2.75	1.49	1.43
19	A2	818	CLA	C1B-C2B	2.75	1.49	1.43
19	A	831	CLA	C4B-NB	2.75	1.41	1.37
19	A	840	CLA	C4B-NB	2.75	1.41	1.37
19	AA	805	CLA	C4B-NB	2.75	1.41	1.37
19	A2	812	CLA	C1B-C2B	2.75	1.49	1.43
19	XX	101	CLA	C1B-C2B	2.75	1.49	1.43
19	B1	825	CLA	C4B-NB	2.75	1.41	1.37
19	BB	828	CLA	C1B-C2B	2.75	1.49	1.43
19	J1	101	CLA	C1B-C2B	2.75	1.49	1.43
19	A	821	CLA	C1B-C2B	2.75	1.49	1.43
19	B2	837	CLA	C1B-C2B	2.75	1.49	1.43
19	A	834	CLA	C1B-C2B	2.75	1.49	1.43
19	A1	822	CLA	C4B-NB	2.75	1.41	1.37
24	L1	203	AJP	C04-C05	2.75	1.56	1.51
19	AA	840	CLA	C4B-NB	2.75	1.41	1.37
19	K1	103	CLA	C1B-C2B	2.75	1.49	1.43
19	BB	819	CLA	C1B-C2B	2.75	1.49	1.43
19	B2	850	CLA	C4B-NB	2.75	1.41	1.37
19	A	804	CLA	C4B-NB	2.75	1.41	1.37
19	B	828	CLA	C1B-C2B	2.74	1.49	1.43
19	A1	815	CLA	C4B-NB	2.74	1.41	1.37
19	B	854	CLA	C4B-NB	2.74	1.41	1.37
19	J2	101	CLA	C1B-C2B	2.74	1.49	1.43
19	AA	839	CLA	C4B-NB	2.74	1.41	1.37
24	K	104	AJP	C07-C08	-2.74	1.49	1.53
19	B1	848	CLA	CMB-C2B	-2.74	1.45	1.50
19	B1	848	CLA	C4B-NB	2.74	1.41	1.37
19	AA	809	CLA	C4B-NB	2.74	1.41	1.37
19	L2	204	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A2	854	AJP	C04-C05	2.74	1.56	1.51
19	B2	852	CLA	C1B-C2B	2.74	1.49	1.43
19	A2	839	CLA	C4B-NB	2.74	1.41	1.37
19	BB	830	CLA	C1B-C2B	2.74	1.49	1.43
19	BB	830	CLA	C4B-NB	2.74	1.41	1.37
19	AA	804	CLA	C4B-NB	2.74	1.41	1.37
19	AA	816	CLA	C4B-NB	2.74	1.41	1.37
19	A2	826	CLA	C1B-C2B	2.74	1.49	1.43
19	B2	824	CLA	C4B-NB	2.74	1.41	1.37
19	A	839	CLA	C4B-NB	2.74	1.41	1.37
19	AA	834	CLA	C4B-NB	2.74	1.41	1.37
19	L1	205	CLA	C1B-C2B	2.73	1.49	1.43
19	X	101	CLA	C1B-C2B	2.73	1.49	1.43
19	A1	807	CLA	C1B-C2B	2.73	1.49	1.43
19	B1	821	CLA	C1B-C2B	2.73	1.49	1.43
19	A1	838	CLA	C4B-NB	2.73	1.41	1.37
19	B1	829	CLA	C4B-NB	2.73	1.41	1.37
19	A2	836	CLA	C4B-NB	2.73	1.41	1.37
19	A	805	CLA	C4B-NB	2.73	1.41	1.37
19	AA	830	CLA	C4B-NB	2.73	1.41	1.37
24	I2	104	AJP	C07-C08	-2.73	1.49	1.53
19	A1	825	CLA	C1B-C2B	2.73	1.49	1.43
19	B2	830	CLA	C1B-C2B	2.73	1.49	1.43
19	K2	104	CLA	C1B-C2B	2.73	1.49	1.43
19	B2	826	CLA	CMB-C2B	-2.73	1.45	1.50
19	B1	813	CLA	C1B-C2B	2.73	1.49	1.43
19	B1	836	CLA	C1B-C2B	2.73	1.49	1.43
19	A1	804	CLA	C4B-NB	2.73	1.41	1.37
19	A2	804	CLA	C4B-NB	2.73	1.41	1.37
19	A2	836	CLA	C1B-C2B	2.73	1.49	1.43
24	A	855	AJP	C83-C06	2.73	1.58	1.53
19	B2	825	CLA	C4B-NB	2.73	1.41	1.37
19	A1	833	CLA	C1B-C2B	2.73	1.49	1.43
19	A1	839	CLA	C4B-NB	2.73	1.41	1.37
19	A1	829	CLA	C4B-NB	2.73	1.41	1.37
19	A2	829	CLA	C4B-NB	2.73	1.41	1.37
19	B1	807	CLA	CMD-C2D	-2.73	1.45	1.50
19	A1	814	CLA	C4B-NB	2.72	1.41	1.37
19	BB	814	CLA	C4B-NB	2.72	1.41	1.37
19	B1	810	CLA	C1B-C2B	2.72	1.49	1.43
24	AA	856	AJP	C83-C06	2.72	1.58	1.53
19	A	813	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	844	CLA	C1B-C2B	2.72	1.49	1.43
19	B	812	CLA	C4B-NB	2.72	1.41	1.37
19	B	811	CLA	C1B-C2B	2.72	1.49	1.43
19	B1	806	CLA	C1B-C2B	2.72	1.49	1.43
19	A2	808	CLA	C1B-C2B	2.72	1.49	1.43
19	AA	801	CLA	C1B-C2B	2.72	1.49	1.43
19	BB	856	CLA	C4B-NB	2.72	1.41	1.37
19	B	831	CLA	C1B-C2B	2.72	1.49	1.43
19	X2	101	CLA	C1B-C2B	2.72	1.49	1.43
19	AA	834	CLA	C1B-C2B	2.72	1.49	1.43
19	A2	822	CLA	C1B-C2B	2.72	1.49	1.43
19	B	803	CLA	C4B-NB	2.72	1.41	1.37
19	B	815	CLA	C4B-NB	2.71	1.41	1.37
19	A	828	CLA	C1B-C2B	2.71	1.49	1.43
19	A2	840	CLA	C4B-NB	2.71	1.41	1.37
19	A1	821	CLA	C1B-C2B	2.71	1.49	1.43
19	AA	839	CLA	C1B-C2B	2.71	1.49	1.43
19	B2	802	CLA	C4B-NB	2.71	1.41	1.37
19	B2	821	CLA	C4B-NB	2.71	1.41	1.37
19	LL	201	CLA	C1B-C2B	2.71	1.49	1.43
19	BB	815	CLA	C4B-NB	2.71	1.41	1.37
19	A	826	CLA	C1B-C2B	2.71	1.49	1.43
19	B	860	CLA	C1B-C2B	2.71	1.49	1.43
19	AA	821	CLA	C4B-NB	2.71	1.41	1.37
19	BB	806	CLA	C1B-C2B	2.71	1.49	1.43
24	M2	101	AJP	C17-C16	2.71	1.58	1.53
19	AA	831	CLA	C4B-NB	2.71	1.41	1.37
19	A2	834	CLA	C1B-C2B	2.71	1.49	1.43
19	B2	813	CLA	C1B-C2B	2.71	1.49	1.43
19	A	801	CLA	C1B-C2B	2.71	1.49	1.43
19	A2	815	CLA	C4B-NB	2.70	1.41	1.37
19	B1	834	CLA	C1B-C2B	2.70	1.49	1.43
19	A1	830	CLA	C4B-NB	2.70	1.41	1.37
19	AA	807	CLA	C1B-C2B	2.70	1.49	1.43
19	BB	825	CLA	C4B-NB	2.70	1.41	1.37
19	A	833	CLA	C1B-C2B	2.70	1.49	1.43
19	BB	852	CLA	CMB-C2B	-2.70	1.45	1.50
19	B2	811	CLA	C1B-C2B	2.70	1.49	1.43
19	B2	846	CLA	C1B-C2B	2.70	1.49	1.43
19	A2	830	CLA	C1B-C2B	2.70	1.49	1.43
19	B2	810	CLA	C1B-C2B	2.70	1.49	1.43
19	AA	832	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	810	CLA	C4B-NB	2.70	1.41	1.37
19	BB	817	CLA	C1B-C2B	2.70	1.49	1.43
19	B2	801	CLA	C1B-C2B	2.70	1.49	1.43
19	A2	839	CLA	C1B-C2B	2.70	1.49	1.43
19	A	839	CLA	C1B-C2B	2.70	1.49	1.43
19	A	809	CLA	C1B-C2B	2.70	1.49	1.43
24	L1	203	AJP	C83-C06	2.70	1.58	1.53
19	AA	826	CLA	C1B-C2B	2.70	1.49	1.43
19	BB	812	CLA	C1B-C2B	2.70	1.49	1.43
19	A	807	CLA	C4B-NB	2.69	1.41	1.37
19	B	810	CLA	C4B-NB	2.69	1.41	1.37
19	A	852	CLA	C1B-C2B	2.69	1.49	1.43
19	B2	815	CLA	C1B-C2B	2.69	1.49	1.43
19	B	812	CLA	C1B-C2B	2.69	1.49	1.43
19	A2	821	CLA	C4B-NB	2.69	1.41	1.37
19	BB	834	CLA	C4B-NB	2.69	1.41	1.37
24	B	849	AJP	C04-C05	2.69	1.56	1.51
24	L	208	AJP	C17-C16	2.69	1.58	1.53
19	B2	835	CLA	C1B-C2B	2.69	1.49	1.43
23	A	854	BCR	C30-C25	-2.69	1.50	1.53
19	A2	852	CLA	C1B-C2B	2.69	1.49	1.43
19	AA	813	CLA	C1B-C2B	2.69	1.49	1.43
19	B1	845	CLA	C1B-C2B	2.69	1.49	1.43
19	K2	102	CLA	C1B-C2B	2.68	1.49	1.43
19	BB	811	CLA	C1B-C2B	2.68	1.49	1.43
19	B2	831	CLA	C1B-C2B	2.68	1.49	1.43
19	A	819	CLA	C1B-C2B	2.68	1.49	1.43
19	LL	203	CLA	CMD-C2D	-2.68	1.45	1.50
19	B	806	CLA	C1B-C2B	2.68	1.49	1.43
19	AA	809	CLA	C1B-C2B	2.68	1.49	1.43
19	A1	852	CLA	C4B-NB	2.68	1.41	1.37
19	B1	834	CLA	C4B-NB	2.68	1.41	1.37
19	B2	818	CLA	C1B-C2B	2.68	1.49	1.43
19	L	204	CLA	C4B-NB	2.68	1.41	1.37
19	B1	815	CLA	C1B-C2B	2.68	1.49	1.43
19	B1	818	CLA	C1B-C2B	2.68	1.49	1.43
19	A1	801	CLA	C1B-C2B	2.68	1.49	1.43
19	AA	816	CLA	C1B-C2B	2.68	1.49	1.43
24	BB	848	AJP	C07-C08	-2.68	1.49	1.53
19	LL	202	CLA	C4B-NB	2.68	1.41	1.37
24	KK	104	AJP	C07-C08	-2.68	1.49	1.53
19	A1	803	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	838	CLA	C1B-C2B	2.68	1.49	1.43
19	B2	823	CLA	C1B-C2B	2.68	1.49	1.43
19	A1	810	CLA	C4B-NB	2.68	1.41	1.37
19	A2	852	CLA	C4B-NB	2.68	1.41	1.37
19	B1	802	CLA	C1B-C2B	2.68	1.49	1.43
19	AA	814	CLA	C1B-C2B	2.67	1.49	1.43
19	A	830	CLA	C4B-NB	2.67	1.41	1.37
19	B1	830	CLA	C1B-C2B	2.67	1.49	1.43
19	A2	804	CLA	C1B-C2B	2.67	1.49	1.43
24	M2	101	AJP	C24-C19	2.67	1.59	1.53
19	B1	806	CLA	C4B-NB	2.67	1.41	1.37
19	B1	801	CLA	C1B-C2B	2.67	1.49	1.43
19	A1	841	CLA	C1B-C2B	2.67	1.49	1.43
19	A2	811	CLA	C4B-NB	2.67	1.41	1.37
19	B2	830	CLA	C4B-NB	2.67	1.41	1.37
19	A	821	CLA	C4B-NB	2.67	1.41	1.37
19	A1	838	CLA	C1B-C2B	2.67	1.49	1.43
19	B2	807	CLA	CMD-C2D	-2.67	1.45	1.50
19	AA	807	CLA	C4B-NB	2.67	1.41	1.37
19	BB	810	CLA	C4B-NB	2.67	1.41	1.37
19	B	820	CLA	C1B-C2B	2.67	1.49	1.43
19	B2	829	CLA	C3B-C4B	2.67	1.50	1.42
19	A	807	CLA	C1B-C2B	2.67	1.49	1.43
19	B	817	CLA	C1B-C2B	2.67	1.49	1.43
24	B	850	AJP	C83-C06	2.67	1.58	1.53
19	A1	803	CLA	C4B-NB	2.67	1.41	1.37
19	A	828	CLA	C4B-NB	2.67	1.41	1.37
19	AA	815	CLA	C4B-NB	2.66	1.41	1.37
19	L	202	CLA	C1B-C2B	2.66	1.49	1.43
19	B1	823	CLA	C1B-C2B	2.66	1.49	1.43
19	A1	824	CLA	C1B-C2B	2.66	1.49	1.43
19	A2	809	CLA	C1B-C2B	2.66	1.49	1.43
19	B2	824	CLA	C1B-C2B	2.66	1.49	1.43
19	B1	833	CLA	C4B-NB	2.66	1.41	1.37
19	B	820	CLA	C4B-NB	2.66	1.41	1.37
19	K1	102	CLA	C1B-C2B	2.66	1.49	1.43
19	A1	828	CLA	C1B-C2B	2.66	1.49	1.43
19	A	822	CLA	C1B-C2B	2.66	1.49	1.43
19	B1	803	CLA	C4B-NB	2.65	1.41	1.37
19	BB	810	CLA	C1B-C2B	2.65	1.49	1.43
19	AA	828	CLA	C1B-C2B	2.65	1.49	1.43
19	FF	305	CLA	C3B-C4B	2.65	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	836	CLA	C1B-C2B	2.65	1.49	1.43
19	BB	806	CLA	C4B-NB	2.65	1.41	1.37
19	A2	831	CLA	C4B-NB	2.65	1.41	1.37
19	A2	825	CLA	C1B-C2B	2.65	1.49	1.43
19	B	821	CLA	C4B-NB	2.65	1.41	1.37
19	A2	814	CLA	C1B-C2B	2.65	1.49	1.43
22	L1	211	LHG	P-O3	2.65	1.69	1.59
19	A	815	CLA	C4B-NB	2.65	1.41	1.37
19	B	824	CLA	C1B-C2B	2.64	1.49	1.43
19	B	825	CLA	C4B-NB	2.64	1.41	1.37
19	A1	826	CLA	C1B-C2B	2.64	1.49	1.43
19	B1	828	CLA	C3B-C4B	2.64	1.50	1.42
19	A	824	CLA	C1B-C2B	2.64	1.49	1.43
19	AA	820	CLA	C4B-NB	2.64	1.41	1.37
19	B1	802	CLA	C4B-NB	2.64	1.41	1.37
19	B	829	CLA	C3B-C4B	2.64	1.50	1.42
24	B	850	AJP	C04-C05	2.64	1.55	1.51
19	A2	832	CLA	C1B-C2B	2.64	1.49	1.43
19	A2	842	CLA	C1B-C2B	2.64	1.49	1.43
19	A1	806	CLA	C4B-NB	2.64	1.41	1.37
19	A1	813	CLA	C1B-C2B	2.64	1.49	1.43
19	L	204	CLA	C1B-C2B	2.64	1.49	1.43
19	AA	853	CLA	C1B-C2B	2.64	1.49	1.43
19	BB	802	CLA	C4B-NB	2.64	1.41	1.37
19	B2	802	CLA	C1B-C2B	2.63	1.49	1.43
19	BB	836	CLA	C4B-NB	2.63	1.41	1.37
19	BB	829	CLA	C1B-C2B	2.63	1.49	1.43
19	B	810	CLA	C1B-C2B	2.63	1.49	1.43
19	BB	808	CLA	C4B-NB	2.63	1.41	1.37
19	BB	834	CLA	C1B-C2B	2.63	1.49	1.43
24	BB	848	AJP	O25-C26	2.63	1.49	1.41
19	B1	809	CLA	C1B-C2B	2.63	1.49	1.43
19	A2	819	CLA	C1B-C2B	2.62	1.49	1.43
19	A	815	CLA	C1B-C2B	2.62	1.49	1.43
19	B	831	CLA	C4B-NB	2.62	1.41	1.37
19	A1	839	CLA	C1B-C2B	2.62	1.49	1.43
19	B	802	CLA	C4B-NB	2.62	1.41	1.37
19	A1	828	CLA	C4B-NB	2.62	1.41	1.37
19	BB	803	CLA	C4B-NB	2.62	1.41	1.37
19	AA	815	CLA	C1B-C2B	2.62	1.49	1.43
20	A2	803	CL0	CBD-CGD	-2.62	1.49	1.52
19	A	814	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	813	CLA	C1B-C2B	2.62	1.49	1.43
19	B	822	CLA	C1B-C2B	2.62	1.49	1.43
19	BB	820	CLA	C1B-C2B	2.62	1.49	1.43
24	L1	204	AJP	O25-C26	2.62	1.49	1.41
19	B	846	CLA	C1B-C2B	2.62	1.49	1.43
19	B1	821	CLA	C4B-NB	2.62	1.41	1.37
19	B2	852	CLA	C4B-NB	2.62	1.41	1.37
19	B	806	CLA	C4B-NB	2.62	1.41	1.37
19	A	820	CLA	C4B-NB	2.61	1.41	1.37
19	A1	820	CLA	C4B-NB	2.61	1.41	1.37
19	AA	811	CLA	C4B-NB	2.61	1.41	1.37
19	B1	829	CLA	C1B-C2B	2.61	1.49	1.43
19	AA	829	CLA	C1B-C2B	2.61	1.49	1.43
19	B	858	CLA	C1B-C2B	2.61	1.49	1.43
19	AA	804	CLA	C1B-C2B	2.61	1.49	1.43
19	AA	824	CLA	C1B-C2B	2.61	1.49	1.43
19	B	835	CLA	C1B-C2B	2.61	1.49	1.43
19	BB	845	CLA	C1B-C2B	2.61	1.49	1.43
19	A2	840	CLA	C1B-C2B	2.61	1.49	1.43
19	A1	808	CLA	C1B-C2B	2.61	1.49	1.43
19	B2	809	CLA	C1B-C2B	2.61	1.49	1.43
19	A	852	CLA	C4B-NB	2.61	1.41	1.37
19	BB	818	CLA	CMD-C2D	-2.61	1.45	1.50
24	L2	203	AJP	O25-C26	2.61	1.49	1.41
19	B1	811	CLA	C1B-C2B	2.61	1.49	1.43
24	B	849	AJP	C05-C06	2.61	1.58	1.53
19	A	812	CLA	C1B-C2B	2.61	1.49	1.43
19	A1	812	CLA	C1B-C2B	2.61	1.49	1.43
19	AA	812	CLA	C1B-C2B	2.61	1.49	1.43
24	A	802	AJP	C04-C05	2.61	1.55	1.51
24	A1	854	AJP	C18-C19	-2.61	1.46	1.53
19	B2	806	CLA	C1B-C2B	2.61	1.49	1.43
19	B2	834	CLA	C3B-C4B	2.60	1.50	1.42
19	B2	825	CLA	C1B-C2B	2.60	1.49	1.43
19	AA	831	CLA	C1B-C2B	2.60	1.49	1.43
19	A1	819	CLA	C4B-NB	2.60	1.41	1.37
19	B2	803	CLA	C4B-NB	2.60	1.41	1.37
24	L	209	AJP	C24-C19	2.60	1.59	1.53
19	B	813	CLA	C1B-C2B	2.60	1.49	1.43
19	AA	819	CLA	C1B-C2B	2.60	1.49	1.43
19	BB	809	CLA	C1B-C2B	2.60	1.49	1.43
24	BB	848	AJP	C81-C12	2.60	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	860	CLA	C4B-NB	2.60	1.41	1.37
19	A1	823	CLA	C1B-C2B	2.60	1.49	1.43
19	A2	817	CLA	C1B-C2B	2.60	1.49	1.43
19	A1	832	CLA	C1B-C2B	2.60	1.49	1.43
24	A1	855	AJP	C05-C06	2.60	1.58	1.53
19	A1	837	CLA	C1B-C2B	2.60	1.49	1.43
24	AA	802	AJP	C04-C05	2.60	1.55	1.51
19	B1	825	CLA	C1B-C2B	2.60	1.49	1.43
19	A1	818	CLA	C1B-C2B	2.59	1.49	1.43
19	BB	813	CLA	C1B-C2B	2.59	1.49	1.43
19	KK	101	CLA	C1B-C2B	2.59	1.49	1.43
24	A1	854	AJP	C07-C08	-2.59	1.49	1.53
19	A2	801	CLA	C4B-NB	2.59	1.41	1.37
19	A2	824	CLA	C1B-C2B	2.59	1.49	1.43
19	AA	841	CLA	C4B-NB	2.59	1.41	1.37
19	B2	834	CLA	CMB-C2B	-2.59	1.45	1.50
19	B	835	CLA	C4B-NB	2.59	1.41	1.37
19	B1	824	CLA	CHC-C1C	2.59	1.43	1.38
19	B2	827	CLA	C1B-C2B	2.59	1.49	1.43
19	B	830	CLA	C4B-NB	2.59	1.41	1.37
24	A1	855	AJP	C04-C05	2.59	1.55	1.51
19	A1	827	CLA	C1B-C2B	2.59	1.49	1.43
19	B1	822	CLA	C1B-C2B	2.58	1.49	1.43
19	A2	828	CLA	C1B-C2B	2.58	1.49	1.43
24	B	857	AJP	C18-C19	-2.58	1.46	1.53
19	B	809	CLA	C1B-C2B	2.58	1.49	1.43
19	A2	805	CLA	C1B-C2B	2.58	1.49	1.43
19	AA	853	CLA	C4B-NB	2.58	1.41	1.37
19	B2	826	CLA	CMD-C2D	-2.58	1.45	1.50
19	A1	830	CLA	C1B-C2B	2.58	1.49	1.43
19	B1	826	CLA	CMD-C2D	-2.58	1.45	1.50
19	A	829	CLA	C1B-C2B	2.58	1.49	1.43
19	F1	302	CLA	C1B-C2B	2.58	1.49	1.43
19	B	834	CLA	CMD-C2D	-2.58	1.45	1.50
19	LL	203	CLA	C1B-C2B	2.58	1.49	1.43
24	B	857	AJP	C07-C08	-2.58	1.49	1.53
19	A1	834	CLA	C1B-C2B	2.57	1.49	1.43
24	B	857	AJP	C05-C06	2.57	1.58	1.53
24	AA	802	AJP	C07-C08	-2.57	1.49	1.53
19	A	840	CLA	C1B-C2B	2.57	1.49	1.43
19	B1	849	CLA	C1B-C2B	2.57	1.49	1.43
24	A2	854	AJP	C05-C06	2.57	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	805	CLA	C1B-C2B	2.57	1.49	1.43
19	A1	816	CLA	C1B-C2B	2.57	1.49	1.43
24	A	802	AJP	C07-C08	-2.57	1.49	1.53
19	A	841	CLA	C4B-NB	2.57	1.41	1.37
19	AA	805	CLA	C1B-C2B	2.57	1.49	1.43
19	AA	829	CLA	C4B-NB	2.57	1.41	1.37
19	AA	801	CLA	C4B-NB	2.56	1.41	1.37
19	A	831	CLA	C1B-C2B	2.56	1.49	1.43
19	B	815	CLA	C1B-C2B	2.56	1.49	1.43
22	A1	845	LHG	O7-C5	-2.56	1.40	1.46
19	A	801	CLA	C4B-NB	2.56	1.41	1.37
19	BB	807	CLA	CMD-C2D	-2.56	1.45	1.50
19	B	808	CLA	C4B-NB	2.56	1.41	1.37
24	L	208	AJP	C04-C05	2.56	1.55	1.51
19	A2	820	CLA	C4B-NB	2.56	1.41	1.37
19	B	807	CLA	CMD-C2D	-2.56	1.45	1.50
19	A	829	CLA	C4B-NB	2.56	1.41	1.37
19	A	804	CLA	C1B-C2B	2.56	1.49	1.43
19	A2	807	CLA	C4B-NB	2.56	1.41	1.37
19	B2	820	CLA	CHC-C1C	2.56	1.43	1.38
19	FF	301	CLA	C1B-C2B	2.56	1.49	1.43
24	I2	104	AJP	C04-C05	2.56	1.55	1.51
19	A1	814	CLA	C1B-C2B	2.56	1.49	1.43
24	B	857	AJP	C04-C05	2.56	1.55	1.51
19	L1	206	CLA	C1B-C2B	2.56	1.49	1.43
19	B2	834	CLA	CHC-C1C	2.56	1.43	1.38
24	M2	101	AJP	C04-C05	2.56	1.55	1.51
19	A1	840	CLA	C4B-NB	2.56	1.41	1.37
19	B1	818	CLA	C3B-C4B	2.56	1.50	1.42
19	K	101	CLA	C1B-C2B	2.56	1.49	1.43
19	B	802	CLA	C1B-C2B	2.56	1.49	1.43
19	A2	815	CLA	C1B-C2B	2.55	1.49	1.43
19	LL	202	CLA	C1B-C2B	2.55	1.49	1.43
19	A2	807	CLA	C1B-C2B	2.55	1.49	1.43
19	BB	804	CLA	C1B-C2B	2.55	1.49	1.43
19	BB	833	CLA	MG-NB	-2.55	2.00	2.05
19	BB	822	CLA	C1B-C2B	2.55	1.49	1.43
19	F	302	CLA	C1B-C2B	2.55	1.49	1.43
24	A1	855	AJP	C07-C08	-2.55	1.49	1.53
19	BB	852	CLA	C1B-C2B	2.55	1.49	1.43
19	A2	841	CLA	C4B-NB	2.55	1.41	1.37
19	AA	830	CLA	C3B-C4B	2.55	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	834	CLA	MG-NB	-2.55	2.00	2.05
19	B1	820	CLA	C1B-C2B	2.55	1.49	1.43
19	A	838	CLA	C1B-C2B	2.55	1.49	1.43
19	A2	815	CLA	C3B-C4B	2.55	1.50	1.42
24	A1	854	AJP	C05-C06	2.54	1.58	1.53
24	B	849	AJP	O25-C26	2.54	1.48	1.41
19	B	804	CLA	C1B-C2B	2.54	1.49	1.43
19	B2	851	CLA	C1B-C2B	2.54	1.49	1.43
19	A1	811	CLA	C1B-C2B	2.54	1.49	1.43
19	FF	302	CLA	C1B-C2B	2.54	1.49	1.43
19	B2	811	CLA	C3B-C4B	2.54	1.50	1.42
19	A1	801	CLA	C4B-NB	2.54	1.41	1.37
24	A1	854	AJP	C04-C05	2.54	1.55	1.51
19	A1	805	CLA	C1B-C2B	2.54	1.49	1.43
19	B	807	CLA	C1B-C2B	2.54	1.49	1.43
19	BB	821	CLA	CMD-C2D	-2.54	1.45	1.50
19	BB	824	CLA	C1B-C2B	2.53	1.49	1.43
19	BB	855	CLA	C1B-C2B	2.53	1.49	1.43
19	B2	835	CLA	C4B-NB	2.53	1.41	1.37
19	BB	823	CLA	C1B-C2B	2.53	1.49	1.43
19	B2	807	CLA	C1B-C2B	2.53	1.49	1.43
19	A1	806	CLA	C1B-C2B	2.53	1.49	1.43
19	B2	818	CLA	C3B-C4B	2.53	1.50	1.42
19	BB	820	CLA	C4B-NB	2.53	1.41	1.37
19	A2	829	CLA	C1B-C2B	2.53	1.49	1.43
19	B1	807	CLA	C1B-C2B	2.53	1.49	1.43
19	BB	825	CLA	C1B-C2B	2.53	1.49	1.43
19	F2	301	CLA	C3B-C4B	2.53	1.50	1.42
19	B1	850	CLA	C1B-C2B	2.53	1.49	1.43
19	B	823	CLA	C1B-C2B	2.53	1.49	1.43
19	A1	842	CLA	C4B-NB	2.53	1.41	1.37
19	A	835	CLA	C1B-C2B	2.53	1.49	1.43
19	A1	819	CLA	CMD-C2D	-2.53	1.45	1.50
19	AA	842	CLA	C1B-C2B	2.53	1.49	1.43
19	B1	804	CLA	C1B-C2B	2.53	1.49	1.43
19	A2	833	CLA	C1B-C2B	2.52	1.49	1.43
19	B2	804	CLA	C1B-C2B	2.52	1.49	1.43
19	L2	205	CLA	C1B-C2B	2.52	1.49	1.43
19	B	825	CLA	C1B-C2B	2.52	1.49	1.43
24	BB	849	AJP	C81-C12	2.52	1.58	1.54
19	A1	829	CLA	CMD-C2D	-2.52	1.45	1.50
19	L	203	CLA	CMB-C2B	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	801	CLA	CMC-C2C	-2.52	1.45	1.50
19	A	811	CLA	C4B-NB	2.52	1.41	1.37
19	A	820	CLA	CMD-C2D	-2.52	1.45	1.50
19	A1	822	CLA	C1B-C2B	2.52	1.49	1.43
19	B1	816	CLA	C1B-C2B	2.52	1.49	1.43
19	F2	302	CLA	C1B-C2B	2.52	1.49	1.43
19	B	824	CLA	CMD-C2D	-2.52	1.45	1.50
22	A	845	LHG	O7-C5	-2.52	1.40	1.46
19	B	827	CLA	CMD-C2D	-2.52	1.45	1.50
19	AA	843	CLA	C4B-NB	2.52	1.41	1.37
19	A2	820	CLA	CMD-C2D	-2.52	1.45	1.50
19	AA	838	CLA	C1B-C2B	2.52	1.49	1.43
19	A2	804	CLA	CMD-C2D	-2.52	1.45	1.50
19	BB	835	CLA	C1B-C2B	2.51	1.49	1.43
19	A	804	CLA	CMD-C2D	-2.51	1.45	1.50
19	A1	801	CLA	CMC-C2C	-2.51	1.45	1.50
19	A1	832	CLA	CMD-C2D	-2.51	1.45	1.50
19	A	842	CLA	C1B-C2B	2.51	1.49	1.43
19	F1	301	CLA	C3B-C4B	2.51	1.50	1.42
19	BB	815	CLA	C1B-C2B	2.51	1.49	1.43
19	BB	833	CLA	CMB-C2B	-2.51	1.45	1.50
19	B2	814	CLA	C1B-C2B	2.51	1.49	1.43
19	BB	808	CLA	C1B-C2B	2.51	1.49	1.43
19	AA	820	CLA	MG-NB	-2.51	2.00	2.05
19	B1	811	CLA	C3B-C4B	2.50	1.50	1.42
19	A2	835	CLA	C1B-C2B	2.50	1.49	1.43
19	F2	301	CLA	C1B-C2B	2.50	1.49	1.43
19	B1	822	CLA	C3B-C4B	2.50	1.50	1.42
19	A2	831	CLA	C1B-C2B	2.50	1.49	1.43
19	B2	816	CLA	C1B-C2B	2.50	1.49	1.43
19	BB	824	CLA	CMD-C2D	-2.50	1.45	1.50
19	A2	830	CLA	C4B-NB	2.50	1.41	1.37
19	A2	837	CLA	CMB-C2B	-2.50	1.45	1.50
24	L1	203	AJP	O25-C26	2.50	1.48	1.41
19	BB	807	CLA	C1B-C2B	2.50	1.49	1.43
19	B2	805	CLA	C1B-C2B	2.50	1.49	1.43
19	BB	833	CLA	CMD-C2D	-2.50	1.45	1.50
19	A	805	CLA	CMD-C2D	-2.50	1.45	1.50
19	B	833	CLA	C1B-C2B	2.49	1.49	1.43
19	B	801	CLA	CMD-C2D	-2.49	1.45	1.50
19	B1	833	CLA	CMD-C2D	-2.49	1.45	1.50
19	B	834	CLA	CMB-C2B	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	846	LHG	O7-C5	-2.49	1.40	1.46
24	A2	854	AJP	C07-C08	-2.49	1.49	1.53
19	B2	822	CLA	C1B-C2B	2.49	1.49	1.43
22	X1	102	LHG	P-O3	2.49	1.69	1.59
19	F	301	CLA	C3B-C4B	2.49	1.50	1.42
24	BB	849	AJP	C04-C05	2.49	1.55	1.51
19	A1	814	CLA	C3B-C4B	2.49	1.50	1.42
19	B	836	CLA	C1B-C2B	2.49	1.49	1.43
19	B	837	CLA	C3B-C4B	2.49	1.50	1.42
19	B2	820	CLA	C1B-C2B	2.49	1.49	1.43
19	A	829	CLA	MG-NB	-2.48	2.00	2.05
19	B1	805	CLA	C1B-C2B	2.48	1.49	1.43
19	B	811	CLA	C3B-C4B	2.48	1.50	1.42
24	L	208	AJP	C24-C19	2.48	1.59	1.53
19	A1	836	CLA	C1B-C2B	2.48	1.48	1.43
19	AA	820	CLA	CMD-C2D	-2.48	1.45	1.50
19	BB	827	CLA	CMD-C2D	-2.48	1.45	1.50
19	A2	815	CLA	CHC-C1C	2.48	1.43	1.38
19	B1	848	CLA	CMD-C2D	-2.48	1.45	1.50
19	A1	829	CLA	C3B-C4B	2.48	1.49	1.42
19	AA	837	CLA	C1B-C2B	2.48	1.48	1.43
19	B1	814	CLA	C1B-C2B	2.48	1.48	1.43
22	X2	102	LHG	P-O3	2.47	1.69	1.59
19	L2	206	CLA	CMD-C2D	-2.47	1.45	1.50
19	A2	831	CLA	MG-NB	-2.47	2.00	2.05
19	F1	301	CLA	C1B-C2B	2.47	1.48	1.43
19	A	837	CLA	C1B-C2B	2.47	1.48	1.43
19	AA	842	CLA	C3B-C4B	2.47	1.49	1.42
19	B2	822	CLA	C3B-C4B	2.47	1.49	1.42
19	A2	806	CLA	CHC-C1C	2.47	1.43	1.38
19	BB	821	CLA	C3B-C4B	2.47	1.49	1.42
19	B	821	CLA	CMD-C2D	-2.47	1.45	1.50
22	B2	848	LHG	P-O3	2.47	1.69	1.59
19	B1	833	CLA	MG-NB	-2.47	2.00	2.05
19	BB	807	CLA	C3B-C4B	2.47	1.49	1.42
19	B1	828	CLA	C1B-C2B	2.47	1.48	1.43
19	BB	829	CLA	MG-NB	-2.47	2.00	2.05
19	BB	816	CLA	CMB-C2B	-2.47	1.45	1.50
19	B2	820	CLA	C3B-C4B	2.47	1.49	1.42
19	B	815	CLA	C3B-C4B	2.47	1.49	1.42
19	BB	804	CLA	C3B-C4B	2.47	1.49	1.42
19	B	805	CLA	C1B-C2B	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	822	CLA	C3B-C4B	2.46	1.49	1.42
19	B	807	CLA	C3B-C4B	2.46	1.49	1.42
19	A1	807	CLA	CMD-C2D	-2.46	1.45	1.50
19	F	301	CLA	C1B-C2B	2.46	1.48	1.43
19	AA	804	CLA	CMD-C2D	-2.46	1.45	1.50
19	A1	809	CLA	C1B-C2B	2.46	1.48	1.43
19	A2	806	CLA	C3B-C4B	2.46	1.49	1.42
19	B1	803	CLA	C1B-C2B	2.46	1.48	1.43
19	AA	811	CLA	C1B-C2B	2.46	1.48	1.43
19	B2	826	CLA	C3B-C4B	2.46	1.49	1.42
19	BB	856	CLA	C1B-C2B	2.46	1.48	1.43
19	A2	806	CLA	C1B-C2B	2.46	1.48	1.43
19	A	811	CLA	C1B-C2B	2.46	1.48	1.43
19	A	804	CLA	CHC-C1C	2.46	1.43	1.38
19	B2	824	CLA	CMD-C2D	-2.46	1.45	1.50
19	B1	807	CLA	C3B-C4B	2.46	1.49	1.42
19	L	202	CLA	CMD-C2D	-2.46	1.45	1.50
19	A	810	CLA	CHC-C1C	2.46	1.43	1.38
19	A	801	CLA	CMC-C2C	-2.46	1.45	1.50
19	B2	835	CLA	MG-NB	-2.46	2.00	2.05
19	B1	833	CLA	CMB-C2B	-2.46	1.45	1.50
19	X2	101	CLA	C3B-C4B	2.46	1.49	1.42
19	B	804	CLA	C3B-C4B	2.45	1.49	1.42
19	A1	810	CLA	C1B-C2B	2.45	1.48	1.43
19	BB	805	CLA	C1B-C2B	2.45	1.48	1.43
19	B2	829	CLA	CHC-C1C	2.45	1.43	1.38
19	A2	836	CLA	CMB-C2B	-2.45	1.45	1.50
19	B2	850	CLA	C1B-C2B	2.45	1.48	1.43
19	A1	813	CLA	C3B-C4B	2.45	1.49	1.42
19	A1	842	CLA	C1B-C2B	2.45	1.48	1.43
24	B	850	AJP	C05-C06	2.45	1.58	1.53
19	B1	824	CLA	C3B-C4B	2.45	1.49	1.42
19	B2	804	CLA	C3B-C4B	2.45	1.49	1.42
19	B1	804	CLA	C3B-C4B	2.44	1.49	1.42
19	A1	814	CLA	CHC-C1C	2.44	1.43	1.38
19	B	859	CLA	C1B-C2B	2.44	1.48	1.43
19	A2	811	CLA	C1B-C2B	2.44	1.48	1.43
22	XX	102	LHG	P-O3	2.44	1.68	1.59
24	M2	101	AJP	C05-C06	2.44	1.58	1.53
19	BB	852	CLA	CMD-C2D	-2.44	1.45	1.50
19	FF	302	CLA	C3B-C4B	2.44	1.49	1.42
19	B1	824	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	805	CLA	CMD-C2D	-2.44	1.45	1.50
19	BB	813	CLA	C3B-C4B	2.44	1.49	1.42
19	A1	828	CLA	CMD-C2D	-2.44	1.45	1.50
24	A	855	AJP	C18-C19	-2.44	1.47	1.53
19	A	842	CLA	C3B-C4B	2.44	1.49	1.42
19	F2	302	CLA	C3B-C4B	2.44	1.49	1.42
19	A1	830	CLA	MG-NB	-2.44	2.01	2.05
19	B1	850	CLA	CHC-C1C	2.44	1.43	1.38
19	A	827	CLA	CMD-C2D	-2.44	1.45	1.50
19	A2	814	CLA	C3B-C4B	2.44	1.49	1.42
19	BB	821	CLA	CHC-C1C	2.43	1.43	1.38
19	B2	822	CLA	CMD-C2D	-2.43	1.45	1.50
19	FF	305	CLA	CHC-C1C	2.43	1.43	1.38
19	B2	829	CLA	C1B-C2B	2.43	1.48	1.43
19	A2	804	CLA	CHC-C1C	2.43	1.43	1.38
19	AA	806	CLA	C3B-C4B	2.43	1.49	1.42
24	K	104	AJP	O25-C26	2.43	1.48	1.41
19	A1	830	CLA	CMD-C2D	-2.43	1.45	1.50
19	L1	207	CLA	CMD-C2D	-2.43	1.45	1.50
19	A2	831	CLA	CMD-C2D	-2.43	1.45	1.50
19	F	302	CLA	C3B-C4B	2.43	1.49	1.42
24	AA	856	AJP	C18-C19	-2.43	1.47	1.53
19	A	806	CLA	C1B-C2B	2.42	1.48	1.43
19	AA	835	CLA	C1B-C2B	2.42	1.48	1.43
19	BB	823	CLA	C3B-C4B	2.42	1.49	1.42
19	A2	837	CLA	C1B-C2B	2.42	1.48	1.43
19	BB	811	CLA	C3B-C4B	2.42	1.49	1.42
19	AA	804	CLA	CHC-C1C	2.42	1.43	1.38
19	AA	806	CLA	CHC-C1C	2.42	1.43	1.38
24	L	208	AJP	C05-C06	2.42	1.58	1.53
19	B2	801	CLA	CMD-C2D	-2.42	1.45	1.50
19	L1	207	CLA	MG-NB	-2.42	2.01	2.05
19	B	816	CLA	CMB-C2B	-2.41	1.45	1.50
19	B2	809	CLA	C3B-C4B	2.41	1.49	1.42
19	B	823	CLA	C3B-C4B	2.41	1.49	1.42
19	L2	206	CLA	C3B-C4B	2.41	1.49	1.42
19	B1	820	CLA	C3B-C4B	2.41	1.49	1.42
19	B1	820	CLA	CHC-C1C	2.41	1.43	1.38
19	BB	802	CLA	C1B-C2B	2.41	1.48	1.43
19	B2	807	CLA	C3B-C4B	2.41	1.49	1.42
19	AA	823	CLA	C1B-C2B	2.41	1.48	1.43
19	B	829	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	836	CLA	CMB-C2B	-2.41	1.45	1.50
19	BB	826	CLA	MG-NB	-2.41	2.01	2.05
19	AA	829	CLA	MG-NB	-2.41	2.01	2.05
19	B1	828	CLA	CHC-C1C	2.41	1.43	1.38
19	A	831	CLA	MG-NB	-2.40	2.01	2.05
19	A	814	CLA	C3B-C4B	2.40	1.49	1.42
19	AA	827	CLA	CMD-C2D	-2.40	1.45	1.50
19	B1	809	CLA	C3B-C4B	2.40	1.49	1.42
22	X	102	LHG	P-O3	2.40	1.68	1.59
19	A2	827	CLA	C1B-C2B	2.40	1.48	1.43
19	A	806	CLA	C3B-C4B	2.40	1.49	1.42
19	A2	829	CLA	MG-NB	-2.40	2.01	2.05
19	B2	803	CLA	C1B-C2B	2.40	1.48	1.43
19	A1	803	CLA	CMD-C2D	-2.40	1.45	1.50
19	A1	840	CLA	CMD-C2D	-2.40	1.45	1.50
19	B	803	CLA	C1B-C2B	2.40	1.48	1.43
24	KK	104	AJP	O25-C26	2.40	1.48	1.41
19	A1	818	CLA	C3B-C4B	2.40	1.49	1.42
19	L	204	CLA	CMD-C2D	-2.40	1.45	1.50
19	LL	201	CLA	CMD-C2D	-2.40	1.45	1.50
24	AA	856	AJP	C24-C23	2.40	1.56	1.52
19	FF	305	CLA	C1B-C2B	2.40	1.48	1.43
19	B2	827	CLA	CHC-C1C	2.40	1.43	1.38
19	B	821	CLA	C3B-C4B	2.40	1.49	1.42
19	AA	816	CLA	CHC-C1C	2.40	1.43	1.38
19	BB	808	CLA	CMB-C2B	-2.40	1.45	1.50
19	A	823	CLA	C1B-C2B	2.39	1.48	1.43
19	A2	820	CLA	MG-NB	-2.39	2.01	2.05
19	B1	815	CLA	C3B-C4B	2.39	1.49	1.42
19	A2	813	CLA	C3B-C4B	2.39	1.49	1.42
19	A	806	CLA	CHC-C1C	2.39	1.43	1.38
19	A2	821	CLA	C3B-C4B	2.39	1.49	1.42
19	BB	815	CLA	C3B-C4B	2.39	1.49	1.42
19	B2	823	CLA	C3B-C4B	2.39	1.49	1.42
19	A1	812	CLA	C3B-C4B	2.39	1.49	1.42
19	AA	831	CLA	MG-NB	-2.39	2.01	2.05
19	B2	816	CLA	C3B-C4B	2.39	1.49	1.42
19	A1	806	CLA	CHC-C1C	2.39	1.43	1.38
19	B2	851	CLA	CHC-C1C	2.39	1.43	1.38
19	A	833	CLA	C3B-C4B	2.39	1.49	1.42
19	X1	101	CLA	C3B-C4B	2.39	1.49	1.42
19	A1	836	CLA	C3B-C4B	2.39	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	823	CLA	CHC-C1C	2.39	1.43	1.38
19	AA	806	CLA	C1B-C2B	2.39	1.48	1.43
19	A	837	CLA	C3B-C4B	2.38	1.49	1.42
19	AA	810	CLA	CHC-C1C	2.38	1.43	1.38
19	A1	820	CLA	C3B-C4B	2.38	1.49	1.42
24	A	855	AJP	C04-C05	2.38	1.55	1.51
19	B1	826	CLA	C3B-C4B	2.38	1.49	1.42
19	X	101	CLA	C3B-C4B	2.38	1.49	1.42
19	BB	814	CLA	C1B-C2B	2.38	1.48	1.43
24	A	855	AJP	C24-C23	2.38	1.56	1.52
19	A	808	CLA	CMD-C2D	-2.38	1.45	1.50
24	AA	856	AJP	C04-C05	2.38	1.55	1.51
19	A	823	CLA	CHC-C1C	2.38	1.43	1.38
19	AA	837	CLA	C3B-C4B	2.38	1.49	1.42
19	B2	816	CLA	CHC-C1C	2.38	1.43	1.38
19	F1	302	CLA	C3B-C4B	2.38	1.49	1.42
19	BB	818	CLA	CHC-C1C	2.38	1.43	1.38
19	B	816	CLA	C1B-C2B	2.38	1.48	1.43
19	B2	821	CLA	CMD-C2D	-2.38	1.45	1.50
19	A1	825	CLA	CMD-C2D	-2.38	1.45	1.50
19	A	831	CLA	CMD-C2D	-2.38	1.45	1.50
24	L	209	AJP	C04-C05	2.38	1.55	1.51
19	A2	811	CLA	MG-NB	-2.38	2.01	2.05
19	A2	823	CLA	C1B-C2B	2.38	1.48	1.43
19	BB	803	CLA	C1B-C2B	2.38	1.48	1.43
19	A2	804	CLA	C3B-C4B	2.37	1.49	1.42
24	BB	848	AJP	C04-C05	2.37	1.55	1.51
19	B	814	CLA	C1B-C2B	2.37	1.48	1.43
19	B	822	CLA	CHC-C1C	2.37	1.43	1.38
19	BB	801	CLA	CMD-C2D	-2.37	1.45	1.50
19	B	835	CLA	CMD-C2D	-2.37	1.45	1.50
19	B	854	CLA	CMB-C2B	-2.37	1.45	1.50
19	BB	802	CLA	MG-NB	-2.37	2.01	2.05
19	A1	832	CLA	C3B-C4B	2.37	1.49	1.42
19	B1	850	CLA	C3B-C4B	2.37	1.49	1.42
19	B	835	CLA	MG-NB	-2.37	2.01	2.05
19	A2	833	CLA	CMD-C2D	-2.37	1.45	1.50
19	AA	831	CLA	CMD-C2D	-2.37	1.45	1.50
19	A1	816	CLA	C3B-C4B	2.37	1.49	1.42
19	B2	834	CLA	CMD-C2D	-2.37	1.45	1.50
19	A2	807	CLA	CHC-C1C	2.37	1.43	1.38
19	A2	819	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	850	CLA	CMB-C2B	-2.37	1.45	1.50
19	A1	841	CLA	C3B-C4B	2.37	1.49	1.42
24	L2	202	AJP	O25-C26	2.37	1.48	1.41
19	AA	837	CLA	CMB-C2B	-2.37	1.45	1.50
19	A1	828	CLA	MG-NB	-2.37	2.01	2.05
19	A	830	CLA	C3B-C4B	2.37	1.49	1.42
19	AA	801	CLA	CMC-C2C	-2.37	1.45	1.50
19	B2	851	CLA	C3B-C4B	2.37	1.49	1.42
19	BB	852	CLA	MG-NB	-2.36	2.01	2.05
19	B	813	CLA	CHC-C1C	2.36	1.43	1.38
19	A2	830	CLA	C3B-C4B	2.36	1.49	1.42
19	A2	805	CLA	CMD-C2D	-2.36	1.45	1.50
19	A	831	CLA	CMB-C2B	-2.36	1.45	1.50
19	B	805	CLA	CMD-C2D	-2.36	1.45	1.50
24	L1	204	AJP	C17-C16	2.36	1.57	1.53
19	A1	836	CLA	CMD-C2D	-2.36	1.45	1.50
19	A1	819	CLA	MG-NB	-2.36	2.01	2.05
19	A2	833	CLA	C3B-C4B	2.36	1.49	1.42
19	B	802	CLA	MG-NB	-2.36	2.01	2.05
19	A2	842	CLA	CMC-C2C	-2.36	1.45	1.50
19	L	203	CLA	C1B-C2B	2.36	1.48	1.43
19	AA	823	CLA	C3B-C4B	2.36	1.49	1.42
19	B2	802	CLA	CHC-C1C	2.36	1.43	1.38
19	A	823	CLA	C3B-C4B	2.36	1.49	1.42
19	AA	810	CLA	C1B-C2B	2.36	1.48	1.43
24	KK	104	AJP	C17-C16	2.36	1.57	1.53
22	L	207	LHG	P-O3	2.36	1.68	1.59
19	A2	827	CLA	MG-NB	-2.36	2.01	2.05
19	A2	823	CLA	C3B-C4B	2.36	1.49	1.42
19	A2	829	CLA	CMD-C2D	-2.36	1.45	1.50
19	AA	820	CLA	CMB-C2B	-2.36	1.45	1.50
19	B2	813	CLA	C3B-C4B	2.36	1.49	1.42
19	BB	856	CLA	CHC-C1C	2.36	1.43	1.38
22	BB	850	LHG	P-O3	2.36	1.68	1.59
22	LL	205	LHG	P-O3	2.36	1.68	1.59
19	B	816	CLA	CMD-C2D	-2.36	1.45	1.50
19	A	804	CLA	MG-NB	-2.36	2.01	2.05
19	BB	816	CLA	MG-NB	-2.36	2.01	2.05
19	BB	805	CLA	C3B-C4B	2.36	1.49	1.42
19	B1	821	CLA	CMD-C2D	-2.35	1.45	1.50
19	BB	816	CLA	C1B-C2B	2.35	1.48	1.43
19	AA	833	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	810	CLA	CHC-C1C	2.35	1.43	1.38
19	K2	104	CLA	C3B-C4B	2.35	1.49	1.42
24	L1	203	AJP	C81-C12	2.35	1.58	1.54
24	L2	203	AJP	C17-C16	2.35	1.57	1.53
19	BB	808	CLA	MG-NB	-2.35	2.01	2.05
19	A2	837	CLA	CMD-C2D	-2.35	1.46	1.50
19	BB	802	CLA	CMB-C2B	-2.35	1.46	1.50
19	B1	813	CLA	CHC-C1C	2.35	1.43	1.38
19	FF	301	CLA	C3B-C4B	2.35	1.49	1.42
19	F1	305	CLA	C3B-C4B	2.35	1.49	1.42
19	B1	836	CLA	C3B-C4B	2.35	1.49	1.42
19	B1	836	CLA	CMD-C2D	-2.35	1.46	1.50
19	B2	849	CLA	CMD-C2D	-2.35	1.46	1.50
19	B1	801	CLA	CMD-C2D	-2.35	1.46	1.50
19	A2	810	CLA	C1B-C2B	2.35	1.48	1.43
19	A2	823	CLA	CHC-C1C	2.35	1.43	1.38
19	A	837	CLA	CMB-C2B	-2.35	1.46	1.50
19	AA	813	CLA	C3B-C4B	2.35	1.49	1.42
19	B1	827	CLA	CHC-C1C	2.35	1.43	1.38
19	AA	814	CLA	C3B-C4B	2.35	1.49	1.42
19	B1	816	CLA	CMD-C2D	-2.35	1.46	1.50
19	L1	207	CLA	C3B-C4B	2.35	1.49	1.42
19	B2	837	CLA	C3B-C4B	2.35	1.49	1.42
19	AA	832	CLA	CMB-C2B	-2.35	1.46	1.50
19	BB	814	CLA	CMD-C2D	-2.35	1.46	1.50
19	A	805	CLA	MG-NB	-2.35	2.01	2.05
19	A2	801	CLA	CMD-C2D	-2.35	1.46	1.50
19	B1	816	CLA	C3B-C4B	2.35	1.49	1.42
24	L2	202	AJP	C04-C05	2.34	1.55	1.51
19	B2	811	CLA	CHC-C1C	2.34	1.43	1.38
19	AA	833	CLA	CMD-C2D	-2.34	1.46	1.50
19	B	822	CLA	CMD-C2D	-2.34	1.46	1.50
19	A2	817	CLA	C3B-C4B	2.34	1.49	1.42
19	B	859	CLA	CHC-C1C	2.34	1.43	1.38
19	B2	849	CLA	MG-NB	-2.34	2.01	2.05
19	B2	850	CLA	MG-NB	-2.34	2.01	2.05
19	L2	205	CLA	CMB-C2B	-2.34	1.46	1.50
19	A1	805	CLA	CHC-C1C	2.34	1.43	1.38
19	A1	815	CLA	CHC-C1C	2.34	1.43	1.38
19	BB	822	CLA	CHC-C1C	2.34	1.43	1.38
19	AA	819	CLA	C3B-C4B	2.34	1.49	1.42
19	B2	834	CLA	MG-NB	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	827	CLA	CMD-C2D	-2.34	1.46	1.50
19	A	820	CLA	MG-NB	-2.34	2.01	2.05
19	BB	836	CLA	CMD-C2D	-2.34	1.46	1.50
19	A	842	CLA	CMD-C2D	-2.34	1.46	1.50
19	L1	206	CLA	CMB-C2B	-2.34	1.46	1.50
19	B1	811	CLA	CHC-C1C	2.34	1.43	1.38
19	AA	801	CLA	CMD-C2D	-2.34	1.46	1.50
19	B1	821	CLA	C3B-C4B	2.34	1.49	1.42
19	B2	813	CLA	CHC-C1C	2.34	1.43	1.38
19	B	829	CLA	CHC-C1C	2.34	1.43	1.38
19	BB	826	CLA	C3B-C4B	2.34	1.49	1.42
19	XX	101	CLA	C3B-C4B	2.34	1.49	1.42
19	L2	206	CLA	MG-NB	-2.34	2.01	2.05
19	A2	828	CLA	CMD-C2D	-2.34	1.46	1.50
19	B2	852	CLA	CMB-C2B	-2.34	1.46	1.50
19	B	814	CLA	CMD-C2D	-2.34	1.46	1.50
19	AA	808	CLA	CMD-C2D	-2.34	1.46	1.50
19	A1	803	CLA	MG-NB	-2.34	2.01	2.05
24	L	208	AJP	O79-C22	-2.34	1.36	1.43
19	A1	842	CLA	CMD-C2D	-2.34	1.46	1.50
19	B1	823	CLA	C3B-C4B	2.34	1.49	1.42
19	J1	103	CLA	C3B-C4B	2.34	1.49	1.42
19	A1	842	CLA	C3B-C4B	2.34	1.49	1.42
19	B1	802	CLA	CHC-C1C	2.34	1.43	1.38
19	AA	815	CLA	C3B-C4B	2.34	1.49	1.42
19	B	805	CLA	C3B-C4B	2.33	1.49	1.42
19	A	829	CLA	CMD-C2D	-2.33	1.46	1.50
19	BB	823	CLA	CMD-C2D	-2.33	1.46	1.50
19	B	802	CLA	CMB-C2B	-2.33	1.46	1.50
19	B2	830	CLA	MG-NB	-2.33	2.01	2.05
19	B	826	CLA	CMC-C2C	-2.33	1.46	1.50
19	A2	827	CLA	CMB-C2B	-2.33	1.46	1.50
19	B	860	CLA	CMB-C2B	-2.33	1.46	1.50
19	A2	835	CLA	C3B-C4B	2.33	1.49	1.42
19	A1	805	CLA	C3B-C4B	2.33	1.49	1.42
24	AA	802	AJP	C05-C06	2.33	1.58	1.53
19	B2	814	CLA	CMB-C2B	-2.33	1.46	1.50
19	A	811	CLA	MG-NB	-2.33	2.01	2.05
19	L	203	CLA	MG-NB	-2.33	2.01	2.05
19	B2	837	CLA	CMD-C2D	-2.33	1.46	1.50
19	AA	805	CLA	MG-NB	-2.33	2.01	2.05
19	B2	809	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	837	CLA	C3B-C4B	2.33	1.49	1.42
22	X2	103	LHG	P-O3	2.33	1.68	1.59
19	B1	819	CLA	C3B-C4B	2.33	1.49	1.42
19	A1	838	CLA	CMD-C2D	-2.33	1.46	1.50
19	A2	836	CLA	MG-NB	-2.33	2.01	2.05
19	B	816	CLA	MG-NB	-2.33	2.01	2.05
19	B	854	CLA	CMD-C2D	-2.33	1.46	1.50
19	B	816	CLA	CHC-C1C	2.33	1.43	1.38
24	M2	101	AJP	O79-C22	-2.33	1.36	1.43
19	A	801	CLA	CMD-C2D	-2.33	1.46	1.50
19	B1	827	CLA	CMD-C2D	-2.32	1.46	1.50
19	B1	809	CLA	CHC-C1C	2.32	1.43	1.38
19	A2	835	CLA	CHC-C1C	2.32	1.43	1.38
19	BB	829	CLA	C4B-NB	2.32	1.40	1.37
19	A2	833	CLA	MG-NB	-2.32	2.01	2.05
19	A	827	CLA	C3B-C4B	2.32	1.49	1.42
19	B2	846	CLA	C3B-C4B	2.32	1.49	1.42
24	A2	854	AJP	C81-C12	2.32	1.58	1.54
19	B2	831	CLA	C3B-C4B	2.32	1.49	1.42
19	A2	829	CLA	CHC-C1C	2.32	1.43	1.38
19	B	813	CLA	C3B-C4B	2.32	1.49	1.42
19	B	811	CLA	CHC-C1C	2.32	1.43	1.38
19	K	101	CLA	C3B-C4B	2.32	1.49	1.42
19	B	836	CLA	CMD-C2D	-2.32	1.46	1.50
19	A1	810	CLA	MG-NB	-2.32	2.01	2.05
19	J2	103	CLA	C3B-C4B	2.32	1.49	1.42
19	A2	808	CLA	CMD-C2D	-2.32	1.46	1.50
19	B1	849	CLA	C3B-C4B	2.32	1.49	1.42
19	FF	301	CLA	CMD-C2D	-2.32	1.46	1.50
19	B1	816	CLA	CHC-C1C	2.32	1.43	1.38
19	A1	824	CLA	CMB-C2B	-2.32	1.46	1.50
19	A	820	CLA	CMB-C2B	-2.32	1.46	1.50
19	AA	843	CLA	CMD-C2D	-2.32	1.46	1.50
24	L2	202	AJP	C05-C06	2.32	1.58	1.53
19	B2	827	CLA	CMD-C2D	-2.32	1.46	1.50
19	A2	816	CLA	CHC-C1C	2.32	1.43	1.38
19	BB	832	CLA	C1B-C2B	2.32	1.48	1.43
19	A	815	CLA	C3B-C4B	2.32	1.49	1.42
19	AA	815	CLA	CHC-C1C	2.32	1.43	1.38
22	B	852	LHG	P-O3	2.32	1.68	1.59
19	A2	831	CLA	CMB-C2B	-2.31	1.46	1.50
19	BB	827	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	C3B-C4B	2.31	1.49	1.42
19	B	846	CLA	C3B-C4B	2.31	1.49	1.42
19	A	815	CLA	CHC-C1C	2.31	1.43	1.38
19	AA	842	CLA	CMC-C2C	-2.31	1.46	1.50
19	A2	824	CLA	MG-NB	-2.31	2.01	2.05
19	L	204	CLA	MG-NB	-2.31	2.01	2.05
24	K	104	AJP	C17-C16	2.31	1.57	1.53
19	B2	828	CLA	C3B-C4B	2.31	1.49	1.42
19	BB	813	CLA	CHC-C1C	2.31	1.43	1.38
19	A	835	CLA	CMD-C2D	-2.31	1.46	1.50
19	J1	101	CLA	C3B-C4B	2.31	1.49	1.42
19	B1	848	CLA	MG-NB	-2.31	2.01	2.05
19	J1	101	CLA	CHC-C1C	2.31	1.43	1.38
19	A	816	CLA	CHC-C1C	2.31	1.43	1.38
19	BB	820	CLA	CHC-C1C	2.31	1.43	1.38
19	B1	845	CLA	C3B-C4B	2.31	1.49	1.42
19	A2	836	CLA	CMD-C2D	-2.31	1.46	1.50
19	BB	836	CLA	C3B-C4B	2.31	1.49	1.42
19	BB	834	CLA	CMD-C2D	-2.31	1.46	1.50
24	L	209	AJP	O79-C22	-2.31	1.36	1.43
19	AA	831	CLA	CMB-C2B	-2.31	1.46	1.50
19	J2	101	CLA	C3B-C4B	2.31	1.49	1.42
24	L	209	AJP	C81-C12	2.31	1.58	1.54
19	B1	834	CLA	MG-NB	-2.31	2.01	2.05
19	B1	813	CLA	C3B-C4B	2.31	1.49	1.42
19	A1	822	CLA	CHC-C1C	2.31	1.43	1.38
19	A1	804	CLA	CMD-C2D	-2.31	1.46	1.50
19	B	837	CLA	CMD-C2D	-2.31	1.46	1.50
19	A2	842	CLA	C3B-C4B	2.31	1.49	1.42
19	B	830	CLA	MG-NB	-2.31	2.01	2.05
19	BB	814	CLA	MG-NB	-2.31	2.01	2.05
19	A	814	CLA	CHC-C1C	2.31	1.43	1.38
19	AA	842	CLA	CHC-C1C	2.31	1.43	1.38
19	A2	841	CLA	CMD-C2D	-2.31	1.46	1.50
19	BB	845	CLA	C3B-C4B	2.31	1.49	1.42
19	B	834	CLA	C4B-NB	2.31	1.40	1.37
19	J2	101	CLA	CHC-C1C	2.31	1.43	1.38
19	B	806	CLA	CMD-C2D	-2.31	1.46	1.50
24	A	802	AJP	C05-C06	2.31	1.58	1.53
19	AA	817	CLA	C3B-C4B	2.31	1.49	1.42
19	AA	835	CLA	C3B-C4B	2.31	1.49	1.42
19	A1	842	CLA	MG-NB	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	842	CLA	CHC-C1C	2.31	1.43	1.38
19	A1	841	CLA	CMD-C2D	-2.31	1.46	1.50
19	A	813	CLA	C3B-C4B	2.31	1.49	1.42
19	B	806	CLA	MG-NB	-2.31	2.01	2.05
19	BB	802	CLA	CHC-C1C	2.31	1.43	1.38
19	B2	816	CLA	CMD-C2D	-2.31	1.46	1.50
19	A	810	CLA	C1B-C2B	2.30	1.48	1.43
19	B	823	CLA	CMD-C2D	-2.30	1.46	1.50
19	B	832	CLA	CMD-C2D	-2.30	1.46	1.50
19	B	811	CLA	CMD-C2D	-2.30	1.46	1.50
22	X1	103	LHG	P-O3	2.30	1.68	1.59
19	A2	842	CLA	CMD-C2D	-2.30	1.46	1.50
19	A2	825	CLA	CMB-C2B	-2.30	1.46	1.50
19	B2	852	CLA	CMD-C2D	-2.30	1.46	1.50
19	AA	829	CLA	CMD-C2D	-2.30	1.46	1.50
19	LL	202	CLA	CMB-C2B	-2.30	1.46	1.50
19	B	817	CLA	C3B-C4B	2.30	1.49	1.42
19	AA	835	CLA	CMD-C2D	-2.30	1.46	1.50
19	A1	837	CLA	C3B-C4B	2.30	1.49	1.42
19	B1	816	CLA	CMB-C2B	-2.30	1.46	1.50
19	K1	105	CLA	CMD-C2D	-2.30	1.46	1.50
19	AA	821	CLA	C3B-C4B	2.30	1.49	1.42
19	KK	102	CLA	C3B-C4B	2.30	1.49	1.42
19	A1	830	CLA	CMB-C2B	-2.30	1.46	1.50
19	A2	839	CLA	CMD-C2D	-2.30	1.46	1.50
19	A	811	CLA	CMD-C2D	-2.30	1.46	1.50
19	A	819	CLA	C3B-C4B	2.30	1.49	1.42
19	JJ	101	CLA	C3B-C4B	2.30	1.49	1.42
19	B1	805	CLA	CMD-C2D	-2.30	1.46	1.50
22	BB	851	LHG	P-O3	2.30	1.68	1.59
19	B	826	CLA	C3B-C4B	2.30	1.49	1.42
19	A	807	CLA	CHC-C1C	2.30	1.43	1.38
22	L	207	LHG	C6-C5	2.30	1.58	1.50
19	K1	103	CLA	C3B-C4B	2.30	1.49	1.42
19	A2	802	CLA	C3B-C4B	2.30	1.49	1.42
19	A2	837	CLA	MG-NB	-2.30	2.01	2.05
19	AA	824	CLA	CMD-C2D	-2.30	1.46	1.50
19	K	101	CLA	CHC-C1C	2.30	1.43	1.38
19	B1	835	CLA	CMD-C2D	-2.30	1.46	1.50
19	A	835	CLA	CHC-C1C	2.30	1.43	1.38
19	B1	814	CLA	C3B-C4B	2.30	1.49	1.42
19	BB	856	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	816	CLA	C3B-C4B	2.29	1.49	1.42
19	K2	102	CLA	CMD-C2D	-2.29	1.46	1.50
19	A2	805	CLA	MG-NB	-2.29	2.01	2.05
19	A1	827	CLA	CMD-C2D	-2.29	1.46	1.50
19	B1	849	CLA	CMD-C2D	-2.29	1.46	1.50
19	B	826	CLA	CMD-C2D	-2.29	1.46	1.50
19	B	859	CLA	C3B-C4B	2.29	1.49	1.42
19	AA	835	CLA	CHC-C1C	2.29	1.43	1.38
19	B	819	CLA	C3B-C4B	2.29	1.49	1.42
19	A1	824	CLA	CMD-C2D	-2.29	1.46	1.50
19	AA	842	CLA	CMD-C2D	-2.29	1.46	1.50
19	A1	806	CLA	C3B-C4B	2.29	1.49	1.42
19	B1	824	CLA	MG-NB	-2.29	2.01	2.05
19	A2	839	CLA	C3B-C4B	2.29	1.49	1.42
19	LL	203	CLA	MG-NB	-2.29	2.01	2.05
19	B	860	CLA	CMD-C2D	-2.29	1.46	1.50
22	LL	205	LHG	C6-C5	2.29	1.58	1.50
19	AA	814	CLA	CHC-C1C	2.29	1.43	1.38
19	B1	819	CLA	CHC-C1C	2.29	1.43	1.38
19	BB	811	CLA	CHC-C1C	2.29	1.43	1.38
19	BB	834	CLA	MG-NB	-2.29	2.01	2.05
19	A1	806	CLA	MG-NB	-2.29	2.01	2.05
19	B2	821	CLA	C3B-C4B	2.29	1.49	1.42
26	B	841	ECH	C1-C6	-2.29	1.50	1.53
19	A1	801	CLA	CMD-C2D	-2.29	1.46	1.50
19	A1	831	CLA	CMB-C2B	-2.29	1.46	1.50
19	B	828	CLA	C3B-C4B	2.29	1.49	1.42
19	BB	801	CLA	C3B-C4B	2.29	1.49	1.42
19	B2	807	CLA	CHC-C1C	2.29	1.43	1.38
24	L	209	AJP	C05-C06	2.29	1.58	1.53
19	BB	823	CLA	CHC-C1C	2.29	1.43	1.38
19	BB	817	CLA	C3B-C4B	2.29	1.49	1.42
19	B	831	CLA	C3B-C4B	2.29	1.49	1.42
19	B1	829	CLA	MG-NB	-2.29	2.01	2.05
19	B1	830	CLA	C3B-C4B	2.29	1.49	1.42
19	B	824	CLA	C3B-C4B	2.29	1.49	1.42
19	B	804	CLA	CHC-C1C	2.29	1.43	1.38
19	B2	850	CLA	CMD-C2D	-2.29	1.46	1.50
19	B1	817	CLA	C3B-C4B	2.29	1.49	1.42
19	L2	205	CLA	C3B-C4B	2.29	1.49	1.42
19	KK	101	CLA	C3B-C4B	2.29	1.49	1.42
19	A1	835	CLA	CMD-C2D	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	836	CLA	CMD-C2D	-2.29	1.46	1.50
19	B	815	CLA	CMD-C2D	-2.29	1.46	1.50
19	A1	852	CLA	CMD-C2D	-2.29	1.46	1.50
19	BB	824	CLA	MG-NB	-2.28	2.01	2.05
19	B2	805	CLA	C3B-C4B	2.28	1.49	1.42
19	BB	828	CLA	C3B-C4B	2.28	1.49	1.42
19	B1	833	CLA	CHC-C1C	2.28	1.43	1.38
19	A1	826	CLA	CMD-C2D	-2.28	1.46	1.50
19	K	102	CLA	C3B-C4B	2.28	1.49	1.42
19	K2	102	CLA	CHC-C1C	2.28	1.43	1.38
19	AA	836	CLA	CMD-C2D	-2.28	1.46	1.50
19	A1	841	CLA	CMC-C2C	-2.28	1.46	1.50
19	B1	834	CLA	CMD-C2D	-2.28	1.46	1.50
19	AA	820	CLA	C3B-C4B	2.28	1.49	1.42
19	A1	823	CLA	MG-NB	-2.28	2.01	2.05
19	A	832	CLA	C3B-C4B	2.28	1.49	1.42
19	A2	832	CLA	CMB-C2B	-2.28	1.46	1.50
19	B2	805	CLA	CMD-C2D	-2.28	1.46	1.50
19	A2	820	CLA	CMB-C2B	-2.28	1.46	1.50
19	A1	822	CLA	C3B-C4B	2.28	1.49	1.42
19	B2	815	CLA	C3B-C4B	2.28	1.49	1.42
19	BB	832	CLA	CMD-C2D	-2.28	1.46	1.50
19	A1	834	CLA	CHC-C1C	2.28	1.43	1.38
19	B	802	CLA	CHC-C1C	2.28	1.43	1.38
19	KK	101	CLA	CHC-C1C	2.28	1.43	1.38
19	JJ	103	CLA	C3B-C4B	2.28	1.49	1.42
19	B2	846	CLA	CHC-C1C	2.28	1.43	1.38
19	B	808	CLA	MG-NB	-2.28	2.01	2.05
19	B1	814	CLA	CMD-C2D	-2.28	1.46	1.50
19	B	820	CLA	CHC-C1C	2.28	1.43	1.38
19	B	819	CLA	CMD-C2D	-2.28	1.46	1.50
19	A1	837	CLA	CHC-C1C	2.28	1.43	1.38
19	B1	845	CLA	CHC-C1C	2.28	1.43	1.38
19	A2	817	CLA	CHC-C1C	2.28	1.43	1.38
19	J	101	CLA	C3B-C4B	2.28	1.49	1.42
19	A2	823	CLA	CMB-C2B	-2.28	1.46	1.50
19	A2	822	CLA	C3B-C4B	2.28	1.49	1.42
19	A	817	CLA	C3B-C4B	2.28	1.49	1.42
19	B2	817	CLA	C3B-C4B	2.28	1.49	1.42
19	A2	836	CLA	CMC-C2C	-2.28	1.46	1.50
19	F2	302	CLA	CMB-C2B	-2.28	1.46	1.50
19	AA	839	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	830	CLA	CMD-C2D	-2.27	1.46	1.50
19	B1	805	CLA	C3B-C4B	2.27	1.49	1.42
19	A2	807	CLA	C3B-C4B	2.27	1.49	1.42
19	B	809	CLA	C3B-C4B	2.27	1.49	1.42
19	A1	809	CLA	CHC-C1C	2.27	1.43	1.38
19	AA	827	CLA	C3B-C4B	2.27	1.49	1.42
19	L1	206	CLA	CMD-C2D	-2.27	1.46	1.50
19	B1	807	CLA	CHC-C1C	2.27	1.43	1.38
19	B	809	CLA	CHC-C1C	2.27	1.43	1.38
19	BB	830	CLA	C3B-C4B	2.27	1.49	1.42
19	BB	832	CLA	C3B-C4B	2.27	1.49	1.42
19	AA	819	CLA	CMD-C2D	-2.27	1.46	1.50
19	B2	806	CLA	MG-NB	-2.27	2.01	2.05
19	B2	815	CLA	CMD-C2D	-2.27	1.46	1.50
19	AA	834	CLA	CMD-C2D	-2.27	1.46	1.50
19	K1	102	CLA	CMD-C2D	-2.27	1.46	1.50
19	A1	808	CLA	C3B-C4B	2.27	1.49	1.42
22	L2	208	LHG	P-O3	2.27	1.68	1.59
23	B1	843	BCR	C38-C26	-2.27	1.47	1.50
19	B1	803	CLA	CMB-C2B	-2.27	1.46	1.50
24	I2	104	AJP	O79-C22	-2.27	1.36	1.43
24	A	802	AJP	C81-C12	2.27	1.58	1.54
20	A1	802	CL0	CBD-CGD	-2.27	1.49	1.52
19	A	822	CLA	C3B-C4B	2.27	1.49	1.42
19	L2	205	CLA	CMD-C2D	-2.27	1.46	1.50
19	A1	821	CLA	C3B-C4B	2.27	1.49	1.42
19	A2	809	CLA	C3B-C4B	2.27	1.49	1.42
19	AA	807	CLA	CHC-C1C	2.27	1.43	1.38
19	B1	818	CLA	CMD-C2D	-2.27	1.46	1.50
19	A2	838	CLA	C3B-C4B	2.27	1.49	1.42
19	A2	823	CLA	CMD-C2D	-2.27	1.46	1.50
19	A	828	CLA	CMD-C2D	-2.27	1.46	1.50
22	X2	102	LHG	P-O6	2.27	1.68	1.59
19	A1	840	CLA	MG-NB	-2.27	2.01	2.05
19	BB	806	CLA	MG-NB	-2.27	2.01	2.05
19	A1	822	CLA	CMD-C2D	-2.27	1.46	1.50
19	A	840	CLA	MG-NB	-2.27	2.01	2.05
19	A2	840	CLA	CMD-C2D	-2.27	1.46	1.50
19	A2	828	CLA	MG-NB	-2.27	2.01	2.05
19	A2	834	CLA	MG-NB	-2.27	2.01	2.05
19	BB	855	CLA	MG-NB	-2.27	2.01	2.05
19	A1	819	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	834	CLA	MG-NB	-2.27	2.01	2.05
19	A2	824	CLA	CMB-C2B	-2.27	1.46	1.50
19	BB	829	CLA	CMD-C2D	-2.27	1.46	1.50
19	A1	827	CLA	C3B-C4B	2.27	1.49	1.42
19	B2	807	CLA	MG-NB	-2.27	2.01	2.05
19	AA	820	CLA	CHC-C1C	2.27	1.43	1.38
19	A1	821	CLA	CMD-C2D	-2.27	1.46	1.50
19	A2	804	CLA	MG-NB	-2.26	2.01	2.05
19	A1	834	CLA	C3B-C4B	2.26	1.49	1.42
19	AA	809	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	809	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	816	CLA	C3B-C4B	2.26	1.49	1.42
19	LL	202	CLA	C3B-C4B	2.26	1.49	1.42
19	B	814	CLA	CMB-C2B	-2.26	1.46	1.50
19	FF	301	CLA	CMB-C2B	-2.26	1.46	1.50
19	BB	818	CLA	C3B-C4B	2.26	1.49	1.42
19	B1	822	CLA	CMD-C2D	-2.26	1.46	1.50
19	A	807	CLA	C3B-C4B	2.26	1.49	1.42
19	AA	828	CLA	C3B-C4B	2.26	1.49	1.42
24	AA	802	AJP	C81-C12	2.26	1.58	1.54
19	A1	852	CLA	MG-NB	-2.26	2.01	2.05
19	A2	807	CLA	MG-NB	-2.26	2.01	2.05
19	A	841	CLA	CMD-C2D	-2.26	1.46	1.50
23	B2	844	BCR	C38-C26	-2.26	1.47	1.50
19	A2	840	CLA	C3B-C4B	2.26	1.49	1.42
19	AA	804	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	829	CLA	CHC-C1C	2.26	1.43	1.38
19	BB	835	CLA	CMD-C2D	-2.26	1.46	1.50
19	A1	803	CLA	C3B-C4B	2.26	1.49	1.42
19	B2	827	CLA	C3B-C4B	2.26	1.49	1.42
19	B2	836	CLA	CMD-C2D	-2.26	1.46	1.50
19	A2	832	CLA	C3B-C4B	2.26	1.49	1.42
19	B1	823	CLA	CHC-C1C	2.26	1.43	1.38
19	B	805	CLA	CHC-C1C	2.26	1.43	1.38
19	B	810	CLA	C3B-C4B	2.26	1.49	1.42
19	FF	301	CLA	CHC-C1C	2.26	1.43	1.38
19	A1	810	CLA	CMD-C2D	-2.26	1.46	1.50
19	A1	835	CLA	CMC-C2C	-2.26	1.46	1.50
19	BB	810	CLA	CMD-C2D	-2.26	1.46	1.50
19	BB	815	CLA	CMD-C2D	-2.26	1.46	1.50
19	A	835	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	810	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	846	LHG	P-O3	2.26	1.68	1.59
19	B1	832	CLA	CMD-C2D	-2.26	1.46	1.50
19	A2	811	CLA	CMD-C2D	-2.26	1.46	1.50
19	AA	823	CLA	MG-NB	-2.26	2.01	2.05
19	A1	841	CLA	CHC-C1C	2.26	1.43	1.38
19	A	804	CLA	C3B-C4B	2.26	1.49	1.42
19	A2	806	CLA	CMC-C2C	-2.26	1.46	1.50
19	AA	811	CLA	CMD-C2D	-2.26	1.46	1.50
19	BB	822	CLA	CMD-C2D	-2.26	1.46	1.50
19	AA	807	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	834	CLA	C3B-C4B	2.26	1.49	1.42
19	BB	816	CLA	CHC-C1C	2.26	1.43	1.38
19	B2	829	CLA	CMD-C2D	-2.26	1.46	1.50
19	B	860	CLA	MG-NB	-2.26	2.01	2.05
19	A2	809	CLA	CHC-C1C	2.26	1.43	1.38
19	BB	809	CLA	CHC-C1C	2.26	1.43	1.38
19	BB	855	CLA	CMB-C2B	-2.26	1.46	1.50
19	AA	824	CLA	MG-NB	-2.26	2.01	2.05
19	B	801	CLA	C3B-C4B	2.26	1.49	1.42
19	B	817	CLA	CMD-C2D	-2.26	1.46	1.50
19	B1	832	CLA	C3B-C4B	2.26	1.49	1.42
24	A	855	AJP	C05-C06	2.26	1.58	1.53
19	A	839	CLA	C3B-C4B	2.26	1.49	1.42
19	AA	822	CLA	C3B-C4B	2.26	1.49	1.42
19	A1	824	CLA	MG-NB	-2.26	2.01	2.05
19	F1	301	CLA	CHC-C1C	2.26	1.43	1.38
19	A	834	CLA	CMD-C2D	-2.26	1.46	1.50
19	B	804	CLA	CMD-C2D	-2.26	1.46	1.50
19	A	852	CLA	CHC-C1C	2.26	1.43	1.38
19	A1	816	CLA	CHC-C1C	2.25	1.43	1.38
19	B	833	CLA	CMD-C2D	-2.25	1.46	1.50
19	BB	814	CLA	CMB-C2B	-2.25	1.46	1.50
19	A	823	CLA	MG-NB	-2.25	2.01	2.05
19	A2	811	CLA	CMB-C2B	-2.25	1.46	1.50
19	B2	819	CLA	C3B-C4B	2.25	1.49	1.42
19	B	831	CLA	CHC-C1C	2.25	1.43	1.38
19	B1	811	CLA	CMD-C2D	-2.25	1.46	1.50
19	A1	822	CLA	MG-NB	-2.25	2.01	2.05
24	AA	856	AJP	C05-C06	2.25	1.58	1.53
19	AA	836	CLA	CMC-C2C	-2.25	1.46	1.50
19	AA	839	CLA	CMD-C2D	-2.25	1.46	1.50
19	BB	819	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	826	CLA	C1B-C2B	2.25	1.48	1.43
19	AA	809	CLA	CHC-C1C	2.25	1.43	1.38
19	A2	816	CLA	C3B-C4B	2.25	1.49	1.42
19	A	812	CLA	C3B-C4B	2.25	1.49	1.42
19	B	846	CLA	CHC-C1C	2.25	1.43	1.38
19	A1	834	CLA	CMD-C2D	-2.25	1.46	1.50
19	B2	818	CLA	CMD-C2D	-2.25	1.46	1.50
19	A1	811	CLA	MG-NB	-2.25	2.01	2.05
19	F	301	CLA	CMD-C2D	-2.25	1.46	1.50
19	BB	804	CLA	CMD-C2D	-2.25	1.46	1.50
19	A1	839	CLA	C3B-C4B	2.25	1.49	1.42
19	A	822	CLA	CMB-C2B	-2.25	1.46	1.50
19	A1	838	CLA	C3B-C4B	2.25	1.49	1.42
19	AA	830	CLA	CMD-C2D	-2.25	1.46	1.50
19	LL	201	CLA	CMB-C2B	-2.25	1.46	1.50
19	A1	803	CLA	CHC-C1C	2.25	1.43	1.38
19	B1	818	CLA	CHC-C1C	2.25	1.43	1.38
19	A1	826	CLA	MG-NB	-2.25	2.01	2.05
19	B2	803	CLA	CMB-C2B	-2.25	1.46	1.50
19	B2	814	CLA	CMD-C2D	-2.25	1.46	1.50
19	LL	202	CLA	CMD-C2D	-2.25	1.46	1.50
19	A1	817	CLA	CHC-C1C	2.25	1.43	1.38
19	B2	818	CLA	CHC-C1C	2.25	1.43	1.38
19	A1	817	CLA	C3B-C4B	2.25	1.49	1.42
19	B1	807	CLA	MG-NB	-2.25	2.01	2.05
19	A2	826	CLA	CMD-C2D	-2.25	1.46	1.50
19	A2	835	CLA	CMD-C2D	-2.25	1.46	1.50
19	B	803	CLA	CMB-C2B	-2.25	1.46	1.50
19	A	834	CLA	MG-NB	-2.25	2.01	2.05
19	B	823	CLA	MG-NB	-2.25	2.01	2.05
19	LL	201	CLA	MG-NB	-2.25	2.01	2.05
19	FF	302	CLA	CMD-C2D	-2.25	1.46	1.50
22	X1	102	LHG	P-O6	2.25	1.68	1.59
19	A1	838	CLA	MG-NB	-2.25	2.01	2.05
19	B2	815	CLA	MG-NB	-2.25	2.01	2.05
19	AA	811	CLA	MG-NB	-2.25	2.01	2.05
19	BB	812	CLA	CMD-C2D	-2.25	1.46	1.50
19	B	802	CLA	CMD-C2D	-2.25	1.46	1.50
24	BB	848	AJP	C05-C06	2.25	1.58	1.53
19	L	203	CLA	C3B-C4B	2.25	1.49	1.42
19	A1	832	CLA	MG-NB	-2.25	2.01	2.05
19	A2	822	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	812	CLA	CMB-C2B	-2.25	1.46	1.50
19	BB	818	CLA	MG-NB	-2.24	2.01	2.05
19	A2	824	CLA	CMD-C2D	-2.24	1.46	1.50
19	B2	824	CLA	MG-NB	-2.24	2.01	2.05
19	A	807	CLA	MG-NB	-2.24	2.01	2.05
19	AA	804	CLA	MG-NB	-2.24	2.01	2.05
19	BB	803	CLA	MG-NB	-2.24	2.01	2.05
19	BB	823	CLA	MG-NB	-2.24	2.01	2.05
19	A1	823	CLA	CMB-C2B	-2.24	1.46	1.50
19	F1	302	CLA	CMB-C2B	-2.24	1.46	1.50
19	A2	821	CLA	CMC-C2C	-2.24	1.46	1.50
19	A	841	CLA	MG-NB	-2.24	2.01	2.05
19	B2	812	CLA	C3B-C4B	2.24	1.49	1.42
19	A	801	CLA	C3B-C4B	2.24	1.49	1.42
19	J	103	CLA	C3B-C4B	2.24	1.49	1.42
19	A2	828	CLA	C3B-C4B	2.24	1.49	1.42
19	B1	804	CLA	CMD-C2D	-2.24	1.46	1.50
19	A	833	CLA	CMD-C2D	-2.24	1.46	1.50
19	AA	841	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	814	CLA	MG-NB	-2.24	2.01	2.05
19	BB	807	CLA	MG-NB	-2.24	2.01	2.05
19	BB	810	CLA	MG-NB	-2.24	2.01	2.05
19	A	830	CLA	CMD-C2D	-2.24	1.46	1.50
19	BB	806	CLA	CMD-C2D	-2.24	1.46	1.50
19	B1	810	CLA	C3B-C4B	2.24	1.49	1.42
19	B	829	CLA	CMB-C2B	-2.24	1.46	1.50
19	A1	827	CLA	MG-NB	-2.24	2.01	2.05
19	BB	824	CLA	C3B-C4B	2.24	1.49	1.42
24	L1	204	AJP	C05-C06	2.24	1.58	1.53
19	B1	829	CLA	CHC-C1C	2.24	1.43	1.38
19	BB	811	CLA	CMD-C2D	-2.24	1.46	1.50
22	B	853	LHG	P-O3	2.24	1.68	1.59
19	BB	816	CLA	CMD-C2D	-2.24	1.46	1.50
19	BB	804	CLA	CHC-C1C	2.24	1.43	1.38
19	B1	808	CLA	C3B-C4B	2.24	1.49	1.42
19	A	825	CLA	C3B-C4B	2.24	1.49	1.42
19	A2	825	CLA	CMD-C2D	-2.24	1.46	1.50
19	B1	812	CLA	C3B-C4B	2.24	1.49	1.42
19	B2	802	CLA	C3B-C4B	2.24	1.49	1.42
19	B	807	CLA	MG-NB	-2.24	2.01	2.05
19	B2	823	CLA	CMD-C2D	-2.24	1.46	1.50
19	BB	845	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	833	CLA	C3B-C4B	2.24	1.49	1.42
19	A	836	CLA	CMC-C2C	-2.24	1.46	1.50
19	F	302	CLA	CMB-C2B	-2.24	1.46	1.50
19	AA	835	CLA	CMB-C2B	-2.24	1.46	1.50
19	L1	206	CLA	MG-NB	-2.24	2.01	2.05
19	B2	829	CLA	MG-NB	-2.24	2.01	2.05
19	A1	826	CLA	C3B-C4B	2.24	1.49	1.42
19	A	836	CLA	CMB-C2B	-2.24	1.46	1.50
19	L1	206	CLA	C3B-C4B	2.24	1.49	1.42
19	A1	826	CLA	CHC-C1C	2.24	1.43	1.38
19	B1	814	CLA	CHC-C1C	2.24	1.43	1.38
19	A1	831	CLA	C3B-C4B	2.24	1.49	1.42
19	K2	102	CLA	C3B-C4B	2.24	1.49	1.42
19	B1	803	CLA	CMD-C2D	-2.24	1.46	1.50
19	A1	839	CLA	MG-NB	-2.24	2.01	2.05
19	B1	821	CLA	MG-NB	-2.24	2.01	2.05
19	A	844	CLA	MG-NB	-2.24	2.01	2.05
19	BB	815	CLA	MG-NB	-2.24	2.01	2.05
19	B	810	CLA	CMD-C2D	-2.24	1.46	1.50
19	AA	828	CLA	CMD-C2D	-2.24	1.46	1.50
19	A2	818	CLA	C3B-C4B	2.24	1.49	1.42
19	B1	816	CLA	MG-NB	-2.24	2.01	2.05
19	B2	801	CLA	C3B-C4B	2.24	1.49	1.42
19	B	823	CLA	CHC-C1C	2.24	1.43	1.38
19	B1	803	CLA	MG-NB	-2.24	2.01	2.05
19	AA	825	CLA	C3B-C4B	2.24	1.49	1.42
19	FF	301	CLA	MG-NB	-2.24	2.01	2.05
19	B	828	CLA	CMD-C2D	-2.24	1.46	1.50
19	B	820	CLA	C3B-C4B	2.24	1.49	1.42
19	BB	833	CLA	C4B-NB	2.24	1.40	1.37
19	AA	816	CLA	MG-NB	-2.23	2.01	2.05
19	A	820	CLA	C1B-C2B	2.23	1.48	1.43
19	B2	827	CLA	MG-NB	-2.23	2.01	2.05
19	A1	839	CLA	CMD-C2D	-2.23	1.46	1.50
19	A	832	CLA	CMB-C2B	-2.23	1.46	1.50
19	B	836	CLA	MG-NB	-2.23	2.01	2.05
19	B2	804	CLA	CMD-C2D	-2.23	1.46	1.50
19	B2	805	CLA	CMB-C2B	-2.23	1.46	1.50
19	A	824	CLA	MG-NB	-2.23	2.01	2.05
19	AA	853	CLA	MG-NB	-2.23	2.01	2.05
19	BB	828	CLA	CMD-C2D	-2.23	1.46	1.50
19	AA	812	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	858	CLA	CMB-C2B	-2.23	1.46	1.50
19	BB	803	CLA	CMB-C2B	-2.23	1.46	1.50
19	B2	822	CLA	CHC-C1C	2.23	1.43	1.38
19	BB	831	CLA	CHC-C1C	2.23	1.43	1.38
19	B2	803	CLA	MG-NB	-2.23	2.01	2.05
19	AA	834	CLA	CMB-C2B	-2.23	1.46	1.50
19	AA	836	CLA	CMB-C2B	-2.23	1.46	1.50
19	B	858	CLA	MG-NB	-2.23	2.01	2.05
19	B1	825	CLA	C3B-C4B	2.23	1.49	1.42
19	A2	810	CLA	CMD-C2D	-2.23	1.46	1.50
19	B2	816	CLA	CMB-C2B	-2.23	1.46	1.50
19	A	806	CLA	CMD-C2D	-2.23	1.46	1.50
19	AA	806	CLA	CMD-C2D	-2.23	1.46	1.50
19	BB	805	CLA	CMB-C2B	-2.23	1.46	1.50
19	L	204	CLA	C3B-C4B	2.23	1.49	1.42
19	A	840	CLA	C3B-C4B	2.23	1.49	1.42
19	B	836	CLA	CMB-C2B	-2.23	1.46	1.50
19	BB	805	CLA	CMD-C2D	-2.23	1.46	1.50
19	F1	305	CLA	CHC-C1C	2.23	1.43	1.38
24	K	104	AJP	C81-C12	2.23	1.58	1.54
19	B1	834	CLA	C3B-C4B	2.23	1.49	1.42
19	AA	808	CLA	C3B-C4B	2.23	1.49	1.42
24	L2	203	AJP	C07-C08	-2.23	1.50	1.53
19	A1	833	CLA	MG-NB	-2.23	2.01	2.05
19	K1	102	CLA	MG-NB	-2.23	2.01	2.05
19	BB	807	CLA	CHC-C1C	2.23	1.43	1.38
19	B	814	CLA	C3B-C4B	2.23	1.49	1.42
19	A1	807	CLA	MG-NB	-2.23	2.01	2.05
19	AA	841	CLA	MG-NB	-2.23	2.01	2.05
19	A1	811	CLA	CMB-C2B	-2.23	1.46	1.50
19	A1	801	CLA	C3B-C4B	2.23	1.49	1.42
19	A2	827	CLA	C3B-C4B	2.23	1.49	1.42
19	B2	802	CLA	MG-NB	-2.23	2.01	2.05
19	BB	805	CLA	CHC-C1C	2.23	1.43	1.38
19	A1	811	CLA	C3B-C4B	2.23	1.49	1.42
19	B	803	CLA	CMD-C2D	-2.23	1.46	1.50
19	B	812	CLA	CMD-C2D	-2.23	1.46	1.50
19	A2	823	CLA	MG-NB	-2.23	2.01	2.05
19	B	813	CLA	MG-NB	-2.23	2.01	2.05
19	B	828	CLA	CHC-C1C	2.23	1.42	1.38
19	AA	801	CLA	CHC-C1C	2.23	1.42	1.38
19	KK	101	CLA	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	826	CLA	C1B-C2B	2.23	1.48	1.43
22	A1	845	LHG	P-O3	2.23	1.68	1.59
19	K1	102	CLA	CHC-C1C	2.23	1.42	1.38
19	B	827	CLA	CHC-C1C	2.23	1.42	1.38
19	A	835	CLA	MG-NB	-2.23	2.01	2.05
19	B	823	CLA	CMC-C2C	-2.23	1.46	1.50
19	F	302	CLA	CMD-C2D	-2.23	1.46	1.50
19	L	202	CLA	MG-NB	-2.23	2.01	2.05
19	BB	802	CLA	C3B-C4B	2.23	1.49	1.42
19	AA	819	CLA	CHC-C1C	2.23	1.42	1.38
19	AA	807	CLA	MG-NB	-2.23	2.01	2.05
19	B1	814	CLA	MG-NB	-2.23	2.01	2.05
19	K2	102	CLA	MG-NB	-2.23	2.01	2.05
19	BB	808	CLA	CHC-C1C	2.22	1.42	1.38
19	A2	844	CLA	CMD-C2D	-2.22	1.46	1.50
19	AA	824	CLA	CMB-C2B	-2.22	1.46	1.50
19	FF	305	CLA	CMD-C2D	-2.22	1.46	1.50
19	BB	809	CLA	MG-NB	-2.22	2.01	2.05
22	B1	847	LHG	P-O3	2.22	1.68	1.59
19	BB	824	CLA	CHC-C1C	2.22	1.42	1.38
19	A	812	CLA	CMB-C2B	-2.22	1.46	1.50
19	BB	855	CLA	C3B-C4B	2.22	1.49	1.42
19	B1	828	CLA	MG-NB	-2.22	2.01	2.05
19	A2	818	CLA	CHC-C1C	2.22	1.42	1.38
19	JJ	101	CLA	CHC-C1C	2.22	1.42	1.38
19	B1	805	CLA	CMB-C2B	-2.22	1.46	1.50
19	B1	815	CLA	CMD-C2D	-2.22	1.46	1.50
19	B2	808	CLA	C3B-C4B	2.22	1.49	1.42
19	BB	803	CLA	C3B-C4B	2.22	1.49	1.42
19	A1	810	CLA	CMC-C2C	-2.22	1.46	1.50
19	F2	302	CLA	CMD-C2D	-2.22	1.46	1.50
19	AA	810	CLA	CMD-C2D	-2.22	1.46	1.50
19	A1	836	CLA	MG-NB	-2.22	2.01	2.05
19	A	824	CLA	CMB-C2B	-2.22	1.46	1.50
19	B	832	CLA	CMB-C2B	-2.22	1.46	1.50
19	A	837	CLA	MG-NB	-2.22	2.01	2.05
19	B2	814	CLA	C3B-C4B	2.22	1.49	1.42
19	A1	809	CLA	CMD-C2D	-2.22	1.46	1.50
19	B	825	CLA	CMB-C2B	-2.22	1.46	1.50
19	A	852	CLA	MG-NB	-2.22	2.01	2.05
19	AA	801	CLA	MG-NB	-2.22	2.01	2.05
19	A1	852	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K1	102	CLA	C3B-C4B	2.22	1.49	1.42
19	A1	805	CLA	CMD-C2D	-2.22	1.46	1.50
19	A1	808	CLA	CHC-C1C	2.22	1.42	1.38
19	B	832	CLA	CHC-C1C	2.22	1.42	1.38
19	A	839	CLA	CMD-C2D	-2.22	1.46	1.50
19	B	829	CLA	CMD-C2D	-2.22	1.46	1.50
19	B2	852	CLA	C3B-C4B	2.22	1.49	1.42
24	BB	849	AJP	C05-C06	2.22	1.57	1.53
19	A2	840	CLA	MG-NB	-2.22	2.01	2.05
19	B	815	CLA	MG-NB	-2.22	2.01	2.05
19	AA	837	CLA	CMD-C2D	-2.22	1.46	1.50
19	A2	838	CLA	CHC-C1C	2.22	1.42	1.38
19	A	818	CLA	C3B-C4B	2.22	1.49	1.42
19	A1	815	CLA	MG-NB	-2.22	2.01	2.05
19	AA	812	CLA	MG-NB	-2.22	2.01	2.05
19	A	823	CLA	CMB-C2B	-2.22	1.46	1.50
19	AA	829	CLA	CMB-C2B	-2.22	1.46	1.50
19	B	807	CLA	CHC-C1C	2.22	1.42	1.38
19	B	833	CLA	C3B-C4B	2.22	1.49	1.42
19	B	808	CLA	CHC-C1C	2.22	1.42	1.38
24	A1	854	AJP	C81-C12	2.22	1.58	1.54
19	A	836	CLA	MG-NB	-2.22	2.01	2.05
26	B1	840	ECH	C1-C6	-2.22	1.50	1.53
19	B2	835	CLA	CMD-C2D	-2.22	1.46	1.50
19	BB	802	CLA	CMD-C2D	-2.22	1.46	1.50
19	A2	808	CLA	C3B-C4B	2.22	1.49	1.42
19	B2	810	CLA	C3B-C4B	2.22	1.49	1.42
19	B2	803	CLA	CMD-C2D	-2.22	1.46	1.50
19	A	837	CLA	CMD-C2D	-2.22	1.46	1.50
19	A	844	CLA	CHC-C1C	2.22	1.42	1.38
19	B	810	CLA	MG-NB	-2.22	2.01	2.05
19	A1	814	CLA	CMD-C2D	-2.22	1.46	1.50
19	A2	852	CLA	CMB-C2B	-2.22	1.46	1.50
19	A1	813	CLA	CHC-C1C	2.22	1.42	1.38
19	A2	814	CLA	CHC-C1C	2.22	1.42	1.38
19	AA	832	CLA	C3B-C4B	2.22	1.49	1.42
19	B	805	CLA	CMB-C2B	-2.22	1.46	1.50
19	BB	856	CLA	CMD-C2D	-2.22	1.46	1.50
19	F2	301	CLA	CHC-C1C	2.22	1.42	1.38
19	B1	802	CLA	MG-NB	-2.22	2.01	2.05
19	B	831	CLA	MG-NB	-2.22	2.01	2.05
19	A	834	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	809	CLA	CMD-C2D	-2.22	1.46	1.50
19	B1	827	CLA	C3B-C4B	2.22	1.49	1.42
19	B1	810	CLA	CHC-C1C	2.22	1.42	1.38
19	BB	825	CLA	C3B-C4B	2.22	1.49	1.42
19	B	826	CLA	C1B-C2B	2.22	1.48	1.43
19	A1	825	CLA	MG-NB	-2.22	2.01	2.05
19	A2	841	CLA	MG-NB	-2.22	2.01	2.05
19	B2	810	CLA	MG-NB	-2.22	2.01	2.05
19	B	812	CLA	MG-NB	-2.21	2.01	2.05
19	AA	809	CLA	CMD-C2D	-2.21	1.46	1.50
19	BB	825	CLA	CMB-C2B	-2.21	1.46	1.50
19	AA	853	CLA	CHC-C1C	2.21	1.42	1.38
19	A1	810	CLA	CMB-C2B	-2.21	1.46	1.50
19	AA	823	CLA	CMB-C2B	-2.21	1.46	1.50
22	L1	211	LHG	O7-C5	-2.21	1.41	1.46
19	A	810	CLA	CMD-C2D	-2.21	1.46	1.50
19	BB	835	CLA	MG-NB	-2.21	2.01	2.05
19	A	808	CLA	C3B-C4B	2.21	1.49	1.42
19	AA	818	CLA	C3B-C4B	2.21	1.49	1.42
23	B	844	BCR	C38-C26	-2.21	1.47	1.50
19	A1	820	CLA	CMC-C2C	-2.21	1.46	1.50
19	A1	832	CLA	CMB-C2B	-2.21	1.46	1.50
19	AA	841	CLA	C3B-C4B	2.21	1.49	1.42
19	A	805	CLA	CMB-C2B	-2.21	1.46	1.50
19	BB	803	CLA	CMD-C2D	-2.21	1.46	1.50
19	A2	852	CLA	MG-NB	-2.21	2.01	2.05
19	K	101	CLA	CMD-C2D	-2.21	1.46	1.50
19	AA	838	CLA	C3B-C4B	2.21	1.49	1.42
19	A1	837	CLA	MG-NB	-2.21	2.01	2.05
19	BB	855	CLA	CMD-C2D	-2.21	1.46	1.50
19	B2	820	CLA	MG-NB	-2.21	2.01	2.05
19	B2	823	CLA	CHC-C1C	2.21	1.42	1.38
19	J	101	CLA	CHC-C1C	2.21	1.42	1.38
22	A	845	LHG	P-O3	2.21	1.68	1.59
19	B2	811	CLA	CMD-C2D	-2.21	1.46	1.50
19	KK	101	CLA	CMD-C2D	-2.21	1.46	1.50
19	B	819	CLA	CHC-C1C	2.21	1.42	1.38
19	A	809	CLA	C3B-C4B	2.21	1.49	1.42
19	B1	849	CLA	MG-NB	-2.21	2.01	2.05
19	FF	305	CLA	MG-NB	-2.21	2.01	2.05
19	B1	801	CLA	C3B-C4B	2.21	1.49	1.42
19	B1	802	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	816	CLA	C3B-C4B	2.21	1.49	1.42
19	B1	820	CLA	MG-NB	-2.21	2.01	2.05
19	B	817	CLA	CHC-C1C	2.21	1.42	1.38
19	B1	828	CLA	CMD-C2D	-2.21	1.46	1.50
19	AA	805	CLA	C3B-C4B	2.21	1.49	1.42
19	A	838	CLA	C3B-C4B	2.21	1.49	1.42
19	B	812	CLA	C3B-C4B	2.21	1.49	1.42
19	AA	816	CLA	C3B-C4B	2.21	1.49	1.42
19	A	815	CLA	CMD-C2D	-2.21	1.46	1.50
19	A	840	CLA	CMB-C2B	-2.21	1.46	1.50
19	AA	805	CLA	CMB-C2B	-2.21	1.46	1.50
19	AA	837	CLA	MG-NB	-2.21	2.01	2.05
19	BB	820	CLA	MG-NB	-2.21	2.01	2.05
19	BB	809	CLA	CMD-C2D	-2.21	1.46	1.50
19	A	828	CLA	C3B-C4B	2.21	1.49	1.42
19	A	819	CLA	MG-NB	-2.21	2.01	2.05
19	A	828	CLA	MG-NB	-2.21	2.01	2.05
19	BB	828	CLA	CHC-C1C	2.21	1.42	1.38
19	B2	803	CLA	C3B-C4B	2.21	1.49	1.42
24	BB	849	AJP	C17-C16	2.21	1.57	1.53
19	B1	822	CLA	CHC-C1C	2.21	1.42	1.38
19	B2	829	CLA	CMB-C2B	-2.21	1.46	1.50
19	B	858	CLA	CMD-C2D	-2.21	1.46	1.50
19	A2	833	CLA	CMB-C2B	-2.21	1.46	1.50
19	B2	825	CLA	CMB-C2B	-2.21	1.46	1.50
19	B	836	CLA	C3B-C4B	2.21	1.49	1.42
19	A	812	CLA	MG-NB	-2.21	2.01	2.05
19	A1	810	CLA	CHC-C1C	2.21	1.42	1.38
19	B1	824	CLA	C1B-C2B	2.21	1.48	1.43
19	A1	812	CLA	CHC-C1C	2.21	1.42	1.38
19	AA	821	CLA	CMD-C2D	-2.21	1.46	1.50
19	A1	822	CLA	CMB-C2B	-2.21	1.46	1.50
19	A	821	CLA	CMD-C2D	-2.21	1.46	1.50
19	A	829	CLA	CMB-C2B	-2.21	1.46	1.50
19	B	806	CLA	CMC-C2C	-2.21	1.46	1.50
19	AA	815	CLA	CMD-C2D	-2.21	1.46	1.50
19	B	805	CLA	MG-NB	-2.21	2.01	2.05
19	B	809	CLA	MG-NB	-2.21	2.01	2.05
19	A2	852	CLA	CMD-C2D	-2.21	1.46	1.50
24	A1	855	AJP	C81-C12	2.21	1.58	1.54
19	B1	805	CLA	MG-NB	-2.21	2.01	2.05
19	A	814	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	822	CLA	CMD-C2D	-2.21	1.46	1.50
19	BB	817	CLA	CMD-C2D	-2.21	1.46	1.50
19	AA	817	CLA	CHC-C1C	2.20	1.42	1.38
19	A	841	CLA	C3B-C4B	2.20	1.49	1.42
19	B	858	CLA	C3B-C4B	2.20	1.49	1.42
19	A	801	CLA	MG-NB	-2.20	2.01	2.05
19	BB	817	CLA	CHC-C1C	2.20	1.42	1.38
19	BB	803	CLA	CMC-C2C	-2.20	1.46	1.50
19	K1	105	CLA	C3B-C4B	2.20	1.49	1.42
19	B	824	CLA	MG-NB	-2.20	2.01	2.05
19	B2	828	CLA	CHC-C1C	2.20	1.42	1.38
19	A2	806	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	835	CLA	CMB-C2B	-2.20	1.46	1.50
19	B2	816	CLA	MG-NB	-2.20	2.01	2.05
19	A	829	CLA	MG-ND	-2.20	2.01	2.05
19	A	817	CLA	CHC-C1C	2.20	1.42	1.38
19	B2	807	CLA	CMB-C2B	-2.20	1.46	1.50
19	B	825	CLA	CMD-C2D	-2.20	1.46	1.50
19	BB	825	CLA	CMD-C2D	-2.20	1.46	1.50
26	B2	841	ECH	C1-C6	-2.20	1.51	1.53
24	BB	849	AJP	O25-C26	2.20	1.48	1.41
19	BB	827	CLA	C3B-C4B	2.20	1.49	1.42
19	A	824	CLA	C3B-C4B	2.20	1.49	1.42
19	B1	817	CLA	CHC-C1C	2.20	1.42	1.38
19	K1	103	CLA	CHC-C1C	2.20	1.42	1.38
19	A	811	CLA	CHC-C1C	2.20	1.42	1.38
19	A	826	CLA	C3B-C4B	2.20	1.49	1.42
19	B2	804	CLA	CHC-C1C	2.20	1.42	1.38
19	A	819	CLA	CMD-C2D	-2.20	1.46	1.50
19	B	859	CLA	CMD-C2D	-2.20	1.46	1.50
19	BB	813	CLA	CMD-C2D	-2.20	1.46	1.50
19	AA	801	CLA	C3B-C4B	2.20	1.49	1.42
19	B1	804	CLA	CHC-C1C	2.20	1.42	1.38
19	KK	102	CLA	CHC-C1C	2.20	1.42	1.38
19	A2	815	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	835	CLA	CMB-C2B	-2.20	1.46	1.50
19	A2	852	CLA	CHC-C1C	2.20	1.42	1.38
19	K	101	CLA	MG-NB	-2.20	2.01	2.05
19	AA	823	CLA	CMD-C2D	-2.20	1.46	1.50
19	A1	815	CLA	C3B-C4B	2.20	1.49	1.42
19	A2	825	CLA	C3B-C4B	2.20	1.49	1.42
19	BB	835	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	820	CLA	CMD-C2D	-2.20	1.46	1.50
19	B1	850	CLA	CMD-C2D	-2.20	1.46	1.50
19	B	813	CLA	CMB-C2B	-2.20	1.46	1.50
19	B	803	CLA	MG-NB	-2.20	2.01	2.05
19	A2	801	CLA	C3B-C4B	2.20	1.49	1.42
19	B	803	CLA	C3B-C4B	2.20	1.49	1.42
19	B2	851	CLA	CMD-C2D	-2.20	1.46	1.50
19	BB	830	CLA	CMD-C2D	-2.20	1.46	1.50
19	K2	104	CLA	CHC-C1C	2.20	1.42	1.38
19	A2	839	CLA	MG-NB	-2.20	2.01	2.05
19	AA	839	CLA	MG-NB	-2.20	2.01	2.05
19	B1	810	CLA	CMD-C2D	-2.20	1.46	1.50
19	A	823	CLA	CMD-C2D	-2.20	1.46	1.50
19	B	803	CLA	CMC-C2C	-2.20	1.46	1.50
19	A1	801	CLA	MG-NB	-2.20	2.01	2.05
19	B2	817	CLA	CHC-C1C	2.20	1.42	1.38
19	AA	843	CLA	C3B-C4B	2.20	1.49	1.42
19	F1	302	CLA	CMD-C2D	-2.20	1.46	1.50
19	L	202	CLA	CMB-C2B	-2.20	1.46	1.50
19	BB	819	CLA	CMD-C2D	-2.20	1.46	1.50
19	B1	823	CLA	MG-NB	-2.20	2.01	2.05
19	A2	808	CLA	MG-NB	-2.20	2.01	2.05
19	A1	824	CLA	C3B-C4B	2.20	1.49	1.42
19	FF	302	CLA	CMB-C2B	-2.20	1.46	1.50
19	A1	852	CLA	CHC-C1C	2.20	1.42	1.38
19	B2	825	CLA	C3B-C4B	2.20	1.49	1.42
19	A	805	CLA	C3B-C4B	2.20	1.49	1.42
19	B2	821	CLA	MG-NB	-2.20	2.01	2.05
19	B	825	CLA	C3B-C4B	2.20	1.49	1.42
19	B1	828	CLA	CMB-C2B	-2.20	1.46	1.50
19	A2	814	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	806	CLA	CMD-C2D	-2.20	1.46	1.50
19	AA	814	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	833	CLA	C3B-C4B	2.20	1.49	1.42
19	B1	823	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	810	CLA	CMD-C2D	-2.20	1.46	1.50
19	B2	830	CLA	CMD-C2D	-2.20	1.46	1.50
19	A2	802	CLA	CHC-C1C	2.20	1.42	1.38
24	B	857	AJP	C81-C12	2.20	1.57	1.54
19	A1	835	CLA	C3B-C4B	2.20	1.49	1.42
19	A2	805	CLA	C3B-C4B	2.20	1.49	1.42
19	AA	824	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	833	CLA	CMB-C2B	-2.19	1.46	1.50
19	A2	821	CLA	CMD-C2D	-2.19	1.46	1.50
19	A	842	CLA	CMC-C2C	-2.19	1.46	1.50
19	BB	836	CLA	CMB-C2B	-2.19	1.46	1.50
19	A	839	CLA	MG-NB	-2.19	2.01	2.05
19	A1	828	CLA	C3B-C4B	2.19	1.49	1.42
19	BB	820	CLA	C3B-C4B	2.19	1.49	1.42
22	A2	846	LHG	P-O3	2.19	1.68	1.59
19	B2	833	CLA	CMD-C2D	-2.19	1.46	1.50
19	BB	809	CLA	CMB-C2B	-2.19	1.46	1.50
19	A1	818	CLA	MG-NB	-2.19	2.01	2.05
19	B2	852	CLA	MG-NB	-2.19	2.01	2.05
19	B1	806	CLA	C3B-C4B	2.19	1.49	1.42
19	F	301	CLA	CMB-C2B	-2.19	1.46	1.50
19	A1	823	CLA	CMD-C2D	-2.19	1.46	1.50
19	A	801	CLA	CHC-C1C	2.19	1.42	1.38
19	A2	819	CLA	MG-NB	-2.19	2.01	2.05
19	A2	838	CLA	MG-NB	-2.19	2.01	2.05
19	B2	825	CLA	MG-NB	-2.19	2.01	2.05
19	A2	834	CLA	CMB-C2B	-2.19	1.46	1.50
19	A1	807	CLA	C3B-C4B	2.19	1.49	1.42
19	A2	840	CLA	CHC-C1C	2.19	1.42	1.38
19	A	826	CLA	MG-NB	-2.19	2.01	2.05
19	AA	814	CLA	MG-NB	-2.19	2.01	2.05
19	A1	801	CLA	CHC-C1C	2.19	1.42	1.38
19	A1	823	CLA	C3B-C4B	2.19	1.49	1.42
19	A2	812	CLA	C3B-C4B	2.19	1.49	1.42
19	B2	814	CLA	MG-NB	-2.19	2.01	2.05
19	B	833	CLA	MG-NB	-2.19	2.01	2.05
19	AA	835	CLA	MG-NB	-2.19	2.01	2.05
19	B	860	CLA	C3B-C4B	2.19	1.49	1.42
24	L1	204	AJP	C07-C08	-2.19	1.50	1.53
19	A1	844	CLA	MG-NB	-2.19	2.01	2.05
19	A2	822	CLA	CMB-C2B	-2.19	1.46	1.50
19	B	859	CLA	CMB-C2B	-2.19	1.46	1.50
24	B	850	AJP	C81-C12	2.19	1.57	1.54
19	A2	844	CLA	MG-NB	-2.19	2.01	2.05
19	B	827	CLA	MG-NB	-2.19	2.01	2.05
19	B1	817	CLA	CMD-C2D	-2.19	1.46	1.50
19	AA	813	CLA	CMD-C2D	-2.19	1.46	1.50
19	BB	812	CLA	MG-NB	-2.19	2.01	2.05
19	A1	837	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L2	205	CLA	MG-NB	-2.19	2.01	2.05
19	B1	805	CLA	CMC-C2C	-2.19	1.46	1.50
19	AA	828	CLA	MG-NB	-2.19	2.01	2.05
19	A2	820	CLA	CMC-C2C	-2.19	1.46	1.50
19	L2	204	CLA	CMB-C2B	-2.19	1.46	1.50
19	AA	836	CLA	MG-NB	-2.19	2.01	2.05
19	B1	804	CLA	CMB-C2B	-2.19	1.46	1.50
19	A2	817	CLA	CMD-C2D	-2.19	1.46	1.50
19	A	825	CLA	CMD-C2D	-2.19	1.46	1.50
19	AA	840	CLA	CMD-C2D	-2.19	1.46	1.50
19	A	821	CLA	CMC-C2C	-2.19	1.46	1.50
19	BB	831	CLA	CMB-C2B	-2.19	1.46	1.50
19	A1	839	CLA	CHC-C1C	2.19	1.42	1.38
19	A2	813	CLA	CHC-C1C	2.19	1.42	1.38
19	B2	805	CLA	MG-NB	-2.19	2.01	2.05
19	A1	816	CLA	CMD-C2D	-2.19	1.46	1.50
19	B	808	CLA	CMD-C2D	-2.19	1.46	1.50
19	A1	818	CLA	CHC-C1C	2.19	1.42	1.38
19	B2	819	CLA	CHC-C1C	2.19	1.42	1.38
19	A	814	CLA	MG-NB	-2.19	2.01	2.05
19	B1	819	CLA	CMD-C2D	-2.19	1.46	1.50
19	A1	810	CLA	C3B-C4B	2.19	1.49	1.42
19	AA	838	CLA	CHC-C1C	2.19	1.42	1.38
19	AA	833	CLA	MG-NB	-2.19	2.01	2.05
19	BB	827	CLA	MG-NB	-2.19	2.01	2.05
19	AA	825	CLA	CMD-C2D	-2.19	1.46	1.50
19	BB	813	CLA	CMB-C2B	-2.19	1.46	1.50
19	A2	818	CLA	CMB-C2B	-2.18	1.46	1.50
19	XX	101	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	809	CLA	CHC-C1C	2.18	1.42	1.38
19	A1	821	CLA	CMB-C2B	-2.18	1.46	1.50
19	B	830	CLA	CMD-C2D	-2.18	1.46	1.50
19	B2	819	CLA	CMC-C2C	-2.18	1.46	1.50
19	AA	811	CLA	CMB-C2B	-2.18	1.46	1.50
19	B1	808	CLA	MG-NB	-2.18	2.01	2.05
19	B1	830	CLA	CHC-C1C	2.18	1.42	1.38
19	B2	810	CLA	CHC-C1C	2.18	1.42	1.38
19	A1	818	CLA	CMD-C2D	-2.18	1.46	1.50
19	A1	834	CLA	CMB-C2B	-2.18	1.46	1.50
19	BB	812	CLA	C3B-C4B	2.18	1.49	1.42
19	A	818	CLA	CHC-C1C	2.18	1.42	1.38
19	AA	818	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	809	CLA	CMD-C2D	-2.18	1.46	1.50
19	AA	830	CLA	CMC-C2C	-2.18	1.46	1.50
19	A	827	CLA	CHC-C1C	2.18	1.42	1.38
19	B1	814	CLA	CMB-C2B	-2.18	1.46	1.50
19	A2	824	CLA	C3B-C4B	2.18	1.49	1.42
19	B	828	CLA	MG-NB	-2.18	2.01	2.05
19	L1	205	CLA	C3B-C4B	2.18	1.49	1.42
19	B1	807	CLA	CMB-C2B	-2.18	1.46	1.50
19	A	813	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	840	CLA	CMD-C2D	-2.18	1.46	1.50
19	A1	821	CLA	MG-NB	-2.18	2.01	2.05
19	B	854	CLA	MG-NB	-2.18	2.01	2.05
22	A2	845	LHG	P-O3	2.18	1.67	1.59
19	A2	804	CLA	CMC-C2C	-2.18	1.46	1.50
19	A2	834	CLA	CMD-C2D	-2.18	1.46	1.50
19	A2	829	CLA	C3B-C4B	2.18	1.49	1.42
19	B	831	CLA	CMD-C2D	-2.18	1.46	1.50
19	A2	832	CLA	MG-NB	-2.18	2.01	2.05
19	A1	834	CLA	MG-NB	-2.18	2.01	2.05
19	AA	845	CLA	MG-NB	-2.18	2.01	2.05
19	A1	812	CLA	CMD-C2D	-2.18	1.46	1.50
19	B1	808	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	844	CLA	CMD-C2D	-2.18	1.46	1.50
19	X	101	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	838	CLA	CHC-C1C	2.18	1.42	1.38
19	A2	838	CLA	CMD-C2D	-2.18	1.46	1.50
19	B	836	CLA	CHC-C1C	2.18	1.42	1.38
19	LL	202	CLA	CHC-C1C	2.18	1.42	1.38
19	B2	804	CLA	CMB-C2B	-2.18	1.46	1.50
19	A2	842	CLA	CHC-C1C	2.18	1.42	1.38
19	A1	833	CLA	CMD-C2D	-2.18	1.46	1.50
19	B2	819	CLA	CMD-C2D	-2.18	1.46	1.50
19	BB	835	CLA	CMB-C2B	-2.18	1.46	1.50
19	L	202	CLA	C3B-C4B	2.18	1.49	1.42
23	FF	306	BCR	C33-C5	-2.18	1.47	1.50
19	A1	825	CLA	C3B-C4B	2.18	1.49	1.42
19	AA	840	CLA	C3B-C4B	2.18	1.49	1.42
19	A	811	CLA	CMB-C2B	-2.18	1.46	1.50
19	B	809	CLA	CMB-C2B	-2.18	1.46	1.50
22	A1	846	LHG	P-O3	2.18	1.67	1.59
19	A1	842	CLA	CMB-C2B	-2.18	1.46	1.50
19	B1	830	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	813	CLA	CMD-C2D	-2.18	1.46	1.50
19	B	830	CLA	CMC-C2C	-2.18	1.46	1.50
19	BB	812	CLA	CMB-C2B	-2.18	1.46	1.50
19	A	837	CLA	CHC-C1C	2.17	1.42	1.38
19	BB	835	CLA	CHC-C1C	2.17	1.42	1.38
19	B1	811	CLA	MG-NB	-2.17	2.01	2.05
19	B	829	CLA	MG-NB	-2.17	2.01	2.05
19	LL	203	CLA	CMB-C2B	-2.17	1.46	1.50
19	B2	824	CLA	CHC-C1C	2.17	1.42	1.38
19	L1	207	CLA	MG-ND	-2.17	2.01	2.05
19	B2	851	CLA	CMB-C2B	-2.17	1.46	1.50
19	A	838	CLA	MG-NB	-2.17	2.01	2.05
19	B1	831	CLA	CMB-C2B	-2.17	1.46	1.50
19	L1	205	CLA	CMB-C2B	-2.17	1.46	1.50
19	L	203	CLA	CMD-C2D	-2.17	1.46	1.50
19	AA	833	CLA	CMC-C2C	-2.17	1.46	1.50
19	A2	841	CLA	C3B-C4B	2.17	1.49	1.42
19	BB	819	CLA	MG-NB	-2.17	2.01	2.05
19	A2	801	CLA	CHC-C1C	2.17	1.42	1.38
19	AA	826	CLA	MG-NB	-2.17	2.01	2.05
19	A1	827	CLA	CHC-C1C	2.17	1.42	1.38
19	A2	844	CLA	C3B-C4B	2.17	1.49	1.42
23	BB	843	BCR	C38-C26	-2.17	1.47	1.50
19	B1	824	CLA	CMB-C2B	-2.17	1.46	1.50
19	A2	833	CLA	CMC-C2C	-2.17	1.46	1.50
19	B2	808	CLA	MG-NB	-2.17	2.01	2.05
19	B1	809	CLA	CMD-C2D	-2.17	1.46	1.50
19	A	807	CLA	CMB-C2B	-2.17	1.46	1.50
19	A	812	CLA	CMD-C2D	-2.17	1.46	1.50
19	BB	826	CLA	CMC-C2C	-2.17	1.46	1.50
19	A2	835	CLA	MG-NB	-2.17	2.01	2.05
23	F	305	BCR	C33-C5	-2.17	1.47	1.50
19	B	835	CLA	C3B-C4B	2.17	1.49	1.42
19	A	808	CLA	MG-NB	-2.17	2.01	2.05
19	BB	813	CLA	MG-NB	-2.17	2.01	2.05
19	A2	813	CLA	CMD-C2D	-2.17	1.46	1.50
19	J1	103	CLA	CHC-C1C	2.17	1.42	1.38
19	B2	806	CLA	C3B-C4B	2.17	1.49	1.42
19	FF	305	CLA	CMB-C2B	-2.17	1.46	1.50
19	J2	103	CLA	CHC-C1C	2.17	1.42	1.38
19	AA	845	CLA	CHC-C1C	2.17	1.42	1.38
22	AA	847	LHG	P-O3	2.17	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L2	204	CLA	C3B-C4B	2.17	1.49	1.42
19	AA	853	CLA	C3B-C4B	2.17	1.49	1.42
19	K1	103	CLA	CMD-C2D	-2.17	1.46	1.50
19	AA	812	CLA	CMD-C2D	-2.17	1.46	1.50
19	A1	831	CLA	MG-NB	-2.17	2.01	2.05
19	A	832	CLA	CMC-C2C	-2.17	1.46	1.50
19	A2	811	CLA	CHC-C1C	2.17	1.42	1.38
19	AA	843	CLA	CMB-C2B	-2.17	1.46	1.50
24	L1	204	AJP	C04-C05	2.17	1.55	1.51
24	L2	203	AJP	C04-C05	2.17	1.55	1.51
19	B1	826	CLA	CMC-C2C	-2.17	1.46	1.50
19	B1	810	CLA	MG-NB	-2.17	2.01	2.05
19	A2	820	CLA	C1B-C2B	2.17	1.48	1.43
19	B1	813	CLA	MG-NB	-2.17	2.01	2.05
19	L2	204	CLA	MG-NB	-2.17	2.01	2.05
19	A1	811	CLA	CMD-C2D	-2.17	1.46	1.50
19	B2	813	CLA	MG-NB	-2.17	2.01	2.05
19	B2	822	CLA	MG-NB	-2.17	2.01	2.05
19	A1	811	CLA	CHC-C1C	2.17	1.42	1.38
19	B1	808	CLA	CHC-C1C	2.17	1.42	1.38
19	B1	806	CLA	CMD-C2D	-2.17	1.46	1.50
19	BB	808	CLA	C3B-C4B	2.17	1.49	1.42
19	BB	810	CLA	CHC-C1C	2.17	1.42	1.38
19	LL	202	CLA	MG-NB	-2.17	2.01	2.05
19	A2	852	CLA	C3B-C4B	2.17	1.49	1.42
19	B	802	CLA	C3B-C4B	2.17	1.49	1.42
19	B1	829	CLA	CMC-C2C	-2.17	1.46	1.50
19	B2	809	CLA	CMD-C2D	-2.17	1.46	1.50
19	B2	825	CLA	CMD-C2D	-2.17	1.46	1.50
19	AA	832	CLA	MG-NB	-2.17	2.01	2.05
19	BB	817	CLA	MG-NB	-2.17	2.01	2.05
19	B1	849	CLA	CMB-C2B	-2.16	1.46	1.50
19	B2	820	CLA	CMD-C2D	-2.16	1.46	1.50
19	BB	806	CLA	CMC-C2C	-2.16	1.46	1.50
19	A	844	CLA	C3B-C4B	2.16	1.49	1.42
19	K	102	CLA	CHC-C1C	2.16	1.42	1.38
19	AA	837	CLA	CHC-C1C	2.16	1.42	1.38
19	B1	803	CLA	C3B-C4B	2.16	1.49	1.42
19	A1	804	CLA	MG-NB	-2.16	2.01	2.05
19	AA	825	CLA	MG-NB	-2.16	2.01	2.05
19	AA	838	CLA	MG-NB	-2.16	2.01	2.05
19	B2	817	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	814	CLA	C3B-C4B	2.16	1.49	1.42
19	B1	829	CLA	CMD-C2D	-2.16	1.46	1.50
19	A1	819	CLA	C1B-C2B	2.16	1.48	1.43
19	A1	831	CLA	CMC-C2C	-2.16	1.46	1.50
19	A2	819	CLA	CMD-C2D	-2.16	1.46	1.50
19	F1	302	CLA	MG-NB	-2.16	2.01	2.05
19	B	810	CLA	CHC-C1C	2.16	1.42	1.38
24	I2	104	AJP	C05-C06	2.16	1.57	1.53
19	B	846	CLA	CMD-C2D	-2.16	1.46	1.50
19	A2	825	CLA	MG-NB	-2.16	2.01	2.05
19	A	816	CLA	MG-NB	-2.16	2.01	2.05
19	A	818	CLA	CMD-C2D	-2.16	1.46	1.50
19	BB	808	CLA	CMD-C2D	-2.16	1.46	1.50
19	A2	834	CLA	C3B-C4B	2.16	1.49	1.42
24	B	850	AJP	O25-C26	2.16	1.47	1.41
19	AA	828	CLA	CHC-C1C	2.16	1.42	1.38
19	F1	301	CLA	CMD-C2D	-2.16	1.46	1.50
19	B2	850	CLA	CMC-C2C	-2.16	1.46	1.50
19	BB	824	CLA	CMB-C2B	-2.16	1.46	1.50
19	B2	850	CLA	C3B-C4B	2.16	1.49	1.42
19	A2	801	CLA	MG-NB	-2.16	2.01	2.05
19	A2	805	CLA	CHC-C1C	2.16	1.42	1.38
19	A1	844	CLA	C3B-C4B	2.16	1.49	1.42
19	B	832	CLA	MG-NB	-2.16	2.01	2.05
19	B2	831	CLA	CHC-C1C	2.16	1.42	1.38
19	A	826	CLA	CMD-C2D	-2.16	1.46	1.50
19	A1	833	CLA	C3B-C4B	2.16	1.49	1.42
19	B1	825	CLA	CMB-C2B	-2.16	1.46	1.50
19	A2	827	CLA	CHC-C1C	2.16	1.42	1.38
19	A2	802	CLA	CMD-C2D	-2.16	1.46	1.50
19	B2	808	CLA	CMD-C2D	-2.16	1.46	1.50
19	AA	840	CLA	MG-NB	-2.16	2.01	2.05
19	AA	818	CLA	CMD-C2D	-2.16	1.46	1.50
19	B2	823	CLA	MG-NB	-2.16	2.01	2.05
19	B	830	CLA	C3B-C4B	2.16	1.49	1.42
19	A2	811	CLA	CMC-C2C	-2.16	1.46	1.50
19	A2	812	CLA	CMD-C2D	-2.16	1.46	1.50
19	A2	812	CLA	MG-NB	-2.16	2.01	2.05
19	AA	843	CLA	MG-NB	-2.16	2.01	2.05
19	A2	805	CLA	CMB-C2B	-2.16	1.46	1.50
19	A2	842	CLA	CMB-C2B	-2.16	1.46	1.50
19	F2	302	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	826	CLA	C3B-C4B	2.16	1.49	1.42
19	A2	822	CLA	MG-NB	-2.16	2.01	2.05
19	BB	828	CLA	MG-NB	-2.16	2.01	2.05
19	LL	201	CLA	C3B-C4B	2.16	1.49	1.42
19	BB	856	CLA	CMB-C2B	-2.16	1.46	1.50
19	B	817	CLA	MG-NB	-2.16	2.01	2.05
19	A2	819	CLA	CHC-C1C	2.16	1.42	1.38
19	A	852	CLA	C3B-C4B	2.16	1.49	1.42
19	X1	101	CLA	CMD-C2D	-2.15	1.46	1.50
19	B2	802	CLA	CMB-C2B	-2.15	1.46	1.50
19	B2	828	CLA	CMD-C2D	-2.15	1.46	1.50
19	F	302	CLA	MG-NB	-2.15	2.01	2.05
19	L	203	CLA	CHC-C1C	2.15	1.42	1.38
19	B1	820	CLA	CMD-C2D	-2.15	1.46	1.50
19	XX	101	CLA	MG-NB	-2.15	2.01	2.05
19	B2	824	CLA	C3B-C4B	2.15	1.49	1.42
19	B1	812	CLA	CHC-C1C	2.15	1.42	1.38
19	A2	817	CLA	MG-NB	-2.15	2.01	2.05
19	B2	826	CLA	MG-NB	-2.15	2.01	2.05
19	AA	822	CLA	CMB-C2B	-2.15	1.46	1.50
19	BB	829	CLA	CMB-C2B	-2.15	1.46	1.50
19	A	822	CLA	MG-NB	-2.15	2.01	2.05
19	A	842	CLA	CMB-C2B	-2.15	1.46	1.50
19	BB	831	CLA	MG-NB	-2.15	2.01	2.05
19	B1	835	CLA	C3B-C4B	2.15	1.49	1.42
19	KK	102	CLA	CMD-C2D	-2.15	1.46	1.50
19	B1	812	CLA	MG-NB	-2.15	2.01	2.05
19	B2	830	CLA	CHC-C1C	2.15	1.42	1.38
19	B2	836	CLA	C3B-C4B	2.15	1.49	1.42
19	A	811	CLA	CMC-C2C	-2.15	1.46	1.50
19	A	825	CLA	MG-NB	-2.15	2.01	2.05
19	B1	825	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	850	AJP	C17-C16	2.15	1.57	1.53
19	L1	205	CLA	MG-NB	-2.15	2.01	2.05
19	B2	831	CLA	MG-NB	-2.15	2.01	2.05
19	AA	808	CLA	MG-NB	-2.15	2.01	2.05
19	FF	302	CLA	MG-NB	-2.15	2.01	2.05
19	BB	820	CLA	CMB-C2B	-2.15	1.46	1.50
19	A	833	CLA	MG-NB	-2.15	2.01	2.05
19	B	821	CLA	MG-NB	-2.15	2.01	2.05
19	A1	825	CLA	CMB-C2B	-2.15	1.46	1.50
19	JJ	103	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XX	102	LHG	P-O6	2.15	1.67	1.59
19	F1	305	CLA	CMD-C2D	-2.15	1.46	1.50
19	AA	842	CLA	CMB-C2B	-2.15	1.46	1.50
19	A2	826	CLA	C3B-C4B	2.15	1.49	1.42
19	BB	826	CLA	C1B-NB	-2.15	1.35	1.37
19	AA	845	CLA	C3B-C4B	2.15	1.49	1.42
19	A2	826	CLA	CMB-C2B	-2.15	1.46	1.50
19	A	814	CLA	CMB-C2B	-2.15	1.46	1.50
19	B	854	CLA	CMC-C2C	-2.15	1.46	1.50
19	B	833	CLA	CMB-C2B	-2.15	1.46	1.50
19	B2	812	CLA	MG-NB	-2.15	2.01	2.05
19	AA	807	CLA	CMB-C2B	-2.15	1.46	1.50
19	B1	815	CLA	CHC-C1C	2.15	1.42	1.38
19	AA	811	CLA	CHC-C1C	2.15	1.42	1.38
19	A	833	CLA	CMC-C2C	-2.15	1.46	1.50
19	AA	838	CLA	CMB-C2B	-2.15	1.46	1.50
19	A2	811	CLA	C3B-C4B	2.15	1.49	1.42
24	M2	101	AJP	C81-C12	2.15	1.57	1.54
19	A2	822	CLA	CHC-C1C	2.15	1.42	1.38
19	B	837	CLA	CHC-C1C	2.15	1.42	1.38
19	B1	827	CLA	MG-NB	-2.15	2.01	2.05
19	BB	825	CLA	MG-NB	-2.15	2.01	2.05
19	A2	829	CLA	CMB-C2B	-2.14	1.46	1.50
19	L1	206	CLA	CHC-C1C	2.14	1.42	1.38
19	AA	827	CLA	CHC-C1C	2.14	1.42	1.38
19	B1	804	CLA	MG-NB	-2.14	2.01	2.05
19	BB	805	CLA	MG-NB	-2.14	2.01	2.05
19	BB	832	CLA	CMB-C2B	-2.14	1.46	1.50
19	B2	837	CLA	CHC-C1C	2.14	1.42	1.38
19	JJ	103	CLA	CMD-C2D	-2.14	1.46	1.50
19	A1	824	CLA	CHC-C1C	2.14	1.42	1.38
19	A	834	CLA	C3B-C4B	2.14	1.49	1.42
19	AA	829	CLA	MG-ND	-2.14	2.01	2.05
19	B2	815	CLA	CMB-C2B	-2.14	1.46	1.50
19	B2	835	CLA	C3B-C4B	2.14	1.49	1.42
19	B	820	CLA	CMB-C2B	-2.14	1.46	1.50
19	AA	821	CLA	CMC-C2C	-2.14	1.46	1.50
19	B1	809	CLA	MG-NB	-2.14	2.01	2.05
19	B	825	CLA	MG-NB	-2.14	2.01	2.05
24	A1	855	AJP	C10-C08	2.14	1.57	1.53
19	B	806	CLA	C3B-C4B	2.14	1.49	1.42
19	B1	815	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	829	CLA	CMC-C2C	-2.14	1.46	1.50
19	BB	845	CLA	CMD-C2D	-2.14	1.46	1.50
19	A1	807	CLA	CMB-C2B	-2.14	1.46	1.50
19	B1	801	CLA	CMB-C2B	-2.14	1.46	1.50
19	B1	806	CLA	CMC-C2C	-2.14	1.46	1.50
24	A2	854	AJP	C10-C08	2.14	1.57	1.53
25	B2	847	LMG	O7-C8	-2.14	1.41	1.46
19	B2	822	CLA	CMB-C2B	-2.14	1.46	1.50
19	B2	830	CLA	CMC-C2C	-2.14	1.46	1.50
19	A	819	CLA	CMC-C2C	-2.14	1.46	1.50
19	A2	814	CLA	MG-NB	-2.14	2.01	2.05
19	B1	845	CLA	CBD-CAD	2.14	1.56	1.51
24	L	208	AJP	C21-C20	2.14	1.57	1.54
19	AA	836	CLA	C3B-C4B	2.14	1.49	1.42
19	A	826	CLA	CHC-C1C	2.14	1.42	1.38
19	B2	808	CLA	CMB-C2B	-2.14	1.46	1.50
19	A1	816	CLA	MG-NB	-2.14	2.01	2.05
19	F1	305	CLA	MG-NB	-2.14	2.01	2.05
19	A2	812	CLA	CHC-C1C	2.14	1.42	1.38
19	B2	846	CLA	CBD-CAD	2.14	1.56	1.51
19	A2	832	CLA	CMC-C2C	-2.14	1.46	1.50
19	J1	101	CLA	MG-NB	-2.14	2.01	2.05
19	B2	812	CLA	CHC-C1C	2.14	1.42	1.38
22	A	846	LHG	P-O3	2.14	1.67	1.59
19	B1	806	CLA	MG-NB	-2.14	2.01	2.05
19	A	827	CLA	MG-NB	-2.14	2.01	2.05
19	B	827	CLA	C3B-C4B	2.14	1.49	1.42
19	L2	205	CLA	CHC-C1C	2.14	1.42	1.38
19	B1	813	CLA	CMD-C2D	-2.14	1.46	1.50
19	B2	836	CLA	CMC-C2C	-2.14	1.46	1.50
19	AA	819	CLA	MG-NB	-2.14	2.01	2.05
19	B2	808	CLA	CHC-C1C	2.14	1.42	1.38
24	B	857	AJP	O25-C26	2.14	1.47	1.41
19	AA	811	CLA	C3B-C4B	2.14	1.49	1.42
19	AA	817	CLA	CMD-C2D	-2.14	1.46	1.50
19	B1	817	CLA	MG-NB	-2.14	2.01	2.05
19	K1	105	CLA	CHC-C1C	2.14	1.42	1.38
19	B	820	CLA	MG-NB	-2.14	2.01	2.05
19	X2	101	CLA	CMD-C2D	-2.14	1.46	1.50
19	B	819	CLA	MG-NB	-2.14	2.01	2.05
19	B2	815	CLA	CHC-C1C	2.14	1.42	1.38
19	B2	809	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	836	CLA	MG-NB	-2.14	2.01	2.05
19	A1	819	CLA	CMC-C2C	-2.14	1.46	1.50
19	A2	826	CLA	CMC-C2C	-2.14	1.46	1.50
19	A	828	CLA	CHC-C1C	2.14	1.42	1.38
19	B2	813	CLA	CMD-C2D	-2.14	1.46	1.50
24	L2	203	AJP	C81-C12	2.14	1.57	1.54
19	A	817	CLA	CMD-C2D	-2.13	1.46	1.50
19	AA	827	CLA	MG-NB	-2.13	2.01	2.05
19	A	838	CLA	CMB-C2B	-2.13	1.46	1.50
19	A2	818	CLA	MG-NB	-2.13	2.01	2.05
19	B2	828	CLA	MG-NB	-2.13	2.01	2.05
19	F2	302	CLA	CHC-C1C	2.13	1.42	1.38
19	A1	844	CLA	CMD-C2D	-2.13	1.46	1.50
19	B2	824	CLA	CMB-C2B	-2.13	1.46	1.50
19	A	836	CLA	C3B-C4B	2.13	1.49	1.42
19	A1	808	CLA	MG-NB	-2.13	2.01	2.05
19	BB	830	CLA	MG-NB	-2.13	2.01	2.05
24	A1	854	AJP	O25-C26	2.13	1.47	1.41
19	B2	802	CLA	CMD-C2D	-2.13	1.46	1.50
19	A	825	CLA	CMB-C2B	-2.13	1.46	1.50
19	A	812	CLA	CHC-C1C	2.13	1.42	1.38
19	B1	850	CLA	CMB-C2B	-2.13	1.46	1.50
19	BB	807	CLA	CMB-C2B	-2.13	1.46	1.50
19	X	101	CLA	MG-NB	-2.13	2.01	2.05
19	B1	802	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	817	CLA	CMB-C2B	-2.13	1.46	1.50
19	J	101	CLA	CMD-C2D	-2.13	1.46	1.50
19	A1	813	CLA	MG-NB	-2.13	2.01	2.05
19	B	822	CLA	MG-NB	-2.13	2.01	2.05
19	A2	818	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	825	CLA	CMC-C2C	-2.13	1.46	1.50
19	A1	832	CLA	CMC-C2C	-2.13	1.46	1.50
19	JJ	101	CLA	CMD-C2D	-2.13	1.46	1.50
19	A1	821	CLA	CHC-C1C	2.13	1.42	1.38
19	B2	818	CLA	MG-NB	-2.13	2.01	2.05
19	B	811	CLA	MG-NB	-2.13	2.01	2.05
19	F1	301	CLA	CMB-C2B	-2.13	1.46	1.50
19	B	827	CLA	CMB-C2B	-2.13	1.46	1.50
19	B1	802	CLA	CMB-C2B	-2.13	1.46	1.50
19	B1	808	CLA	CMB-C2B	-2.13	1.46	1.50
19	A1	804	CLA	CHC-C1C	2.13	1.42	1.38
19	K	102	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	825	CLA	CMB-C2B	-2.13	1.46	1.50
19	B	826	CLA	MG-NB	-2.13	2.01	2.05
19	B	859	CLA	MG-NB	-2.13	2.01	2.05
19	AA	829	CLA	C3B-C4B	2.13	1.48	1.42
19	A2	807	CLA	CMB-C2B	-2.13	1.46	1.50
19	B	808	CLA	CMB-C2B	-2.13	1.46	1.50
19	AA	842	CLA	MG-NB	-2.13	2.01	2.05
19	A1	815	CLA	CMD-C2D	-2.13	1.46	1.50
19	B1	849	CLA	CMC-C2C	-2.13	1.46	1.50
19	A2	835	CLA	CMC-C2C	-2.13	1.46	1.50
19	AA	845	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	816	CLA	CMD-C2D	-2.13	1.46	1.50
19	A2	819	CLA	CMB-C2B	-2.13	1.46	1.50
19	A2	819	CLA	CMC-C2C	-2.13	1.46	1.50
19	A	852	CLA	CMD-C2D	-2.13	1.46	1.50
19	AA	820	CLA	CMC-C2C	-2.13	1.46	1.50
19	A1	816	CLA	CMB-C2B	-2.13	1.46	1.50
19	A1	817	CLA	CMD-C2D	-2.13	1.46	1.50
19	BB	806	CLA	C3B-C4B	2.13	1.48	1.42
19	A2	828	CLA	CMB-C2B	-2.13	1.46	1.50
19	J	103	CLA	CMD-C2D	-2.13	1.46	1.50
19	F	301	CLA	CHC-C1C	2.13	1.42	1.38
19	A2	829	CLA	MG-ND	-2.13	2.01	2.05
19	X1	101	CLA	CHC-C1C	2.13	1.42	1.38
19	A	844	CLA	CMB-C2B	-2.13	1.46	1.50
19	B1	836	CLA	CHC-C1C	2.13	1.42	1.38
19	A1	834	CLA	CMC-C2C	-2.13	1.46	1.50
19	BB	827	CLA	CMB-C2B	-2.13	1.46	1.50
19	A	811	CLA	C3B-C4B	2.12	1.48	1.42
19	A1	806	CLA	CMB-C2B	-2.12	1.46	1.50
19	B2	830	CLA	CMB-C2B	-2.12	1.46	1.50
19	B	846	CLA	MG-NB	-2.12	2.01	2.05
19	A1	817	CLA	MG-NB	-2.12	2.01	2.05
19	A	815	CLA	MG-NB	-2.12	2.01	2.05
19	A1	830	CLA	C3B-C4B	2.12	1.48	1.42
19	B1	829	CLA	CMB-C2B	-2.12	1.46	1.50
19	F2	301	CLA	CMB-C2B	-2.12	1.46	1.50
19	F2	301	CLA	CMD-C2D	-2.12	1.46	1.50
19	AA	838	CLA	CMD-C2D	-2.12	1.46	1.50
24	K	104	AJP	C05-C06	2.12	1.57	1.53
19	A	816	CLA	CMD-C2D	-2.12	1.46	1.50
19	A	840	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	824	CLA	CHC-C1C	2.12	1.42	1.38
19	B1	829	CLA	C3B-C4B	2.12	1.48	1.42
19	A1	818	CLA	CMB-C2B	-2.12	1.46	1.50
19	B1	826	CLA	MG-NB	-2.12	2.01	2.05
19	X1	101	CLA	MG-NB	-2.12	2.01	2.05
19	AA	813	CLA	CHC-C1C	2.12	1.42	1.38
19	A1	835	CLA	CMB-C2B	-2.12	1.46	1.50
19	BB	834	CLA	CMC-C2C	-2.12	1.46	1.50
19	AA	820	CLA	C1B-C2B	2.12	1.48	1.43
23	MM	101	BCR	C33-C5	-2.12	1.47	1.50
19	A1	803	CLA	CMB-C2B	-2.12	1.46	1.50
19	L2	204	CLA	CMD-C2D	-2.12	1.46	1.50
19	A2	830	CLA	MG-NB	-2.12	2.01	2.05
19	AA	812	CLA	CHC-C1C	2.12	1.42	1.38
19	A1	808	CLA	CMD-C2D	-2.12	1.46	1.50
19	L1	205	CLA	CMD-C2D	-2.12	1.46	1.50
19	B1	801	CLA	CHC-C1C	2.12	1.42	1.38
19	A	826	CLA	CMC-C2C	-2.12	1.46	1.50
19	B1	822	CLA	MG-NB	-2.12	2.01	2.05
19	A1	813	CLA	CMD-C2D	-2.12	1.46	1.50
19	B1	812	CLA	CMD-C2D	-2.12	1.46	1.50
19	B1	820	CLA	CMB-C2B	-2.12	1.46	1.50
19	BB	814	CLA	CMC-C2C	-2.12	1.46	1.50
19	BB	820	CLA	CMD-C2D	-2.12	1.46	1.50
19	BB	845	CLA	CBD-CAD	2.12	1.56	1.51
19	B1	801	CLA	MG-NB	-2.12	2.01	2.05
19	X2	101	CLA	CHC-C1C	2.12	1.42	1.38
19	A	822	CLA	CHC-C1C	2.12	1.42	1.38
19	AA	816	CLA	CMB-C2B	-2.12	1.46	1.50
19	A1	840	CLA	C3B-C4B	2.12	1.48	1.42
19	A	838	CLA	CMD-C2D	-2.12	1.46	1.50
19	BB	823	CLA	CMC-C2C	-2.12	1.46	1.50
19	A1	838	CLA	CHC-C1C	2.12	1.42	1.38
19	A1	808	CLA	CMB-C2B	-2.12	1.46	1.50
19	AA	845	CLA	CMB-C2B	-2.12	1.46	1.50
19	A1	828	CLA	MG-ND	-2.12	2.01	2.05
19	B2	817	CLA	MG-NB	-2.12	2.01	2.05
19	AA	818	CLA	MG-NB	-2.12	2.01	2.05
22	B2	848	LHG	P-O6	2.12	1.67	1.59
19	B2	837	CLA	CMB-C2B	-2.12	1.46	1.50
19	AA	834	CLA	C3B-C4B	2.12	1.48	1.42
19	A1	836	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	844	CLA	CMB-C2B	-2.12	1.46	1.50
19	B1	836	CLA	CMB-C2B	-2.12	1.46	1.50
22	BB	851	LHG	P-O6	2.12	1.67	1.59
19	A2	828	CLA	CHC-C1C	2.12	1.42	1.38
19	A1	840	CLA	CMB-C2B	-2.12	1.46	1.50
19	BB	811	CLA	CMC-C2C	-2.12	1.46	1.50
19	BB	834	CLA	CMB-C2B	-2.12	1.46	1.50
19	B1	819	CLA	MG-NB	-2.12	2.01	2.05
19	A	818	CLA	MG-NB	-2.12	2.01	2.05
19	A	809	CLA	MG-NB	-2.12	2.01	2.05
19	B	805	CLA	CMC-C2C	-2.12	1.46	1.50
19	L	204	CLA	CMB-C2B	-2.12	1.46	1.50
19	AA	853	CLA	CMB-C2B	-2.12	1.46	1.50
19	B	814	CLA	CHC-C1C	2.12	1.42	1.38
19	B	808	CLA	C3B-C4B	2.12	1.48	1.42
19	B	811	CLA	CMC-C2C	-2.12	1.46	1.50
19	A1	804	CLA	C3B-C4B	2.12	1.48	1.42
22	A2	845	LHG	O7-C5	-2.12	1.41	1.46
19	J2	101	CLA	MG-NB	-2.12	2.01	2.05
19	BB	826	CLA	MG-ND	-2.12	2.01	2.05
19	BB	845	CLA	MG-NB	-2.12	2.01	2.05
19	AA	815	CLA	MG-NB	-2.11	2.01	2.05
19	B2	812	CLA	CMD-C2D	-2.11	1.46	1.50
19	B1	825	CLA	MG-NB	-2.11	2.01	2.05
19	B2	804	CLA	MG-NB	-2.11	2.01	2.05
19	J	101	CLA	MG-NB	-2.11	2.01	2.05
24	B	849	AJP	C81-C12	2.11	1.57	1.54
22	X	102	LHG	P-O6	2.11	1.67	1.59
19	AA	822	CLA	MG-NB	-2.11	2.01	2.05
19	A2	809	CLA	CMD-C2D	-2.11	1.46	1.50
19	B1	818	CLA	MG-NB	-2.11	2.01	2.05
19	K1	102	CLA	CMB-C2B	-2.11	1.46	1.50
19	A	808	CLA	CHC-C1C	2.11	1.42	1.38
19	B	846	CLA	CBD-CAD	2.11	1.56	1.51
19	B2	836	CLA	CMB-C2B	-2.11	1.46	1.50
19	B	807	CLA	CMB-C2B	-2.11	1.46	1.50
19	BB	845	CLA	CMB-C2B	-2.11	1.46	1.50
19	X	101	CLA	CHC-C1C	2.11	1.42	1.38
19	B	832	CLA	C3B-C4B	2.11	1.48	1.42
19	A1	828	CLA	CMB-C2B	-2.11	1.46	1.50
19	B2	801	CLA	CMB-C2B	-2.11	1.46	1.50
19	A1	806	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	808	CLA	CMB-C2B	-2.11	1.46	1.50
19	AA	808	CLA	CMB-C2B	-2.11	1.46	1.50
19	A2	826	CLA	MG-NB	-2.11	2.01	2.05
19	A	804	CLA	CMB-C2B	-2.11	1.46	1.50
19	A	807	CLA	CMD-C2D	-2.11	1.46	1.50
19	J1	103	CLA	CMD-C2D	-2.11	1.46	1.50
23	K2	103	BCR	C33-C5	-2.11	1.47	1.50
23	M	101	BCR	C33-C5	-2.11	1.47	1.50
19	A1	827	CLA	CMB-C2B	-2.11	1.46	1.50
19	B2	814	CLA	CHC-C1C	2.11	1.42	1.38
19	B2	819	CLA	MG-NB	-2.11	2.01	2.05
19	AA	816	CLA	CMD-C2D	-2.11	1.46	1.50
19	BB	804	CLA	CMC-C2C	-2.11	1.46	1.50
19	B2	801	CLA	CHC-C1C	2.11	1.42	1.38
19	A	805	CLA	CHC-C1C	2.11	1.42	1.38
19	AA	814	CLA	CMB-C2B	-2.11	1.46	1.50
19	BB	805	CLA	CMC-C2C	-2.11	1.46	1.50
19	A2	831	CLA	C3B-C4B	2.11	1.48	1.42
19	A2	809	CLA	MG-NB	-2.11	2.01	2.05
19	AA	825	CLA	CHC-C1C	2.11	1.42	1.38
19	BB	827	CLA	CMC-C2C	-2.11	1.46	1.50
19	KK	102	CLA	MG-NB	-2.11	2.01	2.05
19	FF	302	CLA	CHC-C1C	2.11	1.42	1.38
19	B	804	CLA	CMB-C2B	-2.11	1.46	1.50
19	BB	811	CLA	MG-NB	-2.11	2.01	2.05
19	BB	856	CLA	MG-NB	-2.11	2.01	2.05
19	A	841	CLA	CMB-C2B	-2.11	1.46	1.50
19	A	829	CLA	C3B-C4B	2.10	1.48	1.42
19	AA	809	CLA	MG-NB	-2.10	2.01	2.05
19	A	833	CLA	CHC-C1C	2.10	1.42	1.38
19	A1	839	CLA	CMB-C2B	-2.10	1.46	1.50
19	J1	101	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	817	CLA	CMB-C2B	-2.10	1.46	1.50
19	JJ	101	CLA	MG-NB	-2.10	2.01	2.05
22	L	207	LHG	P-O6	2.10	1.67	1.59
19	BB	804	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	842	CLA	MG-NB	-2.10	2.01	2.05
19	B2	805	CLA	CHC-C1C	2.10	1.42	1.38
19	A1	838	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	830	CLA	CMC-C2C	-2.10	1.46	1.50
19	B	846	CLA	CMB-C2B	-2.10	1.46	1.50
19	AA	840	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	834	CLA	CHC-C1C	2.10	1.42	1.38
19	J2	103	CLA	CMD-C2D	-2.10	1.46	1.50
22	LL	205	LHG	P-O6	2.10	1.67	1.59
19	B	835	CLA	CMB-C2B	-2.10	1.46	1.50
19	B	818	CLA	CHC-C1C	2.10	1.42	1.38
19	AA	841	CLA	CMB-C2B	-2.10	1.46	1.50
19	AA	853	CLA	CMC-C2C	-2.10	1.46	1.50
19	J	103	CLA	CHC-C1C	2.10	1.42	1.38
19	A	824	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	814	CLA	CMC-C2C	-2.10	1.46	1.50
19	AA	807	CLA	CMD-C2D	-2.10	1.46	1.50
19	BB	806	CLA	CMB-C2B	-2.10	1.46	1.50
19	B2	836	CLA	CHC-C1C	2.10	1.42	1.38
19	B2	803	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	813	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	826	CLA	CMB-C2B	-2.10	1.46	1.50
19	BB	828	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	831	CLA	C3B-C4B	2.10	1.48	1.42
19	B2	801	CLA	MG-NB	-2.10	2.01	2.05
19	K2	104	CLA	CMD-C2D	-2.10	1.46	1.50
19	A	827	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	852	CLA	CMC-C2C	-2.10	1.46	1.50
19	AA	826	CLA	CMB-C2B	-2.10	1.46	1.50
23	II	102	BCR	C33-C5	-2.10	1.47	1.50
19	XX	101	CLA	CHC-C1C	2.10	1.42	1.38
19	A2	834	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	833	CLA	CMB-C2B	-2.10	1.46	1.50
19	A2	837	CLA	CHC-C1C	2.10	1.42	1.38
19	B2	823	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	808	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	816	CLA	CMB-C2B	-2.10	1.46	1.50
19	AA	810	CLA	CMB-C2B	-2.10	1.46	1.50
19	AA	813	CLA	CMB-C2B	-2.10	1.46	1.50
19	B2	832	CLA	CMB-C2B	-2.10	1.46	1.50
19	AA	834	CLA	CMC-C2C	-2.10	1.46	1.50
19	B2	832	CLA	CHC-C1C	2.10	1.42	1.38
19	A2	844	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	819	CLA	CMB-C2B	-2.10	1.46	1.50
19	A2	833	CLA	CHC-C1C	2.10	1.42	1.38
19	AA	805	CLA	CHC-C1C	2.10	1.42	1.38
19	A1	817	CLA	CMB-C2B	-2.10	1.46	1.50
19	B1	823	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	831	CLA	CMD-C2D	-2.10	1.46	1.50
19	A1	805	CLA	MG-NB	-2.10	2.01	2.05
19	A2	832	CLA	CMD-C2D	-2.10	1.46	1.50
19	BB	822	CLA	CMC-C2C	-2.10	1.46	1.50
22	L2	208	LHG	O7-C5	-2.10	1.41	1.46
19	B1	848	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	825	CLA	CHC-C1C	2.10	1.42	1.38
19	BB	817	CLA	CMB-C2B	-2.09	1.46	1.50
19	A	832	CLA	MG-NB	-2.09	2.01	2.05
19	B1	803	CLA	CMC-C2C	-2.09	1.46	1.50
19	BB	855	CLA	CMC-C2C	-2.09	1.46	1.50
24	KK	104	AJP	C05-C06	2.09	1.57	1.53
19	J2	101	CLA	CMD-C2D	-2.09	1.46	1.50
19	L2	205	CLA	CMC-C2C	-2.09	1.46	1.50
19	B	828	CLA	CMC-C2C	-2.09	1.46	1.50
19	AA	833	CLA	CMB-C2B	-2.09	1.46	1.50
19	B1	835	CLA	CMC-C2C	-2.09	1.46	1.50
19	BB	815	CLA	CMB-C2B	-2.09	1.46	1.50
19	B1	805	CLA	CHC-C1C	2.09	1.42	1.38
23	M1	101	BCR	C33-C5	-2.09	1.47	1.50
19	B2	813	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	853	CLA	CMD-C2D	-2.09	1.46	1.50
19	AA	806	CLA	MG-NB	-2.09	2.01	2.05
23	K1	104	BCR	C33-C5	-2.09	1.47	1.50
19	A2	807	CLA	CMD-C2D	-2.09	1.46	1.50
19	A1	833	CLA	CMC-C2C	-2.09	1.46	1.50
19	B2	827	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	818	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	832	CLA	CMD-C2D	-2.09	1.46	1.50
19	AA	840	CLA	CHC-C1C	2.09	1.42	1.38
19	B2	811	CLA	MG-NB	-2.09	2.01	2.05
19	A1	852	CLA	CMB-C2B	-2.09	1.46	1.50
19	A2	841	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	819	CLA	CMB-C2B	-2.09	1.46	1.50
19	A1	814	CLA	MG-NB	-2.09	2.01	2.05
19	B	801	CLA	CMB-C2B	-2.09	1.46	1.50
19	B	836	CLA	CMC-C2C	-2.09	1.46	1.50
19	AA	833	CLA	CHC-C1C	2.09	1.42	1.38
23	K	103	BCR	C33-C5	-2.09	1.47	1.50
19	B1	813	CLA	CMB-C2B	-2.09	1.46	1.50
19	K2	102	CLA	CMB-C2B	-2.09	1.46	1.50
19	A2	820	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	CHC-C1C	2.09	1.42	1.38
19	B1	835	CLA	MG-NB	-2.09	2.01	2.05
19	AA	831	CLA	C3B-C4B	2.09	1.48	1.42
23	BB	843	BCR	C33-C5	-2.09	1.47	1.50
19	A1	822	CLA	CMC-C2C	-2.09	1.46	1.50
19	B1	831	CLA	CMD-C2D	-2.09	1.46	1.50
19	BB	836	CLA	CHC-C1C	2.09	1.42	1.38
19	A	828	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	826	CLA	CMC-C2C	-2.09	1.46	1.50
25	M	102	LMG	O7-C8	-2.09	1.41	1.46
19	F	301	CLA	MG-NB	-2.09	2.01	2.05
24	B	857	AJP	C10-C08	2.09	1.57	1.53
19	A2	812	CLA	CMB-C2B	-2.09	1.46	1.50
19	K1	103	CLA	MG-NB	-2.09	2.01	2.05
19	B2	832	CLA	MG-NB	-2.09	2.01	2.05
19	B1	821	CLA	CHC-C1C	2.09	1.42	1.38
19	A2	825	CLA	CHC-C1C	2.09	1.42	1.38
19	A	813	CLA	MG-NB	-2.09	2.01	2.05
19	B	823	CLA	CMB-C2B	-2.09	1.46	1.50
19	AA	828	CLA	CMB-C2B	-2.09	1.46	1.50
19	F1	302	CLA	CHC-C1C	2.09	1.42	1.38
19	A	819	CLA	CHC-C1C	2.09	1.42	1.38
19	A1	835	CLA	MG-NB	-2.09	2.01	2.05
19	AA	813	CLA	MG-NB	-2.09	2.01	2.05
19	B	820	CLA	CMD-C2D	-2.09	1.46	1.50
19	A1	805	CLA	CMC-C2C	-2.09	1.46	1.50
19	A	840	CLA	CMC-C2C	-2.09	1.46	1.50
19	L	202	CLA	CMC-C2C	-2.09	1.46	1.50
19	A	820	CLA	C3B-C4B	2.09	1.48	1.42
19	AA	806	CLA	CMB-C2B	-2.08	1.46	1.50
19	A2	834	CLA	CHC-C1C	2.08	1.42	1.38
19	BB	832	CLA	MG-NB	-2.08	2.01	2.05
19	AA	826	CLA	CMD-C2D	-2.08	1.46	1.50
23	JJ	104	BCR	C33-C5	-2.08	1.47	1.50
19	A1	812	CLA	CMB-C2B	-2.08	1.46	1.50
19	A	852	CLA	CMB-C2B	-2.08	1.46	1.50
19	A	806	CLA	MG-NB	-2.08	2.01	2.05
19	L	203	CLA	CMC-C2C	-2.08	1.46	1.50
19	AA	832	CLA	CMC-C2C	-2.08	1.46	1.50
19	AA	808	CLA	CHC-C1C	2.08	1.42	1.38
19	A	806	CLA	CMB-C2B	-2.08	1.46	1.50
19	A	810	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	810	CLA	CMC-C2C	-2.08	1.46	1.50
19	F	302	CLA	CHC-C1C	2.08	1.42	1.38
24	BB	848	AJP	C17-C16	2.08	1.57	1.53
19	A2	814	CLA	CMB-C2B	-2.08	1.46	1.50
19	AA	804	CLA	CMB-C2B	-2.08	1.46	1.50
19	BB	823	CLA	CMB-C2B	-2.08	1.46	1.50
23	M2	102	BCR	C33-C5	-2.08	1.47	1.50
19	B2	804	CLA	CMC-C2C	-2.08	1.46	1.50
19	A2	842	CLA	MG-NB	-2.08	2.01	2.05
19	BB	818	CLA	CMB-C2B	-2.08	1.46	1.50
19	A2	808	CLA	CMC-C2C	-2.08	1.46	1.50
19	B2	832	CLA	CMD-C2D	-2.08	1.46	1.50
26	BB	840	ECH	C30-C25	-2.08	1.51	1.53
24	B	849	AJP	C17-C16	2.08	1.57	1.53
19	A	820	CLA	CMC-C2C	-2.08	1.46	1.50
19	B1	835	CLA	CHC-C1C	2.08	1.42	1.38
19	B2	832	CLA	C3B-C4B	2.08	1.48	1.42
19	A1	841	CLA	CMB-C2B	-2.08	1.46	1.50
19	A2	844	CLA	CMC-C2C	-2.08	1.46	1.50
19	A2	839	CLA	CHC-C1C	2.08	1.42	1.38
19	A	813	CLA	CHC-C1C	2.08	1.42	1.38
19	B2	820	CLA	CMB-C2B	-2.08	1.46	1.50
19	A	820	CLA	CHC-C1C	2.08	1.42	1.38
19	AA	826	CLA	CHC-C1C	2.08	1.42	1.38
19	K1	105	CLA	MG-NB	-2.08	2.01	2.05
23	B	844	BCR	C33-C5	-2.08	1.47	1.50
19	A1	828	CLA	CHC-C1C	2.08	1.42	1.38
19	A1	833	CLA	CHC-C1C	2.08	1.42	1.38
19	BB	801	CLA	CMB-C2B	-2.08	1.46	1.50
19	A1	826	CLA	CMB-C2B	-2.08	1.46	1.50
19	B	812	CLA	CMB-C2B	-2.08	1.46	1.50
19	A1	829	CLA	CHC-C1C	2.07	1.42	1.38
19	L1	206	CLA	CMC-C2C	-2.07	1.46	1.50
19	A2	813	CLA	CMB-C2B	-2.07	1.46	1.50
19	A1	841	CLA	MG-NB	-2.07	2.01	2.05
19	AA	840	CLA	CMB-C2B	-2.07	1.46	1.50
19	A	832	CLA	CMD-C2D	-2.07	1.46	1.50
19	AA	822	CLA	CHC-C1C	2.07	1.42	1.38
19	A2	802	CLA	MG-NB	-2.07	2.01	2.05
19	B2	806	CLA	CMC-C2C	-2.07	1.46	1.50
19	LL	202	CLA	CMC-C2C	-2.07	1.46	1.50
19	A	817	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	809	CLA	CMB-C2B	-2.07	1.46	1.50
19	B	812	CLA	CHC-C1C	2.07	1.42	1.38
22	L1	211	LHG	P-O6	2.07	1.67	1.59
19	A	821	CLA	MG-NB	-2.07	2.01	2.05
19	A2	844	CLA	CHC-C1C	2.07	1.42	1.38
19	A2	840	CLA	CMC-C2C	-2.07	1.46	1.50
19	BB	825	CLA	CHC-C1C	2.07	1.42	1.38
19	JJ	101	CLA	CMB-C2B	-2.07	1.46	1.50
19	B1	834	CLA	CHC-C1C	2.07	1.42	1.38
19	L1	207	CLA	CMB-C2B	-2.07	1.46	1.50
19	B2	805	CLA	CMC-C2C	-2.07	1.46	1.50
19	BB	835	CLA	CMC-C2C	-2.07	1.46	1.50
19	A2	839	CLA	CMB-C2B	-2.07	1.46	1.50
19	B1	831	CLA	MG-NB	-2.07	2.01	2.05
19	B	801	CLA	MG-NB	-2.07	2.01	2.05
19	B2	827	CLA	CMC-C2C	-2.07	1.46	1.50
19	A	834	CLA	CMC-C2C	-2.07	1.46	1.50
19	BB	819	CLA	CHC-C1C	2.07	1.42	1.38
19	A1	844	CLA	CHC-C1C	2.07	1.42	1.38
19	A1	805	CLA	CMB-C2B	-2.07	1.46	1.50
19	J	101	CLA	CMB-C2B	-2.07	1.46	1.50
19	BB	814	CLA	CHC-C1C	2.07	1.42	1.38
23	F2	304	BCR	C33-C5	-2.07	1.47	1.50
19	A2	809	CLA	CMB-C2B	-2.07	1.46	1.50
19	A	839	CLA	CMB-C2B	-2.07	1.46	1.50
19	B	818	CLA	CMD-C2D	-2.07	1.46	1.50
19	B2	809	CLA	CMB-C2B	-2.07	1.46	1.50
19	A2	821	CLA	CHC-C1C	2.06	1.42	1.38
19	B1	804	CLA	CMC-C2C	-2.06	1.46	1.50
19	A	818	CLA	CMB-C2B	-2.06	1.46	1.50
19	B	819	CLA	CMC-C2C	-2.06	1.46	1.50
19	A1	825	CLA	CHC-C1C	2.06	1.42	1.38
19	A1	809	CLA	CMB-C2B	-2.06	1.46	1.50
19	AA	811	CLA	CMC-C2C	-2.06	1.46	1.50
23	F1	304	BCR	C38-C26	-2.06	1.47	1.50
19	AA	821	CLA	CHC-C1C	2.06	1.42	1.38
19	B1	827	CLA	CMB-C2B	-2.06	1.46	1.50
19	B	827	CLA	CMC-C2C	-2.06	1.46	1.50
19	A2	820	CLA	C3B-C4B	2.06	1.48	1.42
19	B1	845	CLA	MG-NB	-2.06	2.01	2.05
19	A1	825	CLA	CMC-C2C	-2.06	1.46	1.50
19	A	809	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AA	855	BCR	C33-C5	-2.06	1.47	1.50
23	KK	103	BCR	C33-C5	-2.06	1.47	1.50
19	A2	816	CLA	MG-NB	-2.06	2.01	2.05
19	AA	839	CLA	CHC-C1C	2.06	1.42	1.38
19	A1	831	CLA	CMD-C2D	-2.06	1.46	1.50
19	A1	837	CLA	CMB-C2B	-2.06	1.46	1.50
19	A1	823	CLA	CMC-C2C	-2.06	1.46	1.50
19	A2	838	CLA	CMB-C2B	-2.06	1.46	1.50
19	A1	807	CLA	CMC-C2C	-2.06	1.46	1.50
19	A2	817	CLA	CMC-C2C	-2.06	1.46	1.50
19	B	801	CLA	CHC-C1C	2.06	1.42	1.38
19	AA	824	CLA	CHC-C1C	2.06	1.42	1.38
19	BB	803	CLA	CHC-C1C	2.06	1.42	1.38
19	AA	806	CLA	CMC-C2C	-2.06	1.46	1.50
19	B2	846	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	806	CLA	CMB-C2B	-2.06	1.46	1.50
19	AA	805	CLA	CMC-C2C	-2.06	1.46	1.50
19	B2	831	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	824	CLA	CMB-C2B	-2.06	1.46	1.50
19	BB	804	CLA	MG-NB	-2.06	2.01	2.05
19	X2	101	CLA	MG-NB	-2.06	2.01	2.05
19	LL	201	CLA	CMC-C2C	-2.06	1.46	1.50
24	L	208	AJP	C81-C12	2.06	1.57	1.54
23	F	304	BCR	C33-C5	-2.06	1.47	1.50
19	A1	812	CLA	MG-NB	-2.06	2.01	2.05
19	K	102	CLA	MG-NB	-2.06	2.01	2.05
24	L1	204	AJP	C81-C12	2.06	1.57	1.54
19	A	830	CLA	MG-NB	-2.06	2.01	2.05
19	A1	819	CLA	CHC-C1C	2.06	1.42	1.38
19	B	825	CLA	CHC-C1C	2.06	1.42	1.38
19	A	806	CLA	CMC-C2C	-2.06	1.46	1.50
19	L2	206	CLA	MG-ND	-2.06	2.01	2.05
19	B1	827	CLA	CMC-C2C	-2.06	1.46	1.50
19	A	804	CLA	CMC-C2C	-2.06	1.46	1.50
23	I	102	BCR	C33-C5	-2.06	1.47	1.50
19	A	834	CLA	CHC-C1C	2.06	1.42	1.38
19	BB	830	CLA	CHC-C1C	2.06	1.42	1.38
19	A1	839	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	824	CLA	CMC-C2C	-2.05	1.46	1.50
19	K	101	CLA	CMB-C2B	-2.05	1.46	1.50
19	B	803	CLA	CHC-C1C	2.05	1.42	1.38
19	AA	830	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	813	CLA	MG-NB	-2.05	2.01	2.05
19	B2	826	CLA	CMC-C2C	-2.05	1.46	1.50
19	A2	824	CLA	CHC-C1C	2.05	1.42	1.38
23	B2	844	BCR	C33-C5	-2.05	1.47	1.50
19	B	815	CLA	CMC-C2C	-2.05	1.46	1.50
19	F1	301	CLA	MG-NB	-2.05	2.01	2.05
19	A1	829	CLA	CMC-C2C	-2.05	1.46	1.50
23	B1	843	BCR	C33-C5	-2.05	1.47	1.50
19	B	834	CLA	C3B-C4B	2.05	1.48	1.42
19	B	858	CLA	CMC-C2C	-2.05	1.46	1.50
19	AA	839	CLA	CMB-C2B	-2.05	1.46	1.50
19	B	804	CLA	MG-NB	-2.05	2.01	2.05
19	B2	830	CLA	C3B-C4B	2.05	1.48	1.42
19	A1	828	CLA	CMC-C2C	-2.05	1.46	1.50
19	B	824	CLA	CMC-C2C	-2.05	1.46	1.50
19	A	824	CLA	CHC-C1C	2.05	1.42	1.38
19	A	839	CLA	CHC-C1C	2.05	1.42	1.38
19	B1	812	CLA	CMB-C2B	-2.05	1.46	1.50
19	A	805	CLA	CMC-C2C	-2.05	1.46	1.50
19	B	822	CLA	CMB-C2B	-2.05	1.46	1.50
19	A2	815	CLA	MG-NB	-2.05	2.01	2.05
19	B2	846	CLA	MG-NB	-2.05	2.01	2.05
23	F1	306	BCR	C33-C5	-2.05	1.47	1.50
19	B1	817	CLA	CMB-C2B	-2.05	1.46	1.50
19	B2	817	CLA	CMB-C2B	-2.05	1.46	1.50
19	A	823	CLA	CMC-C2C	-2.05	1.46	1.50
19	B2	835	CLA	CMB-C2B	-2.05	1.46	1.50
19	A	822	CLA	CMD-C2D	-2.05	1.46	1.50
19	K2	104	CLA	CBD-CAD	2.05	1.56	1.51
19	A1	842	CLA	C4C-C3C	2.05	1.48	1.45
19	A1	832	CLA	CHC-C1C	2.05	1.42	1.38
19	A1	813	CLA	CMB-C2B	-2.05	1.46	1.50
19	AA	827	CLA	CMC-C2C	-2.05	1.46	1.50
19	A2	810	CLA	CMB-C2B	-2.05	1.46	1.50
19	A2	824	CLA	CMC-C2C	-2.05	1.46	1.50
19	F2	301	CLA	MG-NB	-2.05	2.01	2.05
24	A1	854	AJP	C10-C08	2.05	1.57	1.53
19	B	804	CLA	CMC-C2C	-2.05	1.46	1.50
19	A1	820	CLA	CHC-C1C	2.05	1.42	1.38
19	L1	205	CLA	CHC-C1C	2.05	1.42	1.38
19	A2	840	CLA	CMB-C2B	-2.05	1.46	1.50
19	AA	834	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	845	CLA	CMD-C2D	-2.05	1.46	1.50
23	A2	850	BCR	C33-C5	-2.05	1.47	1.50
19	BB	819	CLA	CMC-C2C	-2.05	1.46	1.50
19	JJ	103	CLA	MG-NB	-2.05	2.01	2.05
19	B1	830	CLA	CMB-C2B	-2.04	1.46	1.50
19	BB	836	CLA	MG-NB	-2.04	2.01	2.05
23	FF	304	BCR	C38-C26	-2.04	1.47	1.50
19	B	854	CLA	C3B-C4B	2.04	1.48	1.42
19	L2	204	CLA	CHC-C1C	2.04	1.42	1.38
19	A1	818	CLA	CMC-C2C	-2.04	1.46	1.50
19	B1	835	CLA	CMB-C2B	-2.04	1.46	1.50
25	B1	846	LMG	O7-C8	-2.04	1.41	1.46
19	B2	837	CLA	MG-NB	-2.04	2.01	2.05
19	KK	101	CLA	CMB-C2B	-2.04	1.46	1.50
19	LL	203	CLA	CMC-C2C	-2.04	1.46	1.50
19	B2	851	CLA	MG-NB	-2.04	2.01	2.05
19	A1	819	CLA	C3B-C4B	2.04	1.48	1.42
19	A1	820	CLA	MG-NB	-2.04	2.01	2.05
19	B2	849	CLA	CMC-C2C	-2.04	1.46	1.50
19	AA	845	CLA	CMC-C2C	-2.04	1.46	1.50
19	A	827	CLA	CMB-C2B	-2.04	1.46	1.50
25	I2	105	LMG	C4-C5	2.04	1.57	1.53
22	L2	208	LHG	P-O6	2.04	1.67	1.59
23	A	854	BCR	C33-C5	-2.04	1.47	1.50
19	A1	823	CLA	CHC-C1C	2.04	1.42	1.38
19	B2	849	CLA	MG-ND	-2.04	2.01	2.05
19	L2	206	CLA	CHC-C1C	2.04	1.42	1.38
20	AA	803	CL0	CBD-CGD	-2.04	1.49	1.52
19	K2	104	CLA	MG-NB	-2.04	2.01	2.05
19	BB	810	CLA	CMC-C2C	-2.04	1.46	1.50
19	A2	808	CLA	CHC-C1C	2.04	1.42	1.38
19	AA	836	CLA	CHC-C1C	2.04	1.42	1.38
19	B1	836	CLA	MG-NB	-2.04	2.01	2.05
19	B	810	CLA	CMB-C2B	-2.04	1.46	1.50
23	F1	304	BCR	C33-C5	-2.04	1.47	1.50
19	B1	825	CLA	CHC-C1C	2.04	1.42	1.38
19	L	204	CLA	CHC-C1C	2.04	1.42	1.38
19	B2	835	CLA	CMC-C2C	-2.04	1.46	1.50
19	AA	801	CLA	CMB-C2B	-2.04	1.46	1.50
19	AA	831	CLA	CMC-C2C	-2.04	1.46	1.50
19	BB	812	CLA	CHC-C1C	2.04	1.42	1.38
19	A2	839	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	831	CLA	C3B-C4B	2.03	1.48	1.42
19	B1	831	CLA	C3B-C4B	2.03	1.48	1.42
19	A1	844	CLA	CMC-C2C	-2.03	1.46	1.50
23	A1	850	BCR	C33-C5	-2.03	1.47	1.50
23	I1	101	BCR	C38-C26	-2.03	1.47	1.50
19	A2	806	CLA	CMB-C2B	-2.03	1.46	1.50
19	LL	203	CLA	C3B-C4B	2.03	1.48	1.42
19	A	844	CLA	CMC-C2C	-2.03	1.46	1.50
19	A1	807	CLA	CHC-C1C	2.03	1.42	1.38
19	A1	815	CLA	CMB-C2B	-2.03	1.46	1.50
19	B1	825	CLA	CMC-C2C	-2.03	1.46	1.50
19	B1	806	CLA	CHC-C1C	2.03	1.42	1.38
19	B1	849	CLA	CHC-C1C	2.03	1.42	1.38
19	B	806	CLA	CHC-C1C	2.03	1.42	1.38
19	A1	824	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	815	CLA	CMB-C2B	-2.03	1.46	1.50
19	B	815	CLA	CHC-C1C	2.03	1.42	1.38
19	J2	101	CLA	CMB-C2B	-2.03	1.46	1.50
19	A2	830	CLA	CHC-C1C	2.03	1.42	1.38
23	B	839	BCR	C33-C5	-2.03	1.47	1.50
25	B1	852	LMG	O1-C1	2.03	1.43	1.40
19	B1	850	CLA	MG-NB	-2.03	2.01	2.05
19	AA	809	CLA	CMB-C2B	-2.03	1.46	1.50
19	J1	101	CLA	CMB-C2B	-2.03	1.46	1.50
19	B2	835	CLA	CHC-C1C	2.03	1.42	1.38
19	BB	821	CLA	MG-NB	-2.03	2.01	2.05
19	B1	834	CLA	CMB-C2B	-2.03	1.46	1.50
19	A2	821	CLA	MG-NB	-2.03	2.01	2.05
19	B2	803	CLA	CHC-C1C	2.03	1.42	1.38
19	A1	801	CLA	CMB-C2B	-2.03	1.46	1.50
19	A	831	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	821	CLA	CHC-C1C	2.03	1.42	1.38
19	A	825	CLA	CMC-C2C	-2.02	1.46	1.50
19	B1	830	CLA	CMD-C2D	-2.02	1.46	1.50
19	L2	204	CLA	CMC-C2C	-2.02	1.46	1.50
23	AA	851	BCR	C33-C5	-2.02	1.47	1.50
23	BB	838	BCR	C33-C5	-2.02	1.47	1.50
23	FF	304	BCR	C33-C5	-2.02	1.47	1.50
19	B1	824	CLA	CMC-C2C	-2.02	1.46	1.50
25	B2	854	LMG	O1-C1	2.02	1.43	1.40
19	BB	815	CLA	CHC-C1C	2.02	1.42	1.38
19	B1	822	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	835	CLA	CMC-C2C	-2.02	1.46	1.50
19	A1	826	CLA	CMC-C2C	-2.02	1.46	1.50
19	B1	808	CLA	CMC-C2C	-2.02	1.46	1.50
19	A2	814	CLA	CMC-C2C	-2.02	1.46	1.50
19	A	829	CLA	CMC-C2C	-2.02	1.46	1.50
23	A1	847	BCR	C33-C5	-2.02	1.47	1.50
19	B1	832	CLA	MG-NB	-2.02	2.01	2.05
19	B2	812	CLA	CMB-C2B	-2.02	1.46	1.50
23	A	850	BCR	C33-C5	-2.02	1.47	1.50
19	B2	812	CLA	CMC-C2C	-2.02	1.46	1.50
19	B1	831	CLA	CHC-C1C	2.02	1.42	1.38
19	L1	207	CLA	CHC-C1C	2.02	1.42	1.38
19	A	812	CLA	CMC-C2C	-2.02	1.46	1.50
19	AA	817	CLA	MG-NB	-2.02	2.01	2.05
19	B2	851	CLA	CMC-C2C	-2.02	1.46	1.50
19	A	808	CLA	CMC-C2C	-2.02	1.46	1.50
19	XX	101	CLA	CMB-C2B	-2.02	1.46	1.50
19	B	801	CLA	CMC-C2C	-2.02	1.46	1.50
19	A2	820	CLA	MG-ND	-2.02	2.01	2.05
23	F2	305	BCR	C33-C5	-2.02	1.47	1.50
19	L1	205	CLA	CMC-C2C	-2.02	1.46	1.50
19	AA	823	CLA	CMC-C2C	-2.02	1.46	1.50
19	B2	824	CLA	CMC-C2C	-2.02	1.46	1.50
23	F2	304	BCR	C38-C26	-2.02	1.47	1.50
23	L	206	BCR	C33-C5	-2.02	1.47	1.50
19	B2	850	CLA	CHC-C1C	2.02	1.42	1.38
19	BB	834	CLA	CHC-C1C	2.02	1.42	1.38
19	A1	816	CLA	CMC-C2C	-2.02	1.46	1.50
19	B2	814	CLA	CMC-C2C	-2.02	1.46	1.50
19	A2	805	CLA	CMC-C2C	-2.02	1.46	1.50
19	A1	813	CLA	CMC-C2C	-2.01	1.46	1.50
19	K2	102	CLA	CMC-C2C	-2.01	1.46	1.50
19	AA	812	CLA	CMC-C2C	-2.01	1.46	1.50
19	A1	842	CLA	MG-ND	-2.01	2.01	2.05
19	BB	814	CLA	MG-ND	-2.01	2.01	2.05
19	B2	801	CLA	CMC-C2C	-2.01	1.46	1.50
19	A	801	CLA	CMB-C2B	-2.01	1.46	1.50
19	BB	801	CLA	CMC-C2C	-2.01	1.46	1.50
19	A1	840	CLA	CMC-C2C	-2.01	1.46	1.50
19	AA	821	CLA	MG-NB	-2.01	2.01	2.05
19	B	815	CLA	CMB-C2B	-2.01	1.46	1.50
23	B2	839	BCR	C33-C5	-2.01	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	803	CLA	CMC-C2C	-2.01	1.46	1.50
19	A2	831	CLA	CMC-C2C	-2.01	1.46	1.50
19	BB	830	CLA	CMB-C2B	-2.01	1.46	1.50
19	B1	845	CLA	CMB-C2B	-2.01	1.46	1.50
19	BB	806	CLA	CHC-C1C	2.01	1.42	1.38
22	X2	103	LHG	P-O6	2.01	1.67	1.59
19	BB	829	CLA	C3B-C4B	2.01	1.48	1.42
19	A2	806	CLA	MG-NB	-2.01	2.01	2.05
19	B	831	CLA	CMB-C2B	-2.01	1.46	1.50
23	L	205	BCR	C33-C5	-2.01	1.47	1.50
19	B1	834	CLA	CMC-C2C	-2.01	1.46	1.50
19	AA	815	CLA	CMB-C2B	-2.01	1.46	1.50
19	B2	821	CLA	CHC-C1C	2.01	1.42	1.38
23	K2	105	BCR	C33-C5	-2.01	1.47	1.50
19	A1	838	CLA	CMC-C2C	-2.01	1.46	1.50
19	B1	815	CLA	CMB-C2B	-2.01	1.46	1.50
19	A2	816	CLA	CMB-C2B	-2.01	1.46	1.50
19	A2	852	CLA	CMC-C2C	-2.01	1.46	1.50
19	BB	810	CLA	CMB-C2B	-2.01	1.46	1.50
19	AA	837	CLA	CMC-C2C	-2.01	1.46	1.50
23	BB	842	BCR	C33-C5	-2.01	1.47	1.50
19	B1	803	CLA	CHC-C1C	2.01	1.42	1.38
19	X	101	CLA	CMB-C2B	-2.00	1.46	1.50
19	AA	808	CLA	CMC-C2C	-2.00	1.46	1.50
19	AA	825	CLA	CMC-C2C	-2.00	1.46	1.50
19	A1	819	CLA	MG-ND	-2.00	2.01	2.05
19	AA	843	CLA	C4C-C3C	2.00	1.48	1.45
23	B1	838	BCR	C33-C5	-2.00	1.47	1.50
19	AA	838	CLA	CMC-C2C	-2.00	1.46	1.50
19	B1	810	CLA	CMB-C2B	-2.00	1.46	1.50
19	B1	812	CLA	CMC-C2C	-2.00	1.46	1.50
19	X1	101	CLA	CMB-C2B	-2.00	1.46	1.50
23	K1	106	BCR	C33-C5	-2.00	1.47	1.50
19	B2	823	CLA	CMC-C2C	-2.00	1.46	1.50
19	AA	817	CLA	CMB-C2B	-2.00	1.46	1.50
19	JJ	103	CLA	CMB-C2B	-2.00	1.46	1.50
19	BB	815	CLA	CMC-C2C	-2.00	1.46	1.50
23	L1	201	BCR	C33-C5	-2.00	1.47	1.50
23	II	104	BCR	C33-C5	-2.00	1.47	1.50
19	K1	102	CLA	CMC-C2C	-2.00	1.46	1.50
19	A	838	CLA	CMC-C2C	-2.00	1.46	1.50
23	A	848	BCR	C33-C5	-2.00	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	829	CLA	CMC-C2C	-2.00	1.46	1.50
19	A	837	CLA	CMC-C2C	-2.00	1.46	1.50
19	X2	101	CLA	CMB-C2B	-2.00	1.46	1.50

All (4054) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	857	AJP	C21-C20-C19	14.02	120.63	107.23
24	M2	101	AJP	C21-C20-C19	13.84	120.47	107.23
24	A1	854	AJP	C80-C20-C21	-13.73	88.84	108.99
24	A1	854	AJP	C21-C20-C19	13.72	120.35	107.23
24	B	857	AJP	C80-C20-C21	-13.64	88.97	108.99
24	L	209	AJP	C21-C20-C19	13.62	120.26	107.23
24	L1	203	AJP	C80-C20-C21	-13.55	89.10	108.99
20	AA	803	CL0	O2D-CGD-CBD	13.53	125.81	110.95
24	L2	202	AJP	C80-C20-C21	-13.18	89.64	108.99
24	L	208	AJP	C80-C20-C21	-13.12	89.73	108.99
24	B	849	AJP	C80-C20-C21	-13.07	89.81	108.99
24	AA	856	AJP	C21-C20-C19	13.06	119.72	107.23
24	A	855	AJP	C21-C20-C19	13.04	119.70	107.23
24	L2	203	AJP	C21-C20-C19	12.93	119.60	107.23
24	L	208	AJP	C21-C20-C15	12.64	127.09	110.10
24	B	850	AJP	C21-C20-C19	12.56	119.24	107.23
20	A	803	CL0	O2D-CGD-CBD	12.54	124.73	110.95
24	AA	856	AJP	C80-C20-C21	-12.49	90.66	108.99
24	A	855	AJP	C80-C20-C21	-12.47	90.68	108.99
24	BB	848	AJP	C80-C20-C21	-12.44	90.72	108.99
24	I2	104	AJP	C80-C20-C21	-12.33	90.89	108.99
24	L	209	AJP	C80-C20-C21	-12.32	90.90	108.99
24	BB	849	AJP	O09-C08-C10	12.32	135.15	110.20
24	BB	849	AJP	C21-C20-C19	12.23	118.93	107.23
24	KK	104	AJP	C80-C20-C21	-12.20	91.09	108.99
24	L1	204	AJP	C21-C20-C19	12.19	118.89	107.23
24	L1	204	AJP	C80-C20-C21	-12.16	91.15	108.99
24	L	208	AJP	C21-C20-C19	12.15	118.85	107.23
24	K	104	AJP	C80-C20-C21	-12.07	91.27	108.99
24	M2	101	AJP	C80-C20-C21	-12.04	91.32	108.99
24	BB	848	AJP	C21-C20-C15	12.01	126.24	110.10
24	A2	854	AJP	C21-C20-C19	12.00	118.71	107.23
24	L2	203	AJP	C80-C20-C21	-12.00	91.37	108.99
24	A1	855	AJP	C80-C20-C21	-11.85	91.59	108.99
24	A2	854	AJP	C80-C20-C21	-11.84	91.62	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	104	AJP	C21-C20-C19	11.74	118.46	107.23
24	A1	855	AJP	C21-C20-C19	11.74	118.45	107.23
24	L1	203	AJP	C21-C20-C15	11.69	125.81	110.10
24	L	209	AJP	O09-C08-C10	11.69	133.86	110.20
24	BB	849	AJP	C80-C20-C21	-11.66	91.88	108.99
24	KK	104	AJP	C21-C20-C19	11.66	118.38	107.23
24	B	850	AJP	C80-C20-C21	-11.64	91.90	108.99
24	B	849	AJP	C21-C20-C15	11.64	125.74	110.10
24	KK	104	AJP	O09-C08-C10	11.57	133.62	110.20
24	KK	104	AJP	C21-C20-C15	11.56	125.64	110.10
24	L	209	AJP	C21-C20-C15	11.53	125.59	110.10
24	A	802	AJP	O09-C08-C10	11.39	133.26	110.20
24	I2	104	AJP	C21-C20-C15	11.37	125.38	110.10
24	B	850	AJP	O09-C08-C10	11.36	133.20	110.20
24	M2	101	AJP	O09-C08-C10	11.36	133.19	110.20
24	AA	802	AJP	O09-C08-C10	11.36	133.19	110.20
24	K	104	AJP	C21-C20-C15	11.35	125.35	110.10
24	I2	104	AJP	O09-C08-C10	11.31	133.10	110.20
24	L2	202	AJP	C21-C20-C15	11.30	125.28	110.10
24	BB	848	AJP	C21-C20-C19	11.29	118.03	107.23
24	B	849	AJP	C21-C20-C19	11.21	117.95	107.23
24	L	208	AJP	O09-C08-C10	11.20	132.87	110.20
24	K	104	AJP	O09-C08-C10	11.17	132.81	110.20
24	AA	802	AJP	C80-C20-C21	-11.15	90.58	108.31
24	A	802	AJP	C80-C20-C21	-11.11	90.64	108.31
24	B	849	AJP	O09-C08-C10	11.10	132.68	110.20
20	A2	803	CL0	O2D-CGD-CBD	11.05	123.09	110.95
24	L2	202	AJP	O09-C08-C10	11.03	132.53	110.20
24	BB	848	AJP	O09-C08-C10	10.99	132.44	110.20
24	L1	204	AJP	C21-C20-C15	10.93	124.79	110.10
24	I2	104	AJP	C21-C20-C19	10.86	117.61	107.23
24	L2	202	AJP	C21-C20-C19	10.80	117.56	107.23
24	B	850	AJP	C03-C02-C85	10.64	121.50	108.59
24	M2	101	AJP	C21-C20-C15	10.62	124.38	110.10
24	L2	202	AJP	C03-C02-C85	10.51	121.34	108.59
24	L2	203	AJP	C21-C20-C15	10.45	124.14	110.10
24	A1	854	AJP	C21-C20-C15	10.32	123.97	110.10
24	BB	849	AJP	C21-C20-C15	10.06	123.62	110.10
26	B	841	ECH	C16-C17-C18	-10.04	113.19	127.28
24	KK	104	AJP	C03-C02-C85	10.01	120.74	108.59
26	B1	840	ECH	C16-C17-C18	-9.99	113.27	127.28
26	B2	841	ECH	C16-C17-C18	-9.96	113.30	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	C1B-CHB-C4A	9.94	127.72	121.32
24	L1	203	AJP	C21-C20-C19	9.92	116.72	107.23
24	K	104	AJP	C03-C02-C85	9.90	120.61	108.59
24	B	857	AJP	C21-C20-C15	9.87	123.36	110.10
24	B	850	AJP	C21-C20-C15	9.72	123.16	110.10
26	BB	840	ECH	C16-C17-C18	-9.68	113.70	127.28
20	AA	803	CL0	C1B-CHB-C4A	9.59	127.49	121.32
20	A2	803	CL0	C1B-CHB-C4A	9.58	127.49	121.32
24	B	849	AJP	C03-C02-C85	9.49	120.10	108.59
24	A1	855	AJP	C21-C20-C15	9.49	122.85	110.10
24	A2	854	AJP	C21-C20-C15	9.34	122.65	110.10
20	A1	802	CL0	O2D-CGD-CBD	9.25	121.11	110.95
24	A	802	AJP	C14-C15-C20	8.95	123.99	113.91
24	AA	802	AJP	C14-C15-C20	8.93	123.97	113.91
24	KK	104	AJP	O09-C05-C04	8.87	126.55	108.54
24	A	855	AJP	C21-C20-C15	8.86	122.01	110.10
24	AA	856	AJP	C21-C20-C15	8.86	122.00	110.10
24	I2	104	AJP	C14-C15-C20	8.68	123.69	113.91
24	AA	802	AJP	C21-C20-C15	8.61	124.70	111.34
24	A	802	AJP	C21-C20-C15	8.56	124.63	111.34
20	A	803	CL0	C1B-CHB-C4A	8.36	126.70	121.32
24	L2	202	AJP	O31-C30-C29	8.33	124.72	109.70
19	BB	801	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	K	104	AJP	O09-C05-C04	8.26	125.30	108.54
24	AA	802	AJP	C80-C20-C15	-8.23	100.11	111.18
24	A	802	AJP	C80-C20-C15	-8.22	100.12	111.18
24	BB	848	AJP	C80-C20-C15	-8.15	100.22	111.18
19	B	801	CLA	C4A-NA-C1A	8.04	110.35	106.68
24	L2	203	AJP	O09-C05-C04	8.02	124.81	108.54
24	A1	854	AJP	C80-C20-C15	-8.00	100.42	111.18
24	AA	856	AJP	O09-C05-C04	7.96	124.70	108.54
19	B1	848	CLA	C4A-NA-C1A	7.96	110.31	106.68
24	A	855	AJP	O09-C05-C04	7.95	124.68	108.54
24	L	208	AJP	C14-C15-C20	7.92	122.83	113.91
24	B	849	AJP	C80-C20-C15	-7.83	100.66	111.18
24	B	857	AJP	C80-C20-C15	-7.80	100.69	111.18
19	L2	205	CLA	C4A-NA-C1A	7.79	110.23	106.68
19	B2	801	CLA	C4A-NA-C1A	7.78	110.23	106.68
24	B	850	AJP	C05-C06-C07	7.73	114.76	103.37
24	M2	101	AJP	C14-C15-C16	7.73	122.56	111.78
19	B1	801	CLA	C4A-NA-C1A	7.72	110.20	106.68
19	B	805	CLA	C4A-NA-C1A	7.70	110.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L1	203	AJP	C80-C20-C15	-7.69	100.84	111.18
24	L2	202	AJP	C05-C06-C07	7.66	114.66	103.37
24	A	802	AJP	O09-C05-C04	7.66	124.09	108.54
24	L2	202	AJP	C80-C20-C15	-7.66	100.88	111.18
19	A2	836	CLA	C4A-NA-C1A	7.62	110.16	106.68
24	BB	849	AJP	C80-C20-C15	-7.60	100.97	111.18
24	AA	802	AJP	O09-C05-C04	7.59	123.94	108.54
19	BB	852	CLA	C4A-NA-C1A	7.56	110.13	106.68
24	BB	849	AJP	O09-C05-C04	7.55	123.87	108.54
24	A2	854	AJP	O09-C05-C04	7.55	123.86	108.54
24	AA	856	AJP	C80-C20-C15	-7.52	101.08	111.18
19	B	854	CLA	C4A-NA-C1A	7.51	110.11	106.68
19	BB	805	CLA	C4A-NA-C1A	7.51	110.11	106.68
24	A	855	AJP	C80-C20-C15	-7.51	101.08	111.18
24	BB	848	AJP	C14-C15-C20	7.48	122.34	113.91
24	K	104	AJP	C80-C20-C15	-7.48	101.12	111.18
24	BB	848	AJP	C01-C02-C85	7.46	122.52	111.03
24	L	209	AJP	C80-C20-C15	-7.45	101.16	111.18
24	M2	101	AJP	C80-C20-C15	-7.44	101.18	111.18
24	L1	204	AJP	C80-C20-C15	-7.43	101.19	111.18
24	BB	849	AJP	C14-C15-C16	7.42	122.13	111.78
19	L1	206	CLA	C4A-NA-C1A	7.42	110.06	106.68
24	KK	104	AJP	C80-C20-C15	-7.41	101.22	111.18
19	B2	805	CLA	C4A-NA-C1A	7.41	110.06	106.68
24	B	849	AJP	C05-C06-C07	7.41	114.28	103.37
24	A1	855	AJP	C80-C20-C15	-7.38	101.25	111.18
24	B	849	AJP	C14-C15-C16	7.37	122.06	111.78
24	L2	203	AJP	C80-C20-C15	-7.37	101.28	111.18
19	LL	202	CLA	C4A-NA-C1A	7.36	110.03	106.68
24	L1	204	AJP	C14-C15-C20	7.33	122.17	113.91
19	L	204	CLA	C4A-NA-C1A	7.33	110.02	106.68
24	L2	203	AJP	O09-C08-C10	7.32	125.02	110.20
19	A2	801	CLA	C4A-NA-C1A	7.32	110.02	106.68
19	B1	805	CLA	C4A-NA-C1A	7.31	110.01	106.68
19	A	836	CLA	C4A-NA-C1A	7.31	110.01	106.68
24	B	849	AJP	O84-C05-O09	-7.31	92.49	109.88
19	A1	835	CLA	C4A-NA-C1A	7.31	110.01	106.68
19	B	859	CLA	C4A-NA-C1A	7.30	110.01	106.68
24	B	850	AJP	C80-C20-C15	-7.30	101.37	111.18
24	A1	855	AJP	C14-C15-C20	7.28	122.11	113.91
24	A2	854	AJP	C80-C20-C15	-7.28	101.39	111.18
19	A	832	CLA	C4A-NA-C1A	7.26	109.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	856	CLA	C4A-NA-C1A	7.25	109.99	106.68
24	L	208	AJP	C05-C06-C07	7.24	114.04	103.37
24	L	209	AJP	C14-C15-C16	7.24	121.88	111.78
24	L2	203	AJP	C03-C02-C85	7.23	117.36	108.59
19	A2	842	CLA	C4A-NA-C1A	7.22	109.97	106.68
24	L2	202	AJP	C14-C15-C16	7.21	121.84	111.78
19	A2	813	CLA	C4A-NA-C1A	7.20	109.96	106.68
24	L1	203	AJP	O31-C30-C29	7.20	122.67	109.70
19	AA	813	CLA	C4A-NA-C1A	7.19	109.96	106.68
19	B2	849	CLA	C4A-NA-C1A	7.17	109.95	106.68
19	A1	829	CLA	C4A-NA-C1A	7.17	109.95	106.68
24	K	104	AJP	C05-C06-C07	7.16	113.92	103.37
19	B	817	CLA	C4A-NA-C1A	7.16	109.94	106.68
19	A1	801	CLA	C4A-NA-C1A	7.15	109.94	106.68
19	AA	836	CLA	C4A-NA-C1A	7.15	109.94	106.68
19	B2	851	CLA	C4A-NA-C1A	7.14	109.94	106.68
24	L2	203	AJP	C14-C15-C16	7.14	121.74	111.78
24	I2	104	AJP	O09-C05-C04	7.13	123.02	108.54
19	A	825	CLA	C4A-NA-C1A	7.13	109.93	106.68
24	L	208	AJP	C80-C20-C15	-7.13	101.60	111.18
24	BB	848	AJP	C14-C15-C16	7.12	121.72	111.78
19	B1	826	CLA	C4A-NA-C1A	7.11	109.92	106.68
24	B	850	AJP	C14-C15-C20	7.11	121.92	113.91
19	B2	826	CLA	C4A-NA-C1A	7.10	109.92	106.68
19	B1	836	CLA	C4A-NA-C1A	7.10	109.92	106.68
19	A	801	CLA	C4A-NA-C1A	7.10	109.92	106.68
19	A	813	CLA	C4A-NA-C1A	7.10	109.92	106.68
24	M2	101	AJP	O09-C05-C04	7.10	122.94	108.54
19	A1	841	CLA	C4A-NA-C1A	7.08	109.91	106.68
24	M2	101	AJP	C05-C06-C07	7.08	113.80	103.37
24	AA	802	AJP	C05-C06-C07	7.08	113.80	103.37
19	AA	801	CLA	C4A-NA-C1A	7.07	109.91	106.68
24	L2	202	AJP	O84-C05-O09	-7.07	93.06	109.88
19	A2	838	CLA	C4A-NA-C1A	7.07	109.90	106.68
24	I2	104	AJP	C05-C06-C07	7.06	113.77	103.37
19	B	833	CLA	C4A-NA-C1A	7.06	109.90	106.68
19	BB	822	CLA	C4A-NA-C1A	7.06	109.90	106.68
24	L	209	AJP	O09-C05-C04	7.05	122.86	108.54
24	A	802	AJP	C05-C06-C07	7.05	113.75	103.37
19	A1	831	CLA	C4A-NA-C1A	7.02	109.88	106.68
24	BB	848	AJP	O09-C05-C04	7.02	122.79	108.54
19	B2	837	CLA	C4A-NA-C1A	7.01	109.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	104	AJP	C14-C15-C20	7.00	121.80	113.91
24	A2	854	AJP	C14-C15-C20	7.00	121.79	113.91
19	B1	850	CLA	C4A-NA-C1A	6.99	109.87	106.68
19	B	822	CLA	C4A-NA-C1A	6.99	109.87	106.68
24	KK	104	AJP	C05-C06-C07	6.97	113.63	103.37
24	A1	854	AJP	O84-C05-O09	-6.96	93.33	109.88
24	KK	104	AJP	C14-C15-C20	6.95	121.74	113.91
19	B1	832	CLA	C4A-NA-C1A	6.93	109.84	106.68
19	A	830	CLA	C4A-NA-C1A	6.93	109.84	106.68
19	BB	817	CLA	C4A-NA-C1A	6.92	109.84	106.68
19	A2	832	CLA	C4A-NA-C1A	6.92	109.83	106.68
19	AA	845	CLA	C4A-NA-C1A	6.90	109.83	106.68
19	A2	823	CLA	C4A-NA-C1A	6.90	109.83	106.68
19	AA	825	CLA	C4A-NA-C1A	6.90	109.83	106.68
19	A2	825	CLA	C4A-NA-C1A	6.89	109.82	106.68
19	A1	807	CLA	C4A-NA-C1A	6.89	109.82	106.68
24	A1	854	AJP	O09-C05-C04	6.88	122.51	108.54
19	K2	104	CLA	C4A-NA-C1A	6.88	109.82	106.68
24	L2	202	AJP	O09-C05-C04	6.88	122.50	108.54
19	B	821	CLA	C4A-NA-C1A	6.88	109.82	106.68
19	A	808	CLA	C4A-NA-C1A	6.87	109.81	106.68
19	B	826	CLA	C4A-NA-C1A	6.87	109.81	106.68
24	AA	856	AJP	C80-C20-C19	-6.87	98.96	110.44
24	A	855	AJP	C80-C20-C19	-6.86	98.97	110.44
19	B2	821	CLA	C4A-NA-C1A	6.86	109.81	106.68
19	A	819	CLA	C4A-NA-C1A	6.86	109.81	106.68
24	L	209	AJP	C05-C06-C07	6.85	113.46	103.37
19	A1	803	CLA	C4A-NA-C1A	6.85	109.80	106.68
24	A	802	AJP	O84-C05-O09	-6.84	93.59	109.88
19	B1	803	CLA	C4A-NA-C1A	6.84	109.80	106.68
19	B2	823	CLA	C4A-NA-C1A	6.83	109.80	106.68
19	AA	832	CLA	C4A-NA-C1A	6.83	109.80	106.68
19	A1	825	CLA	C4A-NA-C1A	6.83	109.79	106.68
24	B	857	AJP	O09-C05-C04	6.83	122.40	108.54
19	AA	842	CLA	C4A-NA-C1A	6.82	109.79	106.68
24	B	857	AJP	O84-C05-O09	-6.82	93.65	109.88
19	B1	823	CLA	C4A-NA-C1A	6.82	109.79	106.68
20	A2	803	CL0	O1D-CGD-CBD	-6.82	114.39	124.72
19	A1	812	CLA	C4A-NA-C1A	6.81	109.79	106.68
19	A1	837	CLA	C4A-NA-C1A	6.81	109.79	106.68
24	B	850	AJP	C14-C15-C16	6.81	121.28	111.78
24	A	802	AJP	C11-C16-C15	-6.81	97.14	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BB	848	AJP	O84-C05-O09	-6.81	93.67	109.88
19	A	828	CLA	C4A-NA-C1A	6.81	109.79	106.68
19	A1	822	CLA	C4A-NA-C1A	6.81	109.78	106.68
24	I2	104	AJP	C80-C20-C15	-6.81	102.03	111.18
19	B2	833	CLA	C4A-NA-C1A	6.80	109.78	106.68
19	B2	836	CLA	C4A-NA-C1A	6.80	109.78	106.68
24	AA	802	AJP	O84-C05-O09	-6.80	93.71	109.88
19	AA	828	CLA	C4A-NA-C1A	6.79	109.78	106.68
19	B1	821	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	L	208	AJP	C11-C16-C15	-6.78	97.20	109.17
24	KK	104	AJP	C14-C15-C16	6.78	121.23	111.78
19	A2	822	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	AA	802	AJP	C11-C16-C15	-6.77	97.21	109.17
19	A2	826	CLA	C4A-NA-C1A	6.77	109.77	106.68
19	B	823	CLA	C4A-NA-C1A	6.77	109.77	106.68
19	AA	822	CLA	C4A-NA-C1A	6.77	109.77	106.68
24	K	104	AJP	C14-C15-C16	6.77	121.22	111.78
19	A2	808	CLA	C4A-NA-C1A	6.76	109.76	106.68
19	AA	821	CLA	C4A-NA-C1A	6.76	109.76	106.68
19	AA	823	CLA	C4A-NA-C1A	6.76	109.76	106.68
19	B	812	CLA	C4A-NA-C1A	6.75	109.76	106.68
19	A1	821	CLA	C4A-NA-C1A	6.74	109.75	106.68
19	K	102	CLA	C4A-NA-C1A	6.74	109.75	106.68
24	I2	104	AJP	C01-C02-C85	6.74	121.40	111.03
19	A2	827	CLA	C4A-NA-C1A	6.74	109.75	106.68
19	AA	818	CLA	C4A-NA-C1A	6.74	109.75	106.68
19	A1	823	CLA	C4A-NA-C1A	6.73	109.75	106.68
19	A	817	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	L1	204	AJP	C01-C02-C85	6.73	121.39	111.03
19	B1	806	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	BB	849	AJP	O31-C30-C29	6.73	121.82	109.70
19	A	844	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	B	803	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	A1	826	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	B	802	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	B2	817	CLA	C4A-NA-C1A	6.72	109.74	106.68
19	F	301	CLA	C4A-NA-C1A	6.72	109.74	106.68
19	A2	828	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	X1	101	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	B1	817	CLA	C4A-NA-C1A	6.70	109.74	106.68
19	B1	804	CLA	C4A-NA-C1A	6.70	109.73	106.68
19	B1	835	CLA	C4A-NA-C1A	6.69	109.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	825	CLA	C4A-NA-C1A	6.69	109.73	106.68
19	A	818	CLA	C4A-NA-C1A	6.69	109.73	106.68
19	B2	830	CLA	C4A-NA-C1A	6.69	109.73	106.68
19	A	821	CLA	C4A-NA-C1A	6.69	109.73	106.68
24	L1	203	AJP	C14-C15-C16	6.69	121.11	111.78
24	BB	849	AJP	C03-C02-C85	6.69	116.70	108.59
19	A	815	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	F1	302	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	A1	838	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	BB	832	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	A	824	CLA	C4A-NA-C1A	6.68	109.72	106.68
24	L1	204	AJP	C14-C15-C16	6.67	121.09	111.78
19	B2	804	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	A2	802	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	B	830	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	AA	830	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	A	823	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	BB	823	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	A2	841	CLA	C4A-NA-C1A	6.66	109.72	106.68
19	B	809	CLA	C4A-NA-C1A	6.65	109.72	106.68
19	L	202	CLA	C4A-NA-C1A	6.65	109.72	106.68
24	B	849	AJP	O25-C26-C27	6.65	124.46	108.09
19	AA	804	CLA	C4A-NA-C1A	6.65	109.71	106.68
24	L1	203	AJP	O25-C26-C27	6.64	124.43	108.09
19	A1	840	CLA	C4A-NA-C1A	6.64	109.71	106.68
19	AA	839	CLA	C4A-NA-C1A	6.64	109.71	106.68
24	B	849	AJP	O09-C05-C04	6.64	122.01	108.54
19	B2	824	CLA	C4A-NA-C1A	6.63	109.70	106.68
19	BB	809	CLA	C4A-NA-C1A	6.63	109.70	106.68
24	L	208	AJP	O09-C05-C04	6.63	122.00	108.54
24	AA	802	AJP	C01-C02-C85	6.62	121.22	111.03
19	B2	803	CLA	C4A-NA-C1A	6.62	109.70	106.68
19	A1	844	CLA	C4A-NA-C1A	6.62	109.70	106.68
19	A1	808	CLA	C4A-NA-C1A	6.61	109.70	106.68
19	B1	815	CLA	C4A-NA-C1A	6.61	109.70	106.68
19	L1	205	CLA	C4A-NA-C1A	6.61	109.69	106.68
19	BB	831	CLA	C4A-NA-C1A	6.61	109.69	106.68
24	A	802	AJP	C01-C02-C85	6.60	121.19	111.03
19	A2	824	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	A2	830	CLA	C4A-NA-C1A	6.60	109.69	106.68
24	B	850	AJP	O09-C05-C04	6.60	121.94	108.54
19	A1	818	CLA	C4A-NA-C1A	6.60	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	812	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	A2	809	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	AA	817	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	BB	828	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	XX	101	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	A2	819	CLA	C4A-NA-C1A	6.59	109.69	106.68
19	A1	827	CLA	C4A-NA-C1A	6.59	109.69	106.68
19	X	101	CLA	C4A-NA-C1A	6.59	109.69	106.68
19	KK	102	CLA	C4A-NA-C1A	6.59	109.69	106.68
19	B1	807	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	L2	204	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	B	807	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	AA	815	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	B2	831	CLA	C4A-NA-C1A	6.57	109.68	106.68
19	B	836	CLA	C4A-NA-C1A	6.57	109.68	106.68
19	A	838	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	B2	812	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	BB	803	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	BB	812	CLA	C4A-NA-C1A	6.56	109.67	106.68
24	BB	848	AJP	O25-C26-C27	6.56	124.23	108.09
19	A1	817	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	A2	821	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	A	839	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	BB	836	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	A2	852	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	AA	805	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	AA	838	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	K1	103	CLA	C4A-NA-C1A	6.55	109.67	106.68
24	A1	855	AJP	O09-C05-C04	6.55	121.83	108.54
19	A	805	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	BB	807	CLA	C4A-NA-C1A	6.54	109.66	106.68
19	BB	830	CLA	C4A-NA-C1A	6.54	109.66	106.68
24	L1	204	AJP	C03-C02-C85	6.54	116.52	108.59
19	B2	807	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	A2	839	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	AA	841	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	L1	204	AJP	O09-C08-C10	6.53	123.42	110.20
19	A2	818	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	A2	844	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	A	841	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	A2	816	CLA	C4A-NA-C1A	6.52	109.66	106.68
19	BB	804	CLA	C4A-NA-C1A	6.52	109.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	813	CLA	C4A-NA-C1A	6.52	109.65	106.68
19	AA	808	CLA	C4A-NA-C1A	6.52	109.65	106.68
24	BB	849	AJP	C05-C06-C07	6.51	112.96	103.37
19	A	812	CLA	C4A-NA-C1A	6.51	109.65	106.68
19	A	842	CLA	C4A-NA-C1A	6.51	109.65	106.68
19	B1	822	CLA	C4A-NA-C1A	6.50	109.65	106.68
19	F2	302	CLA	C4A-NA-C1A	6.50	109.64	106.68
19	B2	808	CLA	C4A-NA-C1A	6.50	109.64	106.68
19	B	806	CLA	C4A-NA-C1A	6.50	109.64	106.68
19	A1	824	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	AA	824	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	B	860	CLA	CAC-C3C-C4C	6.49	133.23	124.79
19	B1	825	CLA	C4A-NA-C1A	6.48	109.64	106.68
19	JJ	101	CLA	C4A-NA-C1A	6.48	109.64	106.68
24	A2	854	AJP	O84-C05-O09	-6.48	94.45	109.88
19	J	101	CLA	C4A-NA-C1A	6.48	109.64	106.68
24	L1	204	AJP	O09-C05-C04	6.48	121.69	108.54
24	L1	203	AJP	C14-C15-C20	6.47	121.19	113.91
19	A2	805	CLA	C4A-NA-C1A	6.47	109.63	106.68
19	X2	101	CLA	C4A-NA-C1A	6.46	109.63	106.68
19	B1	808	CLA	C4A-NA-C1A	6.46	109.63	106.68
24	L1	203	AJP	O84-C05-O09	-6.46	94.51	109.88
19	A	804	CLA	C4A-NA-C1A	6.46	109.62	106.68
19	B	810	CLA	C4A-NA-C1A	6.46	109.62	106.68
19	B	829	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	A2	817	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	L2	203	AJP	C14-C15-C20	6.45	121.17	113.91
24	M2	101	AJP	C03-C02-C85	6.45	116.41	108.59
19	A1	820	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	A1	832	CLA	C4A-NA-C1A	6.44	109.62	106.68
24	A2	854	AJP	C80-C20-C19	-6.44	99.67	110.44
19	B1	802	CLA	C4A-NA-C1A	6.44	109.62	106.68
24	A1	855	AJP	O84-C05-O09	-6.44	94.56	109.88
19	B1	830	CLA	C4A-NA-C1A	6.44	109.62	106.68
19	A	829	CLA	C4A-NA-C1A	6.44	109.62	106.68
19	B	804	CLA	C4A-NA-C1A	6.43	109.61	106.68
19	A	816	CLA	C4A-NA-C1A	6.43	109.61	106.68
19	AA	843	CLA	CAC-C3C-C4C	6.42	133.15	124.79
19	A1	828	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	A1	855	AJP	C80-C20-C19	-6.42	99.70	110.44
19	BB	835	CLA	C4A-NA-C1A	6.42	109.61	106.68
19	B1	809	CLA	C4A-NA-C1A	6.41	109.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FF	302	CLA	C4A-NA-C1A	6.41	109.60	106.68
19	A1	842	CLA	CAC-C3C-C4C	6.41	133.13	124.79
19	B1	831	CLA	C4A-NA-C1A	6.40	109.60	106.68
19	B2	809	CLA	C4A-NA-C1A	6.40	109.60	106.68
19	AA	829	CLA	C4A-NA-C1A	6.40	109.60	106.68
19	A2	806	CLA	C4A-NA-C1A	6.40	109.60	106.68
24	I2	104	AJP	C80-C20-C19	-6.40	99.75	110.44
19	FF	301	CLA	C4A-NA-C1A	6.39	109.60	106.68
19	BB	821	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	B2	819	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	AA	812	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	BB	806	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	LL	201	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	B1	829	CLA	C4A-NA-C1A	6.38	109.59	106.68
19	F1	301	CLA	C4A-NA-C1A	6.38	109.59	106.68
19	B	827	CLA	C4A-NA-C1A	6.38	109.59	106.68
24	L2	203	AJP	C01-C02-C85	6.38	120.84	111.03
19	A1	815	CLA	C4A-NA-C1A	6.37	109.59	106.68
24	L	209	AJP	C03-C02-C85	6.37	116.32	108.59
19	B2	802	CLA	C4A-NA-C1A	6.37	109.59	106.68
19	BB	845	CLA	C4A-NA-C1A	6.37	109.58	106.68
19	F	302	CLA	C4A-NA-C1A	6.36	109.58	106.68
19	A	833	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	AA	819	CLA	C4A-NA-C1A	6.35	109.58	106.68
24	K	104	AJP	C80-C20-C19	-6.35	99.83	110.44
19	A	831	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	A1	804	CLA	C4A-NA-C1A	6.35	109.57	106.68
24	L	208	AJP	C01-C02-C85	6.34	120.80	111.03
19	B2	806	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	B2	828	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	A	822	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	BB	824	CLA	C4A-NA-C1A	6.34	109.57	106.68
24	B	857	AJP	C80-C20-C19	-6.34	99.84	110.44
19	B2	832	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	BB	826	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	A2	804	CLA	C4A-NA-C1A	6.33	109.56	106.68
19	A2	807	CLA	C4A-NA-C1A	6.32	109.56	106.68
19	B	831	CLA	C4A-NA-C1A	6.32	109.56	106.68
19	AA	809	CLA	C4A-NA-C1A	6.32	109.56	106.68
19	A1	816	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	KK	104	AJP	C80-C20-C19	-6.31	99.88	110.44
19	A1	814	CLA	C4A-NA-C1A	6.31	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	846	CLA	C4A-NA-C1A	6.31	109.56	106.68
19	AA	831	CLA	C4A-NA-C1A	6.31	109.56	106.68
19	B2	822	CLA	C4A-NA-C1A	6.30	109.56	106.68
19	B	828	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	L	203	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	BB	827	CLA	C4A-NA-C1A	6.30	109.55	106.68
24	A1	854	AJP	C80-C20-C19	-6.30	99.91	110.44
19	B2	815	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	A	809	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	AA	827	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	M2	101	AJP	O84-C05-O09	-6.26	94.97	109.88
19	K1	105	CLA	C4A-NA-C1A	6.26	109.54	106.68
19	A2	812	CLA	C4A-NA-C1A	6.26	109.54	106.68
19	B1	834	CLA	C4A-NA-C1A	6.26	109.53	106.68
19	F2	301	CLA	C4A-NA-C1A	6.26	109.53	106.68
19	B1	813	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	L1	204	AJP	O31-C30-C29	6.25	120.97	109.70
24	L	209	AJP	C01-C02-C85	6.25	120.65	111.03
19	B	816	CLA	C4A-NA-C1A	6.25	109.53	106.68
19	AA	826	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	KK	104	AJP	O09-C08-C07	6.25	118.46	104.08
24	A	802	AJP	C20-C15-C16	6.25	118.78	112.43
19	K1	102	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	BB	825	CLA	C4A-NA-C1A	6.24	109.53	106.68
24	AA	802	AJP	C20-C15-C16	6.24	118.77	112.43
24	B	850	AJP	O84-C05-O09	-6.24	95.03	109.88
19	A	826	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	AA	840	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	B	813	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	B	824	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	B	825	CLA	C4A-NA-C1A	6.23	109.52	106.68
19	B	819	CLA	C4A-NA-C1A	6.23	109.52	106.68
19	A2	835	CLA	C4A-NA-C1A	6.23	109.52	106.68
19	B2	852	CLA	CAC-C3C-C4C	6.22	132.89	124.79
24	B	849	AJP	O31-C30-C29	6.22	120.91	109.70
19	B	837	CLA	C4A-NA-C1A	6.22	109.52	106.68
19	A1	806	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	I2	104	AJP	C03-C02-C85	6.22	116.13	108.59
24	L	208	AJP	C03-C02-C85	6.22	116.13	108.59
19	J1	103	CLA	C4A-NA-C1A	6.21	109.51	106.68
19	A2	814	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	B	850	AJP	O31-C30-C29	6.21	120.90	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	M2	101	AJP	C01-C02-C85	6.21	120.59	111.03
19	B	832	CLA	C4A-NA-C1A	6.21	109.51	106.68
19	A2	811	CLA	C4A-NA-C1A	6.21	109.51	106.68
19	A	840	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	L	208	AJP	O84-C05-O09	-6.20	95.11	109.88
19	FF	305	CLA	C4A-NA-C1A	6.20	109.51	106.68
24	L2	202	AJP	O09-C08-C07	6.20	118.35	104.08
19	A	806	CLA	C4A-NA-C1A	6.20	109.51	106.68
19	B2	814	CLA	C4A-NA-C1A	6.19	109.50	106.68
24	A	802	AJP	C03-C02-C85	6.19	116.10	108.59
19	A1	833	CLA	C4A-NA-C1A	6.19	109.50	106.68
24	AA	802	AJP	C03-C02-C85	6.19	116.10	108.59
19	BB	808	CLA	C4A-NA-C1A	6.18	109.50	106.68
19	B2	813	CLA	C4A-NA-C1A	6.18	109.50	106.68
19	A	827	CLA	C4A-NA-C1A	6.18	109.50	106.68
19	F1	305	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	BB	848	AJP	O31-C30-C29	6.17	120.83	109.70
19	A1	813	CLA	C4A-NA-C1A	6.17	109.50	106.68
19	B2	810	CLA	C4A-NA-C1A	6.17	109.49	106.68
19	B2	846	CLA	C4A-NA-C1A	6.17	109.49	106.68
19	B2	835	CLA	C4A-NA-C1A	6.17	109.49	106.68
19	B1	845	CLA	C4A-NA-C1A	6.16	109.49	106.68
19	AA	833	CLA	C4A-NA-C1A	6.15	109.49	106.68
24	BB	849	AJP	O84-C05-O09	-6.15	95.24	109.88
19	J1	101	CLA	C4A-NA-C1A	6.14	109.48	106.68
19	J2	103	CLA	C4A-NA-C1A	6.14	109.48	106.68
19	B	814	CLA	C4A-NA-C1A	6.14	109.48	106.68
19	LL	203	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	B1	819	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	B	835	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	AA	814	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	BB	810	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	BB	834	CLA	C4A-NA-C1A	6.12	109.47	106.68
24	B	849	AJP	O09-C08-C07	6.11	118.16	104.08
24	BB	849	AJP	C01-C02-C85	6.11	120.44	111.03
19	A2	834	CLA	C4A-NA-C1A	6.11	109.47	106.68
19	BB	814	CLA	C4A-NA-C1A	6.11	109.47	106.68
19	A1	810	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	A1	836	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	B	808	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	AA	837	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	A1	830	CLA	C4A-NA-C1A	6.10	109.46	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	834	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	JJ	103	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	J	103	CLA	C4A-NA-C1A	6.10	109.46	106.68
19	B1	828	CLA	C4A-NA-C1A	6.09	109.46	106.68
19	A	837	CLA	C4A-NA-C1A	6.09	109.46	106.68
24	B	857	AJP	C24-C23-C22	6.09	117.44	111.07
24	K	104	AJP	O09-C08-C07	6.09	118.10	104.08
19	AA	806	CLA	C4A-NA-C1A	6.09	109.46	106.68
24	BB	849	AJP	O09-C08-C07	6.09	118.09	104.08
19	A1	839	CLA	C4A-NA-C1A	6.09	109.46	106.68
24	A1	855	AJP	O09-C08-C10	6.09	122.52	110.20
19	B1	827	CLA	C4A-NA-C1A	6.08	109.45	106.68
19	AA	816	CLA	C4A-NA-C1A	6.08	109.45	106.68
19	A	814	CLA	C4A-NA-C1A	6.08	109.45	106.68
19	A1	834	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	B	849	AJP	C14-C15-C20	6.07	120.74	113.91
24	L1	203	AJP	C21-C22-C23	6.06	118.57	110.46
19	A2	820	CLA	C4A-NA-C1A	6.05	109.44	106.68
19	BB	819	CLA	C4A-NA-C1A	6.05	109.44	106.68
24	BB	849	AJP	O82-C10-C08	6.05	128.11	111.19
19	J2	101	CLA	C4A-NA-C1A	6.05	109.44	106.68
19	AA	807	CLA	C4A-NA-C1A	6.04	109.44	106.68
19	BB	802	CLA	C4A-NA-C1A	6.04	109.44	106.68
19	K2	102	CLA	C4A-NA-C1A	6.03	109.43	106.68
24	KK	104	AJP	O82-C10-C08	6.03	128.06	111.19
19	B1	810	CLA	C4A-NA-C1A	6.02	109.43	106.68
19	AA	834	CLA	C4A-NA-C1A	6.02	109.42	106.68
19	A2	837	CLA	C4A-NA-C1A	6.01	109.42	106.68
19	A	807	CLA	C4A-NA-C1A	5.99	109.41	106.68
19	B1	818	CLA	C4A-NA-C1A	5.99	109.41	106.68
24	A	802	AJP	O09-C08-C07	5.99	117.86	104.08
24	AA	802	AJP	O09-C08-C07	5.98	117.86	104.08
19	BB	816	CLA	C4A-NA-C1A	5.98	109.41	106.68
24	L	209	AJP	O84-C05-O09	-5.98	95.65	109.88
24	L	209	AJP	C80-C20-C19	-5.98	100.44	110.44
24	L	209	AJP	O82-C10-C08	5.98	127.92	111.19
19	L2	206	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	A2	840	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	B2	816	CLA	C4A-NA-C1A	5.98	109.41	106.68
24	M2	101	AJP	C80-C20-C19	-5.97	100.45	110.44
24	AA	856	AJP	O84-C05-O09	-5.97	95.68	109.88
24	BB	848	AJP	C05-C06-C07	5.97	112.16	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	M2	101	AJP	O09-C08-C07	5.96	117.81	104.08
19	BB	855	CLA	C4A-NA-C1A	5.96	109.40	106.68
24	A	855	AJP	O84-C05-O09	-5.96	95.71	109.88
19	A2	815	CLA	C4A-NA-C1A	5.95	109.39	106.68
19	K	101	CLA	C4A-NA-C1A	5.95	109.39	106.68
19	BB	836	CLA	CAC-C3C-C4C	5.95	132.53	124.79
24	B	850	AJP	O09-C08-C07	5.95	117.77	104.08
24	B	850	AJP	C80-C20-C19	-5.95	100.50	110.44
24	I2	104	AJP	O09-C08-C07	5.94	117.76	104.08
19	B1	814	CLA	C4A-NA-C1A	5.94	109.39	106.68
19	B2	818	CLA	C4A-NA-C1A	5.93	109.39	106.68
19	KK	101	CLA	C4A-NA-C1A	5.92	109.38	106.68
20	AA	803	CL0	O1D-CGD-CBD	-5.92	115.74	124.72
24	A	802	AJP	O82-C10-C08	5.92	127.76	111.19
19	BB	815	CLA	C4A-NA-C1A	5.92	109.38	106.68
19	B2	850	CLA	C4A-NA-C1A	5.92	109.38	106.68
19	A	835	CLA	C4A-NA-C1A	5.92	109.38	106.68
19	A2	831	CLA	C4A-NA-C1A	5.91	109.38	106.68
19	B	818	CLA	C4A-NA-C1A	5.91	109.38	106.68
24	L	208	AJP	C20-C15-C16	5.91	118.43	112.43
24	AA	802	AJP	O82-C10-C08	5.91	127.72	111.19
24	K	104	AJP	O25-C26-C27	5.90	122.61	108.09
24	BB	849	AJP	C83-C06-C05	5.90	124.45	114.94
24	L	209	AJP	O09-C08-C07	5.90	117.67	104.08
19	B	811	CLA	C4A-NA-C1A	5.90	109.37	106.68
19	B1	849	CLA	C4A-NA-C1A	5.89	109.37	106.68
24	B	849	AJP	O82-C10-C08	5.89	127.66	111.19
24	L2	203	AJP	O31-C30-C29	5.88	120.30	109.70
19	B	815	CLA	C4A-NA-C1A	5.87	109.36	106.68
24	L	209	AJP	C18-C17-C16	5.87	121.52	112.16
24	A2	854	AJP	O09-C08-C10	5.86	122.06	110.20
24	L2	203	AJP	C80-C20-C19	-5.86	100.65	110.44
24	L1	204	AJP	C80-C20-C19	-5.85	100.66	110.44
19	A	852	CLA	C4A-NA-C1A	5.85	109.35	106.68
19	A2	829	CLA	C4A-NA-C1A	5.85	109.35	106.68
19	A2	833	CLA	C4A-NA-C1A	5.85	109.35	106.68
19	A1	809	CLA	C4A-NA-C1A	5.85	109.35	106.68
19	BB	811	CLA	C4A-NA-C1A	5.85	109.35	106.68
24	L2	202	AJP	C14-C15-C20	5.84	120.49	113.91
24	BB	849	AJP	C14-C15-C20	5.83	120.48	113.91
19	B2	829	CLA	C4A-NA-C1A	5.82	109.33	106.68
19	A1	811	CLA	C4A-NA-C1A	5.81	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	860	CLA	C4A-NA-C1A	5.80	109.33	106.68
24	K	104	AJP	O82-C10-C08	5.80	127.43	111.19
19	A1	852	CLA	C4A-NA-C1A	5.80	109.32	106.68
19	L1	207	CLA	C4A-NA-C1A	5.79	109.32	106.68
24	L	208	AJP	C18-C17-C16	5.79	121.39	112.16
19	BB	829	CLA	C4A-NA-C1A	5.79	109.32	106.68
19	B2	827	CLA	C4A-NA-C1A	5.76	109.31	106.68
19	B2	811	CLA	C4A-NA-C1A	5.76	109.31	106.68
24	L1	204	AJP	C83-C06-C05	5.76	124.22	114.94
24	KK	104	AJP	O84-C05-O09	-5.76	96.18	109.88
24	B	850	AJP	O82-C10-C08	5.75	127.28	111.19
24	B	857	AJP	O09-C08-C10	5.74	121.82	110.20
24	M2	101	AJP	O82-C10-C08	5.74	127.25	111.19
19	B1	816	CLA	C4A-NA-C1A	5.73	109.29	106.68
24	L2	202	AJP	O82-C10-C08	5.71	127.18	111.19
19	AA	820	CLA	C4A-NA-C1A	5.71	109.28	106.68
24	BB	849	AJP	C80-C20-C19	-5.71	100.90	110.44
19	AA	843	CLA	C4A-NA-C1A	5.71	109.28	106.68
19	A	811	CLA	C4A-NA-C1A	5.70	109.28	106.68
24	I2	104	AJP	O82-C10-C08	5.69	127.11	111.19
19	BB	818	CLA	C4A-NA-C1A	5.69	109.27	106.68
19	B2	852	CLA	C4A-NA-C1A	5.68	109.27	106.68
24	L1	203	AJP	C24-C23-C22	5.67	117.00	111.07
24	L	209	AJP	C83-C06-C05	5.67	124.06	114.94
19	AA	811	CLA	C4A-NA-C1A	5.66	109.26	106.68
19	LL	201	CLA	C4-C3-C5	5.65	125.04	115.23
24	BB	848	AJP	C80-C20-C19	-5.63	101.02	110.44
24	L2	203	AJP	O82-C10-C08	5.63	126.95	111.19
24	KK	104	AJP	O31-C26-C27	5.63	118.58	109.99
19	AA	810	CLA	C4A-NA-C1A	5.63	109.25	106.68
24	L	209	AJP	C14-C15-C20	5.62	120.25	113.91
19	B1	820	CLA	C4A-NA-C1A	5.62	109.24	106.68
24	A1	854	AJP	C24-C23-C22	5.62	116.94	111.07
24	L	208	AJP	O09-C08-C07	5.60	116.98	104.08
24	BB	848	AJP	O09-C08-C07	5.59	116.95	104.08
19	B	820	CLA	C4A-NA-C1A	5.59	109.23	106.68
24	KK	104	AJP	O25-C26-C27	5.59	121.85	108.09
24	M2	101	AJP	C83-C06-C05	5.58	123.93	114.94
24	L2	202	AJP	O25-C26-C27	5.57	121.79	108.09
19	A1	805	CLA	C4A-NA-C1A	5.56	109.22	106.68
24	A1	854	AJP	O09-C08-C10	5.56	121.46	110.20
24	L2	203	AJP	C83-C06-C05	5.55	123.88	114.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L1	204	AJP	O31-C26-C27	5.55	121.77	110.37
19	AA	853	CLA	C4A-NA-C1A	5.53	109.20	106.68
19	AA	835	CLA	C4A-NA-C1A	5.51	109.19	106.68
24	A	855	AJP	O09-C08-C10	5.51	121.36	110.20
19	B	834	CLA	C4A-NA-C1A	5.50	109.19	106.68
24	AA	856	AJP	O09-C08-C10	5.49	121.32	110.20
19	A	810	CLA	C4A-NA-C1A	5.49	109.18	106.68
19	A	820	CLA	C4A-NA-C1A	5.49	109.18	106.68
24	I2	104	AJP	C14-C15-C16	5.48	119.42	111.78
19	A1	842	CLA	C4A-NA-C1A	5.48	109.18	106.68
19	B1	811	CLA	C4A-NA-C1A	5.47	109.17	106.68
24	B	849	AJP	C80-C20-C19	-5.46	101.32	110.44
24	L	208	AJP	C80-C20-C19	-5.45	101.32	110.44
26	B	841	ECH	C19-C18-C17	5.45	127.58	119.01
24	L1	204	AJP	O82-C10-C08	5.45	126.43	111.19
24	L1	203	AJP	O09-C05-C04	5.44	119.59	108.54
24	L2	202	AJP	C80-C20-C19	-5.44	101.35	110.44
19	B	858	CLA	C4A-NA-C1A	5.44	109.16	106.68
24	AA	802	AJP	C80-C20-C19	-5.41	101.39	110.44
24	K	104	AJP	O31-C26-C27	5.41	118.25	109.99
24	A1	854	AJP	C14-C15-C20	5.41	120.00	113.91
24	A	802	AJP	C80-C20-C19	-5.39	101.42	110.44
24	L2	202	AJP	C21-C22-C23	5.38	117.66	110.46
24	K	104	AJP	O84-C05-O09	-5.38	97.08	109.88
24	L2	202	AJP	C24-C23-C22	5.36	116.68	111.07
24	I2	104	AJP	C83-C06-C05	5.36	123.57	114.94
24	L1	204	AJP	O84-C05-O09	-5.35	97.14	109.88
24	L1	203	AJP	O09-C08-C10	5.34	121.01	110.20
19	BB	820	CLA	C4A-NA-C1A	5.33	109.11	106.68
24	L	208	AJP	O82-C10-C08	5.33	126.10	111.19
24	L1	203	AJP	C80-C20-C19	-5.31	101.55	110.44
19	A1	819	CLA	C4A-NA-C1A	5.31	109.10	106.68
24	A1	855	AJP	C11-C12-C07	-5.31	92.16	100.16
24	AA	856	AJP	C21-C22-C23	5.30	117.56	110.46
24	L1	203	AJP	O78-C27-C26	5.30	122.70	110.08
24	A2	854	AJP	C11-C12-C07	-5.30	92.17	100.16
24	A	855	AJP	C14-C15-C20	5.29	119.87	113.91
19	BB	833	CLA	C4A-NA-C1A	5.28	109.09	106.68
24	BB	848	AJP	O31-C30-C32	5.28	119.52	106.44
24	A	855	AJP	C21-C22-C23	5.27	117.51	110.46
19	B1	833	CLA	C4A-NA-C1A	5.26	109.08	106.68
24	AA	856	AJP	C17-C16-C15	-5.26	104.21	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AA	856	AJP	C14-C15-C20	5.26	119.83	113.91
24	BB	848	AJP	C03-C02-C85	5.26	114.97	108.59
19	A2	810	CLA	C4A-NA-C1A	5.25	109.08	106.68
19	B1	824	CLA	C4A-NA-C1A	5.25	109.07	106.68
24	B	849	AJP	C01-C02-C85	5.24	119.10	111.03
24	B	857	AJP	C17-C16-C15	-5.24	104.24	110.52
24	A	855	AJP	C17-C16-C15	-5.24	104.24	110.52
24	L2	203	AJP	O31-C30-C32	5.24	119.42	106.44
24	I2	104	AJP	O84-C05-O09	-5.23	97.43	109.88
24	M2	101	AJP	C14-C15-C20	5.22	119.79	113.91
19	L	202	CLA	C4-C3-C5	5.21	124.27	115.23
24	BB	848	AJP	O78-C27-C26	5.21	122.48	110.08
24	B	849	AJP	O78-C27-C26	5.20	122.48	110.08
26	B2	841	ECH	C19-C18-C17	5.20	127.20	119.01
24	L	209	AJP	C20-C15-C16	5.20	117.72	112.43
19	B2	820	CLA	CAC-C3C-C4C	5.20	131.55	124.79
24	A1	854	AJP	C17-C16-C15	-5.19	104.30	110.52
19	BB	820	CLA	CAC-C3C-C4C	5.18	131.53	124.79
24	AA	802	AJP	C83-C06-C05	5.17	123.27	114.94
24	B	857	AJP	C14-C15-C20	5.17	119.73	113.91
24	L1	204	AJP	O31-C30-C32	5.16	119.23	106.44
19	B	820	CLA	CAC-C3C-C4C	5.16	131.50	124.79
24	M2	101	AJP	C18-C17-C16	5.16	120.39	112.16
24	A	802	AJP	C83-C06-C05	5.14	123.22	114.94
24	L2	202	AJP	C20-C15-C16	5.14	117.65	112.43
24	L1	203	AJP	C20-C15-C16	5.14	117.65	112.43
24	K	104	AJP	C01-C02-C85	5.14	118.94	111.03
26	B1	840	ECH	C19-C18-C17	5.13	127.09	119.01
26	BB	840	ECH	C19-C18-C17	5.13	127.09	119.01
26	B1	840	ECH	C24-C23-C22	-5.12	118.66	126.23
24	KK	104	AJP	O77-C28-C29	5.12	120.50	110.05
24	BB	848	AJP	O82-C10-C08	5.12	125.51	111.19
20	A1	802	CL0	O1D-CGD-CBD	-5.12	116.97	124.72
24	K	104	AJP	O77-C28-C29	5.10	120.46	110.05
26	B	841	ECH	C24-C23-C22	-5.08	118.71	126.23
24	A	802	AJP	C21-C20-C19	5.08	115.04	107.75
24	AA	802	AJP	C15-C20-C19	5.07	115.56	108.51
24	M2	101	AJP	C20-C15-C16	5.07	117.58	112.43
24	A	802	AJP	C15-C20-C19	5.06	115.54	108.51
24	L2	203	AJP	O31-C26-C27	5.06	120.76	110.37
24	B	850	AJP	O31-C30-C32	5.04	118.94	106.44
24	AA	802	AJP	C21-C20-C19	5.04	114.99	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	104	AJP	O78-C27-C26	4.98	121.95	110.08
24	KK	104	AJP	C01-C02-C85	4.98	118.69	111.03
24	BB	848	AJP	C83-C06-C05	4.96	122.93	114.94
24	AA	856	AJP	C11-C12-C07	-4.95	92.70	100.16
24	A	855	AJP	C11-C12-C07	-4.94	92.71	100.16
24	BB	848	AJP	C29-C28-C27	4.94	119.50	110.83
26	BB	840	ECH	C24-C23-C22	-4.93	118.95	126.23
24	BB	849	AJP	O31-C30-C32	4.91	118.61	106.44
24	A1	854	AJP	C11-C12-C07	-4.91	92.76	100.16
24	B	850	AJP	O31-C26-C27	4.91	120.45	110.37
24	B	850	AJP	C83-C06-C05	4.90	122.83	114.94
20	A	803	CL0	O1D-CGD-CBD	-4.89	117.31	124.72
26	B	841	ECH	C36-C18-C19	-4.88	110.63	118.09
24	KK	104	AJP	O78-C27-C26	4.88	121.70	110.08
28	BB	854	DGD	O3G-C3G-C2G	-4.86	99.00	110.82
20	A2	803	CL0	C4D-CHA-CBD	-4.86	104.07	108.97
24	B	850	AJP	C01-C02-C85	4.86	118.51	111.03
24	B	849	AJP	O31-C30-C32	4.85	118.47	106.44
24	KK	104	AJP	C83-C06-C05	4.85	122.75	114.94
24	B	849	AJP	C29-C28-C27	4.84	119.32	110.83
24	BB	849	AJP	C20-C15-C16	4.84	117.34	112.43
19	B2	834	CLA	C4A-NA-C1A	4.83	108.88	106.68
26	B2	841	ECH	C24-C23-C22	-4.82	119.11	126.23
19	B2	820	CLA	C4A-NA-C1A	4.80	108.87	106.68
24	B	850	AJP	C24-C23-C22	4.79	116.08	111.07
24	B	857	AJP	C21-C22-C23	4.79	116.86	110.46
24	B	849	AJP	C83-C06-C05	4.78	122.64	114.94
24	B	857	AJP	C11-C12-C07	-4.78	92.96	100.16
24	I2	104	AJP	C17-C16-C15	-4.77	104.80	110.52
24	L	208	AJP	C14-C15-C16	4.76	118.42	111.78
24	K	104	AJP	C83-C06-C05	4.74	122.58	114.94
24	A1	854	AJP	C21-C22-C23	4.74	116.80	110.46
24	L2	203	AJP	O09-C05-C06	-4.72	98.28	104.56
24	L2	202	AJP	O31-C26-C27	4.72	120.06	110.37
24	L1	203	AJP	O31-C30-C32	4.70	118.09	106.44
28	B	856	DGD	O3G-C3G-C2G	-4.70	99.39	110.82
24	B	849	AJP	C20-C15-C16	4.69	117.19	112.43
24	KK	104	AJP	O25-C26-O31	4.68	118.60	108.92
20	A	803	CL0	CHA-C1A-C2A	-4.67	122.34	133.31
24	L1	204	AJP	C83-C06-C07	4.65	123.79	114.50
24	L	209	AJP	C11-C16-C15	-4.64	100.98	109.17
24	L2	202	AJP	C01-C02-C85	4.63	118.16	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L1	204	AJP	O09-C05-C06	-4.61	98.43	104.56
24	L	208	AJP	C18-C19-C20	4.61	120.04	112.31
19	A2	810	CLA	CAA-C2A-C1A	-4.60	96.91	111.97
24	L2	202	AJP	O78-C27-C26	4.59	121.02	110.08
26	BB	840	ECH	C36-C18-C19	-4.57	111.11	118.09
19	AA	810	CLA	CAA-C2A-C1A	-4.56	97.02	111.97
24	L2	203	AJP	C83-C06-C07	4.56	123.61	114.50
24	L2	203	AJP	C20-C15-C16	4.56	117.06	112.43
24	BB	849	AJP	O31-C26-C27	4.56	119.74	110.37
26	B2	841	ECH	C36-C18-C19	-4.55	111.14	118.09
20	AA	803	CL0	CMA-C3A-C4A	-4.55	104.81	114.61
24	BB	849	AJP	O25-C26-C27	4.53	119.23	108.09
24	KK	104	AJP	C20-C15-C16	4.52	117.03	112.43
20	A2	803	CL0	CMC-C2C-C1C	4.51	132.85	124.73
20	A2	803	CL0	O2D-CGD-O1D	-4.51	115.07	123.85
26	B1	840	ECH	C36-C18-C19	-4.50	111.21	118.09
24	AA	856	AJP	C24-C23-C22	4.50	115.78	111.07
20	AA	803	CL0	C4D-CHA-CBD	-4.49	104.44	108.97
24	L	208	AJP	C83-C06-C05	4.49	122.17	114.94
24	L1	203	AJP	C11-C12-C07	-4.48	93.41	100.16
24	K	104	AJP	C20-C15-C16	4.48	116.98	112.43
24	I2	104	AJP	C13-C14-C15	4.48	120.74	113.14
24	A	855	AJP	C24-C23-C22	4.47	115.75	111.07
24	BB	848	AJP	O82-C10-C11	4.46	129.07	113.68
24	K	104	AJP	O25-C26-O31	4.45	118.14	108.92
24	L2	202	AJP	C26-O31-C30	4.45	122.41	113.72
24	B	850	AJP	O25-C26-C27	4.43	119.00	108.09
24	BB	849	AJP	C24-C23-C22	4.40	115.68	111.07
24	BB	849	AJP	C29-C28-C27	4.40	118.55	110.83
20	A	803	CL0	O2A-CGA-CBA	4.39	125.21	111.83
24	L2	203	AJP	O25-C26-C27	4.39	118.88	108.09
24	L	208	AJP	O82-C10-C11	4.38	128.80	113.68
24	L2	203	AJP	O78-C27-C28	4.38	120.70	110.38
24	L2	203	AJP	C05-C06-C07	4.38	109.82	103.37
19	B2	834	CLA	C3B-C4B-NB	-4.38	106.62	110.53
24	B	850	AJP	C29-C28-C27	4.37	118.51	110.83
24	L1	204	AJP	O78-C27-C28	4.34	120.62	110.38
24	L	209	AJP	C18-C19-C20	4.33	119.58	112.31
20	AA	803	CL0	O2D-CGD-O1D	-4.32	115.43	123.85
24	BB	849	AJP	O82-C10-C11	4.32	128.58	113.68
26	BB	840	ECH	C16-C15-C14	-4.32	114.69	123.52
24	L2	203	AJP	C29-C28-C27	4.30	118.38	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I2	104	AJP	C20-C15-C16	4.30	116.80	112.43
24	B	850	AJP	C20-C15-C16	4.30	116.80	112.43
24	L2	202	AJP	C83-C06-C05	4.29	121.86	114.94
24	AA	802	AJP	O82-C10-C11	4.29	128.49	113.68
24	A	802	AJP	O82-C10-C11	4.29	128.48	113.68
24	L1	203	AJP	C04-C05-C06	4.29	123.43	115.66
24	BB	849	AJP	O78-C27-C26	4.29	120.29	110.08
24	K	104	AJP	O77-C28-C27	4.26	120.42	110.38
21	A1	843	PQN	C14-C13-C15	4.26	122.62	115.23
24	L1	204	AJP	C13-C14-C15	4.25	120.37	113.14
24	BB	848	AJP	C83-C06-C07	4.25	122.99	114.50
24	KK	104	AJP	O77-C28-C27	4.25	120.39	110.38
24	M2	101	AJP	C11-C16-C15	-4.24	101.69	109.17
24	KK	104	AJP	O78-C27-C28	4.23	120.36	110.38
19	A	810	CLA	CAA-C2A-C1A	-4.23	98.13	111.97
19	B2	807	CLA	O2D-CGD-CBD	4.22	118.61	111.23
24	B	849	AJP	C11-C16-C15	-4.22	101.72	109.17
24	BB	848	AJP	O77-C28-C29	4.22	120.32	110.38
24	AA	802	AJP	C21-C22-C23	4.22	117.92	111.35
24	B	850	AJP	O78-C27-C26	4.21	120.10	110.08
20	A1	802	CL0	CMA-C3A-C4A	-4.21	105.55	114.61
24	L1	203	AJP	C29-C28-C27	4.21	118.22	110.83
24	L1	204	AJP	C20-C15-C16	4.20	116.70	112.43
20	AA	803	CL0	CHA-C1A-C2A	-4.20	123.44	133.31
24	L1	204	AJP	O77-C28-C27	4.19	120.26	110.38
21	A2	843	PQN	C14-C13-C15	4.19	122.50	115.23
24	L2	202	AJP	O31-C30-C32	4.18	116.80	106.44
24	A	802	AJP	C21-C22-C23	4.17	117.85	111.35
24	L2	203	AJP	O78-C27-C26	4.17	120.01	110.08
23	F1	306	BCR	C15-C16-C17	-4.17	114.99	123.52
24	L2	202	AJP	O77-C28-C29	4.17	120.20	110.38
24	B	850	AJP	O78-C27-C28	4.17	120.20	110.38
24	L1	203	AJP	O77-C28-C29	4.17	120.19	110.38
23	F2	305	BCR	C15-C16-C17	-4.16	115.00	123.52
24	L2	202	AJP	O77-C28-C27	4.15	120.16	110.38
20	A1	802	CL0	CHA-C1A-C2A	-4.14	123.60	133.31
24	K	104	AJP	O78-C27-C28	4.14	120.12	110.38
24	L1	204	AJP	C05-C06-C07	4.13	109.46	103.37
24	L1	203	AJP	O77-C28-C27	4.13	120.11	110.38
19	A	852	CLA	C7-C6-C5	4.13	124.27	113.26
21	A	843	PQN	C14-C13-C15	4.12	122.38	115.23
24	L1	204	AJP	O77-C28-C29	4.11	120.07	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L2	202	AJP	O82-C10-C11	4.10	127.83	113.68
24	L2	202	AJP	C29-C28-C27	4.10	118.03	110.83
24	L2	203	AJP	C13-C14-C15	4.10	120.11	113.14
24	B	850	AJP	O77-C28-C27	4.10	120.03	110.38
20	A2	803	CL0	C3D-C4D-CHA	4.09	114.75	108.54
24	BB	849	AJP	O77-C28-C27	4.07	119.98	110.38
24	M2	101	AJP	O82-C10-C11	4.07	127.72	113.68
24	B	850	AJP	C13-C14-C15	4.07	120.05	113.14
24	L1	204	AJP	O78-C27-C26	4.06	119.75	110.08
24	L2	203	AJP	O77-C28-C27	4.06	119.95	110.38
19	B1	807	CLA	O2D-CGD-CBD	4.06	118.32	111.23
24	L1	204	AJP	C29-C28-C27	4.06	117.95	110.83
24	BB	849	AJP	O78-C27-C28	4.05	119.93	110.38
19	BB	807	CLA	O2D-CGD-CBD	4.05	118.32	111.23
19	B	860	CLA	CAC-C3C-C2C	-4.05	120.11	127.56
24	L2	203	AJP	O77-C28-C29	4.05	119.92	110.38
24	L1	203	AJP	C26-O31-C30	4.05	121.62	113.72
24	A	855	AJP	C15-C20-C19	4.05	114.14	108.51
24	AA	856	AJP	C15-C20-C19	4.04	114.13	108.51
24	B	850	AJP	O82-C10-C11	4.02	127.55	113.68
23	J	104	BCR	C2-C1-C6	4.02	116.28	110.44
24	KK	104	AJP	O82-C10-C11	4.02	127.53	113.68
24	K	104	AJP	C13-C14-C15	4.01	119.96	113.14
24	B	849	AJP	O31-C26-C27	4.01	118.61	110.37
24	K	104	AJP	O82-C10-C11	4.01	127.50	113.68
24	BB	849	AJP	O77-C28-C29	4.01	119.82	110.38
19	AA	843	CLA	CAC-C3C-C2C	-4.00	120.21	127.56
24	L1	203	AJP	O31-C26-C27	4.00	118.58	110.37
24	L	209	AJP	O82-C10-C11	3.98	127.41	113.68
19	A1	842	CLA	CAC-C3C-C2C	-3.98	120.25	127.56
24	B	850	AJP	O77-C28-C29	3.98	119.75	110.38
24	L1	204	AJP	C26-C27-C28	3.98	118.38	110.01
24	B	850	AJP	C26-C27-C28	3.97	118.37	110.01
24	BB	849	AJP	C26-C27-C28	3.97	118.37	110.01
19	A2	852	CLA	C7-C6-C5	3.97	123.85	113.26
24	B	849	AJP	C26-C27-C28	3.97	118.35	110.01
24	I2	104	AJP	O82-C10-C11	3.97	127.36	113.68
24	BB	848	AJP	O31-C26-C27	3.96	118.52	110.37
19	B2	852	CLA	CAC-C3C-C2C	-3.96	120.28	127.56
24	L2	202	AJP	O78-C27-C28	3.96	119.71	110.38
24	BB	848	AJP	C18-C19-C20	3.94	118.93	112.31
24	M2	101	AJP	C18-C19-C20	3.94	118.93	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BB	849	AJP	C13-C14-C15	3.92	119.80	113.14
19	B	807	CLA	O2D-CGD-CBD	3.92	118.08	111.23
24	L2	203	AJP	O84-C05-O09	-3.92	100.56	109.88
19	B2	807	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
20	A1	802	CL0	C4D-CHA-CBD	-3.91	105.03	108.97
26	B	841	ECH	C33-C5-C6	-3.90	120.22	124.48
20	AA	803	CL0	C3D-C4D-CHA	3.90	114.47	108.54
24	B	849	AJP	O82-C10-C11	3.89	127.11	113.68
24	B	849	AJP	O77-C28-C29	3.89	119.55	110.38
24	L	208	AJP	C01-C02-C03	3.89	120.58	112.08
24	B	849	AJP	O77-C28-C27	3.88	119.53	110.38
24	BB	848	AJP	C26-C27-C28	3.88	118.17	110.01
19	A2	823	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
24	L2	202	AJP	C11-C16-C15	-3.87	102.34	109.17
19	B1	807	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
19	B2	833	CLA	CGD-CBD-CAD	-3.83	98.44	110.85
24	L1	204	AJP	O25-C26-C27	3.83	117.51	108.09
19	BB	807	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
24	L2	203	AJP	C26-C27-C28	3.81	118.03	110.01
24	L	208	AJP	C83-C06-C07	3.81	122.11	114.50
24	AA	802	AJP	C14-C15-C16	3.80	117.08	111.78
24	K	104	AJP	C29-C28-C27	3.80	117.54	110.86
20	A1	802	CL0	C3D-C4D-CHA	3.79	114.30	108.54
24	L	209	AJP	C01-C02-C03	3.79	120.36	112.08
19	AA	820	CLA	C3B-C4B-NB	-3.78	107.15	110.53
24	A1	855	AJP	C15-C20-C19	3.78	113.76	108.51
24	KK	104	AJP	C29-C28-C27	3.78	117.50	110.86
24	L1	203	AJP	C11-C16-C15	-3.78	102.50	109.17
23	BB	847	BCR	C15-C16-C17	-3.77	115.80	123.52
26	B1	840	ECH	C16-C15-C14	-3.77	115.80	123.52
24	L2	202	AJP	C26-C27-C28	3.77	117.95	110.01
19	B	807	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
24	M2	101	AJP	C01-C02-C03	3.77	120.32	112.08
24	A	802	AJP	C14-C15-C16	3.77	117.03	111.78
19	B1	825	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
24	BB	849	AJP	C01-C02-C03	3.76	120.30	112.08
24	I2	104	AJP	C20-C21-C22	-3.74	110.32	113.94
23	BB	841	BCR	C15-C14-C13	-3.74	122.03	127.28
24	B	850	AJP	C06-C07-C08	-3.74	98.27	104.28
26	BB	840	ECH	C33-C5-C6	-3.74	120.41	124.48
26	B1	840	ECH	C33-C5-C6	-3.74	120.41	124.48
20	A2	803	CL0	CHA-C1A-C2A	-3.74	124.53	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B2	841	ECH	C33-C5-C6	-3.74	120.41	124.48
24	I2	104	AJP	C06-C07-C08	-3.73	98.28	104.28
19	B2	827	CLA	C3B-C4B-NB	-3.73	107.20	110.53
23	B	842	BCR	C15-C14-C13	-3.73	122.04	127.28
23	B	848	BCR	C15-C16-C17	-3.72	115.91	123.52
19	B1	833	CLA	O2D-CGD-CBD	3.72	117.73	111.23
19	B	825	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
24	A2	854	AJP	C15-C20-C19	3.70	113.66	108.51
19	B	801	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
19	A2	811	CLA	C3B-C4B-NB	-3.70	107.23	110.53
23	F1	306	BCR	C15-C14-C13	-3.69	122.10	127.28
23	B2	842	BCR	C1-C6-C5	-3.69	117.59	122.64
23	F2	305	BCR	C15-C14-C13	-3.69	122.10	127.28
23	F	305	BCR	C15-C16-C17	-3.69	115.96	123.52
19	B2	834	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
19	BB	825	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
24	L1	204	AJP	C06-C07-C08	-3.68	98.36	104.28
24	L1	203	AJP	C26-C27-C28	3.68	117.75	110.01
26	B1	840	ECH	C7-C8-C9	-3.66	120.82	126.23
26	B2	841	ECH	C16-C15-C14	-3.66	116.03	123.52
19	BB	822	CLA	C3B-C4B-NB	-3.66	107.27	110.53
19	B	812	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
24	A	802	AJP	C01-C02-C03	3.65	120.06	112.08
19	LL	201	CLA	C6-C5-C3	3.65	122.35	113.47
21	AA	844	PQN	C14-C13-C15	3.64	121.54	115.23
24	BB	849	AJP	O25-C26-O31	3.64	120.26	110.69
26	B2	841	ECH	C7-C8-C9	-3.64	120.86	126.23
26	BB	840	ECH	C12-C13-C14	-3.64	113.29	119.01
24	AA	802	AJP	C01-C02-C03	3.63	120.03	112.08
24	L1	204	AJP	O25-C26-O31	3.63	120.25	110.69
19	B2	834	CLA	O2D-CGD-CBD	3.63	117.58	111.23
19	B1	824	CLA	C3B-C4B-NB	-3.63	107.29	110.53
19	B2	801	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
20	A	803	CL0	C3D-C4D-CHA	3.62	114.05	108.54
19	B	801	CLA	C4-C3-C2	-3.62	114.33	123.63
24	BB	849	AJP	C21-C22-C23	3.62	115.30	110.46
24	B	849	AJP	O84-C05-C04	3.61	113.91	110.76
23	J1	102	BCR	C15-C16-C17	-3.61	116.13	123.52
24	B	849	AJP	C18-C19-C20	3.60	118.36	112.31
23	A	851	BCR	C2-C1-C6	3.60	115.67	110.44
23	FF	306	BCR	C15-C16-C17	-3.60	116.15	123.52
23	F1	304	BCR	C24-C23-C22	-3.60	120.91	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	825	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
24	L1	203	AJP	C24-C19-C20	3.59	116.48	112.66
24	L	208	AJP	C17-C18-C19	3.58	118.77	111.84
26	B	841	ECH	C7-C8-C9	-3.58	120.94	126.23
23	J	102	BCR	C15-C16-C17	-3.57	116.21	123.52
24	A1	854	AJP	C18-C19-C20	3.57	118.30	112.31
26	B	841	ECH	C16-C15-C14	-3.57	116.22	123.52
24	L2	202	AJP	C83-C06-C07	3.57	121.62	114.50
23	FF	306	BCR	C15-C14-C13	-3.56	122.28	127.28
23	A1	850	BCR	C15-C16-C17	-3.56	116.24	123.52
24	I2	104	AJP	C01-C02-C03	3.56	119.86	112.08
28	BB	854	DGD	O6D-C1D-O3G	-3.56	101.64	110.04
19	BB	801	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
24	L	208	AJP	C06-C07-C08	-3.55	98.58	104.28
23	B2	842	BCR	C15-C16-C17	-3.55	116.26	123.52
19	A2	823	CLA	O2D-CGD-CBD	3.55	117.43	111.23
19	BB	801	CLA	O2D-CGD-CBD	3.53	117.41	111.23
19	A1	852	CLA	C3B-C4B-NB	-3.53	107.38	110.53
24	L2	203	AJP	O25-C26-O31	3.53	119.98	110.69
23	A2	850	BCR	C15-C16-C17	-3.53	116.30	123.52
23	AA	854	BCR	C15-C16-C17	-3.53	116.30	123.52
23	J2	102	BCR	C15-C16-C17	-3.53	116.31	123.52
19	F	302	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
19	A1	826	CLA	C3B-C4B-NB	-3.52	107.39	110.53
23	A	853	BCR	C15-C16-C17	-3.51	116.33	123.52
19	A1	810	CLA	C3B-C4B-NB	-3.51	107.40	110.53
19	F2	302	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
19	F1	301	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
23	JJ	102	BCR	C15-C16-C17	-3.50	116.35	123.52
19	F	301	CLA	O2D-CGD-CBD	3.50	117.35	111.23
23	F	305	BCR	C15-C14-C13	-3.50	122.38	127.28
24	B	849	AJP	C06-C07-C08	-3.48	98.68	104.28
19	A2	832	CLA	O2D-CGD-O1D	-3.48	117.06	123.85
23	L	205	BCR	C15-C16-C17	-3.48	116.39	123.52
19	B2	812	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
24	L1	204	AJP	C01-C02-C03	3.47	119.67	112.08
19	A	804	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	FF	305	CLA	C3B-C4B-NB	-3.47	107.43	110.53
24	BB	848	AJP	O77-C28-C27	3.47	118.55	110.38
19	KK	101	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
24	BB	848	AJP	C11-C16-C15	-3.46	103.05	109.17
19	AA	838	CLA	O2D-CGD-O1D	-3.46	117.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	857	AJP	C18-C19-C20	3.46	118.12	112.31
23	A1	851	BCR	C2-C1-C6	3.46	115.47	110.44
24	BB	848	AJP	C20-C15-C16	3.46	115.94	112.43
24	BB	848	AJP	C01-C02-C03	3.45	119.63	112.08
24	B	849	AJP	C83-C06-C07	3.45	121.40	114.50
24	KK	104	AJP	C83-C06-C07	3.45	121.40	114.50
19	K	101	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
19	F1	301	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
24	KK	104	AJP	C24-C19-C20	3.45	116.33	112.66
23	B1	841	BCR	C15-C14-C13	-3.44	122.45	127.28
28	B	856	DGD	O6D-C1D-O3G	-3.44	101.91	110.04
19	A	838	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
19	K1	102	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
19	A	811	CLA	C3B-C4B-NB	-3.44	107.46	110.53
20	A	803	CL0	C1C-CHC-C4B	3.44	128.37	116.07
19	B	858	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
24	L2	202	AJP	C06-C07-C08	-3.44	98.76	104.28
24	B	850	AJP	O25-C26-O31	3.43	119.73	110.69
19	BB	809	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
19	AA	810	CLA	C3B-C4B-NB	-3.43	107.47	110.53
20	AA	803	CL0	C1C-CHC-C4B	3.43	128.35	116.07
19	BB	833	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
19	A2	833	CLA	C3B-C4B-NB	-3.43	107.47	110.53
19	B	801	CLA	O2D-CGD-CBD	3.43	117.23	111.23
19	FF	302	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
20	A	803	CL0	C4D-CHA-CBD	-3.42	105.52	108.97
19	A	832	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
24	L	208	AJP	C13-C12-C07	-3.42	110.50	115.36
23	F	304	BCR	C24-C23-C22	-3.41	121.19	126.23
19	A1	852	CLA	C7-C6-C5	3.41	122.35	113.26
23	A2	851	BCR	C2-C1-C6	3.41	115.39	110.44
20	A2	803	CL0	C1C-CHC-C4B	3.40	128.25	116.07
19	B2	829	CLA	C3B-C4B-NB	-3.40	107.49	110.53
24	KK	104	AJP	C13-C14-C15	3.40	118.92	113.14
23	FF	304	BCR	C24-C23-C22	-3.40	121.20	126.23
24	B	849	AJP	C03-C04-C05	3.40	117.26	111.93
20	A1	802	CL0	O2D-CGD-O1D	-3.40	117.23	123.85
20	A1	802	CL0	C1C-CHC-C4B	3.40	128.22	116.07
19	A	823	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
19	F2	301	CLA	CAA-C2A-C3A	-3.39	103.83	113.00
24	L2	203	AJP	C01-C02-C03	3.39	119.49	112.08
19	A	827	CLA	C3B-C4B-NB	-3.39	107.50	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L2	202	AJP	C13-C14-C15	3.39	118.89	113.14
19	A2	806	CLA	CAA-C2A-C1A	-3.39	100.88	111.97
23	J1	104	BCR	C2-C1-C6	3.38	115.35	110.44
24	L1	204	AJP	O84-C05-C04	3.38	113.71	110.76
19	BB	827	CLA	C3B-C4B-NB	-3.38	107.51	110.53
24	BB	848	AJP	C06-C07-C08	-3.38	98.84	104.28
19	B1	801	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
23	A1	849	BCR	C2-C1-C6	3.38	115.35	110.44
19	B1	827	CLA	C3B-C4B-NB	-3.38	107.52	110.53
19	B	820	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
20	A	803	CL0	O2A-CGA-O1A	-3.37	115.20	123.63
19	A1	831	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
19	F1	302	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
19	BB	836	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
26	B	841	ECH	C28-C27-C26	-3.37	115.62	118.64
23	AA	850	BCR	C2-C1-C6	3.37	115.33	110.44
19	BB	836	CLA	CAC-C3C-C2C	-3.36	121.38	127.56
19	B1	812	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
19	A1	805	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
23	A2	849	BCR	C2-C1-C6	3.35	115.31	110.44
23	AA	852	BCR	C2-C1-C6	3.35	115.31	110.44
19	B1	836	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	I2	103	BCR	C15-C16-C17	-3.35	116.67	123.52
19	B2	837	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
19	K2	102	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
26	BB	840	ECH	C7-C8-C9	-3.34	121.29	126.23
19	L	203	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
24	B	849	AJP	C13-C14-C15	3.33	118.80	113.14
24	BB	848	AJP	C21-C22-C23	3.33	114.92	110.46
19	A2	804	CLA	C3B-C4B-NB	-3.33	107.56	110.53
23	F2	304	BCR	C24-C23-C22	-3.33	121.31	126.23
19	L	202	CLA	C6-C5-C3	3.33	121.57	113.47
19	AA	823	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
19	BB	856	CLA	CHB-C4A-NA	3.32	129.20	124.40
19	B	816	CLA	C3B-C4B-NB	-3.32	107.57	110.53
19	B1	822	CLA	C3B-C4B-NB	-3.32	107.57	110.53
19	A1	809	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
24	A	802	AJP	C83-C06-C07	3.31	121.12	114.50
19	A2	827	CLA	C3B-C4B-NB	-3.31	107.58	110.53
19	BB	820	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
19	BB	823	CLA	C3B-C4B-NB	-3.30	107.58	110.53
19	B2	822	CLA	C3B-C4B-NB	-3.30	107.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	806	CLA	C3B-C4B-NB	-3.30	107.58	110.53
19	LL	202	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
19	B	809	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
24	L2	202	AJP	C24-C19-C20	3.30	116.17	112.66
24	K	104	AJP	C18-C19-C20	3.29	117.83	112.31
19	B	859	CLA	CHB-C4A-NA	3.29	129.15	124.40
24	L1	203	AJP	C15-C20-C19	3.29	113.08	108.51
19	B	837	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
19	B2	801	CLA	O2D-CGD-CBD	3.29	116.97	111.23
24	K	104	AJP	C24-C19-C20	3.29	116.16	112.66
19	AA	833	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	K	101	CLA	CAA-C2A-C3A	-3.28	104.13	113.00
24	M2	101	AJP	C13-C14-C15	3.28	118.71	113.14
19	F	301	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
23	L1	208	BCR	C15-C16-C17	-3.28	116.81	123.52
23	B2	842	BCR	C30-C25-C26	-3.28	118.16	122.64
19	AA	832	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
19	AA	806	CLA	CBA-CAA-C2A	3.27	123.54	113.79
19	BB	802	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	L2	203	AJP	C11-C16-C15	-3.27	103.39	109.17
19	A1	832	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	L2	203	AJP	C18-C19-C20	3.27	117.80	112.31
23	K1	106	BCR	C24-C23-C22	-3.27	121.40	126.23
19	B1	833	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
23	A	849	BCR	C2-C1-C6	3.27	115.19	110.44
19	A2	806	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	K	104	AJP	C83-C06-C07	3.26	121.02	114.50
19	BB	855	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
19	B	823	CLA	C3B-C4B-NB	-3.26	107.62	110.53
23	B2	842	BCR	C15-C14-C13	-3.26	122.71	127.28
24	L	209	AJP	C83-C06-C07	3.26	121.01	114.50
24	AA	802	AJP	C83-C06-C07	3.26	121.01	114.50
19	B2	816	CLA	C3B-C4B-NB	-3.25	107.62	110.53
19	B2	820	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
19	BB	816	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	B1	820	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
19	A	806	CLA	CBA-CAA-C2A	3.25	123.47	113.79
19	A2	829	CLA	C3B-C4B-NB	-3.25	107.63	110.53
20	A2	803	CL0	C9-C8-C10	3.25	122.86	111.27
19	BB	805	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
23	J2	104	BCR	C24-C23-C22	-3.25	121.43	126.23
19	A2	810	CLA	O2D-CGD-O1D	-3.24	117.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	805	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
19	B	834	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
24	A2	854	AJP	C24-C23-C22	3.24	114.39	110.38
19	KK	101	CLA	CAA-C2A-C3A	-3.24	104.24	113.00
19	AA	827	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	F1	301	CLA	C3B-C4B-NB	-3.24	107.64	110.53
19	B1	828	CLA	C3B-C4B-NB	-3.23	107.64	110.53
19	A	833	CLA	C3B-C4B-NB	-3.23	107.64	110.53
19	AA	804	CLA	C3B-C4B-NB	-3.23	107.65	110.53
19	BB	801	CLA	CHB-C4A-NA	3.22	129.05	124.40
23	A1	853	BCR	C15-C16-C17	-3.22	116.93	123.52
19	B	859	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
19	BB	836	CLA	CHB-C4A-NA	3.22	129.05	124.40
19	F2	301	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
19	B1	816	CLA	C3B-C4B-NB	-3.22	107.66	110.53
23	A2	853	BCR	C15-C16-C17	-3.22	116.94	123.52
19	B1	850	CLA	CHB-C4A-NA	3.22	129.04	124.40
19	F2	301	CLA	C3B-C4B-NB	-3.21	107.66	110.53
19	A	810	CLA	C3B-C4B-NB	-3.21	107.66	110.53
19	L1	206	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
19	B	805	CLA	C3B-C4B-NB	-3.21	107.66	110.53
19	A1	822	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
19	B2	809	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
19	AA	823	CLA	C3B-C4B-NB	-3.21	107.67	110.53
25	I1	102	LMG	O6-C1-O1	-3.21	102.47	110.04
19	B2	851	CLA	CHB-C4A-NA	3.20	129.02	124.40
19	AA	842	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	BB	829	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
19	B1	809	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
19	B	834	CLA	CAA-C2A-C3A	-3.20	104.35	113.00
19	B1	821	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	A	823	CLA	C3B-C4B-NB	-3.20	107.67	110.53
24	B	849	AJP	C21-C22-C23	3.20	114.74	110.46
19	BB	856	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
24	KK	104	AJP	C18-C19-C20	3.20	117.67	112.31
19	B	834	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
23	A	850	BCR	C15-C16-C17	-3.20	116.98	123.52
24	L1	203	AJP	O78-C27-C28	3.19	117.91	110.38
19	B2	826	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
23	M	101	BCR	C15-C16-C17	-3.19	116.99	123.52
19	L2	205	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
24	L	209	AJP	C13-C12-C07	-3.19	110.82	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	850	AJP	C21-C22-C23	3.19	114.73	110.46
23	F2	304	BCR	C2-C1-C6	3.19	115.07	110.44
19	BB	826	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
19	B1	826	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
19	B1	815	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
19	A1	806	CLA	C3B-C4B-NB	-3.19	107.69	110.53
19	B	822	CLA	C3B-C4B-NB	-3.18	107.69	110.53
23	K	103	BCR	C15-C16-C17	-3.18	117.01	123.52
19	A1	816	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	B	829	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	LL	201	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	L1	203	AJP	C13-C14-C15	3.18	118.54	113.14
24	B	850	AJP	O09-C05-C06	-3.18	100.33	104.56
19	B1	805	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	L	208	AJP	C24-C19-C18	-3.18	107.17	112.75
24	A1	855	AJP	C24-C23-C22	3.17	114.30	110.38
23	A	854	BCR	C24-C23-C22	-3.17	121.54	126.23
19	A2	810	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	A	806	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	A2	817	CLA	C3B-C4B-NB	-3.17	107.70	110.53
23	FF	304	BCR	C2-C1-C6	3.17	115.05	110.44
24	K	104	AJP	C06-C07-C08	-3.17	99.19	104.28
19	B1	818	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	B2	833	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
19	A1	837	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
26	B1	840	ECH	C12-C13-C14	-3.16	114.03	119.01
19	A2	810	CLA	O2D-CGD-CBD	3.16	116.76	111.23
24	I2	104	AJP	O09-C05-C06	-3.16	100.36	104.56
19	BB	833	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
19	AA	811	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
23	J1	104	BCR	C24-C23-C22	-3.16	121.56	126.23
19	B	826	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
19	B	859	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
19	A1	832	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
19	AA	801	CLA	C3B-C4B-NB	-3.16	107.71	110.53
19	B	805	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
19	A	852	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	AA	811	CLA	C3B-C4B-NB	-3.15	107.72	110.53
23	II	104	BCR	C15-C16-C17	-3.15	117.07	123.52
19	BB	813	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
19	A2	838	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
19	B1	833	CLA	C3B-C4B-NB	-3.15	107.72	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BB	848	AJP	O78-C27-C28	3.15	117.80	110.38
23	F1	304	BCR	C2-C1-C6	3.15	115.01	110.44
26	B2	841	ECH	C12-C13-C14	-3.15	114.06	119.01
23	AA	851	BCR	C15-C16-C17	-3.15	117.08	123.52
19	A	809	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
19	B1	832	CLA	CHB-C4A-NA	3.14	128.94	124.40
19	B	801	CLA	CHB-C4A-NA	3.14	128.94	124.40
20	A2	803	CL0	O2A-CGA-CBA	3.14	121.41	111.83
19	AA	853	CLA	C3B-C4B-NB	-3.14	107.73	110.53
19	L1	205	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
19	F	301	CLA	C3B-C4B-NB	-3.14	107.73	110.53
24	B	849	AJP	O78-C27-C28	3.13	117.77	110.38
19	BB	805	CLA	C3B-C4B-NB	-3.13	107.73	110.53
19	A2	852	CLA	C3B-C4B-NB	-3.13	107.73	110.53
19	AA	841	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
19	L	202	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
23	F	305	BCR	C11-C10-C9	-3.12	122.90	127.28
19	B	827	CLA	C3B-C4B-NB	-3.12	107.74	110.53
19	A	808	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
19	A2	806	CLA	CBA-CAA-C2A	3.12	123.08	113.79
26	B	841	ECH	C12-C13-C14	-3.12	114.10	119.01
19	B2	818	CLA	C3B-C4B-NB	-3.12	107.74	110.53
19	A	810	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
19	B	832	CLA	C3B-C4B-NB	-3.12	107.75	110.53
24	BB	849	AJP	C83-C06-C07	3.12	120.73	114.50
19	A2	805	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
19	B1	850	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
19	AA	805	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
19	B1	836	CLA	CHB-C4A-NA	3.12	128.90	124.40
19	A	810	CLA	CBA-CAA-C2A	3.11	123.06	113.79
19	B1	805	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	B2	814	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
19	A	801	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	B1	807	CLA	C3B-C4B-NB	-3.11	107.75	110.53
19	AA	819	CLA	C3B-C4B-NB	-3.11	107.76	110.53
23	J1	104	BCR	C1-C6-C5	-3.11	118.39	122.64
19	A1	803	CLA	C3B-C4B-NB	-3.11	107.76	110.53
19	A	841	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
19	B	817	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
19	A2	823	CLA	C3B-C4B-NB	-3.10	107.76	110.53
19	A1	804	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
19	A2	822	CLA	O2D-CGD-O1D	-3.10	117.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A2	854	AJP	C18-C19-C20	3.10	117.51	112.31
24	M2	101	AJP	C06-C07-C08	-3.10	99.30	104.28
19	B1	814	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
19	AA	845	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
19	B1	823	CLA	C3B-C4B-NB	-3.10	107.77	110.53
19	F	301	CLA	CHB-C4A-NA	3.10	128.87	124.40
19	A	839	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
24	L1	204	AJP	O82-C10-C11	3.09	124.35	113.68
19	B2	837	CLA	CHB-C4A-NA	3.09	128.87	124.40
19	BB	814	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
19	AA	804	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
19	J1	101	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	B	830	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
19	A1	809	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	A1	813	CLA	C3B-C4B-NB	-3.09	107.77	110.53
19	BB	856	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
23	B	848	BCR	C1-C6-C5	-3.09	118.42	122.64
19	A	832	CLA	O2D-CGD-CBD	3.08	116.62	111.23
24	KK	104	AJP	C26-C27-C28	3.08	116.50	110.01
19	A	808	CLA	C1-O2A-CGA	3.08	124.11	116.65
19	AA	853	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
19	B	804	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
19	K1	102	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
23	F2	305	BCR	C11-C10-C9	-3.08	122.96	127.28
23	J	104	BCR	C24-C23-C22	-3.08	121.68	126.23
19	B2	807	CLA	C3B-C4B-NB	-3.08	107.78	110.53
19	A	814	CLA	C3B-C4B-NB	-3.08	107.78	110.53
24	A1	855	AJP	C24-C19-C20	3.08	115.93	112.66
24	K	104	AJP	C26-C27-C28	3.08	116.48	110.01
19	BB	804	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
19	A	829	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	A1	855	AJP	C18-C19-C20	3.07	117.46	112.31
19	A1	834	CLA	C1-C2-C3	-3.07	121.17	126.20
24	AA	856	AJP	C14-C15-C16	3.07	116.06	111.78
19	AA	816	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	A1	807	CLA	O2A-CGA-O1A	-3.07	115.96	123.63
19	A	844	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
24	L2	202	AJP	C18-C19-C20	3.07	117.45	112.31
19	B	814	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
19	A	837	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	L	208	AJP	C20-C21-C22	3.07	116.92	113.94
23	F1	306	BCR	C11-C10-C9	-3.07	122.98	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	844	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
19	B1	833	CLA	O2A-CGA-O1A	-3.06	115.96	123.63
23	I2	103	BCR	C24-C23-C22	-3.06	121.70	126.23
19	B	807	CLA	C3B-C4B-NB	-3.06	107.80	110.53
19	B	806	CLA	C5-C3-C2	3.06	128.04	121.17
24	L	208	AJP	C17-C16-C15	3.06	114.19	110.52
19	K2	102	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
24	B	850	AJP	C11-C16-C15	-3.06	103.77	109.17
19	B2	851	CLA	CBA-CAA-C2A	3.06	122.89	113.79
19	AA	814	CLA	C3B-C4B-NB	-3.06	107.80	110.53
19	A1	808	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
23	B1	843	BCR	C33-C5-C6	-3.05	121.15	124.48
19	F1	301	CLA	CHB-C4A-NA	3.05	128.81	124.40
19	A2	835	CLA	C1-C2-C3	-3.05	121.19	126.20
19	B2	817	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
19	A1	818	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	AA	809	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
19	A1	841	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	A2	814	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	A	805	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	L	209	AJP	C17-C18-C19	3.05	117.73	111.84
19	A2	844	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
24	L	208	AJP	C17-C16-C11	3.05	116.59	112.29
23	F	304	BCR	C2-C1-C6	3.05	114.86	110.44
19	B1	801	CLA	O2D-CGD-CBD	3.05	116.55	111.23
19	J2	101	CLA	C3B-C4B-NB	-3.04	107.81	110.53
24	K	104	AJP	C11-C16-C15	-3.04	103.79	109.17
20	AA	803	CL0	CMC-C2C-C1C	3.04	130.21	124.73
24	L1	204	AJP	C18-C19-C20	3.04	117.41	112.31
24	AA	856	AJP	C18-C19-C20	3.04	117.41	112.31
19	BB	807	CLA	C3B-C4B-NB	-3.04	107.82	110.53
24	A	855	AJP	C18-C19-C20	3.04	117.41	112.31
19	A1	840	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
20	A	803	CL0	O2D-CGD-O1D	-3.04	117.93	123.85
24	L2	203	AJP	O82-C10-C11	3.04	124.16	113.68
19	B	802	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
23	K2	105	BCR	C24-C23-C22	-3.04	121.74	126.23
19	B2	834	CLA	O2A-CGA-O1A	-3.04	116.03	123.63
19	A2	809	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	A	855	AJP	C14-C15-C16	3.03	116.01	111.78
19	A	842	CLA	C3B-C4B-NB	-3.03	107.82	110.53
19	A	833	CLA	O2D-CGD-O1D	-3.03	117.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B2	844	BCR	C33-C5-C6	-3.03	121.17	124.48
19	A1	822	CLA	C3B-C4B-NB	-3.03	107.82	110.53
24	BB	849	AJP	O09-C05-C06	-3.03	100.53	104.56
19	A1	809	CLA	O2D-CGD-CBD	3.03	116.53	111.23
19	B1	804	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	A	821	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	A	844	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	B1	829	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
19	AA	814	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
19	BB	852	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
23	A1	853	BCR	C27-C26-C25	3.03	126.79	122.70
19	AA	837	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	B	813	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
19	FF	301	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	A2	853	BCR	C27-C26-C25	3.02	126.79	122.70
19	B1	813	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
23	BB	843	BCR	C33-C5-C6	-3.02	121.19	124.48
19	A	852	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
19	A2	821	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
19	B	813	CLA	C3B-C4B-NB	-3.02	107.83	110.53
19	A2	824	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
23	J2	104	BCR	C1-C6-C5	-3.02	118.51	122.64
19	A2	840	CLA	C3B-C4B-NB	-3.02	107.83	110.53
19	K	101	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	B	844	BCR	C33-C5-C6	-3.02	121.19	124.48
19	AA	810	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
23	KK	103	BCR	C15-C16-C17	-3.02	117.34	123.52
19	L2	204	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
19	AA	821	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
19	A1	821	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
19	B2	852	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
24	M2	101	AJP	C83-C06-C07	3.02	120.52	114.50
19	B2	804	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
19	BB	828	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
19	A	815	CLA	CHB-C4A-NA	3.01	128.75	124.40
23	A	853	BCR	C27-C26-C25	3.01	126.78	122.70
23	AA	854	BCR	C27-C26-C25	3.01	126.78	122.70
24	L	209	AJP	C17-C16-C15	3.01	114.13	110.52
19	A2	807	CLA	C3B-C4B-NB	-3.01	107.84	110.53
19	AA	821	CLA	CHB-C4A-NA	3.01	128.75	124.40
19	B1	817	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	A2	833	CLA	O2D-CGD-O1D	-3.01	117.99	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	832	CLA	O2D-CGD-CBD	3.01	116.49	111.23
19	A2	840	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	AA	839	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	BB	806	CLA	C5-C3-C2	3.01	127.92	121.17
19	B2	823	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	BB	849	AJP	O84-C05-C04	3.01	113.38	110.76
19	B2	810	CLA	C3B-C4B-NB	-3.01	107.84	110.53
19	A1	814	CLA	CHB-C4A-NA	3.01	128.74	124.40
19	B	818	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
19	B2	801	CLA	CHB-C4A-NA	3.01	128.74	124.40
19	A2	852	CLA	C6-C5-C3	3.01	120.79	113.47
19	A2	815	CLA	CHB-C4A-NA	3.00	128.74	124.40
23	J	102	BCR	C15-C14-C13	-3.00	123.06	127.28
19	A1	828	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	A2	819	CLA	C3B-C4B-NB	-3.00	107.85	110.53
24	L2	203	AJP	O84-C05-C04	3.00	113.38	110.76
19	B1	814	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	B1	810	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	B	802	CLA	C3B-C4B-NB	-3.00	107.86	110.53
19	BB	813	CLA	C3B-C4B-NB	-3.00	107.86	110.53
19	A2	830	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
24	K	104	AJP	C20-C21-C22	-3.00	109.25	114.17
23	FF	306	BCR	C11-C10-C9	-2.99	123.08	127.28
19	LL	203	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
19	A1	839	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	B2	839	BCR	C15-C14-C13	-2.99	123.08	127.28
19	B1	819	CLA	C3B-C4B-NB	-2.99	107.86	110.53
19	BB	835	CLA	C3B-C4B-NB	-2.99	107.86	110.53
19	B2	833	CLA	CHB-C4A-NA	2.99	128.71	124.40
19	A2	820	CLA	C3B-C4B-NB	-2.98	107.87	110.53
19	A2	834	CLA	C3B-C4B-NB	-2.98	107.87	110.53
23	F1	306	BCR	C24-C23-C22	-2.98	121.82	126.23
19	AA	820	CLA	O2A-CGA-O1A	-2.98	116.17	123.63
19	AA	815	CLA	CHB-C4A-NA	2.98	128.70	124.40
24	AA	802	AJP	C24-C19-C20	2.98	117.31	112.31
19	BB	856	CLA	CAA-CBA-CGA	2.98	121.67	113.21
19	B2	802	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
19	A1	809	CLA	CAA-C2A-C1A	-2.98	102.22	111.97
19	B1	816	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
19	B1	806	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
19	A2	801	CLA	CHB-C4A-NA	2.97	128.69	124.40
19	BB	856	CLA	C3B-C4B-NB	-2.97	107.88	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BB	849	AJP	C24-C19-C20	2.97	115.83	112.66
19	B1	802	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
19	A2	841	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
19	B	828	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
23	AA	855	BCR	C24-C23-C22	-2.97	121.84	126.23
19	B2	805	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	AA	801	CLA	CHB-C4A-NA	2.97	128.69	124.40
19	KK	101	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	A	801	CLA	CHB-C4A-NA	2.97	128.69	124.40
19	B	837	CLA	CHB-C4A-NA	2.97	128.69	124.40
19	B2	821	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
19	F2	301	CLA	CHB-C4A-NA	2.97	128.68	124.40
26	BB	840	ECH	C29-C30-C25	-2.97	106.13	110.44
19	B	816	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
19	B	819	CLA	C3B-C4B-NB	-2.96	107.88	110.53
19	B2	851	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
19	F	302	CLA	C3B-C4B-NB	-2.96	107.89	110.53
23	B1	838	BCR	C15-C14-C13	-2.96	123.12	127.28
24	L	209	AJP	C06-C07-C08	-2.96	99.52	104.28
19	B1	813	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B	803	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
19	A1	817	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	A	819	CLA	C3B-C4B-NB	-2.96	107.89	110.53
23	FF	306	BCR	C33-C5-C6	-2.96	121.25	124.48
19	B1	806	CLA	C5-C3-C2	2.96	127.81	121.17
19	A	842	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
19	B	828	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B1	850	CLA	CBA-CAA-C2A	2.96	122.59	113.79
24	L2	202	AJP	C15-C20-C19	2.96	112.62	108.51
19	B2	807	CLA	CHB-C4A-NA	2.96	128.67	124.40
19	A2	812	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B2	813	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B2	806	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	AA	802	AJP	C06-C07-C08	-2.95	99.53	104.28
19	B	830	CLA	C3B-C4B-NB	-2.95	107.89	110.53
24	I2	104	AJP	C83-C06-C07	2.95	120.40	114.50
19	AA	842	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
19	A1	829	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
25	B2	847	LMG	O6-C1-O1	-2.95	103.08	110.04
24	B	850	AJP	C24-C19-C20	2.95	115.80	112.66
24	A	802	AJP	C24-C19-C20	2.95	117.26	112.31
19	A1	820	CLA	O2D-CGD-O1D	-2.95	118.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A1	850	BCR	C33-C5-C6	-2.95	121.27	124.48
19	F2	302	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	A	807	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	A1	801	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	B	859	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	A	821	CLA	CHB-C4A-NA	2.94	128.65	124.40
19	B	859	CLA	CBA-CAA-C2A	2.94	122.55	113.79
23	L1	208	BCR	C24-C23-C22	-2.94	121.88	126.23
24	KK	104	AJP	C20-C21-C22	-2.94	109.33	114.17
19	BB	831	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
19	B1	820	CLA	C3B-C4B-NB	-2.94	107.91	110.53
19	B	833	CLA	CHB-C4A-NA	2.94	128.64	124.40
23	B1	839	BCR	C1-C6-C5	-2.94	118.62	122.64
19	B2	836	CLA	C3B-C4B-NB	-2.94	107.91	110.53
19	A	817	CLA	C3B-C4B-NB	-2.94	107.91	110.53
24	A2	854	AJP	C17-C16-C15	-2.93	107.00	110.52
19	BB	818	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
19	A	805	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	A1	801	CLA	CHB-C4A-NA	2.93	128.63	124.40
19	A1	833	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	J	101	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	B2	804	CLA	C1-C2-C3	-2.93	121.39	126.20
23	B2	840	BCR	C1-C6-C5	-2.93	118.63	122.64
19	B2	830	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
19	BB	814	CLA	CHB-C4A-NA	2.93	128.63	124.40
24	L1	204	AJP	C81-C12-C11	2.93	117.95	111.58
19	B1	850	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
19	A	804	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
20	A1	802	CL0	C9-C8-C7	2.93	121.71	111.27
24	K	104	AJP	C18-C17-C16	2.93	116.83	112.16
19	B1	830	CLA	C3B-C4B-NB	-2.93	107.92	110.53
19	AA	819	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
19	B2	813	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
25	I1	102	LMG	O6-C5-C4	2.93	114.97	109.70
19	A1	826	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
19	F2	302	CLA	O2D-CGD-CBD	2.93	116.34	111.23
19	B2	809	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	BB	804	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	A2	818	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	B2	831	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	A1	812	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	BB	831	CLA	C3B-C4B-NB	-2.92	107.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	806	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
19	F1	305	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	B1	801	CLA	CHB-C4A-NA	2.92	128.61	124.40
19	B	831	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	JJ	101	CLA	C3B-C4B-NB	-2.92	107.93	110.53
19	BB	820	CLA	O2D-CGD-CBD	2.92	116.33	111.23
19	B2	835	CLA	C3B-C4B-NB	-2.92	107.93	110.53
24	A	802	AJP	C06-C07-C08	-2.92	99.59	104.28
19	JJ	103	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	A1	831	CLA	O2D-CGD-CBD	2.92	116.33	111.23
19	A	818	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	B	840	BCR	C1-C6-C5	-2.91	118.65	122.64
19	BB	856	CLA	CBA-CAA-C2A	2.91	122.47	113.79
19	A	825	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
19	A2	823	CLA	CHB-C4A-NA	2.91	128.60	124.40
19	B	815	CLA	CMB-C2B-C1B	-2.91	120.98	125.42
19	AA	816	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	B	836	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A	827	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	BB	840	ECH	C8-C7-C6	-2.91	119.22	127.00
19	B	801	CLA	C4-C3-C5	2.91	120.28	115.23
19	A	806	CLA	CAA-C2A-C1A	-2.91	102.43	111.97
19	B1	804	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A2	801	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	B2	802	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	B	804	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	AA	829	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A2	837	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	AA	817	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	A1	811	CLA	C3B-C4B-NB	-2.91	107.94	110.53
19	A1	836	CLA	C3B-C4B-NB	-2.91	107.94	110.53
19	AA	845	CLA	C3B-C4B-NB	-2.91	107.94	110.53
19	A1	810	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
19	B	827	CLA	CHB-C4A-NA	2.91	128.59	124.40
19	B	834	CLA	O2D-CGD-CBD	2.91	116.31	111.23
19	B2	851	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
24	I2	104	AJP	C24-C19-C20	2.91	117.18	112.31
19	BB	833	CLA	O2D-CGD-CBD	2.90	116.31	111.23
19	B	808	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	A	840	CLA	C3B-C4B-NB	-2.90	107.94	110.53
23	B1	843	BCR	C27-C26-C25	2.90	126.63	122.70
19	KK	102	CLA	O2D-CGD-O1D	-2.90	118.20	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	823	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
19	L	203	CLA	C3B-C4B-NB	-2.90	107.94	110.53
23	BB	847	BCR	C1-C6-C5	-2.90	118.67	122.64
19	A1	815	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
19	AA	807	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	B	859	CLA	CAA-CBA-CGA	2.90	121.44	113.21
19	BB	818	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	BB	828	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	A1	807	CLA	C1-O2A-CGA	2.90	123.66	116.65
19	A	823	CLA	O2D-CGD-CBD	2.90	116.29	111.23
19	A2	844	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	A	820	CLA	C3B-C4B-NB	-2.90	107.94	110.53
26	B	841	ECH	C8-C7-C6	-2.90	119.26	127.00
19	A1	803	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
23	AA	855	BCR	C33-C5-C6	-2.89	121.33	124.48
19	B2	806	CLA	C5-C3-C2	2.89	127.66	121.17
19	A1	838	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
19	BB	816	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
23	MM	101	BCR	C27-C26-C25	2.89	126.61	122.70
24	A2	854	AJP	C24-C19-C20	2.89	115.74	112.66
23	B1	842	BCR	C15-C16-C17	-2.89	117.60	123.52
23	JJ	104	BCR	C24-C23-C22	-2.89	121.96	126.23
19	B1	834	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	B1	835	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	B1	809	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	FF	302	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	L2	203	AJP	C06-C07-C08	-2.89	99.63	104.28
19	K	102	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
23	F1	306	BCR	C33-C5-C6	-2.89	121.33	124.48
23	I2	101	BCR	C33-C5-C6	-2.89	121.33	124.48
19	B1	810	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
19	AA	825	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
23	AA	852	BCR	C28-C27-C26	-2.89	108.91	114.06
19	B2	816	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
19	B2	821	CLA	C3B-C4B-NB	-2.89	107.95	110.53
23	AA	851	BCR	C33-C5-C6	-2.89	121.33	124.48
23	A	851	BCR	C28-C27-C26	-2.89	108.91	114.06
24	BB	848	AJP	C13-C14-C15	2.89	118.04	113.14
19	B1	807	CLA	CHB-C4A-NA	2.89	128.56	124.40
23	F2	303	BCR	C2-C1-C6	2.88	114.63	110.44
19	B2	807	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
19	B1	821	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	812	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	B1	841	BCR	C30-C25-C26	-2.88	118.70	122.64
23	MM	101	BCR	C33-C5-C6	-2.88	121.34	124.48
19	L	203	CLA	O2D-CGD-CBD	2.88	116.27	111.23
23	F	305	BCR	C33-C5-C6	-2.88	121.34	124.48
19	BB	808	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
19	A1	844	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	A2	825	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	A	850	BCR	C33-C5-C6	-2.88	121.34	124.48
19	AA	834	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	K2	103	BCR	C33-C5-C6	-2.88	121.34	124.48
19	F1	301	CLA	O2D-CGD-CBD	2.88	116.26	111.23
23	I	102	BCR	C2-C1-C6	2.88	114.62	110.44
23	I1	101	BCR	C33-C5-C6	-2.88	121.34	124.48
23	K	103	BCR	C33-C5-C6	-2.88	121.34	124.48
19	A1	815	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	B2	808	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	A2	815	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	A2	806	CLA	CHB-C4A-NA	2.87	128.55	124.40
19	B1	848	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
24	B	857	AJP	C04-C05-C06	2.87	120.86	115.66
19	B1	824	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
19	A1	824	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	BB	826	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
19	A2	842	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	K1	104	BCR	C33-C5-C6	-2.87	121.35	124.48
19	BB	827	CLA	CHB-C4A-NA	2.87	128.54	124.40
23	A2	850	BCR	C33-C5-C6	-2.87	121.35	124.48
19	B2	804	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	A1	811	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
19	AA	827	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	B1	838	BCR	C33-C5-C6	-2.87	121.36	124.48
23	II	101	BCR	C33-C5-C6	-2.87	121.36	124.48
23	A	854	BCR	C33-C5-C6	-2.86	121.36	124.48
23	FF	303	BCR	C35-C13-C14	-2.86	118.17	122.82
19	BB	807	CLA	CHB-C4A-NA	2.86	128.53	124.40
19	A2	805	CLA	C3B-C4B-NB	-2.86	107.97	110.53
19	B2	819	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
19	BB	821	CLA	C3B-C4B-NB	-2.86	107.97	110.53
19	A	820	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
19	B2	850	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	AA	818	CLA	C3B-C4B-NB	-2.86	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	820	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	A	836	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	L1	203	AJP	C12-C07-C06	2.86	128.95	120.50
23	I	101	BCR	C33-C5-C6	-2.86	121.36	124.48
19	A1	839	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	B2	823	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	A	819	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	BB	802	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	A2	827	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	B	814	CLA	CHB-C4A-NA	2.86	128.52	124.40
19	B1	802	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	M	101	BCR	C33-C5-C6	-2.85	121.37	124.48
19	LL	202	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	X	101	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	BB	817	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	B	832	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	B2	839	BCR	C33-C5-C6	-2.85	121.37	124.48
19	B1	806	CLA	CHB-C4A-NA	2.85	128.51	124.40
19	B	810	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	B	817	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	A2	839	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	A	851	BCR	C3-C4-C5	-2.85	108.98	114.06
23	II	104	BCR	C24-C23-C22	-2.85	122.02	126.23
24	A	855	AJP	C11-C16-C15	-2.85	104.14	109.17
19	A1	819	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	A1	827	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	A1	821	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	B1	808	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	BB	841	BCR	C15-C16-C17	-2.84	117.70	123.52
19	B	806	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	B1	818	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
19	A1	820	CLA	CHB-C4A-NA	2.84	128.50	124.40
19	B1	815	CLA	CHB-C4A-NA	2.84	128.50	124.40
24	AA	856	AJP	C11-C16-C15	-2.84	104.15	109.17
19	A2	813	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	B2	812	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	XX	101	CLA	C3B-C4B-NB	-2.84	107.99	110.53
19	A2	828	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	M2	102	BCR	C33-C5-C6	-2.84	121.39	124.48
19	X1	101	CLA	C3B-C4B-NB	-2.84	108.00	110.53
19	A	824	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
19	AA	804	CLA	C1-C2-C3	-2.84	121.55	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	827	CLA	CHB-C4A-NA	2.84	128.49	124.40
19	AA	817	CLA	CHB-C4A-NA	2.84	128.49	124.40
25	L1	210	LMG	O6-C1-O1	-2.84	103.34	110.04
19	B2	818	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
19	A2	816	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
19	B1	812	CLA	C3B-C4B-NB	-2.84	108.00	110.53
19	A2	831	CLA	C3B-C4B-NB	-2.84	108.00	110.53
19	AA	835	CLA	C1-C2-C3	-2.84	121.55	126.20
26	B1	840	ECH	C40-C30-C25	2.83	114.69	110.24
19	BB	806	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
19	A1	814	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	A2	835	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	A	809	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	B1	802	CLA	CHB-C4A-NA	2.83	128.49	124.40
19	B	806	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
23	J1	102	BCR	C15-C14-C13	-2.83	123.31	127.28
19	B2	824	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	A1	841	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	F1	302	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	B	835	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	A	817	CLA	CHB-C4A-NA	2.83	128.48	124.40
19	B1	822	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	B2	814	CLA	CHB-C4A-NA	2.83	128.48	124.40
25	B	851	LMG	O6-C1-O1	-2.83	103.36	110.04
19	A	842	CLA	C4-C3-C5	2.83	120.14	115.23
19	A	835	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	B	827	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	L2	203	AJP	C18-C17-C16	2.83	116.67	112.16
19	AA	840	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	A	812	CLA	C3B-C4B-NB	-2.83	108.01	110.53
23	M	101	BCR	C27-C26-C25	2.82	126.52	122.70
19	BB	823	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	B1	840	ECH	C8-C7-C6	-2.82	119.45	127.00
19	B2	830	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	B	820	CLA	C3B-C4B-NB	-2.82	108.01	110.53
23	BB	839	BCR	C1-C6-C5	-2.82	118.78	122.64
19	B	812	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	B2	841	ECH	C8-C7-C6	-2.82	119.46	127.00
19	BB	832	CLA	CHB-C4A-NA	2.82	128.47	124.40
19	B2	834	CLA	C3A-C2A-C1A	2.82	105.56	101.34
19	A2	811	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	B2	803	CLA	O2D-CGD-O1D	-2.82	118.36	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	842	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	BB	814	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	A	811	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	A1	835	CLA	CHB-C4A-NA	2.82	128.47	124.40
19	B	807	CLA	CHB-C4A-NA	2.82	128.47	124.40
19	A2	804	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	AA	824	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	BB	803	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	B2	828	CLA	C3B-C4B-NB	-2.82	108.02	110.53
19	A	834	CLA	C3B-C4B-NB	-2.82	108.02	110.53
19	A1	819	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	F2	303	BCR	C33-C5-C6	-2.82	121.41	124.48
19	B1	811	CLA	C3B-C4B-NB	-2.82	108.02	110.53
24	B	857	AJP	C15-C20-C19	2.82	112.42	108.51
19	B	822	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
19	B1	819	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
19	B	829	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
19	B	834	CLA	C3B-C4B-NB	-2.82	108.02	110.53
23	F2	305	BCR	C33-C5-C6	-2.81	121.41	124.48
19	A	812	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	AA	840	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	A2	822	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	L	206	BCR	C33-C5-C6	-2.81	121.41	124.48
19	AA	825	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	AA	833	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	B1	833	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
19	J2	103	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	BB	833	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
19	A	835	CLA	C1-C2-C3	-2.81	121.59	126.20
23	JJ	104	BCR	C33-C5-C6	-2.81	121.42	124.48
19	A2	828	CLA	CHB-C4A-NA	2.81	128.46	124.40
19	A	828	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	MM	101	BCR	C15-C16-C17	-2.81	117.77	123.52
19	AA	830	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	B1	833	CLA	C3A-C2A-C1A	2.81	105.55	101.34
19	A	817	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	KK	103	BCR	C33-C5-C6	-2.81	121.42	124.48
19	A	840	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	B2	820	CLA	CAC-C3C-C2C	-2.81	122.40	127.56
23	A	848	BCR	C33-C5-C6	-2.81	121.42	124.48
19	BB	819	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
19	B2	834	CLA	CHB-C4A-NA	2.81	128.45	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	842	BCR	C15-C16-C17	-2.81	117.78	123.52
23	BB	847	BCR	C33-C5-C6	-2.81	121.42	124.48
19	B2	833	CLA	C2A-C1A-CHA	2.81	128.74	123.87
19	A1	827	CLA	CHB-C4A-NA	2.80	128.45	124.40
19	A2	819	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
19	A2	816	CLA	CHB-C4A-NA	2.80	128.44	124.40
19	LL	201	CLA	C4-C3-C2	-2.80	116.43	123.63
23	AA	849	BCR	C33-C5-C6	-2.80	121.43	124.48
19	JJ	101	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	A2	803	CL0	CMA-C3A-C4A	-2.80	108.58	114.61
19	A1	823	CLA	CHB-C4A-NA	2.80	128.44	124.40
19	A	825	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	B	815	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
19	B	860	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	F	303	BCR	C2-C1-C6	2.80	114.50	110.44
19	XX	101	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	B	844	BCR	C27-C26-C25	2.80	126.49	122.70
23	B1	841	BCR	C15-C16-C17	-2.80	117.80	123.52
19	BB	820	CLA	CAC-C3C-C2C	-2.80	122.42	127.56
19	A1	842	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	B2	834	CLA	CHB-C1B-NB	2.80	128.25	124.05
24	L	209	AJP	O84-C05-C04	2.79	113.19	110.76
19	B1	850	CLA	CAA-CBA-CGA	2.79	121.14	113.21
20	AA	803	CL0	CMB-C2B-C3B	2.79	130.27	124.68
19	B1	829	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	B1	807	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
19	K2	102	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	FF	303	BCR	C33-C5-C6	-2.79	121.44	124.48
24	L1	203	AJP	O09-C05-C06	-2.79	100.85	104.56
19	AA	817	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	A1	855	AJP	C17-C16-C15	-2.79	107.17	110.52
19	K2	104	CLA	CHB-C4A-NA	2.79	128.43	124.40
23	B	842	BCR	C28-C27-C26	-2.79	109.08	114.06
24	A1	855	AJP	C11-C16-C15	-2.79	104.24	109.17
24	L1	204	AJP	C11-C16-C15	-2.79	104.24	109.17
19	BB	829	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	B1	850	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	L1	206	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	AA	809	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	L1	205	CLA	C4-C3-C2	-2.79	116.47	123.63
19	J2	101	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	A2	851	BCR	C28-C27-C26	-2.79	109.08	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J2	102	BCR	C15-C14-C13	-2.79	123.37	127.28
19	B1	849	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	AA	812	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	AA	812	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	A2	820	CLA	O2A-CGA-O1A	-2.79	116.66	123.63
19	AA	843	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	BB	841	BCR	C30-C25-C26	-2.79	118.83	122.64
19	B	817	CLA	CHB-C4A-NA	2.79	128.42	124.40
19	B1	827	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
19	B2	810	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	F	303	BCR	C35-C13-C14	-2.78	118.31	122.82
23	F	303	BCR	C33-C5-C6	-2.78	121.45	124.48
19	A	818	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
19	AA	805	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	B1	850	CLA	C6-C5-C3	2.78	120.25	113.47
19	J1	103	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
19	A1	838	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	B2	820	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	L2	203	AJP	C81-C12-C11	2.78	117.63	111.58
19	A2	809	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	A2	842	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	A1	854	AJP	C12-C07-C06	2.78	128.72	120.50
19	A	816	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
20	A	803	CL0	CMC-C2C-C1C	2.78	129.73	124.73
19	BB	821	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
19	F	302	CLA	O2D-CGD-CBD	2.78	116.09	111.23
19	J1	101	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
19	AA	842	CLA	C6-C5-C3	2.78	120.23	113.47
19	A	830	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	F1	303	BCR	C33-C5-C6	-2.78	121.45	124.48
19	A2	836	CLA	CHB-C4A-NA	2.78	128.41	124.40
19	A1	818	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
19	BB	836	CLA	CBC-CAC-C3C	2.78	119.94	112.42
19	BB	817	CLA	CHB-C4A-NA	2.78	128.41	124.40
24	B	857	AJP	C12-C07-C06	2.77	128.70	120.50
19	AA	806	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
19	BB	833	CLA	CAA-C2A-C3A	-2.77	105.50	113.00
19	A2	808	CLA	C3B-C4B-NB	-2.77	108.05	110.53
19	B1	825	CLA	O2D-CGD-CBD	2.77	116.08	111.23
19	A1	807	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	B1	817	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	B2	851	CLA	C6-C5-C3	2.77	120.22	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	FF	301	CLA	O2D-CGD-CBD	2.77	116.08	111.23
19	A1	819	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
19	BB	804	CLA	C1-C2-C3	-2.77	121.66	126.20
19	B	819	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
19	A	806	CLA	CHB-C4A-NA	2.77	128.40	124.40
26	B	841	ECH	C40-C30-C25	2.77	114.59	110.24
19	B1	833	CLA	CHB-C4A-NA	2.77	128.40	124.40
19	AA	818	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
19	AA	829	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
26	BB	840	ECH	C40-C30-C25	2.77	114.58	110.24
19	A	835	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	B1	804	CLA	C1-C2-C3	-2.77	121.66	126.20
23	I1	101	BCR	C8-C7-C6	-2.77	119.60	127.00
19	B	823	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
19	BB	815	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
19	A	823	CLA	CHB-C4A-NA	2.77	128.39	124.40
23	FF	303	BCR	C2-C1-C6	2.77	114.46	110.44
23	F1	304	BCR	C38-C26-C25	-2.77	121.47	124.48
23	B	848	BCR	C27-C26-C25	2.77	126.44	122.70
23	F	305	BCR	C24-C23-C22	-2.77	122.14	126.23
19	B1	845	CLA	C3B-C4B-NB	-2.76	108.06	110.53
19	A	822	CLA	C3B-C4B-NB	-2.76	108.06	110.53
23	J	104	BCR	C1-C6-C5	-2.76	118.86	122.64
19	A1	828	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
23	B2	844	BCR	C27-C26-C25	2.76	126.44	122.70
19	A	816	CLA	C3B-C4B-NB	-2.76	108.06	110.53
19	BB	801	CLA	C4-C3-C2	-2.76	116.53	123.63
19	B2	827	CLA	CHB-C4A-NA	2.76	128.39	124.40
23	II	102	BCR	C2-C1-C6	2.76	114.45	110.44
19	J	101	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	A1	836	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	A2	801	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	A	802	AJP	C81-C12-C11	2.76	117.59	111.58
19	AA	828	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
19	AA	828	CLA	CHB-C4A-NA	2.76	128.38	124.40
19	LL	202	CLA	O2D-CGD-CBD	2.76	116.05	111.23
19	A2	821	CLA	CHB-C4A-NA	2.76	128.38	124.40
19	B	836	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
19	AA	828	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	A2	846	LHG	O4-P-O5	2.76	125.26	112.44
26	B	841	ECH	C21-C20-C19	-2.76	115.22	123.20
22	A1	846	LHG	O4-P-O5	2.75	125.26	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A2	803	CL0	O2A-CGA-O1A	-2.75	116.74	123.63
19	K1	105	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
19	B	824	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
23	M1	101	BCR	C33-C5-C6	-2.75	121.48	124.48
19	BB	802	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	AA	836	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
19	AA	836	CLA	CHB-C4A-NA	2.75	128.37	124.40
23	II	101	BCR	C8-C7-C6	-2.75	119.65	127.00
22	A	846	LHG	O4-P-O5	2.75	125.24	112.44
19	A1	804	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	L2	204	CLA	C4-C3-C2	-2.75	116.56	123.63
23	L	206	BCR	C27-C26-C25	2.75	126.42	122.70
19	A2	829	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	BB	827	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	BB	835	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	L1	208	BCR	C2-C1-C6	2.75	114.43	110.44
23	BB	847	BCR	C27-C26-C25	2.75	126.42	122.70
23	B	848	BCR	C33-C5-C6	-2.75	121.49	124.48
19	AA	835	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	AA	826	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	A2	828	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	AA	806	CLA	CHB-C4A-NA	2.75	128.36	124.40
19	B	831	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	A	836	CLA	CHB-C4A-NA	2.74	128.36	124.40
19	BB	824	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
19	X2	101	CLA	C3B-C4B-NB	-2.74	108.08	110.53
26	BB	840	ECH	C21-C20-C19	-2.74	115.25	123.20
19	AA	823	CLA	O2D-CGD-CBD	2.74	116.03	111.23
19	BB	810	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	AA	809	CLA	CHB-C4A-NA	2.74	128.36	124.40
19	B2	851	CLA	CAA-CBA-CGA	2.74	120.99	113.21
23	A1	851	BCR	C28-C27-C26	-2.74	109.17	114.06
19	B	805	CLA	CHB-C4A-NA	2.74	128.35	124.40
19	A	808	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	F1	305	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
19	A2	818	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
22	X1	103	LHG	O4-P-O5	2.74	125.18	112.44
19	F1	302	CLA	CHB-C4A-NA	2.74	128.35	124.40
19	AA	823	CLA	CHB-C4A-NA	2.74	128.35	124.40
23	K1	106	BCR	C38-C26-C25	-2.74	121.50	124.48
23	L2	207	BCR	C15-C16-C17	-2.74	117.92	123.52
19	A1	827	CLA	C3B-C4B-NB	-2.74	108.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	846	CLA	C3B-C4B-NB	-2.74	108.09	110.53
19	B	854	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
19	K2	104	CLA	C3B-C4B-NB	-2.74	108.09	110.53
19	X	101	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
24	A2	854	AJP	C11-C16-C15	-2.73	104.34	109.17
24	L1	204	AJP	C21-C22-C23	2.73	114.12	110.46
19	A1	820	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	A1	824	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	A2	806	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	B2	805	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	AA	802	AJP	C81-C12-C11	2.73	117.52	111.58
20	AA	803	CL0	C9-C8-C7	2.73	121.01	111.27
23	LL	204	BCR	C27-C26-C25	2.73	126.39	122.70
19	KK	101	CLA	O2D-CGD-CBD	2.73	116.00	111.23
23	I2	101	BCR	C8-C7-C6	-2.73	119.71	127.00
19	A	809	CLA	CHB-C4A-NA	2.73	128.34	124.40
19	B2	819	CLA	C3B-C4B-NB	-2.73	108.10	110.53
19	KK	102	CLA	C3B-C4B-NB	-2.73	108.10	110.53
24	B	849	AJP	C01-C02-C03	2.73	118.04	112.08
19	K1	102	CLA	O2D-CGD-CBD	2.73	115.99	111.23
23	I2	102	BCR	C2-C1-C6	2.72	114.40	110.44
19	A2	824	CLA	CHB-C4A-NA	2.72	128.33	124.40
19	B1	814	CLA	CHB-C4A-NA	2.72	128.33	124.40
19	B1	803	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	A	834	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	FF	305	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	BB	848	AJP	C24-C19-C20	2.72	115.56	112.66
19	B2	814	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	BB	806	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	F	301	CLA	C2A-C1A-CHA	2.72	128.59	123.87
19	BB	809	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	BB	832	CLA	CED-O2D-CGD	2.72	122.09	115.92
19	A2	835	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	B2	849	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	A2	807	CLA	CHB-C4A-NA	2.72	128.33	124.40
19	BB	819	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	B	834	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
19	A1	817	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	A2	837	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	A	807	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
22	L2	208	LHG	O4-P-O5	2.72	125.09	112.44
22	B	853	LHG	O4-P-O5	2.72	125.09	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	834	CLA	CAA-C2A-C3A	-2.72	105.66	113.00
19	F2	302	CLA	CHB-C4A-NA	2.72	128.32	124.40
19	A1	816	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	A	829	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	X2	101	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	A	810	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
23	L1	209	BCR	C33-C5-C6	-2.71	121.52	124.48
23	L2	207	BCR	C33-C5-C6	-2.71	121.52	124.48
22	X2	103	LHG	O4-P-O5	2.71	125.07	112.44
19	B2	811	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	AA	822	CLA	C3B-C4B-NB	-2.71	108.11	110.53
24	KK	104	AJP	C01-C02-C03	2.71	118.01	112.08
19	K1	103	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	AA	847	LHG	O4-P-O5	2.71	125.07	112.44
19	A1	805	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A1	837	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A	816	CLA	CHB-C4A-NA	2.71	128.31	124.40
19	AA	815	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	B2	851	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A	811	CLA	CHB-C4A-NA	2.71	128.31	124.40
19	A	828	CLA	CHB-C4A-NA	2.71	128.31	124.40
19	F	301	CLA	CAA-C2A-C3A	-2.71	105.68	113.00
19	K1	102	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A2	802	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
19	A2	842	CLA	CHB-C4A-NA	2.71	128.31	124.40
23	F1	303	BCR	C2-C1-C6	2.71	114.37	110.44
19	BB	811	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	BB	841	BCR	C28-C27-C26	-2.71	109.23	114.06
24	L1	204	AJP	C24-C19-C20	2.70	115.54	112.66
19	A1	833	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
19	B1	836	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	J	104	BCR	C27-C26-C25	2.70	126.36	122.70
23	FF	304	BCR	C27-C26-C25	2.70	126.36	122.70
19	B2	822	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	AA	846	LHG	O4-P-O5	2.70	125.02	112.44
19	A1	822	CLA	CHB-C4A-NA	2.70	128.30	124.40
19	AA	843	CLA	CHD-C4C-C3C	2.70	128.71	124.77
23	F2	304	BCR	C27-C26-C25	2.70	126.36	122.70
19	B1	808	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
23	K2	103	BCR	C27-C26-C25	2.70	126.35	122.70
19	B	806	CLA	CHB-C4A-NA	2.70	128.30	124.40
19	K	102	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	L1	201	BCR	C2-C1-C6	2.70	114.36	110.44
19	BB	825	CLA	O2D-CGD-CBD	2.70	115.95	111.23
23	F1	304	BCR	C27-C26-C25	2.70	126.35	122.70
19	A	842	CLA	CHB-C4A-NA	2.70	128.30	124.40
19	A1	830	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
19	A1	808	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	B1	847	LHG	O4-P-O5	2.70	125.00	112.44
23	A1	851	BCR	C3-C4-C5	-2.70	109.24	114.06
23	L1	209	BCR	C15-C16-C17	-2.70	118.00	123.52
19	B1	805	CLA	CHB-C4A-NA	2.70	128.29	124.40
19	B1	830	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
19	B2	817	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	I1	101	BCR	C38-C26-C25	-2.70	121.54	124.48
23	F	303	BCR	C27-C26-C25	2.70	126.35	122.70
22	A	845	LHG	O4-P-O5	2.70	124.98	112.44
24	A1	855	AJP	C04-C05-C06	2.69	120.54	115.66
19	B2	837	CLA	C3B-C4B-NB	-2.69	108.12	110.53
22	A1	845	LHG	O4-P-O5	2.69	124.98	112.44
22	LL	205	LHG	O4-P-O5	2.69	124.98	112.44
22	L	207	LHG	O4-P-O5	2.69	124.97	112.44
19	A1	841	CLA	CHB-C4A-NA	2.69	128.29	124.40
19	B2	806	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	BB	808	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	J2	102	BCR	C1-C6-C5	-2.69	118.96	122.64
19	A1	835	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	A2	816	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	BB	825	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	A2	815	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
23	K1	104	BCR	C27-C26-C25	2.69	126.34	122.70
23	J2	104	BCR	C27-C26-C25	2.69	126.34	122.70
23	II	104	BCR	C33-C5-C6	-2.69	121.55	124.48
19	B2	820	CLA	CBC-CAC-C3C	2.69	119.71	112.42
19	A1	801	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	B	846	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	BB	845	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	A2	842	CLA	C4-C3-C5	2.69	119.89	115.23
19	BB	824	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	L1	203	AJP	C18-C19-C20	2.69	116.82	112.31
19	AA	810	CLA	CBA-CAA-C2A	2.69	121.79	113.79
19	A2	834	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
22	XX	102	LHG	O4-P-O5	2.69	124.94	112.44
19	L	202	CLA	CHB-C4A-NA	2.69	128.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	817	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
23	K1	106	BCR	C33-C5-C6	-2.68	121.56	124.48
23	B2	843	BCR	C15-C16-C17	-2.68	118.03	123.52
19	AA	808	CLA	C3B-C4B-NB	-2.68	108.13	110.53
19	F1	302	CLA	O2D-CGD-CBD	2.68	115.92	111.23
19	L1	206	CLA	O2D-CGD-CBD	2.68	115.92	111.23
24	A1	854	AJP	C04-C05-C06	2.68	120.52	115.66
19	X	101	CLA	CHB-C4A-NA	2.68	128.27	124.40
23	A2	848	BCR	C15-C16-C17	-2.68	118.03	123.52
19	AA	831	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	A2	845	LHG	O4-P-O5	2.68	124.92	112.44
22	X	102	LHG	O4-P-O5	2.68	124.92	112.44
19	B	834	CLA	CHB-C4A-NA	2.68	128.27	124.40
19	AA	835	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
19	BB	811	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
19	A1	841	CLA	C4-C3-C5	2.68	119.88	115.23
23	J1	102	BCR	C1-C6-C5	-2.68	118.97	122.64
19	A2	817	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	A	803	CL0	CMD-C2D-C3D	-2.68	119.33	124.68
19	A	836	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	A1	842	CLA	CHD-C4C-C3C	2.68	128.68	124.77
19	L1	206	CLA	C1-O2A-CGA	2.68	123.13	116.65
19	AA	811	CLA	CHB-C4A-NA	2.68	128.26	124.40
19	B2	808	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	A1	834	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	B2	806	CLA	CHB-C4A-NA	2.68	128.26	124.40
19	B2	817	CLA	CHB-C4A-NA	2.68	128.26	124.40
19	B	832	CLA	CHB-C4A-NA	2.68	128.26	124.40
19	BB	805	CLA	CHB-C4A-NA	2.68	128.26	124.40
19	BB	833	CLA	CHB-C4A-NA	2.68	128.26	124.40
24	BB	848	AJP	C18-C17-C16	2.68	116.42	112.16
19	BB	815	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	F1	301	CLA	C2A-C1A-CHA	2.67	128.51	123.87
24	A1	854	AJP	C15-C20-C19	2.67	112.23	108.51
19	BB	831	CLA	CHB-C4A-NA	2.67	128.26	124.40
26	B2	841	ECH	C21-C20-C19	-2.67	115.45	123.20
23	A1	848	BCR	C33-C5-C6	-2.67	121.57	124.48
19	B	820	CLA	CBC-CAC-C3C	2.67	119.67	112.42
19	B1	848	CLA	CHB-C4A-NA	2.67	128.26	124.40
23	AA	854	BCR	C2-C1-C6	2.67	114.32	110.44
19	A1	806	CLA	CHB-C4A-NA	2.67	128.26	124.40
19	AA	836	CLA	C3B-C4B-NB	-2.67	108.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	L	205	BCR	C2-C1-C6	2.67	114.32	110.44
22	BB	851	LHG	O4-P-O5	2.67	124.86	112.44
24	A1	855	AJP	C12-C07-C06	2.67	128.39	120.50
23	A	853	BCR	C2-C1-C6	2.67	114.32	110.44
23	A2	848	BCR	C33-C5-C6	-2.67	121.57	124.48
25	II	105	LMG	O6-C1-O1	-2.67	103.74	110.04
23	BB	843	BCR	C27-C26-C25	2.67	126.31	122.70
24	L	208	AJP	C81-C12-C11	2.67	117.39	111.58
19	AA	816	CLA	CHB-C4A-NA	2.67	128.25	124.40
19	B	814	CLA	C3B-C4B-NB	-2.67	108.15	110.53
19	BB	833	CLA	C3A-C2A-C1A	2.67	105.33	101.34
19	L1	205	CLA	CHB-C4A-NA	2.67	128.25	124.40
23	I2	103	BCR	C2-C1-C6	2.67	114.31	110.44
19	A1	830	CLA	C3B-C4B-NB	-2.67	108.15	110.53
19	A1	815	CLA	CHB-C4A-NA	2.67	128.25	124.40
19	B1	817	CLA	CHB-C4A-NA	2.67	128.25	124.40
19	X1	101	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
19	A2	839	CLA	C3B-C4B-NB	-2.66	108.15	110.53
19	L	202	CLA	C3B-C4B-NB	-2.66	108.15	110.53
19	A	813	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
19	B2	802	CLA	CHB-C4A-NA	2.66	128.25	124.40
23	K2	105	BCR	C33-C5-C6	-2.66	121.58	124.48
23	FF	306	BCR	C24-C23-C22	-2.66	122.29	126.23
22	X1	102	LHG	O4-P-O5	2.66	124.84	112.44
19	A	820	CLA	CHB-C4A-NA	2.66	128.24	124.40
24	M2	101	AJP	C17-C18-C19	2.66	116.99	111.84
24	B	850	AJP	C83-C06-C07	2.66	119.82	114.50
19	A1	823	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
24	M2	101	AJP	C13-C12-C07	-2.66	111.57	115.36
19	B	807	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
23	FF	303	BCR	C27-C26-C25	2.66	126.30	122.70
24	K	104	AJP	C01-C02-C03	2.66	117.90	112.08
24	L1	204	AJP	C04-C03-C02	-2.66	106.36	111.67
22	X2	102	LHG	O4-P-O5	2.66	124.82	112.44
19	A	815	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	B1	840	ECH	C21-C20-C19	-2.66	115.50	123.20
23	I	101	BCR	C8-C7-C6	-2.66	119.89	127.00
19	B1	833	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
24	L2	202	AJP	C03-C04-C05	2.66	116.10	111.93
23	B	842	BCR	C30-C25-C26	-2.66	119.00	122.64
23	II	104	BCR	C27-C26-C25	2.66	126.30	122.70
19	B	804	CLA	C1-C2-C3	-2.66	121.84	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	853	BCR	C33-C5-C6	-2.66	121.58	124.48
19	K	101	CLA	CHB-C4A-NA	2.66	128.24	124.40
24	A2	854	AJP	C20-C21-C22	-2.66	109.80	114.17
19	A	829	CLA	CHB-C4A-NA	2.66	128.23	124.40
19	B	823	CLA	CHB-C4A-NA	2.66	128.23	124.40
19	AA	843	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	F	302	CLA	CHB-C4A-NA	2.66	128.23	124.40
23	A1	853	BCR	C15-C14-C13	-2.65	123.56	127.28
23	F1	303	BCR	C27-C26-C25	2.65	126.29	122.70
19	A	826	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	XX	101	CLA	CHB-C4A-NA	2.65	128.23	124.40
19	A1	803	CLA	C1-C2-C3	-2.65	121.85	126.20
19	B	810	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	AA	854	BCR	C33-C5-C6	-2.65	121.59	124.48
23	A2	851	BCR	C3-C4-C5	-2.65	109.33	114.06
19	AA	821	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	A1	805	CLA	O2D-CGD-CBD	2.65	115.86	111.23
24	L2	202	AJP	O84-C05-C04	2.65	113.07	110.76
23	K	103	BCR	C24-C23-C22	-2.65	122.31	126.23
19	B	810	CLA	CHB-C4A-NA	2.65	128.22	124.40
23	A2	853	BCR	C2-C1-C6	2.65	114.29	110.44
19	L2	204	CLA	CHB-C4A-NA	2.65	128.22	124.40
24	M2	101	AJP	O84-C05-C04	2.65	113.07	110.76
19	AA	813	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
19	A	842	CLA	C6-C5-C3	2.65	119.92	113.47
19	B2	815	CLA	C3B-C4B-NB	-2.65	108.17	110.53
19	BB	820	CLA	C3B-C4B-NB	-2.65	108.17	110.53
26	B2	841	ECH	C40-C30-C25	2.65	114.39	110.24
23	F2	303	BCR	C27-C26-C25	2.65	126.28	122.70
19	A1	816	CLA	CHB-C4A-NA	2.65	128.22	124.40
19	X1	101	CLA	CHB-C4A-NA	2.65	128.22	124.40
19	A2	841	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	B2	841	ECH	C29-C30-C25	-2.65	106.59	110.44
19	BB	834	CLA	C3B-C4B-NB	-2.65	108.17	110.53
23	J1	104	BCR	C27-C26-C25	2.65	126.28	122.70
19	BB	856	CLA	C6-C5-C3	2.64	119.91	113.47
19	LL	203	CLA	CAC-C3C-C4C	2.64	128.23	124.79
19	A2	807	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
19	B1	835	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
23	A2	847	BCR	C2-C1-C6	2.64	114.28	110.44
19	BB	821	CLA	CHB-C4A-NA	2.64	128.22	124.40
19	B	809	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	809	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	AA	842	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	B2	804	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	AA	804	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	A2	824	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	A1	847	BCR	C23-C22-C21	-2.64	118.61	124.72
19	A2	825	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	A	853	BCR	C33-C5-C6	-2.64	121.60	124.48
22	BB	850	LHG	O4-P-O5	2.64	124.73	112.44
19	B	808	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	II	104	BCR	C2-C1-C6	2.64	114.27	110.44
26	B1	840	ECH	C29-C30-C25	-2.64	106.61	110.44
19	BB	823	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	B2	852	CLA	CHD-C4C-C3C	2.64	128.62	124.77
19	A1	825	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
19	A2	817	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
19	L2	205	CLA	C3B-C4B-NB	-2.64	108.17	110.53
19	B	825	CLA	C3B-C4B-NB	-2.64	108.17	110.53
19	AA	845	CLA	CHB-C4A-NA	2.64	128.21	124.40
19	A	822	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	L	205	BCR	C27-C26-C25	2.64	126.27	122.70
23	A2	847	BCR	C23-C22-C21	-2.64	118.62	124.72
23	A1	847	BCR	C2-C1-C6	2.64	114.27	110.44
19	BB	804	CLA	CHB-C4A-NA	2.64	128.21	124.40
24	B	850	AJP	C15-C20-C19	2.64	112.18	108.51
19	A2	813	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
19	BB	832	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
19	J	103	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
19	A2	809	CLA	CHB-C4A-NA	2.64	128.20	124.40
19	B2	815	CLA	CHB-C4A-NA	2.64	128.20	124.40
19	AA	820	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	A1	840	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	BB	833	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	A	801	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
25	B1	846	LMG	O6-C1-O1	-2.63	103.82	110.04
19	B1	833	CLA	C2A-C1A-CHA	2.63	128.44	123.87
22	B	852	LHG	O4-P-O5	2.63	124.69	112.44
19	BB	806	CLA	CHB-C4A-NA	2.63	128.20	124.40
19	A1	840	CLA	CHB-C4A-NA	2.63	128.20	124.40
19	B1	813	CLA	CHB-C4A-NA	2.63	128.20	124.40
19	BB	810	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	B	804	CLA	CHB-C4A-NA	2.63	128.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	I1	101	BCR	C24-C23-C22	-2.63	122.34	126.23
19	B	821	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	B1	820	CLA	O2D-CGD-CBD	2.63	115.83	111.23
19	A1	812	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
23	LL	204	BCR	C33-C5-C6	-2.63	121.61	124.48
19	B	818	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	I2	104	AJP	O84-C05-C04	2.63	113.05	110.76
23	KK	103	BCR	C24-C23-C22	-2.63	122.35	126.23
19	LL	203	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	AA	842	CLA	C4-C3-C5	2.63	119.79	115.23
19	FF	302	CLA	CHB-C4A-NA	2.63	128.19	124.40
23	L1	209	BCR	C11-C10-C9	-2.62	123.60	127.28
19	B1	806	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	A2	821	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	A	806	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
23	I2	103	BCR	C7-C8-C9	-2.62	122.36	126.23
24	B	850	AJP	C18-C17-C16	2.62	116.34	112.16
19	A	820	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
23	FF	304	BCR	C15-C16-C17	-2.62	118.16	123.52
19	B2	811	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
23	B1	841	BCR	C28-C27-C26	-2.62	109.38	114.06
19	A1	823	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	AA	803	CL0	C9-C8-C10	2.62	120.61	111.27
19	B	811	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
24	A2	854	AJP	C12-C07-C06	2.62	128.24	120.50
19	A1	838	CLA	CHB-C4A-NA	2.62	128.18	124.40
19	B1	811	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	AA	839	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	A1	834	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	A	826	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	A2	838	CLA	C3B-C4B-NB	-2.62	108.19	110.53
20	AA	803	CL0	C1-O2A-CGA	-2.62	110.32	116.65
23	A2	851	BCR	C24-C23-C22	-2.62	122.36	126.23
19	FF	302	CLA	O2D-CGD-CBD	2.62	115.80	111.23
19	A2	808	CLA	CHB-C4A-NA	2.62	128.18	124.40
19	A	828	CLA	C3B-C4B-NB	-2.62	108.19	110.53
23	I	102	BCR	C33-C5-C6	-2.62	121.63	124.48
19	A1	841	CLA	C6-C5-C3	2.62	119.84	113.47
19	B1	809	CLA	CHB-C4A-NA	2.62	128.17	124.40
19	B	859	CLA	C6-C5-C3	2.61	119.84	113.47
19	LL	201	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	BB	807	CLA	O2A-CGA-O1A	-2.61	117.09	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	II	102	BCR	C7-C8-C9	-2.61	122.37	126.23
19	A1	808	CLA	CHB-C4A-NA	2.61	128.17	124.40
19	BB	836	CLA	O2D-CGD-CBD	2.61	115.80	111.23
23	FF	303	BCR	C8-C7-C6	-2.61	120.02	127.00
20	A1	802	CL0	CMB-C2B-C3B	2.61	129.90	124.68
19	K1	102	CLA	CHB-C4A-NA	2.61	128.17	124.40
23	AA	848	BCR	C23-C22-C21	-2.61	118.69	124.72
22	L1	211	LHG	O4-P-O5	2.61	124.58	112.44
23	L	205	BCR	C33-C5-C6	-2.61	121.64	124.48
23	B	843	BCR	C15-C16-C17	-2.61	118.18	123.52
19	AA	843	CLA	CHB-C4A-NA	2.61	128.16	124.40
24	BB	849	AJP	C18-C19-C20	2.61	116.69	112.31
24	L2	202	AJP	C01-C02-C03	2.61	117.78	112.08
23	K	103	BCR	C38-C26-C25	-2.61	121.64	124.48
19	A2	811	CLA	CHB-C4A-NA	2.61	128.16	124.40
19	AA	834	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
19	B	834	CLA	C3A-C2A-C1A	2.61	105.24	101.34
19	A2	825	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	A2	839	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	AA	807	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
23	AA	852	BCR	C1-C6-C5	-2.60	119.08	122.64
23	F1	306	BCR	C27-C26-C25	2.60	126.22	122.70
19	AA	822	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
19	A1	835	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	AA	808	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	B1	836	CLA	O2D-CGD-CBD	2.60	115.78	111.23
23	F	305	BCR	C7-C8-C9	-2.60	122.38	126.23
23	KK	103	BCR	C38-C26-C25	-2.60	121.64	124.48
19	BB	812	CLA	C3B-C4B-NB	-2.60	108.21	110.53
23	I2	103	BCR	C33-C5-C6	-2.60	121.64	124.48
19	A	838	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	B	850	AJP	C18-C19-C20	2.60	116.67	112.31
19	B	833	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
19	F2	301	CLA	C2A-C1A-CHA	2.60	128.38	123.87
24	I2	104	AJP	C18-C19-C20	2.60	116.67	112.31
19	B1	815	CLA	O2D-CGD-CBD	2.60	115.77	111.23
19	B1	835	CLA	CHB-C4A-NA	2.60	128.15	124.40
19	B2	837	CLA	O2D-CGD-CBD	2.60	115.77	111.23
19	B	803	CLA	CHB-C4A-NA	2.60	128.15	124.40
23	L	205	BCR	C24-C23-C22	-2.60	122.39	126.23
19	A2	842	CLA	C6-C5-C3	2.60	119.79	113.47
24	A1	854	AJP	C13-C14-C15	2.60	117.55	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A1	855	AJP	C20-C21-C22	-2.60	109.90	114.17
23	A1	853	BCR	C2-C1-C6	2.60	114.21	110.44
23	I2	103	BCR	C27-C26-C25	2.60	126.21	122.70
19	X2	101	CLA	CHB-C4A-NA	2.60	128.15	124.40
19	B	854	CLA	CHB-C4A-NA	2.60	128.15	124.40
19	B	825	CLA	O2D-CGD-CBD	2.59	115.77	111.23
23	AA	848	BCR	C2-C1-C6	2.59	114.21	110.44
19	K2	102	CLA	O2D-CGD-CBD	2.59	115.76	111.23
19	BB	852	CLA	CHB-C4A-NA	2.59	128.14	124.40
23	AA	854	BCR	C15-C14-C13	-2.59	123.64	127.28
19	AA	831	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
19	BB	833	CLA	CMB-C2B-C3B	2.59	132.64	126.55
19	A1	852	CLA	C6-C5-C3	2.59	119.78	113.47
23	II	101	BCR	C2-C1-C6	2.59	114.20	110.44
19	KK	101	CLA	CHB-C4A-NA	2.59	128.14	124.40
19	B2	825	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	AA	813	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	LL	201	CLA	CHB-C4A-NA	2.59	128.13	124.40
19	A2	810	CLA	CBA-CAA-C2A	2.59	121.49	113.79
19	B2	832	CLA	CHB-C4A-NA	2.59	128.13	124.40
23	L1	208	BCR	C33-C5-C6	-2.59	121.66	124.48
19	BB	822	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	AA	810	CLA	O2D-CGD-CBD	2.59	115.75	111.23
19	A2	832	CLA	CHB-C4A-NA	2.59	128.13	124.40
19	B2	828	CLA	O2D-CGD-O1D	-2.59	118.82	123.85
23	BB	838	BCR	C33-C5-C6	-2.58	121.66	124.48
23	F2	305	BCR	C27-C26-C25	2.58	126.20	122.70
23	J	102	BCR	C1-C6-C5	-2.58	119.11	122.64
19	A	830	CLA	C3B-C4B-NB	-2.58	108.22	110.53
23	I	101	BCR	C2-C1-C6	2.58	114.19	110.44
19	B2	815	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
19	B	860	CLA	CHD-C4C-C3C	2.58	128.54	124.77
19	A	842	CLA	C5-C3-C2	-2.58	115.37	121.17
23	I	102	BCR	C7-C8-C9	-2.58	122.42	126.23
23	A	853	BCR	C15-C14-C13	-2.58	123.66	127.28
20	A1	802	CL0	CMC-C2C-C1C	2.58	129.38	124.73
23	A2	853	BCR	C15-C14-C13	-2.58	123.66	127.28
19	B	831	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	AA	810	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	BB	845	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	B	820	CLA	CAC-C3C-C2C	-2.58	122.82	127.56
23	B1	842	BCR	C2-C1-C6	2.58	114.19	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	809	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	BB	809	CLA	O2D-CGD-CBD	2.58	115.74	111.23
19	B1	845	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	BB	810	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	B2	834	CLA	C2A-C1A-CHA	2.58	128.34	123.87
19	B2	833	CLA	C5-C3-C2	2.58	126.95	121.17
23	A	847	BCR	C23-C22-C21	-2.58	118.76	124.72
19	A1	806	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	A	839	CLA	C3B-C4B-NB	-2.58	108.23	110.53
23	I2	101	BCR	C38-C26-C25	-2.57	121.67	124.48
23	B	839	BCR	C33-C5-C6	-2.57	121.68	124.48
23	II	102	BCR	C33-C5-C6	-2.57	121.68	124.48
19	B	811	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	J	102	BCR	C27-C26-C25	2.57	126.18	122.70
24	L2	202	AJP	C85-O84-C05	2.57	118.13	113.69
19	B	833	CLA	CED-O2D-CGD	2.57	121.75	115.92
19	B2	833	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
19	B	820	CLA	O2D-CGD-CBD	2.57	115.73	111.23
19	B2	846	CLA	CHB-C4A-NA	2.57	128.11	124.40
19	B2	835	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	AA	856	AJP	C17-C18-C19	2.57	116.81	111.84
19	A	810	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	A	847	BCR	C2-C1-C6	2.57	114.17	110.44
19	BB	826	CLA	CHB-C1B-NB	2.57	127.91	124.05
23	M	101	BCR	C15-C14-C13	-2.57	123.67	127.28
19	A	844	CLA	CHB-C4A-NA	2.57	128.11	124.40
19	AA	832	CLA	O2D-CGD-CBD	2.57	115.72	111.23
19	AA	801	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
23	J	104	BCR	C15-C16-C17	-2.57	118.26	123.52
23	K	103	BCR	C2-C1-C6	2.57	114.17	110.44
19	LL	202	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	A1	814	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	AA	826	CLA	C3B-C4B-NB	-2.57	108.24	110.53
19	A2	831	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	AA	829	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	JJ	103	CLA	C3B-C4B-NB	-2.57	108.24	110.53
19	A1	810	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	B	815	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	B	809	CLA	O2D-CGD-CBD	2.56	115.71	111.23
23	BB	839	BCR	C8-C7-C6	-2.56	120.15	127.00
19	BB	815	CLA	CHB-C4A-NA	2.56	128.10	124.40
23	L1	201	BCR	C33-C5-C6	-2.56	121.69	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J1	103	CLA	C3B-C4B-NB	-2.56	108.24	110.53
19	B1	823	CLA	CHB-C4A-NA	2.56	128.10	124.40
19	A	821	CLA	C3B-C4B-NB	-2.56	108.24	110.53
24	BB	849	AJP	C11-C16-C15	-2.56	104.64	109.17
19	B1	832	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
24	KK	104	AJP	C06-C07-C08	-2.56	100.16	104.28
23	J1	104	BCR	C15-C16-C17	-2.56	118.28	123.52
19	B	859	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
19	B	824	CLA	C3B-C4B-NB	-2.56	108.25	110.53
19	A2	822	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	A2	814	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
23	B2	842	BCR	C28-C27-C26	-2.56	109.50	114.06
19	A	831	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
23	A	850	BCR	C8-C7-C6	-2.56	120.17	127.00
19	AA	838	CLA	O2D-CGD-CBD	2.56	115.70	111.23
19	BB	830	CLA	C3B-C4B-NB	-2.56	108.25	110.53
19	BB	830	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	B2	836	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
19	A	813	CLA	C3B-C4B-NB	-2.56	108.25	110.53
19	L	202	CLA	C4-C3-C2	-2.55	117.07	123.63
24	L1	204	AJP	C18-C17-C16	2.55	116.23	112.16
22	B2	848	LHG	O4-P-O5	2.55	124.32	112.44
19	K	101	CLA	O2D-CGD-CBD	2.55	115.69	111.23
23	A2	847	BCR	C33-C5-C6	-2.55	121.70	124.48
23	FF	304	BCR	C38-C26-C25	-2.55	121.70	124.48
19	B	821	CLA	C5-C3-C2	2.55	126.89	121.17
19	AA	838	CLA	C3B-C4B-NB	-2.55	108.25	110.53
19	A1	828	CLA	CHB-C4A-NA	2.55	128.08	124.40
23	F	303	BCR	C8-C7-C6	-2.55	120.19	127.00
24	I2	104	AJP	C15-C20-C19	2.55	112.06	108.51
23	JJ	102	BCR	C2-C1-C6	2.55	114.14	110.44
23	A	847	BCR	C33-C5-C6	-2.55	121.70	124.48
19	AA	807	CLA	CHB-C4A-NA	2.55	128.08	124.40
24	L2	203	AJP	C11-C12-C07	-2.55	96.32	100.16
24	BB	849	AJP	C15-C20-C19	2.55	112.05	108.51
19	A1	803	CLA	CHB-C4A-NA	2.55	128.07	124.40
19	A1	809	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
19	B	802	CLA	CHB-C4A-NA	2.54	128.07	124.40
19	AA	810	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	A	855	AJP	C17-C18-C19	2.54	116.76	111.84
19	B2	803	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	I2	105	LMG	O6-C1-O1	-2.54	104.04	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K1	106	BCR	C28-C27-C26	-2.54	109.53	114.06
19	B2	810	CLA	C4-C3-C5	2.54	119.64	115.23
23	B	840	BCR	C28-C27-C26	-2.54	109.53	114.06
26	B2	841	ECH	C37-C22-C21	2.54	126.93	122.82
23	AA	851	BCR	C8-C7-C6	-2.54	120.21	127.00
19	B1	804	CLA	CHB-C4A-NA	2.54	128.06	124.40
23	A1	848	BCR	C15-C16-C17	-2.54	118.33	123.52
23	L	206	BCR	C11-C10-C9	-2.54	123.72	127.28
23	F2	304	BCR	C33-C5-C6	-2.53	121.72	124.48
23	L1	208	BCR	C27-C26-C25	2.53	126.13	122.70
19	B	820	CLA	CHB-C4A-NA	2.53	128.06	124.40
19	B	846	CLA	CHB-C4A-NA	2.53	128.06	124.40
19	L2	204	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	B	815	CLA	CMB-C2B-C3B	2.53	132.51	126.55
23	JJ	104	BCR	C15-C16-C17	-2.53	118.34	123.52
23	B1	839	BCR	C33-C5-C6	-2.53	121.72	124.48
19	B	833	CLA	C2A-C1A-CHA	2.53	128.26	123.87
23	F1	304	BCR	C15-C16-C17	-2.53	118.34	123.52
19	BB	832	CLA	C2A-C1A-CHA	2.53	128.26	123.87
19	AA	821	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
23	I	101	BCR	C24-C23-C22	-2.53	122.50	126.23
23	B2	843	BCR	C2-C1-C6	2.53	114.11	110.44
23	KK	103	BCR	C2-C1-C6	2.53	114.11	110.44
22	B1	847	LHG	P-O3-C3	-2.53	106.86	121.35
19	J2	103	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	A2	842	CLA	C5-C3-C2	-2.53	115.50	121.17
23	BB	838	BCR	C15-C16-C17	-2.53	118.35	123.52
19	AA	815	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
19	B1	832	CLA	C5-C3-C2	2.52	126.83	121.17
19	K1	103	CLA	C3B-C4B-NB	-2.52	108.28	110.53
19	BB	856	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
23	A2	851	BCR	C1-C6-C5	-2.52	119.19	122.64
23	B1	842	BCR	C27-C26-C25	2.52	126.11	122.70
20	A1	802	CL0	C4C-C3C-C2C	-2.52	103.41	113.37
19	A1	821	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	BB	813	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	B2	820	CLA	O2D-CGD-CBD	2.52	115.64	111.23
19	A	832	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	A2	802	CLA	C3B-C4B-NB	-2.52	108.28	110.53
26	B	841	ECH	C37-C22-C21	2.52	126.90	122.82
24	AA	856	AJP	C12-C07-C06	2.52	127.94	120.50
19	B	835	CLA	CED-O2D-CGD	2.52	121.63	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	JJ	102	BCR	C27-C26-C25	2.52	126.11	122.70
19	B1	825	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	A	855	AJP	C12-C07-C06	2.52	127.94	120.50
19	A2	836	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	K2	102	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	A2	826	CLA	CHB-C4A-NA	2.52	128.03	124.40
23	K2	105	BCR	C1-C6-C5	-2.52	119.20	122.64
19	A1	809	CLA	CHB-C4A-NA	2.51	128.03	124.40
24	L1	204	AJP	C12-C07-C06	2.51	127.93	120.50
19	B2	836	CLA	CHB-C4A-NA	2.51	128.03	124.40
19	A2	844	CLA	CHB-C4A-NA	2.51	128.03	124.40
23	I2	101	BCR	C24-C23-C22	-2.51	122.52	126.23
19	BB	835	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	JJ	102	BCR	C1-C6-C5	-2.51	119.21	122.64
19	A1	844	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	B1	821	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	B1	831	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	B	834	CLA	CMB-C2B-C3B	2.51	132.45	126.55
19	B	860	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	A	854	BCR	C1-C6-C5	-2.51	119.21	122.64
19	B	836	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	M2	102	BCR	C35-C13-C14	-2.51	118.75	122.82
23	BB	839	BCR	C28-C27-C26	-2.51	109.58	114.06
19	B2	834	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
19	B	837	CLA	C3B-C4B-NB	-2.51	108.29	110.53
19	BB	820	CLA	CBC-CAC-C3C	2.51	119.21	112.42
23	I2	102	BCR	C15-C16-C17	-2.51	118.39	123.52
20	AA	803	CL0	C4C-C3C-C2C	-2.51	103.47	113.37
23	M	101	BCR	C24-C23-C22	-2.51	122.53	126.23
19	A	824	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	JJ	104	BCR	C27-C26-C25	2.50	126.09	122.70
19	A2	826	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
23	I	101	BCR	C15-C16-C17	-2.50	118.40	123.52
23	F	304	BCR	C38-C26-C25	-2.50	121.75	124.48
19	A1	841	CLA	C5-C3-C2	-2.50	115.55	121.17
19	AA	822	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	BB	849	AJP	C06-C07-C08	-2.50	100.26	104.28
23	L1	201	BCR	C7-C8-C9	-2.50	122.54	126.23
19	BB	828	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	B1	832	CLA	CED-O2D-CGD	2.50	121.58	115.92
23	B2	840	BCR	C28-C27-C26	-2.50	109.60	114.06
19	A	831	CLA	C3B-C4B-NB	-2.50	108.30	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B2	823	CLA	CHB-C4A-NA	2.50	128.00	124.40
19	B1	828	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
21	A	843	PQN	C15-C13-C12	-2.50	115.56	121.17
24	KK	104	AJP	C81-C12-C11	2.50	117.01	111.58
24	L1	204	AJP	C11-C12-C07	-2.50	96.40	100.16
23	AA	855	BCR	C28-C27-C26	-2.50	109.60	114.06
19	B	834	CLA	C2A-C1A-CHA	2.50	128.20	123.87
24	BB	849	AJP	C13-C12-C07	-2.49	111.81	115.36
24	B	850	AJP	C81-C12-C11	2.49	117.01	111.58
19	B1	833	CLA	CMB-C2B-C3B	2.49	132.42	126.55
19	A2	813	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	L1	205	CLA	C3B-C4B-NB	-2.49	108.30	110.53
24	L	209	AJP	C24-C19-C18	-2.49	108.37	112.75
24	KK	104	AJP	O84-C05-C04	-2.49	108.59	110.76
19	A1	829	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	A	841	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	B	837	CLA	O2D-CGD-CBD	2.49	115.59	111.23
23	L1	201	BCR	C15-C16-C17	-2.49	118.42	123.52
23	F1	306	BCR	C7-C8-C9	-2.49	122.55	126.23
23	F1	303	BCR	C11-C10-C9	-2.49	123.78	127.28
19	B2	831	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	M2	102	BCR	C24-C23-C22	-2.49	122.55	126.23
23	B	843	BCR	C33-C5-C6	-2.49	121.77	124.48
19	BB	820	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	B2	825	CLA	O2D-CGD-CBD	2.49	115.58	111.23
19	A1	811	CLA	CBA-CAA-C2A	2.49	121.20	113.79
19	BB	826	CLA	O2D-CGD-CBD	2.49	115.58	111.23
19	BB	805	CLA	O2D-CGD-CBD	2.49	115.58	111.23
19	L	204	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
19	AA	841	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	B2	812	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	A	841	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	AA	841	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	AA	848	BCR	C15-C16-C17	-2.49	118.43	123.52
23	MM	101	BCR	C15-C14-C13	-2.49	123.79	127.28
19	FF	301	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
19	K	102	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	BB	821	CLA	C5-C3-C2	2.49	126.75	121.17
19	AA	838	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	F1	304	BCR	C33-C5-C6	-2.48	121.77	124.48
23	M1	101	BCR	C24-C23-C22	-2.48	122.56	126.23
19	AA	824	CLA	CHB-C4A-NA	2.48	127.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A1	847	BCR	C33-C5-C6	-2.48	121.78	124.48
23	A1	853	BCR	C33-C5-C6	-2.48	121.78	124.48
23	F	304	BCR	C15-C16-C17	-2.48	118.44	123.52
23	F	303	BCR	C11-C10-C9	-2.48	123.80	127.28
24	B	849	AJP	C85-O84-C05	2.48	117.97	113.69
23	I2	101	BCR	C15-C16-C17	-2.48	118.44	123.52
19	A2	841	CLA	C3B-C4B-NB	-2.48	108.32	110.53
23	F2	305	BCR	C7-C8-C9	-2.48	122.57	126.23
19	A	807	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	L2	202	AJP	O25-C23-C24	-2.48	104.82	109.64
23	A1	849	BCR	C33-C5-C6	-2.48	121.78	124.48
23	BB	839	BCR	C33-C5-C6	-2.48	121.78	124.48
19	A	810	CLA	O2D-CGD-CBD	2.48	115.56	111.23
19	A1	837	CLA	CHB-C4A-NA	2.48	127.97	124.40
23	LL	204	BCR	C38-C26-C25	-2.48	121.78	124.48
23	L1	209	BCR	C27-C26-C25	2.48	126.05	122.70
23	A	847	BCR	C15-C16-C17	-2.48	118.45	123.52
19	A2	804	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	K	104	AJP	C81-C12-C11	2.48	116.97	111.58
23	J1	104	BCR	C38-C26-C25	-2.48	121.78	124.48
23	J2	102	BCR	C38-C26-C25	-2.48	121.78	124.48
23	L	205	BCR	C7-C8-C9	-2.47	122.57	126.23
23	B	843	BCR	C2-C1-C6	2.47	114.03	110.44
19	A	838	CLA	O2D-CGD-CBD	2.47	115.56	111.23
19	A1	831	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	A1	847	BCR	C15-C16-C17	-2.47	118.46	123.52
19	A	838	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	BB	842	BCR	C2-C1-C6	2.47	114.03	110.44
19	BB	826	CLA	C2D-C1D-ND	-2.47	107.68	110.13
23	J2	104	BCR	C33-C5-C6	-2.47	121.79	124.48
19	A2	820	CLA	CBA-CAA-C2A	2.47	121.15	113.79
19	B1	833	CLA	CHB-C1B-NB	2.47	127.76	124.05
19	B2	829	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
23	K2	105	BCR	C28-C27-C26	-2.47	109.65	114.06
23	I1	101	BCR	C15-C16-C17	-2.47	118.46	123.52
19	B2	849	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	AA	813	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	A2	830	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	L	204	CLA	CAC-C3C-C4C	2.47	128.00	124.79
19	BB	813	CLA	O2D-CGD-CBD	2.47	115.55	111.23
19	B	825	CLA	CHB-C4A-NA	2.47	127.96	124.40
23	J2	104	BCR	C38-C26-C25	-2.47	121.79	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	F	304	BCR	C27-C26-C25	2.47	126.04	122.70
19	B	826	CLA	C6-C5-C3	2.47	119.48	113.47
19	B1	812	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	B1	830	CLA	CHB-C4A-NA	2.47	127.96	124.40
23	BB	842	BCR	C27-C26-C25	2.47	126.04	122.70
19	B1	826	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	B	821	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	B	822	CLA	CHB-C4A-NA	2.46	127.96	124.40
23	M1	101	BCR	C35-C13-C14	-2.46	118.82	122.82
23	A2	853	BCR	C30-C25-C26	-2.46	119.27	122.64
24	A	802	AJP	C85-O84-C05	2.46	117.94	113.69
19	B2	852	CLA	CHB-C4A-NA	2.46	127.96	124.40
22	A	846	LHG	P-O3-C3	-2.46	107.23	121.35
19	A	804	CLA	C1-C2-C3	-2.46	122.16	126.20
23	FF	306	BCR	C7-C8-C9	-2.46	122.59	126.23
23	F	304	BCR	C33-C5-C6	-2.46	121.80	124.48
19	BB	834	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	B1	850	CLA	C4-C3-C5	2.46	119.50	115.23
19	B2	832	CLA	C3B-C4B-NB	-2.46	108.33	110.53
19	B1	824	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	B2	840	BCR	C8-C7-C6	-2.46	120.42	127.00
24	L	209	AJP	C13-C14-C15	2.46	117.32	113.14
19	B2	826	CLA	C3B-C4B-NB	-2.46	108.33	110.53
19	AA	840	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	K1	106	BCR	C1-C6-C5	-2.46	119.28	122.64
24	AA	856	AJP	C13-C14-C15	2.46	117.32	113.14
19	A1	829	CLA	CAC-C3C-C4C	2.46	127.99	124.79
23	K2	105	BCR	C20-C21-C22	-2.46	123.83	127.28
23	JJ	102	BCR	C15-C14-C13	-2.46	123.83	127.28
19	A	804	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	AA	847	LHG	P-O3-C3	-2.46	107.27	121.35
25	II	105	LMG	O1-C1-C2	-2.46	104.54	108.27
19	A1	820	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
23	AA	848	BCR	C33-C5-C6	-2.46	121.81	124.48
19	A2	802	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	A1	845	LHG	P-O6-C4	-2.45	107.29	121.35
23	J	104	BCR	C38-C26-C25	-2.45	121.81	124.48
23	J	102	BCR	C38-C26-C25	-2.45	121.81	124.48
19	B	819	CLA	CHB-C4A-NA	2.45	127.94	124.40
19	B2	803	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	B	805	CLA	O2D-CGD-CBD	2.45	115.52	111.23
19	B2	807	CLA	C1-O2A-CGA	2.45	122.58	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L	208	AJP	C85-O84-C05	2.45	117.92	113.69
23	J1	102	BCR	C27-C26-C25	2.45	126.02	122.70
19	B1	803	CLA	CHB-C4A-NA	2.45	127.94	124.40
19	A1	822	CLA	O2D-CGD-CBD	2.45	115.51	111.23
23	F2	304	BCR	C15-C16-C17	-2.45	118.50	123.52
19	B1	815	CLA	C3B-C4B-NB	-2.45	108.34	110.53
23	L1	209	BCR	C38-C26-C25	-2.45	121.81	124.48
20	A	803	CL0	C9-C8-C7	2.45	120.01	111.27
19	BB	830	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	B1	839	BCR	C8-C7-C6	-2.45	120.45	127.00
19	A1	801	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
19	AA	830	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	B1	831	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	A2	854	AJP	O84-C05-C06	-2.45	99.96	107.26
23	B	840	BCR	C8-C7-C6	-2.45	120.46	127.00
19	A2	836	CLA	C3B-C4B-NB	-2.45	108.35	110.53
23	I1	101	BCR	C27-C26-C25	2.45	126.01	122.70
23	I2	102	BCR	C7-C8-C9	-2.45	122.62	126.23
19	B	809	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	B	812	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	A	820	CLA	C1-C2-C3	-2.45	122.19	126.20
23	F	305	BCR	C27-C26-C25	2.44	126.01	122.70
24	A	855	AJP	C13-C14-C15	2.44	117.29	113.14
23	A1	851	BCR	C1-C6-C5	-2.44	119.30	122.64
23	F2	303	BCR	C35-C13-C14	-2.44	118.86	122.82
19	B	815	CLA	C5-C3-C2	2.44	126.65	121.17
24	L2	202	AJP	C81-C12-C11	2.44	116.90	111.58
19	FF	301	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	BB	842	BCR	C33-C5-C6	-2.44	121.82	124.48
19	B2	851	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
23	J1	102	BCR	C38-C26-C25	-2.44	121.82	124.48
23	K1	104	BCR	C38-C26-C25	-2.44	121.82	124.48
23	B2	840	BCR	C33-C5-C6	-2.44	121.82	124.48
23	B	843	BCR	C27-C26-C25	2.44	126.00	122.70
19	B	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	B1	803	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	BB	849	AJP	C17-C16-C15	-2.44	107.60	110.52
19	AA	820	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	A1	853	BCR	C30-C25-C26	-2.44	119.30	122.64
25	M	102	LMG	C38-C37-C36	-2.44	102.04	114.37
19	A	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	I2	101	BCR	C27-C26-C25	2.44	126.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	810	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	B2	819	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	B	806	CLA	O2A-CGA-O1A	-2.44	117.54	123.63
23	F2	304	BCR	C38-C26-C25	-2.44	121.83	124.48
19	A2	830	CLA	CHB-C4A-NA	2.44	127.91	124.40
22	L	207	LHG	P-O3-C3	-2.43	107.40	121.35
19	B	833	CLA	C5-C3-C2	2.43	126.63	121.17
23	L2	207	BCR	C27-C26-C25	2.43	125.99	122.70
23	KK	103	BCR	C35-C13-C14	-2.43	118.87	122.82
19	B1	805	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
22	A2	846	LHG	P-O3-C3	-2.43	107.41	121.35
19	JJ	101	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	LL	205	LHG	P-O3-C3	-2.43	107.42	121.35
19	B2	813	CLA	CHB-C4A-NA	2.43	127.91	124.40
19	B1	806	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
23	II	101	BCR	C38-C26-C25	-2.43	121.83	124.48
19	J	101	CLA	CHB-C4A-NA	2.43	127.91	124.40
19	A2	820	CLA	CHB-C4A-NA	2.43	127.91	124.40
19	B	835	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	L2	202	AJP	O25-C26-O31	2.43	117.08	110.69
20	A1	802	CL0	CGD-CBD-CAD	-2.43	102.98	110.85
23	L2	207	BCR	C38-C26-C25	-2.43	121.83	124.48
19	B1	850	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
19	BB	836	CLA	C3B-C4B-NB	-2.43	108.36	110.53
23	F2	303	BCR	C11-C10-C9	-2.43	123.87	127.28
19	A2	804	CLA	C1-C2-C3	-2.43	122.22	126.20
19	A1	819	CLA	CHB-C4A-NA	2.43	127.90	124.40
19	B1	832	CLA	C3B-C4B-NB	-2.43	108.36	110.53
19	B2	805	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
23	MM	101	BCR	C11-C10-C9	-2.43	123.88	127.28
22	A2	845	LHG	P-O6-C4	-2.43	107.45	121.35
19	BB	826	CLA	C6-C5-C3	2.43	119.38	113.47
19	B2	826	CLA	CHB-C4A-NA	2.43	127.90	124.40
19	B2	830	CLA	C5-C3-C2	2.42	126.61	121.17
23	F1	303	BCR	C15-C16-C17	-2.42	118.56	123.52
19	B2	821	CLA	CHB-C4A-NA	2.42	127.90	124.40
19	A2	838	CLA	CHB-C4A-NA	2.42	127.89	124.40
19	BB	806	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	A1	850	BCR	C8-C7-C6	-2.42	120.53	127.00
19	A	830	CLA	CAC-C3C-C4C	2.42	127.94	124.79
19	B	821	CLA	C3B-C4B-NB	-2.42	108.37	110.53
19	AA	830	CLA	CHB-C4A-NA	2.42	127.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	815	CLA	C3B-C4B-NB	-2.42	108.37	110.53
19	B2	806	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
20	A2	803	CL0	CAC-C3C-C4C	2.42	130.25	124.03
19	K1	105	CLA	C3A-C2A-C1A	-2.42	103.83	106.30
24	B	849	AJP	C81-C12-C11	2.42	116.84	111.58
19	B2	833	CLA	O2D-CGD-CBD	2.42	115.46	111.23
19	A1	825	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	B	849	AJP	C24-C19-C20	2.42	115.23	112.66
19	A	839	CLA	CHB-C4A-NA	2.42	127.89	124.40
23	A	849	BCR	C33-C5-C6	-2.41	121.85	124.48
24	BB	849	AJP	C18-C17-C16	2.41	116.01	112.16
23	BB	847	BCR	C15-C14-C13	-2.41	123.89	127.28
19	L2	205	CLA	CHB-C4A-NA	2.41	127.88	124.40
19	A2	812	CLA	CBA-CAA-C2A	2.41	120.97	113.79
19	A2	808	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
26	BB	840	ECH	C37-C22-C21	2.41	126.72	122.82
19	AA	831	CLA	CHB-C4A-NA	2.41	127.88	124.40
19	A2	832	CLA	C3B-C4B-NB	-2.41	108.38	110.53
23	I2	101	BCR	C2-C1-C6	2.41	113.94	110.44
23	F1	303	BCR	C8-C7-C6	-2.41	120.56	127.00
24	B	849	AJP	C32-C30-C29	2.41	118.93	113.02
19	B2	825	CLA	CHB-C4A-NA	2.41	127.88	124.40
19	A	830	CLA	CHB-C4A-NA	2.41	127.88	124.40
19	A	821	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
23	J2	102	BCR	C27-C26-C25	2.41	125.96	122.70
19	L	204	CLA	C1-C2-C3	-2.41	122.25	126.20
28	BB	854	DGD	C1D-C2D-C3D	-2.41	104.95	110.01
25	M	102	LMG	O1-C7-C8	-2.41	104.97	110.82
19	A	808	CLA	CHB-C4A-NA	2.41	127.87	124.40
19	AA	832	CLA	CHB-C4A-NA	2.41	127.87	124.40
23	F2	305	BCR	C24-C23-C22	-2.41	122.68	126.23
24	AA	802	AJP	O84-C05-C04	2.41	112.86	110.76
19	BB	801	CLA	C5-C3-C2	2.40	126.56	121.17
23	A1	848	BCR	C2-C1-C6	2.40	113.93	110.44
23	A2	848	BCR	C2-C1-C6	2.40	113.93	110.44
19	B	833	CLA	C3B-C4B-NB	-2.40	108.38	110.53
23	A1	851	BCR	C24-C23-C22	-2.40	122.68	126.23
23	BB	838	BCR	C7-C8-C9	-2.40	122.68	126.23
23	A	847	BCR	C8-C7-C6	-2.40	120.58	127.00
23	L1	208	BCR	C7-C8-C9	-2.40	122.68	126.23
23	B2	839	BCR	C35-C13-C14	-2.40	118.92	122.82
23	B2	840	BCR	C29-C30-C25	2.40	113.93	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	853	LHG	P-O3-C3	-2.40	107.59	121.35
19	B	860	CLA	CBC-CAC-C3C	2.40	118.93	112.42
23	B2	843	BCR	C27-C26-C25	2.40	125.95	122.70
24	L	208	AJP	O84-C05-C04	2.40	112.85	110.76
23	F2	303	BCR	C8-C7-C6	-2.40	120.58	127.00
23	JJ	102	BCR	C38-C26-C25	-2.40	121.86	124.48
19	B1	832	CLA	C2A-C1A-CHA	2.40	128.03	123.87
20	A	803	CL0	C4C-C3C-C2C	-2.40	103.89	113.37
19	B	805	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
19	B1	807	CLA	C11-C12-C13	-2.40	107.99	115.97
19	A1	825	CLA	CHB-C4A-NA	2.40	127.86	124.40
19	A	833	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	KK	103	BCR	C8-C7-C6	-2.40	120.59	127.00
23	B1	842	BCR	C33-C5-C6	-2.40	121.87	124.48
23	L	206	BCR	C38-C26-C25	-2.40	121.87	124.48
24	M2	101	AJP	C81-C12-C11	2.40	116.80	111.58
19	B1	825	CLA	CHB-C4A-NA	2.40	127.86	124.40
19	B	834	CLA	C4-C3-C5	2.40	119.39	115.23
25	B	851	LMG	O1-C7-C8	-2.40	104.99	110.82
23	FF	303	BCR	C11-C10-C9	-2.40	123.92	127.28
19	L1	207	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
26	BB	840	ECH	C8-C9-C10	2.39	122.78	119.01
19	K1	103	CLA	CHB-C4A-NA	2.39	127.86	124.40
23	K1	106	BCR	C15-C14-C13	-2.39	123.92	127.28
19	AA	833	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	K2	105	BCR	C15-C14-C13	-2.39	123.92	127.28
19	A1	817	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	B	849	AJP	C15-C20-C19	2.39	111.84	108.51
19	B2	824	CLA	C3B-C4B-NB	-2.39	108.39	110.53
23	K1	104	BCR	C2-C1-C6	2.39	113.91	110.44
19	A1	819	CLA	CBA-CAA-C2A	2.39	120.91	113.79
19	B2	850	CLA	C3B-C4B-NB	-2.39	108.40	110.53
20	AA	803	CL0	CAC-C3C-C4C	2.39	130.17	124.03
19	A1	835	CLA	O2D-CGD-CBD	2.39	115.41	111.23
19	A1	812	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	B	857	AJP	C11-C16-C15	-2.39	104.95	109.17
23	B	840	BCR	C29-C30-C25	2.39	113.91	110.44
19	A2	812	CLA	CHB-C4A-NA	2.39	127.85	124.40
19	KK	102	CLA	CHB-C4A-NA	2.39	127.85	124.40
19	A2	816	CLA	C1-C2-C3	-2.39	122.90	126.76
19	BB	815	CLA	C3B-C4B-NB	-2.39	108.40	110.53
19	AA	818	CLA	CHB-C4A-NA	2.39	127.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	801	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
19	BB	825	CLA	CHB-C4A-NA	2.39	127.84	124.40
23	A2	850	BCR	C8-C7-C6	-2.38	120.63	127.00
23	BB	839	BCR	C29-C30-C25	2.38	113.90	110.44
19	BB	856	CLA	C2A-C1A-CHA	2.38	128.00	123.87
19	B2	852	CLA	C3B-C4B-NB	-2.38	108.40	110.53
23	B1	843	BCR	C24-C23-C22	-2.38	122.71	126.23
23	K2	103	BCR	C38-C26-C25	-2.38	121.89	124.48
19	B2	821	CLA	C4-C3-C2	-2.38	117.51	123.63
19	A2	821	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
23	M2	102	BCR	C2-C1-C6	2.38	113.90	110.44
19	A1	820	CLA	CBA-CAA-C2A	2.38	120.88	113.79
23	M2	102	BCR	C7-C8-C9	-2.38	122.71	126.23
19	B2	831	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	B	859	CLA	O2D-CGD-CBD	2.38	115.39	111.23
23	I1	101	BCR	C2-C1-C6	2.38	113.89	110.44
23	B	848	BCR	C15-C14-C13	-2.38	123.94	127.28
19	BB	815	CLA	CMB-C2B-C3B	2.38	132.14	126.55
26	B	841	ECH	C7-C6-C5	-2.38	116.08	121.56
23	AA	852	BCR	C24-C23-C22	-2.38	122.72	126.23
19	B2	805	CLA	O2D-CGD-CBD	2.38	115.39	111.23
19	B1	820	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	KK	104	AJP	C18-C17-C16	2.38	115.95	112.16
19	F2	301	CLA	O2D-CGD-CBD	2.38	115.39	111.23
23	AA	849	BCR	C2-C1-C6	2.38	113.89	110.44
23	L1	209	BCR	C16-C15-C14	-2.38	118.66	123.52
23	II	104	BCR	C7-C8-C9	-2.38	122.72	126.23
19	A1	813	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	A	811	CLA	CAC-C3C-C4C	2.38	127.88	124.79
23	BB	843	BCR	C16-C15-C14	-2.37	118.66	123.52
23	A	851	BCR	C1-C6-C5	-2.37	119.39	122.64
19	BB	812	CLA	CHB-C4A-NA	2.37	127.83	124.40
19	L	203	CLA	C1-O2A-CGA	2.37	122.39	116.65
23	K1	106	BCR	C15-C16-C17	-2.37	118.66	123.52
19	A	812	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	B1	824	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
19	A2	810	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
23	FF	306	BCR	C35-C13-C14	-2.37	118.97	122.82
22	A1	846	LHG	P-O3-C3	-2.37	107.76	121.35
20	A1	802	CL0	C9-C8-C10	2.37	119.73	111.27
19	B1	809	CLA	O2D-CGD-CBD	2.37	115.38	111.23
19	B2	809	CLA	O2D-CGD-CBD	2.37	115.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	847	BCR	C8-C7-C6	-2.37	120.67	127.00
19	B2	833	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	B1	815	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
23	BB	842	BCR	C15-C16-C17	-2.37	118.67	123.52
19	AA	832	CLA	C3B-C4B-NB	-2.37	108.42	110.53
25	B	851	LMG	O1-C1-C2	-2.37	104.67	108.27
19	A2	819	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
23	B	848	BCR	C38-C26-C25	-2.37	121.90	124.48
24	L2	203	AJP	C32-C30-C29	2.37	118.83	113.02
23	JJ	104	BCR	C2-C1-C6	2.37	113.88	110.44
19	A1	818	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
19	A1	826	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	B2	807	CLA	C11-C12-C13	-2.37	108.10	115.97
23	II	102	BCR	C15-C16-C17	-2.37	118.68	123.52
22	X1	103	LHG	P-O3-C3	-2.37	107.79	121.35
23	B	844	BCR	C16-C15-C14	-2.37	118.68	123.52
23	A	848	BCR	C2-C1-C6	2.37	113.88	110.44
22	L2	208	LHG	P-O3-C3	-2.37	107.80	121.35
19	A	836	CLA	O2D-CGD-CBD	2.37	115.36	111.23
23	B2	843	BCR	C33-C5-C6	-2.36	121.90	124.48
19	AA	837	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	BB	840	ECH	C7-C6-C5	-2.36	116.11	121.56
19	B2	851	CLA	C4-C3-C5	2.36	119.33	115.23
19	A2	838	CLA	O2D-CGD-CBD	2.36	115.36	111.23
19	BB	856	CLA	O2D-CGD-CBD	2.36	115.36	111.23
19	B1	810	CLA	CHB-C4A-NA	2.36	127.81	124.40
19	BB	845	CLA	CAC-C3C-C4C	2.36	127.86	124.79
19	BB	815	CLA	C5-C3-C2	2.36	126.47	121.17
23	A1	849	BCR	C7-C8-C9	-2.36	122.74	126.23
19	AA	816	CLA	O2D-CGD-CBD	2.36	115.36	111.23
22	BB	851	LHG	P-O3-C3	-2.36	107.83	121.35
19	BB	812	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	L1	203	AJP	C20-C21-C22	2.36	118.05	114.17
19	B2	824	CLA	CHB-C4A-NA	2.36	127.81	124.40
19	B1	833	CLA	C4-C3-C5	2.36	119.32	115.23
19	A	837	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
19	A1	809	CLA	CBA-CAA-C2A	2.36	120.81	113.79
23	JJ	104	BCR	C38-C26-C25	-2.36	121.91	124.48
19	A1	807	CLA	CHB-C4A-NA	2.36	127.80	124.40
19	AA	830	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	M1	101	BCR	C27-C26-C25	2.36	125.89	122.70
23	L2	207	BCR	C24-C23-C22	-2.36	122.75	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	II	101	BCR	C24-C23-C22	-2.36	122.75	126.23
23	B1	843	BCR	C16-C15-C14	-2.35	118.70	123.52
19	B	829	CLA	CHB-C4A-NA	2.35	127.80	124.40
19	BB	826	CLA	CHB-C4A-NA	2.35	127.80	124.40
23	A2	849	BCR	C33-C5-C6	-2.35	121.92	124.48
19	A1	820	CLA	CAC-C3C-C4C	2.35	127.85	124.79
24	B	850	AJP	C26-O25-C23	-2.35	111.33	115.27
19	AA	842	CLA	C5-C3-C2	-2.35	115.89	121.17
19	BB	824	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	AA	855	BCR	C1-C6-C5	-2.35	119.42	122.64
20	A1	802	CL0	C4-C3-C5	2.35	119.31	115.23
24	A	802	AJP	O84-C05-C04	2.35	112.81	110.76
23	B1	838	BCR	C27-C26-C25	2.35	125.88	122.70
19	A1	837	CLA	O2D-CGD-CBD	2.35	115.34	111.23
23	BB	838	BCR	C24-C23-C22	-2.35	122.76	126.23
19	B	846	CLA	CAC-C3C-C4C	2.35	127.85	124.79
19	BB	822	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	A2	849	BCR	C7-C8-C9	-2.35	122.76	126.23
24	I2	104	AJP	C04-C03-C02	-2.35	106.98	111.67
19	A2	840	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	B2	810	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	AA	802	AJP	C85-O84-C05	2.35	117.74	113.69
23	A	849	BCR	C7-C8-C9	-2.35	122.76	126.23
19	L2	205	CLA	O2D-CGD-CBD	2.35	115.33	111.23
26	B1	840	ECH	C28-C27-C26	-2.35	116.54	118.64
24	L2	203	AJP	C04-C03-C02	-2.35	106.99	111.67
19	AA	836	CLA	O2D-CGD-CBD	2.35	115.33	111.23
23	A	848	BCR	C38-C26-C25	-2.35	121.92	124.48
23	B1	838	BCR	C35-C13-C14	-2.34	119.02	122.82
19	B2	832	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
24	B	850	AJP	C85-O84-C05	2.34	117.73	113.69
19	BB	832	CLA	C5-C3-C2	2.34	126.43	121.17
23	J	102	BCR	C33-C5-C6	-2.34	121.93	124.48
19	A	824	CLA	C3B-C4B-NB	-2.34	108.44	110.53
19	BB	836	CLA	CHD-C4C-C3C	2.34	128.19	124.77
23	B	844	BCR	C15-C16-C17	-2.34	118.73	123.52
19	A1	828	CLA	C4-C3-C5	2.34	119.29	115.23
21	A	843	PQN	C21-C22-C23	-2.34	108.18	115.97
19	A1	815	CLA	C1-C2-C3	-2.34	122.97	126.76
24	L1	203	AJP	O25-C23-C24	-2.34	105.08	109.64
23	B2	839	BCR	C27-C26-C25	2.34	125.87	122.70
19	B2	826	CLA	O2A-CGA-O1A	-2.34	117.78	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A1	812	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	I2	103	BCR	C11-C10-C9	-2.34	124.00	127.28
25	I2	105	LMG	O3-C3-C2	-2.34	104.86	110.38
19	AA	824	CLA	C3B-C4B-NB	-2.34	108.44	110.53
19	BB	803	CLA	C3B-C4B-NB	-2.34	108.44	110.53
24	L	209	AJP	O09-C05-C06	-2.34	101.45	104.56
19	A1	819	CLA	C1-C2-C3	-2.34	122.37	126.20
23	B2	839	BCR	C15-C16-C17	-2.34	118.74	123.52
23	II	101	BCR	C15-C16-C17	-2.34	118.74	123.52
19	AA	853	CLA	C7-C6-C5	2.34	119.49	113.26
23	B	844	BCR	C8-C7-C6	-2.34	120.76	127.00
19	B2	824	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
19	B1	806	CLA	C4-C3-C2	-2.34	117.63	123.63
24	L	209	AJP	C81-C12-C11	2.34	116.66	111.58
23	B2	844	BCR	C16-C15-C14	-2.34	118.74	123.52
19	L1	207	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
20	AA	803	CL0	CBC-CAC-C3C	-2.33	109.53	112.87
19	B2	801	CLA	CBA-CAA-C2A	2.33	120.74	113.79
19	BB	820	CLA	CHD-C4C-C3C	2.33	128.18	124.77
23	F2	303	BCR	C38-C26-C25	-2.33	121.94	124.48
22	A	845	LHG	P-O6-C4	-2.33	107.97	121.35
23	K2	105	BCR	C15-C16-C17	-2.33	118.75	123.52
19	A1	832	CLA	CHB-C4A-NA	2.33	127.77	124.40
19	A1	836	CLA	CHB-C4A-NA	2.33	127.77	124.40
19	B2	821	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
23	AA	849	BCR	C38-C26-C25	-2.33	121.94	124.48
23	K1	104	BCR	C15-C16-C17	-2.33	118.75	123.52
23	A	854	BCR	C15-C16-C17	-2.33	118.75	123.52
23	AA	852	BCR	C15-C16-C17	-2.33	118.75	123.52
19	B1	850	CLA	O2D-CGD-CBD	2.33	115.31	111.23
19	A	822	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	B1	801	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
19	B1	819	CLA	CHB-C4A-NA	2.33	127.76	124.40
22	B	852	LHG	P-O6-C4	-2.33	108.02	121.35
26	B2	841	ECH	C7-C6-C5	-2.33	116.19	121.56
19	BB	803	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	B1	831	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	J2	101	CLA	CHB-C4A-NA	2.33	127.76	124.40
19	B	828	CLA	CHB-C4A-NA	2.33	127.76	124.40
23	B2	839	BCR	C24-C23-C22	-2.33	122.79	126.23
23	A1	851	BCR	C15-C16-C17	-2.33	118.76	123.52
19	B	816	CLA	CHB-C4A-NA	2.33	127.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	F2	303	BCR	C15-C16-C17	-2.33	118.76	123.52
19	B1	810	CLA	C6-C5-C3	2.32	119.13	113.47
19	A2	814	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A	819	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A2	821	CLA	CBA-CAA-C2A	2.32	120.71	113.79
23	B1	843	BCR	C8-C7-C6	-2.32	120.79	127.00
19	B2	826	CLA	O2D-CGD-CBD	2.32	115.29	111.23
23	B2	839	BCR	C7-C8-C9	-2.32	122.80	126.23
23	B2	844	BCR	C8-C7-C6	-2.32	120.80	127.00
23	B1	838	BCR	C7-C8-C9	-2.32	122.80	126.23
19	B2	815	CLA	C4-C3-C2	-2.32	117.67	123.63
23	MM	101	BCR	C24-C23-C22	-2.32	122.80	126.23
19	A	818	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A	837	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A	819	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
19	B1	834	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	A2	829	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	JJ	103	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	F2	305	BCR	C20-C21-C22	-2.32	124.03	127.28
19	A2	811	CLA	C1-O2A-CGA	2.32	122.26	116.65
23	II	101	BCR	C16-C15-C14	-2.32	118.78	123.52
19	BB	827	CLA	CBA-CAA-C2A	2.32	120.69	113.79
19	B	812	CLA	CMA-C3A-C2A	-2.32	110.91	116.23
24	B	850	AJP	C01-C02-C03	2.32	117.15	112.08
23	AA	848	BCR	C8-C7-C6	-2.32	120.81	127.00
19	A	815	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
19	BB	805	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
26	B1	840	ECH	C7-C6-C5	-2.32	116.22	121.56
19	A2	823	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	M2	102	BCR	C27-C26-C25	2.32	125.83	122.70
19	A1	839	CLA	CHB-C4A-NA	2.32	127.74	124.40
19	A1	842	CLA	CHB-C4A-NA	2.32	127.74	124.40
19	A	840	CLA	CHB-C4A-NA	2.32	127.74	124.40
19	A2	852	CLA	CHB-C4A-NA	2.32	127.74	124.40
23	FF	304	BCR	C33-C5-C6	-2.31	121.96	124.48
19	B1	805	CLA	O2D-CGD-CBD	2.31	115.28	111.23
24	A1	855	AJP	O09-C05-C06	-2.31	101.48	104.56
19	B	824	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
23	JJ	102	BCR	C8-C7-C6	-2.31	120.81	127.00
23	F1	304	BCR	C20-C21-C22	-2.31	124.03	127.28
23	A1	850	BCR	C2-C1-C6	2.31	113.80	110.44
19	B1	822	CLA	CHB-C4A-NA	2.31	127.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	858	CLA	O2D-CGD-CBD	2.31	115.28	111.23
22	X2	103	LHG	P-O3-C3	-2.31	108.09	121.35
19	A1	822	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
19	A	821	CLA	CBA-CAA-C2A	2.31	120.67	113.79
22	A	845	LHG	P-O3-C3	-2.31	108.10	121.35
23	B1	838	BCR	C24-C23-C22	-2.31	122.81	126.23
19	FF	305	CLA	CHB-C4A-NA	2.31	127.74	124.40
24	L2	202	AJP	C20-C21-C22	2.31	117.97	114.17
19	B2	827	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
19	A1	833	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	AA	839	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	B1	815	CLA	C5-C3-C2	2.31	126.35	121.17
19	A2	818	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	L1	205	CLA	C6-C5-C3	2.31	119.09	113.47
19	AA	812	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	B2	820	CLA	CHB-C4A-NA	2.31	127.73	124.40
19	B2	815	CLA	O2D-CGD-CBD	2.31	115.27	111.23
19	A	807	CLA	C1-C2-C3	-2.31	122.42	126.20
23	BB	843	BCR	C8-C7-C6	-2.31	120.83	127.00
25	L1	210	LMG	O1-C7-C8	-2.31	105.21	110.82
19	B	801	CLA	C6-C5-C3	2.31	119.09	113.47
19	B	806	CLA	C4-C3-C2	-2.31	117.70	123.63
19	J	103	CLA	C3B-C4B-NB	-2.31	108.47	110.53
19	B1	835	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
23	B1	838	BCR	C15-C16-C17	-2.31	118.80	123.52
24	L1	204	AJP	O25-C23-C24	-2.31	105.15	109.64
23	B1	842	BCR	C38-C26-C25	-2.31	121.97	124.48
19	BB	816	CLA	CHB-C4A-NA	2.31	127.73	124.40
23	F	304	BCR	C20-C21-C22	-2.31	124.05	127.28
28	B	856	DGD	O5D-C6D-C5D	-2.31	104.22	109.42
23	A2	851	BCR	C8-C7-C6	-2.30	120.84	127.00
19	B1	801	CLA	CBA-CAA-C2A	2.30	120.65	113.79
19	AA	853	CLA	O2D-CGD-CBD	2.30	115.26	111.23
24	L1	204	AJP	C26-O25-C23	2.30	119.12	115.27
19	A1	832	CLA	O2D-CGD-CBD	2.30	115.26	111.23
23	I	102	BCR	C15-C16-C17	-2.30	118.81	123.52
19	AA	821	CLA	CBA-CAA-C2A	2.30	120.64	113.79
23	A2	850	BCR	C2-C1-C6	2.30	113.78	110.44
20	A2	803	CL0	C4C-C3C-C2C	-2.30	104.28	113.37
22	BB	850	LHG	P-O6-C4	-2.30	108.16	121.35
19	B2	833	CLA	CHA-C1A-NA	-2.30	121.18	126.39
19	B	859	CLA	C2A-C1A-CHA	2.30	127.86	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	824	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	AA	806	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
22	AA	846	LHG	P-O6-C4	-2.30	108.16	121.35
23	F	303	BCR	C15-C16-C17	-2.30	118.81	123.52
23	K2	103	BCR	C2-C1-C6	2.30	113.78	110.44
19	B2	816	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	B2	828	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	A1	801	CLA	O1D-CGD-CBD	2.30	129.06	124.52
19	A2	806	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
19	A	806	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
21	A2	843	PQN	C15-C13-C12	-2.30	116.00	121.17
22	A2	845	LHG	P-O3-C3	-2.30	108.17	121.35
23	BB	843	BCR	C15-C16-C17	-2.30	118.81	123.52
19	L1	205	CLA	C4-C3-C5	2.30	119.22	115.23
23	K2	103	BCR	C15-C16-C17	-2.30	118.81	123.52
19	AA	826	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	AA	820	CLA	C1-C2-C3	-2.30	122.43	126.20
20	A1	802	CL0	C1-C2-C3	2.30	129.97	126.20
23	L1	208	BCR	C11-C10-C9	-2.30	124.05	127.28
19	A2	852	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
19	A2	834	CLA	CHB-C4A-NA	2.30	127.72	124.40
23	K	103	BCR	C8-C7-C6	-2.30	120.86	127.00
19	AA	801	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
24	BB	848	AJP	O84-C05-C06	-2.30	100.41	107.26
23	A	850	BCR	C27-C26-C25	2.30	125.81	122.70
21	A1	843	PQN	C15-C13-C12	-2.30	116.01	121.17
23	A2	847	BCR	C15-C16-C17	-2.30	118.82	123.52
23	BB	847	BCR	C38-C26-C25	-2.30	121.98	124.48
24	A2	854	AJP	C04-C05-C06	2.30	119.82	115.66
19	A	852	CLA	O2D-CGD-CBD	2.30	115.24	111.23
23	KK	103	BCR	C16-C15-C14	-2.30	118.82	123.52
24	I2	104	AJP	C81-C12-C11	2.30	116.58	111.58
23	JJ	104	BCR	C8-C7-C6	-2.30	120.87	127.00
23	I1	101	BCR	C16-C15-C14	-2.30	118.82	123.52
23	AA	850	BCR	C7-C8-C9	-2.29	122.84	126.23
23	B	839	BCR	C7-C8-C9	-2.29	122.84	126.23
19	BB	833	CLA	C2A-C1A-CHA	2.29	127.85	123.87
19	K1	105	CLA	CHB-C4A-NA	2.29	127.71	124.40
19	L1	206	CLA	CHB-C4A-NA	2.29	127.71	124.40
23	B2	843	BCR	C38-C26-C25	-2.29	121.98	124.48
19	B2	802	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
24	A1	854	AJP	C11-C16-C15	-2.29	105.12	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	AA	805	CLA	O2D-CGD-CBD	2.29	115.24	111.23
24	L1	203	AJP	C85-O84-C05	2.29	117.64	113.69
19	A2	813	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
23	M	101	BCR	C8-C7-C6	-2.29	120.88	127.00
20	AA	803	CL0	C4C-CHD-C1D	2.29	124.27	116.07
26	B	841	ECH	C29-C30-C25	-2.29	107.11	110.44
23	JJ	102	BCR	C33-C5-C6	-2.29	121.98	124.48
23	A	848	BCR	C27-C26-C25	2.29	125.80	122.70
19	J1	103	CLA	CHB-C4A-NA	2.29	127.70	124.40
19	B1	826	CLA	O2D-CGD-CBD	2.29	115.23	111.23
24	L2	203	AJP	C85-O84-C05	2.29	117.64	113.69
19	AA	823	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
19	F1	305	CLA	CHB-C4A-NA	2.29	127.70	124.40
19	A	831	CLA	CHB-C4A-NA	2.29	127.70	124.40
19	BB	824	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
23	A1	848	BCR	C27-C26-C25	2.29	125.79	122.70
19	B	827	CLA	O2A-CGA-O1A	-2.29	117.45	123.33
19	B1	849	CLA	C3B-C4B-NB	-2.29	108.49	110.53
19	LL	202	CLA	C1-O2A-CGA	2.28	122.18	116.65
19	B	854	CLA	C3B-C4B-NB	-2.28	108.49	110.53
23	F1	304	BCR	C8-C7-C6	-2.28	120.90	127.00
19	AA	843	CLA	CBC-CAC-C3C	2.28	118.61	112.42
23	AA	849	BCR	C27-C26-C25	2.28	125.79	122.70
19	A1	820	CLA	C6-C5-C3	2.28	119.03	113.47
23	FF	303	BCR	C15-C16-C17	-2.28	118.85	123.52
19	L2	206	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
23	BB	839	BCR	C15-C16-C17	-2.28	118.85	123.52
19	A	825	CLA	CHB-C4A-NA	2.28	127.69	124.40
19	BB	806	CLA	C4-C3-C2	-2.28	117.77	123.63
19	B2	806	CLA	C4-C3-C2	-2.28	117.78	123.63
23	B	840	BCR	C33-C5-C6	-2.28	122.00	124.48
19	B2	815	CLA	C5-C3-C2	2.28	126.28	121.17
23	F2	304	BCR	C8-C7-C6	-2.28	120.92	127.00
19	J2	103	CLA	CHB-C4A-NA	2.28	127.69	124.40
19	AA	819	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	FF	306	BCR	C35-C13-C12	2.28	121.56	118.09
23	B	839	BCR	C15-C16-C17	-2.28	118.86	123.52
19	A	826	CLA	CHB-C4A-NA	2.28	127.68	124.40
23	LL	204	BCR	C15-C16-C17	-2.28	118.86	123.52
19	B1	807	CLA	C1-O2A-CGA	2.27	122.16	116.65
19	L2	204	CLA	C6-C5-C3	2.27	119.01	113.47
26	BB	840	ECH	C23-C24-C25	-2.27	120.92	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A1	802	CL0	CMD-C2D-C3D	-2.27	120.14	124.68
19	A	801	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	A1	855	AJP	C85-O84-C05	2.27	117.61	113.69
20	A1	802	CL0	C4C-CHD-C1D	2.27	124.20	116.07
22	X1	103	LHG	P-O6-C4	-2.27	108.33	121.35
22	BB	850	LHG	P-O3-C3	-2.27	108.34	121.35
19	A1	842	CLA	CBC-CAC-C3C	2.27	118.58	112.42
19	B	818	CLA	CHB-C4A-NA	2.27	127.68	124.40
19	J	103	CLA	CHB-C4A-NA	2.27	127.68	124.40
19	B2	830	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
19	A	832	CLA	C1-C2-C3	-2.27	122.48	126.20
23	J	102	BCR	C8-C7-C6	-2.27	120.94	127.00
19	B	834	CLA	C4-C3-C2	-2.27	117.80	123.63
19	A2	831	CLA	CHB-C4A-NA	2.27	127.67	124.40
23	L1	209	BCR	C8-C7-C6	-2.27	120.94	127.00
19	BB	818	CLA	CHB-C4A-NA	2.27	127.67	124.40
23	A2	851	BCR	C15-C16-C17	-2.27	118.88	123.52
19	B2	826	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
23	AA	855	BCR	C20-C21-C22	-2.27	124.10	127.28
22	X2	103	LHG	P-O6-C4	-2.27	108.35	121.35
23	J	104	BCR	C3-C4-C5	-2.27	110.01	114.06
19	AA	832	CLA	C1-C2-C3	-2.27	122.48	126.20
23	AA	851	BCR	C27-C26-C25	2.27	125.77	122.70
19	AA	819	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
23	F	305	BCR	C35-C13-C14	-2.27	119.14	122.82
19	A2	829	CLA	C4-C3-C2	-2.27	117.81	123.63
23	L	206	BCR	C15-C16-C17	-2.26	118.89	123.52
23	A2	848	BCR	C38-C26-C25	-2.26	122.01	124.48
23	J1	102	BCR	C2-C1-C6	2.26	113.73	110.44
19	BB	832	CLA	CHA-C1A-NA	-2.26	121.26	126.39
26	BB	840	ECH	C35-C13-C14	2.26	126.48	122.82
23	MM	101	BCR	C8-C7-C6	-2.26	120.95	127.00
19	B	836	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	AA	850	BCR	C33-C5-C6	-2.26	122.02	124.48
20	A2	803	CL0	C4C-CHD-C1D	2.26	124.16	116.07
24	B	850	AJP	C32-C30-C29	2.26	118.57	113.02
23	F1	306	BCR	C35-C13-C14	-2.26	119.15	122.82
19	A	814	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
19	A2	821	CLA	CAC-C3C-C4C	2.26	127.73	124.79
19	AA	834	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	F2	305	BCR	C35-C13-C14	-2.26	119.15	122.82
19	B	813	CLA	O2D-CGD-CBD	2.26	115.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	827	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
19	A1	805	CLA	CHB-C4A-NA	2.26	127.66	124.40
25	I1	102	LMG	O3-C3-C2	-2.26	105.05	110.38
19	A	823	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
19	B	826	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	J2	102	BCR	C33-C5-C6	-2.26	122.02	124.48
24	B	857	AJP	C17-C18-C19	2.26	116.21	111.84
23	II	101	BCR	C27-C26-C25	2.26	125.75	122.70
23	A2	847	BCR	C21-C20-C19	-2.26	119.31	124.65
19	A1	830	CLA	CHB-C4A-NA	2.26	127.66	124.40
19	A1	831	CLA	C3B-C4B-NB	-2.26	108.52	110.53
25	M	102	LMG	C7-O1-C1	2.26	118.63	113.80
23	A	851	BCR	C24-C23-C22	-2.26	122.90	126.23
23	I2	102	BCR	C8-C7-C6	-2.26	120.97	127.00
24	B	857	AJP	C13-C14-C15	2.26	116.97	113.14
23	A	851	BCR	C15-C16-C17	-2.25	118.91	123.52
23	B	844	BCR	C24-C23-C22	-2.25	122.90	126.23
19	A2	826	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	B2	801	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	B	826	CLA	O2D-CGD-CBD	2.25	115.17	111.23
19	A	813	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
23	MM	101	BCR	C7-C8-C9	-2.25	122.90	126.23
23	M2	102	BCR	C15-C16-C17	-2.25	118.91	123.52
19	BB	803	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
23	FF	303	BCR	C38-C26-C25	-2.25	122.03	124.48
19	B	860	CLA	CHB-C4A-NA	2.25	127.65	124.40
19	B2	822	CLA	CHB-C4A-NA	2.25	127.65	124.40
19	B	803	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	AA	820	CLA	CBA-CAA-C2A	2.25	120.49	113.79
23	A	848	BCR	C15-C16-C17	-2.25	118.92	123.52
22	AA	846	LHG	P-O3-C3	-2.25	108.46	121.35
23	A2	848	BCR	C27-C26-C25	2.25	125.74	122.70
19	BB	835	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
19	B	821	CLA	C4-C3-C2	-2.25	117.85	123.63
19	B1	815	CLA	C4-C3-C2	-2.25	117.85	123.63
23	M1	101	BCR	C15-C16-C17	-2.25	118.92	123.52
19	AA	827	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
19	A	816	CLA	C1-C2-C3	-2.25	123.13	126.76
19	A2	823	CLA	C5-C3-C2	2.25	126.21	121.17
23	AA	848	BCR	C21-C20-C19	-2.25	119.33	124.65
19	LL	203	CLA	C2D-C1D-ND	-2.25	107.90	110.13
19	BB	833	CLA	CHB-C1B-NB	2.25	127.42	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	L2	207	BCR	C8-C7-C6	-2.25	121.00	127.00
23	FF	306	BCR	C27-C26-C25	2.25	125.74	122.70
20	A	803	CL0	O2A-C1-C2	2.24	116.75	108.11
23	F1	303	BCR	C35-C13-C14	-2.24	119.18	122.82
23	A1	853	BCR	C7-C8-C9	-2.24	122.92	126.23
23	A1	848	BCR	C38-C26-C25	-2.24	122.04	124.48
23	B	842	BCR	C1-C6-C5	-2.24	119.57	122.64
19	A2	827	CLA	CHB-C4A-NA	2.24	127.64	124.40
22	X	102	LHG	P-O3-C3	-2.24	108.50	121.35
19	B	816	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
21	AA	844	PQN	C21-C22-C23	-2.24	108.51	115.97
19	A1	824	CLA	CHB-C4A-NA	2.24	127.64	124.40
19	A1	810	CLA	C1-O2A-CGA	2.24	122.08	116.65
19	BB	852	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	B1	840	ECH	C37-C22-C21	2.24	126.44	122.82
23	J1	102	BCR	C33-C5-C6	-2.24	122.04	124.48
21	A1	843	PQN	C21-C22-C23	-2.24	108.52	115.97
25	II	105	LMG	O2-C2-C1	-2.24	104.74	110.08
22	X2	102	LHG	P-O3-C3	-2.24	108.52	121.35
24	A1	855	AJP	C21-C22-C23	2.24	113.89	111.40
19	L1	207	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
23	A1	849	BCR	C38-C26-C25	-2.24	122.04	124.48
23	A2	849	BCR	C15-C16-C17	-2.24	118.94	123.52
23	I2	101	BCR	C16-C15-C14	-2.24	118.94	123.52
19	A1	818	CLA	CHB-C4A-NA	2.24	127.63	124.40
23	JJ	102	BCR	C11-C10-C9	-2.24	124.14	127.28
23	A1	847	BCR	C8-C7-C6	-2.24	121.02	127.00
24	I2	104	AJP	C24-C19-C18	-2.24	108.82	112.75
19	AA	829	CLA	C4-C3-C2	-2.24	117.89	123.63
19	AA	813	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
19	A2	836	CLA	O2D-CGD-CBD	2.24	115.14	111.23
19	BB	856	CLA	O2A-CGA-CBA	2.24	118.65	111.83
22	L2	208	LHG	O7-C7-C8	2.23	116.32	111.48
23	J2	104	BCR	C15-C16-C17	-2.23	118.95	123.52
19	B2	827	CLA	O2A-CGA-O1A	-2.23	117.58	123.33
19	A	805	CLA	O2D-CGD-CBD	2.23	115.14	111.23
23	J2	102	BCR	C8-C7-C6	-2.23	121.03	127.00
24	L1	203	AJP	C81-C12-C11	2.23	116.44	111.58
19	AA	837	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
19	BB	833	CLA	C4-C3-C5	2.23	119.10	115.23
23	K	103	BCR	C27-C26-C25	2.23	125.72	122.70
19	A2	807	CLA	C1-C2-C3	-2.23	122.54	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	821	CLA	O2D-CGD-CBD	2.23	115.13	111.23
20	A2	803	CL0	C2C-C1C-NC	2.23	116.78	110.46
24	A2	854	AJP	C21-C22-C23	2.23	113.89	111.40
19	B1	806	CLA	C1-C2-C3	2.23	129.85	126.20
23	BB	841	BCR	C35-C13-C14	-2.23	119.20	122.82
19	B1	826	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
23	A	854	BCR	C20-C21-C22	-2.23	124.15	127.28
19	B	826	CLA	C4-C3-C5	2.23	119.10	115.23
19	B1	803	CLA	C11-C12-C13	-2.23	108.55	115.97
19	LL	203	CLA	CMB-C2B-C3B	2.23	131.80	126.55
19	B	801	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	KK	103	BCR	C27-C26-C25	2.23	125.72	122.70
19	A	834	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	B	834	CLA	CHB-C1B-NB	2.23	127.39	124.05
21	A2	843	PQN	C21-C22-C23	-2.23	108.56	115.97
19	B1	801	CLA	C3B-C4B-NB	-2.23	108.54	110.53
19	A1	811	CLA	CHB-C4A-NA	2.23	127.61	124.40
19	A	829	CLA	C5-C3-C2	2.23	126.17	121.17
19	B1	850	CLA	C2A-C1A-CHA	2.23	127.73	123.87
23	I2	103	BCR	C15-C14-C13	-2.23	124.16	127.28
23	A1	847	BCR	C21-C20-C19	-2.23	119.38	124.65
19	FF	301	CLA	CGD-CBD-CAD	-2.23	103.64	110.85
19	A2	820	CLA	O2D-CGD-CBD	2.23	115.12	111.23
19	LL	203	CLA	CHB-C4A-NA	2.23	127.61	124.40
19	B2	822	CLA	C5-C3-C2	2.23	126.16	121.17
19	A1	804	CLA	CHB-C4A-NA	2.22	127.61	124.40
19	J1	101	CLA	CHB-C4A-NA	2.22	127.61	124.40
23	FF	304	BCR	C20-C21-C22	-2.22	124.16	127.28
23	A1	850	BCR	C27-C26-C25	2.22	125.71	122.70
22	B	852	LHG	P-O3-C3	-2.22	108.61	121.35
19	BB	819	CLA	CMA-C3A-C2A	-2.22	111.13	116.23
19	B	830	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
25	B	851	LMG	O2-C2-C1	-2.22	104.78	110.08
19	AA	809	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
26	B2	841	ECH	C23-C24-C25	-2.22	121.07	127.00
25	B1	846	LMG	O3-C3-C2	-2.22	105.14	110.38
19	B1	827	CLA	O2A-CGA-O1A	-2.22	117.62	123.33
19	A2	835	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	BB	848	AJP	C81-C12-C11	2.22	116.41	111.58
25	B2	847	LMG	O3-C3-C2	-2.22	105.15	110.38
19	L2	204	CLA	C4-C3-C5	2.22	119.08	115.23
23	B	840	BCR	C15-C16-C17	-2.22	118.98	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B1	818	CLA	CHB-C4A-NA	2.22	127.60	124.40
23	II	104	BCR	C15-C14-C13	-2.22	124.17	127.28
19	B	808	CLA	CHB-C4A-NA	2.22	127.60	124.40
22	BB	851	LHG	O7-C7-C8	2.22	116.28	111.48
23	A	847	BCR	C21-C20-C19	-2.22	119.41	124.65
19	BB	833	CLA	C4-C3-C2	-2.22	117.94	123.63
19	AA	808	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
24	BB	848	AJP	C04-C03-C02	-2.22	107.25	111.67
23	AA	849	BCR	C15-C16-C17	-2.22	118.99	123.52
23	L	206	BCR	C8-C7-C6	-2.22	121.08	127.00
23	F2	304	BCR	C20-C21-C22	-2.21	124.17	127.28
23	J1	102	BCR	C8-C7-C6	-2.21	121.08	127.00
23	A2	850	BCR	C27-C26-C25	2.21	125.70	122.70
23	BB	841	BCR	C1-C6-C5	-2.21	119.61	122.64
19	B2	808	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	I	101	BCR	C16-C15-C14	-2.21	118.99	123.52
25	M	102	LMG	C1-C2-C3	-2.21	105.36	110.01
23	AA	850	BCR	C15-C16-C17	-2.21	118.99	123.52
19	A	830	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
19	A1	813	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	A	848	BCR	C8-C7-C6	-2.21	121.09	127.00
22	X1	102	LHG	P-O3-C3	-2.21	108.68	121.35
23	A	853	BCR	C38-C26-C25	-2.21	122.07	124.48
23	AA	849	BCR	C8-C7-C6	-2.21	121.09	127.00
19	B2	852	CLA	CBC-CAC-C3C	2.21	118.41	112.42
19	A1	806	CLA	C1-C2-C3	-2.21	122.58	126.20
19	A1	822	CLA	C5-C3-C2	2.21	126.13	121.17
19	B	833	CLA	CHA-C1A-NA	-2.21	121.39	126.39
19	B2	836	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
25	L1	210	LMG	O1-C1-C2	-2.21	104.92	108.27
19	A	821	CLA	CAC-C3C-C4C	2.21	127.66	124.79
23	B	843	BCR	C8-C7-C6	-2.21	121.10	127.00
19	A2	805	CLA	O2D-CGD-CBD	2.21	115.09	111.23
25	B1	844	LMG	C40-C39-C38	-2.21	103.20	114.37
19	B	815	CLA	CBA-CAA-C2A	2.21	120.36	113.79
19	A2	830	CLA	CAC-C3C-C4C	2.21	127.66	124.79
19	BB	827	CLA	O2A-CGA-O1A	-2.21	117.66	123.33
22	XX	102	LHG	P-O3-C3	-2.21	108.70	121.35
19	BB	816	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	A2	811	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
25	B2	854	LMG	O3-C3-C2	-2.21	105.18	110.38
25	L1	210	LMG	O2-C2-C1	-2.21	104.82	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B1	852	LMG	O3-C3-C2	-2.21	105.18	110.38
19	B1	829	CLA	C5-C3-C2	2.21	126.12	121.17
19	B2	801	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	A1	834	CLA	CHB-C4A-NA	2.20	127.58	124.40
20	A2	803	CL0	CGD-CBD-CAD	-2.20	103.71	110.85
24	L1	204	AJP	C85-O84-C05	2.20	117.49	113.69
23	L1	201	BCR	C24-C23-C22	-2.20	122.97	126.23
19	A	814	CLA	CHB-C4A-NA	2.20	127.58	124.40
25	B1	844	LMG	O2-C2-C1	-2.20	104.83	110.08
23	A	847	BCR	C15-C14-C13	-2.20	124.19	127.28
23	A	848	BCR	C16-C15-C14	-2.20	119.01	123.52
19	B	827	CLA	CBA-CAA-C2A	2.20	120.34	113.79
25	B	845	LMG	C40-C39-C38	-2.20	103.24	114.37
19	B1	845	CLA	CAC-C3C-C4C	2.20	127.65	124.79
23	F	303	BCR	C38-C26-C25	-2.20	122.08	124.48
22	B2	848	LHG	P-O3-C3	-2.20	108.74	121.35
19	AA	827	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	F	305	BCR	C20-C21-C22	-2.20	124.19	127.28
19	A	801	CLA	O1D-CGD-CBD	2.20	128.86	124.52
19	B1	828	CLA	CHB-C4A-NA	2.20	127.58	124.40
26	B	841	ECH	C10-C11-C12	-2.20	116.83	123.20
19	B2	834	CLA	C4-C3-C5	2.20	119.05	115.23
19	BB	801	CLA	C2A-C1A-CHA	2.20	127.68	123.87
25	B	845	LMG	O3-C3-C2	-2.20	105.19	110.38
23	L2	207	BCR	C11-C10-C9	-2.20	124.19	127.28
22	B	853	LHG	P-O6-C4	-2.20	108.76	121.35
22	A1	845	LHG	P-O3-C3	-2.20	108.76	121.35
23	M1	101	BCR	C7-C8-C9	-2.20	122.99	126.23
23	AA	848	BCR	C23-C24-C25	-2.20	123.31	126.28
23	L	205	BCR	C15-C14-C13	-2.20	124.20	127.28
19	AA	805	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
26	B2	841	ECH	C10-C11-C12	-2.19	116.84	123.20
23	AA	854	BCR	C38-C26-C25	-2.19	122.09	124.48
19	BB	830	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
19	B2	834	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
23	A2	848	BCR	C8-C7-C6	-2.19	121.14	127.00
19	A	809	CLA	C1-C2-C3	-2.19	123.22	126.76
19	B	812	CLA	O1D-CGD-CBD	2.19	128.84	124.52
19	A	835	CLA	CHB-C4A-NA	2.19	127.56	124.40
19	AA	809	CLA	CAC-C3C-C4C	2.19	127.64	124.79
25	BB	844	LMG	O2-C2-C1	-2.19	104.86	110.08
23	FF	303	BCR	C15-C14-C13	-2.19	124.21	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	I	102	BCR	C24-C23-C22	-2.19	123.00	126.23
19	A	827	CLA	CHB-C4A-NA	2.19	127.56	124.40
19	B	803	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
19	B1	850	CLA	O2A-CGA-CBA	2.19	118.51	111.83
23	L	205	BCR	C8-C7-C6	-2.19	121.15	127.00
23	L1	208	BCR	C8-C7-C6	-2.19	121.15	127.00
19	A	805	CLA	CHB-C4A-NA	2.19	127.56	124.40
19	B2	810	CLA	CAC-C3C-C4C	2.19	127.64	124.79
19	B1	813	CLA	O2D-CGD-CBD	2.19	115.05	111.23
19	B1	832	CLA	CHA-C1A-NA	-2.19	121.44	126.39
19	A	829	CLA	C4-C3-C2	-2.19	118.01	123.63
23	I2	102	BCR	C33-C5-C6	-2.19	122.10	124.48
21	A	843	PQN	C11-C3-C2	-2.19	121.14	124.89
19	BB	815	CLA	CBA-CAA-C2A	2.19	120.30	113.79
25	B2	845	LMG	O2-C2-C1	-2.19	104.86	110.08
19	BB	834	CLA	O2A-CGA-O1A	-2.19	117.71	123.33
28	B	856	DGD	O6E-C1E-O5D	-2.19	104.88	110.04
23	A1	847	BCR	C16-C15-C14	-2.19	119.05	123.52
26	B1	840	ECH	C10-C11-C12	-2.19	116.87	123.20
19	B	825	CLA	C1-O2A-CGA	2.19	121.94	116.65
19	B2	850	CLA	CHB-C4A-NA	2.19	127.55	124.40
19	AA	814	CLA	CHB-C4A-NA	2.19	127.55	124.40
19	B2	837	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
23	AA	855	BCR	C15-C16-C17	-2.18	119.05	123.52
24	KK	104	AJP	C24-C23-C22	2.18	113.35	111.07
19	B	814	CLA	C4-C3-C5	-2.18	111.44	115.23
23	AA	855	BCR	C29-C30-C25	2.18	113.61	110.44
25	BB	844	LMG	O1-C1-C2	-2.18	104.96	108.27
19	BB	831	CLA	O2D-CGD-CBD	2.18	115.05	111.23
23	A1	848	BCR	C8-C7-C6	-2.18	121.17	127.00
19	B	835	CLA	O2A-CGA-O1A	-2.18	117.72	123.33
23	L	206	BCR	C16-C15-C14	-2.18	119.06	123.52
25	L1	210	LMG	C38-C37-C36	-2.18	103.34	114.37
19	B	830	CLA	CHB-C4A-NA	2.18	127.55	124.40
25	M	102	LMG	O3-C3-C2	-2.18	105.23	110.38
26	B	841	ECH	C23-C24-C25	-2.18	121.17	127.00
23	AA	848	BCR	C38-C26-C25	-2.18	122.10	124.48
19	B2	818	CLA	CHB-C4A-NA	2.18	127.55	124.40
23	K2	103	BCR	C8-C7-C6	-2.18	121.18	127.00
23	II	104	BCR	C8-C7-C6	-2.18	121.18	127.00
19	B	805	CLA	C3A-C2A-C1A	2.18	104.60	101.34
19	B1	819	CLA	CMA-C3A-C2A	-2.18	111.24	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A2	834	CLA	CAA-C2A-C3A	-2.18	111.24	116.23
20	AA	803	CL0	CMD-C2D-C3D	-2.18	120.33	124.68
19	A	809	CLA	CAC-C3C-C4C	2.18	127.62	124.79
19	B2	829	CLA	CHB-C4A-NA	2.18	127.54	124.40
24	A1	854	AJP	O25-C23-C24	-2.18	105.41	109.64
23	A	854	BCR	C28-C27-C26	-2.18	110.18	114.06
23	A	847	BCR	C38-C26-C25	-2.17	122.11	124.48
25	B2	845	LMG	O3-C3-C2	-2.17	105.25	110.38
25	BB	844	LMG	O3-C3-C2	-2.17	105.25	110.38
23	BB	838	BCR	C8-C7-C6	-2.17	121.19	127.00
25	B1	852	LMG	C1-C2-C3	-2.17	105.44	110.01
24	I2	104	AJP	C12-C07-C06	2.17	126.92	120.50
24	B	850	AJP	C03-C04-C05	2.17	115.34	111.93
19	AA	816	CLA	C1-C2-C3	-2.17	123.25	126.76
24	A	802	AJP	C13-C12-C07	-2.17	112.27	115.36
25	B1	844	LMG	O3-C3-C2	-2.17	105.25	110.38
19	LL	203	CLA	CHB-C1B-NB	2.17	127.31	124.05
19	B2	825	CLA	C1-O2A-CGA	2.17	121.91	116.65
19	BB	826	CLA	C3A-C2A-C1A	2.17	104.59	101.34
19	A	808	CLA	CED-O2D-CGD	2.17	120.84	115.92
25	B	845	LMG	O2-C2-C1	-2.17	104.90	110.08
24	BB	849	AJP	C85-O84-C05	2.17	117.43	113.69
19	A2	805	CLA	CHB-C4A-NA	2.17	127.53	124.40
19	FF	301	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	L1	210	LMG	O3-C3-C2	-2.17	105.26	110.38
23	FF	304	BCR	C8-C7-C6	-2.17	121.20	127.00
19	B	859	CLA	O2A-CGA-CBA	2.17	118.45	111.83
23	A1	851	BCR	C8-C7-C6	-2.17	121.21	127.00
23	B2	844	BCR	C15-C16-C17	-2.17	119.08	123.52
19	B	837	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	B1	826	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
19	A2	819	CLA	CHB-C4A-NA	2.17	127.53	124.40
19	BB	829	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
19	BB	808	CLA	CHB-C4A-NA	2.17	127.53	124.40
19	BB	819	CLA	CHB-C4A-NA	2.17	127.53	124.40
19	B2	815	CLA	CBA-CAA-C2A	2.17	120.24	113.79
24	A1	854	AJP	C17-C18-C19	2.17	116.03	111.84
19	B1	836	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
23	B1	843	BCR	C15-C16-C17	-2.17	119.09	123.52
21	AA	844	PQN	C15-C13-C12	-2.16	116.31	121.17
23	LL	204	BCR	C11-C10-C9	-2.16	124.24	127.28
28	B	856	DGD	C1D-C2D-C3D	-2.16	105.46	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B2	854	LMG	O2-C2-C1	-2.16	104.92	110.08
24	BB	848	AJP	O84-C85-C02	-2.16	109.39	112.17
19	B1	829	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	B2	835	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	A2	854	AJP	C85-O84-C05	2.16	117.42	113.69
23	AA	854	BCR	C7-C8-C9	-2.16	123.03	126.23
19	BB	836	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	L	203	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	AA	802	AJP	C13-C12-C07	-2.16	112.28	115.36
23	FF	306	BCR	C4-C5-C6	2.16	125.62	122.70
25	B2	854	LMG	C1-C2-C3	-2.16	105.46	110.01
24	BB	848	AJP	O79-C22-C23	-2.16	105.60	110.08
20	A	803	CL0	CBC-CAC-C3C	-2.16	109.78	112.87
19	A	839	CLA	O2D-CGD-CBD	2.16	115.01	111.23
19	BB	805	CLA	C3A-C2A-C1A	2.16	104.57	101.34
23	A2	849	BCR	C38-C26-C25	-2.16	122.13	124.48
25	B	851	LMG	O3-C3-C2	-2.16	105.29	110.38
19	B1	804	CLA	CBA-CAA-C2A	2.16	120.22	113.79
25	B	851	LMG	C38-C37-C36	-2.16	103.46	114.37
24	BB	848	AJP	O25-C26-O31	2.16	116.37	110.69
19	B	804	CLA	CBA-CAA-C2A	2.16	120.21	113.79
19	A1	804	CLA	O2D-CGD-CBD	2.16	115.00	111.23
23	AA	851	BCR	C2-C1-C6	2.16	113.57	110.44
23	BB	842	BCR	C8-C7-C6	-2.16	121.23	127.00
22	L1	211	LHG	P-O6-C4	-2.16	108.99	121.35
19	B2	851	CLA	C2A-C1A-CHA	2.16	127.61	123.87
19	AA	825	CLA	CHB-C4A-NA	2.16	127.51	124.40
19	AA	835	CLA	CHB-C4A-NA	2.16	127.51	124.40
19	B2	804	CLA	CBA-CAA-C2A	2.16	120.21	113.79
19	J	103	CLA	CAC-C3C-C4C	2.16	127.59	124.79
23	K1	104	BCR	C8-C7-C6	-2.16	121.24	127.00
23	A	849	BCR	C38-C26-C25	-2.16	122.13	124.48
20	A2	803	CL0	C9-C8-C7	2.16	118.96	111.27
23	L	205	BCR	C11-C10-C9	-2.15	124.26	127.28
19	A2	808	CLA	O1D-CGD-CBD	2.15	128.77	124.52
19	B1	826	CLA	C3A-C2A-C1A	2.15	104.57	101.34
22	A2	846	LHG	P-O6-C4	-2.15	109.01	121.35
19	A1	810	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
23	AA	854	BCR	C11-C10-C9	-2.15	124.26	127.28
19	B1	816	CLA	CHB-C4A-NA	2.15	127.51	124.40
23	A	847	BCR	C23-C24-C25	-2.15	123.37	126.28
25	B1	852	LMG	O2-C2-C1	-2.15	104.94	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	BB	829	CLA	C5-C3-C2	2.15	126.00	121.17
19	BB	803	CLA	CMB-C2B-C3B	2.15	131.61	126.55
19	B	817	CLA	O2D-CGD-CBD	2.15	114.99	111.23
23	AA	850	BCR	C38-C26-C25	-2.15	122.14	124.48
19	B2	849	CLA	C3B-C4B-NB	-2.15	108.61	110.53
23	A	849	BCR	C16-C15-C14	-2.15	119.12	123.52
23	A1	853	BCR	C8-C7-C6	-2.15	121.25	127.00
23	L1	209	BCR	C24-C23-C22	-2.15	123.05	126.23
23	A1	849	BCR	C15-C16-C17	-2.15	119.12	123.52
23	A2	851	BCR	C16-C15-C14	-2.15	119.12	123.52
19	BB	822	CLA	O2D-CGD-CBD	2.15	114.99	111.23
19	B	835	CLA	O2D-CGD-CBD	2.15	114.99	111.23
23	A2	847	BCR	C16-C15-C14	-2.15	119.12	123.52
19	A1	828	CLA	C4-C3-C2	-2.15	118.11	123.63
19	BB	804	CLA	CBA-CAA-C2A	2.15	120.18	113.79
19	AA	829	CLA	C5-C3-C2	2.15	125.98	121.17
19	BB	826	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
19	B1	807	CLA	C16-C15-C13	-2.14	108.84	115.97
19	B2	803	CLA	C11-C12-C13	-2.14	108.84	115.97
22	L	207	LHG	P-O6-C4	-2.14	109.06	121.35
22	LL	205	LHG	P-O6-C4	-2.14	109.06	121.35
23	B	844	BCR	C38-C26-C25	-2.14	122.14	124.48
19	B	830	CLA	C5-C3-C2	2.14	125.98	121.17
19	B1	808	CLA	CHB-C4A-NA	2.14	127.49	124.40
19	AA	805	CLA	CHB-C4A-NA	2.14	127.49	124.40
23	J2	104	BCR	C2-C3-C4	2.14	115.99	111.28
19	B	801	CLA	CBA-CAA-C2A	2.14	120.17	113.79
25	M	102	LMG	O2-C2-C1	-2.14	104.97	110.08
19	A2	833	CLA	CHB-C4A-NA	2.14	127.49	124.40
25	B1	846	LMG	O1-C7-C8	-2.14	105.61	110.82
19	A1	829	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
20	A2	803	CL0	CBC-CAC-C3C	-2.14	109.81	112.87
23	A2	853	BCR	C8-C7-C6	-2.14	121.28	127.00
19	A	832	CLA	C3B-C4B-NB	-2.14	108.62	110.53
25	II	105	LMG	O3-C3-C2	-2.14	105.33	110.38
19	B2	803	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
23	M1	101	BCR	C2-C1-C6	2.14	113.55	110.44
23	B2	839	BCR	C38-C26-C25	-2.14	122.15	124.48
19	B2	834	CLA	CMB-C2B-C3B	2.14	131.58	126.55
19	B1	848	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	A2	803	CL0	CMD-C2D-C3D	-2.14	120.41	124.68
23	K1	106	BCR	C20-C21-C22	-2.14	124.28	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AA	848	BCR	C15-C14-C13	-2.14	124.28	127.28
23	A	849	BCR	C24-C23-C22	-2.14	123.07	126.23
24	KK	104	AJP	C17-C16-C15	-2.14	107.96	110.52
23	B	842	BCR	C35-C13-C14	-2.14	119.36	122.82
19	A2	834	CLA	CMA-C3A-C2A	-2.14	111.33	116.23
19	B2	846	CLA	CAC-C3C-C4C	2.14	127.57	124.79
19	BB	826	CLA	C16-C15-C13	-2.14	108.87	115.97
24	L1	204	AJP	C32-C30-C29	2.14	118.26	113.02
22	A1	846	LHG	P-O6-C4	-2.14	109.11	121.35
28	BB	854	DGD	C3G-C2G-C1G	-2.13	106.81	111.78
23	BB	838	BCR	C11-C10-C9	-2.13	124.28	127.28
19	BB	856	CLA	C4-C3-C5	2.13	118.93	115.23
19	B1	815	CLA	CBA-CAA-C2A	2.13	120.14	113.79
19	L2	206	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
23	B	839	BCR	C8-C7-C6	-2.13	121.30	127.00
23	A	853	BCR	C7-C8-C9	-2.13	123.08	126.23
19	B	831	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
19	B2	812	CLA	O1D-CGD-CBD	2.13	128.72	124.52
23	A	851	BCR	C8-C7-C6	-2.13	121.30	127.00
24	BB	848	AJP	O84-C05-C04	2.13	112.62	110.76
23	I2	101	BCR	C16-C17-C18	-2.13	124.29	127.28
19	A	805	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
23	AA	849	BCR	C16-C15-C14	-2.13	119.16	123.52
23	B2	842	BCR	C29-C30-C25	2.13	113.53	110.44
23	B1	838	BCR	C38-C26-C25	-2.13	122.16	124.48
22	AA	847	LHG	P-O6-C4	-2.13	109.16	121.35
19	A2	839	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
20	A	803	CL0	C9-C8-C10	2.13	118.86	111.27
19	A1	833	CLA	CAA-C2A-C3A	-2.13	111.35	116.23
23	L	206	BCR	C24-C23-C22	-2.13	123.09	126.23
24	K	104	AJP	C15-C20-C19	2.13	111.47	108.51
26	B	841	ECH	C23-C22-C21	-2.13	115.67	119.01
19	A2	829	CLA	C5-C3-C2	2.13	125.94	121.17
23	B2	844	BCR	C38-C26-C25	-2.13	122.17	124.48
23	AA	850	BCR	C3-C4-C5	-2.13	110.27	114.06
19	AA	841	CLA	O2D-CGD-CBD	2.13	114.94	111.23
23	I	101	BCR	C27-C26-C25	2.12	125.58	122.70
20	AA	803	CL0	C5-C3-C2	-2.12	116.40	121.17
19	B1	821	CLA	C4-C3-C2	-2.12	118.17	123.63
23	AA	852	BCR	C33-C5-C6	-2.12	122.17	124.48
20	A	803	CL0	C4C-CHD-C1D	2.12	123.67	116.07
26	B1	840	ECH	C23-C24-C25	-2.12	121.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	815	CLA	C4-C3-C2	-2.12	118.17	123.63
19	B1	802	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	B2	821	CLA	C5-C3-C2	2.12	125.93	121.17
19	B2	805	CLA	C3A-C2A-C1A	2.12	104.52	101.34
19	B	826	CLA	C16-C15-C13	-2.12	108.91	115.97
22	B	853	LHG	O7-C7-C8	2.12	116.07	111.48
19	B2	830	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	B1	841	BCR	C36-C18-C19	2.12	121.33	118.09
19	B1	815	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	A	853	BCR	C8-C7-C6	-2.12	121.33	127.00
23	L1	208	BCR	C15-C14-C13	-2.12	124.30	127.28
23	J	102	BCR	C2-C1-C6	2.12	113.52	110.44
23	F	303	BCR	C15-C14-C13	-2.12	124.30	127.28
22	A	846	LHG	P-O6-C4	-2.12	109.20	121.35
19	BB	855	CLA	CHB-C4A-NA	2.12	127.46	124.40
19	AA	811	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
19	A1	821	CLA	O2D-CGD-CBD	2.12	114.94	111.23
25	I2	105	LMG	C1-C2-C3	-2.12	105.55	110.01
20	A1	802	CL0	C2C-C1C-NC	2.12	116.46	110.46
19	B	837	CLA	C1-C2-C3	-2.12	122.72	126.20
19	BB	829	CLA	CHB-C4A-NA	2.12	127.46	124.40
19	B1	805	CLA	C3A-C2A-C1A	2.12	104.51	101.34
19	BB	833	CLA	C1D-ND-C4D	-2.12	104.83	106.31
25	BB	844	LMG	C40-C39-C38	-2.12	103.67	114.37
19	B	834	CLA	C1D-ND-C4D	-2.12	104.83	106.31
19	L	204	CLA	CHB-C4A-NA	2.12	127.45	124.40
19	B1	833	CLA	C4-C3-C2	-2.12	118.19	123.63
23	L	206	BCR	C10-C11-C12	-2.12	117.07	123.20
23	M	101	BCR	C16-C15-C14	-2.12	119.19	123.52
19	AA	839	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
19	B1	810	CLA	C1-C2-C3	-2.11	122.73	126.20
19	B1	833	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
24	BB	849	AJP	C12-C07-C06	2.11	126.74	120.50
19	A1	827	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
19	AA	831	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
19	BB	803	CLA	C11-C12-C13	-2.11	108.95	115.97
23	AA	850	BCR	C24-C23-C22	-2.11	123.11	126.23
23	A2	849	BCR	C11-C10-C9	-2.11	124.32	127.28
19	B	810	CLA	C1-C2-C3	-2.11	122.74	126.20
26	B	841	ECH	C33-C5-C4	2.11	118.10	113.60
28	BB	854	DGD	O3E-C3E-C2E	-2.11	105.40	110.38
19	B1	810	CLA	CAC-C3C-C4C	2.11	127.53	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	839	BCR	C15-C14-C13	-2.11	124.32	127.28
26	B2	841	ECH	C8-C9-C10	2.11	122.33	119.01
19	B	834	CLA	C1-O2A-CGA	2.11	121.75	116.65
23	AA	848	BCR	C16-C15-C14	-2.11	119.21	123.52
24	A	855	AJP	C24-C19-C20	2.11	114.90	112.66
19	A	839	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
19	AA	808	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
19	BB	832	CLA	C3B-C4B-NB	-2.11	108.65	110.53
19	B1	833	CLA	C1-O2A-CGA	2.11	121.75	116.65
19	B	846	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
21	A1	843	PQN	C11-C3-C2	-2.11	121.28	124.89
28	BB	854	DGD	O6E-C5E-C4E	2.11	113.49	109.70
23	A	850	BCR	C2-C1-C6	2.11	113.50	110.44
19	A2	822	CLA	O2D-CGD-CBD	2.11	114.91	111.23
19	B2	807	CLA	C16-C15-C13	-2.11	108.97	115.97
19	B2	834	CLA	C1-O2A-CGA	2.10	121.75	116.65
23	A	849	BCR	C35-C13-C12	2.10	121.30	118.09
19	A	834	CLA	CMA-C3A-C2A	-2.10	111.40	116.23
24	L2	203	AJP	C26-O25-C23	2.10	118.79	115.27
20	AA	803	CL0	C2C-C1C-NC	2.10	116.41	110.46
19	A2	837	CLA	CHB-C4A-NA	2.10	127.44	124.40
23	I2	103	BCR	C8-C7-C6	-2.10	121.38	127.00
19	BB	810	CLA	CAC-C3C-C4C	2.10	127.52	124.79
20	A	803	CL0	CGD-CBD-CAD	-2.10	104.04	110.85
19	A2	833	CLA	O2D-CGD-CBD	2.10	114.90	111.23
19	BB	801	CLA	C6-C5-C3	2.10	118.59	113.47
23	AA	854	BCR	C8-C7-C6	-2.10	121.39	127.00
19	B1	849	CLA	CHB-C4A-NA	2.10	127.43	124.40
19	AA	826	CLA	O2A-CGA-O1A	-2.10	117.93	123.33
19	B	815	CLA	O2D-CGD-CBD	2.10	114.90	111.23
23	L1	201	BCR	C8-C7-C6	-2.10	121.39	127.00
19	AA	807	CLA	C1-C2-C3	-2.10	122.76	126.20
24	B	849	AJP	C18-C17-C16	2.10	115.51	112.16
19	BB	826	CLA	C3B-C4B-NB	-2.10	108.66	110.53
23	M	101	BCR	C7-C8-C9	-2.10	123.13	126.23
24	BB	849	AJP	C04-C03-C02	-2.10	107.48	111.67
23	F	304	BCR	C8-C7-C6	-2.10	121.39	127.00
23	A	849	BCR	C15-C16-C17	-2.10	119.23	123.52
19	AA	824	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
19	B	819	CLA	CMA-C3A-C2A	-2.10	111.42	116.23
23	M	101	BCR	C11-C10-C9	-2.10	124.34	127.28
19	A1	830	CLA	O2A-CGA-O1A	-2.10	118.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	M2	102	BCR	C35-C13-C12	2.10	121.29	118.09
22	L1	211	LHG	O7-C7-C8	2.10	116.02	111.48
19	B2	851	CLA	O2A-CGA-CBA	2.10	118.23	111.83
19	A	809	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
19	B	806	CLA	C1-O2A-CGA	2.10	121.72	116.65
19	B2	813	CLA	O2D-CGD-CBD	2.10	114.89	111.23
24	L	208	AJP	O09-C05-C06	-2.10	101.77	104.56
19	B1	833	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	B	857	AJP	O25-C23-C24	-2.09	105.56	109.64
23	MM	101	BCR	C35-C13-C14	-2.09	119.42	122.82
19	B	858	CLA	CHB-C4A-NA	2.09	127.42	124.40
19	L2	206	CLA	C3B-C4B-NB	-2.09	108.66	110.53
19	A2	828	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	II	102	BCR	C24-C23-C22	-2.09	123.14	126.23
19	AA	828	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	AA	856	AJP	C24-C19-C20	2.09	114.89	112.66
23	B	839	BCR	C11-C10-C9	-2.09	124.34	127.28
23	AA	850	BCR	C16-C15-C14	-2.09	119.24	123.52
19	B1	821	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
19	AA	810	CLA	CAA-CBA-CGA	-2.09	107.27	113.21
19	B2	803	CLA	CMB-C2B-C3B	2.09	131.47	126.55
28	B	856	DGD	O3E-C3E-C2E	-2.09	105.45	110.38
19	B	858	CLA	C3B-C4B-NB	-2.09	108.66	110.53
19	B2	851	CLA	O2D-CGD-CBD	2.09	114.88	111.23
23	B	839	BCR	C24-C23-C22	-2.09	123.14	126.23
19	K1	102	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
23	AA	854	BCR	C30-C25-C26	-2.09	119.78	122.64
23	B	848	BCR	C7-C8-C9	-2.09	123.14	126.23
19	A	842	CLA	C1-O2A-CGA	2.09	121.71	116.65
23	A1	850	BCR	C24-C23-C22	-2.09	123.14	126.23
19	A	820	CLA	CBA-CAA-C2A	2.09	120.00	113.79
23	A	853	BCR	C11-C10-C9	-2.09	124.35	127.28
19	A	805	CLA	C5-C3-C2	2.09	125.85	121.17
24	BB	848	AJP	C32-C30-C29	2.09	118.14	113.02
19	BB	845	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
19	B1	801	CLA	C5-C3-C2	2.09	125.85	121.17
19	B1	829	CLA	CHB-C4A-NA	2.09	127.41	124.40
19	B	804	CLA	O2D-CGD-CBD	2.09	114.88	111.23
19	B	814	CLA	O2D-CGD-CBD	2.09	114.88	111.23
23	MM	101	BCR	C16-C15-C14	-2.08	119.25	123.52
19	A2	831	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	A	851	BCR	C38-C26-C25	-2.08	122.21	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A1	849	BCR	C11-C10-C9	-2.08	124.36	127.28
19	B1	827	CLA	CBA-CAA-C2A	2.08	119.99	113.79
19	B2	826	CLA	C6-C5-C3	2.08	118.54	113.47
23	A2	849	BCR	C16-C15-C14	-2.08	119.26	123.52
19	LL	202	CLA	CHD-C1D-ND	-2.08	121.87	124.80
22	B1	847	LHG	P-O6-C4	-2.08	109.42	121.35
19	B1	816	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	A2	827	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	F	305	BCR	C35-C13-C12	2.08	121.27	118.09
19	A1	808	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	FF	306	BCR	C20-C21-C22	-2.08	124.36	127.28
19	L1	205	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	A2	830	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	B1	826	CLA	C3B-C4B-NB	-2.08	108.67	110.53
23	J	102	BCR	C2-C3-C4	2.08	115.85	111.28
19	A	828	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	B2	819	CLA	CMA-C3A-C2A	-2.08	111.46	116.23
19	A	811	CLA	C1-O2A-CGA	2.08	121.68	116.65
19	L2	204	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
26	B1	840	ECH	C8-C9-C10	2.08	122.28	119.01
19	K	101	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
25	B1	844	LMG	O1-C1-C2	-2.08	105.12	108.27
23	J2	102	BCR	C2-C1-C6	2.08	113.46	110.44
23	B	839	BCR	C27-C26-C25	2.08	125.51	122.70
19	BB	802	CLA	C4-C3-C5	2.08	118.83	115.23
19	A1	821	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	B	803	CLA	CMB-C2B-C3B	2.08	131.44	126.55
19	A	811	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
22	BB	851	LHG	P-O6-C4	-2.08	109.45	121.35
19	K1	105	CLA	CAC-C3C-C4C	2.08	127.49	124.79
19	K1	105	CLA	C2A-C1A-CHA	2.08	125.93	122.71
21	B	838	PQN	C26-C25-C23	-2.08	109.06	115.97
23	L2	207	BCR	C15-C14-C13	-2.08	124.37	127.28
19	A2	826	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
19	B1	822	CLA	O2D-CGD-CBD	2.08	114.86	111.23
23	A2	850	BCR	C24-C23-C22	-2.07	123.17	126.23
23	B2	842	BCR	C24-C23-C22	-2.07	123.17	126.23
24	L2	202	AJP	C12-C07-C06	2.07	126.63	120.50
19	B	833	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
19	L	204	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
19	A2	812	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
19	A	823	CLA	C5-C3-C2	2.07	125.82	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	854	BCR	C8-C7-C6	-2.07	121.46	127.00
24	L	209	AJP	C04-C03-C02	-2.07	107.53	111.67
23	M2	102	BCR	C38-C26-C25	-2.07	122.22	124.48
23	KK	103	BCR	C35-C13-C12	2.07	121.25	118.09
23	BB	843	BCR	C24-C23-C22	-2.07	123.17	126.23
28	BB	854	DGD	O5D-C6D-C5D	-2.07	104.75	109.42
24	BB	849	AJP	C26-O25-C23	-2.07	111.81	115.27
19	A2	833	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	J2	102	BCR	C2-C3-C4	2.07	115.83	111.28
19	A	808	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
25	II	105	LMG	O7-C10-O9	-2.07	118.87	123.70
19	A2	822	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	A2	849	BCR	C8-C7-C6	-2.07	121.47	127.00
23	M	101	BCR	C38-C26-C25	-2.07	122.23	124.48
19	A	834	CLA	CAA-C2A-C3A	-2.07	111.49	116.23
19	A	826	CLA	O2A-CGA-O1A	-2.07	118.01	123.33
26	B	841	ECH	C8-C9-C10	2.07	122.26	119.01
23	I2	103	BCR	C40-C30-C25	2.07	113.49	110.24
19	BB	814	CLA	O2D-CGD-CBD	2.07	114.84	111.23
19	KK	101	CLA	O2A-CGA-O1A	-2.07	118.01	123.33
19	B	801	CLA	C2A-C1A-CHA	2.07	127.45	123.87
22	X2	103	LHG	O7-C7-C8	2.07	115.95	111.48
26	B	841	ECH	C39-C30-C25	-2.07	107.00	110.24
19	K2	102	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
23	J2	104	BCR	C8-C7-C6	-2.07	121.48	127.00
19	B2	821	CLA	CBA-CAA-C2A	2.07	119.94	113.79
19	B	859	CLA	C4-C3-C5	2.07	118.81	115.23
25	I2	105	LMG	O2-C2-C1	-2.07	105.15	110.08
19	F1	301	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
19	B2	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
19	A2	824	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
19	B	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
25	B2	845	LMG	C40-C39-C38	-2.06	103.94	114.37
23	K1	106	BCR	C8-C7-C6	-2.06	121.49	127.00
19	A1	830	CLA	CAC-C3C-C4C	2.06	127.47	124.79
19	A1	823	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
19	AA	830	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	BB	821	CLA	C4-C3-C2	-2.06	118.33	123.63
19	B2	835	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
23	M1	101	BCR	C35-C13-C12	2.06	121.24	118.09
19	J1	101	CLA	CMA-C3A-C2A	-2.06	111.50	116.23
19	A1	826	CLA	CAA-C2A-C3A	-2.06	107.43	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	102	LMG	O6-C1-O1	-2.06	105.18	110.04
19	BB	804	CLA	O2D-CGD-CBD	2.06	114.83	111.23
23	BB	838	BCR	C27-C26-C25	2.06	125.49	122.70
19	F2	301	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	B1	807	CLA	CHA-C4D-ND	2.06	136.79	132.55
19	A	852	CLA	CHB-C4A-NA	2.06	127.37	124.40
23	A1	849	BCR	C27-C26-C25	2.06	125.48	122.70
23	A	847	BCR	C16-C15-C14	-2.06	119.31	123.52
23	B1	842	BCR	C8-C7-C6	-2.06	121.50	127.00
23	M1	101	BCR	C38-C26-C25	-2.06	122.24	124.48
19	A	841	CLA	O2D-CGD-CBD	2.06	114.82	111.23
19	K2	104	CLA	CHA-C1A-NA	-2.06	121.74	126.39
23	AA	850	BCR	C35-C13-C12	2.06	121.23	118.09
21	AA	844	PQN	C2M-C2-C3	-2.06	121.07	124.45
19	BB	802	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
19	AA	805	CLA	C5-C3-C2	2.05	125.78	121.17
23	A1	849	BCR	C16-C15-C14	-2.05	119.32	123.52
23	J2	104	BCR	C16-C15-C14	-2.05	119.32	123.52
19	B	834	CLA	C6-C7-C8	-2.05	109.14	115.97
25	B	851	LMG	C40-C39-C38	-2.05	104.00	114.37
19	A1	838	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	A2	809	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
21	B1	837	PQN	C11-C3-C2	-2.05	121.37	124.89
23	A2	849	BCR	C27-C26-C25	2.05	125.48	122.70
19	B1	826	CLA	CHB-C1B-NB	2.05	127.12	124.05
23	K2	105	BCR	C8-C7-C6	-2.05	121.52	127.00
19	A1	826	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	BB	840	ECH	C33-C5-C4	2.05	117.97	113.60
19	B2	821	CLA	O2D-CGD-CBD	2.05	114.81	111.23
19	BB	820	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
19	BB	829	CLA	CBC-CAC-C3C	2.05	117.97	112.42
19	A2	842	CLA	C1-O2A-CGA	2.05	121.61	116.65
25	B1	846	LMG	O2-C2-C1	-2.05	105.19	110.08
23	A	848	BCR	C24-C23-C22	-2.05	123.21	126.23
23	A	854	BCR	C29-C30-C25	2.05	113.41	110.44
23	J	104	BCR	C16-C15-C14	-2.05	119.33	123.52
19	B1	814	CLA	O2D-CGD-CBD	2.05	114.81	111.23
19	B1	848	CLA	O2D-CGD-CBD	2.05	114.81	111.23
19	B2	834	CLA	CBA-CAA-C2A	2.05	119.88	113.79
19	BB	806	CLA	C1-C2-C3	2.05	129.55	126.20
23	J	102	BCR	C11-C10-C9	-2.05	124.41	127.28
19	L2	206	CLA	CHB-C4A-NA	2.05	127.35	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L2	203	AJP	C24-C19-C20	2.05	114.84	112.66
19	F	301	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
23	JJ	104	BCR	C16-C15-C14	-2.05	119.33	123.52
24	AA	856	AJP	C81-C12-C11	2.05	116.03	111.58
19	AA	834	CLA	CAA-C2A-C3A	-2.04	111.54	116.23
19	B2	826	CLA	CHB-C1B-NB	2.04	127.12	124.05
25	B1	846	LMG	C1-C2-C3	-2.04	105.71	110.01
23	B1	838	BCR	C8-C7-C6	-2.04	121.54	127.00
23	B2	843	BCR	C8-C7-C6	-2.04	121.54	127.00
19	B1	834	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
23	AA	855	BCR	C8-C7-C6	-2.04	121.54	127.00
19	B1	802	CLA	C4-C3-C5	2.04	118.77	115.23
19	A	827	CLA	O1D-CGD-CBD	2.04	128.55	124.52
19	AA	801	CLA	O1D-CGD-CBD	2.04	128.55	124.52
24	A	855	AJP	C81-C12-C11	2.04	116.03	111.58
19	L	204	CLA	C6-C5-C3	2.04	118.44	113.47
19	B2	831	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	A	833	CLA	O2D-CGD-CBD	2.04	114.80	111.23
21	A2	843	PQN	C11-C3-C2	-2.04	121.39	124.89
23	B2	839	BCR	C8-C7-C6	-2.04	121.55	127.00
19	B	818	CLA	CAA-C2A-C3A	-2.04	111.55	116.23
23	B1	841	BCR	C35-C13-C14	-2.04	119.51	122.82
19	B	802	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	BB	801	CLA	C3B-C4B-NB	-2.04	108.71	110.53
19	BB	825	CLA	C1-O2A-CGA	2.04	121.58	116.65
23	AA	852	BCR	C8-C7-C6	-2.04	121.55	127.00
22	L	207	LHG	O7-C7-C8	2.04	115.89	111.48
19	A1	834	CLA	C11-C10-C8	-2.04	109.19	115.97
19	A	852	CLA	C6-C5-C3	2.04	118.43	113.47
19	B2	807	CLA	CHA-C4D-ND	2.04	136.75	132.55
23	A1	849	BCR	C8-C7-C6	-2.04	121.56	127.00
19	AA	834	CLA	CMA-C3A-C2A	-2.04	111.56	116.23
23	A1	851	BCR	C10-C11-C12	-2.04	117.30	123.20
19	A	844	CLA	O1D-CGD-CBD	2.04	128.53	124.52
19	B2	827	CLA	CBA-CAA-C2A	2.04	119.85	113.79
19	A1	832	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
19	A2	829	CLA	CAC-C3C-C4C	2.04	127.44	124.79
19	B2	823	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
19	A1	825	CLA	O2A-CGA-O1A	-2.03	118.10	123.33
25	II	105	LMG	C38-C37-C36	-2.03	104.09	114.37
20	A	803	CL0	C2C-C1C-NC	2.03	116.21	110.46
19	BB	812	CLA	CMA-C3A-C2A	-2.03	111.57	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	851	BCR	C33-C5-C6	-2.03	122.27	124.48
24	K	104	AJP	C13-C12-C07	-2.03	112.47	115.36
19	LL	201	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	LL	205	LHG	O7-C7-C8	2.03	115.88	111.48
23	L2	207	BCR	C10-C11-C12	-2.03	117.31	123.20
23	A	849	BCR	C3-C4-C5	-2.03	110.43	114.06
23	I	102	BCR	C38-C26-C25	-2.03	122.27	124.48
19	JJ	103	CLA	CAC-C3C-C4C	2.03	127.43	124.79
19	B1	834	CLA	O2D-CGD-CBD	2.03	114.78	111.23
23	B1	838	BCR	C11-C10-C9	-2.03	124.43	127.28
23	A	854	BCR	C15-C14-C13	-2.03	124.43	127.28
23	BB	838	BCR	C20-C21-C22	-2.03	124.43	127.28
19	A1	804	CLA	C5-C3-C2	2.03	125.72	121.17
19	A2	827	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
19	A2	820	CLA	C1-C2-C3	-2.03	122.87	126.20
25	B2	845	LMG	C1-C2-C3	-2.03	105.74	110.01
19	B1	832	CLA	CAA-C2A-C1A	2.03	118.62	111.97
19	B	814	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
19	BB	835	CLA	O2D-CGD-CBD	2.03	114.77	111.23
24	B	849	AJP	C12-C07-C06	2.03	126.49	120.50
24	L	208	AJP	C24-C23-C22	-2.03	108.29	111.53
19	A1	833	CLA	CMA-C3A-C2A	-2.03	111.59	116.23
25	B2	845	LMG	C42-C41-C40	-2.02	104.14	114.37
19	A	824	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
23	B2	839	BCR	C11-C10-C9	-2.02	124.44	127.28
19	AA	811	CLA	CAC-C3C-C4C	2.02	127.42	124.79
19	B	830	CLA	O2D-CGD-CBD	2.02	114.77	111.23
19	BB	833	CLA	C6-C7-C8	-2.02	109.25	115.97
25	B	845	LMG	O1-C7-C8	-2.02	105.90	110.82
19	A	828	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
23	F	305	BCR	C4-C5-C6	2.02	125.43	122.70
19	B1	834	CLA	CED-O2D-CGD	2.02	120.50	115.92
19	A	825	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
23	A	853	BCR	C30-C25-C26	-2.02	119.88	122.64
23	LL	204	BCR	C8-C7-C6	-2.02	121.60	127.00
23	A	850	BCR	C24-C23-C22	-2.02	123.25	126.23
23	LL	204	BCR	C24-C23-C22	-2.02	123.25	126.23
19	F2	301	CLA	CHA-C1A-NA	-2.02	121.82	126.39
20	A1	802	CL0	C5-C3-C2	-2.02	116.64	121.17
26	B2	841	ECH	C28-C27-C26	-2.02	116.83	118.64
19	B	815	CLA	CHA-C1A-NA	-2.02	121.82	126.39
19	B	810	CLA	CAC-C3C-C4C	2.02	127.42	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	804	CLA	C6-C5-C3	-2.02	108.55	113.47
23	AA	849	BCR	C24-C23-C22	-2.02	123.25	126.23
23	B	843	BCR	C38-C26-C25	-2.02	122.28	124.48
19	B	820	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
24	I2	104	AJP	C21-C22-C23	2.02	113.48	110.89
23	AA	850	BCR	C27-C26-C25	2.02	125.43	122.70
19	B2	815	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
19	AA	826	CLA	O1A-CGA-CBA	2.02	129.49	123.09
23	A	849	BCR	C27-C26-C25	2.02	125.43	122.70
24	L2	203	AJP	C12-C07-C06	2.02	126.46	120.50
23	LL	204	BCR	C4-C5-C6	2.02	125.43	122.70
19	LL	203	CLA	CHC-C1C-NC	2.02	127.35	124.31
23	B1	843	BCR	C38-C26-C25	-2.02	122.28	124.48
19	BB	815	CLA	O2D-CGD-CBD	2.02	114.75	111.23
19	AA	821	CLA	CAC-C3C-C4C	2.01	127.41	124.79
19	AA	805	CLA	C4-C3-C2	-2.01	118.45	123.63
19	AA	853	CLA	CHB-C4A-NA	2.01	127.31	124.40
19	BB	806	CLA	C1-O2A-CGA	2.01	121.53	116.65
24	M2	101	AJP	O09-C05-C06	-2.01	101.88	104.56
19	B	806	CLA	C1-C2-C3	2.01	129.50	126.20
19	AA	823	CLA	C5-C3-C2	2.01	125.69	121.17
20	A1	802	CL0	O2A-CGA-CBA	2.01	117.97	111.83
28	BB	854	DGD	O6E-C1E-O5D	-2.01	105.29	110.04
23	A	849	BCR	C8-C7-C6	-2.01	121.62	127.00
19	J2	103	CLA	CAC-C3C-C4C	2.01	127.41	124.79
23	I2	102	BCR	C16-C15-C14	-2.01	119.40	123.52
19	A1	807	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
25	B2	854	LMG	C7-O1-C1	2.01	118.11	113.80
23	A1	847	BCR	C15-C14-C13	-2.01	124.46	127.28
19	B2	806	CLA	C1-C2-C3	2.01	129.49	126.20
23	AA	852	BCR	C38-C26-C25	-2.01	122.29	124.48
25	B1	852	LMG	O6-C1-O1	-2.01	105.30	110.04
19	B1	833	CLA	CBC-CAC-C3C	2.01	117.87	112.42
19	B1	829	CLA	O2D-CGD-CBD	2.01	114.74	111.23
19	B2	809	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
19	B	820	CLA	CHD-C4C-C3C	2.01	127.70	124.77
23	AA	852	BCR	C39-C30-C25	2.01	113.39	110.24
19	B1	809	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
19	A1	829	CLA	C3B-C4B-NB	-2.01	108.74	110.53
19	B2	824	CLA	O2D-CGD-CBD	2.01	114.74	111.23
23	F1	306	BCR	C35-C13-C12	2.01	121.16	118.09
19	A1	840	CLA	O2D-CGD-CBD	2.01	114.74	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	836	CLA	O2D-CGD-CBD	2.01	114.74	111.23
19	AA	811	CLA	O2D-CGD-CBD	2.01	114.74	111.23
19	BB	852	CLA	O2D-CGD-CBD	2.01	114.74	111.23
23	L1	201	BCR	C16-C15-C14	-2.01	119.41	123.52
19	A2	835	CLA	C11-C10-C8	-2.01	109.29	115.97
19	A2	826	CLA	O1A-CGA-CBA	2.01	129.46	123.09
19	J2	103	CLA	CMA-C3A-C2A	-2.01	111.63	116.23
19	BB	818	CLA	CMA-C3A-C2A	-2.01	111.63	116.23
19	B1	825	CLA	C1-O2A-CGA	2.01	121.51	116.65
23	A1	851	BCR	C40-C30-C25	2.01	113.39	110.24
23	I	102	BCR	C8-C7-C6	-2.01	121.64	127.00
19	B	860	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
23	MM	101	BCR	C4-C5-C6	2.01	125.41	122.70
19	AA	828	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
19	B	803	CLA	C11-C12-C13	-2.01	109.30	115.97
24	L1	204	AJP	C17-C16-C15	-2.00	108.12	110.52
19	BB	833	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
19	A	832	CLA	C3A-C2A-C1A	2.00	104.34	101.34
19	A1	852	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
19	AA	825	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
19	BB	833	CLA	CHA-C4D-ND	2.00	136.68	132.55
19	A2	811	CLA	O2D-CGD-CBD	2.00	114.73	111.23
24	L1	204	AJP	C15-C20-C19	2.00	111.30	108.51
19	BB	815	CLA	C4-C3-C2	-2.00	118.49	123.63
23	J	102	BCR	C7-C8-C9	-2.00	123.27	126.23
19	BB	833	CLA	C1-O2A-CGA	2.00	121.50	116.65
23	A	848	BCR	C11-C10-C9	-2.00	124.47	127.28
19	B1	833	CLA	C6-C7-C8	-2.00	109.32	115.97
24	L	208	AJP	C12-C07-C06	2.00	126.41	120.50

All (703) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A1	801	CLA	ND
19	A1	803	CLA	ND
19	A1	804	CLA	ND
19	A1	806	CLA	ND
19	A1	807	CLA	ND
19	A1	808	CLA	ND
19	A1	809	CLA	ND
19	A1	810	CLA	ND
19	A1	811	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A1	812	CLA	ND
19	A1	813	CLA	ND
19	A1	814	CLA	ND
19	A1	815	CLA	ND
19	A1	816	CLA	ND
19	A1	817	CLA	ND
19	A1	818	CLA	ND
19	A1	820	CLA	ND
19	A1	821	CLA	ND
19	A1	822	CLA	ND
19	A1	823	CLA	ND
19	A1	824	CLA	ND
19	A1	825	CLA	ND
19	A1	826	CLA	ND
19	A1	827	CLA	ND
19	A1	828	CLA	ND
19	A1	829	CLA	ND
19	A1	830	CLA	ND
19	A1	831	CLA	ND
19	A1	832	CLA	ND
19	A1	833	CLA	ND
19	A1	834	CLA	ND
19	A1	835	CLA	ND
19	A1	836	CLA	ND
19	A1	837	CLA	ND
19	A1	838	CLA	ND
19	A1	839	CLA	ND
19	A1	840	CLA	ND
19	A1	841	CLA	ND
19	A1	842	CLA	ND
19	A1	844	CLA	ND
19	A1	852	CLA	ND
19	B1	801	CLA	ND
19	B1	802	CLA	ND
19	B1	803	CLA	ND
19	B1	804	CLA	ND
19	B1	805	CLA	ND
19	B1	806	CLA	ND
19	B1	807	CLA	ND
19	B1	808	CLA	ND
19	B1	809	CLA	ND
19	B1	810	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B1	811	CLA	ND
19	B1	812	CLA	ND
19	B1	813	CLA	ND
19	B1	814	CLA	ND
19	B1	815	CLA	ND
19	B1	816	CLA	ND
19	B1	817	CLA	ND
19	B1	818	CLA	ND
19	B1	819	CLA	ND
19	B1	820	CLA	ND
19	B1	821	CLA	ND
19	B1	822	CLA	ND
19	B1	823	CLA	ND
19	B1	824	CLA	ND
19	B1	825	CLA	ND
19	B1	826	CLA	ND
19	B1	827	CLA	ND
19	B1	828	CLA	ND
19	B1	829	CLA	ND
19	B1	830	CLA	ND
19	B1	831	CLA	ND
19	B1	832	CLA	ND
19	B1	833	CLA	ND
19	B1	834	CLA	ND
19	B1	835	CLA	ND
19	B1	836	CLA	ND
19	B1	845	CLA	ND
19	B1	848	CLA	ND
19	B1	849	CLA	ND
19	B1	850	CLA	ND
19	F1	301	CLA	ND
19	F1	302	CLA	ND
19	F1	305	CLA	ND
19	J1	101	CLA	ND
19	J1	103	CLA	ND
19	K1	102	CLA	ND
19	K1	103	CLA	ND
19	K1	105	CLA	ND
19	L1	205	CLA	ND
19	L1	206	CLA	ND
19	L1	207	CLA	ND
19	X1	101	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A2	801	CLA	ND
19	A2	802	CLA	ND
19	A2	804	CLA	ND
19	A2	805	CLA	ND
19	A2	806	CLA	ND
19	A2	807	CLA	ND
19	A2	808	CLA	ND
19	A2	809	CLA	ND
19	A2	810	CLA	ND
19	A2	811	CLA	ND
19	A2	812	CLA	ND
19	A2	813	CLA	ND
19	A2	814	CLA	ND
19	A2	815	CLA	ND
19	A2	816	CLA	ND
19	A2	817	CLA	ND
19	A2	818	CLA	ND
19	A2	819	CLA	ND
19	A2	820	CLA	ND
19	A2	821	CLA	ND
19	A2	822	CLA	ND
19	A2	823	CLA	ND
19	A2	824	CLA	ND
19	A2	825	CLA	ND
19	A2	826	CLA	ND
19	A2	827	CLA	ND
19	A2	828	CLA	ND
19	A2	829	CLA	ND
19	A2	830	CLA	ND
19	A2	831	CLA	ND
19	A2	832	CLA	ND
19	A2	833	CLA	ND
19	A2	834	CLA	ND
19	A2	835	CLA	ND
19	A2	837	CLA	ND
19	A2	838	CLA	ND
19	A2	839	CLA	ND
19	A2	840	CLA	ND
19	A2	841	CLA	ND
19	A2	842	CLA	ND
19	A2	844	CLA	ND
19	A2	852	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B2	801	CLA	ND
19	B2	802	CLA	ND
19	B2	803	CLA	ND
19	B2	804	CLA	ND
19	B2	805	CLA	ND
19	B2	806	CLA	ND
19	B2	807	CLA	ND
19	B2	808	CLA	ND
19	B2	809	CLA	ND
19	B2	810	CLA	ND
19	B2	811	CLA	ND
19	B2	812	CLA	ND
19	B2	813	CLA	ND
19	B2	814	CLA	ND
19	B2	815	CLA	ND
19	B2	816	CLA	ND
19	B2	817	CLA	ND
19	B2	818	CLA	ND
19	B2	819	CLA	ND
19	B2	820	CLA	ND
19	B2	821	CLA	ND
19	B2	822	CLA	ND
19	B2	823	CLA	ND
19	B2	824	CLA	ND
19	B2	825	CLA	ND
19	B2	826	CLA	ND
19	B2	827	CLA	ND
19	B2	828	CLA	ND
19	B2	829	CLA	ND
19	B2	830	CLA	ND
19	B2	831	CLA	ND
19	B2	832	CLA	ND
19	B2	834	CLA	ND
19	B2	835	CLA	ND
19	B2	836	CLA	ND
19	B2	837	CLA	ND
19	B2	846	CLA	ND
19	B2	849	CLA	ND
19	B2	850	CLA	ND
19	B2	851	CLA	ND
19	B2	852	CLA	ND
19	F2	301	CLA	ND

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Mol	Chain	Res	Type	Atom
19	F2	302	CLA	ND
19	J2	101	CLA	ND
19	J2	103	CLA	ND
19	K2	102	CLA	ND
19	K2	104	CLA	ND
19	L2	204	CLA	ND
19	L2	205	CLA	ND
19	L2	206	CLA	ND
19	X2	101	CLA	ND
19	A	801	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND
19	A	811	CLA	ND
19	A	812	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	817	CLA	ND
19	A	818	CLA	ND
19	A	819	CLA	ND
19	A	821	CLA	ND
19	A	822	CLA	ND
19	A	823	CLA	ND
19	A	824	CLA	ND
19	A	825	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	831	CLA	ND
19	A	832	CLA	ND
19	A	833	CLA	ND
19	A	834	CLA	ND
19	A	835	CLA	ND
19	A	836	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	841	CLA	ND
19	A	842	CLA	ND
19	A	844	CLA	ND
19	A	852	CLA	ND
19	B	801	CLA	ND
19	B	802	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	805	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
19	B	816	CLA	ND
19	B	817	CLA	ND
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	820	CLA	ND
19	B	821	CLA	ND
19	B	822	CLA	ND
19	B	823	CLA	ND
19	B	824	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND
19	B	827	CLA	ND
19	B	828	CLA	ND
19	B	829	CLA	ND
19	B	830	CLA	ND
19	B	831	CLA	ND
19	B	832	CLA	ND
19	B	834	CLA	ND
19	B	835	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	846	CLA	ND
19	B	854	CLA	ND
19	B	858	CLA	ND
19	B	859	CLA	ND
19	B	860	CLA	ND
19	F	301	CLA	ND
19	F	302	CLA	ND
19	J	101	CLA	ND
19	K	101	CLA	ND
19	K	102	CLA	ND
19	L	202	CLA	ND
19	L	203	CLA	ND
19	L	204	CLA	ND
19	X	101	CLA	ND
19	AA	801	CLA	ND
19	AA	804	CLA	ND
19	AA	805	CLA	ND
19	AA	806	CLA	ND
19	AA	807	CLA	ND
19	AA	808	CLA	ND
19	AA	809	CLA	ND
19	AA	810	CLA	ND
19	AA	811	CLA	ND
19	AA	812	CLA	ND
19	AA	813	CLA	ND
19	AA	814	CLA	ND
19	AA	815	CLA	ND
19	AA	816	CLA	ND
19	AA	817	CLA	ND
19	AA	818	CLA	ND
19	AA	819	CLA	ND
19	AA	820	CLA	ND
19	AA	821	CLA	ND
19	AA	823	CLA	ND
19	AA	824	CLA	ND
19	AA	825	CLA	ND
19	AA	826	CLA	ND
19	AA	827	CLA	ND
19	AA	828	CLA	ND
19	AA	829	CLA	ND

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Mol	Chain	Res	Type	Atom
19	AA	830	CLA	ND
19	AA	831	CLA	ND
19	AA	832	CLA	ND
19	AA	833	CLA	ND
19	AA	834	CLA	ND
19	AA	835	CLA	ND
19	AA	836	CLA	ND
19	AA	837	CLA	ND
19	AA	838	CLA	ND
19	AA	839	CLA	ND
19	AA	840	CLA	ND
19	AA	841	CLA	ND
19	AA	842	CLA	ND
19	AA	843	CLA	ND
19	AA	845	CLA	ND
19	AA	853	CLA	ND
19	BB	801	CLA	ND
19	BB	802	CLA	ND
19	BB	803	CLA	ND
19	BB	804	CLA	ND
19	BB	805	CLA	ND
19	BB	806	CLA	ND
19	BB	807	CLA	ND
19	BB	808	CLA	ND
19	BB	809	CLA	ND
19	BB	810	CLA	ND
19	BB	811	CLA	ND
19	BB	812	CLA	ND
19	BB	813	CLA	ND
19	BB	814	CLA	ND
19	BB	815	CLA	ND
19	BB	816	CLA	ND
19	BB	817	CLA	ND
19	BB	818	CLA	ND
19	BB	819	CLA	ND
19	BB	820	CLA	ND
19	BB	821	CLA	ND
19	BB	822	CLA	ND
19	BB	823	CLA	ND
19	BB	824	CLA	ND
19	BB	825	CLA	ND
19	BB	826	CLA	ND

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Mol	Chain	Res	Type	Atom
19	BB	827	CLA	ND
19	BB	828	CLA	ND
19	BB	829	CLA	ND
19	BB	830	CLA	ND
19	BB	831	CLA	ND
19	BB	833	CLA	ND
19	BB	834	CLA	ND
19	BB	835	CLA	ND
19	BB	836	CLA	ND
19	BB	845	CLA	ND
19	BB	852	CLA	ND
19	BB	855	CLA	ND
19	BB	856	CLA	ND
19	FF	301	CLA	ND
19	FF	302	CLA	ND
19	FF	305	CLA	ND
19	JJ	101	CLA	ND
19	JJ	103	CLA	ND
19	KK	101	CLA	ND
19	KK	102	CLA	ND
19	LL	201	CLA	ND
19	LL	202	CLA	ND
19	LL	203	CLA	ND
19	XX	101	CLA	ND
20	A1	802	CL0	C8
20	A1	802	CL0	ND
20	A1	802	CL0	NC
20	A1	802	CL0	NA
20	A2	803	CL0	C8
20	A2	803	CL0	ND
20	A2	803	CL0	NC
20	A2	803	CL0	NA
20	A	803	CL0	C8
20	A	803	CL0	ND
20	A	803	CL0	NC
20	A	803	CL0	NA
20	AA	803	CL0	C8
20	AA	803	CL0	ND
20	AA	803	CL0	NC
20	AA	803	CL0	NA
24	A1	854	AJP	C26
24	A1	854	AJP	C05

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Mol	Chain	Res	Type	Atom
24	A1	854	AJP	C10
24	A1	854	AJP	C11
24	A1	854	AJP	C12
24	A1	854	AJP	C19
24	A1	854	AJP	C28
24	A1	854	AJP	C30
24	A1	854	AJP	C15
24	A1	854	AJP	C27
24	A1	854	AJP	C16
24	A1	854	AJP	C07
24	A1	854	AJP	C20
24	A1	854	AJP	C22
24	A1	854	AJP	C02
24	A1	854	AJP	C23
24	A1	855	AJP	C05
24	A1	855	AJP	C10
24	A1	855	AJP	C11
24	A1	855	AJP	C12
24	A1	855	AJP	C19
24	A1	855	AJP	C15
24	A1	855	AJP	C16
24	A1	855	AJP	C07
24	A1	855	AJP	C20
24	A1	855	AJP	C22
24	A1	855	AJP	C02
24	A1	855	AJP	C23
24	L1	203	AJP	C26
24	L1	203	AJP	C05
24	L1	203	AJP	C10
24	L1	203	AJP	C11
24	L1	203	AJP	C12
24	L1	203	AJP	C19
24	L1	203	AJP	C28
24	L1	203	AJP	C30
24	L1	203	AJP	C15
24	L1	203	AJP	C27
24	L1	203	AJP	C16
24	L1	203	AJP	C07
24	L1	203	AJP	C20
24	L1	203	AJP	C22
24	L1	203	AJP	C02
24	L1	203	AJP	C23

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Mol	Chain	Res	Type	Atom
24	L1	204	AJP	C26
24	L1	204	AJP	C05
24	L1	204	AJP	C10
24	L1	204	AJP	C11
24	L1	204	AJP	C12
24	L1	204	AJP	C19
24	L1	204	AJP	C28
24	L1	204	AJP	C30
24	L1	204	AJP	C15
24	L1	204	AJP	C27
24	L1	204	AJP	C16
24	L1	204	AJP	C07
24	L1	204	AJP	C20
24	L1	204	AJP	C22
24	L1	204	AJP	C02
24	L1	204	AJP	C23
24	A2	854	AJP	C05
24	A2	854	AJP	C10
24	A2	854	AJP	C11
24	A2	854	AJP	C12
24	A2	854	AJP	C19
24	A2	854	AJP	C15
24	A2	854	AJP	C16
24	A2	854	AJP	C07
24	A2	854	AJP	C20
24	A2	854	AJP	C22
24	A2	854	AJP	C02
24	A2	854	AJP	C23
24	I2	104	AJP	C05
24	I2	104	AJP	C11
24	I2	104	AJP	C12
24	I2	104	AJP	C19
24	I2	104	AJP	C08
24	I2	104	AJP	C15
24	I2	104	AJP	C22
24	I2	104	AJP	C16
24	I2	104	AJP	C07
24	I2	104	AJP	C20
24	I2	104	AJP	C10
24	I2	104	AJP	C02
24	L2	202	AJP	C26
24	L2	202	AJP	C05

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Mol	Chain	Res	Type	Atom
24	L2	202	AJP	C11
24	L2	202	AJP	C12
24	L2	202	AJP	C19
24	L2	202	AJP	C28
24	L2	202	AJP	C08
24	L2	202	AJP	C30
24	L2	202	AJP	C15
24	L2	202	AJP	C27
24	L2	202	AJP	C22
24	L2	202	AJP	C16
24	L2	202	AJP	C07
24	L2	202	AJP	C20
24	L2	202	AJP	C10
24	L2	202	AJP	C02
24	L2	202	AJP	C23
24	L2	203	AJP	C26
24	L2	203	AJP	C05
24	L2	203	AJP	C11
24	L2	203	AJP	C12
24	L2	203	AJP	C19
24	L2	203	AJP	C28
24	L2	203	AJP	C30
24	L2	203	AJP	C15
24	L2	203	AJP	C27
24	L2	203	AJP	C22
24	L2	203	AJP	C16
24	L2	203	AJP	C07
24	L2	203	AJP	C20
24	L2	203	AJP	C10
24	L2	203	AJP	C02
24	L2	203	AJP	C23
24	M2	101	AJP	C05
24	M2	101	AJP	C11
24	M2	101	AJP	C12
24	M2	101	AJP	C19
24	M2	101	AJP	C08
24	M2	101	AJP	C15
24	M2	101	AJP	C22
24	M2	101	AJP	C16
24	M2	101	AJP	C07
24	M2	101	AJP	C20
24	M2	101	AJP	C10

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Mol	Chain	Res	Type	Atom
24	M2	101	AJP	C02
24	A	802	AJP	C05
24	A	802	AJP	C11
24	A	802	AJP	C12
24	A	802	AJP	C19
24	A	802	AJP	C08
24	A	802	AJP	C15
24	A	802	AJP	C16
24	A	802	AJP	C07
24	A	802	AJP	C20
24	A	802	AJP	C10
24	A	802	AJP	C02
24	A	855	AJP	C05
24	A	855	AJP	C10
24	A	855	AJP	C11
24	A	855	AJP	C12
24	A	855	AJP	C19
24	A	855	AJP	C15
24	A	855	AJP	C16
24	A	855	AJP	C07
24	A	855	AJP	C20
24	A	855	AJP	C22
24	A	855	AJP	C02
24	A	855	AJP	C23
24	B	849	AJP	C26
24	B	849	AJP	C05
24	B	849	AJP	C06
24	B	849	AJP	C11
24	B	849	AJP	C12
24	B	849	AJP	C19
24	B	849	AJP	C28
24	B	849	AJP	C08
24	B	849	AJP	C30
24	B	849	AJP	C15
24	B	849	AJP	C27
24	B	849	AJP	C22
24	B	849	AJP	C16
24	B	849	AJP	C07
24	B	849	AJP	C20
24	B	849	AJP	C10
24	B	849	AJP	C02
24	B	849	AJP	C23

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Mol	Chain	Res	Type	Atom
24	B	850	AJP	C26
24	B	850	AJP	C05
24	B	850	AJP	C11
24	B	850	AJP	C12
24	B	850	AJP	C19
24	B	850	AJP	C28
24	B	850	AJP	C08
24	B	850	AJP	C30
24	B	850	AJP	C15
24	B	850	AJP	C27
24	B	850	AJP	C22
24	B	850	AJP	C16
24	B	850	AJP	C07
24	B	850	AJP	C20
24	B	850	AJP	C10
24	B	850	AJP	C02
24	B	850	AJP	C23
24	B	857	AJP	C26
24	B	857	AJP	C05
24	B	857	AJP	C10
24	B	857	AJP	C11
24	B	857	AJP	C12
24	B	857	AJP	C19
24	B	857	AJP	C28
24	B	857	AJP	C30
24	B	857	AJP	C15
24	B	857	AJP	C27
24	B	857	AJP	C16
24	B	857	AJP	C07
24	B	857	AJP	C20
24	B	857	AJP	C22
24	B	857	AJP	C02
24	B	857	AJP	C23
24	K	104	AJP	C26
24	K	104	AJP	C05
24	K	104	AJP	C11
24	K	104	AJP	C12
24	K	104	AJP	C19
24	K	104	AJP	C28
24	K	104	AJP	C08
24	K	104	AJP	C15
24	K	104	AJP	C27

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Mol	Chain	Res	Type	Atom
24	K	104	AJP	C22
24	K	104	AJP	C16
24	K	104	AJP	C07
24	K	104	AJP	C20
24	K	104	AJP	C10
24	K	104	AJP	C02
24	K	104	AJP	C23
24	L	208	AJP	C05
24	L	208	AJP	C06
24	L	208	AJP	C11
24	L	208	AJP	C12
24	L	208	AJP	C19
24	L	208	AJP	C08
24	L	208	AJP	C15
24	L	208	AJP	C22
24	L	208	AJP	C16
24	L	208	AJP	C07
24	L	208	AJP	C20
24	L	208	AJP	C10
24	L	208	AJP	C02
24	L	209	AJP	C05
24	L	209	AJP	C06
24	L	209	AJP	C11
24	L	209	AJP	C12
24	L	209	AJP	C19
24	L	209	AJP	C08
24	L	209	AJP	C15
24	L	209	AJP	C22
24	L	209	AJP	C16
24	L	209	AJP	C07
24	L	209	AJP	C20
24	L	209	AJP	C10
24	L	209	AJP	C02
24	AA	802	AJP	C05
24	AA	802	AJP	C11
24	AA	802	AJP	C12
24	AA	802	AJP	C19
24	AA	802	AJP	C08
24	AA	802	AJP	C15
24	AA	802	AJP	C16
24	AA	802	AJP	C07
24	AA	802	AJP	C20

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Mol	Chain	Res	Type	Atom
24	AA	802	AJP	C10
24	AA	802	AJP	C02
24	AA	856	AJP	C05
24	AA	856	AJP	C10
24	AA	856	AJP	C11
24	AA	856	AJP	C12
24	AA	856	AJP	C19
24	AA	856	AJP	C15
24	AA	856	AJP	C16
24	AA	856	AJP	C07
24	AA	856	AJP	C20
24	AA	856	AJP	C22
24	AA	856	AJP	C02
24	AA	856	AJP	C23
24	BB	848	AJP	C26
24	BB	848	AJP	C05
24	BB	848	AJP	C11
24	BB	848	AJP	C12
24	BB	848	AJP	C19
24	BB	848	AJP	C28
24	BB	848	AJP	C08
24	BB	848	AJP	C30
24	BB	848	AJP	C15
24	BB	848	AJP	C27
24	BB	848	AJP	C22
24	BB	848	AJP	C16
24	BB	848	AJP	C07
24	BB	848	AJP	C20
24	BB	848	AJP	C10
24	BB	848	AJP	C02
24	BB	848	AJP	C23
24	BB	849	AJP	C26
24	BB	849	AJP	C05
24	BB	849	AJP	C11
24	BB	849	AJP	C12
24	BB	849	AJP	C19
24	BB	849	AJP	C28
24	BB	849	AJP	C08
24	BB	849	AJP	C30
24	BB	849	AJP	C15
24	BB	849	AJP	C27
24	BB	849	AJP	C22

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Mol	Chain	Res	Type	Atom
24	BB	849	AJP	C16
24	BB	849	AJP	C07
24	BB	849	AJP	C20
24	BB	849	AJP	C10
24	BB	849	AJP	C02
24	BB	849	AJP	C23
24	KK	104	AJP	C26
24	KK	104	AJP	C05
24	KK	104	AJP	C11
24	KK	104	AJP	C12
24	KK	104	AJP	C19
24	KK	104	AJP	C28
24	KK	104	AJP	C08
24	KK	104	AJP	C15
24	KK	104	AJP	C27
24	KK	104	AJP	C22
24	KK	104	AJP	C16
24	KK	104	AJP	C07
24	KK	104	AJP	C20
24	KK	104	AJP	C10
24	KK	104	AJP	C02
24	KK	104	AJP	C23

All (5701) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	CBD-CGD-O2D-CED
19	A1	804	CLA	C1A-C2A-CAA-CBA
19	A1	804	CLA	C3A-C2A-CAA-CBA
19	A1	804	CLA	CHA-CBD-CGD-O1D
19	A1	804	CLA	CHA-CBD-CGD-O2D
19	A1	805	CLA	C1A-C2A-CAA-CBA
19	A1	805	CLA	C3A-C2A-CAA-CBA
19	A1	805	CLA	C2B-C3B-CAB-CBB
19	A1	805	CLA	C4B-C3B-CAB-CBB
19	A1	806	CLA	C1A-C2A-CAA-CBA
19	A1	806	CLA	C3A-C2A-CAA-CBA
19	A1	806	CLA	CAD-CBD-CGD-O1D
19	A1	806	CLA	CAD-CBD-CGD-O2D
19	A1	807	CLA	O1A-CGA-O2A-C1
19	A1	809	CLA	C3A-C2A-CAA-CBA
19	A1	810	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A1	810	CLA	C4B-C3B-CAB-CBB
19	A1	810	CLA	CBD-CGD-O2D-CED
19	A1	810	CLA	C2-C3-C5-C6
19	A1	810	CLA	C4-C3-C5-C6
19	A1	811	CLA	C1A-C2A-CAA-CBA
19	A1	811	CLA	C3A-C2A-CAA-CBA
19	A1	811	CLA	CBD-CGD-O2D-CED
19	A1	813	CLA	C1A-C2A-CAA-CBA
19	A1	815	CLA	C1A-C2A-CAA-CBA
19	A1	815	CLA	C3A-C2A-CAA-CBA
19	A1	815	CLA	CBD-CGD-O2D-CED
19	A1	819	CLA	C3A-C2A-CAA-CBA
19	A1	819	CLA	C4B-C3B-CAB-CBB
19	A1	820	CLA	C1A-C2A-CAA-CBA
19	A1	820	CLA	C3A-C2A-CAA-CBA
19	A1	822	CLA	CBD-CGD-O2D-CED
19	A1	824	CLA	C1A-C2A-CAA-CBA
19	A1	825	CLA	C1A-C2A-CAA-CBA
19	A1	825	CLA	C3A-C2A-CAA-CBA
19	A1	827	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C3A-C2A-CAA-CBA
19	A1	828	CLA	C11-C10-C8-C9
19	A1	832	CLA	CHA-CBD-CGD-O1D
19	A1	832	CLA	CHA-CBD-CGD-O2D
19	A1	833	CLA	CBD-CGD-O2D-CED
19	A1	835	CLA	CHA-CBD-CGD-O1D
19	A1	835	CLA	CHA-CBD-CGD-O2D
19	A1	837	CLA	CHA-CBD-CGD-O1D
19	A1	837	CLA	CHA-CBD-CGD-O2D
19	A1	838	CLA	CHA-CBD-CGD-O1D
19	A1	838	CLA	CHA-CBD-CGD-O2D
19	A1	842	CLA	C2C-C3C-CAC-CBC
19	A1	842	CLA	C4C-C3C-CAC-CBC
19	A1	844	CLA	CBD-CGD-O2D-CED
19	A1	852	CLA	CAD-CBD-CGD-O1D
19	A1	852	CLA	CAD-CBD-CGD-O2D
19	B1	801	CLA	CHA-CBD-CGD-O2D
19	B1	802	CLA	CAD-CBD-CGD-O2D
19	B1	805	CLA	CHA-CBD-CGD-O1D
19	B1	805	CLA	CHA-CBD-CGD-O2D
19	B1	807	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B1	807	CLA	C6-C7-C8-C9
19	B1	809	CLA	CAD-CBD-CGD-O1D
19	B1	809	CLA	CAD-CBD-CGD-O2D
19	B1	811	CLA	CAD-CBD-CGD-O2D
19	B1	812	CLA	CAD-CBD-CGD-O1D
19	B1	812	CLA	CAD-CBD-CGD-O2D
19	B1	813	CLA	C1A-C2A-CAA-CBA
19	B1	813	CLA	CHA-CBD-CGD-O1D
19	B1	813	CLA	CHA-CBD-CGD-O2D
19	B1	814	CLA	C4B-C3B-CAB-CBB
19	B1	815	CLA	C3A-C2A-CAA-CBA
19	B1	815	CLA	CHA-CBD-CGD-O2D
19	B1	815	CLA	C14-C13-C15-C16
19	B1	816	CLA	C4B-C3B-CAB-CBB
19	B1	817	CLA	CHA-CBD-CGD-O1D
19	B1	817	CLA	CHA-CBD-CGD-O2D
19	B1	820	CLA	CHA-CBD-CGD-O1D
19	B1	820	CLA	CHA-CBD-CGD-O2D
19	B1	821	CLA	CHA-CBD-CGD-O1D
19	B1	821	CLA	CHA-CBD-CGD-O2D
19	B1	824	CLA	C1A-C2A-CAA-CBA
19	B1	824	CLA	C3A-C2A-CAA-CBA
19	B1	824	CLA	C2B-C3B-CAB-CBB
19	B1	824	CLA	C4B-C3B-CAB-CBB
19	B1	824	CLA	CBD-CGD-O2D-CED
19	B1	825	CLA	CAD-CBD-CGD-O1D
19	B1	825	CLA	CAD-CBD-CGD-O2D
19	B1	826	CLA	CHA-CBD-CGD-O1D
19	B1	826	CLA	CHA-CBD-CGD-O2D
19	B1	827	CLA	C3A-C2A-CAA-CBA
19	B1	827	CLA	CBD-CGD-O2D-CED
19	B1	831	CLA	C1A-C2A-CAA-CBA
19	B1	831	CLA	C3A-C2A-CAA-CBA
19	B1	832	CLA	CBD-CGD-O2D-CED
19	B1	833	CLA	C1A-C2A-CAA-CBA
19	B1	833	CLA	C2B-C3B-CAB-CBB
19	B1	833	CLA	C4B-C3B-CAB-CBB
19	B1	833	CLA	CHA-CBD-CGD-O1D
19	B1	833	CLA	CHA-CBD-CGD-O2D
19	B1	835	CLA	C6-C7-C8-C9
19	B1	836	CLA	CHA-CBD-CGD-O1D
19	B1	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B1	848	CLA	CBD-CGD-O2D-CED
19	B1	850	CLA	C4B-C3B-CAB-CBB
19	F1	301	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C3A-C2A-CAA-CBA
19	F1	302	CLA	CBD-CGD-O2D-CED
19	K1	103	CLA	C1A-C2A-CAA-CBA
19	K1	103	CLA	C3A-C2A-CAA-CBA
19	K1	103	CLA	CBA-CGA-O2A-C1
19	K1	105	CLA	CBD-CGD-O2D-CED
19	L1	206	CLA	C2B-C3B-CAB-CBB
19	L1	206	CLA	C4B-C3B-CAB-CBB
19	A2	802	CLA	C1A-C2A-CAA-CBA
19	A2	802	CLA	C3A-C2A-CAA-CBA
19	A2	802	CLA	CBA-CGA-O2A-C1
19	A2	802	CLA	CAD-CBD-CGD-O1D
19	A2	802	CLA	CAD-CBD-CGD-O2D
19	A2	804	CLA	CBD-CGD-O2D-CED
19	A2	805	CLA	C1A-C2A-CAA-CBA
19	A2	805	CLA	C3A-C2A-CAA-CBA
19	A2	805	CLA	CHA-CBD-CGD-O1D
19	A2	805	CLA	CHA-CBD-CGD-O2D
19	A2	806	CLA	C1A-C2A-CAA-CBA
19	A2	806	CLA	CAD-CBD-CGD-O1D
19	A2	806	CLA	CAD-CBD-CGD-O2D
19	A2	807	CLA	C1A-C2A-CAA-CBA
19	A2	807	CLA	C3A-C2A-CAA-CBA
19	A2	807	CLA	CAD-CBD-CGD-O1D
19	A2	807	CLA	CAD-CBD-CGD-O2D
19	A2	811	CLA	C3A-C2A-CAA-CBA
19	A2	811	CLA	C2-C3-C5-C6
19	A2	811	CLA	C4-C3-C5-C6
19	A2	812	CLA	C1A-C2A-CAA-CBA
19	A2	812	CLA	C3A-C2A-CAA-CBA
19	A2	812	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	C1A-C2A-CAA-CBA
19	A2	816	CLA	C1A-C2A-CAA-CBA
19	A2	816	CLA	C3A-C2A-CAA-CBA
19	A2	820	CLA	C3A-C2A-CAA-CBA
19	A2	820	CLA	C2B-C3B-CAB-CBB
19	A2	820	CLA	C4B-C3B-CAB-CBB
19	A2	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A2	821	CLA	C3A-C2A-CAA-CBA
19	A2	823	CLA	CBD-CGD-O2D-CED
19	A2	825	CLA	CBD-CGD-O2D-CED
19	A2	826	CLA	C1A-C2A-CAA-CBA
19	A2	828	CLA	C1A-C2A-CAA-CBA
19	A2	828	CLA	CBD-CGD-O2D-CED
19	A2	829	CLA	C1A-C2A-CAA-CBA
19	A2	829	CLA	C3A-C2A-CAA-CBA
19	A2	832	CLA	CHA-CBD-CGD-O2D
19	A2	834	CLA	CBD-CGD-O2D-CED
19	A2	835	CLA	CBD-CGD-O2D-CED
19	A2	836	CLA	C2B-C3B-CAB-CBB
19	A2	836	CLA	C4B-C3B-CAB-CBB
19	A2	836	CLA	CHA-CBD-CGD-O1D
19	A2	836	CLA	CHA-CBD-CGD-O2D
19	A2	838	CLA	CHA-CBD-CGD-O1D
19	A2	838	CLA	CHA-CBD-CGD-O2D
19	A2	839	CLA	CHA-CBD-CGD-O1D
19	A2	839	CLA	CHA-CBD-CGD-O2D
19	A2	844	CLA	CBD-CGD-O2D-CED
19	B2	802	CLA	CAD-CBD-CGD-O1D
19	B2	802	CLA	CAD-CBD-CGD-O2D
19	B2	805	CLA	CHA-CBD-CGD-O1D
19	B2	805	CLA	CHA-CBD-CGD-O2D
19	B2	806	CLA	CBD-CGD-O2D-CED
19	B2	807	CLA	CHA-CBD-CGD-O1D
19	B2	807	CLA	CHA-CBD-CGD-O2D
19	B2	809	CLA	CAD-CBD-CGD-O1D
19	B2	809	CLA	CAD-CBD-CGD-O2D
19	B2	810	CLA	CBD-CGD-O2D-CED
19	B2	811	CLA	CAD-CBD-CGD-O1D
19	B2	811	CLA	CAD-CBD-CGD-O2D
19	B2	812	CLA	CAD-CBD-CGD-O1D
19	B2	812	CLA	CAD-CBD-CGD-O2D
19	B2	813	CLA	C1A-C2A-CAA-CBA
19	B2	813	CLA	CHA-CBD-CGD-O1D
19	B2	813	CLA	CHA-CBD-CGD-O2D
19	B2	815	CLA	C3A-C2A-CAA-CBA
19	B2	815	CLA	C14-C13-C15-C16
19	B2	816	CLA	CBD-CGD-O2D-CED
19	B2	817	CLA	CHA-CBD-CGD-O1D
19	B2	817	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B2	820	CLA	C2C-C3C-CAC-CBC
19	B2	820	CLA	C4C-C3C-CAC-CBC
19	B2	820	CLA	CHA-CBD-CGD-O1D
19	B2	820	CLA	CHA-CBD-CGD-O2D
19	B2	821	CLA	C1A-C2A-CAA-CBA
19	B2	821	CLA	C3A-C2A-CAA-CBA
19	B2	821	CLA	CHA-CBD-CGD-O1D
19	B2	821	CLA	CHA-CBD-CGD-O2D
19	B2	823	CLA	C6-C7-C8-C9
19	B2	824	CLA	C1A-C2A-CAA-CBA
19	B2	824	CLA	C3A-C2A-CAA-CBA
19	B2	825	CLA	CAD-CBD-CGD-O1D
19	B2	825	CLA	CAD-CBD-CGD-O2D
19	B2	826	CLA	CHA-CBD-CGD-O1D
19	B2	826	CLA	CHA-CBD-CGD-O2D
19	B2	826	CLA	C2-C3-C5-C6
19	B2	826	CLA	C4-C3-C5-C6
19	B2	827	CLA	C3A-C2A-CAA-CBA
19	B2	831	CLA	CAD-CBD-CGD-O1D
19	B2	831	CLA	CAD-CBD-CGD-O2D
19	B2	832	CLA	C1A-C2A-CAA-CBA
19	B2	832	CLA	C3A-C2A-CAA-CBA
19	B2	833	CLA	CHA-CBD-CGD-O1D
19	B2	833	CLA	CHA-CBD-CGD-O2D
19	B2	834	CLA	C1A-C2A-CAA-CBA
19	B2	834	CLA	CHA-CBD-CGD-O1D
19	B2	834	CLA	CHA-CBD-CGD-O2D
19	B2	837	CLA	CHA-CBD-CGD-O1D
19	B2	837	CLA	CHA-CBD-CGD-O2D
19	B2	849	CLA	CBD-CGD-O2D-CED
19	B2	851	CLA	CBD-CGD-O2D-CED
19	B2	852	CLA	C2C-C3C-CAC-CBC
19	B2	852	CLA	C4C-C3C-CAC-CBC
19	F2	301	CLA	C1A-C2A-CAA-CBA
19	F2	302	CLA	C1A-C2A-CAA-CBA
19	F2	302	CLA	C3A-C2A-CAA-CBA
19	F2	302	CLA	CBD-CGD-O2D-CED
19	K2	104	CLA	C3A-C2A-CAA-CBA
19	L2	205	CLA	C2B-C3B-CAB-CBB
19	L2	205	CLA	C4B-C3B-CAB-CBB
19	L2	206	CLA	CBD-CGD-O2D-CED
19	A	805	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	805	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C4B-C3B-CAB-CBB
19	A	806	CLA	CAD-CBD-CGD-O1D
19	A	806	CLA	CAD-CBD-CGD-O2D
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	CAD-CBD-CGD-O2D
19	A	808	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	C4B-C3B-CAB-CBB
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C2-C3-C5-C6
19	A	811	CLA	C4-C3-C5-C6
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C2B-C3B-CAB-CBB
19	A	820	CLA	C4B-C3B-CAB-CBB
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	CAD-CBD-CGD-O1D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	A	826	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	835	CLA	C2B-C3B-CAB-CBB
19	A	835	CLA	C4B-C3B-CAB-CBB
19	A	835	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	839	CLA	CHA-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O1D
19	A	844	CLA	CAD-CBD-CGD-O2D
19	B	801	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	C1A-C2A-CAA-CBA
19	B	803	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	O1A-CGA-O2A-C1
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CAD-CBD-CGD-O1D
19	B	809	CLA	CAD-CBD-CGD-O2D
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CAD-CBD-CGD-O1D
19	B	811	CLA	CAD-CBD-CGD-O2D
19	B	812	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	C2B-C3B-CAB-CBB
19	B	814	CLA	C4B-C3B-CAB-CBB
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	C14-C13-C15-C16
19	B	817	CLA	CHA-CBD-CGD-O1D
19	B	817	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	C4B-C3B-CAB-CBB
19	B	820	CLA	C2C-C3C-CAC-CBC
19	B	820	CLA	C4C-C3C-CAC-CBC
19	B	820	CLA	CHA-CBD-CGD-O1D
19	B	820	CLA	CHA-CBD-CGD-O2D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	C6-C7-C8-C9
19	B	825	CLA	CAD-CBD-CGD-O1D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	B	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	CHA-CBD-CGD-O2D
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C4B-C3B-CAB-CBB
19	B	833	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	836	CLA	C2B-C3B-CAB-CBB
19	B	836	CLA	C4B-C3B-CAB-CBB
19	B	837	CLA	CHA-CBD-CGD-O1D
19	B	837	CLA	CHA-CBD-CGD-O2D
19	B	859	CLA	C4B-C3B-CAB-CBB
19	B	860	CLA	C2C-C3C-CAC-CBC
19	B	860	CLA	C4C-C3C-CAC-CBC
19	F	301	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C3A-C2A-CAA-CBA
19	F	302	CLA	CBD-CGD-O2D-CED
19	K	102	CLA	C1A-C2A-CAA-CBA
19	K	102	CLA	C3A-C2A-CAA-CBA
19	K	102	CLA	CBA-CGA-O2A-C1
19	K	102	CLA	O1A-CGA-O2A-C1
19	K	102	CLA	CAD-CBD-CGD-O1D
19	K	102	CLA	CAD-CBD-CGD-O2D
19	L	202	CLA	CAD-CBD-CGD-O1D
19	L	202	CLA	CAD-CBD-CGD-O2D
19	L	203	CLA	C1A-C2A-CAA-CBA
19	L	203	CLA	C3A-C2A-CAA-CBA
19	L	204	CLA	CBD-CGD-O2D-CED
19	AA	804	CLA	CBD-CGD-O2D-CED
19	AA	805	CLA	C3A-C2A-CAA-CBA
19	AA	805	CLA	CHA-CBD-CGD-O1D
19	AA	805	CLA	CHA-CBD-CGD-O2D
19	AA	806	CLA	C1A-C2A-CAA-CBA
19	AA	806	CLA	C3A-C2A-CAA-CBA
19	AA	806	CLA	C2B-C3B-CAB-CBB
19	AA	806	CLA	C4B-C3B-CAB-CBB
19	AA	806	CLA	CAD-CBD-CGD-O2D
19	AA	807	CLA	C1A-C2A-CAA-CBA
19	AA	807	CLA	C3A-C2A-CAA-CBA
19	AA	807	CLA	CAD-CBD-CGD-O1D
19	AA	807	CLA	CAD-CBD-CGD-O2D
19	AA	808	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	AA	811	CLA	C2B-C3B-CAB-CBB
19	AA	811	CLA	C4B-C3B-CAB-CBB
19	AA	811	CLA	CBD-CGD-O2D-CED
19	AA	811	CLA	C2-C3-C5-C6
19	AA	811	CLA	C4-C3-C5-C6
19	AA	812	CLA	C1A-C2A-CAA-CBA
19	AA	812	CLA	C3A-C2A-CAA-CBA
19	AA	812	CLA	CBD-CGD-O2D-CED
19	AA	814	CLA	C1A-C2A-CAA-CBA
19	AA	816	CLA	C1A-C2A-CAA-CBA
19	AA	816	CLA	C3A-C2A-CAA-CBA
19	AA	816	CLA	CBD-CGD-O2D-CED
19	AA	820	CLA	C3A-C2A-CAA-CBA
19	AA	821	CLA	C1A-C2A-CAA-CBA
19	AA	821	CLA	C3A-C2A-CAA-CBA
19	AA	824	CLA	C1A-C2A-CAA-CBA
19	AA	824	CLA	C3A-C2A-CAA-CBA
19	AA	824	CLA	CAD-CBD-CGD-O1D
19	AA	824	CLA	CAD-CBD-CGD-O2D
19	AA	826	CLA	C1A-C2A-CAA-CBA
19	AA	826	CLA	C3A-C2A-CAA-CBA
19	AA	828	CLA	C1A-C2A-CAA-CBA
19	AA	828	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	C1A-C2A-CAA-CBA
19	AA	829	CLA	C3A-C2A-CAA-CBA
19	AA	830	CLA	CBD-CGD-O2D-CED
19	AA	832	CLA	CHA-CBD-CGD-O1D
19	AA	832	CLA	CHA-CBD-CGD-O2D
19	AA	835	CLA	C2B-C3B-CAB-CBB
19	AA	835	CLA	C4B-C3B-CAB-CBB
19	AA	835	CLA	CBD-CGD-O2D-CED
19	AA	836	CLA	CHA-CBD-CGD-O1D
19	AA	836	CLA	CHA-CBD-CGD-O2D
19	AA	838	CLA	CHA-CBD-CGD-O1D
19	AA	838	CLA	CHA-CBD-CGD-O2D
19	AA	839	CLA	CHA-CBD-CGD-O1D
19	AA	839	CLA	CHA-CBD-CGD-O2D
19	AA	843	CLA	C2C-C3C-CAC-CBC
19	AA	843	CLA	C4C-C3C-CAC-CBC
19	AA	845	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	C1A-C2A-CAA-CBA
19	BB	801	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	BB	801	CLA	CHA-CBD-CGD-O1D
19	BB	801	CLA	CHA-CBD-CGD-O2D
19	BB	802	CLA	C2B-C3B-CAB-CBB
19	BB	802	CLA	C4B-C3B-CAB-CBB
19	BB	802	CLA	CAD-CBD-CGD-O1D
19	BB	802	CLA	CAD-CBD-CGD-O2D
19	BB	803	CLA	CBD-CGD-O2D-CED
19	BB	805	CLA	CHA-CBD-CGD-O1D
19	BB	805	CLA	CHA-CBD-CGD-O2D
19	BB	806	CLA	CBD-CGD-O2D-CED
19	BB	807	CLA	CHA-CBD-CGD-O1D
19	BB	807	CLA	CHA-CBD-CGD-O2D
19	BB	809	CLA	CAD-CBD-CGD-O1D
19	BB	809	CLA	CAD-CBD-CGD-O2D
19	BB	810	CLA	CBD-CGD-O2D-CED
19	BB	811	CLA	CAD-CBD-CGD-O1D
19	BB	811	CLA	CAD-CBD-CGD-O2D
19	BB	812	CLA	CAD-CBD-CGD-O1D
19	BB	812	CLA	CAD-CBD-CGD-O2D
19	BB	813	CLA	C1A-C2A-CAA-CBA
19	BB	813	CLA	CHA-CBD-CGD-O1D
19	BB	813	CLA	CHA-CBD-CGD-O2D
19	BB	814	CLA	C2B-C3B-CAB-CBB
19	BB	814	CLA	C4B-C3B-CAB-CBB
19	BB	815	CLA	C1A-C2A-CAA-CBA
19	BB	815	CLA	C3A-C2A-CAA-CBA
19	BB	820	CLA	C4B-C3B-CAB-CBB
19	BB	820	CLA	C2C-C3C-CAC-CBC
19	BB	820	CLA	C4C-C3C-CAC-CBC
19	BB	821	CLA	CHA-CBD-CGD-O1D
19	BB	821	CLA	CHA-CBD-CGD-O2D
19	BB	825	CLA	CAD-CBD-CGD-O1D
19	BB	825	CLA	CAD-CBD-CGD-O2D
19	BB	826	CLA	CHA-CBD-CGD-O1D
19	BB	826	CLA	CHA-CBD-CGD-O2D
19	BB	827	CLA	C3A-C2A-CAA-CBA
19	BB	830	CLA	CAD-CBD-CGD-O2D
19	BB	831	CLA	C4B-C3B-CAB-CBB
19	BB	832	CLA	CBD-CGD-O2D-CED
19	BB	833	CLA	C1A-C2A-CAA-CBA
19	BB	835	CLA	C2B-C3B-CAB-CBB
19	BB	835	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	BB	836	CLA	C2C-C3C-CAC-CBC
19	BB	836	CLA	C4C-C3C-CAC-CBC
19	BB	836	CLA	CHA-CBD-CGD-O1D
19	BB	836	CLA	CHA-CBD-CGD-O2D
19	BB	852	CLA	CBD-CGD-O2D-CED
19	BB	856	CLA	C2B-C3B-CAB-CBB
19	BB	856	CLA	C4B-C3B-CAB-CBB
19	FF	302	CLA	C1A-C2A-CAA-CBA
19	FF	302	CLA	C3A-C2A-CAA-CBA
19	FF	302	CLA	CBD-CGD-O2D-CED
19	KK	102	CLA	C1A-C2A-CAA-CBA
19	KK	102	CLA	C3A-C2A-CAA-CBA
19	KK	102	CLA	CBA-CGA-O2A-C1
19	KK	102	CLA	CAD-CBD-CGD-O2D
19	LL	202	CLA	C4B-C3B-CAB-CBB
19	LL	203	CLA	C1A-C2A-CAA-CBA
19	LL	203	CLA	C3A-C2A-CAA-CBA
20	A1	802	CL0	C2-C1-O2A-CGA
20	A1	802	CL0	C2-C3-C5-C6
20	A1	802	CL0	C4-C3-C5-C6
20	A2	803	CL0	C6-C7-C8-C9
20	A	803	CL0	C1A-C2A-CAA-CBA
20	A	803	CL0	C2-C1-O2A-CGA
20	AA	803	CL0	C2-C1-O2A-CGA
20	AA	803	CL0	C4C-C3C-CAC-CBC
22	A1	846	LHG	O1-C1-C2-C3
22	B1	847	LHG	C3-O3-P-O5
22	L1	211	LHG	C3-O3-P-O6
22	L1	211	LHG	O9-C7-O7-C5
22	X1	102	LHG	O1-C1-C2-O2
22	X1	102	LHG	O1-C1-C2-C3
22	X1	102	LHG	C3-O3-P-O5
22	X1	102	LHG	C4-O6-P-O3
22	X1	102	LHG	C4-O6-P-O4
22	X1	102	LHG	C4-O6-P-O5
22	X1	103	LHG	C3-O3-P-O5
22	X1	103	LHG	O9-C7-O7-C5
22	X1	103	LHG	C8-C7-O7-C5
22	A2	845	LHG	C1-C2-C3-O3
22	A2	845	LHG	O2-C2-C3-O3
22	A2	846	LHG	O1-C1-C2-C3
22	L2	208	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	L2	208	LHG	C4-O6-P-O3
22	L2	208	LHG	O9-C7-O7-C5
22	X2	102	LHG	O1-C1-C2-O2
22	X2	102	LHG	O1-C1-C2-C3
22	X2	102	LHG	C3-O3-P-O5
22	X2	102	LHG	C4-O6-P-O3
22	X2	102	LHG	C4-O6-P-O4
22	X2	103	LHG	C3-O3-P-O5
22	X2	103	LHG	O9-C7-O7-C5
22	X2	103	LHG	C8-C7-O7-C5
22	A	845	LHG	C1-C2-C3-O3
22	A	845	LHG	O2-C2-C3-O3
22	A	846	LHG	O1-C1-C2-C3
22	B	853	LHG	C3-O3-P-O5
22	B	853	LHG	O9-C7-O7-C5
22	B	853	LHG	C8-C7-O7-C5
22	L	207	LHG	O9-C7-O7-C5
22	X	102	LHG	O1-C1-C2-O2
22	X	102	LHG	O1-C1-C2-C3
22	X	102	LHG	C3-O3-P-O5
22	AA	846	LHG	C1-C2-C3-O3
22	AA	846	LHG	O2-C2-C3-O3
22	AA	847	LHG	O1-C1-C2-C3
22	BB	851	LHG	C3-O3-P-O5
22	BB	851	LHG	C3-O3-P-O6
22	BB	851	LHG	O9-C7-O7-C5
22	BB	851	LHG	C8-C7-O7-C5
22	LL	205	LHG	O9-C7-O7-C5
22	XX	102	LHG	O1-C1-C2-O2
22	XX	102	LHG	O1-C1-C2-C3
22	XX	102	LHG	C4-O6-P-O3
22	XX	102	LHG	C4-O6-P-O4
22	XX	102	LHG	C4-O6-P-O5
23	A1	847	BCR	C11-C10-C9-C34
23	A1	847	BCR	C11-C12-C13-C35
23	A1	848	BCR	C7-C8-C9-C10
23	A1	848	BCR	C11-C12-C13-C14
23	A1	848	BCR	C11-C12-C13-C35
23	A1	848	BCR	C16-C17-C18-C36
23	A1	848	BCR	C37-C22-C23-C24
23	A1	849	BCR	C11-C10-C9-C34
23	A1	849	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A1	849	BCR	C17-C18-C19-C20
23	A1	849	BCR	C20-C21-C22-C37
23	A1	849	BCR	C37-C22-C23-C24
23	A1	850	BCR	C11-C10-C9-C8
23	A1	850	BCR	C11-C10-C9-C34
23	A1	850	BCR	C10-C11-C12-C13
23	A1	850	BCR	C11-C12-C13-C14
23	A1	850	BCR	C16-C17-C18-C19
23	A1	850	BCR	C16-C17-C18-C36
23	A1	850	BCR	C37-C22-C23-C24
23	A1	851	BCR	C11-C10-C9-C8
23	A1	851	BCR	C11-C10-C9-C34
23	A1	851	BCR	C10-C11-C12-C13
23	A1	851	BCR	C16-C17-C18-C19
23	A1	851	BCR	C16-C17-C18-C36
23	A1	851	BCR	C18-C19-C20-C21
23	A1	851	BCR	C20-C21-C22-C37
23	A1	851	BCR	C37-C22-C23-C24
23	A1	851	BCR	C22-C23-C24-C25
23	A1	853	BCR	C16-C17-C18-C36
23	A1	853	BCR	C36-C18-C19-C20
23	A1	853	BCR	C18-C19-C20-C21
23	A1	853	BCR	C20-C21-C22-C37
23	B1	838	BCR	C1-C6-C7-C8
23	B1	838	BCR	C5-C6-C7-C8
23	B1	838	BCR	C7-C8-C9-C10
23	B1	838	BCR	C11-C12-C13-C35
23	B1	838	BCR	C16-C17-C18-C36
23	B1	838	BCR	C17-C18-C19-C20
23	B1	838	BCR	C20-C21-C22-C37
23	B1	839	BCR	C35-C13-C14-C15
23	B1	839	BCR	C20-C21-C22-C37
23	B1	841	BCR	C6-C7-C8-C9
23	B1	841	BCR	C35-C13-C14-C15
23	B1	841	BCR	C16-C17-C18-C19
23	B1	841	BCR	C36-C18-C19-C20
23	B1	841	BCR	C18-C19-C20-C21
23	B1	841	BCR	C21-C22-C23-C24
23	B1	841	BCR	C23-C24-C25-C26
23	B1	841	BCR	C23-C24-C25-C30
23	B1	842	BCR	C6-C7-C8-C9
23	B1	842	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	B1	842	BCR	C7-C8-C9-C34
23	B1	842	BCR	C11-C10-C9-C8
23	B1	842	BCR	C11-C12-C13-C14
23	B1	842	BCR	C17-C18-C19-C20
23	B1	842	BCR	C36-C18-C19-C20
23	B1	842	BCR	C20-C21-C22-C23
23	B1	842	BCR	C20-C21-C22-C37
23	B1	843	BCR	C11-C12-C13-C35
23	B1	843	BCR	C14-C15-C16-C17
23	B1	843	BCR	C16-C17-C18-C36
23	B1	843	BCR	C20-C21-C22-C37
23	B1	843	BCR	C22-C23-C24-C25
23	F1	303	BCR	C7-C8-C9-C34
23	F1	303	BCR	C11-C10-C9-C8
23	F1	303	BCR	C11-C10-C9-C34
23	F1	303	BCR	C10-C11-C12-C13
23	F1	303	BCR	C12-C13-C14-C15
23	F1	303	BCR	C16-C17-C18-C36
23	F1	304	BCR	C7-C8-C9-C10
23	F1	304	BCR	C7-C8-C9-C34
23	F1	304	BCR	C11-C10-C9-C34
23	F1	304	BCR	C18-C19-C20-C21
23	F1	304	BCR	C20-C21-C22-C23
23	F1	304	BCR	C21-C22-C23-C24
23	F1	306	BCR	C1-C6-C7-C8
23	F1	306	BCR	C5-C6-C7-C8
23	F1	306	BCR	C6-C7-C8-C9
23	F1	306	BCR	C7-C8-C9-C10
23	F1	306	BCR	C11-C10-C9-C8
23	F1	306	BCR	C10-C11-C12-C13
23	F1	306	BCR	C11-C12-C13-C14
23	F1	306	BCR	C11-C12-C13-C35
23	F1	306	BCR	C16-C17-C18-C19
23	F1	306	BCR	C16-C17-C18-C36
23	F1	306	BCR	C18-C19-C20-C21
23	F1	306	BCR	C21-C22-C23-C24
23	F1	306	BCR	C37-C22-C23-C24
23	F1	306	BCR	C22-C23-C24-C25
23	I1	101	BCR	C11-C10-C9-C34
23	I1	101	BCR	C16-C17-C18-C36
23	I1	101	BCR	C20-C21-C22-C37
23	I1	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	J1	102	BCR	C11-C10-C9-C34
23	J1	102	BCR	C11-C12-C13-C14
23	J1	102	BCR	C35-C13-C14-C15
23	J1	102	BCR	C16-C17-C18-C36
23	J1	102	BCR	C36-C18-C19-C20
23	J1	102	BCR	C21-C22-C23-C24
23	J1	102	BCR	C37-C22-C23-C24
23	J1	104	BCR	C11-C10-C9-C34
23	J1	104	BCR	C11-C12-C13-C35
23	J1	104	BCR	C16-C17-C18-C36
23	J1	104	BCR	C21-C22-C23-C24
23	J1	104	BCR	C23-C24-C25-C26
23	K1	104	BCR	C11-C12-C13-C35
23	K1	104	BCR	C20-C21-C22-C23
23	K1	104	BCR	C20-C21-C22-C37
23	K1	104	BCR	C21-C22-C23-C24
23	K1	106	BCR	C7-C8-C9-C10
23	K1	106	BCR	C35-C13-C14-C15
23	K1	106	BCR	C36-C18-C19-C20
23	K1	106	BCR	C18-C19-C20-C21
23	K1	106	BCR	C20-C21-C22-C37
23	K1	106	BCR	C22-C23-C24-C25
23	L1	201	BCR	C11-C12-C13-C35
23	L1	201	BCR	C17-C18-C19-C20
23	L1	201	BCR	C36-C18-C19-C20
23	L1	208	BCR	C7-C8-C9-C10
23	L1	208	BCR	C7-C8-C9-C34
23	L1	208	BCR	C11-C10-C9-C34
23	L1	208	BCR	C16-C17-C18-C36
23	L1	208	BCR	C37-C22-C23-C24
23	L1	208	BCR	C23-C24-C25-C26
23	L1	208	BCR	C23-C24-C25-C30
23	L1	209	BCR	C1-C6-C7-C8
23	L1	209	BCR	C5-C6-C7-C8
23	L1	209	BCR	C11-C10-C9-C8
23	L1	209	BCR	C11-C10-C9-C34
23	L1	209	BCR	C9-C10-C11-C12
23	L1	209	BCR	C10-C11-C12-C13
23	L1	209	BCR	C11-C12-C13-C14
23	L1	209	BCR	C11-C12-C13-C35
23	L1	209	BCR	C16-C17-C18-C36
23	L1	209	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	L1	209	BCR	C21-C22-C23-C24
23	M1	101	BCR	C6-C7-C8-C9
23	M1	101	BCR	C7-C8-C9-C10
23	M1	101	BCR	C11-C10-C9-C8
23	M1	101	BCR	C11-C10-C9-C34
23	M1	101	BCR	C10-C11-C12-C13
23	M1	101	BCR	C12-C13-C14-C15
23	M1	101	BCR	C35-C13-C14-C15
23	M1	101	BCR	C14-C15-C16-C17
23	M1	101	BCR	C17-C18-C19-C20
23	M1	101	BCR	C36-C18-C19-C20
23	M1	101	BCR	C18-C19-C20-C21
23	M1	101	BCR	C21-C22-C23-C24
23	M1	101	BCR	C37-C22-C23-C24
23	A2	847	BCR	C11-C10-C9-C34
23	A2	847	BCR	C11-C12-C13-C35
23	A2	848	BCR	C7-C8-C9-C10
23	A2	848	BCR	C11-C12-C13-C35
23	A2	848	BCR	C37-C22-C23-C24
23	A2	849	BCR	C7-C8-C9-C34
23	A2	849	BCR	C11-C10-C9-C34
23	A2	849	BCR	C18-C19-C20-C21
23	A2	849	BCR	C21-C22-C23-C24
23	A2	849	BCR	C37-C22-C23-C24
23	A2	850	BCR	C11-C10-C9-C8
23	A2	850	BCR	C11-C10-C9-C34
23	A2	850	BCR	C10-C11-C12-C13
23	A2	850	BCR	C11-C12-C13-C14
23	A2	850	BCR	C16-C17-C18-C19
23	A2	850	BCR	C16-C17-C18-C36
23	A2	850	BCR	C37-C22-C23-C24
23	A2	851	BCR	C11-C10-C9-C8
23	A2	851	BCR	C11-C10-C9-C34
23	A2	851	BCR	C10-C11-C12-C13
23	A2	851	BCR	C35-C13-C14-C15
23	A2	851	BCR	C18-C19-C20-C21
23	A2	851	BCR	C20-C21-C22-C37
23	A2	851	BCR	C37-C22-C23-C24
23	A2	851	BCR	C22-C23-C24-C25
23	A2	853	BCR	C16-C17-C18-C36
23	A2	853	BCR	C36-C18-C19-C20
23	A2	853	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	A2	853	BCR	C20-C21-C22-C37
23	B2	839	BCR	C1-C6-C7-C8
23	B2	839	BCR	C5-C6-C7-C8
23	B2	839	BCR	C7-C8-C9-C10
23	B2	839	BCR	C11-C12-C13-C35
23	B2	839	BCR	C16-C17-C18-C36
23	B2	839	BCR	C17-C18-C19-C20
23	B2	839	BCR	C20-C21-C22-C37
23	B2	840	BCR	C35-C13-C14-C15
23	B2	840	BCR	C16-C17-C18-C36
23	B2	840	BCR	C21-C22-C23-C24
23	B2	840	BCR	C37-C22-C23-C24
23	B2	842	BCR	C6-C7-C8-C9
23	B2	842	BCR	C11-C10-C9-C34
23	B2	842	BCR	C10-C11-C12-C13
23	B2	842	BCR	C11-C12-C13-C35
23	B2	842	BCR	C35-C13-C14-C15
23	B2	842	BCR	C14-C15-C16-C17
23	B2	842	BCR	C18-C19-C20-C21
23	B2	842	BCR	C20-C21-C22-C37
23	B2	842	BCR	C22-C23-C24-C25
23	B2	843	BCR	C6-C7-C8-C9
23	B2	843	BCR	C7-C8-C9-C10
23	B2	843	BCR	C7-C8-C9-C34
23	B2	843	BCR	C11-C10-C9-C8
23	B2	843	BCR	C10-C11-C12-C13
23	B2	843	BCR	C11-C12-C13-C14
23	B2	843	BCR	C17-C18-C19-C20
23	B2	843	BCR	C36-C18-C19-C20
23	B2	843	BCR	C20-C21-C22-C37
23	B2	844	BCR	C16-C17-C18-C36
23	B2	844	BCR	C20-C21-C22-C23
23	B2	844	BCR	C20-C21-C22-C37
23	B2	844	BCR	C22-C23-C24-C25
23	F2	303	BCR	C7-C8-C9-C34
23	F2	303	BCR	C11-C10-C9-C8
23	F2	303	BCR	C11-C10-C9-C34
23	F2	303	BCR	C10-C11-C12-C13
23	F2	303	BCR	C11-C12-C13-C35
23	F2	303	BCR	C16-C17-C18-C36
23	F2	303	BCR	C21-C22-C23-C24
23	F2	304	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	F2	304	BCR	C7-C8-C9-C34
23	F2	304	BCR	C11-C10-C9-C8
23	F2	304	BCR	C11-C10-C9-C34
23	F2	304	BCR	C18-C19-C20-C21
23	F2	304	BCR	C20-C21-C22-C23
23	F2	304	BCR	C21-C22-C23-C24
23	F2	305	BCR	C1-C6-C7-C8
23	F2	305	BCR	C5-C6-C7-C8
23	F2	305	BCR	C7-C8-C9-C10
23	F2	305	BCR	C7-C8-C9-C34
23	F2	305	BCR	C11-C10-C9-C8
23	F2	305	BCR	C10-C11-C12-C13
23	F2	305	BCR	C11-C12-C13-C14
23	F2	305	BCR	C11-C12-C13-C35
23	F2	305	BCR	C15-C16-C17-C18
23	F2	305	BCR	C16-C17-C18-C19
23	F2	305	BCR	C16-C17-C18-C36
23	F2	305	BCR	C17-C18-C19-C20
23	F2	305	BCR	C18-C19-C20-C21
23	F2	305	BCR	C20-C21-C22-C23
23	F2	305	BCR	C20-C21-C22-C37
23	F2	305	BCR	C22-C23-C24-C25
23	I2	101	BCR	C11-C10-C9-C34
23	I2	101	BCR	C16-C17-C18-C36
23	I2	101	BCR	C20-C21-C22-C37
23	I2	101	BCR	C21-C22-C23-C24
23	I2	102	BCR	C36-C18-C19-C20
23	I2	103	BCR	C7-C8-C9-C10
23	I2	103	BCR	C7-C8-C9-C34
23	I2	103	BCR	C11-C10-C9-C34
23	I2	103	BCR	C10-C11-C12-C13
23	I2	103	BCR	C16-C17-C18-C36
23	I2	103	BCR	C37-C22-C23-C24
23	I2	103	BCR	C23-C24-C25-C26
23	I2	103	BCR	C23-C24-C25-C30
23	J2	102	BCR	C11-C10-C9-C34
23	J2	102	BCR	C11-C12-C13-C14
23	J2	102	BCR	C35-C13-C14-C15
23	J2	102	BCR	C36-C18-C19-C20
23	J2	102	BCR	C21-C22-C23-C24
23	J2	102	BCR	C37-C22-C23-C24
23	J2	104	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	J2	104	BCR	C11-C10-C9-C34
23	J2	104	BCR	C11-C12-C13-C35
23	J2	104	BCR	C16-C17-C18-C19
23	J2	104	BCR	C16-C17-C18-C36
23	J2	104	BCR	C21-C22-C23-C24
23	J2	104	BCR	C23-C24-C25-C26
23	K2	103	BCR	C18-C19-C20-C21
23	K2	103	BCR	C20-C21-C22-C23
23	K2	103	BCR	C20-C21-C22-C37
23	K2	105	BCR	C7-C8-C9-C10
23	K2	105	BCR	C35-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C36
23	K2	105	BCR	C17-C18-C19-C20
23	K2	105	BCR	C36-C18-C19-C20
23	K2	105	BCR	C18-C19-C20-C21
23	K2	105	BCR	C20-C21-C22-C23
23	K2	105	BCR	C20-C21-C22-C37
23	L2	207	BCR	C1-C6-C7-C8
23	L2	207	BCR	C5-C6-C7-C8
23	L2	207	BCR	C11-C10-C9-C8
23	L2	207	BCR	C11-C10-C9-C34
23	L2	207	BCR	C10-C11-C12-C13
23	L2	207	BCR	C11-C12-C13-C14
23	L2	207	BCR	C11-C12-C13-C35
23	L2	207	BCR	C16-C17-C18-C36
23	L2	207	BCR	C20-C21-C22-C37
23	L2	207	BCR	C21-C22-C23-C24
23	M2	102	BCR	C6-C7-C8-C9
23	M2	102	BCR	C7-C8-C9-C10
23	M2	102	BCR	C11-C10-C9-C8
23	M2	102	BCR	C11-C10-C9-C34
23	M2	102	BCR	C10-C11-C12-C13
23	M2	102	BCR	C12-C13-C14-C15
23	M2	102	BCR	C35-C13-C14-C15
23	M2	102	BCR	C14-C15-C16-C17
23	M2	102	BCR	C17-C18-C19-C20
23	M2	102	BCR	C36-C18-C19-C20
23	M2	102	BCR	C18-C19-C20-C21
23	M2	102	BCR	C37-C22-C23-C24
23	A	847	BCR	C11-C10-C9-C34
23	A	848	BCR	C7-C8-C9-C10
23	A	848	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	A	848	BCR	C16-C17-C18-C36
23	A	848	BCR	C21-C22-C23-C24
23	A	849	BCR	C7-C8-C9-C34
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C35-C13-C14-C15
23	A	849	BCR	C17-C18-C19-C20
23	A	849	BCR	C20-C21-C22-C37
23	A	849	BCR	C37-C22-C23-C24
23	A	850	BCR	C7-C8-C9-C34
23	A	850	BCR	C11-C10-C9-C8
23	A	850	BCR	C11-C10-C9-C34
23	A	850	BCR	C11-C12-C13-C14
23	A	850	BCR	C11-C12-C13-C35
23	A	850	BCR	C16-C17-C18-C19
23	A	850	BCR	C16-C17-C18-C36
23	A	850	BCR	C20-C21-C22-C37
23	A	850	BCR	C37-C22-C23-C24
23	A	851	BCR	C11-C10-C9-C8
23	A	851	BCR	C10-C11-C12-C13
23	A	851	BCR	C12-C13-C14-C15
23	A	851	BCR	C16-C17-C18-C19
23	A	851	BCR	C16-C17-C18-C36
23	A	851	BCR	C18-C19-C20-C21
23	A	851	BCR	C20-C21-C22-C37
23	A	851	BCR	C37-C22-C23-C24
23	A	851	BCR	C22-C23-C24-C25
23	A	853	BCR	C13-C14-C15-C16
23	A	853	BCR	C16-C17-C18-C36
23	A	853	BCR	C36-C18-C19-C20
23	A	853	BCR	C18-C19-C20-C21
23	A	854	BCR	C7-C8-C9-C10
23	A	854	BCR	C35-C13-C14-C15
23	A	854	BCR	C14-C15-C16-C17
23	A	854	BCR	C17-C18-C19-C20
23	A	854	BCR	C36-C18-C19-C20
23	A	854	BCR	C18-C19-C20-C21
23	A	854	BCR	C19-C20-C21-C22
23	A	854	BCR	C20-C21-C22-C23
23	A	854	BCR	C20-C21-C22-C37
23	B	839	BCR	C1-C6-C7-C8
23	B	839	BCR	C5-C6-C7-C8
23	B	839	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	B	839	BCR	C16-C17-C18-C36
23	B	839	BCR	C17-C18-C19-C20
23	B	839	BCR	C18-C19-C20-C21
23	B	839	BCR	C20-C21-C22-C37
23	B	840	BCR	C37-C22-C23-C24
23	B	842	BCR	C6-C7-C8-C9
23	B	842	BCR	C11-C12-C13-C35
23	B	842	BCR	C35-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C36
23	B	842	BCR	C21-C22-C23-C24
23	B	842	BCR	C23-C24-C25-C26
23	B	842	BCR	C23-C24-C25-C30
23	B	843	BCR	C6-C7-C8-C9
23	B	843	BCR	C7-C8-C9-C10
23	B	843	BCR	C11-C10-C9-C8
23	B	843	BCR	C11-C10-C9-C34
23	B	843	BCR	C10-C11-C12-C13
23	B	843	BCR	C11-C12-C13-C14
23	B	843	BCR	C36-C18-C19-C20
23	B	843	BCR	C20-C21-C22-C23
23	B	843	BCR	C20-C21-C22-C37
23	B	844	BCR	C11-C12-C13-C35
23	B	844	BCR	C16-C17-C18-C36
23	B	844	BCR	C20-C21-C22-C23
23	B	844	BCR	C20-C21-C22-C37
23	B	844	BCR	C22-C23-C24-C25
23	B	848	BCR	C7-C8-C9-C10
23	B	848	BCR	C7-C8-C9-C34
23	B	848	BCR	C12-C13-C14-C15
23	B	848	BCR	C16-C17-C18-C36
23	B	848	BCR	C36-C18-C19-C20
23	B	848	BCR	C19-C20-C21-C22
23	F	303	BCR	C7-C8-C9-C34
23	F	303	BCR	C11-C10-C9-C8
23	F	303	BCR	C11-C10-C9-C34
23	F	303	BCR	C10-C11-C12-C13
23	F	303	BCR	C12-C13-C14-C15
23	F	303	BCR	C16-C17-C18-C36
23	F	304	BCR	C7-C8-C9-C10
23	F	304	BCR	C11-C10-C9-C8
23	F	304	BCR	C11-C12-C13-C35
23	F	304	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	F	304	BCR	C17-C18-C19-C20
23	F	304	BCR	C18-C19-C20-C21
23	F	304	BCR	C20-C21-C22-C23
23	F	304	BCR	C21-C22-C23-C24
23	F	305	BCR	C1-C6-C7-C8
23	F	305	BCR	C5-C6-C7-C8
23	F	305	BCR	C6-C7-C8-C9
23	F	305	BCR	C7-C8-C9-C10
23	F	305	BCR	C10-C11-C12-C13
23	F	305	BCR	C11-C12-C13-C14
23	F	305	BCR	C11-C12-C13-C35
23	F	305	BCR	C15-C16-C17-C18
23	F	305	BCR	C16-C17-C18-C19
23	F	305	BCR	C16-C17-C18-C36
23	F	305	BCR	C17-C18-C19-C20
23	F	305	BCR	C18-C19-C20-C21
23	F	305	BCR	C21-C22-C23-C24
23	F	305	BCR	C37-C22-C23-C24
23	F	305	BCR	C22-C23-C24-C25
23	I	101	BCR	C11-C10-C9-C34
23	I	101	BCR	C35-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C36
23	I	101	BCR	C20-C21-C22-C37
23	I	101	BCR	C21-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
23	J	102	BCR	C11-C10-C9-C34
23	J	102	BCR	C9-C10-C11-C12
23	J	102	BCR	C11-C12-C13-C14
23	J	102	BCR	C12-C13-C14-C15
23	J	102	BCR	C35-C13-C14-C15
23	J	102	BCR	C16-C17-C18-C36
23	J	102	BCR	C17-C18-C19-C20
23	J	102	BCR	C21-C22-C23-C24
23	J	102	BCR	C37-C22-C23-C24
23	J	104	BCR	C6-C7-C8-C9
23	J	104	BCR	C11-C10-C9-C34
23	J	104	BCR	C11-C12-C13-C35
23	J	104	BCR	C16-C17-C18-C36
23	J	104	BCR	C17-C18-C19-C20
23	J	104	BCR	C21-C22-C23-C24
23	J	104	BCR	C23-C24-C25-C26
23	K	103	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	K	103	BCR	C10-C11-C12-C13
23	K	103	BCR	C16-C17-C18-C36
23	K	103	BCR	C17-C18-C19-C20
23	K	103	BCR	C20-C21-C22-C37
23	K	103	BCR	C21-C22-C23-C24
23	K	103	BCR	C37-C22-C23-C24
23	L	205	BCR	C7-C8-C9-C10
23	L	205	BCR	C7-C8-C9-C34
23	L	205	BCR	C11-C10-C9-C34
23	L	205	BCR	C37-C22-C23-C24
23	L	205	BCR	C23-C24-C25-C26
23	L	205	BCR	C23-C24-C25-C30
23	L	206	BCR	C1-C6-C7-C8
23	L	206	BCR	C5-C6-C7-C8
23	L	206	BCR	C11-C10-C9-C8
23	L	206	BCR	C11-C10-C9-C34
23	L	206	BCR	C9-C10-C11-C12
23	L	206	BCR	C10-C11-C12-C13
23	L	206	BCR	C11-C12-C13-C14
23	L	206	BCR	C11-C12-C13-C35
23	L	206	BCR	C16-C17-C18-C36
23	L	206	BCR	C17-C18-C19-C20
23	L	206	BCR	C20-C21-C22-C37
23	L	206	BCR	C21-C22-C23-C24
23	M	101	BCR	C7-C8-C9-C10
23	M	101	BCR	C7-C8-C9-C34
23	M	101	BCR	C11-C10-C9-C8
23	M	101	BCR	C11-C10-C9-C34
23	M	101	BCR	C10-C11-C12-C13
23	M	101	BCR	C11-C12-C13-C14
23	M	101	BCR	C11-C12-C13-C35
23	M	101	BCR	C12-C13-C14-C15
23	M	101	BCR	C35-C13-C14-C15
23	M	101	BCR	C14-C15-C16-C17
23	M	101	BCR	C15-C16-C17-C18
23	M	101	BCR	C16-C17-C18-C19
23	M	101	BCR	C16-C17-C18-C36
23	M	101	BCR	C18-C19-C20-C21
23	M	101	BCR	C21-C22-C23-C24
23	M	101	BCR	C37-C22-C23-C24
23	M	101	BCR	C23-C24-C25-C26
23	AA	848	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	AA	848	BCR	C10-C11-C12-C13
23	AA	849	BCR	C7-C8-C9-C10
23	AA	849	BCR	C11-C10-C9-C34
23	AA	849	BCR	C16-C17-C18-C36
23	AA	849	BCR	C21-C22-C23-C24
23	AA	850	BCR	C7-C8-C9-C34
23	AA	850	BCR	C11-C10-C9-C34
23	AA	850	BCR	C35-C13-C14-C15
23	AA	850	BCR	C17-C18-C19-C20
23	AA	850	BCR	C20-C21-C22-C37
23	AA	850	BCR	C37-C22-C23-C24
23	AA	851	BCR	C7-C8-C9-C34
23	AA	851	BCR	C11-C10-C9-C8
23	AA	851	BCR	C11-C10-C9-C34
23	AA	851	BCR	C10-C11-C12-C13
23	AA	851	BCR	C11-C12-C13-C14
23	AA	851	BCR	C11-C12-C13-C35
23	AA	851	BCR	C16-C17-C18-C19
23	AA	851	BCR	C16-C17-C18-C36
23	AA	851	BCR	C20-C21-C22-C37
23	AA	851	BCR	C37-C22-C23-C24
23	AA	852	BCR	C11-C10-C9-C8
23	AA	852	BCR	C10-C11-C12-C13
23	AA	852	BCR	C12-C13-C14-C15
23	AA	852	BCR	C16-C17-C18-C19
23	AA	852	BCR	C16-C17-C18-C36
23	AA	852	BCR	C18-C19-C20-C21
23	AA	852	BCR	C20-C21-C22-C37
23	AA	852	BCR	C37-C22-C23-C24
23	AA	852	BCR	C22-C23-C24-C25
23	AA	854	BCR	C11-C12-C13-C35
23	AA	854	BCR	C13-C14-C15-C16
23	AA	854	BCR	C16-C17-C18-C36
23	AA	854	BCR	C36-C18-C19-C20
23	AA	854	BCR	C18-C19-C20-C21
23	AA	854	BCR	C20-C21-C22-C37
23	AA	854	BCR	C21-C22-C23-C24
23	AA	855	BCR	C7-C8-C9-C10
23	AA	855	BCR	C35-C13-C14-C15
23	AA	855	BCR	C36-C18-C19-C20
23	AA	855	BCR	C18-C19-C20-C21
23	AA	855	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	AA	855	BCR	C20-C21-C22-C23
23	AA	855	BCR	C20-C21-C22-C37
23	BB	838	BCR	C1-C6-C7-C8
23	BB	838	BCR	C5-C6-C7-C8
23	BB	838	BCR	C7-C8-C9-C10
23	BB	838	BCR	C16-C17-C18-C36
23	BB	838	BCR	C18-C19-C20-C21
23	BB	838	BCR	C20-C21-C22-C23
23	BB	838	BCR	C20-C21-C22-C37
23	BB	839	BCR	C37-C22-C23-C24
23	BB	841	BCR	C6-C7-C8-C9
23	BB	841	BCR	C11-C12-C13-C35
23	BB	841	BCR	C35-C13-C14-C15
23	BB	841	BCR	C16-C17-C18-C36
23	BB	841	BCR	C17-C18-C19-C20
23	BB	841	BCR	C21-C22-C23-C24
23	BB	841	BCR	C37-C22-C23-C24
23	BB	841	BCR	C23-C24-C25-C26
23	BB	841	BCR	C23-C24-C25-C30
23	BB	842	BCR	C6-C7-C8-C9
23	BB	842	BCR	C7-C8-C9-C10
23	BB	842	BCR	C11-C10-C9-C8
23	BB	842	BCR	C11-C10-C9-C34
23	BB	842	BCR	C11-C12-C13-C14
23	BB	842	BCR	C16-C17-C18-C36
23	BB	842	BCR	C36-C18-C19-C20
23	BB	842	BCR	C20-C21-C22-C23
23	BB	842	BCR	C20-C21-C22-C37
23	BB	843	BCR	C35-C13-C14-C15
23	BB	843	BCR	C16-C17-C18-C36
23	BB	843	BCR	C36-C18-C19-C20
23	BB	843	BCR	C20-C21-C22-C23
23	BB	843	BCR	C20-C21-C22-C37
23	BB	843	BCR	C22-C23-C24-C25
23	BB	847	BCR	C7-C8-C9-C10
23	BB	847	BCR	C7-C8-C9-C34
23	BB	847	BCR	C12-C13-C14-C15
23	BB	847	BCR	C36-C18-C19-C20
23	BB	847	BCR	C19-C20-C21-C22
23	FF	303	BCR	C6-C7-C8-C9
23	FF	303	BCR	C7-C8-C9-C34
23	FF	303	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	FF	303	BCR	C11-C10-C9-C34
23	FF	303	BCR	C10-C11-C12-C13
23	FF	303	BCR	C12-C13-C14-C15
23	FF	303	BCR	C16-C17-C18-C36
23	FF	303	BCR	C21-C22-C23-C24
23	FF	304	BCR	C7-C8-C9-C10
23	FF	304	BCR	C7-C8-C9-C34
23	FF	304	BCR	C11-C10-C9-C8
23	FF	304	BCR	C11-C10-C9-C34
23	FF	304	BCR	C11-C12-C13-C35
23	FF	304	BCR	C35-C13-C14-C15
23	FF	304	BCR	C18-C19-C20-C21
23	FF	304	BCR	C20-C21-C22-C23
23	FF	304	BCR	C21-C22-C23-C24
23	FF	306	BCR	C1-C6-C7-C8
23	FF	306	BCR	C5-C6-C7-C8
23	FF	306	BCR	C6-C7-C8-C9
23	FF	306	BCR	C7-C8-C9-C10
23	FF	306	BCR	C11-C10-C9-C8
23	FF	306	BCR	C10-C11-C12-C13
23	FF	306	BCR	C11-C12-C13-C14
23	FF	306	BCR	C11-C12-C13-C35
23	FF	306	BCR	C15-C16-C17-C18
23	FF	306	BCR	C16-C17-C18-C19
23	FF	306	BCR	C16-C17-C18-C36
23	FF	306	BCR	C17-C18-C19-C20
23	FF	306	BCR	C18-C19-C20-C21
23	FF	306	BCR	C21-C22-C23-C24
23	FF	306	BCR	C37-C22-C23-C24
23	FF	306	BCR	C22-C23-C24-C25
23	II	101	BCR	C11-C10-C9-C34
23	II	101	BCR	C16-C17-C18-C36
23	II	101	BCR	C21-C22-C23-C24
23	II	101	BCR	C37-C22-C23-C24
23	II	102	BCR	C35-C13-C14-C15
23	II	102	BCR	C17-C18-C19-C20
23	II	102	BCR	C36-C18-C19-C20
23	II	104	BCR	C7-C8-C9-C10
23	II	104	BCR	C7-C8-C9-C34
23	II	104	BCR	C11-C10-C9-C34
23	II	104	BCR	C16-C17-C18-C36
23	II	104	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	II	104	BCR	C23-C24-C25-C26
23	II	104	BCR	C23-C24-C25-C30
23	JJ	102	BCR	C11-C10-C9-C34
23	JJ	102	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C11-C12-C13-C14
23	JJ	102	BCR	C35-C13-C14-C15
23	JJ	102	BCR	C16-C17-C18-C36
23	JJ	102	BCR	C36-C18-C19-C20
23	JJ	102	BCR	C21-C22-C23-C24
23	JJ	102	BCR	C37-C22-C23-C24
23	JJ	104	BCR	C11-C10-C9-C34
23	JJ	104	BCR	C11-C12-C13-C35
23	JJ	104	BCR	C16-C17-C18-C36
23	JJ	104	BCR	C17-C18-C19-C20
23	JJ	104	BCR	C23-C24-C25-C26
23	KK	103	BCR	C11-C10-C9-C34
23	KK	103	BCR	C16-C17-C18-C36
23	KK	103	BCR	C17-C18-C19-C20
23	KK	103	BCR	C20-C21-C22-C37
23	KK	103	BCR	C21-C22-C23-C24
23	KK	103	BCR	C37-C22-C23-C24
23	LL	204	BCR	C1-C6-C7-C8
23	LL	204	BCR	C5-C6-C7-C8
23	LL	204	BCR	C6-C7-C8-C9
23	LL	204	BCR	C11-C10-C9-C8
23	LL	204	BCR	C11-C10-C9-C34
23	LL	204	BCR	C11-C12-C13-C14
23	LL	204	BCR	C11-C12-C13-C35
23	LL	204	BCR	C16-C17-C18-C36
23	LL	204	BCR	C17-C18-C19-C20
23	LL	204	BCR	C20-C21-C22-C37
23	LL	204	BCR	C21-C22-C23-C24
23	MM	101	BCR	C7-C8-C9-C10
23	MM	101	BCR	C11-C10-C9-C8
23	MM	101	BCR	C11-C10-C9-C34
23	MM	101	BCR	C10-C11-C12-C13
23	MM	101	BCR	C11-C12-C13-C14
23	MM	101	BCR	C12-C13-C14-C15
23	MM	101	BCR	C35-C13-C14-C15
23	MM	101	BCR	C14-C15-C16-C17
23	MM	101	BCR	C16-C17-C18-C19
23	MM	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	MM	101	BCR	C18-C19-C20-C21
23	MM	101	BCR	C20-C21-C22-C23
23	MM	101	BCR	C20-C21-C22-C37
23	MM	101	BCR	C21-C22-C23-C24
23	MM	101	BCR	C37-C22-C23-C24
24	L1	203	AJP	C27-C26-O25-C23
24	B	849	AJP	C27-C26-O25-C23
24	K	104	AJP	C27-C26-O25-C23
24	BB	848	AJP	C27-C26-O25-C23
25	B1	844	LMG	C2-C1-O1-C7
25	B1	844	LMG	O6-C1-O1-C7
25	B1	846	LMG	C2-C1-O1-C7
25	I1	102	LMG	O6-C1-O1-C7
25	B2	845	LMG	C2-C1-O1-C7
25	B2	845	LMG	O6-C1-O1-C7
25	B2	847	LMG	C2-C1-O1-C7
25	B2	847	LMG	O6-C1-O1-C7
25	B	845	LMG	C2-C1-O1-C7
25	B	845	LMG	O6-C1-O1-C7
25	BB	844	LMG	C2-C1-O1-C7
25	BB	844	LMG	O6-C1-O1-C7
25	II	105	LMG	C11-C10-O7-C8
26	B1	840	ECH	C5-C6-C7-C8
26	B1	840	ECH	C7-C8-C9-C10
26	B1	840	ECH	C7-C8-C9-C34
26	B1	840	ECH	C11-C12-C13-C14
26	B2	841	ECH	C5-C6-C7-C8
26	B2	841	ECH	C7-C8-C9-C10
26	B2	841	ECH	C7-C8-C9-C34
26	B2	841	ECH	C11-C12-C13-C14
26	B	841	ECH	C5-C6-C7-C8
26	B	841	ECH	C7-C8-C9-C10
26	B	841	ECH	C7-C8-C9-C34
26	BB	840	ECH	C5-C6-C7-C8
26	BB	840	ECH	C7-C8-C9-C10
26	BB	840	ECH	C7-C8-C9-C34
26	BB	840	ECH	C11-C12-C13-C14
26	BB	840	ECH	C11-C12-C13-C35
26	BB	840	ECH	C13-C14-C15-C16
28	B	856	DGD	C2D-C1D-O3G-C3G
28	B	856	DGD	O6D-C1D-O3G-C3G
28	B	856	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
28	B	856	DGD	O6E-C1E-O5D-C6D
28	BB	854	DGD	C2D-C1D-O3G-C3G
28	BB	854	DGD	O6D-C1D-O3G-C3G
28	BB	854	DGD	C2E-C1E-O5D-C6D
28	BB	854	DGD	O6E-C1E-O5D-C6D
19	B1	833	CLA	C4C-C3C-CAC-CBC
19	BB	829	CLA	C4C-C3C-CAC-CBC
19	A1	827	CLA	O1D-CGD-O2D-CED
19	B1	803	CLA	O1D-CGD-O2D-CED
19	B1	832	CLA	O1D-CGD-O2D-CED
19	A2	801	CLA	O1D-CGD-O2D-CED
19	A2	812	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	O1D-CGD-O2D-CED
19	B	854	CLA	O1D-CGD-O2D-CED
19	AA	812	CLA	O1D-CGD-O2D-CED
19	AA	823	CLA	O1D-CGD-O2D-CED
19	BB	806	CLA	O1D-CGD-O2D-CED
19	BB	816	CLA	O1D-CGD-O2D-CED
19	BB	832	CLA	O1D-CGD-O2D-CED
19	BB	833	CLA	C4C-C3C-CAC-CBC
19	B1	833	CLA	C2C-C3C-CAC-CBC
19	A1	811	CLA	O1D-CGD-O2D-CED
19	A1	822	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	O1D-CGD-O2D-CED
19	B1	816	CLA	O1D-CGD-O2D-CED
19	B1	848	CLA	O1D-CGD-O2D-CED
19	F1	301	CLA	O1D-CGD-O2D-CED
19	A2	828	CLA	O1D-CGD-O2D-CED
19	B2	803	CLA	O1D-CGD-O2D-CED
19	B2	806	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1D-CGD-O2D-CED
19	B	816	CLA	O1D-CGD-O2D-CED
19	B	833	CLA	O1D-CGD-O2D-CED
19	B	859	CLA	O1D-CGD-O2D-CED
19	AA	828	CLA	O1D-CGD-O2D-CED
19	BB	803	CLA	O1D-CGD-O2D-CED
19	BB	808	CLA	O1D-CGD-O2D-CED
19	BB	852	CLA	O1D-CGD-O2D-CED
19	BB	856	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	CBD-CGD-O2D-CED
19	A1	827	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A1	829	CLA	CBD-CGD-O2D-CED
19	A1	830	CLA	CBD-CGD-O2D-CED
19	A1	834	CLA	CBD-CGD-O2D-CED
19	A1	836	CLA	CBD-CGD-O2D-CED
19	B1	801	CLA	CBD-CGD-O2D-CED
19	B1	803	CLA	CBD-CGD-O2D-CED
19	B1	806	CLA	CBD-CGD-O2D-CED
19	B1	810	CLA	CBD-CGD-O2D-CED
19	B1	816	CLA	CBD-CGD-O2D-CED
19	B1	850	CLA	CBD-CGD-O2D-CED
19	F1	301	CLA	CBD-CGD-O2D-CED
19	J1	101	CLA	CBD-CGD-O2D-CED
19	L1	207	CLA	CBD-CGD-O2D-CED
19	A2	801	CLA	CBD-CGD-O2D-CED
19	A2	811	CLA	CBD-CGD-O2D-CED
19	A2	816	CLA	CBD-CGD-O2D-CED
19	A2	830	CLA	CBD-CGD-O2D-CED
19	A2	831	CLA	CBD-CGD-O2D-CED
19	A2	837	CLA	CBD-CGD-O2D-CED
19	B2	801	CLA	CBD-CGD-O2D-CED
19	B2	803	CLA	CBD-CGD-O2D-CED
19	B2	812	CLA	CBD-CGD-O2D-CED
19	B2	824	CLA	CBD-CGD-O2D-CED
19	B2	827	CLA	CBD-CGD-O2D-CED
19	F2	301	CLA	CBD-CGD-O2D-CED
19	J2	101	CLA	CBD-CGD-O2D-CED
19	A	801	CLA	CBD-CGD-O2D-CED
19	A	804	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	823	CLA	CBD-CGD-O2D-CED
19	A	824	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	824	CLA	CBD-CGD-O2D-CED
19	B	827	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	B	854	CLA	CBD-CGD-O2D-CED
19	B	859	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	CBD-CGD-O2D-CED
19	J	103	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	AA	822	CLA	CBD-CGD-O2D-CED
19	AA	823	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	CBD-CGD-O2D-CED
19	BB	801	CLA	CBD-CGD-O2D-CED
19	BB	808	CLA	CBD-CGD-O2D-CED
19	BB	816	CLA	CBD-CGD-O2D-CED
19	BB	820	CLA	CBD-CGD-O2D-CED
19	BB	824	CLA	CBD-CGD-O2D-CED
19	BB	830	CLA	CBD-CGD-O2D-CED
19	BB	831	CLA	CBD-CGD-O2D-CED
19	BB	856	CLA	CBD-CGD-O2D-CED
19	FF	301	CLA	CBD-CGD-O2D-CED
19	LL	203	CLA	CBD-CGD-O2D-CED
24	L2	202	AJP	C27-C26-O25-C23
24	KK	104	AJP	C27-C26-O25-C23
19	B1	806	CLA	O1A-CGA-O2A-C1
19	B1	807	CLA	O1A-CGA-O2A-C1
19	B2	806	CLA	O1A-CGA-O2A-C1
19	B2	807	CLA	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
19	BB	806	CLA	O1A-CGA-O2A-C1
20	A1	802	CL0	O1A-CGA-O2A-C1
22	L1	211	LHG	O10-C23-O8-C6
19	K1	103	CLA	O1A-CGA-O2A-C1
19	A2	802	CLA	O1A-CGA-O2A-C1
19	KK	102	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	C4C-C3C-CAC-CBC
19	BB	833	CLA	C2C-C3C-CAC-CBC
19	B2	849	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	O1D-CGD-O2D-CED
25	I2	105	LMG	C4-C5-C6-O5
19	BB	829	CLA	C2C-C3C-CAC-CBC
19	B1	810	CLA	O1D-CGD-O2D-CED
19	B1	850	CLA	O1D-CGD-O2D-CED
19	K1	105	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	F	301	CLA	O1D-CGD-O2D-CED
19	BB	824	CLA	O1D-CGD-O2D-CED
19	FF	301	CLA	O1D-CGD-O2D-CED
19	LL	203	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	CBA-CGA-O2A-C1
19	B1	807	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B2	806	CLA	CBA-CGA-O2A-C1
19	B2	807	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	BB	806	CLA	CBA-CGA-O2A-C1
25	B1	844	LMG	C29-C28-O8-C9
25	B1	852	LMG	C29-C28-O8-C9
25	B2	845	LMG	C29-C28-O8-C9
25	B2	854	LMG	C29-C28-O8-C9
25	B	845	LMG	C29-C28-O8-C9
19	A2	832	CLA	CBD-CGD-O2D-CED
19	B2	852	CLA	CBD-CGD-O2D-CED
19	AA	801	CLA	CBD-CGD-O2D-CED
19	A1	814	CLA	O1A-CGA-O2A-C1
19	B1	833	CLA	O1A-CGA-O2A-C1
19	A2	815	CLA	O1A-CGA-O2A-C1
19	A2	839	CLA	O1A-CGA-O2A-C1
19	B2	802	CLA	O1A-CGA-O2A-C1
19	B2	834	CLA	O1A-CGA-O2A-C1
19	A	815	CLA	O1A-CGA-O2A-C1
19	A	839	CLA	O1A-CGA-O2A-C1
19	B	826	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	O1A-CGA-O2A-C1
19	AA	815	CLA	O1A-CGA-O2A-C1
19	AA	839	CLA	O1A-CGA-O2A-C1
19	BB	802	CLA	O1A-CGA-O2A-C1
19	BB	807	CLA	O1A-CGA-O2A-C1
19	BB	833	CLA	O1A-CGA-O2A-C1
19	FF	301	CLA	O1A-CGA-O2A-C1
20	AA	803	CL0	O1A-CGA-O2A-C1
22	L2	208	LHG	O10-C23-O8-C6
25	B1	846	LMG	O10-C28-O8-C9
25	B1	852	LMG	O10-C28-O8-C9
25	I1	102	LMG	O10-C28-O8-C9
25	B2	847	LMG	O10-C28-O8-C9
25	B2	854	LMG	O10-C28-O8-C9
28	B	856	DGD	O1A-C1A-O1G-C1G
28	BB	854	DGD	O1A-C1A-O1G-C1G
19	B2	834	CLA	C4C-C3C-CAC-CBC
19	B	834	CLA	C2C-C3C-CAC-CBC
19	A1	815	CLA	O1D-CGD-O2D-CED
19	L1	207	CLA	O1D-CGD-O2D-CED
19	A2	816	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A2	823	CLA	O1D-CGD-O2D-CED
19	B2	810	CLA	O1D-CGD-O2D-CED
19	B2	824	CLA	O1D-CGD-O2D-CED
19	F2	301	CLA	O1D-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	B	824	CLA	O1D-CGD-O2D-CED
19	F	302	CLA	O1D-CGD-O2D-CED
19	L	204	CLA	O1D-CGD-O2D-CED
19	AA	811	CLA	O1D-CGD-O2D-CED
19	A1	810	CLA	O1D-CGD-O2D-CED
19	B1	824	CLA	O1D-CGD-O2D-CED
19	F1	302	CLA	O1D-CGD-O2D-CED
19	A2	804	CLA	O1D-CGD-O2D-CED
19	A2	825	CLA	O1D-CGD-O2D-CED
19	A2	844	CLA	O1D-CGD-O2D-CED
19	F2	302	CLA	O1D-CGD-O2D-CED
19	L2	206	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	AA	816	CLA	O1D-CGD-O2D-CED
19	AA	845	CLA	O1D-CGD-O2D-CED
19	BB	810	CLA	O1D-CGD-O2D-CED
19	FF	302	CLA	O1D-CGD-O2D-CED
19	B1	815	CLA	CBD-CGD-O2D-CED
19	A2	836	CLA	CBD-CGD-O2D-CED
19	BB	826	CLA	O1A-CGA-O2A-C1
25	B	845	LMG	O10-C28-O8-C9
25	I1	102	LMG	O9-C10-O7-C8
25	II	105	LMG	O9-C10-O7-C8
28	B	856	DGD	O1B-C1B-O2G-C2G
28	BB	854	DGD	O1B-C1B-O2G-C2G
19	A1	844	CLA	O1D-CGD-O2D-CED
24	L2	203	AJP	C29-C30-C32-O33
19	A1	822	CLA	C3-C5-C6-C7
19	A2	823	CLA	C3-C5-C6-C7
19	B2	804	CLA	C3-C5-C6-C7
19	L2	205	CLA	C3-C5-C6-C7
19	A	823	CLA	C3-C5-C6-C7
19	A	835	CLA	C3-C5-C6-C7
19	B	804	CLA	C3-C5-C6-C7
19	AA	808	CLA	C3-C5-C6-C7
19	AA	823	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	AA	835	CLA	C3-C5-C6-C7
19	BB	804	CLA	C3-C5-C6-C7
19	FF	301	CLA	C3-C5-C6-C7
19	A1	803	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	CBA-CGA-O2A-C1
19	A1	814	CLA	CBA-CGA-O2A-C1
19	A1	821	CLA	CBA-CGA-O2A-C1
19	B1	833	CLA	CBA-CGA-O2A-C1
19	A2	801	CLA	CBA-CGA-O2A-C1
19	A2	815	CLA	CBA-CGA-O2A-C1
19	B2	834	CLA	CBA-CGA-O2A-C1
19	A	801	CLA	CBA-CGA-O2A-C1
19	A	813	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	B	834	CLA	CBA-CGA-O2A-C1
19	AA	813	CLA	CBA-CGA-O2A-C1
19	AA	815	CLA	CBA-CGA-O2A-C1
19	BB	816	CLA	CBA-CGA-O2A-C1
19	BB	833	CLA	CBA-CGA-O2A-C1
20	A1	802	CL0	CBA-CGA-O2A-C1
20	AA	803	CL0	CBA-CGA-O2A-C1
22	L1	211	LHG	C24-C23-O8-C6
22	L2	208	LHG	C24-C23-O8-C6
25	B1	846	LMG	C29-C28-O8-C9
25	B2	847	LMG	C29-C28-O8-C9
25	BB	844	LMG	C29-C28-O8-C9
24	B	849	AJP	O31-C30-C32-O33
19	A1	819	CLA	CBD-CGD-O2D-CED
19	A1	823	CLA	CBD-CGD-O2D-CED
19	A1	825	CLA	CBD-CGD-O2D-CED
19	A1	828	CLA	CBD-CGD-O2D-CED
19	A1	831	CLA	CBD-CGD-O2D-CED
19	A1	835	CLA	CBD-CGD-O2D-CED
19	A1	837	CLA	CBD-CGD-O2D-CED
19	A1	852	CLA	CBD-CGD-O2D-CED
19	B1	820	CLA	CBD-CGD-O2D-CED
19	B1	831	CLA	CBD-CGD-O2D-CED
19	B1	836	CLA	CBD-CGD-O2D-CED
19	A2	808	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A2	826	CLA	CBD-CGD-O2D-CED
19	A2	829	CLA	CBD-CGD-O2D-CED
19	A2	838	CLA	CBD-CGD-O2D-CED
19	B2	829	CLA	CBD-CGD-O2D-CED
19	B2	832	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	CBD-CGD-O2D-CED
19	A	834	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	A	844	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
19	J	101	CLA	CBD-CGD-O2D-CED
19	K	102	CLA	CBD-CGD-O2D-CED
19	AA	820	CLA	CBD-CGD-O2D-CED
19	AA	831	CLA	CBD-CGD-O2D-CED
19	AA	834	CLA	CBD-CGD-O2D-CED
19	AA	836	CLA	CBD-CGD-O2D-CED
19	BB	815	CLA	CBD-CGD-O2D-CED
19	JJ	101	CLA	CBD-CGD-O2D-CED
19	KK	102	CLA	CBD-CGD-O2D-CED
22	L1	211	LHG	C8-C7-O7-C5
22	L2	208	LHG	C8-C7-O7-C5
22	L	207	LHG	C8-C7-O7-C5
22	LL	205	LHG	C8-C7-O7-C5
19	A1	833	CLA	O1D-CGD-O2D-CED
19	A1	834	CLA	O1D-CGD-O2D-CED
19	A1	836	CLA	O1D-CGD-O2D-CED
19	B1	827	CLA	O1D-CGD-O2D-CED
19	A2	834	CLA	O1D-CGD-O2D-CED
19	B2	801	CLA	O1D-CGD-O2D-CED
19	B2	816	CLA	O1D-CGD-O2D-CED
19	B2	851	CLA	O1D-CGD-O2D-CED
19	A	835	CLA	O1D-CGD-O2D-CED
19	AA	830	CLA	O1D-CGD-O2D-CED
19	A1	812	CLA	O1A-CGA-O2A-C1
19	A1	820	CLA	O1A-CGA-O2A-C1
19	B2	834	CLA	C2C-C3C-CAC-CBC
24	L1	204	AJP	C29-C30-C32-O33
19	A1	830	CLA	O1D-CGD-O2D-CED
19	A2	835	CLA	O1D-CGD-O2D-CED
19	B	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	AA	804	CLA	O1D-CGD-O2D-CED
19	AA	835	CLA	O1D-CGD-O2D-CED
19	A1	809	CLA	C4-C3-C5-C6
19	A1	841	CLA	C4-C3-C5-C6
19	A2	810	CLA	C4-C3-C5-C6
19	A2	842	CLA	C4-C3-C5-C6
19	B2	849	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	B	826	CLA	C4-C3-C5-C6
19	B	834	CLA	C4-C3-C5-C6
19	B	854	CLA	C4-C3-C5-C6
19	BB	826	CLA	C4-C3-C5-C6
19	BB	852	CLA	C4-C3-C5-C6
21	A1	843	PQN	C14-C13-C15-C16
21	A2	843	PQN	C14-C13-C15-C16
21	A	843	PQN	C14-C13-C15-C16
21	AA	844	PQN	C14-C13-C15-C16
19	A1	809	CLA	C2-C3-C5-C6
19	B1	826	CLA	C2-C3-C5-C6
19	A2	810	CLA	C2-C3-C5-C6
19	B2	849	CLA	C2-C3-C5-C6
19	B	854	CLA	C2-C3-C5-C6
19	BB	826	CLA	C2-C3-C5-C6
21	A1	843	PQN	C12-C13-C15-C16
21	AA	844	PQN	C12-C13-C15-C16
19	B2	837	CLA	CBD-CGD-O2D-CED
19	AA	817	CLA	CBD-CGD-O2D-CED
19	A2	811	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	O1D-CGD-O2D-CED
19	BB	801	CLA	O1D-CGD-O2D-CED
25	I2	105	LMG	O6-C5-C6-O5
19	A2	829	CLA	C2A-CAA-CBA-CGA
19	A	825	CLA	C3-C5-C6-C7
19	AA	825	CLA	C3-C5-C6-C7
19	AA	853	CLA	C2A-CAA-CBA-CGA
19	A1	838	CLA	O1A-CGA-O2A-C1
19	A2	808	CLA	O1A-CGA-O2A-C1
19	B2	801	CLA	O1A-CGA-O2A-C1
19	AA	808	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	O10-C28-O8-C9
25	B2	845	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
19	B1	804	CLA	C3-C5-C6-C7
19	A2	808	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	BB	807	CLA	C3-C5-C6-C7
20	A	803	CL0	C3-C5-C6-C7
19	A1	807	CLA	CBA-CGA-O2A-C1
19	A1	812	CLA	CBA-CGA-O2A-C1
19	A2	813	CLA	CBA-CGA-O2A-C1
19	A2	839	CLA	CBA-CGA-O2A-C1
19	B2	801	CLA	CBA-CGA-O2A-C1
19	B2	802	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	CBA-CGA-O2A-C1
19	A	819	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CBA-CGA-O2A-C1
19	F	301	CLA	CBA-CGA-O2A-C1
19	AA	801	CLA	CBA-CGA-O2A-C1
19	AA	819	CLA	CBA-CGA-O2A-C1
19	AA	839	CLA	CBA-CGA-O2A-C1
19	AA	843	CLA	CBA-CGA-O2A-C1
19	BB	801	CLA	CBA-CGA-O2A-C1
19	BB	802	CLA	CBA-CGA-O2A-C1
19	BB	807	CLA	CBA-CGA-O2A-C1
19	BB	826	CLA	CBA-CGA-O2A-C1
19	BB	832	CLA	CBA-CGA-O2A-C1
19	FF	301	CLA	CBA-CGA-O2A-C1
20	A	803	CL0	CBA-CGA-O2A-C1
25	II	105	LMG	C29-C28-O8-C9
28	B	856	DGD	C2A-C1A-O1G-C1G
28	BB	854	DGD	C2A-C1A-O1G-C1G
24	BB	848	AJP	O31-C30-C32-O33
25	B1	846	LMG	C4-C5-C6-O5
23	A1	853	BCR	C13-C14-C15-C16
23	F1	306	BCR	C15-C16-C17-C18
23	A2	853	BCR	C13-C14-C15-C16
23	A2	853	BCR	C15-C16-C17-C18
23	I2	101	BCR	C9-C10-C11-C12
23	L2	207	BCR	C9-C10-C11-C12
23	A	853	BCR	C15-C16-C17-C18
23	AA	854	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	LL	204	BCR	C9-C10-C11-C12
23	MM	101	BCR	C19-C20-C21-C22
19	A1	818	CLA	O1A-CGA-O2A-C1
19	A1	821	CLA	O1A-CGA-O2A-C1
19	B1	801	CLA	O1A-CGA-O2A-C1
19	B1	802	CLA	O1A-CGA-O2A-C1
19	B1	826	CLA	O1A-CGA-O2A-C1
19	A2	813	CLA	O1A-CGA-O2A-C1
19	A2	819	CLA	O1A-CGA-O2A-C1
19	A2	821	CLA	O1A-CGA-O2A-C1
19	A2	822	CLA	O1A-CGA-O2A-C1
19	B2	826	CLA	O1A-CGA-O2A-C1
19	B2	852	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	O1A-CGA-O2A-C1
19	B	801	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	O1A-CGA-O2A-C1
19	B	860	CLA	O1A-CGA-O2A-C1
19	AA	819	CLA	O1A-CGA-O2A-C1
19	AA	821	CLA	O1A-CGA-O2A-C1
19	AA	843	CLA	O1A-CGA-O2A-C1
25	M	102	LMG	O10-C28-O8-C9
25	BB	844	LMG	O10-C28-O8-C9
19	A1	829	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	O1D-CGD-O2D-CED
19	A2	837	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	CBD-CGD-O2D-CED
19	A	817	CLA	CBD-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	AA	813	CLA	CBD-CGD-O2D-CED
22	A1	845	LHG	O2-C2-C3-O3
22	B1	847	LHG	O2-C2-C3-O3
22	B2	848	LHG	O2-C2-C3-O3
22	L2	208	LHG	O2-C2-C3-O3
22	B	853	LHG	O2-C2-C3-O3
22	BB	851	LHG	O2-C2-C3-O3
19	A1	801	CLA	O1D-CGD-O2D-CED
19	B1	801	CLA	O1D-CGD-O2D-CED
19	J1	101	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	O1D-CGD-O2D-CED
19	J	103	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	BB	820	CLA	O1D-CGD-O2D-CED
19	A1	809	CLA	CBA-CGA-O2A-C1
19	A1	822	CLA	CBA-CGA-O2A-C1
19	A1	835	CLA	CBA-CGA-O2A-C1
19	A1	838	CLA	CBA-CGA-O2A-C1
19	B1	830	CLA	CBA-CGA-O2A-C1
19	B1	832	CLA	CBA-CGA-O2A-C1
19	A2	808	CLA	CBA-CGA-O2A-C1
19	A2	819	CLA	CBA-CGA-O2A-C1
19	A2	820	CLA	CBA-CGA-O2A-C1
19	A2	823	CLA	CBA-CGA-O2A-C1
19	B2	823	CLA	CBA-CGA-O2A-C1
19	B2	826	CLA	CBA-CGA-O2A-C1
19	B2	831	CLA	CBA-CGA-O2A-C1
19	B2	833	CLA	CBA-CGA-O2A-C1
19	B2	852	CLA	CBA-CGA-O2A-C1
19	F2	301	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
19	B	833	CLA	CBA-CGA-O2A-C1
19	B	860	CLA	CBA-CGA-O2A-C1
19	AA	808	CLA	CBA-CGA-O2A-C1
19	AA	820	CLA	CBA-CGA-O2A-C1
19	AA	821	CLA	CBA-CGA-O2A-C1
19	BB	823	CLA	CBA-CGA-O2A-C1
19	BB	830	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	C29-C28-O8-C9
25	M	102	LMG	C29-C28-O8-C9
19	A1	801	CLA	O1A-CGA-O2A-C1
19	A1	842	CLA	O1A-CGA-O2A-C1
19	A2	801	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	O1A-CGA-O2A-C1
19	A	813	CLA	O1A-CGA-O2A-C1
19	F	301	CLA	O1A-CGA-O2A-C1
19	AA	801	CLA	O1A-CGA-O2A-C1
19	AA	813	CLA	O1A-CGA-O2A-C1
19	BB	816	CLA	O1A-CGA-O2A-C1
25	II	105	LMG	O10-C28-O8-C9
19	B2	827	CLA	O1D-CGD-O2D-CED
19	AA	822	CLA	O1D-CGD-O2D-CED
24	B	850	AJP	O31-C30-C32-O33

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Mol	Chain	Res	Type	Atoms
25	M	102	LMG	O6-C5-C6-O5
19	A1	812	CLA	CBD-CGD-O2D-CED
19	B1	808	CLA	CBD-CGD-O2D-CED
19	B1	812	CLA	CBD-CGD-O2D-CED
19	A2	820	CLA	CBD-CGD-O2D-CED
19	B2	831	CLA	CBD-CGD-O2D-CED
19	BB	812	CLA	CBD-CGD-O2D-CED
19	A1	840	CLA	CBA-CGA-O2A-C1
19	A2	841	CLA	CBA-CGA-O2A-C1
19	BB	831	CLA	O1D-CGD-O2D-CED
23	B2	844	BCR	C14-C15-C16-C17
23	A	848	BCR	C14-C15-C16-C17
23	AA	849	BCR	C14-C15-C16-C17
19	A2	830	CLA	O1D-CGD-O2D-CED
19	A	801	CLA	O1D-CGD-O2D-CED
19	BB	830	CLA	O1D-CGD-O2D-CED
19	B1	815	CLA	C3-C5-C6-C7
19	A2	805	CLA	C3-C5-C6-C7
19	B2	815	CLA	C3-C5-C6-C7
19	A2	813	CLA	CBD-CGD-O2D-CED
19	B2	834	CLA	CBD-CGD-O2D-CED
19	AA	808	CLA	CBD-CGD-O2D-CED
19	AA	838	CLA	CBD-CGD-O2D-CED
19	A2	831	CLA	O1D-CGD-O2D-CED
19	B	812	CLA	O1D-CGD-O2D-CED
19	AA	829	CLA	O1D-CGD-O2D-CED
19	A1	818	CLA	CBA-CGA-O2A-C1
19	A1	820	CLA	CBA-CGA-O2A-C1
19	A1	842	CLA	CBA-CGA-O2A-C1
19	B1	801	CLA	CBA-CGA-O2A-C1
19	B1	802	CLA	CBA-CGA-O2A-C1
19	B1	826	CLA	CBA-CGA-O2A-C1
19	A2	821	CLA	CBA-CGA-O2A-C1
19	A2	822	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	B	801	CLA	CBA-CGA-O2A-C1
19	B	802	CLA	CBA-CGA-O2A-C1
19	AA	823	CLA	CBA-CGA-O2A-C1
19	A1	818	CLA	C4-C3-C5-C6
19	B1	811	CLA	C4-C3-C5-C6
19	B1	823	CLA	C4-C3-C5-C6
19	B1	826	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B1	833	CLA	C4-C3-C5-C6
19	B1	850	CLA	C4-C3-C5-C6
19	A2	819	CLA	C4-C3-C5-C6
19	B2	811	CLA	C4-C3-C5-C6
19	B2	816	CLA	C4-C3-C5-C6
19	B2	823	CLA	C4-C3-C5-C6
19	B2	834	CLA	C4-C3-C5-C6
19	B2	851	CLA	C4-C3-C5-C6
19	A	819	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	B	823	CLA	C4-C3-C5-C6
19	B	859	CLA	C4-C3-C5-C6
19	L	202	CLA	C4-C3-C5-C6
19	BB	811	CLA	C4-C3-C5-C6
19	BB	823	CLA	C4-C3-C5-C6
19	BB	833	CLA	C4-C3-C5-C6
19	BB	856	CLA	C4-C3-C5-C6
19	LL	201	CLA	C4-C3-C5-C6
19	A1	818	CLA	C2-C3-C5-C6
19	B1	811	CLA	C2-C3-C5-C6
19	B1	816	CLA	C2-C3-C5-C6
19	B1	823	CLA	C2-C3-C5-C6
19	B1	833	CLA	C2-C3-C5-C6
19	B1	850	CLA	C2-C3-C5-C6
19	A2	819	CLA	C2-C3-C5-C6
19	B2	811	CLA	C2-C3-C5-C6
19	B2	816	CLA	C2-C3-C5-C6
19	B2	823	CLA	C2-C3-C5-C6
19	B2	834	CLA	C2-C3-C5-C6
19	B2	851	CLA	C2-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	B	823	CLA	C2-C3-C5-C6
19	B	826	CLA	C2-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	B	859	CLA	C2-C3-C5-C6
19	L	202	CLA	C2-C3-C5-C6
19	AA	819	CLA	C2-C3-C5-C6
19	BB	811	CLA	C2-C3-C5-C6
19	BB	823	CLA	C2-C3-C5-C6
19	BB	852	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	BB	856	CLA	C2-C3-C5-C6
19	LL	201	CLA	C2-C3-C5-C6
21	A2	843	PQN	C12-C13-C15-C16
21	A	843	PQN	C12-C13-C15-C16
19	A1	809	CLA	O1A-CGA-O2A-C1
19	B1	832	CLA	O1A-CGA-O2A-C1
19	B2	823	CLA	O1A-CGA-O2A-C1
19	B2	833	CLA	O1A-CGA-O2A-C1
19	B	816	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	O1A-CGA-O2A-C1
19	AA	820	CLA	O1A-CGA-O2A-C1
19	BB	801	CLA	O1A-CGA-O2A-C1
19	BB	823	CLA	O1A-CGA-O2A-C1
25	L1	210	LMG	O10-C28-O8-C9
24	L2	202	AJP	O31-C30-C32-O33
24	A1	854	AJP	C29-C30-C32-O33
25	M	102	LMG	C4-C5-C6-O5
19	AA	812	CLA	CBA-CGA-O2A-C1
19	B2	820	CLA	CBD-CGD-O2D-CED
19	B	860	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	CBD-CGD-O2D-CED
19	BB	819	CLA	CBD-CGD-O2D-CED
19	XX	101	CLA	CBD-CGD-O2D-CED
19	A1	828	CLA	C2A-CAA-CBA-CGA
19	A1	852	CLA	C2A-CAA-CBA-CGA
19	A	852	CLA	C2A-CAA-CBA-CGA
20	AA	803	CL0	C2A-CAA-CBA-CGA
24	B	849	AJP	O31-C26-O25-C23
19	B1	815	CLA	O1D-CGD-O2D-CED
19	A2	832	CLA	O1D-CGD-O2D-CED
19	A2	836	CLA	O1D-CGD-O2D-CED
19	J2	101	CLA	O1D-CGD-O2D-CED
19	A1	822	CLA	O1A-CGA-O2A-C1
19	A1	835	CLA	O1A-CGA-O2A-C1
19	B1	830	CLA	O1A-CGA-O2A-C1
19	A2	823	CLA	O1A-CGA-O2A-C1
19	B2	831	CLA	O1A-CGA-O2A-C1
19	F2	301	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	O1A-CGA-O2A-C1
19	BB	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	BB	832	CLA	O1A-CGA-O2A-C1
20	A	803	CL0	O1A-CGA-O2A-C1
25	B1	846	LMG	O6-C1-O1-C7
24	A1	854	AJP	O31-C30-C32-O33
25	B1	846	LMG	O6-C5-C6-O5
19	A1	819	CLA	CBA-CGA-O2A-C1
19	F1	301	CLA	CBA-CGA-O2A-C1
19	B2	811	CLA	CBA-CGA-O2A-C1
19	B	811	CLA	CBA-CGA-O2A-C1
19	L	202	CLA	CBA-CGA-O2A-C1
20	A2	803	CL0	CBA-CGA-O2A-C1
22	A2	846	LHG	C24-C23-O8-C6
22	B2	848	LHG	C24-C23-O8-C6
19	A1	807	CLA	CBD-CGD-O2D-CED
19	A1	814	CLA	CBD-CGD-O2D-CED
19	A1	842	CLA	CBD-CGD-O2D-CED
19	B1	819	CLA	CBD-CGD-O2D-CED
19	B1	830	CLA	CBD-CGD-O2D-CED
19	A2	815	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	CBD-CGD-O2D-CED
19	A	852	CLA	CBD-CGD-O2D-CED
19	AA	815	CLA	CBD-CGD-O2D-CED
19	BB	813	CLA	CBD-CGD-O2D-CED
19	BB	836	CLA	CBD-CGD-O2D-CED
20	A2	803	CL0	CBD-CGD-O2D-CED
20	AA	803	CL0	CBD-CGD-O2D-CED
19	A2	830	CLA	C2C-C3C-CAC-CBC
19	A2	820	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	O1A-CGA-O2A-C1
19	AA	823	CLA	O1A-CGA-O2A-C1
19	A1	835	CLA	O1D-CGD-O2D-CED
19	B2	852	CLA	O1D-CGD-O2D-CED
19	AA	831	CLA	O1D-CGD-O2D-CED
19	AA	834	CLA	O1D-CGD-O2D-CED
19	B2	823	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	AA	826	CLA	CBD-CGD-O2D-CED
19	BB	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A2	815	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
24	L1	203	AJP	C29-C30-C32-O33
23	A1	853	BCR	C15-C16-C17-C18
23	B1	841	BCR	C13-C14-C15-C16
23	I1	101	BCR	C9-C10-C11-C12
23	B	842	BCR	C13-C14-C15-C16
26	BB	840	ECH	C15-C16-C17-C18
19	A1	819	CLA	O1A-CGA-O2A-C1
19	F1	301	CLA	O1A-CGA-O2A-C1
20	A2	803	CL0	O1A-CGA-O2A-C1
22	B1	847	LHG	C1-C2-C3-O3
19	A1	804	CLA	CBA-CGA-O2A-C1
19	B1	821	CLA	CBA-CGA-O2A-C1
19	B1	823	CLA	CBA-CGA-O2A-C1
19	A2	805	CLA	CBA-CGA-O2A-C1
19	A2	810	CLA	CBA-CGA-O2A-C1
19	A2	836	CLA	CBA-CGA-O2A-C1
19	B2	821	CLA	CBA-CGA-O2A-C1
19	A	805	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	CBA-CGA-O2A-C1
19	AA	805	CLA	CBA-CGA-O2A-C1
19	AA	810	CLA	CBA-CGA-O2A-C1
19	AA	827	CLA	CBA-CGA-O2A-C1
19	BB	803	CLA	CBA-CGA-O2A-C1
19	LL	201	CLA	CBA-CGA-O2A-C1
22	A1	846	LHG	C24-C23-O8-C6
22	X2	103	LHG	C24-C23-O8-C6
22	B	853	LHG	C24-C23-O8-C6
22	BB	851	LHG	C24-C23-O8-C6
25	L1	210	LMG	C29-C28-O8-C9
19	B	823	CLA	CBD-CGD-O2D-CED
24	BB	849	AJP	C29-C30-C32-O33
19	A1	823	CLA	O1D-CGD-O2D-CED
19	B2	812	CLA	O1D-CGD-O2D-CED
19	B	837	CLA	O1D-CGD-O2D-CED
19	AA	801	CLA	O1D-CGD-O2D-CED
19	A1	828	CLA	C4-C3-C5-C6
19	B1	816	CLA	C4-C3-C5-C6
19	A	810	CLA	C4-C3-C5-C6
19	A	842	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	AA	810	CLA	C4-C3-C5-C6
19	AA	819	CLA	C4-C3-C5-C6
19	AA	842	CLA	C4-C3-C5-C6
19	BB	816	CLA	C4-C3-C5-C6
20	AA	803	CL0	C4-C3-C5-C6
19	A1	828	CLA	C2-C3-C5-C6
19	A1	841	CLA	C2-C3-C5-C6
19	A2	842	CLA	C2-C3-C5-C6
19	A	810	CLA	C2-C3-C5-C6
19	A	842	CLA	C2-C3-C5-C6
19	AA	810	CLA	C2-C3-C5-C6
19	AA	842	CLA	C2-C3-C5-C6
19	BB	816	CLA	C2-C3-C5-C6
19	BB	833	CLA	C2-C3-C5-C6
20	AA	803	CL0	C2-C3-C5-C6
19	F1	301	CLA	C3-C5-C6-C7
19	A1	826	CLA	CBD-CGD-O2D-CED
19	AA	843	CLA	CBD-CGD-O2D-CED
19	A1	803	CLA	C6-C7-C8-C9
19	A1	852	CLA	C11-C10-C8-C9
19	B1	816	CLA	C6-C7-C8-C9
19	B1	823	CLA	C6-C7-C8-C9
19	B1	825	CLA	C14-C13-C15-C16
19	B1	833	CLA	C14-C13-C15-C16
19	A2	804	CLA	C6-C7-C8-C9
19	A2	813	CLA	C6-C7-C8-C9
19	A2	829	CLA	C11-C10-C8-C9
19	A2	852	CLA	C11-C10-C8-C9
19	B2	807	CLA	C6-C7-C8-C9
19	B2	816	CLA	C6-C7-C8-C9
19	B2	825	CLA	C14-C13-C15-C16
19	B2	836	CLA	C6-C7-C8-C9
19	L2	205	CLA	C6-C7-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	A	827	CLA	C14-C13-C15-C16
19	A	829	CLA	C11-C10-C8-C9
19	A	852	CLA	C11-C10-C8-C9
19	B	807	CLA	C6-C7-C8-C9
19	B	807	CLA	C14-C13-C15-C16
19	B	825	CLA	C14-C13-C15-C16
19	B	834	CLA	C14-C13-C15-C16
19	B	836	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	AA	804	CLA	C6-C7-C8-C9
19	AA	829	CLA	C11-C10-C8-C9
19	AA	853	CLA	C11-C10-C8-C9
19	BB	807	CLA	C6-C7-C8-C9
19	BB	807	CLA	C14-C13-C15-C16
19	BB	815	CLA	C14-C13-C15-C16
19	BB	823	CLA	C6-C7-C8-C9
19	BB	825	CLA	C14-C13-C15-C16
19	BB	835	CLA	C6-C7-C8-C9
20	A2	803	CL0	C11-C10-C8-C9
20	AA	803	CL0	C6-C7-C8-C9
24	L1	204	AJP	O31-C30-C32-O33
19	A1	825	CLA	O1D-CGD-O2D-CED
19	A1	831	CLA	O1D-CGD-O2D-CED
19	A1	837	CLA	O1D-CGD-O2D-CED
19	A1	852	CLA	O1D-CGD-O2D-CED
19	B1	831	CLA	O1D-CGD-O2D-CED
25	I1	102	LMG	C2-C1-O1-C7
19	K1	105	CLA	C2C-C3C-CAC-CBC
19	A2	808	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	O1D-CGD-O2D-CED
19	AA	820	CLA	O1D-CGD-O2D-CED
24	BB	849	AJP	O31-C30-C32-O33
25	II	105	LMG	O6-C5-C6-O5
19	B1	823	CLA	O1A-CGA-O2A-C1
19	A2	810	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	O1A-CGA-O2A-C1
25	B	851	LMG	O10-C28-O8-C9
19	B1	820	CLA	O1D-CGD-O2D-CED
19	A2	838	CLA	O1D-CGD-O2D-CED
23	A1	847	BCR	C36-C18-C19-C20
23	A1	848	BCR	C7-C8-C9-C34
23	A1	848	BCR	C36-C18-C19-C20
23	A1	849	BCR	C7-C8-C9-C34
23	A1	849	BCR	C11-C12-C13-C35
23	A1	850	BCR	C7-C8-C9-C34
23	A1	850	BCR	C11-C12-C13-C35
23	A1	851	BCR	C7-C8-C9-C34
23	A1	851	BCR	C36-C18-C19-C20
23	A1	853	BCR	C7-C8-C9-C34
23	A1	853	BCR	C11-C12-C13-C35
23	A1	853	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	B1	838	BCR	C7-C8-C9-C34
23	B1	838	BCR	C37-C22-C23-C24
23	B1	839	BCR	C37-C22-C23-C24
23	B1	841	BCR	C7-C8-C9-C34
23	B1	841	BCR	C11-C12-C13-C35
23	B1	841	BCR	C37-C22-C23-C24
23	B1	842	BCR	C11-C12-C13-C35
23	B1	843	BCR	C36-C18-C19-C20
23	F1	303	BCR	C11-C12-C13-C35
23	F1	304	BCR	C11-C12-C13-C35
23	F1	304	BCR	C36-C18-C19-C20
23	F1	306	BCR	C7-C8-C9-C34
23	F1	306	BCR	C36-C18-C19-C20
23	I1	101	BCR	C11-C12-C13-C35
23	I1	101	BCR	C36-C18-C19-C20
23	J1	102	BCR	C7-C8-C9-C34
23	J1	102	BCR	C11-C12-C13-C35
23	J1	104	BCR	C36-C18-C19-C20
23	K1	104	BCR	C7-C8-C9-C34
23	K1	104	BCR	C36-C18-C19-C20
23	K1	106	BCR	C7-C8-C9-C34
23	L1	201	BCR	C7-C8-C9-C34
23	L1	201	BCR	C37-C22-C23-C24
23	L1	208	BCR	C11-C12-C13-C35
23	M1	101	BCR	C7-C8-C9-C34
23	A2	847	BCR	C36-C18-C19-C20
23	A2	848	BCR	C7-C8-C9-C34
23	A2	848	BCR	C36-C18-C19-C20
23	A2	849	BCR	C11-C12-C13-C35
23	A2	850	BCR	C7-C8-C9-C34
23	A2	850	BCR	C11-C12-C13-C35
23	A2	851	BCR	C7-C8-C9-C34
23	A2	853	BCR	C7-C8-C9-C34
23	A2	853	BCR	C11-C12-C13-C35
23	A2	853	BCR	C37-C22-C23-C24
23	B2	839	BCR	C7-C8-C9-C34
23	B2	839	BCR	C37-C22-C23-C24
23	B2	842	BCR	C7-C8-C9-C34
23	B2	844	BCR	C11-C12-C13-C35
23	B2	844	BCR	C36-C18-C19-C20
23	F2	304	BCR	C11-C12-C13-C35
23	F2	305	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	I2	101	BCR	C11-C12-C13-C35
23	I2	101	BCR	C36-C18-C19-C20
23	I2	102	BCR	C11-C12-C13-C35
23	I2	102	BCR	C37-C22-C23-C24
23	I2	103	BCR	C11-C12-C13-C35
23	J2	102	BCR	C7-C8-C9-C34
23	J2	102	BCR	C11-C12-C13-C35
23	J2	104	BCR	C36-C18-C19-C20
23	J2	104	BCR	C37-C22-C23-C24
23	K2	103	BCR	C11-C12-C13-C35
23	K2	103	BCR	C36-C18-C19-C20
23	K2	105	BCR	C7-C8-C9-C34
23	L2	207	BCR	C7-C8-C9-C34
23	M2	102	BCR	C7-C8-C9-C34
23	A	847	BCR	C11-C12-C13-C35
23	A	848	BCR	C11-C12-C13-C35
23	A	848	BCR	C36-C18-C19-C20
23	A	848	BCR	C37-C22-C23-C24
23	A	851	BCR	C7-C8-C9-C34
23	A	853	BCR	C11-C12-C13-C35
23	A	854	BCR	C7-C8-C9-C34
23	A	854	BCR	C37-C22-C23-C24
23	B	839	BCR	C7-C8-C9-C34
23	B	839	BCR	C11-C12-C13-C35
23	B	839	BCR	C37-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C34
23	B	842	BCR	C37-C22-C23-C24
23	B	843	BCR	C7-C8-C9-C34
23	B	843	BCR	C11-C12-C13-C35
23	B	844	BCR	C7-C8-C9-C34
23	B	844	BCR	C36-C18-C19-C20
23	B	848	BCR	C37-C22-C23-C24
23	F	304	BCR	C7-C8-C9-C34
23	F	304	BCR	C36-C18-C19-C20
23	F	305	BCR	C7-C8-C9-C34
23	I	101	BCR	C11-C12-C13-C35
23	I	101	BCR	C36-C18-C19-C20
23	I	102	BCR	C7-C8-C9-C34
23	I	102	BCR	C11-C12-C13-C35
23	I	102	BCR	C36-C18-C19-C20
23	J	102	BCR	C7-C8-C9-C34
23	J	102	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	J	102	BCR	C36-C18-C19-C20
23	J	104	BCR	C36-C18-C19-C20
23	L	205	BCR	C11-C12-C13-C35
23	M	101	BCR	C36-C18-C19-C20
23	AA	848	BCR	C11-C12-C13-C35
23	AA	849	BCR	C11-C12-C13-C35
23	AA	849	BCR	C36-C18-C19-C20
23	AA	849	BCR	C37-C22-C23-C24
23	AA	850	BCR	C36-C18-C19-C20
23	AA	852	BCR	C7-C8-C9-C34
23	AA	852	BCR	C36-C18-C19-C20
23	AA	855	BCR	C7-C8-C9-C34
23	AA	855	BCR	C37-C22-C23-C24
23	BB	838	BCR	C7-C8-C9-C34
23	BB	838	BCR	C37-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C34
23	BB	842	BCR	C7-C8-C9-C34
23	BB	842	BCR	C11-C12-C13-C35
23	BB	843	BCR	C7-C8-C9-C34
23	BB	843	BCR	C11-C12-C13-C35
23	BB	847	BCR	C37-C22-C23-C24
23	FF	304	BCR	C36-C18-C19-C20
23	FF	306	BCR	C7-C8-C9-C34
23	II	101	BCR	C11-C12-C13-C35
23	II	101	BCR	C36-C18-C19-C20
23	II	102	BCR	C7-C8-C9-C34
23	II	102	BCR	C11-C12-C13-C35
23	II	104	BCR	C11-C12-C13-C35
23	JJ	102	BCR	C7-C8-C9-C34
23	JJ	102	BCR	C11-C12-C13-C35
23	JJ	104	BCR	C36-C18-C19-C20
23	JJ	104	BCR	C37-C22-C23-C24
23	KK	103	BCR	C7-C8-C9-C34
23	KK	103	BCR	C11-C12-C13-C35
23	MM	101	BCR	C7-C8-C9-C34
23	MM	101	BCR	C36-C18-C19-C20
26	B1	840	ECH	C11-C12-C13-C35
26	B2	841	ECH	C11-C12-C13-C35
23	A1	853	BCR	C7-C8-C9-C10
23	A1	853	BCR	C21-C22-C23-C24
23	B1	838	BCR	C21-C22-C23-C24
23	B1	841	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	F1	306	BCR	C17-C18-C19-C20
23	K1	106	BCR	C17-C18-C19-C20
23	L1	201	BCR	C7-C8-C9-C10
23	A2	853	BCR	C7-C8-C9-C10
23	A2	853	BCR	C21-C22-C23-C24
23	B2	839	BCR	C21-C22-C23-C24
23	F2	305	BCR	C21-C22-C23-C24
23	I2	102	BCR	C7-C8-C9-C10
23	M2	102	BCR	C21-C22-C23-C24
23	A	853	BCR	C7-C8-C9-C10
23	A	853	BCR	C21-C22-C23-C24
23	B	839	BCR	C21-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C10
23	B	848	BCR	C17-C18-C19-C20
23	B	848	BCR	C21-C22-C23-C24
23	I	102	BCR	C7-C8-C9-C10
23	AA	854	BCR	C7-C8-C9-C10
23	AA	855	BCR	C17-C18-C19-C20
23	BB	838	BCR	C21-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C10
23	BB	847	BCR	C17-C18-C19-C20
23	BB	847	BCR	C21-C22-C23-C24
23	II	102	BCR	C7-C8-C9-C10
23	JJ	104	BCR	C21-C22-C23-C24
19	AA	829	CLA	C2A-CAA-CBA-CGA
19	K	102	CLA	O1D-CGD-O2D-CED
19	A1	804	CLA	O1A-CGA-O2A-C1
19	B1	821	CLA	O1A-CGA-O2A-C1
19	A2	805	CLA	O1A-CGA-O2A-C1
19	B2	821	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	O1A-CGA-O2A-C1
19	AA	810	CLA	O1A-CGA-O2A-C1
19	BB	815	CLA	C3-C5-C6-C7
19	A	821	CLA	C8-C10-C11-C12
25	I1	102	LMG	C11-C10-O7-C8
28	B	856	DGD	C2B-C1B-O2G-C2G
28	BB	854	DGD	C2B-C1B-O2G-C2G
28	B	856	DGD	O6E-C5E-C6E-O5E
19	A1	831	CLA	CBA-CGA-O2A-C1
19	B1	803	CLA	CBA-CGA-O2A-C1
19	A2	827	CLA	CBA-CGA-O2A-C1
19	BB	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	846	LHG	C24-C23-O8-C6
25	B	851	LMG	C29-C28-O8-C9
19	A1	801	CLA	C8-C10-C11-C12
19	LL	203	CLA	C2C-C3C-CAC-CBC
19	A1	807	CLA	C2-C1-O2A-CGA
19	A1	826	CLA	C2-C1-O2A-CGA
19	B1	807	CLA	C2-C1-O2A-CGA
19	A2	827	CLA	C2-C1-O2A-CGA
19	B2	807	CLA	C2-C1-O2A-CGA
19	A	808	CLA	C2-C1-O2A-CGA
19	A1	828	CLA	O1D-CGD-O2D-CED
19	A2	826	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	O1D-CGD-O2D-CED
19	A	844	CLA	O1D-CGD-O2D-CED
19	J	101	CLA	O1D-CGD-O2D-CED
19	AA	836	CLA	O1D-CGD-O2D-CED
19	JJ	101	CLA	O1D-CGD-O2D-CED
19	A1	813	CLA	CBD-CGD-O2D-CED
23	AA	855	BCR	C14-C15-C16-C17
19	B	837	CLA	C2C-C3C-CAC-CBC
19	B1	807	CLA	C15-C16-C17-C18
19	A2	821	CLA	C8-C10-C11-C12
19	A2	829	CLA	C10-C11-C12-C13
19	B2	807	CLA	C15-C16-C17-C18
19	A	808	CLA	C10-C11-C12-C13
19	B	815	CLA	C10-C11-C12-C13
19	AA	808	CLA	C10-C11-C12-C13
19	BB	803	CLA	C8-C10-C11-C12
24	BB	848	AJP	O31-C26-O25-C23
19	A1	819	CLA	O1D-CGD-O2D-CED
19	A2	814	CLA	O1D-CGD-O2D-CED
19	B	815	CLA	O1D-CGD-O2D-CED
22	A1	846	LHG	O10-C23-O8-C6
19	AA	821	CLA	C8-C10-C11-C12
19	B1	835	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	C11-C10-C8-C7
21	A1	843	PQN	C16-C17-C18-C20
21	A2	843	PQN	C16-C17-C18-C20
19	A1	826	CLA	CBA-CGA-O2A-C1
19	B1	811	CLA	CBA-CGA-O2A-C1
19	A	836	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	X1	103	LHG	C24-C23-O8-C6
19	B1	821	CLA	C4-C3-C5-C6
19	B1	801	CLA	C5-C6-C7-C8
19	B	822	CLA	C13-C15-C16-C17
19	KK	102	CLA	O1D-CGD-O2D-CED
23	F1	306	BCR	C9-C10-C11-C12
23	F1	306	BCR	C19-C20-C21-C22
23	J1	102	BCR	C9-C10-C11-C12
23	K1	106	BCR	C13-C14-C15-C16
23	J2	102	BCR	C9-C10-C11-C12
23	K2	105	BCR	C13-C14-C15-C16
23	A	853	BCR	C19-C20-C21-C22
23	F	305	BCR	C9-C10-C11-C12
23	AA	854	BCR	C19-C20-C21-C22
23	FF	306	BCR	C9-C10-C11-C12
23	II	101	BCR	C9-C10-C11-C12
23	MM	101	BCR	C15-C16-C17-C18
26	B	841	ECH	C13-C14-C15-C16
24	AA	856	AJP	O25-C26-C27-O78
19	BB	815	CLA	O1D-CGD-O2D-CED
19	A1	834	CLA	C3-C5-C6-C7
19	A2	835	CLA	C3-C5-C6-C7
19	A1	803	CLA	C13-C15-C16-C17
19	B1	803	CLA	C13-C15-C16-C17
19	B2	801	CLA	C10-C11-C12-C13
19	B2	803	CLA	C8-C10-C11-C12
21	B1	837	PQN	C25-C26-C27-C28
22	X1	102	LHG	C7-C8-C9-C10
22	A2	846	LHG	C7-C8-C9-C10
22	X	102	LHG	C7-C8-C9-C10
19	A2	836	CLA	O1A-CGA-O2A-C1
19	B2	811	CLA	O1A-CGA-O2A-C1
19	AA	805	CLA	O1A-CGA-O2A-C1
19	BB	803	CLA	O1A-CGA-O2A-C1
19	LL	201	CLA	O1A-CGA-O2A-C1
22	X2	103	LHG	O10-C23-O8-C6
22	BB	851	LHG	O10-C23-O8-C6
19	B2	819	CLA	CBD-CGD-O2D-CED
19	A	837	CLA	CBD-CGD-O2D-CED
19	B1	836	CLA	O1D-CGD-O2D-CED
19	A2	829	CLA	O1D-CGD-O2D-CED
19	B2	832	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	813	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	A1	807	CLA	C10-C11-C12-C13
19	A1	835	CLA	C5-C6-C7-C8
19	B1	806	CLA	C8-C10-C11-C12
19	B1	822	CLA	C13-C15-C16-C17
19	B1	826	CLA	C10-C11-C12-C13
19	B1	832	CLA	C15-C16-C17-C18
19	A2	801	CLA	C10-C11-C12-C13
19	A2	807	CLA	C5-C6-C7-C8
19	B2	806	CLA	C8-C10-C11-C12
19	B2	823	CLA	C13-C15-C16-C17
19	B2	825	CLA	C10-C11-C12-C13
19	B	803	CLA	C8-C10-C11-C12
19	B	806	CLA	C8-C10-C11-C12
19	AA	804	CLA	C10-C11-C12-C13
19	AA	807	CLA	C5-C6-C7-C8
19	BB	815	CLA	C10-C11-C12-C13
19	BB	822	CLA	C13-C15-C16-C17
21	B2	838	PQN	C25-C26-C27-C28
21	A	843	PQN	C23-C25-C26-C27
24	L2	203	AJP	O31-C30-C32-O33
19	A1	811	CLA	C2A-CAA-CBA-CGA
19	A1	829	CLA	C2A-CAA-CBA-CGA
19	B1	835	CLA	C2A-CAA-CBA-CGA
19	B1	836	CLA	C2A-CAA-CBA-CGA
19	A2	830	CLA	C2A-CAA-CBA-CGA
19	A2	852	CLA	C2A-CAA-CBA-CGA
19	B2	822	CLA	C2A-CAA-CBA-CGA
19	B2	836	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
19	B	822	CLA	C2A-CAA-CBA-CGA
19	AA	830	CLA	C2A-CAA-CBA-CGA
19	BB	835	CLA	C2A-CAA-CBA-CGA
19	BB	836	CLA	C2A-CAA-CBA-CGA
19	FF	301	CLA	C2A-CAA-CBA-CGA
20	A1	802	CL0	C2A-CAA-CBA-CGA
19	B2	829	CLA	O1D-CGD-O2D-CED
23	A1	847	BCR	C10-C11-C12-C13
23	A1	849	BCR	C18-C19-C20-C21
23	B1	842	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	K1	104	BCR	C18-C19-C20-C21
23	A2	847	BCR	C10-C11-C12-C13
23	A2	847	BCR	C18-C19-C20-C21
23	A	847	BCR	C10-C11-C12-C13
23	A	850	BCR	C10-C11-C12-C13
23	L	205	BCR	C10-C11-C12-C13
23	BB	842	BCR	C10-C11-C12-C13
23	II	104	BCR	C10-C11-C12-C13
23	KK	103	BCR	C10-C11-C12-C13
23	LL	204	BCR	C10-C11-C12-C13
19	A1	842	CLA	C13-C15-C16-C17
19	B1	801	CLA	C10-C11-C12-C13
19	B1	823	CLA	C8-C10-C11-C12
19	B1	825	CLA	C10-C11-C12-C13
19	A2	840	CLA	C5-C6-C7-C8
19	B2	801	CLA	C5-C6-C7-C8
19	A	801	CLA	C10-C11-C12-C13
19	A	829	CLA	C10-C11-C12-C13
19	AA	819	CLA	C8-C10-C11-C12
19	BB	803	CLA	C13-C15-C16-C17
28	BB	854	DGD	O6E-C5E-C6E-O5E
22	X2	102	LHG	C7-C8-C9-C10
22	XX	102	LHG	C7-C8-C9-C10
25	I1	102	LMG	C10-C11-C12-C13
25	B	851	LMG	C28-C29-C30-C31
19	AA	841	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	O1A-CGA-O2A-C1
19	L	202	CLA	O1A-CGA-O2A-C1
19	AA	827	CLA	O1A-CGA-O2A-C1
19	B2	808	CLA	CBD-CGD-O2D-CED
23	J1	104	BCR	C6-C7-C8-C9
23	M1	101	BCR	C22-C23-C24-C25
23	F2	305	BCR	C6-C7-C8-C9
23	M2	102	BCR	C22-C23-C24-C25
19	A1	801	CLA	C10-C11-C12-C13
19	A1	803	CLA	C10-C11-C12-C13
19	A1	806	CLA	C5-C6-C7-C8
19	B1	803	CLA	C8-C10-C11-C12
19	L1	207	CLA	C13-C15-C16-C17
19	A2	801	CLA	C8-C10-C11-C12
19	A2	804	CLA	C10-C11-C12-C13
19	A2	808	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B2	803	CLA	C13-C15-C16-C17
19	B2	822	CLA	C13-C15-C16-C17
19	B2	833	CLA	C15-C16-C17-C18
19	A	801	CLA	C8-C10-C11-C12
19	A	804	CLA	C8-C10-C11-C12
19	A	804	CLA	C10-C11-C12-C13
19	A	807	CLA	C5-C6-C7-C8
19	B	814	CLA	C5-C6-C7-C8
19	B	826	CLA	C10-C11-C12-C13
19	B	829	CLA	C13-C15-C16-C17
19	B	860	CLA	C13-C15-C16-C17
19	AA	801	CLA	C8-C10-C11-C12
19	AA	801	CLA	C10-C11-C12-C13
19	AA	804	CLA	C8-C10-C11-C12
19	AA	804	CLA	C13-C15-C16-C17
19	AA	829	CLA	C10-C11-C12-C13
19	AA	853	CLA	C13-C15-C16-C17
19	BB	801	CLA	C5-C6-C7-C8
19	BB	806	CLA	C8-C10-C11-C12
19	BB	832	CLA	C15-C16-C17-C18
20	AA	803	CL0	C13-C15-C16-C17
19	BB	821	CLA	CBA-CGA-O2A-C1
19	B1	813	CLA	CBD-CGD-O2D-CED
19	B1	823	CLA	CBD-CGD-O2D-CED
19	B	813	CLA	CBD-CGD-O2D-CED
19	B	825	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	O1A-CGA-O2A-C1
22	A2	846	LHG	O10-C23-O8-C6
22	B2	848	LHG	O10-C23-O8-C6
22	B	853	LHG	O10-C23-O8-C6
19	A1	828	CLA	C10-C11-C12-C13
19	B2	834	CLA	C13-C15-C16-C17
19	B	801	CLA	C5-C6-C7-C8
19	B	836	CLA	C13-C15-C16-C17
19	AA	831	CLA	C5-C6-C7-C8
20	A1	802	CL0	C13-C15-C16-C17
20	A	803	CL0	C8-C10-C11-C12
19	B	819	CLA	O1D-CGD-O2D-CED
19	B1	805	CLA	C3-C5-C6-C7
19	B	805	CLA	C3-C5-C6-C7
19	B2	831	CLA	O1D-CGD-O2D-CED
19	B2	837	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	AA	817	CLA	O1D-CGD-O2D-CED
19	BB	812	CLA	O1D-CGD-O2D-CED
19	A1	839	CLA	C5-C6-C7-C8
19	B2	826	CLA	C5-C6-C7-C8
19	A	804	CLA	C13-C15-C16-C17
19	B	825	CLA	C10-C11-C12-C13
19	B	833	CLA	C15-C16-C17-C18
21	B	838	PQN	C25-C26-C27-C28
19	BB	822	CLA	CBD-CGD-O2D-CED
19	B1	803	CLA	O1A-CGA-O2A-C1
19	BB	811	CLA	O1A-CGA-O2A-C1
22	A1	846	LHG	C7-C8-C9-C10
22	AA	847	LHG	C7-C8-C9-C10
19	A	817	CLA	O1D-CGD-O2D-CED
19	AA	813	CLA	O1D-CGD-O2D-CED
19	A1	840	CLA	O1A-CGA-O2A-C1
19	A2	841	CLA	O1A-CGA-O2A-C1
19	A1	852	CLA	C13-C15-C16-C17
19	B1	815	CLA	C10-C11-C12-C13
19	B1	826	CLA	C5-C6-C7-C8
19	B1	835	CLA	C8-C10-C11-C12
19	A2	807	CLA	C13-C15-C16-C17
19	A2	829	CLA	C5-C6-C7-C8
19	A	819	CLA	C8-C10-C11-C12
19	BB	825	CLA	C10-C11-C12-C13
19	FF	305	CLA	C13-C15-C16-C17
19	A1	827	CLA	CBA-CGA-O2A-C1
19	B1	816	CLA	CBA-CGA-O2A-C1
19	L1	205	CLA	CBA-CGA-O2A-C1
19	A2	832	CLA	CBA-CGA-O2A-C1
19	B2	808	CLA	CBA-CGA-O2A-C1
19	L2	204	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
22	AA	847	LHG	C24-C23-O8-C6
25	I2	105	LMG	C11-C10-O7-C8
19	B1	811	CLA	O1A-CGA-O2A-C1
19	A2	827	CLA	O1A-CGA-O2A-C1
22	X1	103	LHG	O10-C23-O8-C6
19	A	841	CLA	CBA-CGA-O2A-C1
19	B2	805	CLA	C3-C5-C6-C7
19	BB	805	CLA	C3-C5-C6-C7
23	A1	853	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	A2	853	BCR	C19-C20-C21-C22
23	F2	305	BCR	C9-C10-C11-C12
23	A	854	BCR	C13-C14-C15-C16
23	B	848	BCR	C15-C16-C17-C18
23	AA	855	BCR	C13-C14-C15-C16
23	BB	841	BCR	C13-C14-C15-C16
23	BB	847	BCR	C15-C16-C17-C18
26	B1	840	ECH	C15-C16-C17-C18
26	B2	841	ECH	C15-C16-C17-C18
26	B	841	ECH	C15-C16-C17-C18
19	A1	822	CLA	C8-C10-C11-C12
19	A2	804	CLA	C13-C15-C16-C17
19	A	808	CLA	C15-C16-C17-C18
19	A	823	CLA	C5-C6-C7-C8
19	AA	823	CLA	C5-C6-C7-C8
19	A1	826	CLA	O1A-CGA-O2A-C1
19	A1	831	CLA	O1A-CGA-O2A-C1
24	A	855	AJP	O25-C26-C27-O78
25	L1	210	LMG	O9-C10-O7-C8
25	I2	105	LMG	O9-C10-O7-C8
19	A2	812	CLA	C2A-CAA-CBA-CGA
19	B2	837	CLA	C2A-CAA-CBA-CGA
19	B	836	CLA	C2A-CAA-CBA-CGA
19	B	860	CLA	C2A-CAA-CBA-CGA
19	BB	822	CLA	C2A-CAA-CBA-CGA
19	B1	808	CLA	CBA-CGA-O2A-C1
19	A2	828	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	AA	832	CLA	CBA-CGA-O2A-C1
19	AA	836	CLA	CBA-CGA-O2A-C1
22	B1	847	LHG	C24-C23-O8-C6
19	A1	830	CLA	C5-C6-C7-C8
19	A1	831	CLA	C8-C10-C11-C12
19	B1	828	CLA	C13-C15-C16-C17
19	B1	832	CLA	C5-C6-C7-C8
19	A2	823	CLA	C5-C6-C7-C8
19	B2	814	CLA	C8-C10-C11-C12
19	B2	826	CLA	C10-C11-C12-C13
19	B2	833	CLA	C5-C6-C7-C8
19	A	823	CLA	C8-C10-C11-C12
19	A	831	CLA	C5-C6-C7-C8
19	A	852	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	C10-C11-C12-C13
19	B	834	CLA	C10-C11-C12-C13
19	B	836	CLA	C8-C10-C11-C12
19	AA	804	CLA	C5-C6-C7-C8
19	AA	807	CLA	C13-C15-C16-C17
19	AA	827	CLA	C5-C6-C7-C8
19	BB	814	CLA	C5-C6-C7-C8
19	BB	826	CLA	C10-C11-C12-C13
21	A1	843	PQN	C23-C25-C26-C27
21	B	838	PQN	C15-C16-C17-C18
19	B2	836	CLA	CBD-CGD-O2D-CED
19	F2	301	CLA	C3-C5-C6-C7
19	A1	812	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	O1D-CGD-O2D-CED
19	AA	838	CLA	O1D-CGD-O2D-CED
19	A1	806	CLA	C13-C15-C16-C17
19	A1	807	CLA	C15-C16-C17-C18
19	A1	818	CLA	C8-C10-C11-C12
19	B1	806	CLA	C15-C16-C17-C18
19	B1	810	CLA	C8-C10-C11-C12
19	B1	814	CLA	C5-C6-C7-C8
19	B1	814	CLA	C8-C10-C11-C12
19	A2	832	CLA	C8-C10-C11-C12
19	A2	852	CLA	C13-C15-C16-C17
19	B2	806	CLA	C15-C16-C17-C18
19	L2	204	CLA	C5-C6-C7-C8
19	A	804	CLA	C5-C6-C7-C8
19	A	807	CLA	C10-C11-C12-C13
19	B	823	CLA	C15-C16-C17-C18
19	B	833	CLA	C5-C6-C7-C8
19	AA	823	CLA	C8-C10-C11-C12
19	AA	843	CLA	C13-C15-C16-C17
19	BB	814	CLA	C8-C10-C11-C12
21	BB	837	PQN	C25-C26-C27-C28
19	A1	820	CLA	C8-C10-C11-C12
19	A1	820	CLA	C15-C16-C17-C18
19	B1	823	CLA	C13-C15-C16-C17
19	A2	808	CLA	C15-C16-C17-C18
19	A2	819	CLA	C8-C10-C11-C12
19	B2	810	CLA	C8-C10-C11-C12
19	B2	852	CLA	C13-C15-C16-C17
19	A	807	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	803	CLA	C13-C15-C16-C17
19	BB	801	CLA	C10-C11-C12-C13
19	BB	823	CLA	C15-C16-C17-C18
21	A2	843	PQN	C25-C26-C27-C28
19	B1	829	CLA	CBA-CGA-O2A-C1
19	A2	831	CLA	CBA-CGA-O2A-C1
19	B	859	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	O6-C5-C6-O5
19	B1	808	CLA	O1D-CGD-O2D-CED
19	AA	812	CLA	O1A-CGA-O2A-C1
19	A2	823	CLA	C8-C10-C11-C12
19	B2	834	CLA	C10-C11-C12-C13
19	L2	206	CLA	C13-C15-C16-C17
19	A	832	CLA	C8-C10-C11-C12
19	AA	808	CLA	C15-C16-C17-C18
19	AA	832	CLA	C8-C10-C11-C12
19	BB	832	CLA	C5-C6-C7-C8
21	A1	843	PQN	C25-C26-C27-C28
21	A2	843	PQN	C23-C25-C26-C27
19	B2	814	CLA	C3-C5-C6-C7
19	B	818	CLA	CBD-CGD-O2D-CED
22	A1	845	LHG	C8-C7-O7-C5
19	A2	813	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	O1A-CGA-O2A-C1
25	B	851	LMG	O9-C10-O7-C8
19	A1	803	CLA	C5-C6-C7-C8
19	B1	833	CLA	C10-C11-C12-C13
19	BB	833	CLA	C10-C11-C12-C13
21	A	843	PQN	C25-C26-C27-C28
22	X1	103	LHG	O2-C2-C3-O3
19	A2	820	CLA	O1D-CGD-O2D-CED
19	A1	830	CLA	CBA-CGA-O2A-C1
19	B2	815	CLA	CBA-CGA-O2A-C1
19	B2	830	CLA	CBA-CGA-O2A-C1
19	AA	828	CLA	CBA-CGA-O2A-C1
19	A1	804	CLA	C8-C10-C11-C12
19	B	823	CLA	C8-C10-C11-C12
19	BB	835	CLA	C13-C15-C16-C17
23	A1	847	BCR	C16-C17-C18-C36
23	A1	848	BCR	C11-C10-C9-C34
23	A1	848	BCR	C20-C21-C22-C37
23	A1	850	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	A1	851	BCR	C35-C13-C14-C15
23	A1	853	BCR	C35-C13-C14-C15
23	B1	839	BCR	C11-C10-C9-C34
23	B1	839	BCR	C16-C17-C18-C36
23	B1	841	BCR	C16-C17-C18-C36
23	B1	842	BCR	C11-C10-C9-C34
23	B1	843	BCR	C35-C13-C14-C15
23	F1	303	BCR	C20-C21-C22-C37
23	F1	304	BCR	C35-C13-C14-C15
23	F1	304	BCR	C16-C17-C18-C36
23	F1	306	BCR	C20-C21-C22-C37
23	I1	101	BCR	C35-C13-C14-C15
23	J1	102	BCR	C20-C21-C22-C37
23	J1	104	BCR	C20-C21-C22-C37
23	K1	104	BCR	C35-C13-C14-C15
23	K1	104	BCR	C16-C17-C18-C36
23	K1	106	BCR	C16-C17-C18-C36
23	L1	201	BCR	C35-C13-C14-C15
23	L1	208	BCR	C35-C13-C14-C15
23	L1	208	BCR	C20-C21-C22-C37
23	A2	847	BCR	C16-C17-C18-C36
23	A2	848	BCR	C11-C10-C9-C34
23	A2	848	BCR	C16-C17-C18-C36
23	A2	848	BCR	C20-C21-C22-C37
23	A2	849	BCR	C20-C21-C22-C37
23	A2	850	BCR	C20-C21-C22-C37
23	A2	853	BCR	C35-C13-C14-C15
23	B2	840	BCR	C11-C10-C9-C34
23	B2	843	BCR	C11-C10-C9-C34
23	B2	843	BCR	C16-C17-C18-C36
23	B2	844	BCR	C35-C13-C14-C15
23	F2	303	BCR	C20-C21-C22-C37
23	F2	304	BCR	C35-C13-C14-C15
23	F2	304	BCR	C16-C17-C18-C36
23	F2	305	BCR	C11-C10-C9-C34
23	I2	101	BCR	C35-C13-C14-C15
23	I2	102	BCR	C11-C10-C9-C34
23	I2	102	BCR	C35-C13-C14-C15
23	I2	103	BCR	C35-C13-C14-C15
23	I2	103	BCR	C20-C21-C22-C37
23	J2	102	BCR	C16-C17-C18-C36
23	J2	104	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	K2	103	BCR	C11-C10-C9-C34
23	K2	103	BCR	C16-C17-C18-C36
23	A	847	BCR	C35-C13-C14-C15
23	A	847	BCR	C16-C17-C18-C36
23	A	848	BCR	C35-C13-C14-C15
23	A	849	BCR	C16-C17-C18-C36
23	A	851	BCR	C11-C10-C9-C34
23	A	851	BCR	C35-C13-C14-C15
23	A	853	BCR	C35-C13-C14-C15
23	A	853	BCR	C20-C21-C22-C37
23	B	839	BCR	C11-C10-C9-C34
23	B	840	BCR	C11-C10-C9-C34
23	B	840	BCR	C35-C13-C14-C15
23	B	840	BCR	C16-C17-C18-C36
23	B	843	BCR	C16-C17-C18-C36
23	B	844	BCR	C35-C13-C14-C15
23	B	848	BCR	C35-C13-C14-C15
23	F	303	BCR	C35-C13-C14-C15
23	F	303	BCR	C20-C21-C22-C37
23	F	305	BCR	C20-C21-C22-C37
23	I	102	BCR	C35-C13-C14-C15
23	J	104	BCR	C20-C21-C22-C37
23	K	103	BCR	C35-C13-C14-C15
23	L	205	BCR	C16-C17-C18-C36
23	L	205	BCR	C20-C21-C22-C37
23	AA	848	BCR	C35-C13-C14-C15
23	AA	848	BCR	C16-C17-C18-C36
23	AA	849	BCR	C35-C13-C14-C15
23	AA	852	BCR	C11-C10-C9-C34
23	AA	852	BCR	C35-C13-C14-C15
23	AA	854	BCR	C35-C13-C14-C15
23	BB	839	BCR	C11-C10-C9-C34
23	BB	839	BCR	C35-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C36
23	BB	841	BCR	C20-C21-C22-C37
23	BB	847	BCR	C35-C13-C14-C15
23	BB	847	BCR	C16-C17-C18-C36
23	FF	303	BCR	C35-C13-C14-C15
23	FF	303	BCR	C20-C21-C22-C37
23	II	101	BCR	C20-C21-C22-C37
19	A1	814	CLA	C3-C5-C6-C7
19	A1	842	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B2	845	LMG	C4-C5-C6-O5
23	F1	304	BCR	C37-C22-C23-C24
23	J1	104	BCR	C37-C22-C23-C24
23	K1	104	BCR	C37-C22-C23-C24
23	B2	843	BCR	C11-C12-C13-C35
23	F2	304	BCR	C37-C22-C23-C24
23	F2	305	BCR	C36-C18-C19-C20
23	I2	102	BCR	C7-C8-C9-C34
23	A	847	BCR	C7-C8-C9-C34
23	A	848	BCR	C7-C8-C9-C34
23	A	851	BCR	C11-C12-C13-C35
23	A	853	BCR	C7-C8-C9-C34
23	A	853	BCR	C37-C22-C23-C24
23	B	848	BCR	C11-C12-C13-C35
23	F	304	BCR	C37-C22-C23-C24
23	J	104	BCR	C37-C22-C23-C24
23	K	103	BCR	C36-C18-C19-C20
23	AA	849	BCR	C7-C8-C9-C34
23	AA	854	BCR	C7-C8-C9-C34
23	AA	854	BCR	C37-C22-C23-C24
23	BB	847	BCR	C11-C12-C13-C35
23	FF	303	BCR	C11-C12-C13-C35
23	FF	304	BCR	C37-C22-C23-C24
23	II	102	BCR	C37-C22-C23-C24
23	KK	103	BCR	C36-C18-C19-C20
19	K1	105	CLA	C4C-C3C-CAC-CBC
23	L1	208	BCR	C21-C22-C23-C24
23	L1	209	BCR	C17-C18-C19-C20
23	A2	849	BCR	C11-C12-C13-C14
23	I2	102	BCR	C17-C18-C19-C20
23	I2	103	BCR	C21-C22-C23-C24
23	F	303	BCR	C21-C22-C23-C24
23	I	102	BCR	C17-C18-C19-C20
23	L	205	BCR	C21-C22-C23-C24
23	II	104	BCR	C21-C22-C23-C24
19	B1	816	CLA	O1A-CGA-O2A-C1
19	A2	828	CLA	O1A-CGA-O2A-C1
19	B2	808	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
22	A	846	LHG	O10-C23-O8-C6
19	F1	301	CLA	C2A-CAA-CBA-CGA
19	F2	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	B	814	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
19	B	858	CLA	C2A-CAA-CBA-CGA
19	F	301	CLA	C2A-CAA-CBA-CGA
19	AA	843	CLA	C2A-CAA-CBA-CGA
19	BB	814	CLA	C2A-CAA-CBA-CGA
19	BB	855	CLA	C2A-CAA-CBA-CGA
20	A	803	CL0	C2A-CAA-CBA-CGA
19	B2	815	CLA	C10-C11-C12-C13
20	A2	803	CL0	C15-C16-C17-C18
22	A1	845	LHG	C7-C8-C9-C10
22	A	846	LHG	C7-C8-C9-C10
19	A1	820	CLA	CBD-CGD-O2D-CED
19	B1	812	CLA	O1D-CGD-O2D-CED
19	B2	834	CLA	O1D-CGD-O2D-CED
23	I	101	BCR	C9-C10-C11-C12
19	A1	812	CLA	C16-C17-C18-C20
19	A1	822	CLA	C11-C12-C13-C15
19	A2	823	CLA	C11-C12-C13-C15
19	A	823	CLA	C11-C12-C13-C15
19	AA	813	CLA	C16-C17-C18-C20
19	AA	823	CLA	C11-C12-C13-C14
19	AA	823	CLA	C11-C12-C13-C15
19	BB	825	CLA	C16-C17-C18-C19
21	B2	838	PQN	C26-C27-C28-C30
21	BB	837	PQN	C26-C27-C28-C29
19	B2	820	CLA	O1D-CGD-O2D-CED
19	AA	808	CLA	O1D-CGD-O2D-CED
19	L1	205	CLA	O1A-CGA-O2A-C1
19	A2	832	CLA	O1A-CGA-O2A-C1
19	L2	204	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
19	BB	821	CLA	O1A-CGA-O2A-C1
19	F	301	CLA	C3-C5-C6-C7
19	A	829	CLA	C5-C6-C7-C8
23	A1	847	BCR	C11-C10-C9-C8
23	A1	849	BCR	C11-C10-C9-C8
23	A1	851	BCR	C12-C13-C14-C15
23	A1	853	BCR	C16-C17-C18-C19
23	B1	838	BCR	C16-C17-C18-C19
23	B1	838	BCR	C20-C21-C22-C23
23	B1	839	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	B1	843	BCR	C20-C21-C22-C23
23	F1	303	BCR	C16-C17-C18-C19
23	F1	304	BCR	C11-C10-C9-C8
23	F1	304	BCR	C16-C17-C18-C19
23	F1	306	BCR	C20-C21-C22-C23
23	I1	101	BCR	C16-C17-C18-C19
23	J1	102	BCR	C12-C13-C14-C15
23	J1	102	BCR	C20-C21-C22-C23
23	J1	104	BCR	C11-C10-C9-C8
23	J1	104	BCR	C12-C13-C14-C15
23	J1	104	BCR	C16-C17-C18-C19
23	K1	106	BCR	C12-C13-C14-C15
23	K1	106	BCR	C16-C17-C18-C19
23	K1	106	BCR	C20-C21-C22-C23
23	L1	208	BCR	C11-C10-C9-C8
23	L1	209	BCR	C20-C21-C22-C23
23	A2	847	BCR	C11-C10-C9-C8
23	A2	849	BCR	C11-C10-C9-C8
23	A2	851	BCR	C12-C13-C14-C15
23	A2	851	BCR	C20-C21-C22-C23
23	A2	853	BCR	C16-C17-C18-C19
23	B2	839	BCR	C20-C21-C22-C23
23	B2	840	BCR	C16-C17-C18-C19
23	B2	842	BCR	C11-C10-C9-C8
23	B2	842	BCR	C12-C13-C14-C15
23	F2	303	BCR	C12-C13-C14-C15
23	F2	303	BCR	C16-C17-C18-C19
23	F2	304	BCR	C16-C17-C18-C19
23	I2	101	BCR	C16-C17-C18-C19
23	I2	102	BCR	C20-C21-C22-C23
23	I2	103	BCR	C11-C10-C9-C8
23	J2	102	BCR	C12-C13-C14-C15
23	J2	104	BCR	C11-C10-C9-C8
23	K2	105	BCR	C12-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C19
23	L2	207	BCR	C16-C17-C18-C19
23	L2	207	BCR	C20-C21-C22-C23
23	A	847	BCR	C11-C10-C9-C8
23	A	849	BCR	C12-C13-C14-C15
23	A	849	BCR	C20-C21-C22-C23
23	A	853	BCR	C16-C17-C18-C19
23	A	854	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	B	839	BCR	C20-C21-C22-C23
23	B	842	BCR	C12-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C19
23	F	303	BCR	C16-C17-C18-C19
23	F	304	BCR	C12-C13-C14-C15
23	F	305	BCR	C11-C10-C9-C8
23	I	101	BCR	C11-C10-C9-C8
23	I	101	BCR	C12-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C19
23	I	101	BCR	C20-C21-C22-C23
23	J	104	BCR	C11-C10-C9-C8
23	J	104	BCR	C16-C17-C18-C19
23	K	103	BCR	C16-C17-C18-C19
23	L	205	BCR	C11-C10-C9-C8
23	L	206	BCR	C16-C17-C18-C19
23	L	206	BCR	C20-C21-C22-C23
23	AA	848	BCR	C11-C10-C9-C8
23	AA	850	BCR	C12-C13-C14-C15
23	AA	850	BCR	C20-C21-C22-C23
23	AA	854	BCR	C16-C17-C18-C19
23	AA	855	BCR	C12-C13-C14-C15
23	BB	838	BCR	C16-C17-C18-C19
23	BB	841	BCR	C16-C17-C18-C19
23	FF	303	BCR	C16-C17-C18-C19
23	II	101	BCR	C11-C10-C9-C8
23	II	101	BCR	C16-C17-C18-C19
23	II	101	BCR	C20-C21-C22-C23
23	II	104	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C12-C13-C14-C15
23	JJ	102	BCR	C20-C21-C22-C23
23	JJ	104	BCR	C11-C10-C9-C8
23	JJ	104	BCR	C16-C17-C18-C19
23	KK	103	BCR	C16-C17-C18-C19
23	LL	204	BCR	C16-C17-C18-C19
23	LL	204	BCR	C20-C21-C22-C23
25	B2	847	LMG	O9-C10-O7-C8
19	BB	819	CLA	O1D-CGD-O2D-CED
24	B	850	AJP	C29-C30-C32-O33
19	B1	835	CLA	C13-C15-C16-C17
21	BB	837	PQN	C15-C16-C17-C18
19	B1	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	XX	101	CLA	O1D-CGD-O2D-CED
19	B2	803	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
19	BB	856	CLA	CBA-CGA-O2A-C1
19	L1	205	CLA	C5-C6-C7-C8
19	B	814	CLA	C8-C10-C11-C12
21	AA	844	PQN	C25-C26-C27-C28
19	A1	807	CLA	C3-C5-C6-C7
19	B2	852	CLA	C3-C5-C6-C7
19	BB	801	CLA	C3-C5-C6-C7
19	AA	853	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	C2-C1-O2A-CGA
19	B1	828	CLA	C2-C1-O2A-CGA
19	B2	829	CLA	C2-C1-O2A-CGA
19	A	827	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C2-C1-O2A-CGA
19	B	807	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
19	AA	827	CLA	C2-C1-O2A-CGA
19	BB	807	CLA	C2-C1-O2A-CGA
19	FF	305	CLA	C2-C1-O2A-CGA
20	A2	803	CL0	C2-C1-O2A-CGA
19	A2	813	CLA	C16-C17-C18-C20
19	A2	823	CLA	C11-C12-C13-C14
19	A	823	CLA	C11-C12-C13-C14
21	B2	838	PQN	C26-C27-C28-C29
21	B	838	PQN	C26-C27-C28-C29
19	A1	827	CLA	O1A-CGA-O2A-C1
19	B	859	CLA	O1A-CGA-O2A-C1
22	AA	847	LHG	O10-C23-O8-C6
19	A1	822	CLA	C5-C6-C7-C8
19	A	827	CLA	C15-C16-C17-C18
19	A	822	CLA	O1D-CGD-O2D-CED
22	AA	846	LHG	C27-C28-C29-C30
25	B1	844	LMG	C30-C31-C32-C33
19	AA	840	CLA	CBD-CGD-O2D-CED
23	B	844	BCR	C14-C15-C16-C17
23	F	305	BCR	C14-C15-C16-C17
23	BB	843	BCR	C14-C15-C16-C17
23	KK	103	BCR	C14-C15-C16-C17
22	X2	103	LHG	C14-C15-C16-C17
22	A	845	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	B1	844	LMG	C22-C23-C24-C25
19	B	860	CLA	O1D-CGD-O2D-CED
28	BB	854	DGD	C1B-C2B-C3B-C4B
19	BB	810	CLA	C10-C11-C12-C13
22	AA	846	LHG	C26-C27-C28-C29
19	AA	832	CLA	O1A-CGA-O2A-C1
19	B2	851	CLA	CBA-CGA-O2A-C1
24	BB	849	AJP	O31-C26-O25-C23
22	X1	103	LHG	C30-C31-C32-C33
22	A	845	LHG	C26-C27-C28-C29
25	M	102	LMG	C32-C33-C34-C35
22	A1	845	LHG	O9-C7-O7-C5
22	A1	846	LHG	O1-C1-C2-O2
22	A	846	LHG	O1-C1-C2-O2
22	AA	847	LHG	O1-C1-C2-O2
22	B	853	LHG	C30-C31-C32-C33
25	I2	105	LMG	C16-C17-C18-C19
19	A	832	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
19	BB	823	CLA	C8-C10-C11-C12
19	B2	830	CLA	C4C-C3C-CAC-CBC
19	A1	811	CLA	C4B-C3B-CAB-CBB
19	B1	802	CLA	C4B-C3B-CAB-CBB
19	B1	827	CLA	C4B-C3B-CAB-CBB
19	B1	831	CLA	C4B-C3B-CAB-CBB
19	A2	806	CLA	C4B-C3B-CAB-CBB
19	A2	811	CLA	C4B-C3B-CAB-CBB
19	A2	812	CLA	C4B-C3B-CAB-CBB
19	B2	814	CLA	C4B-C3B-CAB-CBB
19	B2	816	CLA	C4B-C3B-CAB-CBB
19	B2	827	CLA	C4B-C3B-CAB-CBB
19	A	812	CLA	C4B-C3B-CAB-CBB
19	A	823	CLA	C4B-C3B-CAB-CBB
19	B	802	CLA	C4B-C3B-CAB-CBB
19	B	808	CLA	C4B-C3B-CAB-CBB
19	B	816	CLA	C4B-C3B-CAB-CBB
19	L	203	CLA	C4B-C3B-CAB-CBB
19	AA	812	CLA	C4B-C3B-CAB-CBB
19	AA	823	CLA	C4B-C3B-CAB-CBB
19	BB	808	CLA	C4B-C3B-CAB-CBB
19	BB	816	CLA	C4B-C3B-CAB-CBB
19	BB	833	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	X	102	LHG	C23-C24-C25-C26
22	LL	205	LHG	C23-C24-C25-C26
28	B	856	DGD	C1B-C2B-C3B-C4B
22	BB	851	LHG	C30-C31-C32-C33
19	A1	822	CLA	C11-C12-C13-C14
19	A	804	CLA	C16-C17-C18-C19
19	A	813	CLA	C16-C17-C18-C20
21	B1	837	PQN	C26-C27-C28-C30
21	B	838	PQN	C26-C27-C28-C30
19	A1	814	CLA	O1D-CGD-O2D-CED
19	B1	830	CLA	O1D-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	BB	813	CLA	O1D-CGD-O2D-CED
19	A2	801	CLA	C2A-CAA-CBA-CGA
19	B2	814	CLA	C2A-CAA-CBA-CGA
19	AA	804	CLA	C2A-CAA-CBA-CGA
25	B	851	LMG	C19-C20-C21-C22
19	A2	831	CLA	C5-C6-C7-C8
19	B	810	CLA	C10-C11-C12-C13
22	AA	846	LHG	C8-C7-O7-C5
22	B	853	LHG	C11-C10-C9-C8
19	B1	805	CLA	C6-C7-C8-C10
19	A2	804	CLA	C12-C13-C15-C16
19	B2	805	CLA	C6-C7-C8-C10
19	B	805	CLA	C6-C7-C8-C10
19	BB	805	CLA	C6-C7-C8-C10
21	A	843	PQN	C16-C17-C18-C20
22	XX	102	LHG	C23-C24-C25-C26
19	B	808	CLA	CBA-CGA-O2A-C1
19	BB	829	CLA	CBA-CGA-O2A-C1
22	X2	103	LHG	C11-C10-C9-C8
22	BB	851	LHG	C14-C15-C16-C17
25	B2	845	LMG	C41-C42-C43-C44
19	B2	837	CLA	C3-C5-C6-C7
19	L	202	CLA	C3-C5-C6-C7
24	L1	203	AJP	O31-C26-O25-C23
19	A1	807	CLA	C3A-C2A-CAA-CBA
19	A1	810	CLA	C3A-C2A-CAA-CBA
19	A1	826	CLA	C3A-C2A-CAA-CBA
19	A1	838	CLA	C3A-C2A-CAA-CBA
19	B1	802	CLA	C3A-C2A-CAA-CBA
19	B1	820	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B1	850	CLA	C3A-C2A-CAA-CBA
19	A2	808	CLA	C3A-C2A-CAA-CBA
19	A2	826	CLA	C3A-C2A-CAA-CBA
19	A2	827	CLA	C3A-C2A-CAA-CBA
19	A2	839	CLA	C3A-C2A-CAA-CBA
19	B2	802	CLA	C3A-C2A-CAA-CBA
19	B2	820	CLA	C3A-C2A-CAA-CBA
19	B2	834	CLA	C3A-C2A-CAA-CBA
19	B2	851	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	A	827	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	A	839	CLA	C3A-C2A-CAA-CBA
19	A	852	CLA	C3A-C2A-CAA-CBA
19	B	802	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C3A-C2A-CAA-CBA
19	AA	808	CLA	C3A-C2A-CAA-CBA
19	AA	811	CLA	C3A-C2A-CAA-CBA
19	AA	827	CLA	C3A-C2A-CAA-CBA
19	AA	839	CLA	C3A-C2A-CAA-CBA
19	AA	853	CLA	C3A-C2A-CAA-CBA
19	BB	820	CLA	C3A-C2A-CAA-CBA
19	BB	824	CLA	C3A-C2A-CAA-CBA
19	BB	856	CLA	C3A-C2A-CAA-CBA
19	FF	301	CLA	C3A-C2A-CAA-CBA
20	A	803	CL0	C3A-C2A-CAA-CBA
22	A1	845	LHG	C27-C28-C29-C30
22	B	853	LHG	C14-C15-C16-C17
22	LL	205	LHG	C11-C12-C13-C14
25	B	851	LMG	C30-C31-C32-C33
19	A	812	CLA	CBA-CGA-O2A-C1
19	A1	828	CLA	C5-C6-C7-C8
19	B2	814	CLA	C5-C6-C7-C8
19	B	810	CLA	C8-C10-C11-C12
19	BB	806	CLA	C15-C16-C17-C18
19	BB	836	CLA	O1D-CGD-O2D-CED
22	L	207	LHG	C23-C24-C25-C26
23	A	853	BCR	C9-C10-C11-C12
23	B	842	BCR	C9-C10-C11-C12
23	AA	854	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	BB	841	BCR	C9-C10-C11-C12
23	KK	103	BCR	C9-C10-C11-C12
21	B1	837	PQN	C26-C27-C28-C29
21	BB	837	PQN	C26-C27-C28-C30
19	B1	808	CLA	O1A-CGA-O2A-C1
19	A2	831	CLA	O1A-CGA-O2A-C1
19	B2	851	CLA	O1A-CGA-O2A-C1
19	AA	828	CLA	O1A-CGA-O2A-C1
19	AA	836	CLA	O1A-CGA-O2A-C1
19	BB	856	CLA	O1A-CGA-O2A-C1
22	L	207	LHG	C11-C12-C13-C14
22	BB	851	LHG	C1-C2-C3-O3
19	A1	842	CLA	O1D-CGD-O2D-CED
19	B1	815	CLA	CBA-CGA-O2A-C1
19	B1	850	CLA	CBA-CGA-O2A-C1
19	B2	816	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	CBA-CGA-O2A-C1
19	AA	831	CLA	CBA-CGA-O2A-C1
19	BB	824	CLA	CBA-CGA-O2A-C1
28	BB	854	DGD	C1G-C2G-C3G-O3G
22	BB	851	LHG	C15-C16-C17-C18
25	B	845	LMG	C22-C23-C24-C25
19	AA	843	CLA	C3-C5-C6-C7
25	L1	210	LMG	C28-C29-C30-C31
22	X1	103	LHG	C14-C15-C16-C17
22	X2	103	LHG	C15-C16-C17-C18
25	B1	844	LMG	C18-C19-C20-C21
25	B2	845	LMG	C22-C23-C24-C25
25	B	845	LMG	C29-C30-C31-C32
25	B	851	LMG	C18-C19-C20-C21
25	M	102	LMG	C34-C35-C36-C37
19	A1	830	CLA	O1A-CGA-O2A-C1
19	B1	829	CLA	O1A-CGA-O2A-C1
19	B2	815	CLA	O1A-CGA-O2A-C1
19	B2	830	CLA	O1A-CGA-O2A-C1
19	B	824	CLA	O1A-CGA-O2A-C1
22	B1	847	LHG	O10-C23-O8-C6
22	B	853	LHG	C15-C16-C17-C18
19	A1	807	CLA	O1D-CGD-O2D-CED
19	B2	836	CLA	C13-C15-C16-C17
19	A	808	CLA	O1D-CGD-O2D-CED
19	A	852	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	BB	844	LMG	C22-C23-C24-C25
25	BB	844	LMG	C29-C30-C31-C32
19	B1	850	CLA	O1A-CGA-O2A-C1
19	B2	803	CLA	O1A-CGA-O2A-C1
19	A1	811	CLA	C2B-C3B-CAB-CBB
19	A1	817	CLA	C2B-C3B-CAB-CBB
19	A1	819	CLA	C2B-C3B-CAB-CBB
19	B1	814	CLA	C2B-C3B-CAB-CBB
19	B1	816	CLA	C2B-C3B-CAB-CBB
19	B1	831	CLA	C2B-C3B-CAB-CBB
19	B1	850	CLA	C2B-C3B-CAB-CBB
19	A2	806	CLA	C2B-C3B-CAB-CBB
19	A2	811	CLA	C2B-C3B-CAB-CBB
19	A2	812	CLA	C2B-C3B-CAB-CBB
19	A2	818	CLA	C2B-C3B-CAB-CBB
19	B2	814	CLA	C2B-C3B-CAB-CBB
19	B2	816	CLA	C2B-C3B-CAB-CBB
19	A	806	CLA	C2B-C3B-CAB-CBB
19	A	811	CLA	C2B-C3B-CAB-CBB
19	A	812	CLA	C2B-C3B-CAB-CBB
19	B	802	CLA	C2B-C3B-CAB-CBB
19	B	808	CLA	C2B-C3B-CAB-CBB
19	B	816	CLA	C2B-C3B-CAB-CBB
19	B	820	CLA	C2B-C3B-CAB-CBB
19	B	832	CLA	C2B-C3B-CAB-CBB
19	B	859	CLA	C2B-C3B-CAB-CBB
19	L	203	CLA	C2B-C3B-CAB-CBB
19	AA	812	CLA	C2B-C3B-CAB-CBB
19	AA	818	CLA	C2B-C3B-CAB-CBB
19	BB	808	CLA	C2B-C3B-CAB-CBB
19	BB	816	CLA	C2B-C3B-CAB-CBB
19	BB	820	CLA	C2B-C3B-CAB-CBB
19	BB	831	CLA	C2B-C3B-CAB-CBB
19	LL	202	CLA	C2B-C3B-CAB-CBB
23	A1	851	BCR	C23-C24-C25-C26
23	A1	851	BCR	C23-C24-C25-C30
23	J1	104	BCR	C23-C24-C25-C30
23	A2	851	BCR	C23-C24-C25-C26
23	A2	851	BCR	C23-C24-C25-C30
23	B2	842	BCR	C23-C24-C25-C26
23	B2	842	BCR	C23-C24-C25-C30
23	F2	303	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
23	F2	305	BCR	C23-C24-C25-C26
23	F2	305	BCR	C23-C24-C25-C30
23	J2	104	BCR	C23-C24-C25-C30
23	A	851	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C30
23	J	104	BCR	C23-C24-C25-C30
23	K	103	BCR	C23-C24-C25-C30
23	M	101	BCR	C23-C24-C25-C30
23	JJ	104	BCR	C23-C24-C25-C30
23	KK	103	BCR	C23-C24-C25-C30
26	BB	840	ECH	C1-C6-C7-C8
22	X1	103	LHG	C11-C10-C9-C8
25	L1	210	LMG	C19-C20-C21-C22
22	A	845	LHG	C8-C7-O7-C5
25	B2	847	LMG	C11-C10-O7-C8
19	AA	833	CLA	CBA-CGA-O2A-C1
19	FF	305	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	C15-C16-C17-C18
19	B1	836	CLA	C3-C5-C6-C7
19	A	805	CLA	C3-C5-C6-C7
19	AA	805	CLA	C3-C5-C6-C7
25	I1	102	LMG	C12-C13-C14-C15
19	A	826	CLA	O1D-CGD-O2D-CED
19	AA	815	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	C2A-CAA-CBA-CGA
19	A1	842	CLA	C2A-CAA-CBA-CGA
19	B1	814	CLA	C2A-CAA-CBA-CGA
19	A2	804	CLA	C2A-CAA-CBA-CGA
19	A2	824	CLA	C2A-CAA-CBA-CGA
19	B2	852	CLA	C2A-CAA-CBA-CGA
19	A	801	CLA	C2A-CAA-CBA-CGA
19	A	804	CLA	C2A-CAA-CBA-CGA
19	AA	801	CLA	C2A-CAA-CBA-CGA
19	AA	829	CLA	C5-C6-C7-C8
22	A2	845	LHG	C27-C28-C29-C30
22	X2	103	LHG	C30-C31-C32-C33
25	B2	845	LMG	C30-C31-C32-C33
19	BB	824	CLA	O1A-CGA-O2A-C1
22	BB	851	LHG	C17-C18-C19-C20
19	B1	849	CLA	C4-C3-C5-C6
19	A	827	CLA	C4-C3-C5-C6
19	A2	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	A1	847	BCR	C18-C19-C20-C21
23	B1	838	BCR	C18-C19-C20-C21
23	I1	101	BCR	C18-C19-C20-C21
23	L1	208	BCR	C10-C11-C12-C13
23	B2	839	BCR	C18-C19-C20-C21
23	I2	102	BCR	C18-C19-C20-C21
23	A	847	BCR	C18-C19-C20-C21
23	A	848	BCR	C10-C11-C12-C13
23	A	849	BCR	C10-C11-C12-C13
23	A	849	BCR	C18-C19-C20-C21
23	B	844	BCR	C18-C19-C20-C21
23	I	101	BCR	C18-C19-C20-C21
23	AA	848	BCR	C18-C19-C20-C21
23	AA	849	BCR	C10-C11-C12-C13
23	AA	850	BCR	C10-C11-C12-C13
23	AA	850	BCR	C18-C19-C20-C21
23	BB	841	BCR	C18-C19-C20-C21
23	II	101	BCR	C18-C19-C20-C21
19	B1	810	CLA	C10-C11-C12-C13
19	A2	831	CLA	C13-C15-C16-C17
19	A	852	CLA	C8-C10-C11-C12
19	BB	810	CLA	C8-C10-C11-C12
19	B1	821	CLA	C2-C3-C5-C6
19	AA	813	CLA	C16-C17-C18-C19
22	B1	847	LHG	C11-C12-C13-C14
25	L1	210	LMG	C15-C16-C17-C18
19	B1	829	CLA	C4C-C3C-CAC-CBC
19	AA	826	CLA	O1D-CGD-O2D-CED
19	B1	824	CLA	CBA-CGA-O2A-C1
19	B1	828	CLA	CBA-CGA-O2A-C1
19	B2	829	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	O1A-CGA-O2A-C1
19	A1	820	CLA	C14-C13-C15-C16
19	BB	833	CLA	C14-C13-C15-C16
20	A1	802	CL0	C6-C7-C8-C9
22	B	852	LHG	C11-C12-C13-C14
22	B	853	LHG	C17-C18-C19-C20
28	B	856	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	C5-C6-C7-C8
19	AA	830	CLA	C2C-C3C-CAC-CBC
22	L1	211	LHG	C9-C10-C11-C12
22	X1	103	LHG	C17-C18-C19-C20
22	A2	845	LHG	C13-C14-C15-C16
23	K2	105	BCR	C22-C23-C24-C25
23	L2	207	BCR	C6-C7-C8-C9
23	A	854	BCR	C22-C23-C24-C25
23	B	839	BCR	C6-C7-C8-C9
23	L	206	BCR	C6-C7-C8-C9
23	AA	855	BCR	C22-C23-C24-C25
23	JJ	104	BCR	C6-C7-C8-C9
23	K1	104	BCR	C14-C15-C16-C17
19	B2	849	CLA	C13-C15-C16-C17
19	A	805	CLA	C8-C10-C11-C12
25	II	105	LMG	C34-C35-C36-C37
22	BB	851	LHG	C11-C10-C9-C8
22	BB	850	LHG	C11-C12-C13-C14
25	L1	210	LMG	C30-C31-C32-C33
19	B	814	CLA	CBA-CGA-O2A-C1
19	AA	804	CLA	CBA-CGA-O2A-C1
22	AA	846	LHG	C24-C23-O8-C6
23	B1	841	BCR	C9-C10-C11-C12
23	B2	842	BCR	C19-C20-C21-C22
23	KK	103	BCR	C15-C16-C17-C18
20	A	803	CL0	CBD-CGD-O2D-CED
22	A1	846	LHG	C8-C7-O7-C5
22	A2	846	LHG	C8-C7-O7-C5
22	A	846	LHG	C8-C7-O7-C5
22	AA	847	LHG	C8-C7-O7-C5
25	L1	210	LMG	C11-C10-O7-C8
19	A1	803	CLA	C8-C10-C11-C12
19	BB	826	CLA	C5-C6-C7-C8
22	A1	846	LHG	O9-C7-O7-C5
22	AA	846	LHG	O9-C7-O7-C5
22	X1	103	LHG	C15-C16-C17-C18
25	B1	844	LMG	C29-C30-C31-C32
25	L1	210	LMG	C11-C12-C13-C14
25	B2	845	LMG	C18-C19-C20-C21
25	B2	845	LMG	C29-C30-C31-C32
19	A	830	CLA	C2C-C3C-CAC-CBC
19	B1	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B2	816	CLA	O1A-CGA-O2A-C1
19	BB	829	CLA	O1A-CGA-O2A-C1
19	B1	848	CLA	C13-C15-C16-C17
23	AA	852	BCR	C11-C12-C13-C35
26	B	841	ECH	C11-C12-C13-C35
19	A2	828	CLA	C3-C5-C6-C7
23	A1	849	BCR	C21-C22-C23-C24
23	F1	304	BCR	C17-C18-C19-C20
23	A2	848	BCR	C11-C12-C13-C14
23	I2	101	BCR	C17-C18-C19-C20
23	A	854	BCR	C21-C22-C23-C24
23	B	842	BCR	C17-C18-C19-C20
23	FF	304	BCR	C17-C18-C19-C20
23	II	101	BCR	C17-C18-C19-C20
19	L2	205	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
19	B1	822	CLA	C2A-CAA-CBA-CGA
19	B1	825	CLA	C16-C17-C18-C19
19	B	825	CLA	C16-C17-C18-C19
25	L1	210	LMG	C18-C19-C20-C21
19	L1	207	CLA	C4-C3-C5-C6
19	B2	814	CLA	C4-C3-C5-C6
19	B2	821	CLA	C4-C3-C5-C6
19	L2	206	CLA	C4-C3-C5-C6
19	B	810	CLA	C4-C3-C5-C6
19	AA	827	CLA	C4-C3-C5-C6
22	B2	848	LHG	C11-C10-C9-C8
22	AA	846	LHG	C13-C14-C15-C16
19	A2	852	CLA	C8-C10-C11-C12
19	B2	836	CLA	C8-C10-C11-C12
19	A2	830	CLA	C4C-C3C-CAC-CBC
19	A	833	CLA	O1A-CGA-O2A-C1
19	AA	831	CLA	O1A-CGA-O2A-C1
19	B2	829	CLA	C3-C5-C6-C7
19	A	815	CLA	C3-C5-C6-C7
19	B	860	CLA	C3-C5-C6-C7
19	B2	806	CLA	C5-C6-C7-C8
19	A	836	CLA	C13-C15-C16-C17
19	BB	835	CLA	C8-C10-C11-C12
19	BB	815	CLA	CBA-CGA-O2A-C1
22	X1	102	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	X2	102	LHG	C23-C24-C25-C26
25	B1	844	LMG	C4-C5-C6-O5
22	L2	208	LHG	C11-C10-C9-C8
22	A	845	LHG	O9-C7-O7-C5
22	A2	846	LHG	O6-C4-C5-O7
22	A	846	LHG	O6-C4-C5-O7
22	AA	847	LHG	O6-C4-C5-O7
22	BB	850	LHG	O6-C4-C5-O7
19	A1	809	CLA	C10-C11-C12-C13
19	B1	828	CLA	C5-C6-C7-C8
19	B2	829	CLA	C13-C15-C16-C17
19	A	827	CLA	C5-C6-C7-C8
19	B	829	CLA	C5-C6-C7-C8
19	A1	812	CLA	C16-C17-C18-C19
25	B	845	LMG	C41-C42-C43-C44
19	B1	824	CLA	O1A-CGA-O2A-C1
19	B2	823	CLA	O1D-CGD-O2D-CED
25	B2	847	LMG	O6-C5-C6-O5
19	B1	806	CLA	C5-C6-C7-C8
19	A2	821	CLA	C15-C16-C17-C18
19	B	823	CLA	C13-C15-C16-C17
19	BB	852	CLA	C13-C15-C16-C17
19	FF	305	CLA	C5-C6-C7-C8
21	B1	837	PQN	C15-C16-C17-C18
19	B1	828	CLA	C3-C5-C6-C7
19	LL	201	CLA	C3-C5-C6-C7
19	AA	824	CLA	CBD-CGD-O2D-CED
19	A1	813	CLA	O1D-CGD-O2D-CED
19	BB	823	CLA	O1D-CGD-O2D-CED
19	B2	824	CLA	CBA-CGA-O2A-C1
19	B2	829	CLA	C5-C6-C7-C8
19	BB	806	CLA	C5-C6-C7-C8
25	B1	852	LMG	O6-C5-C6-O5
19	BB	833	CLA	CBD-CGD-O2D-CED
25	BB	844	LMG	C41-C42-C43-C44
19	B2	806	CLA	C2-C1-O2A-CGA
19	BB	806	CLA	C2-C1-O2A-CGA
25	B2	854	LMG	O6-C5-C6-O5
19	B	823	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	C16-C17-C18-C19
19	A2	827	CLA	C15-C16-C17-C18
22	X2	103	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	A	845	LHG	C13-C14-C15-C16
25	B	845	LMG	C13-C14-C15-C16
22	B1	847	LHG	C11-C10-C9-C8
22	A	845	LHG	C12-C13-C14-C15
19	BB	810	CLA	C4-C3-C5-C6
19	AA	815	CLA	C3-C5-C6-C7
19	B1	849	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
19	BB	810	CLA	C2-C3-C5-C6
22	A1	845	LHG	C1-C2-C3-O3
25	B	845	LMG	C18-C19-C20-C21
28	BB	854	DGD	C2B-C3B-C4B-C5B
19	A1	803	CLA	C2A-CAA-CBA-CGA
19	A1	823	CLA	C2A-CAA-CBA-CGA
19	B1	849	CLA	C2A-CAA-CBA-CGA
19	K1	103	CLA	C2A-CAA-CBA-CGA
19	A2	808	CLA	C2A-CAA-CBA-CGA
19	B2	850	CLA	C2A-CAA-CBA-CGA
19	A	812	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2A-CAA-CBA-CGA
19	A1	832	CLA	CBD-CGD-O2D-CED
19	B2	813	CLA	CBD-CGD-O2D-CED
23	A1	847	BCR	C14-C15-C16-C17
19	BB	855	CLA	C15-C16-C17-C18
22	A2	845	LHG	C8-C7-O7-C5
22	BB	850	LHG	C8-C7-O7-C5
22	A2	846	LHG	O1-C1-C2-O2
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	803	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	AA	833	CLA	O1A-CGA-O2A-C1
19	FF	305	CLA	O1A-CGA-O2A-C1
19	A1	827	CLA	C3-C5-C6-C7
19	B2	822	CLA	C3-C5-C6-C7
25	I1	102	LMG	C11-C12-C13-C14
25	BB	844	LMG	C18-C19-C20-C21
19	A1	807	CLA	C1A-C2A-CAA-CBA
19	A1	809	CLA	C1A-C2A-CAA-CBA
19	A1	810	CLA	C1A-C2A-CAA-CBA
19	A1	817	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A1	819	CLA	C1A-C2A-CAA-CBA
19	A1	822	CLA	C1A-C2A-CAA-CBA
19	A1	826	CLA	C1A-C2A-CAA-CBA
19	A1	838	CLA	C1A-C2A-CAA-CBA
19	B1	804	CLA	C1A-C2A-CAA-CBA
19	B1	815	CLA	C1A-C2A-CAA-CBA
19	B1	820	CLA	C1A-C2A-CAA-CBA
19	B1	825	CLA	C1A-C2A-CAA-CBA
19	B1	827	CLA	C1A-C2A-CAA-CBA
19	B1	828	CLA	C1A-C2A-CAA-CBA
19	B1	834	CLA	C1A-C2A-CAA-CBA
19	B1	850	CLA	C1A-C2A-CAA-CBA
19	A2	808	CLA	C1A-C2A-CAA-CBA
19	A2	811	CLA	C1A-C2A-CAA-CBA
19	A2	818	CLA	C1A-C2A-CAA-CBA
19	A2	820	CLA	C1A-C2A-CAA-CBA
19	A2	823	CLA	C1A-C2A-CAA-CBA
19	A2	827	CLA	C1A-C2A-CAA-CBA
19	A2	839	CLA	C1A-C2A-CAA-CBA
19	B2	802	CLA	C1A-C2A-CAA-CBA
19	B2	804	CLA	C1A-C2A-CAA-CBA
19	B2	815	CLA	C1A-C2A-CAA-CBA
19	B2	820	CLA	C1A-C2A-CAA-CBA
19	B2	825	CLA	C1A-C2A-CAA-CBA
19	B2	827	CLA	C1A-C2A-CAA-CBA
19	B2	835	CLA	C1A-C2A-CAA-CBA
19	B2	851	CLA	C1A-C2A-CAA-CBA
19	K2	104	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C1A-C2A-CAA-CBA
19	A	827	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	A	839	CLA	C1A-C2A-CAA-CBA
19	A	852	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	820	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	859	CLA	C1A-C2A-CAA-CBA
19	AA	805	CLA	C1A-C2A-CAA-CBA
19	AA	811	CLA	C1A-C2A-CAA-CBA
19	AA	818	CLA	C1A-C2A-CAA-CBA
19	AA	820	CLA	C1A-C2A-CAA-CBA
19	AA	822	CLA	C1A-C2A-CAA-CBA
19	AA	825	CLA	C1A-C2A-CAA-CBA
19	AA	827	CLA	C1A-C2A-CAA-CBA
19	AA	839	CLA	C1A-C2A-CAA-CBA
19	BB	804	CLA	C1A-C2A-CAA-CBA
19	BB	808	CLA	C1A-C2A-CAA-CBA
19	BB	824	CLA	C1A-C2A-CAA-CBA
19	BB	825	CLA	C1A-C2A-CAA-CBA
19	BB	827	CLA	C1A-C2A-CAA-CBA
19	BB	856	CLA	C1A-C2A-CAA-CBA
19	FF	301	CLA	C1A-C2A-CAA-CBA
19	B1	850	CLA	C5-C6-C7-C8
19	B2	851	CLA	C5-C6-C7-C8
21	B2	838	PQN	C15-C16-C17-C18
19	B2	824	CLA	O1A-CGA-O2A-C1
19	B2	829	CLA	O1A-CGA-O2A-C1
19	L2	205	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	O1A-CGA-O2A-C1
22	A1	845	LHG	C12-C13-C14-C15
19	A2	804	CLA	C5-C6-C7-C8
22	L1	211	LHG	O6-C4-C5-C6
22	A	846	LHG	O6-C4-C5-C6
25	B2	845	LMG	O6-C5-C6-O5
22	A2	846	LHG	O9-C7-O7-C5
22	A	846	LHG	O9-C7-O7-C5
22	AA	847	LHG	O9-C7-O7-C5
19	B	829	CLA	C3-C5-C6-C7
19	FF	305	CLA	C3-C5-C6-C7
19	A1	803	CLA	C12-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C15
19	A1	822	CLA	C6-C7-C8-C10
19	A1	830	CLA	C6-C7-C8-C10
19	B1	801	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B1	806	CLA	C6-C7-C8-C10
19	B1	815	CLA	C11-C10-C8-C7
19	B1	815	CLA	C12-C13-C15-C16
19	B1	821	CLA	C6-C7-C8-C10
19	B1	832	CLA	C6-C7-C8-C10
19	L1	205	CLA	C6-C7-C8-C10
19	A2	804	CLA	C6-C7-C8-C10
19	A2	807	CLA	C11-C12-C13-C15
19	A2	807	CLA	C12-C13-C15-C16
19	A2	813	CLA	C11-C12-C13-C15
19	A2	823	CLA	C6-C7-C8-C10
19	A2	831	CLA	C6-C7-C8-C10
19	B2	806	CLA	C6-C7-C8-C10
19	B2	810	CLA	C6-C7-C8-C10
19	B2	821	CLA	C6-C7-C8-C10
19	B2	826	CLA	C6-C7-C8-C10
19	B2	833	CLA	C6-C7-C8-C10
19	B2	836	CLA	C6-C7-C8-C10
19	L2	204	CLA	C6-C7-C8-C10
19	A	807	CLA	C11-C12-C13-C15
19	A	807	CLA	C12-C13-C15-C16
19	A	813	CLA	C11-C12-C13-C15
19	A	821	CLA	C11-C12-C13-C15
19	A	823	CLA	C6-C7-C8-C10
19	A	831	CLA	C6-C7-C8-C10
19	A	835	CLA	C12-C13-C15-C16
19	B	806	CLA	C6-C7-C8-C10
19	B	815	CLA	C12-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C10
19	B	826	CLA	C6-C7-C8-C10
19	B	836	CLA	C6-C7-C8-C10
19	AA	804	CLA	C12-C13-C15-C16
19	AA	813	CLA	C11-C12-C13-C15
19	AA	821	CLA	C11-C12-C13-C15
19	AA	823	CLA	C6-C7-C8-C10
19	AA	831	CLA	C6-C7-C8-C10
19	BB	806	CLA	C6-C7-C8-C10
19	BB	821	CLA	C6-C7-C8-C10
19	BB	826	CLA	C6-C7-C8-C10
19	BB	832	CLA	C6-C7-C8-C10
19	BB	835	CLA	C6-C7-C8-C10
21	A	843	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
19	AA	820	CLA	C8-C10-C11-C12
19	B1	828	CLA	O1A-CGA-O2A-C1
22	A1	845	LHG	C13-C14-C15-C16
19	A1	813	CLA	C3A-C2A-CAA-CBA
19	B1	813	CLA	C3A-C2A-CAA-CBA
19	A2	814	CLA	C3A-C2A-CAA-CBA
19	B2	813	CLA	C3A-C2A-CAA-CBA
19	A	814	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	AA	814	CLA	C3A-C2A-CAA-CBA
19	BB	813	CLA	C3A-C2A-CAA-CBA
25	B	845	LMG	C33-C34-C35-C36
19	A	827	CLA	C10-C11-C12-C13
19	AA	805	CLA	C8-C10-C11-C12
19	BB	856	CLA	C5-C6-C7-C8
25	II	105	LMG	C28-C29-C30-C31
19	A1	826	CLA	C4-C3-C5-C6
19	A1	835	CLA	C4-C3-C5-C6
19	B1	814	CLA	C4-C3-C5-C6
19	B2	829	CLA	C4-C3-C5-C6
19	BB	808	CLA	C4-C3-C5-C6
19	A1	826	CLA	C2-C3-C5-C6
19	L1	207	CLA	C2-C3-C5-C6
19	A2	827	CLA	C2-C3-C5-C6
19	B2	829	CLA	C2-C3-C5-C6
19	L2	206	CLA	C2-C3-C5-C6
19	A	827	CLA	C2-C3-C5-C6
19	BB	808	CLA	C2-C3-C5-C6
19	FF	305	CLA	C2-C3-C5-C6
19	LL	203	CLA	C4C-C3C-CAC-CBC
19	B1	802	CLA	C15-C16-C17-C18
19	A2	801	CLA	C5-C6-C7-C8
19	B2	823	CLA	C8-C10-C11-C12
19	B	806	CLA	C5-C6-C7-C8
19	BB	823	CLA	C13-C15-C16-C17
25	II	105	LMG	C4-C5-C6-O5
22	X	102	LHG	C8-C7-O7-C5
25	B	851	LMG	C11-C10-O7-C8
19	A2	826	CLA	C2A-CAA-CBA-CGA
19	AA	812	CLA	C2A-CAA-CBA-CGA
19	A1	803	CLA	C14-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B1	801	CLA	C14-C13-C15-C16
19	B1	806	CLA	C6-C7-C8-C9
19	B1	810	CLA	C11-C10-C8-C9
19	B1	848	CLA	C11-C10-C8-C9
19	L1	205	CLA	C6-C7-C8-C9
19	A2	804	CLA	C14-C13-C15-C16
19	A2	821	CLA	C11-C12-C13-C14
19	A2	831	CLA	C6-C7-C8-C9
19	B2	810	CLA	C6-C7-C8-C9
19	B2	815	CLA	C11-C10-C8-C9
19	B2	849	CLA	C11-C10-C8-C9
19	L2	204	CLA	C6-C7-C8-C9
19	A	807	CLA	C14-C13-C15-C16
19	A	813	CLA	C11-C12-C13-C14
19	A	836	CLA	C14-C13-C15-C16
19	B	801	CLA	C14-C13-C15-C16
19	B	806	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	854	CLA	C11-C10-C8-C9
19	AA	813	CLA	C11-C12-C13-C14
19	AA	821	CLA	C11-C12-C13-C14
19	AA	831	CLA	C6-C7-C8-C9
19	AA	836	CLA	C14-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C14
19	BB	801	CLA	C14-C13-C15-C16
19	BB	806	CLA	C6-C7-C8-C9
19	BB	821	CLA	C6-C7-C8-C9
19	BB	832	CLA	C6-C7-C8-C9
21	A2	843	PQN	C16-C17-C18-C19
19	A	837	CLA	O1D-CGD-O2D-CED
22	LL	205	LHG	C24-C23-O8-C6
19	B	815	CLA	O1A-CGA-O2A-C1
19	A1	826	CLA	O1D-CGD-O2D-CED
25	BB	844	LMG	C30-C31-C32-C33
25	B1	852	LMG	C2-C1-O1-C7
19	A2	810	CLA	C10-C11-C12-C13
19	A	820	CLA	C8-C10-C11-C12
22	B	853	LHG	C23-C24-C25-C26
22	B1	847	LHG	C4-C5-C6-O8
22	L1	211	LHG	C4-C5-C6-O8
22	B2	848	LHG	C4-C5-C6-O8
22	L2	208	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	M	102	LMG	O1-C7-C8-C9
28	B	856	DGD	C1G-C2G-C3G-O3G
22	AA	846	LHG	C12-C13-C14-C15
19	B2	850	CLA	C15-C16-C17-C18
19	B	834	CLA	C13-C15-C16-C17
19	AA	810	CLA	C10-C11-C12-C13
19	AA	843	CLA	O1D-CGD-O2D-CED
19	A1	832	CLA	CBA-CGA-O2A-C1
19	A1	839	CLA	CBA-CGA-O2A-C1
19	A2	804	CLA	CBA-CGA-O2A-C1
19	AA	840	CLA	CBA-CGA-O2A-C1
19	AA	853	CLA	CBA-CGA-O2A-C1
19	BB	808	CLA	CBA-CGA-O2A-C1
22	L	207	LHG	C24-C23-O8-C6
24	L1	203	AJP	O31-C30-C32-O33
19	A2	807	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C20
19	AA	804	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	C41-C42-C43-C44
19	A	841	CLA	O1A-CGA-O2A-C1
20	A1	802	CL0	CHA-CBD-CGD-O2D
23	B1	841	BCR	C20-C21-C22-C37
23	F1	306	BCR	C11-C10-C9-C34
23	K2	103	BCR	C35-C13-C14-C15
23	L	205	BCR	C35-C13-C14-C15
23	AA	849	BCR	C20-C21-C22-C37
23	BB	838	BCR	C35-C13-C14-C15
23	II	104	BCR	C20-C21-C22-C37
19	B1	835	CLA	O1D-CGD-O2D-CED
19	BB	815	CLA	O1A-CGA-O2A-C1
22	AA	846	LHG	O10-C23-O8-C6
19	A2	827	CLA	C4-C3-C5-C6
19	FF	305	CLA	C4-C3-C5-C6
19	A1	835	CLA	C2-C3-C5-C6
19	B1	814	CLA	C2-C3-C5-C6
19	B1	828	CLA	C2-C3-C5-C6
19	B2	814	CLA	C2-C3-C5-C6
19	B	829	CLA	C2-C3-C5-C6
19	AA	827	CLA	C2-C3-C5-C6
19	B1	801	CLA	C13-C15-C16-C17
19	B1	849	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	L1	207	CLA	C10-C11-C12-C13
19	B	826	CLA	C15-C16-C17-C18
19	BB	826	CLA	C15-C16-C17-C18
23	I1	101	BCR	C37-C22-C23-C24
23	I2	101	BCR	C37-C22-C23-C24
26	B1	840	ECH	C37-C22-C23-C24
26	B2	841	ECH	C37-C22-C23-C24
26	B	841	ECH	C37-C22-C23-C24
26	BB	840	ECH	C37-C22-C23-C24
19	B2	825	CLA	C16-C17-C18-C19
22	A1	845	LHG	C26-C27-C28-C29
25	B	851	LMG	C37-C38-C39-C40
23	A1	848	BCR	C21-C22-C23-C24
23	A2	849	BCR	C17-C18-C19-C20
23	A2	850	BCR	C21-C22-C23-C24
23	F2	304	BCR	C17-C18-C19-C20
23	L2	207	BCR	C17-C18-C19-C20
23	AA	854	BCR	C17-C18-C19-C20
23	JJ	102	BCR	C17-C18-C19-C20
26	B1	840	ECH	C21-C22-C23-C24
26	B2	841	ECH	C17-C18-C19-C20
26	B2	841	ECH	C21-C22-C23-C24
26	B	841	ECH	C21-C22-C23-C24
26	BB	840	ECH	C21-C22-C23-C24
19	A1	830	CLA	C13-C15-C16-C17
19	AA	821	CLA	C15-C16-C17-C18
19	A2	802	CLA	C2A-CAA-CBA-CGA
19	A1	804	CLA	C3-C5-C6-C7
19	B1	823	CLA	C15-C16-C17-C18
19	B2	801	CLA	C13-C15-C16-C17
19	B2	819	CLA	O1D-CGD-O2D-CED
19	A1	803	CLA	CBA-CGA-O2A-C1
22	A	845	LHG	C24-C23-O8-C6
25	L1	210	LMG	C9-C8-O7-C10
25	B	851	LMG	C9-C8-O7-C10
28	B	856	DGD	C1G-C2G-O2G-C1B
28	BB	854	DGD	C1G-C2G-O2G-C1B
23	B	842	BCR	C18-C19-C20-C21
23	K	103	BCR	C18-C19-C20-C21
19	B1	803	CLA	C5-C6-C7-C8
19	B1	833	CLA	C13-C15-C16-C17
19	A2	807	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B2	803	CLA	C5-C6-C7-C8
19	B2	810	CLA	C10-C11-C12-C13
19	A	801	CLA	C5-C6-C7-C8
23	K2	105	BCR	C19-C20-C21-C22
23	B	844	BCR	C9-C10-C11-C12
23	J	102	BCR	C15-C16-C17-C18
23	K	103	BCR	C15-C16-C17-C18
23	L	205	BCR	C15-C16-C17-C18
26	B1	840	ECH	C13-C14-C15-C16
26	B2	841	ECH	C13-C14-C15-C16
19	B2	830	CLA	C2C-C3C-CAC-CBC
19	A2	813	CLA	C16-C17-C18-C19
19	B	808	CLA	CBD-CGD-O2D-CED
25	B2	845	LMG	C33-C34-C35-C36
23	A1	851	BCR	C20-C21-C22-C23
23	B1	841	BCR	C11-C10-C9-C8
23	B1	841	BCR	C12-C13-C14-C15
23	L1	209	BCR	C16-C17-C18-C19
23	B2	839	BCR	C16-C17-C18-C19
23	B2	842	BCR	C20-C21-C22-C23
23	M2	102	BCR	C16-C17-C18-C19
23	B	839	BCR	C16-C17-C18-C19
23	B	840	BCR	C16-C17-C18-C19
23	J	102	BCR	C11-C10-C9-C8
23	AA	849	BCR	C16-C17-C18-C19
23	FF	304	BCR	C12-C13-C14-C15
22	B2	848	LHG	C1-C2-C3-O3
22	A1	846	LHG	O6-C4-C5-O7
23	K1	104	BCR	C22-C23-C24-C25
19	A	810	CLA	C8-C10-C11-C12
19	A2	833	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
20	AA	803	CL0	C2C-C3C-CAC-CBC
19	B2	808	CLA	O1D-CGD-O2D-CED
19	B	836	CLA	O1D-CGD-O2D-CED
19	B	830	CLA	C4C-C3C-CAC-CBC
19	A1	807	CLA	C5-C6-C7-C8
19	B	829	CLA	C4-C3-C5-C6
19	BB	821	CLA	C4-C3-C5-C6
19	AA	841	CLA	O1A-CGA-O2A-C1
19	A2	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	C16-C17-C18-C19
19	A2	807	CLA	C16-C17-C18-C20
22	L2	208	LHG	C24-C25-C26-C27
25	B2	854	LMG	C14-C15-C16-C17
25	I2	105	LMG	O1-C7-C8-O7
25	B	845	LMG	C30-C31-C32-C33
19	B	804	CLA	CBA-CGA-O2A-C1
19	BB	804	CLA	CBA-CGA-O2A-C1
19	K	102	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	C3-C5-C6-C7
19	A	830	CLA	C3-C5-C6-C7
25	B1	852	LMG	C14-C15-C16-C17
19	AA	810	CLA	C8-C10-C11-C12
25	L1	210	LMG	C37-C38-C39-C40
19	BB	822	CLA	O1D-CGD-O2D-CED
19	A1	805	CLA	CBA-CGA-O2A-C1
19	A1	815	CLA	CBA-CGA-O2A-C1
19	B2	804	CLA	CBA-CGA-O2A-C1
25	M	102	LMG	C15-C16-C17-C18
19	A1	852	CLA	C8-C10-C11-C12
19	B	803	CLA	C5-C6-C7-C8
19	AA	830	CLA	C5-C6-C7-C8
19	BB	802	CLA	C15-C16-C17-C18
23	A2	848	BCR	C14-C15-C16-C17
23	F2	303	BCR	C14-C15-C16-C17
23	L	205	BCR	C14-C15-C16-C17
23	FF	306	BCR	C14-C15-C16-C17
19	B1	813	CLA	O1D-CGD-O2D-CED
22	BB	850	LHG	C23-C24-C25-C26
25	II	105	LMG	C16-C17-C18-C19
19	L2	206	CLA	C10-C11-C12-C13
19	B	858	CLA	C15-C16-C17-C18
19	BB	803	CLA	C5-C6-C7-C8
19	BB	823	CLA	C10-C11-C12-C13
19	B	813	CLA	O1D-CGD-O2D-CED
19	AA	804	CLA	C16-C17-C18-C19
20	A	803	CL0	C16-C17-C18-C19
19	B1	828	CLA	C4-C3-C5-C6
19	A2	821	CLA	C4-C3-C5-C6
19	B2	850	CLA	C4-C3-C5-C6
19	AA	821	CLA	C4-C3-C5-C6
19	B1	804	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	BB	814	CLA	CBA-CGA-O2A-C1
19	BB	852	CLA	CBA-CGA-O2A-C1
19	B1	810	CLA	C5-C6-C7-C8
19	A	830	CLA	C5-C6-C7-C8
19	AA	827	CLA	C15-C16-C17-C18
19	AA	843	CLA	C15-C16-C17-C18
24	K	104	AJP	O31-C26-O25-C23
25	II	105	LMG	C35-C36-C37-C38
25	B2	845	LMG	C35-C36-C37-C38
22	B	853	LHG	O1-C1-C2-O2
19	A1	806	CLA	C14-C13-C15-C16
19	A1	812	CLA	C11-C12-C13-C14
19	A1	822	CLA	C6-C7-C8-C9
19	A1	830	CLA	C6-C7-C8-C9
19	B1	815	CLA	C11-C10-C8-C9
19	B1	821	CLA	C6-C7-C8-C9
19	B1	826	CLA	C6-C7-C8-C9
19	B1	832	CLA	C6-C7-C8-C9
19	A2	807	CLA	C11-C12-C13-C14
19	A2	807	CLA	C14-C13-C15-C16
19	A2	813	CLA	C11-C12-C13-C14
19	A2	823	CLA	C6-C7-C8-C9
19	A2	830	CLA	C11-C12-C13-C14
19	B2	801	CLA	C14-C13-C15-C16
19	B2	806	CLA	C6-C7-C8-C9
19	B2	821	CLA	C6-C7-C8-C9
19	B2	823	CLA	C11-C12-C13-C14
19	B2	826	CLA	C6-C7-C8-C9
19	B2	833	CLA	C6-C7-C8-C9
19	B2	836	CLA	C14-C13-C15-C16
19	A	804	CLA	C14-C13-C15-C16
19	A	821	CLA	C11-C12-C13-C14
19	A	823	CLA	C6-C7-C8-C9
19	A	835	CLA	C14-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C9
19	AA	804	CLA	C14-C13-C15-C16
19	AA	823	CLA	C6-C7-C8-C9
19	BB	803	CLA	C6-C7-C8-C9
19	BB	826	CLA	C6-C7-C8-C9
19	BB	852	CLA	C11-C10-C8-C9
20	A	803	CL0	C6-C7-C8-C9
21	A	843	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	X2	102	LHG	C25-C26-C27-C28
19	B1	823	CLA	O1D-CGD-O2D-CED
19	A	810	CLA	C10-C11-C12-C13
19	B	859	CLA	C5-C6-C7-C8
19	A1	817	CLA	C4B-C3B-CAB-CBB
19	A1	834	CLA	C4B-C3B-CAB-CBB
19	A2	818	CLA	C4B-C3B-CAB-CBB
19	A2	835	CLA	C4B-C3B-CAB-CBB
19	B2	832	CLA	C4B-C3B-CAB-CBB
19	B2	836	CLA	C4B-C3B-CAB-CBB
19	B2	851	CLA	C4B-C3B-CAB-CBB
19	A	809	CLA	C4B-C3B-CAB-CBB
19	B	827	CLA	C4B-C3B-CAB-CBB
19	B	834	CLA	C4B-C3B-CAB-CBB
19	AA	818	CLA	C4B-C3B-CAB-CBB
19	BB	827	CLA	C4B-C3B-CAB-CBB
19	A2	830	CLA	C5-C6-C7-C8
19	L	204	CLA	C8-C10-C11-C12
19	AA	831	CLA	C13-C15-C16-C17
19	BB	801	CLA	C15-C16-C17-C18
21	B1	837	PQN	C18-C20-C21-C22
20	A2	803	CL0	C2A-CAA-CBA-CGA
19	A1	820	CLA	O1D-CGD-O2D-CED
25	B2	854	LMG	C2-C1-O1-C7
19	A1	826	CLA	C15-C16-C17-C18
22	X1	102	LHG	C25-C26-C27-C28
25	M	102	LMG	C12-C13-C14-C15
25	M	102	LMG	C17-C18-C19-C20
19	AA	830	CLA	C3-C5-C6-C7
28	B	856	DGD	C4B-C5B-C6B-C7B
22	A1	846	LHG	O6-C4-C5-C6
22	A2	846	LHG	O6-C4-C5-C6
22	AA	847	LHG	O6-C4-C5-C6
22	A2	845	LHG	C12-C13-C14-C15
25	B2	845	LMG	C13-C14-C15-C16
19	A1	806	CLA	C12-C13-C15-C16
19	A1	807	CLA	C6-C7-C8-C10
19	A1	828	CLA	C11-C10-C8-C7
19	A1	829	CLA	C11-C10-C8-C7
19	A1	834	CLA	C12-C13-C15-C16
19	B1	803	CLA	C6-C7-C8-C10
19	B1	806	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B1	807	CLA	C6-C7-C8-C10
19	B1	810	CLA	C11-C10-C8-C7
19	B1	811	CLA	C11-C10-C8-C7
19	B1	826	CLA	C6-C7-C8-C10
19	B1	826	CLA	C12-C13-C15-C16
19	B1	835	CLA	C6-C7-C8-C10
19	B1	848	CLA	C11-C10-C8-C7
19	A2	821	CLA	C11-C12-C13-C15
19	A2	830	CLA	C11-C10-C8-C7
19	A2	835	CLA	C12-C13-C15-C16
19	B2	801	CLA	C12-C13-C15-C16
19	B2	806	CLA	C12-C13-C15-C16
19	B2	811	CLA	C11-C10-C8-C7
19	B2	815	CLA	C11-C10-C8-C7
19	B2	815	CLA	C12-C13-C15-C16
19	B2	823	CLA	C6-C7-C8-C10
19	B2	826	CLA	C12-C13-C15-C16
19	B2	836	CLA	C12-C13-C15-C16
19	B2	849	CLA	C11-C10-C8-C7
19	A	804	CLA	C12-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C10
19	A	830	CLA	C11-C10-C8-C7
19	B	801	CLA	C12-C13-C15-C16
19	B	803	CLA	C6-C7-C8-C10
19	B	823	CLA	C6-C7-C8-C10
19	B	833	CLA	C6-C7-C8-C10
19	B	854	CLA	C11-C10-C8-C7
19	AA	807	CLA	C11-C12-C13-C15
19	AA	829	CLA	C11-C10-C8-C7
19	AA	830	CLA	C11-C10-C8-C7
19	AA	835	CLA	C12-C13-C15-C16
19	AA	836	CLA	C12-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C15
19	BB	801	CLA	C12-C13-C15-C16
19	BB	803	CLA	C6-C7-C8-C10
19	BB	815	CLA	C12-C13-C15-C16
19	BB	823	CLA	C6-C7-C8-C10
19	BB	835	CLA	C12-C13-C15-C16
19	BB	852	CLA	C11-C10-C8-C7
20	A	803	CL0	C11-C10-C8-C7
20	A	803	CL0	C12-C13-C15-C16
20	AA	803	CL0	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	B2	838	PQN	C21-C22-C23-C25
21	B	838	PQN	C21-C22-C23-C25
19	A1	829	CLA	C5-C6-C7-C8
19	F1	301	CLA	C10-C11-C12-C13
19	B2	852	CLA	C15-C16-C17-C18
19	AA	853	CLA	O1A-CGA-O2A-C1
22	L2	208	LHG	C13-C14-C15-C16
25	L1	210	LMG	C21-C22-C23-C24
25	B2	845	LMG	C38-C39-C40-C41
19	A1	814	CLA	C3A-C2A-CAA-CBA
19	A1	827	CLA	C3A-C2A-CAA-CBA
19	B1	804	CLA	C3A-C2A-CAA-CBA
19	B1	821	CLA	C3A-C2A-CAA-CBA
19	A2	806	CLA	C3A-C2A-CAA-CBA
19	A2	815	CLA	C3A-C2A-CAA-CBA
19	A2	828	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C4-C3-C5-C6
19	A	824	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C4-C3-C5-C6
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	821	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	859	CLA	C3A-C2A-CAA-CBA
19	AA	815	CLA	C3A-C2A-CAA-CBA
19	AA	828	CLA	C3A-C2A-CAA-CBA
19	AA	828	CLA	C4-C3-C5-C6
19	BB	804	CLA	C3A-C2A-CAA-CBA
19	BB	821	CLA	C3A-C2A-CAA-CBA
19	LL	201	CLA	C3A-C2A-CAA-CBA
19	A1	801	CLA	C5-C6-C7-C8
19	BB	855	CLA	C2-C3-C5-C6
19	B2	836	CLA	O1D-CGD-O2D-CED
19	A1	832	CLA	O1A-CGA-O2A-C1
19	A1	839	CLA	O1A-CGA-O2A-C1
19	A2	804	CLA	O1A-CGA-O2A-C1
19	AA	840	CLA	O1A-CGA-O2A-C1
19	BB	808	CLA	O1A-CGA-O2A-C1
22	LL	205	LHG	O10-C23-O8-C6
19	A1	809	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B2	849	CLA	CBA-CGA-O2A-C1
19	AA	816	CLA	CBA-CGA-O2A-C1
19	A1	829	CLA	C2C-C3C-CAC-CBC
23	B1	843	BCR	C9-C10-C11-C12
23	K1	106	BCR	C19-C20-C21-C22
23	A	848	BCR	C9-C10-C11-C12
23	F	305	BCR	C19-C20-C21-C22
23	J	104	BCR	C9-C10-C11-C12
23	K	103	BCR	C19-C20-C21-C22
23	FF	306	BCR	C19-C20-C21-C22
23	JJ	104	BCR	C9-C10-C11-C12
23	KK	103	BCR	C19-C20-C21-C22
23	MM	101	BCR	C13-C14-C15-C16
26	B1	840	ECH	C9-C10-C11-C12
26	B2	841	ECH	C9-C10-C11-C12
19	A1	803	CLA	C3-C5-C6-C7
19	B1	814	CLA	C3-C5-C6-C7
19	B1	825	CLA	C3-C5-C6-C7
23	F1	303	BCR	C36-C18-C19-C20
23	L1	209	BCR	C7-C8-C9-C34
23	A	847	BCR	C36-C18-C19-C20
23	A	849	BCR	C36-C18-C19-C20
23	K	103	BCR	C7-C8-C9-C34
26	B2	841	ECH	C36-C18-C19-C20
22	L	207	LHG	O10-C23-O8-C6
19	B	818	CLA	O1D-CGD-O2D-CED
25	B1	844	LMG	C16-C17-C18-C19
19	AA	801	CLA	C5-C6-C7-C8
23	B2	842	BCR	C11-C12-C13-C14
23	A	853	BCR	C17-C18-C19-C20
22	B	853	LHG	C1-C2-C3-O3
19	L	202	CLA	C2A-CAA-CBA-CGA
19	A2	816	CLA	CBA-CGA-O2A-C1
22	X1	102	LHG	C4-C5-C6-O8
25	B1	846	LMG	O1-C7-C8-C9
25	I1	102	LMG	O1-C7-C8-C9
25	B2	847	LMG	O1-C7-C8-C9
28	BB	854	DGD	C4B-C5B-C6B-C7B
19	B	801	CLA	C16-C17-C18-C20
19	AA	804	CLA	C16-C17-C18-C20
19	B	805	CLA	C5-C6-C7-C8
19	B	811	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	BB	801	CLA	C8-C10-C11-C12
19	BB	805	CLA	C5-C6-C7-C8
19	B	825	CLA	O1D-CGD-O2D-CED
25	B	851	LMG	C11-C12-C13-C14
25	B	851	LMG	C21-C22-C23-C24
25	BB	844	LMG	C13-C14-C15-C16
19	A1	827	CLA	C4-C3-C5-C6
19	B2	808	CLA	C4-C3-C5-C6
19	BB	855	CLA	C4-C3-C5-C6
22	B	852	LHG	C23-C24-C25-C26
19	AA	821	CLA	C2-C3-C5-C6
19	AA	828	CLA	C2-C3-C5-C6
19	A	804	CLA	O1A-CGA-O2A-C1
19	A2	804	CLA	C3-C5-C6-C7
19	AA	828	CLA	C3-C5-C6-C7
19	BB	833	CLA	C13-C15-C16-C17
19	B2	825	CLA	C16-C17-C18-C20
20	A	803	CL0	C16-C17-C18-C20
19	A2	810	CLA	C8-C10-C11-C12
22	B	852	LHG	O6-C4-C5-O7
22	A	846	LHG	C14-C15-C16-C17
25	L1	210	LMG	C34-C35-C36-C37
25	B1	844	LMG	O6-C5-C6-O5
19	B2	832	CLA	C2B-C3B-CAB-CBB
19	B2	836	CLA	C2B-C3B-CAB-CBB
19	B2	851	CLA	C2B-C3B-CAB-CBB
23	A1	849	BCR	C23-C24-C25-C30
23	B1	843	BCR	C1-C6-C7-C8
23	I1	101	BCR	C1-C6-C7-C8
23	J1	102	BCR	C23-C24-C25-C30
23	K1	106	BCR	C23-C24-C25-C30
23	A2	849	BCR	C23-C24-C25-C30
23	B2	844	BCR	C1-C6-C7-C8
23	I2	101	BCR	C1-C6-C7-C8
23	J2	102	BCR	C23-C24-C25-C30
23	A	849	BCR	C23-C24-C25-C30
23	A	854	BCR	C23-C24-C25-C30
23	B	843	BCR	C23-C24-C25-C30
23	B	844	BCR	C1-C6-C7-C8
23	F	303	BCR	C23-C24-C25-C30
23	J	102	BCR	C23-C24-C25-C30
23	AA	850	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
23	AA	852	BCR	C23-C24-C25-C26
23	AA	855	BCR	C23-C24-C25-C30
23	BB	843	BCR	C1-C6-C7-C8
23	BB	847	BCR	C1-C6-C7-C8
23	FF	303	BCR	C23-C24-C25-C30
23	JJ	102	BCR	C23-C24-C25-C30
26	B1	840	ECH	C1-C6-C7-C8
26	B2	841	ECH	C1-C6-C7-C8
26	B	841	ECH	C1-C6-C7-C8
22	B	852	LHG	C8-C7-O7-C5
19	A	808	CLA	C5-C6-C7-C8
19	AA	832	CLA	C3-C5-C6-C7
22	A2	845	LHG	C29-C30-C31-C32
19	A1	803	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	O10-C23-O8-C6
25	BB	844	LMG	C16-C17-C18-C19
19	F2	301	CLA	C10-C11-C12-C13
19	AA	836	CLA	C13-C15-C16-C17
19	AA	840	CLA	O1D-CGD-O2D-CED
22	B	853	LHG	C34-C35-C36-C37
25	B1	844	LMG	C38-C39-C40-C41
25	BB	844	LMG	C38-C39-C40-C41
25	II	105	LMG	C11-C12-C13-C14
22	AA	847	LHG	C14-C15-C16-C17
19	A1	803	CLA	C16-C17-C18-C20
19	A1	852	CLA	C5-C6-C7-C8
19	B1	801	CLA	C15-C16-C17-C18
19	A	831	CLA	C13-C15-C16-C17
19	B	860	CLA	C15-C16-C17-C18
19	L	202	CLA	C5-C6-C7-C8
19	BB	815	CLA	C13-C15-C16-C17
25	I1	102	LMG	O1-C7-C8-O7
25	M	102	LMG	O1-C7-C8-O7
25	M	102	LMG	O7-C8-C9-O8
28	B	856	DGD	O2G-C2G-C3G-O3G
28	B	856	DGD	C4E-C5E-C6E-O5E
19	AA	830	CLA	C13-C15-C16-C17
19	A1	820	CLA	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	B	858	CLA	C4-C3-C5-C6
23	L2	207	BCR	C18-C19-C20-C21
23	KK	103	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	B1	805	CLA	C5-C6-C7-C8
19	B2	805	CLA	C5-C6-C7-C8
19	B2	850	CLA	C2-C3-C5-C6
19	A	821	CLA	C2-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	B	858	CLA	C2-C3-C5-C6
19	B1	825	CLA	C16-C17-C18-C20
28	B	856	DGD	C1A-C2A-C3A-C4A
19	AA	804	CLA	C3-C5-C6-C7
19	BB	836	CLA	C3-C5-C6-C7
19	B1	803	CLA	C6-C7-C8-C9
19	B1	806	CLA	C14-C13-C15-C16
19	A2	835	CLA	C14-C13-C15-C16
19	B2	803	CLA	C6-C7-C8-C9
19	B2	805	CLA	C11-C12-C13-C14
19	B2	806	CLA	C14-C13-C15-C16
19	B2	826	CLA	C14-C13-C15-C16
19	A	808	CLA	C6-C7-C8-C9
19	A	831	CLA	C6-C7-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	B	805	CLA	C11-C12-C13-C14
19	AA	807	CLA	C14-C13-C15-C16
19	AA	813	CLA	C6-C7-C8-C9
19	AA	835	CLA	C14-C13-C15-C16
19	BB	805	CLA	C11-C12-C13-C14
19	BB	835	CLA	C14-C13-C15-C16
20	A2	803	CL0	C11-C12-C13-C14
21	BB	837	PQN	C21-C22-C23-C24
19	L2	204	CLA	C10-C11-C12-C13
19	B1	820	CLA	C2C-C3C-CAC-CBC
23	L1	209	BCR	C6-C7-C8-C9
23	F	303	BCR	C6-C7-C8-C9
23	BB	838	BCR	C6-C7-C8-C9
23	BB	841	BCR	C22-C23-C24-C25
23	MM	101	BCR	C22-C23-C24-C25
19	B1	804	CLA	O1A-CGA-O2A-C1
19	B2	804	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
23	A1	848	BCR	C14-C15-C16-C17
23	A	847	BCR	C20-C21-C22-C23
23	A	849	BCR	C14-C15-C16-C17
23	B	848	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	AA	848	BCR	C20-C21-C22-C23
23	BB	847	BCR	C14-C15-C16-C17
22	BB	851	LHG	C34-C35-C36-C37
19	A	804	CLA	C16-C17-C18-C20
19	B	825	CLA	C16-C17-C18-C20
19	BB	825	CLA	C16-C17-C18-C20
25	M	102	LMG	C2-C1-O1-C7
25	B	845	LMG	C35-C36-C37-C38
25	B2	845	LMG	C16-C17-C18-C19
19	A2	825	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	O1A-CGA-O2A-C1
19	BB	804	CLA	O1A-CGA-O2A-C1
19	L1	205	CLA	C10-C11-C12-C13
23	I2	103	BCR	C15-C16-C17-C18
23	J2	102	BCR	C15-C16-C17-C18
23	K	103	BCR	C9-C10-C11-C12
23	BB	843	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C15-C16-C17-C18
26	B	841	ECH	C9-C10-C11-C12
19	A1	820	CLA	C2-C3-C5-C6
19	A2	836	CLA	C2-C3-C5-C6
19	B2	808	CLA	C2-C3-C5-C6
19	A	828	CLA	C2-C3-C5-C6
19	A2	804	CLA	C16-C17-C18-C20
19	B	801	CLA	C16-C17-C18-C19
19	B1	829	CLA	C2C-C3C-CAC-CBC
19	B	823	CLA	C10-C11-C12-C13
22	BB	850	LHG	O9-C7-O7-C5
25	B	845	LMG	C38-C39-C40-C41
23	A1	847	BCR	C35-C13-C14-C15
23	B1	838	BCR	C11-C10-C9-C34
23	B1	838	BCR	C35-C13-C14-C15
23	B1	842	BCR	C16-C17-C18-C36
23	K1	104	BCR	C11-C10-C9-C34
23	L1	201	BCR	C11-C10-C9-C34
23	A2	848	BCR	C35-C13-C14-C15
23	B2	843	BCR	C35-C13-C14-C15
23	A	848	BCR	C20-C21-C22-C37
23	B	840	BCR	C20-C21-C22-C37
23	B	842	BCR	C20-C21-C22-C37
23	B	848	BCR	C20-C21-C22-C37
23	F	304	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	BB	838	BCR	C11-C10-C9-C34
23	FF	306	BCR	C20-C21-C22-C37
23	II	101	BCR	C35-C13-C14-C15
23	II	104	BCR	C35-C13-C14-C15
23	JJ	104	BCR	C20-C21-C22-C37
19	B	837	CLA	C4C-C3C-CAC-CBC
19	A	835	CLA	CBA-CGA-O2A-C1
21	B2	838	PQN	C18-C20-C21-C22
19	AA	824	CLA	O1D-CGD-O2D-CED
19	F	301	CLA	C10-C11-C12-C13
23	L	206	BCR	C7-C8-C9-C34
23	L	206	BCR	C37-C22-C23-C24
26	B1	840	ECH	C36-C18-C19-C20
26	B	841	ECH	C36-C18-C19-C20
26	BB	840	ECH	C36-C18-C19-C20
19	A1	812	CLA	C11-C12-C13-C15
19	A1	835	CLA	C12-C13-C15-C16
19	A1	852	CLA	C11-C10-C8-C7
19	B1	823	CLA	C6-C7-C8-C10
19	A2	808	CLA	C6-C7-C8-C10
19	A2	813	CLA	C6-C7-C8-C10
19	B2	803	CLA	C6-C7-C8-C10
19	B2	807	CLA	C6-C7-C8-C10
19	L2	205	CLA	C6-C7-C8-C10
19	A	836	CLA	C12-C13-C15-C16
19	B	825	CLA	C12-C13-C15-C16
19	B	826	CLA	C12-C13-C15-C16
19	AA	801	CLA	C11-C10-C8-C7
19	AA	807	CLA	C12-C13-C15-C16
19	AA	808	CLA	C6-C7-C8-C10
19	BB	806	CLA	C12-C13-C15-C16
19	BB	810	CLA	C11-C10-C8-C7
19	BB	826	CLA	C12-C13-C15-C16
20	A2	803	CL0	C11-C12-C13-C15
21	BB	837	PQN	C21-C22-C23-C25
22	X1	103	LHG	C10-C11-C12-C13
25	B	851	LMG	C32-C33-C34-C35
25	B1	844	LMG	C13-C14-C15-C16
25	BB	844	LMG	C33-C34-C35-C36
19	BB	825	CLA	CBD-CGD-O2D-CED
19	A2	804	CLA	C8-C10-C11-C12
19	B	815	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	BB	811	CLA	C8-C10-C11-C12
23	A1	850	BCR	C21-C22-C23-C24
23	J1	102	BCR	C17-C18-C19-C20
23	J1	104	BCR	C11-C12-C13-C14
23	L1	201	BCR	C11-C12-C13-C14
23	L1	201	BCR	C21-C22-C23-C24
23	M1	101	BCR	C11-C12-C13-C14
23	A2	848	BCR	C21-C22-C23-C24
23	J2	102	BCR	C17-C18-C19-C20
23	M2	102	BCR	C11-C12-C13-C14
23	B	843	BCR	C17-C18-C19-C20
23	AA	851	BCR	C21-C22-C23-C24
23	AA	852	BCR	C7-C8-C9-C10
23	FF	303	BCR	C7-C8-C9-C10
26	B1	840	ECH	C17-C18-C19-C20
26	B	841	ECH	C17-C18-C19-C20
26	BB	840	ECH	C17-C18-C19-C20
19	B1	825	CLA	CBA-CGA-O2A-C1
19	A1	805	CLA	O1A-CGA-O2A-C1
19	A2	816	CLA	O1A-CGA-O2A-C1
19	A2	833	CLA	O1A-CGA-O2A-C1
19	BB	814	CLA	O1A-CGA-O2A-C1
25	I1	102	LMG	C8-C7-O1-C1
22	A	845	LHG	C7-C8-C9-C10
20	A	803	CL0	C5-C6-C7-C8
19	A1	825	CLA	C2A-CAA-CBA-CGA
19	A	826	CLA	C2A-CAA-CBA-CGA
19	AA	808	CLA	C2A-CAA-CBA-CGA
19	AA	843	CLA	C16-C17-C18-C19
19	BB	801	CLA	C16-C17-C18-C20
22	A2	845	LHG	O9-C7-O7-C5
22	X	102	LHG	O9-C7-O7-C5
22	B1	847	LHG	C12-C13-C14-C15
19	B1	808	CLA	C4-C3-C5-C6
19	B1	848	CLA	C4-C3-C5-C6
19	L1	205	CLA	C4-C3-C5-C6
19	B2	849	CLA	O1A-CGA-O2A-C1
19	A1	827	CLA	C2-C3-C5-C6
19	A2	852	CLA	C5-C6-C7-C8
25	B1	844	LMG	C35-C36-C37-C38
19	A2	830	CLA	C3-C5-C6-C7
25	B	851	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	II	105	LMG	C30-C31-C32-C33
22	L	207	LHG	C6-C5-O7-C7
22	LL	205	LHG	C6-C5-O7-C7
19	A1	815	CLA	O1A-CGA-O2A-C1
19	AA	816	CLA	O1A-CGA-O2A-C1
23	A2	853	BCR	C9-C10-C11-C12
19	BB	826	CLA	CBD-CGD-O2D-CED
19	BB	852	CLA	O1A-CGA-O2A-C1
19	A1	829	CLA	C3-C5-C6-C7
23	B1	839	BCR	C20-C21-C22-C23
23	I1	101	BCR	C20-C21-C22-C23
23	L1	208	BCR	C16-C17-C18-C19
23	M1	101	BCR	C16-C17-C18-C19
23	F2	303	BCR	C20-C21-C22-C23
23	I2	101	BCR	C20-C21-C22-C23
23	I2	103	BCR	C16-C17-C18-C19
23	A	848	BCR	C16-C17-C18-C19
23	BB	839	BCR	C12-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C19
23	BB	841	BCR	C12-C13-C14-C15
22	L1	211	LHG	O6-C4-C5-O7
22	X2	102	LHG	C4-C5-C6-O8
22	X	102	LHG	C4-C5-C6-O8
22	XX	102	LHG	C4-C5-C6-O8
25	B2	845	LMG	O1-C7-C8-C9
25	B	845	LMG	O1-C7-C8-C9
25	II	105	LMG	O1-C7-C8-C9
19	L1	206	CLA	C8-C10-C11-C12
19	B2	834	CLA	C15-C16-C17-C18
19	A	808	CLA	C3-C5-C6-C7
19	B1	825	CLA	O1A-CGA-O2A-C1
19	BB	810	CLA	C5-C6-C7-C8
19	A2	828	CLA	C4-C3-C5-C6
19	A2	836	CLA	C4-C3-C5-C6
19	KK	102	CLA	C2A-CAA-CBA-CGA
19	B2	823	CLA	C15-C16-C17-C18
25	BB	844	LMG	C35-C36-C37-C38
19	B1	835	CLA	C3-C5-C6-C7
22	A1	845	LHG	O7-C5-C6-O8
22	B1	847	LHG	O7-C5-C6-O8
22	X1	102	LHG	O7-C5-C6-O8
22	B2	848	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
22	X2	102	LHG	O7-C5-C6-O8
22	X	102	LHG	O7-C5-C6-O8
22	XX	102	LHG	O7-C5-C6-O8
25	B2	845	LMG	O1-C7-C8-O7
25	B	845	LMG	O1-C7-C8-O7
19	A1	834	CLA	C14-C13-C15-C16
19	B1	805	CLA	C11-C12-C13-C14
19	A2	827	CLA	C14-C13-C15-C16
19	B	826	CLA	C6-C7-C8-C9
19	BB	810	CLA	C11-C10-C8-C9
19	BB	816	CLA	C6-C7-C8-C9
19	L	204	CLA	C2C-C3C-CAC-CBC
22	B	852	LHG	O9-C7-O7-C5
25	B	845	LMG	C16-C17-C18-C19
19	A1	826	CLA	C5-C6-C7-C8
19	B1	801	CLA	C8-C10-C11-C12
22	X2	102	LHG	C27-C28-C29-C30
19	B2	813	CLA	O1D-CGD-O2D-CED
19	AA	830	CLA	C4C-C3C-CAC-CBC
23	M	101	BCR	C13-C14-C15-C16
19	B	808	CLA	O1D-CGD-O2D-CED
19	A1	842	CLA	C16-C17-C18-C19
19	L	204	CLA	C16-C17-C18-C20
19	BB	808	CLA	C11-C12-C13-C15
19	B1	815	CLA	C13-C15-C16-C17
19	B	801	CLA	C15-C16-C17-C18
22	A1	845	LHG	C15-C16-C17-C18
19	A	830	CLA	C4C-C3C-CAC-CBC
19	B2	815	CLA	C13-C15-C16-C17
19	BB	801	CLA	C13-C15-C16-C17
19	BB	833	CLA	O1D-CGD-O2D-CED
19	L2	204	CLA	C4-C3-C5-C6
19	B	821	CLA	C4-C3-C5-C6
19	B	824	CLA	C4-C3-C5-C6
19	B1	808	CLA	C2-C3-C5-C6
19	A2	828	CLA	C2-C3-C5-C6
19	A2	827	CLA	C5-C6-C7-C8
22	X2	103	LHG	C10-C11-C12-C13
19	A1	818	CLA	C2A-CAA-CBA-CGA
19	A2	842	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	AA	826	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	845	LHG	C32-C33-C34-C35
19	A1	806	CLA	C16-C17-C18-C19
19	B	808	CLA	C11-C12-C13-C15
19	AA	843	CLA	C16-C17-C18-C20
23	F2	305	BCR	C14-C15-C16-C17
23	A	847	BCR	C14-C15-C16-C17
23	AA	848	BCR	C14-C15-C16-C17
19	B2	825	CLA	CBD-CGD-O2D-CED
20	A2	803	CL0	C4C-C3C-CAC-CBC
22	X1	102	LHG	C27-C28-C29-C30
23	B	848	BCR	C18-C19-C20-C21
25	II	105	LMG	C13-C14-C15-C16
19	B1	808	CLA	C11-C12-C13-C15
19	B2	808	CLA	C11-C12-C13-C15
19	A	812	CLA	O1A-CGA-O2A-C1
19	B1	826	CLA	C15-C16-C17-C18
19	A	835	CLA	O1A-CGA-O2A-C1
20	A2	803	CL0	C3-C5-C6-C7
23	K2	103	BCR	C7-C8-C9-C34
23	AA	848	BCR	C36-C18-C19-C20
19	A1	806	CLA	C4B-C3B-CAB-CBB
19	A1	812	CLA	C4B-C3B-CAB-CBB
19	A1	821	CLA	C4B-C3B-CAB-CBB
19	A1	824	CLA	C4B-C3B-CAB-CBB
19	A1	826	CLA	C4B-C3B-CAB-CBB
19	B1	802	CLA	C1A-C2A-CAA-CBA
19	B1	805	CLA	C4B-C3B-CAB-CBB
19	B1	808	CLA	C4B-C3B-CAB-CBB
19	B1	813	CLA	C4B-C3B-CAB-CBB
19	B1	817	CLA	C4B-C3B-CAB-CBB
19	B1	820	CLA	C4B-C3B-CAB-CBB
19	B1	823	CLA	C4B-C3B-CAB-CBB
19	B1	832	CLA	C4B-C3B-CAB-CBB
19	B1	835	CLA	C4B-C3B-CAB-CBB
19	F1	305	CLA	C1A-C2A-CAA-CBA
19	J1	101	CLA	C4B-C3B-CAB-CBB
19	J1	103	CLA	C4B-C3B-CAB-CBB
19	A2	807	CLA	C4B-C3B-CAB-CBB
19	A2	817	CLA	C4B-C3B-CAB-CBB
19	A2	822	CLA	C4B-C3B-CAB-CBB
19	A2	825	CLA	C4B-C3B-CAB-CBB
19	A2	827	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A2	842	CLA	C4B-C3B-CAB-CBB
19	B2	801	CLA	C1A-C2A-CAA-CBA
19	B2	805	CLA	C4B-C3B-CAB-CBB
19	B2	808	CLA	C4B-C3B-CAB-CBB
19	B2	813	CLA	C4B-C3B-CAB-CBB
19	B2	817	CLA	C4B-C3B-CAB-CBB
19	B2	829	CLA	C1A-C2A-CAA-CBA
19	B2	833	CLA	C1A-C2A-CAA-CBA
19	B2	833	CLA	C4B-C3B-CAB-CBB
19	J2	101	CLA	C4B-C3B-CAB-CBB
19	J2	103	CLA	C4B-C3B-CAB-CBB
19	K2	104	CLA	C4B-C3B-CAB-CBB
19	L2	205	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C4B-C3B-CAB-CBB
19	A	813	CLA	C4B-C3B-CAB-CBB
19	A	814	CLA	C4B-C3B-CAB-CBB
19	A	817	CLA	C4B-C3B-CAB-CBB
19	A	818	CLA	C4B-C3B-CAB-CBB
19	A	819	CLA	C4B-C3B-CAB-CBB
19	A	822	CLA	C4B-C3B-CAB-CBB
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C4B-C3B-CAB-CBB
19	A	836	CLA	C4B-C3B-CAB-CBB
19	B	805	CLA	C4B-C3B-CAB-CBB
19	B	809	CLA	C4B-C3B-CAB-CBB
19	B	813	CLA	C4B-C3B-CAB-CBB
19	B	817	CLA	C4B-C3B-CAB-CBB
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C4B-C3B-CAB-CBB
19	B	835	CLA	C1A-C2A-CAA-CBA
19	J	101	CLA	C4B-C3B-CAB-CBB
19	J	103	CLA	C4B-C3B-CAB-CBB
19	AA	807	CLA	C4B-C3B-CAB-CBB
19	AA	814	CLA	C4B-C3B-CAB-CBB
19	AA	817	CLA	C4B-C3B-CAB-CBB
19	AA	819	CLA	C4B-C3B-CAB-CBB
19	AA	820	CLA	C4B-C3B-CAB-CBB
19	AA	822	CLA	C4B-C3B-CAB-CBB
19	AA	823	CLA	C1A-C2A-CAA-CBA
19	AA	825	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	AA	836	CLA	C4B-C3B-CAB-CBB
19	BB	809	CLA	C4B-C3B-CAB-CBB
19	BB	817	CLA	C4B-C3B-CAB-CBB
19	BB	818	CLA	C4B-C3B-CAB-CBB
19	BB	821	CLA	C1A-C2A-CAA-CBA
19	BB	834	CLA	C1A-C2A-CAA-CBA
19	FF	301	CLA	C4B-C3B-CAB-CBB
19	FF	305	CLA	C1A-C2A-CAA-CBA
19	JJ	101	CLA	C4B-C3B-CAB-CBB
19	JJ	103	CLA	C4B-C3B-CAB-CBB
19	XX	101	CLA	C4B-C3B-CAB-CBB
19	L2	206	CLA	CBA-CGA-O2A-C1
19	BB	824	CLA	C4-C3-C5-C6
19	B	859	CLA	C8-C10-C11-C12
19	L1	205	CLA	C2-C3-C5-C6
23	B1	838	BCR	C11-C12-C13-C14
23	B1	841	BCR	C17-C18-C19-C20
23	I1	101	BCR	C17-C18-C19-C20
23	B2	839	BCR	C11-C12-C13-C14
23	A	850	BCR	C21-C22-C23-C24
23	AA	850	BCR	C21-C22-C23-C24
23	II	101	BCR	C11-C12-C13-C14
23	JJ	104	BCR	C11-C12-C13-C14
23	J1	102	BCR	C15-C16-C17-C18
19	BB	825	CLA	C3-C5-C6-C7
19	AA	806	CLA	C2A-CAA-CBA-CGA
19	A2	842	CLA	C5-C6-C7-C8
19	L	202	CLA	C10-C11-C12-C13
22	B	852	LHG	O6-C4-C5-C6
25	B2	845	LMG	C39-C40-C41-C42
19	BB	835	CLA	CBD-CGD-O2D-CED
22	X	102	LHG	C29-C30-C31-C32
19	L2	206	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	C15-C16-C17-C18
22	A	845	LHG	C15-C16-C17-C18
19	A1	805	CLA	C6-C7-C8-C10
19	A1	852	CLA	C11-C12-C13-C15
19	B1	825	CLA	C6-C7-C8-C10
19	B1	832	CLA	C11-C12-C13-C15
19	B1	835	CLA	C12-C13-C15-C16
19	B1	836	CLA	C6-C7-C8-C10
19	A2	806	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	A2	819	CLA	C11-C10-C8-C7
19	A2	829	CLA	C11-C10-C8-C7
19	A2	836	CLA	C12-C13-C15-C16
19	A2	852	CLA	C11-C10-C8-C7
19	B2	825	CLA	C6-C7-C8-C10
19	B2	825	CLA	C12-C13-C15-C16
19	B2	833	CLA	C11-C12-C13-C15
19	B2	834	CLA	C11-C10-C8-C7
19	B2	837	CLA	C6-C7-C8-C10
19	A	829	CLA	C11-C10-C8-C7
19	A	852	CLA	C11-C10-C8-C7
19	B	806	CLA	C12-C13-C15-C16
19	B	810	CLA	C11-C10-C8-C7
19	B	811	CLA	C11-C10-C8-C7
19	B	815	CLA	C6-C7-C8-C10
19	B	825	CLA	C6-C7-C8-C10
19	B	833	CLA	C11-C12-C13-C15
19	B	836	CLA	C12-C13-C15-C16
19	AA	806	CLA	C6-C7-C8-C10
19	AA	853	CLA	C11-C10-C8-C7
19	BB	811	CLA	C11-C10-C8-C7
19	BB	815	CLA	C6-C7-C8-C10
19	BB	825	CLA	C6-C7-C8-C10
19	BB	832	CLA	C11-C12-C13-C15
19	BB	836	CLA	C6-C7-C8-C10
21	B1	837	PQN	C21-C22-C23-C25
19	B	814	CLA	C10-C11-C12-C13
22	AA	846	LHG	C32-C33-C34-C35
19	A1	829	CLA	C13-C15-C16-C17
19	A2	836	CLA	C5-C6-C7-C8
22	B	853	LHG	C2-C3-O3-P
22	B	853	LHG	C10-C11-C12-C13
25	B	851	LMG	C34-C35-C36-C37
19	B2	804	CLA	C3A-C2A-CAA-CBA
20	A1	802	CL0	C16-C17-C18-C19
21	B	838	PQN	C18-C20-C21-C22
19	A1	842	CLA	C15-C16-C17-C18
19	A1	841	CLA	C2A-CAA-CBA-CGA
19	A2	819	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C2A-CAA-CBA-CGA
19	A1	807	CLA	C6-C7-C8-C9
19	B1	826	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A2	808	CLA	C6-C7-C8-C9
19	A	807	CLA	C11-C12-C13-C14
19	AA	808	CLA	C6-C7-C8-C9
19	BB	806	CLA	C14-C13-C15-C16
19	BB	826	CLA	C14-C13-C15-C16
21	A1	843	PQN	C16-C17-C18-C19
21	B1	837	PQN	C21-C22-C23-C24
21	B2	838	PQN	C21-C22-C23-C24
21	B	838	PQN	C21-C22-C23-C24
19	B1	814	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	C5-C6-C7-C8
19	B	858	CLA	C5-C6-C7-C8
23	A1	848	BCR	C9-C10-C11-C12
23	A1	853	BCR	C9-C10-C11-C12
23	B1	838	BCR	C9-C10-C11-C12
23	B1	838	BCR	C13-C14-C15-C16
23	J1	104	BCR	C15-C16-C17-C18
23	B2	839	BCR	C9-C10-C11-C12
23	B2	839	BCR	C13-C14-C15-C16
23	B2	842	BCR	C15-C16-C17-C18
23	B2	844	BCR	C9-C10-C11-C12
23	F2	305	BCR	C19-C20-C21-C22
23	AA	849	BCR	C9-C10-C11-C12
19	AA	807	CLA	C10-C11-C12-C13
22	AA	846	LHG	C16-C17-C18-C19
19	A1	832	CLA	O1D-CGD-O2D-CED
22	XX	102	LHG	C29-C30-C31-C32
19	BB	829	CLA	C3-C5-C6-C7
19	B1	823	CLA	C10-C11-C12-C13
19	L1	207	CLA	O1A-CGA-O2A-C1
22	L1	211	LHG	O7-C5-C6-O8
22	L2	208	LHG	O7-C5-C6-O8
25	B1	846	LMG	O1-C7-C8-O7
25	B2	847	LMG	O1-C7-C8-O7
25	BB	844	LMG	O1-C7-C8-O7
28	BB	854	DGD	O2G-C2G-C3G-O3G
25	L1	210	LMG	C42-C43-C44-C45
19	A1	841	CLA	C5-C6-C7-C8
19	A2	820	CLA	C8-C10-C11-C12
19	BB	801	CLA	C16-C17-C18-C19
22	L	207	LHG	C4-C5-C6-O8
22	LL	205	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	B1	844	LMG	O1-C7-C8-C9
25	BB	844	LMG	O1-C7-C8-C9
19	BB	814	CLA	C4-C3-C5-C6
22	A	845	LHG	C16-C17-C18-C19
19	B2	801	CLA	C15-C16-C17-C18
20	AA	803	CL0	C8-C10-C11-C12
19	L2	204	CLA	C2-C3-C5-C6
19	B	824	CLA	C2-C3-C5-C6
19	LL	202	CLA	C3-C5-C6-C7
25	II	105	LMG	C37-C38-C39-C40
22	BB	851	LHG	C10-C11-C12-C13
19	A1	815	CLA	CAD-CBD-CGD-O2D
19	A1	823	CLA	CAD-CBD-CGD-O2D
19	A1	844	CLA	CAD-CBD-CGD-O2D
19	B1	810	CLA	CAD-CBD-CGD-O2D
19	B1	830	CLA	CAD-CBD-CGD-O2D
19	K1	103	CLA	CAD-CBD-CGD-O2D
19	A2	824	CLA	CAD-CBD-CGD-O2D
19	A2	844	CLA	CAD-CBD-CGD-O2D
19	A2	852	CLA	CAD-CBD-CGD-O2D
19	B2	810	CLA	CAD-CBD-CGD-O2D
19	L2	204	CLA	CAD-CBD-CGD-O2D
19	B	802	CLA	CAD-CBD-CGD-O2D
19	B	810	CLA	CAD-CBD-CGD-O2D
19	B	831	CLA	CAD-CBD-CGD-O2D
19	AA	845	CLA	CAD-CBD-CGD-O2D
19	BB	810	CLA	CAD-CBD-CGD-O2D
19	LL	201	CLA	CAD-CBD-CGD-O2D
20	A2	803	CL0	CAD-CBD-CGD-O2D
19	BB	826	CLA	O1D-CGD-O2D-CED
25	B	851	LMG	C42-C43-C44-C45
19	BB	825	CLA	O1A-CGA-O2A-C1
19	B1	814	CLA	CBA-CGA-O2A-C1
19	L1	207	CLA	CBA-CGA-O2A-C1
19	A1	806	CLA	C16-C17-C18-C20
19	A1	842	CLA	C16-C17-C18-C20
19	B2	823	CLA	C16-C17-C18-C20
19	B	860	CLA	C16-C17-C18-C19
19	A	806	CLA	C2A-CAA-CBA-CGA
19	B2	825	CLA	O1A-CGA-O2A-C1
19	AA	853	CLA	C5-C6-C7-C8
19	A2	830	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	830	CLA	C2C-C3C-CAC-CBC
19	A1	815	CLA	CAD-CBD-CGD-O1D
19	A1	823	CLA	CAD-CBD-CGD-O1D
19	A1	826	CLA	CHA-CBD-CGD-O1D
19	A1	826	CLA	CHA-CBD-CGD-O2D
19	A1	831	CLA	CHA-CBD-CGD-O1D
19	A1	831	CLA	CHA-CBD-CGD-O2D
19	A1	844	CLA	CAD-CBD-CGD-O1D
19	B1	801	CLA	CHA-CBD-CGD-O1D
19	B1	802	CLA	CAD-CBD-CGD-O1D
19	B1	807	CLA	CHA-CBD-CGD-O1D
19	B1	810	CLA	CAD-CBD-CGD-O1D
19	B1	811	CLA	CAD-CBD-CGD-O1D
19	B1	815	CLA	CHA-CBD-CGD-O1D
19	B1	822	CLA	CHA-CBD-CGD-O1D
19	B1	822	CLA	CHA-CBD-CGD-O2D
19	B1	830	CLA	CAD-CBD-CGD-O1D
19	K1	103	CLA	CAD-CBD-CGD-O1D
19	A2	809	CLA	CHA-CBD-CGD-O1D
19	A2	824	CLA	CAD-CBD-CGD-O1D
19	A2	832	CLA	CHA-CBD-CGD-O1D
19	A2	842	CLA	CHA-CBD-CGD-O1D
19	A2	844	CLA	CAD-CBD-CGD-O1D
19	A2	852	CLA	CAD-CBD-CGD-O1D
19	B2	801	CLA	CHA-CBD-CGD-O1D
19	B2	801	CLA	CHA-CBD-CGD-O2D
19	B2	810	CLA	CAD-CBD-CGD-O1D
19	B2	822	CLA	CHA-CBD-CGD-O1D
19	B2	822	CLA	CHA-CBD-CGD-O2D
19	F2	302	CLA	CHA-CBD-CGD-O1D
19	F2	302	CLA	CHA-CBD-CGD-O2D
19	L2	204	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	CAD-CBD-CGD-O1D
19	B	801	CLA	CHA-CBD-CGD-O1D
19	B	801	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CAD-CBD-CGD-O1D
19	B	819	CLA	CHA-CBD-CGD-O1D
19	B	831	CLA	CAD-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	AA	806	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	AA	809	CLA	CHA-CBD-CGD-O1D
19	AA	816	CLA	CAD-CBD-CGD-O1D
19	AA	833	CLA	CHA-CBD-CGD-O2D
19	AA	845	CLA	CAD-CBD-CGD-O1D
19	BB	810	CLA	CAD-CBD-CGD-O1D
19	BB	830	CLA	CAD-CBD-CGD-O1D
19	BB	833	CLA	CHA-CBD-CGD-O1D
19	BB	833	CLA	CHA-CBD-CGD-O2D
19	KK	102	CLA	CAD-CBD-CGD-O1D
19	LL	201	CLA	CAD-CBD-CGD-O1D
22	A1	845	LHG	C4-O6-P-O5
22	L1	211	LHG	C3-O3-P-O5
22	A2	845	LHG	C4-O6-P-O5
22	L2	208	LHG	C3-O3-P-O5
22	L2	208	LHG	C4-O6-P-O5
22	X2	102	LHG	C4-O6-P-O5
22	X2	103	LHG	C3-O3-P-O6
22	A	845	LHG	C4-O6-P-O5
22	B	852	LHG	C4-O6-P-O5
22	X	102	LHG	C4-O6-P-O3
22	X	102	LHG	C4-O6-P-O4
22	X	102	LHG	C4-O6-P-O5
22	AA	846	LHG	C4-O6-P-O5
22	BB	850	LHG	C3-O3-P-O5
22	XX	102	LHG	C3-O3-P-O5
23	F1	304	BCR	C19-C20-C21-C22
23	L1	208	BCR	C15-C16-C17-C18
23	A2	847	BCR	C35-C13-C14-C15
23	A2	848	BCR	C9-C10-C11-C12
23	B2	843	BCR	C19-C20-C21-C22
23	J2	104	BCR	C15-C16-C17-C18
23	B	839	BCR	C9-C10-C11-C12
23	F	304	BCR	C19-C20-C21-C22
23	I	101	BCR	C13-C14-C15-C16
23	J	104	BCR	C15-C16-C17-C18
23	BB	838	BCR	C9-C10-C11-C12
23	BB	842	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C20-C21-C22-C37
22	L1	211	LHG	C24-C25-C26-C27
19	B1	824	CLA	C4-C3-C5-C6
19	B2	824	CLA	C4-C3-C5-C6
19	AA	836	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A1	821	CLA	C2B-C3B-CAB-CBB
19	A1	824	CLA	C2B-C3B-CAB-CBB
19	A1	834	CLA	C2B-C3B-CAB-CBB
19	A1	835	CLA	C2B-C3B-CAB-CBB
19	B1	802	CLA	C2B-C3B-CAB-CBB
19	B1	827	CLA	C2B-C3B-CAB-CBB
19	B1	835	CLA	C2B-C3B-CAB-CBB
19	J1	101	CLA	C2B-C3B-CAB-CBB
19	A2	822	CLA	C2B-C3B-CAB-CBB
19	A2	825	CLA	C2B-C3B-CAB-CBB
19	A2	827	CLA	C2B-C3B-CAB-CBB
19	A2	835	CLA	C2B-C3B-CAB-CBB
19	B2	805	CLA	C2B-C3B-CAB-CBB
19	B2	808	CLA	C2B-C3B-CAB-CBB
19	B2	827	CLA	C2B-C3B-CAB-CBB
19	B2	833	CLA	C2B-C3B-CAB-CBB
19	J2	101	CLA	C2B-C3B-CAB-CBB
19	K2	104	CLA	C2B-C3B-CAB-CBB
19	A	818	CLA	C2B-C3B-CAB-CBB
19	A	822	CLA	C2B-C3B-CAB-CBB
19	A	823	CLA	C2B-C3B-CAB-CBB
19	A	836	CLA	C2B-C3B-CAB-CBB
19	B	833	CLA	C2B-C3B-CAB-CBB
19	J	101	CLA	C2B-C3B-CAB-CBB
19	J	103	CLA	C2B-C3B-CAB-CBB
19	AA	820	CLA	C2B-C3B-CAB-CBB
19	AA	823	CLA	C2B-C3B-CAB-CBB
19	AA	827	CLA	C2B-C3B-CAB-CBB
19	AA	836	CLA	C2B-C3B-CAB-CBB
19	BB	818	CLA	C2B-C3B-CAB-CBB
19	BB	833	CLA	C2B-C3B-CAB-CBB
19	JJ	103	CLA	C2B-C3B-CAB-CBB
23	F1	303	BCR	C23-C24-C25-C30
23	I	101	BCR	C1-C6-C7-C8
23	BB	842	BCR	C23-C24-C25-C30
19	B2	821	CLA	C2-C3-C5-C6
22	L1	211	LHG	C2-C3-O3-P
22	L2	208	LHG	C2-C3-O3-P
22	X2	103	LHG	C2-C3-O3-P
22	BB	851	LHG	C2-C3-O3-P
23	B1	843	BCR	C7-C8-C9-C34
23	B2	844	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	F2	303	BCR	C37-C22-C23-C24
23	F2	304	BCR	C36-C18-C19-C20
23	F	303	BCR	C11-C12-C13-C35
23	I	102	BCR	C37-C22-C23-C24
19	A	832	CLA	C3-C5-C6-C7
22	XX	102	LHG	O9-C7-O7-C5
19	A	835	CLA	C15-C16-C17-C18
19	B1	814	CLA	C10-C11-C12-C13
19	B	825	CLA	C3-C5-C6-C7
22	BB	851	LHG	C25-C26-C27-C28
19	AA	835	CLA	CBA-CGA-O2A-C1
25	BB	844	LMG	C19-C20-C21-C22
19	AA	840	CLA	C5-C6-C7-C8
25	B1	844	LMG	C19-C20-C21-C22
23	A	847	BCR	C13-C14-C15-C16
23	B	843	BCR	C9-C10-C11-C12
19	B1	801	CLA	C16-C17-C18-C20
19	AA	853	CLA	C8-C10-C11-C12
22	BB	850	LHG	O6-C4-C5-C6
25	B1	844	LMG	C33-C34-C35-C36
19	A1	834	CLA	CBA-CGA-O2A-C1
19	A2	835	CLA	CBA-CGA-O2A-C1
19	A1	829	CLA	C11-C10-C8-C9
19	A1	835	CLA	C14-C13-C15-C16
19	B1	805	CLA	C6-C7-C8-C9
19	B1	811	CLA	C11-C10-C8-C9
19	B1	835	CLA	C14-C13-C15-C16
19	L1	206	CLA	C11-C12-C13-C14
19	A2	806	CLA	C6-C7-C8-C9
19	A2	830	CLA	C11-C10-C8-C9
19	B2	805	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C10-C8-C9
19	A	801	CLA	C11-C10-C8-C9
19	A	813	CLA	C6-C7-C8-C9
19	A	830	CLA	C11-C10-C8-C9
19	B	810	CLA	C11-C10-C8-C9
19	B	816	CLA	C6-C7-C8-C9
19	B	826	CLA	C14-C13-C15-C16
19	L	203	CLA	C11-C12-C13-C14
19	AA	801	CLA	C11-C10-C8-C9
19	AA	807	CLA	C11-C12-C13-C14
19	AA	827	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	AA	830	CLA	C11-C10-C8-C9
19	BB	805	CLA	C6-C7-C8-C9
19	BB	811	CLA	C11-C10-C8-C9
19	LL	202	CLA	C11-C12-C13-C14
20	A	803	CL0	C14-C13-C15-C16
19	L1	206	CLA	C11-C12-C13-C15
19	A	801	CLA	C11-C10-C8-C7
19	L	203	CLA	C11-C12-C13-C15
19	LL	202	CLA	C11-C12-C13-C15
23	B2	843	BCR	C20-C21-C22-C23
23	J2	102	BCR	C11-C10-C9-C8
23	B	840	BCR	C12-C13-C14-C15
23	B	842	BCR	C11-C10-C9-C8
23	B	844	BCR	C16-C17-C18-C19
23	I	102	BCR	C20-C21-C22-C23
23	K	103	BCR	C11-C10-C9-C8
23	BB	841	BCR	C11-C10-C9-C8
23	FF	303	BCR	C20-C21-C22-C23
23	B1	838	BCR	C6-C7-C8-C9
23	BB	847	BCR	C22-C23-C24-C25
19	B2	823	CLA	C16-C17-C18-C19
19	B	808	CLA	C11-C12-C13-C14
19	BB	808	CLA	C11-C12-C13-C14
20	A1	802	CL0	C16-C17-C18-C20
23	A2	847	BCR	C14-C15-C16-C17
19	A1	839	CLA	CBD-CGD-O2D-CED
19	A2	835	CLA	O1A-CGA-O2A-C1
22	AA	846	LHG	C15-C16-C17-C18
19	B2	801	CLA	C16-C17-C18-C20
19	B	860	CLA	C16-C17-C18-C20
25	M	102	LMG	C30-C31-C32-C33
19	A	809	CLA	O1A-CGA-O2A-C1
22	X1	102	LHG	O9-C7-O7-C5
19	A2	827	CLA	C10-C11-C12-C13
19	B	801	CLA	C13-C15-C16-C17
22	X1	103	LHG	C2-C3-O3-P
22	X1	103	LHG	C25-C26-C27-C28
25	B1	844	LMG	O1-C7-C8-O7
25	II	105	LMG	O1-C7-C8-O7
19	BB	856	CLA	C8-C10-C11-C12
19	A1	834	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B2	814	CLA	C11-C12-C13-C14
23	B2	842	BCR	C13-C14-C15-C16
23	F	304	BCR	C15-C16-C17-C18
23	AA	848	BCR	C13-C14-C15-C16
22	A2	845	LHG	C26-C27-C28-C29
19	L	204	CLA	C10-C11-C12-C13
22	X1	102	LHG	C8-C7-O7-C5
22	XX	102	LHG	C8-C7-O7-C5
19	AA	842	CLA	C2A-CAA-CBA-CGA
19	AA	819	CLA	CBD-CGD-O2D-CED
19	A1	820	CLA	C16-C17-C18-C20
25	B	845	LMG	C19-C20-C21-C22
19	B1	814	CLA	C11-C12-C13-C14
22	X2	103	LHG	C23-C24-C25-C26
22	A1	845	LHG	C9-C10-C11-C12
19	B	805	CLA	C16-C17-C18-C19
23	B2	840	BCR	C11-C12-C13-C35
23	A	851	BCR	C36-C18-C19-C20
23	F	303	BCR	C36-C18-C19-C20
23	FF	303	BCR	C36-C18-C19-C20
22	A1	845	LHG	C29-C30-C31-C32
19	B2	808	CLA	C11-C12-C13-C14
19	L	204	CLA	C16-C17-C18-C19
19	AA	835	CLA	O1A-CGA-O2A-C1
23	J1	104	BCR	C17-C18-C19-C20
23	AA	855	BCR	C21-C22-C23-C24
23	BB	839	BCR	C21-C22-C23-C24
23	BB	842	BCR	C17-C18-C19-C20
26	B	841	ECH	C11-C12-C13-C14
19	B2	825	CLA	CBA-CGA-O2A-C1
19	BB	825	CLA	CBA-CGA-O2A-C1
25	B2	845	LMG	C19-C20-C21-C22
19	LL	201	CLA	C5-C6-C7-C8
19	A	831	CLA	C2A-CAA-CBA-CGA
19	L	204	CLA	C2A-CAA-CBA-CGA
19	BB	821	CLA	O1D-CGD-O2D-CED
23	B1	842	BCR	C9-C10-C11-C12
23	F2	304	BCR	C19-C20-C21-C22
23	J2	104	BCR	C9-C10-C11-C12
23	FF	304	BCR	C19-C20-C21-C22
19	A1	801	CLA	C16-C17-C18-C19
19	B1	808	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A2	801	CLA	C16-C17-C18-C19
19	A2	804	CLA	C16-C17-C18-C19
22	AA	846	LHG	C7-C8-C9-C10
19	B1	825	CLA	CBD-CGD-O2D-CED
19	B2	810	CLA	C4-C3-C5-C6
19	A	836	CLA	C4-C3-C5-C6
19	LL	201	CLA	C10-C11-C12-C13
19	A	809	CLA	CBA-CGA-O2A-C1
22	X2	103	LHG	O1-C1-C2-O2
19	B1	823	CLA	C16-C17-C18-C20
22	B2	848	LHG	C12-C13-C14-C15
22	A2	845	LHG	C7-C8-C9-C10
19	A1	805	CLA	C6-C7-C8-C9
19	A1	826	CLA	C11-C10-C8-C9
19	A2	827	CLA	C11-C10-C8-C9
19	B	805	CLA	C6-C7-C8-C9
19	B	811	CLA	C11-C10-C8-C9
19	B	811	CLA	C11-C12-C13-C14
19	B2	826	CLA	C15-C16-C17-C18
19	AA	819	CLA	O1D-CGD-O2D-CED
19	BB	835	CLA	O1D-CGD-O2D-CED
19	A1	808	CLA	C4B-C3B-CAB-CBB
19	A1	835	CLA	C4B-C3B-CAB-CBB
19	X1	101	CLA	C4B-C3B-CAB-CBB
19	A2	809	CLA	C4B-C3B-CAB-CBB
19	A2	813	CLA	C4B-C3B-CAB-CBB
19	A2	823	CLA	C4B-C3B-CAB-CBB
19	A	837	CLA	C4B-C3B-CAB-CBB
19	AA	809	CLA	C4B-C3B-CAB-CBB
19	AA	837	CLA	C4B-C3B-CAB-CBB
19	BB	832	CLA	C4B-C3B-CAB-CBB
19	LL	202	CLA	C8-C10-C11-C12
19	A	807	CLA	C16-C17-C18-C19
22	A1	845	LHG	C24-C23-O8-C6
19	A	840	CLA	C5-C6-C7-C8
22	A1	845	LHG	O10-C23-O8-C6
19	B1	802	CLA	C4-C3-C5-C6
19	A2	808	CLA	C4-C3-C5-C6
19	BB	802	CLA	C4-C3-C5-C6
19	AA	836	CLA	C2-C3-C5-C6
19	BB	824	CLA	C2-C3-C5-C6
22	X1	103	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	AA	846	LHG	C18-C19-C20-C21
22	B	853	LHG	C18-C19-C20-C21
23	II	104	BCR	C15-C16-C17-C18
19	B	825	CLA	CBA-CGA-O2A-C1
19	B1	823	CLA	C16-C17-C18-C19
25	M	102	LMG	C37-C38-C39-C40
19	A1	803	CLA	C6-C7-C8-C10
19	BB	811	CLA	C11-C12-C13-C15
21	A1	843	PQN	C21-C22-C23-C25
23	J	102	BCR	C14-C15-C16-C17
25	II	105	LMG	C32-C33-C34-C35
19	A1	801	CLA	C16-C17-C18-C20
19	A2	801	CLA	C16-C17-C18-C20
19	A1	829	CLA	C4C-C3C-CAC-CBC
19	AA	826	CLA	CAA-CBA-CGA-O1A
19	B1	810	CLA	C3A-C2A-CAA-CBA
19	B2	801	CLA	C3A-C2A-CAA-CBA
19	B2	807	CLA	C3A-C2A-CAA-CBA
19	L2	204	CLA	C3A-C2A-CAA-CBA
19	A	810	CLA	C3A-C2A-CAA-CBA
19	AA	808	CLA	C4-C3-C5-C6
19	AA	836	CLA	C3A-C2A-CAA-CBA
19	BB	801	CLA	C3A-C2A-CAA-CBA
19	BB	802	CLA	C3A-C2A-CAA-CBA
22	BB	851	LHG	C18-C19-C20-C21
19	B1	801	CLA	C16-C17-C18-C19
23	F1	303	BCR	C35-C13-C14-C15
23	L1	201	BCR	C20-C21-C22-C37
23	A2	848	BCR	C22-C23-C24-C25
23	A2	851	BCR	C16-C17-C18-C36
23	B2	839	BCR	C6-C7-C8-C9
23	B2	839	BCR	C11-C10-C9-C34
23	B2	842	BCR	C16-C17-C18-C36
23	F2	303	BCR	C35-C13-C14-C15
23	I	102	BCR	C20-C21-C22-C37
23	II	102	BCR	C20-C21-C22-C37
26	B1	840	ECH	C11-C10-C9-C34
26	B2	841	ECH	C11-C10-C9-C34
26	B	841	ECH	C11-C10-C9-C34
26	BB	840	ECH	C11-C10-C9-C34
24	KK	104	AJP	O31-C26-O25-C23
19	B2	801	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	B2	823	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
19	B1	806	CLA	C10-C11-C12-C13
19	L1	205	CLA	C2-C1-O2A-CGA
19	L2	204	CLA	C2-C1-O2A-CGA
23	J1	104	BCR	C9-C10-C11-C12
23	LL	204	BCR	C13-C14-C15-C16
19	AA	842	CLA	C16-C17-C18-C20
19	B2	806	CLA	C10-C11-C12-C13
19	A	842	CLA	C5-C6-C7-C8
23	F2	303	BCR	C36-C18-C19-C20
19	J	103	CLA	C2C-C3C-CAC-CBC
19	A2	826	CLA	CAA-CBA-CGA-O1A
24	L2	202	AJP	O31-C26-O25-C23
19	BB	805	CLA	C16-C17-C18-C19
19	B2	805	CLA	C16-C17-C18-C19
22	XX	102	LHG	C25-C26-C27-C28
19	A	826	CLA	CAA-CBA-CGA-O1A
19	BB	820	CLA	CAA-CBA-CGA-O1A
23	A	849	BCR	C21-C22-C23-C24
23	A	851	BCR	C7-C8-C9-C10
23	J	104	BCR	C11-C12-C13-C14
23	AA	850	BCR	C7-C8-C9-C10
19	B	829	CLA	C2C-C3C-CAC-CBC
19	B1	824	CLA	C2-C3-C5-C6
19	B2	824	CLA	C2-C3-C5-C6
24	A	855	AJP	C27-C26-O25-C23
24	AA	856	AJP	C27-C26-O25-C23
19	B2	801	CLA	C16-C17-C18-C19
19	B	859	CLA	C10-C11-C12-C13
22	L2	208	LHG	C10-C11-C12-C13
22	X	102	LHG	C25-C26-C27-C28
19	A2	818	CLA	CAA-CBA-CGA-O1A
22	A2	846	LHG	C11-C12-C13-C14
22	A1	846	LHG	C11-C12-C13-C14
25	II	105	LMG	C31-C32-C33-C34
19	BB	806	CLA	C10-C11-C12-C13
22	X2	103	LHG	C25-C26-C27-C28
19	A1	801	CLA	C11-C10-C8-C9
19	A1	820	CLA	C11-C12-C13-C14
19	B1	825	CLA	C6-C7-C8-C9
19	B1	826	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B1	833	CLA	C6-C7-C8-C9
19	A2	836	CLA	C11-C10-C8-C9
19	B2	826	CLA	C11-C12-C13-C14
19	B2	829	CLA	C14-C13-C15-C16
19	B2	834	CLA	C14-C13-C15-C16
19	B2	837	CLA	C6-C7-C8-C9
19	A	830	CLA	C11-C12-C13-C14
19	A	842	CLA	C6-C7-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	B	811	CLA	C6-C7-C8-C9
19	B	825	CLA	C6-C7-C8-C9
19	B	829	CLA	C14-C13-C15-C16
19	AA	842	CLA	C6-C7-C8-C9
19	BB	801	CLA	C6-C7-C8-C9
19	BB	811	CLA	C6-C7-C8-C9
19	BB	811	CLA	C11-C12-C13-C14
19	FF	305	CLA	C14-C13-C15-C16
20	AA	803	CL0	C11-C10-C8-C9
21	A	843	PQN	C16-C17-C18-C19
19	A	807	CLA	C16-C17-C18-C20
19	A	842	CLA	C16-C17-C18-C20
19	A1	828	CLA	C13-C15-C16-C17
19	BB	821	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CAA-CBA-CGA-O2A
25	I1	102	LMG	C7-C8-O7-C10
19	B2	815	CLA	C5-C6-C7-C8
19	B	802	CLA	C15-C16-C17-C18
22	X2	102	LHG	C31-C32-C33-C34
20	A	803	CL0	O1D-CGD-O2D-CED
23	B	840	BCR	C13-C14-C15-C16
19	AA	827	CLA	C10-C11-C12-C13
19	A	836	CLA	C2-C3-C5-C6
19	AA	808	CLA	C2-C3-C5-C6
19	BB	821	CLA	C2-C3-C5-C6
22	X2	103	LHG	C28-C29-C30-C31
25	I1	102	LMG	C19-C20-C21-C22
19	BB	825	CLA	C5-C6-C7-C8
28	BB	854	DGD	O6D-C5D-C6D-O5D
19	AA	819	CLA	C2A-CAA-CBA-CGA
19	A1	819	CLA	C8-C10-C11-C12
19	B1	825	CLA	C5-C6-C7-C8
19	A1	814	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A1	852	CLA	C1A-C2A-CAA-CBA
19	B1	801	CLA	C1A-C2A-CAA-CBA
19	B1	810	CLA	C1A-C2A-CAA-CBA
19	B1	811	CLA	C1A-C2A-CAA-CBA
19	B1	821	CLA	C1A-C2A-CAA-CBA
19	B1	832	CLA	C1A-C2A-CAA-CBA
19	A2	810	CLA	C1A-C2A-CAA-CBA
19	A2	815	CLA	C1A-C2A-CAA-CBA
19	B2	810	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C1A-C2A-CAA-CBA
19	AA	810	CLA	C1A-C2A-CAA-CBA
19	AA	815	CLA	C1A-C2A-CAA-CBA
19	BB	802	CLA	C1A-C2A-CAA-CBA
19	BB	820	CLA	C1A-C2A-CAA-CBA
19	BB	831	CLA	C1A-C2A-CAA-CBA
19	LL	201	CLA	C1A-C2A-CAA-CBA
23	L1	201	BCR	C20-C21-C22-C23
23	B2	842	BCR	C16-C17-C18-C19
23	A	850	BCR	C20-C21-C22-C23
26	B1	840	ECH	C11-C10-C9-C8
26	B2	841	ECH	C11-C10-C9-C8
26	B	841	ECH	C11-C10-C9-C8
26	BB	840	ECH	C11-C10-C9-C8
19	B1	848	CLA	CBA-CGA-O2A-C1
19	A2	842	CLA	C16-C17-C18-C20
19	X1	101	CLA	CAA-CBA-CGA-O1A
19	A2	826	CLA	CAA-CBA-CGA-O2A
19	K2	104	CLA	CAA-CBA-CGA-O1A
22	B1	847	LHG	O6-C4-C5-O7
22	X1	103	LHG	C18-C19-C20-C21
22	A	845	LHG	C18-C19-C20-C21
19	A	829	CLA	C13-C15-C16-C17
19	A1	806	CLA	C2B-C3B-CAB-CBB
19	A1	808	CLA	C2B-C3B-CAB-CBB
19	A1	812	CLA	C2B-C3B-CAB-CBB
19	A1	826	CLA	C2B-C3B-CAB-CBB
19	B1	808	CLA	C2B-C3B-CAB-CBB
19	B1	813	CLA	C2B-C3B-CAB-CBB
19	B1	817	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	B1	820	CLA	C2B-C3B-CAB-CBB
19	B1	823	CLA	C2B-C3B-CAB-CBB
19	B1	832	CLA	C2B-C3B-CAB-CBB
19	J1	103	CLA	C2B-C3B-CAB-CBB
19	A2	807	CLA	C2B-C3B-CAB-CBB
19	A2	809	CLA	C2B-C3B-CAB-CBB
19	A2	817	CLA	C2B-C3B-CAB-CBB
19	A2	823	CLA	C2B-C3B-CAB-CBB
19	A2	842	CLA	C2B-C3B-CAB-CBB
19	B2	813	CLA	C2B-C3B-CAB-CBB
19	B2	817	CLA	C2B-C3B-CAB-CBB
19	J2	103	CLA	C2B-C3B-CAB-CBB
19	A	807	CLA	C2B-C3B-CAB-CBB
19	A	813	CLA	C2B-C3B-CAB-CBB
19	A	814	CLA	C2B-C3B-CAB-CBB
19	A	817	CLA	C2B-C3B-CAB-CBB
19	A	819	CLA	C2B-C3B-CAB-CBB
19	A	825	CLA	C2B-C3B-CAB-CBB
19	B	809	CLA	C2B-C3B-CAB-CBB
19	B	813	CLA	C2B-C3B-CAB-CBB
19	B	817	CLA	C2B-C3B-CAB-CBB
19	B	827	CLA	C2B-C3B-CAB-CBB
19	B	834	CLA	C2B-C3B-CAB-CBB
19	AA	807	CLA	C2B-C3B-CAB-CBB
19	AA	809	CLA	C2B-C3B-CAB-CBB
19	AA	814	CLA	C2B-C3B-CAB-CBB
19	AA	817	CLA	C2B-C3B-CAB-CBB
19	AA	819	CLA	C2B-C3B-CAB-CBB
19	AA	822	CLA	C2B-C3B-CAB-CBB
19	AA	825	CLA	C2B-C3B-CAB-CBB
19	BB	809	CLA	C2B-C3B-CAB-CBB
19	BB	817	CLA	C2B-C3B-CAB-CBB
19	BB	827	CLA	C2B-C3B-CAB-CBB
19	FF	301	CLA	C2B-C3B-CAB-CBB
19	JJ	101	CLA	C2B-C3B-CAB-CBB
19	XX	101	CLA	C2B-C3B-CAB-CBB
23	A1	849	BCR	C23-C24-C25-C26
23	B1	842	BCR	C23-C24-C25-C30
23	B1	843	BCR	C5-C6-C7-C8
23	F1	303	BCR	C1-C6-C7-C8
23	I1	101	BCR	C5-C6-C7-C8
23	J1	102	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	K1	104	BCR	C23-C24-C25-C30
23	K1	106	BCR	C23-C24-C25-C26
23	L1	209	BCR	C23-C24-C25-C30
23	A2	849	BCR	C23-C24-C25-C26
23	B2	843	BCR	C23-C24-C25-C30
23	B2	844	BCR	C5-C6-C7-C8
23	F2	303	BCR	C1-C6-C7-C8
23	F2	303	BCR	C23-C24-C25-C26
23	I2	101	BCR	C5-C6-C7-C8
23	J2	102	BCR	C23-C24-C25-C26
23	K2	105	BCR	C23-C24-C25-C30
23	L2	207	BCR	C23-C24-C25-C30
23	A	849	BCR	C23-C24-C25-C26
23	A	854	BCR	C23-C24-C25-C26
23	B	843	BCR	C23-C24-C25-C26
23	B	844	BCR	C5-C6-C7-C8
23	F	303	BCR	C1-C6-C7-C8
23	F	303	BCR	C23-C24-C25-C26
23	F	305	BCR	C23-C24-C25-C30
23	J	102	BCR	C1-C6-C7-C8
23	K	103	BCR	C23-C24-C25-C26
23	M	101	BCR	C1-C6-C7-C8
23	AA	850	BCR	C23-C24-C25-C26
23	AA	852	BCR	C23-C24-C25-C30
23	AA	855	BCR	C23-C24-C25-C26
23	BB	843	BCR	C5-C6-C7-C8
23	BB	847	BCR	C5-C6-C7-C8
23	FF	303	BCR	C1-C6-C7-C8
23	FF	303	BCR	C23-C24-C25-C26
23	II	101	BCR	C1-C6-C7-C8
23	JJ	102	BCR	C1-C6-C7-C8
23	KK	103	BCR	C23-C24-C25-C26
23	MM	101	BCR	C1-C6-C7-C8
26	B1	840	ECH	C23-C24-C25-C26
26	B2	841	ECH	C23-C24-C25-C26
26	B	841	ECH	C23-C24-C25-C26
26	BB	840	ECH	C23-C24-C25-C26
19	A2	818	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	CAA-CBA-CGA-O2A
19	B	820	CLA	CAA-CBA-CGA-O1A
19	B1	805	CLA	C16-C17-C18-C19
19	BB	807	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	B	854	CLA	CBA-CGA-O2A-C1
19	AA	842	CLA	C5-C6-C7-C8
19	A1	820	CLA	C16-C17-C18-C19
19	BB	822	CLA	C16-C17-C18-C19
19	B	837	CLA	C3-C5-C6-C7
20	A2	803	CL0	C10-C11-C12-C13
19	A	826	CLA	CAA-CBA-CGA-O2A
19	AA	818	CLA	CAA-CBA-CGA-O2A
19	A2	840	CLA	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	BB	807	CLA	C4-C3-C5-C6
19	BB	814	CLA	C10-C11-C12-C13
19	B2	810	CLA	C2-C3-C5-C6
19	A1	839	CLA	O1D-CGD-O2D-CED
19	K2	104	CLA	CAA-CBA-CGA-O2A
19	BB	820	CLA	CAA-CBA-CGA-O2A
19	XX	101	CLA	CAA-CBA-CGA-O2A
23	A1	847	BCR	C13-C14-C15-C16
23	J1	104	BCR	C19-C20-C21-C22
19	A1	801	CLA	C11-C10-C8-C7
19	A1	818	CLA	C11-C10-C8-C7
19	B1	804	CLA	C11-C10-C8-C7
19	B1	807	CLA	C11-C12-C13-C15
19	B1	815	CLA	C6-C7-C8-C10
19	B2	804	CLA	C11-C10-C8-C7
19	B2	807	CLA	C11-C12-C13-C15
19	B2	815	CLA	C6-C7-C8-C10
19	A	806	CLA	C6-C7-C8-C10
19	A	819	CLA	C11-C10-C8-C7
19	B	810	CLA	C6-C7-C8-C10
19	B	811	CLA	C6-C7-C8-C10
19	B	811	CLA	C11-C12-C13-C15
19	B	829	CLA	C12-C13-C15-C16
19	BB	808	CLA	C6-C7-C8-C10
19	FF	305	CLA	C12-C13-C15-C16
19	A1	819	CLA	C2A-CAA-CBA-CGA
19	B	824	CLA	C2A-CAA-CBA-CGA
19	X	101	CLA	C2A-CAA-CBA-CGA
19	AA	824	CLA	C2A-CAA-CBA-CGA
19	BB	825	CLA	O1D-CGD-O2D-CED
19	A1	817	CLA	CAA-CBA-CGA-O2A
19	X2	101	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	L1	204	AJP	C27-C26-O25-C23
25	I1	102	LMG	C17-C18-C19-C20
19	AA	826	CLA	CAA-CBA-CGA-O2A
19	B2	825	CLA	C5-C6-C7-C8
19	AA	829	CLA	C13-C15-C16-C17
23	A2	847	BCR	C7-C8-C9-C34
28	BB	854	DGD	C4D-C5D-C6D-O5D
19	A1	817	CLA	CAA-CBA-CGA-O1A
19	XX	101	CLA	CAA-CBA-CGA-O1A
19	B2	802	CLA	C4-C3-C5-C6
23	I	102	BCR	C18-C19-C20-C21
25	B1	846	LMG	O7-C10-C11-C12
21	BB	837	PQN	C18-C20-C21-C22
19	B1	802	CLA	C2-C3-C5-C6
19	A2	804	CLA	C2-C3-C5-C6
19	A2	808	CLA	C2-C3-C5-C6
19	BB	802	CLA	C2-C3-C5-C6
19	BB	814	CLA	C2-C3-C5-C6
25	II	105	LMG	C29-C30-C31-C32
19	A1	818	CLA	CBD-CGD-O2D-CED
19	A1	806	CLA	C10-C11-C12-C13
19	B2	849	CLA	C8-C10-C11-C12
19	X1	101	CLA	CAA-CBA-CGA-O2A
19	AA	818	CLA	CAA-CBA-CGA-O1A
19	AA	801	CLA	C16-C17-C18-C19
19	B2	837	CLA	C2C-C3C-CAC-CBC
22	B	853	LHG	C12-C13-C14-C15
22	X2	103	LHG	O2-C2-C3-O3
19	BB	802	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	C3-C5-C6-C7
19	A2	801	CLA	C3-C5-C6-C7
19	BB	845	CLA	C2A-CAA-CBA-CGA
19	X2	101	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	CAA-CBA-CGA-O1A
19	A1	812	CLA	C6-C7-C8-C9
19	B1	828	CLA	C14-C13-C15-C16
19	B2	834	CLA	C6-C7-C8-C9
19	A	827	CLA	C11-C10-C8-C9
19	B	834	CLA	C6-C7-C8-C9
21	A1	843	PQN	C21-C22-C23-C24
21	A2	843	PQN	C21-C22-C23-C24
19	B2	807	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	854	CLA	C13-C15-C16-C17
19	BB	804	CLA	C10-C11-C12-C13
19	A2	805	CLA	C8-C10-C11-C12
19	A1	818	CLA	O1D-CGD-O2D-CED
22	X1	102	LHG	C31-C32-C33-C34
23	A2	849	BCR	C6-C7-C8-C9
23	A	850	BCR	C22-C23-C24-C25
19	A2	804	CLA	C4-C3-C5-C6
20	A2	803	CL0	C4-C3-C5-C6
19	B1	833	CLA	C15-C16-C17-C18
22	L	207	LHG	C5-C4-O6-P
22	LL	205	LHG	C5-C4-O6-P
23	F1	303	BCR	C14-C15-C16-C17
19	B1	848	CLA	C2-C3-C5-C6
19	B	834	CLA	CBD-CGD-O2D-CED
19	BB	822	CLA	C16-C17-C18-C20
22	A1	845	LHG	C4-C5-C6-O8
22	X	102	LHG	C31-C32-C33-C34
22	AA	846	LHG	C33-C34-C35-C36
19	B1	848	CLA	O1A-CGA-O2A-C1
19	A2	830	CLA	O1A-CGA-O2A-C1
19	L2	206	CLA	C2A-CAA-CBA-CGA
19	BB	824	CLA	C2A-CAA-CBA-CGA
19	B1	848	CLA	C8-C10-C11-C12
19	F1	305	CLA	CAA-CBA-CGA-O2A
19	A2	837	CLA	CAA-CBA-CGA-O2A
19	B	827	CLA	CAA-CBA-CGA-O2A
22	B	852	LHG	O1-C1-C2-O2
22	BB	850	LHG	O1-C1-C2-O2
19	A	804	CLA	C4-C3-C5-C6
19	A1	825	CLA	CAA-CBA-CGA-O2A
19	A1	836	CLA	CAA-CBA-CGA-O2A
20	A2	803	CL0	C2-C3-C5-C6
19	B1	811	CLA	C8-C10-C11-C12
19	B2	811	CLA	C8-C10-C11-C12
19	B	825	CLA	C5-C6-C7-C8
19	BB	821	CLA	C5-C6-C7-C8
19	BB	833	CLA	C15-C16-C17-C18
22	B	853	LHG	C28-C29-C30-C31
19	B1	803	CLA	C4B-C3B-CAB-CBB
19	B1	809	CLA	C4B-C3B-CAB-CBB
19	B2	823	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	BB	805	CLA	C4B-C3B-CAB-CBB
19	A2	829	CLA	C13-C15-C16-C17
19	B	854	CLA	O1A-CGA-O2A-C1
19	AA	809	CLA	O1A-CGA-O2A-C1
19	A	830	CLA	C13-C15-C16-C17
19	B2	814	CLA	C10-C11-C12-C13
19	A2	809	CLA	O1A-CGA-O2A-C1
19	X	101	CLA	CAA-CBA-CGA-O2A
19	B2	852	CLA	C16-C17-C18-C19
28	B	856	DGD	O6D-C5D-C6D-O5D
23	B1	843	BCR	C11-C10-C9-C34
23	B2	839	BCR	C35-C13-C14-C15
23	B2	844	BCR	C11-C10-C9-C34
23	I2	102	BCR	C20-C21-C22-C37
23	AA	851	BCR	C35-C13-C14-C15
19	A	801	CLA	C3-C5-C6-C7
19	AA	801	CLA	C3-C5-C6-C7
22	A2	845	LHG	C15-C16-C17-C18
22	LL	205	LHG	C10-C11-C12-C13
19	BB	802	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
22	X2	103	LHG	C18-C19-C20-C21
19	B1	801	CLA	C3-C5-C6-C7
28	B	856	DGD	C4D-C5D-C6D-O5D
19	BB	856	CLA	C10-C11-C12-C13
22	X2	103	LHG	C31-C32-C33-C34
19	A1	820	CLA	C11-C10-C8-C7
19	A1	826	CLA	C11-C10-C8-C7
19	A2	801	CLA	C11-C10-C8-C7
19	B2	829	CLA	C12-C13-C15-C16
19	BB	811	CLA	C6-C7-C8-C10
21	A2	843	PQN	C21-C22-C23-C25
19	B	827	CLA	CAA-CBA-CGA-O1A
21	AA	844	PQN	C23-C25-C26-C27
23	BB	839	BCR	C13-C14-C15-C16
22	B	852	LHG	C11-C10-C9-C8
19	AA	801	CLA	C16-C17-C18-C20
19	BB	803	CLA	C3-C5-C6-C7
19	X	101	CLA	CAA-CBA-CGA-O1A
19	A1	820	CLA	C11-C10-C8-C9
19	A1	841	CLA	C6-C7-C8-C9
19	B1	803	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B1	811	CLA	C6-C7-C8-C9
19	B1	811	CLA	C11-C12-C13-C14
19	B1	825	CLA	C11-C10-C8-C9
19	A2	801	CLA	C11-C10-C8-C9
19	A2	819	CLA	C11-C10-C8-C9
19	A2	836	CLA	C14-C13-C15-C16
19	B2	803	CLA	C11-C12-C13-C14
19	B2	811	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C12-C13-C14
19	B2	825	CLA	C6-C7-C8-C9
19	B	815	CLA	C11-C10-C8-C9
19	AA	827	CLA	C11-C10-C8-C9
19	BB	803	CLA	C11-C12-C13-C14
19	BB	810	CLA	C6-C7-C8-C9
19	BB	815	CLA	C6-C7-C8-C9
19	BB	833	CLA	C6-C7-C8-C9
19	BB	836	CLA	C6-C7-C8-C9
22	X	102	LHG	C30-C31-C32-C33
25	I2	105	LMG	C8-C7-O1-C1
28	B	856	DGD	C2G-C3G-O3G-C1D
28	BB	854	DGD	C2G-C3G-O3G-C1D
22	BB	851	LHG	C12-C13-C14-C15
19	A1	825	CLA	CAA-CBA-CGA-O1A
19	B	828	CLA	CAA-CBA-CGA-O2A
19	L1	207	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	C2A-CAA-CBA-CGA
19	XX	101	CLA	C2A-CAA-CBA-CGA
19	B	824	CLA	C2-C1-O2A-CGA
19	BB	824	CLA	C2-C1-O2A-CGA
19	B1	829	CLA	C3-C5-C6-C7
19	B2	807	CLA	C3-C5-C6-C7
19	A1	828	CLA	C16-C17-C18-C20
19	A1	841	CLA	C16-C17-C18-C20
19	AA	821	CLA	C16-C17-C18-C19
19	AA	809	CLA	CBA-CGA-O2A-C1
19	A1	832	CLA	C3A-C2A-CAA-CBA
19	A1	852	CLA	C3A-C2A-CAA-CBA
19	B1	801	CLA	C3A-C2A-CAA-CBA
19	B1	807	CLA	C3A-C2A-CAA-CBA
19	B1	833	CLA	C3A-C2A-CAA-CBA
19	A2	833	CLA	C3A-C2A-CAA-CBA
19	A2	836	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B2	810	CLA	C3A-C2A-CAA-CBA
19	A	836	CLA	C3A-C2A-CAA-CBA
19	B	834	CLA	C3A-C2A-CAA-CBA
19	F	301	CLA	C3A-C2A-CAA-CBA
19	AA	833	CLA	C3A-C2A-CAA-CBA
19	BB	831	CLA	C3A-C2A-CAA-CBA
19	B	807	CLA	C2C-C3C-CAC-CBC
19	B2	820	CLA	CAA-CBA-CGA-O2A
19	B	846	CLA	C2A-CAA-CBA-CGA
19	A	816	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	C2-C3-C5-C6
19	B2	825	CLA	O1D-CGD-O2D-CED
22	X2	103	LHG	C12-C13-C14-C15
19	F1	305	CLA	CAA-CBA-CGA-O1A
22	BB	850	LHG	C11-C10-C9-C8
20	A2	803	CL0	CAA-CBA-CGA-O2A
25	I1	102	LMG	C9-C8-O7-C10
23	F1	303	BCR	C18-C19-C20-C21
23	I2	101	BCR	C18-C19-C20-C21
23	I	101	BCR	C10-C11-C12-C13
19	B1	820	CLA	CAA-CBA-CGA-O2A
22	XX	102	LHG	C31-C32-C33-C34
20	A	803	CL0	CAA-CBA-CGA-O2A
23	B2	843	BCR	C9-C10-C11-C12
23	I2	103	BCR	C14-C15-C16-C17
23	II	104	BCR	C14-C15-C16-C17
19	A1	804	CLA	C11-C12-C13-C15
19	A1	836	CLA	CAA-CBA-CGA-O1A
19	B1	831	CLA	CAA-CBA-CGA-O2A
19	A2	837	CLA	CAA-CBA-CGA-O1A
22	XX	102	LHG	C30-C31-C32-C33
19	AA	842	CLA	C16-C17-C18-C19
23	A1	850	BCR	C20-C21-C22-C23
23	I1	101	BCR	C11-C10-C9-C8
23	A2	851	BCR	C16-C17-C18-C19
23	BB	841	BCR	C20-C21-C22-C23
23	II	102	BCR	C20-C21-C22-C23
19	AA	807	CLA	C15-C16-C17-C18
25	B	845	LMG	C39-C40-C41-C42
23	A1	848	BCR	C22-C23-C24-C25
23	AA	851	BCR	C22-C23-C24-C25
19	A	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	I2	105	LMG	O1-C7-C8-C9
25	I2	105	LMG	C7-C8-C9-O8
28	BB	854	DGD	O1G-C1G-C2G-C3G
19	A1	806	CLA	C15-C16-C17-C18
19	B1	815	CLA	C5-C6-C7-C8
19	L	204	CLA	C13-C15-C16-C17
19	B2	852	CLA	C16-C17-C18-C20
19	B2	832	CLA	CAA-CBA-CGA-O2A
19	B	828	CLA	CAA-CBA-CGA-O1A
19	A1	803	CLA	C4-C3-C5-C6
19	A1	810	CLA	C2A-CAA-CBA-CGA
19	A2	806	CLA	C2A-CAA-CBA-CGA
19	AA	831	CLA	C2A-CAA-CBA-CGA
19	B1	820	CLA	CAA-CBA-CGA-O1A
19	B2	820	CLA	CAA-CBA-CGA-O1A
23	I2	101	BCR	C15-C16-C17-C18
23	JJ	104	BCR	C15-C16-C17-C18
19	B2	836	CLA	C16-C17-C18-C19
19	A	842	CLA	C16-C17-C18-C19
22	L	207	LHG	C10-C11-C12-C13
19	A2	809	CLA	CBA-CGA-O2A-C1
19	AA	822	CLA	CAA-CBA-CGA-O2A
19	AA	831	CLA	CAA-CBA-CGA-O2A
25	B	851	LMG	O7-C10-C11-C12
19	B2	825	CLA	C3-C5-C6-C7
19	A1	852	CLA	C11-C12-C13-C14
19	B1	832	CLA	C11-C12-C13-C14
19	B1	836	CLA	C6-C7-C8-C9
19	B2	833	CLA	C11-C12-C13-C14
19	B2	849	CLA	C6-C7-C8-C9
19	L2	206	CLA	C11-C12-C13-C14
19	B	815	CLA	C6-C7-C8-C9
19	B	833	CLA	C11-C12-C13-C14
19	B	836	CLA	C14-C13-C15-C16
19	AA	806	CLA	C6-C7-C8-C9
19	BB	825	CLA	C6-C7-C8-C9
19	BB	826	CLA	C11-C12-C13-C14
19	BB	832	CLA	C11-C12-C13-C14
19	A1	828	CLA	C16-C17-C18-C19
19	AA	821	CLA	C16-C17-C18-C20
19	A1	838	CLA	CAA-CBA-CGA-O2A
19	A	839	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	B	854	CLA	CAA-CBA-CGA-O2A
19	A2	829	CLA	C2C-C3C-CAC-CBC
23	I1	101	BCR	C11-C12-C13-C14
23	A	849	BCR	C7-C8-C9-C10
23	I	101	BCR	C17-C18-C19-C20
23	BB	843	BCR	C7-C8-C9-C10
19	A1	830	CLA	CAA-CBA-CGA-O2A
19	B1	811	CLA	C6-C7-C8-C10
19	B1	811	CLA	C11-C12-C13-C15
19	B1	828	CLA	C12-C13-C15-C16
19	B1	833	CLA	C6-C7-C8-C10
19	A2	827	CLA	C11-C10-C8-C7
19	A2	852	CLA	C11-C12-C13-C15
19	B2	811	CLA	C6-C7-C8-C10
19	B2	811	CLA	C11-C12-C13-C15
19	B2	834	CLA	C6-C7-C8-C10
19	A	804	CLA	C6-C7-C8-C10
19	A	852	CLA	C11-C12-C13-C15
19	B	808	CLA	C6-C7-C8-C10
19	B	834	CLA	C6-C7-C8-C10
19	B	837	CLA	C6-C7-C8-C10
19	AA	804	CLA	C6-C7-C8-C10
19	AA	807	CLA	C11-C10-C8-C7
19	AA	810	CLA	C11-C12-C13-C15
19	AA	819	CLA	C11-C10-C8-C7
19	AA	842	CLA	C6-C7-C8-C10
19	BB	810	CLA	C6-C7-C8-C10
19	BB	825	CLA	C12-C13-C15-C16
19	BB	833	CLA	C6-C7-C8-C10
25	I2	105	LMG	C13-C14-C15-C16
22	A2	845	LHG	C11-C12-C13-C14
22	A2	845	LHG	C33-C34-C35-C36
19	A1	804	CLA	C2B-C3B-CAB-CBB
19	B1	803	CLA	C2B-C3B-CAB-CBB
19	X1	101	CLA	C2B-C3B-CAB-CBB
19	A2	813	CLA	C2B-C3B-CAB-CBB
19	A	809	CLA	C2B-C3B-CAB-CBB
19	B	805	CLA	C2B-C3B-CAB-CBB
23	A1	850	BCR	C5-C6-C7-C8
23	A1	851	BCR	C1-C6-C7-C8
23	A1	851	BCR	C5-C6-C7-C8
23	F1	303	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	F1	306	BCR	C23-C24-C25-C30
23	J1	102	BCR	C1-C6-C7-C8
23	K1	104	BCR	C23-C24-C25-C26
23	L1	209	BCR	C23-C24-C25-C26
23	A2	850	BCR	C1-C6-C7-C8
23	A2	850	BCR	C5-C6-C7-C8
23	A2	851	BCR	C1-C6-C7-C8
23	A2	851	BCR	C5-C6-C7-C8
23	B2	843	BCR	C23-C24-C25-C26
23	F2	303	BCR	C5-C6-C7-C8
23	J2	102	BCR	C1-C6-C7-C8
23	L2	207	BCR	C23-C24-C25-C26
23	A	848	BCR	C1-C6-C7-C8
23	A	850	BCR	C1-C6-C7-C8
23	A	850	BCR	C5-C6-C7-C8
23	A	851	BCR	C1-C6-C7-C8
23	A	851	BCR	C5-C6-C7-C8
23	F	303	BCR	C5-C6-C7-C8
23	F	305	BCR	C23-C24-C25-C26
23	I	101	BCR	C5-C6-C7-C8
23	J	102	BCR	C5-C6-C7-C8
23	J	102	BCR	C23-C24-C25-C26
23	L	205	BCR	C1-C6-C7-C8
23	L	205	BCR	C5-C6-C7-C8
23	AA	849	BCR	C1-C6-C7-C8
23	AA	851	BCR	C1-C6-C7-C8
23	AA	851	BCR	C5-C6-C7-C8
23	AA	852	BCR	C1-C6-C7-C8
23	AA	852	BCR	C5-C6-C7-C8
23	BB	842	BCR	C23-C24-C25-C26
23	FF	303	BCR	C5-C6-C7-C8
23	II	101	BCR	C5-C6-C7-C8
23	II	104	BCR	C1-C6-C7-C8
23	II	104	BCR	C5-C6-C7-C8
23	JJ	102	BCR	C5-C6-C7-C8
23	JJ	102	BCR	C23-C24-C25-C26
23	MM	101	BCR	C5-C6-C7-C8
19	B1	821	CLA	C5-C6-C7-C8
24	L2	203	AJP	O31-C26-O25-C23
22	X1	103	LHG	C28-C29-C30-C31
19	B2	808	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	BB	801	CLA	C2-C1-O2A-CGA
19	LL	201	CLA	C2-C1-O2A-CGA
19	B2	822	CLA	C16-C17-C18-C19
19	B2	837	CLA	C11-C12-C13-C15
19	L1	205	CLA	C8-C10-C11-C12
19	L2	204	CLA	C8-C10-C11-C12
22	XX	102	LHG	C27-C28-C29-C30
19	A1	827	CLA	CAA-CBA-CGA-O2A
19	A1	852	CLA	CAA-CBA-CGA-O2A
19	B1	810	CLA	CAA-CBA-CGA-O2A
19	B1	848	CLA	CAA-CBA-CGA-O2A
19	A2	830	CLA	CAA-CBA-CGA-O2A
19	A2	839	CLA	CAA-CBA-CGA-O2A
19	A	852	CLA	C5-C6-C7-C8
22	B1	847	LHG	C24-C25-C26-C27
19	A	821	CLA	C16-C17-C18-C19
19	FF	301	CLA	C2C-C3C-CAC-CBC
25	I2	105	LMG	C20-C21-C22-C23
19	A1	828	CLA	CAA-CBA-CGA-O2A
22	A1	846	LHG	C14-C15-C16-C17
19	A2	831	CLA	C2A-CAA-CBA-CGA
19	L	204	CLA	C4C-C3C-CAC-CBC
19	A2	842	CLA	CAA-CBA-CGA-O2A
19	A	842	CLA	CAA-CBA-CGA-O2A
19	BB	852	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	C5-C6-C7-C8
19	A1	829	CLA	CAA-CBA-CGA-O2A
19	A1	841	CLA	CAA-CBA-CGA-O2A
19	A	852	CLA	CAA-CBA-CGA-O2A
19	AA	839	CLA	CAA-CBA-CGA-O2A
19	B1	801	CLA	CAA-CBA-CGA-O2A
19	A2	852	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	CAA-CBA-CGA-O2A
19	L	202	CLA	CAA-CBA-CGA-O2A
19	B1	831	CLA	CAA-CBA-CGA-O1A
22	X	102	LHG	C27-C28-C29-C30
22	B1	847	LHG	C25-C26-C27-C28
19	F	301	CLA	C11-C12-C13-C15
19	A1	807	CLA	C2A-CAA-CBA-CGA
19	A1	830	CLA	C2A-CAA-CBA-CGA
19	B2	832	CLA	CAA-CBA-CGA-O1A
19	A1	821	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	831	CLA	CAA-CBA-CGA-O2A
19	AA	843	CLA	CAA-CBA-CGA-O2A
28	BB	854	DGD	C4E-C5E-C6E-O5E
22	B	853	LHG	C25-C26-C27-C28
19	A1	829	CLA	C11-C12-C13-C14
19	B1	804	CLA	C11-C10-C8-C9
19	B	826	CLA	C11-C12-C13-C14
19	L	204	CLA	C6-C7-C8-C9
22	X2	103	LHG	C34-C35-C36-C37
19	A	807	CLA	C15-C16-C17-C18
19	A1	842	CLA	CAA-CBA-CGA-O2A
19	A2	831	CLA	CAA-CBA-CGA-O2A
19	B2	810	CLA	CAA-CBA-CGA-O2A
19	B2	852	CLA	CAA-CBA-CGA-O2A
19	A	829	CLA	CAA-CBA-CGA-O2A
22	BB	850	LHG	O8-C23-C24-C25
28	B	856	DGD	O1G-C1G-C2G-C3G
19	B	860	CLA	C5-C6-C7-C8
19	A1	804	CLA	C4B-C3B-CAB-CBB
19	A1	813	CLA	C4B-C3B-CAB-CBB
19	A1	831	CLA	C1A-C2A-CAA-CBA
19	A1	836	CLA	C4B-C3B-CAB-CBB
19	B1	804	CLA	C4B-C3B-CAB-CBB
19	B1	807	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C4B-C3B-CAB-CBB
19	L1	207	CLA	C1A-C2A-CAA-CBA
19	X1	101	CLA	C1A-C2A-CAA-CBA
19	A2	814	CLA	C4B-C3B-CAB-CBB
19	A2	819	CLA	C4B-C3B-CAB-CBB
19	A2	832	CLA	C1A-C2A-CAA-CBA
19	A2	837	CLA	C4B-C3B-CAB-CBB
19	A2	852	CLA	C1A-C2A-CAA-CBA
19	B2	804	CLA	C4B-C3B-CAB-CBB
19	B2	807	CLA	C1A-C2A-CAA-CBA
19	B2	807	CLA	C4B-C3B-CAB-CBB
19	B2	809	CLA	C4B-C3B-CAB-CBB
19	B2	811	CLA	C1A-C2A-CAA-CBA
19	B2	820	CLA	C4B-C3B-CAB-CBB
19	B2	837	CLA	C4B-C3B-CAB-CBB
19	L2	204	CLA	C1A-C2A-CAA-CBA
19	L2	206	CLA	C1A-C2A-CAA-CBA
19	X2	101	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	X2	101	CLA	C4B-C3B-CAB-CBB
19	A	827	CLA	C4B-C3B-CAB-CBB
19	A	832	CLA	C1A-C2A-CAA-CBA
19	B	810	CLA	C1A-C2A-CAA-CBA
19	K	101	CLA	C4B-C3B-CAB-CBB
19	X	101	CLA	C4B-C3B-CAB-CBB
19	AA	813	CLA	C4B-C3B-CAB-CBB
19	AA	827	CLA	C4B-C3B-CAB-CBB
19	AA	836	CLA	C1A-C2A-CAA-CBA
19	BB	810	CLA	C1A-C2A-CAA-CBA
19	BB	811	CLA	C1A-C2A-CAA-CBA
19	BB	823	CLA	C4B-C3B-CAB-CBB
19	BB	832	CLA	C1A-C2A-CAA-CBA
19	BB	836	CLA	C4B-C3B-CAB-CBB
19	A2	813	CLA	C3-C5-C6-C7
22	A2	846	LHG	C14-C15-C16-C17
19	B2	801	CLA	CAA-CBA-CGA-O2A
19	A	840	CLA	CAA-CBA-CGA-O2A
19	B	860	CLA	CAA-CBA-CGA-O2A
19	AA	842	CLA	CAA-CBA-CGA-O2A
22	B	852	LHG	O8-C23-C24-C25
22	A	845	LHG	O7-C5-C6-O8
23	A1	847	BCR	C11-C12-C13-C14
23	A1	851	BCR	C7-C8-C9-C10
23	K1	104	BCR	C11-C12-C13-C14
23	A2	847	BCR	C11-C12-C13-C14
23	F2	303	BCR	C7-C8-C9-C10
23	J2	104	BCR	C11-C12-C13-C14
23	J2	104	BCR	C17-C18-C19-C20
23	B	840	BCR	C21-C22-C23-C24
23	F	303	BCR	C7-C8-C9-C10
23	B1	841	BCR	C15-C16-C17-C18
23	K1	106	BCR	C9-C10-C11-C12
23	K2	105	BCR	C9-C10-C11-C12
23	M2	102	BCR	C13-C14-C15-C16
26	BB	840	ECH	C9-C10-C11-C12
19	A1	830	CLA	C8-C10-C11-C12
19	L	203	CLA	C8-C10-C11-C12
19	B	817	CLA	CBD-CGD-O2D-CED
19	AA	807	CLA	C16-C17-C18-C20
22	X1	103	LHG	C31-C32-C33-C34
19	A2	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B1	821	CLA	CAA-CBA-CGA-O2A
19	A2	822	CLA	CAA-CBA-CGA-O2A
19	A2	828	CLA	CAA-CBA-CGA-O2A
19	AA	830	CLA	CAA-CBA-CGA-O2A
19	AA	840	CLA	CAA-CBA-CGA-O2A
19	B1	824	CLA	C2A-CAA-CBA-CGA
19	B2	810	CLA	C2A-CAA-CBA-CGA
22	L	207	LHG	C13-C14-C15-C16
19	A2	829	CLA	C4C-C3C-CAC-CBC
19	B1	804	CLA	C10-C11-C12-C13
19	A1	829	CLA	O1A-CGA-O2A-C1
19	L	203	CLA	C3-C5-C6-C7
19	AA	822	CLA	C2-C3-C5-C6
19	B	821	CLA	C5-C6-C7-C8
19	B	814	CLA	C4-C3-C5-C6
19	B2	821	CLA	CAA-CBA-CGA-O2A
19	A	828	CLA	CAA-CBA-CGA-O2A
19	B1	808	CLA	C6-C7-C8-C10
19	B2	808	CLA	C6-C7-C8-C10
19	B2	816	CLA	C6-C7-C8-C10
19	B2	822	CLA	C11-C10-C8-C7
19	A	810	CLA	C11-C12-C13-C15
19	A	827	CLA	C11-C10-C8-C7
19	A	842	CLA	C6-C7-C8-C10
19	B	807	CLA	C6-C7-C8-C10
19	L	204	CLA	C12-C13-C15-C16
19	BB	804	CLA	C11-C10-C8-C7
19	BB	807	CLA	C6-C7-C8-C10
19	BB	822	CLA	C11-C10-C8-C7
19	A2	840	CLA	C2-C3-C5-C6
19	A	804	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	A1	819	CLA	C5-C6-C7-C8
22	A2	845	LHG	C18-C19-C20-C21
19	B1	836	CLA	C11-C12-C13-C15
19	AA	827	CLA	O2A-C1-C2-C3
19	BB	821	CLA	O2A-C1-C2-C3
22	BB	851	LHG	C28-C29-C30-C31
19	L	204	CLA	CAA-CBA-CGA-O2A
19	AA	828	CLA	CAA-CBA-CGA-O2A
25	L1	210	LMG	O7-C10-C11-C12
19	A2	807	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	A	845	LHG	C33-C34-C35-C36
19	B2	824	CLA	C2A-CAA-CBA-CGA
22	X2	102	LHG	O9-C7-O7-C5
19	A2	842	CLA	C16-C17-C18-C19
19	AA	836	CLA	C16-C17-C18-C20
19	A1	809	CLA	C5-C6-C7-C8
19	A2	829	CLA	C15-C16-C17-C18
19	B2	852	CLA	C5-C6-C7-C8
19	AA	820	CLA	CAA-CBA-CGA-O2A
19	B2	833	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	C3A-C2A-CAA-CBA
19	BB	810	CLA	C3A-C2A-CAA-CBA
19	BB	833	CLA	C3A-C2A-CAA-CBA
19	B1	810	CLA	CAA-CBA-CGA-O1A
19	B	854	CLA	CAA-CBA-CGA-O1A
19	A1	842	CLA	C5-C6-C7-C8
19	B	806	CLA	C13-C15-C16-C17
19	B2	822	CLA	C16-C17-C18-C20
19	AA	807	CLA	C16-C17-C18-C19
19	AA	835	CLA	C16-C17-C18-C20
19	A	830	CLA	CAA-CBA-CGA-O2A
23	A1	853	BCR	C20-C21-C22-C23
23	M1	101	BCR	C20-C21-C22-C23
23	A2	850	BCR	C20-C21-C22-C23
23	K2	103	BCR	C16-C17-C18-C19
23	B	848	BCR	C16-C17-C18-C19
19	A	837	CLA	CAA-CBA-CGA-O2A
23	I	101	BCR	C14-C15-C16-C17
19	B	815	CLA	C5-C6-C7-C8
19	A1	828	CLA	CAA-CBA-CGA-O1A
19	A1	830	CLA	CAA-CBA-CGA-O1A
22	AA	846	LHG	C25-C26-C27-C28
19	L	203	CLA	CAA-CBA-CGA-O2A
19	BB	821	CLA	CAA-CBA-CGA-O2A
19	B1	836	CLA	C2C-C3C-CAC-CBC
19	AA	842	CLA	CAA-CBA-CGA-O1A
19	B	804	CLA	C10-C11-C12-C13
19	A	820	CLA	C2A-CAA-CBA-CGA
19	A	827	CLA	C2A-CAA-CBA-CGA
19	BB	809	CLA	CAA-CBA-CGA-O1A
19	A1	818	CLA	C11-C10-C8-C9
19	B1	808	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B2	804	CLA	C11-C10-C8-C9
19	B2	834	CLA	C11-C10-C8-C9
19	A	806	CLA	C6-C7-C8-C9
19	A	807	CLA	C11-C10-C8-C9
19	A	819	CLA	C11-C10-C8-C9
19	B	803	CLA	C11-C12-C13-C14
19	B	806	CLA	C14-C13-C15-C16
19	B	837	CLA	C6-C7-C8-C9
19	BB	808	CLA	C6-C7-C8-C9
19	BB	815	CLA	C11-C10-C8-C9
19	A1	839	CLA	CAA-CBA-CGA-O2A
19	B1	848	CLA	CAA-CBA-CGA-O1A
19	A2	822	CLA	CAA-CBA-CGA-O1A
19	A2	842	CLA	CAA-CBA-CGA-O1A
19	B2	821	CLA	CAA-CBA-CGA-O1A
19	BB	852	CLA	CAA-CBA-CGA-O1A
22	A	846	LHG	C11-C12-C13-C14
22	LL	205	LHG	C12-C13-C14-C15
23	F2	303	BCR	C9-C10-C11-C12
23	I	101	BCR	C15-C16-C17-C18
23	FF	303	BCR	C9-C10-C11-C12
19	B2	809	CLA	CAA-CBA-CGA-O2A
19	A2	808	CLA	C5-C6-C7-C8
19	L2	206	CLA	C8-C10-C11-C12
19	AA	843	CLA	C5-C6-C7-C8
23	B1	839	BCR	C11-C12-C13-C35
19	B1	801	CLA	CAA-CBA-CGA-O1A
19	A	839	CLA	CAA-CBA-CGA-O1A
19	B	860	CLA	CAA-CBA-CGA-O1A
19	AA	828	CLA	CAA-CBA-CGA-O1A
19	AA	831	CLA	CAA-CBA-CGA-O1A
19	B1	824	CLA	CAA-CBA-CGA-O2A
22	LL	205	LHG	C13-C14-C15-C16
19	A2	810	CLA	C5-C6-C7-C8
19	B1	809	CLA	CAA-CBA-CGA-O2A
19	A1	852	CLA	CAA-CBA-CGA-O1A
19	A2	830	CLA	CAA-CBA-CGA-O1A
19	A2	839	CLA	CAA-CBA-CGA-O1A
19	A	852	CLA	CAA-CBA-CGA-O1A
19	AA	822	CLA	CAA-CBA-CGA-O1A
19	AA	830	CLA	CAA-CBA-CGA-O1A
22	B	852	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	BB	811	CLA	O1D-CGD-O2D-CED
22	X1	102	LHG	C29-C30-C31-C32
22	AA	847	LHG	C11-C12-C13-C14
19	B2	836	CLA	C3-C5-C6-C7
22	L	207	LHG	C12-C13-C14-C15
23	K1	104	BCR	C17-C18-C19-C20
23	A2	853	BCR	C17-C18-C19-C20
19	A	825	CLA	O1D-CGD-O2D-CED
19	A1	841	CLA	CAA-CBA-CGA-O1A
19	B1	821	CLA	CAA-CBA-CGA-O1A
19	A2	828	CLA	CAA-CBA-CGA-O1A
19	B2	801	CLA	CAA-CBA-CGA-O1A
19	A	828	CLA	CAA-CBA-CGA-O1A
19	AA	839	CLA	CAA-CBA-CGA-O1A
22	BB	850	LHG	O10-C23-C24-C25
25	B	845	LMG	O10-C28-C29-C30
25	BB	844	LMG	O10-C28-C29-C30
28	B	856	DGD	O1B-C1B-C2B-C3B
28	BB	854	DGD	O1B-C1B-C2B-C3B
23	LL	204	BCR	C18-C19-C20-C21
19	B2	821	CLA	C13-C15-C16-C17
28	B	856	DGD	C5D-C6D-O5D-C1E
28	BB	854	DGD	C5D-C6D-O5D-C1E
19	A1	821	CLA	CAA-CBA-CGA-O1A
19	A1	829	CLA	CAA-CBA-CGA-O1A
19	A1	838	CLA	CAA-CBA-CGA-O1A
19	A2	852	CLA	CAA-CBA-CGA-O1A
19	L	202	CLA	CAA-CBA-CGA-O1A
19	B2	824	CLA	CAA-CBA-CGA-O2A
19	B2	821	CLA	C5-C6-C7-C8
19	X1	101	CLA	C2A-CAA-CBA-CGA
19	A2	820	CLA	C2A-CAA-CBA-CGA
19	AA	836	CLA	C16-C17-C18-C19
19	J	103	CLA	C4C-C3C-CAC-CBC
19	A1	827	CLA	CAA-CBA-CGA-O1A
25	B1	846	LMG	C14-C15-C16-C17
19	B2	810	CLA	C5-C6-C7-C8
19	AA	831	CLA	C8-C10-C11-C12
22	A1	845	LHG	C16-C17-C18-C19
19	B	829	CLA	C10-C11-C12-C13
19	A1	842	CLA	CAA-CBA-CGA-O1A
19	A	822	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	CAA-CBA-CGA-O1A
19	A	830	CLA	CAA-CBA-CGA-O1A
19	A	842	CLA	CAA-CBA-CGA-O1A
19	A	814	CLA	CAD-CBD-CGD-O2D
19	A	821	CLA	CAD-CBD-CGD-O2D
19	A	823	CLA	CAD-CBD-CGD-O2D
19	B	820	CLA	CAD-CBD-CGD-O2D
19	B	828	CLA	CAD-CBD-CGD-O2D
19	AA	816	CLA	CAD-CBD-CGD-O2D
19	BB	820	CLA	CAD-CBD-CGD-O2D
19	BB	828	CLA	CAD-CBD-CGD-O2D
19	B1	850	CLA	C8-C10-C11-C12
19	AA	836	CLA	C5-C6-C7-C8
19	A2	841	CLA	CAA-CBA-CGA-O2A
19	FF	301	CLA	CAA-CBA-CGA-O2A
19	B2	852	CLA	CAA-CBA-CGA-O1A
22	L1	211	LHG	O2-C2-C3-O3
19	B2	804	CLA	C10-C11-C12-C13
19	B2	814	CLA	O1A-CGA-O2A-C1
24	L2	203	AJP	C27-C26-O25-C23
23	A	848	BCR	C22-C23-C24-C25
23	AA	849	BCR	C22-C23-C24-C25
19	B1	801	CLA	C2-C1-O2A-CGA
19	B1	824	CLA	C2-C1-O2A-CGA
19	AA	843	CLA	CAA-CBA-CGA-O1A
19	A2	821	CLA	O1D-CGD-O2D-CED
19	BB	802	CLA	CAA-CBA-CGA-O2A
19	A1	841	CLA	C16-C17-C18-C19
19	A	821	CLA	C16-C17-C18-C20
19	AA	829	CLA	C16-C17-C18-C19
22	AA	846	LHG	C11-C12-C13-C14
19	B1	809	CLA	CAA-CBA-CGA-O1A
19	A	837	CLA	CAA-CBA-CGA-O1A
19	B2	810	CLA	CAA-CBA-CGA-O1A
19	BB	821	CLA	CAA-CBA-CGA-O1A
19	A1	820	CLA	C12-C13-C15-C16
19	A2	835	CLA	C11-C10-C8-C7
19	BB	829	CLA	C6-C7-C8-C10
19	B1	802	CLA	CAA-CBA-CGA-O2A
19	B	801	CLA	CAA-CBA-CGA-O2A
19	B	821	CLA	CAA-CBA-CGA-O2A
19	BB	824	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	BB	850	LHG	O7-C7-C8-C9
25	II	105	LMG	O8-C28-C29-C30
19	B2	809	CLA	CAA-CBA-CGA-O1A
19	A2	831	CLA	CAA-CBA-CGA-O1A
22	A1	845	LHG	C18-C19-C20-C21
19	A	820	CLA	CAA-CBA-CGA-O2A
19	B	824	CLA	CAA-CBA-CGA-O2A
28	BB	854	DGD	O2G-C1B-C2B-C3B
19	B2	814	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	CAA-CBA-CGA-O2A
19	A	840	CLA	CAA-CBA-CGA-O1A
19	L	203	CLA	CAA-CBA-CGA-O1A
19	L	204	CLA	CAA-CBA-CGA-O1A
19	AA	840	CLA	CAA-CBA-CGA-O1A
25	B2	845	LMG	O10-C28-C29-C30

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	855	AJP	C19-C20-C21-C22-C23-C24

314 monomers are involved in 452 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	AA	841	CLA	1	0
19	A2	840	CLA	1	0
19	X2	101	CLA	1	0
23	K1	106	BCR	2	0
19	B1	821	CLA	1	0
19	A1	834	CLA	2	0
19	A1	842	CLA	1	0
20	A	803	CL0	2	0
19	F1	302	CLA	1	0
19	A1	836	CLA	1	0
23	F	305	BCR	4	0
19	A	833	CLA	1	0
19	B	854	CLA	1	0
19	LL	201	CLA	4	0
19	B	812	CLA	2	0
19	JJ	103	CLA	1	0
19	B	859	CLA	2	0
19	BB	823	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AA	852	BCR	4	0
23	AA	855	BCR	1	0
19	B	858	CLA	1	0
23	A1	851	BCR	3	0
21	A2	843	PQN	1	0
19	B1	806	CLA	1	0
19	A	836	CLA	1	0
23	J2	104	BCR	2	0
23	K2	105	BCR	2	0
23	AA	848	BCR	1	0
23	F2	303	BCR	2	0
19	A1	839	CLA	2	0
19	J	103	CLA	2	0
19	B2	821	CLA	1	0
19	B1	815	CLA	2	0
19	B2	833	CLA	3	0
19	BB	804	CLA	2	0
23	A	851	BCR	4	0
19	BB	834	CLA	6	0
19	B2	834	CLA	4	0
19	A1	811	CLA	1	0
23	J2	102	BCR	1	0
19	J2	103	CLA	1	0
19	A	828	CLA	2	0
19	A	837	CLA	2	0
19	A1	852	CLA	6	0
19	F2	302	CLA	1	0
19	A2	831	CLA	1	0
19	F2	301	CLA	2	0
19	K2	104	CLA	1	0
22	L1	211	LHG	2	0
24	BB	848	AJP	1	0
19	B	833	CLA	6	0
20	AA	803	CL0	1	0
19	B2	849	CLA	2	0
19	A1	824	CLA	1	0
19	A	818	CLA	1	0
19	BB	806	CLA	2	0
21	B	838	PQN	2	0
19	BB	856	CLA	2	0
19	B2	806	CLA	2	0
23	BB	842	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	I2	105	LMG	1	0
27	C	102	SF4	1	0
19	B2	823	CLA	1	0
19	BB	802	CLA	1	0
19	B1	811	CLA	1	0
19	B1	834	CLA	9	0
19	A	815	CLA	3	0
19	A2	833	CLA	1	0
20	A2	803	CL0	4	0
22	B	852	LHG	1	0
19	B2	810	CLA	4	0
19	BB	817	CLA	1	0
19	B1	807	CLA	1	0
19	B	802	CLA	1	0
19	A1	804	CLA	2	0
23	B	843	BCR	4	0
19	B2	837	CLA	1	0
19	A1	817	CLA	2	0
23	J1	104	BCR	1	0
19	A1	828	CLA	3	0
22	L2	208	LHG	1	0
27	C1	102	SF4	1	0
19	B1	802	CLA	1	0
19	BB	822	CLA	2	0
19	BB	815	CLA	2	0
19	AA	853	CLA	3	0
19	B2	836	CLA	1	0
19	A	830	CLA	1	0
23	B2	840	BCR	2	0
19	A2	828	CLA	1	0
23	J	102	BCR	1	0
19	A2	816	CLA	1	0
19	B2	852	CLA	2	0
19	B	837	CLA	1	0
19	AA	843	CLA	1	0
19	B1	836	CLA	1	0
19	L1	207	CLA	1	0
19	A2	836	CLA	1	0
19	A1	801	CLA	1	0
19	B1	825	CLA	1	0
23	A2	847	BCR	1	0
19	A2	802	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B2	839	BCR	1	0
19	A2	818	CLA	2	0
19	F	301	CLA	2	0
19	A1	819	CLA	2	0
23	I1	101	BCR	1	0
23	B	842	BCR	5	0
23	MM	101	BCR	1	0
19	A2	835	CLA	1	0
19	A2	815	CLA	3	0
19	A	834	CLA	2	0
23	BB	839	BCR	1	0
19	A1	815	CLA	2	0
19	AA	821	CLA	2	0
19	L1	206	CLA	1	0
19	A2	837	CLA	1	0
23	AA	851	BCR	1	0
26	B2	841	ECH	1	0
23	J1	102	BCR	1	0
19	A1	840	CLA	1	0
19	L	202	CLA	3	0
23	F1	306	BCR	4	0
19	B1	833	CLA	13	0
19	B1	827	CLA	2	0
19	A	801	CLA	1	0
23	J	104	BCR	1	0
19	B	827	CLA	1	0
19	A2	804	CLA	1	0
19	K1	105	CLA	1	0
19	BB	811	CLA	1	0
19	B	831	CLA	1	0
19	A	804	CLA	1	0
23	A	854	BCR	2	0
19	A	805	CLA	3	0
19	A2	830	CLA	1	0
22	A1	846	LHG	1	0
19	AA	820	CLA	2	0
19	B2	851	CLA	2	0
19	A	806	CLA	1	0
19	A	816	CLA	1	0
19	AA	810	CLA	1	0
19	B	835	CLA	8	0
19	A2	832	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	BB	833	CLA	12	0
19	B	804	CLA	2	0
23	M	101	BCR	2	0
23	K2	103	BCR	1	0
25	L1	210	LMG	1	0
20	A1	802	CL0	4	0
19	B	832	CLA	1	0
19	A2	821	CLA	1	0
23	B1	841	BCR	2	0
21	A1	843	PQN	2	0
19	B2	811	CLA	1	0
19	L1	205	CLA	3	0
22	A	845	LHG	2	0
19	F1	301	CLA	3	0
19	A1	833	CLA	2	0
19	BB	805	CLA	1	0
19	A1	807	CLA	1	0
19	A	822	CLA	3	0
19	A2	834	CLA	1	0
19	A2	842	CLA	4	0
19	BB	829	CLA	2	0
19	BB	801	CLA	1	0
19	AA	831	CLA	1	0
19	BB	821	CLA	1	0
19	B2	822	CLA	1	0
21	A	843	PQN	1	0
23	B1	842	BCR	3	0
19	B	829	CLA	1	0
23	F2	305	BCR	4	0
19	BB	812	CLA	2	0
19	BB	820	CLA	4	0
23	FF	303	BCR	3	0
19	B1	820	CLA	1	0
19	B2	820	CLA	1	0
19	A2	801	CLA	1	0
19	A2	820	CLA	1	0
22	B1	847	LHG	1	0
19	B	828	CLA	3	0
24	B	849	AJP	1	0
19	BB	810	CLA	5	0
19	FF	305	CLA	2	0
19	B1	810	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F1	305	CLA	2	0
19	B	830	CLA	1	0
23	BB	841	BCR	6	0
19	A2	805	CLA	3	0
19	A1	829	CLA	2	0
19	AA	805	CLA	2	0
22	A2	846	LHG	1	0
19	B1	832	CLA	4	0
19	A	826	CLA	1	0
19	AA	830	CLA	3	0
19	A2	806	CLA	2	0
23	A1	847	BCR	2	0
19	A2	841	CLA	1	0
23	B	840	BCR	1	0
19	B	815	CLA	1	0
19	AA	806	CLA	1	0
19	B1	850	CLA	2	0
25	M	102	LMG	1	0
19	B2	850	CLA	1	0
19	A	832	CLA	2	0
19	FF	302	CLA	1	0
19	A2	810	CLA	1	0
19	B	834	CLA	12	0
19	B2	829	CLA	2	0
19	BB	852	CLA	4	0
22	AA	847	LHG	1	0
22	A2	845	LHG	1	0
19	B1	822	CLA	1	0
19	AA	836	CLA	1	0
19	A2	825	CLA	1	0
19	A	842	CLA	2	0
19	AA	828	CLA	3	0
19	A1	814	CLA	3	0
19	B2	809	CLA	1	0
19	AA	842	CLA	2	0
19	L	203	CLA	1	0
19	B	820	CLA	3	0
19	A2	812	CLA	1	0
19	AA	818	CLA	2	0
19	B	811	CLA	1	0
26	BB	840	ECH	2	0
19	B2	827	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B1	839	BCR	1	0
23	B	839	BCR	2	0
23	FF	306	BCR	3	0
26	B	841	ECH	2	0
24	L2	203	AJP	1	0
19	B1	809	CLA	1	0
19	B1	804	CLA	1	0
19	A	820	CLA	3	0
23	JJ	102	BCR	1	0
19	B	810	CLA	3	0
19	AA	815	CLA	3	0
19	B	822	CLA	2	0
19	B	860	CLA	2	0
23	B2	842	BCR	4	0
19	B1	848	CLA	2	0
21	AA	844	PQN	1	0
19	B1	828	CLA	2	0
19	A2	852	CLA	5	0
19	K1	103	CLA	1	0
23	A2	850	BCR	1	0
23	AA	854	BCR	1	0
19	A1	827	CLA	1	0
19	A	821	CLA	1	0
19	BB	832	CLA	6	0
19	AA	827	CLA	1	0
28	B	856	DGD	1	0
19	A1	831	CLA	1	0
22	AA	846	LHG	2	0
26	B1	840	ECH	1	0
19	A1	832	CLA	1	0
19	B2	828	CLA	1	0
19	A	840	CLA	1	0
23	LL	204	BCR	1	0
23	A	847	BCR	1	0
19	FF	301	CLA	2	0
23	F	303	BCR	2	0
23	I2	103	BCR	1	0
19	A	841	CLA	2	0
19	AA	816	CLA	1	0
21	BB	837	PQN	2	0
23	A2	851	BCR	5	0
19	B2	802	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A1	803	CLA	1	0
19	BB	835	CLA	2	0
23	B2	843	BCR	3	0
19	B	826	CLA	2	0
19	BB	826	CLA	2	0
19	BB	828	CLA	3	0
19	B2	835	CLA	3	0
19	AA	834	CLA	1	0
19	B1	826	CLA	1	0
19	B2	826	CLA	2	0
19	A1	835	CLA	1	0
19	B	818	CLA	2	0
19	B	801	CLA	1	0
19	B1	823	CLA	1	0
19	B	823	CLA	1	0
19	AA	804	CLA	2	0
19	AA	822	CLA	1	0
19	AA	832	CLA	1	0
23	L	205	BCR	1	0
23	BB	838	BCR	2	0
19	J1	103	CLA	1	0
19	A	812	CLA	1	0
23	A1	850	BCR	1	0
19	F	302	CLA	1	0
23	B1	838	BCR	1	0
19	AA	826	CLA	1	0
19	B	806	CLA	3	0
19	B1	835	CLA	1	0
23	F1	303	BCR	2	0
19	A	852	CLA	6	0
19	B	836	CLA	2	0
19	A1	844	CLA	1	0
19	A	831	CLA	1	0
23	K1	104	BCR	1	0
19	A1	805	CLA	1	0
19	A2	844	CLA	1	0
19	BB	831	CLA	1	0
24	L1	204	AJP	1	0
19	A1	841	CLA	3	0
19	B2	830	CLA	1	0
19	AA	801	CLA	1	0
23	JJ	104	BCR	1	0

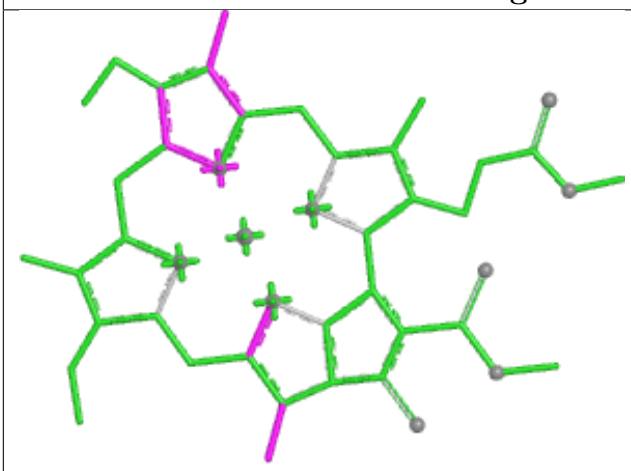
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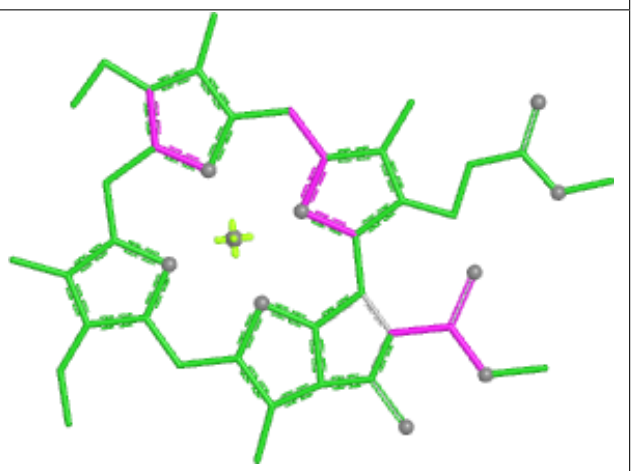
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A1	830	CLA	1	0
19	B	821	CLA	1	0

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

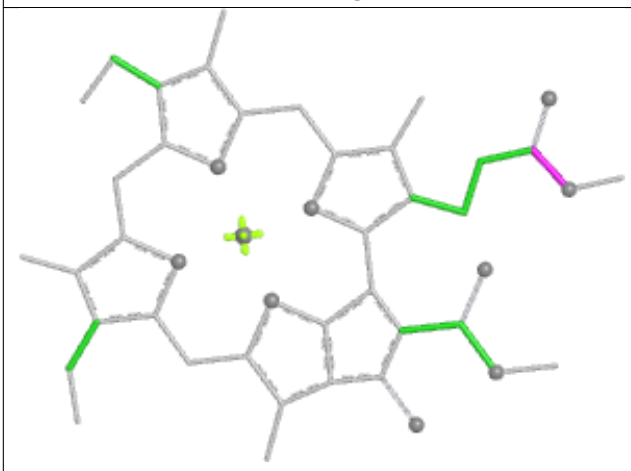
Ligand CLA AA 841



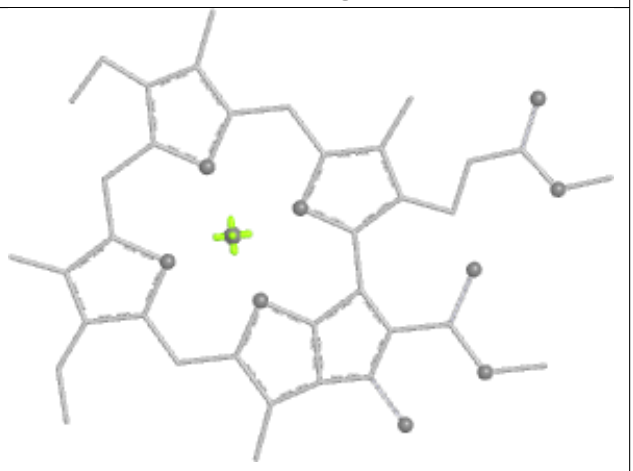
Bond lengths



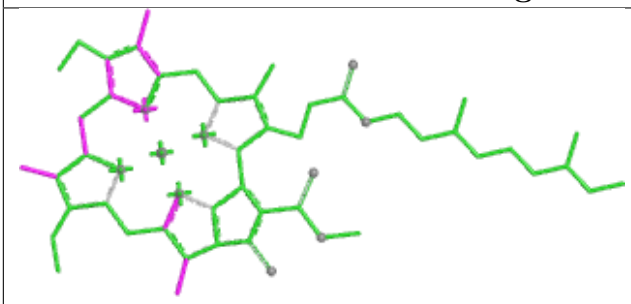
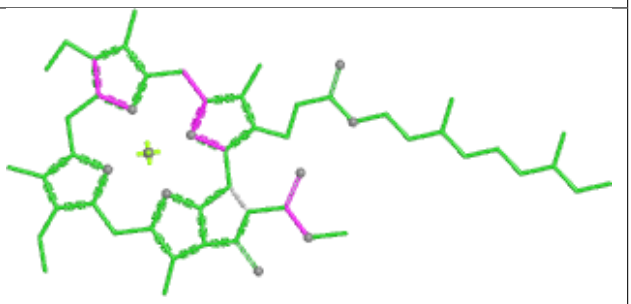
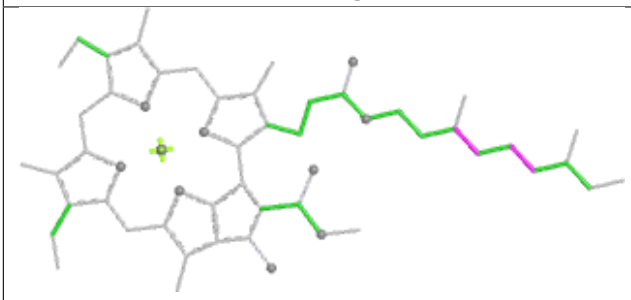
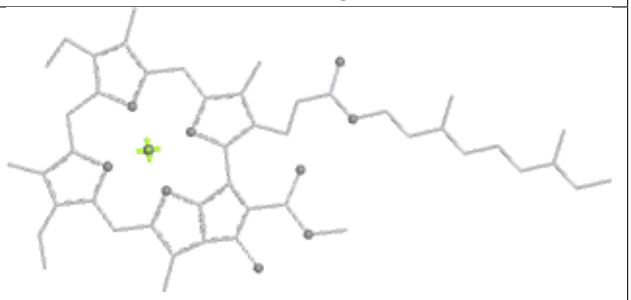
Bond angles



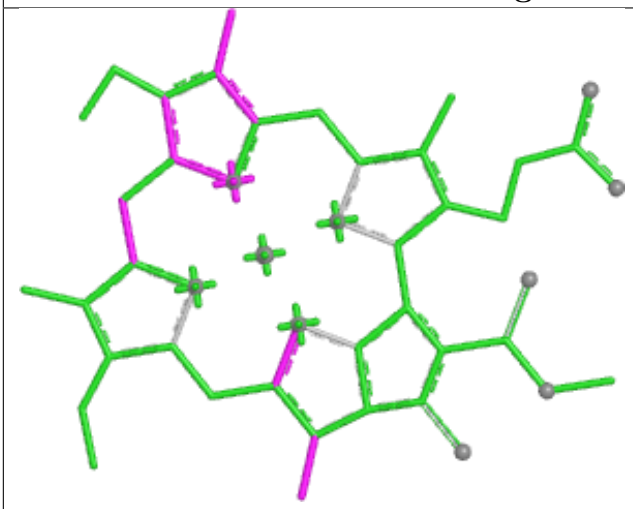
Torsions



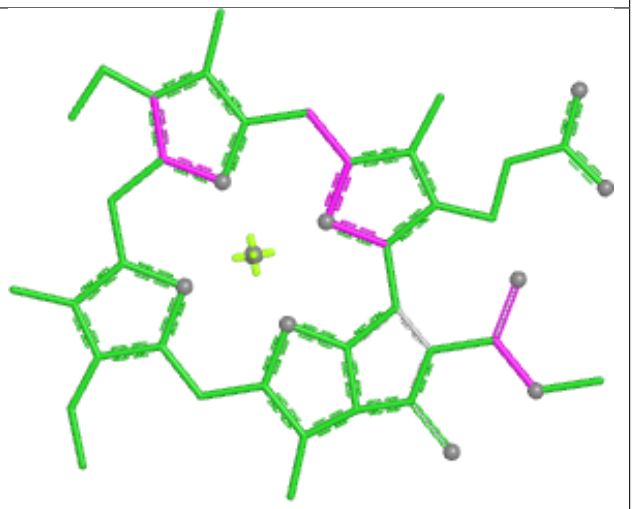
Rings

Ligand CLA A2 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

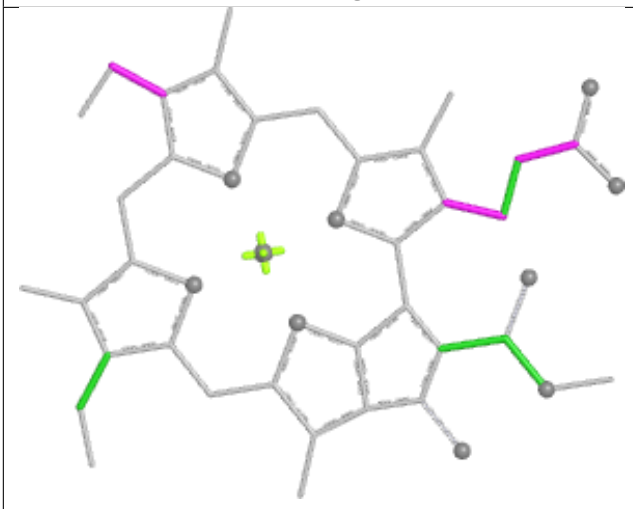
Ligand CLA X2 101



Bond lengths



Bond angles

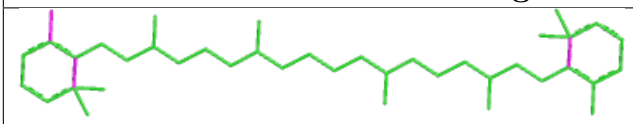


Torsions

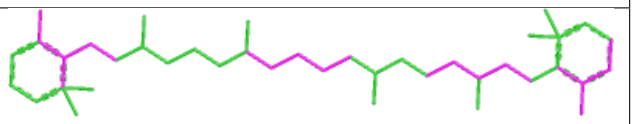


Rings

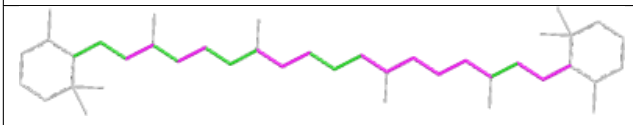
Ligand BCR K1 106



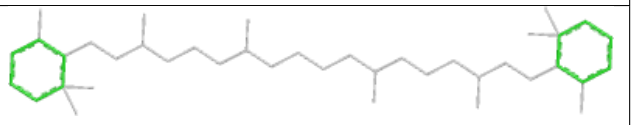
Bond lengths



Bond angles

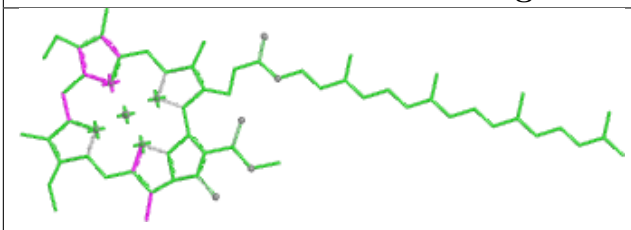


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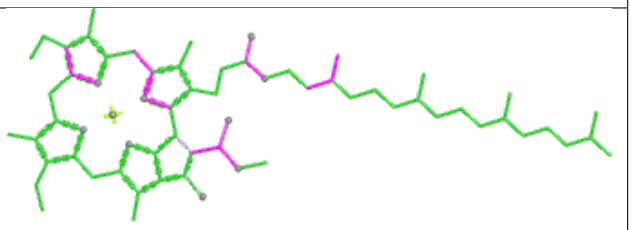


Rings

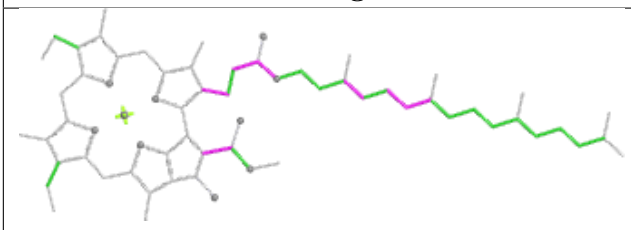
Ligand CLA B1 821



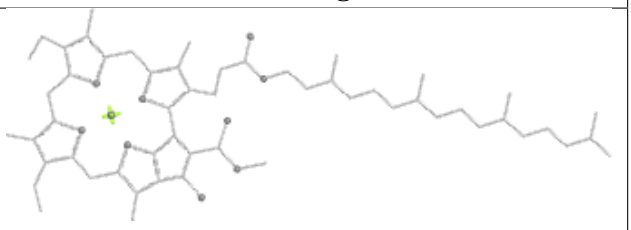
Bond lengths



Bond angles

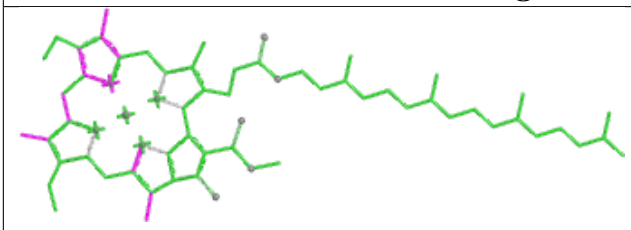


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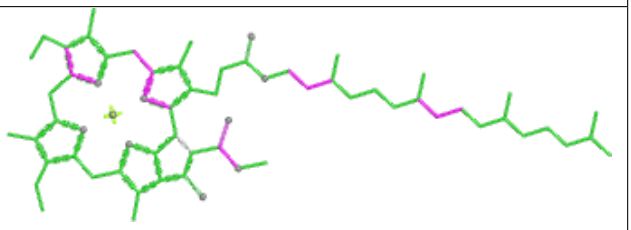


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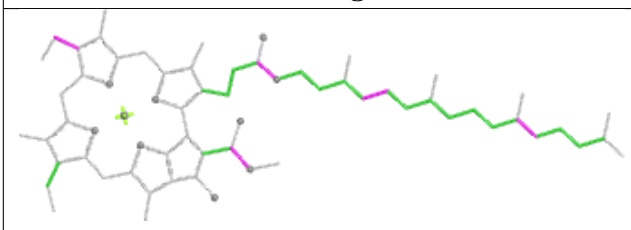
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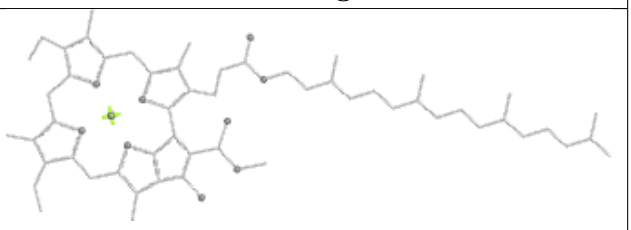
Bond lengths



Bond angles

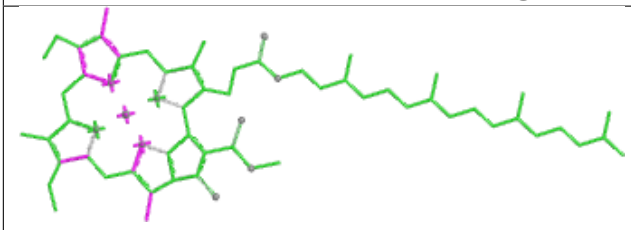


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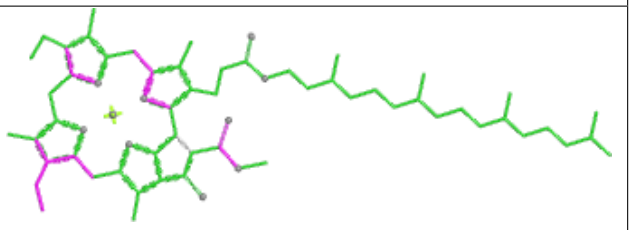


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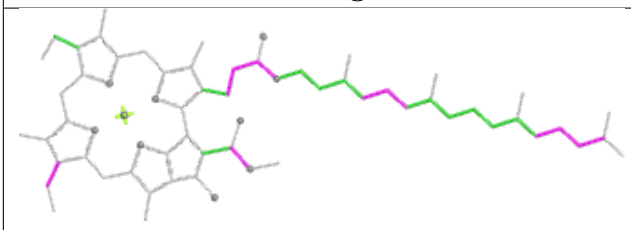
Ligand CLA A1 842



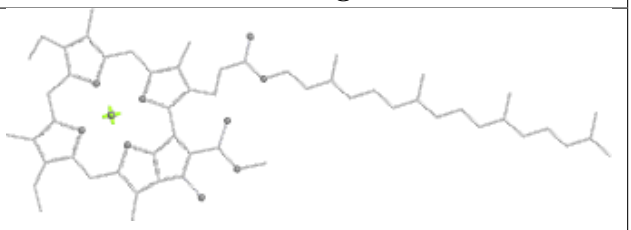
Bond lengths



Bond angles

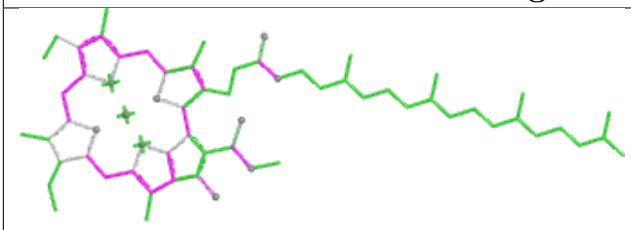


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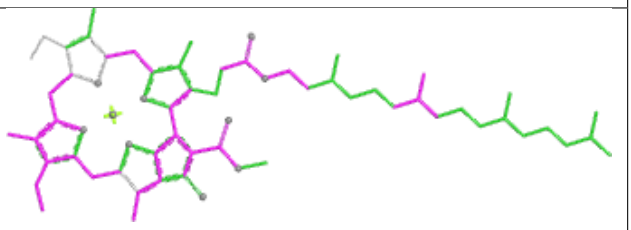


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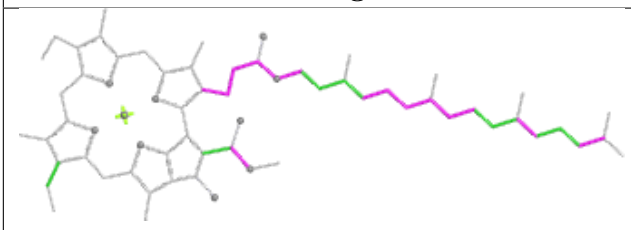
Ligand CL0 A 803



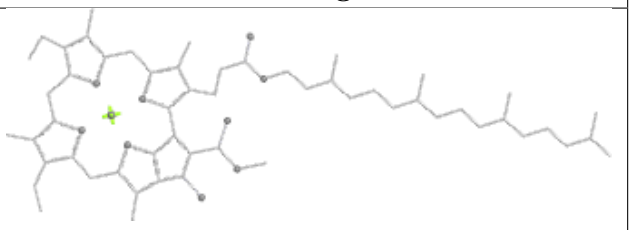
Bond lengths



Bond angles

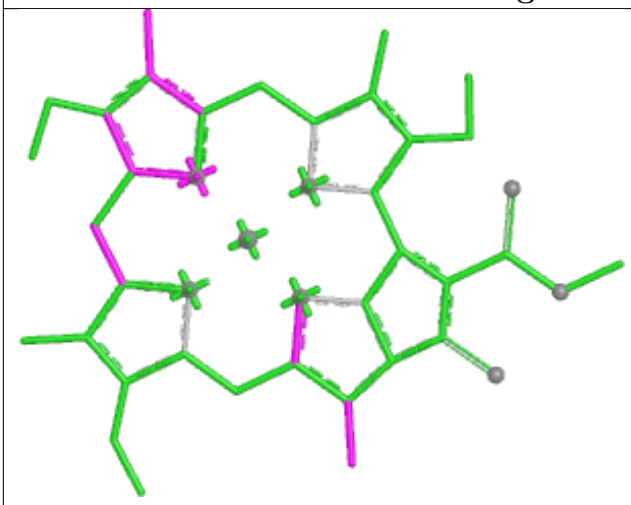


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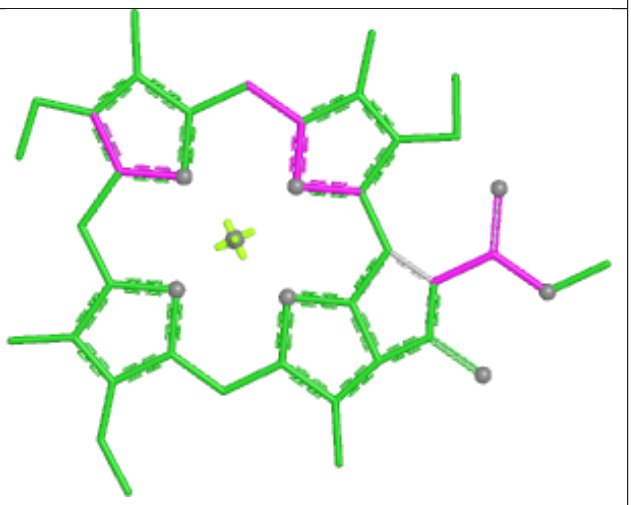


Rings

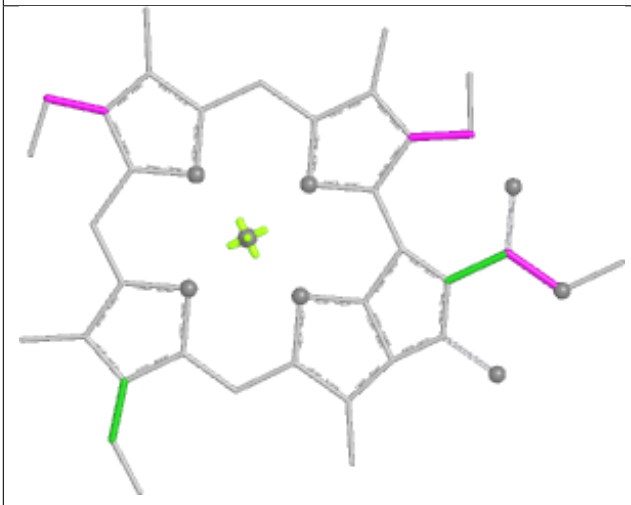
Ligand CLA F1 302



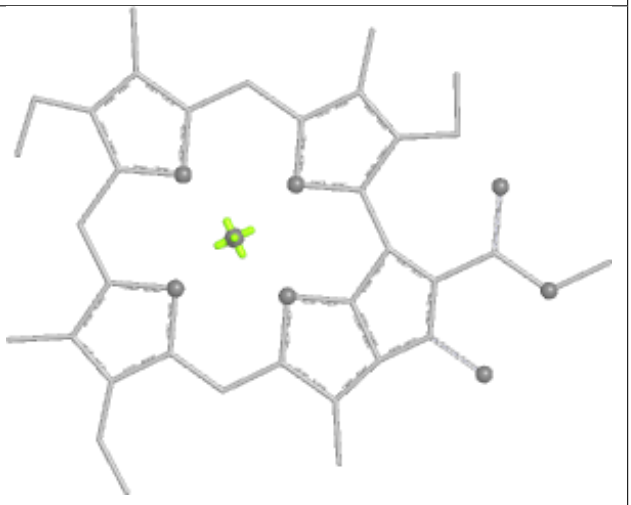
Bond lengths



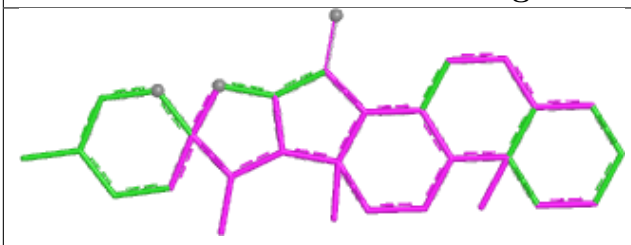
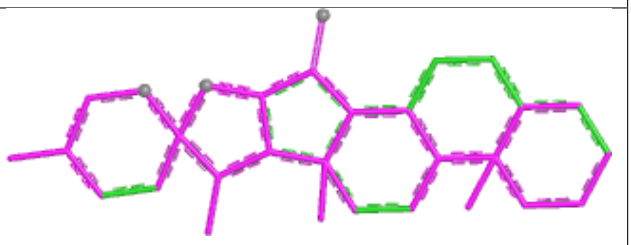
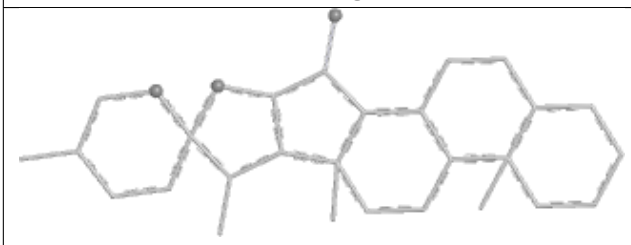
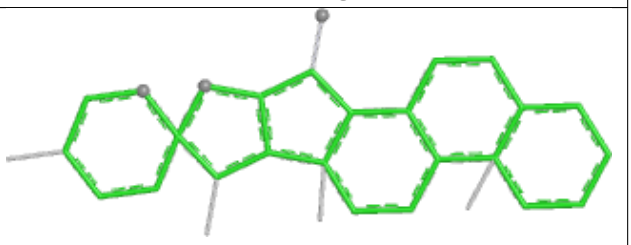
Bond angles

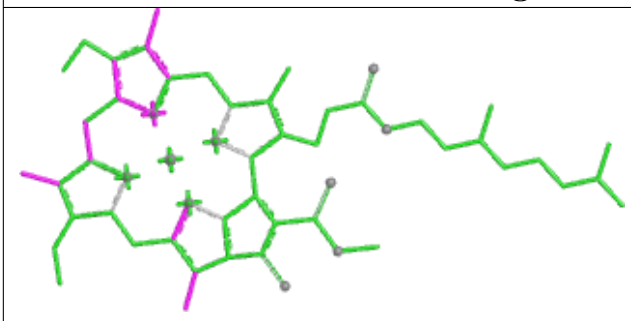
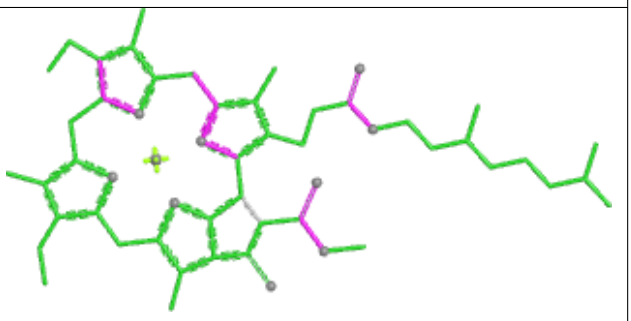
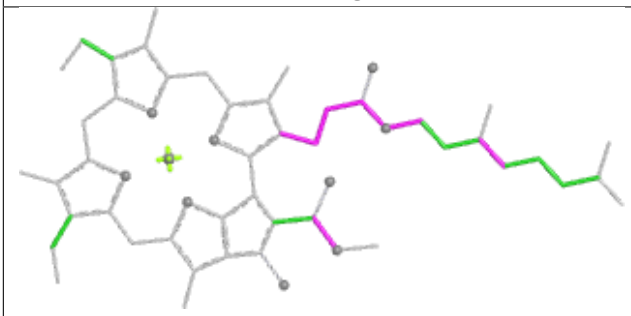
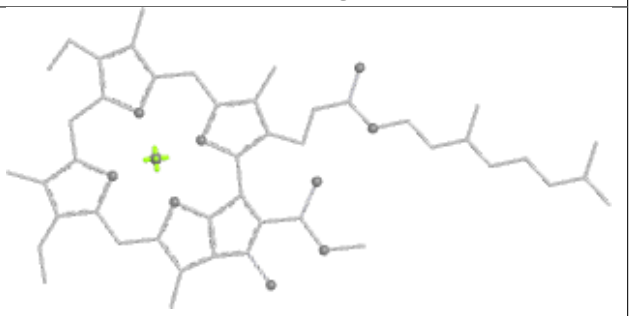


Torsions

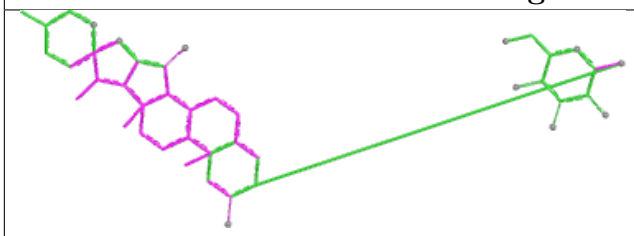


Rings

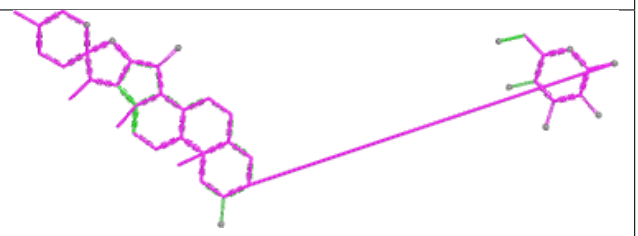
Ligand AJP AA 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

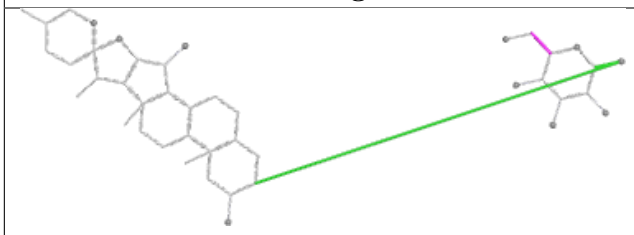
Ligand AJP B 850



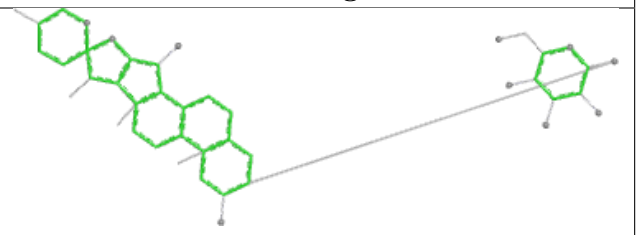
Bond lengths



Bond angles

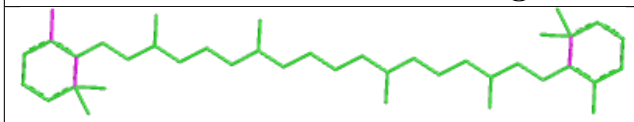


Torsions

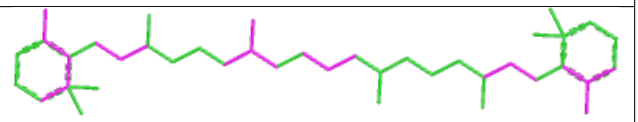


Rings

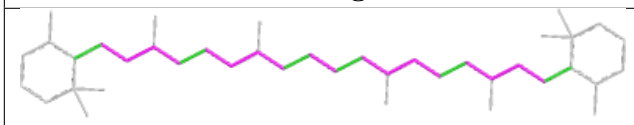
Ligand BCR M1 101



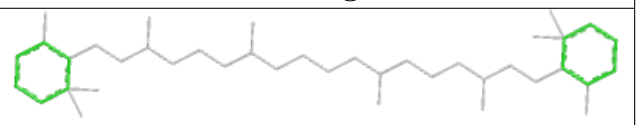
Bond lengths



Bond angles

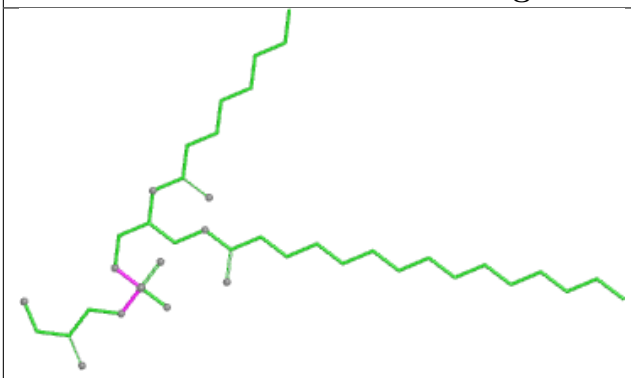


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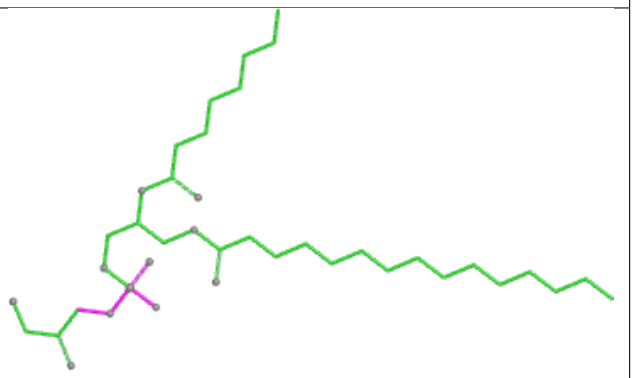


Rings

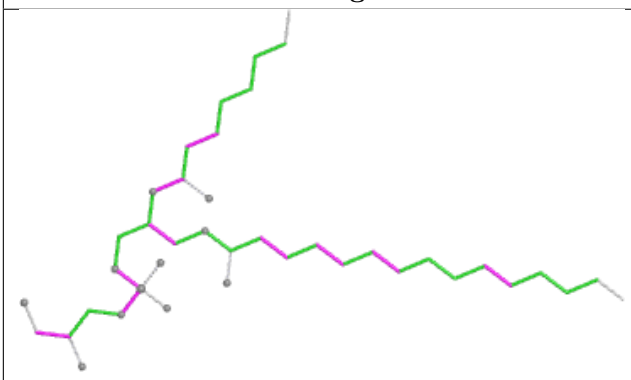
Ligand LHG X2 102



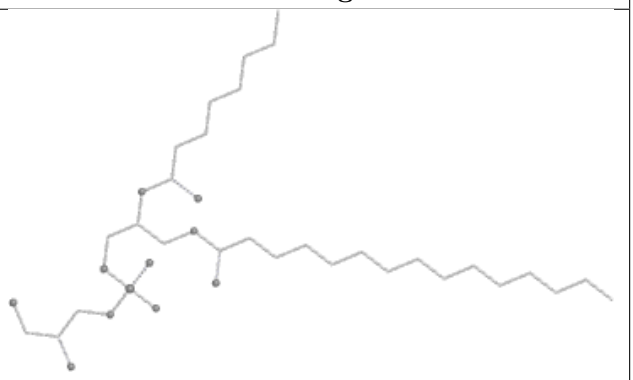
Bond lengths



Bond angles

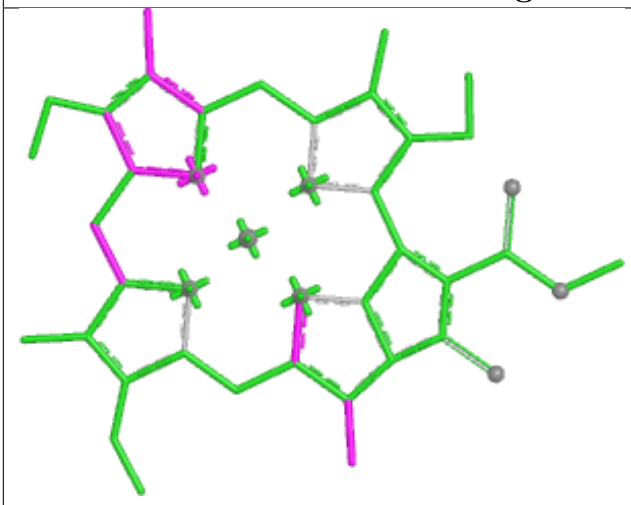


Torsions

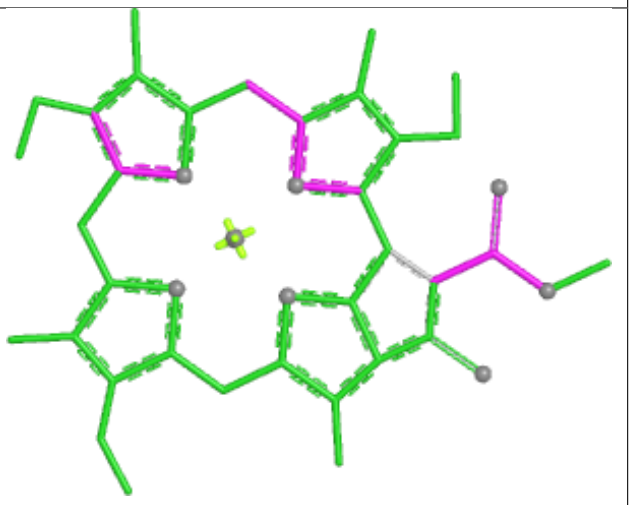


Rings

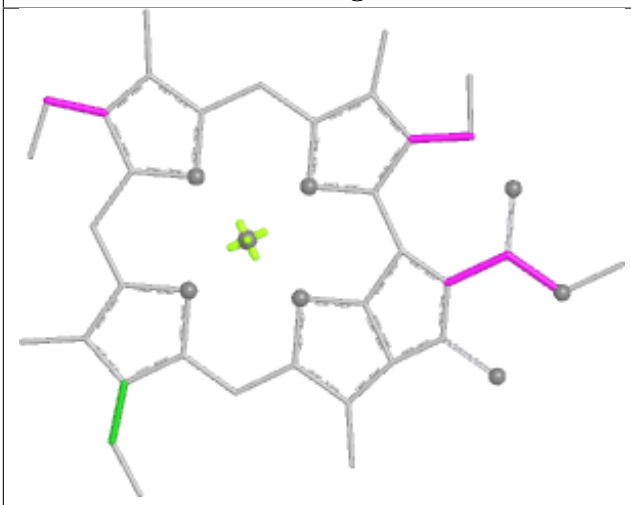
Ligand CLA B1 813



Bond lengths



Bond angles

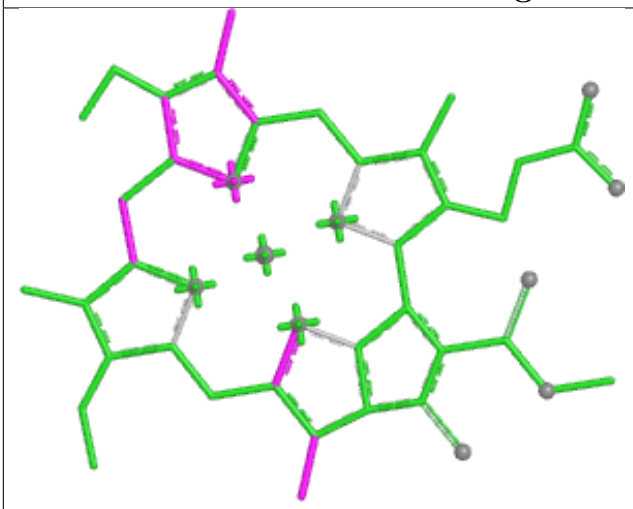


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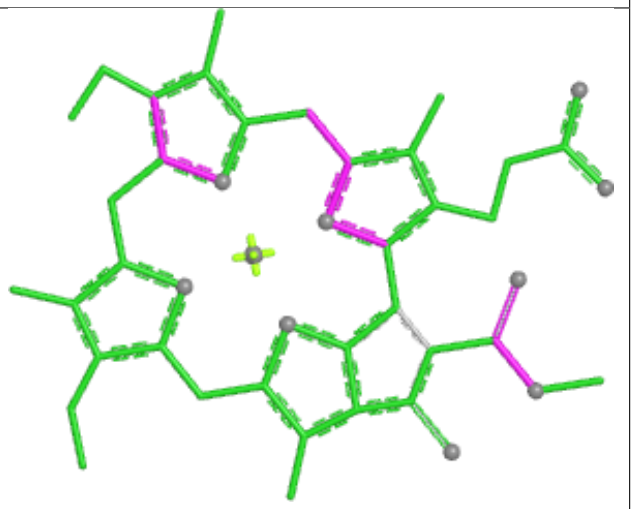


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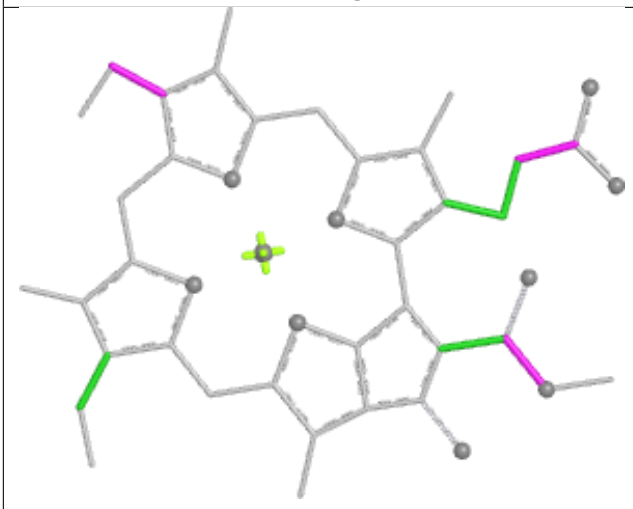
Ligand CLA A1 836



Bond lengths



Bond angles

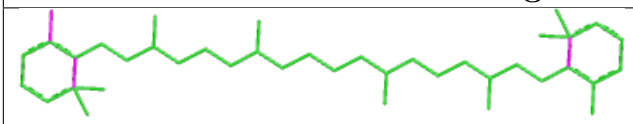


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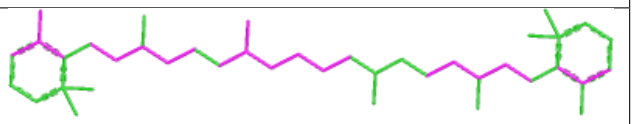


Rings

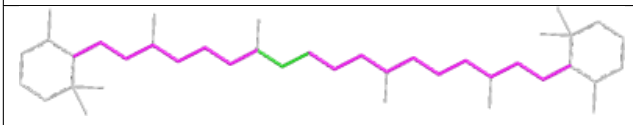
Ligand BCR F 305



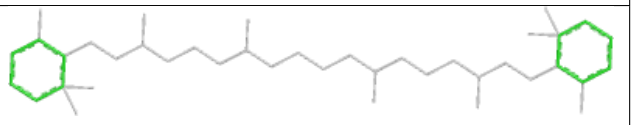
Bond lengths



Bond angles

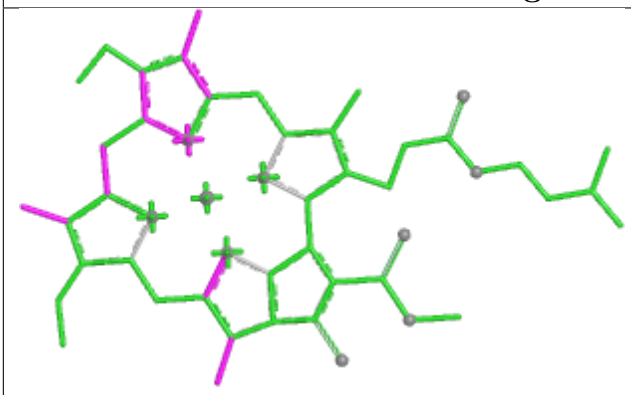


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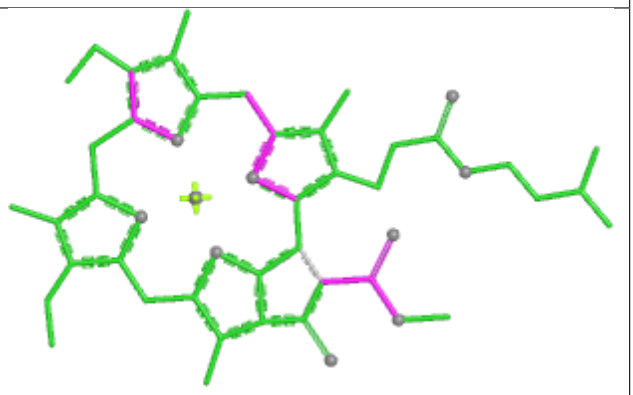


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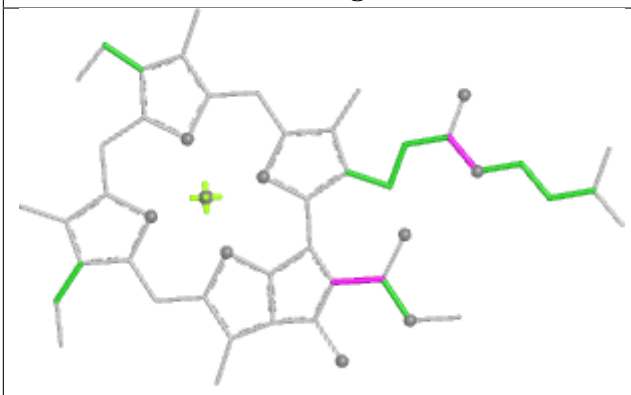
Ligand CLA A 833



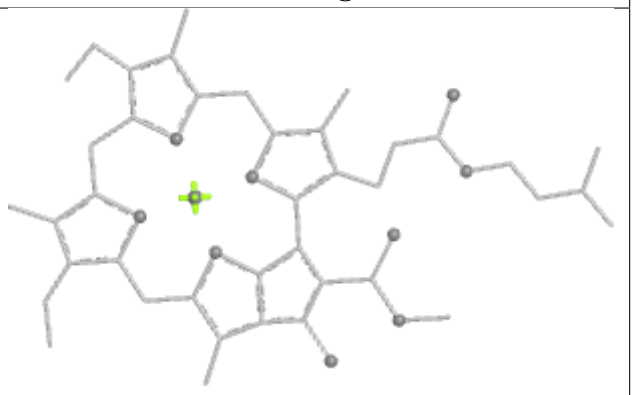
Bond lengths



Bond angles

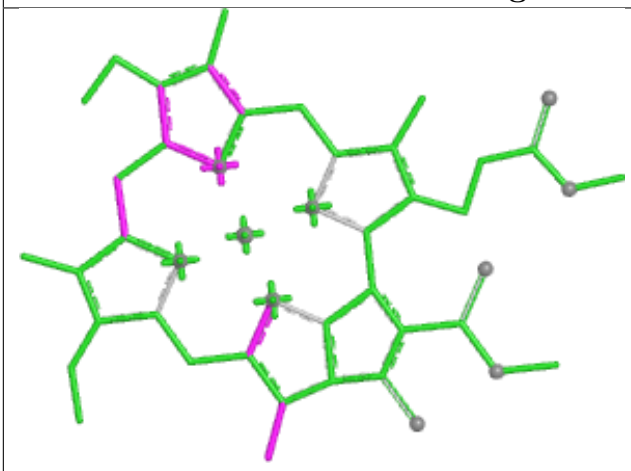


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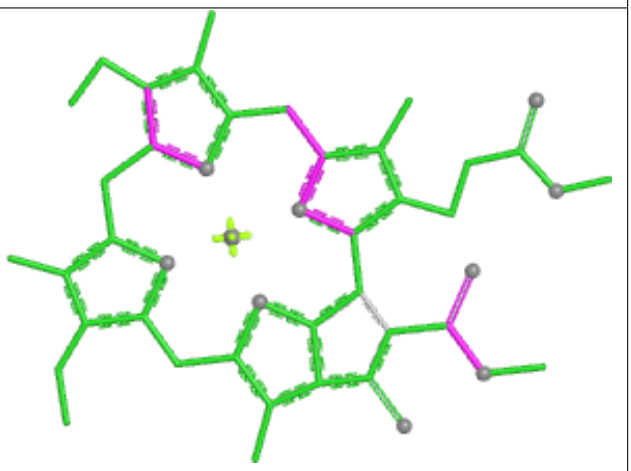


Rings

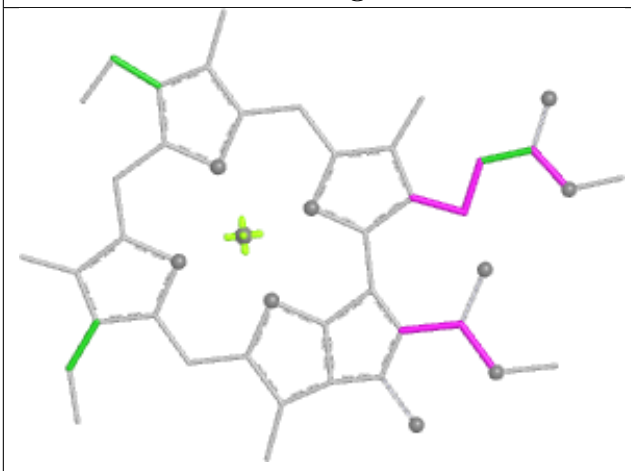
Ligand CLA KK 102



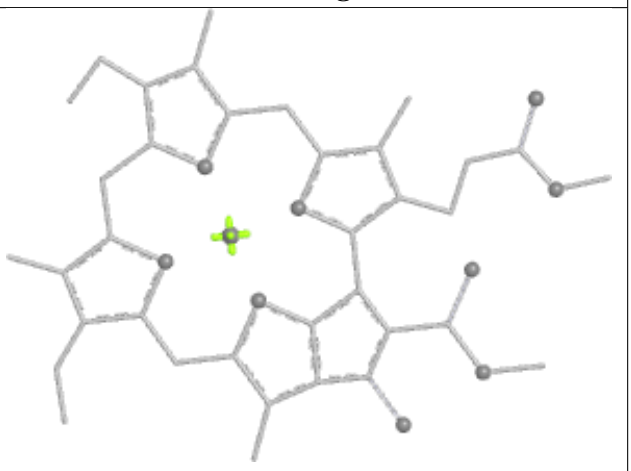
Bond lengths



Bond angles

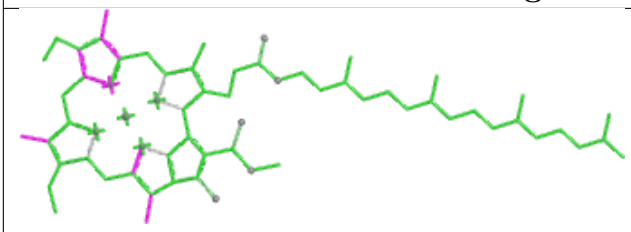


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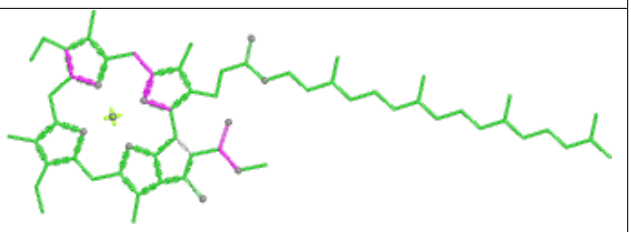


Rings

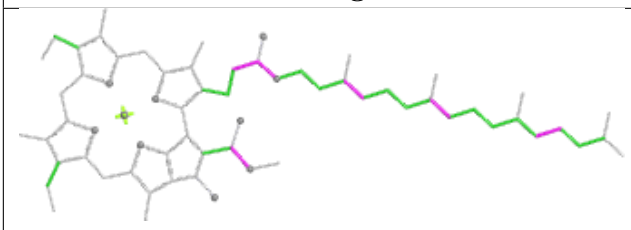
Ligand CLA B 854



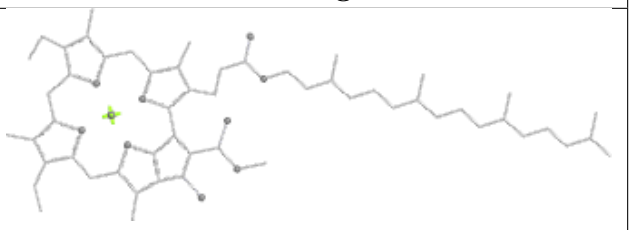
Bond lengths



Bond angles

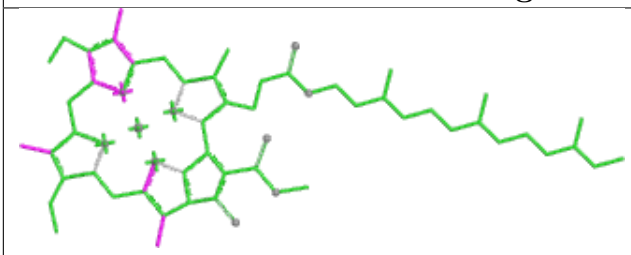


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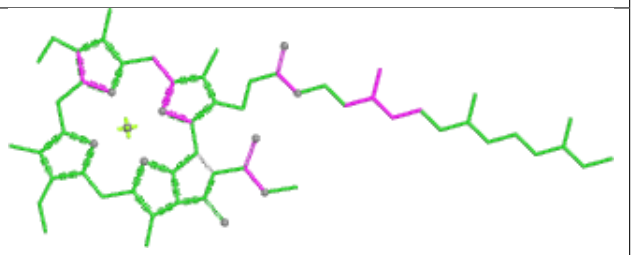


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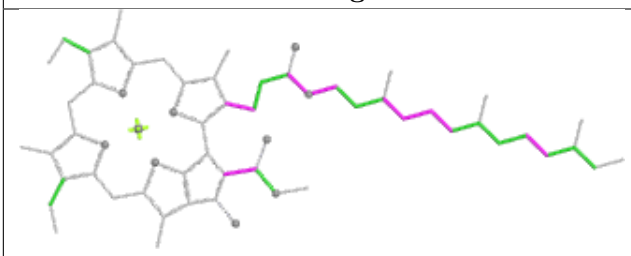
Ligand CLA LL 201



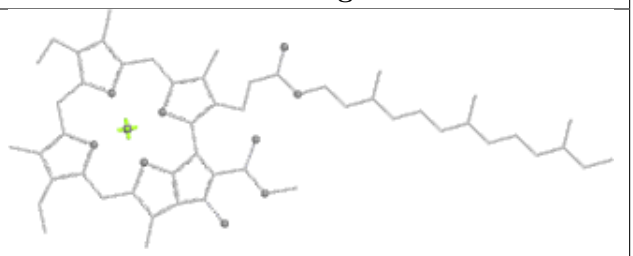
Bond lengths



Bond angles

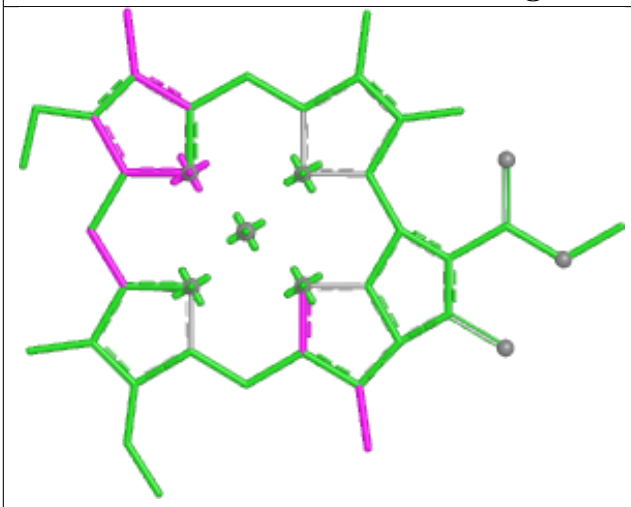


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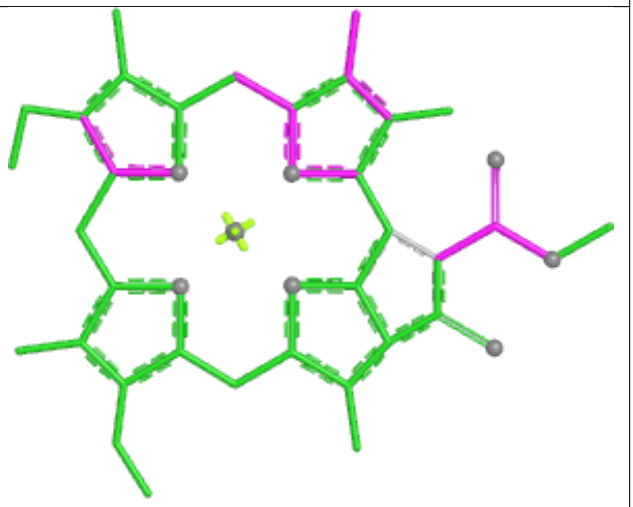


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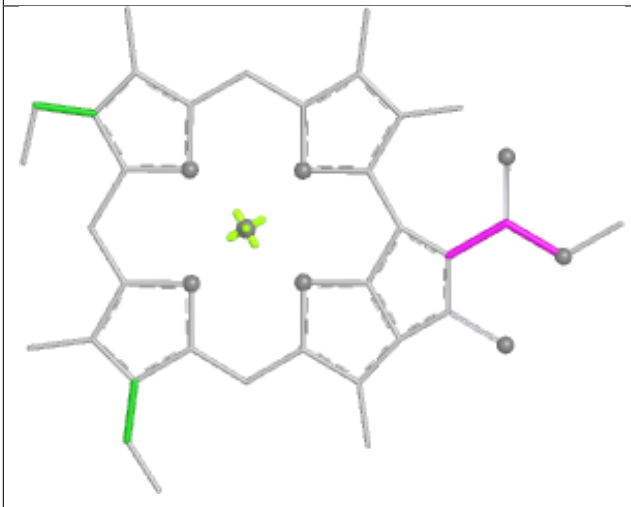
Ligand CLA B 812



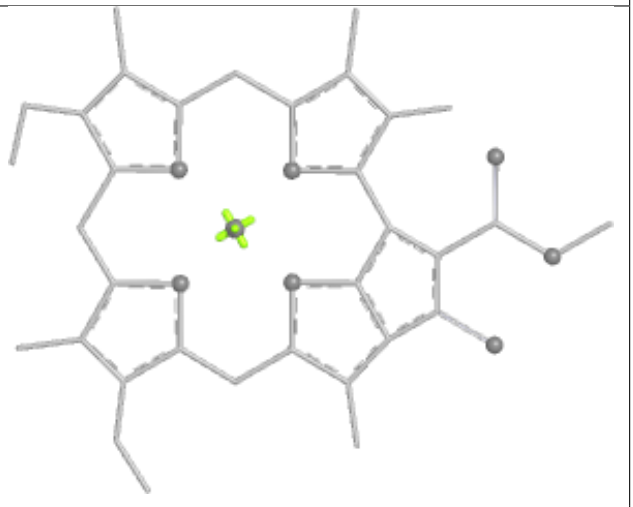
Bond lengths



Bond angles

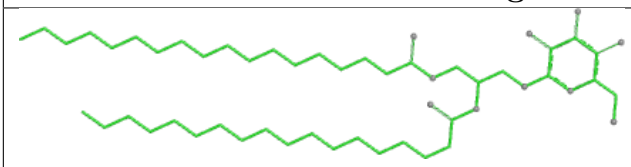


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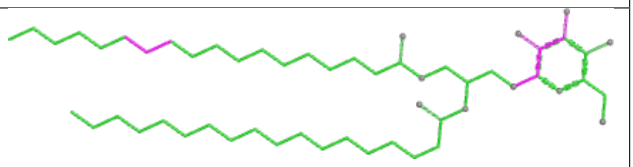


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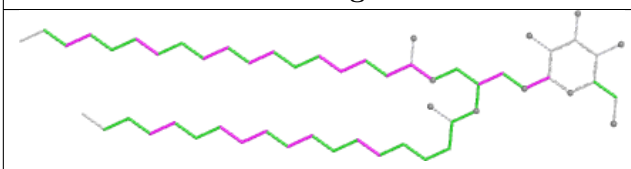
Ligand LMG BB 844



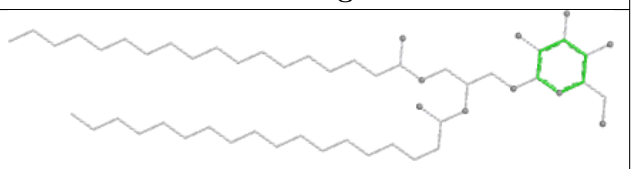
Bond lengths



Bond angles

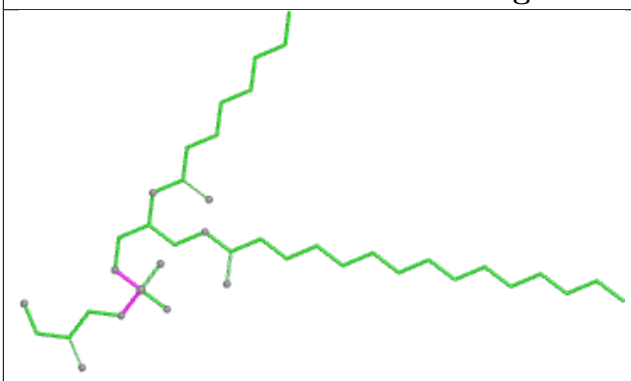


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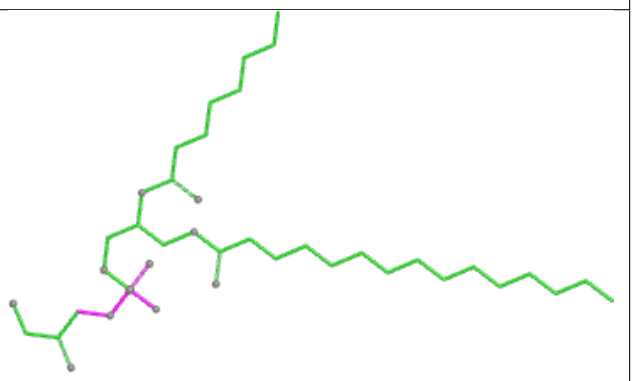


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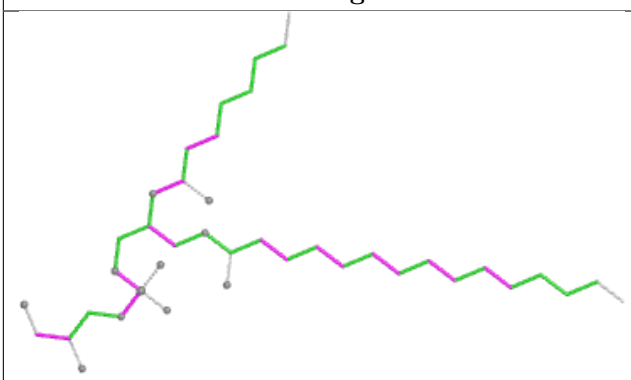
Ligand LHG X1 102



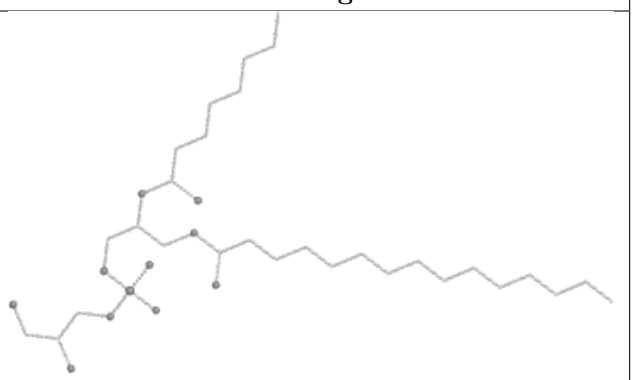
Bond lengths



Bond angles

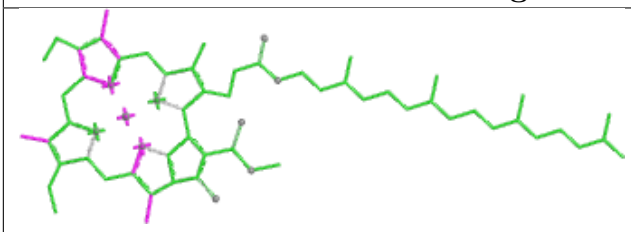


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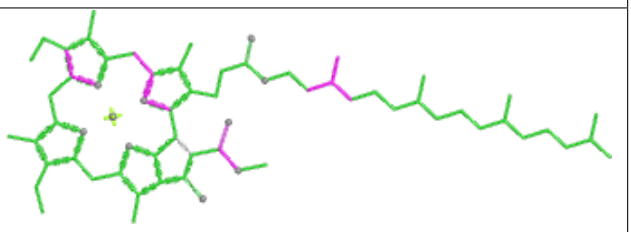


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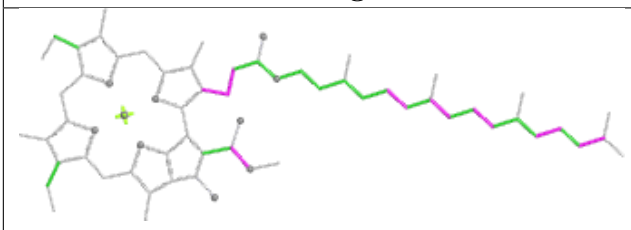
Ligand CLA AA 829



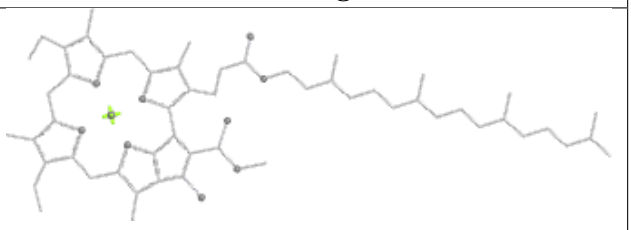
Bond lengths



Bond angles



Torsions

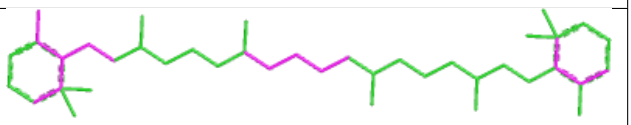


Rings

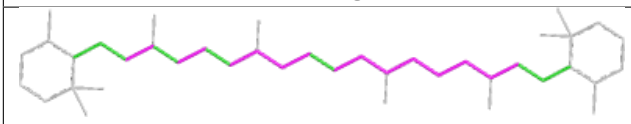
Ligand BCR A2 853



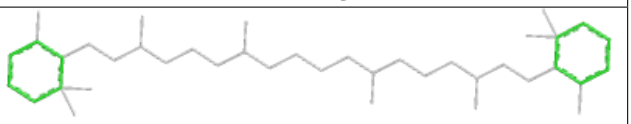
Bond lengths



Bond angles

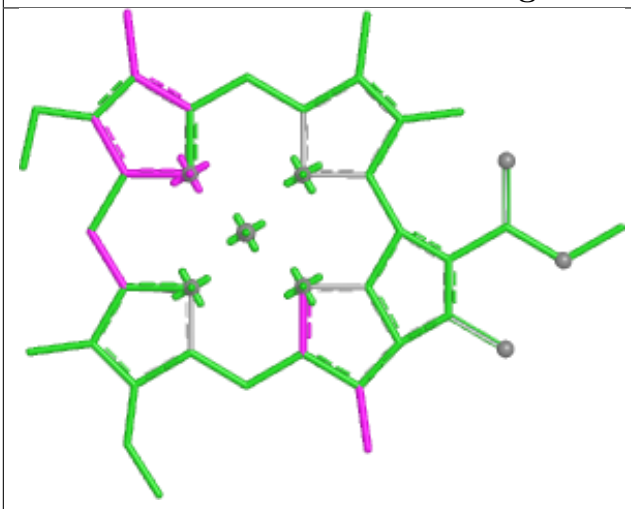


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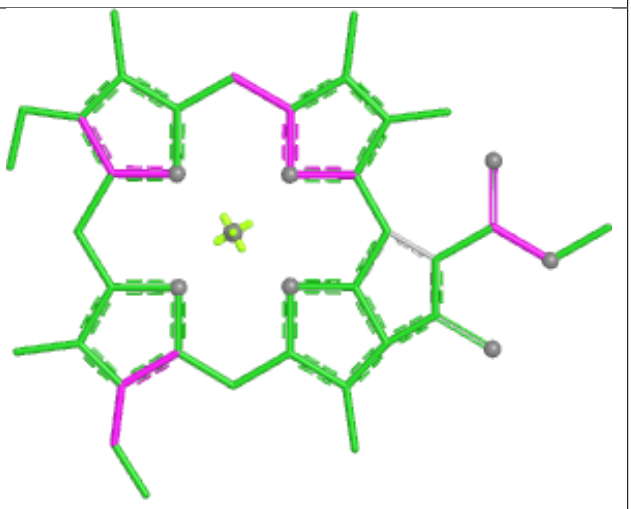


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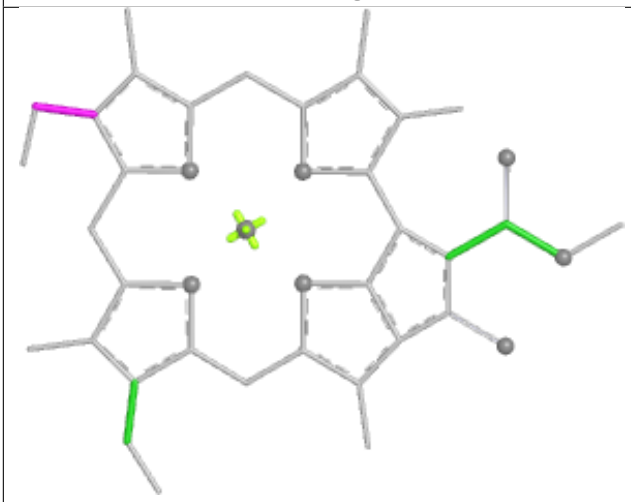
Ligand CLA JJ 103



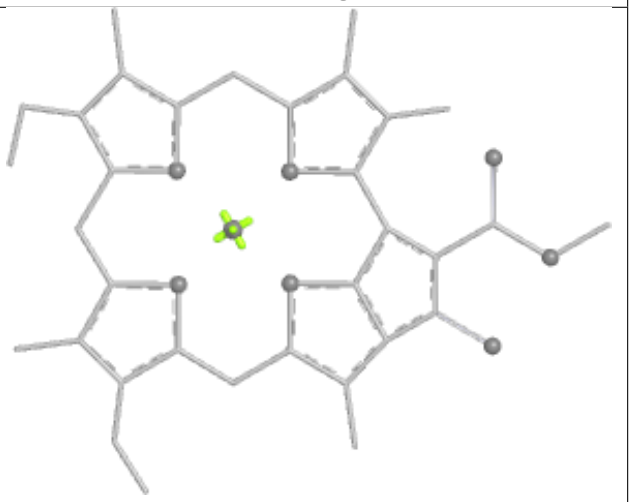
Bond lengths



Bond angles



Torsions

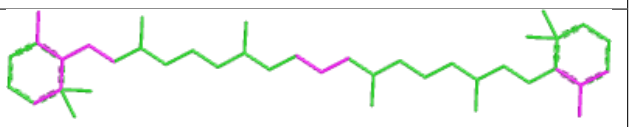


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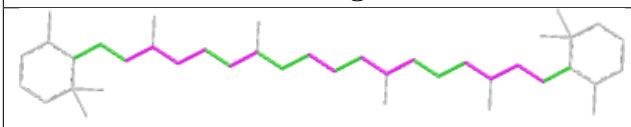
Ligand BCR A1 848



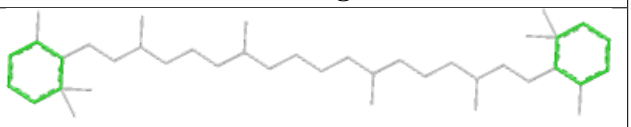
Bond lengths



Bond angles

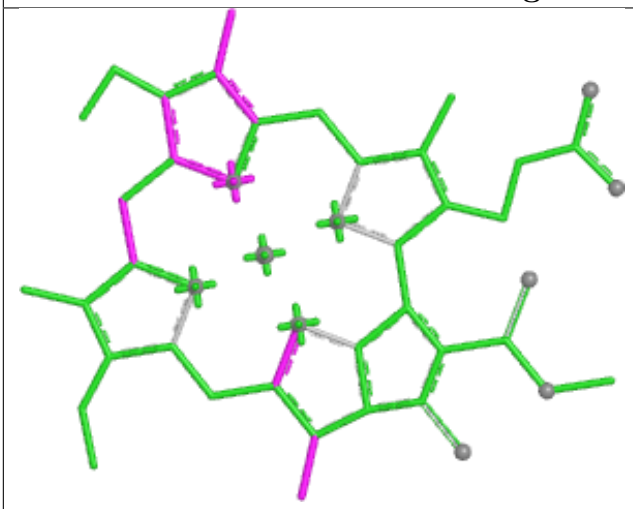


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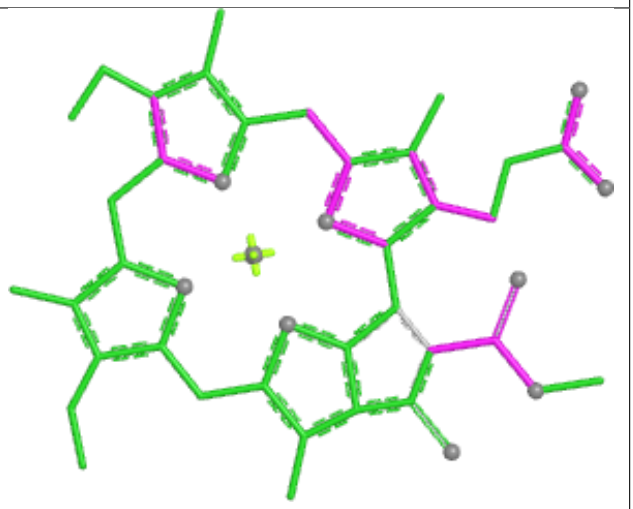


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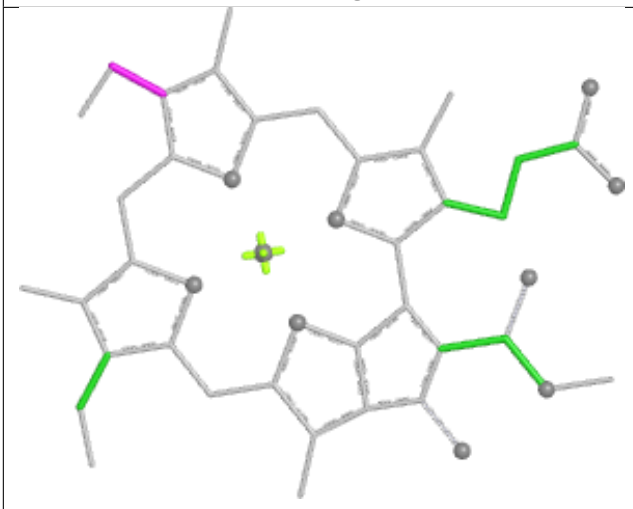
Ligand CLA K 101



Bond lengths



Bond angles

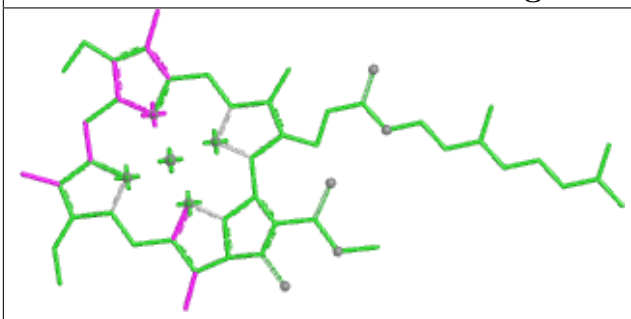


Torsions

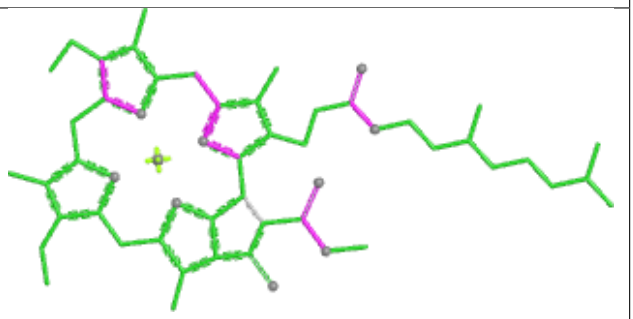


Rings

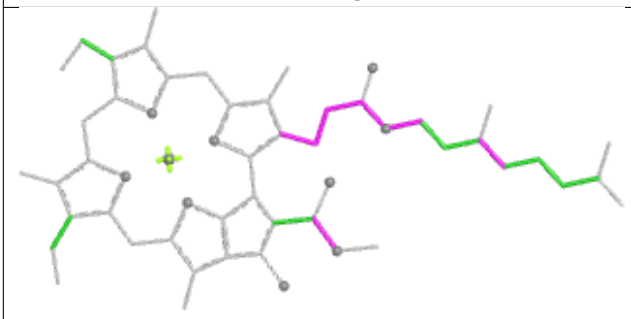
Ligand CLA B 824



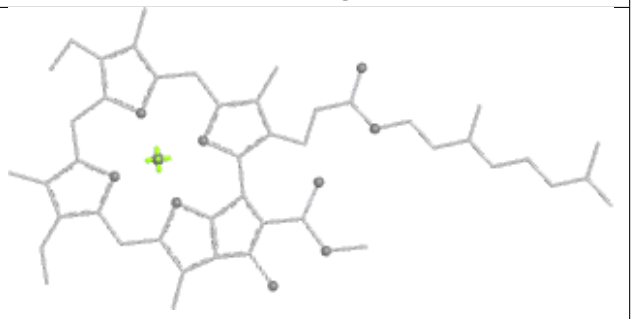
Bond lengths



Bond angles

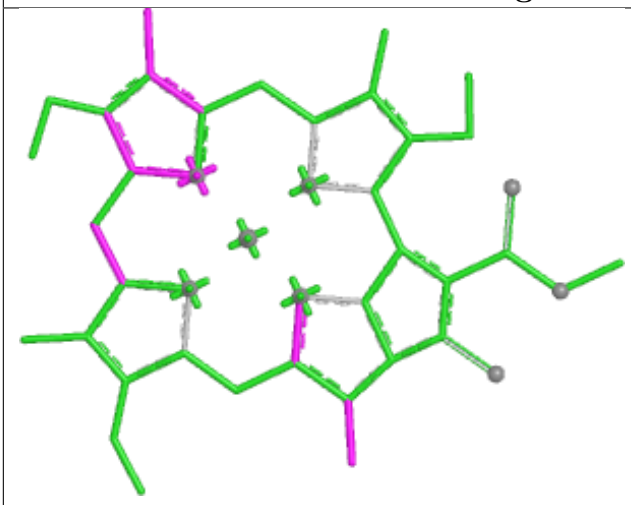


Torsions

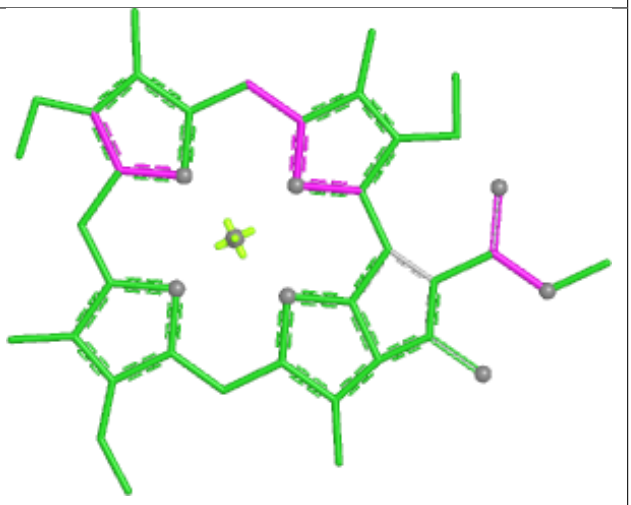


Rings

Ligand CLA B1 817



Bond lengths



Bond angles

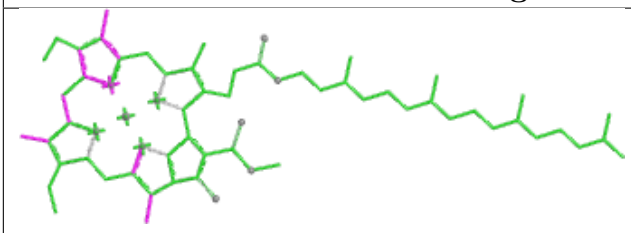


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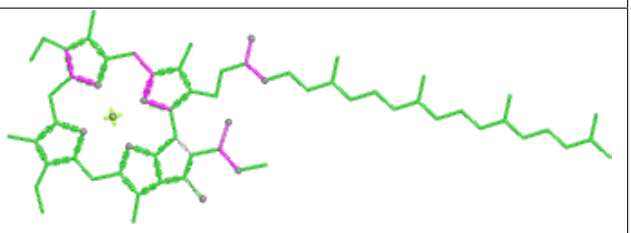


Rings

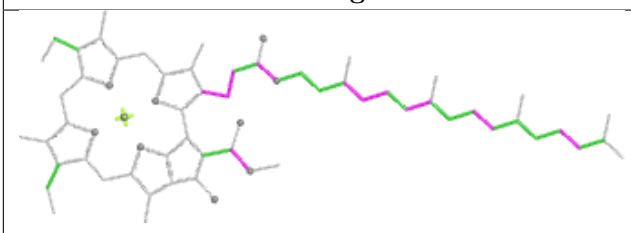
Ligand CLA AA 808



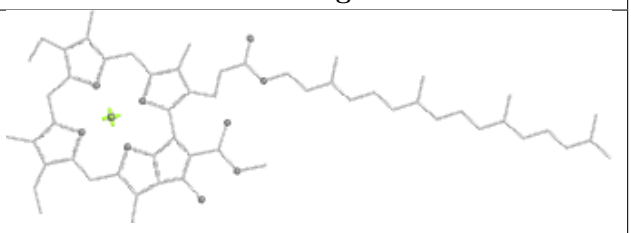
Bond lengths



Bond angles

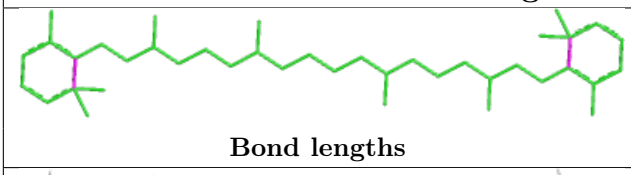


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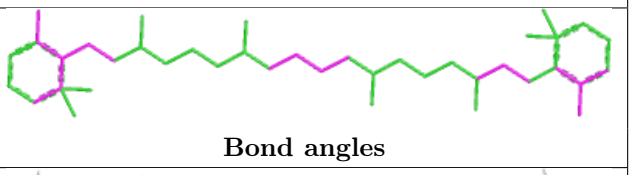


Rings

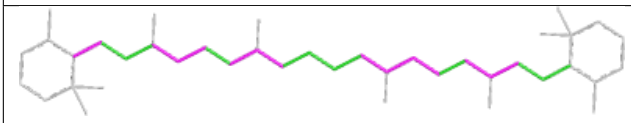
Ligand BCR II 101



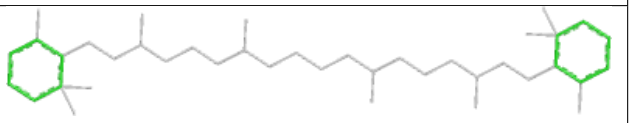
Bond lengths



Bond angles

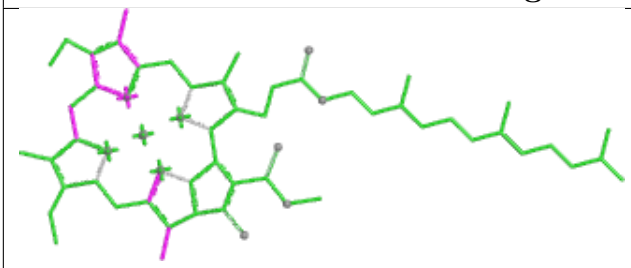


Torsions

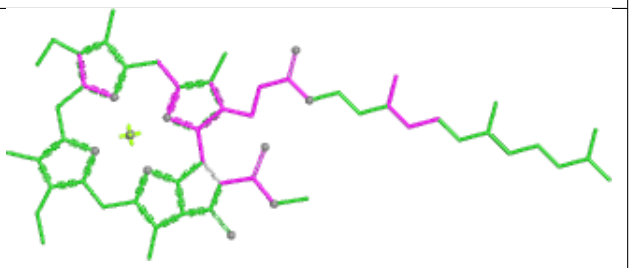


Rings

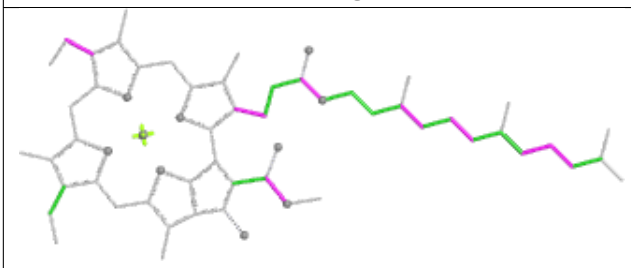
Ligand CLA B 859



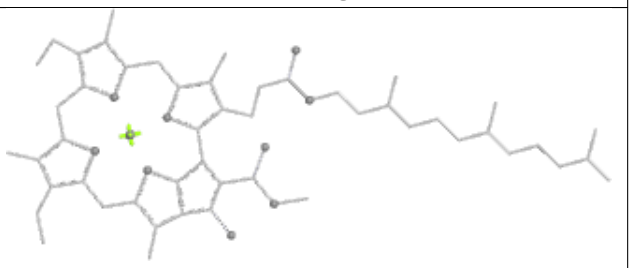
Bond lengths



Bond angles

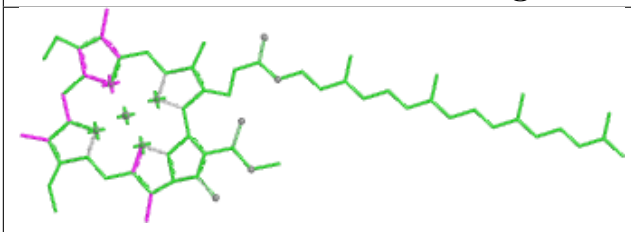


Torsions

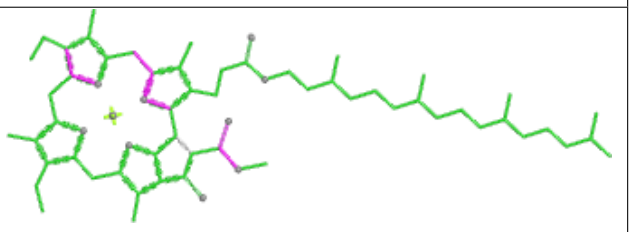


Rings

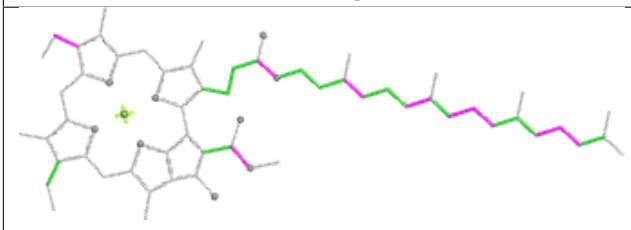
Ligand CLA BB 823



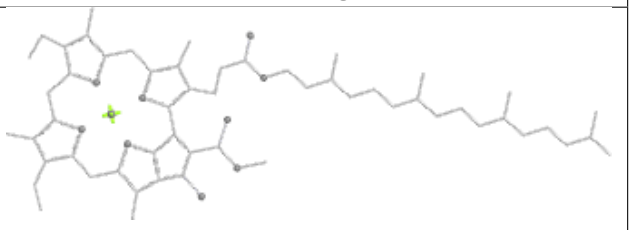
Bond lengths



Bond angles

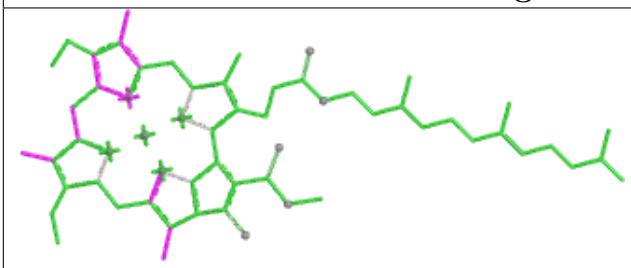


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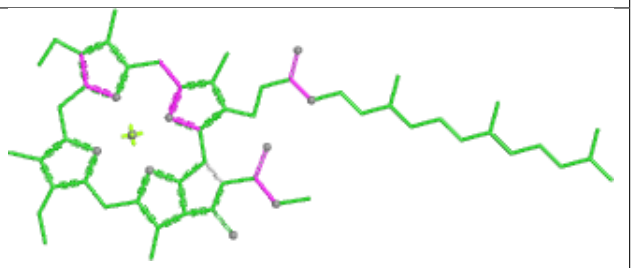


Rings

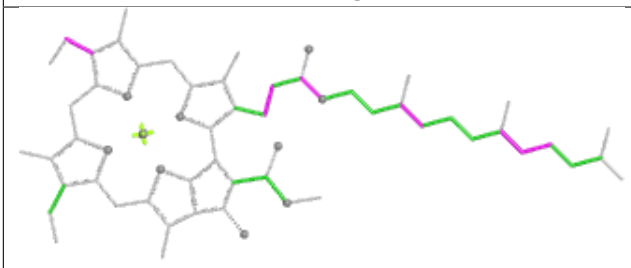
Ligand CLA A2 819



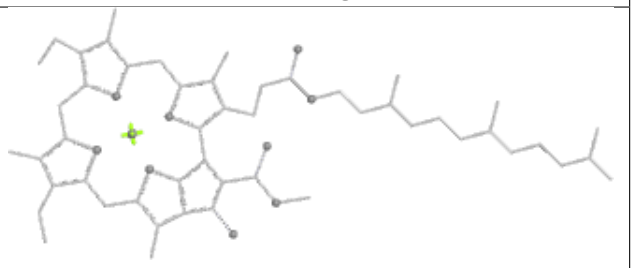
Bond lengths



Bond angles

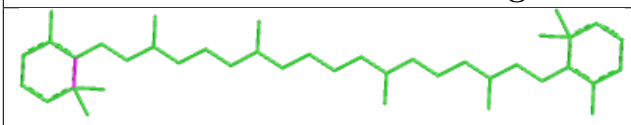


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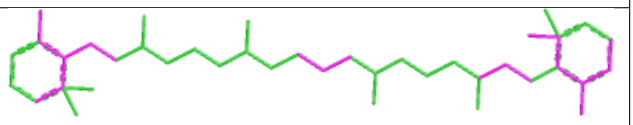


Rings

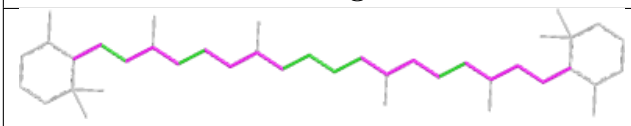
Ligand BCR AA 852



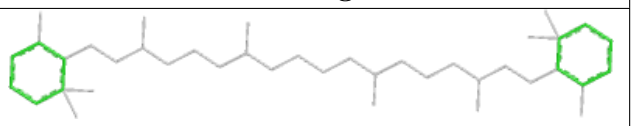
Bond lengths



Bond angles



Torsions

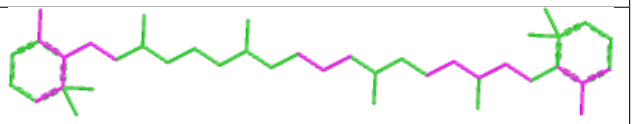


Rings

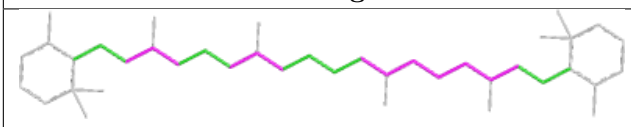
Ligand BCR F2 304



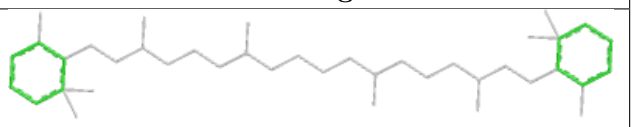
Bond lengths



Bond angles

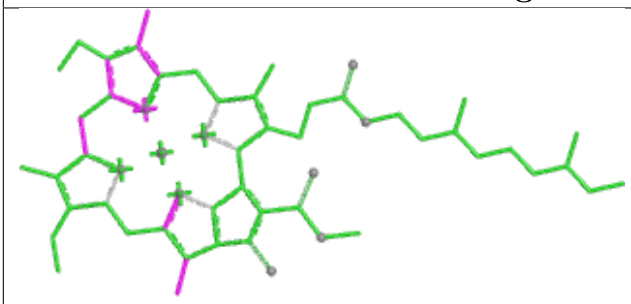


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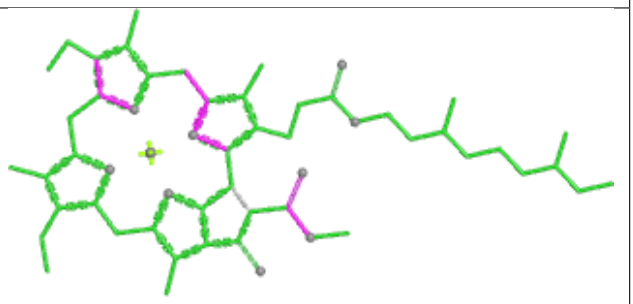


Rings

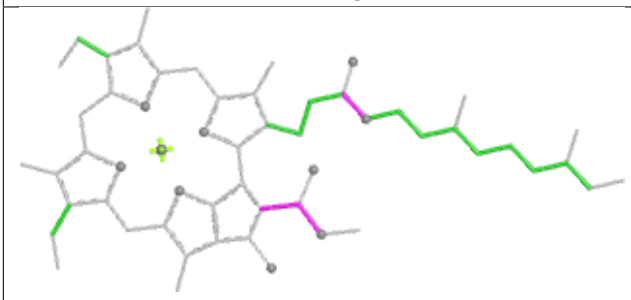
Ligand CLA B1 830



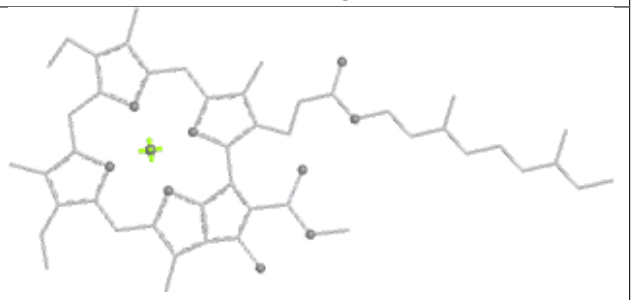
Bond lengths



Bond angles

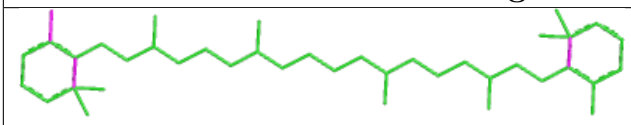


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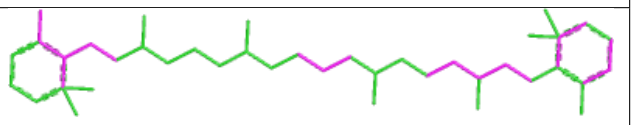


Rings

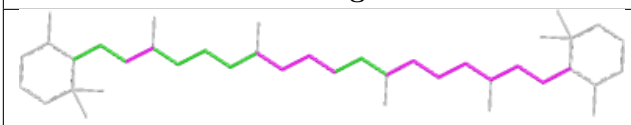
Ligand BCR AA 855



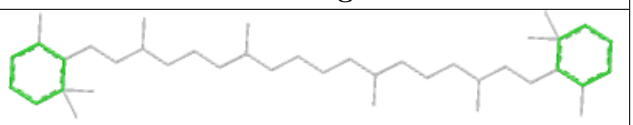
Bond lengths



Bond angles

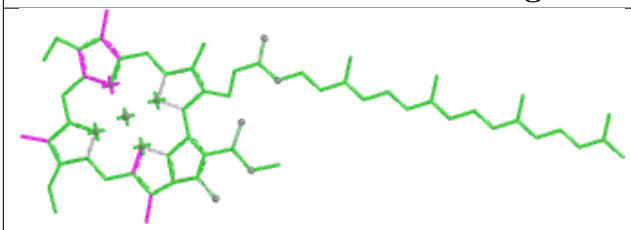


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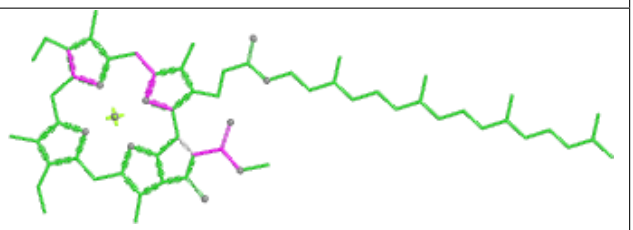


Rings

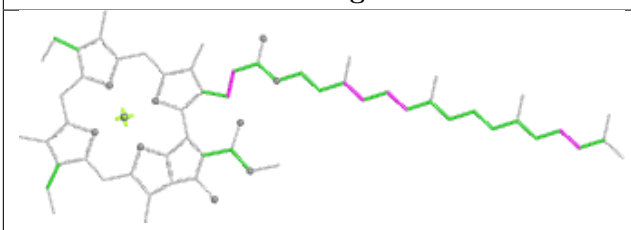
Ligand CLA B 858



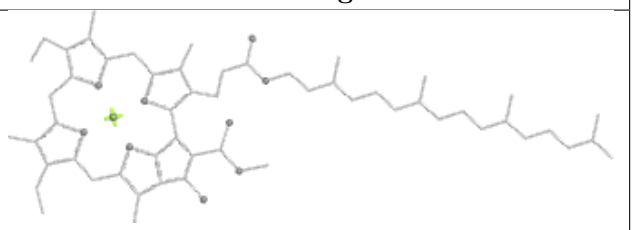
Bond lengths



Bond angles

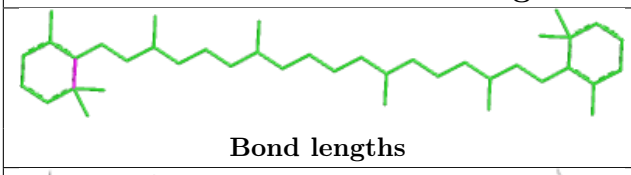


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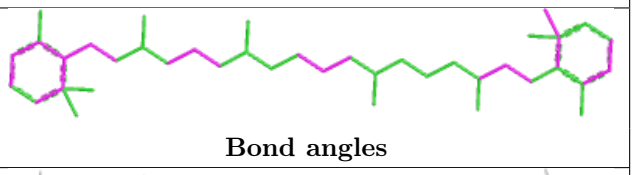


Rings

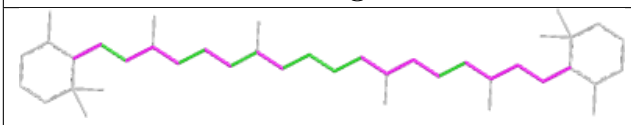
Ligand BCR A1 851



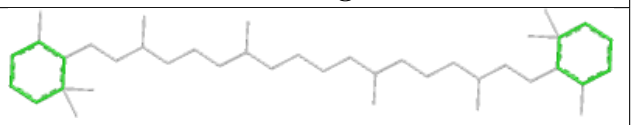
Bond lengths



Bond angles

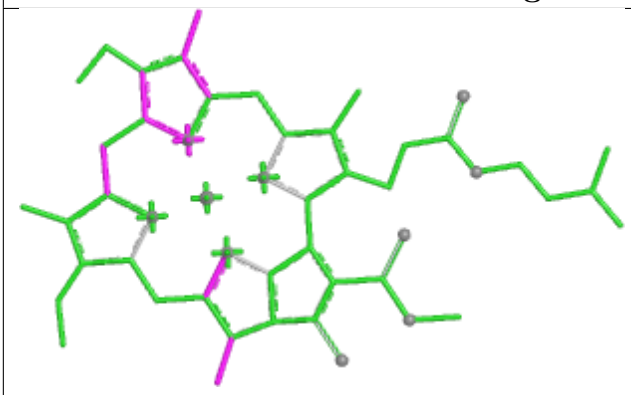


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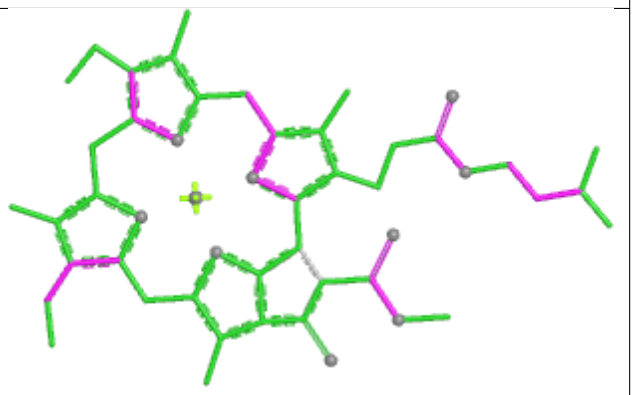


Rings

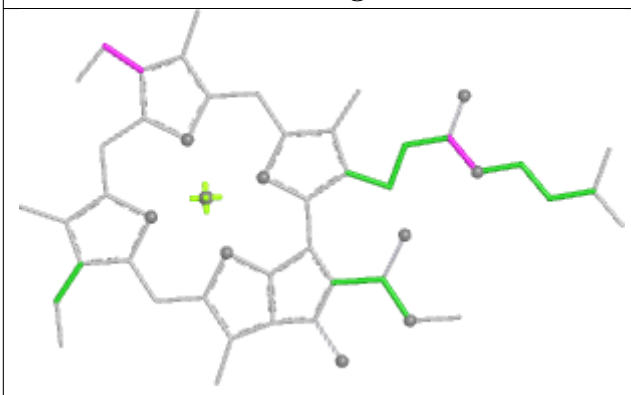
Ligand CLA A 809



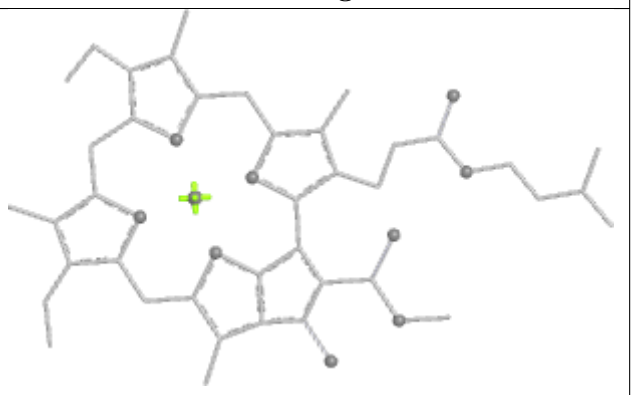
Bond lengths



Bond angles

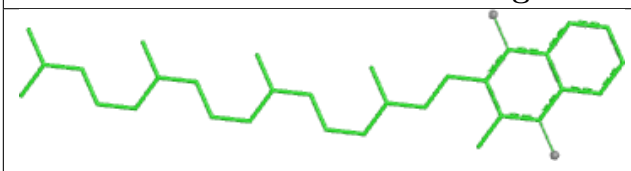


Torsions

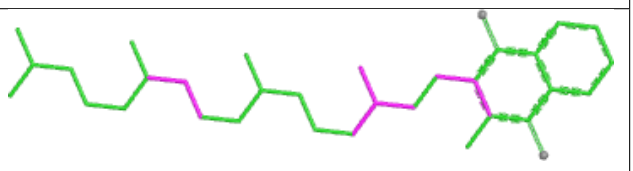


Rings

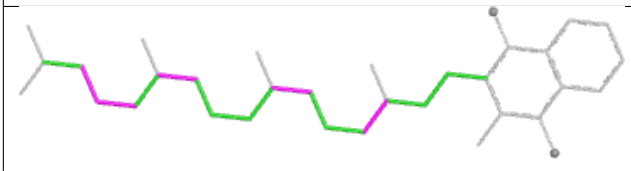
Ligand PQN A2 843



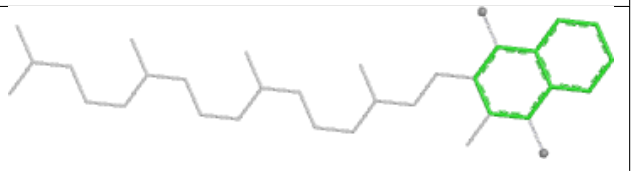
Bond lengths



Bond angles

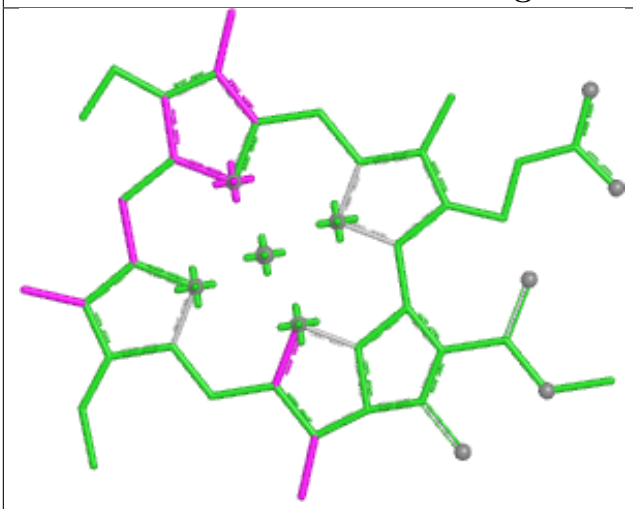


Torsions

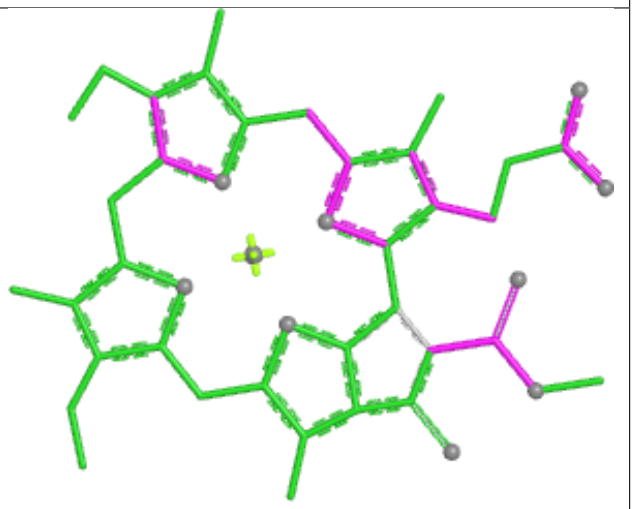


Rings

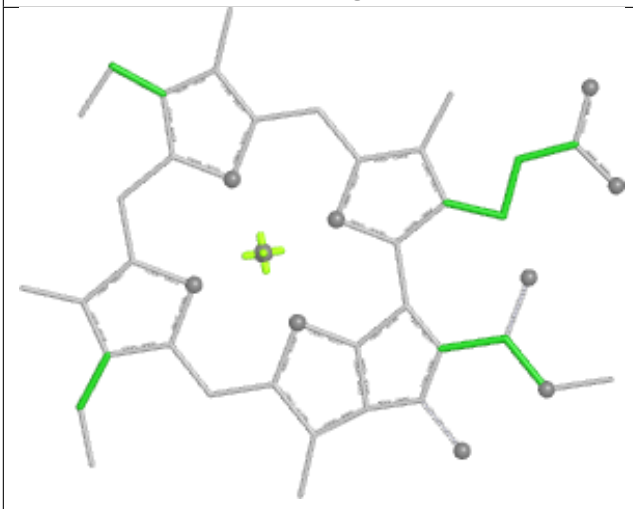
Ligand CLA K1 102



Bond lengths



Bond angles

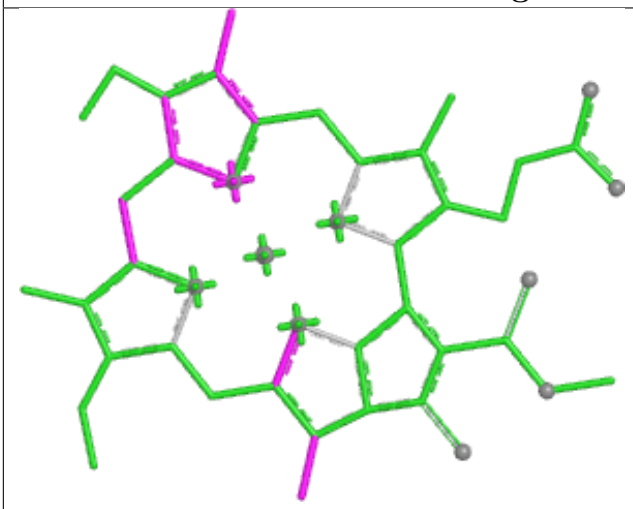


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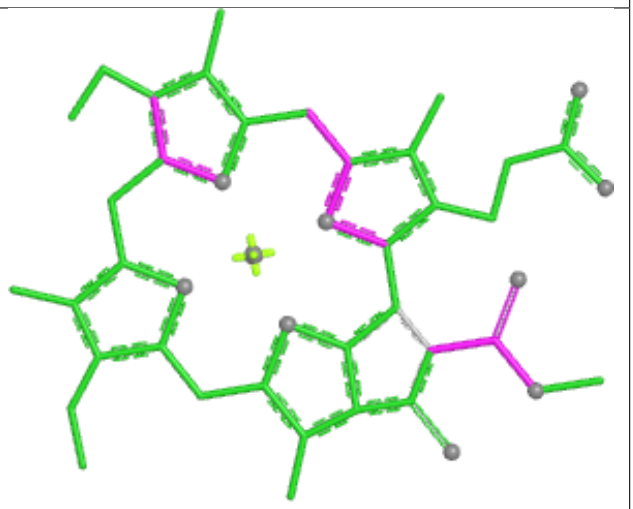


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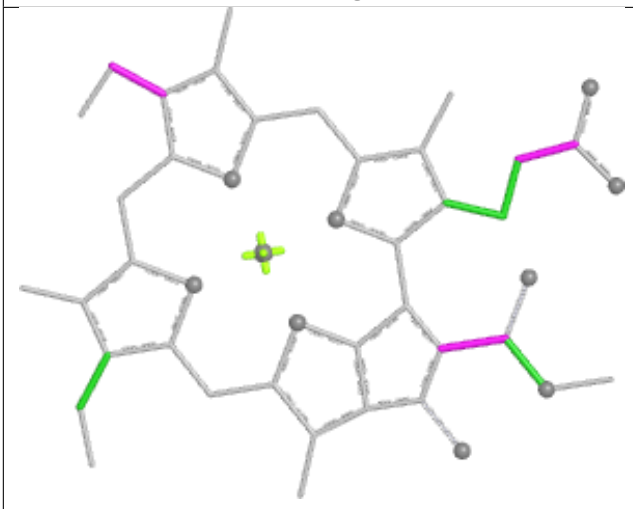
Ligand CLA BB 809



Bond lengths



Bond angles

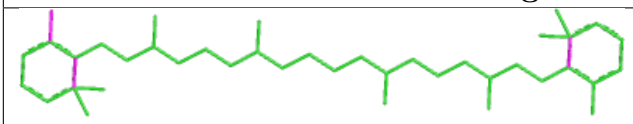


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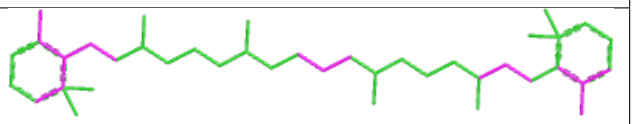


Rings

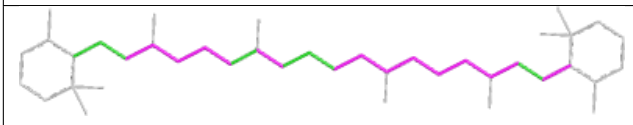
Ligand BCR K 103



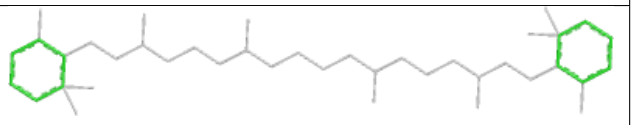
Bond lengths



Bond angles

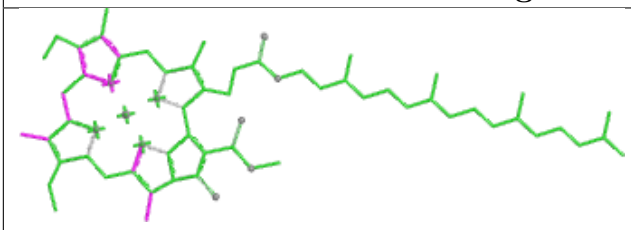


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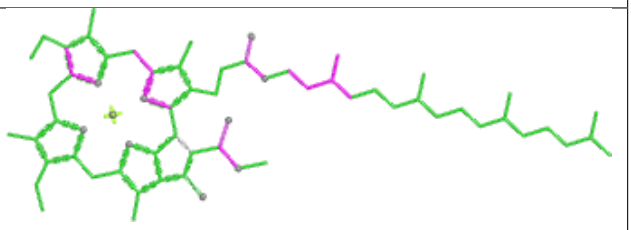


Rings

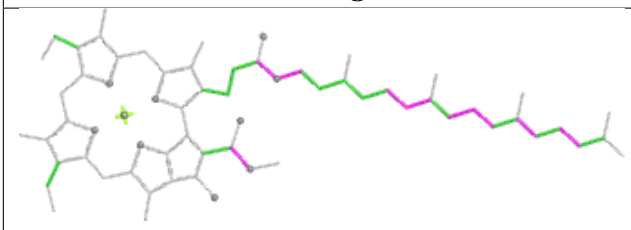
Ligand CLA B1 806



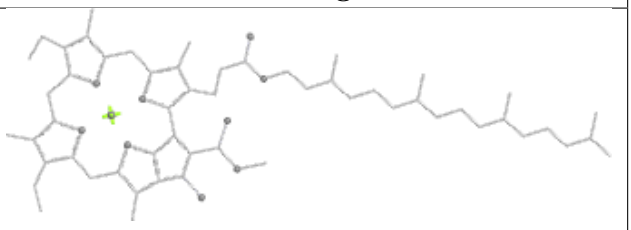
Bond lengths



Bond angles

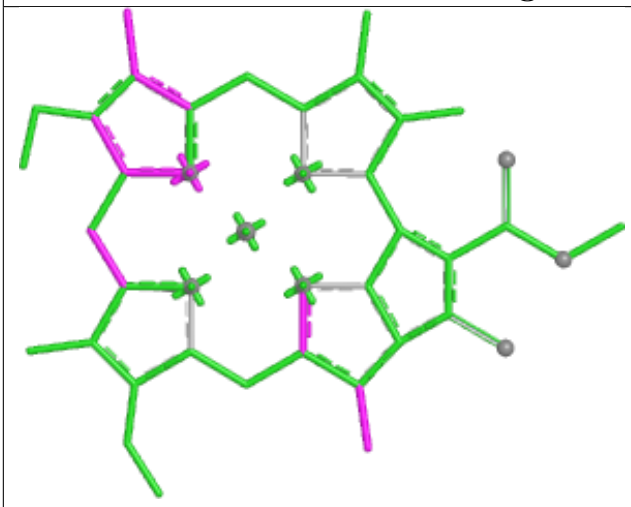


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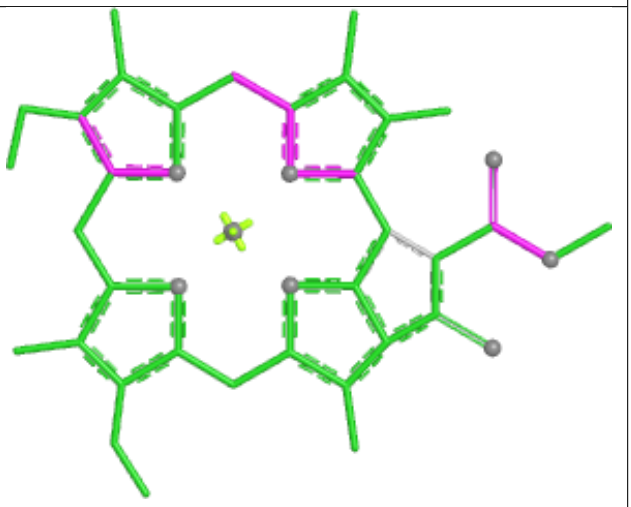


Rings

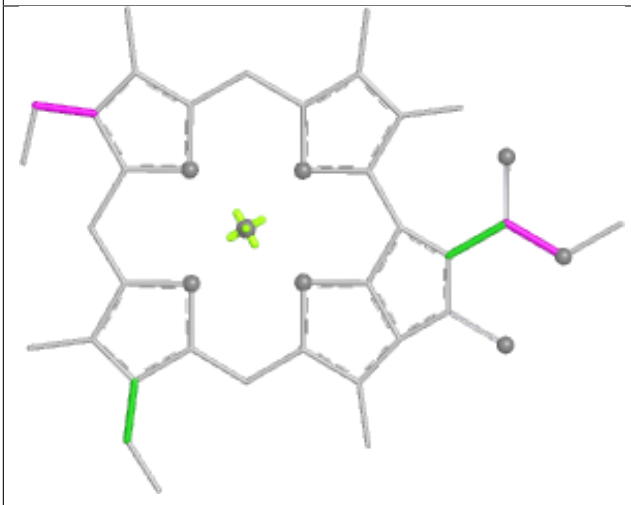
Ligand CLA JJ 101



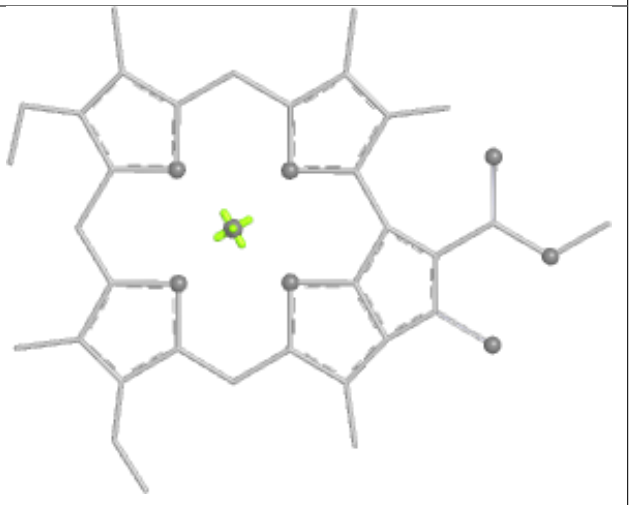
Bond lengths



Bond angles

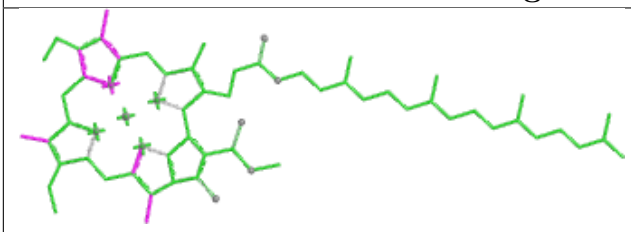


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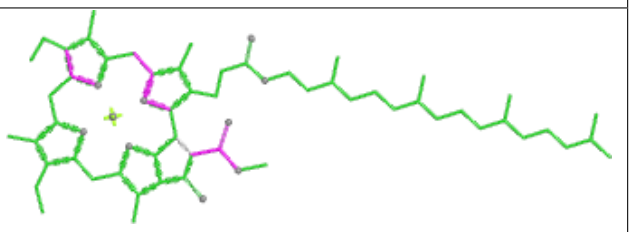


Rings

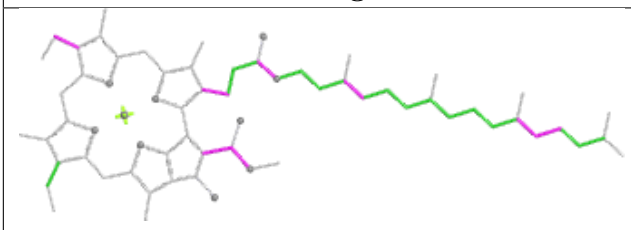
Ligand CLA A 836



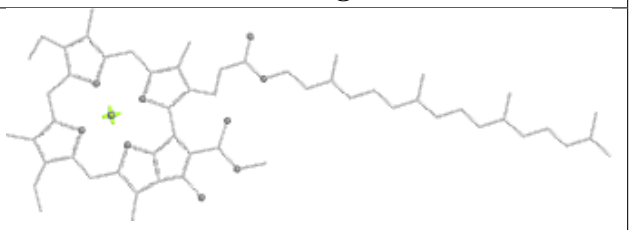
Bond lengths



Bond angles

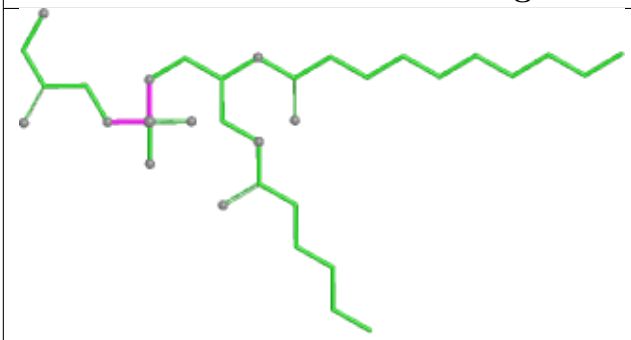


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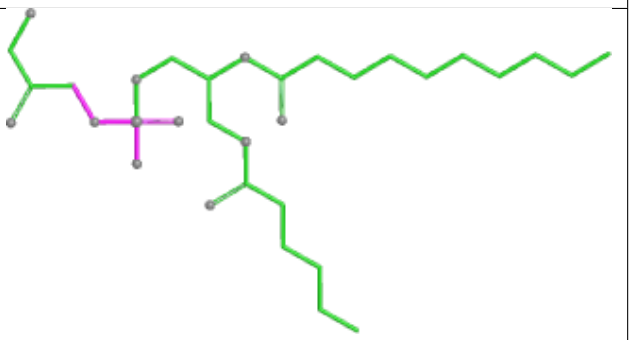


Rings

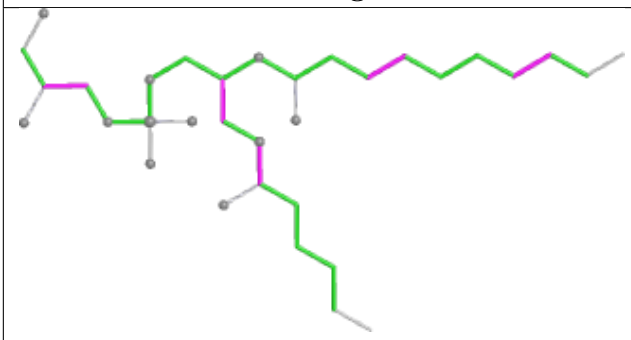
Ligand LHG B2 848



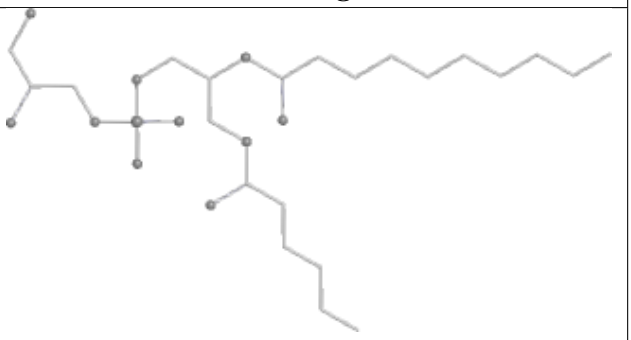
Bond lengths



Bond angles

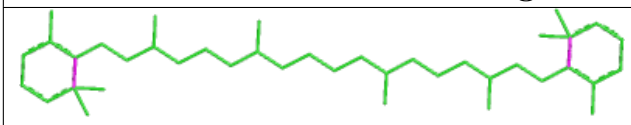


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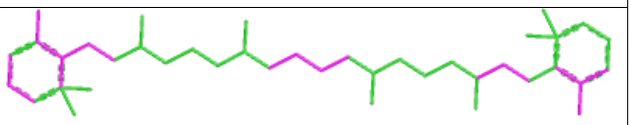


Rings

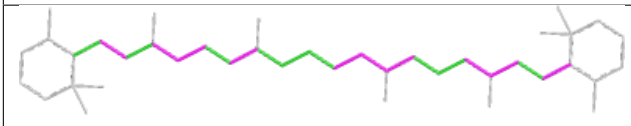
Ligand BCR J2 104



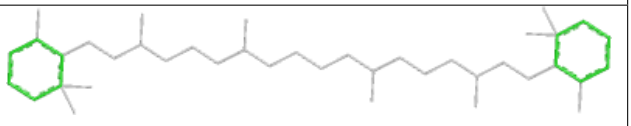
Bond lengths



Bond angles

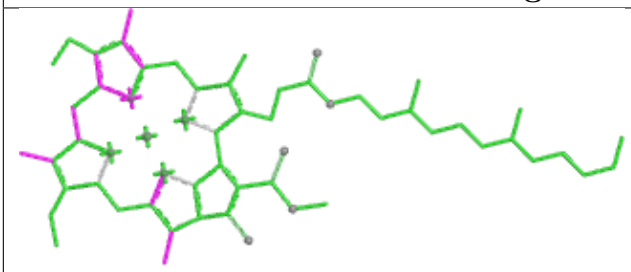


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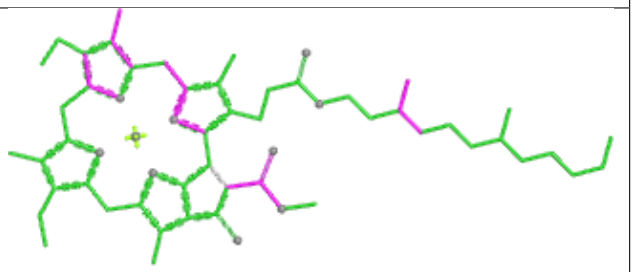


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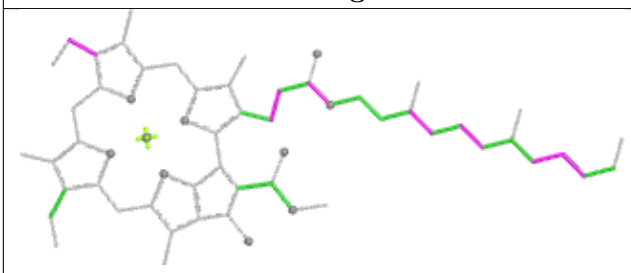
Ligand CLA B 814



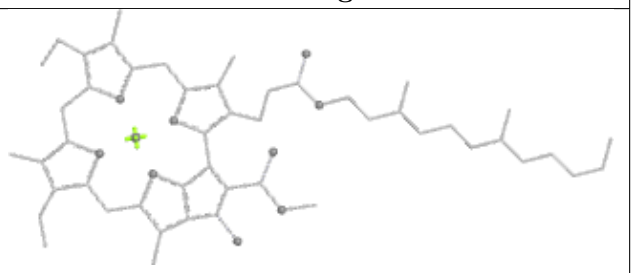
Bond lengths



Bond angles

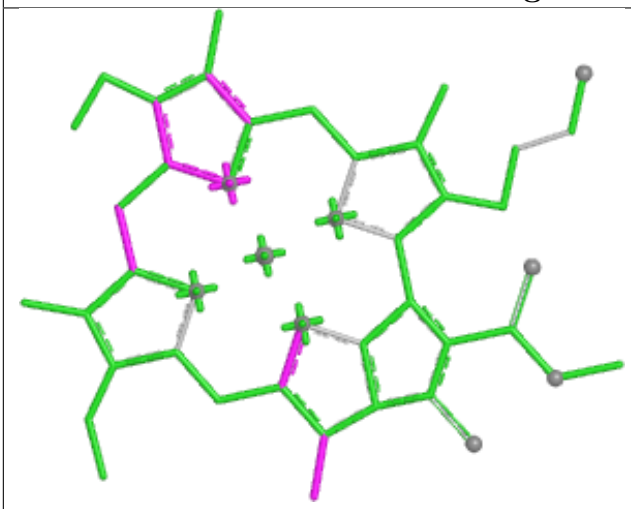


Torsions



Rings

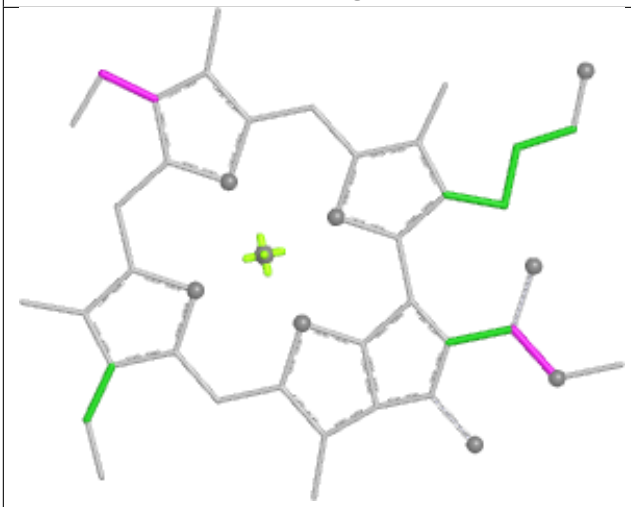
Ligand CLA A 817



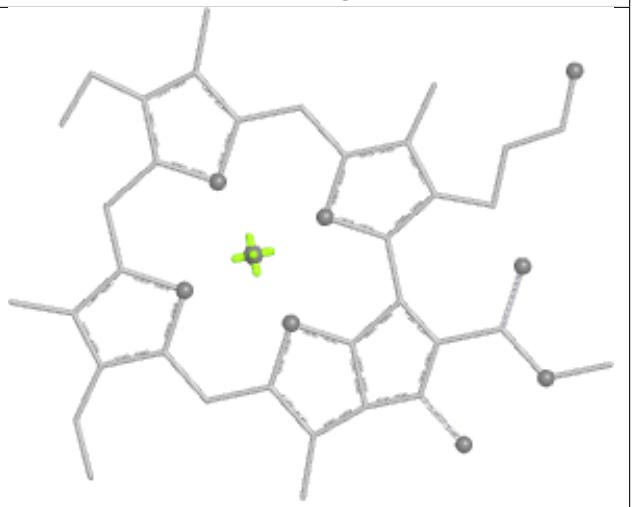
Bond lengths



Bond angles

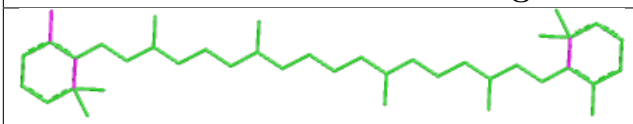


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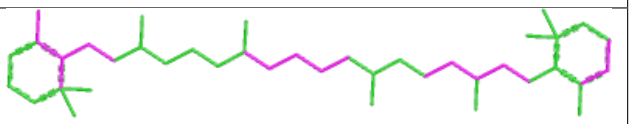


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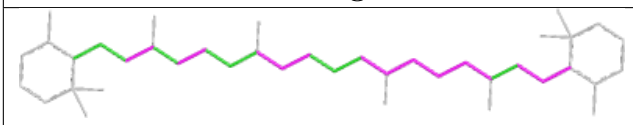
Ligand BCR K2 105



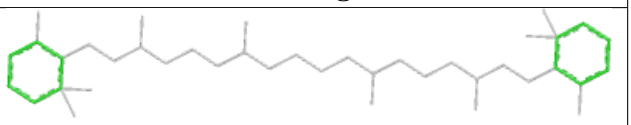
Bond lengths



Bond angles

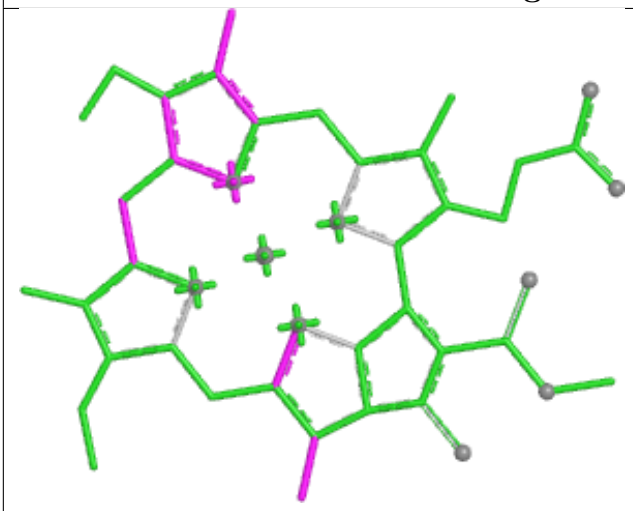


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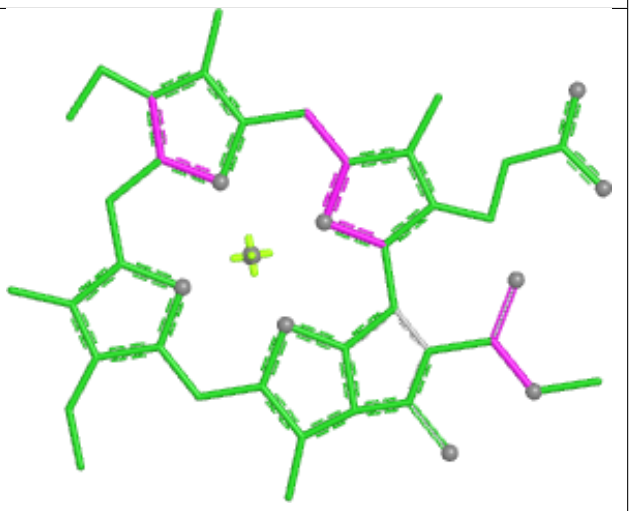


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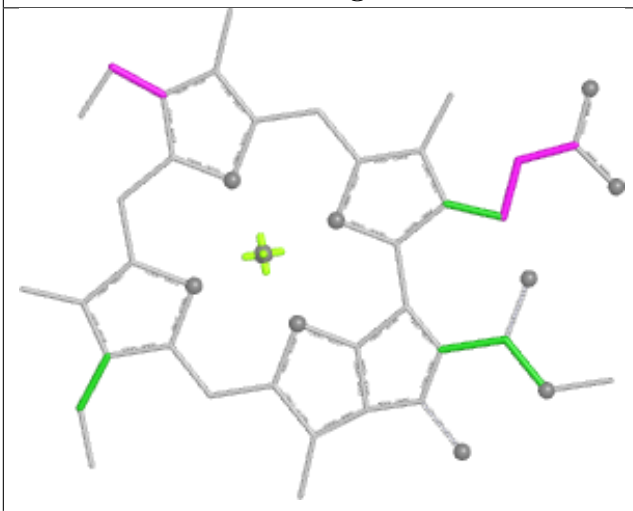
Ligand CLA X 101



Bond lengths



Bond angles

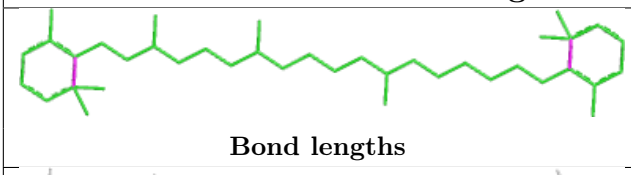


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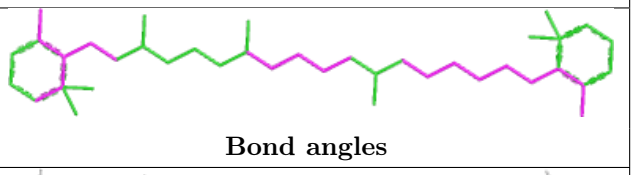


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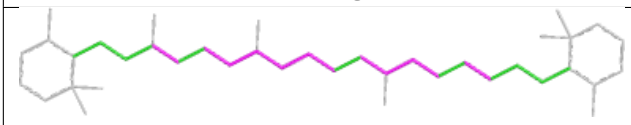
Ligand BCR AA 848



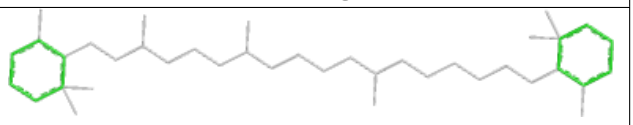
Bond lengths



Bond angles

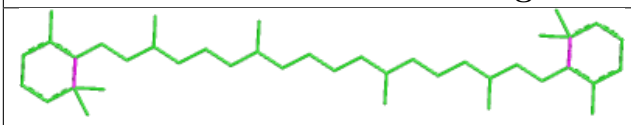


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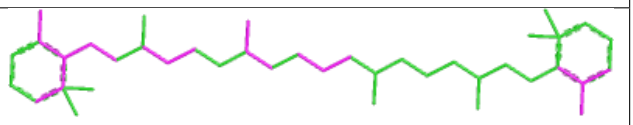


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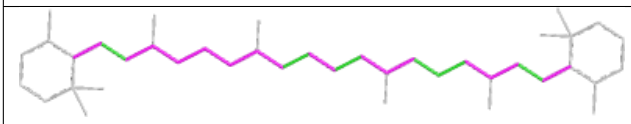
Ligand BCR F2 303



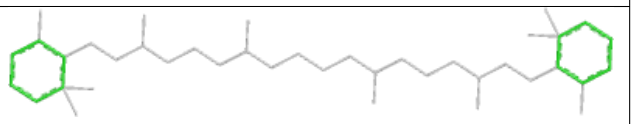
Bond lengths



Bond angles

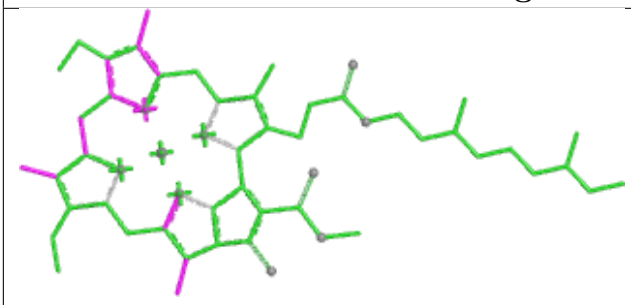


Torsions

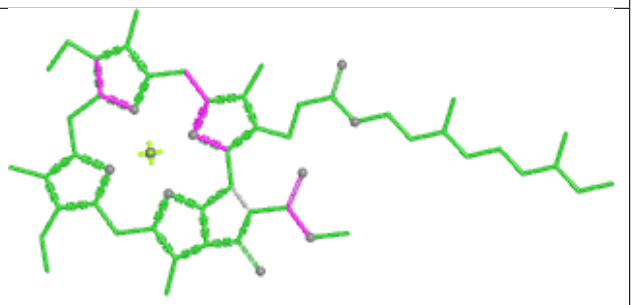


Rings

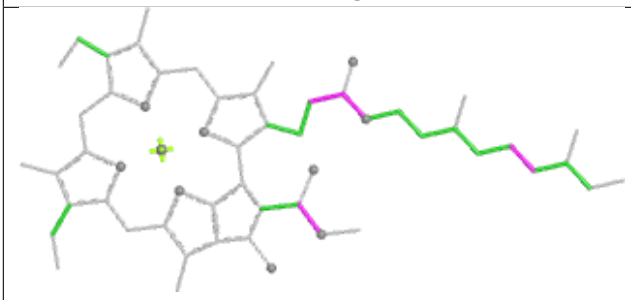
Ligand CLA A1 839



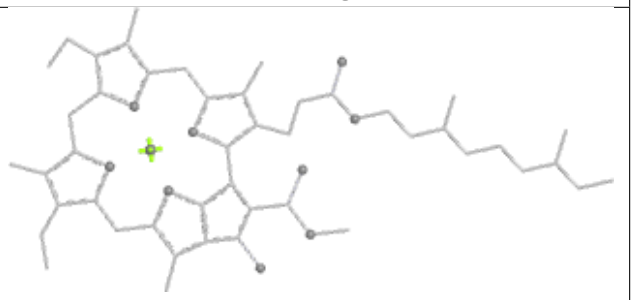
Bond lengths



Bond angles

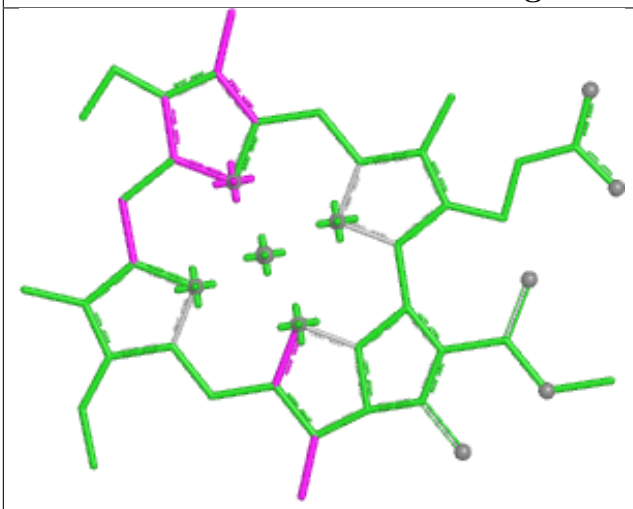


Torsions

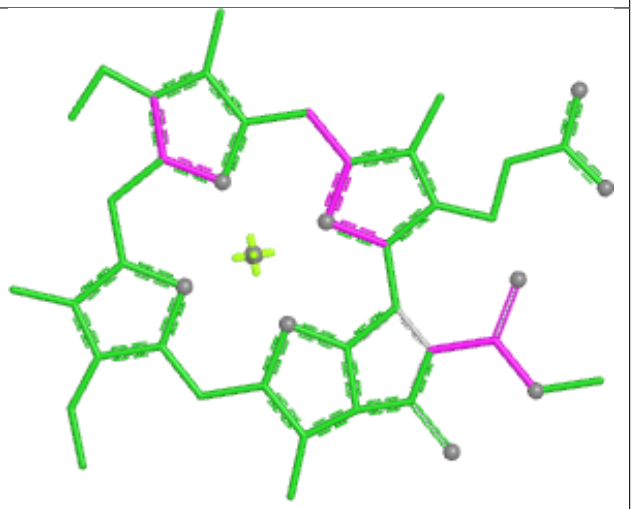


Rings

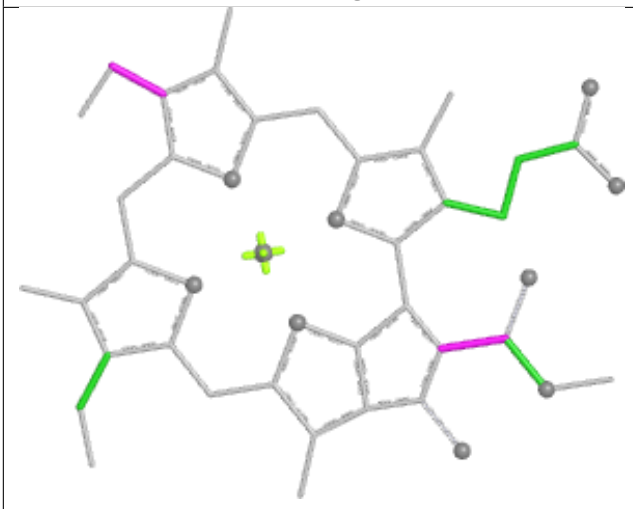
Ligand CLA B 809



Bond lengths



Bond angles

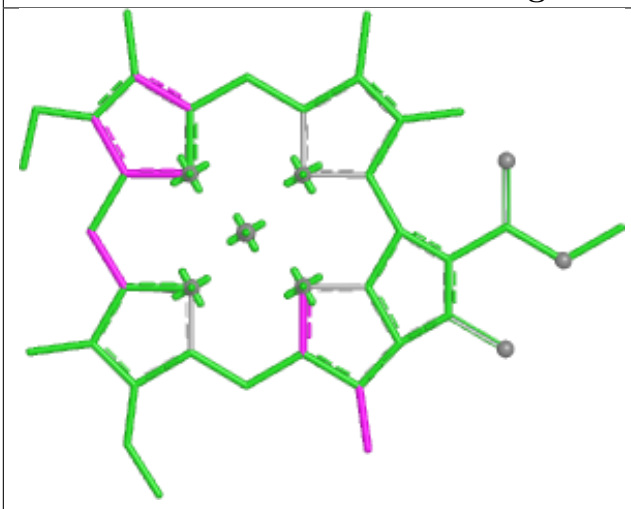


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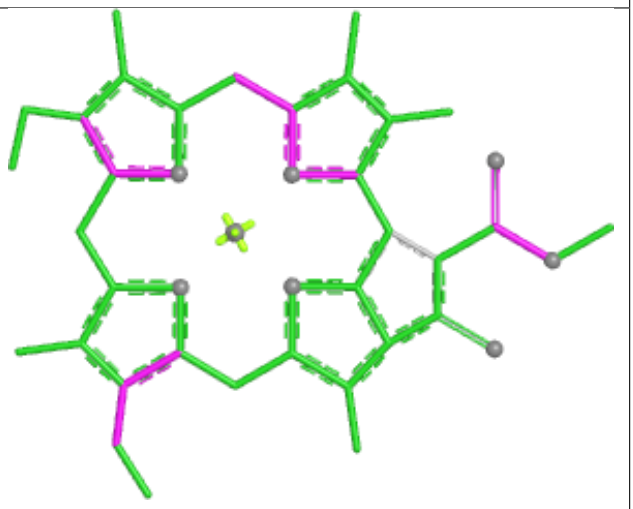


Rings

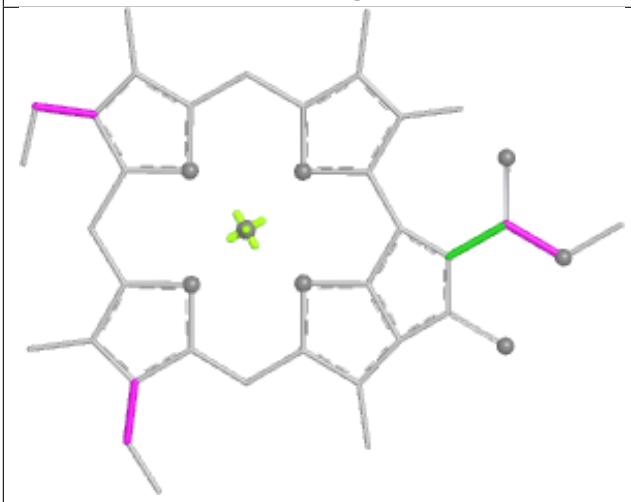
Ligand CLA J 103



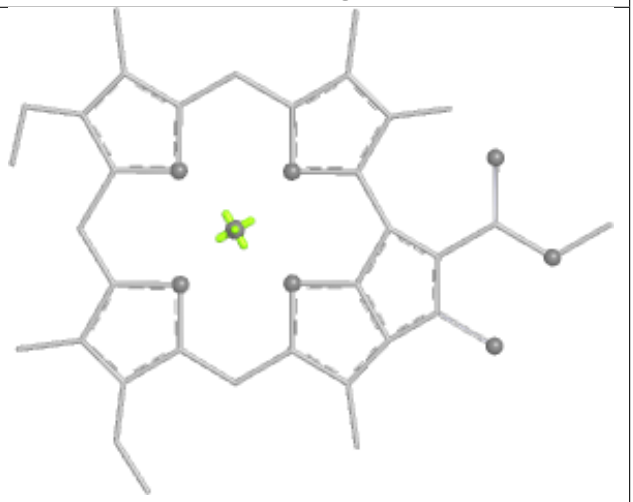
Bond lengths



Bond angles

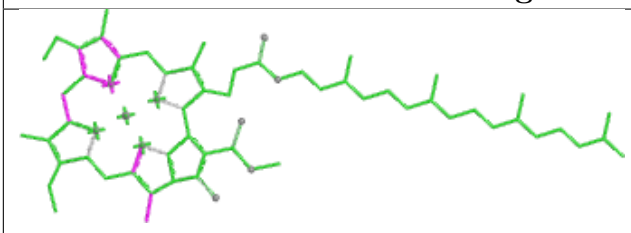


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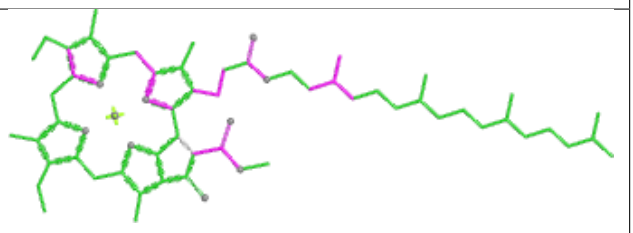


Rings

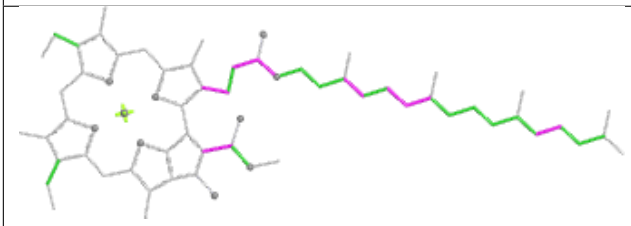
Ligand CLA B2 821



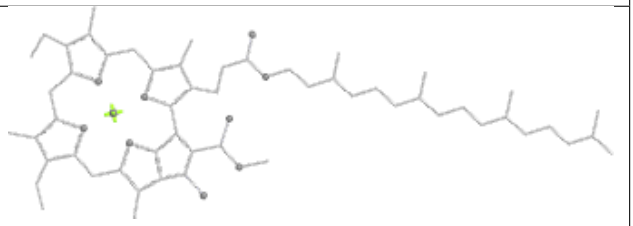
Bond lengths



Bond angles

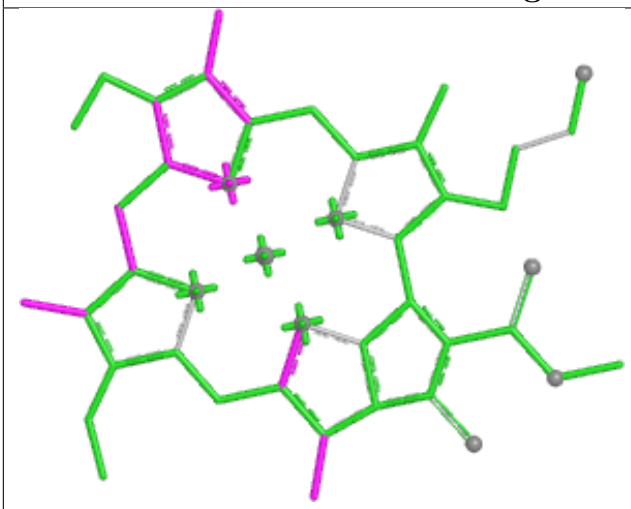


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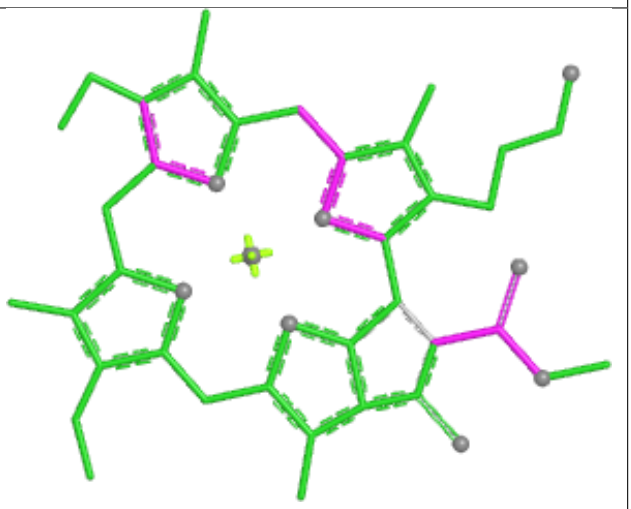


Rings

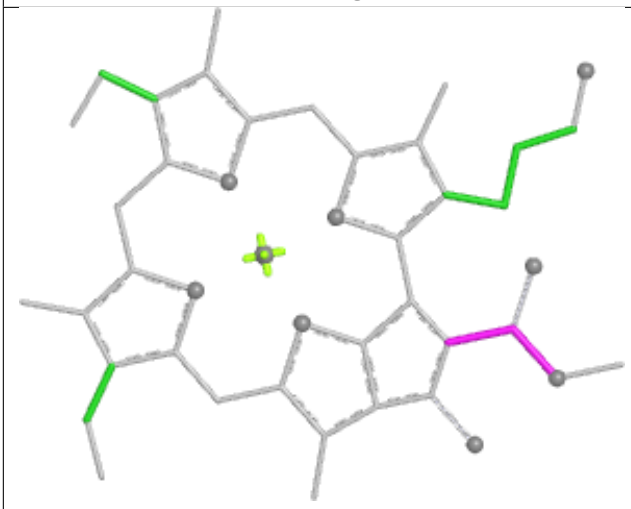
Ligand CLA A 838



Bond lengths



Bond angles

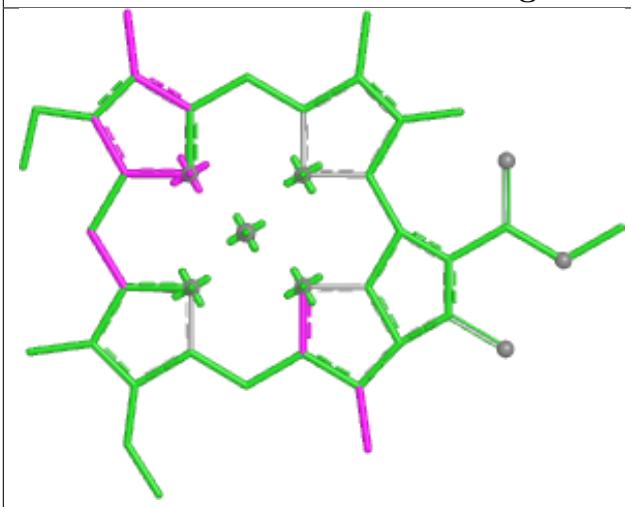


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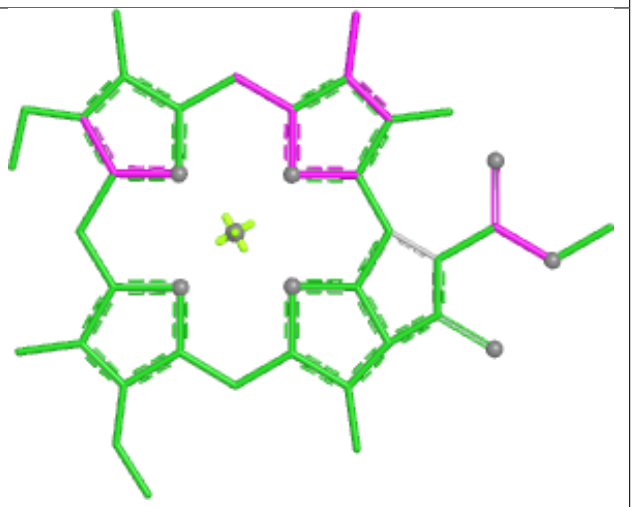


Rings

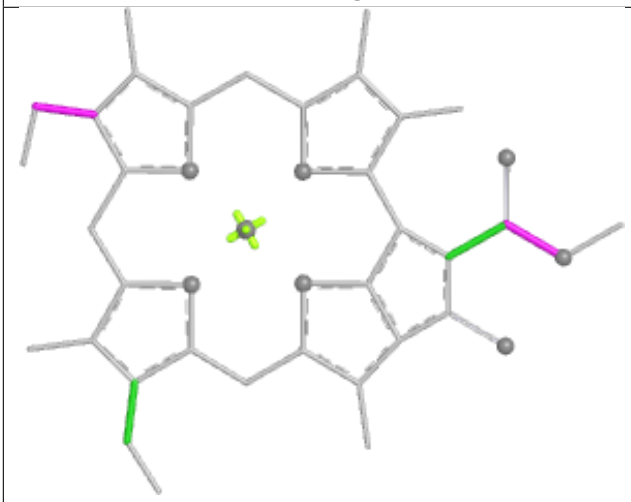
Ligand CLA J1 101



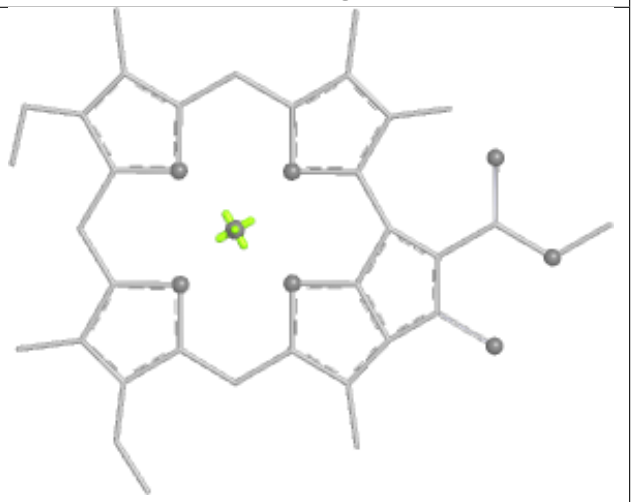
Bond lengths



Bond angles

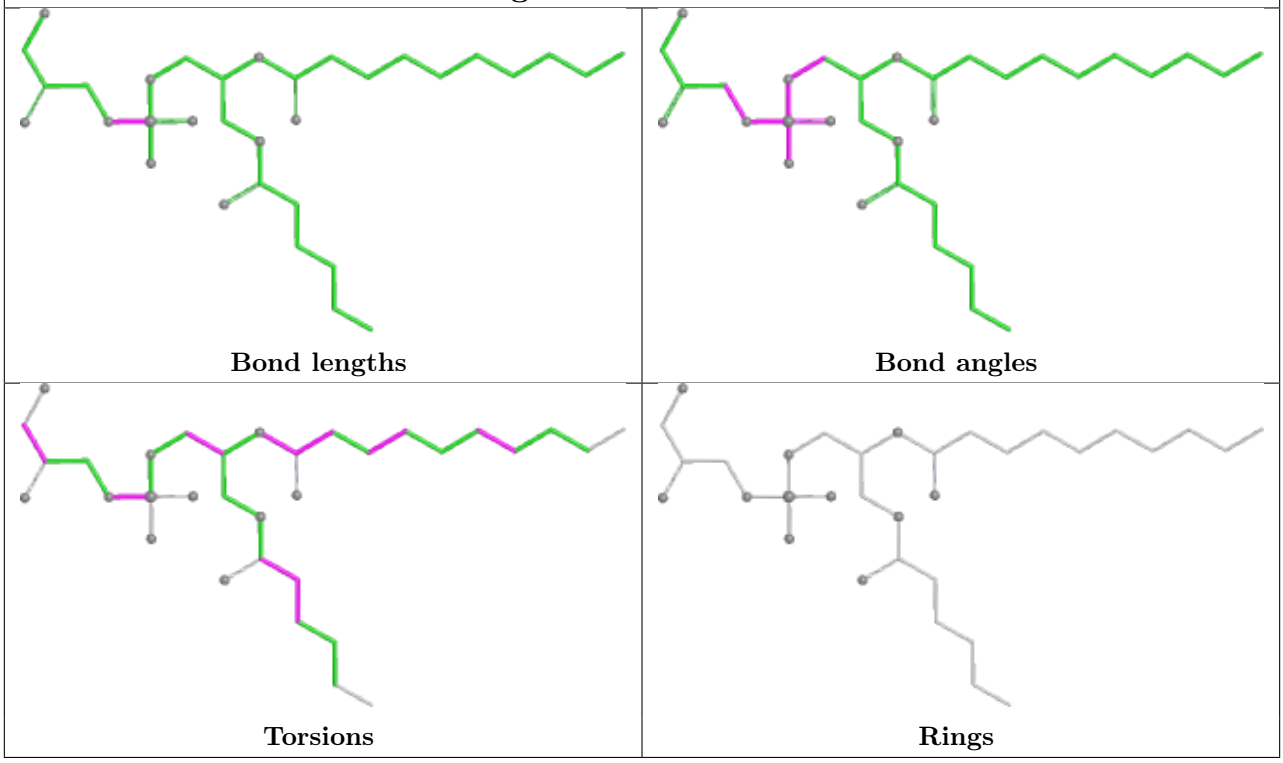


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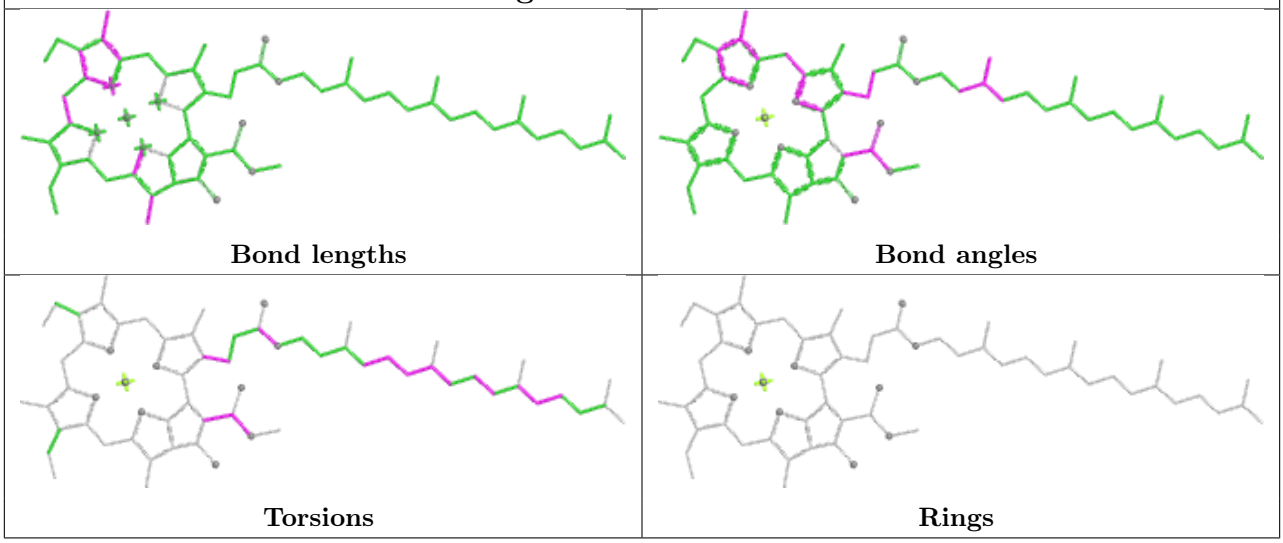


Rings

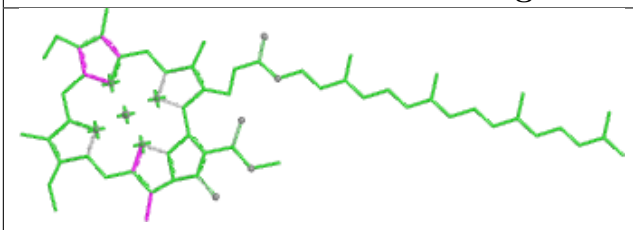
Ligand LHG BB 850



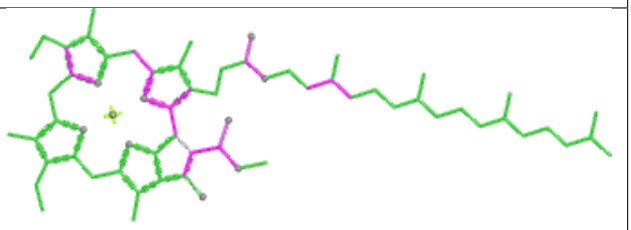
Ligand CLA B1 815



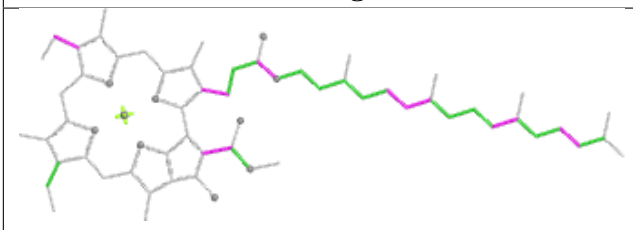
Ligand CLA B2 833



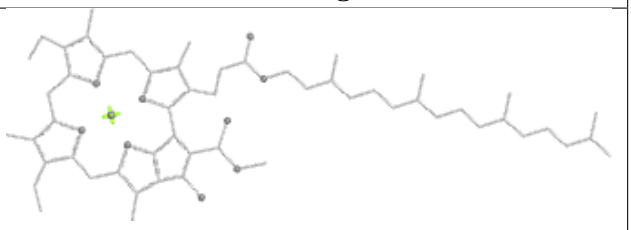
Bond lengths



Bond angles

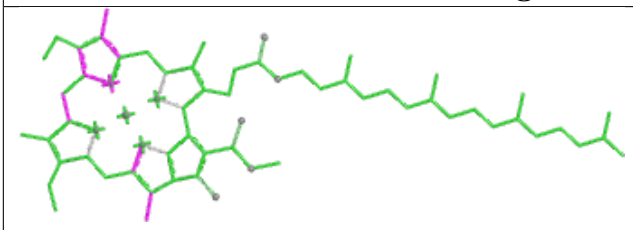


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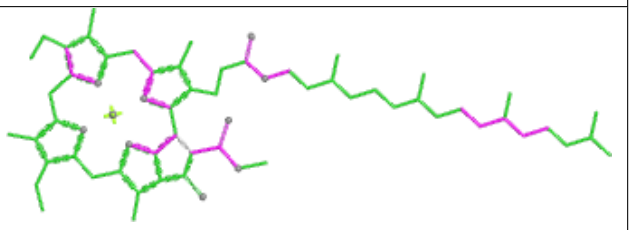


Rings

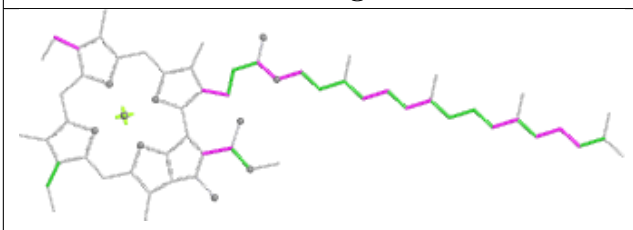
Ligand CLA B2 807



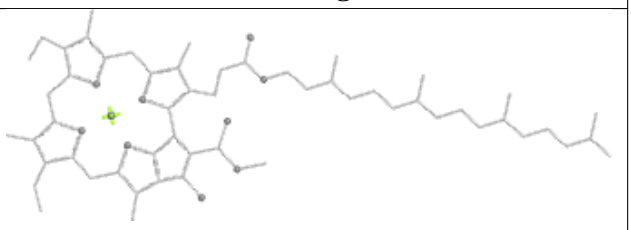
Bond lengths



Bond angles

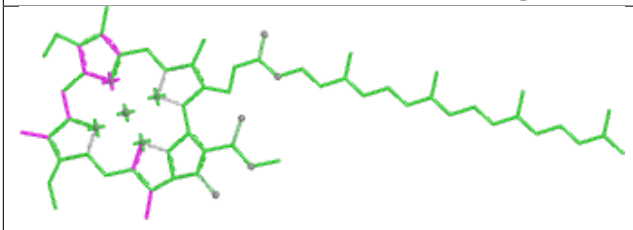


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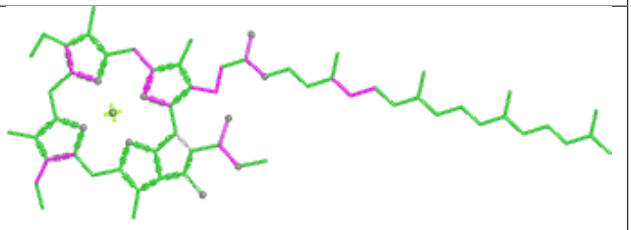


Rings

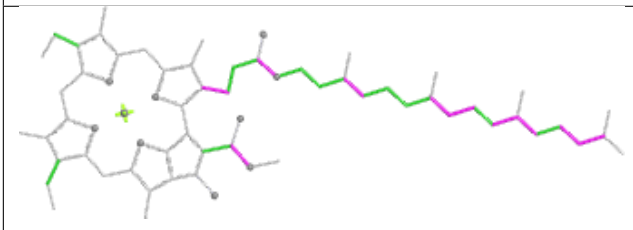
Ligand CLA A1 820



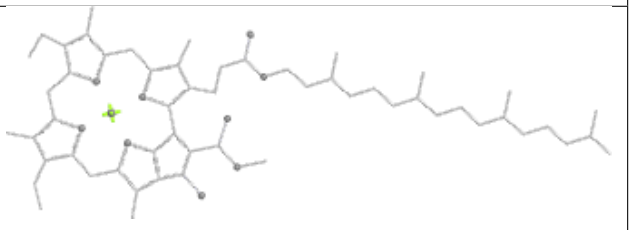
Bond lengths



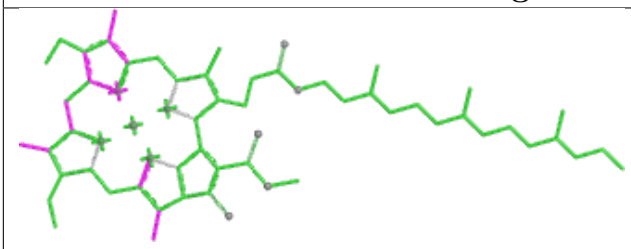
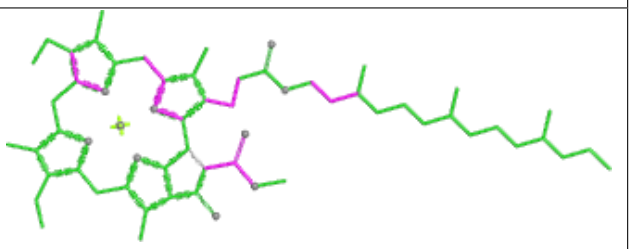
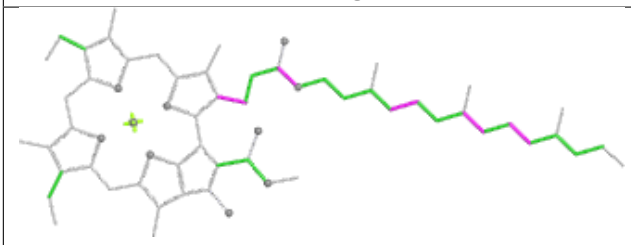
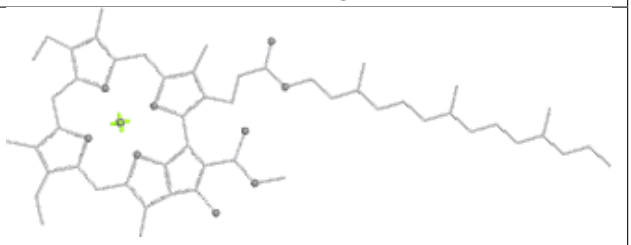
Bond angles

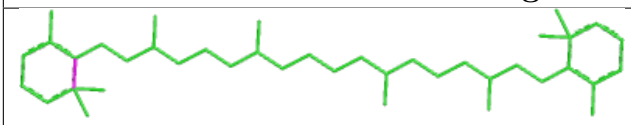
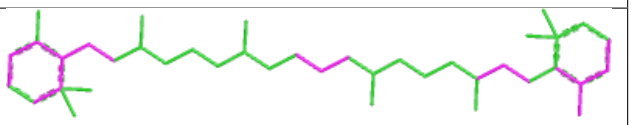
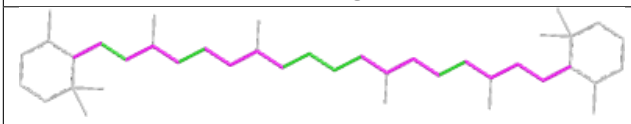
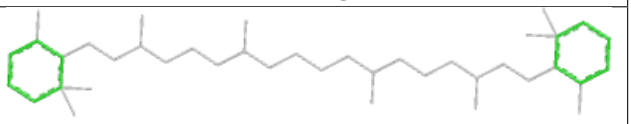


Torsions

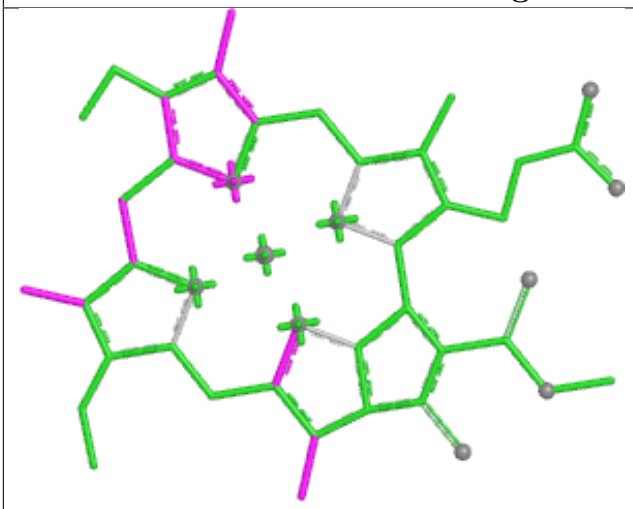


Rings

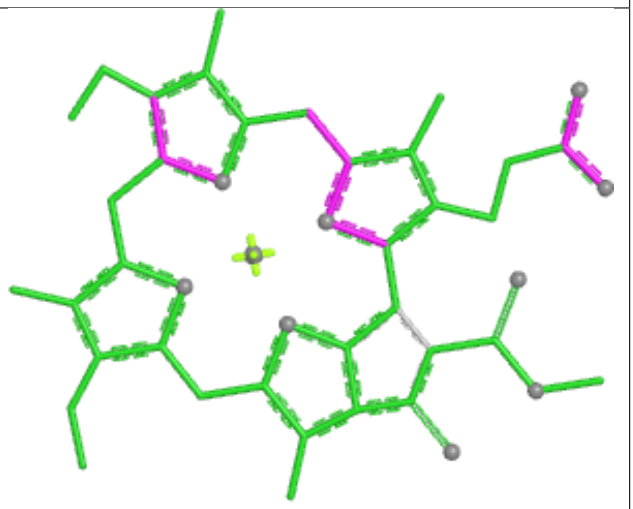
Ligand CLA BB 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

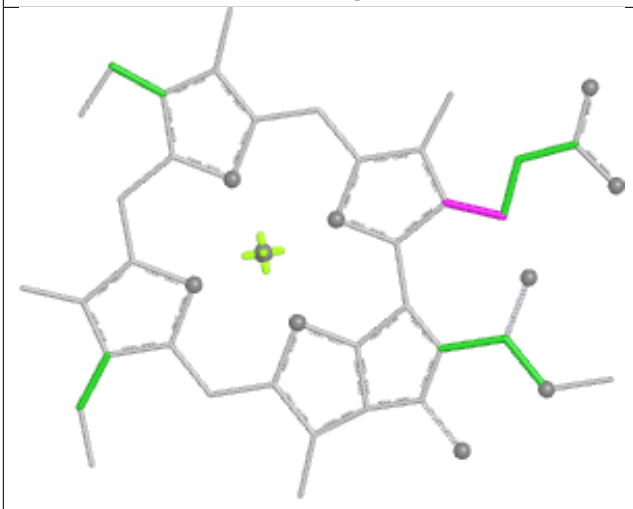
Ligand CLA BB 834



Bond lengths



Bond angles

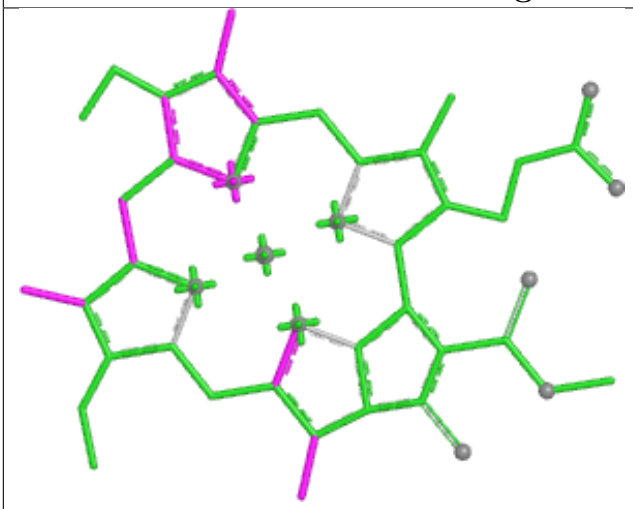


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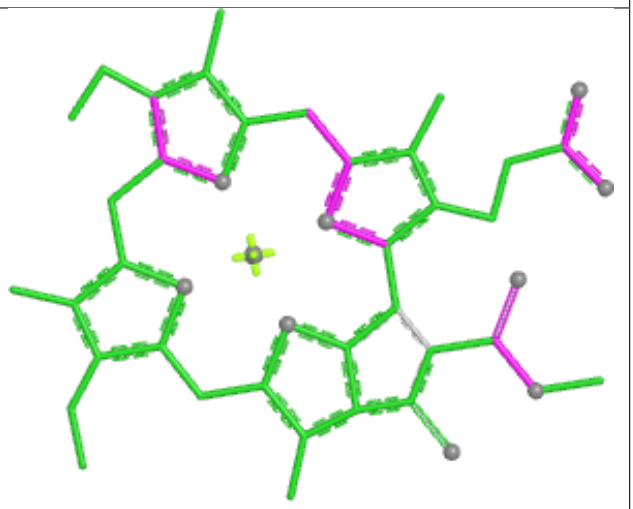


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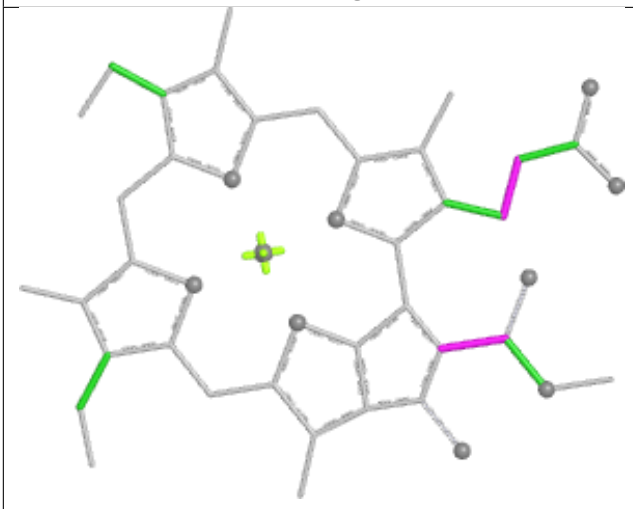
Ligand CLA A2 824



Bond lengths



Bond angles

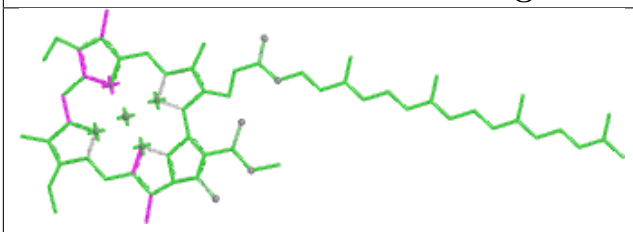


Torsions

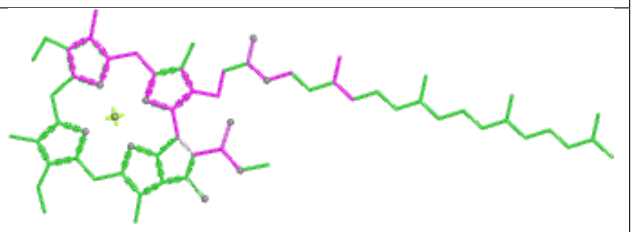


Rings

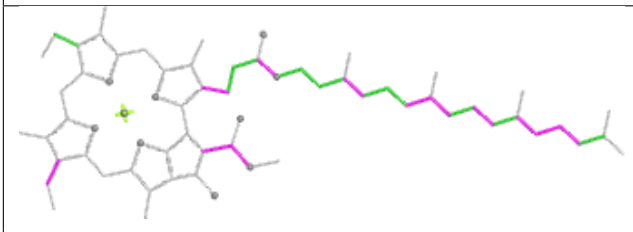
Ligand CLA B2 834



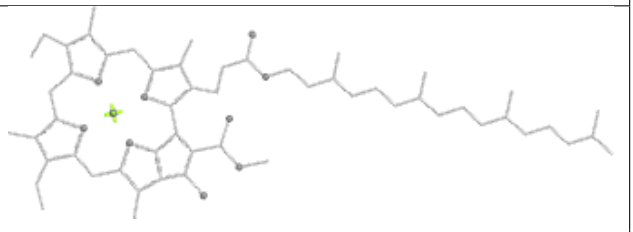
Bond lengths



Bond angles

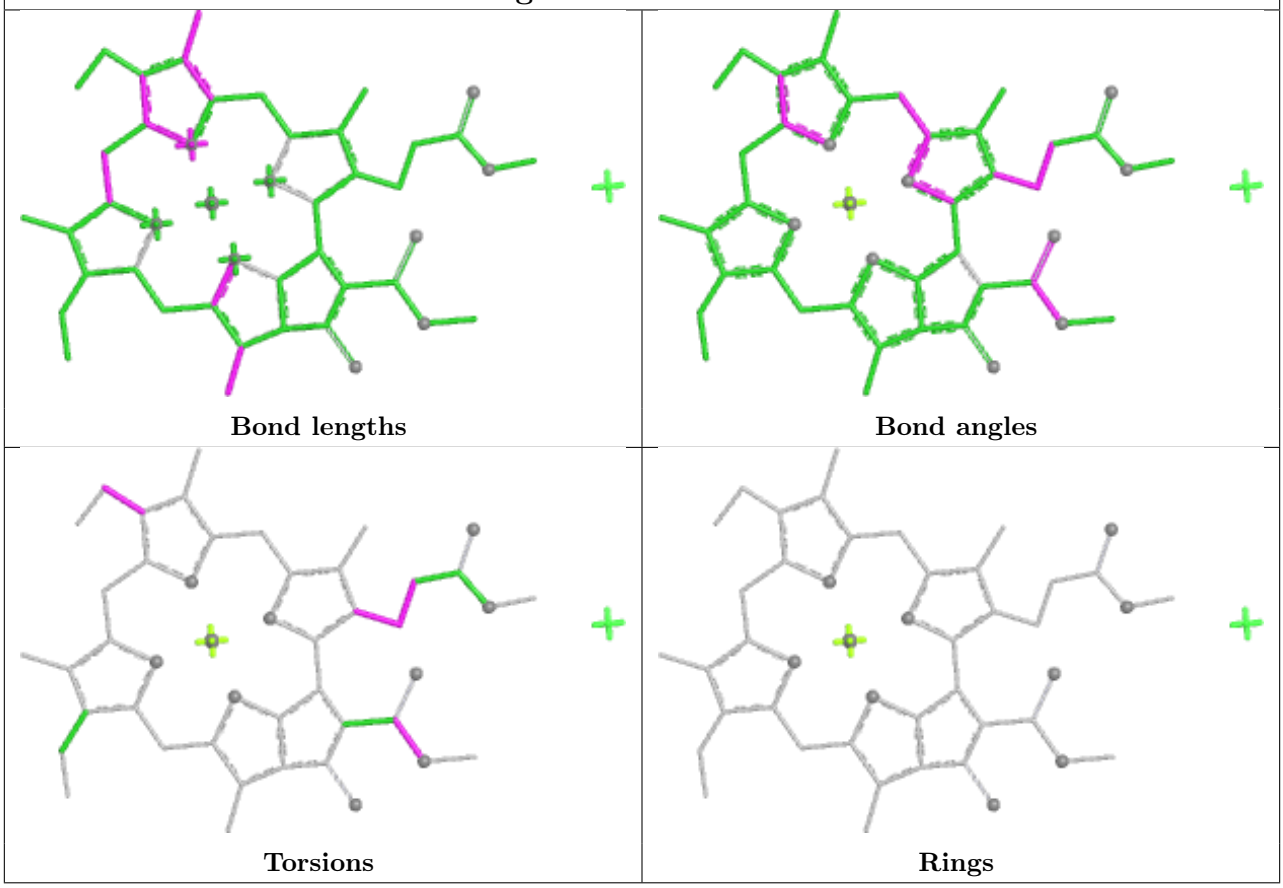


Torsions

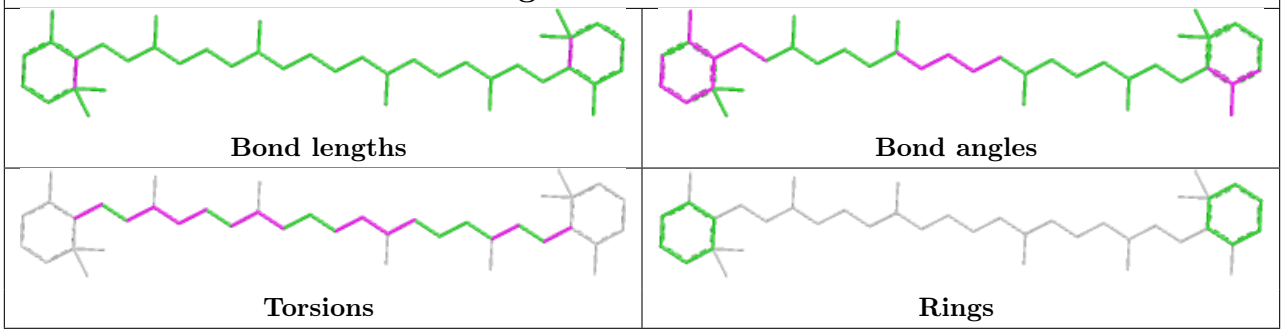


Rings

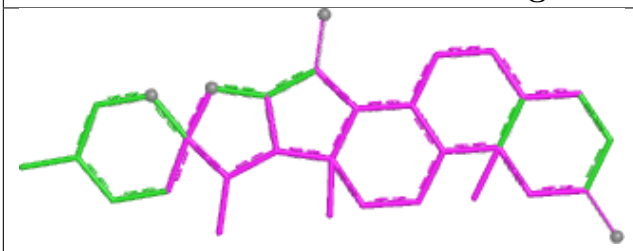
Ligand CLA A1 811



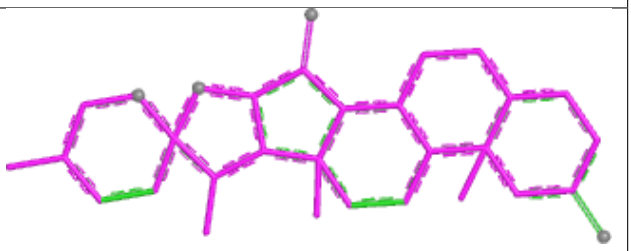
Ligand BCR J2 102



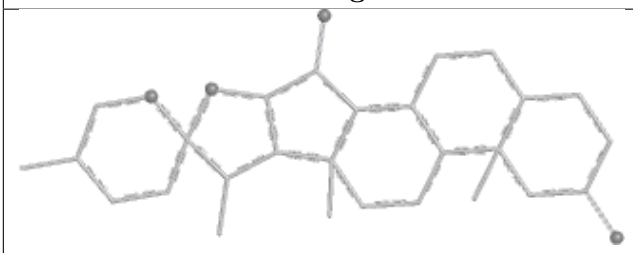
Ligand AJP L 208



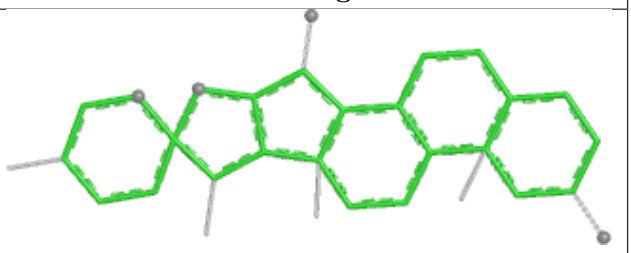
Bond lengths



Bond angles

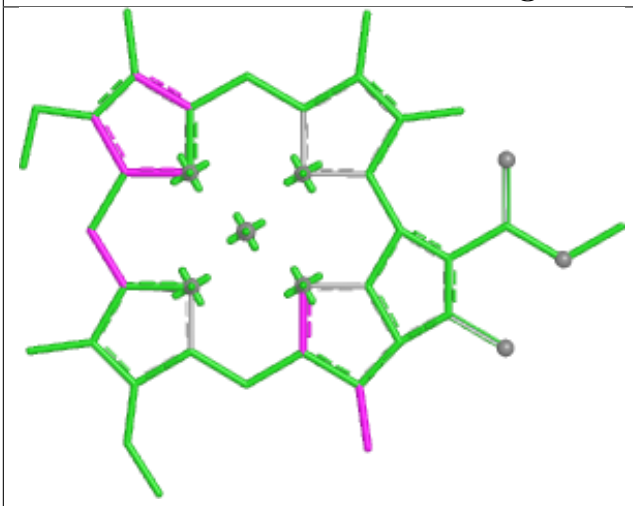


Torsions

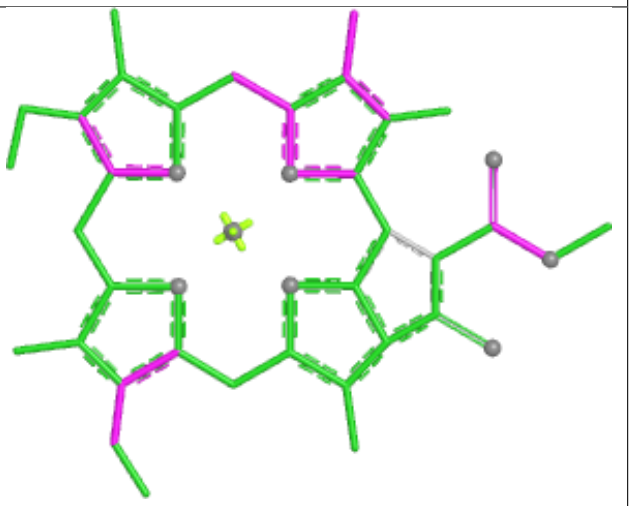


Rings

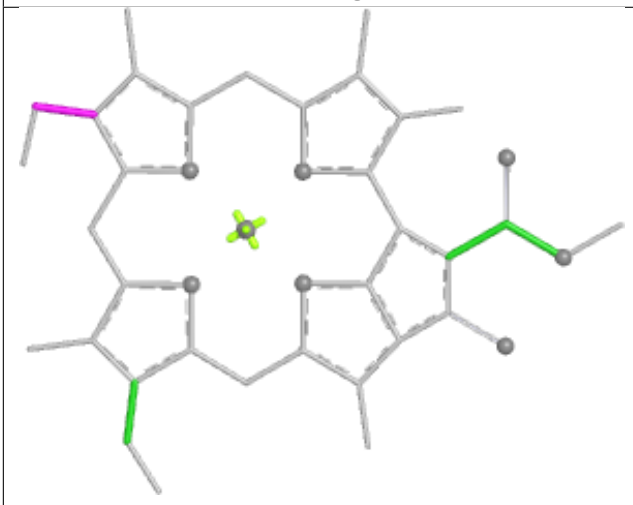
Ligand CLA J2 103



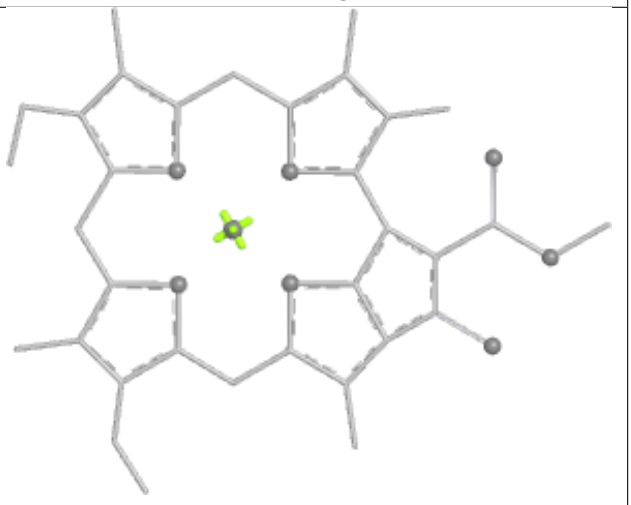
Bond lengths



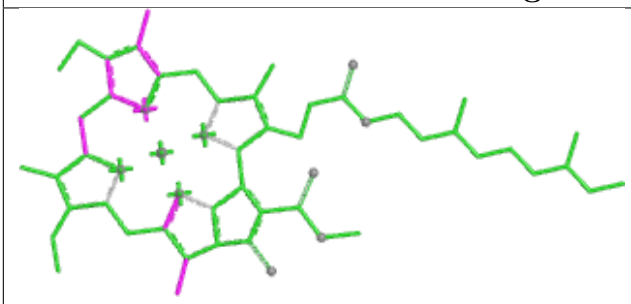
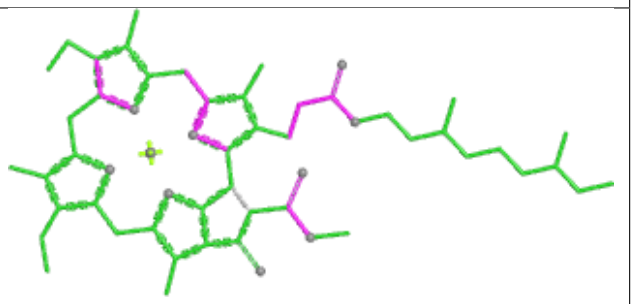
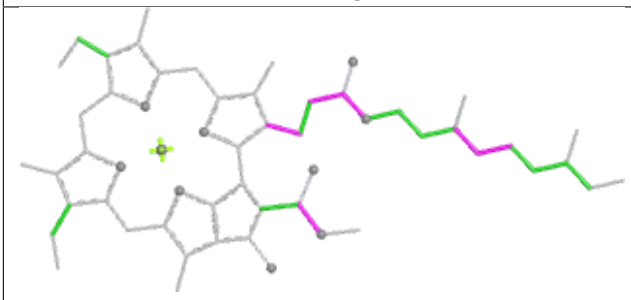
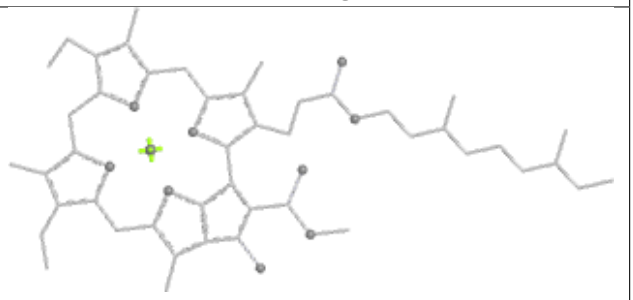
Bond angles



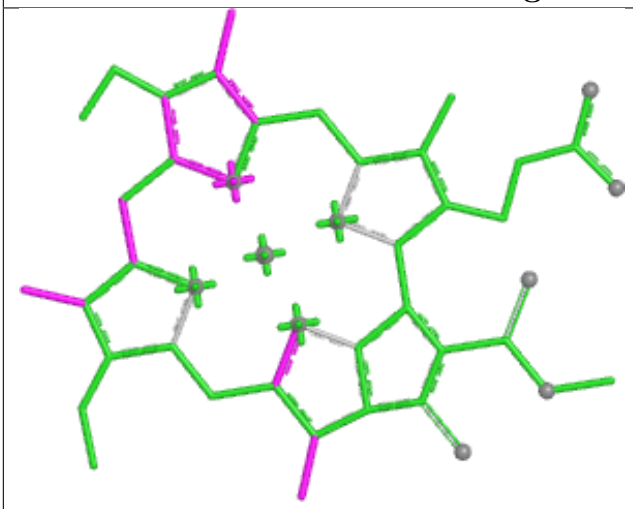
Torsions



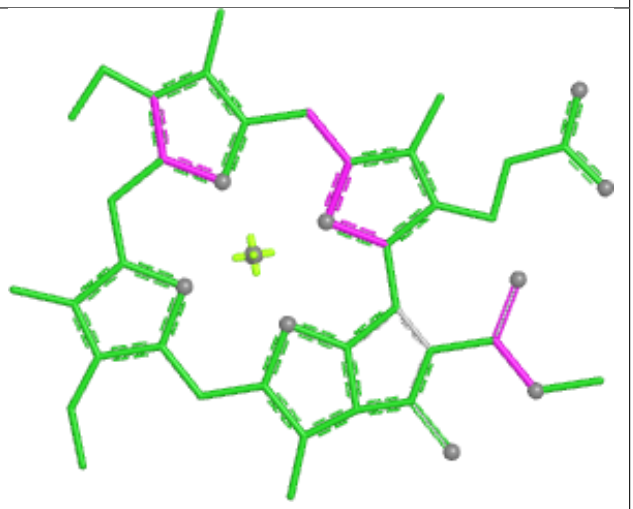
Rings

Ligand CLA A 828	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

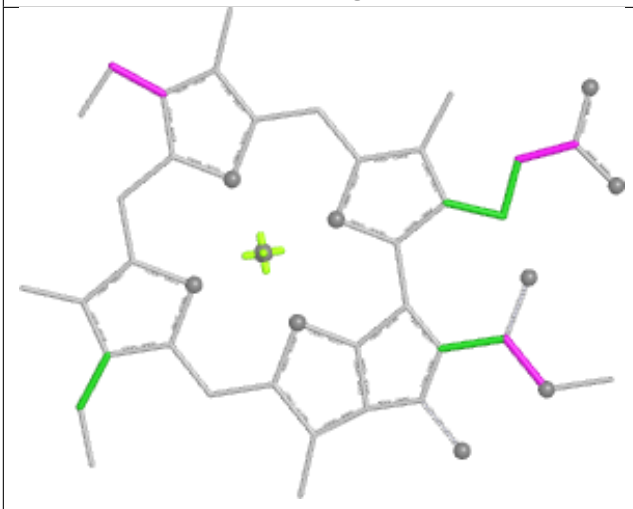
Ligand CLA A 837



Bond lengths



Bond angles

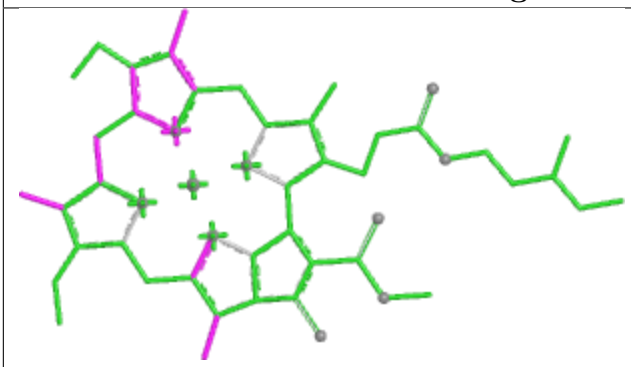


Torsions

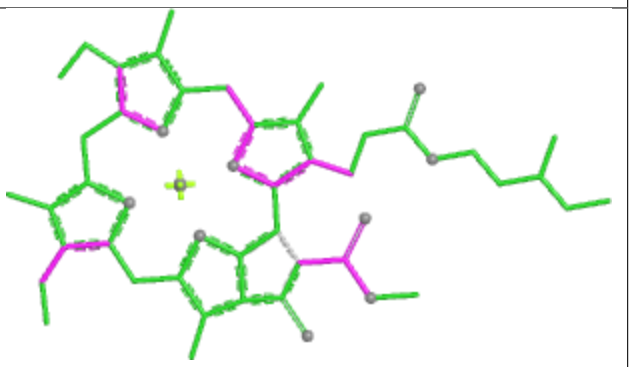


Rings

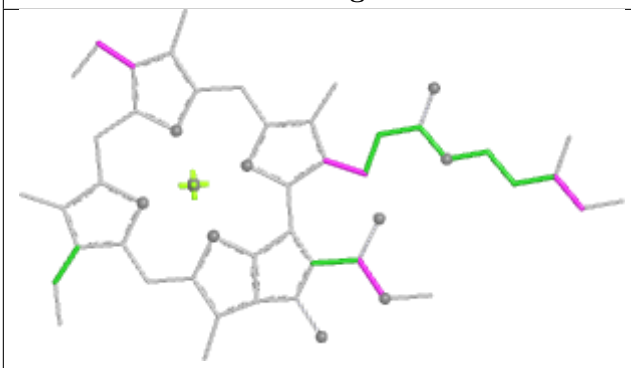
Ligand CLA AA 811



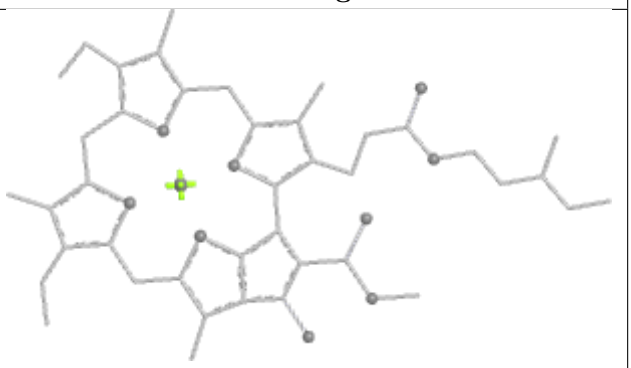
Bond lengths



Bond angles

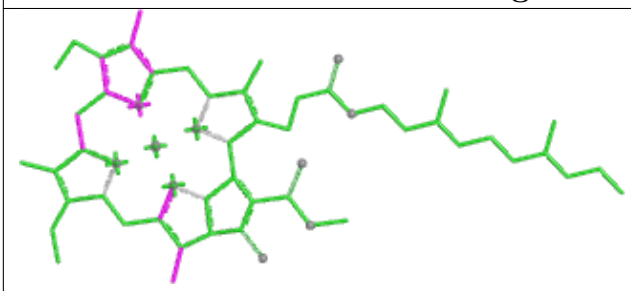


Torsions

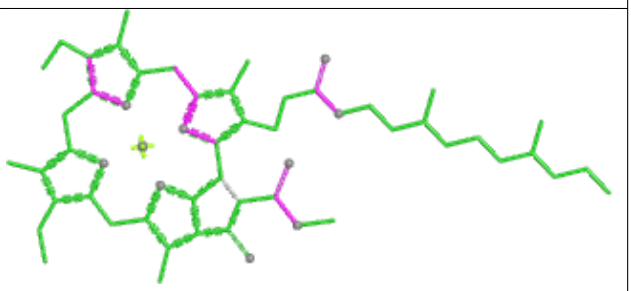


Rings

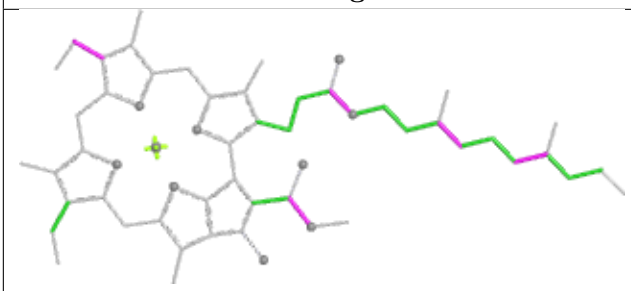
Ligand CLA BB 816



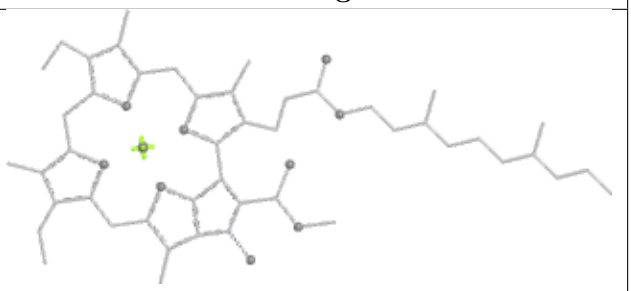
Bond lengths



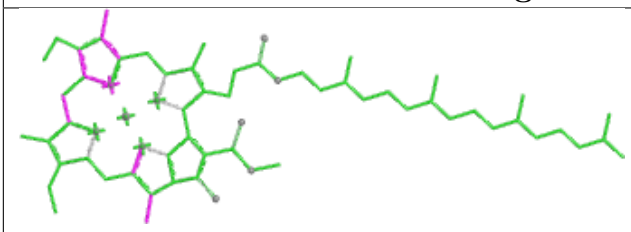
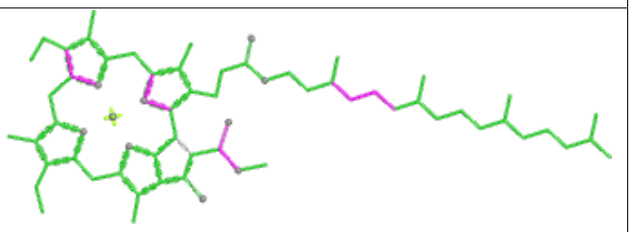
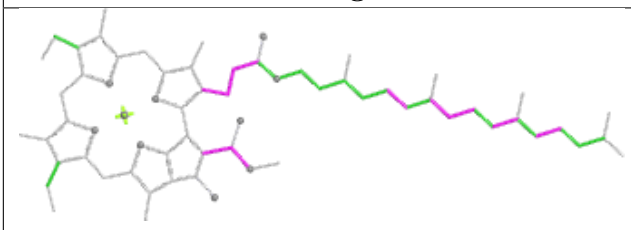
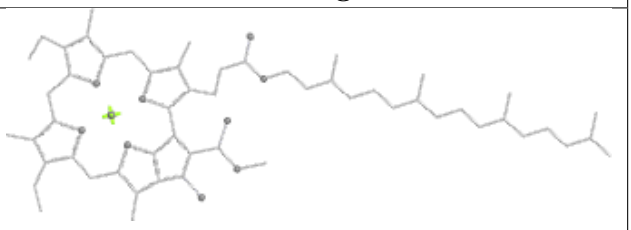
Bond angles

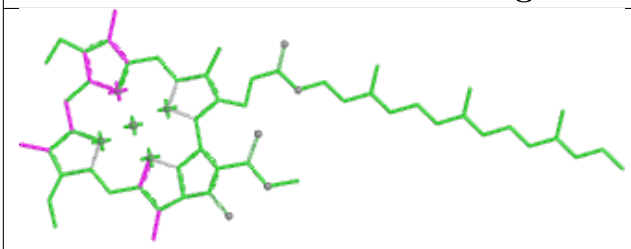
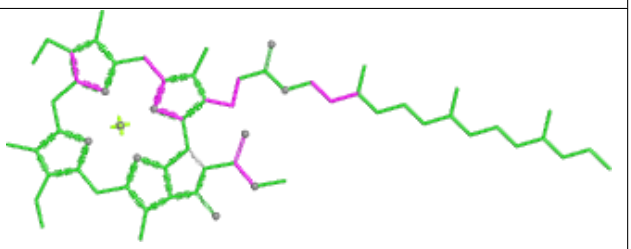
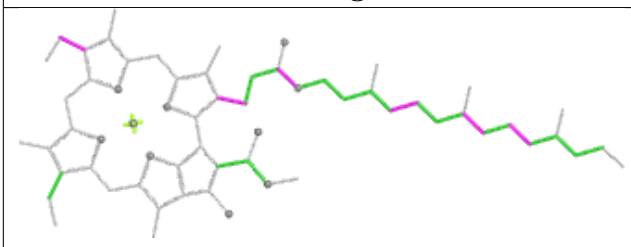
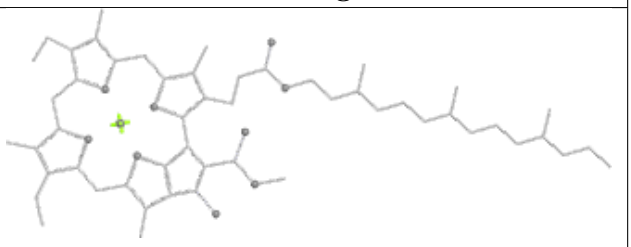


Torsions

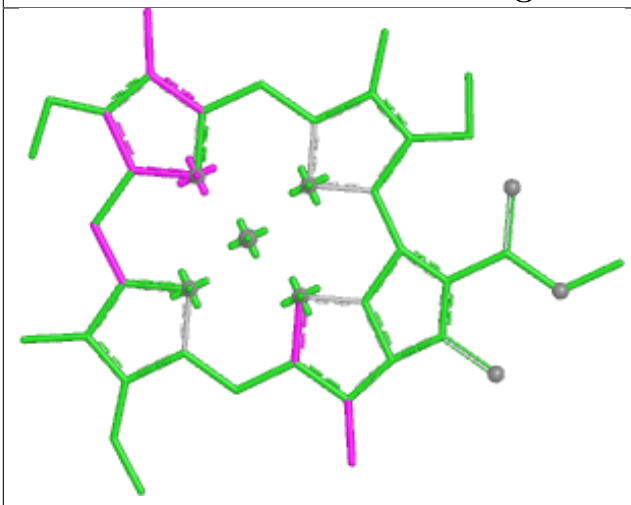


Rings

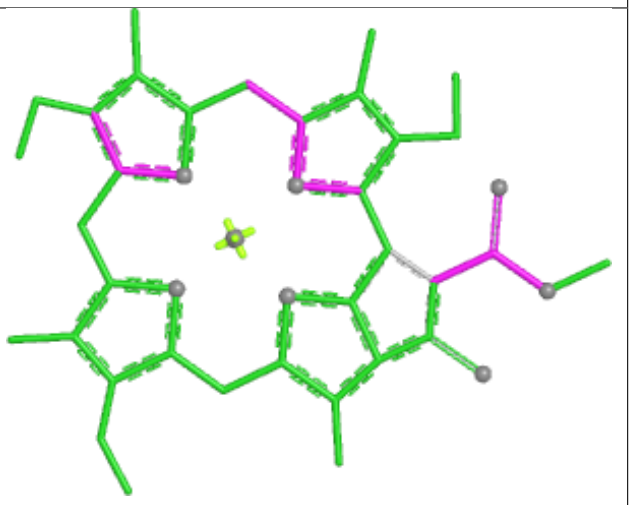
Ligand CLA A1 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

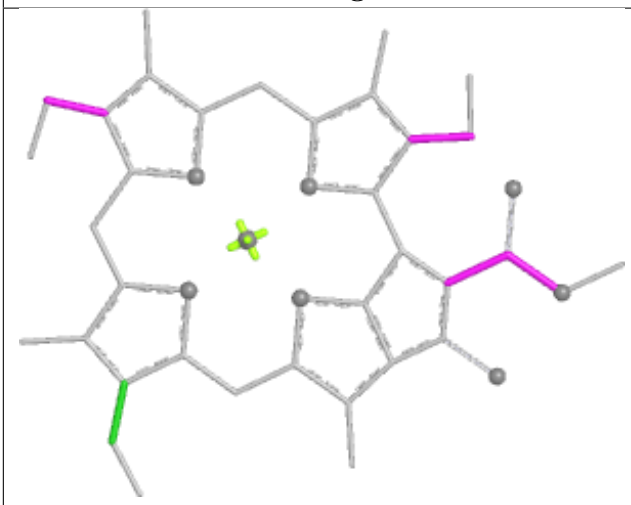
Ligand CLA B2 813



Bond lengths



Bond angles

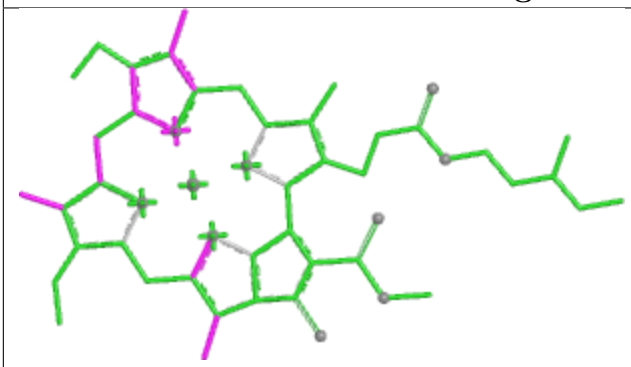


Torsions

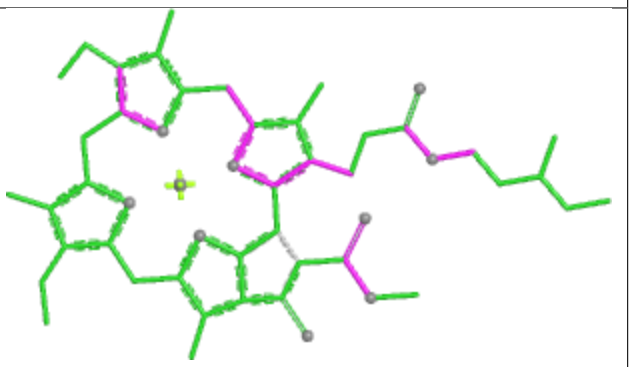


Rings

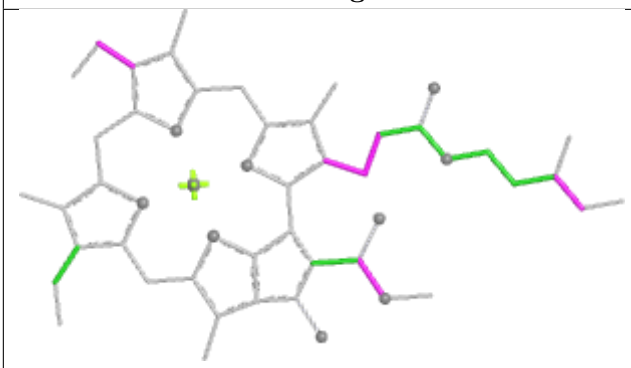
Ligand CLA A1 810



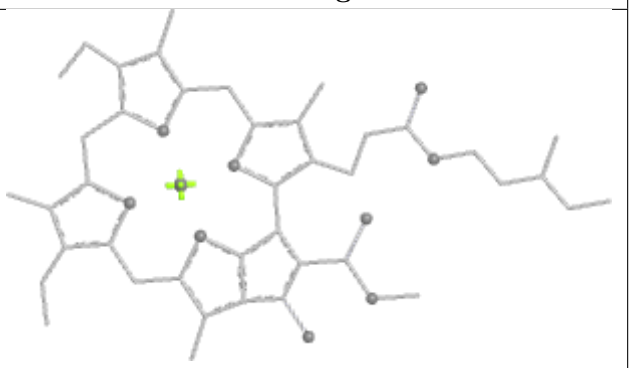
Bond lengths



Bond angles

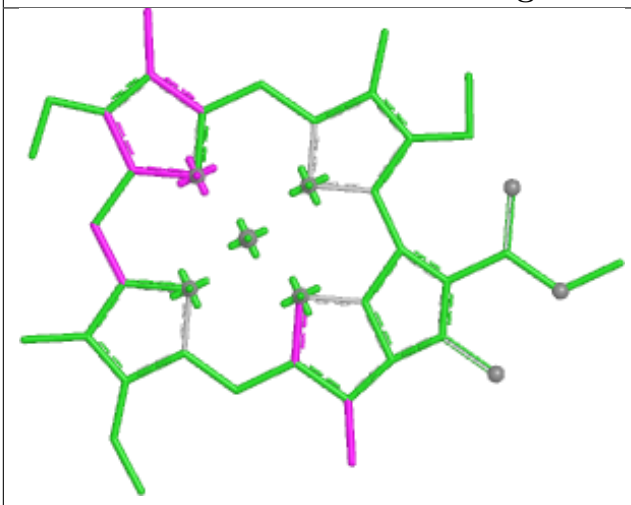


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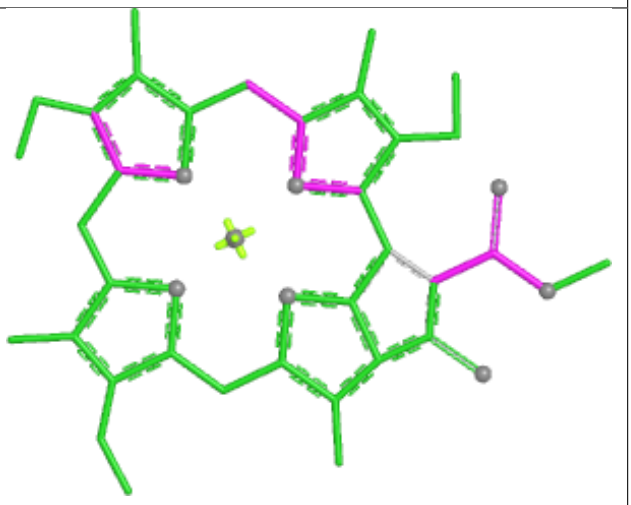


Rings

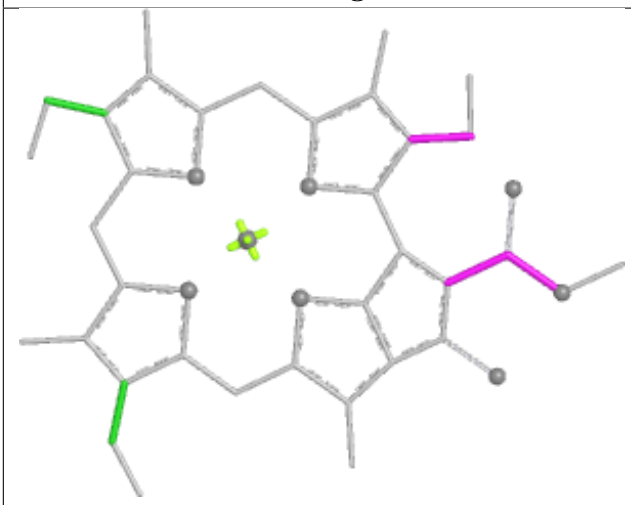
Ligand CLA F2 302



Bond lengths



Bond angles

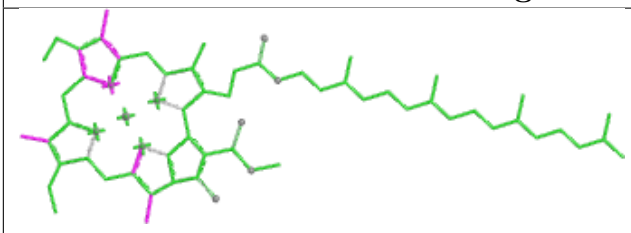


Torsions

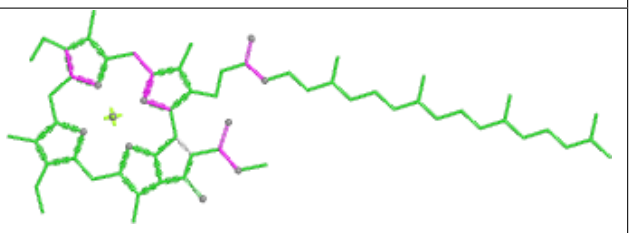


Rings

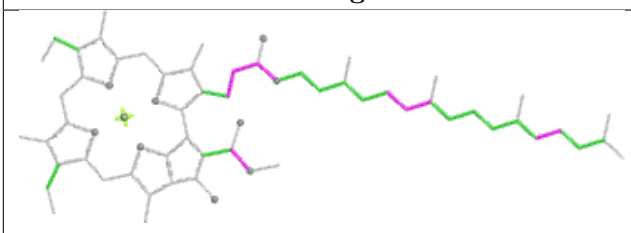
Ligand CLA A2 831



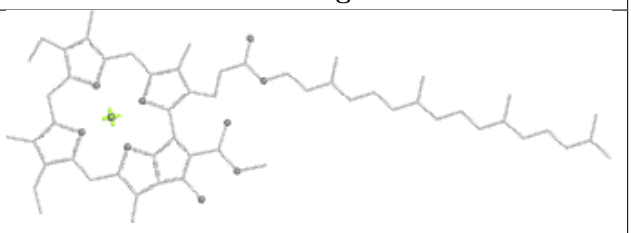
Bond lengths



Bond angles

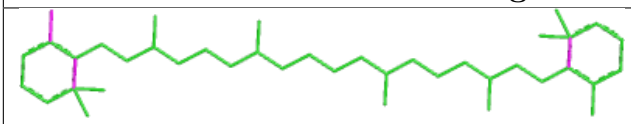


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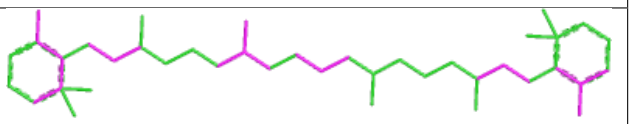


Rings

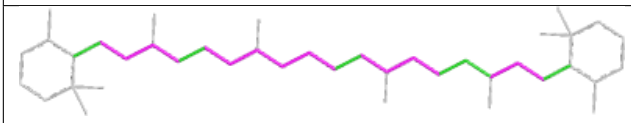
Ligand BCR M2 102



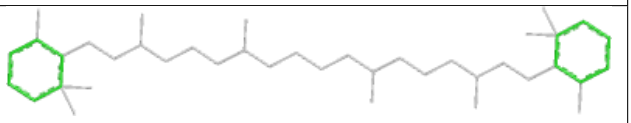
Bond lengths



Bond angles

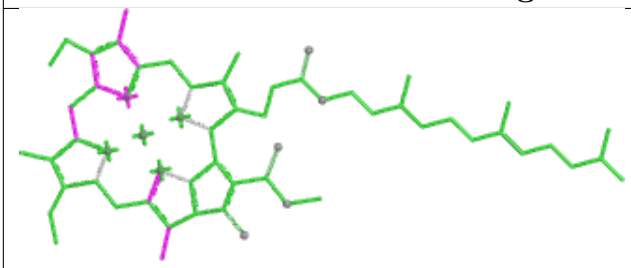


Torsions

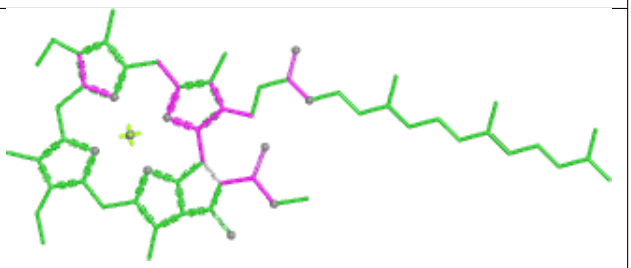


Rings

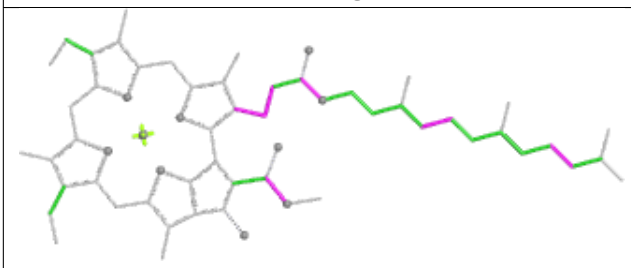
Ligand CLA F2 301



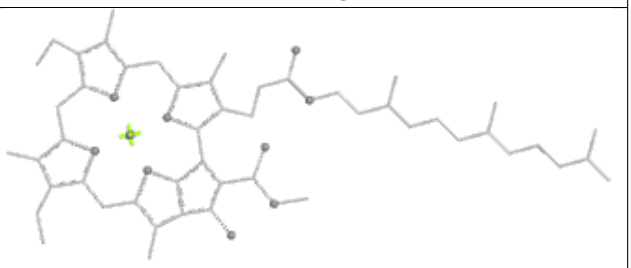
Bond lengths



Bond angles

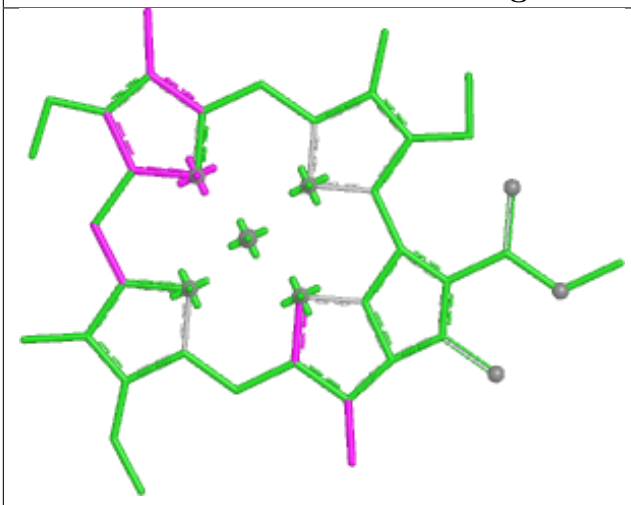


Torsions

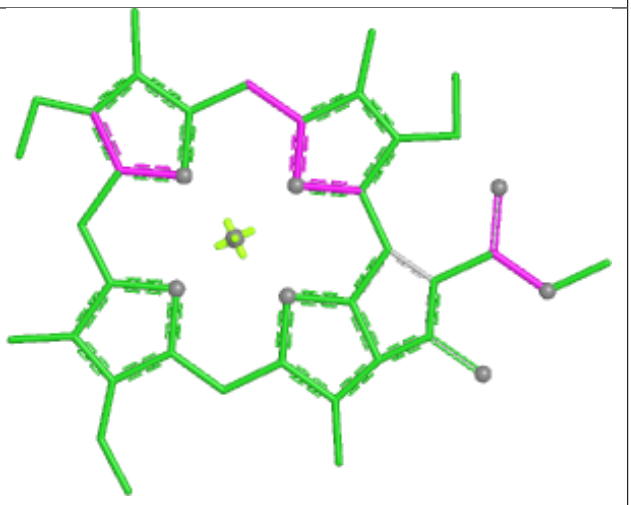


Rings

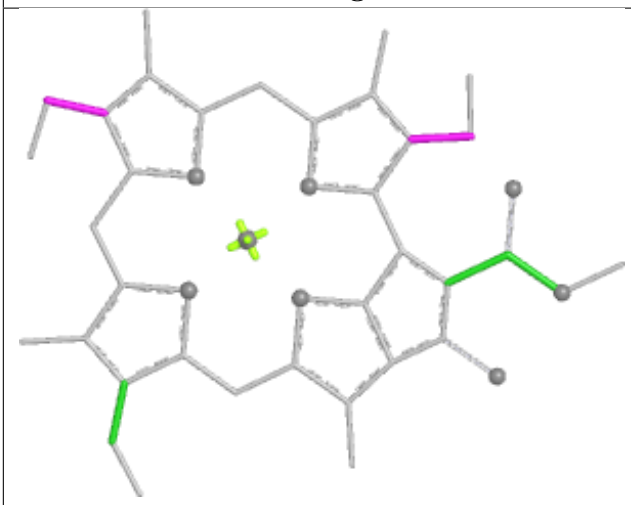
Ligand CLA AA 814



Bond lengths



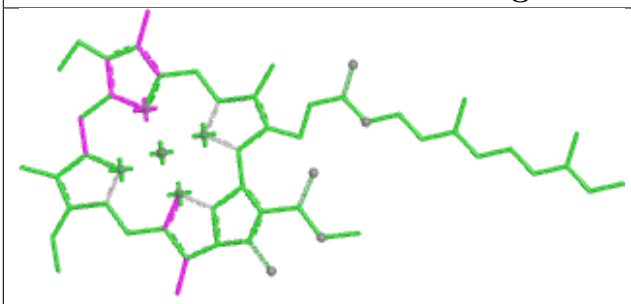
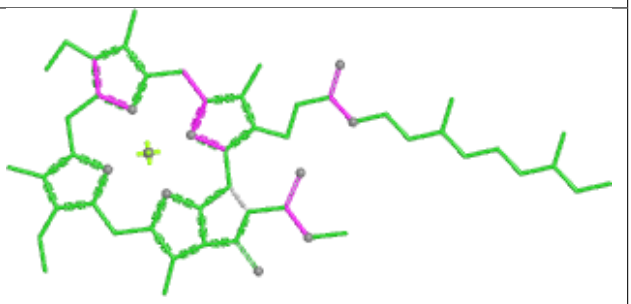
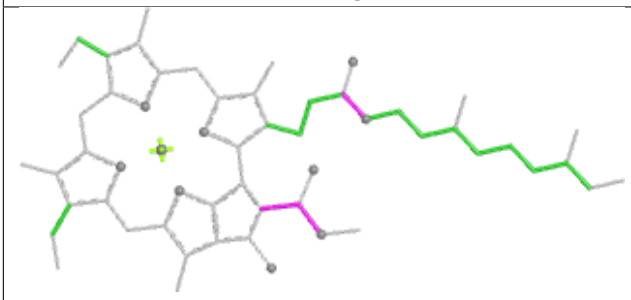
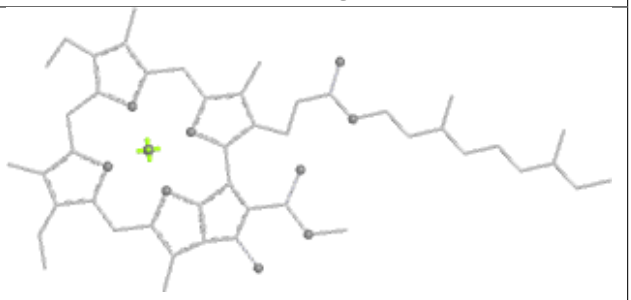
Bond angles

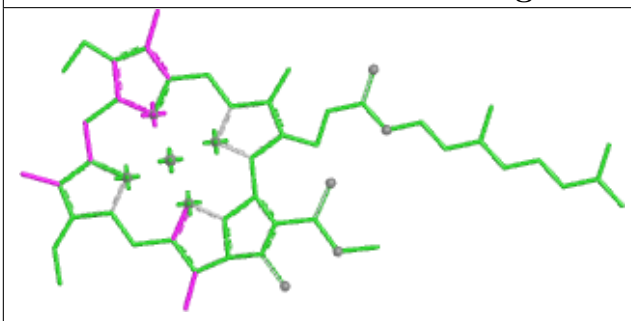
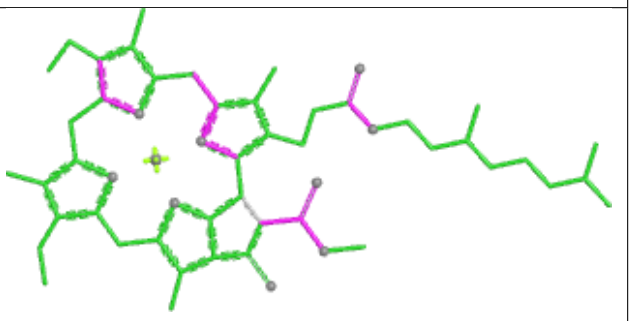
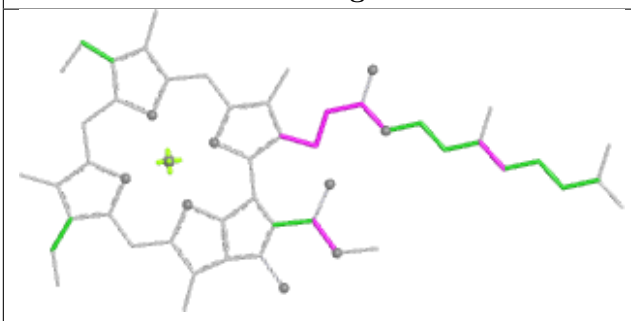
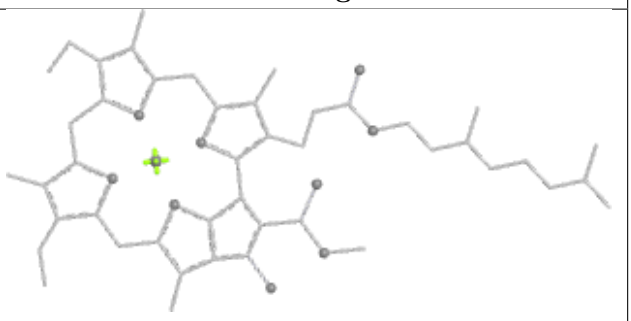


Torsions

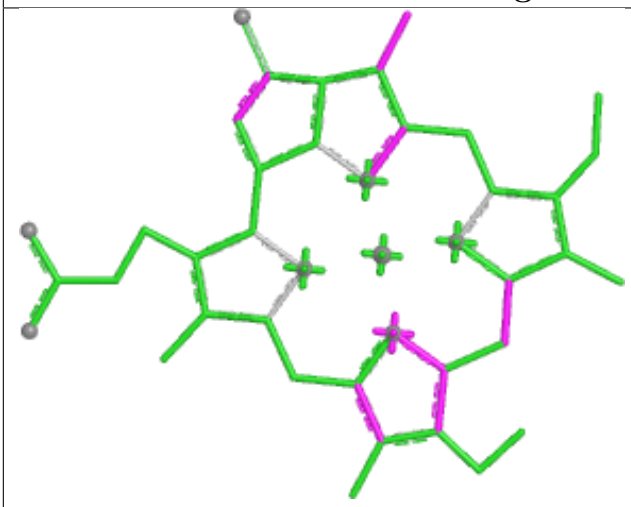


Rings

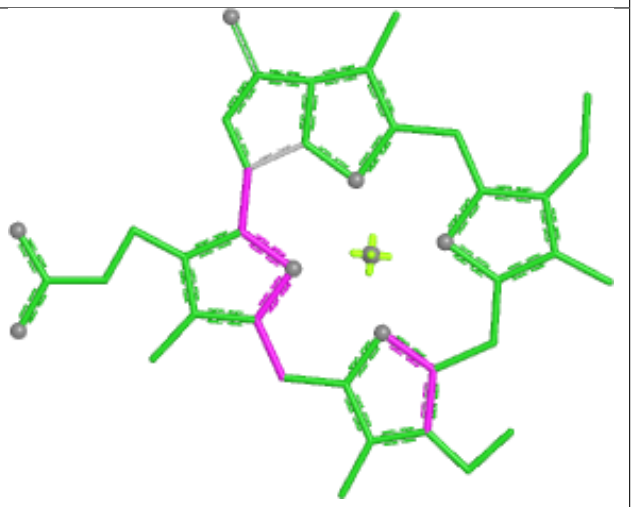
Ligand CLA BB 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

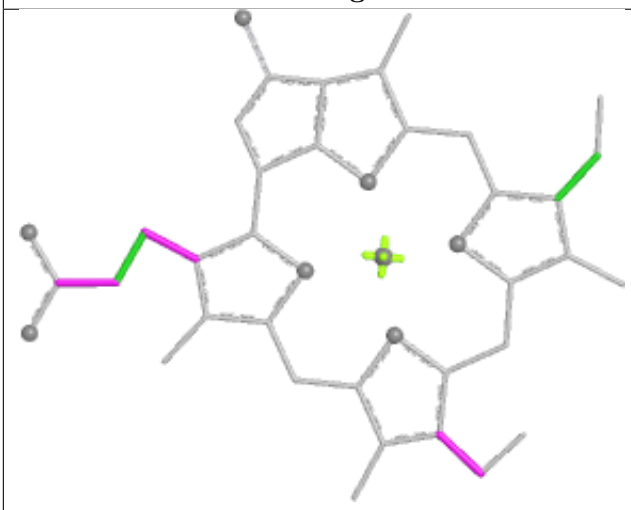
Ligand CLA K2 104



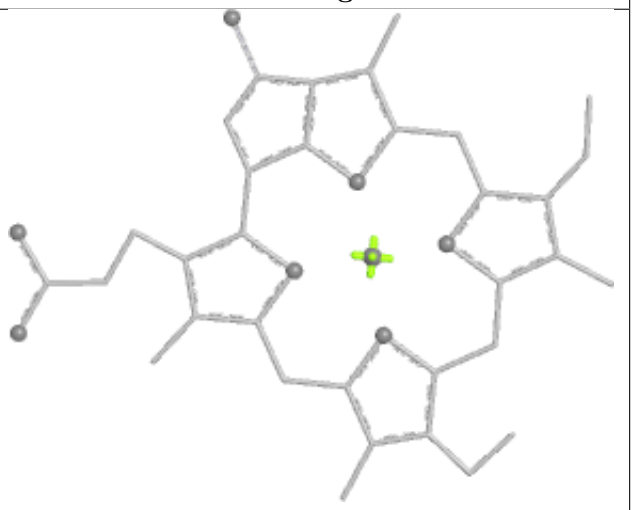
Bond lengths



Bond angles

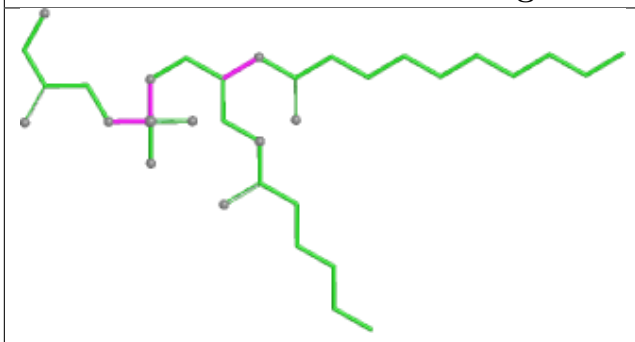


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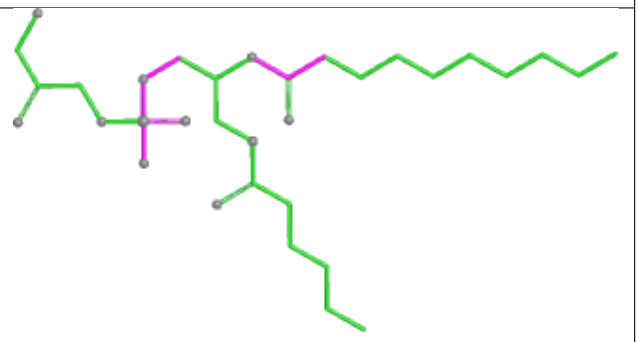


Rings

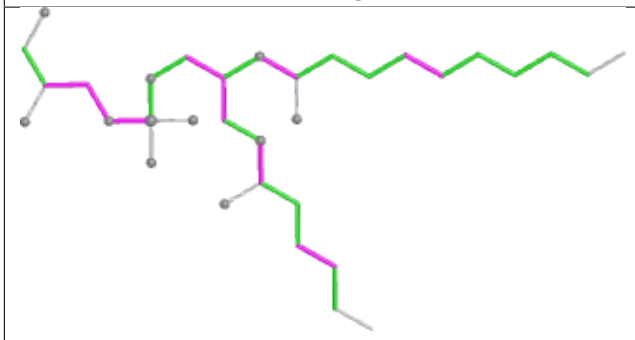
Ligand LHG L1 211



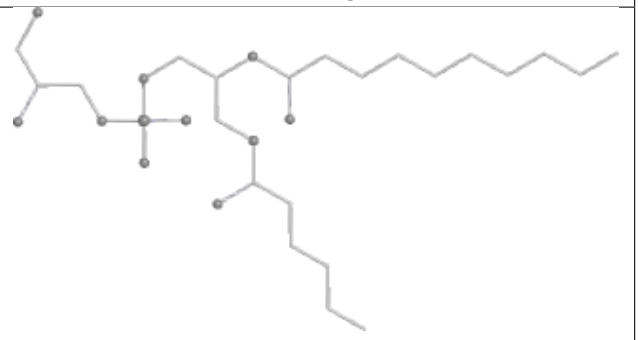
Bond lengths



Bond angles

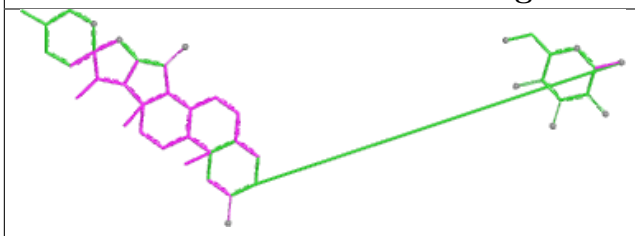


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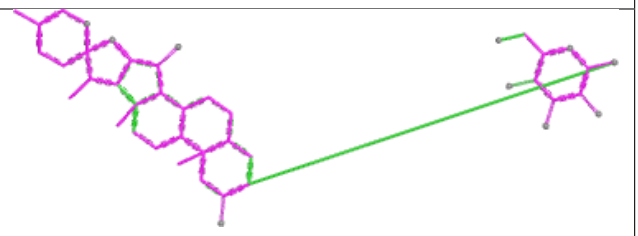


Rings

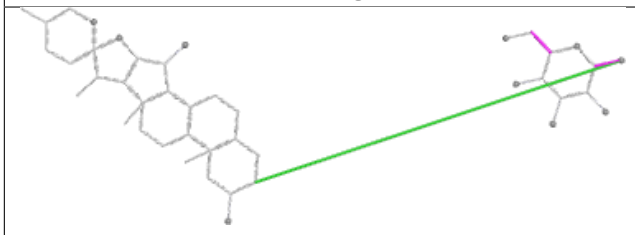
Ligand AJP BB 848



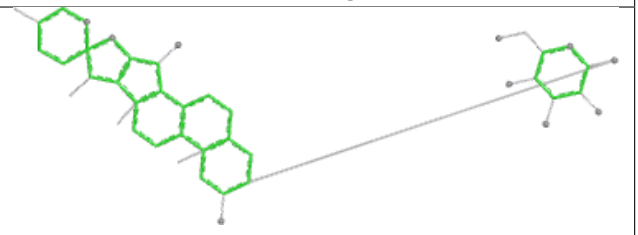
Bond lengths



Bond angles

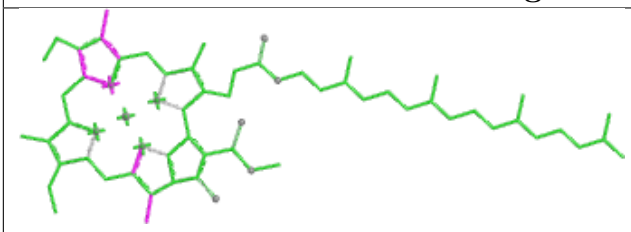


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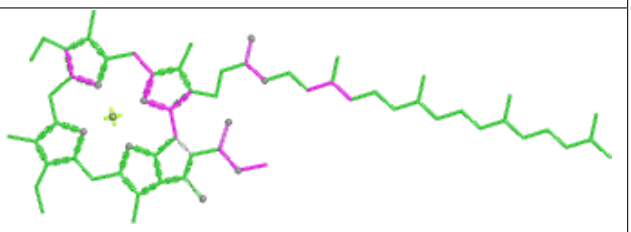


Rings

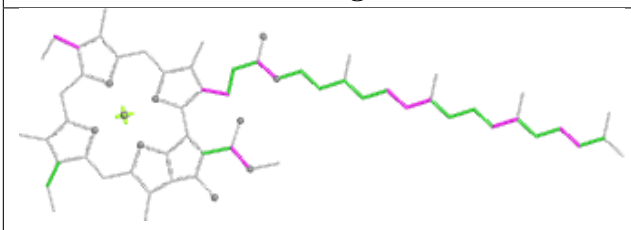
Ligand CLA B 833



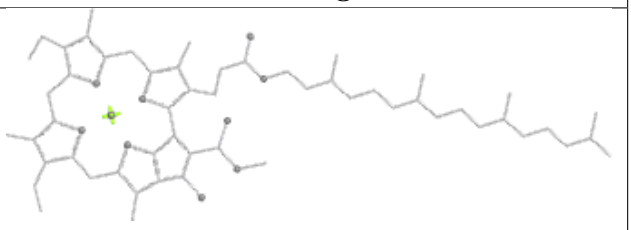
Bond lengths



Bond angles

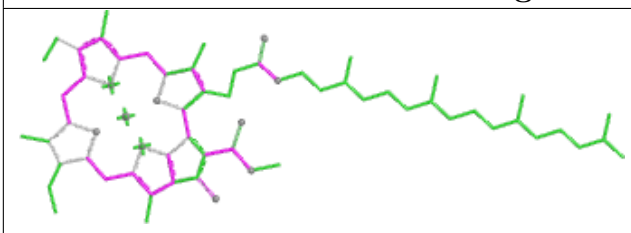


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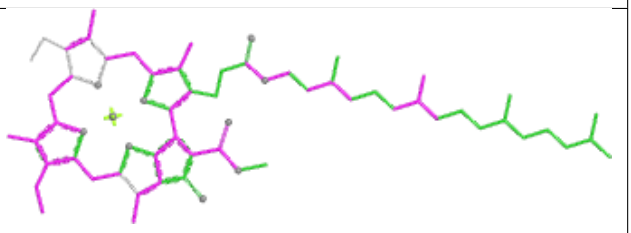


Rings

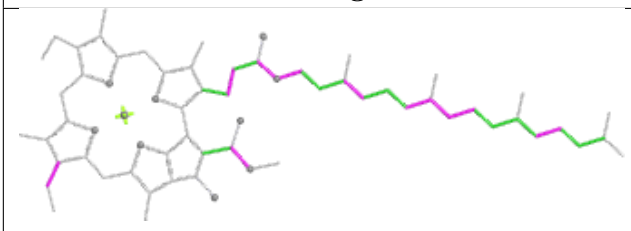
Ligand CL0 AA 803



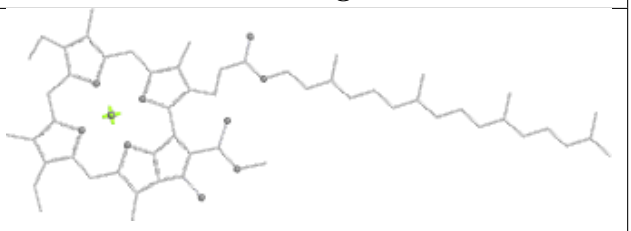
Bond lengths



Bond angles

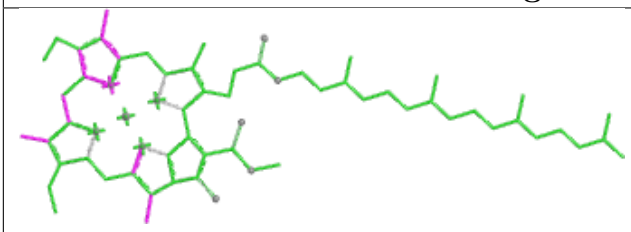


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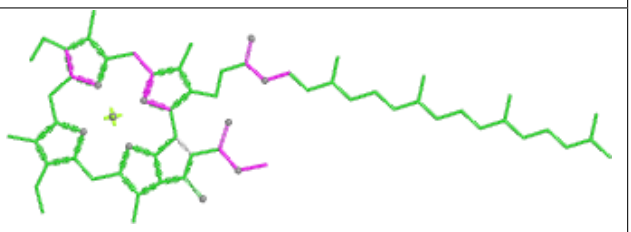


Rings

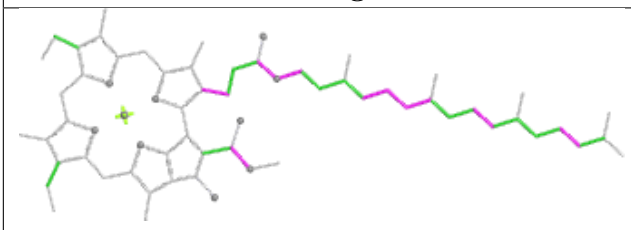
Ligand CLA A 808



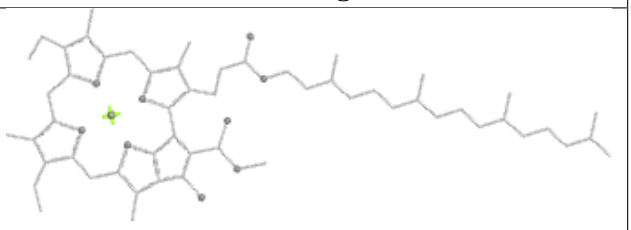
Bond lengths



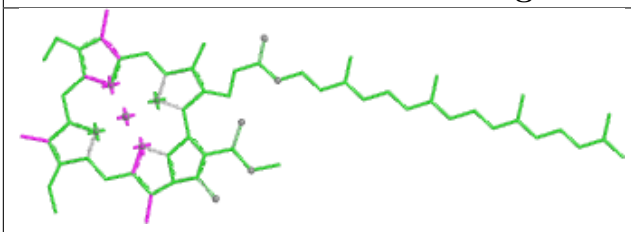
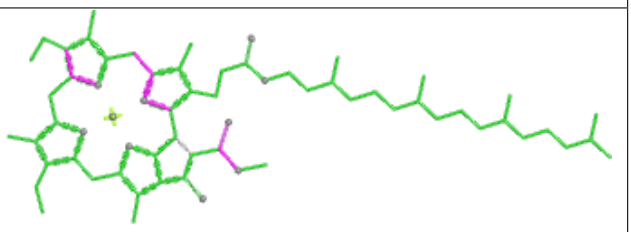
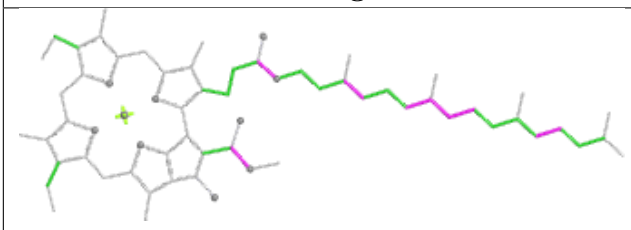
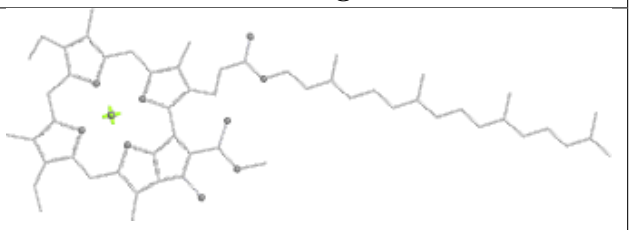
Bond angles

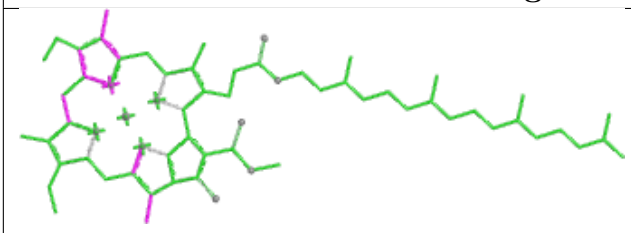
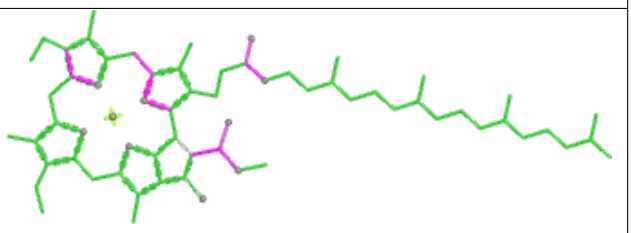
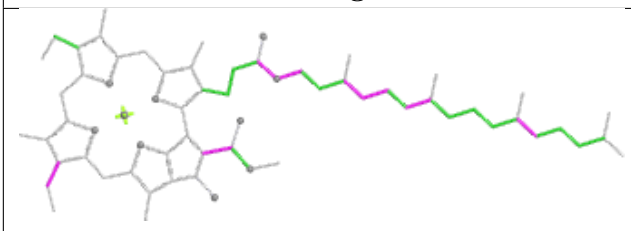
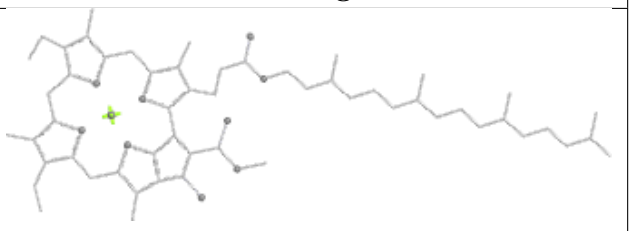


Torsions

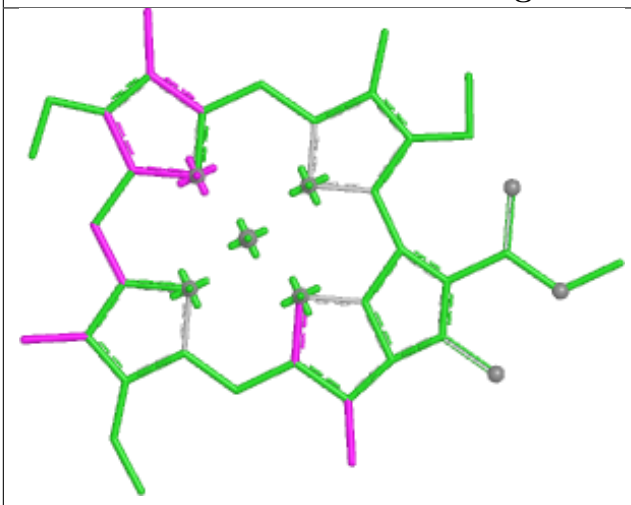


Rings

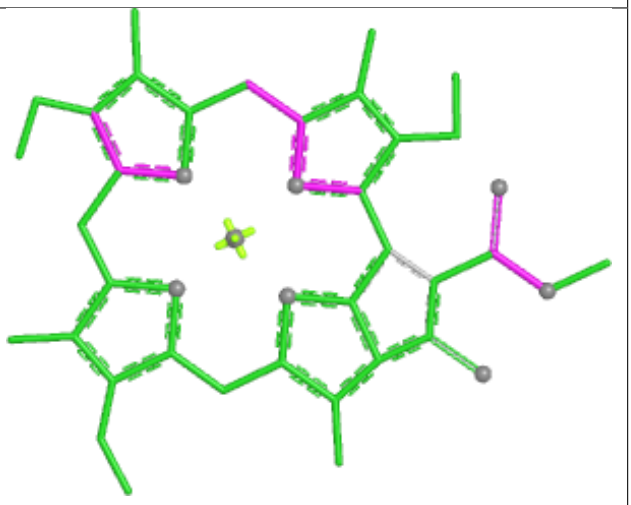
Ligand CLA B2 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

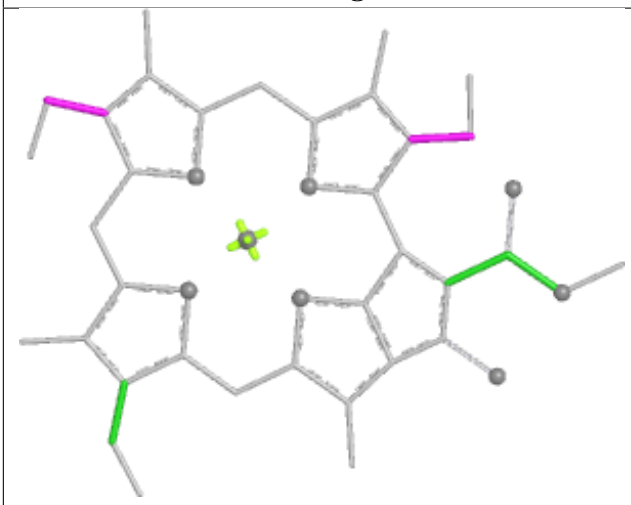
Ligand CLA A1 824



Bond lengths



Bond angles

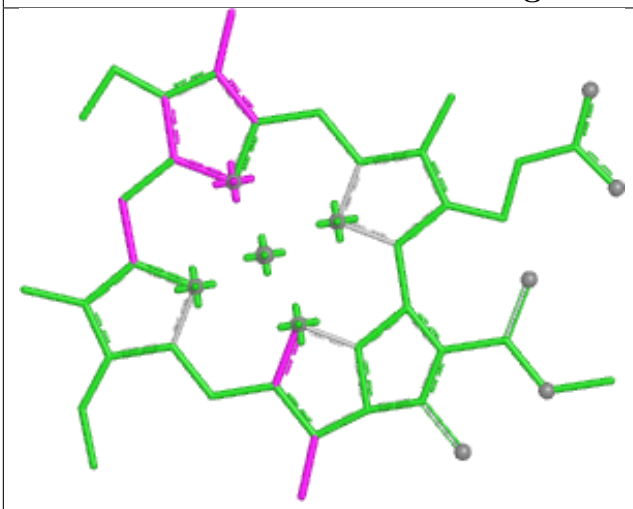


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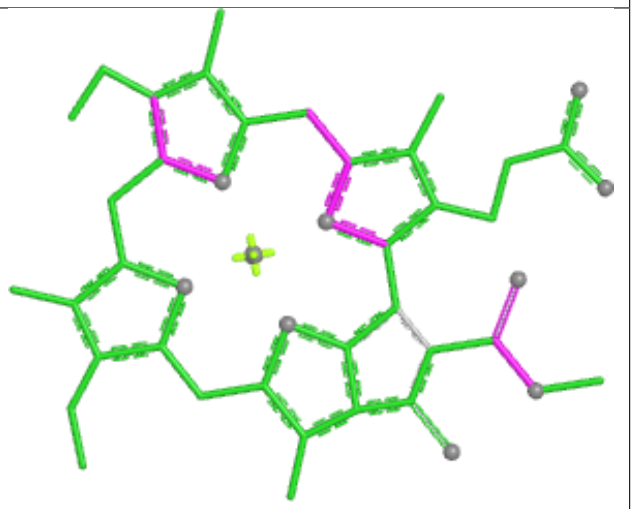


Rings

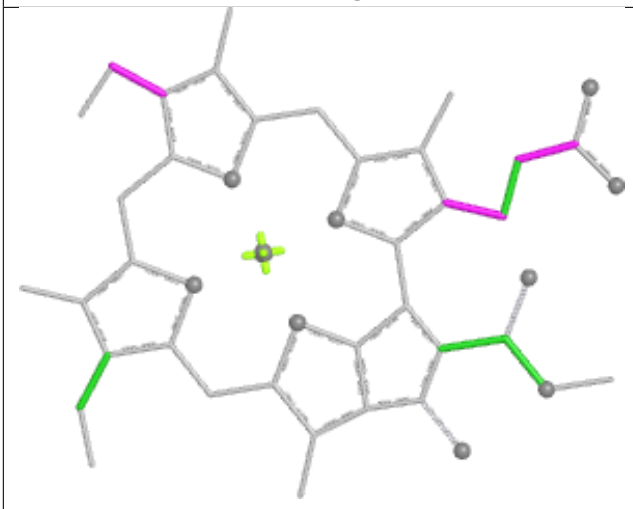
Ligand CLA A 818



Bond lengths



Bond angles

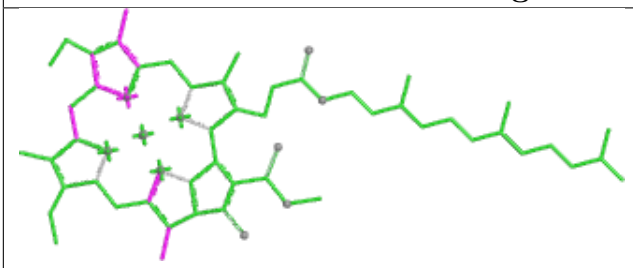


Torsions

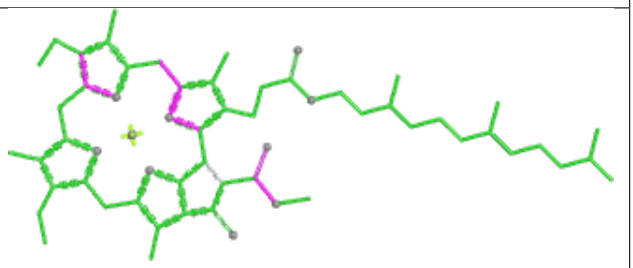


Rings

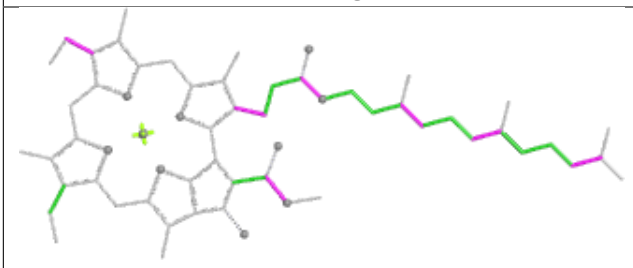
Ligand CLA BB 808



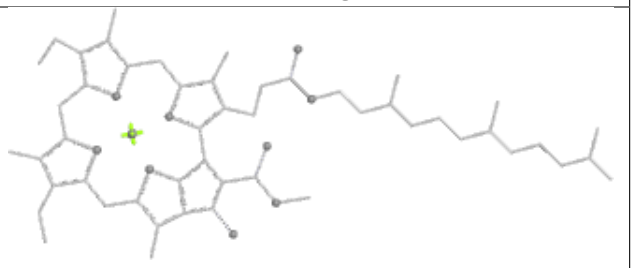
Bond lengths



Bond angles

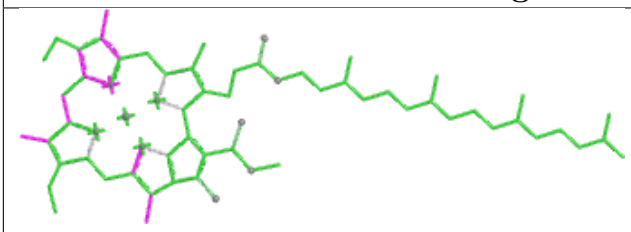


Torsions

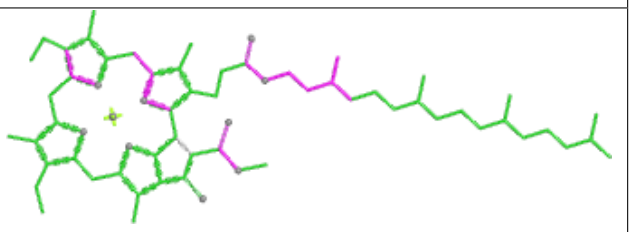


Rings

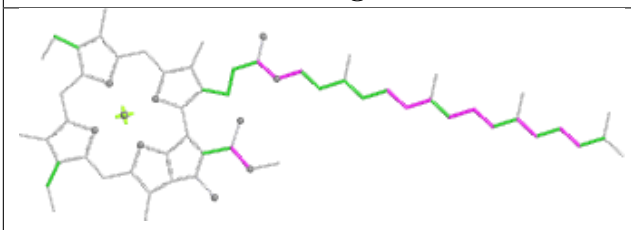
Ligand CLA BB 806



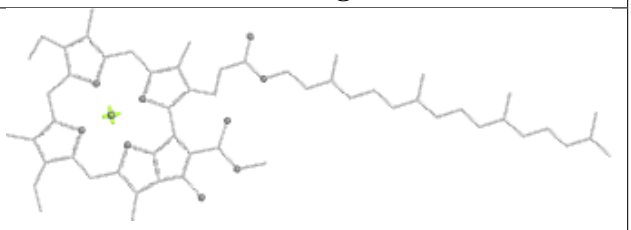
Bond lengths



Bond angles

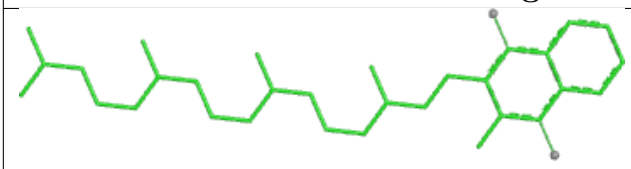


Torsions

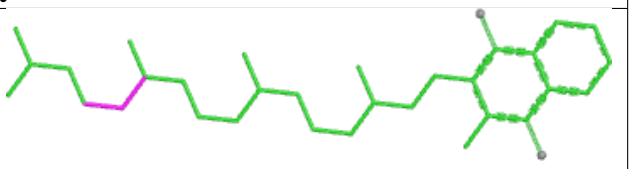


Rings

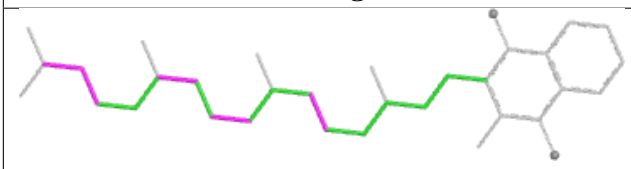
Ligand PQN B 838



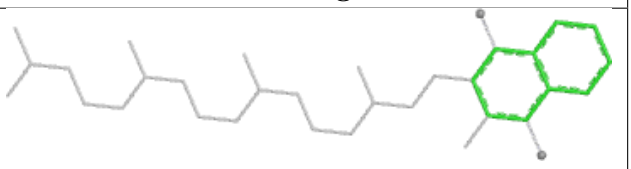
Bond lengths



Bond angles

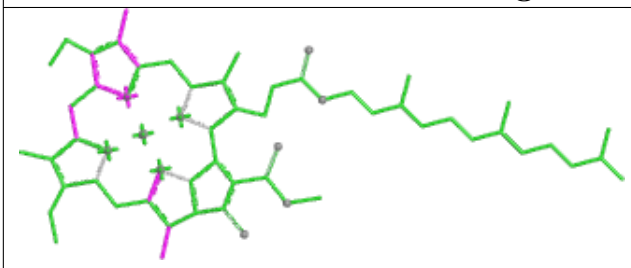


Torsions

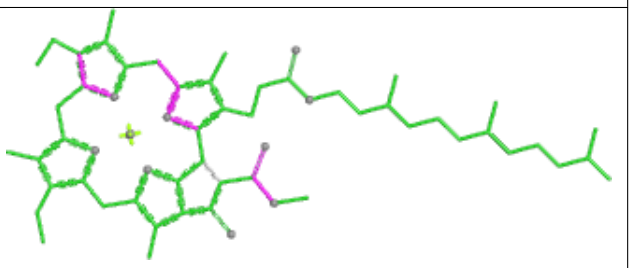


Rings

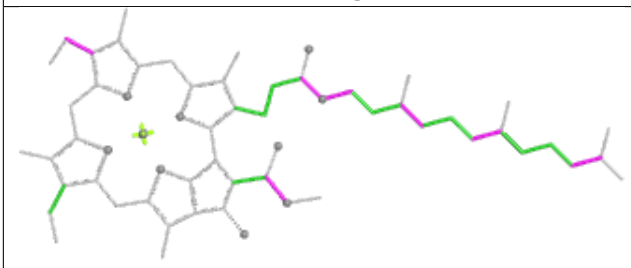
Ligand CLA B2 808



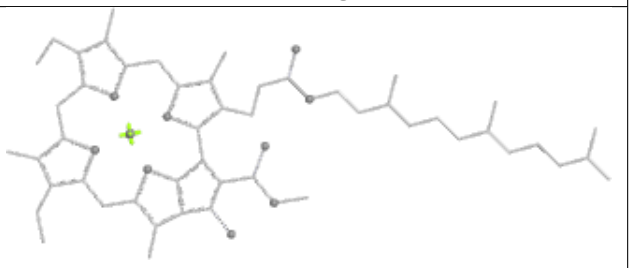
Bond lengths



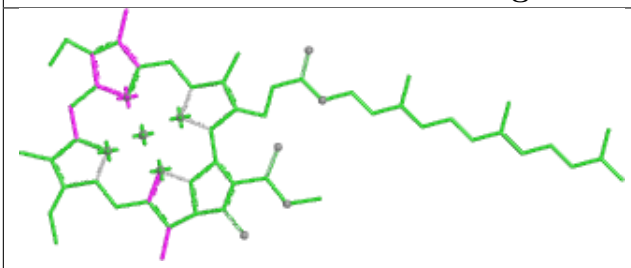
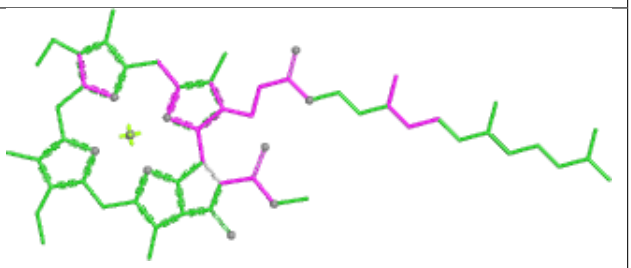
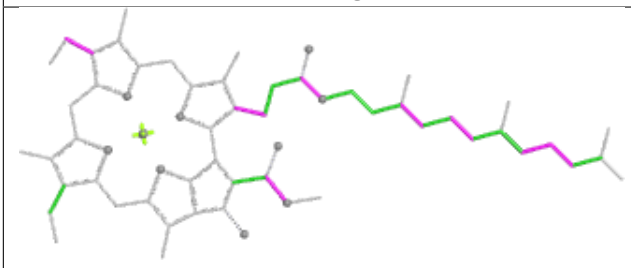
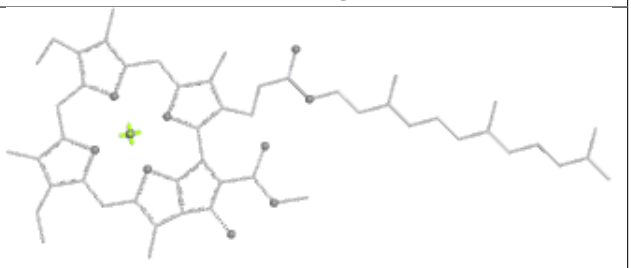
Bond angles

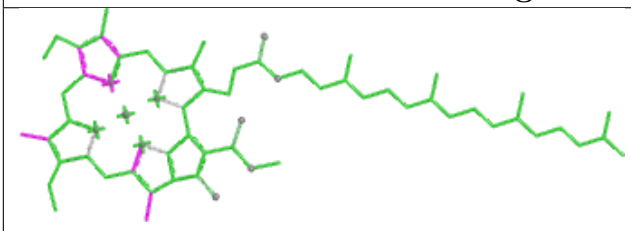
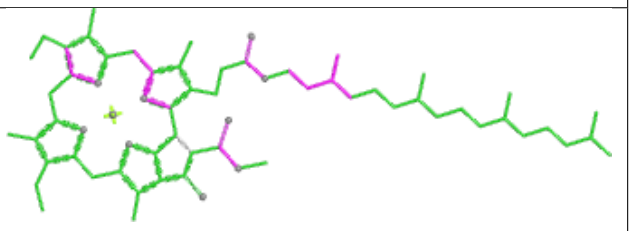
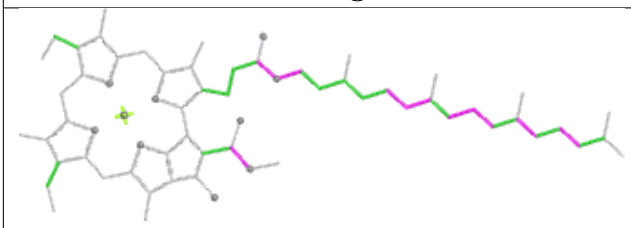
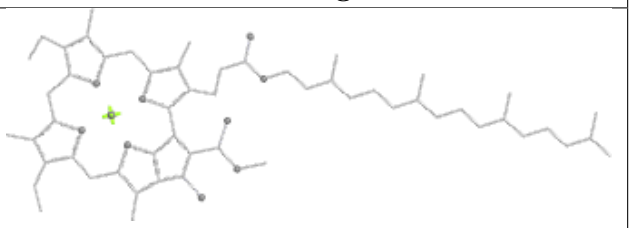


Torsions

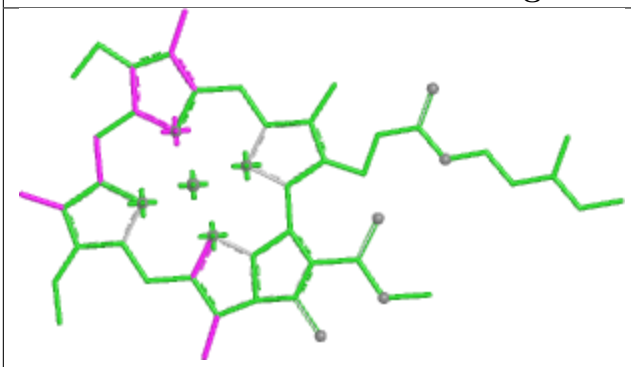


Rings

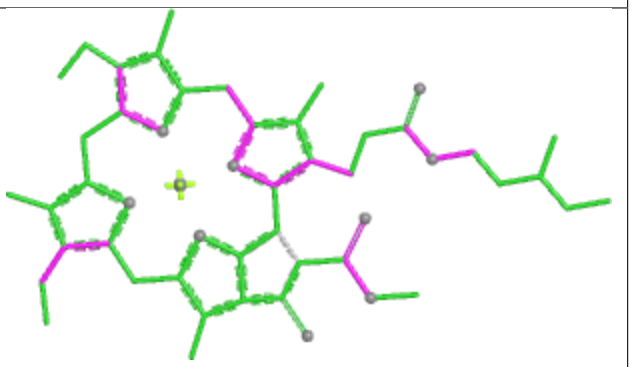
Ligand CLA BB 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B2 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

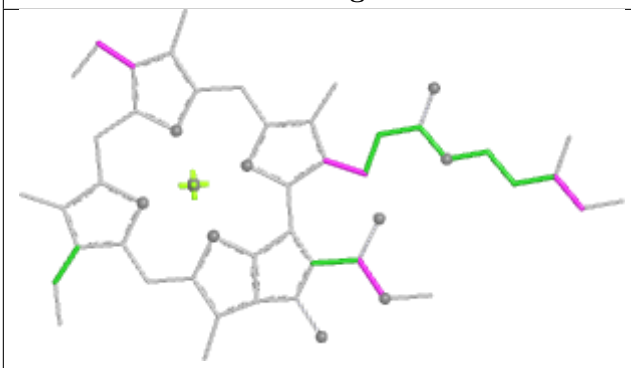
Ligand CLA A 811



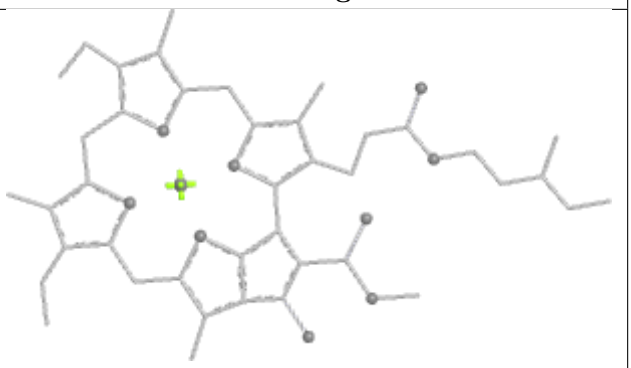
Bond lengths



Bond angles

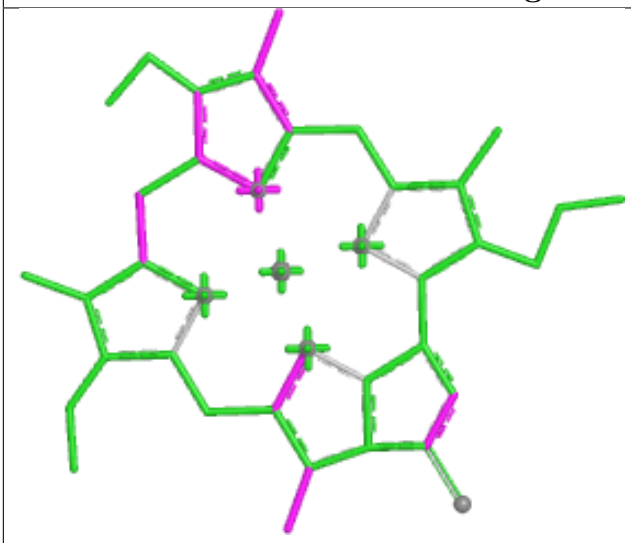


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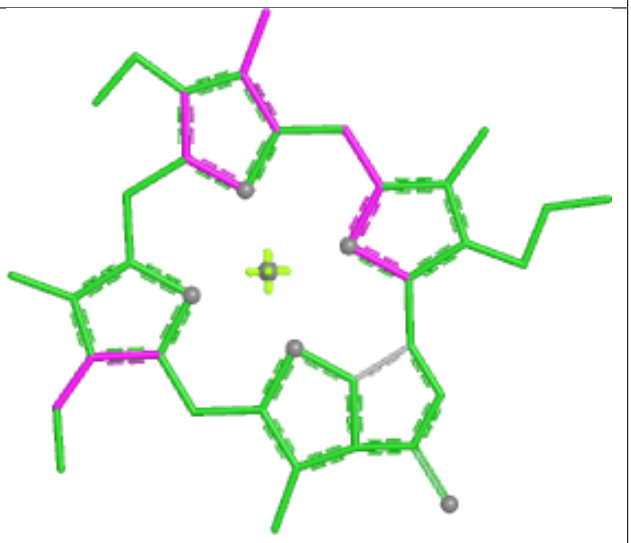


Rings

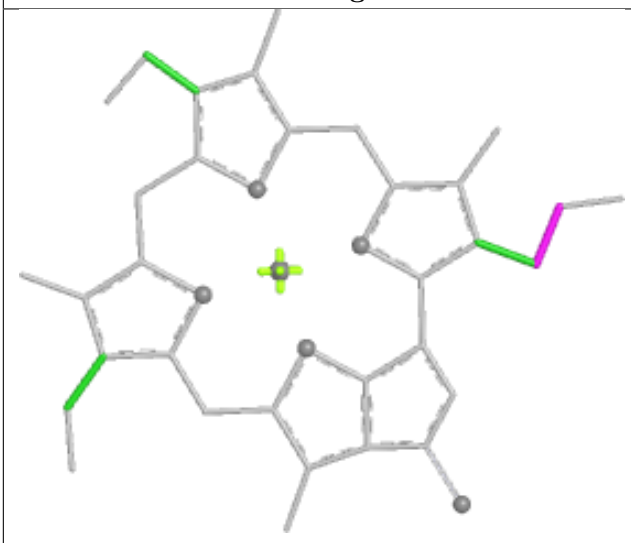
Ligand CLA B 846



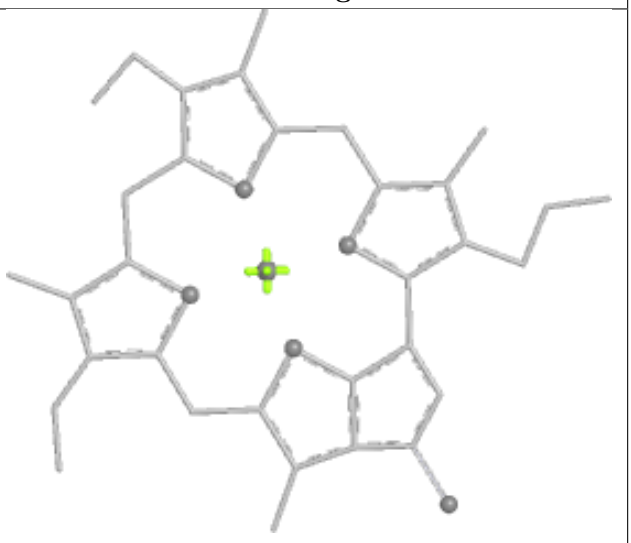
Bond lengths



Bond angles

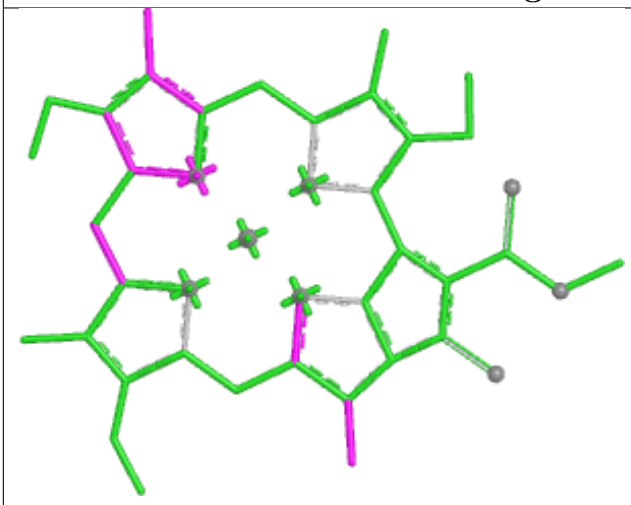


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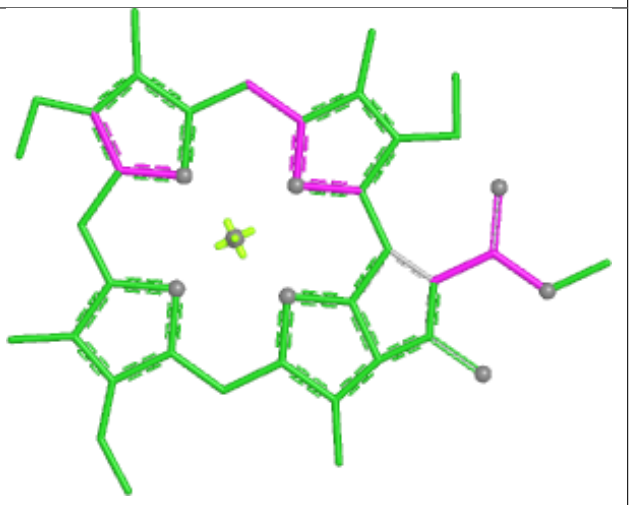


Rings

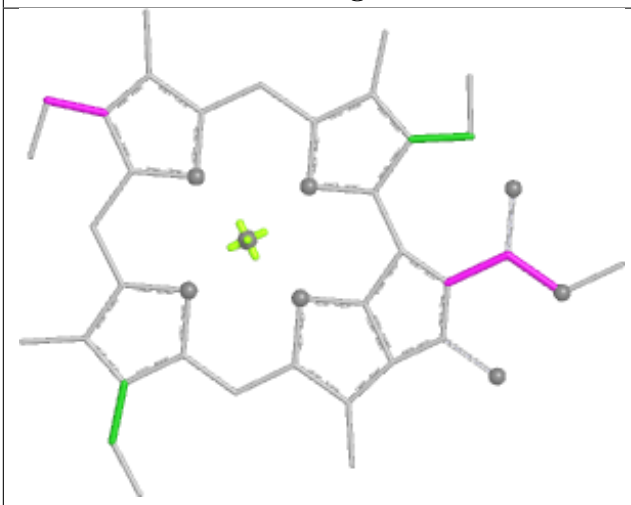
Ligand CLA B 817



Bond lengths



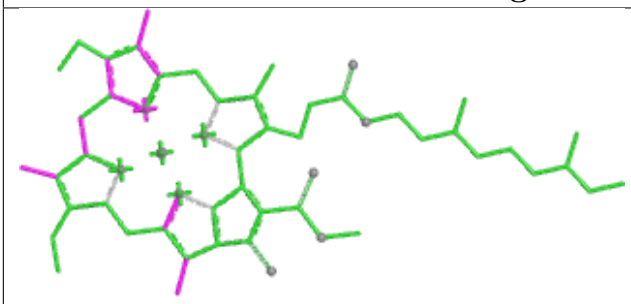
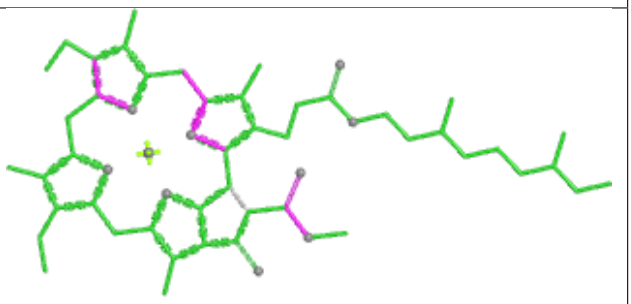
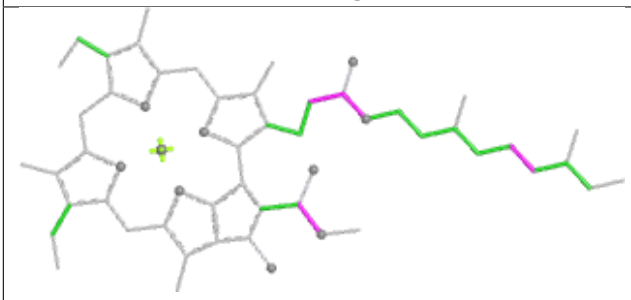
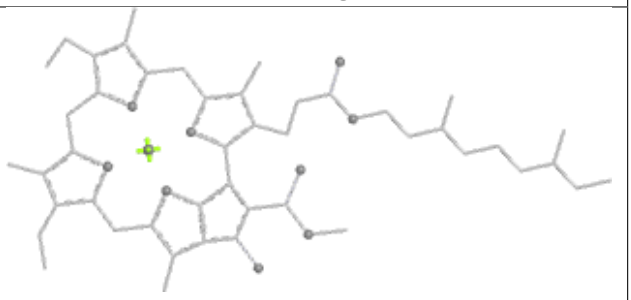
Bond angles



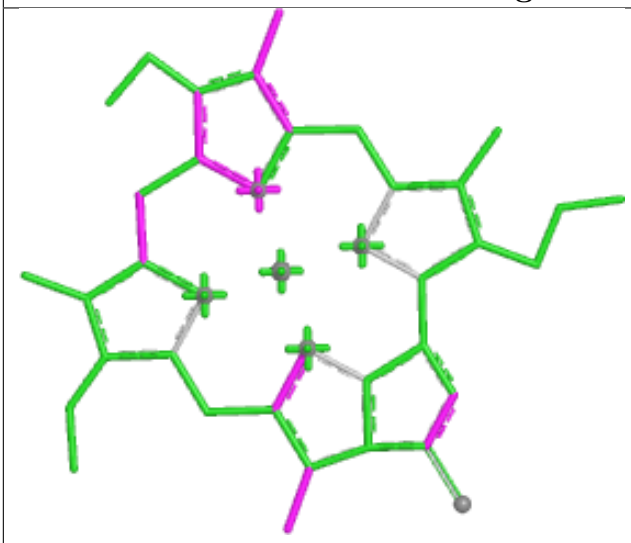
Torsions



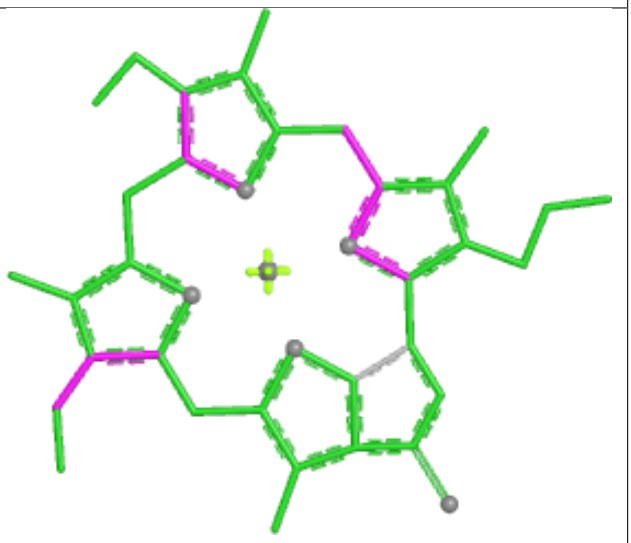
Rings

Ligand CLA AA 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

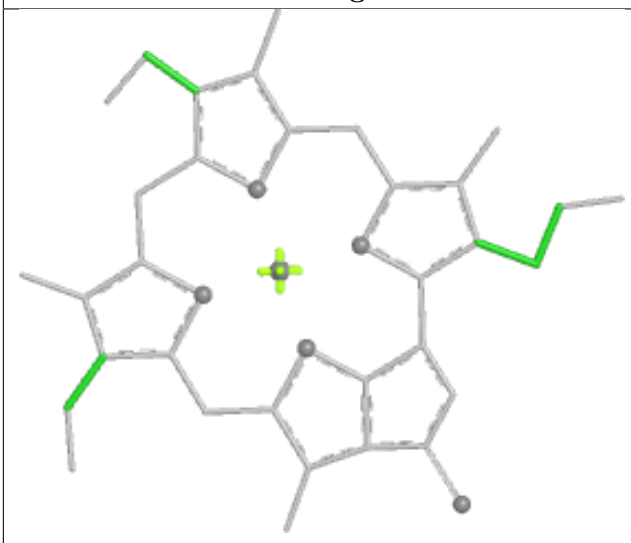
Ligand CLA B1 845



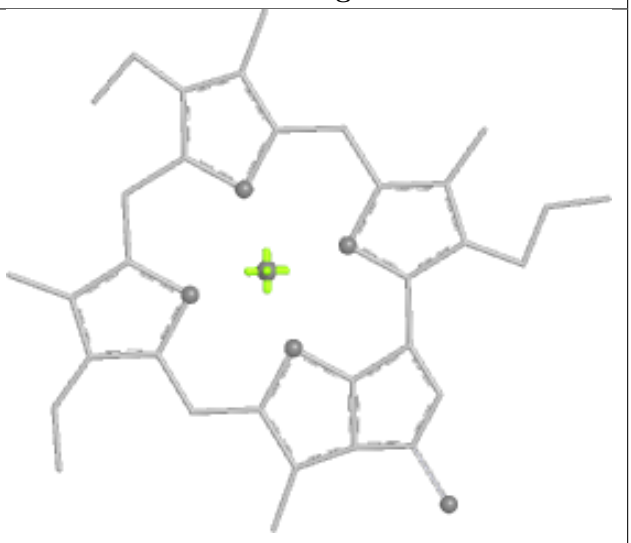
Bond lengths



Bond angles

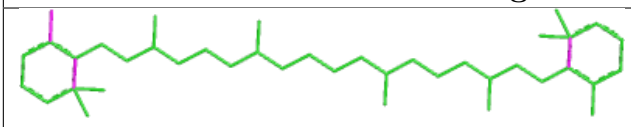


Torsions

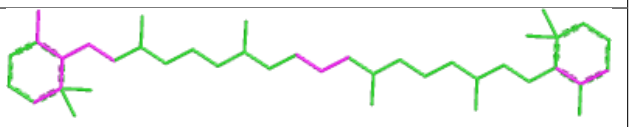


Rings

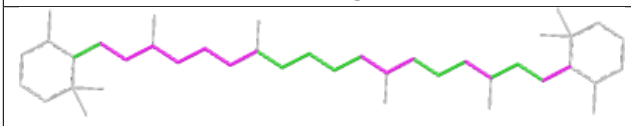
Ligand BCR BB 842



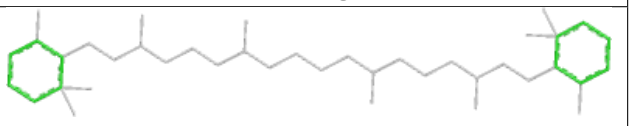
Bond lengths



Bond angles

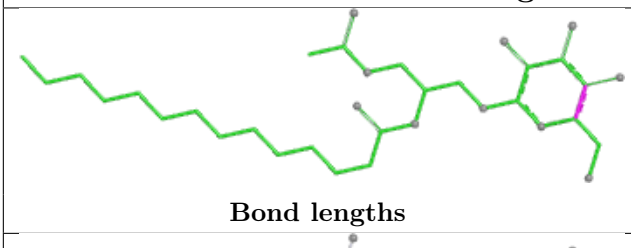


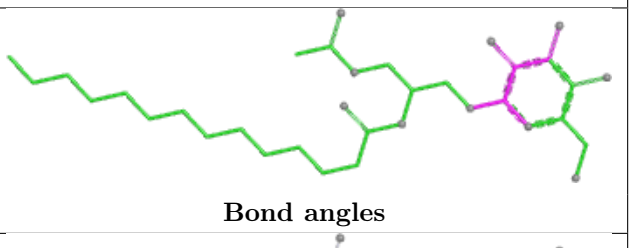
Torsions

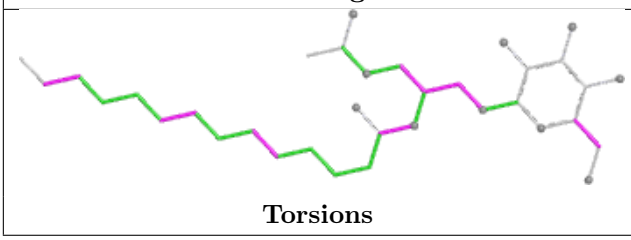


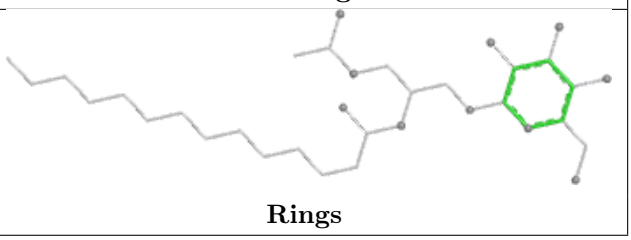
Rings

Ligand LMG I2 105

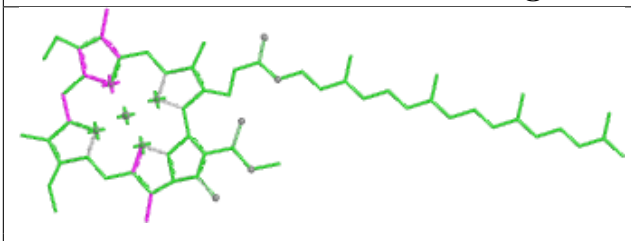

Bond lengths

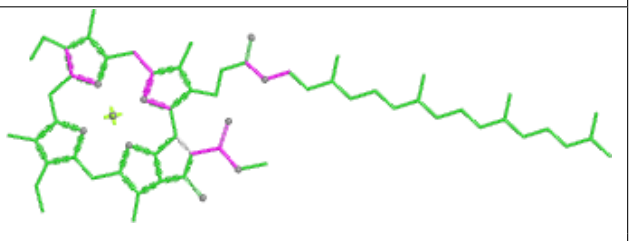

Bond angles

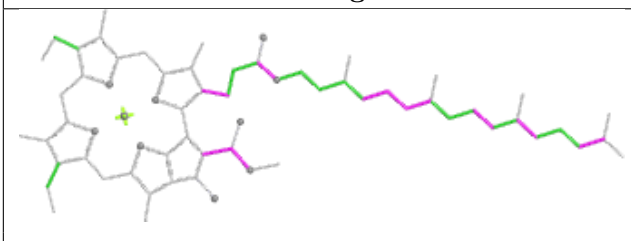

Torsions

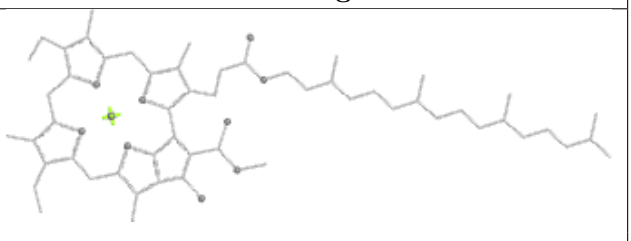

Rings

Ligand CLA B 825

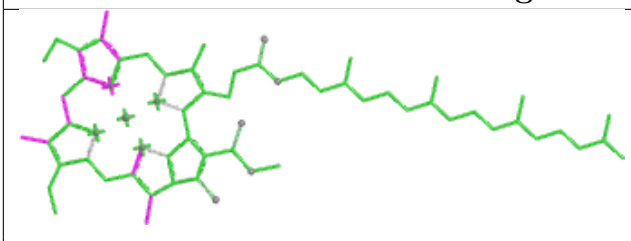

Bond lengths

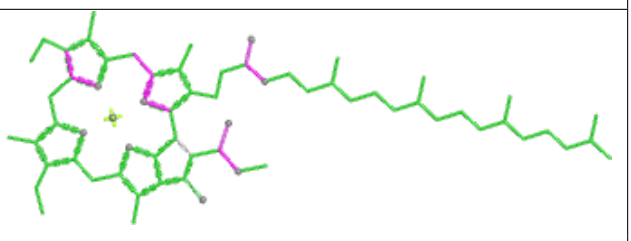

Bond angles

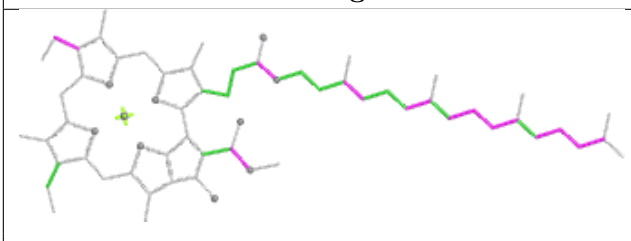

Torsions

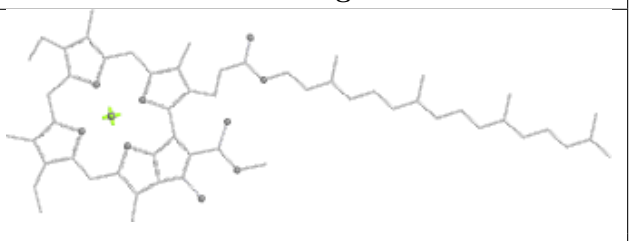

Rings

Ligand CLA B2 823

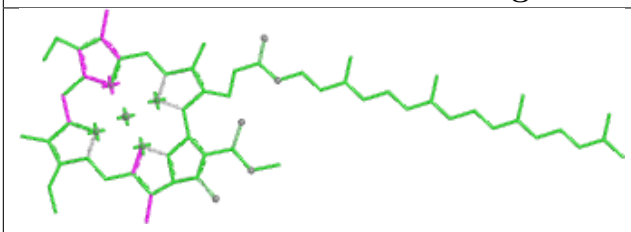

Bond lengths


Bond angles

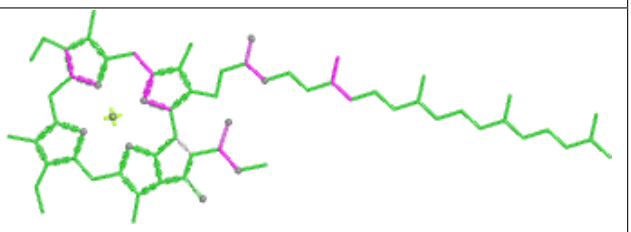

Torsions


Rings

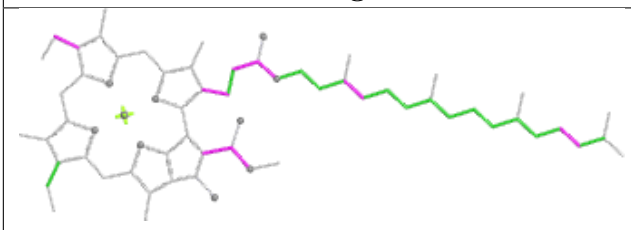
Ligand CLA BB 802



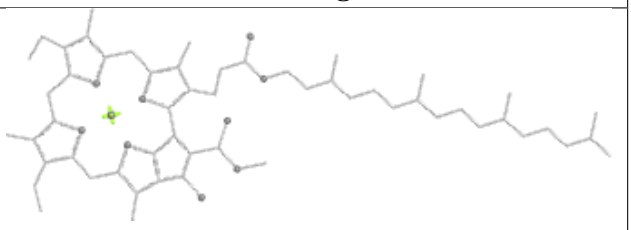
Bond lengths



Bond angles

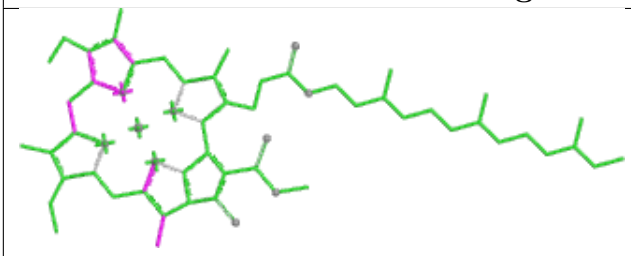


Torsions

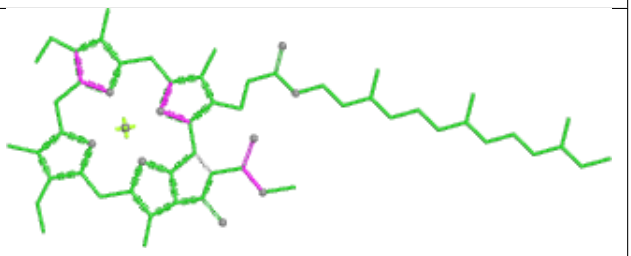


Rings

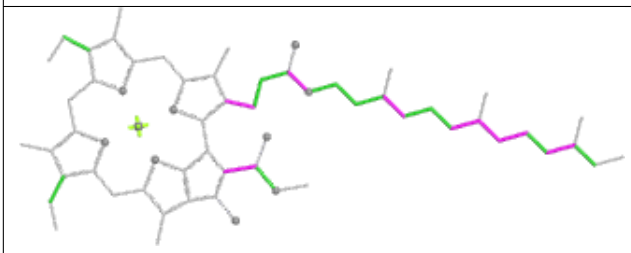
Ligand CLA B1 811



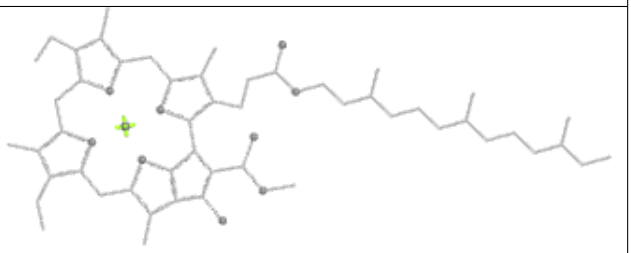
Bond lengths



Bond angles

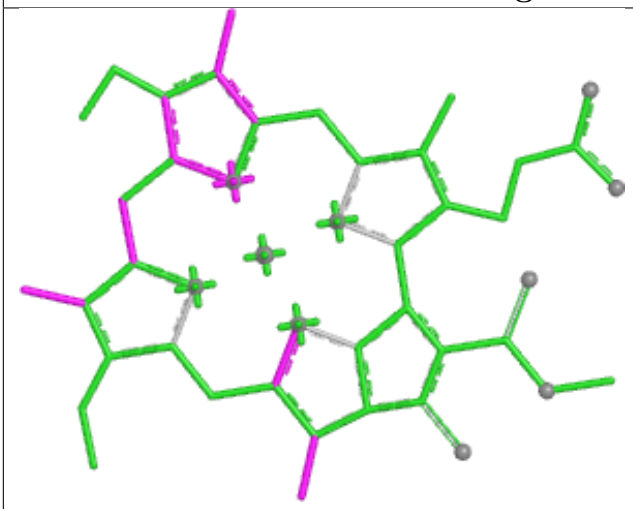


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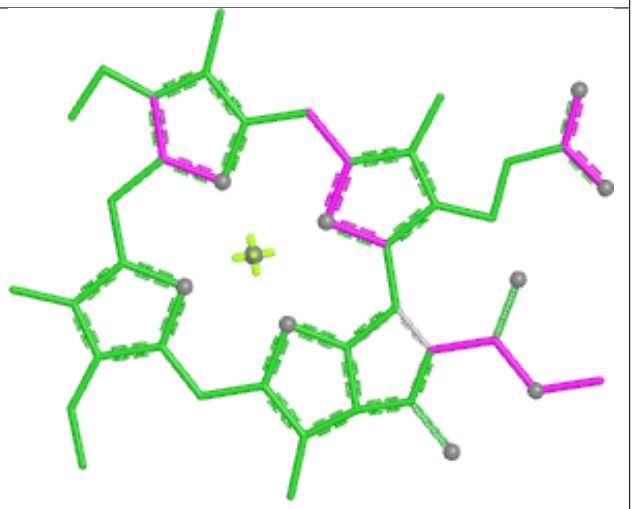


Rings

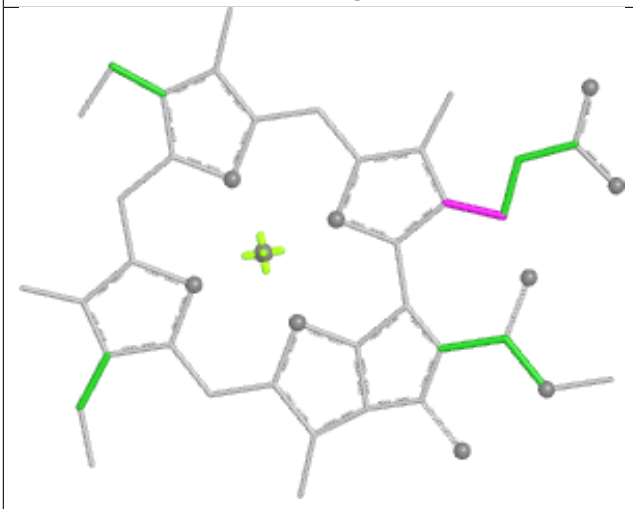
Ligand CLA B1 834



Bond lengths



Bond angles

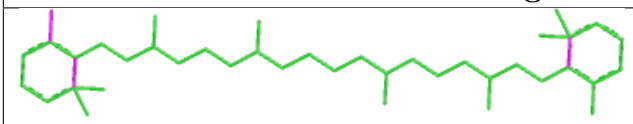


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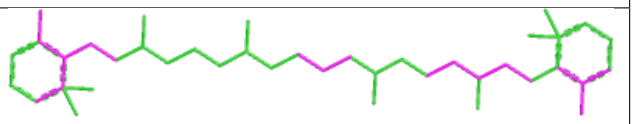


Rings

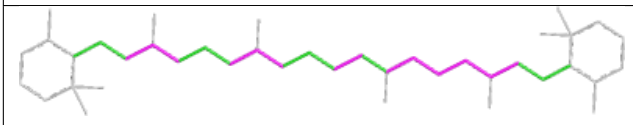
Ligand BCR F 304



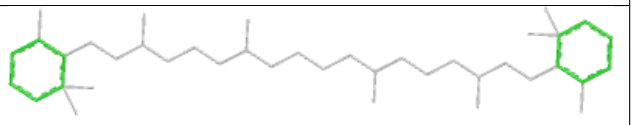
Bond lengths



Bond angles

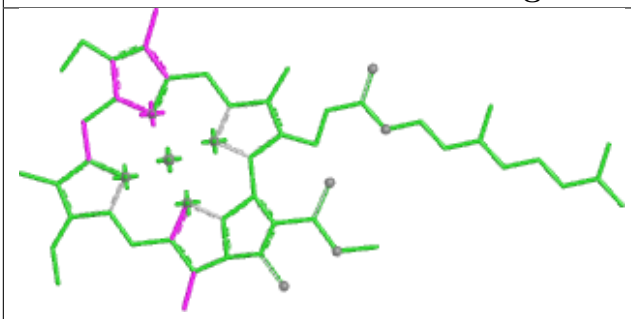


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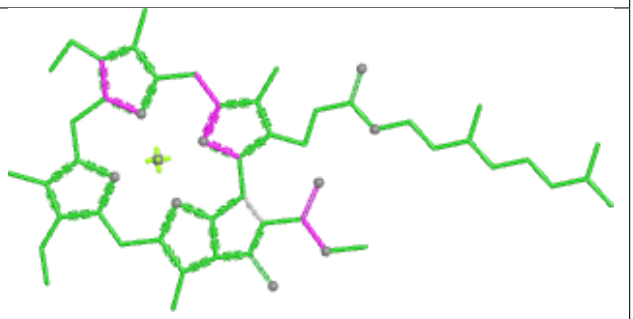


Rings

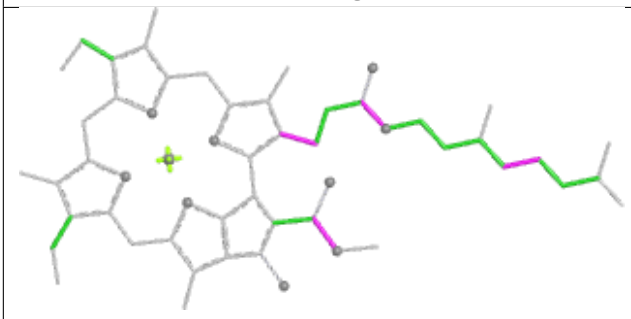
Ligand CLA A 815



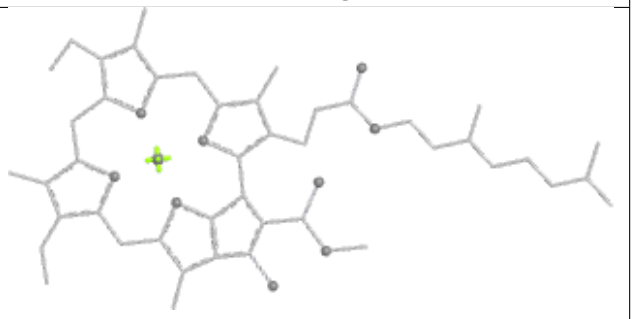
Bond lengths



Bond angles

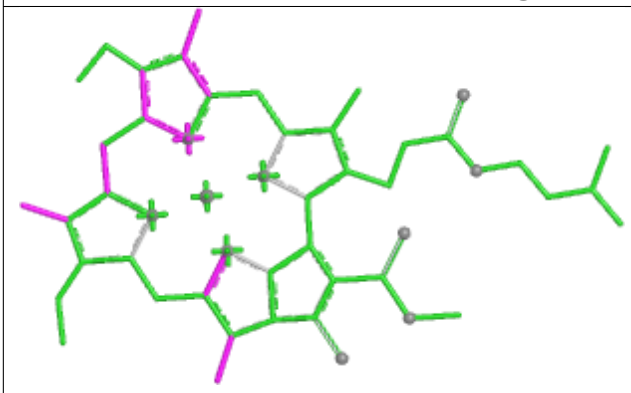


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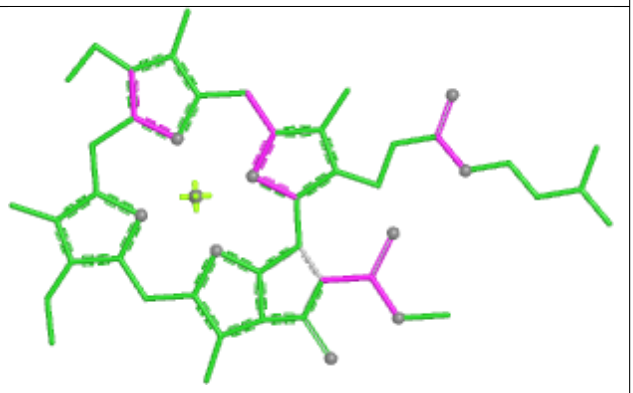


Rings

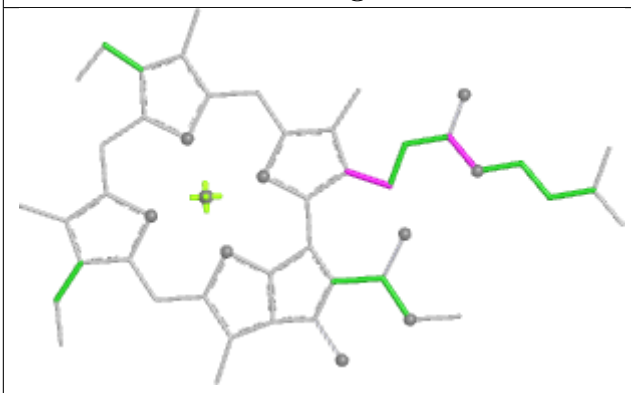
Ligand CLA A2 833



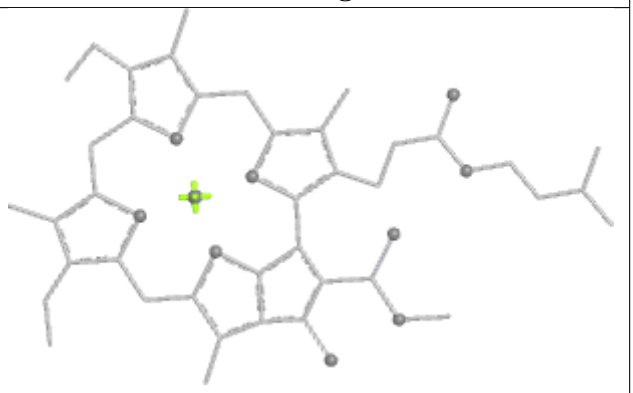
Bond lengths



Bond angles

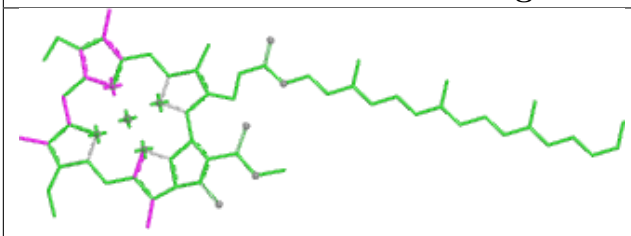


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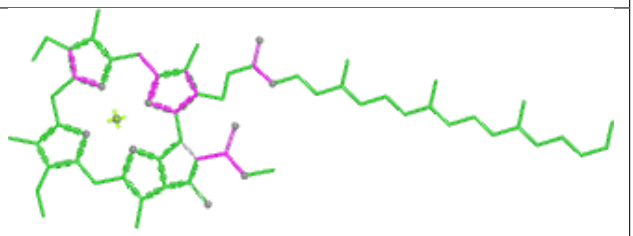


Rings

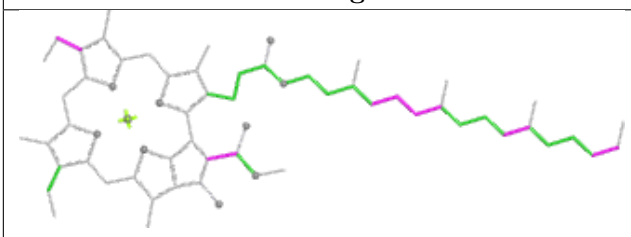
Ligand CLA B2 805



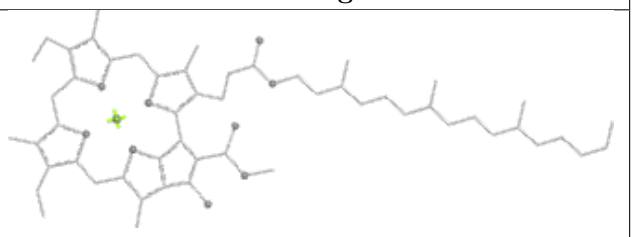
Bond lengths



Bond angles

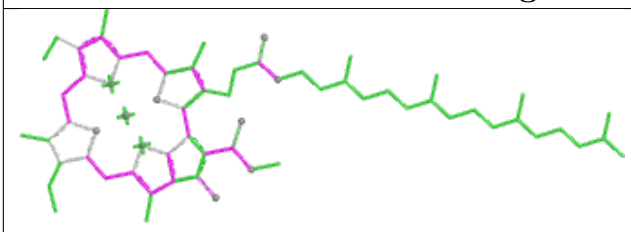


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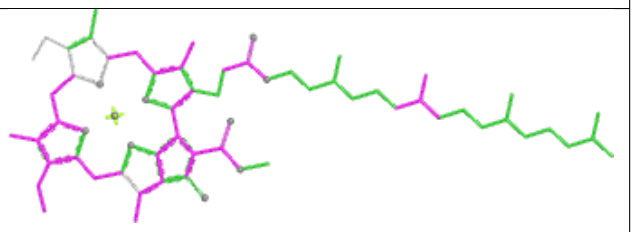


Rings

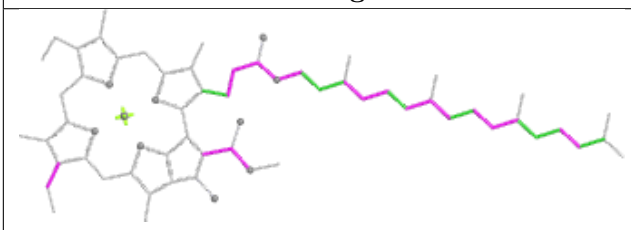
Ligand CL0 A2 803



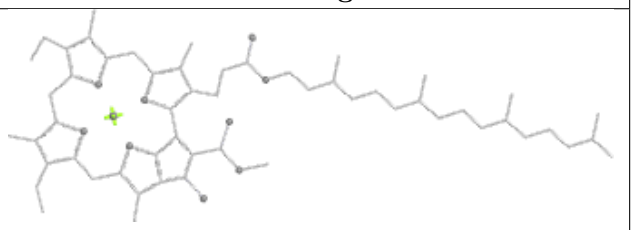
Bond lengths



Bond angles



Torsions

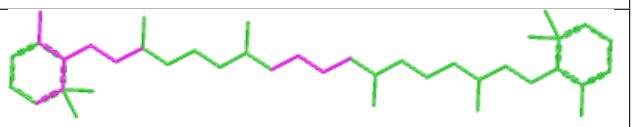


Rings

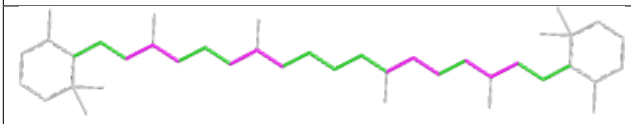
Ligand BCR I2 102



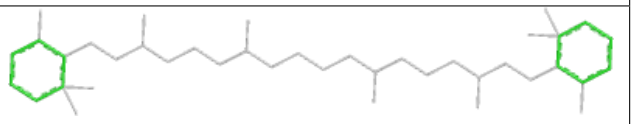
Bond lengths



Bond angles

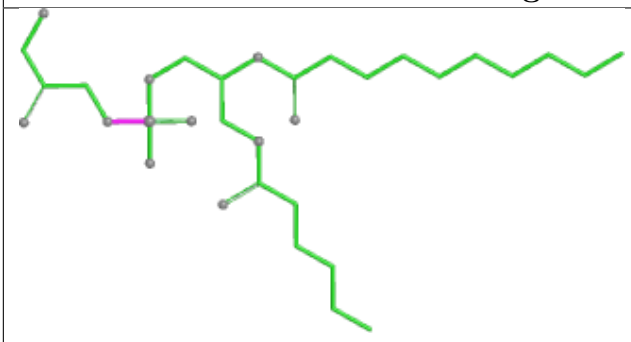


Torsions

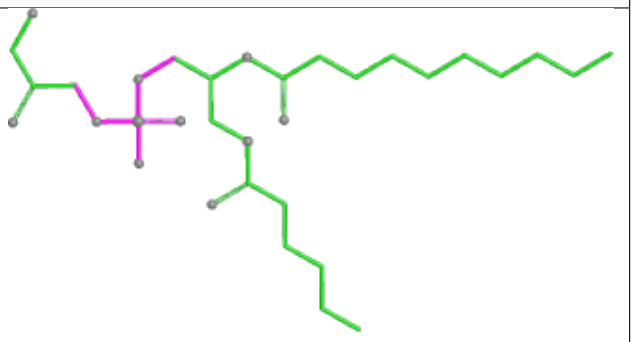


Rings

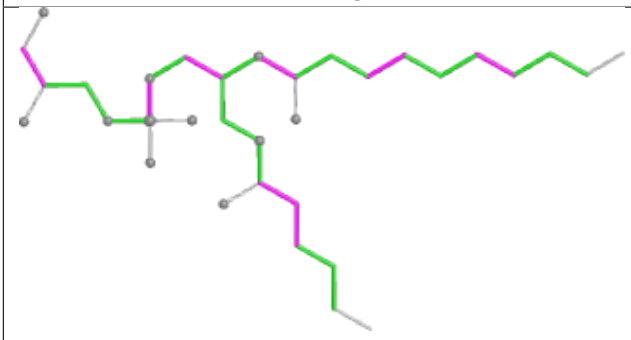
Ligand LHG B 852



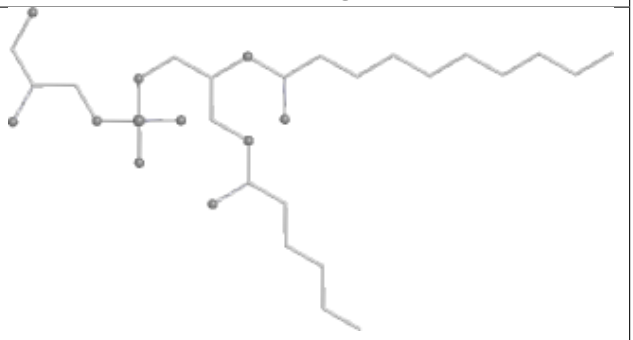
Bond lengths



Bond angles

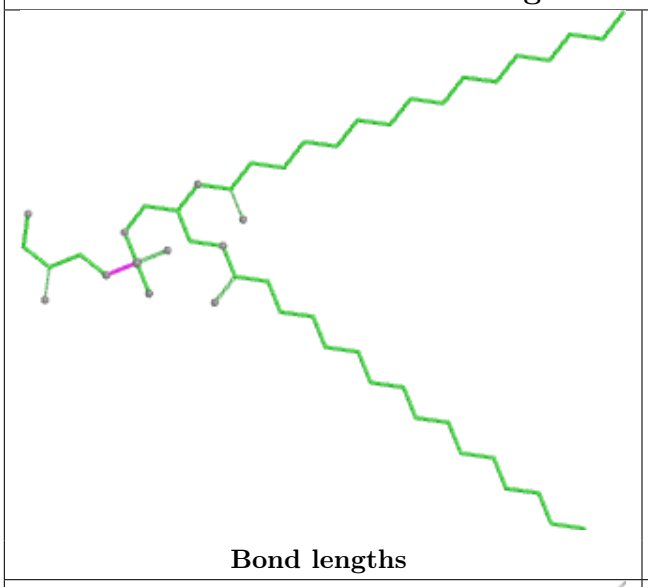


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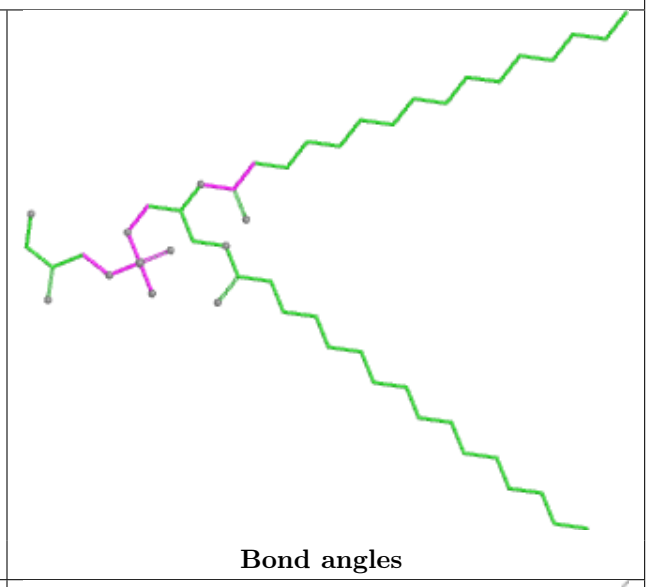


Rings

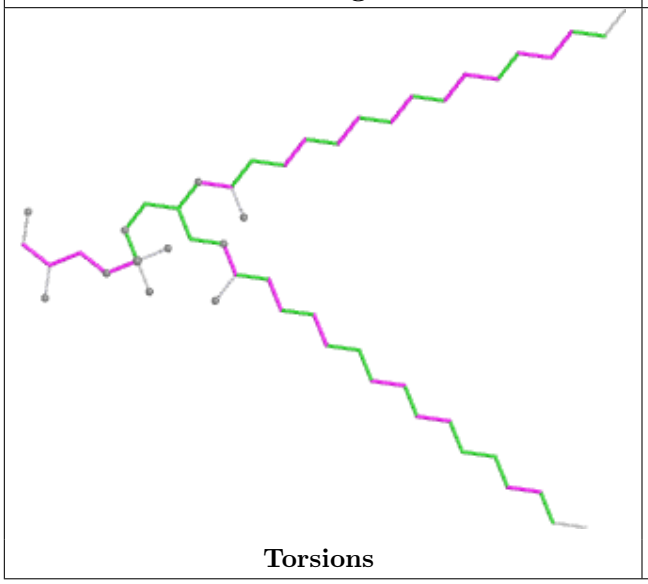
Ligand LHG B 853



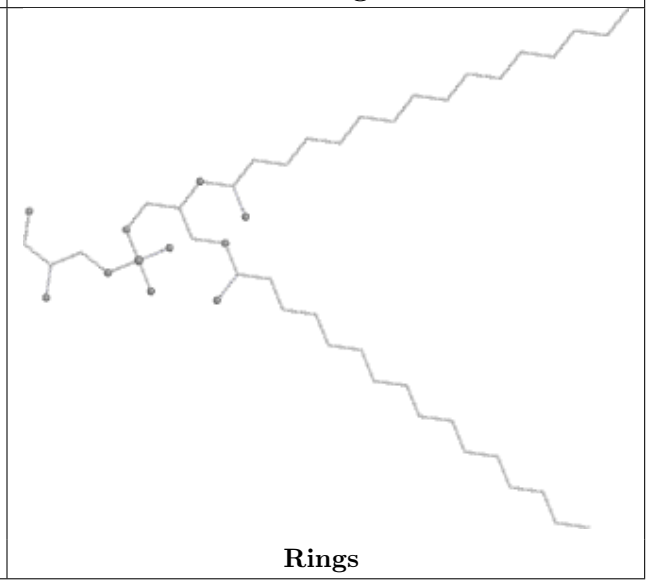
Bond lengths



Bond angles

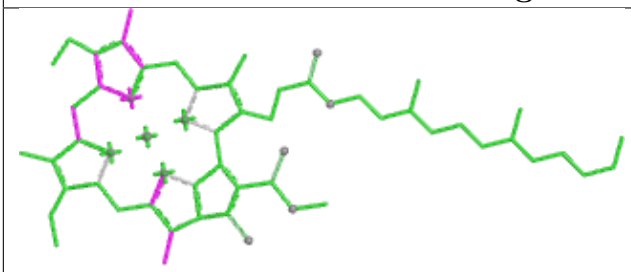


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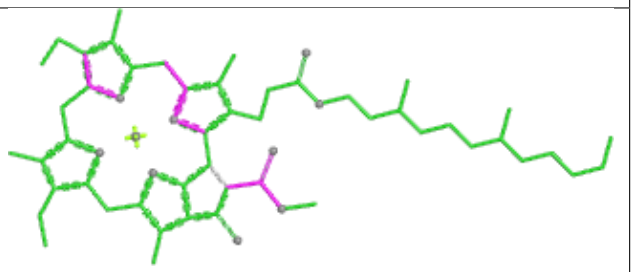


Rings

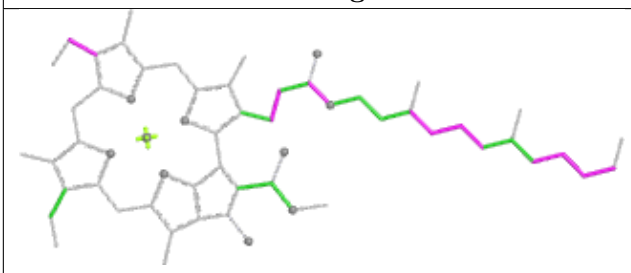
Ligand CLA B1 814



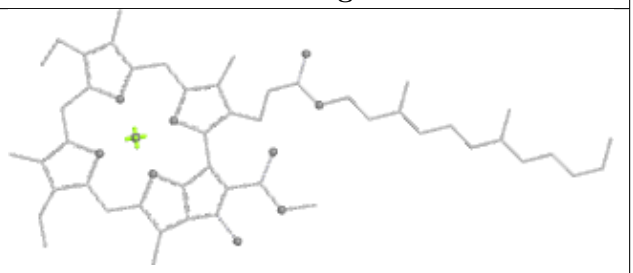
Bond lengths



Bond angles

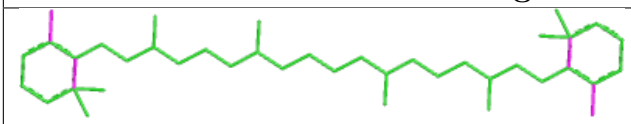


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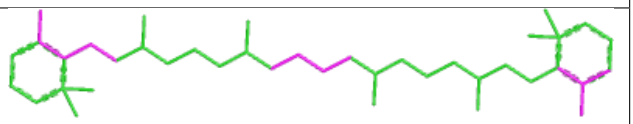


Rings

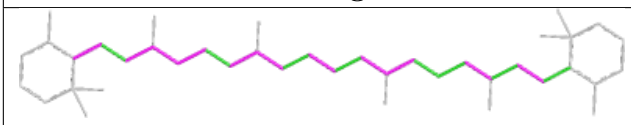
Ligand BCR B2 844



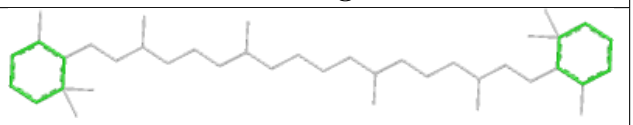
Bond lengths



Bond angles

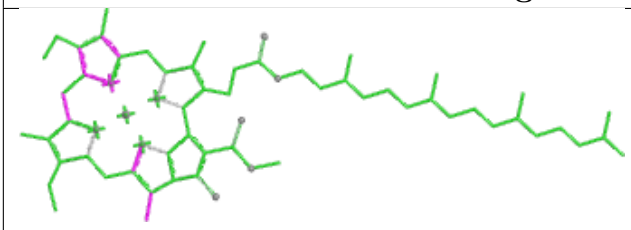


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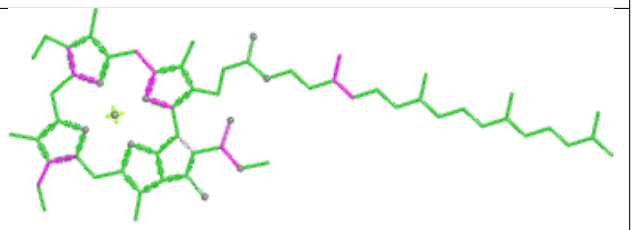


Rings

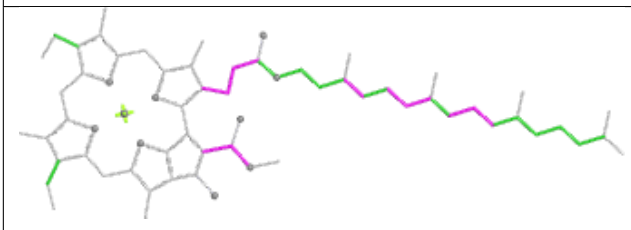
Ligand CLA B2 810



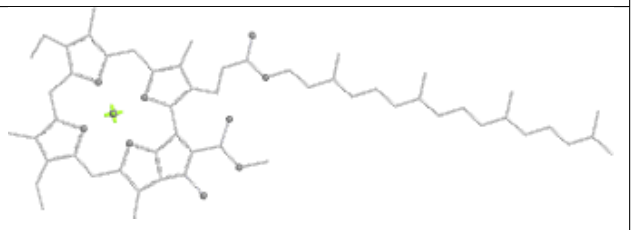
Bond lengths



Bond angles

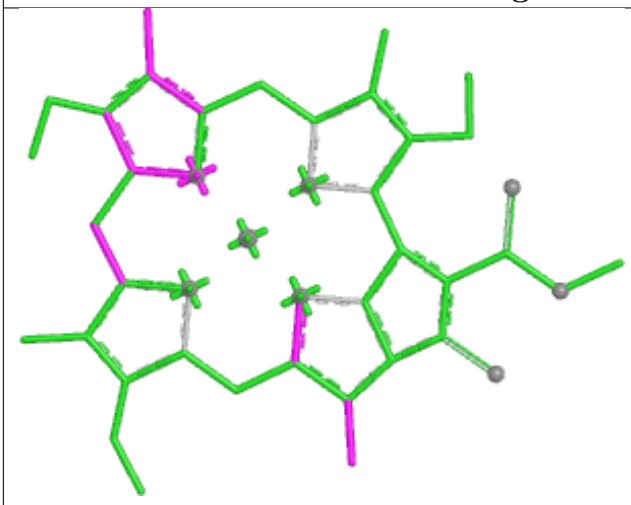


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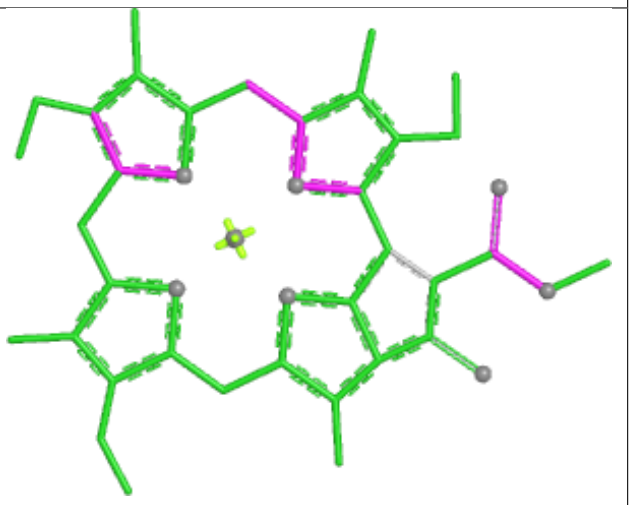


Rings

Ligand CLA BB 817



Bond lengths



Bond angles

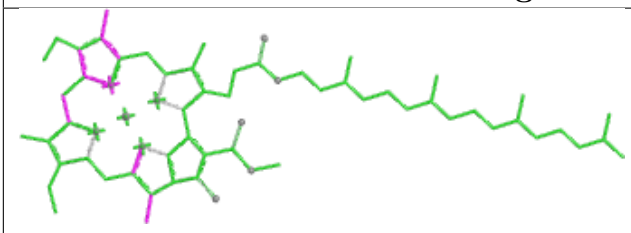


Torsions

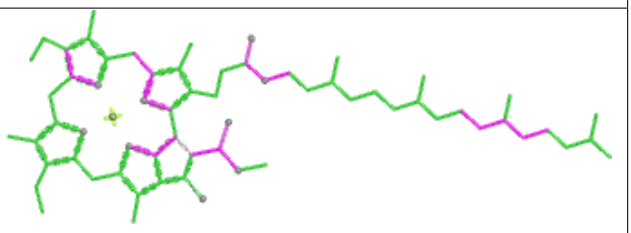


Rings

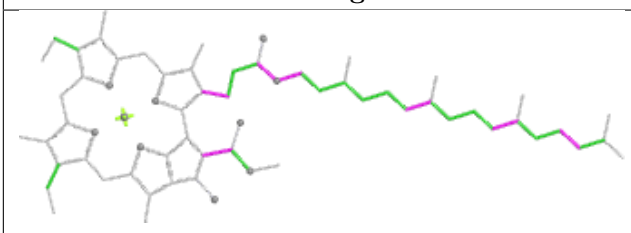
Ligand CLA B1 807



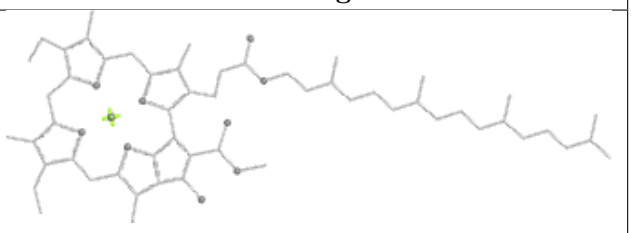
Bond lengths



Bond angles

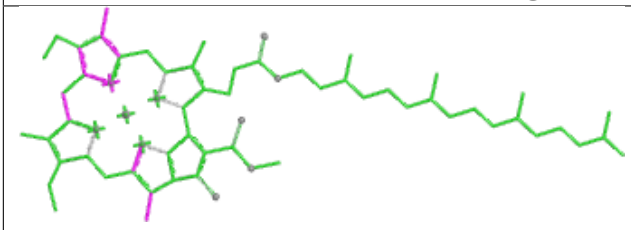


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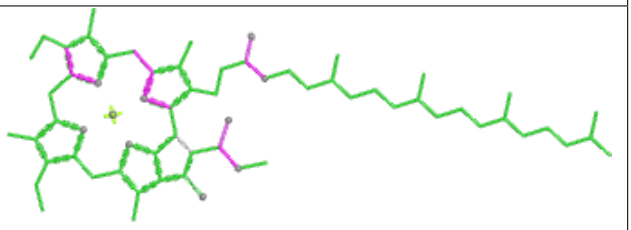


Rings

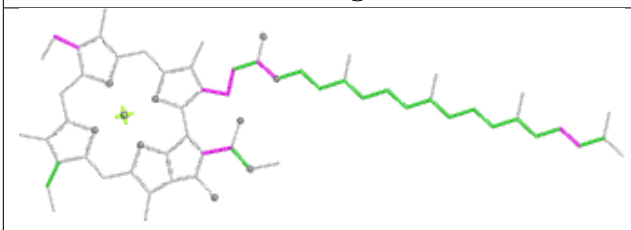
Ligand CLA B 802



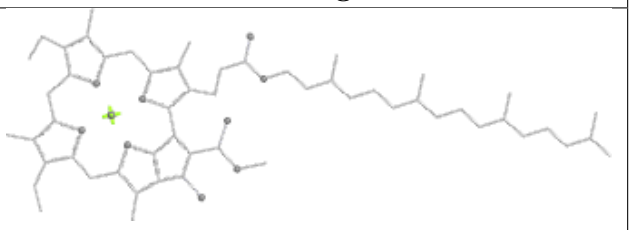
Bond lengths



Bond angles

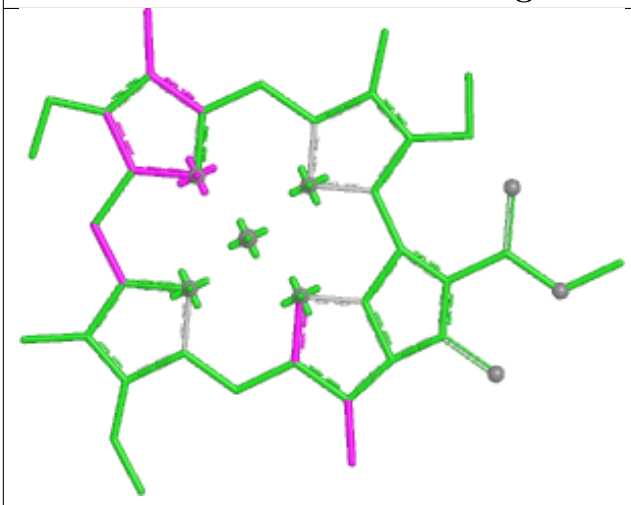


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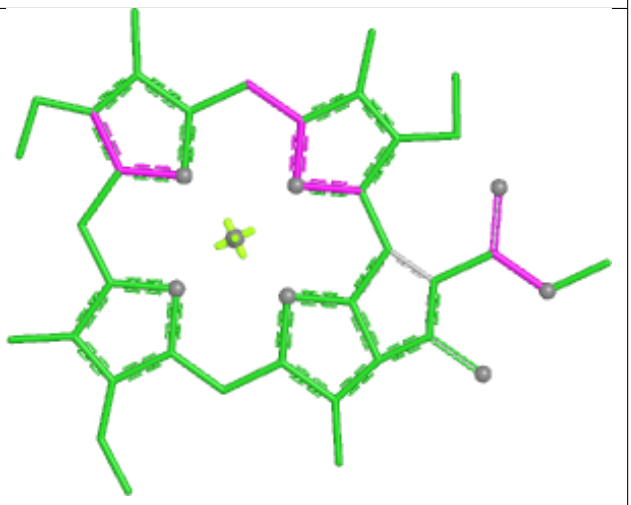


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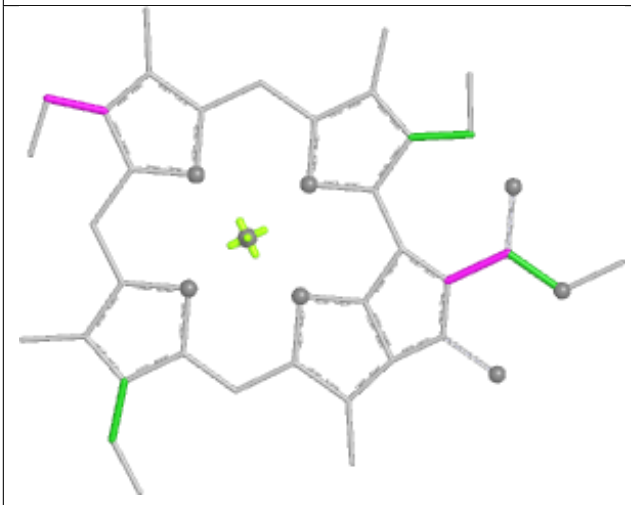
Ligand CLA B2 817



Bond lengths



Bond angles

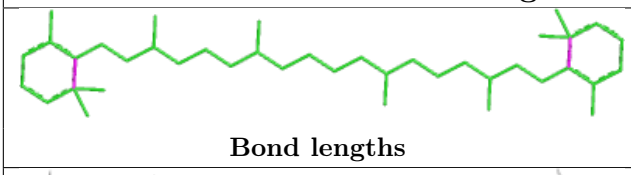


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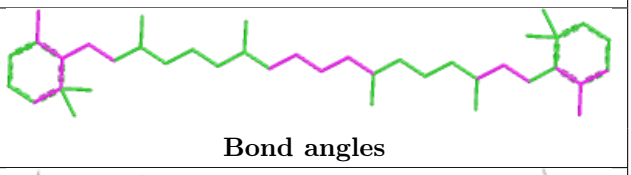


Rings

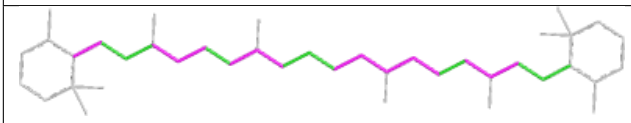
Ligand BCR I2 101



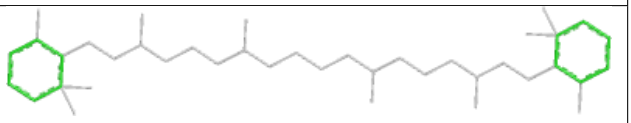
Bond lengths



Bond angles

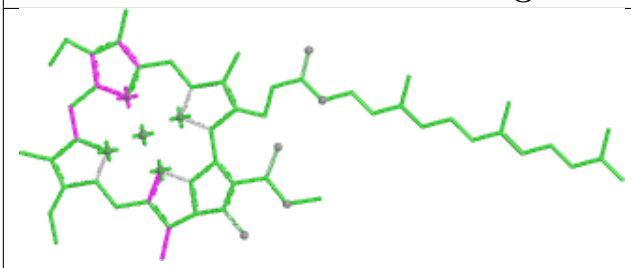


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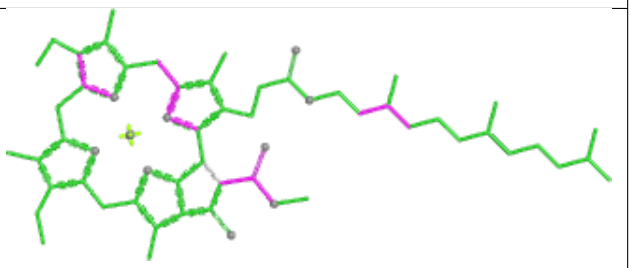


Rings

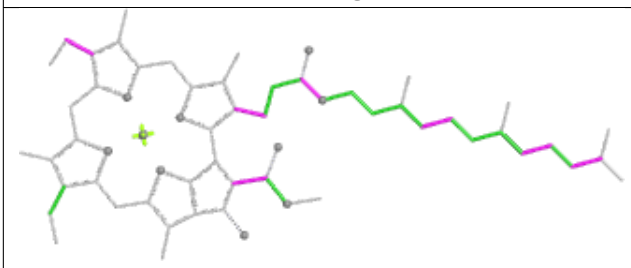
Ligand CLA A1 804



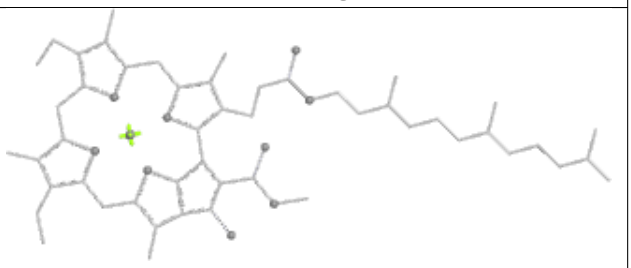
Bond lengths



Bond angles

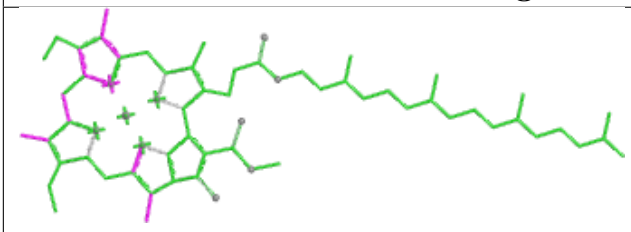


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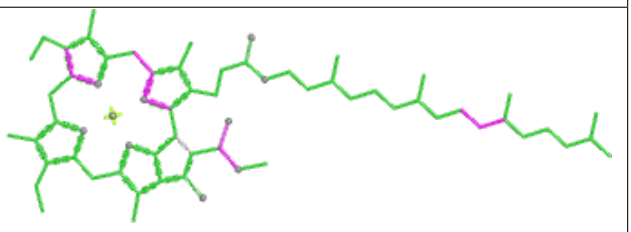


Rings

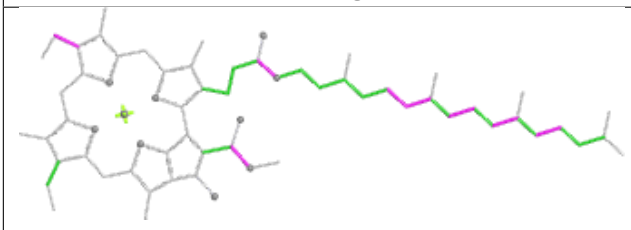
Ligand CLA B1 803



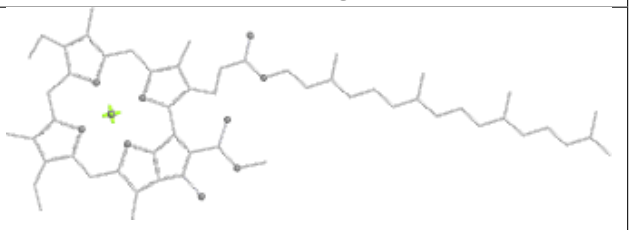
Bond lengths



Bond angles

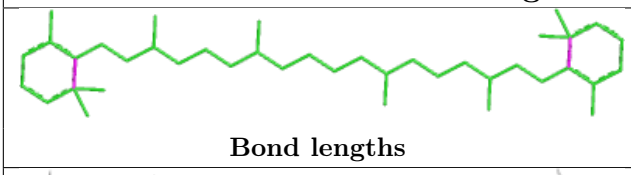


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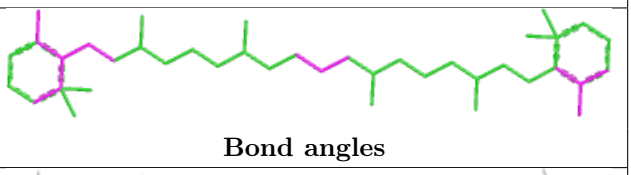


Rings

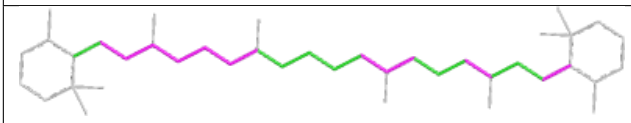
Ligand BCR B 843



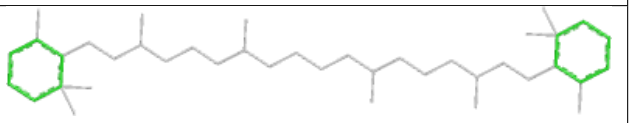
Bond lengths



Bond angles

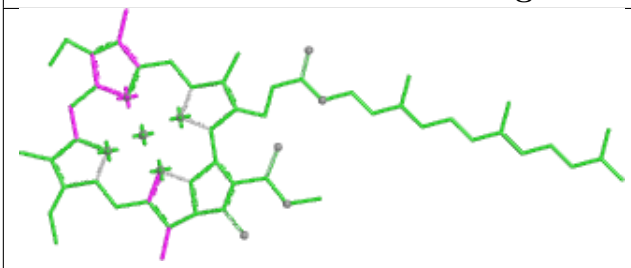


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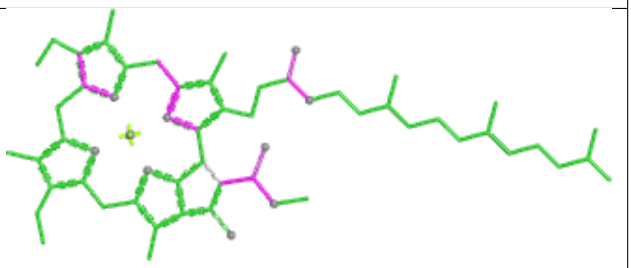


Rings

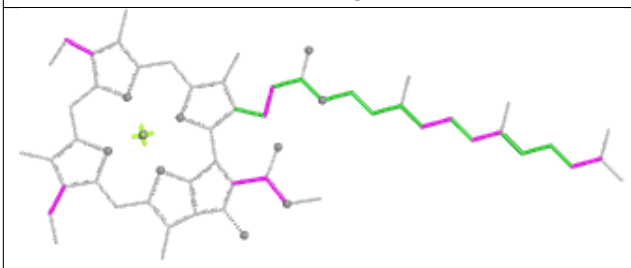
Ligand CLA B2 837



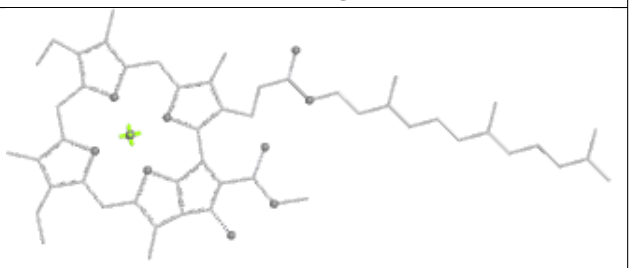
Bond lengths



Bond angles

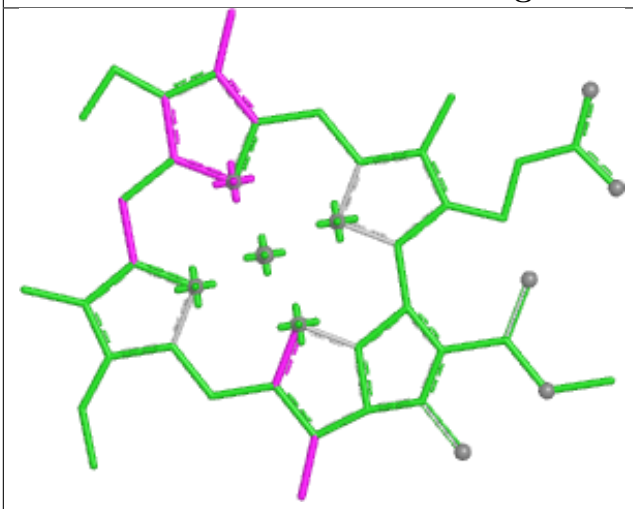


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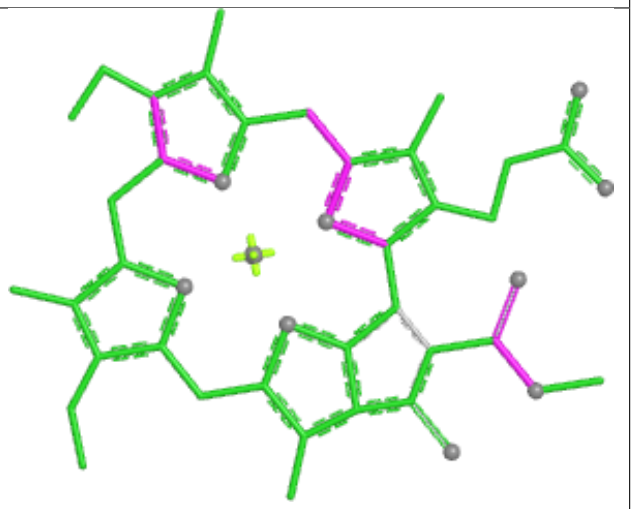


Rings

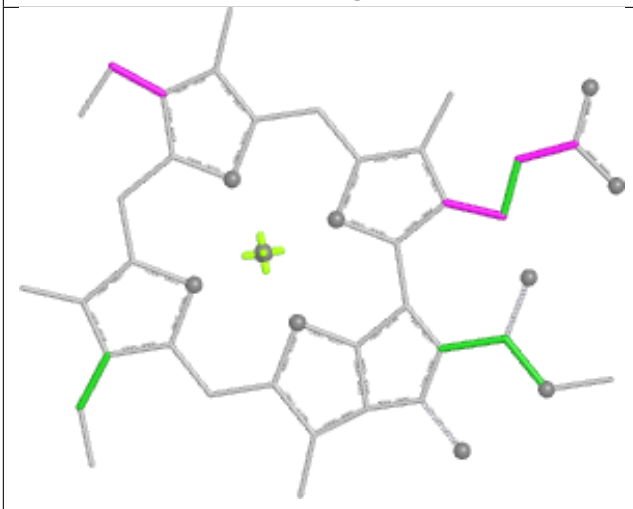
Ligand CLA A1 817



Bond lengths



Bond angles

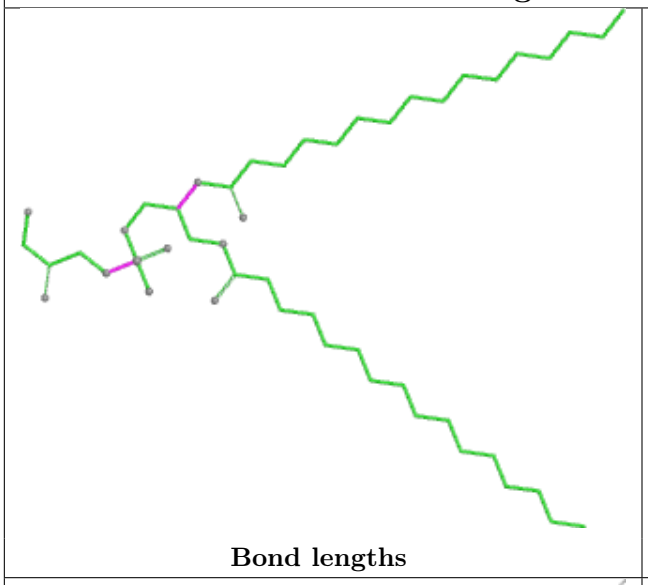


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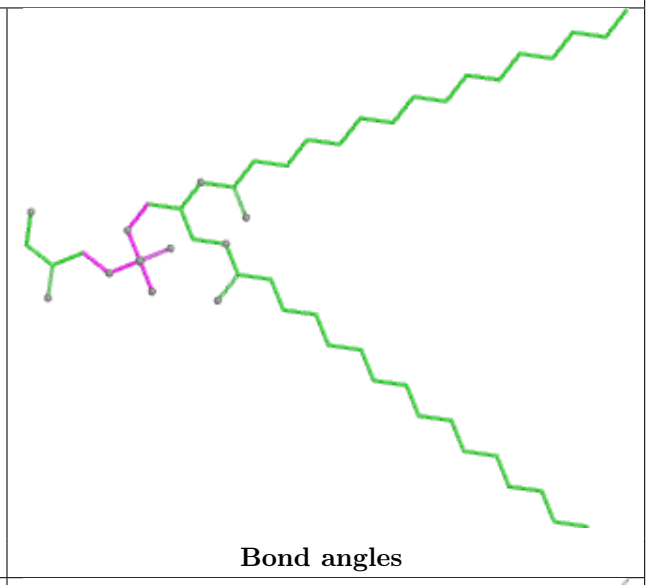


Rings

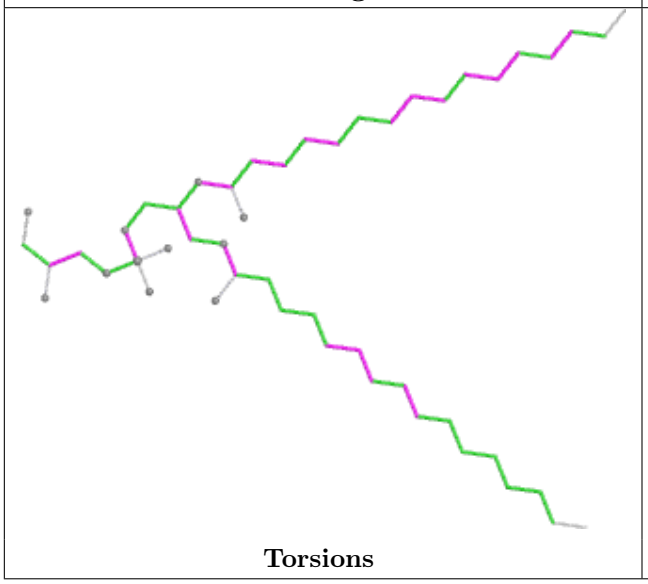
Ligand LHG A1 845



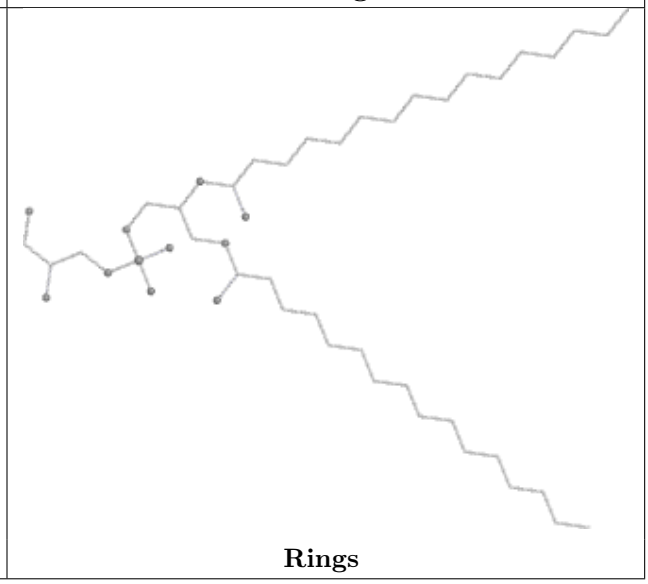
Bond lengths



Bond angles

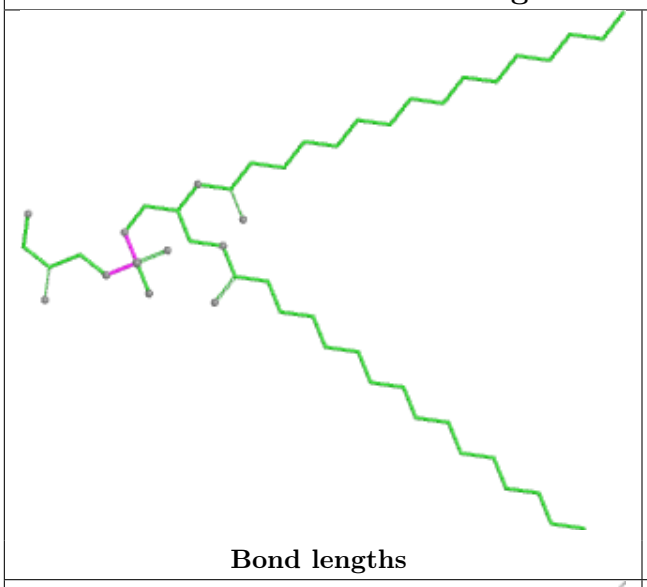


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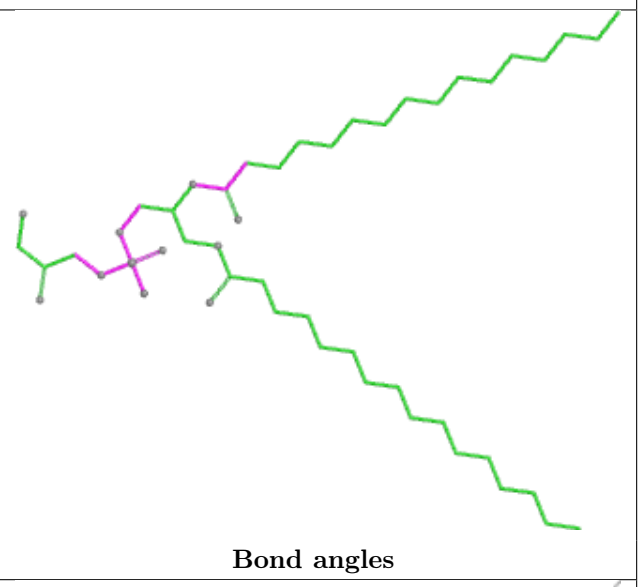


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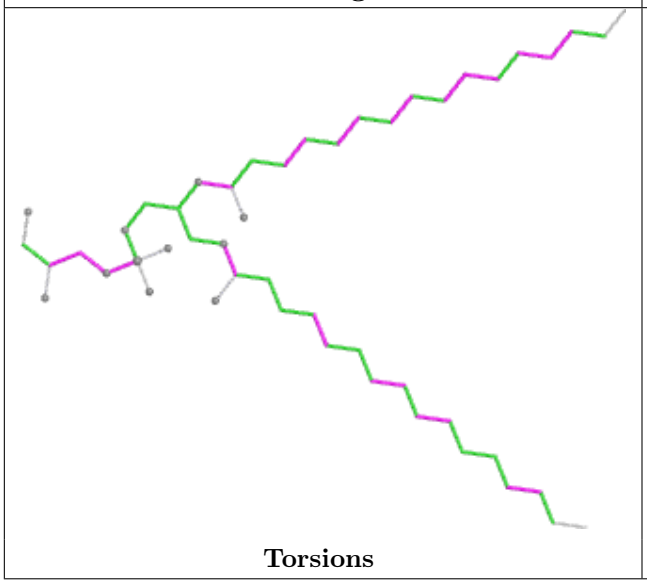
Ligand LHG BB 851



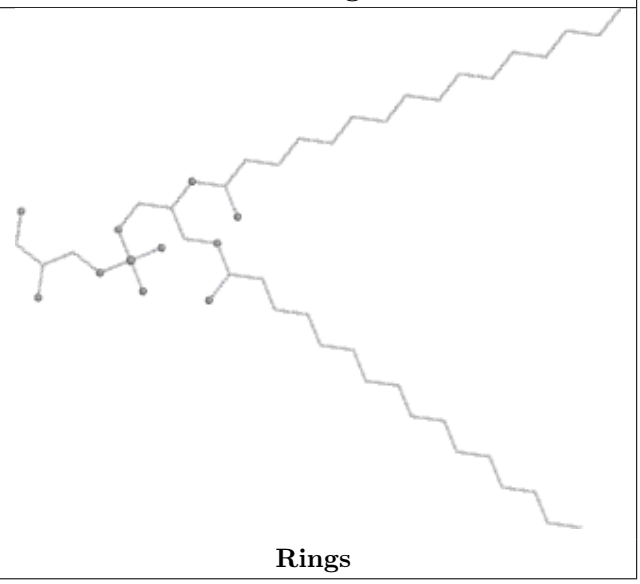
Bond lengths



Bond angles



Torsions

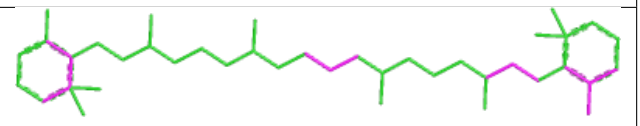


Rings

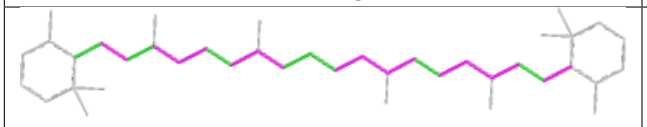
Ligand BCR J1 104



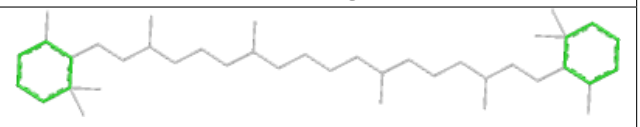
Bond lengths



Bond angles

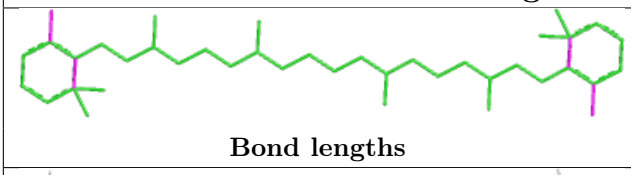


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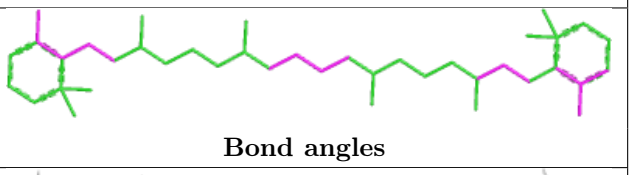


Rings

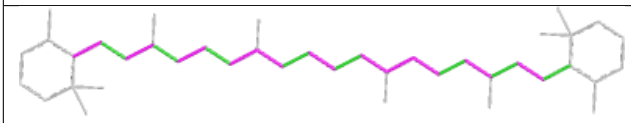
Ligand BCR B 844



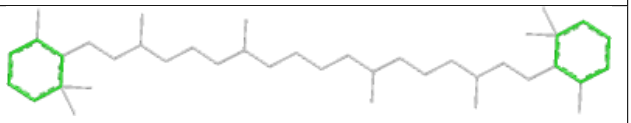
Bond lengths



Bond angles

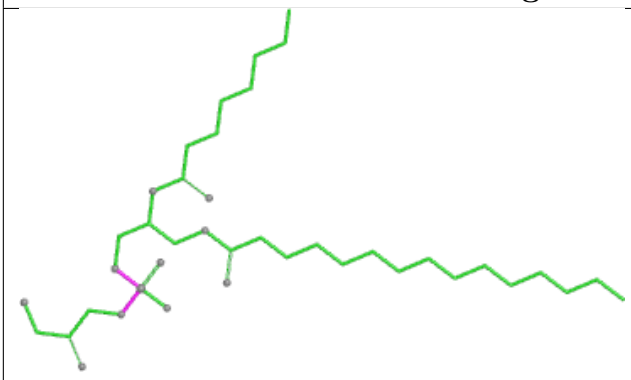


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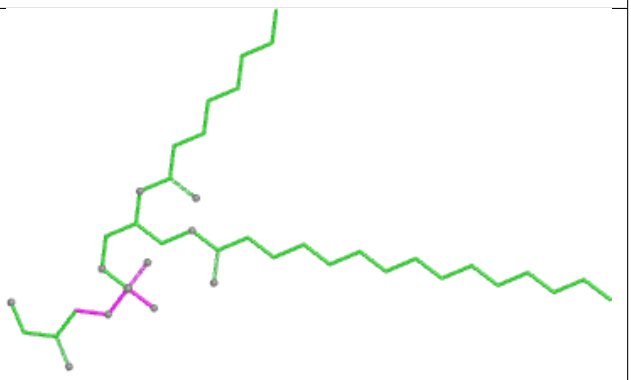


Rings

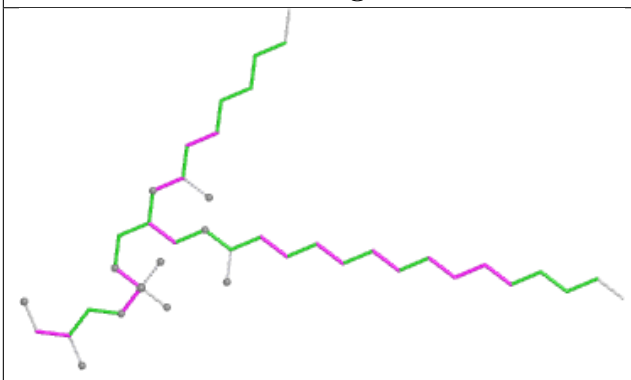
Ligand LHG X 102



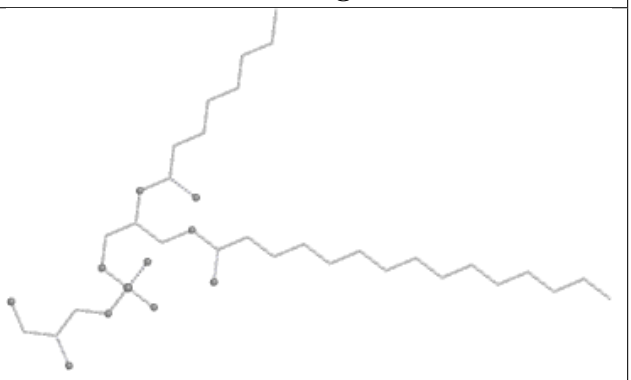
Bond lengths



Bond angles

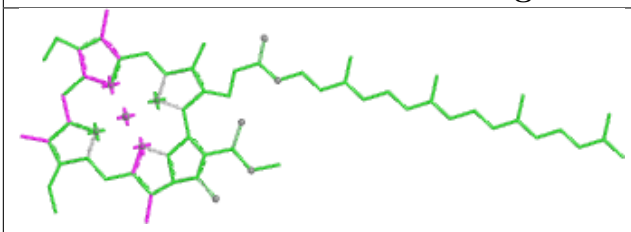


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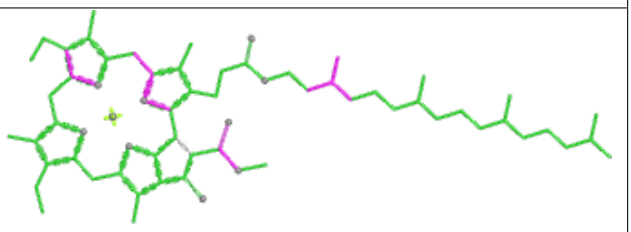


Rings

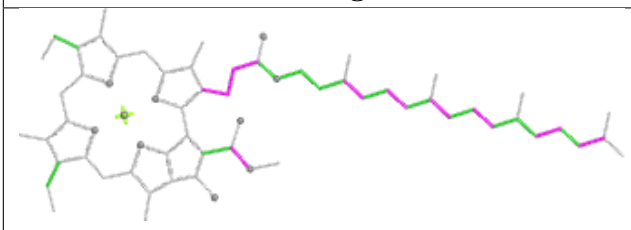
Ligand CLA A1 828



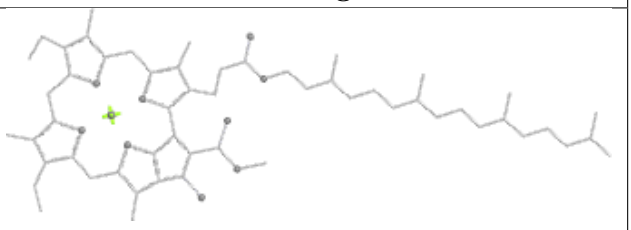
Bond lengths



Bond angles

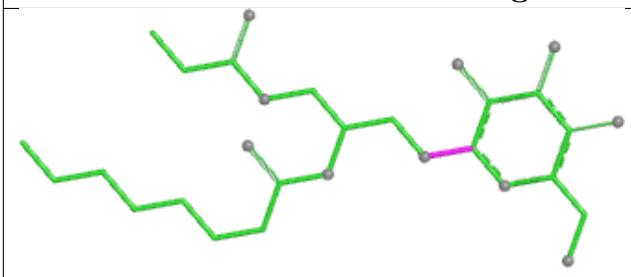


Torsions

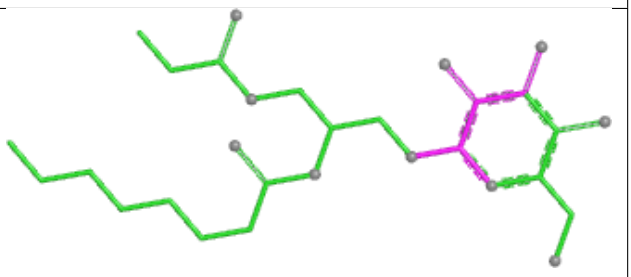


Rings

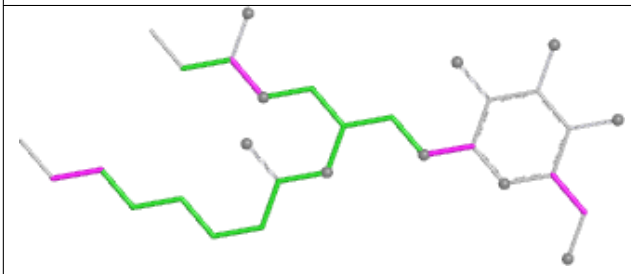
Ligand LMG B1 852



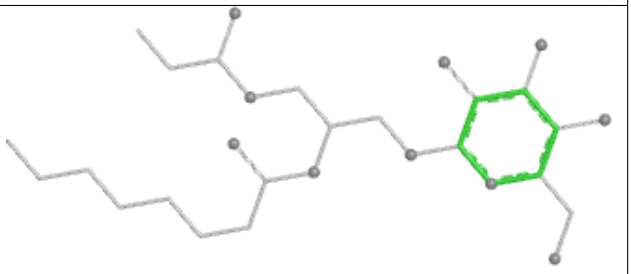
Bond lengths



Bond angles

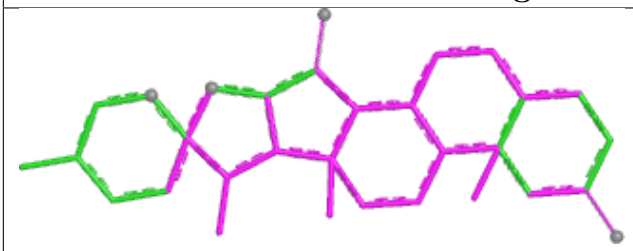


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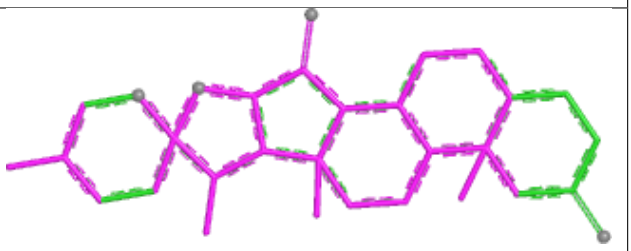


Rings

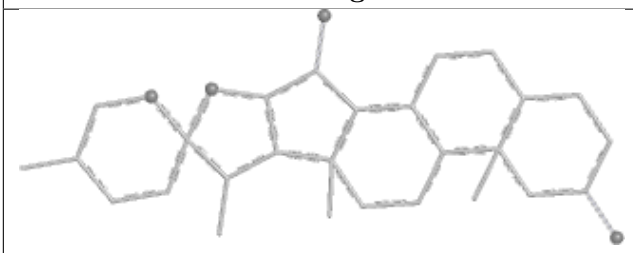
Ligand AJP M2 101



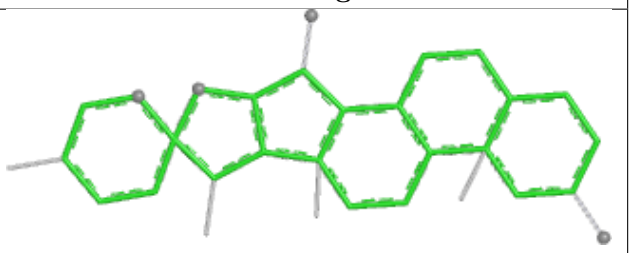
Bond lengths



Bond angles

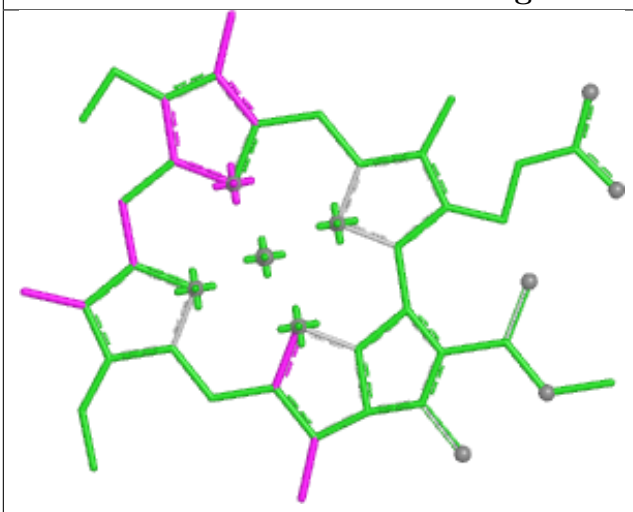


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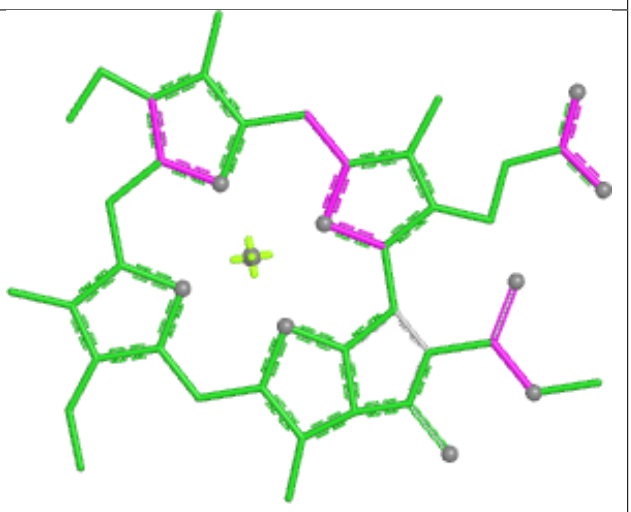


Rings

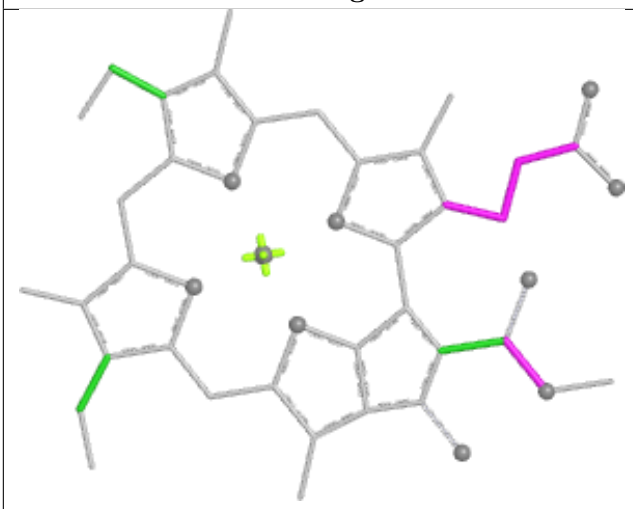
Ligand CLA A1 825



Bond lengths



Bond angles

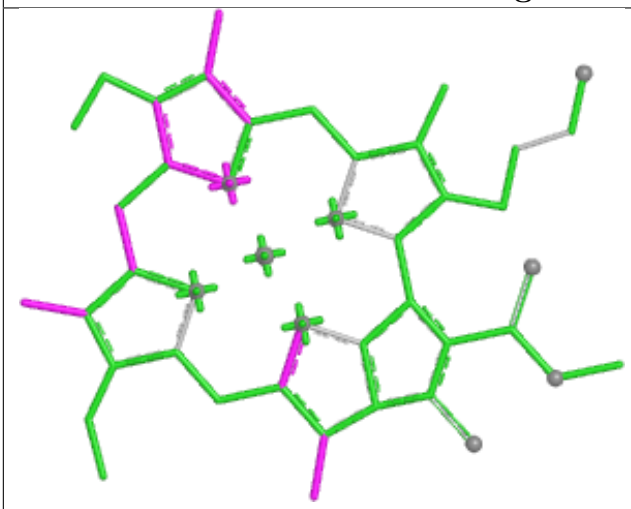


Torsions



Rings

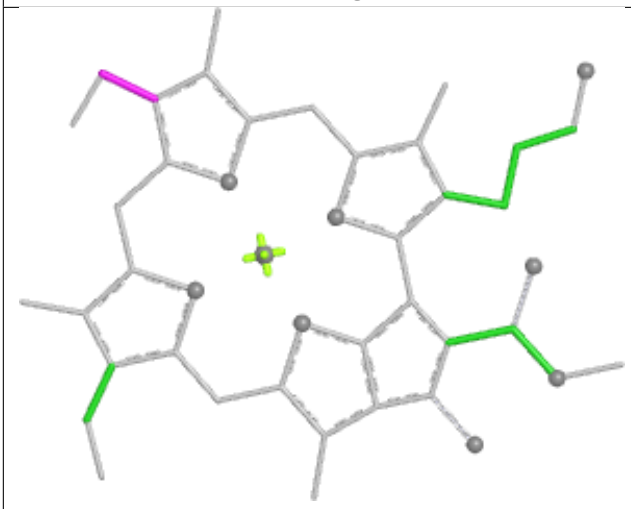
Ligand CLA A2 817



Bond lengths



Bond angles

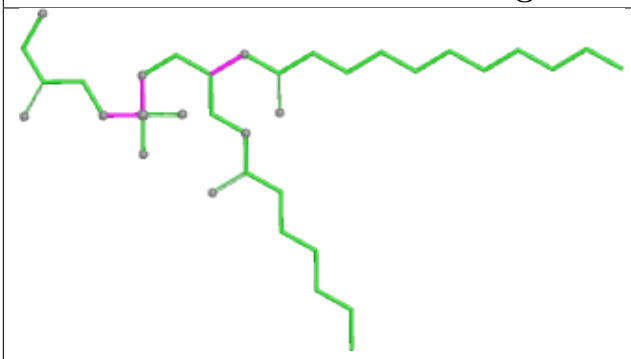


Torsions

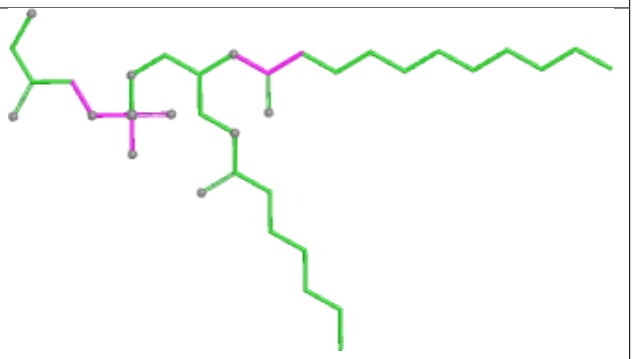


Rings

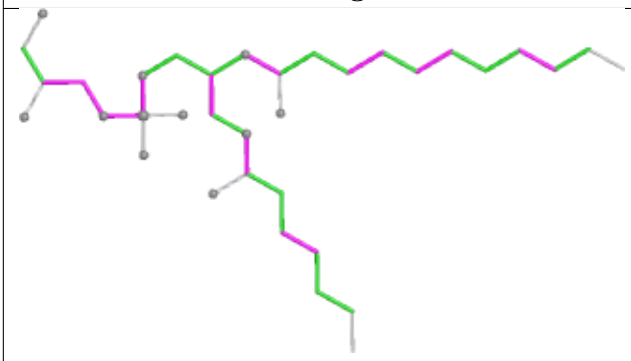
Ligand LHG L2 208



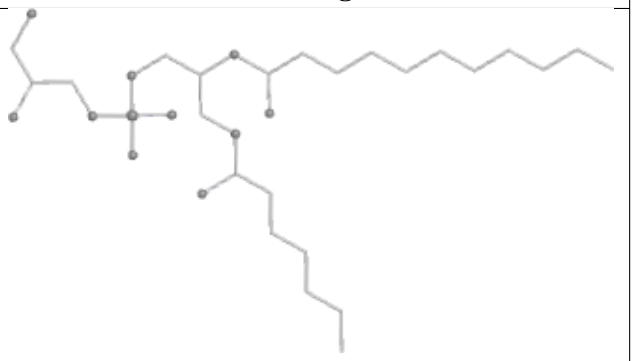
Bond lengths



Bond angles

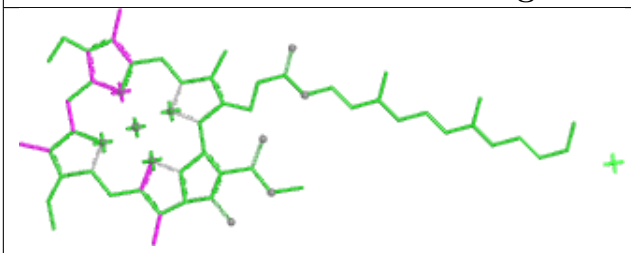


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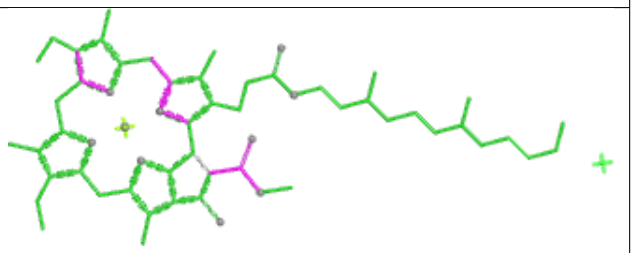


Rings

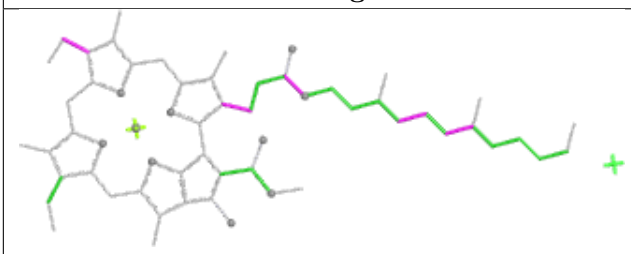
Ligand CLA L2 205



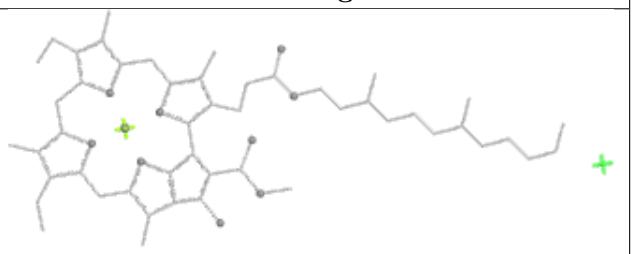
Bond lengths



Bond angles

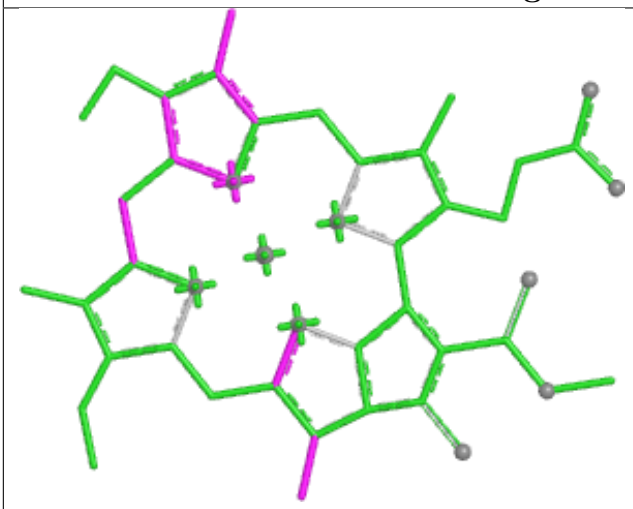


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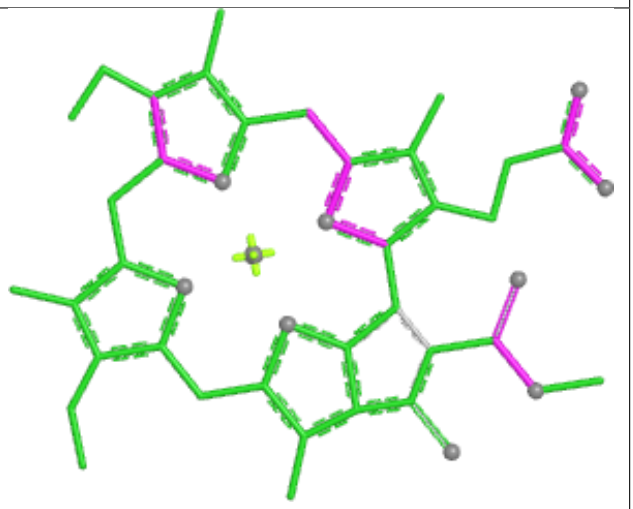


Rings

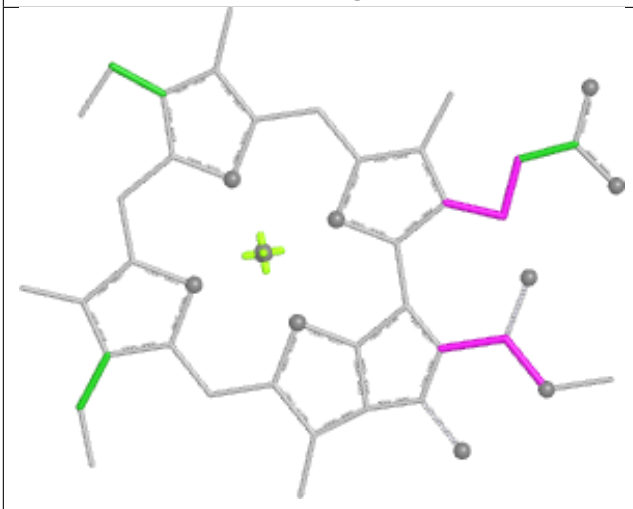
Ligand CLA A 824



Bond lengths



Bond angles

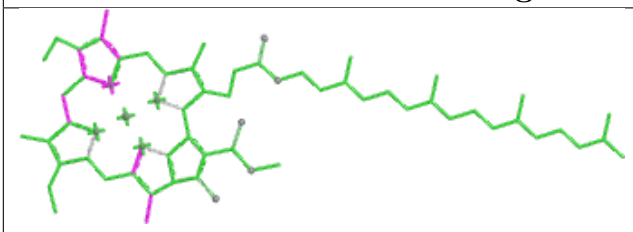


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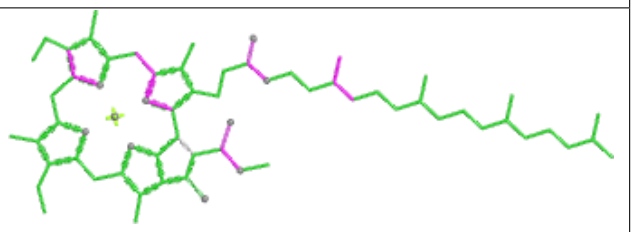


Rings

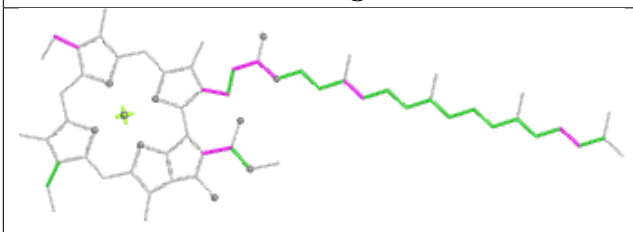
Ligand CLA B1 802



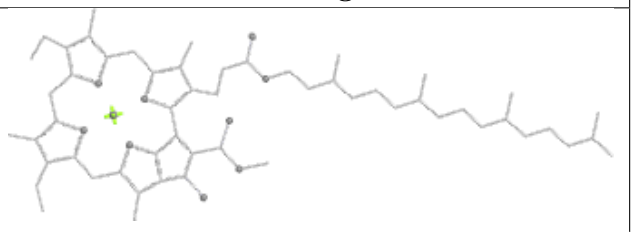
Bond lengths



Bond angles

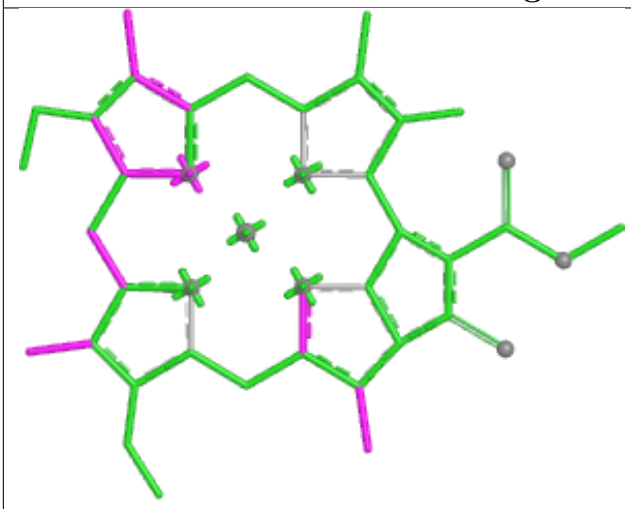


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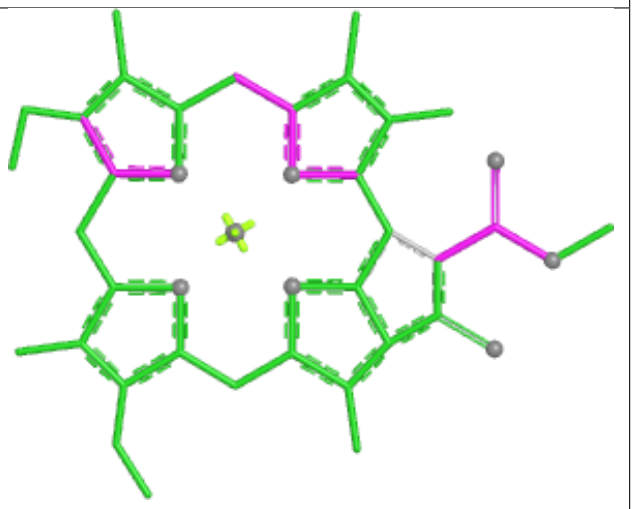


Rings

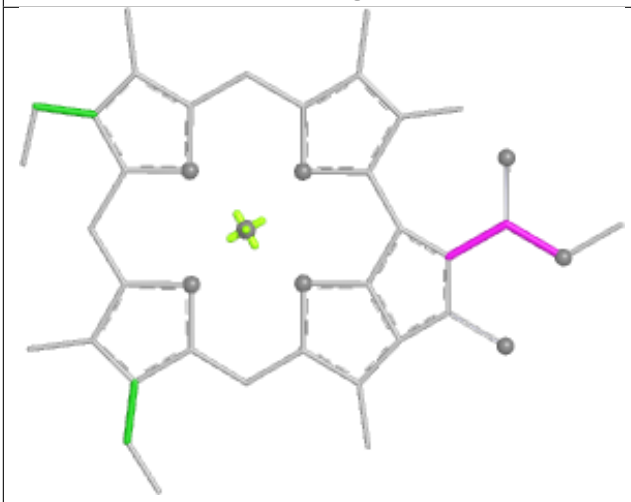
Ligand CLA A 844



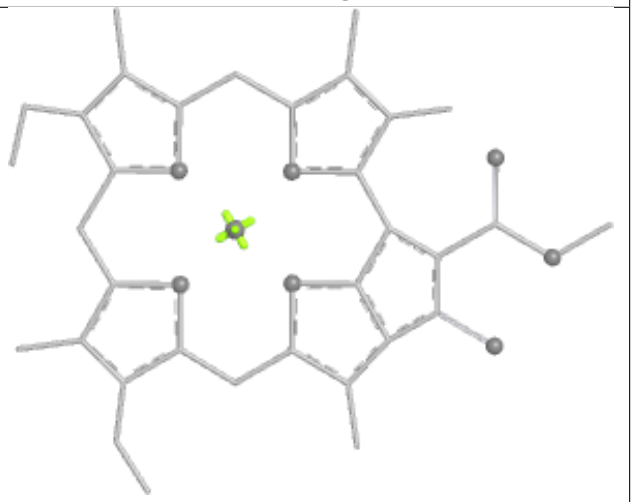
Bond lengths



Bond angles

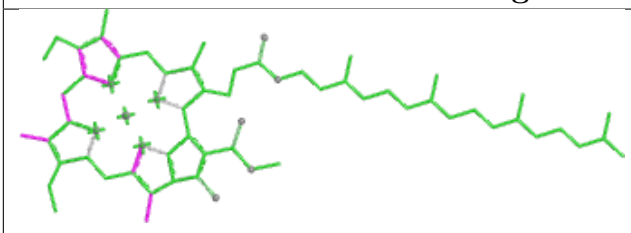


Torsions

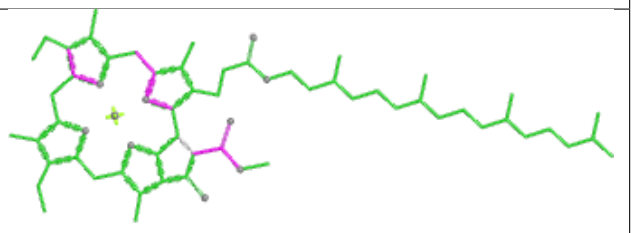


Rings

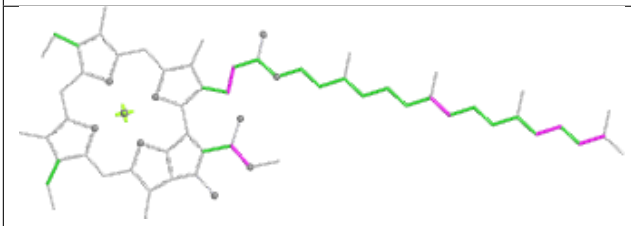
Ligand CLA BB 822



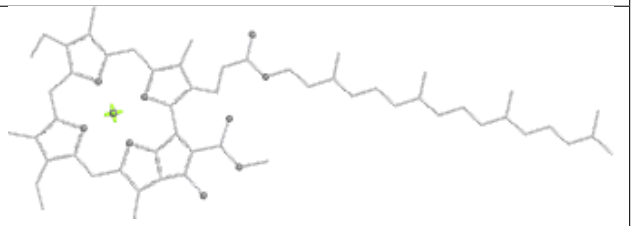
Bond lengths



Bond angles

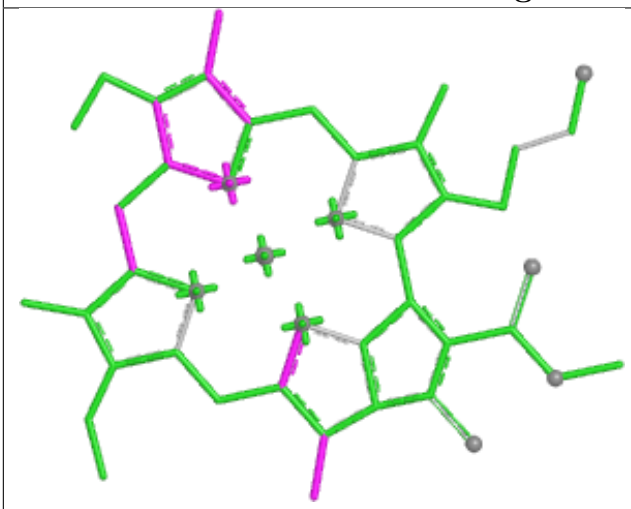


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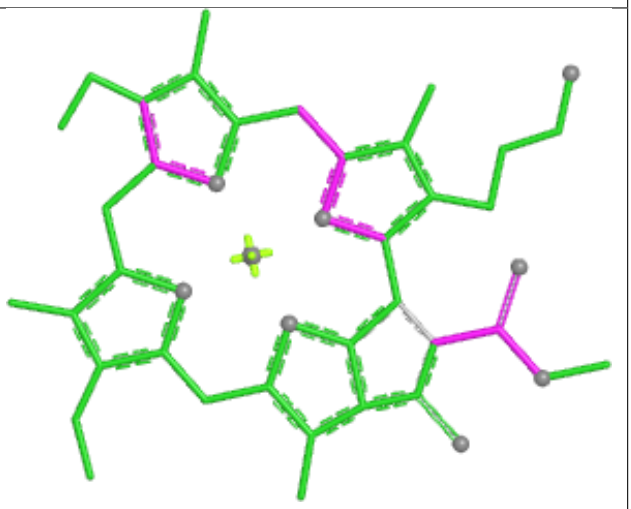


Rings

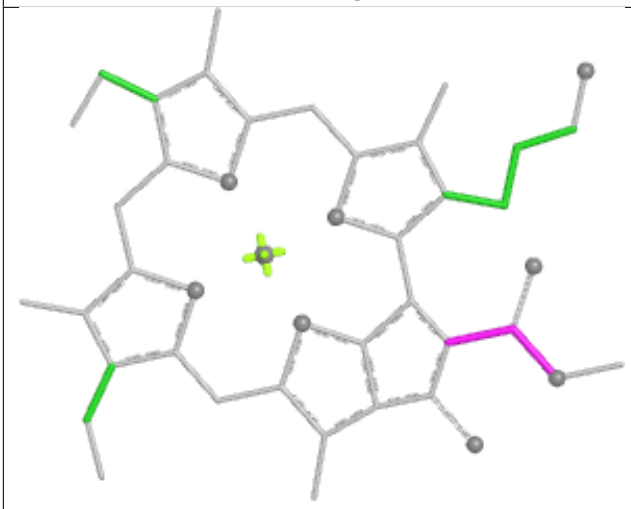
Ligand CLA A2 838



Bond lengths



Bond angles

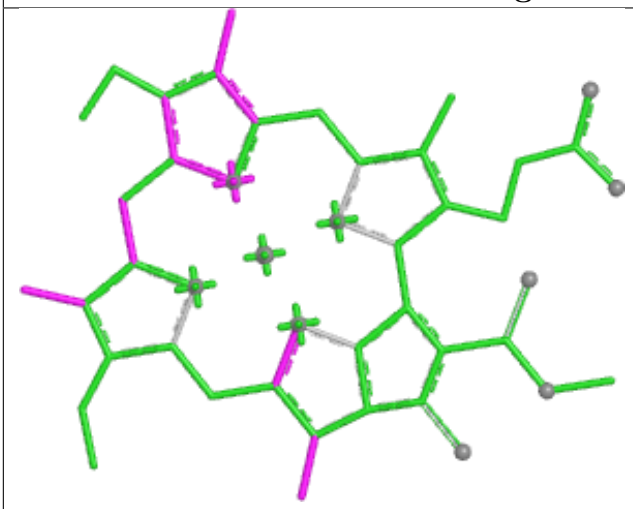


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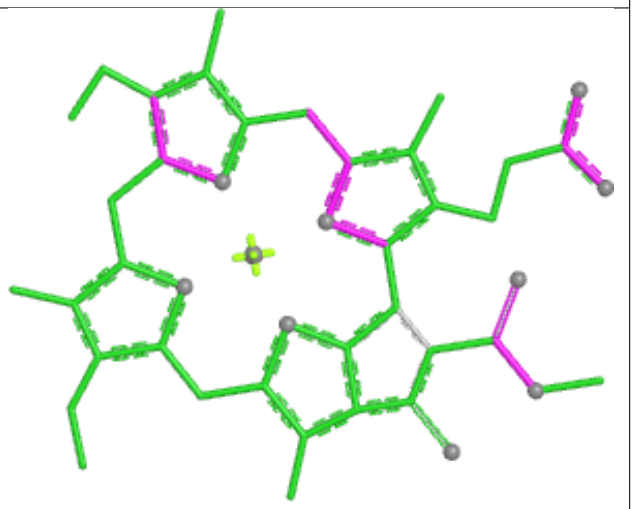


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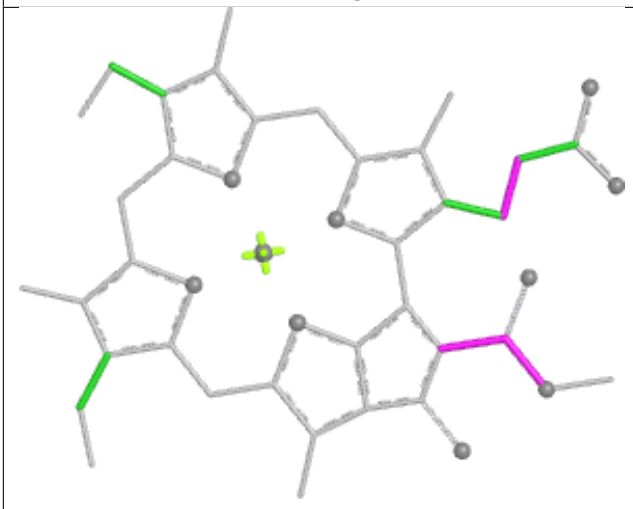
Ligand CLA A1 823



Bond lengths



Bond angles

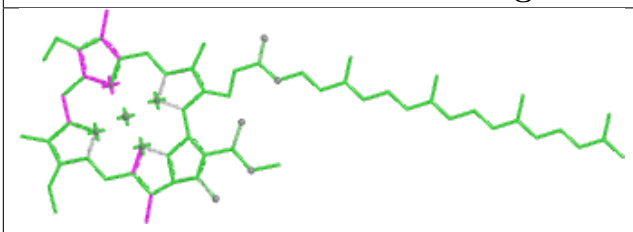


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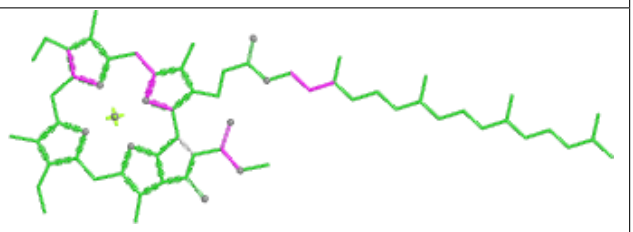


Rings

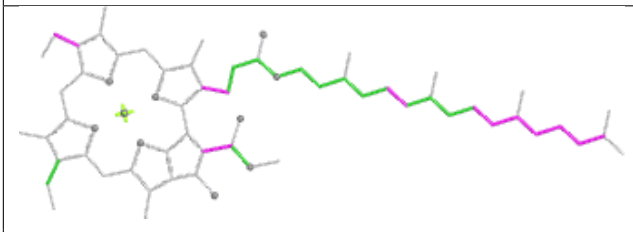
Ligand CLA A2 807



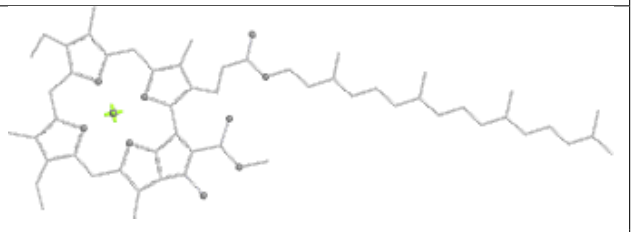
Bond lengths



Bond angles

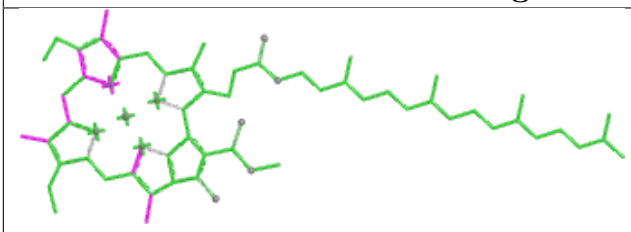


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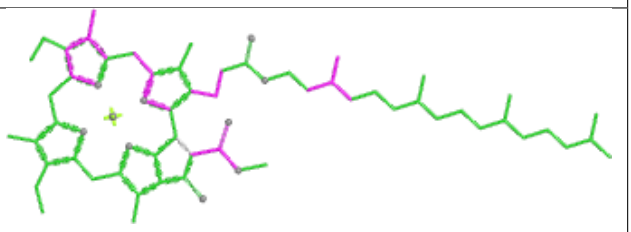


Rings

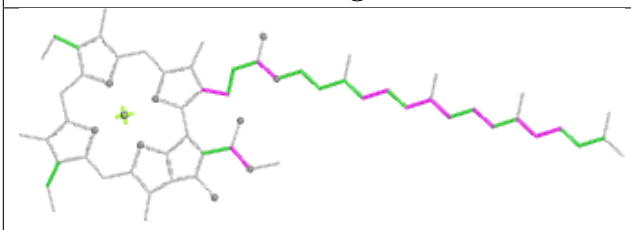
Ligand CLA BB 815



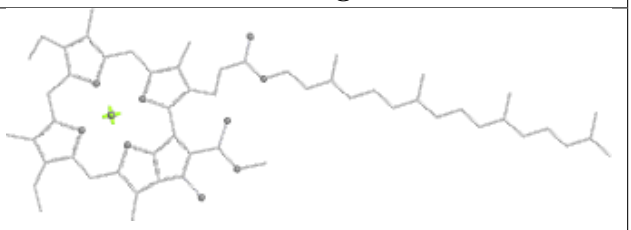
Bond lengths



Bond angles

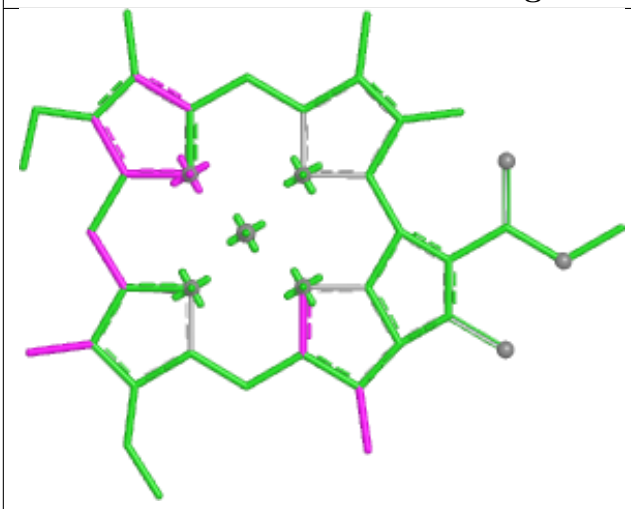


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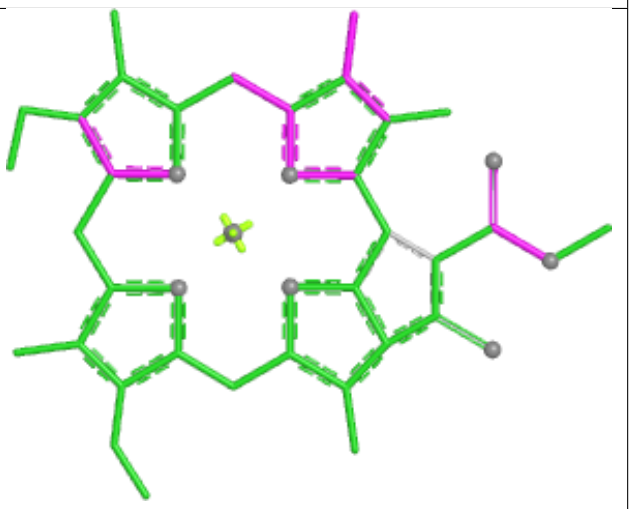


Rings

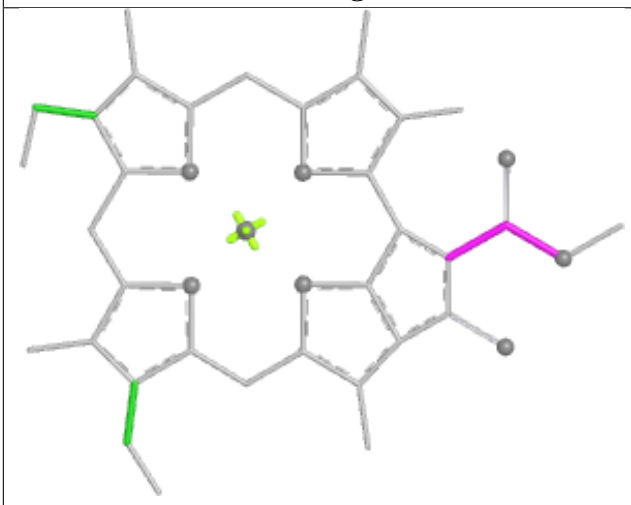
Ligand CLA B 819



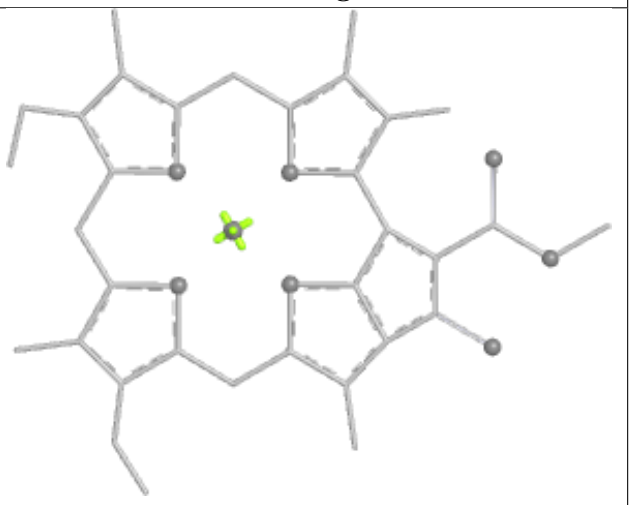
Bond lengths



Bond angles

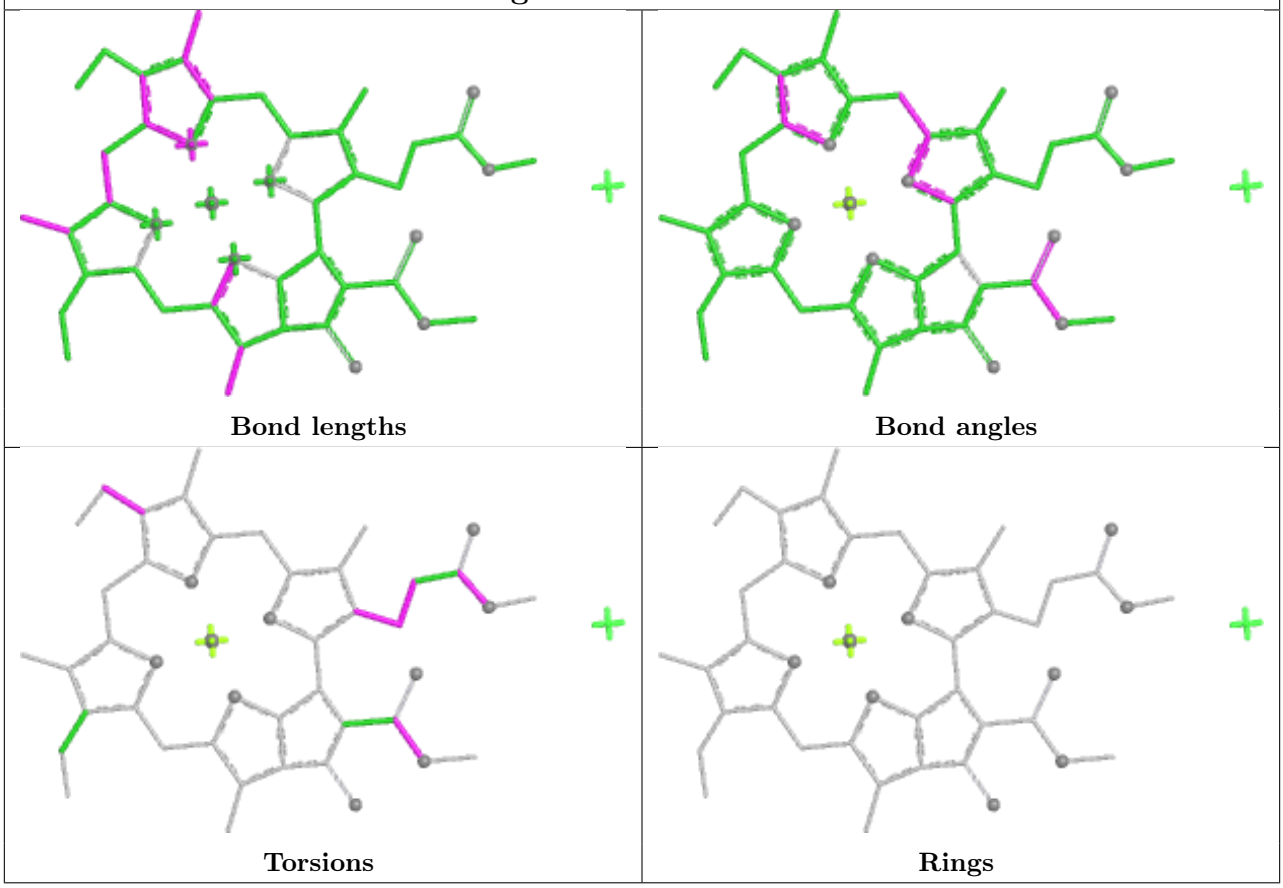


Torsions

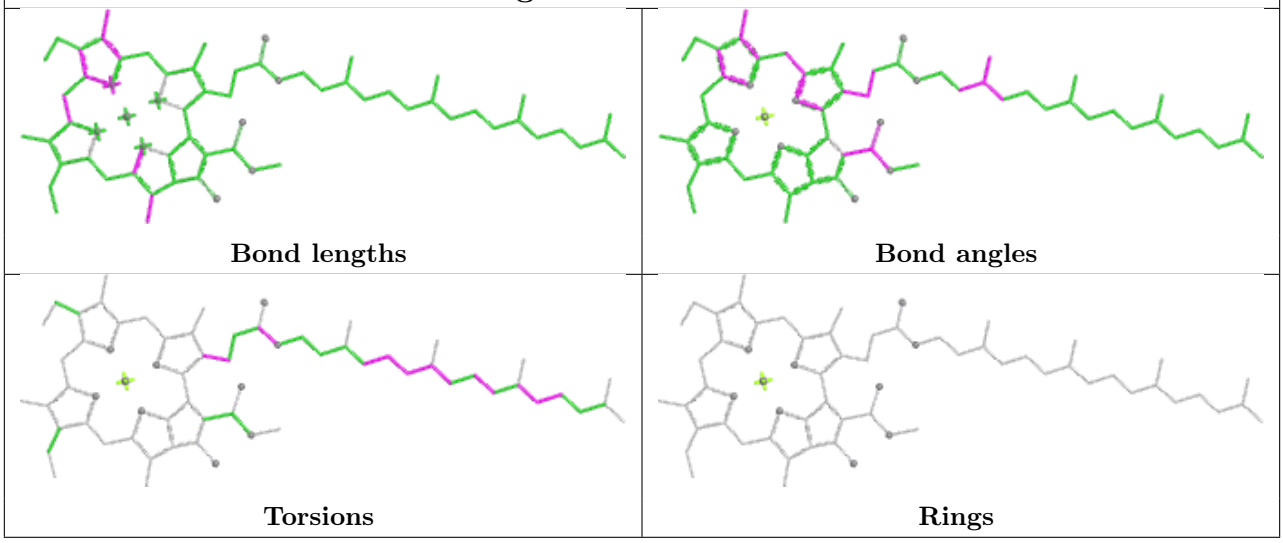


Rings

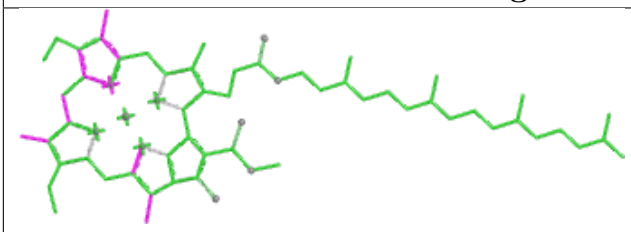
Ligand CLA AA 812



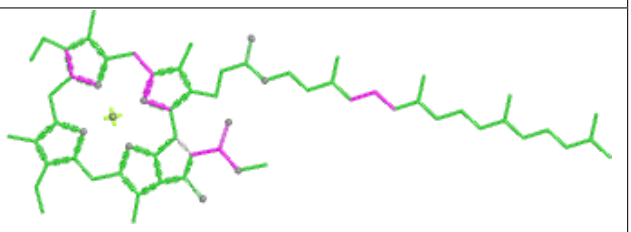
Ligand CLA B2 815



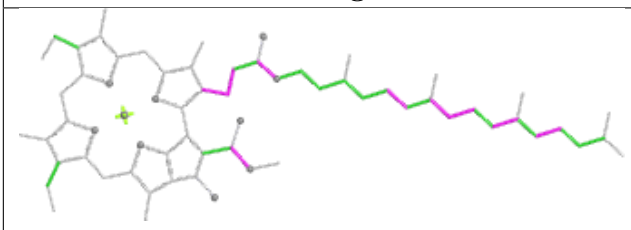
Ligand CLA AA 853



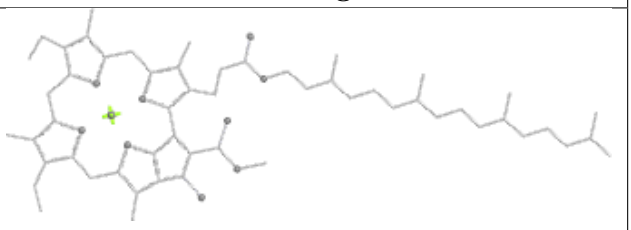
Bond lengths



Bond angles

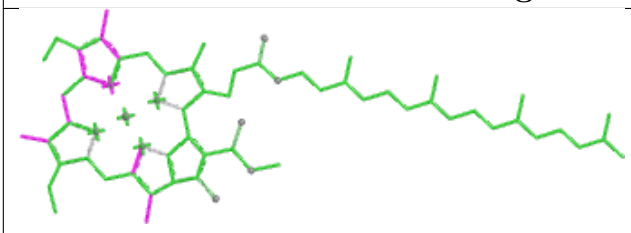


Torsions

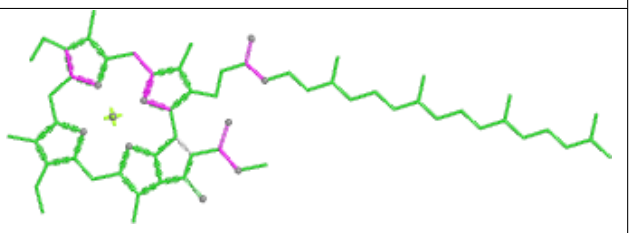


Rings

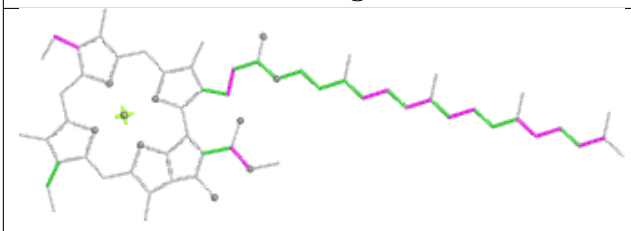
Ligand CLA B2 836



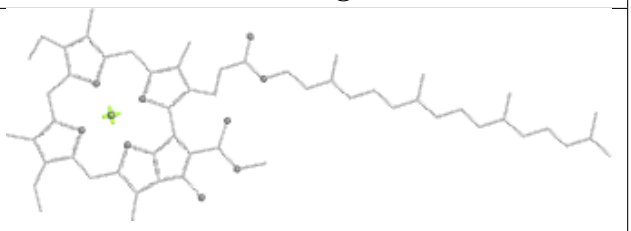
Bond lengths



Bond angles

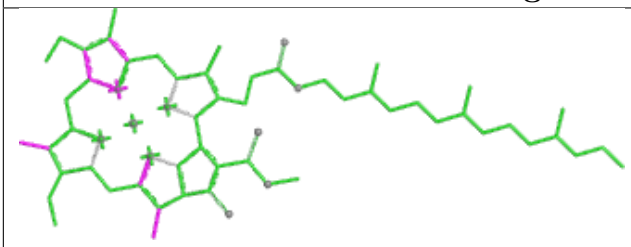


Torsions

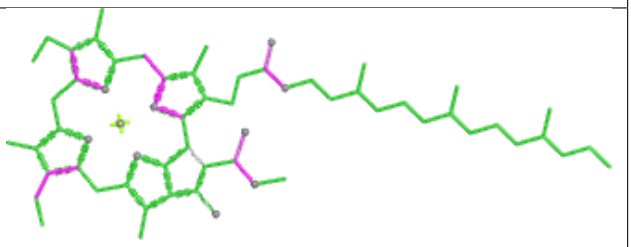


Rings

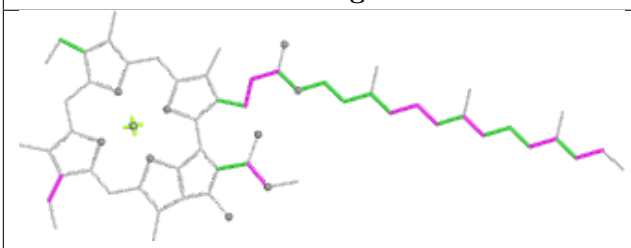
Ligand CLA A 830



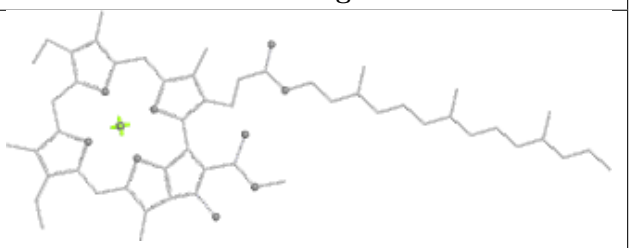
Bond lengths



Bond angles

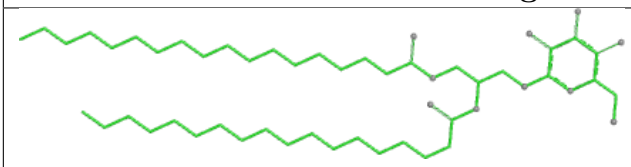


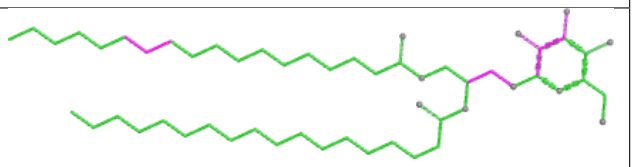
Torsions

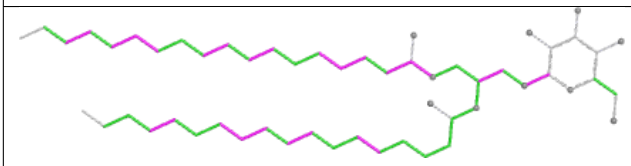


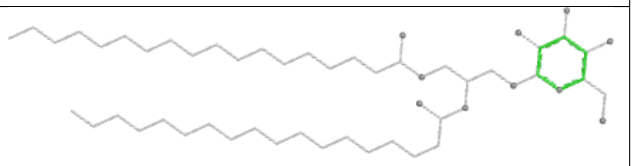
Rings

Ligand LMG B 845

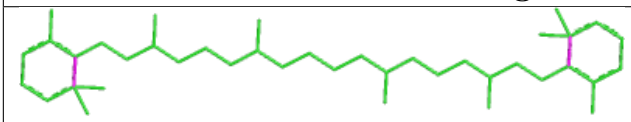

Bond lengths

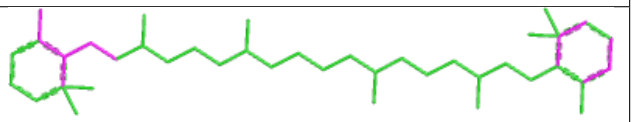

Bond angles

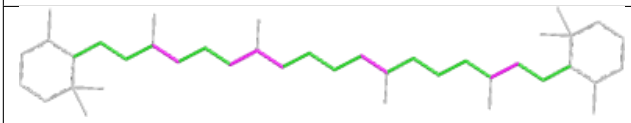

Torsions

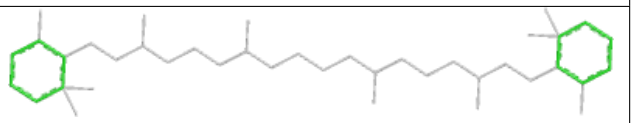

Rings

Ligand BCR B2 840

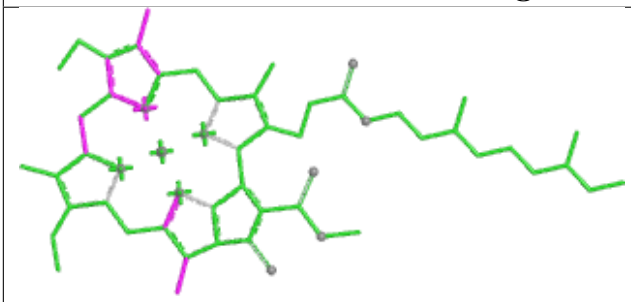

Bond lengths

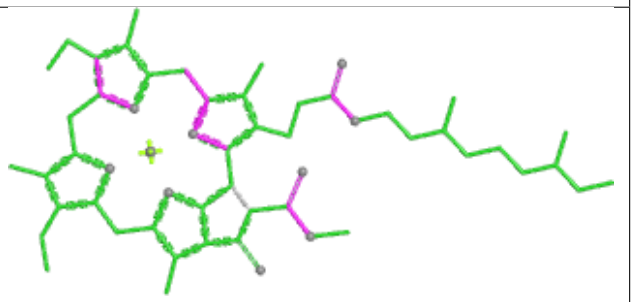

Bond angles

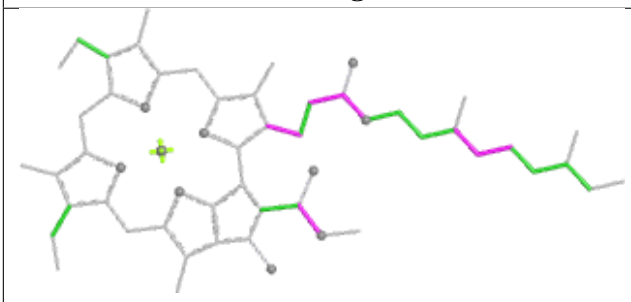

Torsions

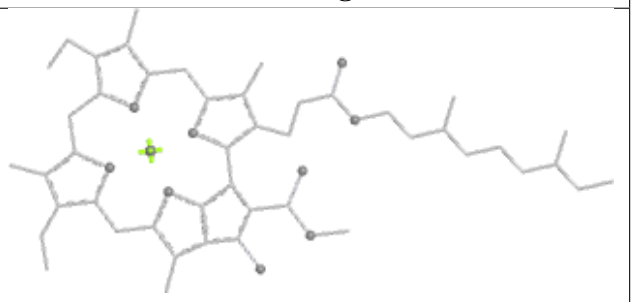

Rings

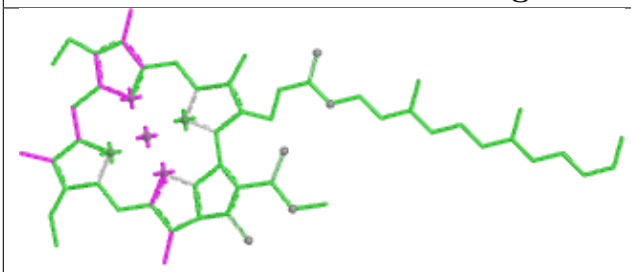
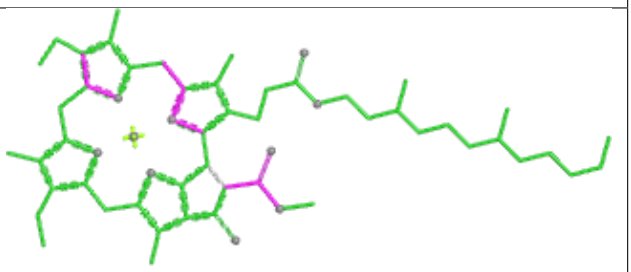
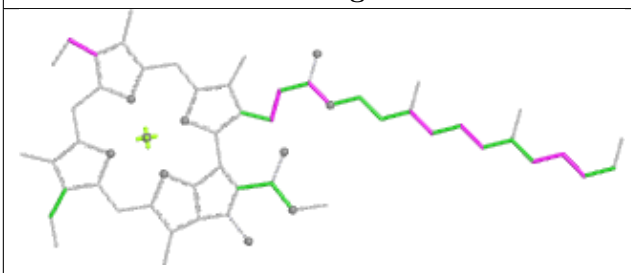
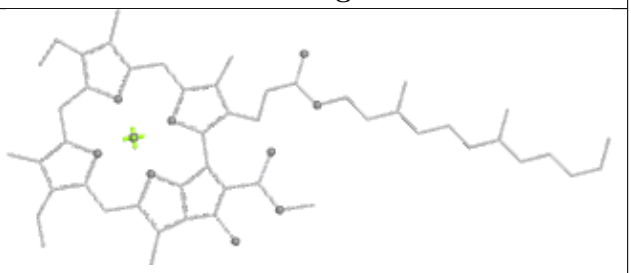
Ligand CLA A2 828

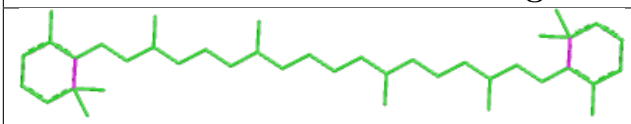
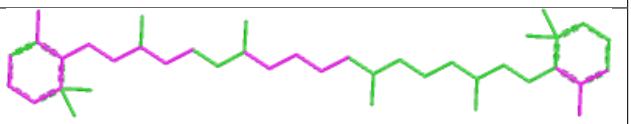
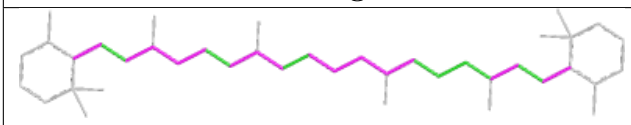
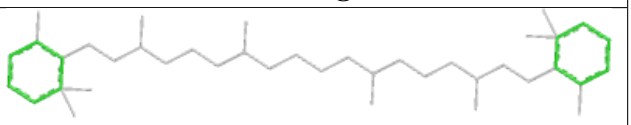

Bond lengths


Bond angles

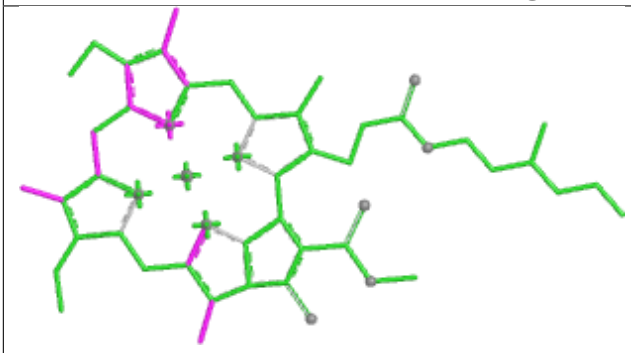

Torsions


Rings

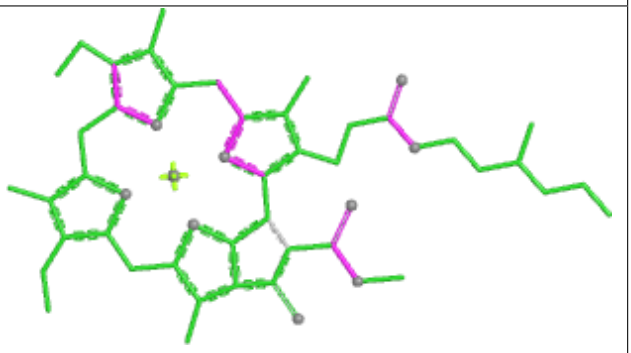
Ligand CLA BB 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

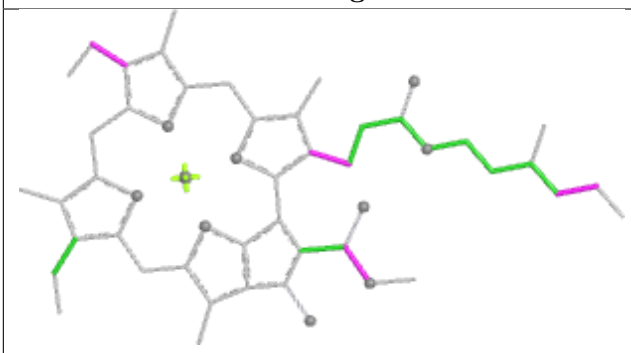
Ligand CLA A 825



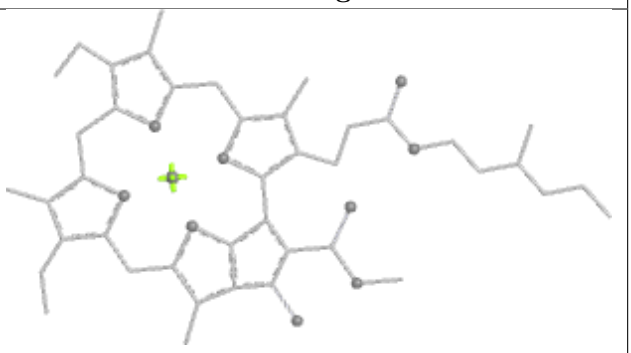
Bond lengths



Bond angles

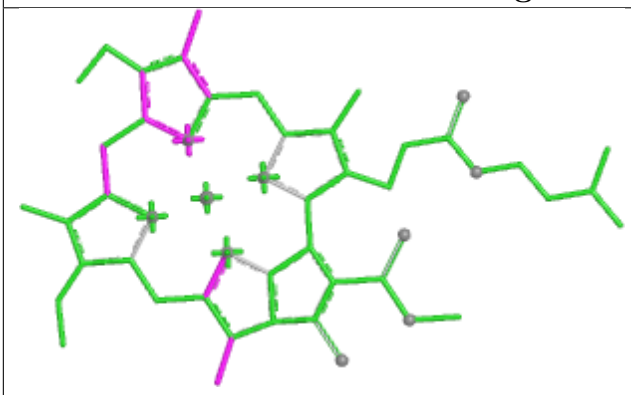


Torsions

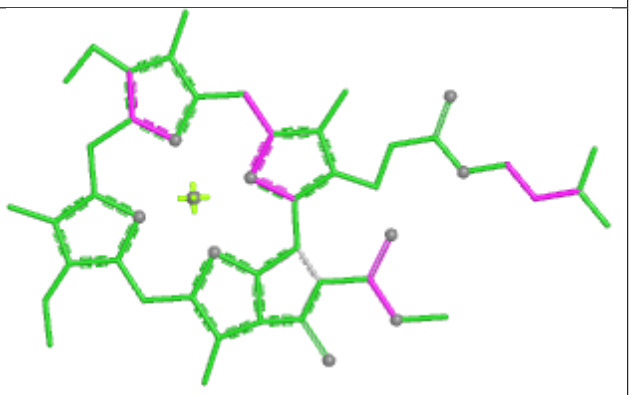


Rings

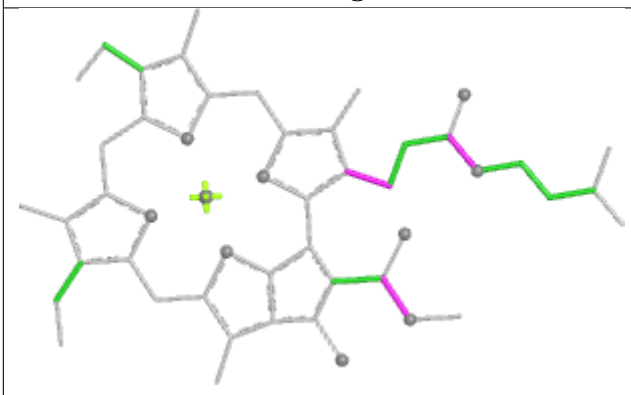
Ligand CLA A2 816



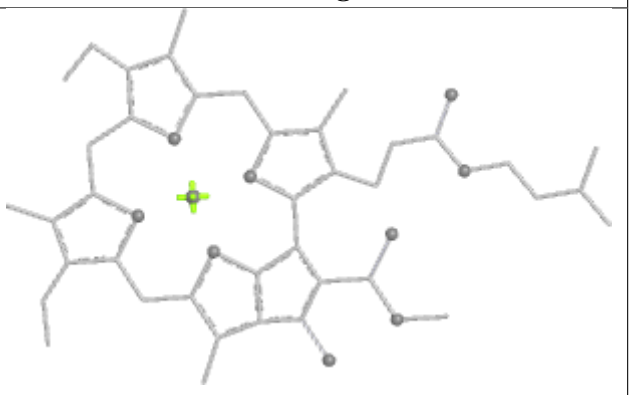
Bond lengths



Bond angles

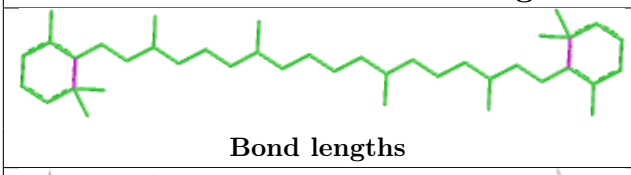


Torsions

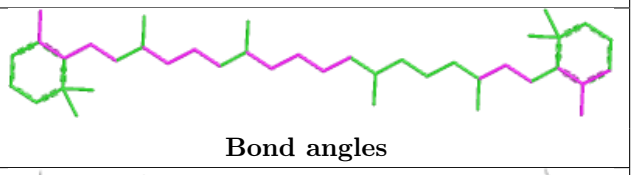


Rings

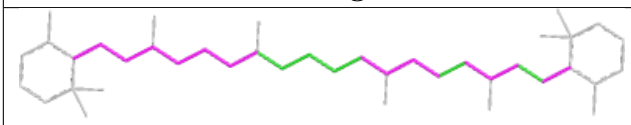
Ligand BCR L2 207



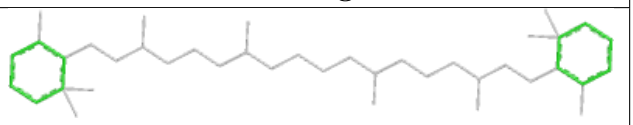
Bond lengths



Bond angles

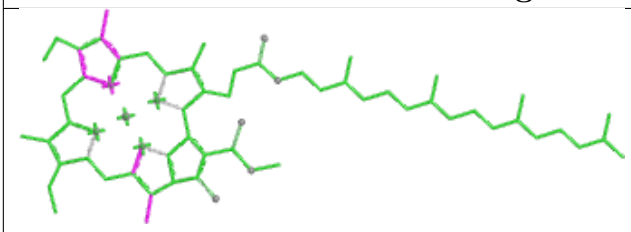


Torsions

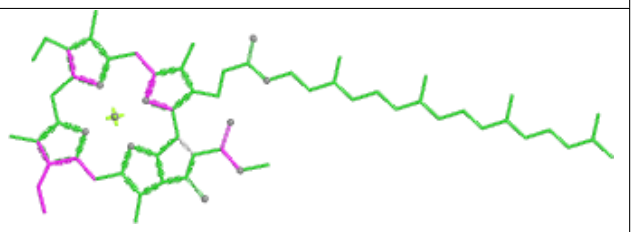


Rings

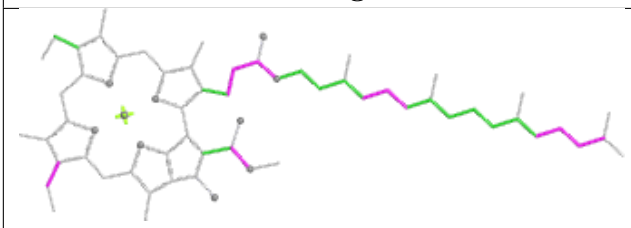
Ligand CLA B2 852



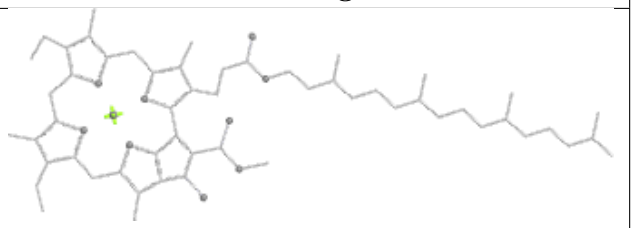
Bond lengths



Bond angles

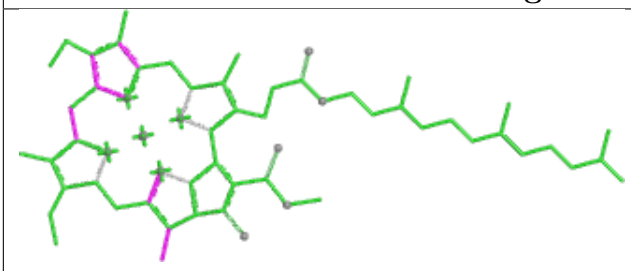


Torsions

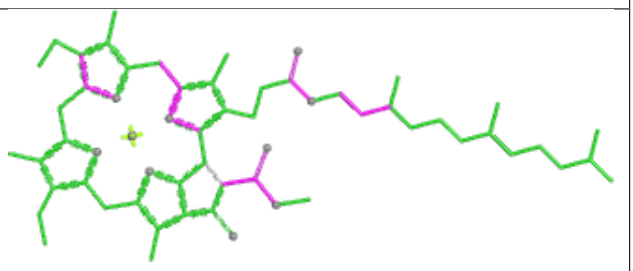


Rings

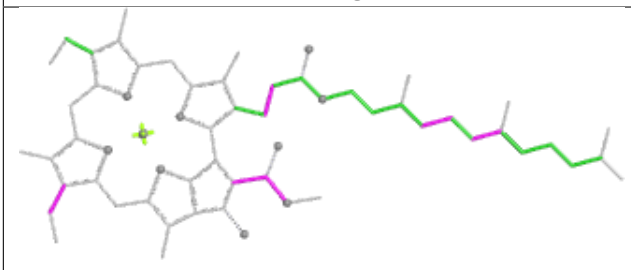
Ligand CLA B 837



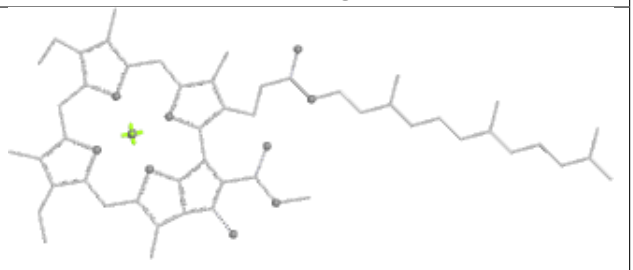
Bond lengths



Bond angles

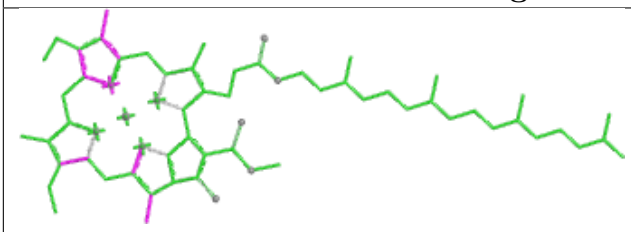


Torsions

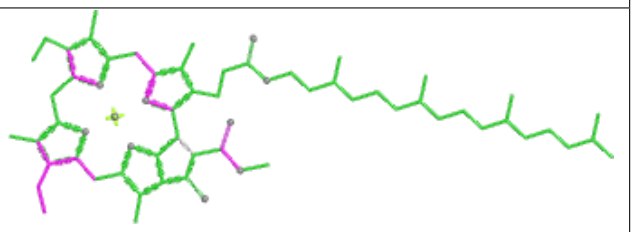


Rings

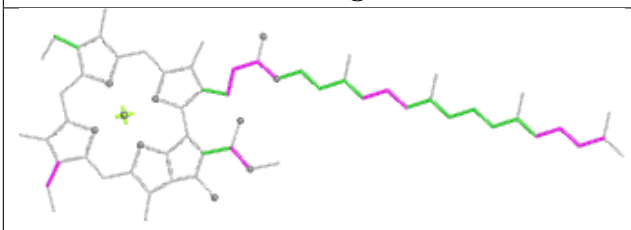
Ligand CLA AA 843



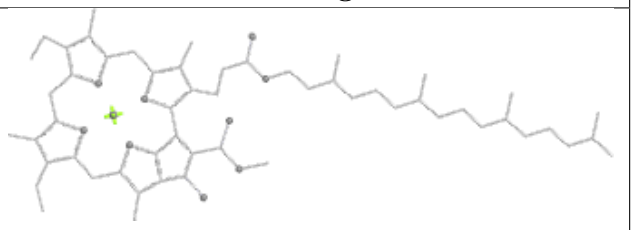
Bond lengths



Bond angles

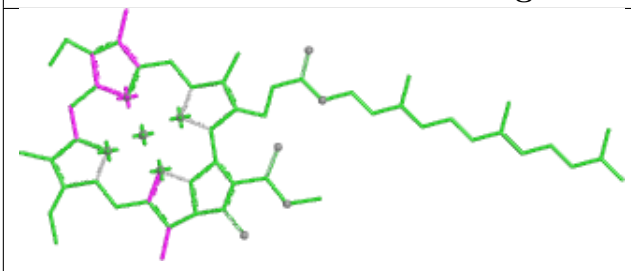


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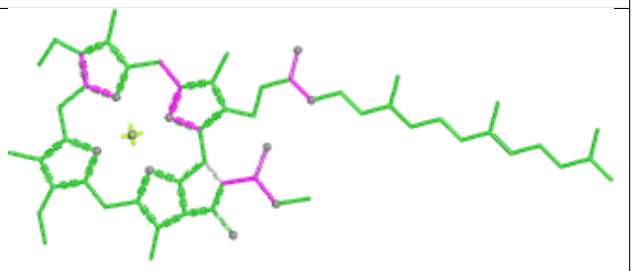


Rings

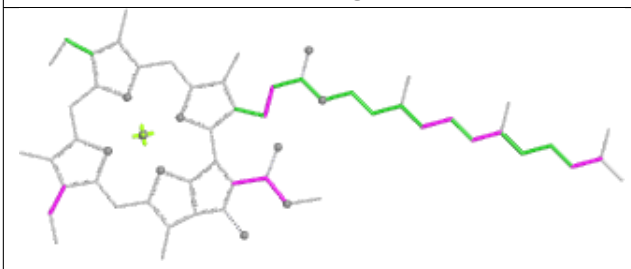
Ligand CLA B1 836



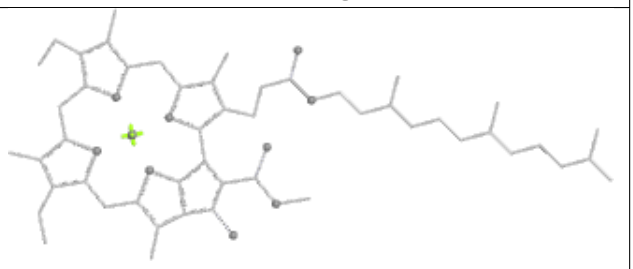
Bond lengths



Bond angles

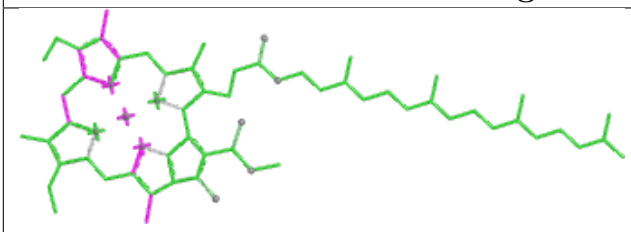


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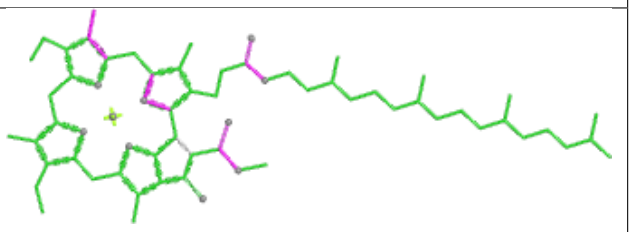


Rings

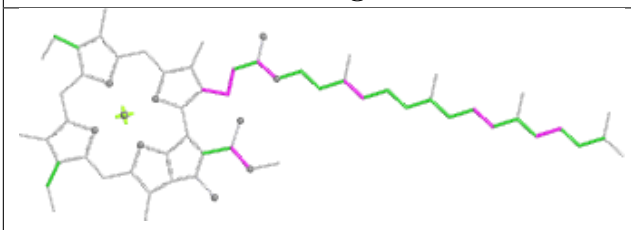
Ligand CLA L1 207



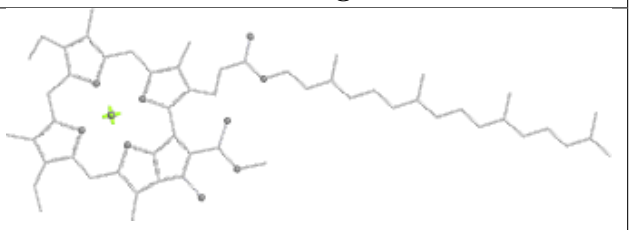
Bond lengths



Bond angles

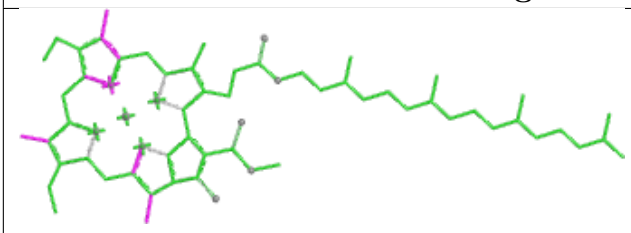


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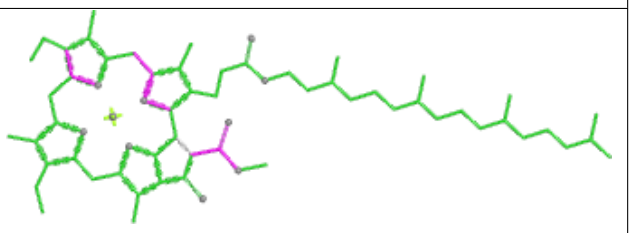


Rings

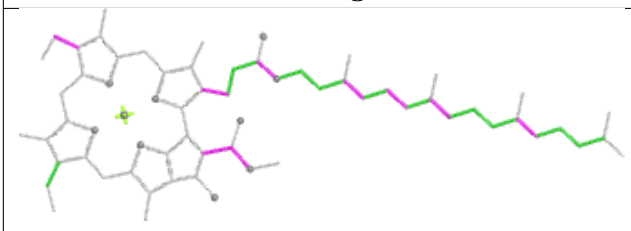
Ligand CLA A2 836



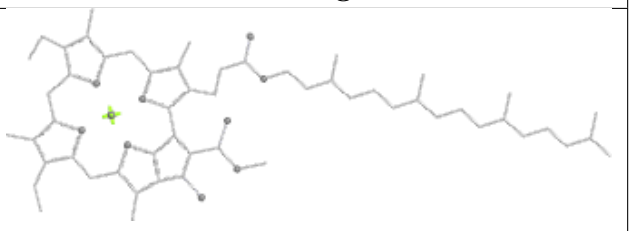
Bond lengths



Bond angles

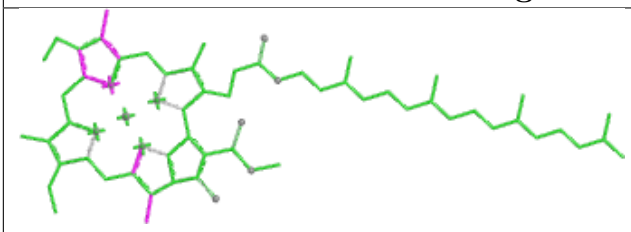


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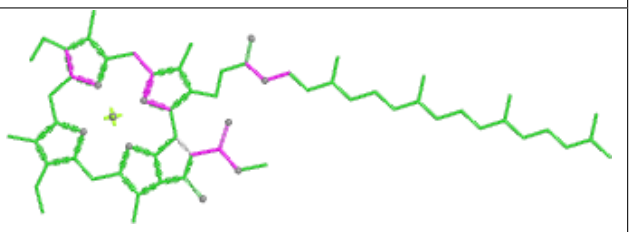


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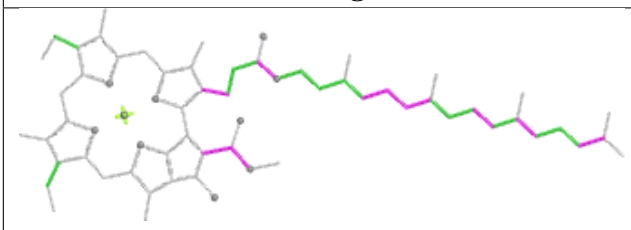
Ligand CLA B2 825



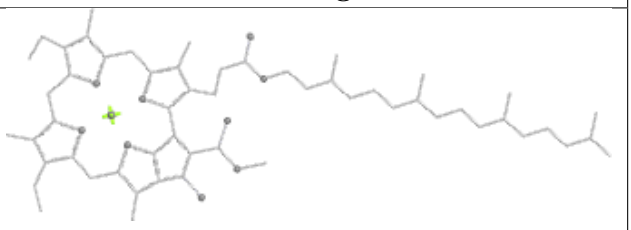
Bond lengths



Bond angles

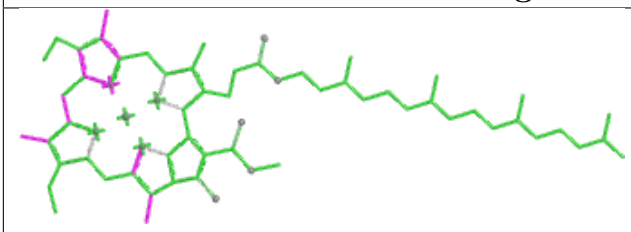


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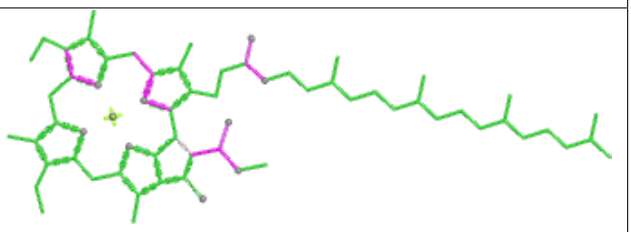


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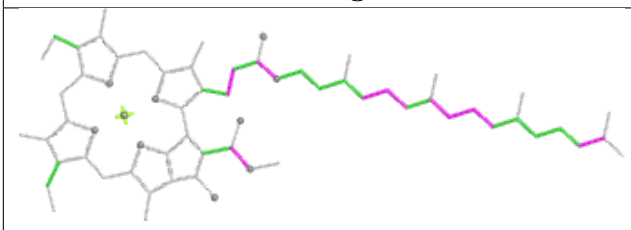
Ligand CLA A1 801



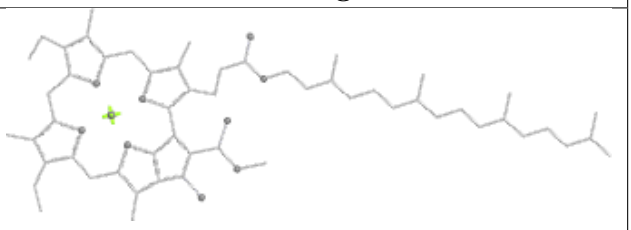
Bond lengths



Bond angles

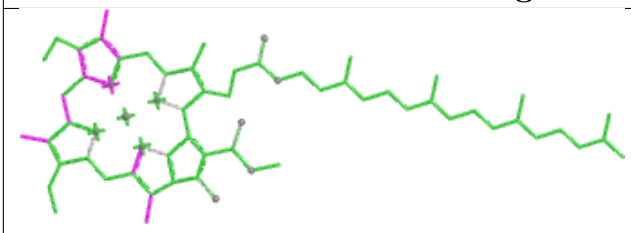


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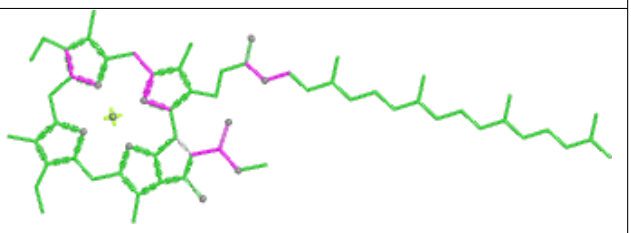


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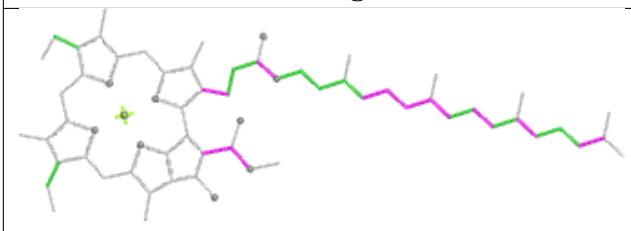
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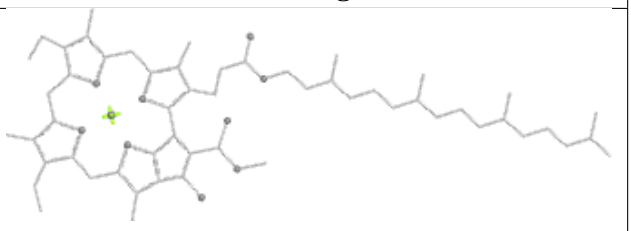
Bond lengths



Bond angles

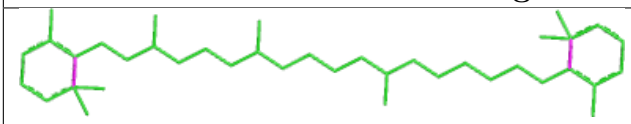


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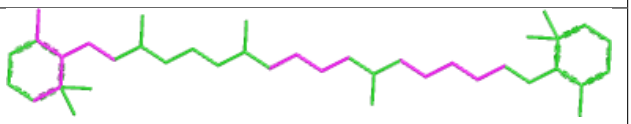


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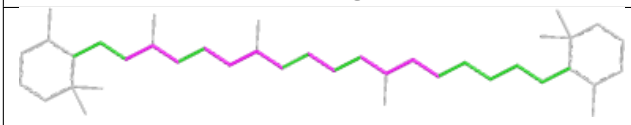
Ligand BCR A2 847



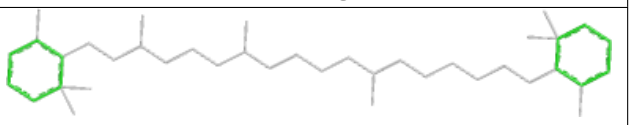
Bond lengths



Bond angles

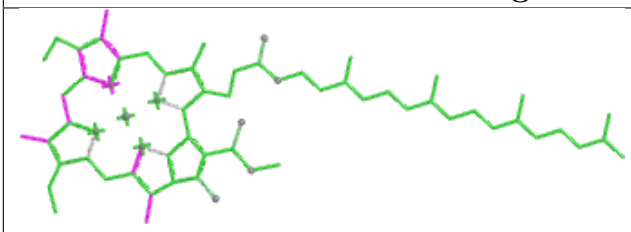


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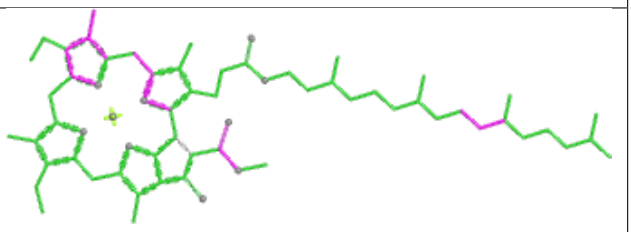


Rings

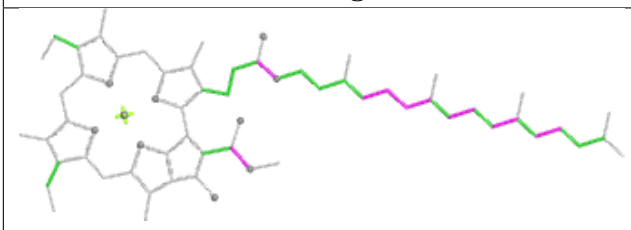
Ligand CLA BB 803



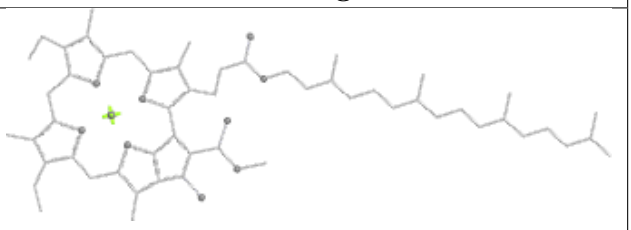
Bond lengths



Bond angles

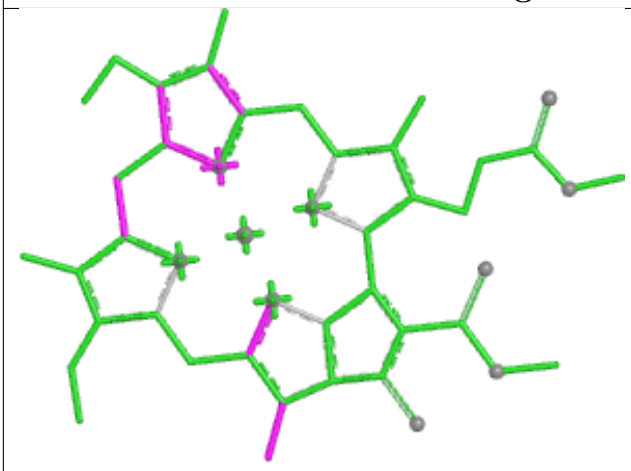


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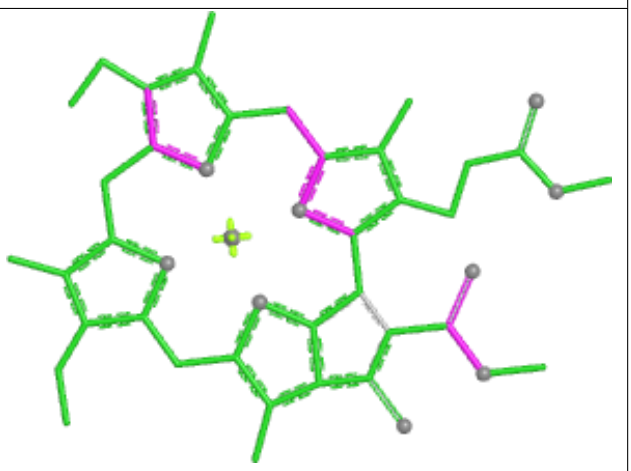


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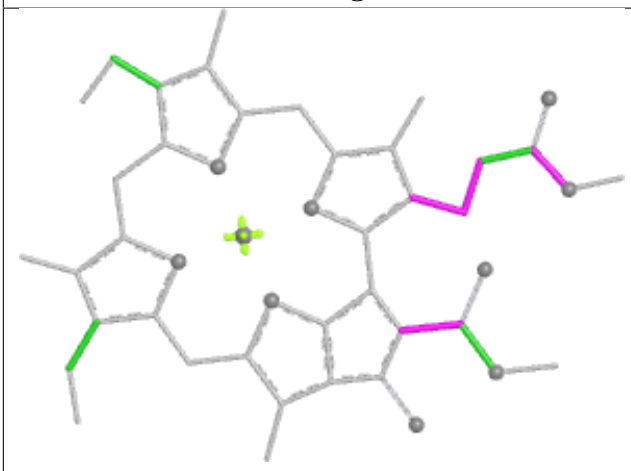
Ligand CLA A2 802



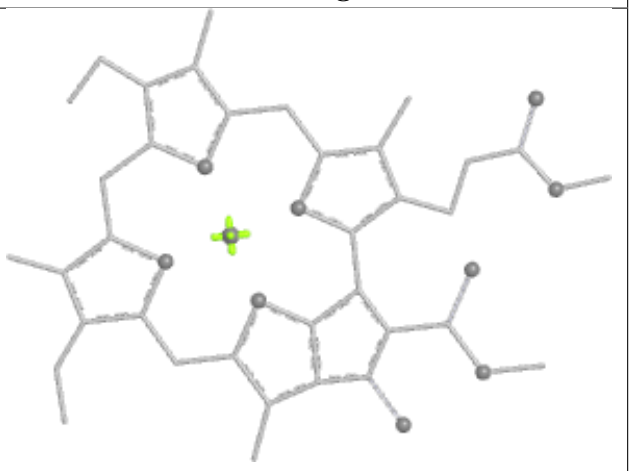
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Bond angles

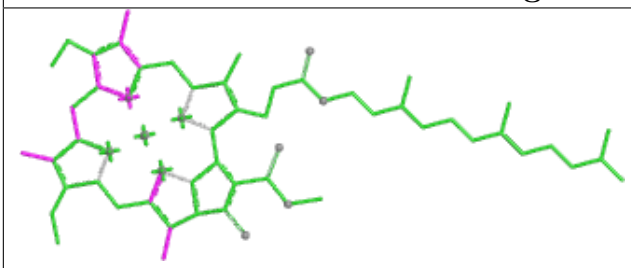


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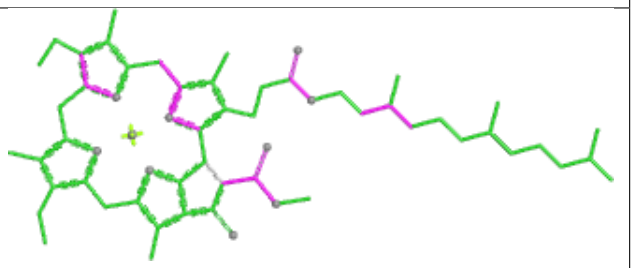


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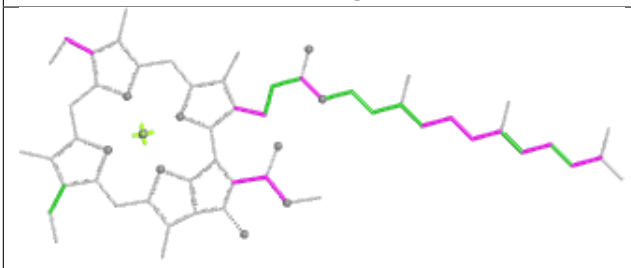
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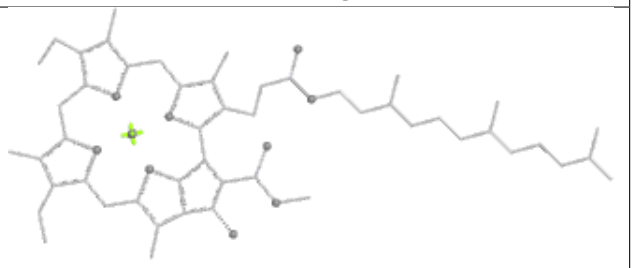
Bond lengths



Bond angles

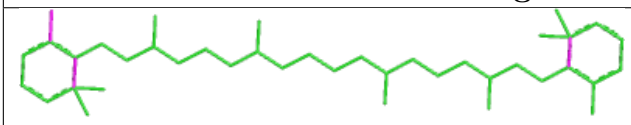


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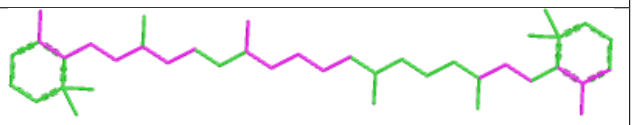


Rings

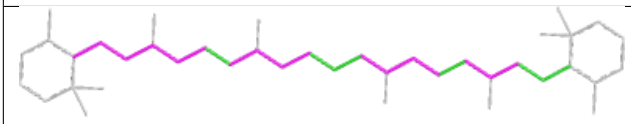
Ligand BCR B2 839



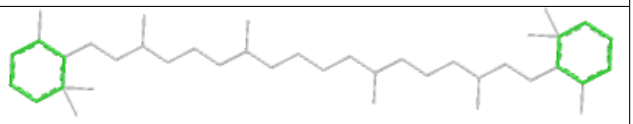
Bond lengths



Bond angles

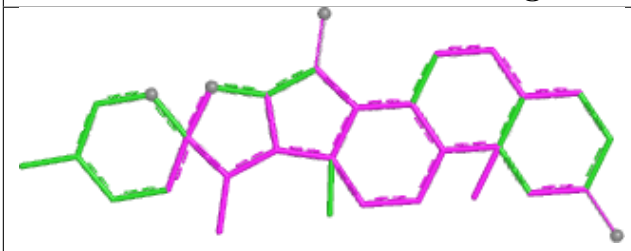


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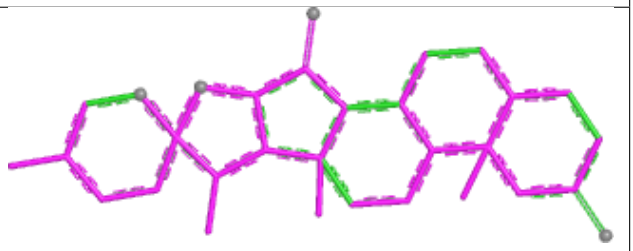


Rings

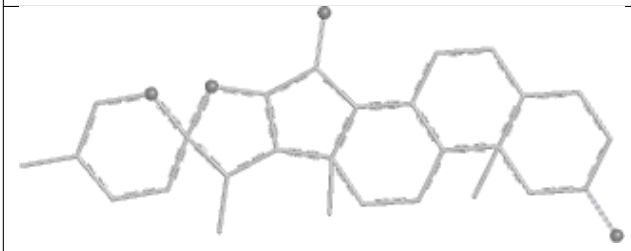
Ligand AJP I2 104



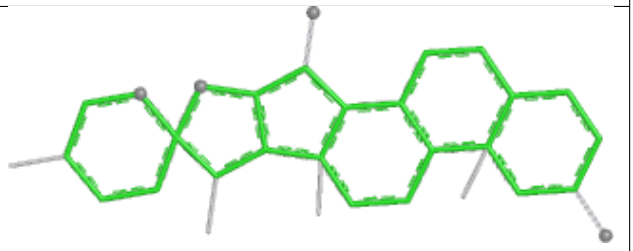
Bond lengths



Bond angles

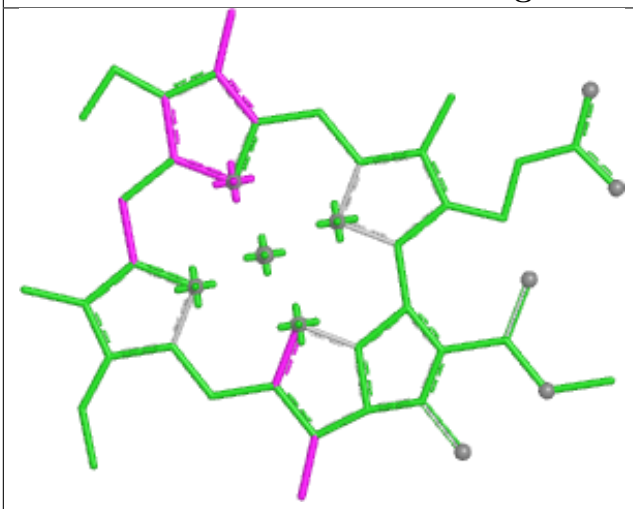


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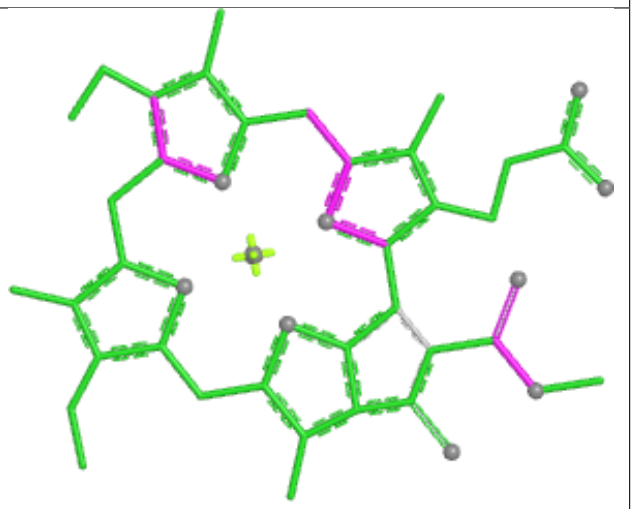


Rings

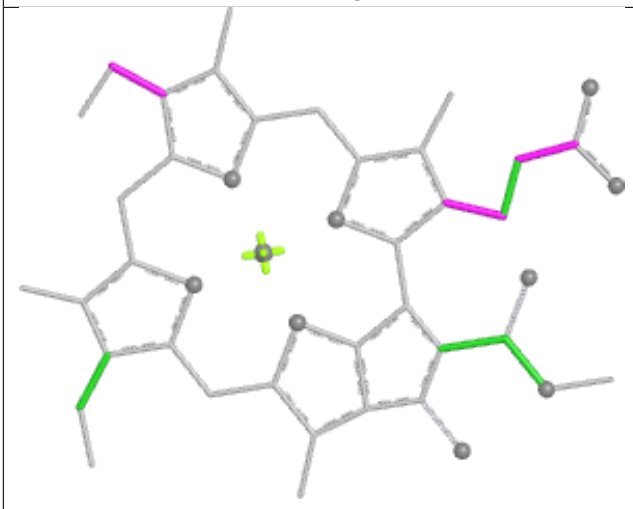
Ligand CLA A2 818



Bond lengths



Bond angles

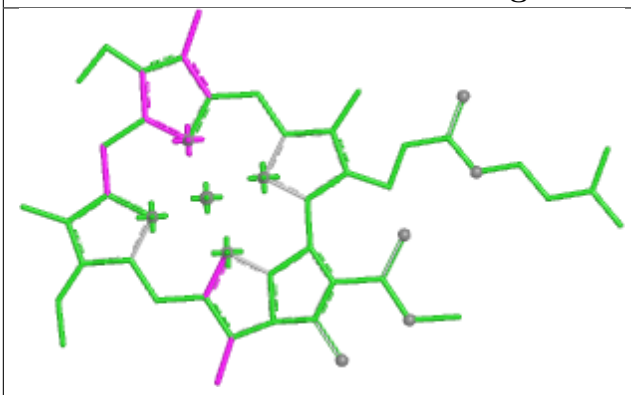


Torsions

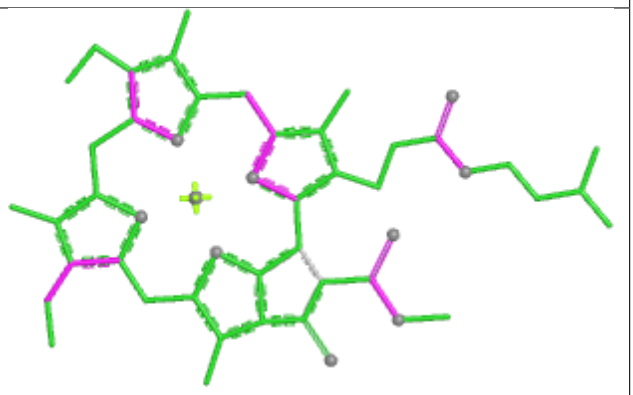


Rings

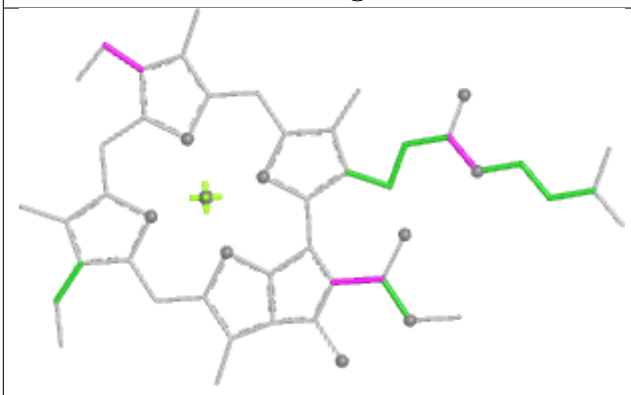
Ligand CLA AA 809



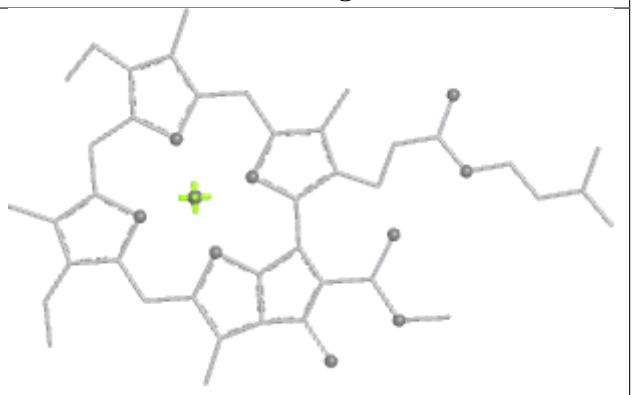
Bond lengths



Bond angles

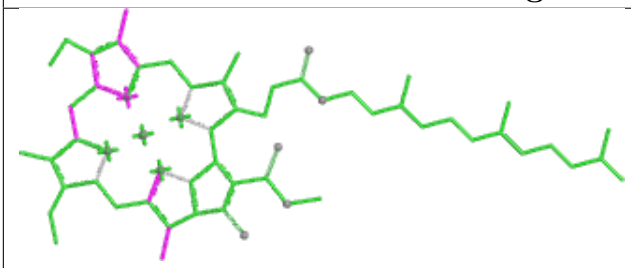


Torsions

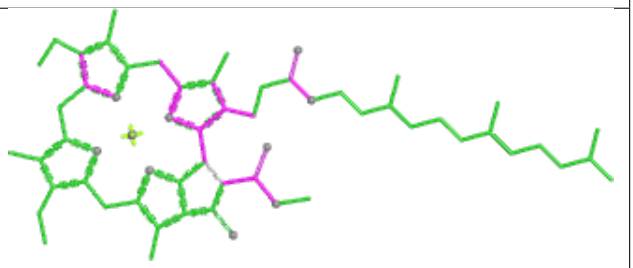


Rings

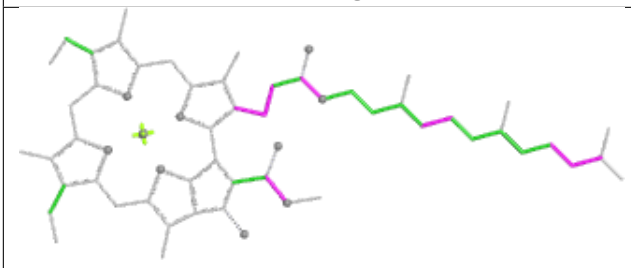
Ligand CLA F 301



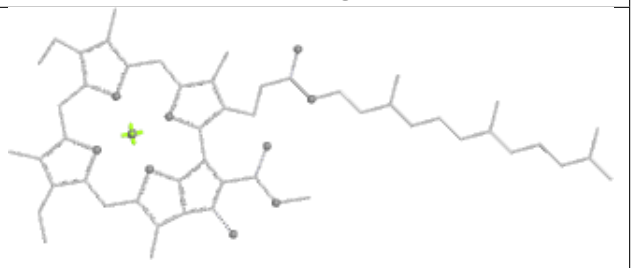
Bond lengths



Bond angles

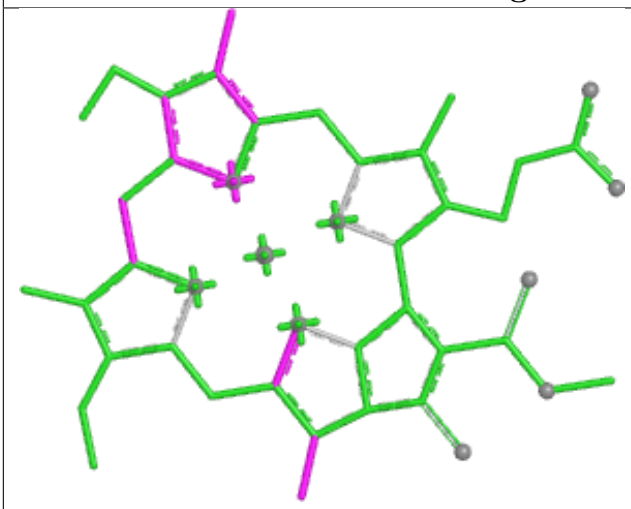


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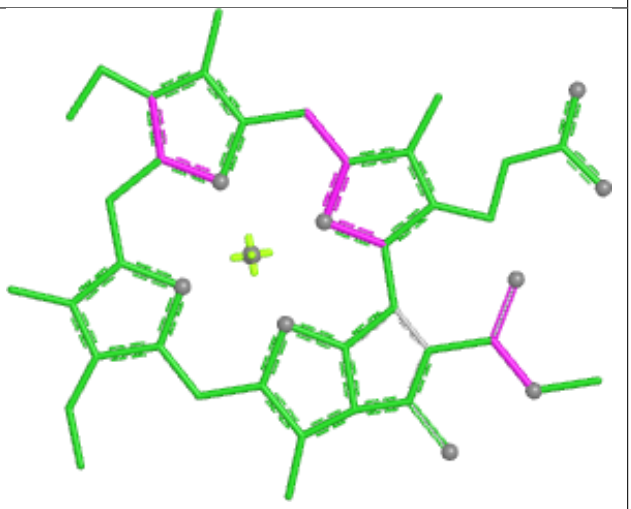


Rings

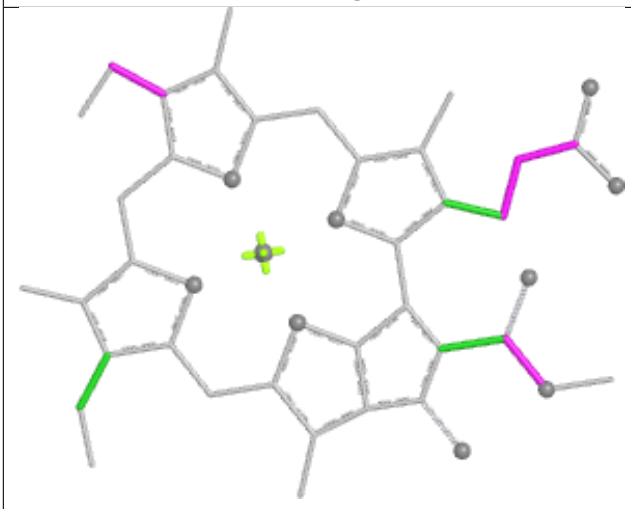
Ligand CLA XX 101



Bond lengths



Bond angles

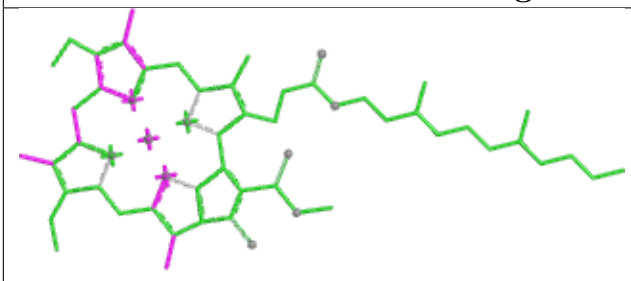


Torsions

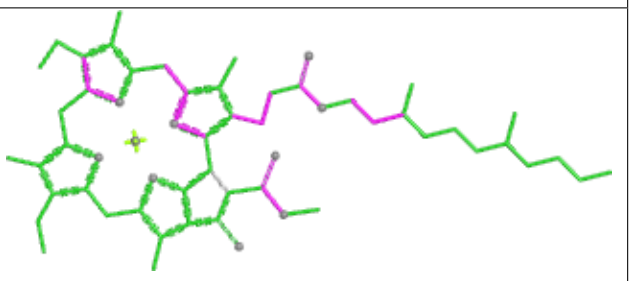


Rings

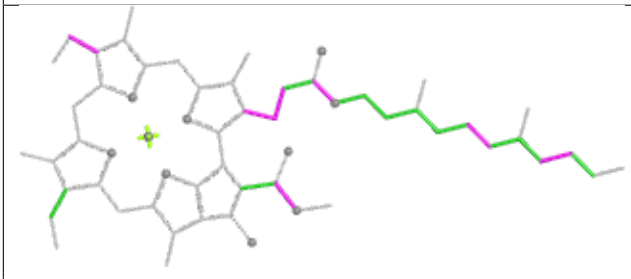
Ligand CLA A1 819



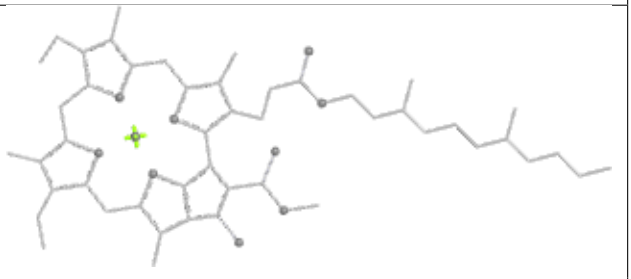
Bond lengths



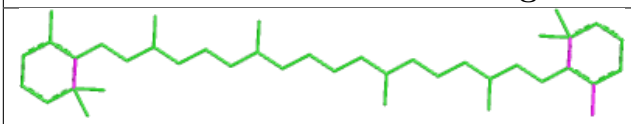
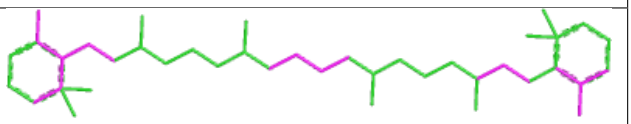
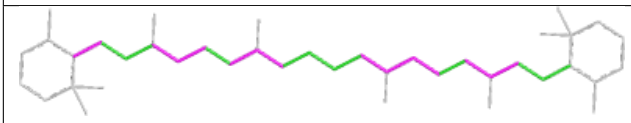
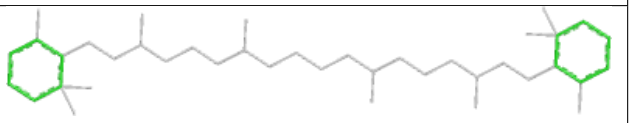
Bond angles

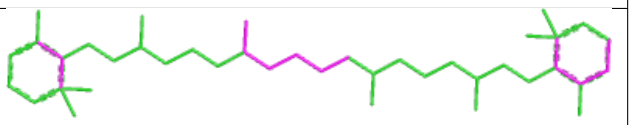
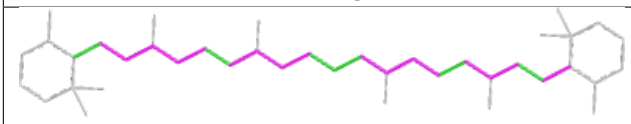
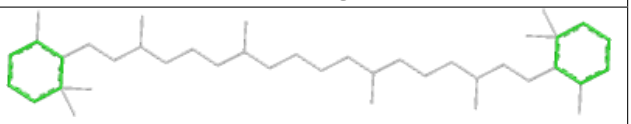


Torsions

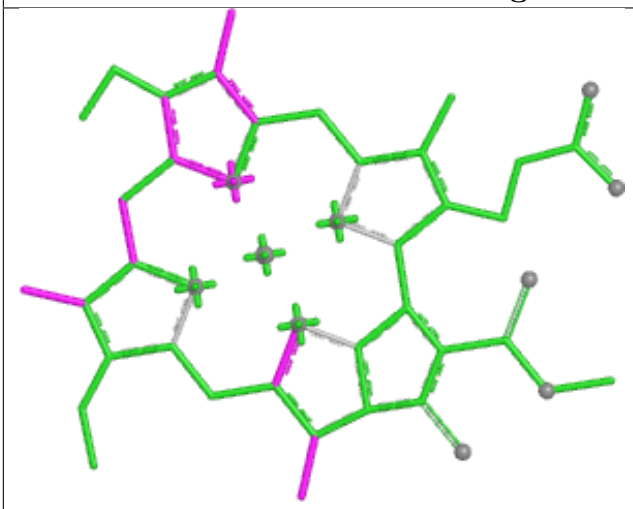


Rings

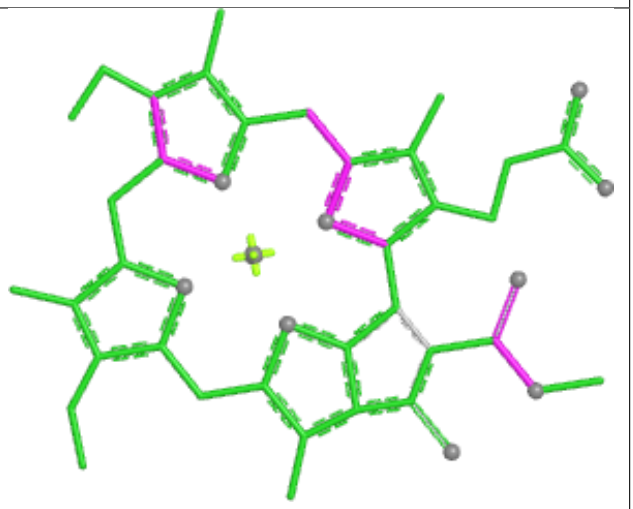
Ligand BCR I1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

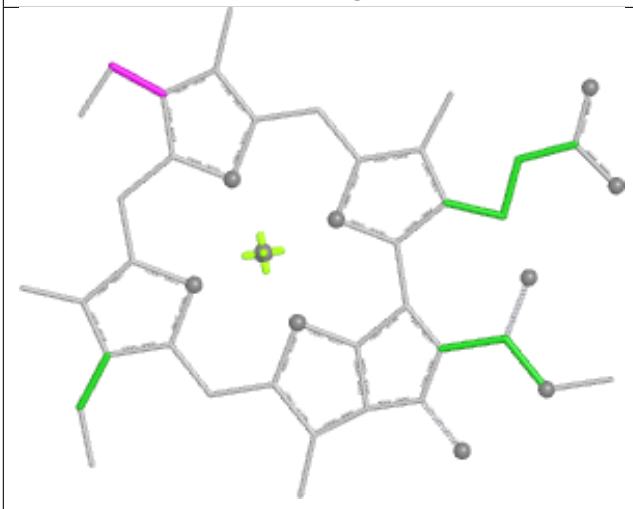
Ligand CLA AA 837



Bond lengths



Bond angles

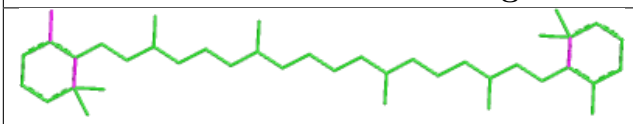


Torsions

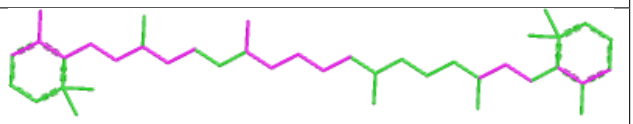


Rings

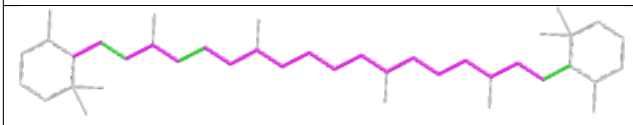
Ligand BCR MM 101



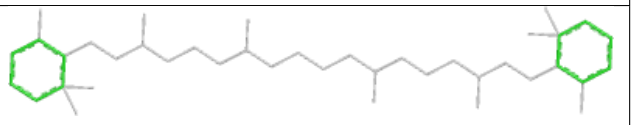
Bond lengths



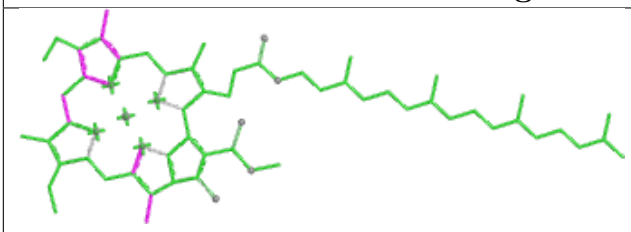
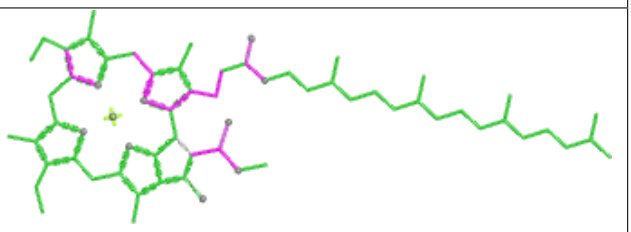
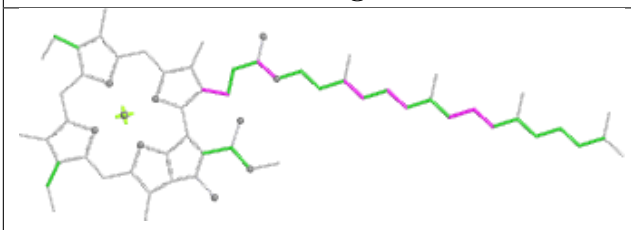
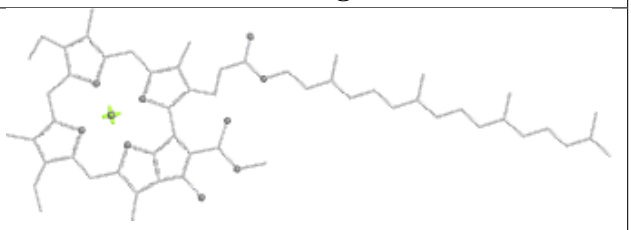
Bond angles

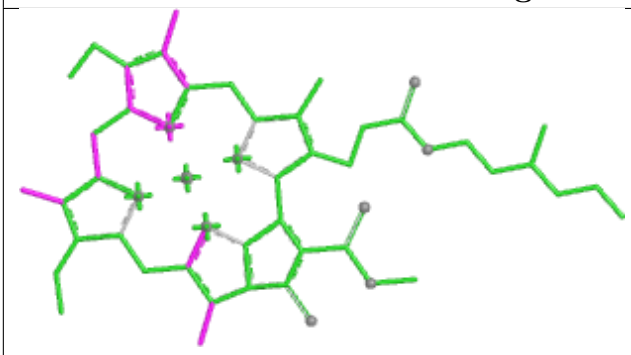
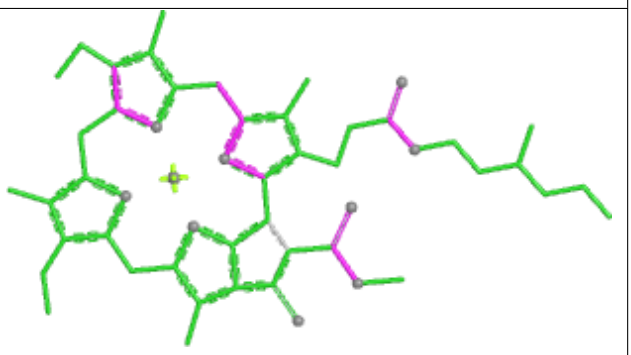
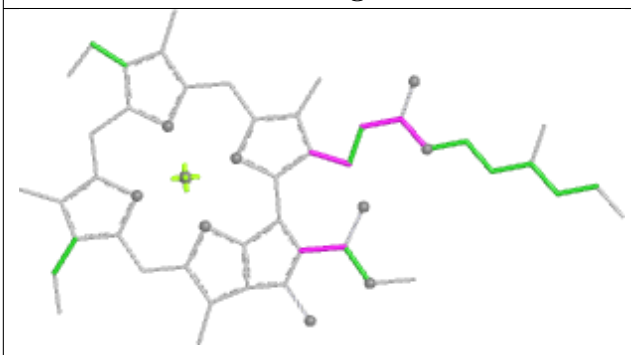
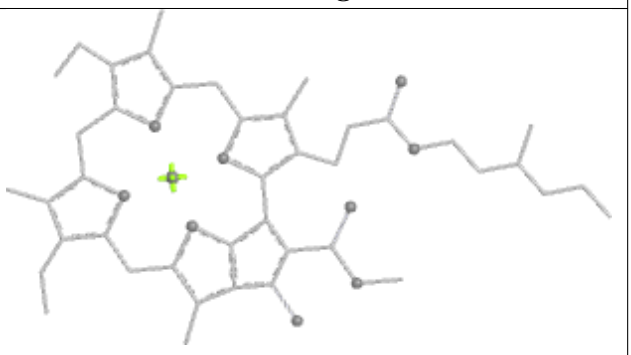


Torsions

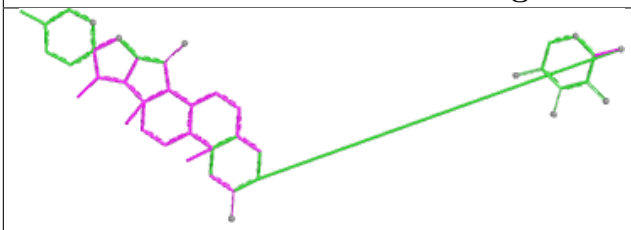


Rings

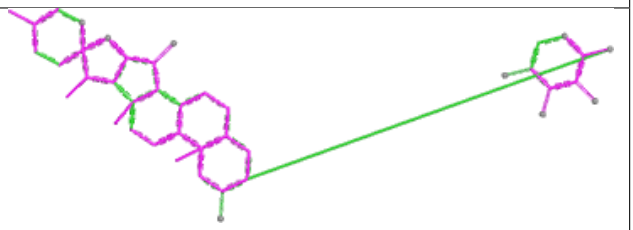
Ligand CLA A1 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A1 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

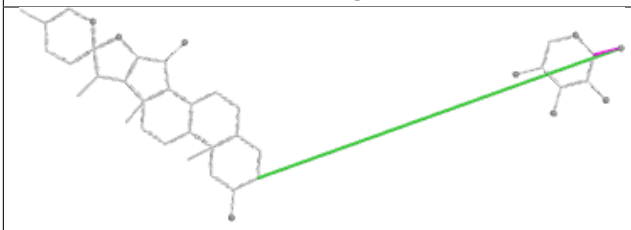
Ligand AJP KK 104



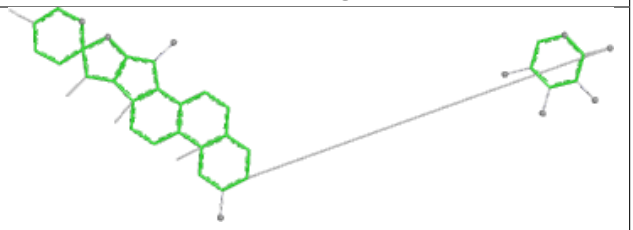
Bond lengths



Bond angles

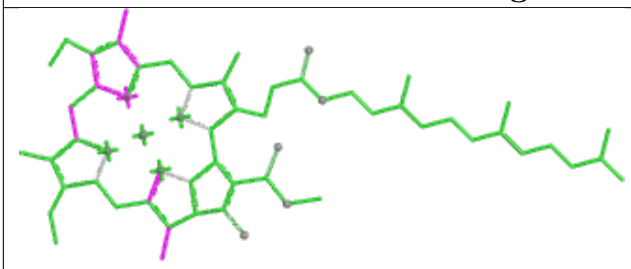


Torsions

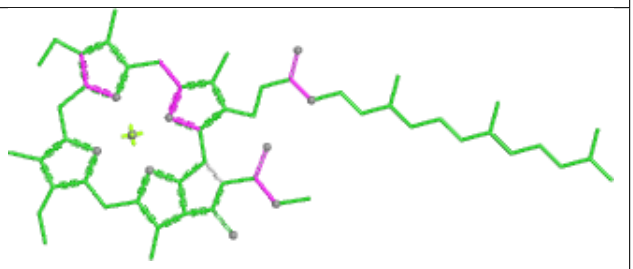


Rings

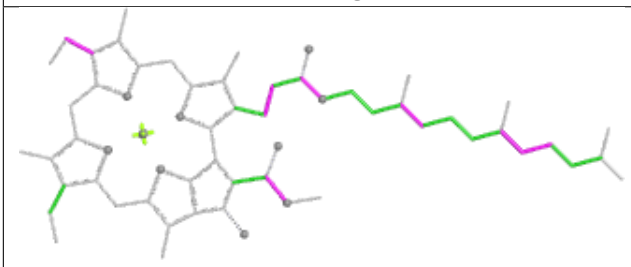
Ligand CLA AA 819



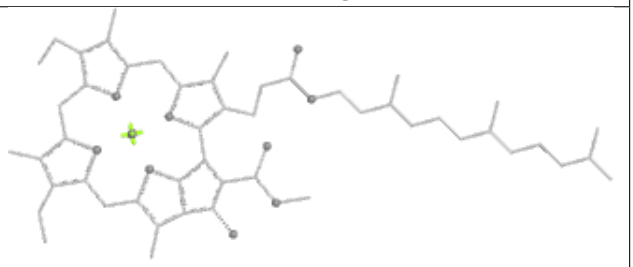
Bond lengths



Bond angles

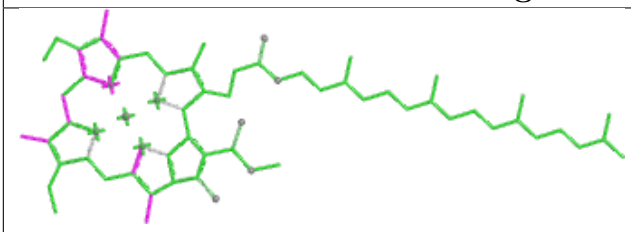


Torsions

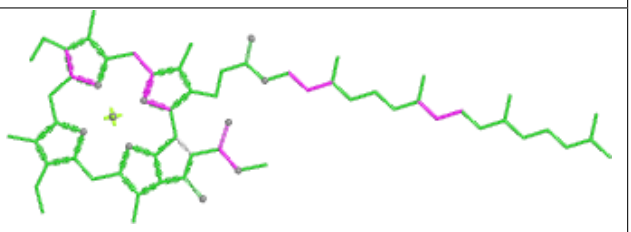


Rings

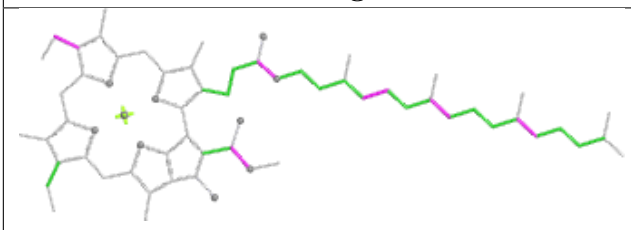
Ligand CLA A2 835



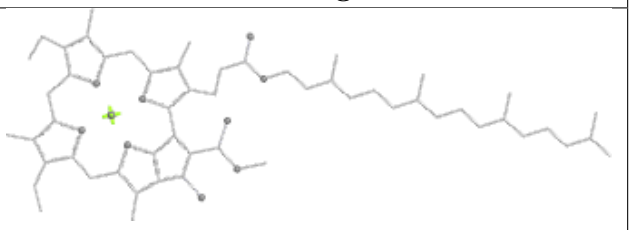
Bond lengths



Bond angles

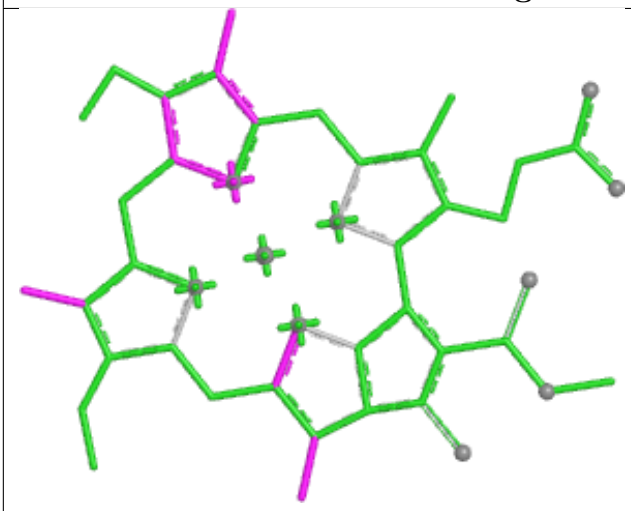


Torsions

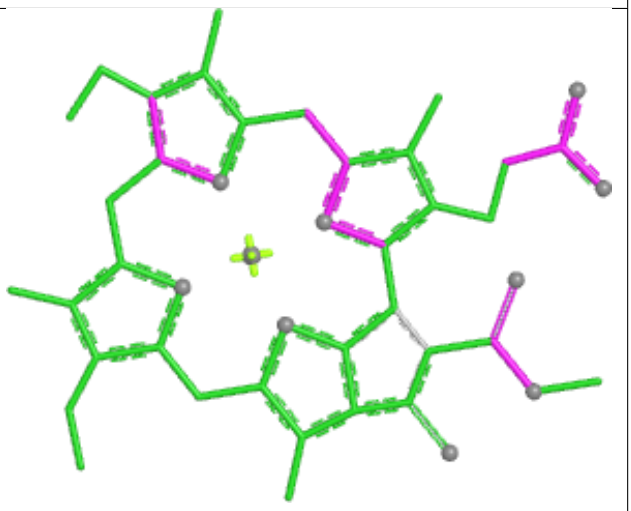


Rings

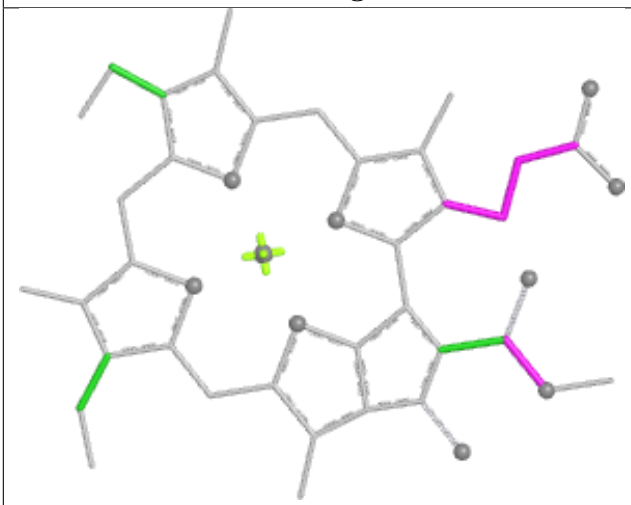
Ligand CLA A2 826



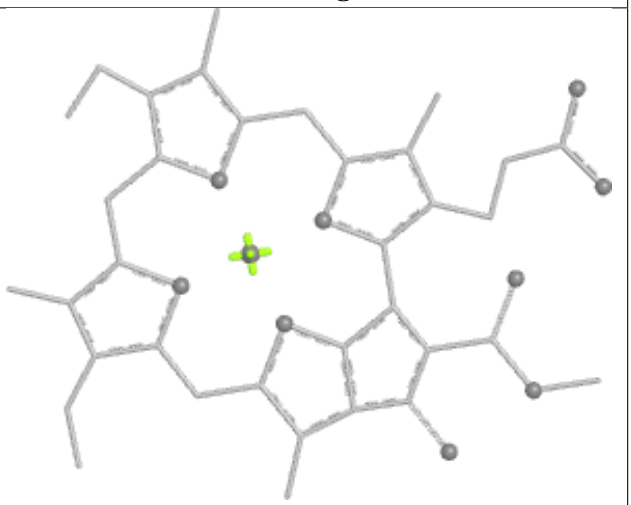
Bond lengths



Bond angles

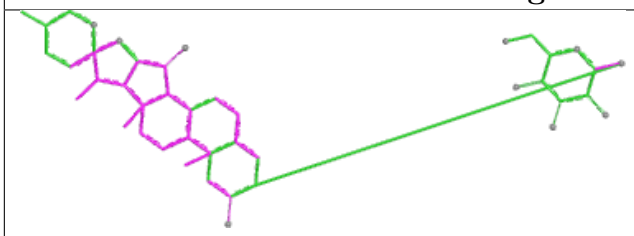


Torsions

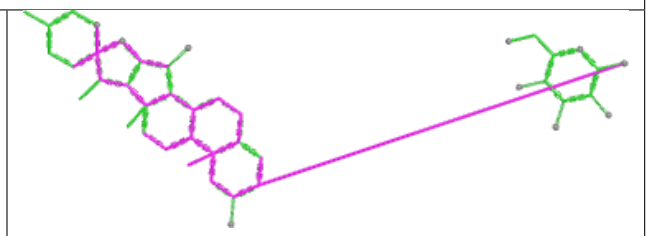


Rings

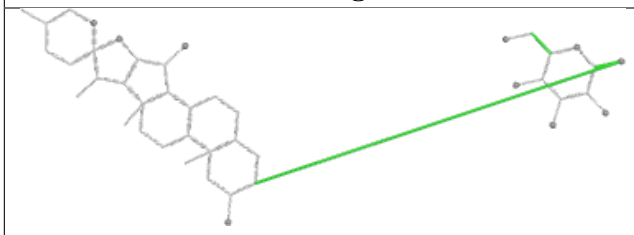
Ligand AJP B 857



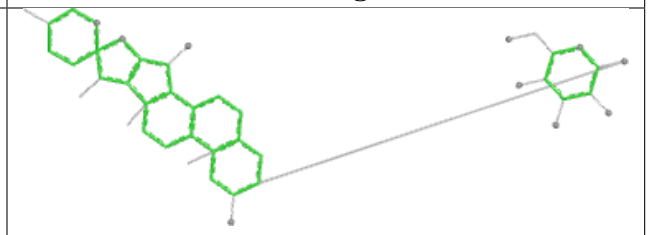
Bond lengths



Bond angles

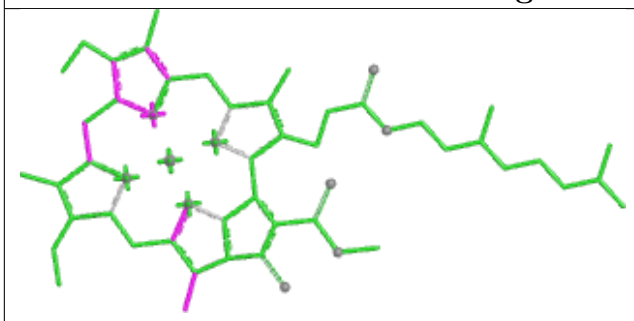


Torsions

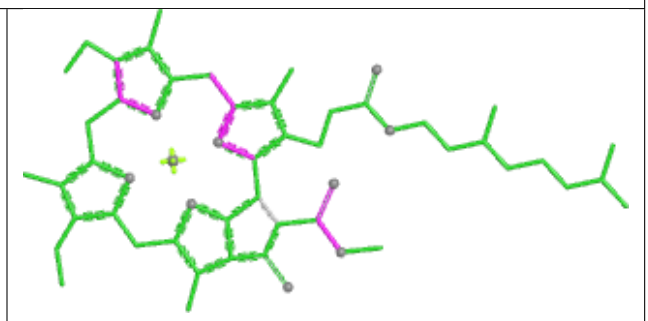


Rings

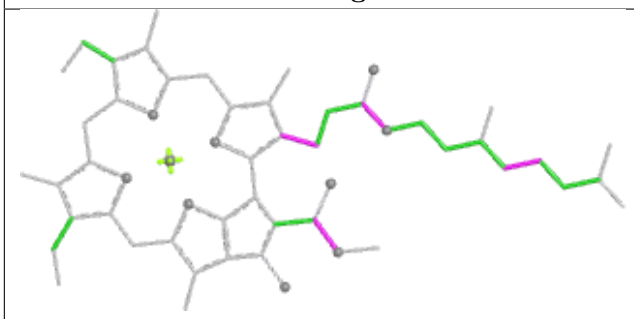
Ligand CLA A2 815



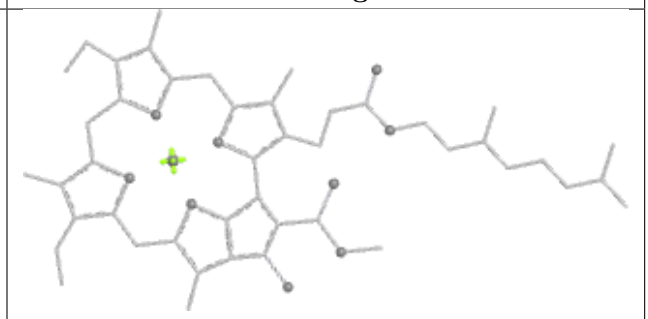
Bond lengths



Bond angles

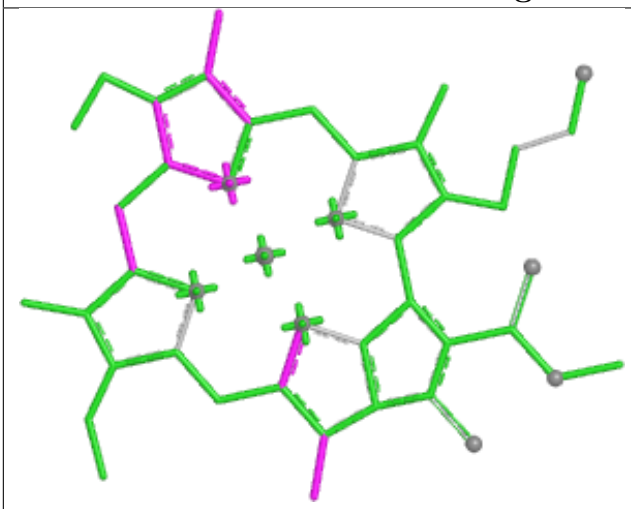


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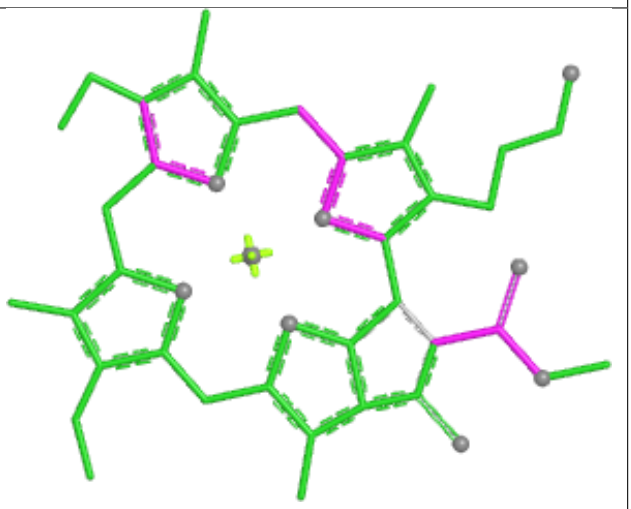


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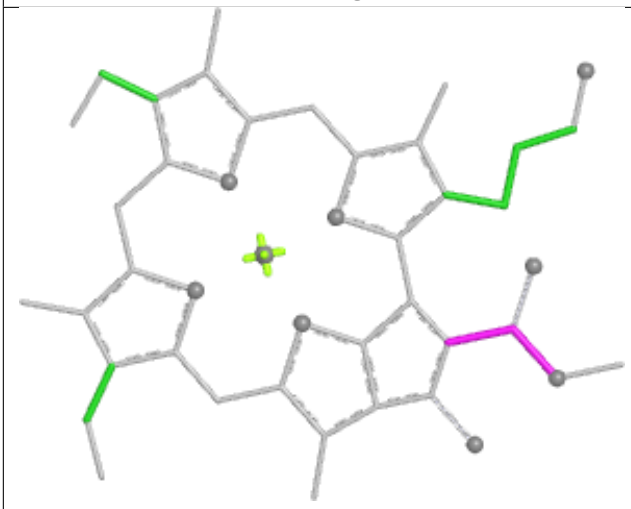
Ligand CLA A1 837



Bond lengths



Bond angles

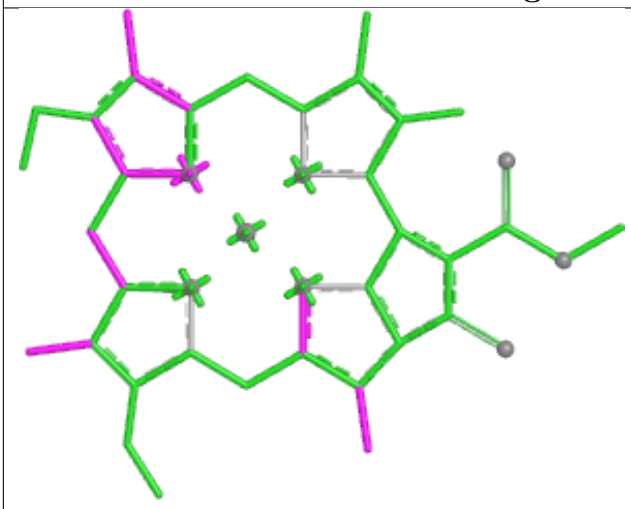


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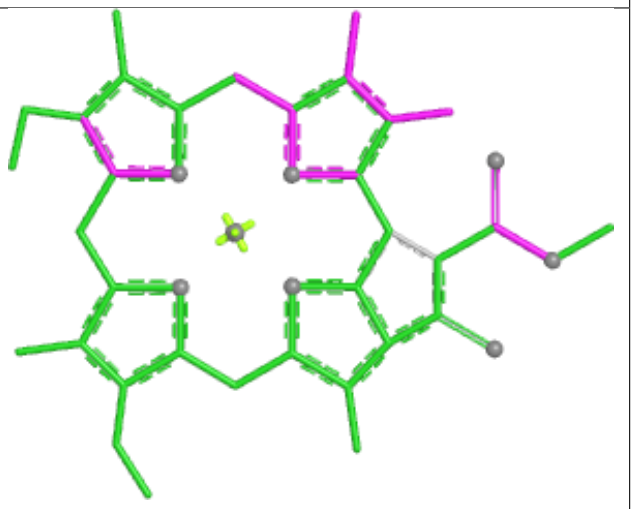


Rings

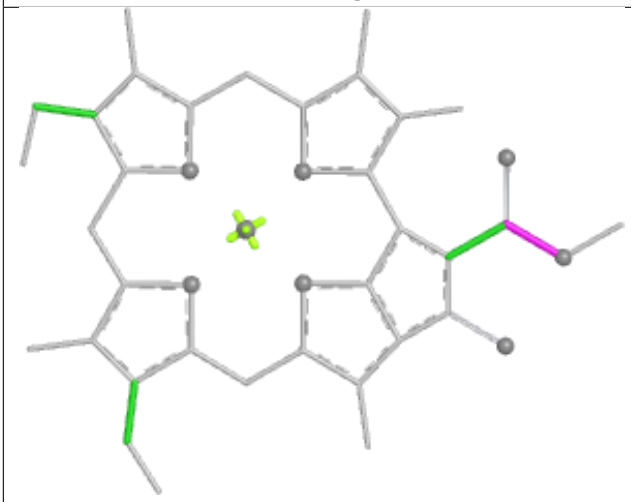
Ligand CLA A 834



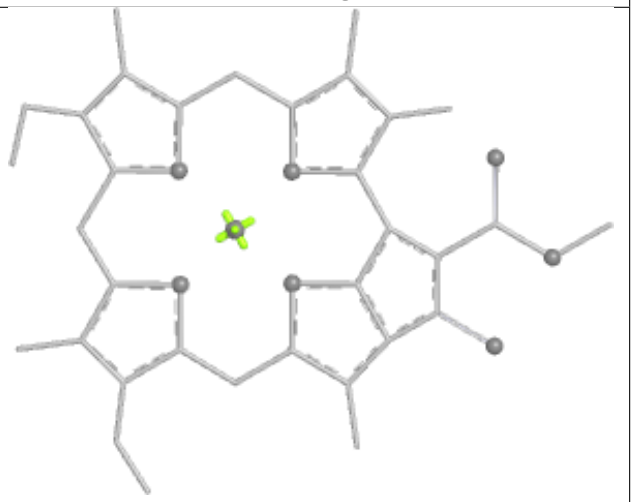
Bond lengths



Bond angles



Torsions

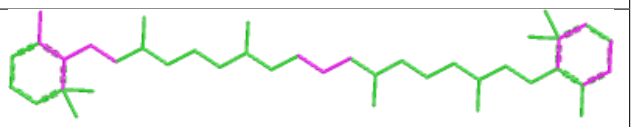


Rings

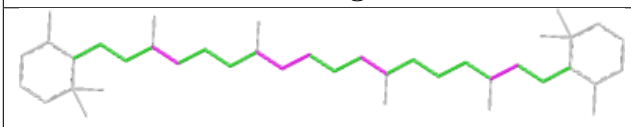
Ligand BCR BB 839



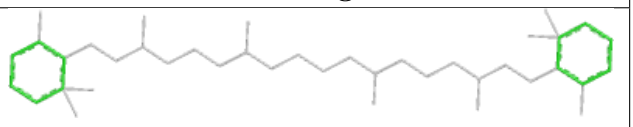
Bond lengths



Bond angles

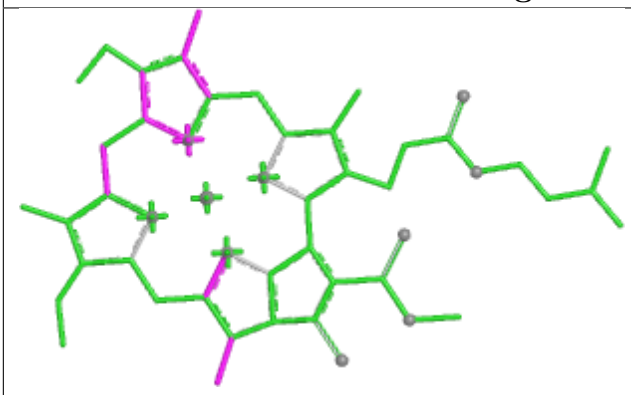


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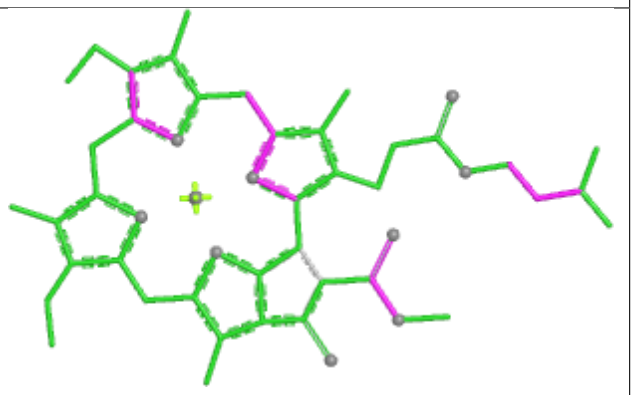


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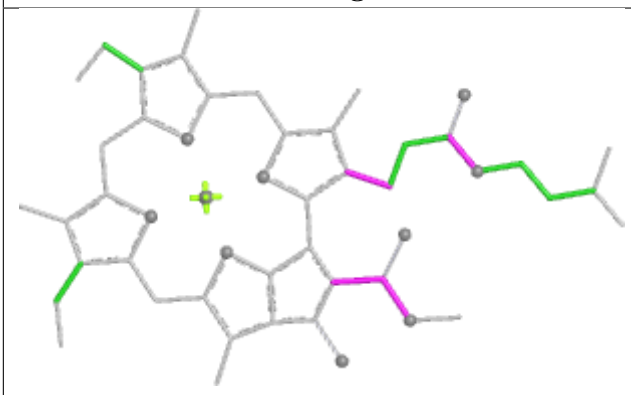
Ligand CLA A1 815



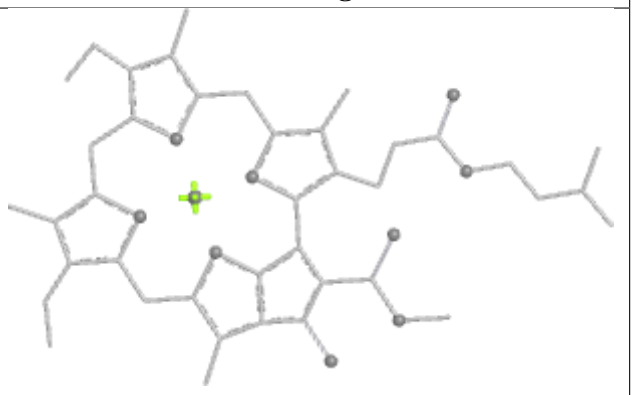
Bond lengths



Bond angles

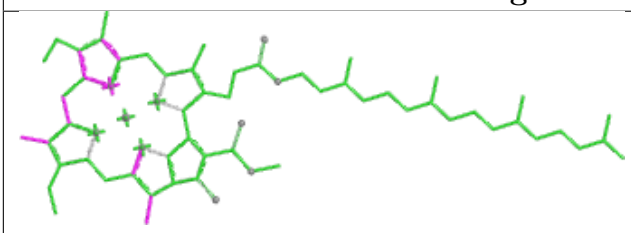


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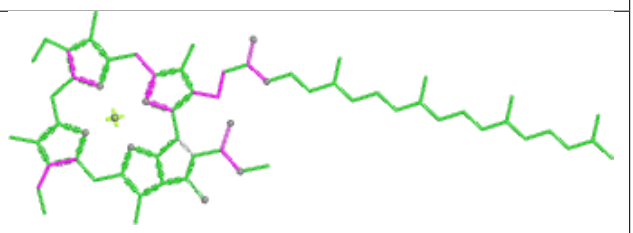


Rings

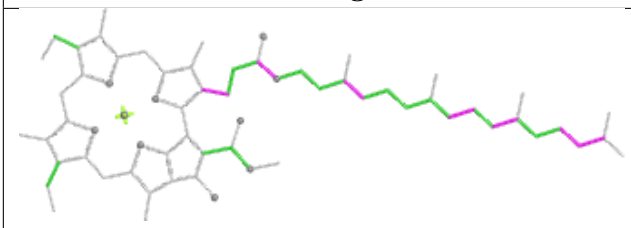
Ligand CLA AA 821



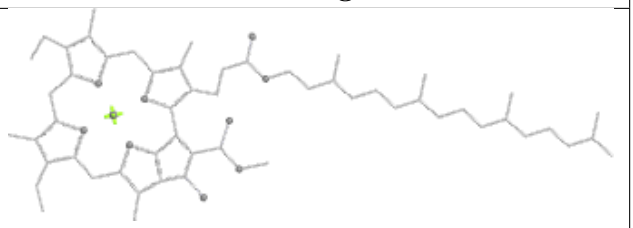
Bond lengths



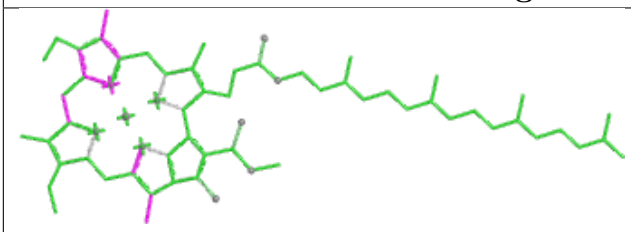
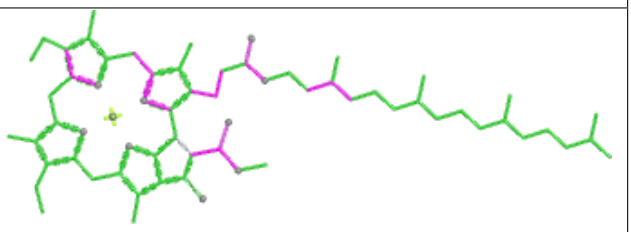
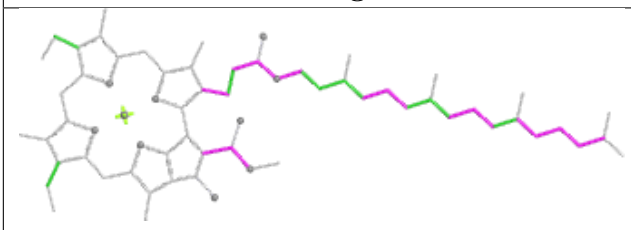
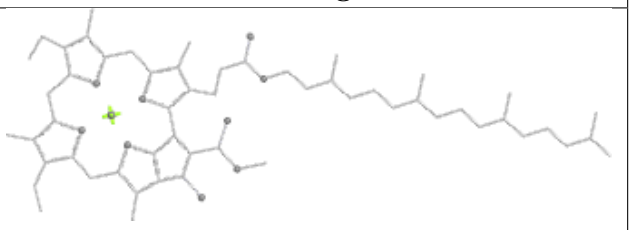
Bond angles

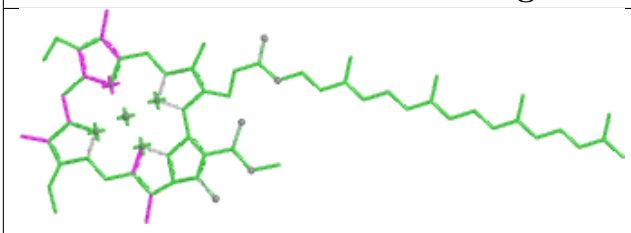
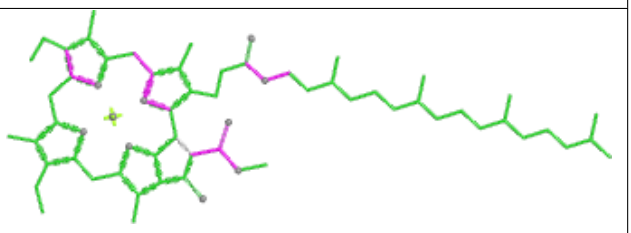
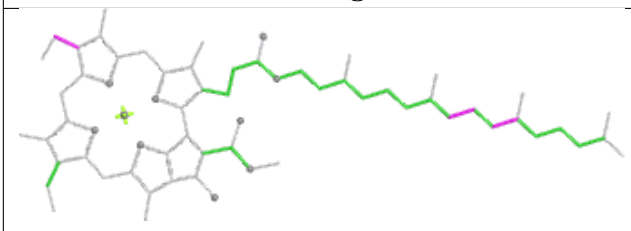
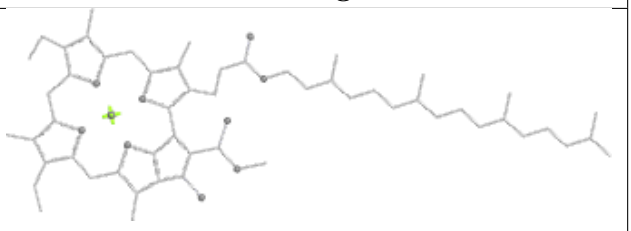


Torsions

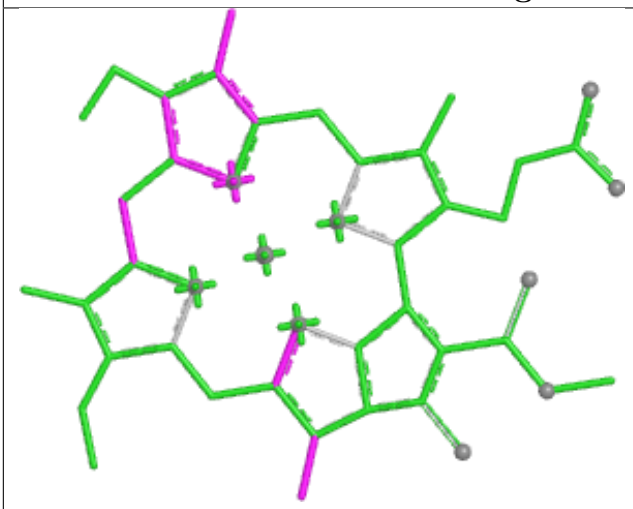


Rings

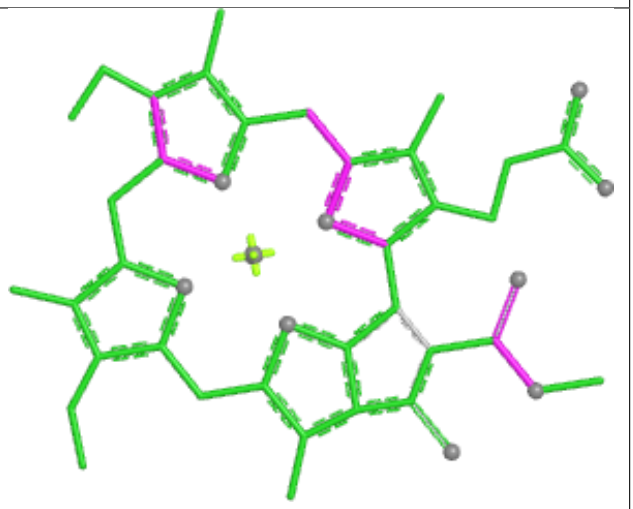
Ligand CLA B1 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L1 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

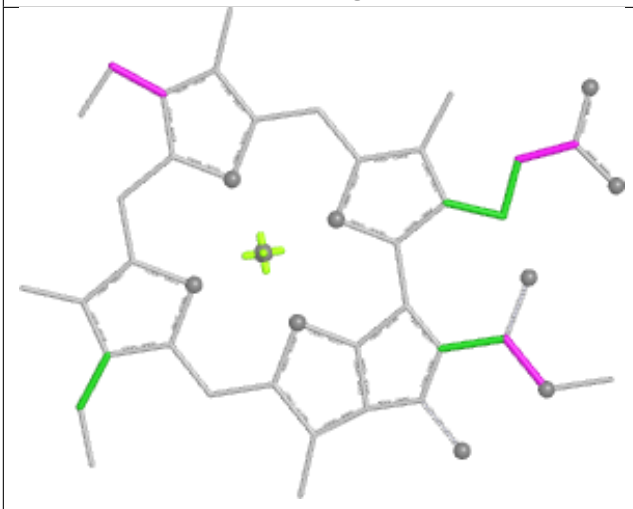
Ligand CLA A2 837



Bond lengths



Bond angles

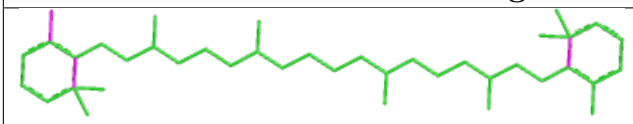


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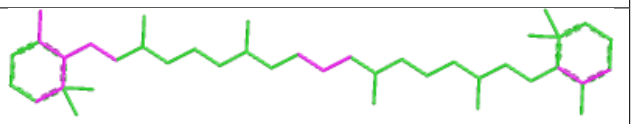


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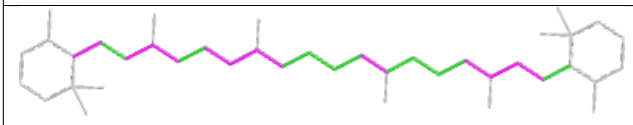
Ligand BCR AA 851



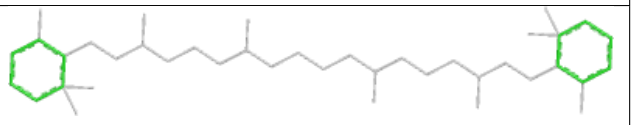
Bond lengths



Bond angles

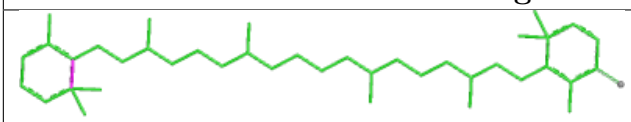


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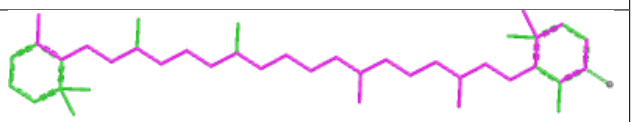


Rings

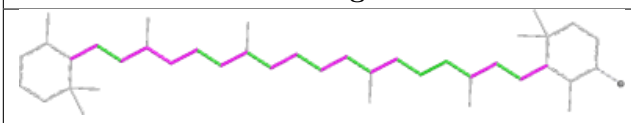
Ligand ECH B2 841



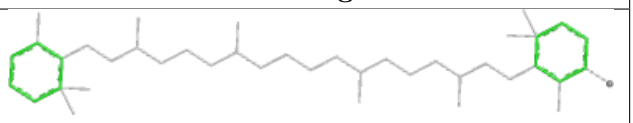
Bond lengths



Bond angles

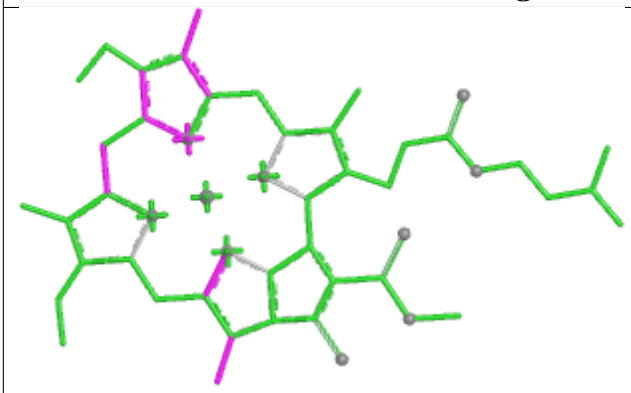


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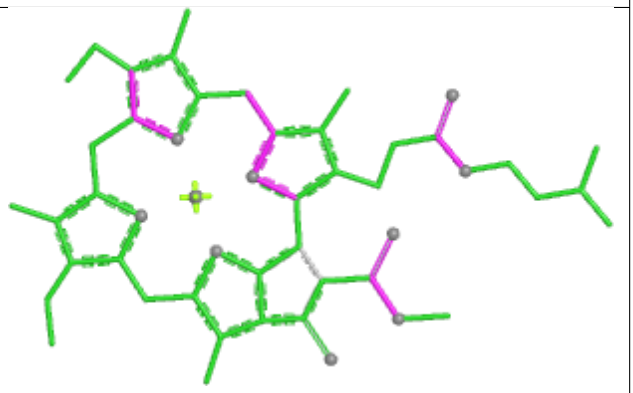


Rings

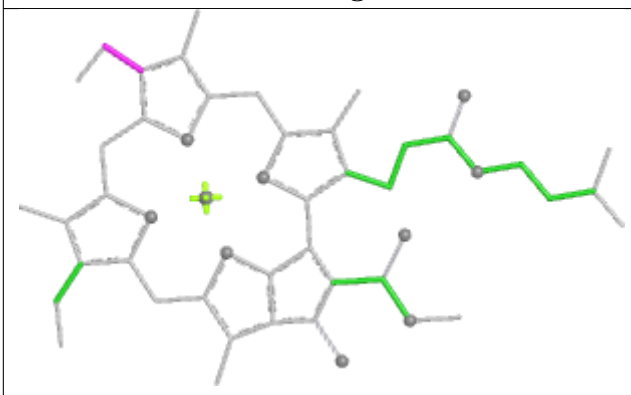
Ligand CLA A1 808



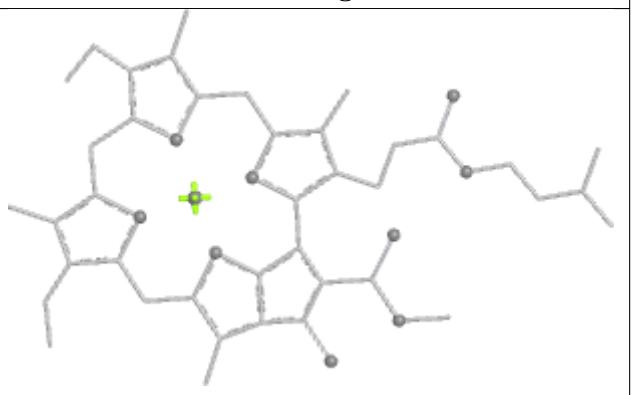
Bond lengths



Bond angles

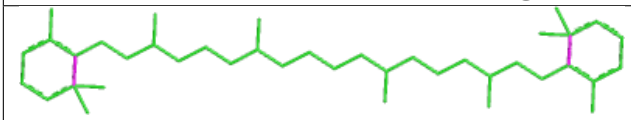


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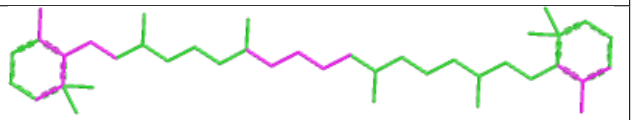


Rings

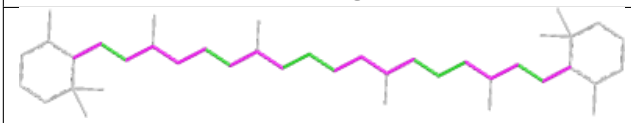
Ligand BCR J1 102



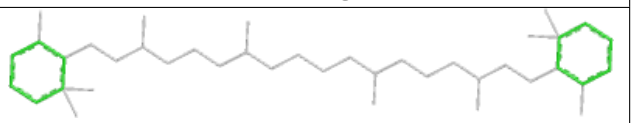
Bond lengths



Bond angles

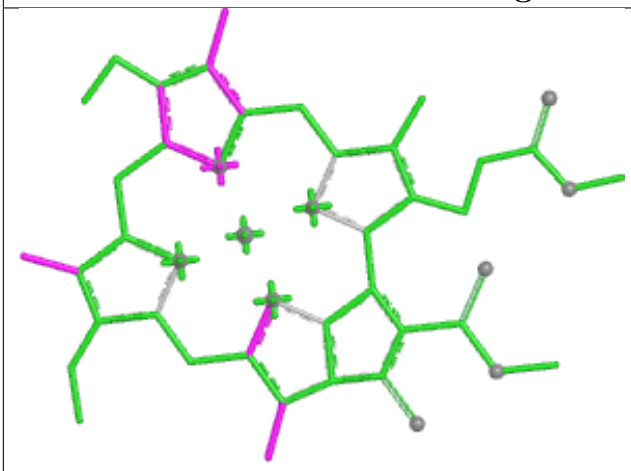


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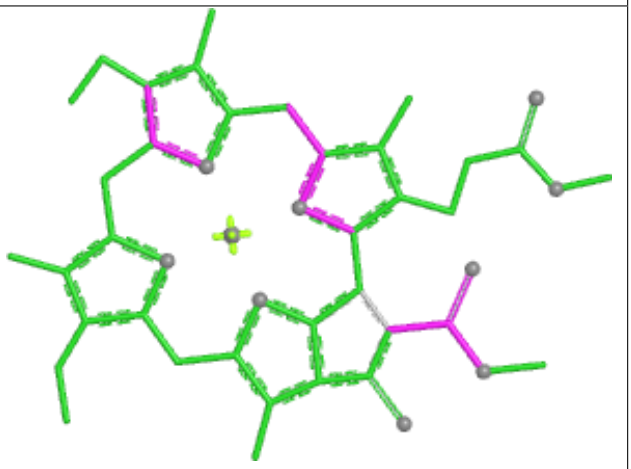


Rings

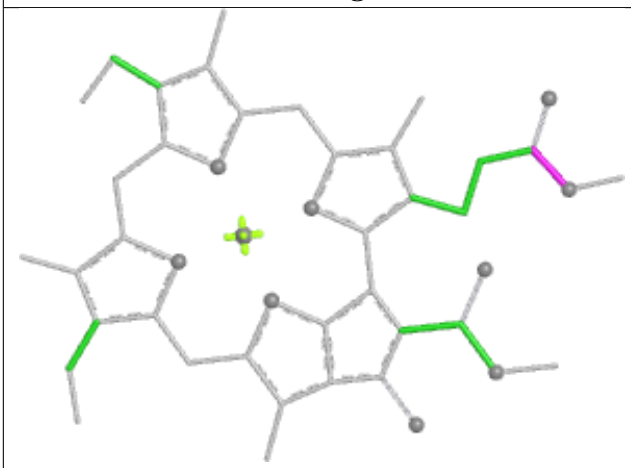
Ligand CLA A1 840



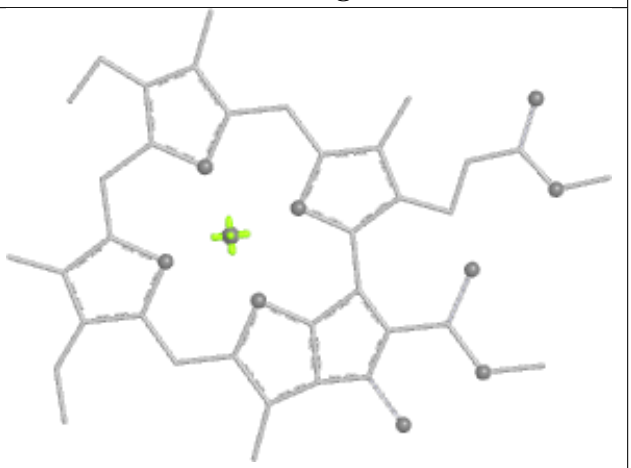
Bond lengths



Bond angles

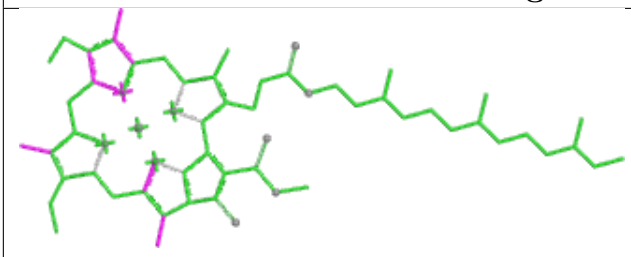


Torsions

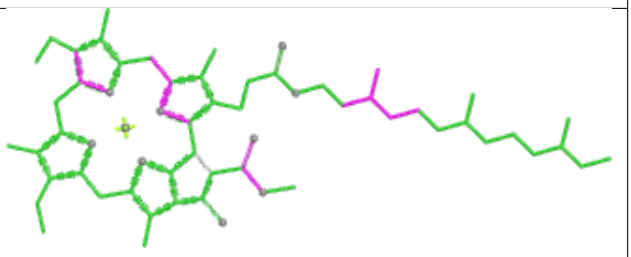


Rings

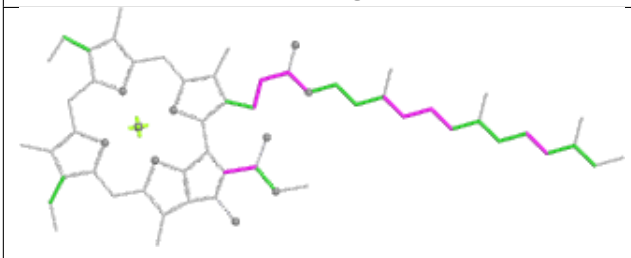
Ligand CLA L 202



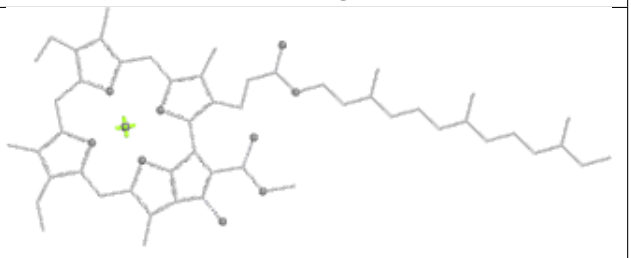
Bond lengths



Bond angles

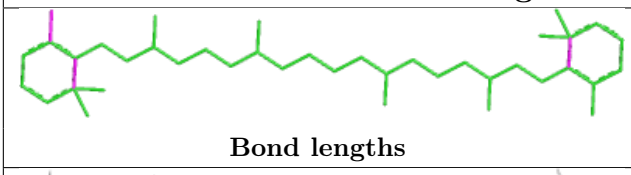


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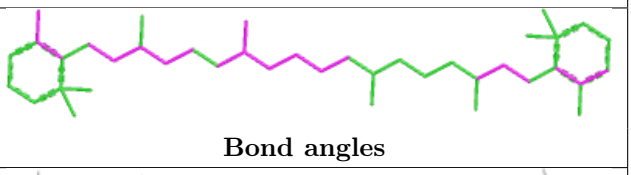


Rings

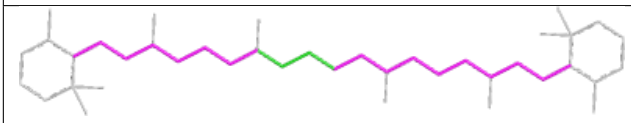
Ligand BCR F1 306



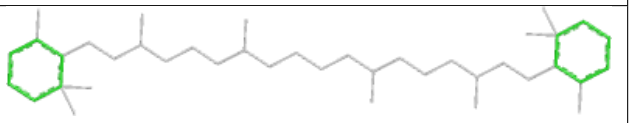
Bond lengths



Bond angles

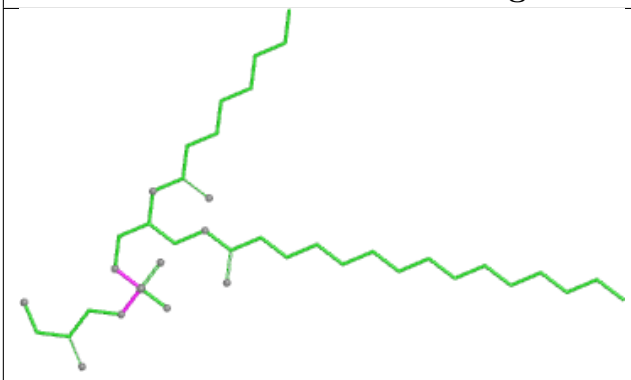


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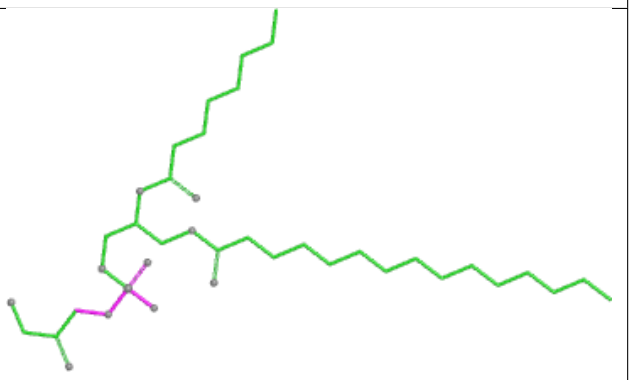


Rings

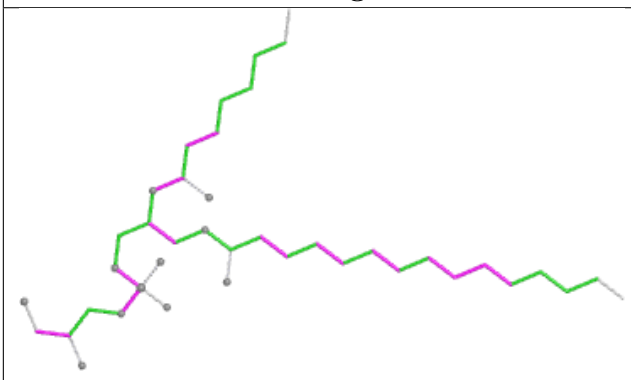
Ligand LHG XX 102



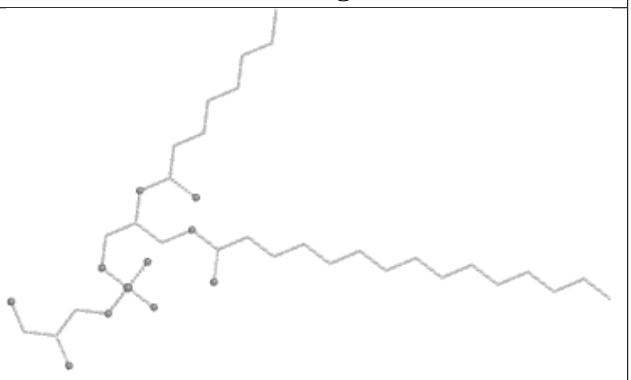
Bond lengths



Bond angles

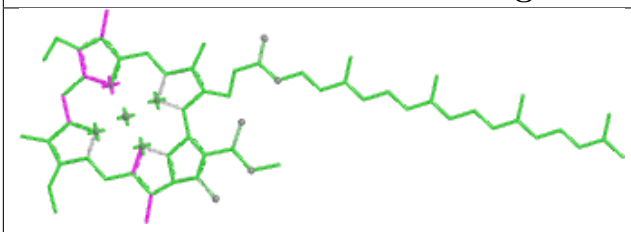


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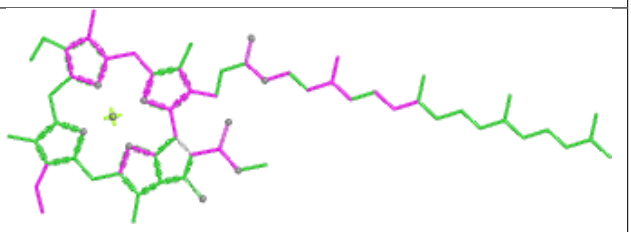


Rings

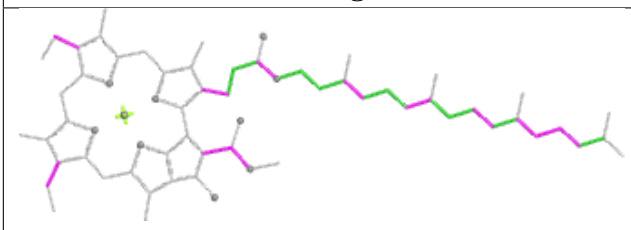
Ligand CLA B1 833



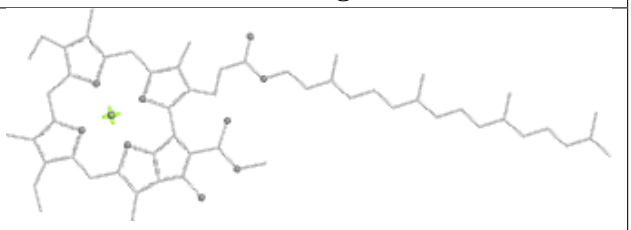
Bond lengths



Bond angles

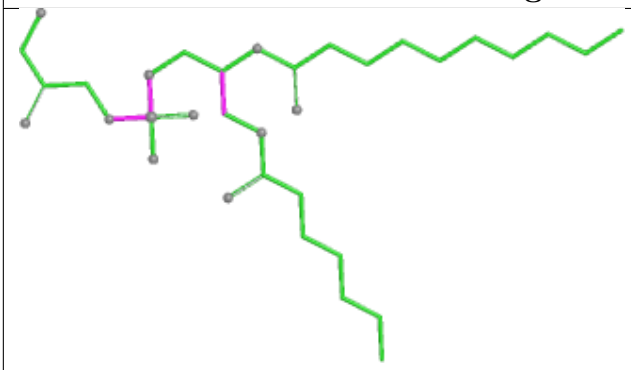


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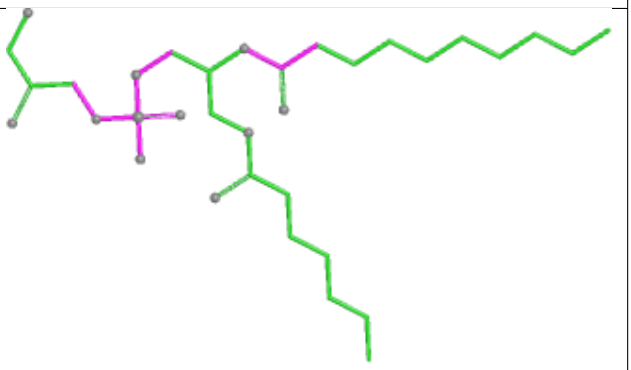


Rings

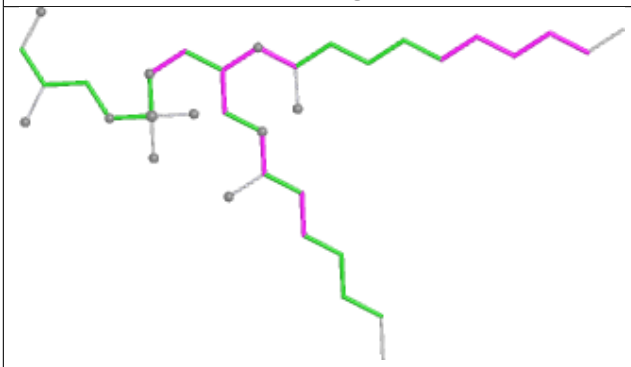
Ligand LHG L 207



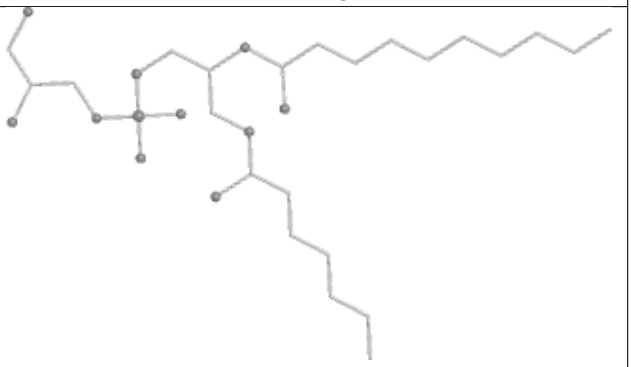
Bond lengths



Bond angles

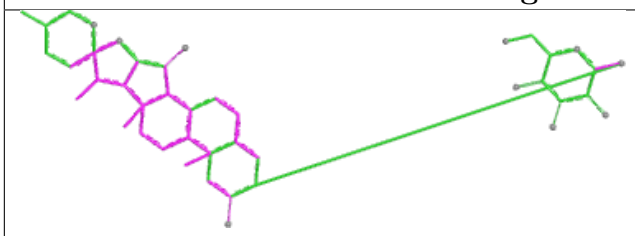


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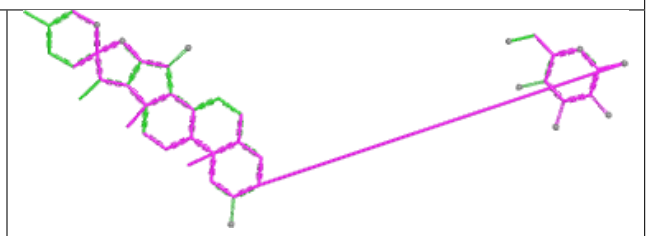


Rings

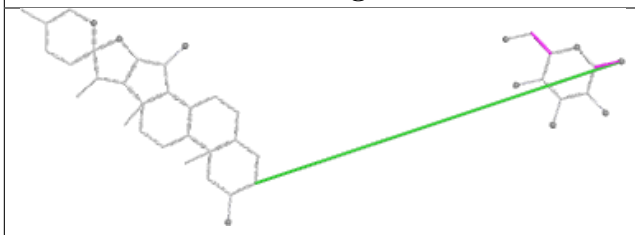
Ligand AJP L1 203



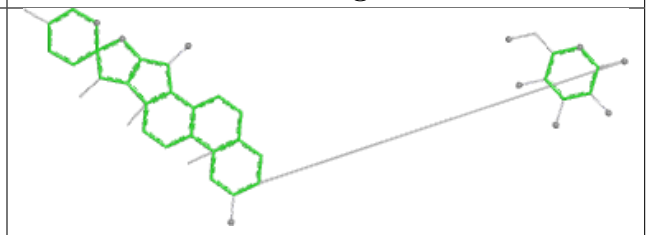
Bond lengths



Bond angles

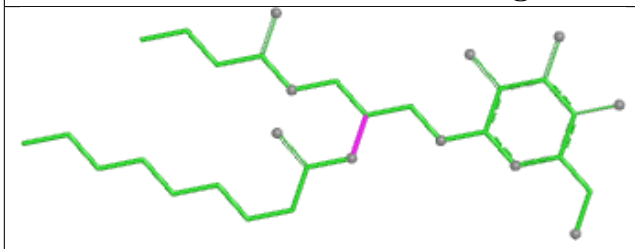


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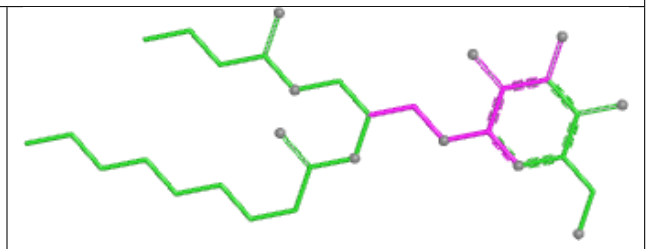


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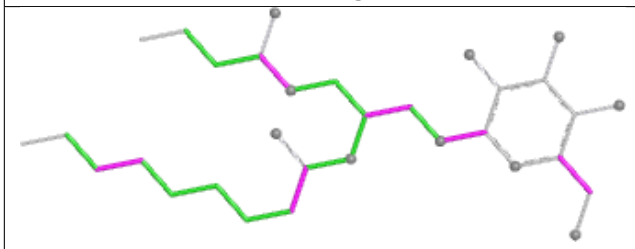
Ligand LMG B1 846



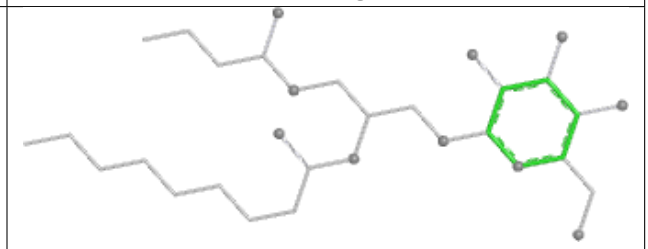
Bond lengths



Bond angles

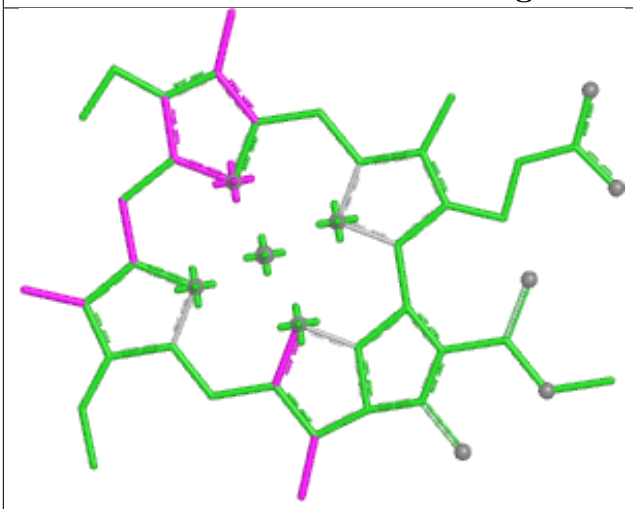


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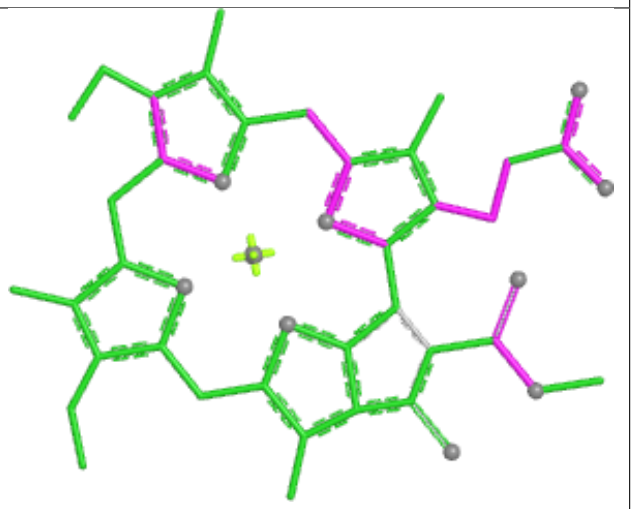


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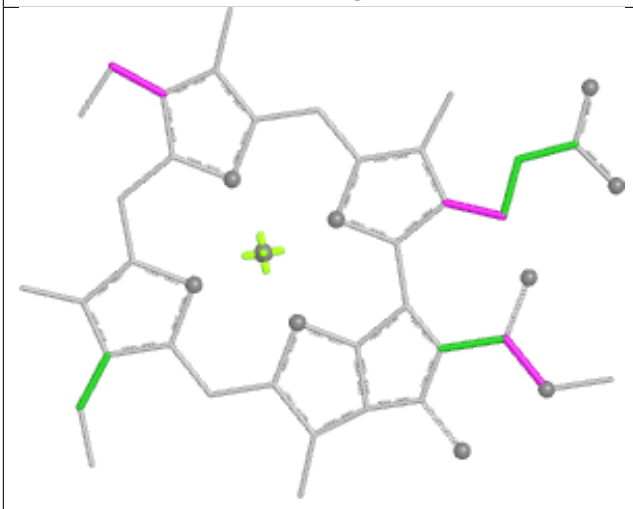
Ligand CLA B1 827



Bond lengths



Bond angles

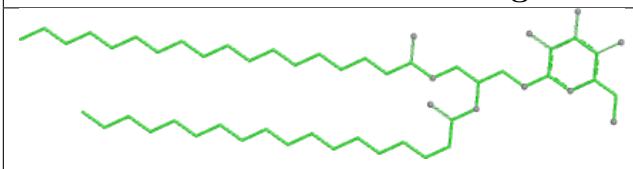


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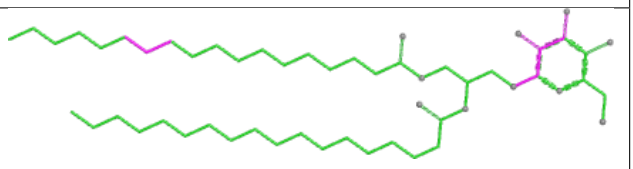


Rings

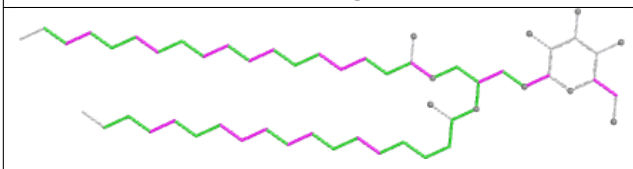
Ligand LMG B1 844



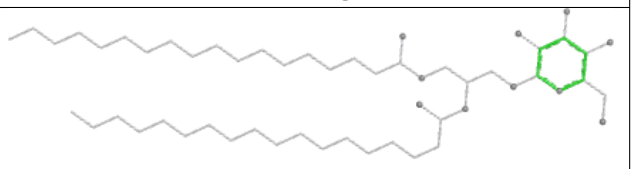
Bond lengths



Bond angles

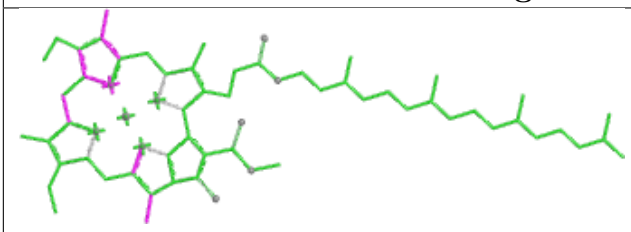


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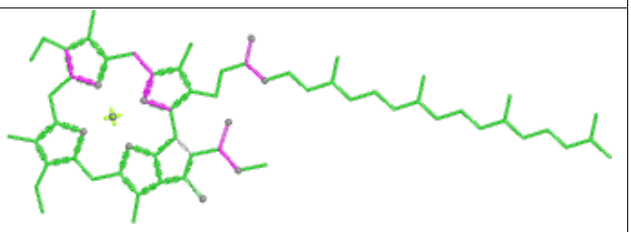


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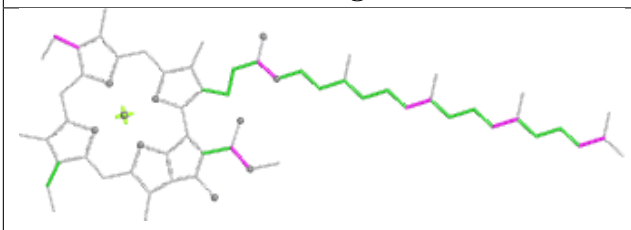
Ligand CLA A1 812



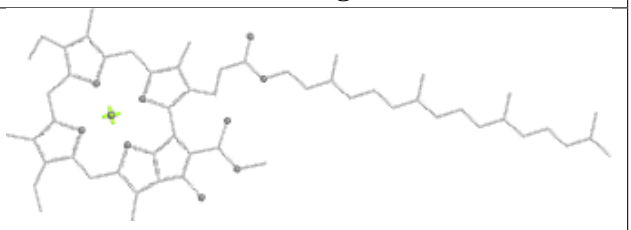
Bond lengths



Bond angles



Torsions

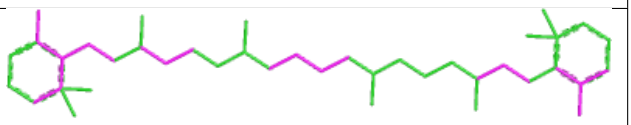


Rings

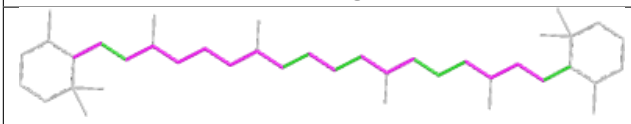
Ligand BCR A 848



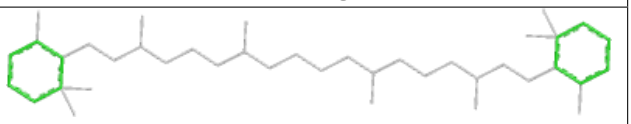
Bond lengths



Bond angles

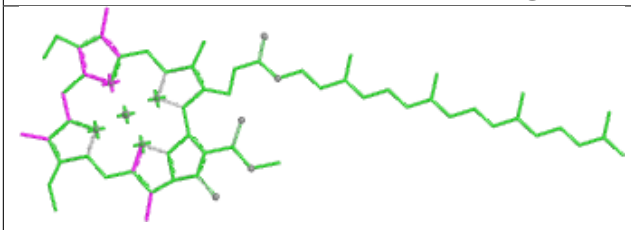


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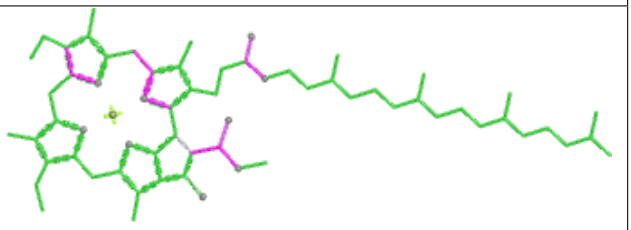


Rings

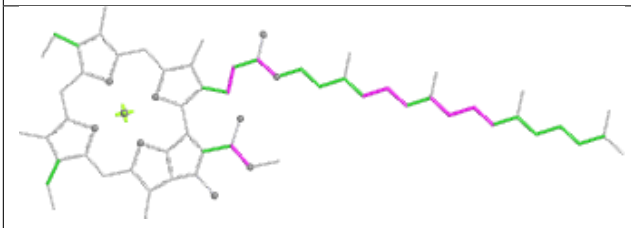
Ligand CLA A 801



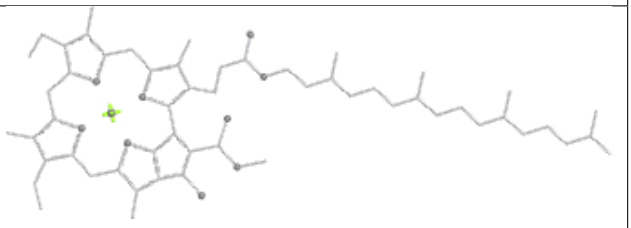
Bond lengths



Bond angles

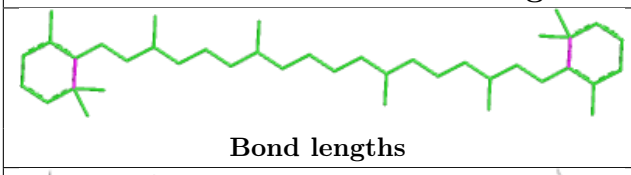


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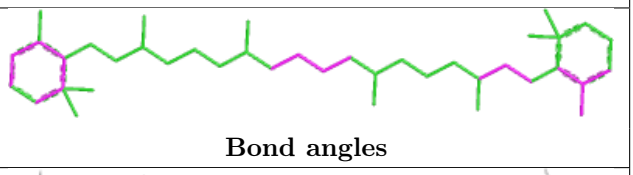


Rings

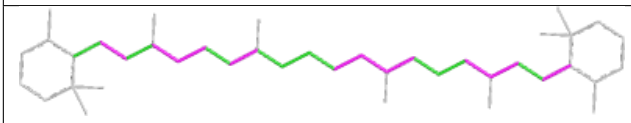
Ligand BCR J 104



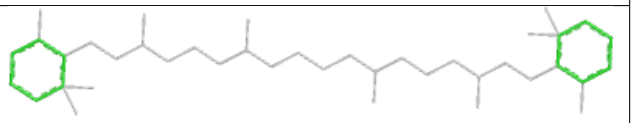
Bond lengths



Bond angles

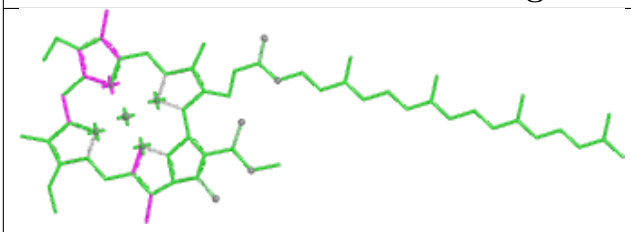


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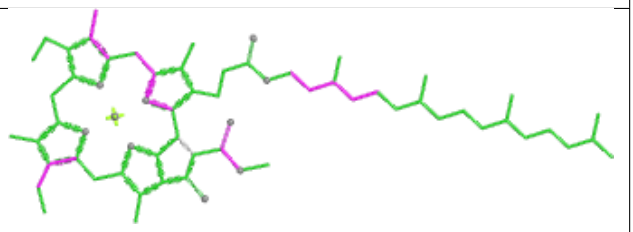


Rings

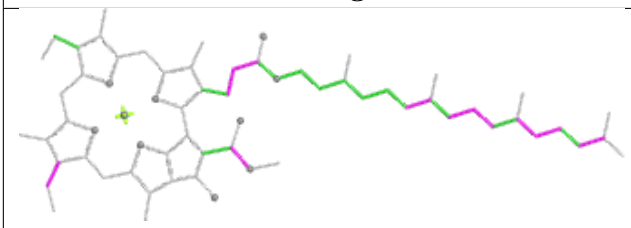
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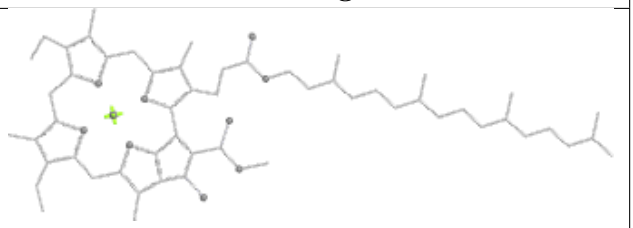
Bond lengths



Bond angles

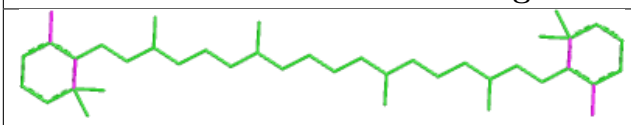


Torsions

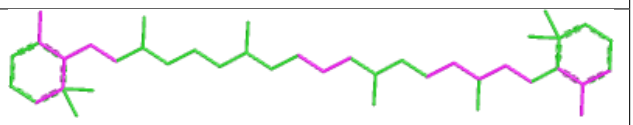


Rings

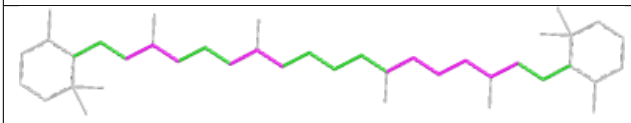
Ligand BCR FF 304



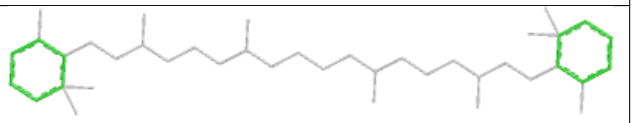
Bond lengths



Bond angles

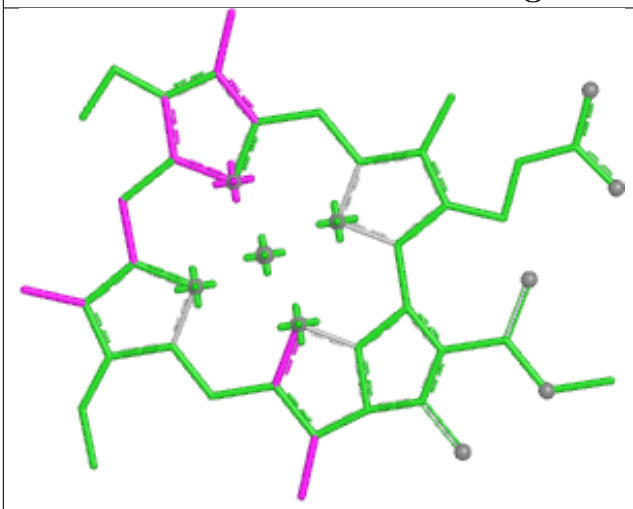


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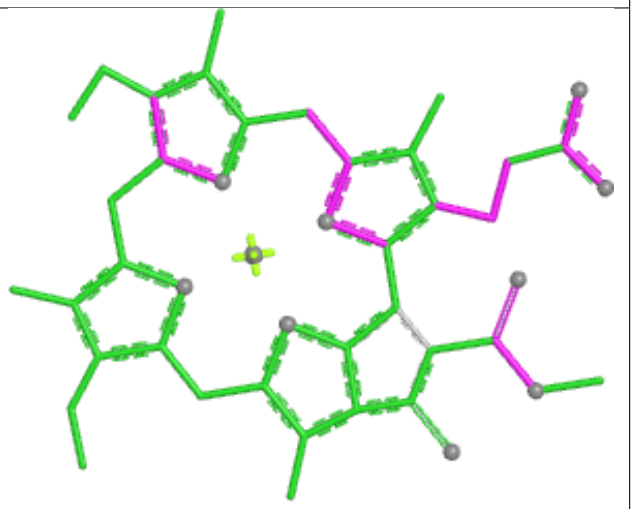


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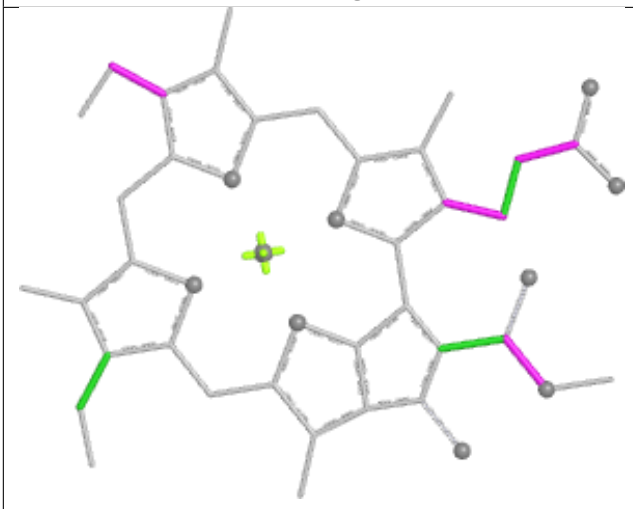
Ligand CLA B 827



Bond lengths



Bond angles

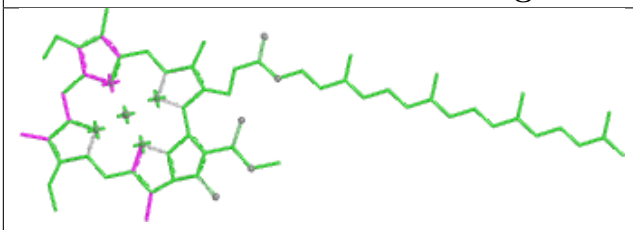


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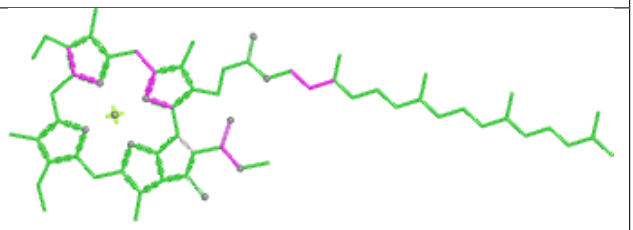


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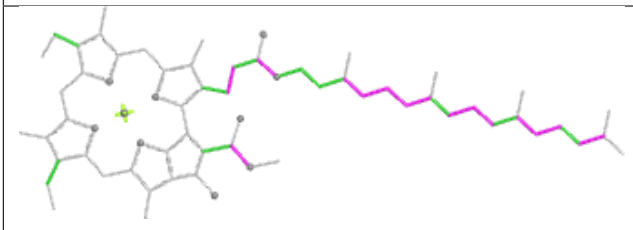
Ligand CLA A2 804



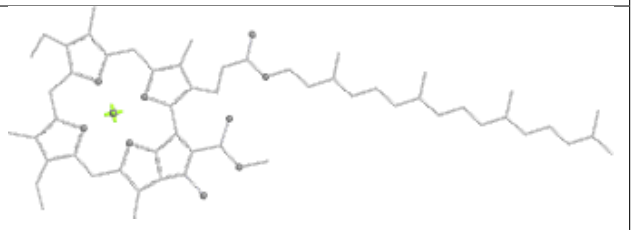
Bond lengths



Bond angles

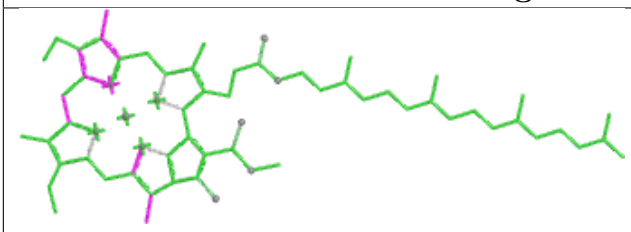


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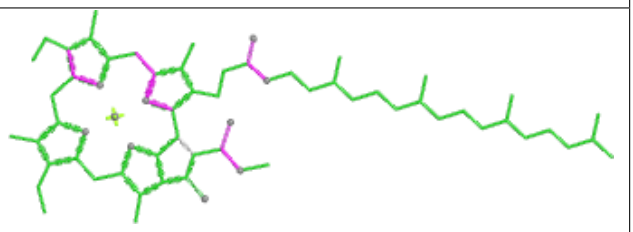


Rings

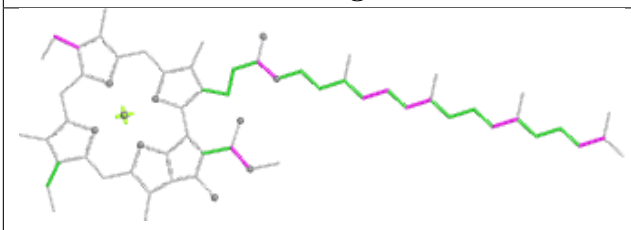
Ligand CLA A2 813



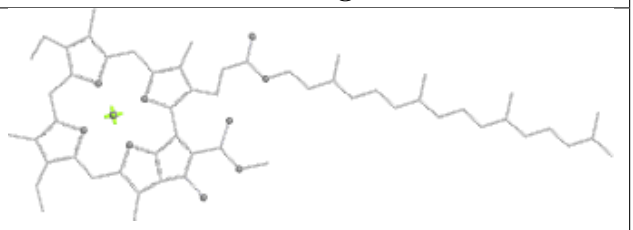
Bond lengths



Bond angles

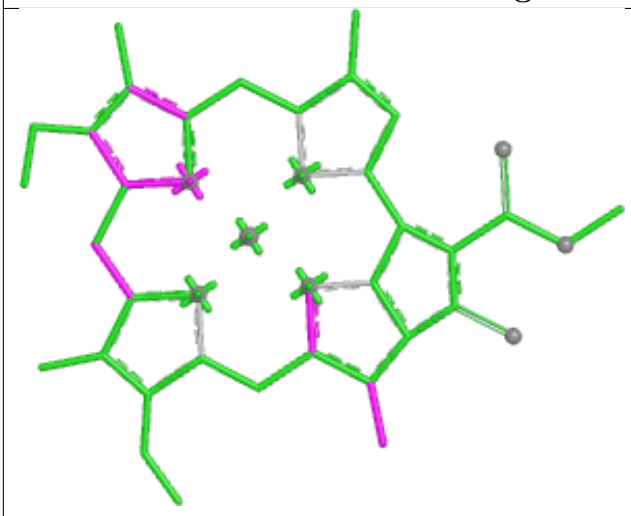


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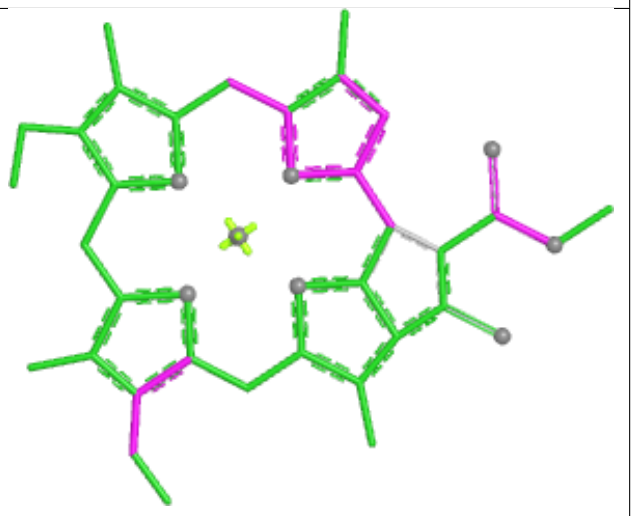


Rings

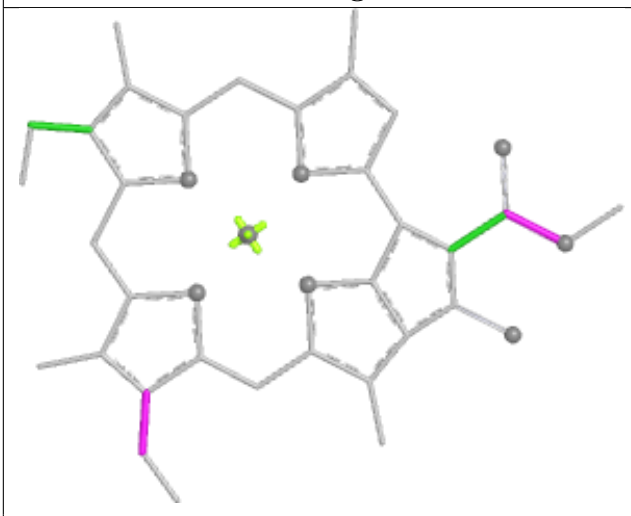
Ligand CLA K1 105



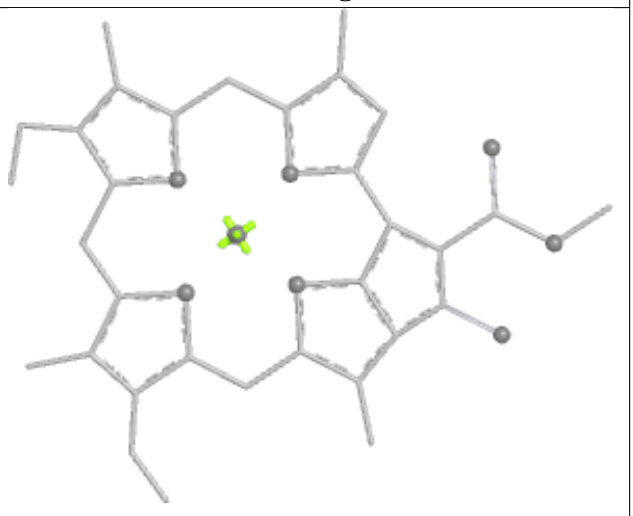
Bond lengths



Bond angles

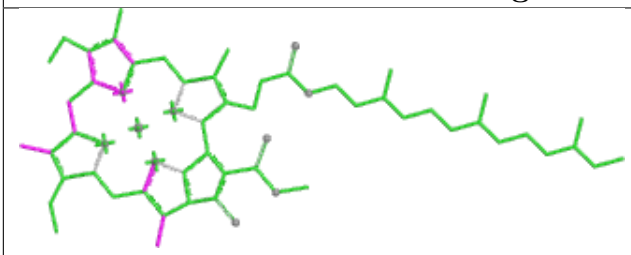


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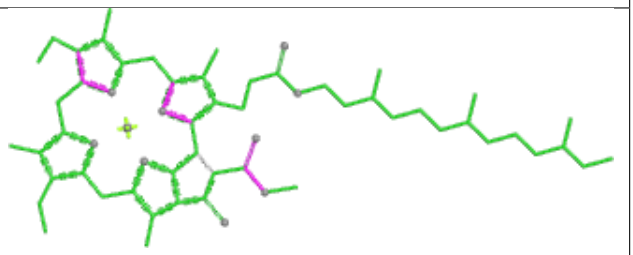


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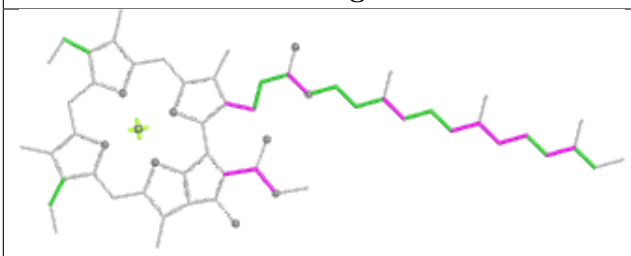
Ligand CLA BB 811



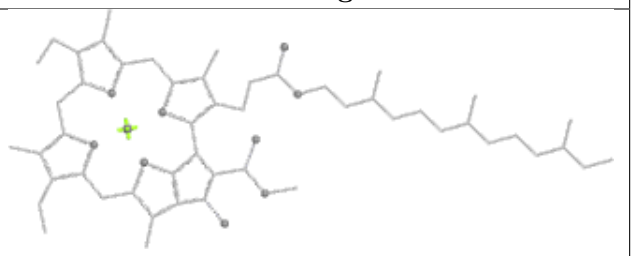
Bond lengths



Bond angles

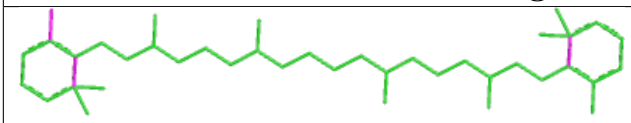


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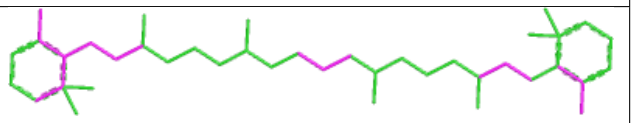


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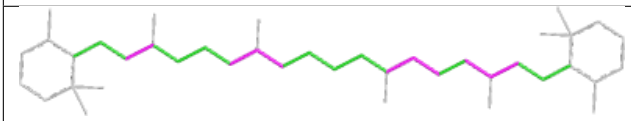
Ligand BCR I 102



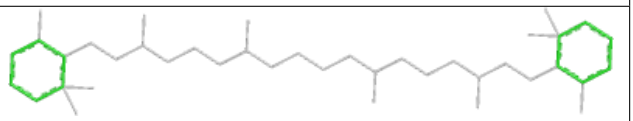
Bond lengths



Bond angles

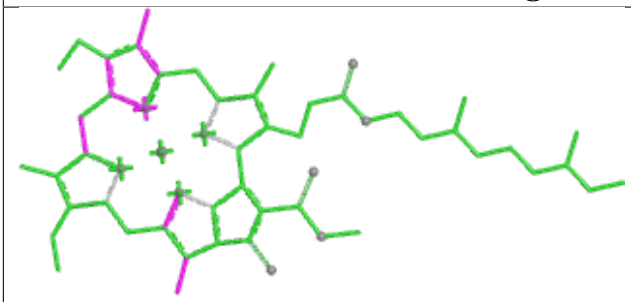


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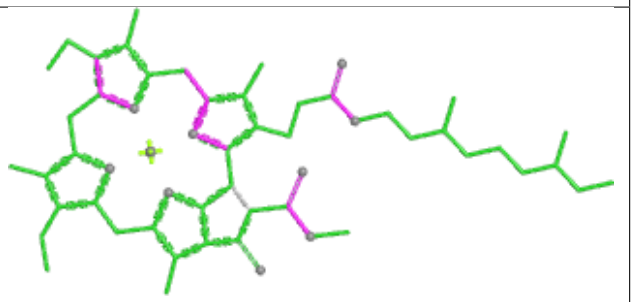


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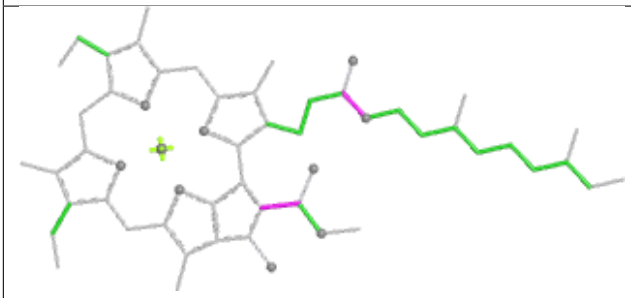
Ligand CLA B 831



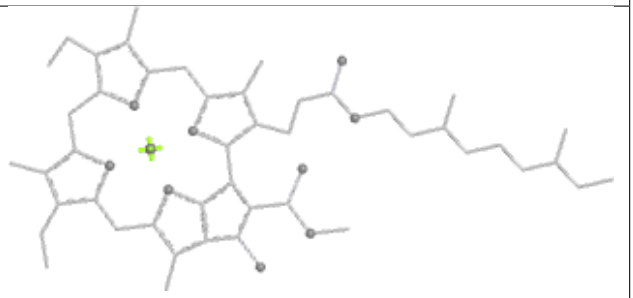
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Bond angles

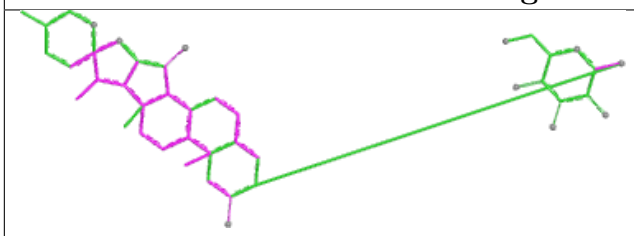


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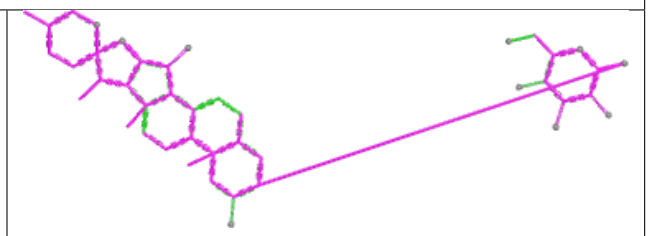


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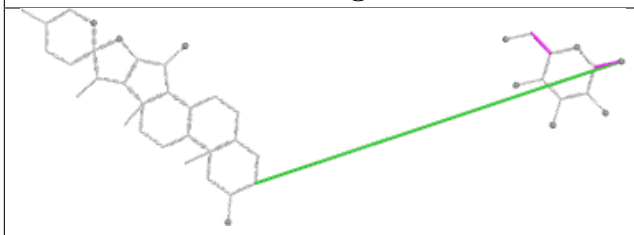
Ligand AJP L2 202



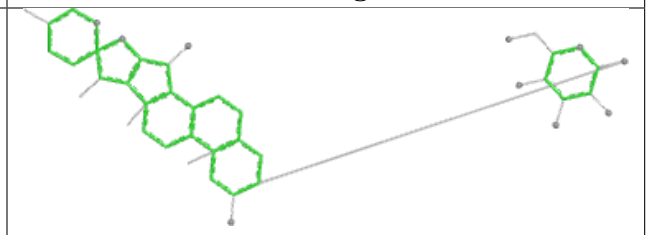
Bond lengths



Bond angles

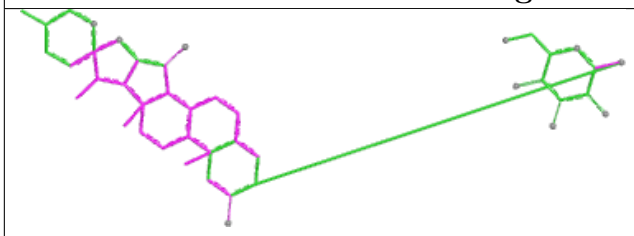


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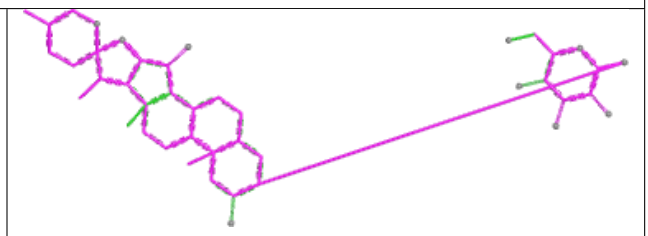


Rings

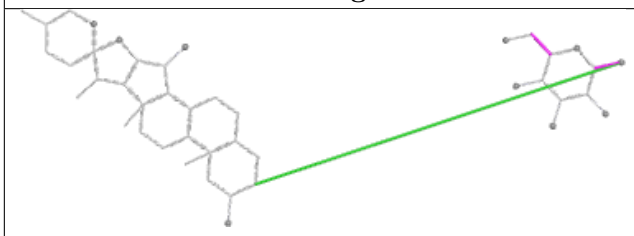
Ligand AJP BB 849



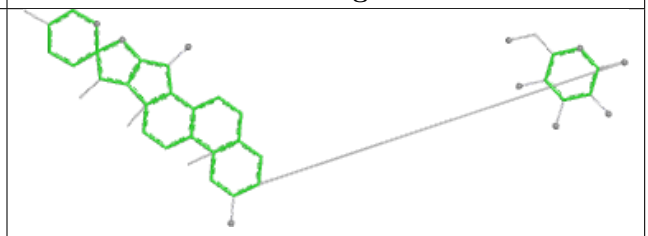
Bond lengths



Bond angles

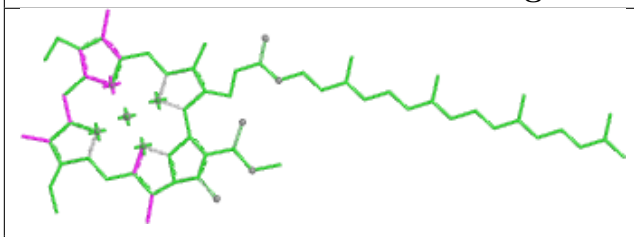


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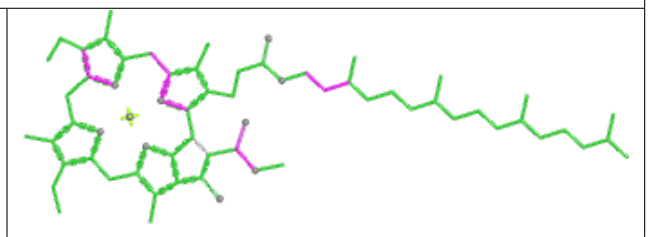


Rings

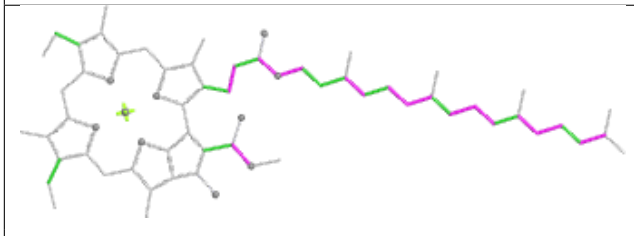
Ligand CLA A 804



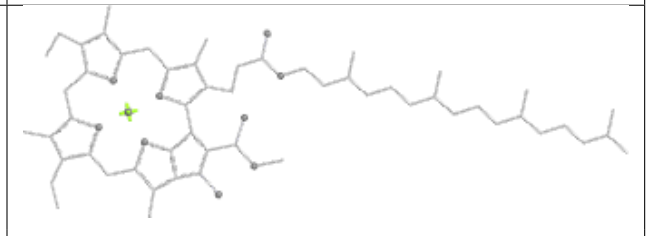
Bond lengths



Bond angles

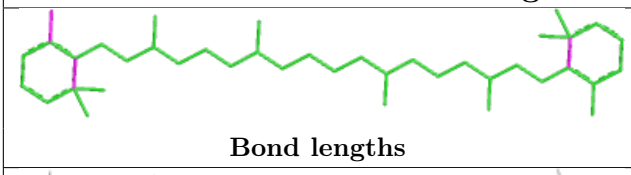


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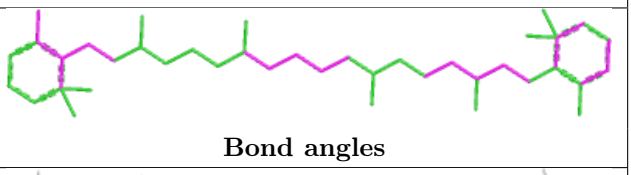


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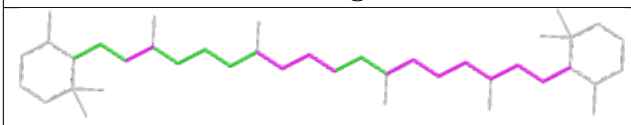
Ligand BCR A 854



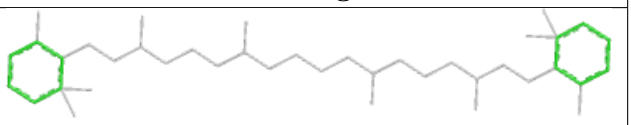
Bond lengths



Bond angles

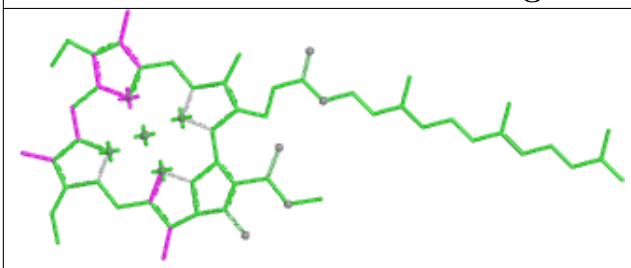


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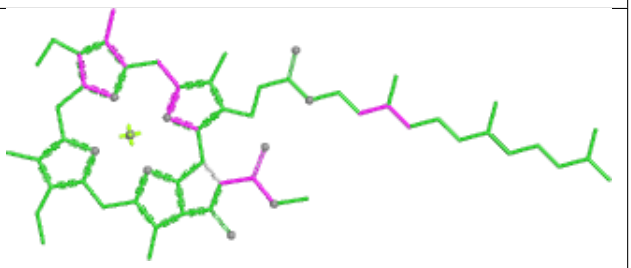


Rings

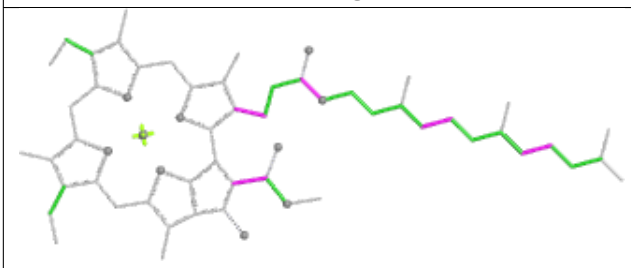
Ligand CLA A 805



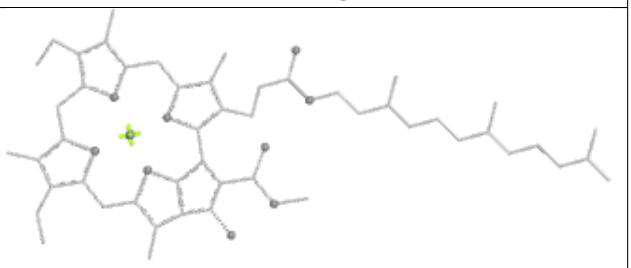
Bond lengths



Bond angles

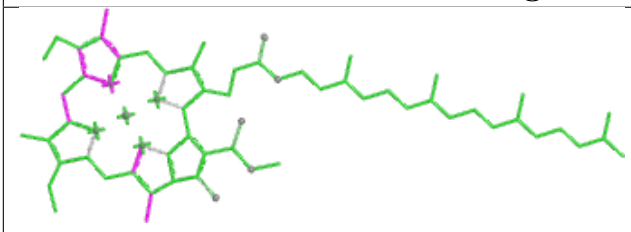


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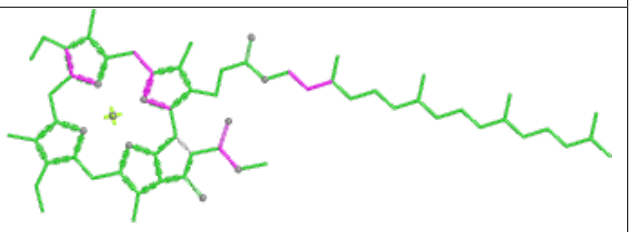


Rings

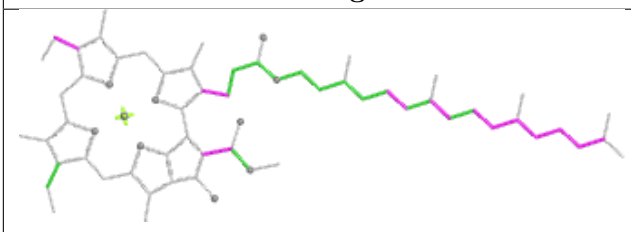
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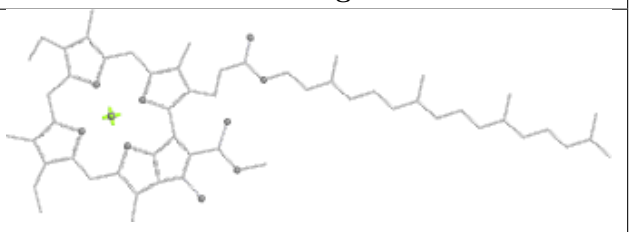
Bond lengths



Bond angles

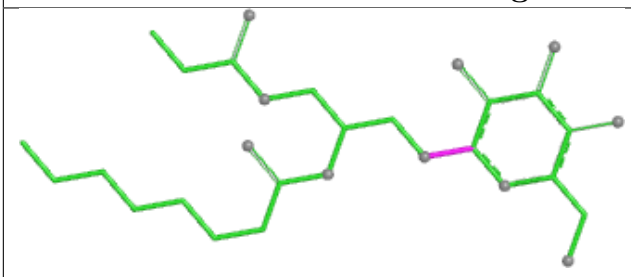


Torsions

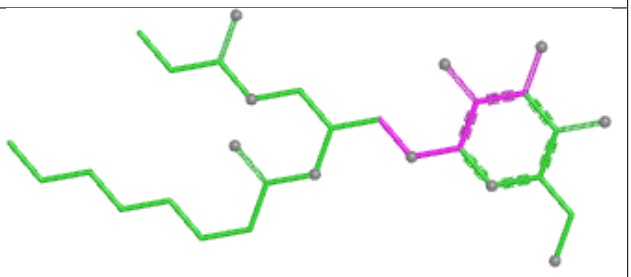


Rings

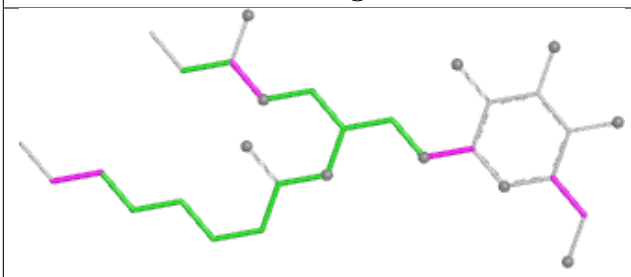
Ligand LMG B2 854



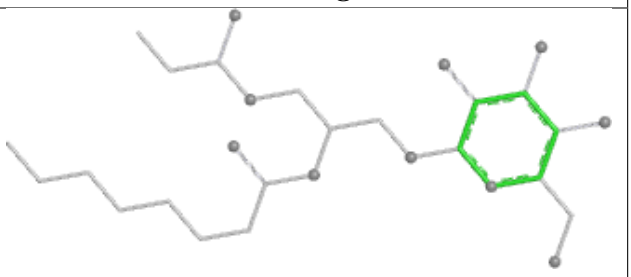
Bond lengths



Bond angles

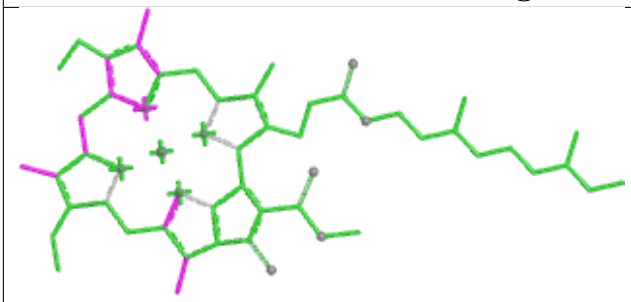


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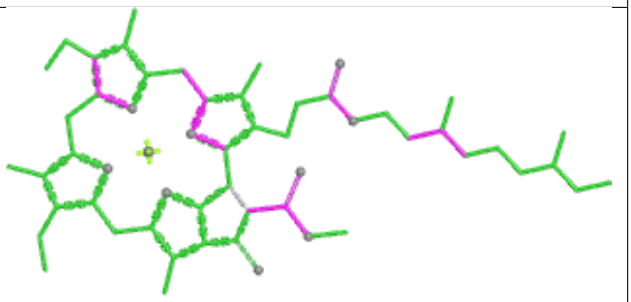


Rings

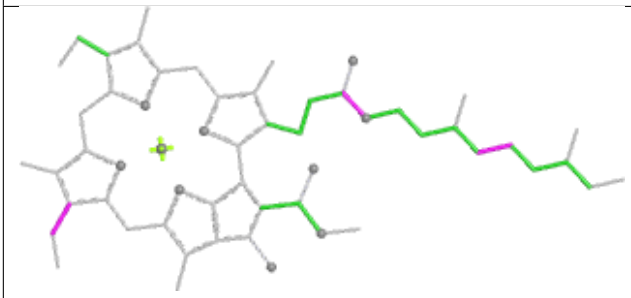
Ligand CLA B1 829



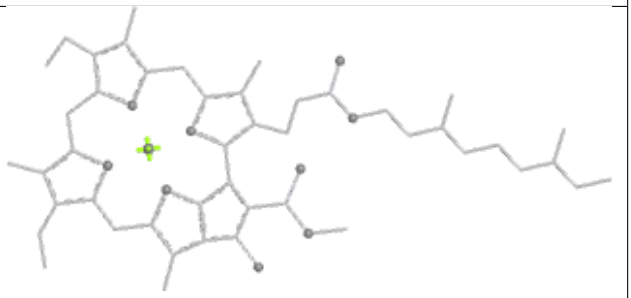
Bond lengths



Bond angles

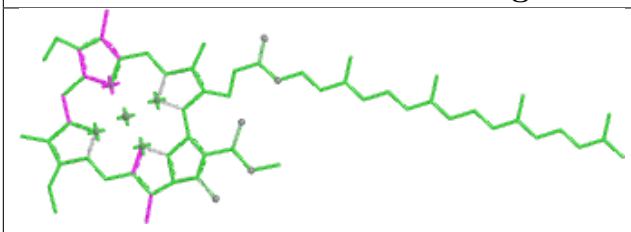


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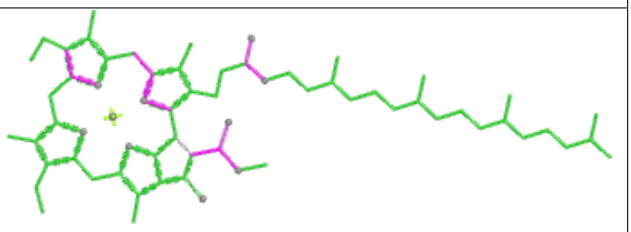


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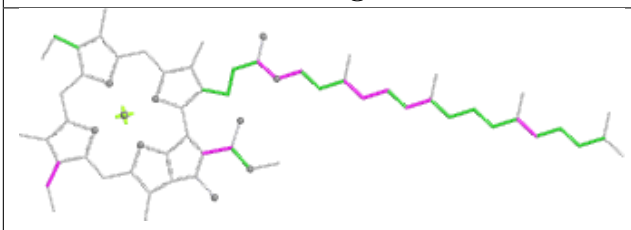
Ligand CLA BB 807



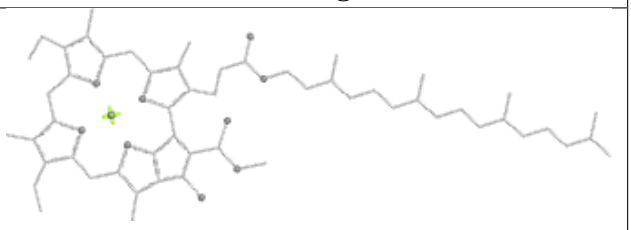
Bond lengths



Bond angles

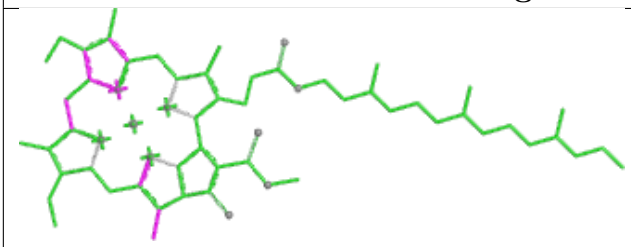


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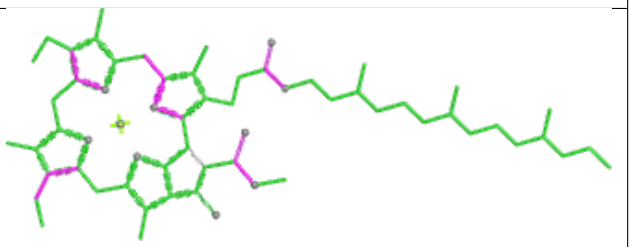


Rings

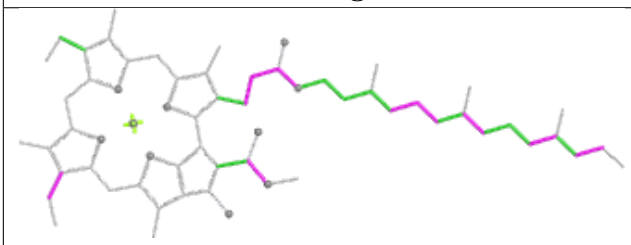
Ligand CLA A2 830



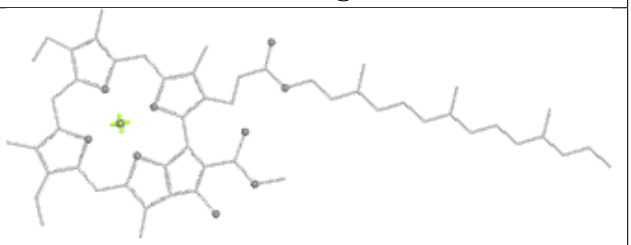
Bond lengths



Bond angles

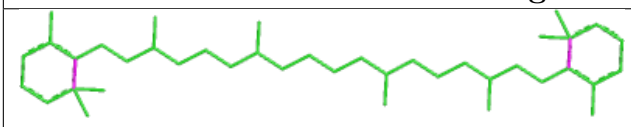


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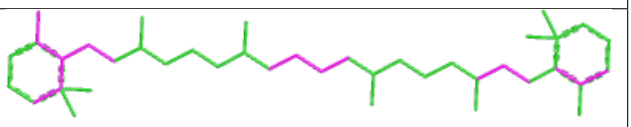


Rings

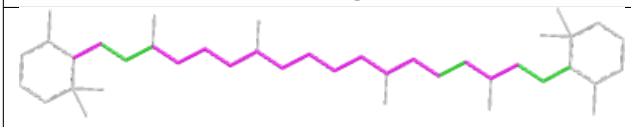
Ligand BCR I 101



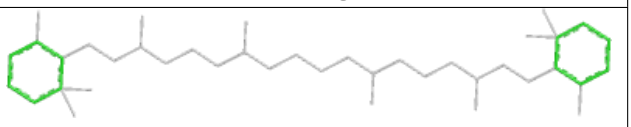
Bond lengths



Bond angles

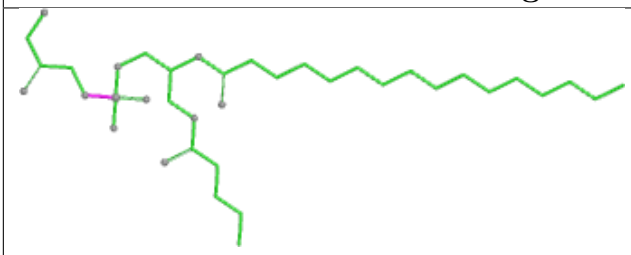


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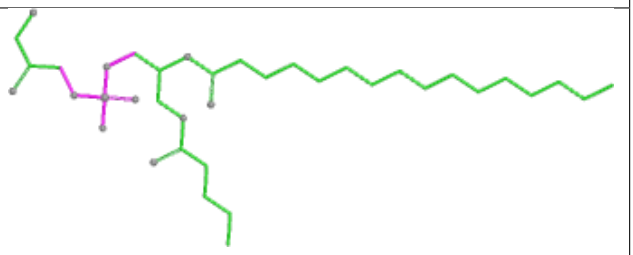


Rings

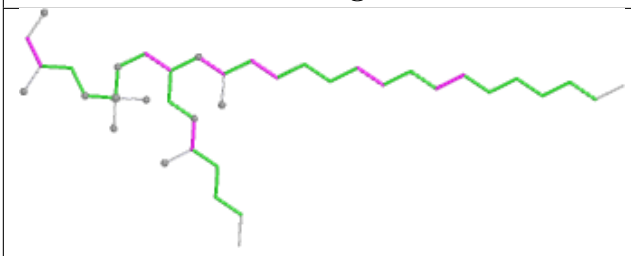
Ligand LHG A 846



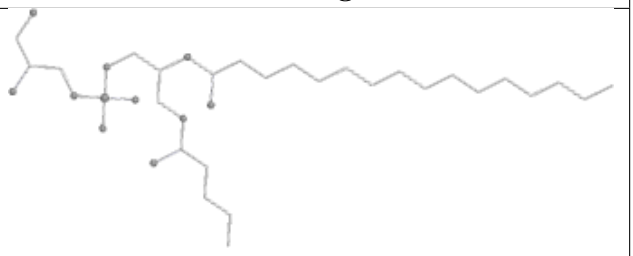
Bond lengths



Bond angles

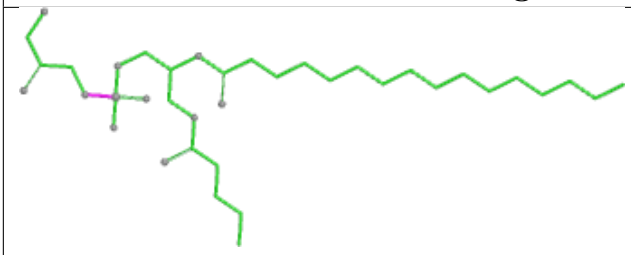


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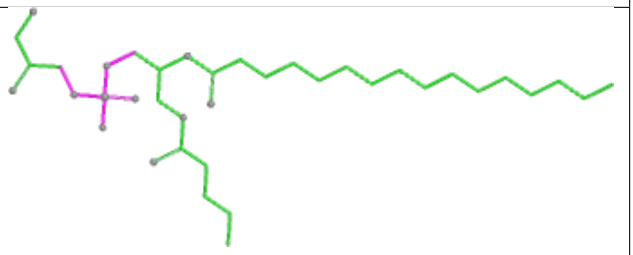


Rings

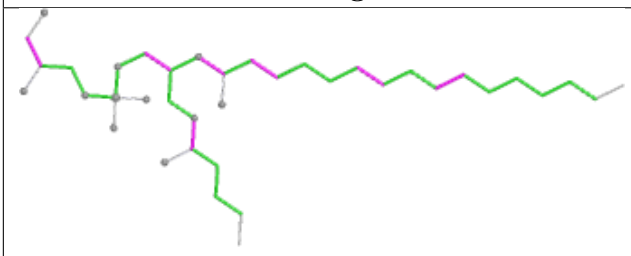
Ligand LHG A1 846



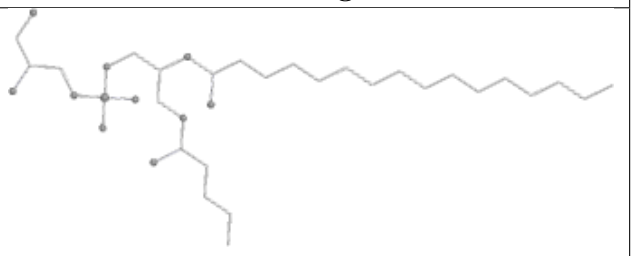
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Bond angles

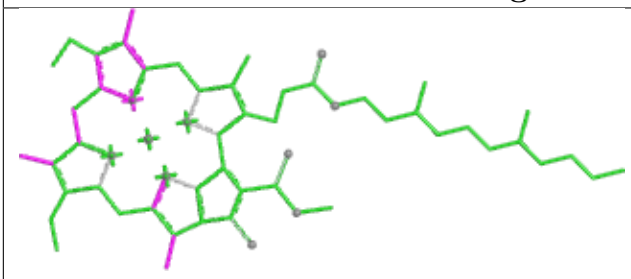


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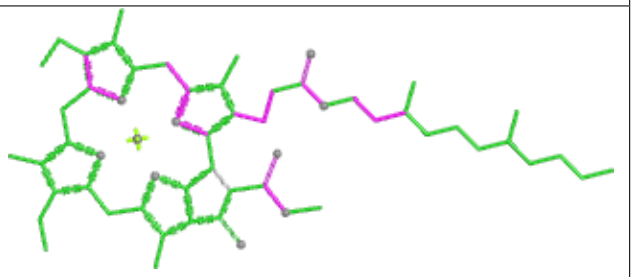


Rings

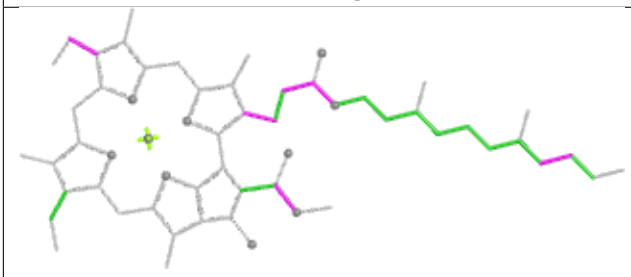
Ligand CLA AA 820



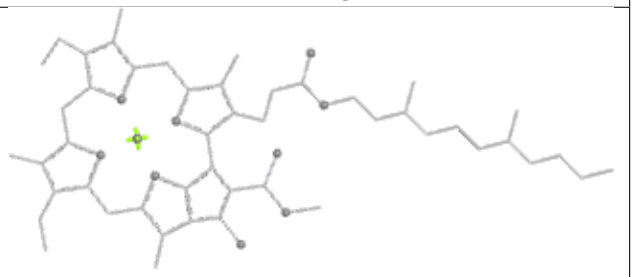
Bond lengths



Bond angles

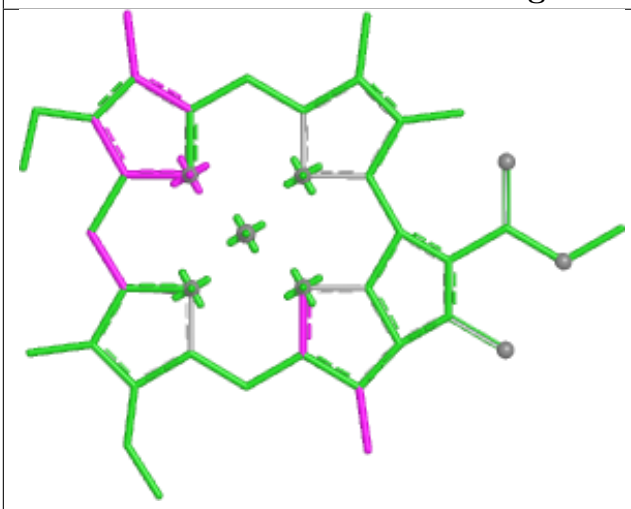


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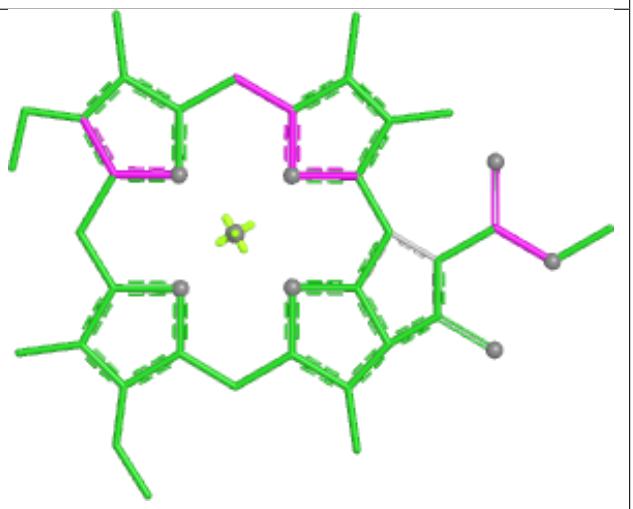


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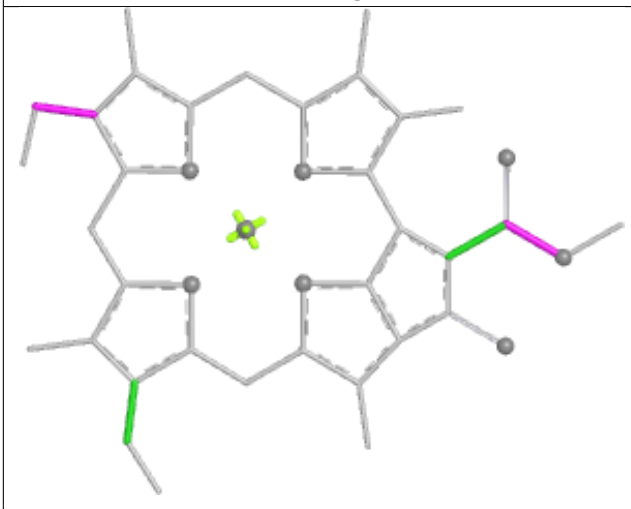
Ligand CLA J 101



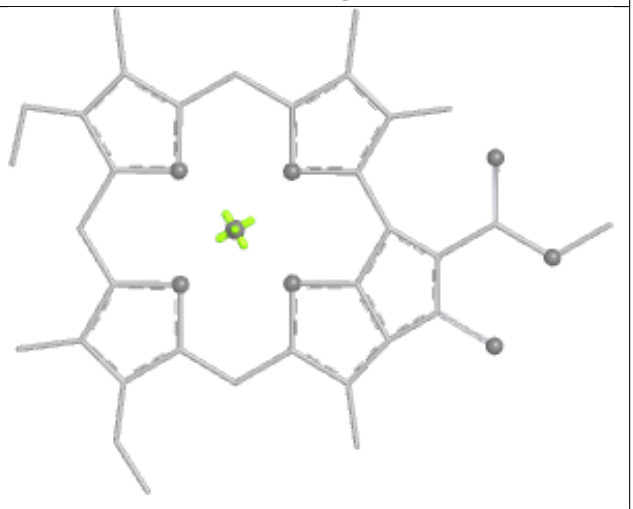
Bond lengths



Bond angles

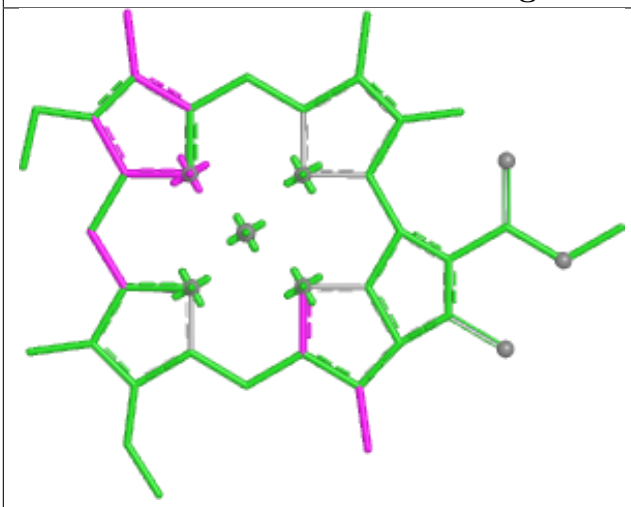


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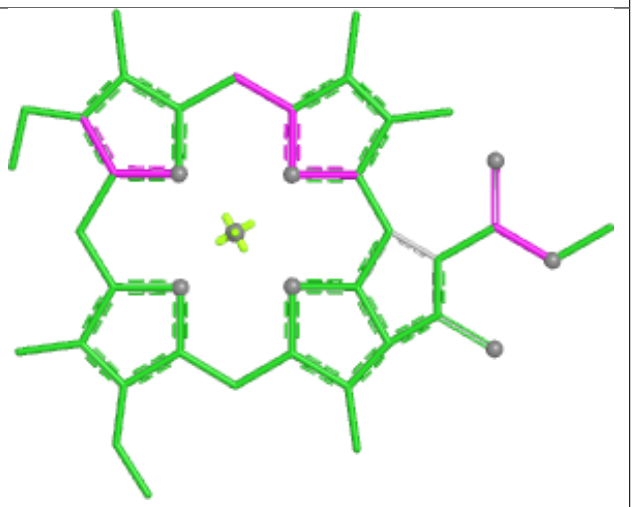


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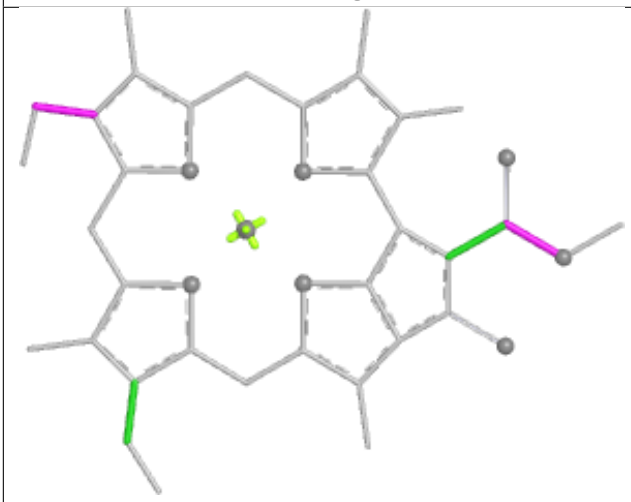
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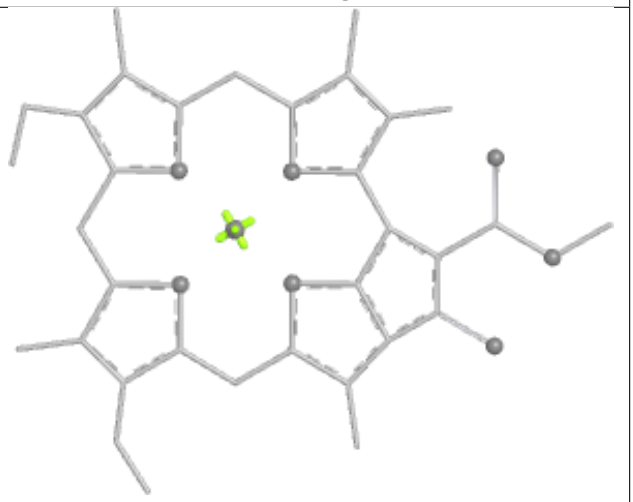
Bond lengths



Bond angles

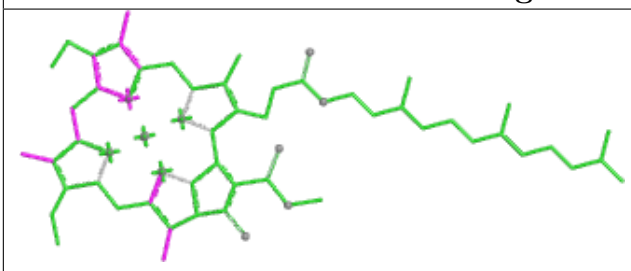


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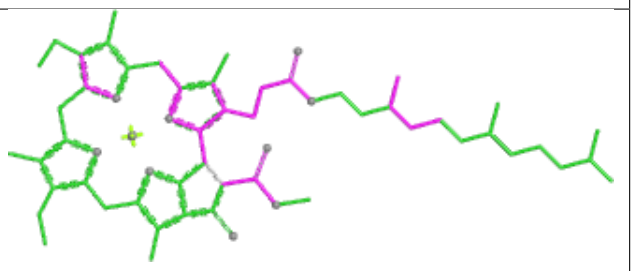


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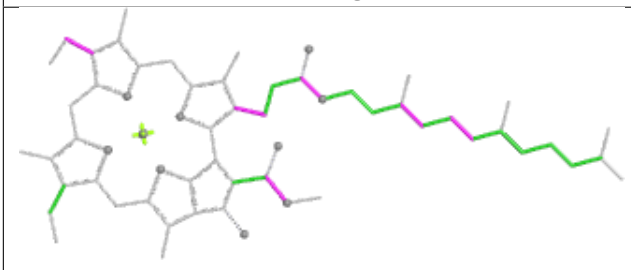
Ligand CLA B2 851



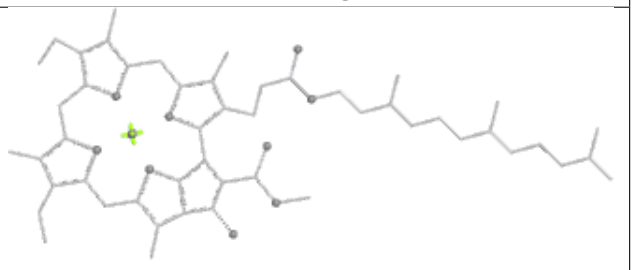
Bond lengths



Bond angles

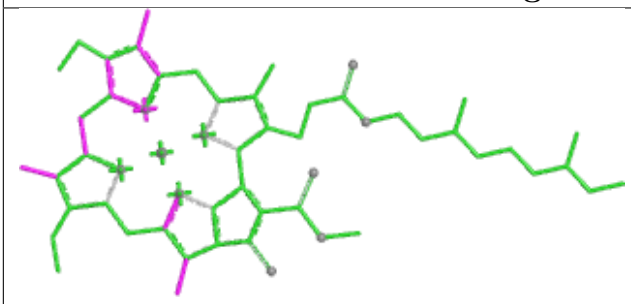


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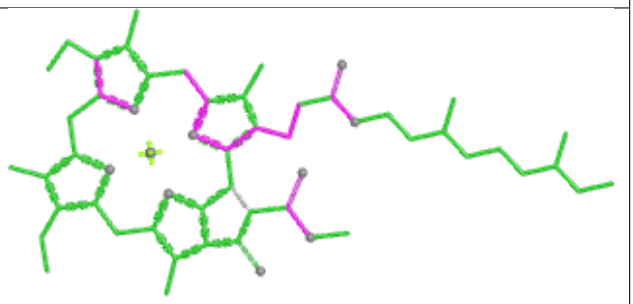


Rings

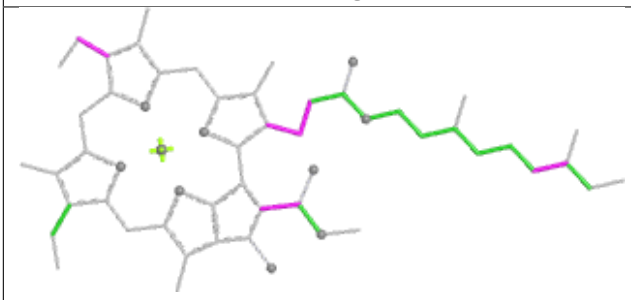
Ligand CLA A 806



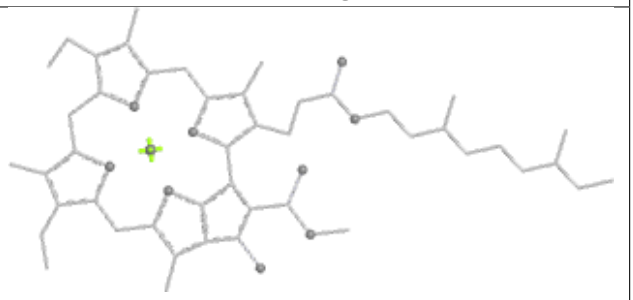
Bond lengths



Bond angles

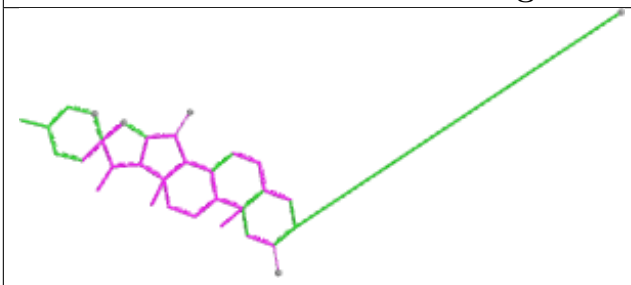


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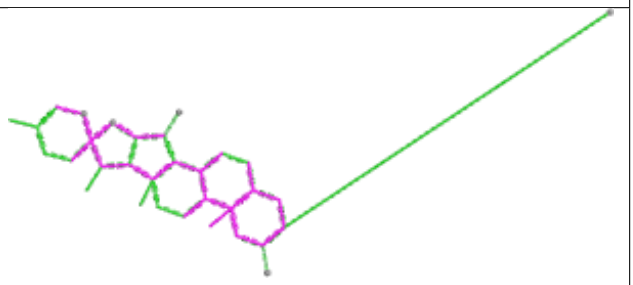


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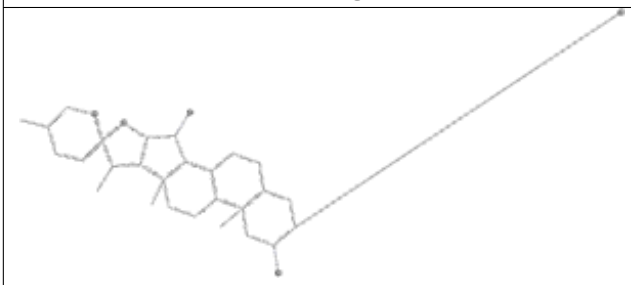
Ligand AJP A2 854



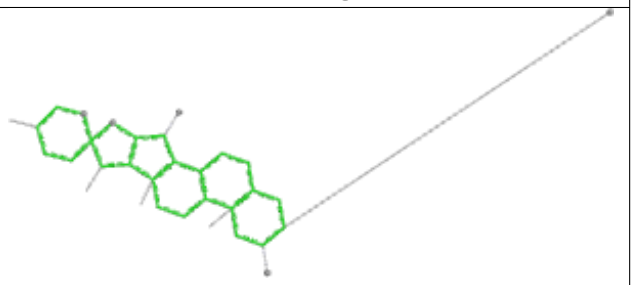
Bond lengths



Bond angles

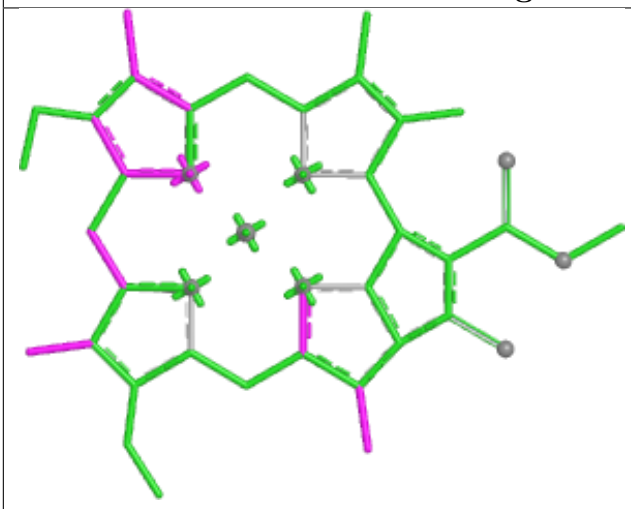


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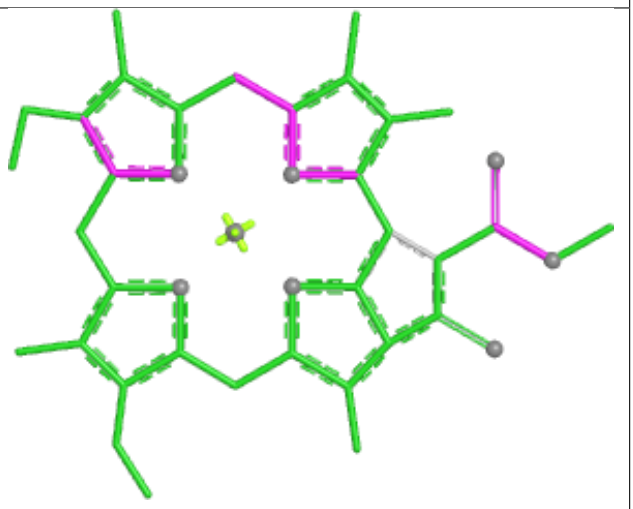


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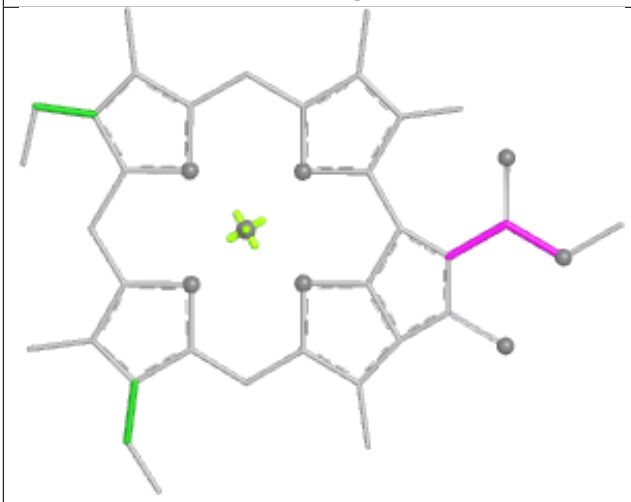
Ligand CLA B1 812



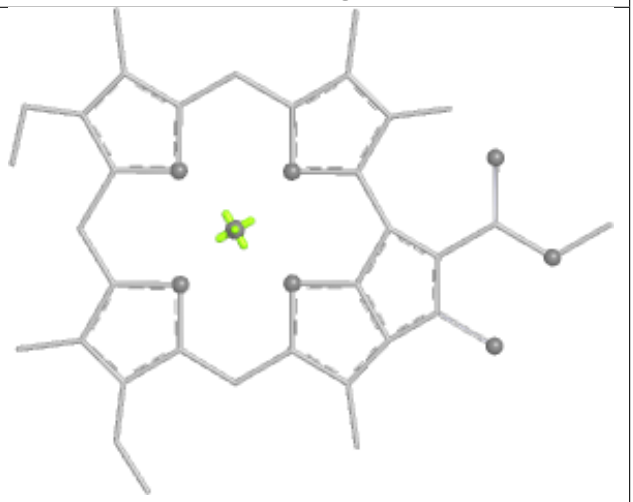
Bond lengths



Bond angles

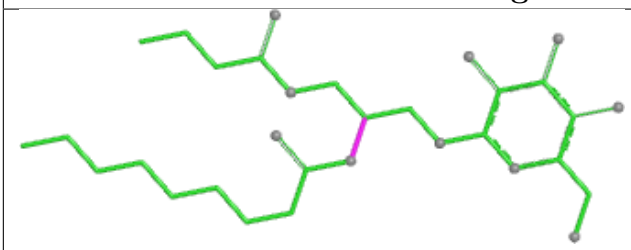


Torsions

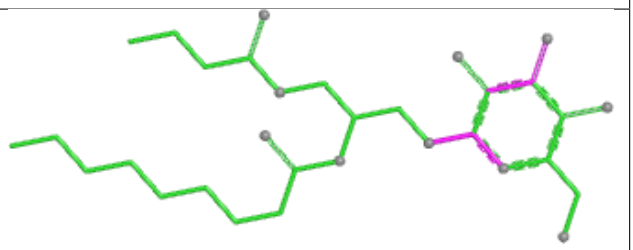


Rings

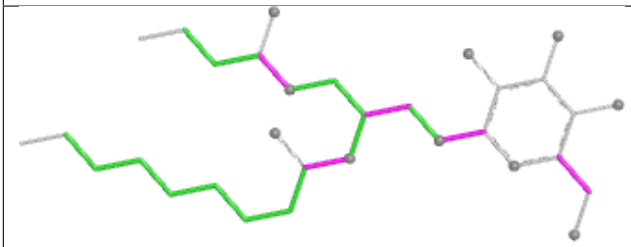
Ligand LMG B2 847



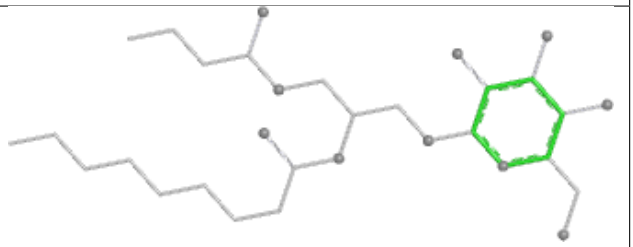
Bond lengths



Bond angles

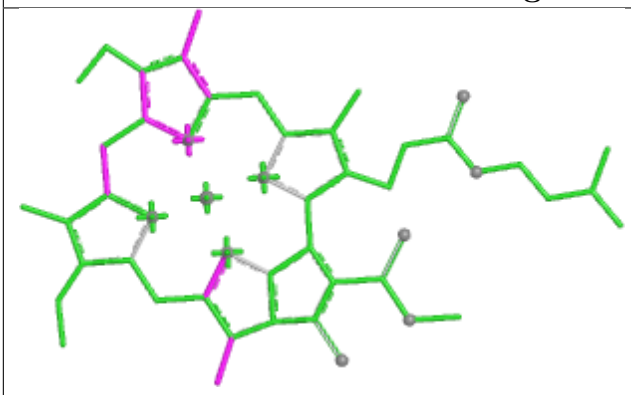


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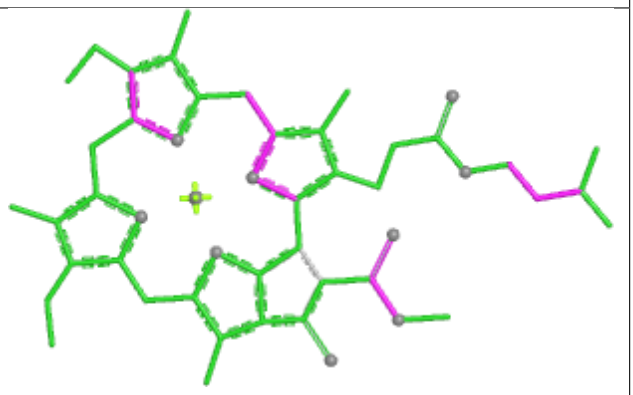


Rings

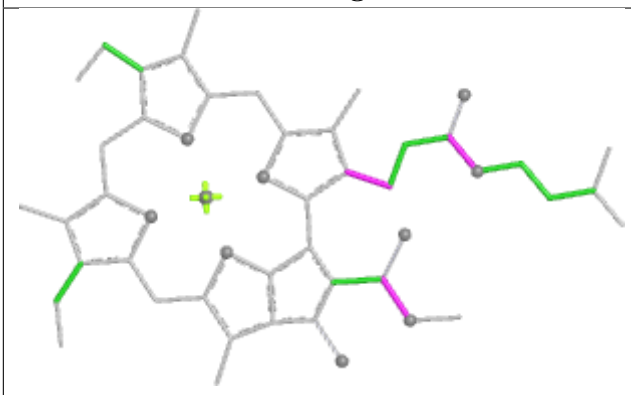
Ligand CLA A 816



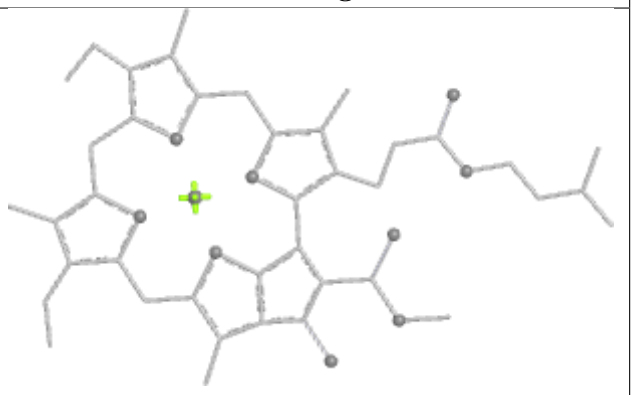
Bond lengths



Bond angles

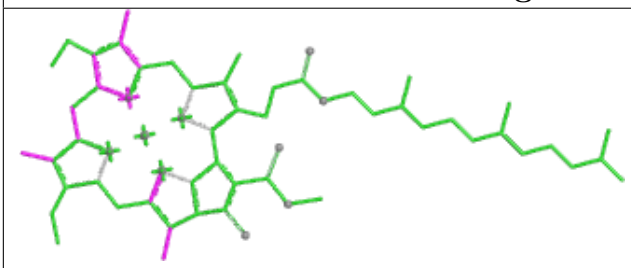


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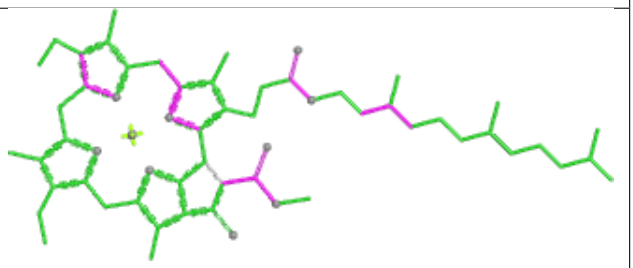


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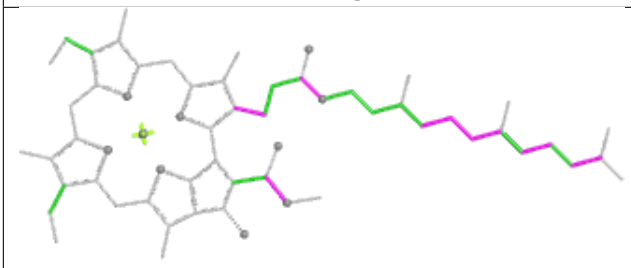
Ligand CLA A1 822



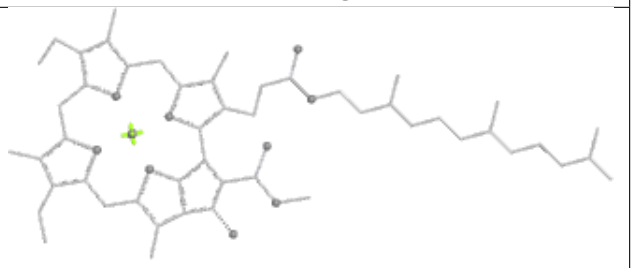
Bond lengths



Bond angles

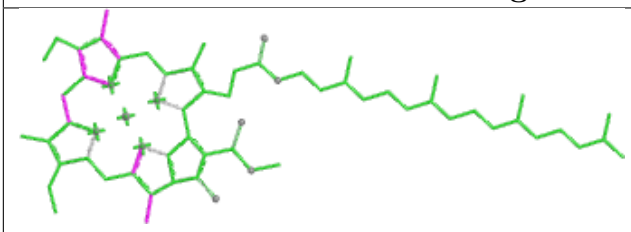


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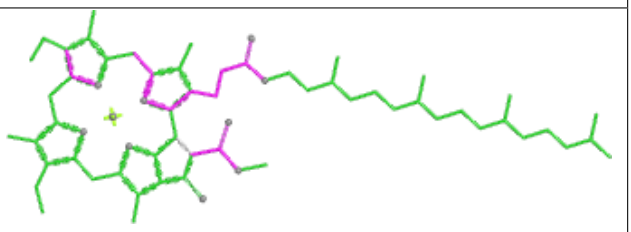


Rings

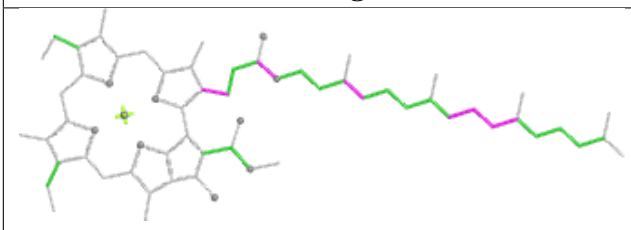
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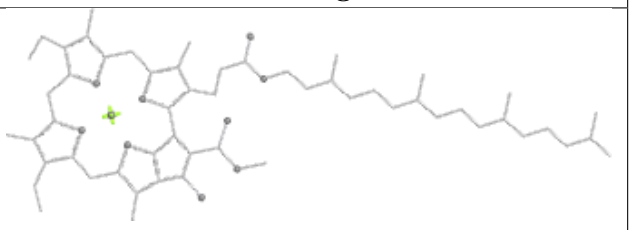
Bond lengths



Bond angles

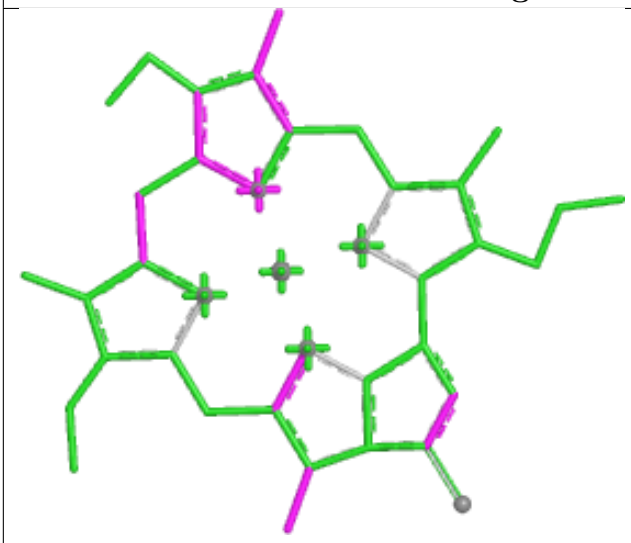


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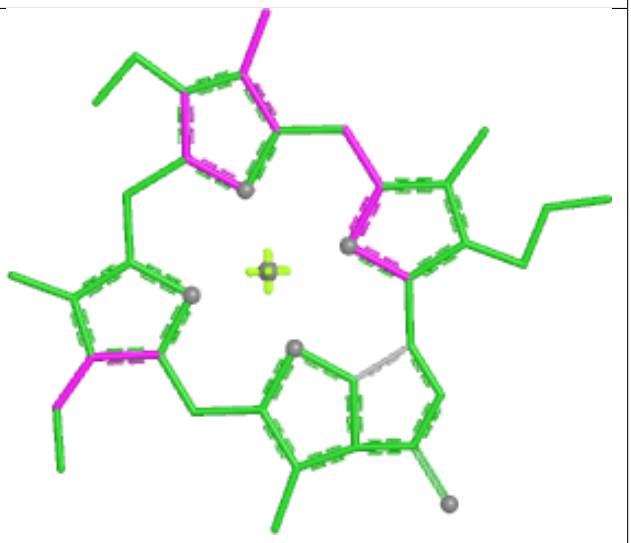


Rings

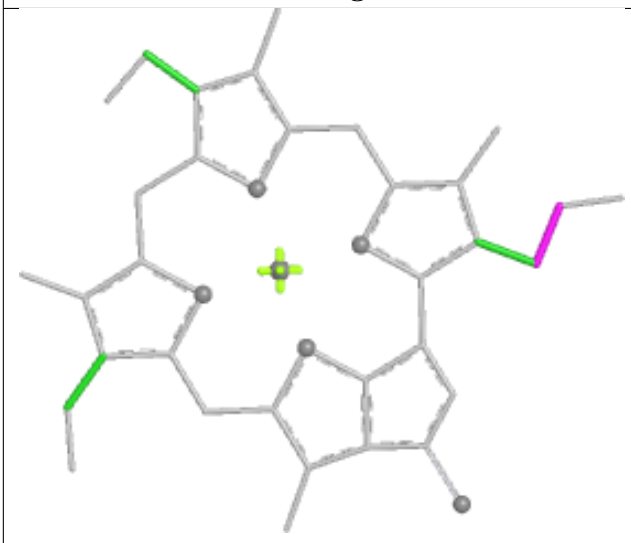
Ligand CLA BB 845



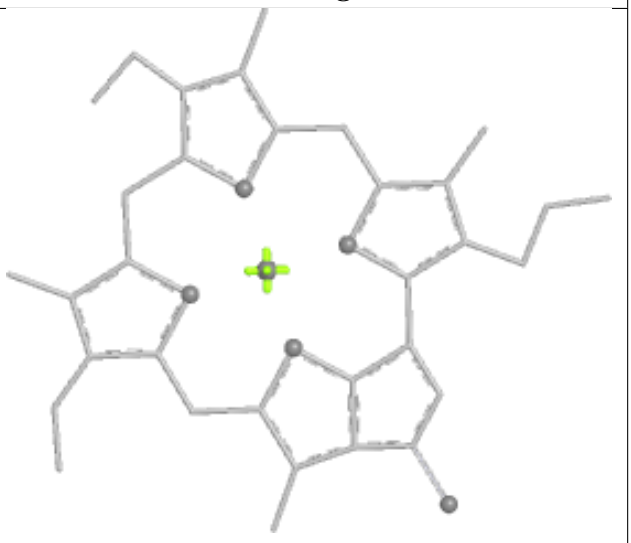
Bond lengths



Bond angles

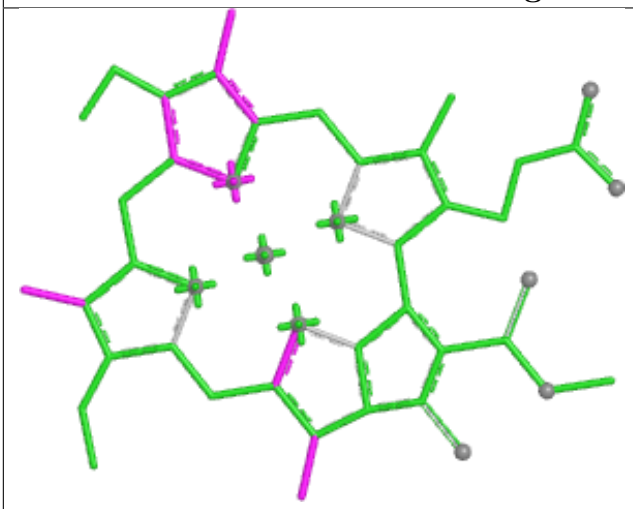


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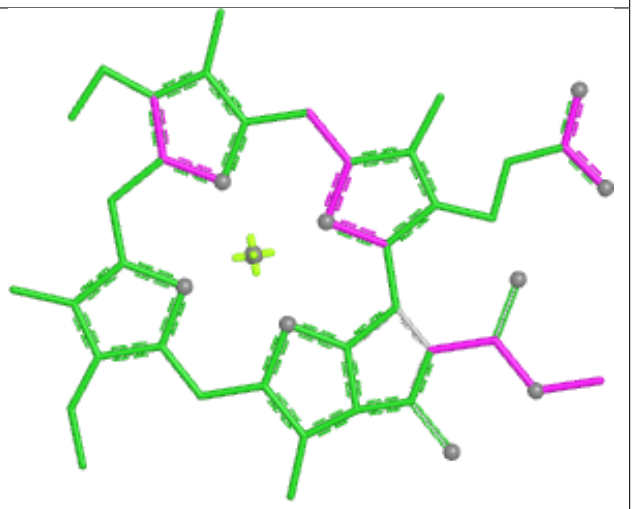


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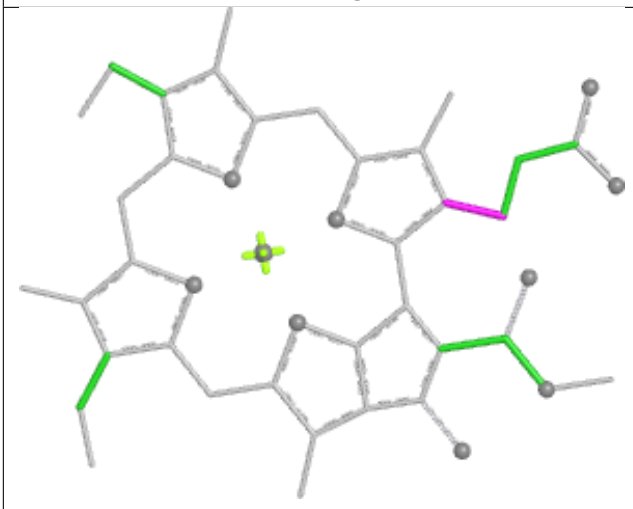
Ligand CLA B 835



Bond lengths



Bond angles

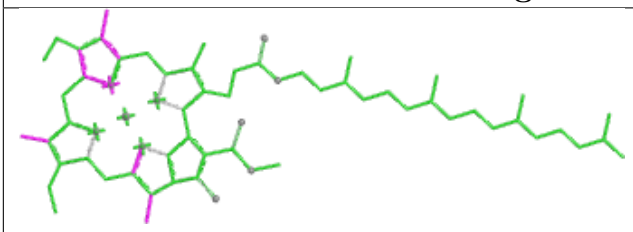


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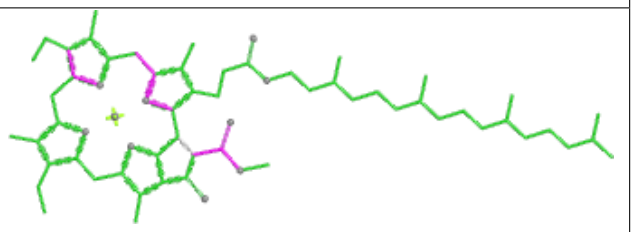


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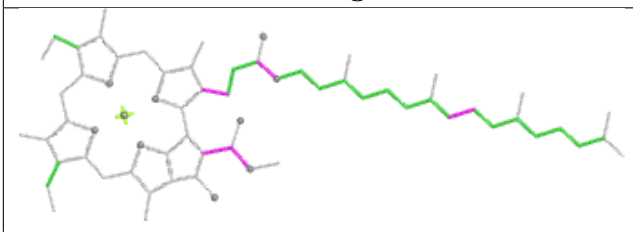
Ligand CLA A2 832



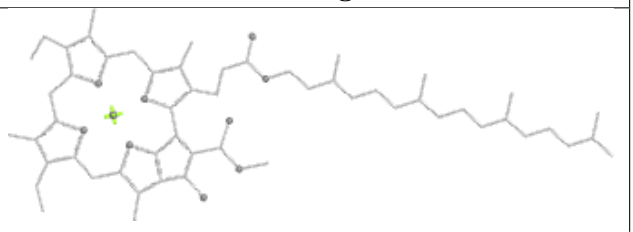
Bond lengths



Bond angles

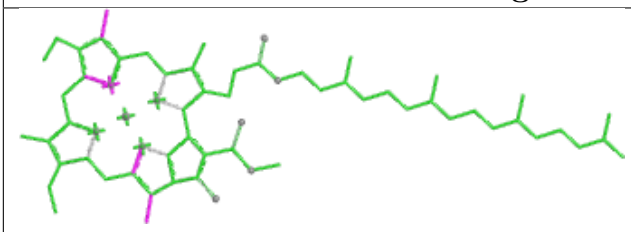


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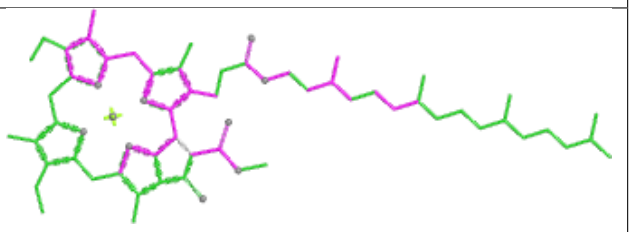


Rings

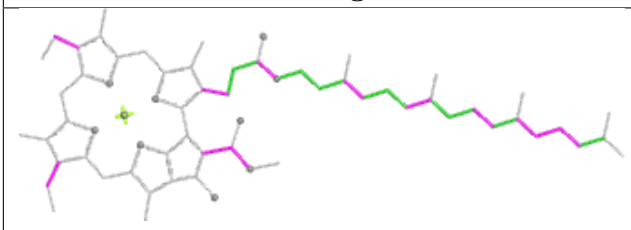
Ligand CLA BB 833



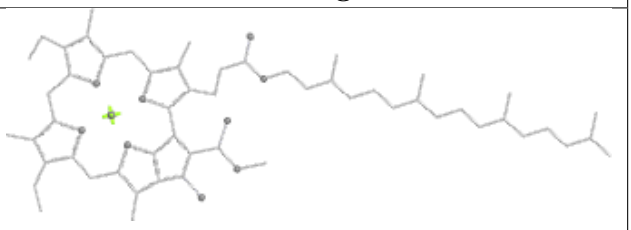
Bond lengths



Bond angles

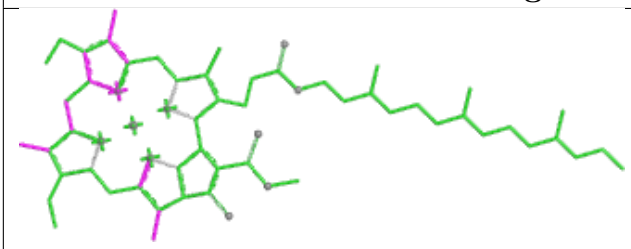


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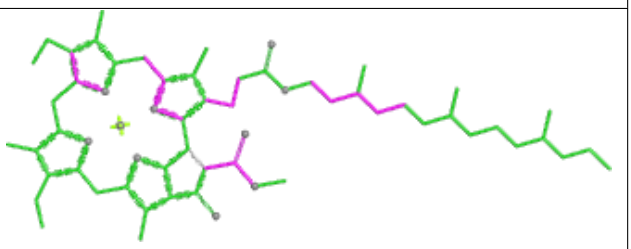


Rings

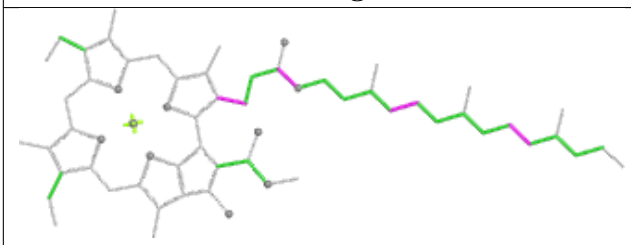
Ligand CLA B 804



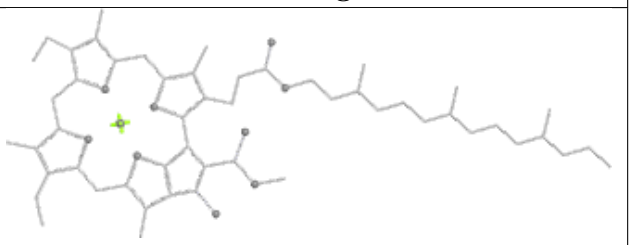
Bond lengths



Bond angles

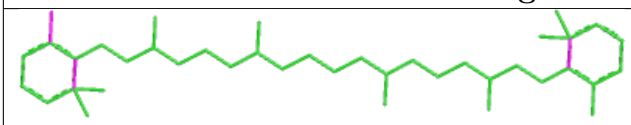


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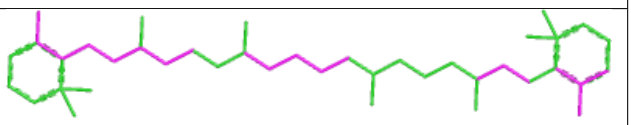


Rings

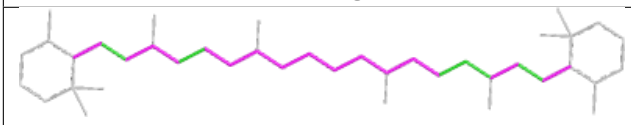
Ligand BCR M 101



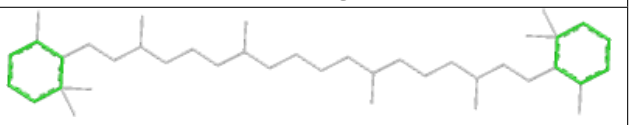
Bond lengths



Bond angles

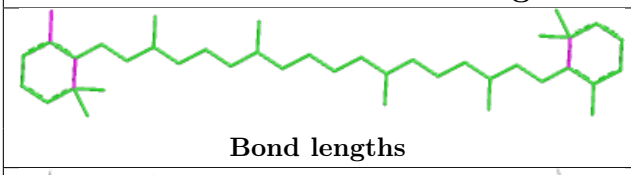


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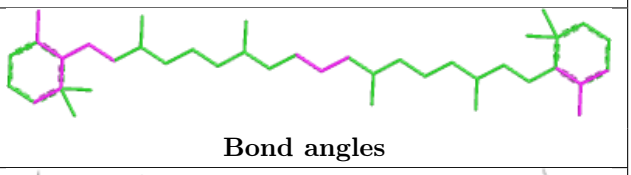


Rings

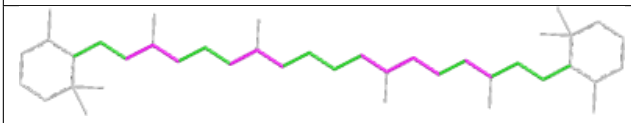
Ligand BCR K2 103



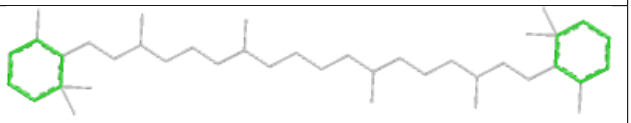
Bond lengths



Bond angles

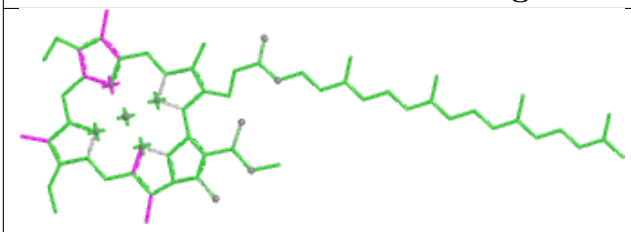


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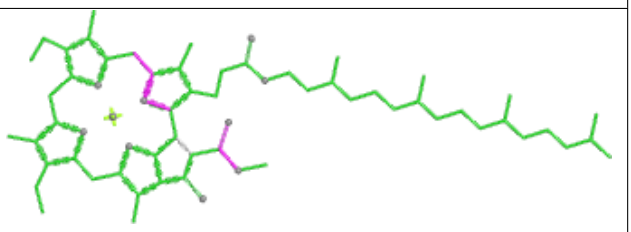


Rings

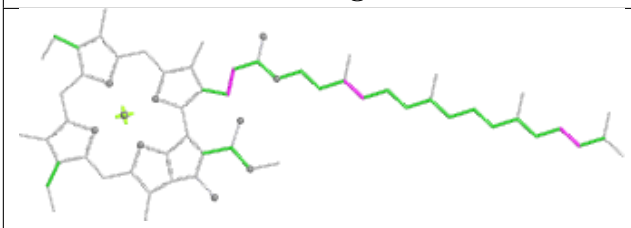
Ligand CLA BB 855



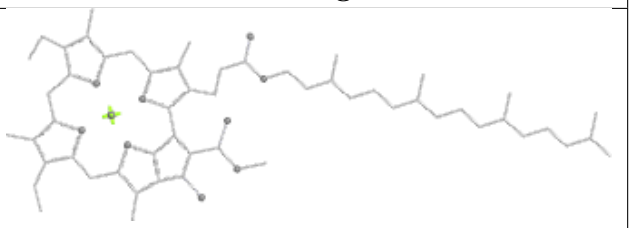
Bond lengths



Bond angles

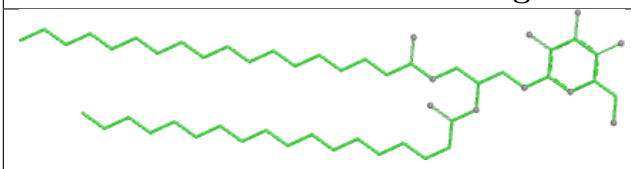


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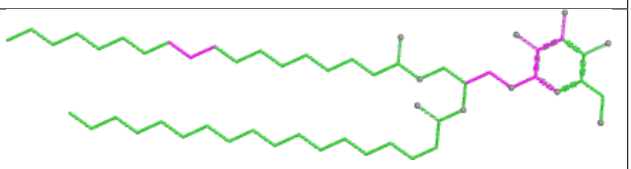


Rings

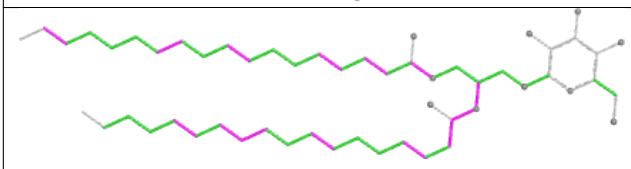
Ligand LMG L1 210



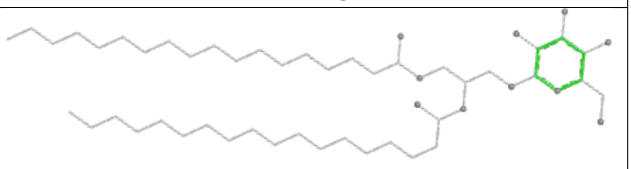
Bond lengths



Bond angles

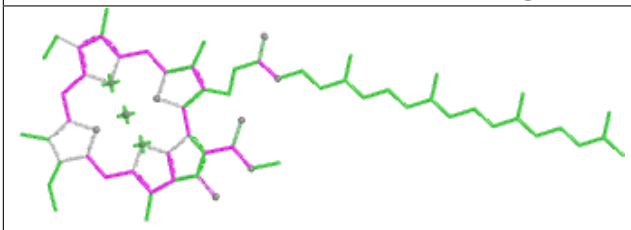


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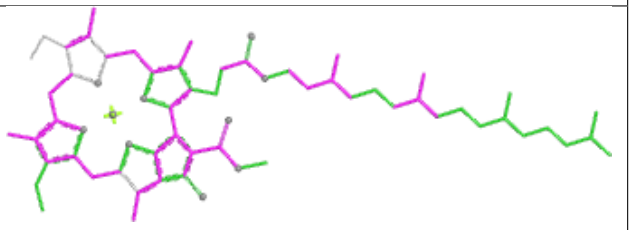


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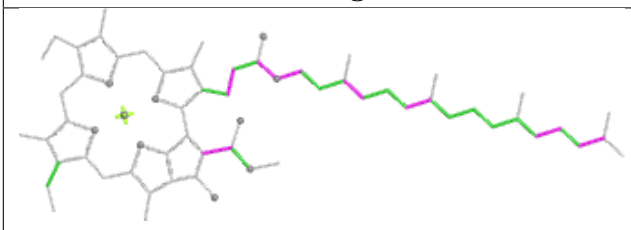
Ligand CL0 A1 802



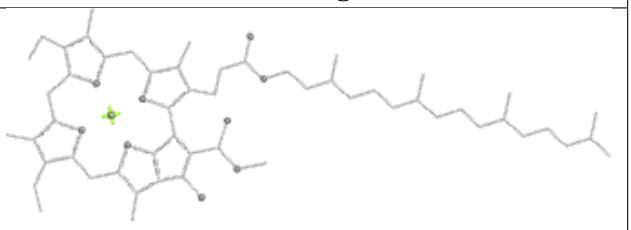
Bond lengths



Bond angles

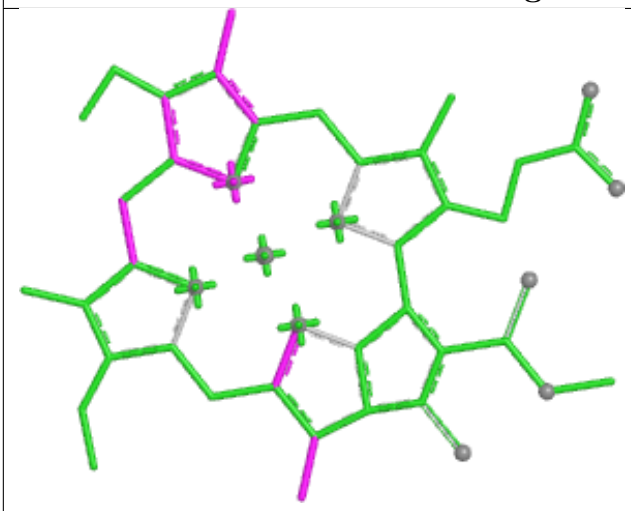


Torsions

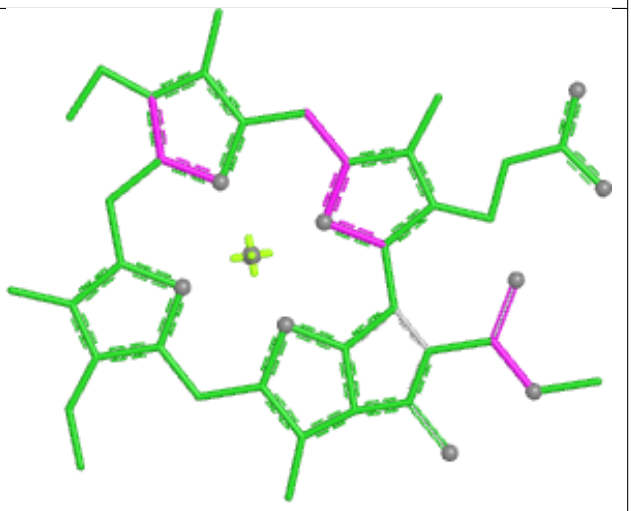


Rings

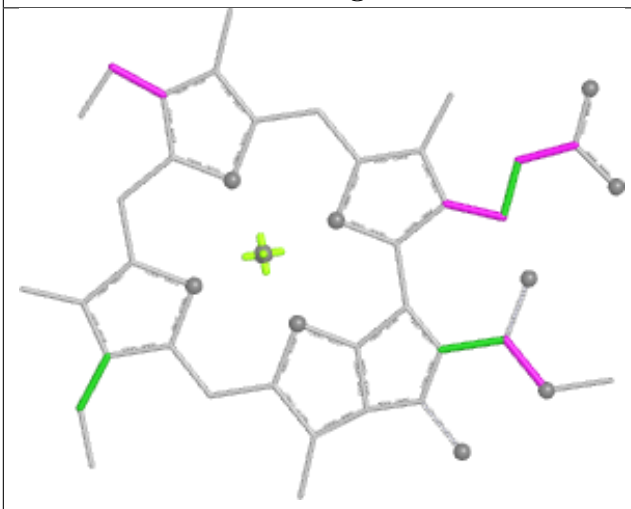
Ligand CLA B 832



Bond lengths



Bond angles

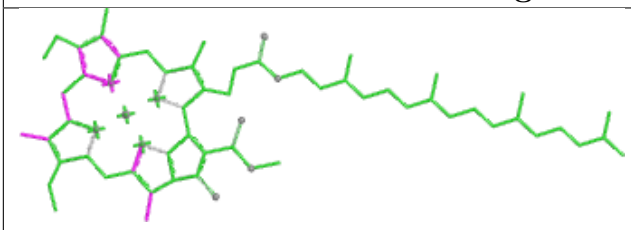


Torsions

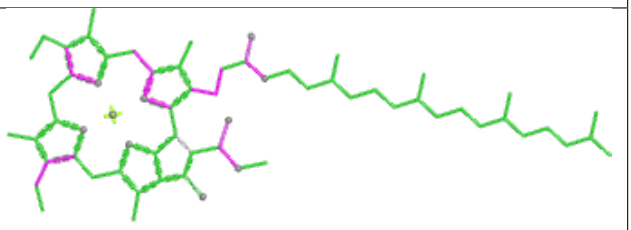


Rings

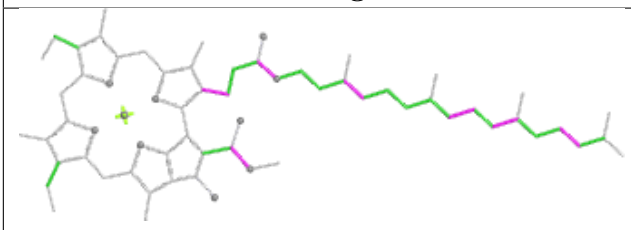
Ligand CLA A2 821



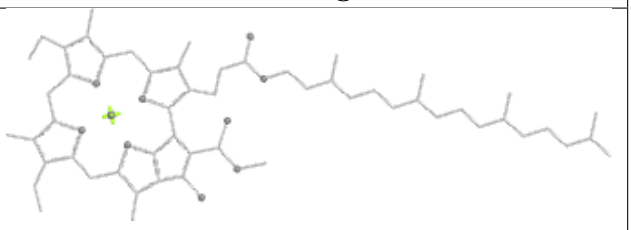
Bond lengths



Bond angles

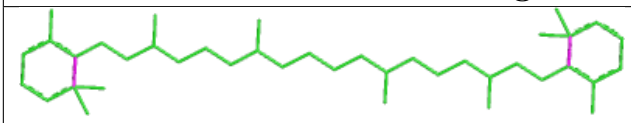


Torsions

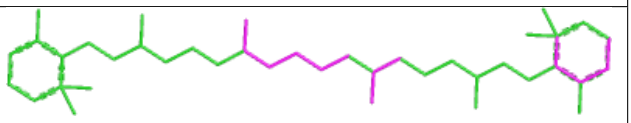


Rings

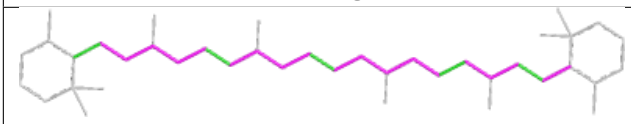
Ligand BCR B1 841



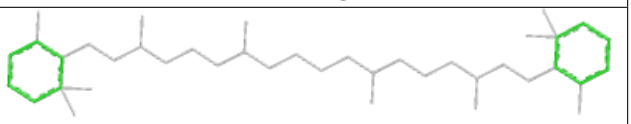
Bond lengths



Bond angles

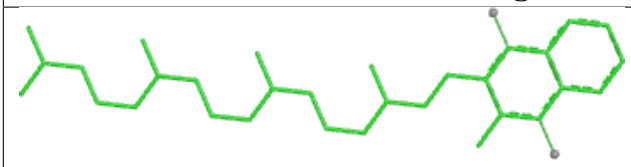


Torsions

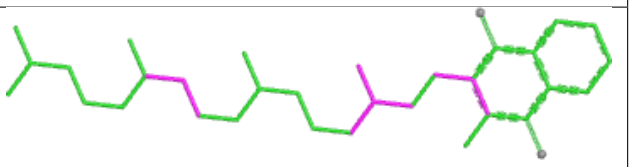


Rings

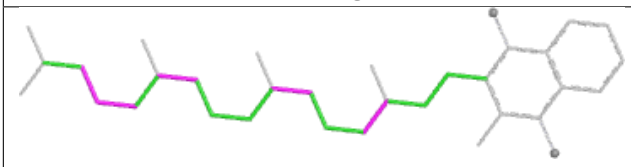
Ligand PQN A1 843



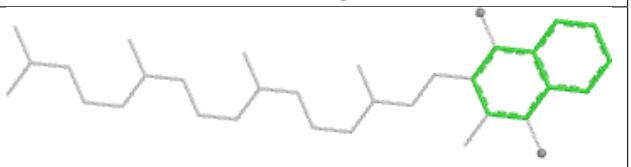
Bond lengths



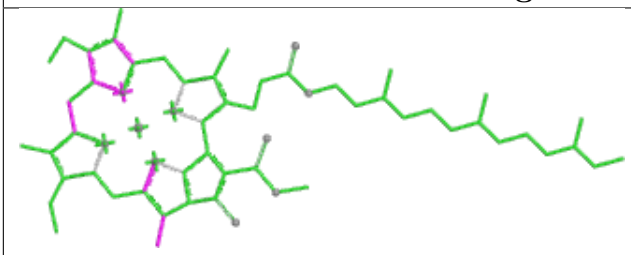
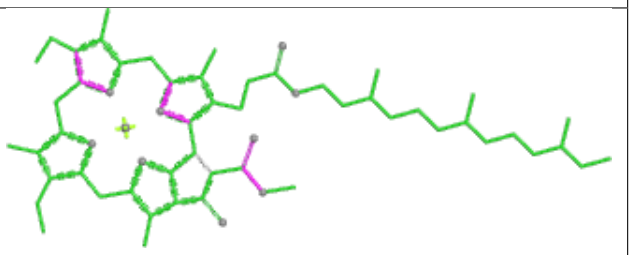
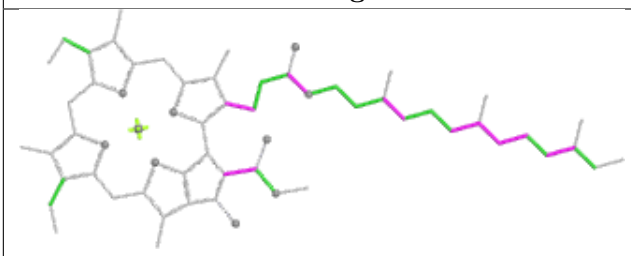
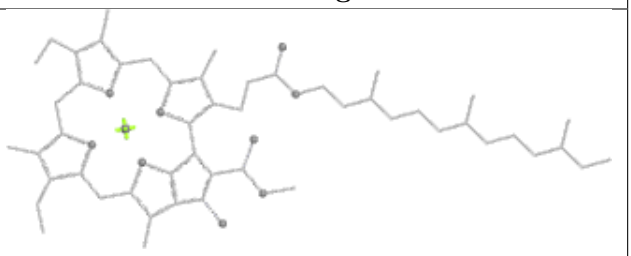
Bond angles

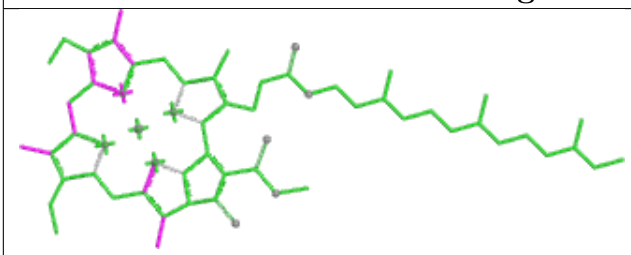
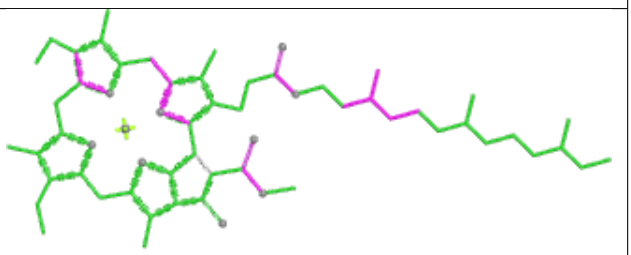
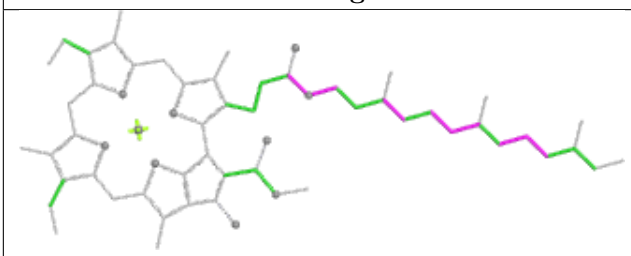
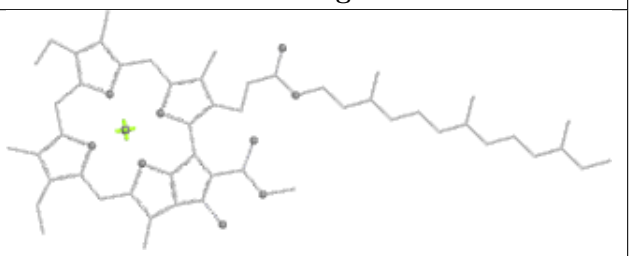


Torsions

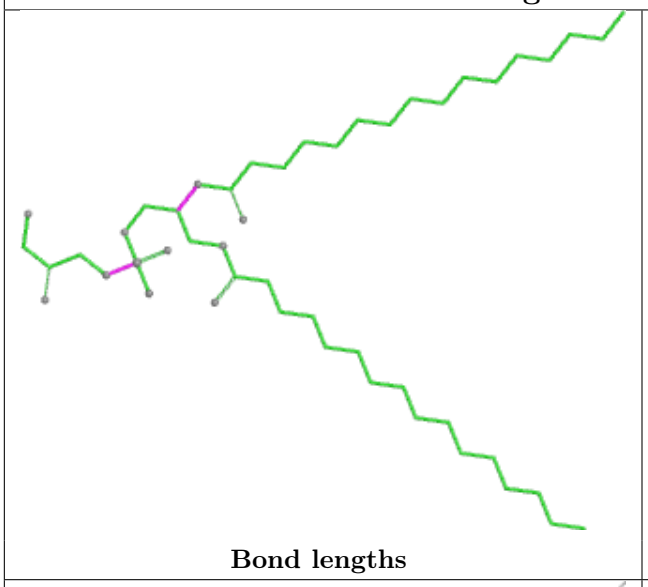


Rings

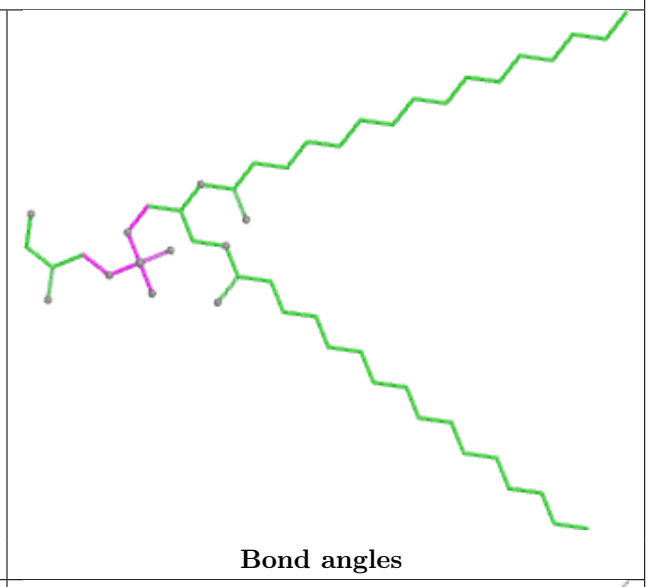
Ligand CLA B2 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L1 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

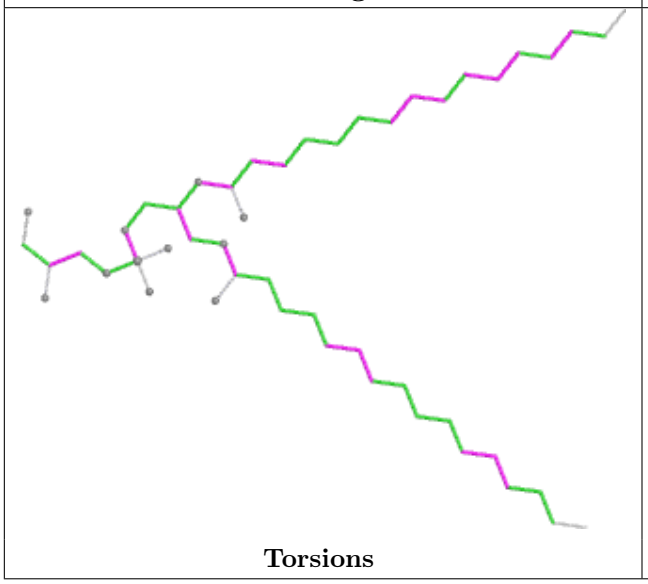
Ligand LHG A 845



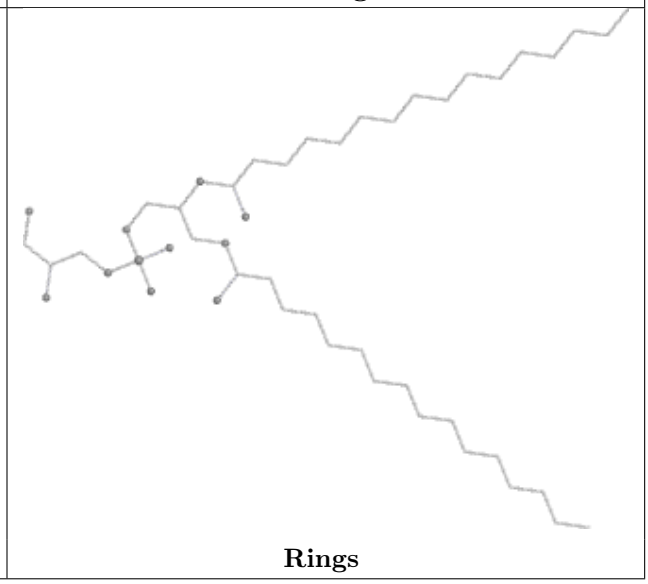
Bond lengths



Bond angles

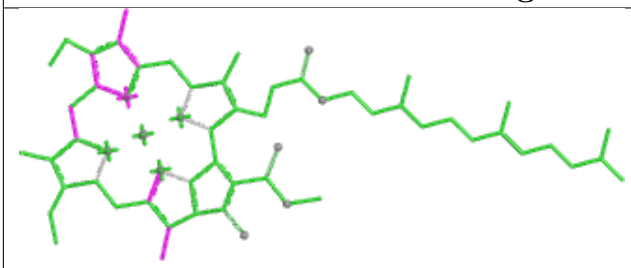


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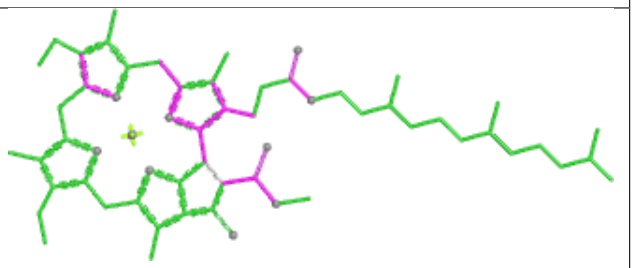


Rings

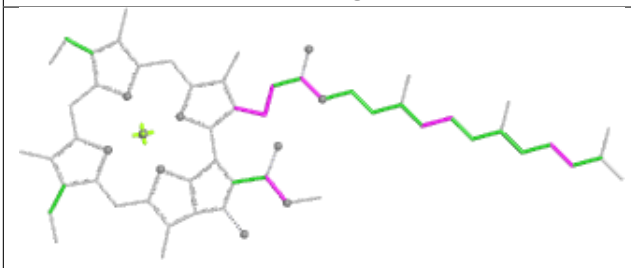
Ligand CLA F1 301



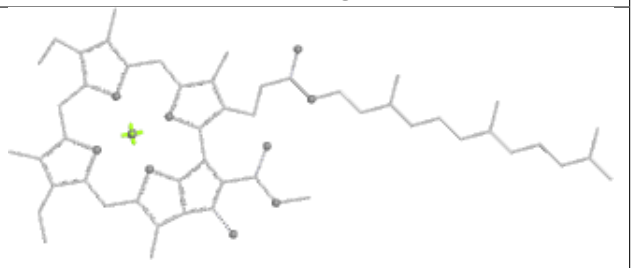
Bond lengths



Bond angles

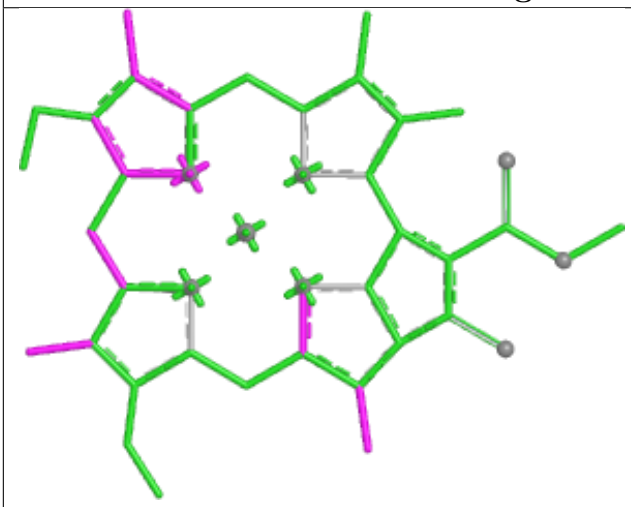


Torsions

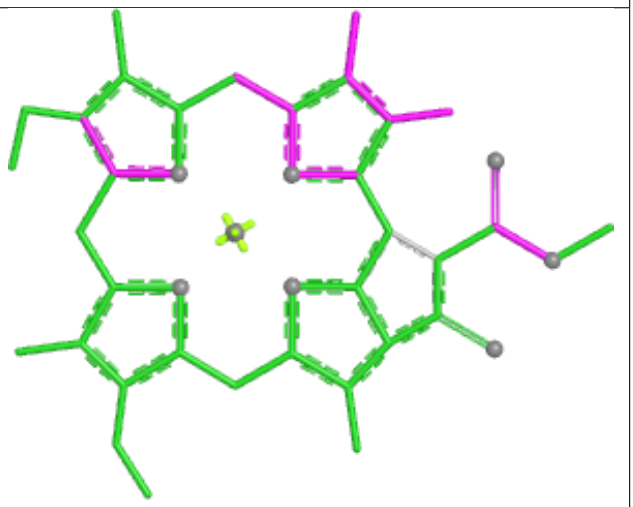


Rings

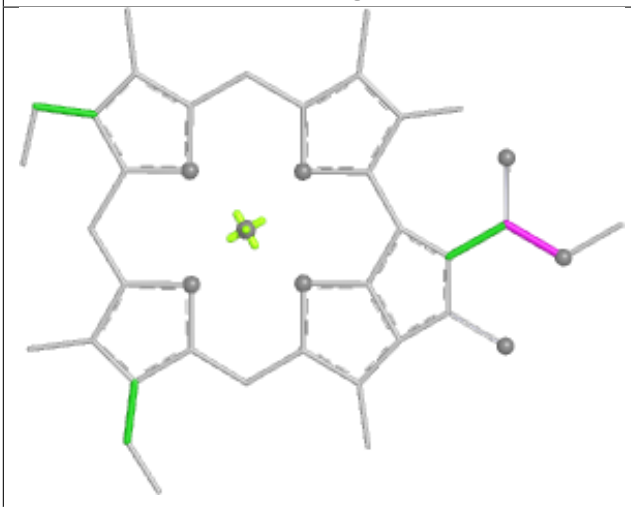
Ligand CLA A1 833



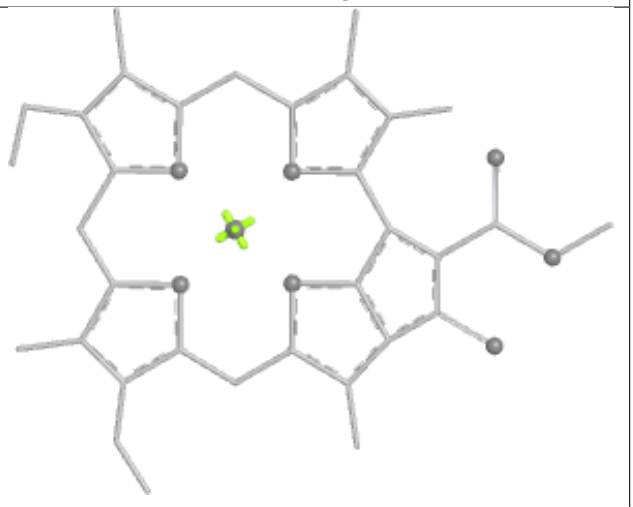
Bond lengths



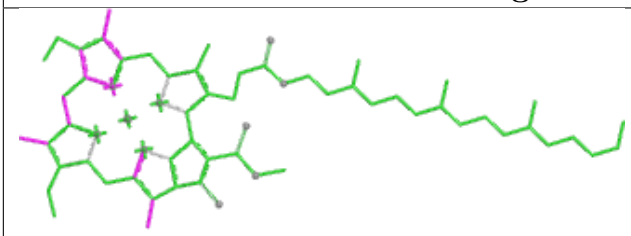
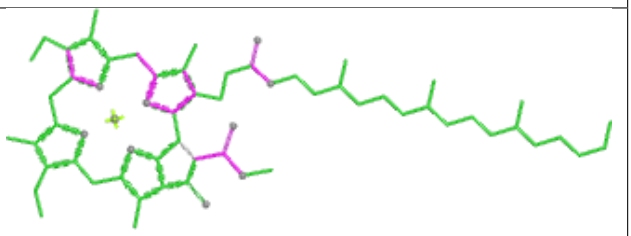
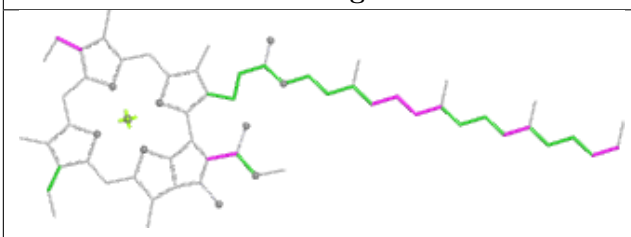
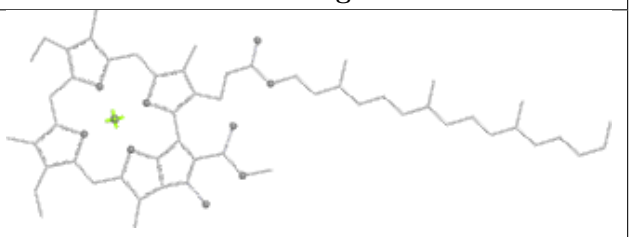
Bond angles

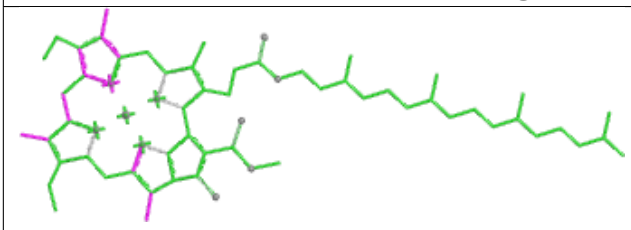
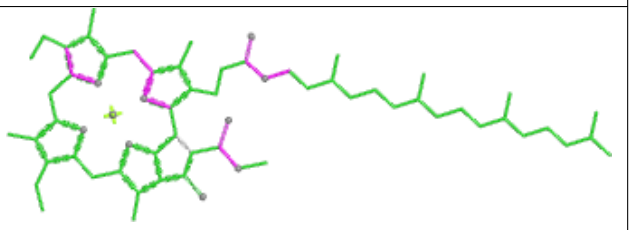
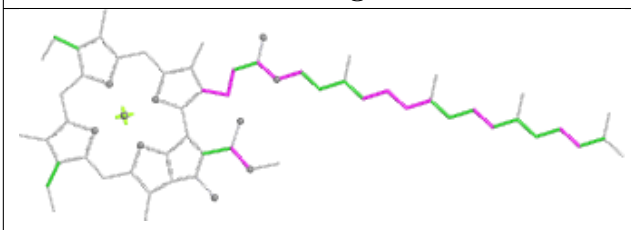
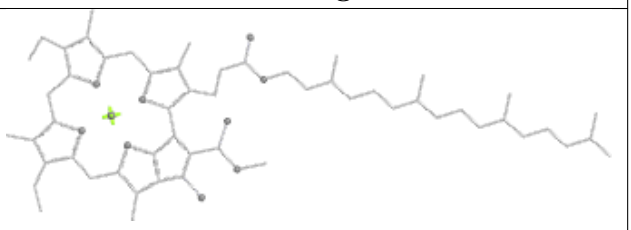


Torsions

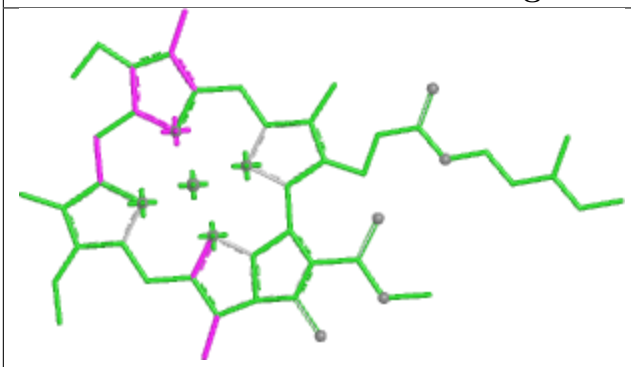


Rings

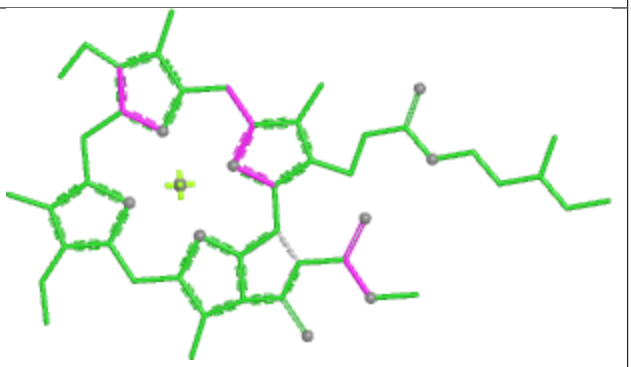
Ligand CLA BB 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

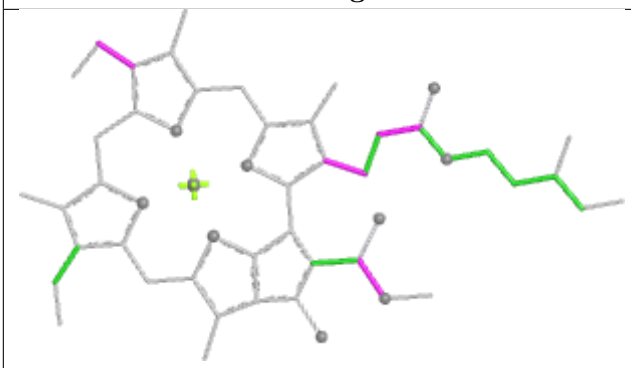
Ligand CLA A 822



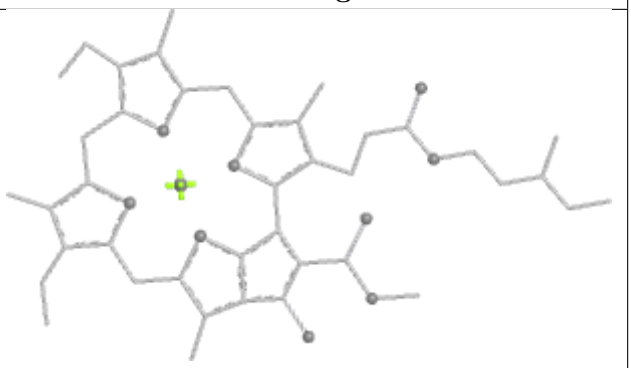
Bond lengths



Bond angles

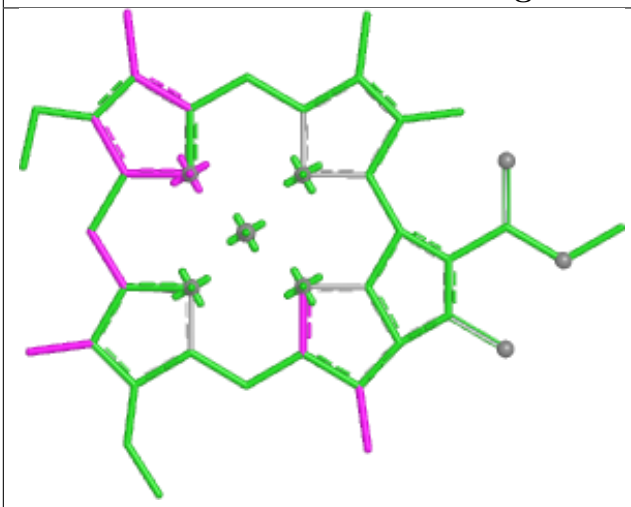


Torsions

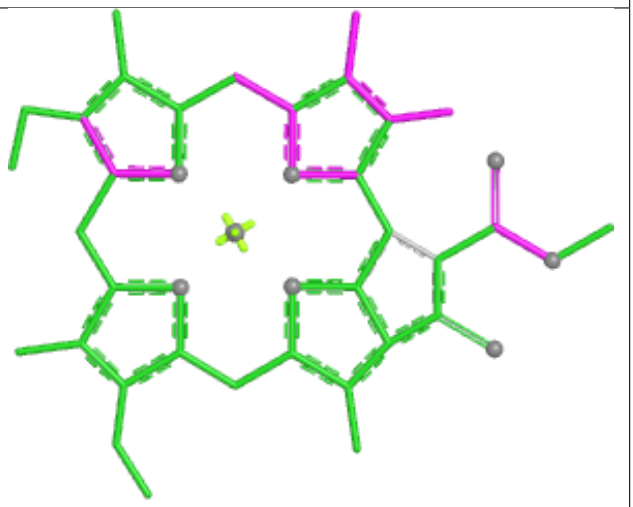


Rings

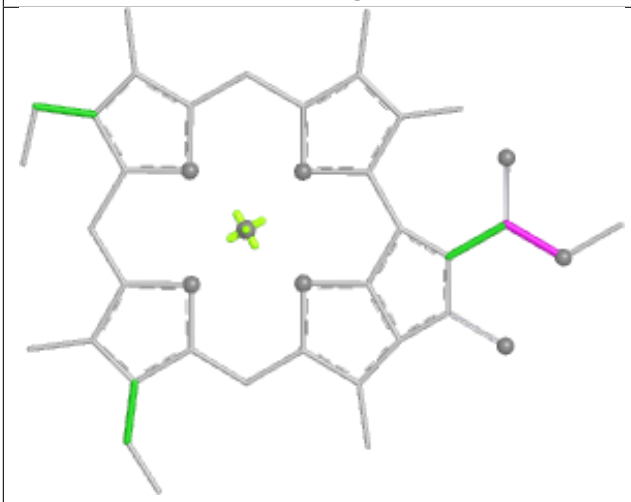
Ligand CLA A2 834



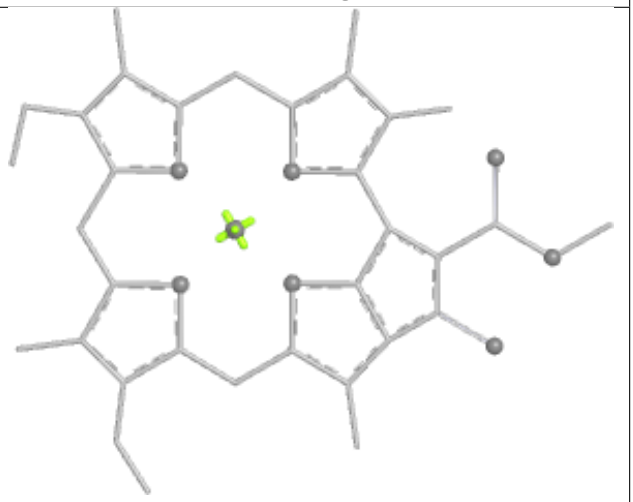
Bond lengths



Bond angles

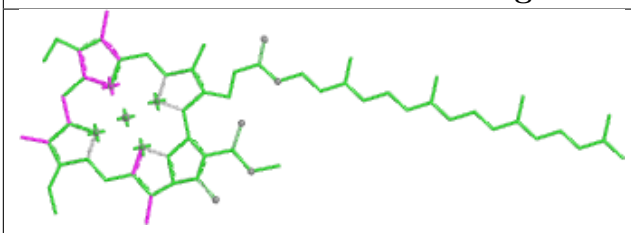


Torsions

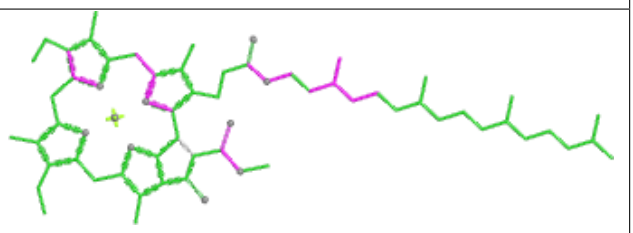


Rings

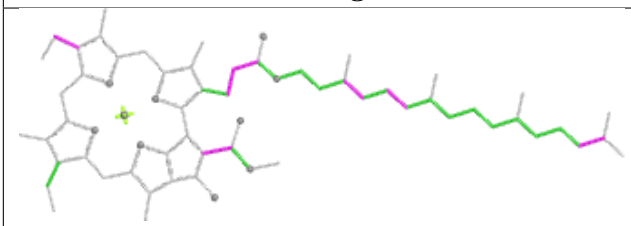
Ligand CLA A2 842



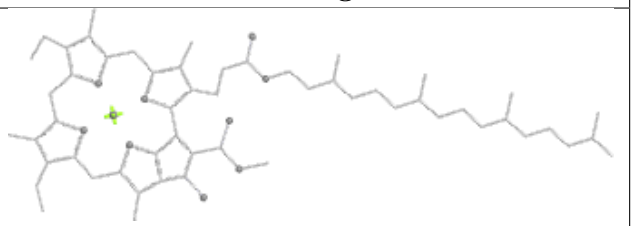
Bond lengths



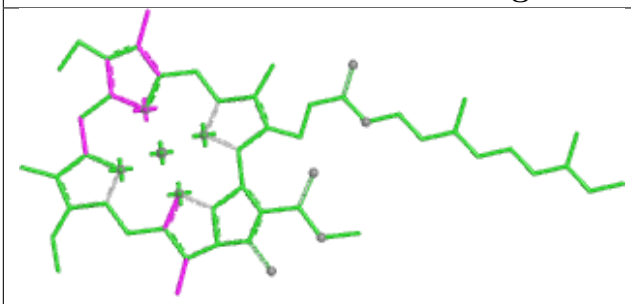
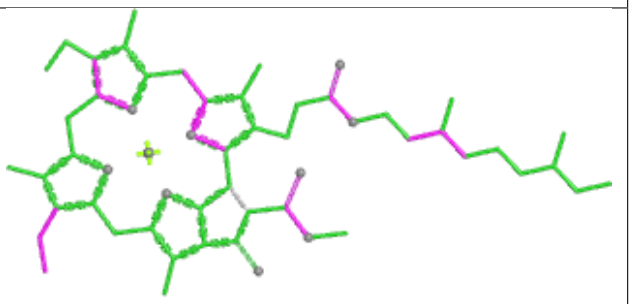
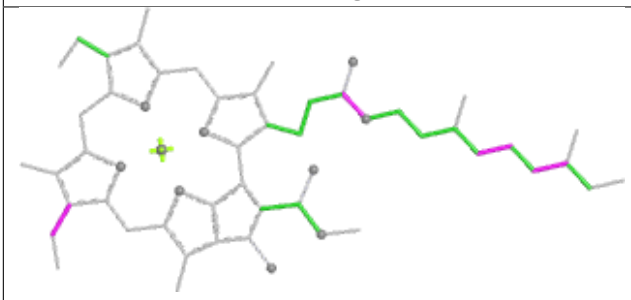
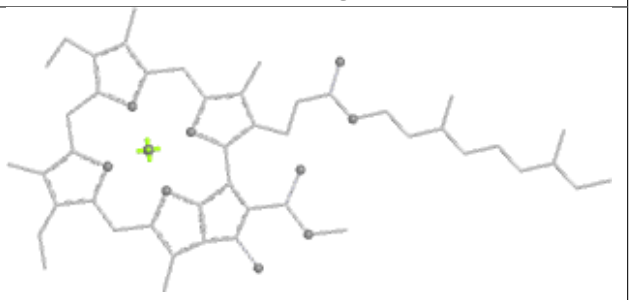
Bond angles

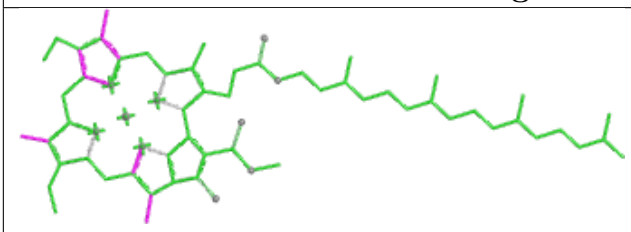
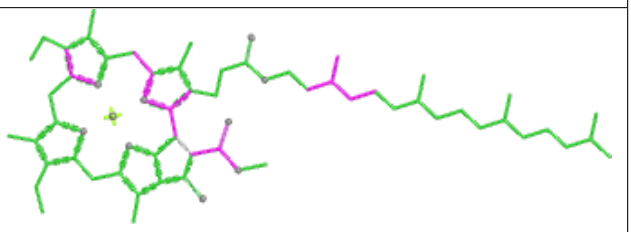
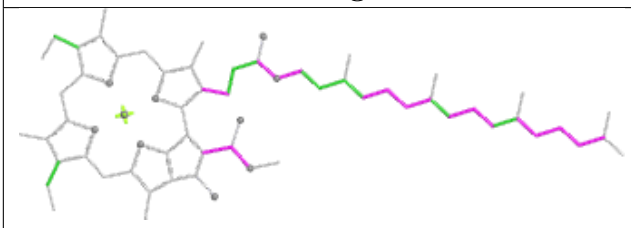
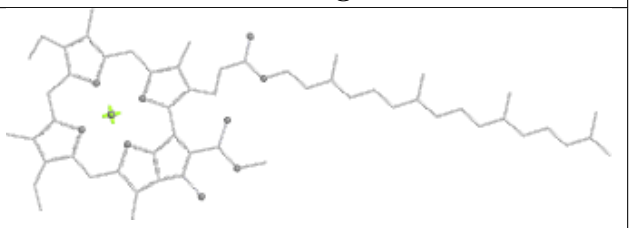


Torsions

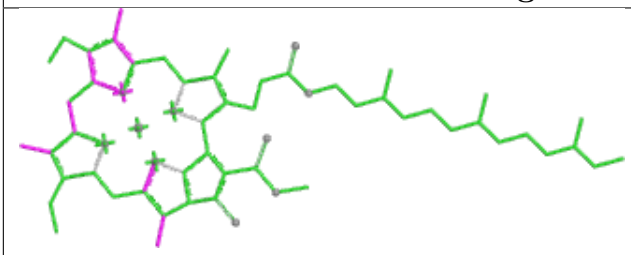


Rings

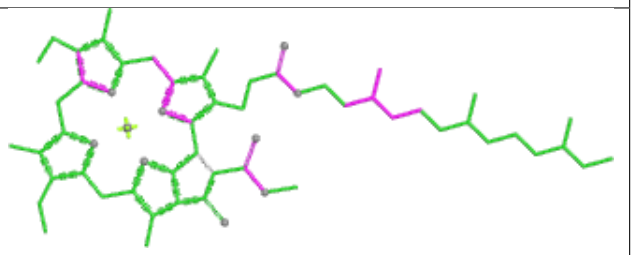
Ligand CLA BB 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BB 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

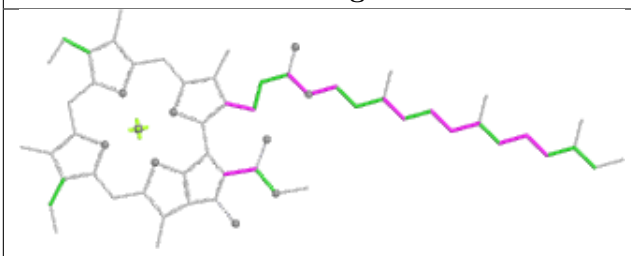
Ligand CLA L2 204



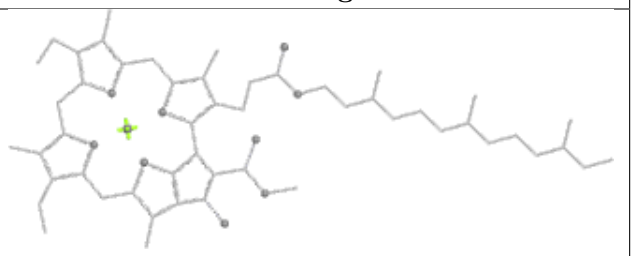
Bond lengths



Bond angles

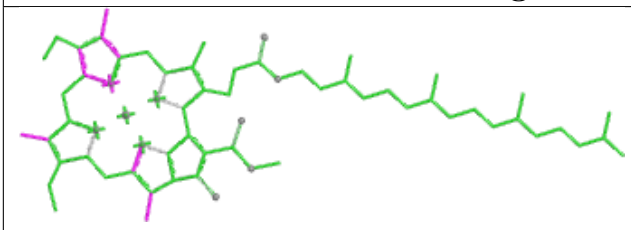


Torsions

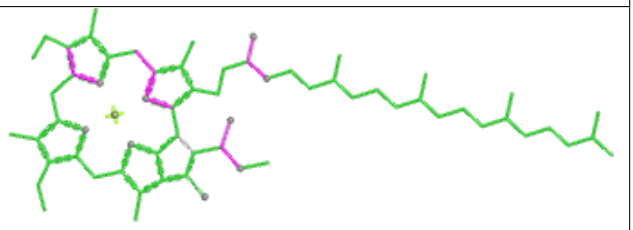


Rings

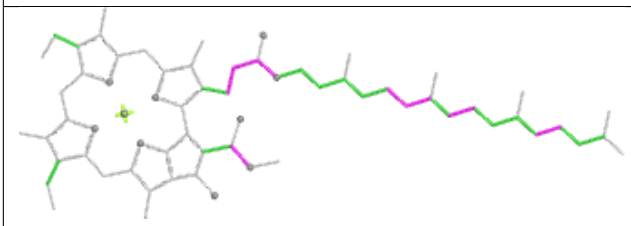
Ligand CLA AA 831



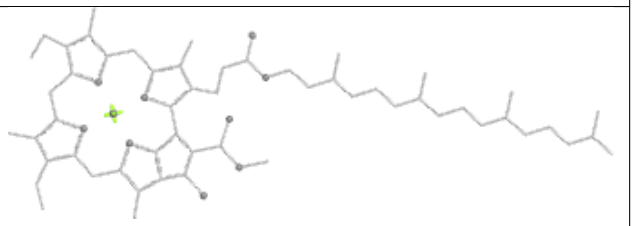
Bond lengths



Bond angles

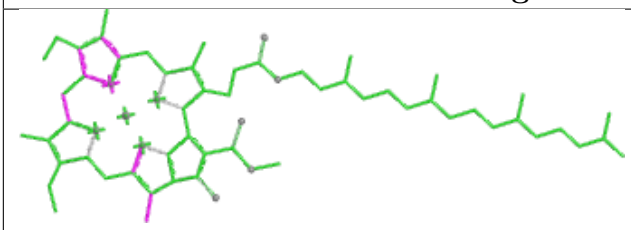


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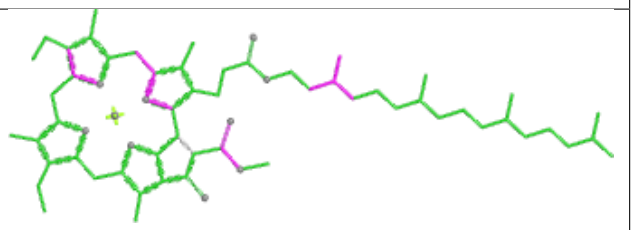


Rings

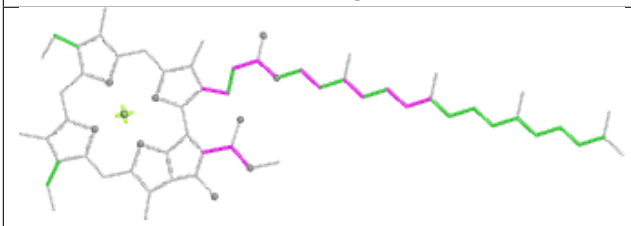
Ligand CLA BB 821



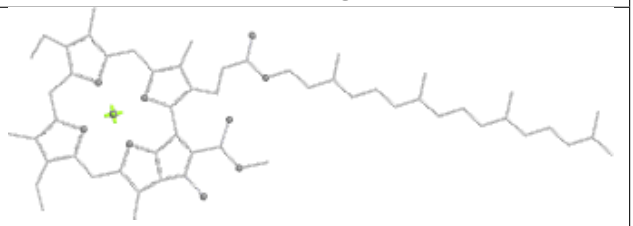
Bond lengths



Bond angles

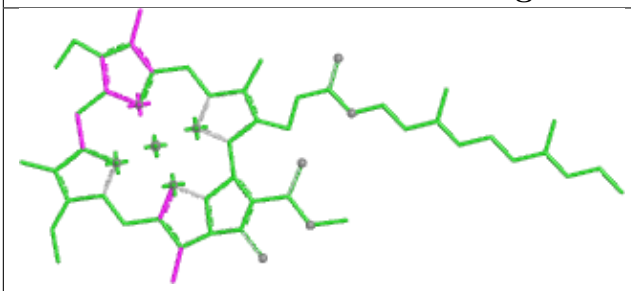


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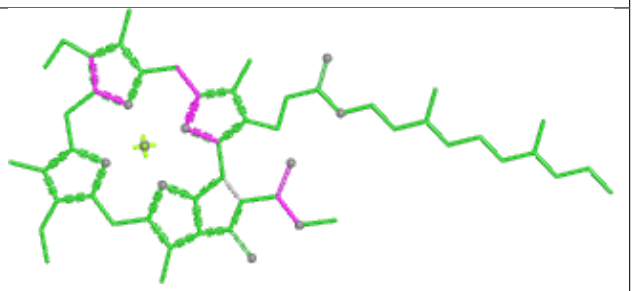


Rings

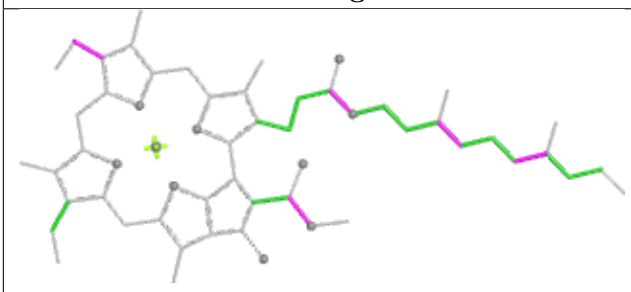
Ligand CLA B2 816



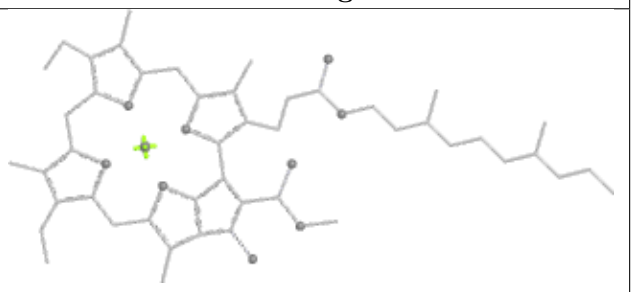
Bond lengths



Bond angles

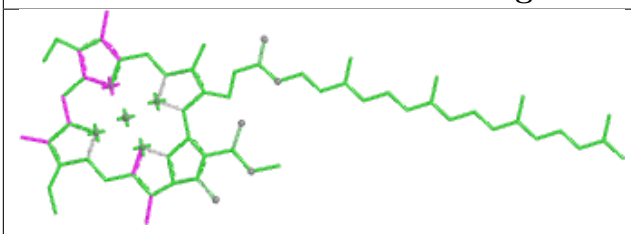


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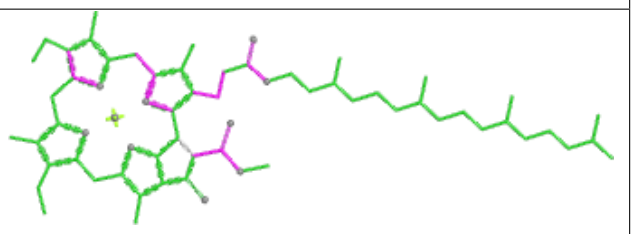


Rings

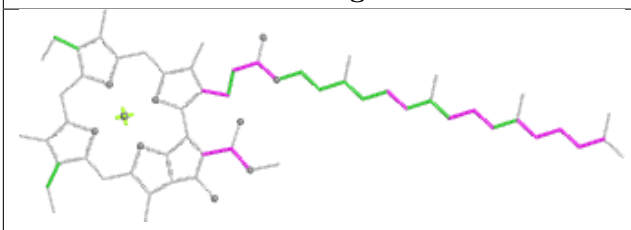
Ligand CLA B2 801



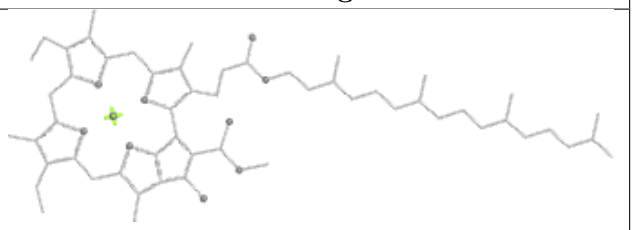
Bond lengths



Bond angles

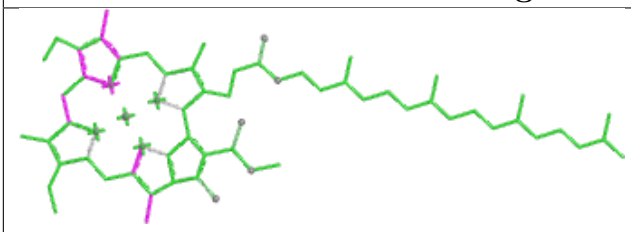


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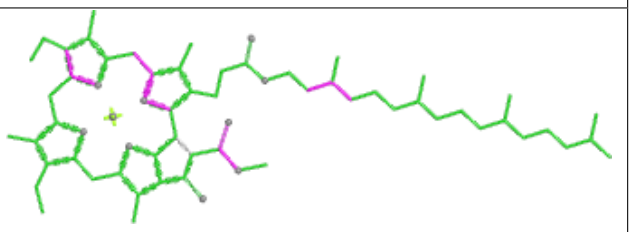


Rings

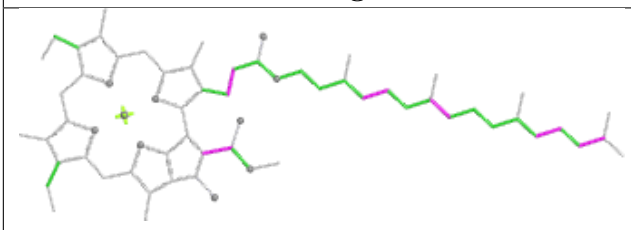
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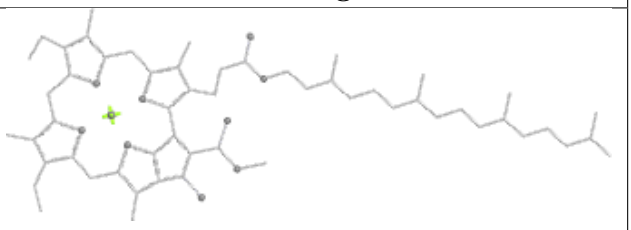
Bond lengths



Bond angles

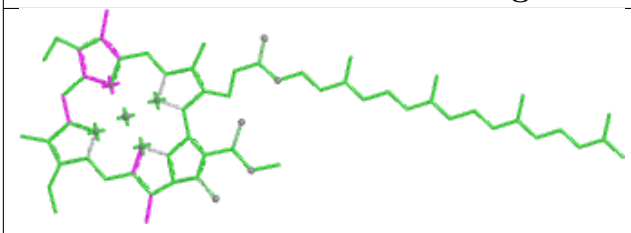


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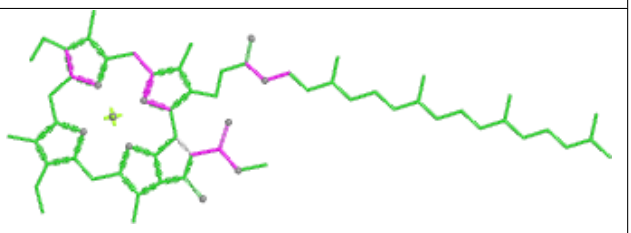


Rings

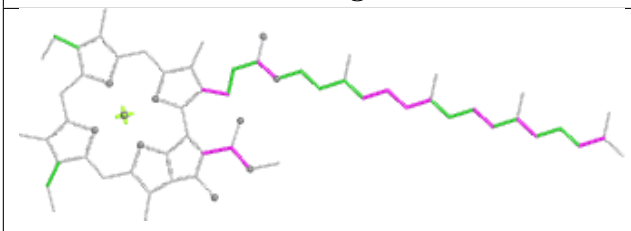
Ligand CLA BB 825



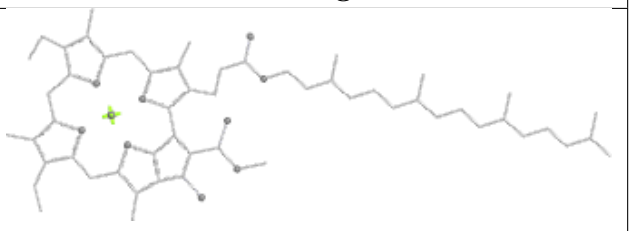
Bond lengths



Bond angles

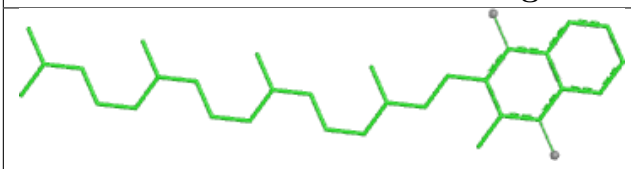


Torsions

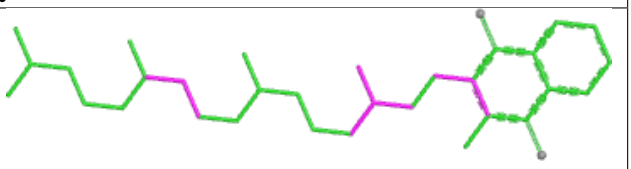


Rings

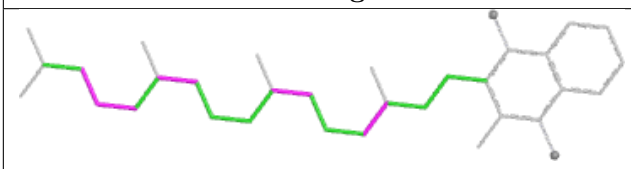
Ligand PQN A 843



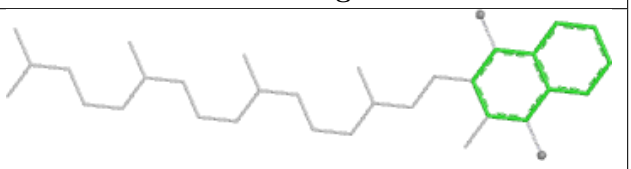
Bond lengths



Bond angles

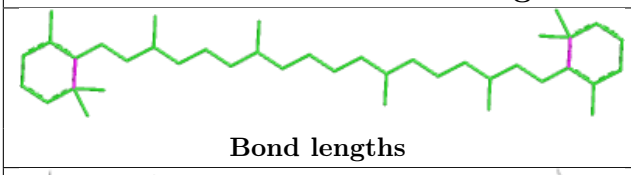


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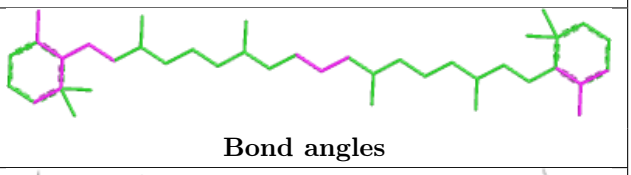


Rings

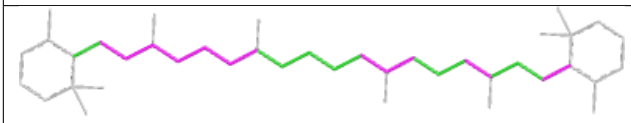
Ligand BCR B1 842



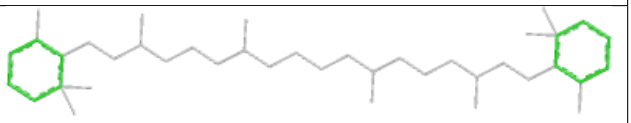
Bond lengths



Bond angles



Torsions

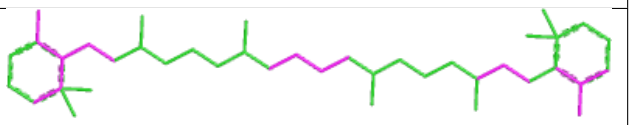


Rings

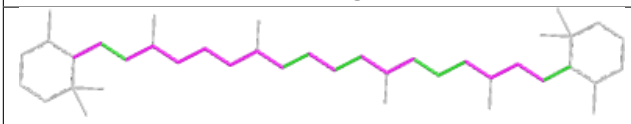
Ligand BCR AA 849



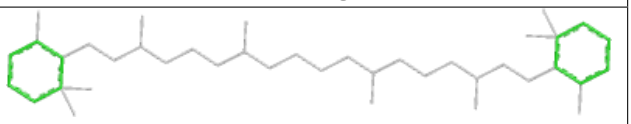
Bond lengths



Bond angles

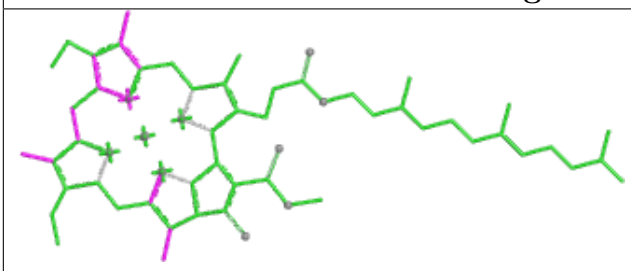


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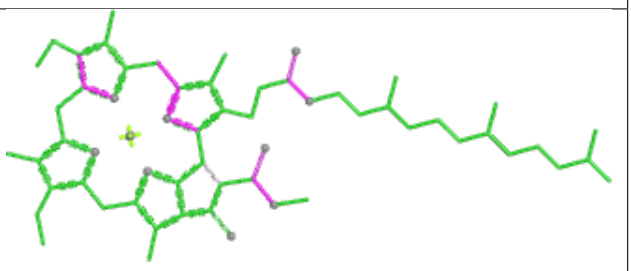


Rings

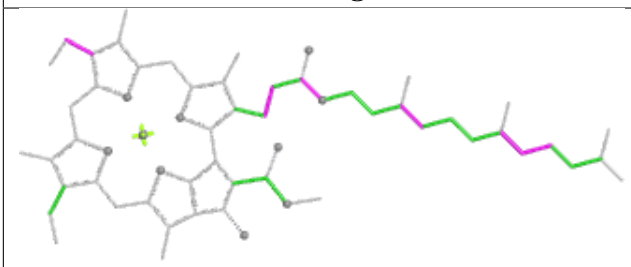
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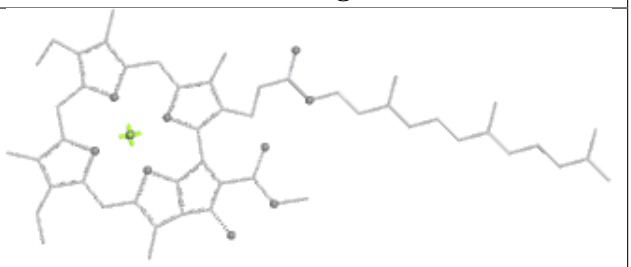
Bond lengths



Bond angles

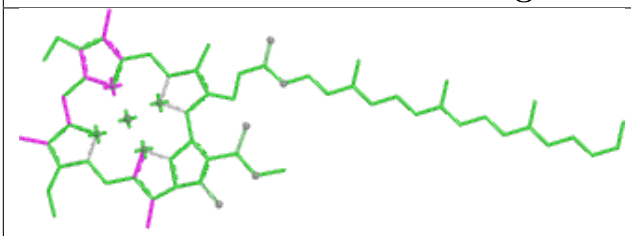


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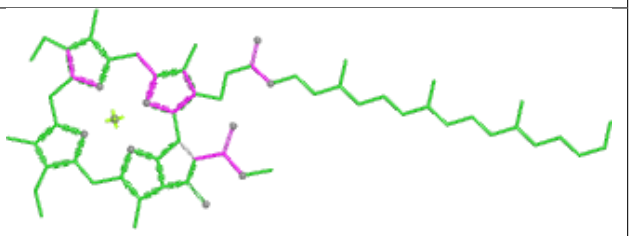


Rings

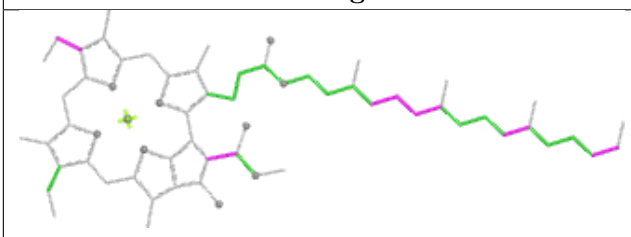
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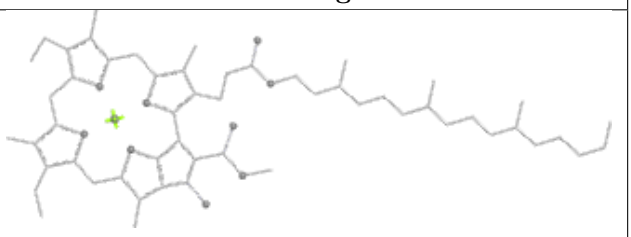
Bond lengths



Bond angles

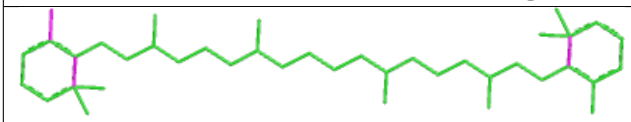


Torsions

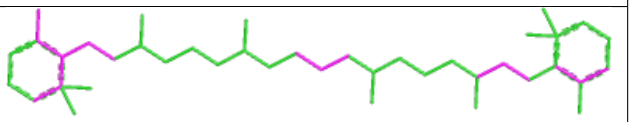


Rings

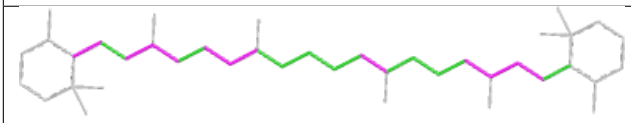
Ligand BCR A 850



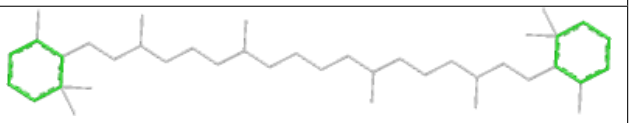
Bond lengths



Bond angles

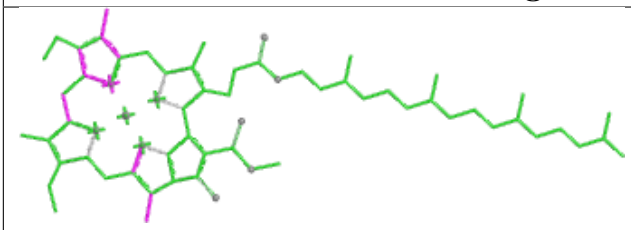


Torsions

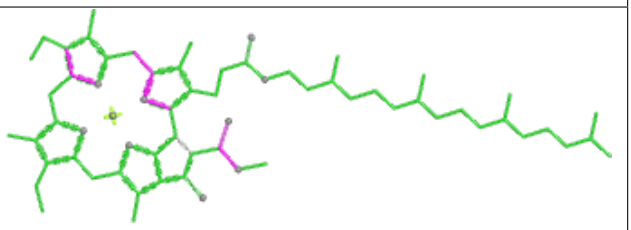


Rings

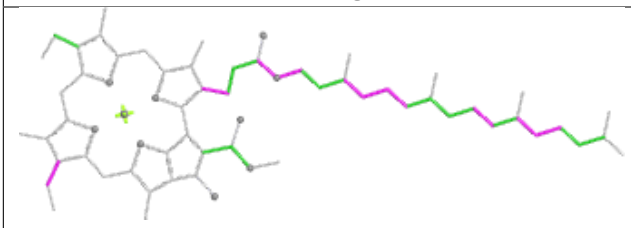
Ligand CLA B 829



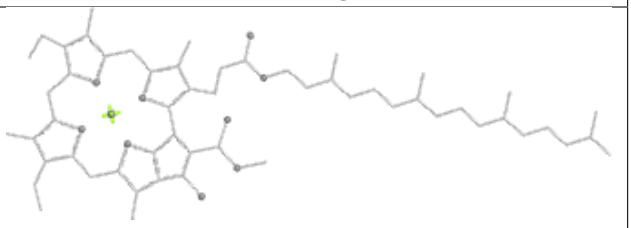
Bond lengths



Bond angles

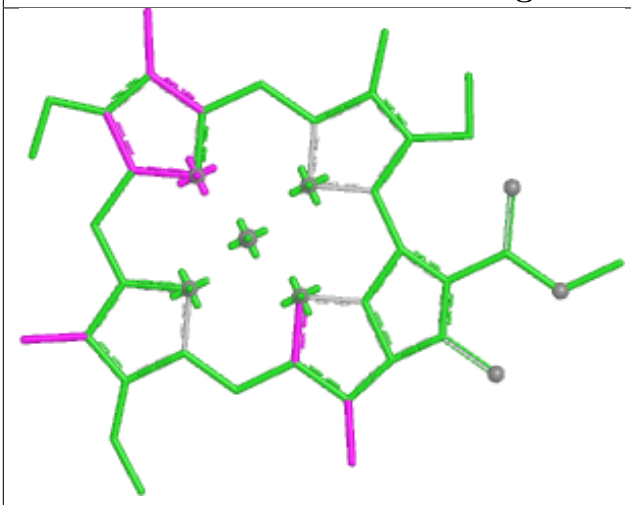


Torsions

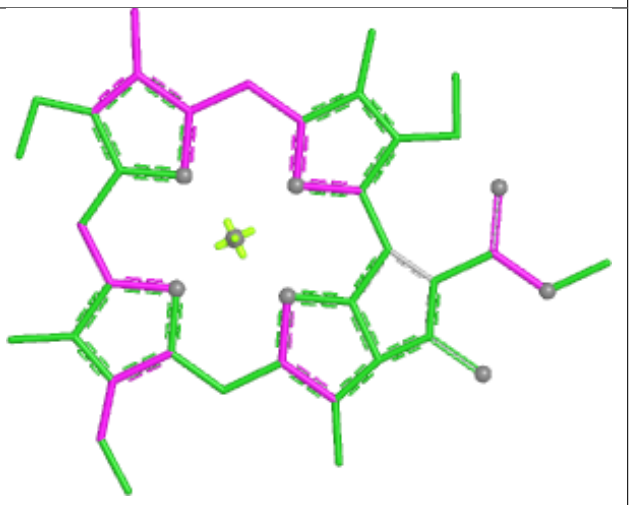


Rings

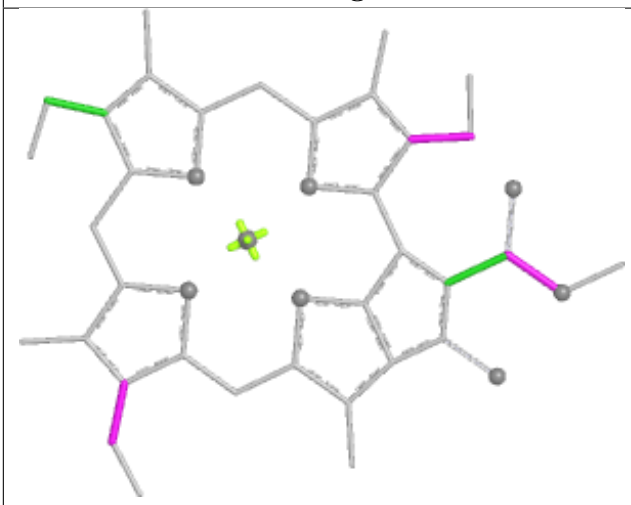
Ligand CLA LL 203



Bond lengths



Bond angles



Torsions

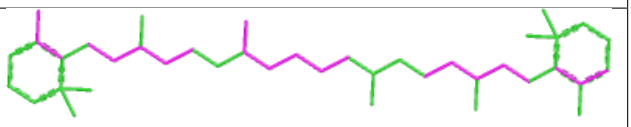


Rings

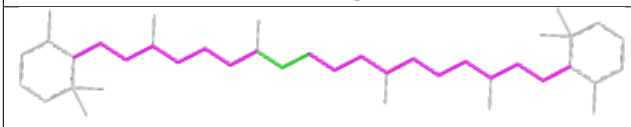
Ligand BCR F2 305



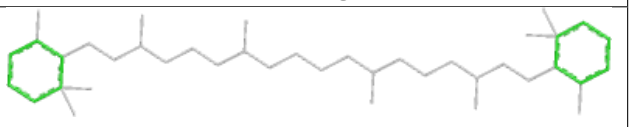
Bond lengths



Bond angles

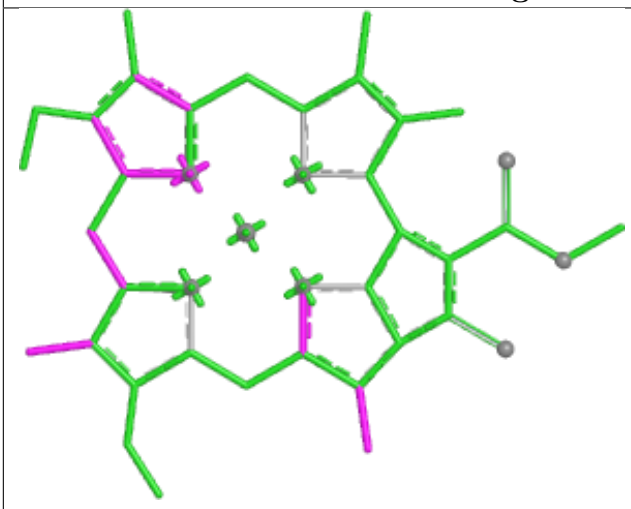


Torsions

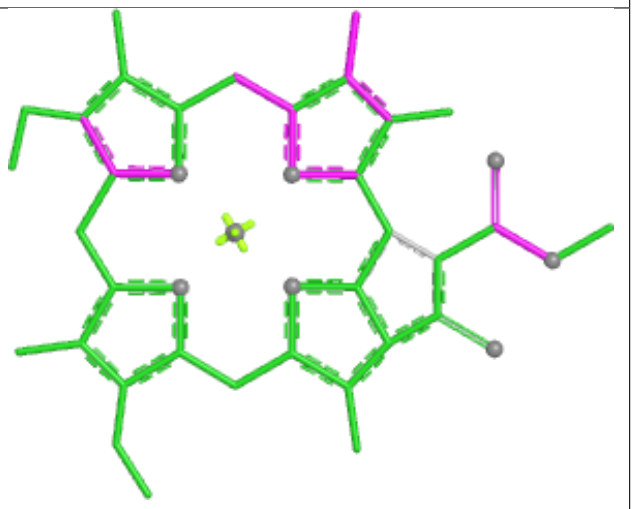


Rings

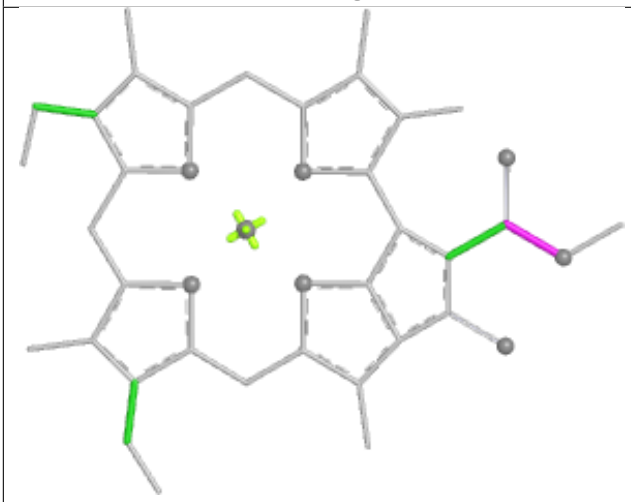
Ligand CLA BB 819



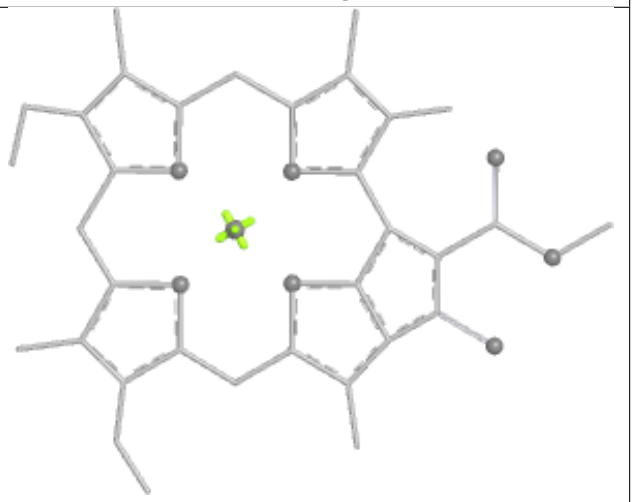
Bond lengths



Bond angles



Torsions

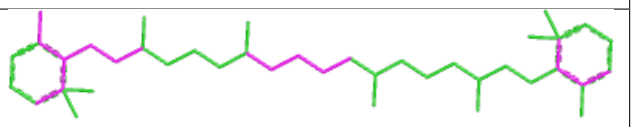


Rings

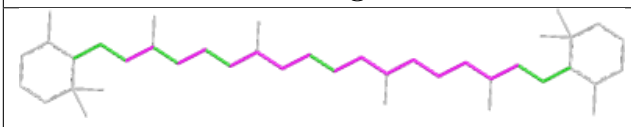
Ligand BCR A1 853



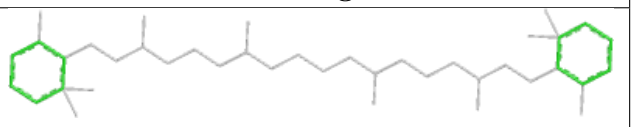
Bond lengths



Bond angles

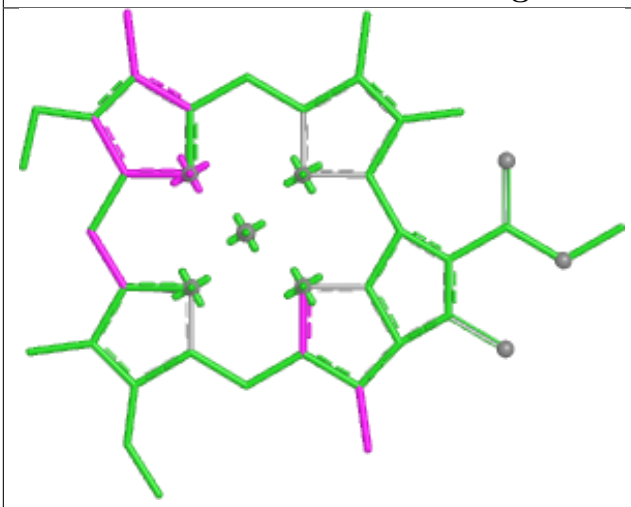


Torsions

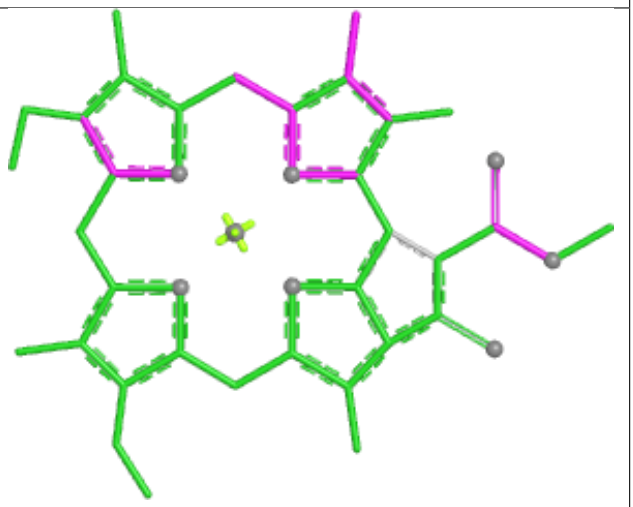


Rings

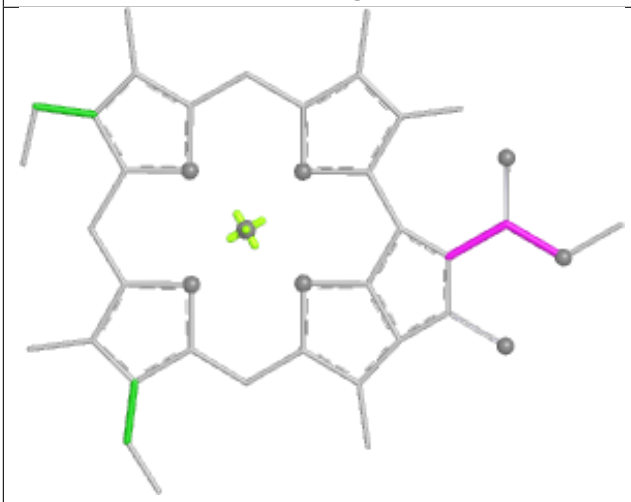
Ligand CLA BB 812



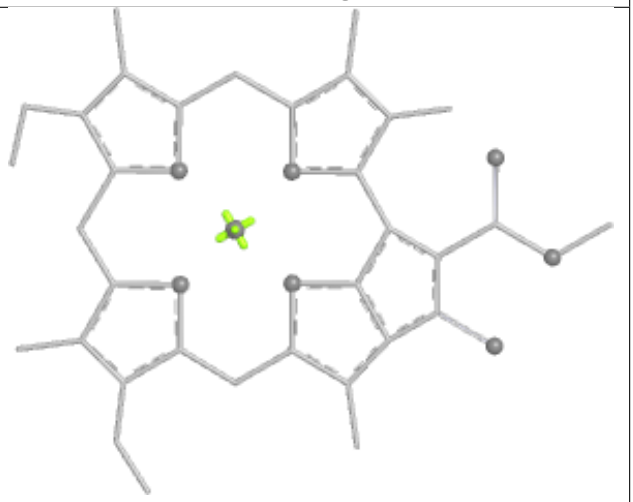
Bond lengths



Bond angles

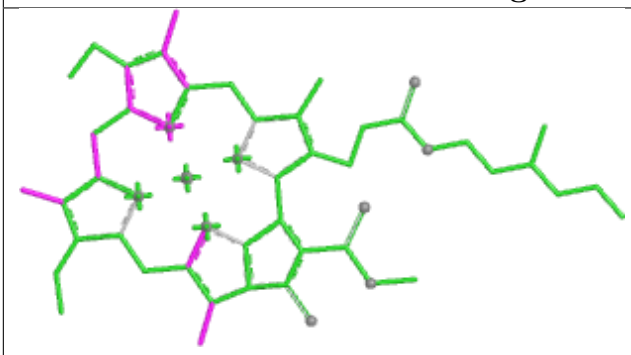


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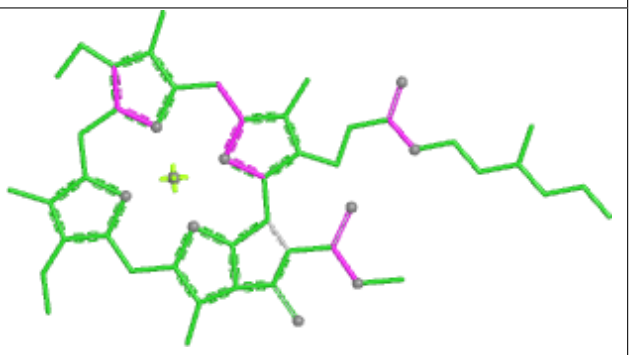


Rings

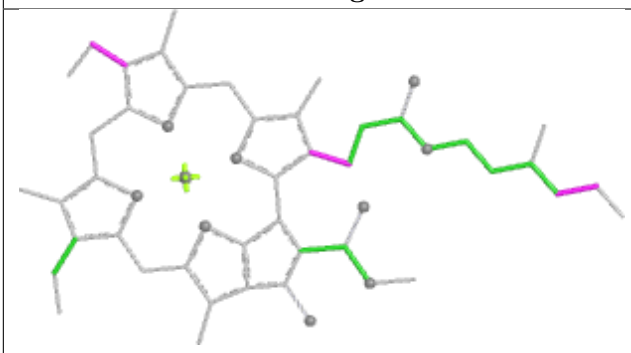
Ligand CLA AA 825



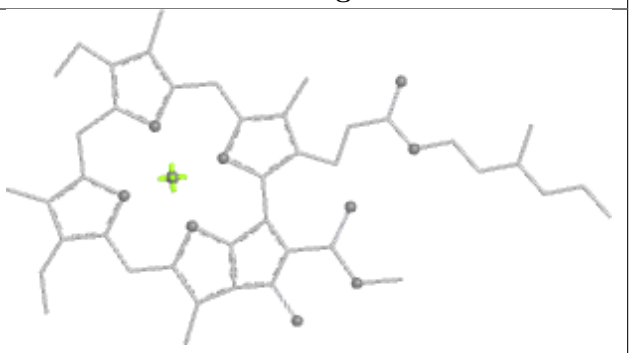
Bond lengths



Bond angles

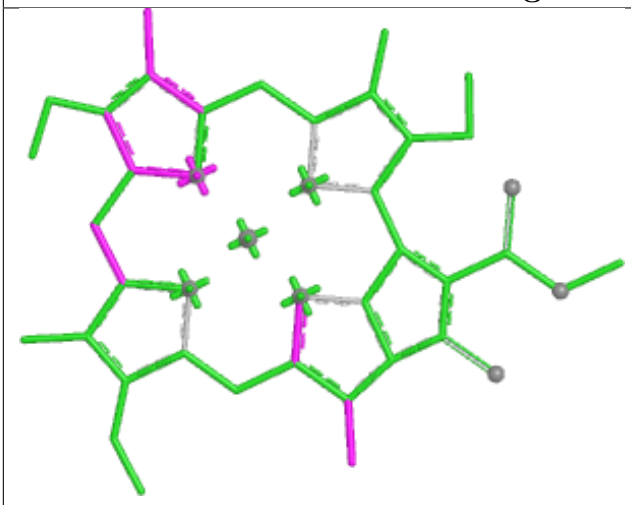


Torsions

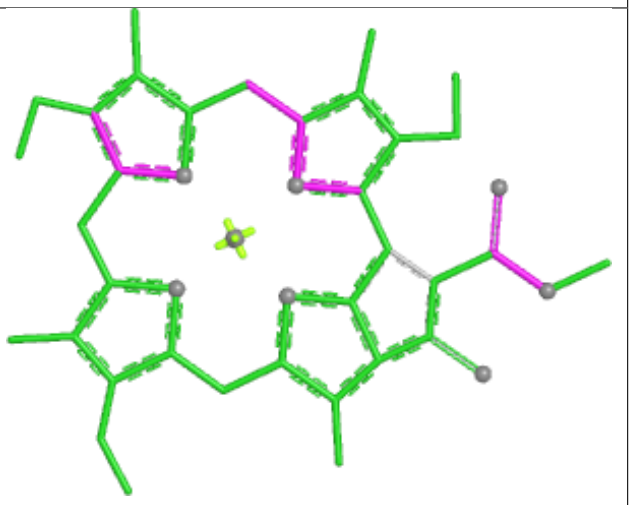


Rings

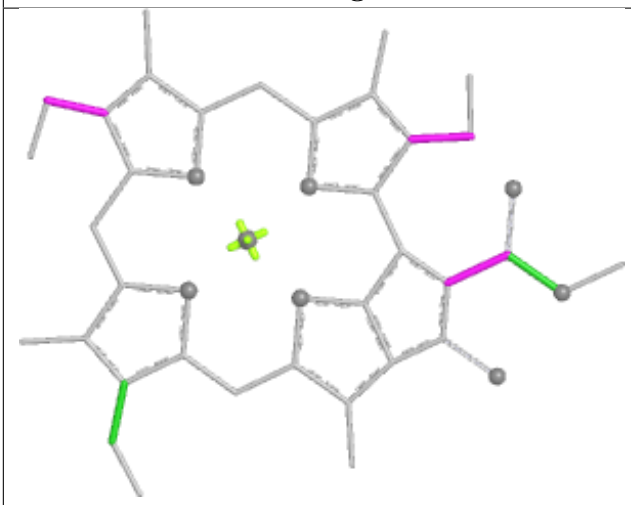
Ligand CLA A 814



Bond lengths



Bond angles

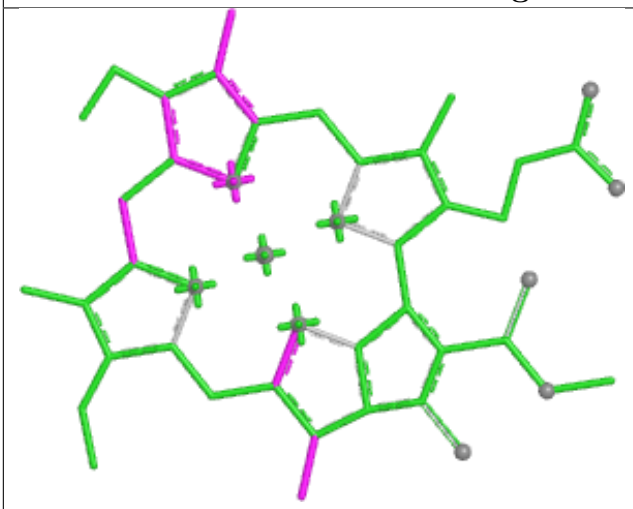


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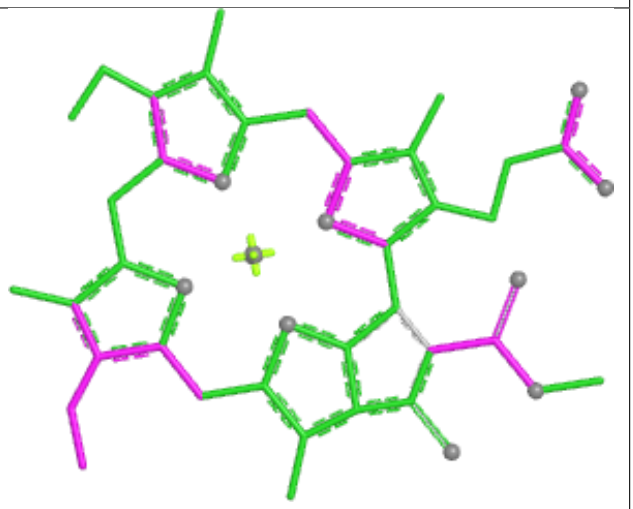


Rings

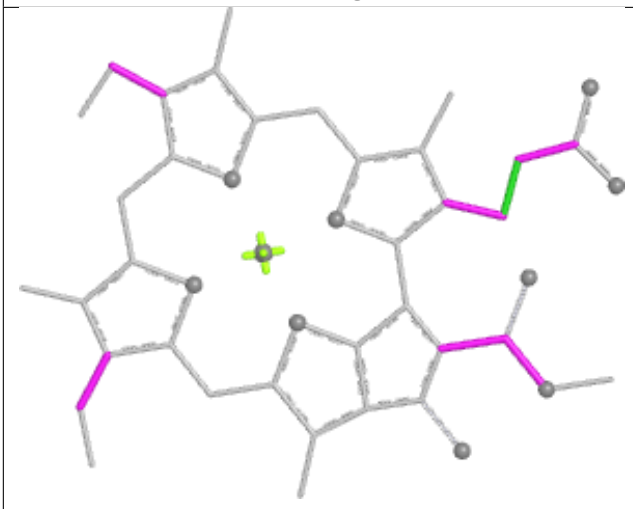
Ligand CLA BB 820



Bond lengths



Bond angles

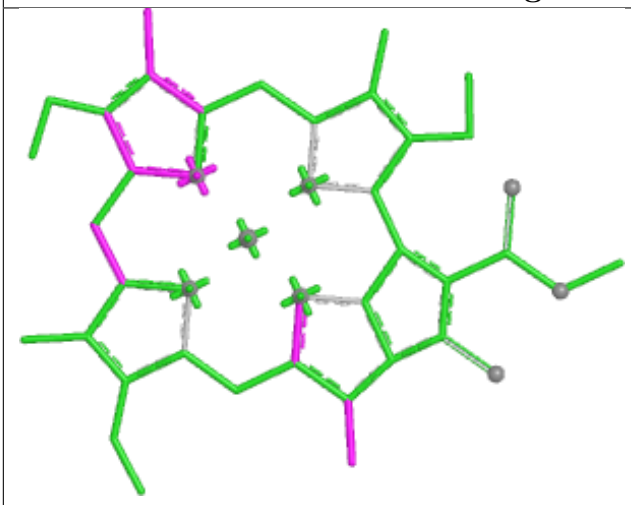


Torsions

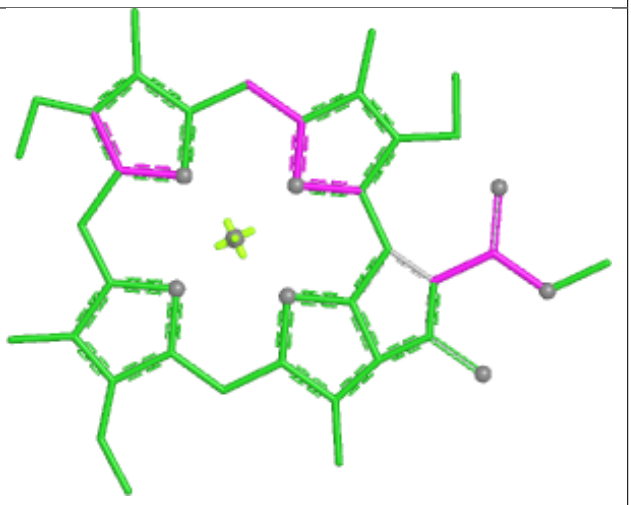


Rings

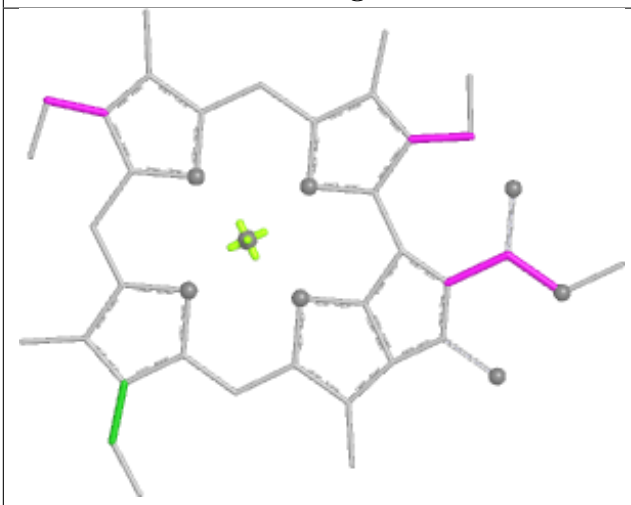
Ligand CLA B 813



Bond lengths



Bond angles

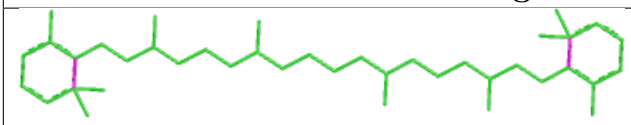


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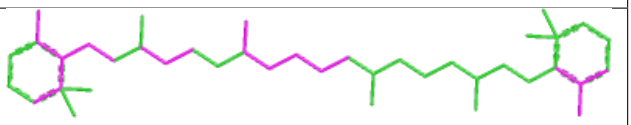


Rings

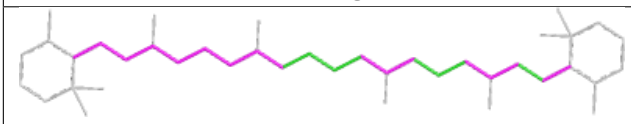
Ligand BCR FF 303



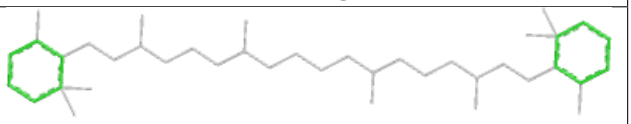
Bond lengths



Bond angles

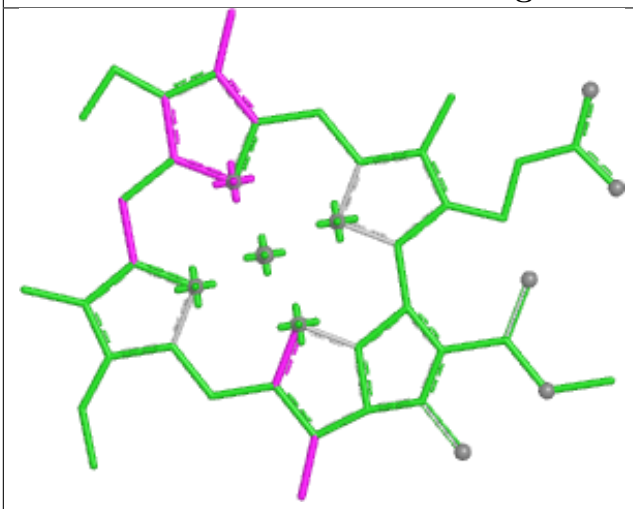


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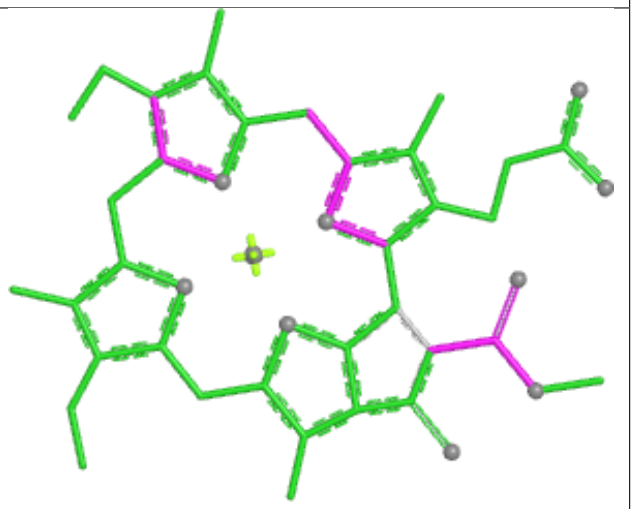


Rings

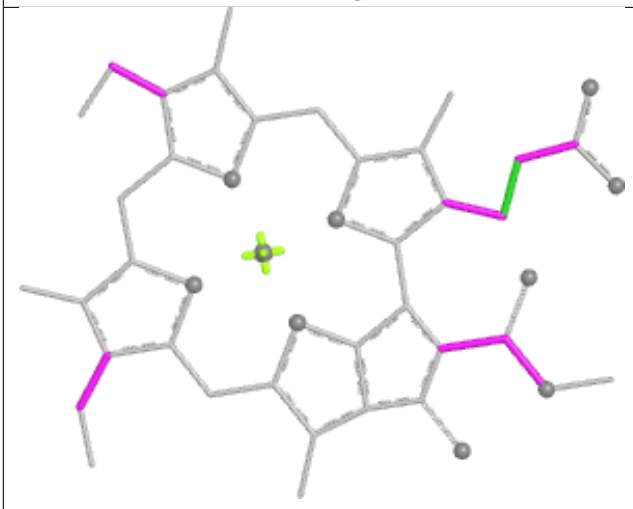
Ligand CLA B1 820



Bond lengths



Bond angles

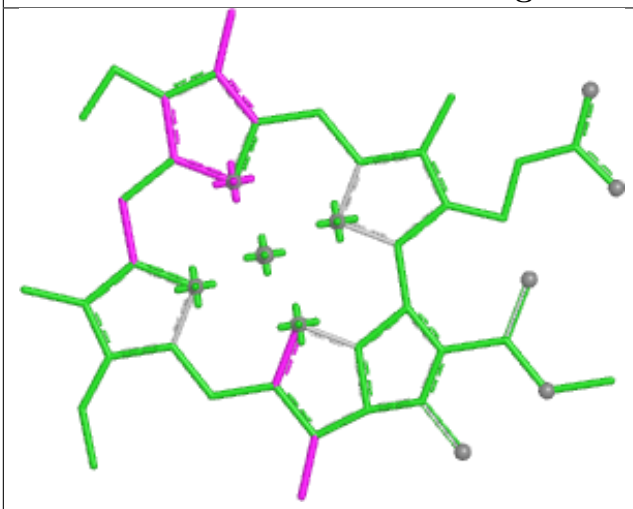


Torsions

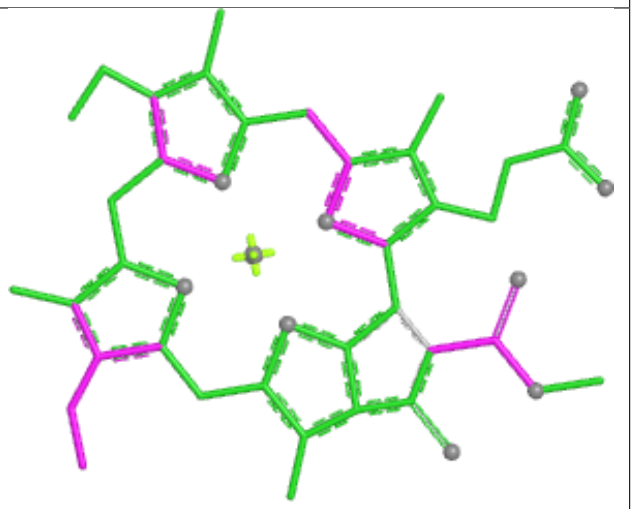


Rings

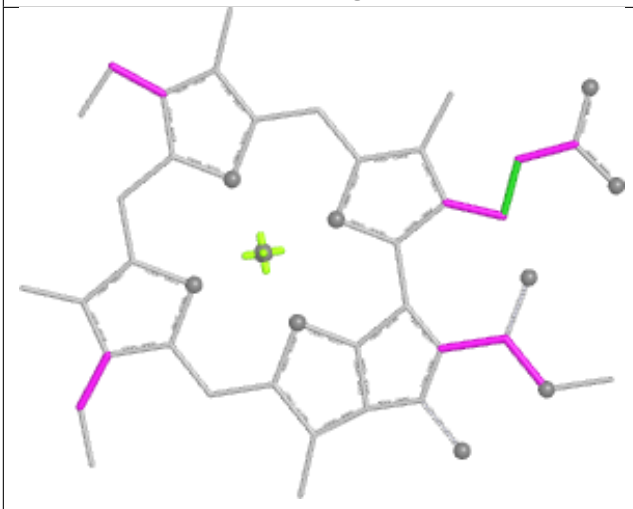
Ligand CLA B2 820



Bond lengths



Bond angles

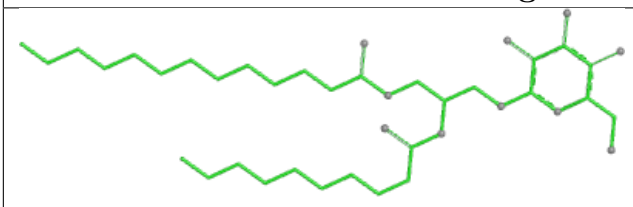


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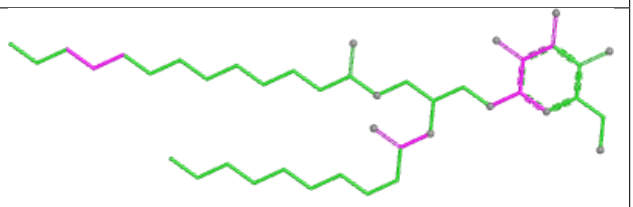


Rings

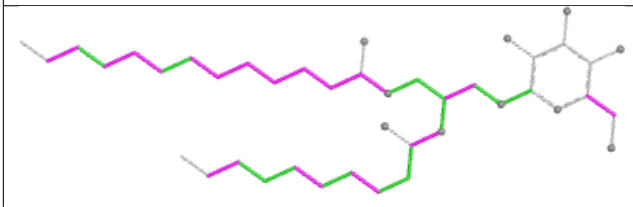
Ligand LMG II 105



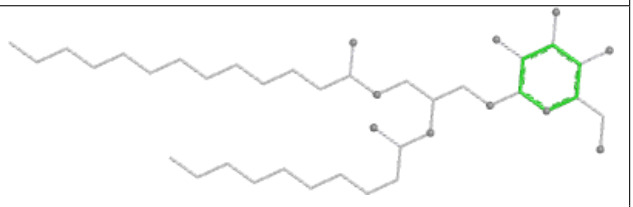
Bond lengths



Bond angles

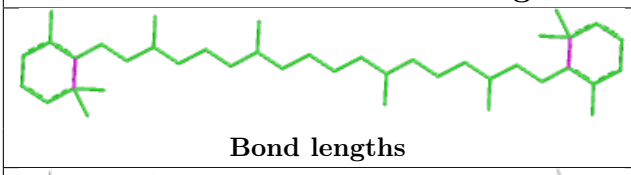


Torsions

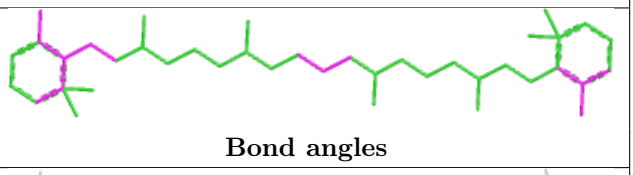


Rings

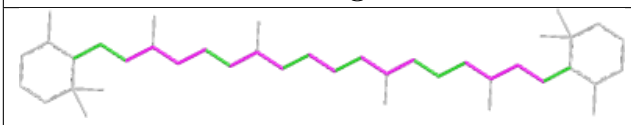
Ligand BCR A2 848



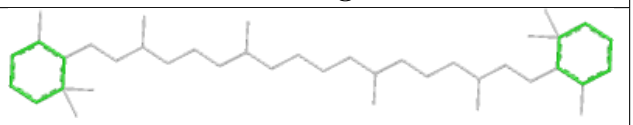
Bond lengths



Bond angles

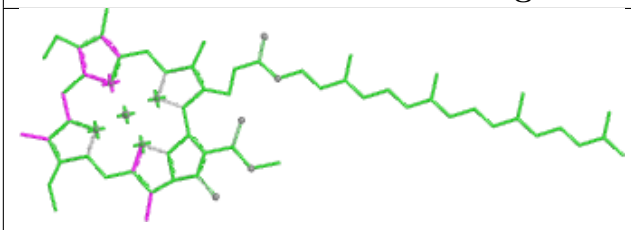


Torsions

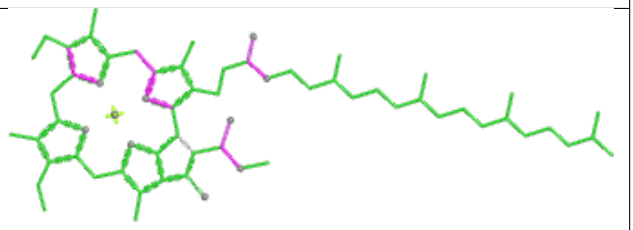


Rings

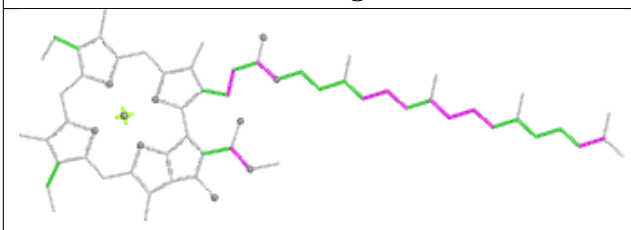
Ligand CLA A2 801



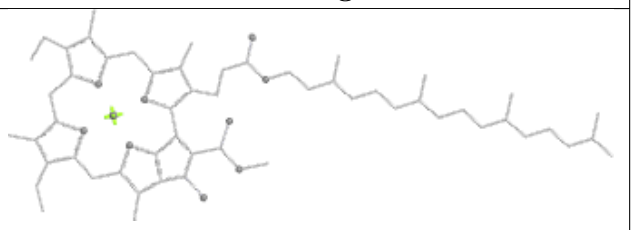
Bond lengths



Bond angles

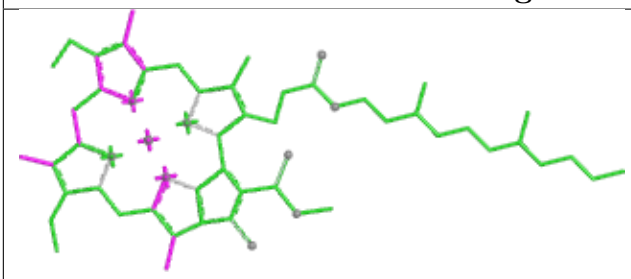


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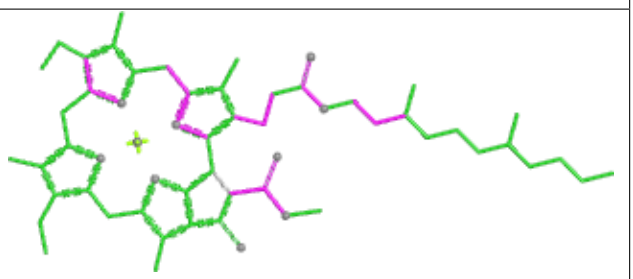


Rings

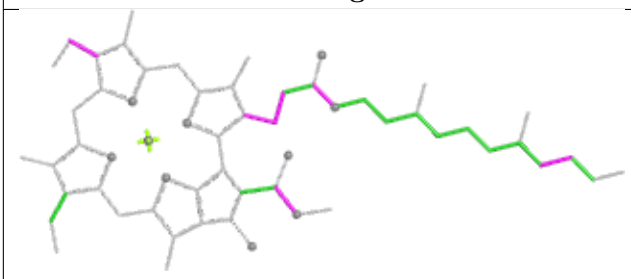
Ligand CLA A2 820



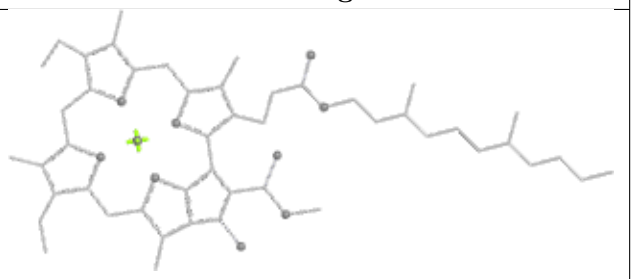
Bond lengths



Bond angles

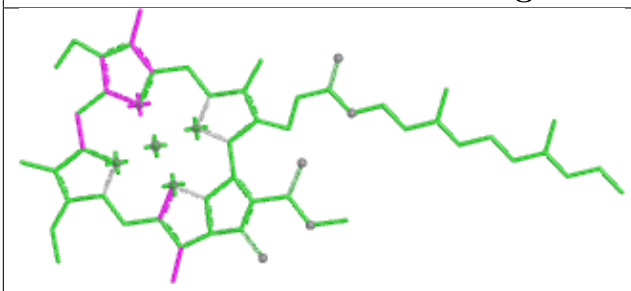


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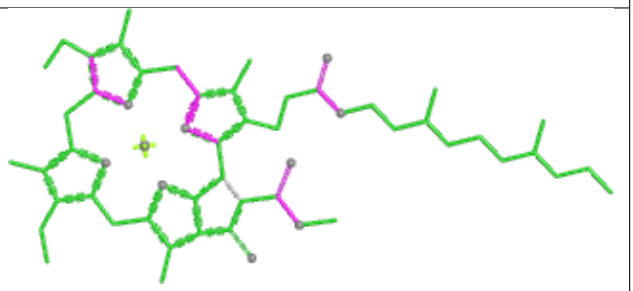


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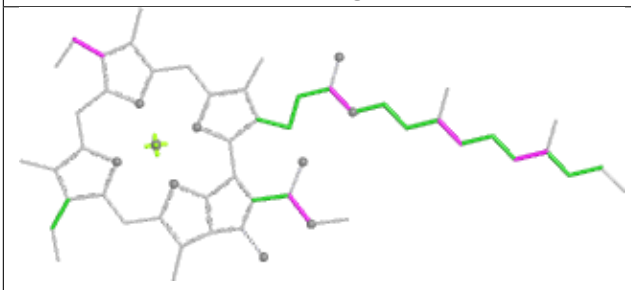
Ligand CLA B1 816



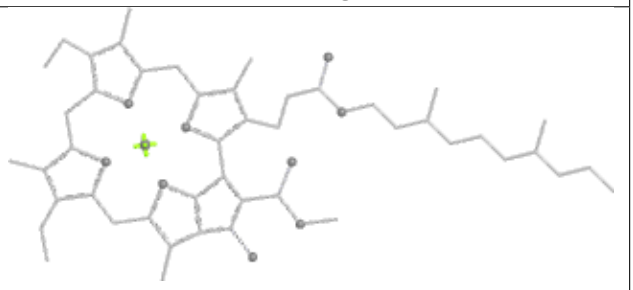
Bond lengths



Bond angles

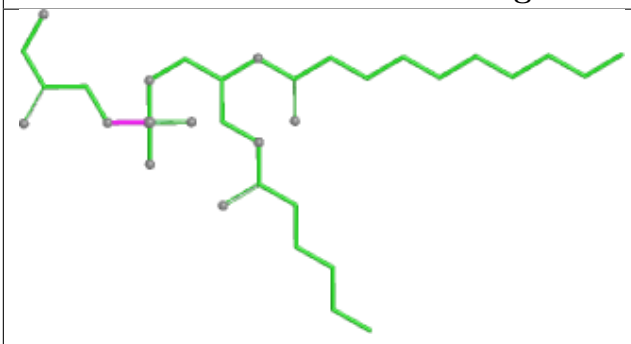


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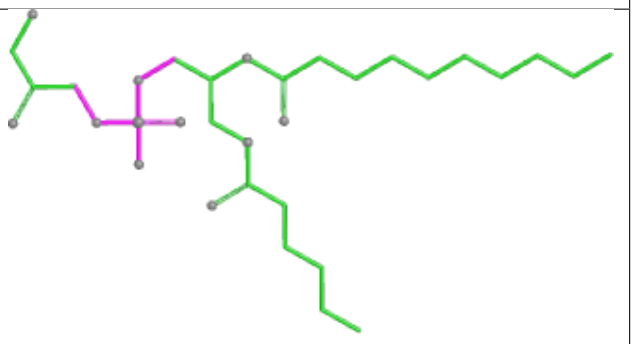


Rings

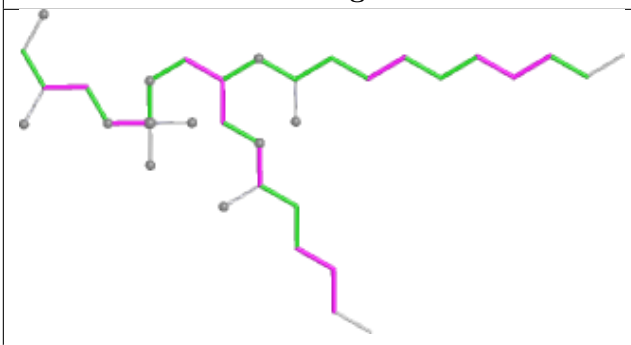
Ligand LHG B1 847



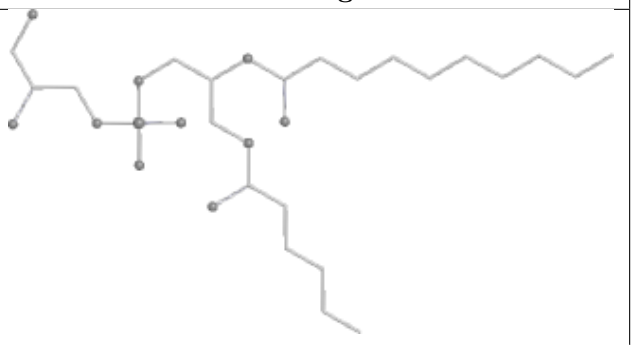
Bond lengths



Bond angles

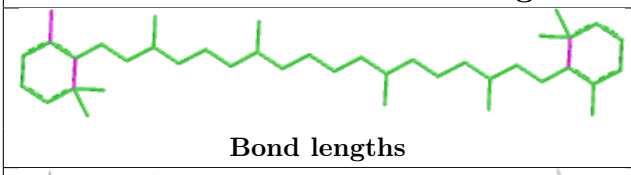


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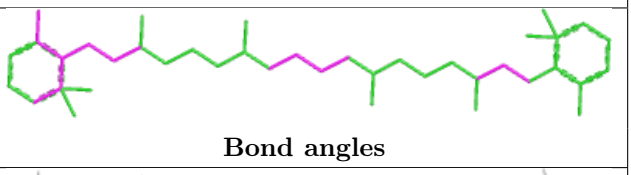


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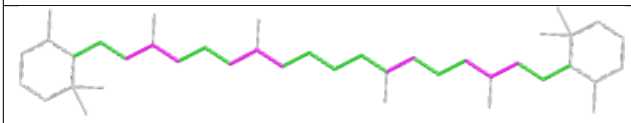
Ligand BCR L1 201



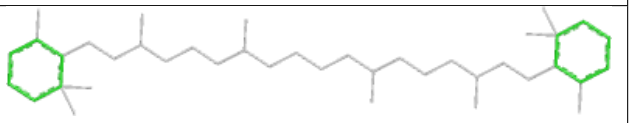
Bond lengths



Bond angles

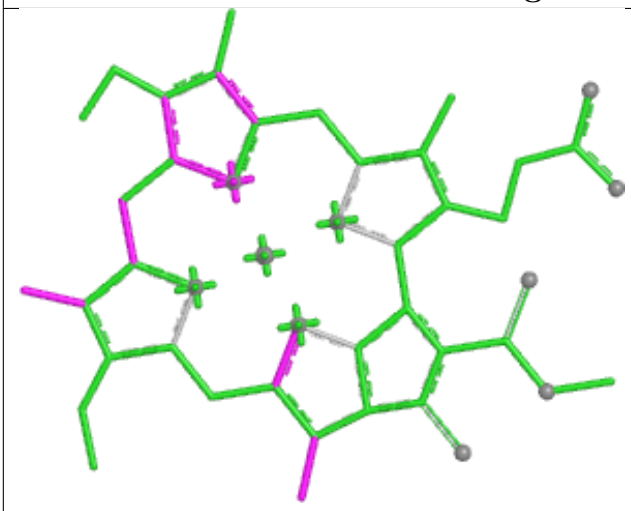


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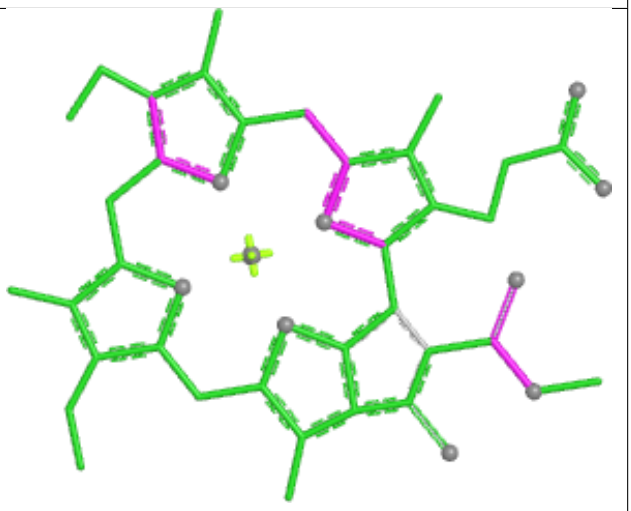


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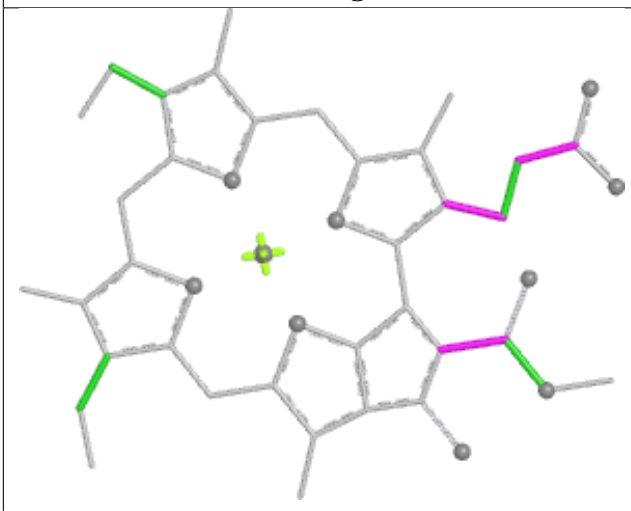
Ligand CLA B 828



Bond lengths



Bond angles

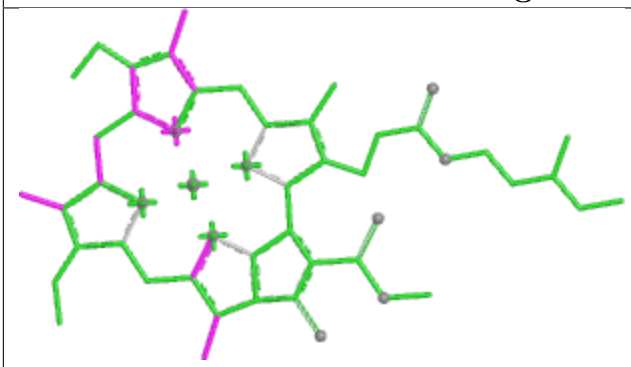


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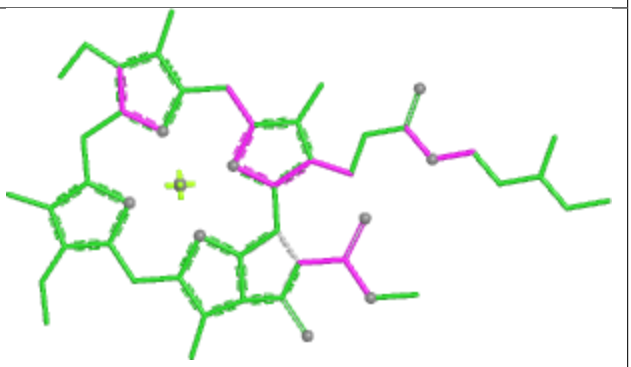


Rings

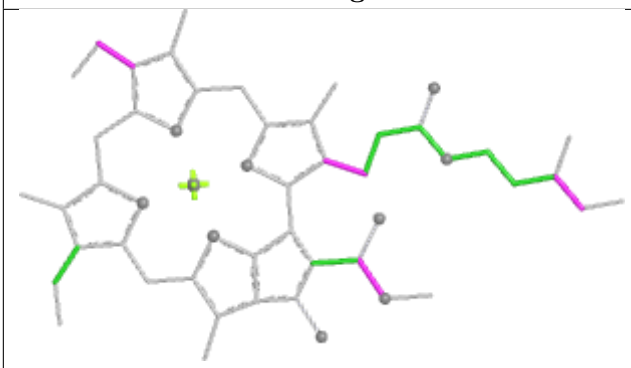
Ligand CLA A2 811



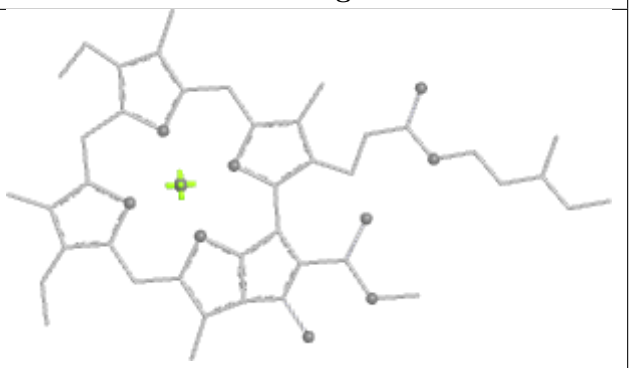
Bond lengths



Bond angles

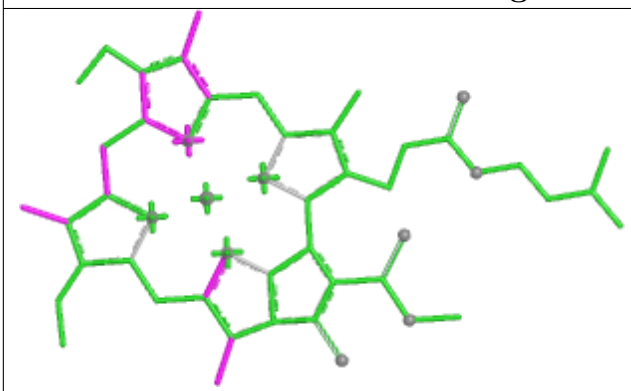


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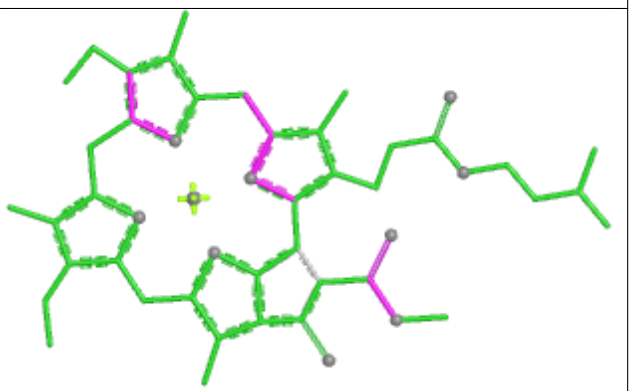


Rings

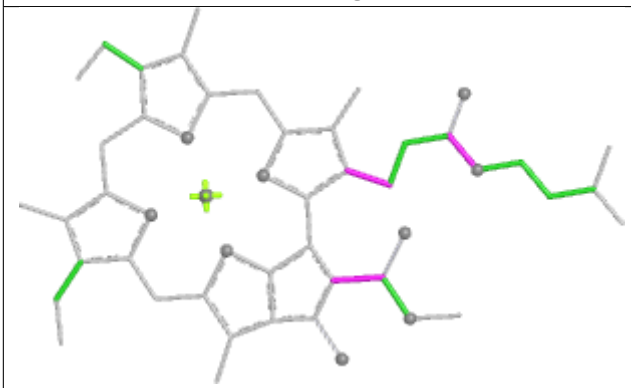
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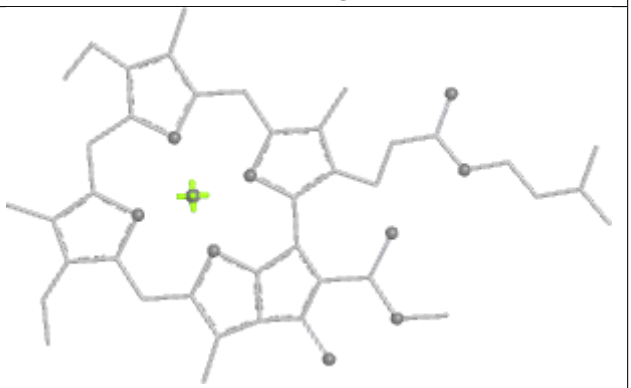
Bond lengths



Bond angles

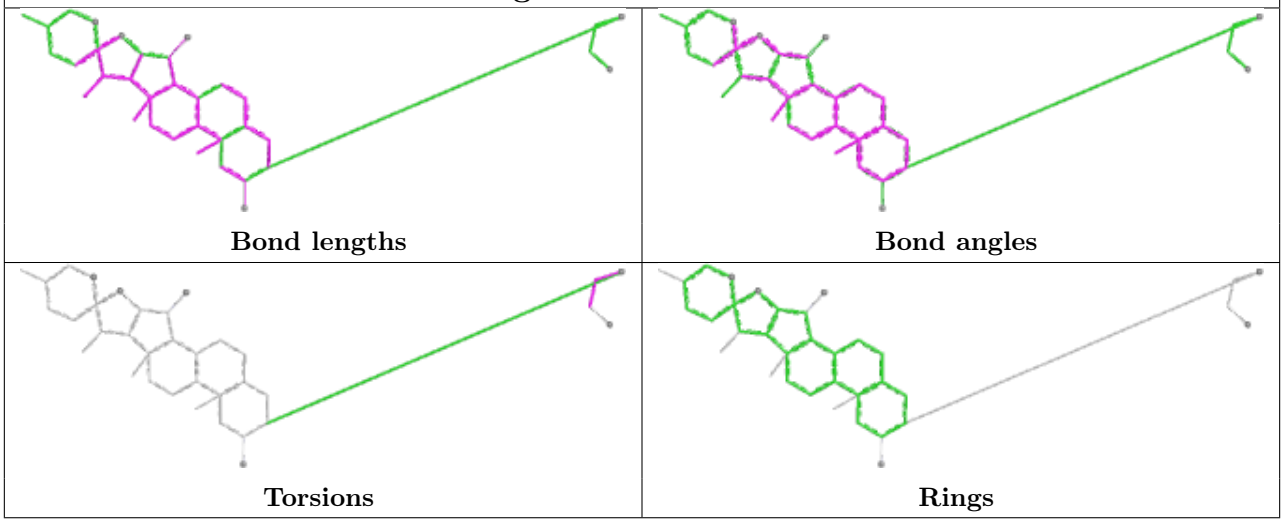


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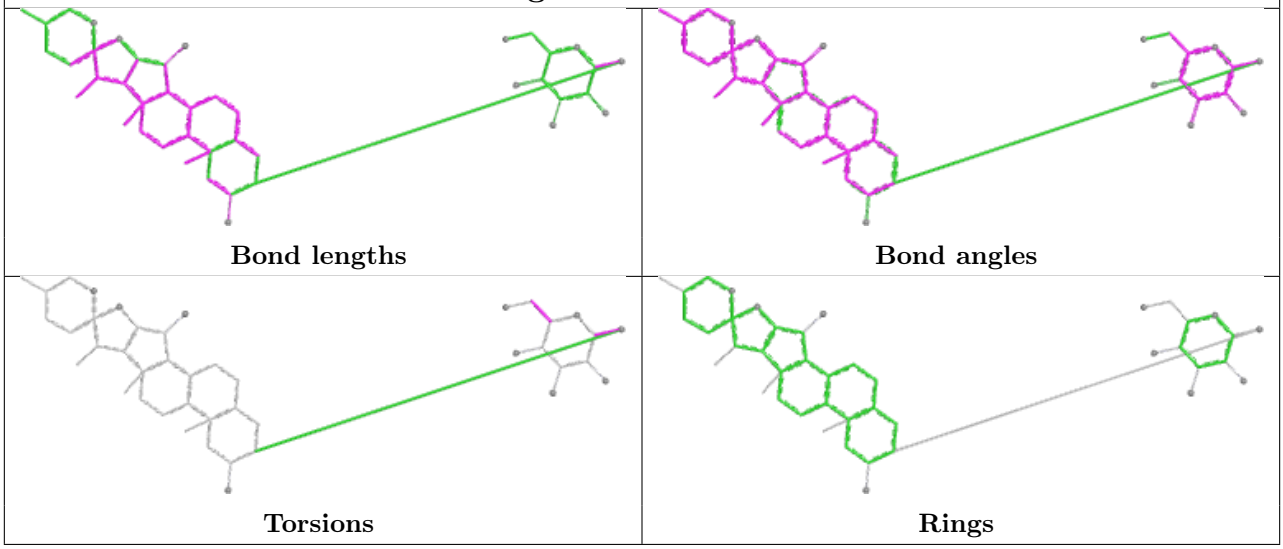


Rings

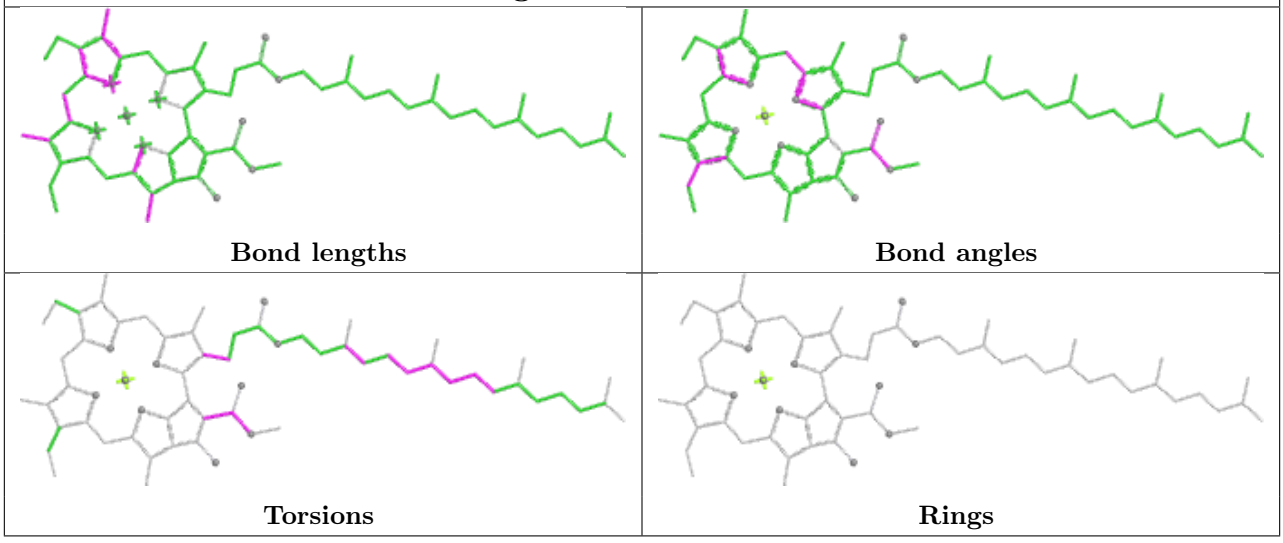
Ligand AJP AA 856



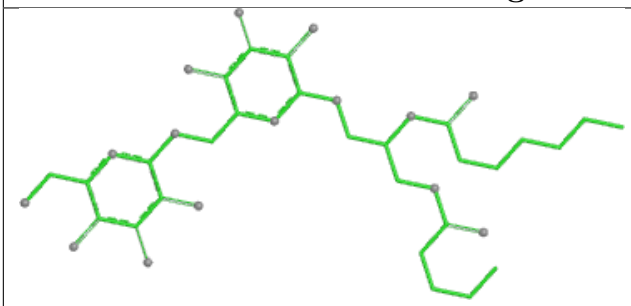
Ligand AJP B 849



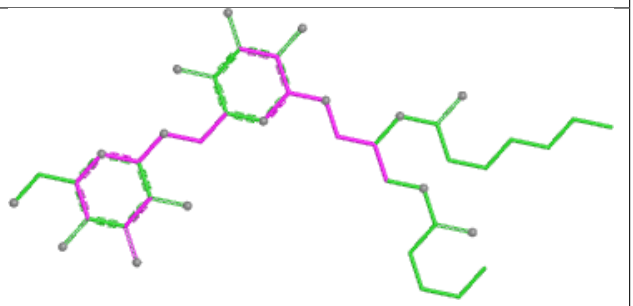
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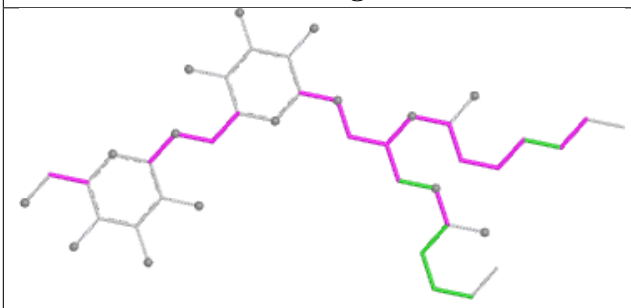
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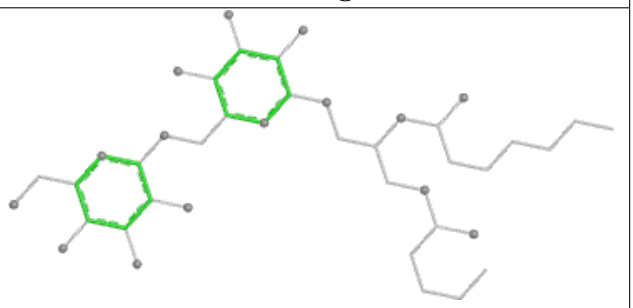
Bond lengths



Bond angles

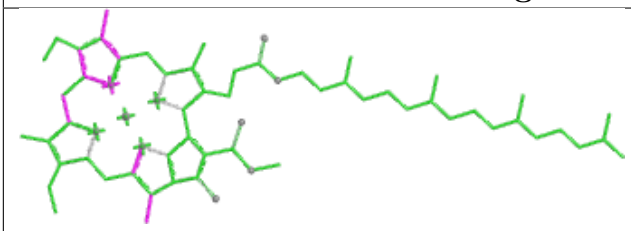


Torsions

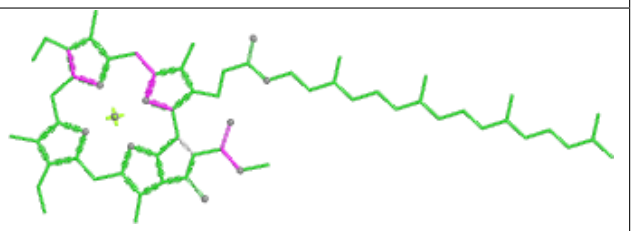


Rings

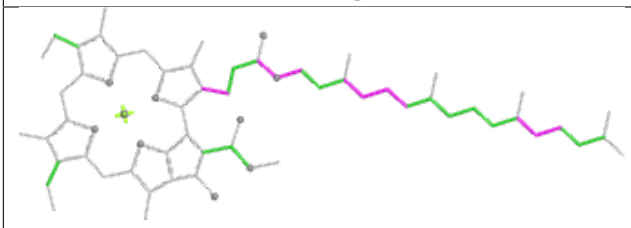
Ligand CLA FF 305



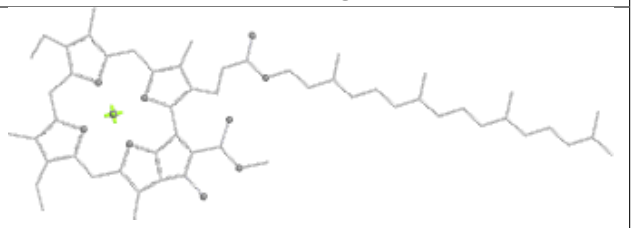
Bond lengths



Bond angles

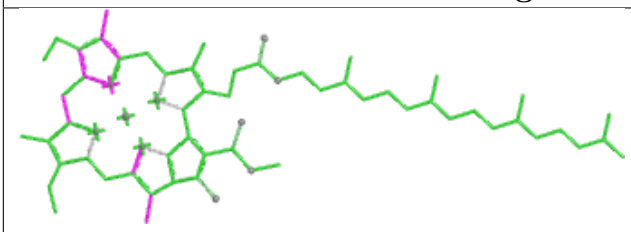


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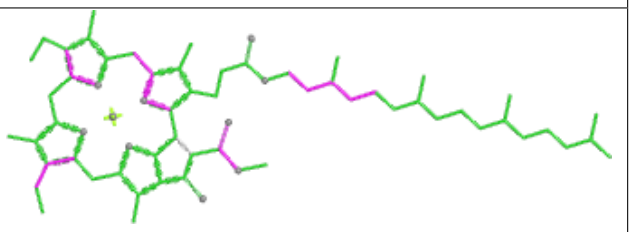


Rings

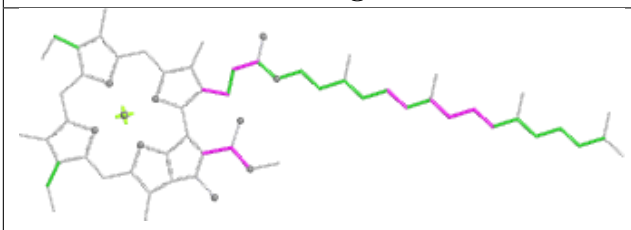
Ligand CLA B1 810



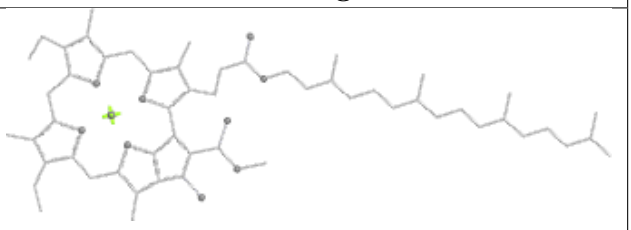
Bond lengths



Bond angles

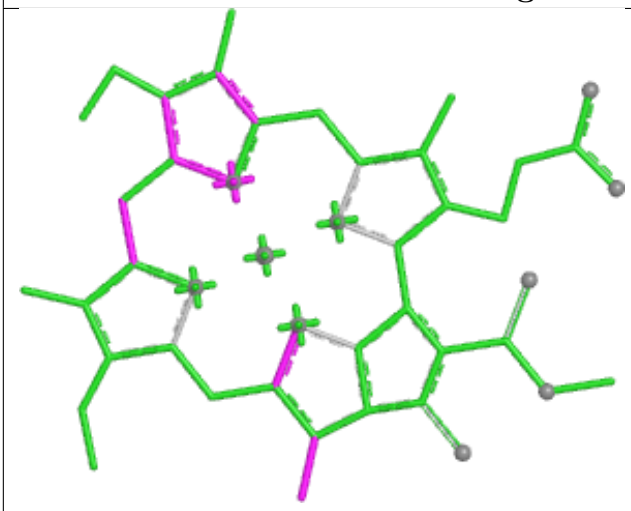


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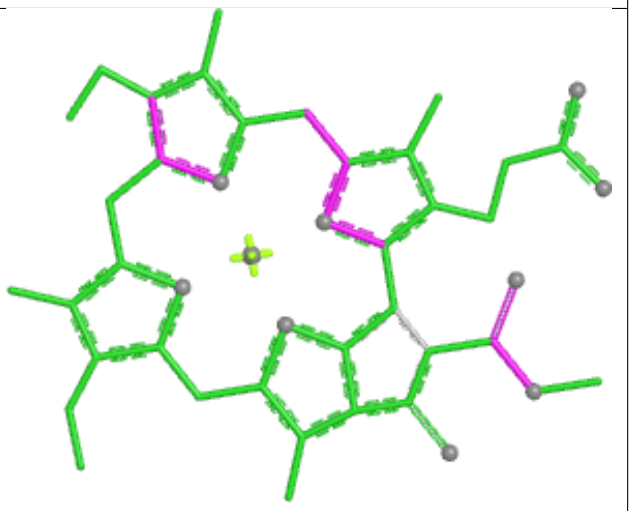


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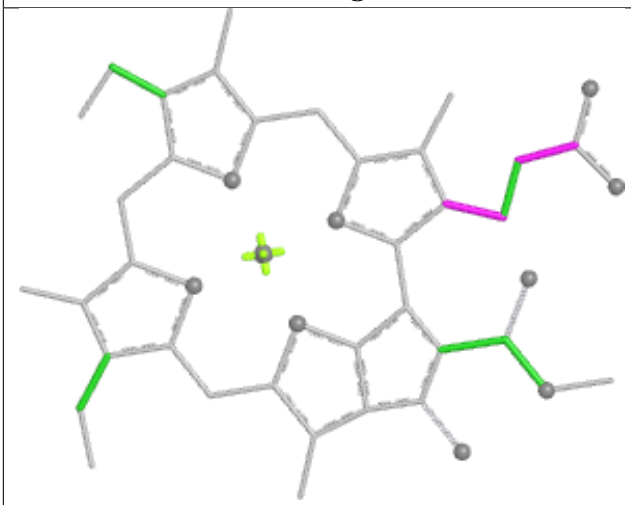
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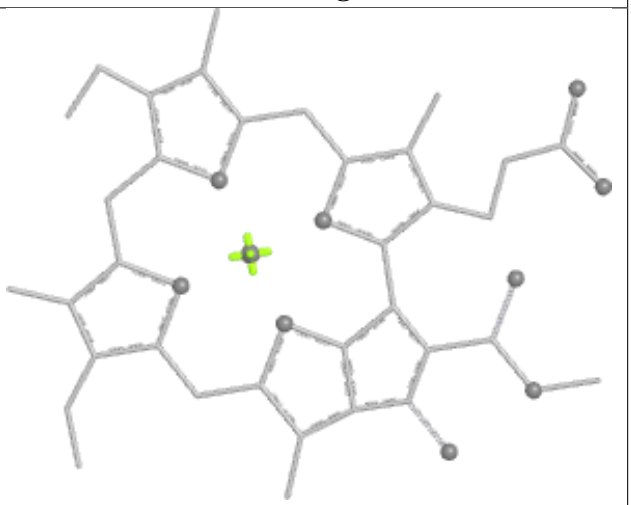
Bond lengths



Bond angles

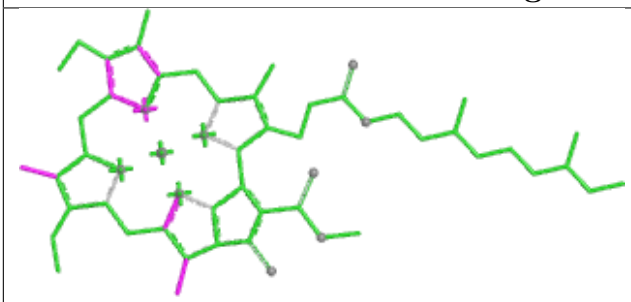


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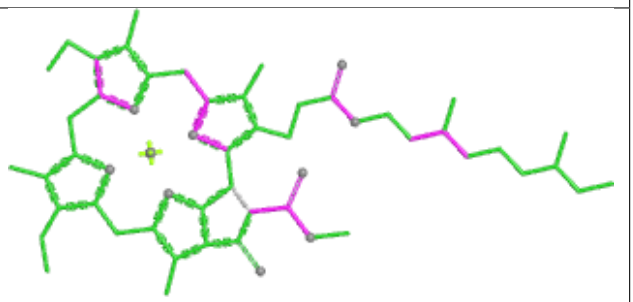


Rings

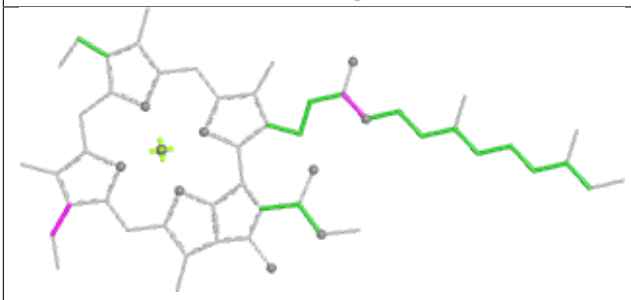
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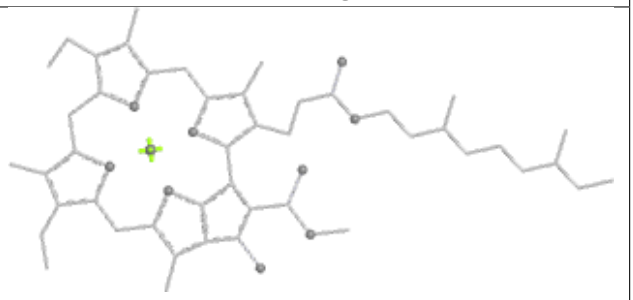
Bond lengths



Bond angles

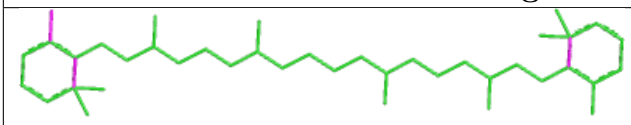


Torsions

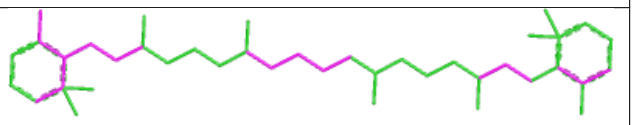


Rings

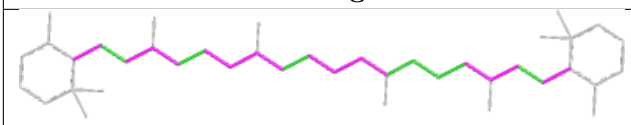
Ligand BCR II 104



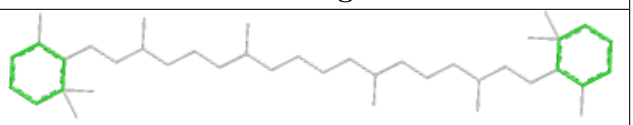
Bond lengths



Bond angles



Torsions

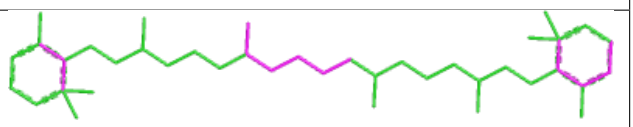


Rings

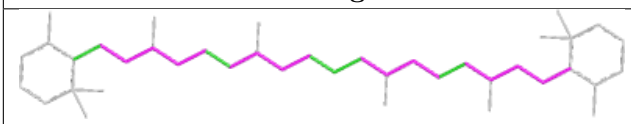
Ligand BCR BB 841



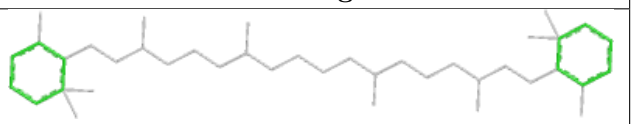
Bond lengths



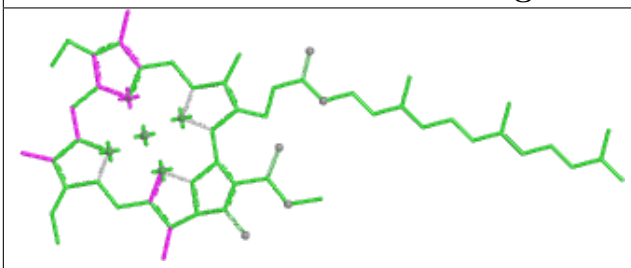
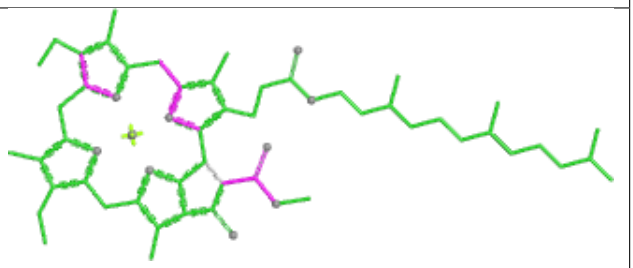
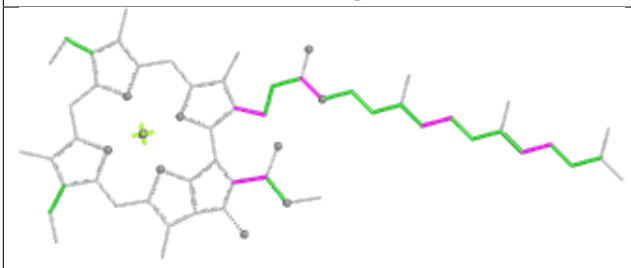
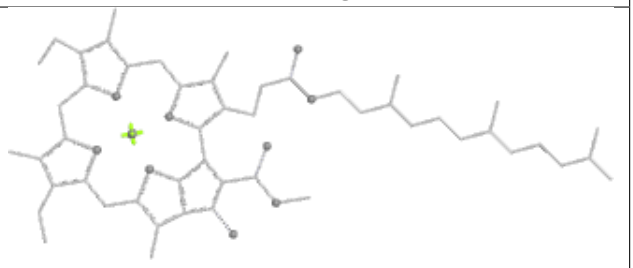
Bond angles

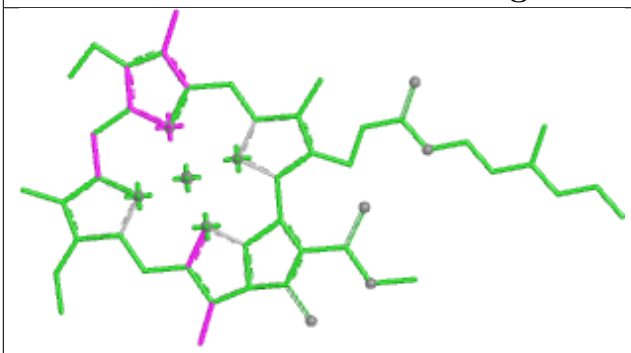
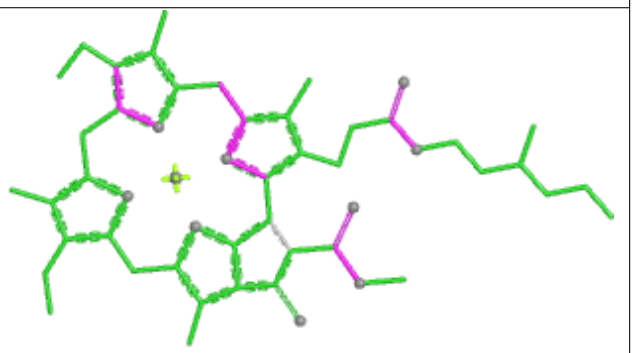
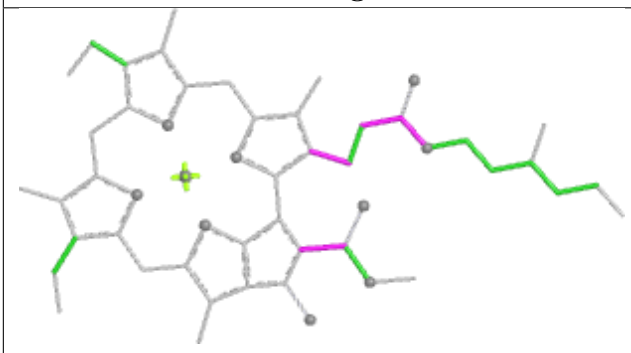
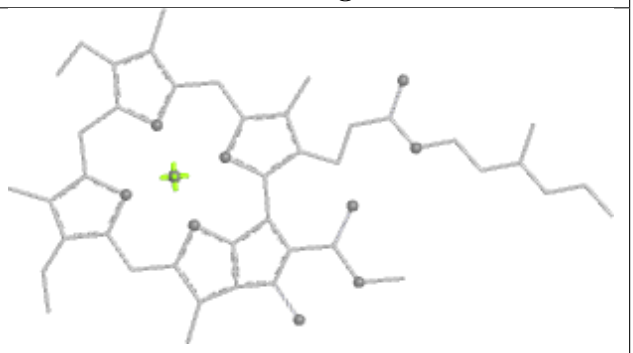


Torsions

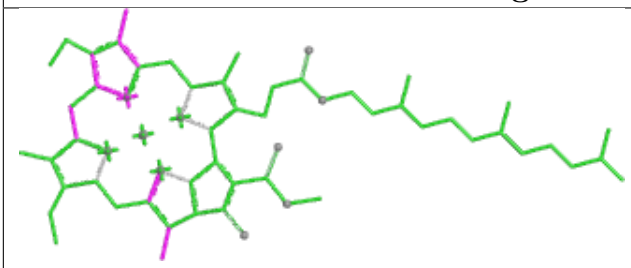


Rings

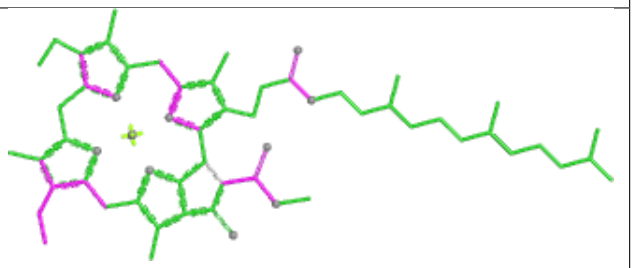
Ligand CLA A2 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

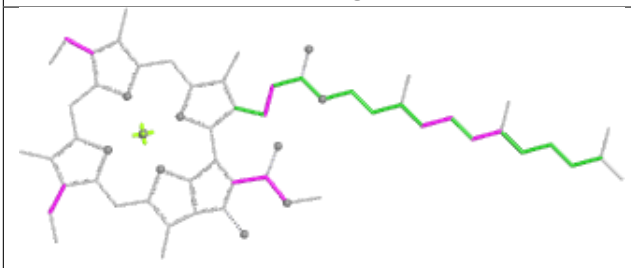
Ligand CLA BB 836



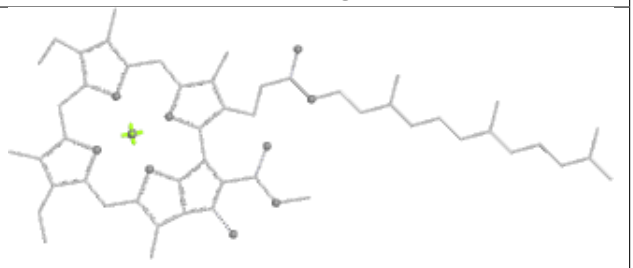
Bond lengths



Bond angles

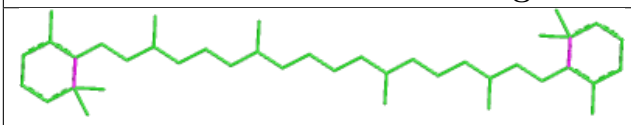


Torsions

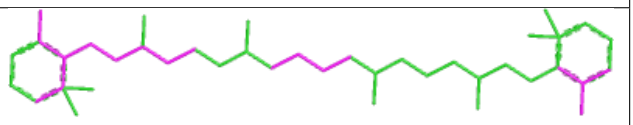


Rings

Ligand BCR A2 849



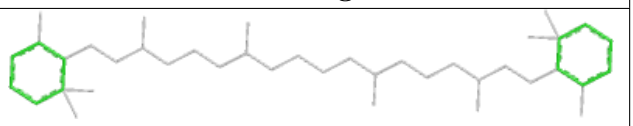
Bond lengths



Bond angles



Torsions

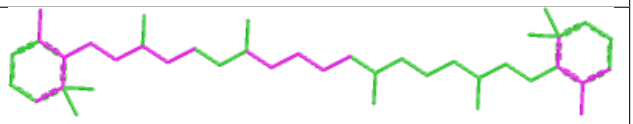


Rings

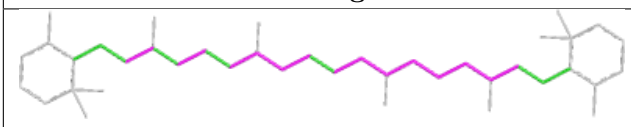
Ligand BCR A 853



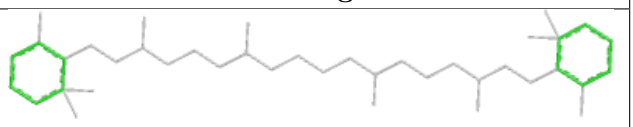
Bond lengths



Bond angles

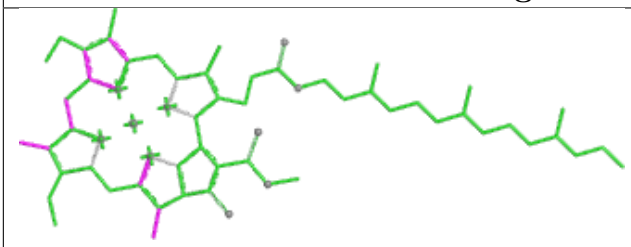


Torsions

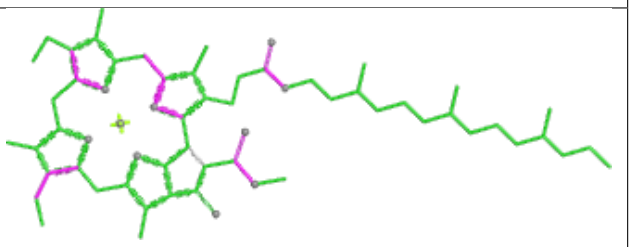


Rings

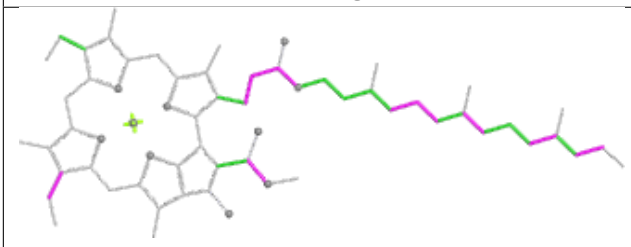
Ligand CLA A1 829



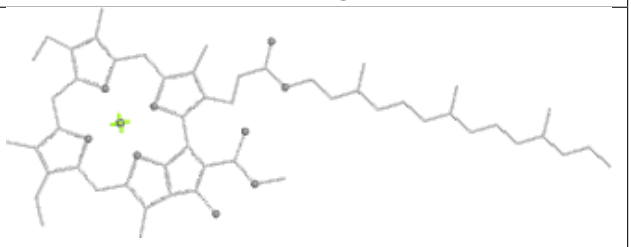
Bond lengths



Bond angles

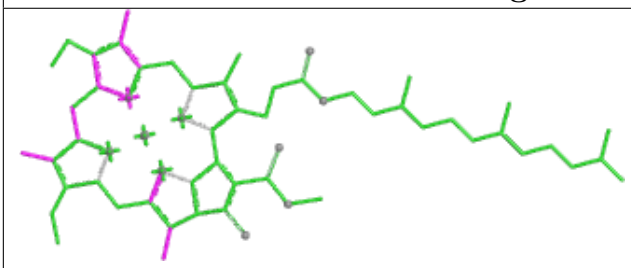


Torsions

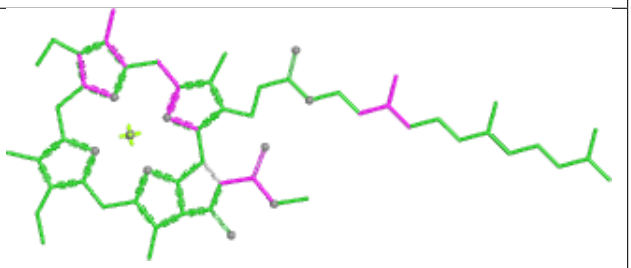


Rings

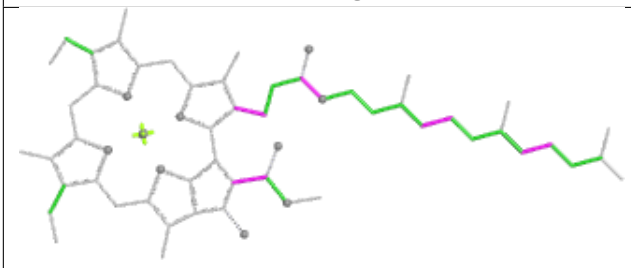
Ligand CLA AA 805



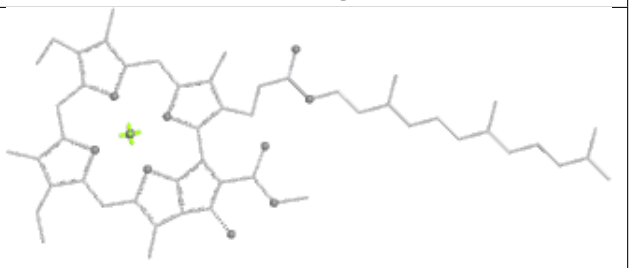
Bond lengths



Bond angles

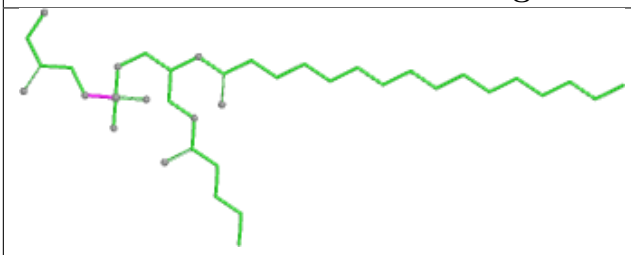


Torsions

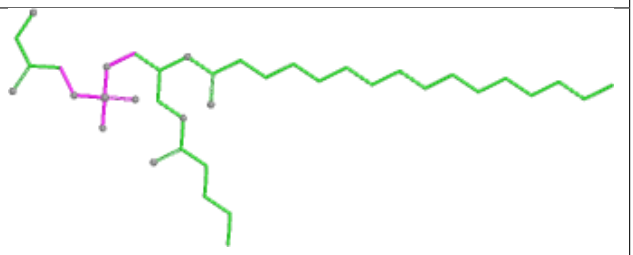


Rings

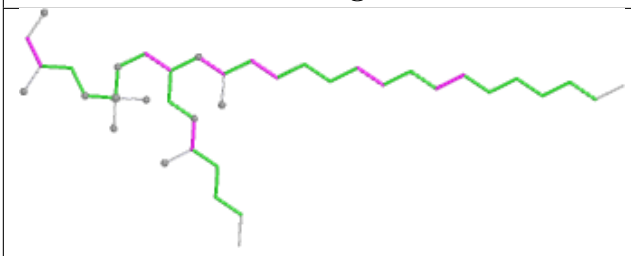
Ligand LHG A2 846



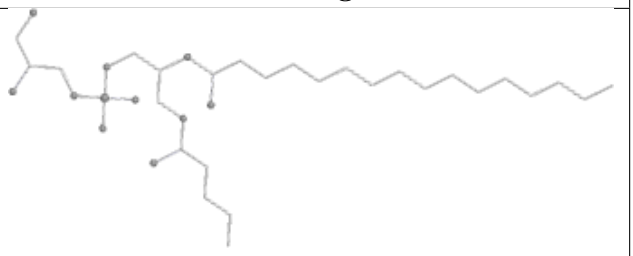
Bond lengths



Bond angles

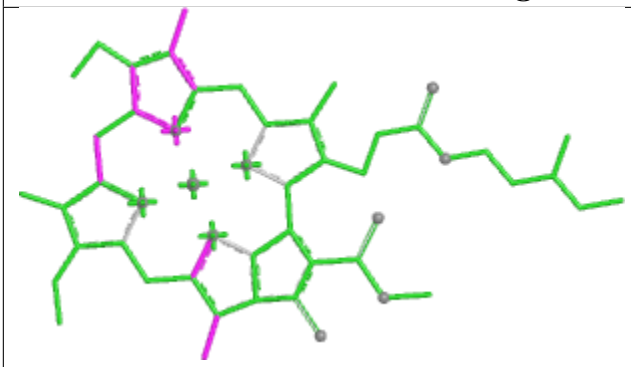


Torsions

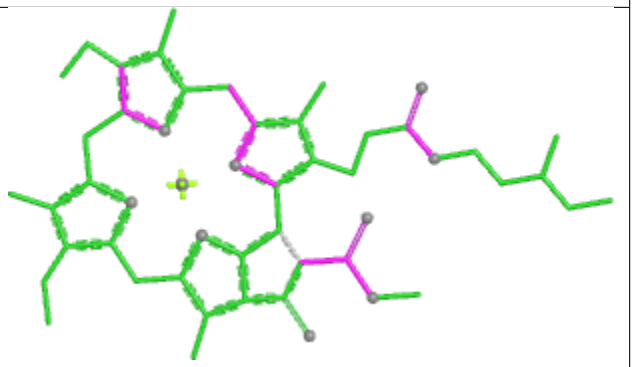


Rings

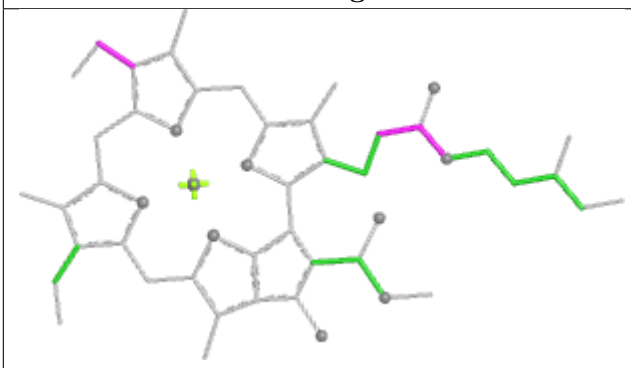
Ligand CLA A1 821



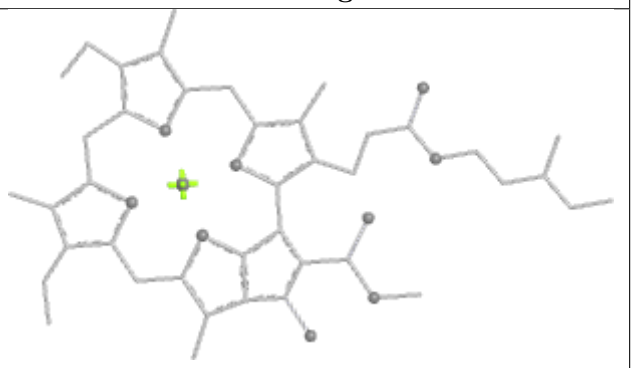
Bond lengths



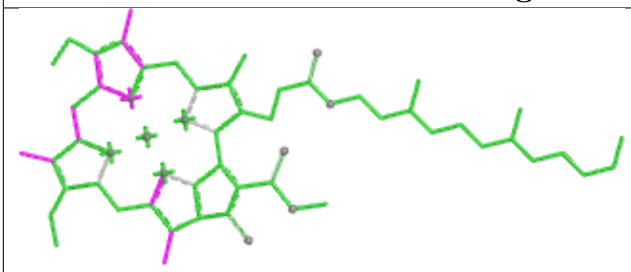
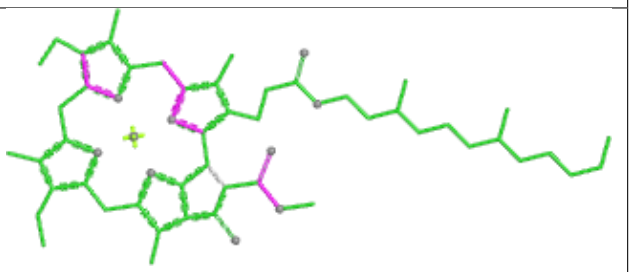
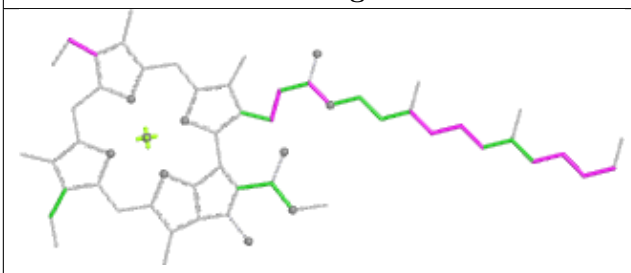
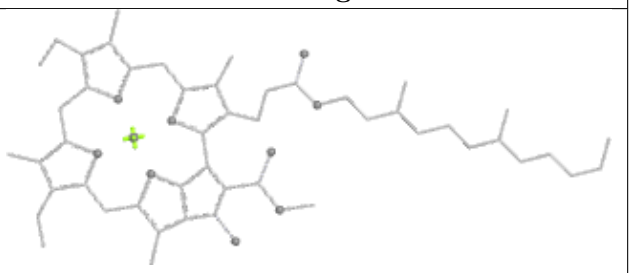
Bond angles

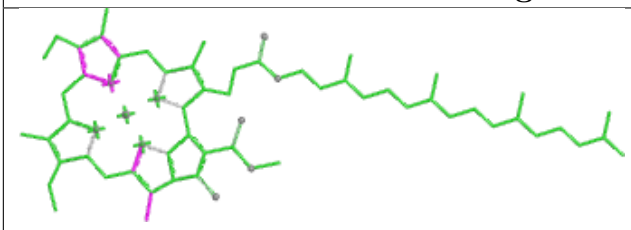
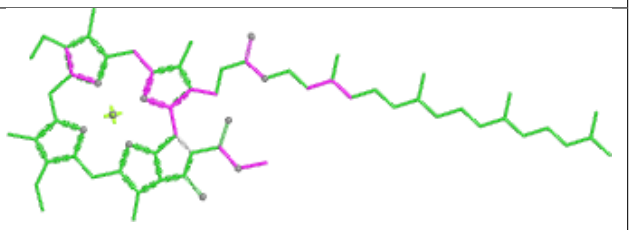
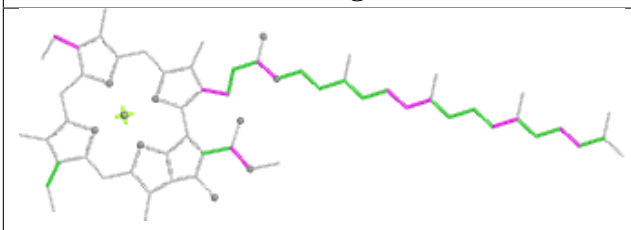
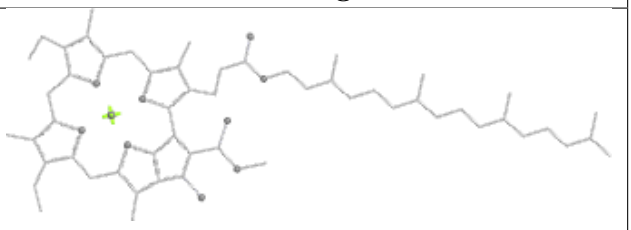


Torsions

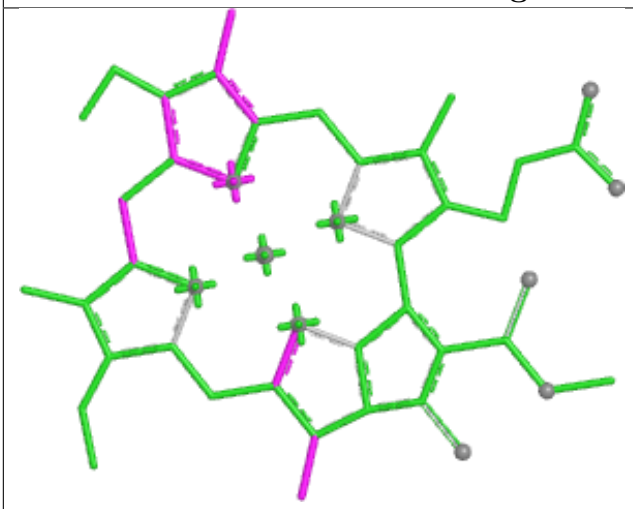


Rings

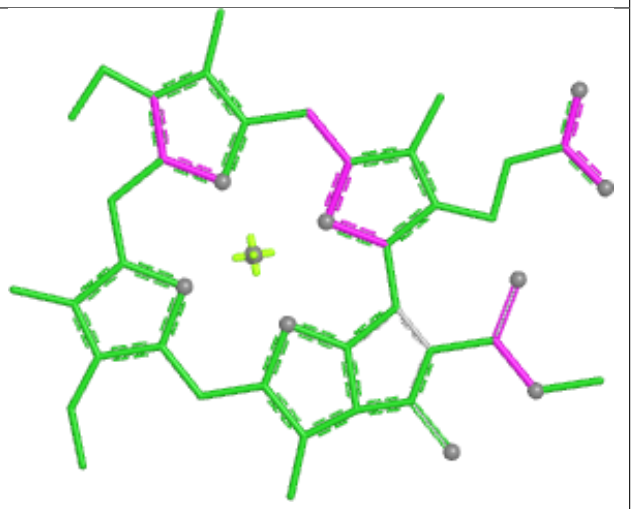
Ligand CLA B2 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B1 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

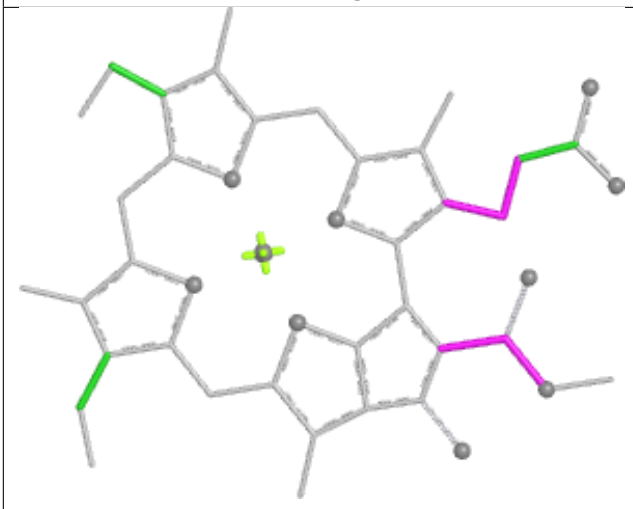
Ligand CLA AA 824



Bond lengths



Bond angles

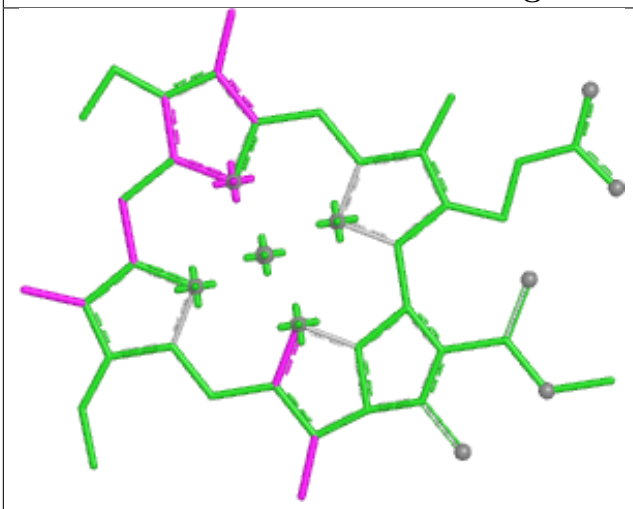


Torsions

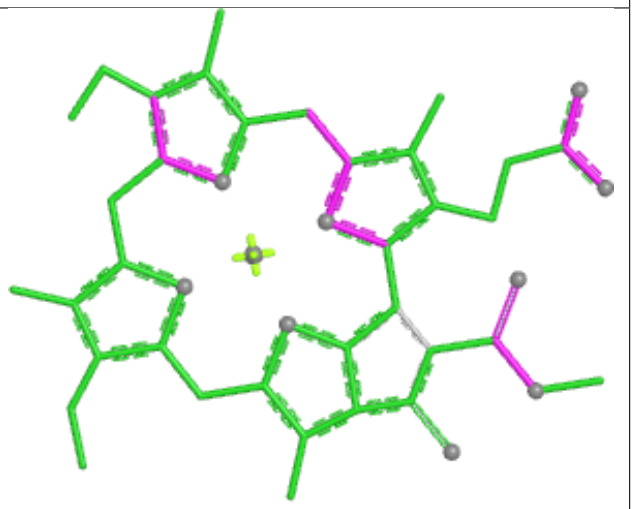


Rings

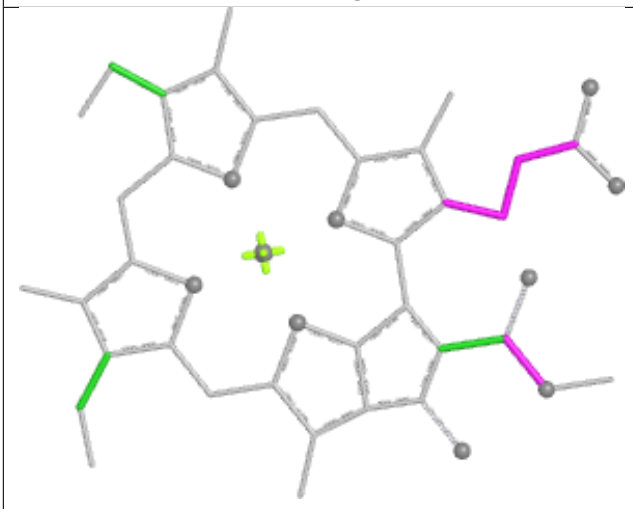
Ligand CLA A 826



Bond lengths



Bond angles

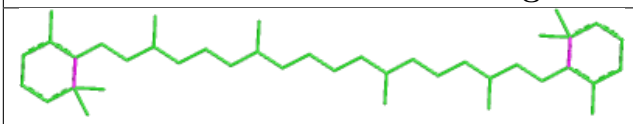


Torsions

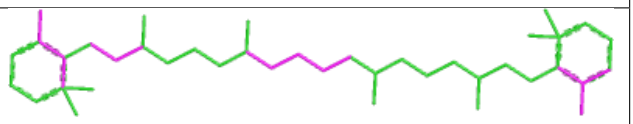


Rings

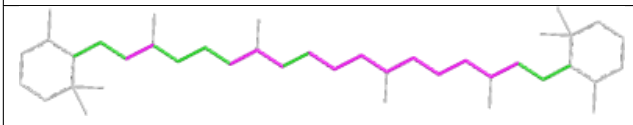
Ligand BCR B 848



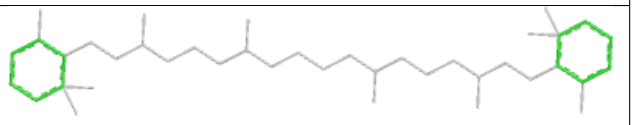
Bond lengths



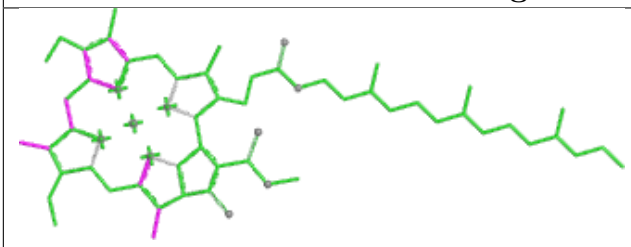
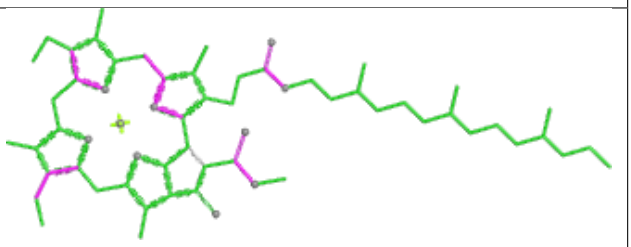
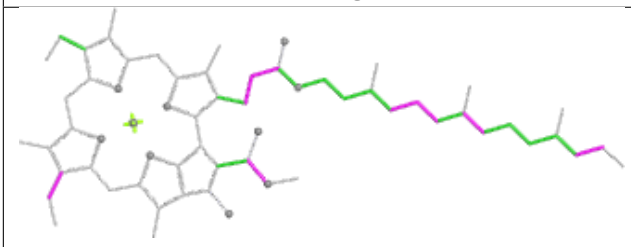
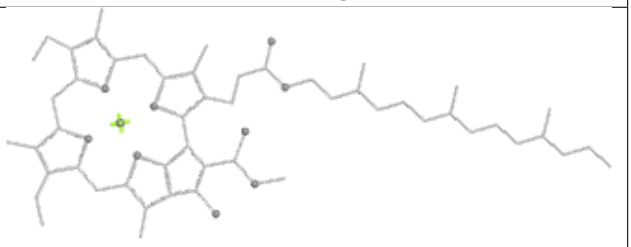
Bond angles

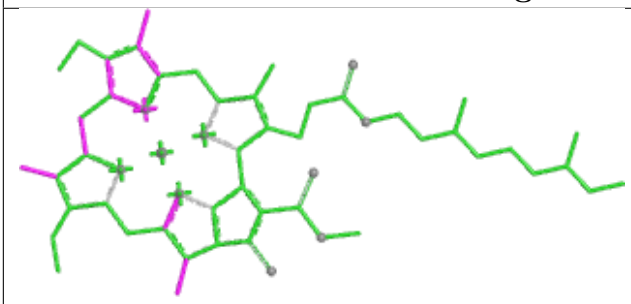
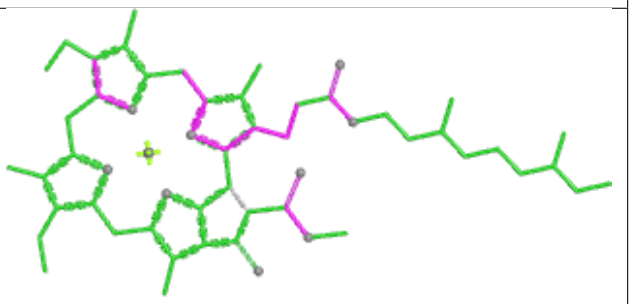
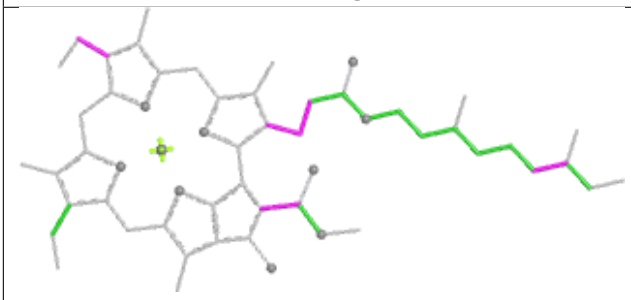
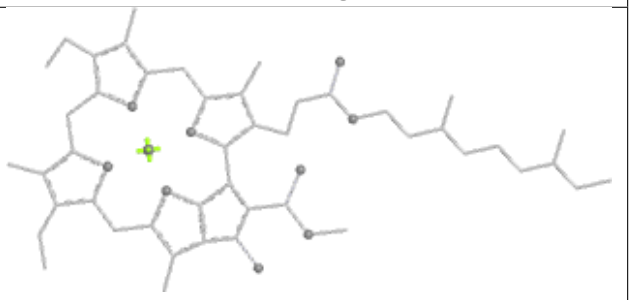


Torsions

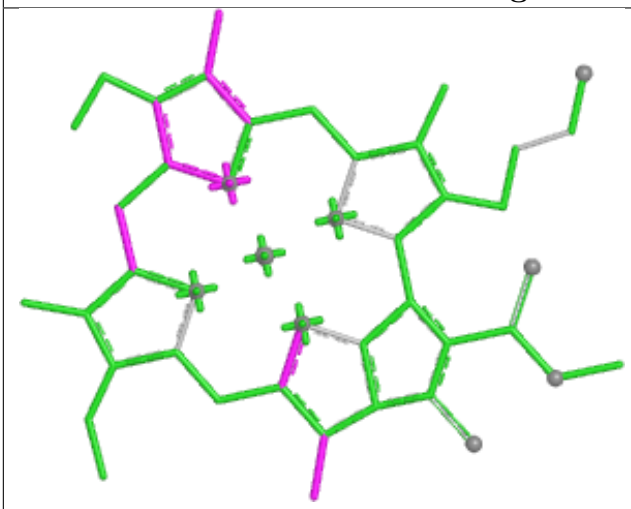


Rings

Ligand CLA AA 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

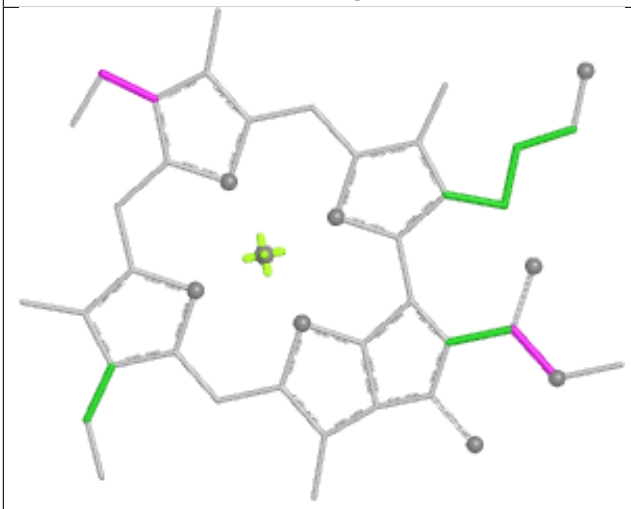
Ligand CLA AA 817



Bond lengths



Bond angles

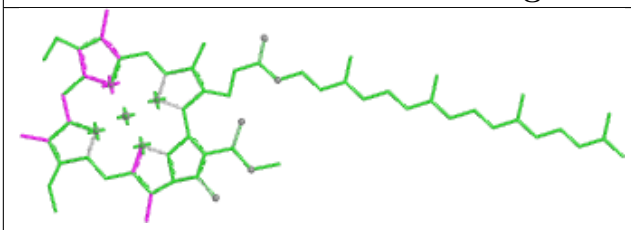


Torsions

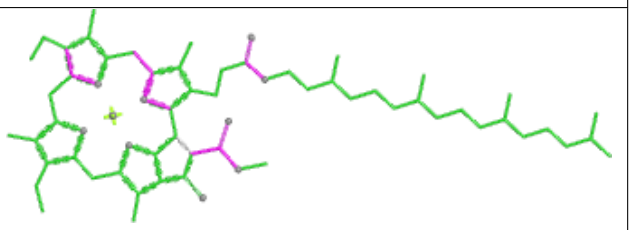


Rings

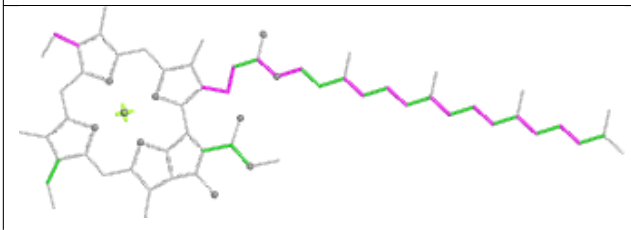
Ligand CLA A 827



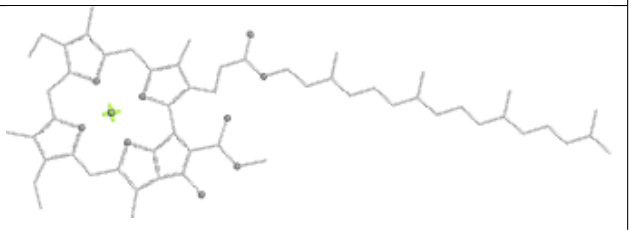
Bond lengths



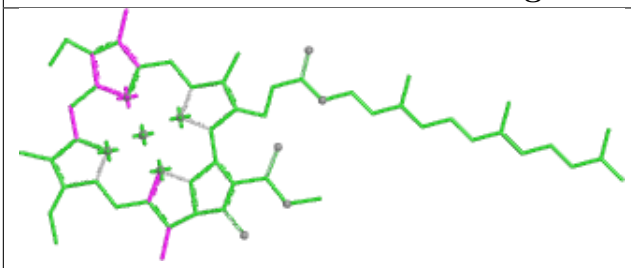
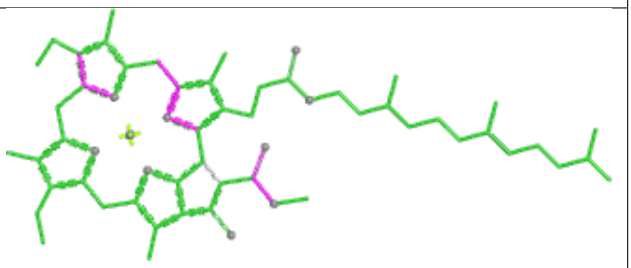
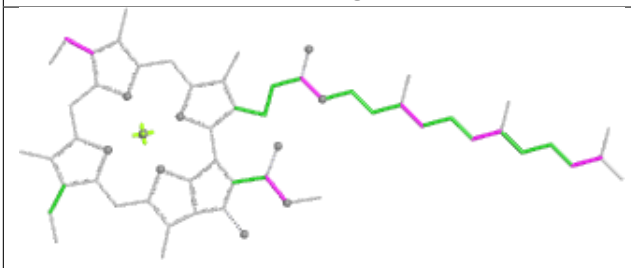
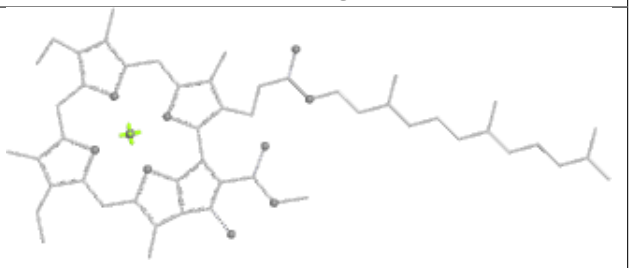
Bond angles

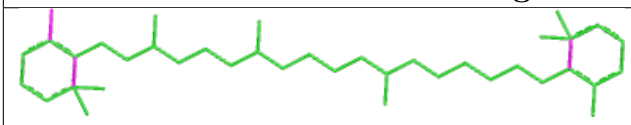
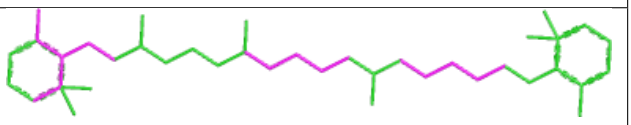
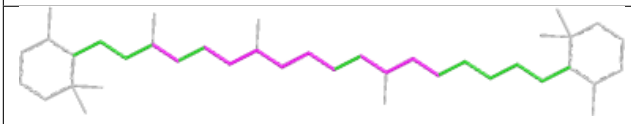
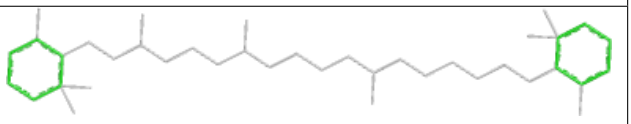


Torsions

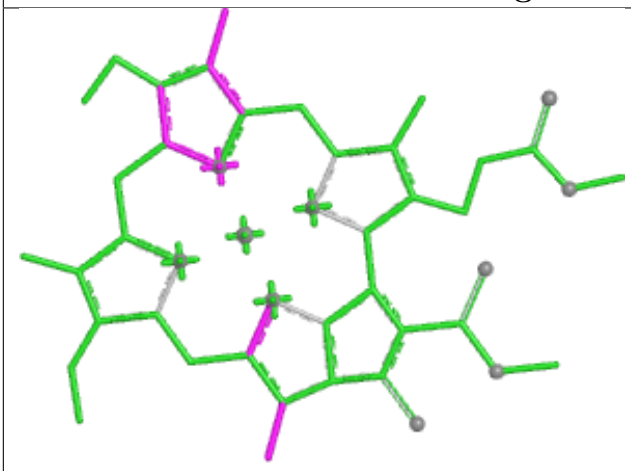


Rings

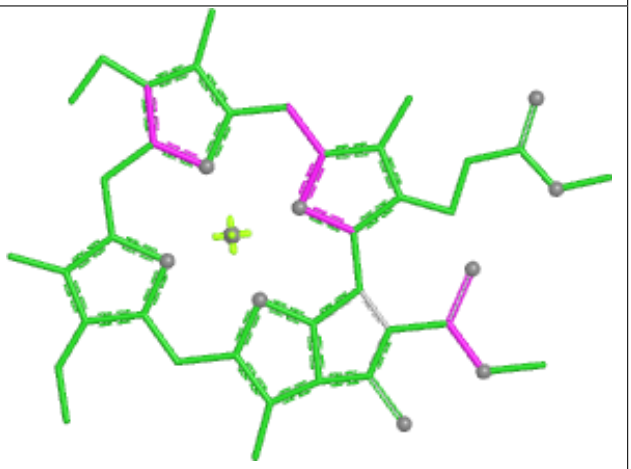
Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A1 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

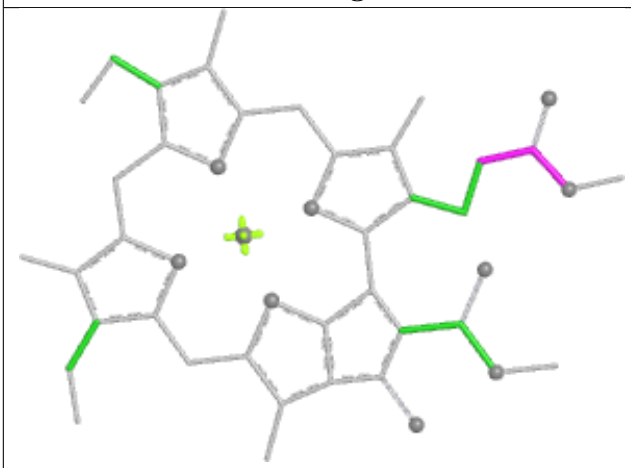
Ligand CLA A2 841



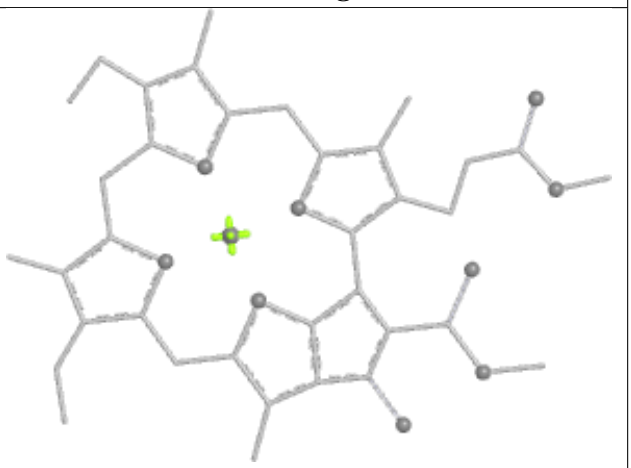
Bond lengths



Bond angles



Torsions

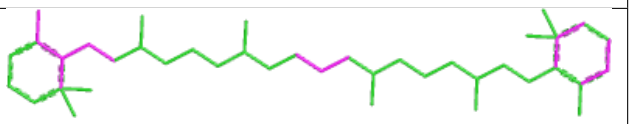


Rings

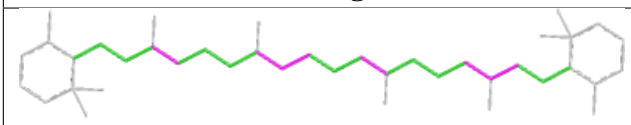
Ligand BCR B 840



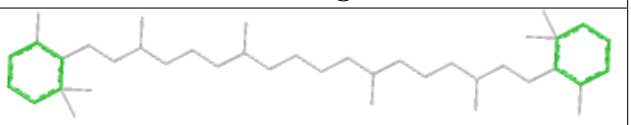
Bond lengths



Bond angles

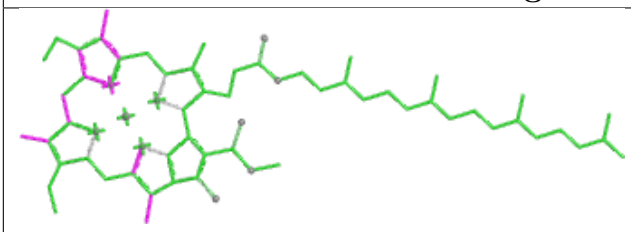


Torsions

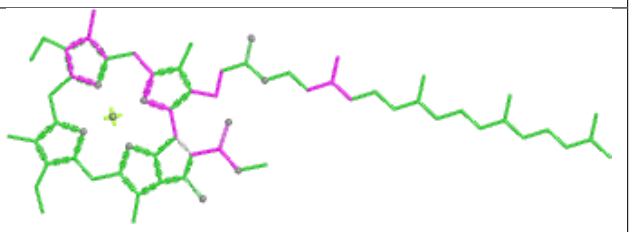


Rings

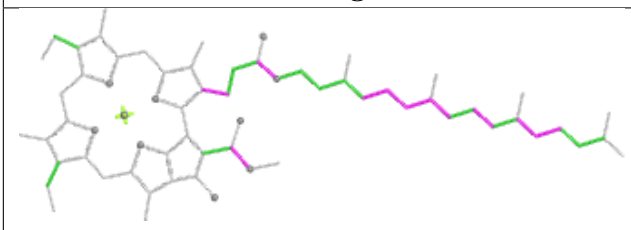
Ligand CLA B 815



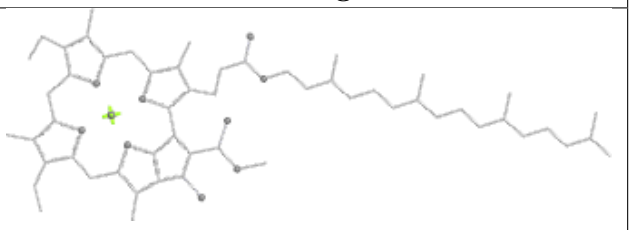
Bond lengths



Bond angles

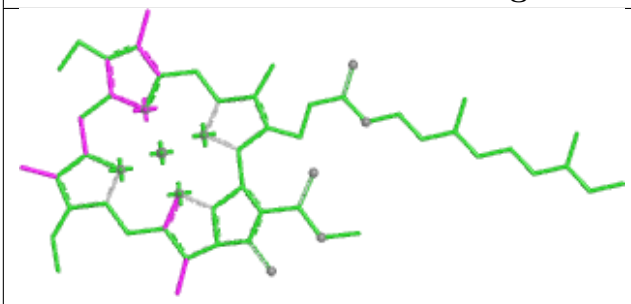


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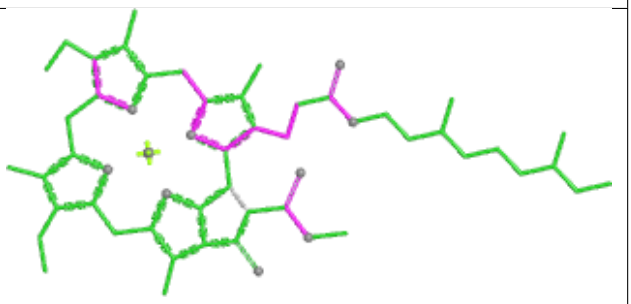


Rings

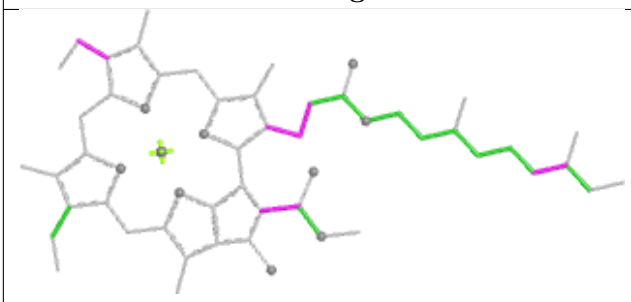
Ligand CLA AA 806



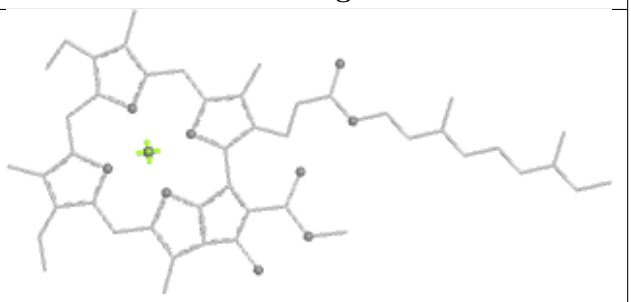
Bond lengths



Bond angles

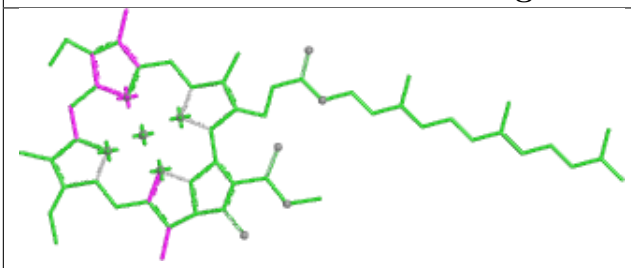


Torsions

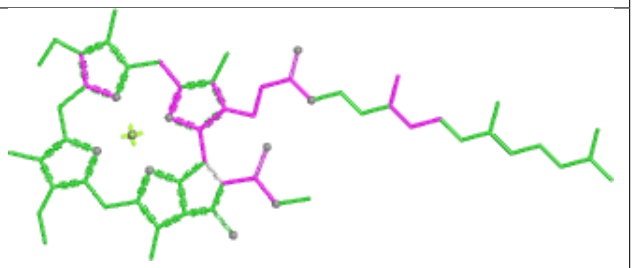


Rings

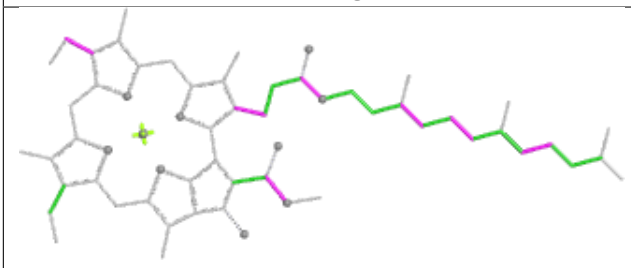
Ligand CLA B1 850



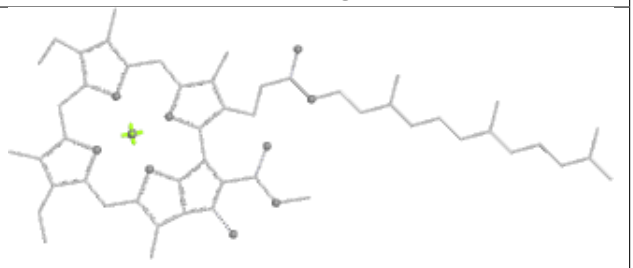
Bond lengths



Bond angles

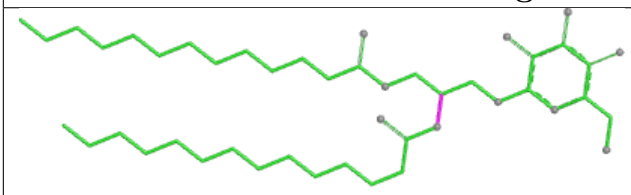


Torsions

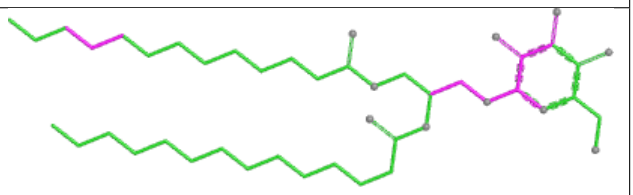


Rings

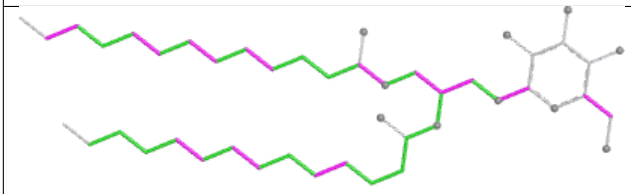
Ligand LMG M 102



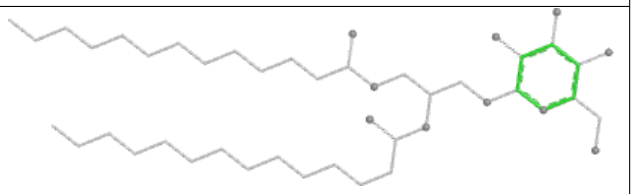
Bond lengths



Bond angles

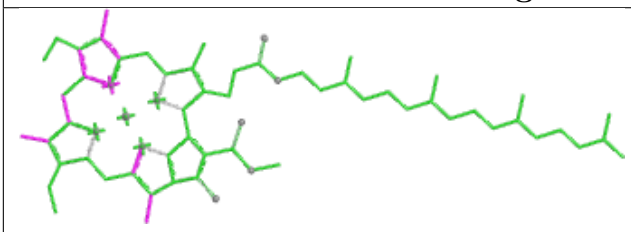


Torsions

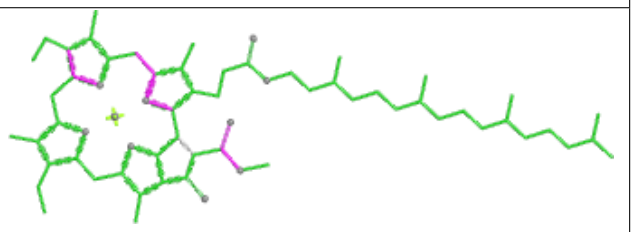


Rings

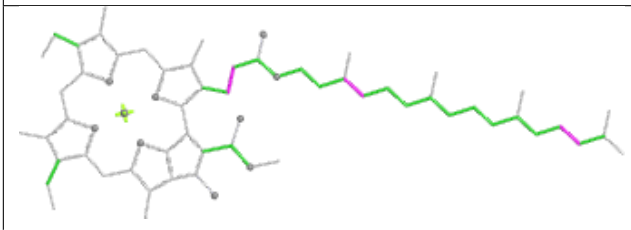
Ligand CLA B2 850



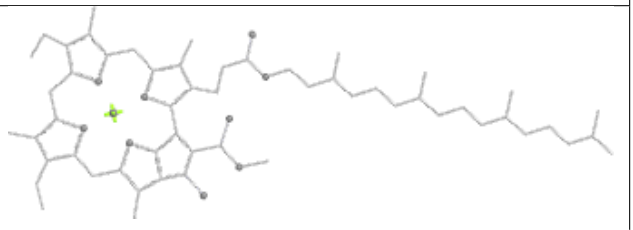
Bond lengths



Bond angles

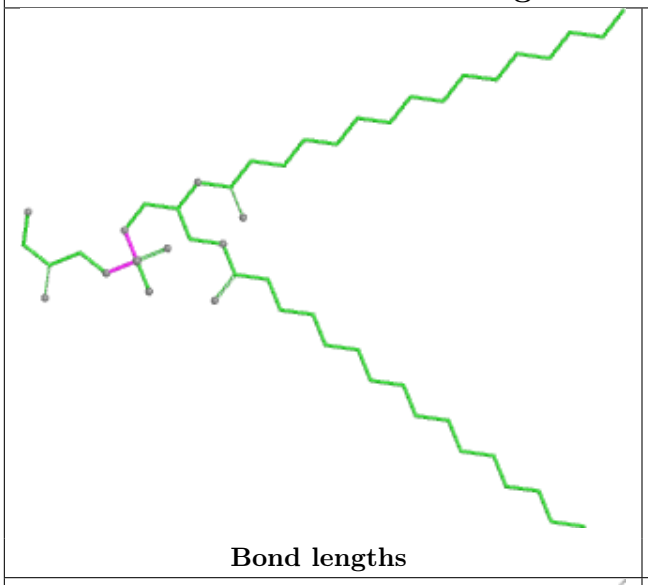


Torsions

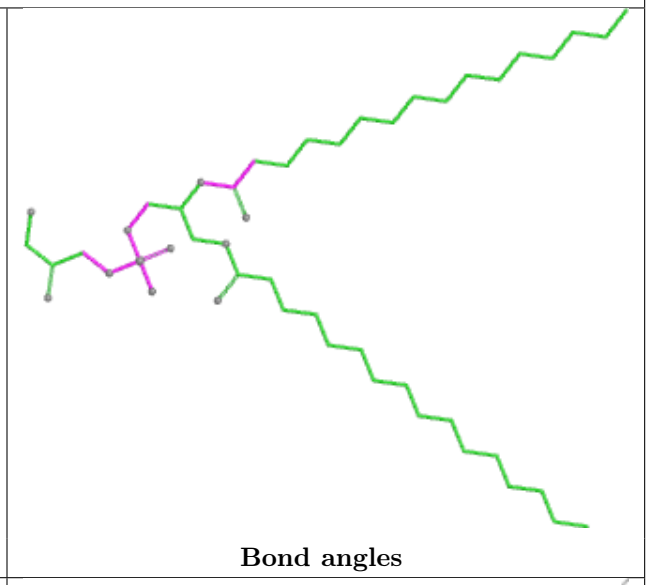


Rings

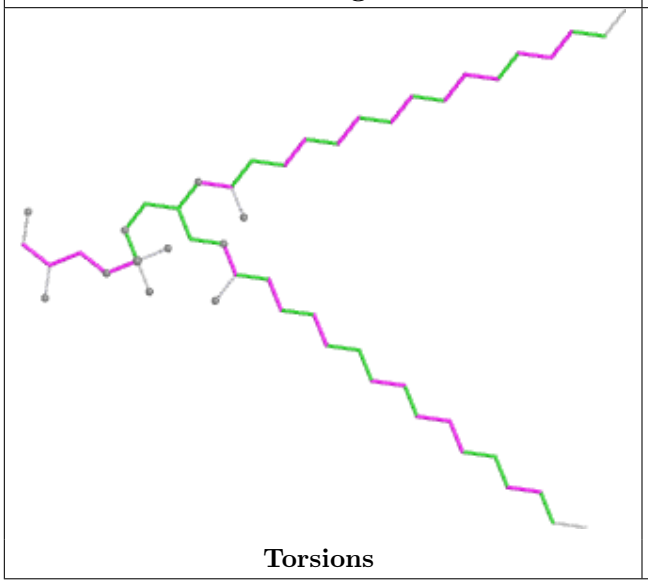
Ligand LHG X2 103



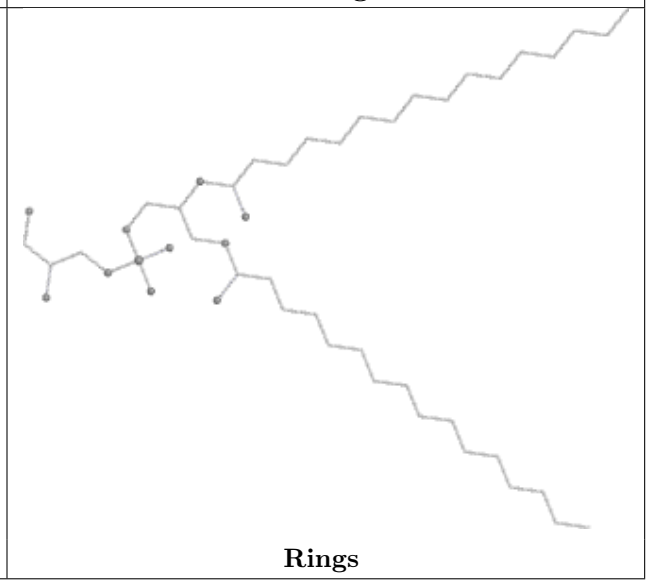
Bond lengths



Bond angles

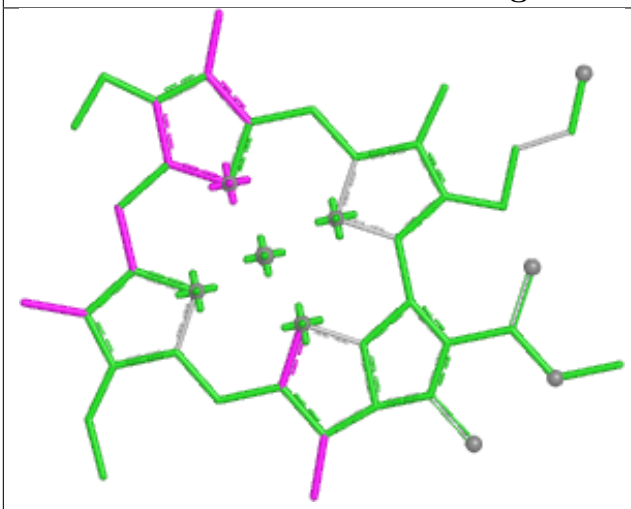


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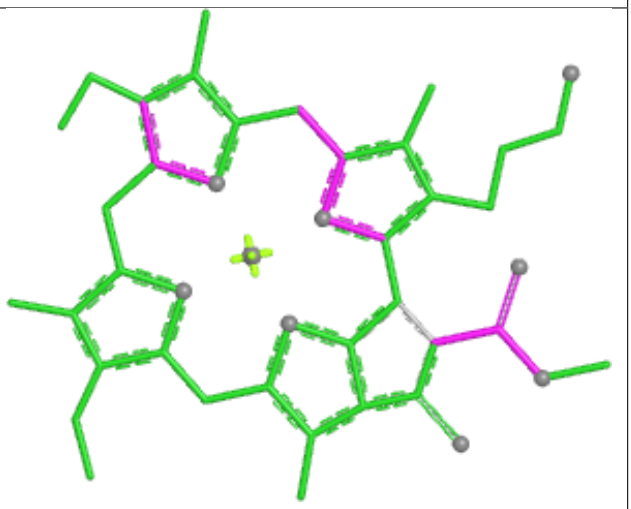


Rings

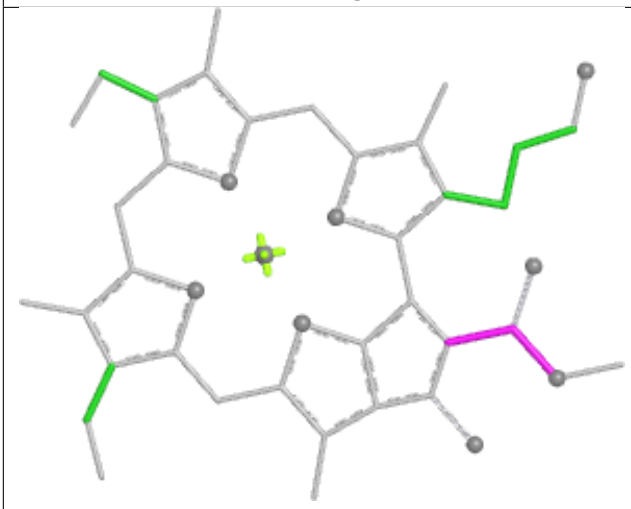
Ligand CLA AA 838



Bond lengths



Bond angles

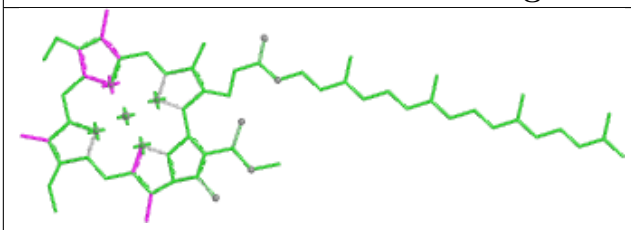


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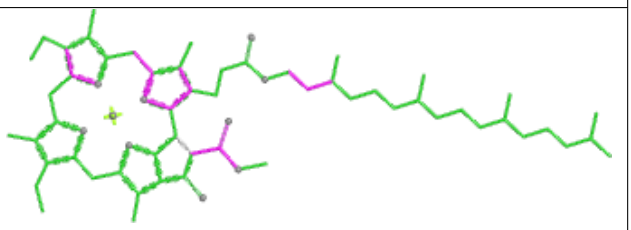


Rings

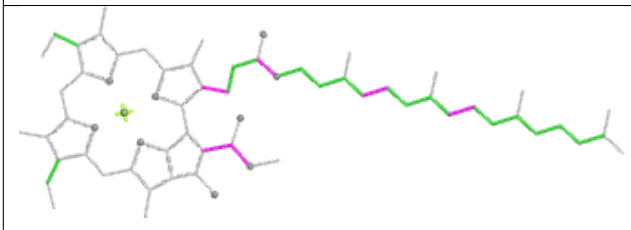
Ligand CLA A 832



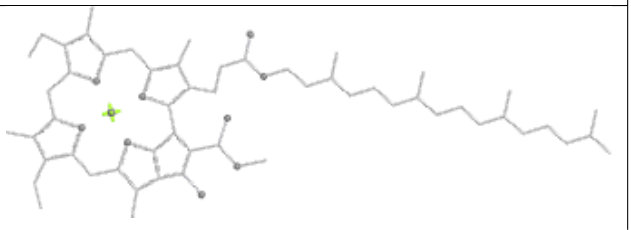
Bond lengths



Bond angles

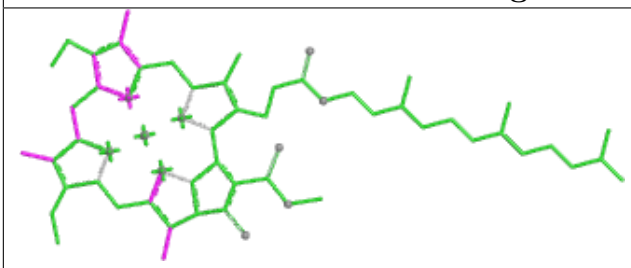


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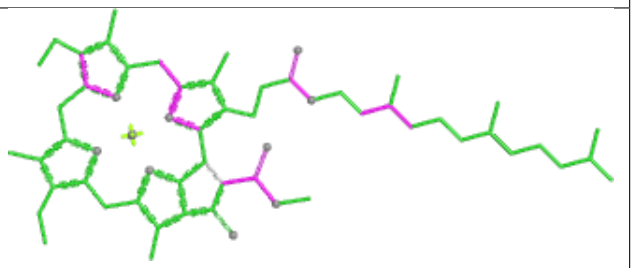


Rings

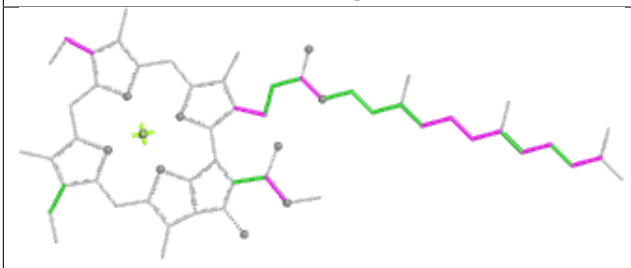
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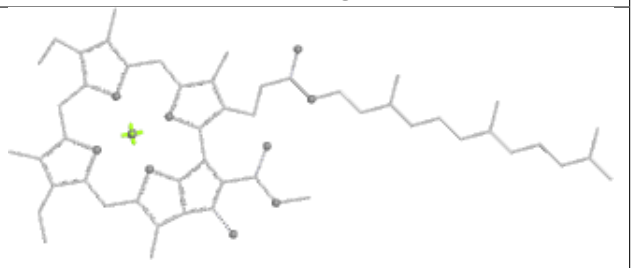
Bond lengths



Bond angles

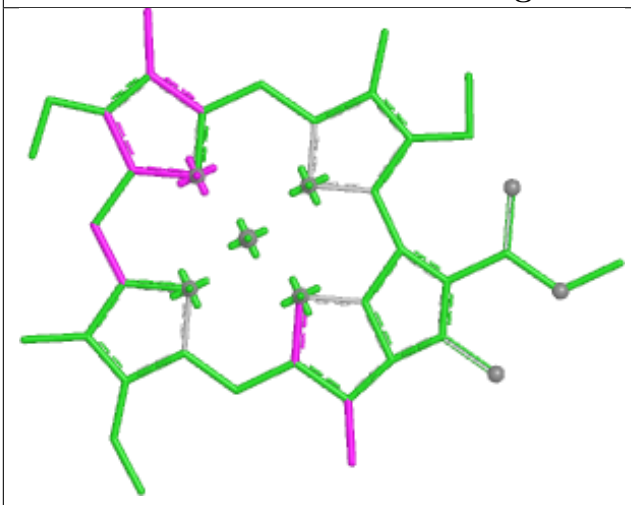


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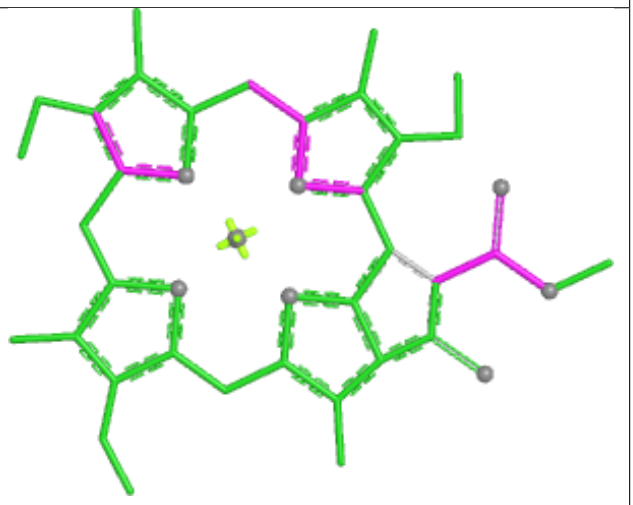


Rings

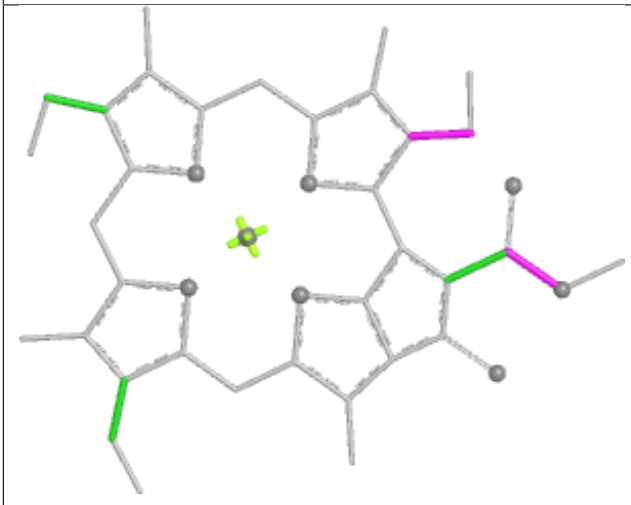
Ligand CLA FF 302



Bond lengths



Bond angles

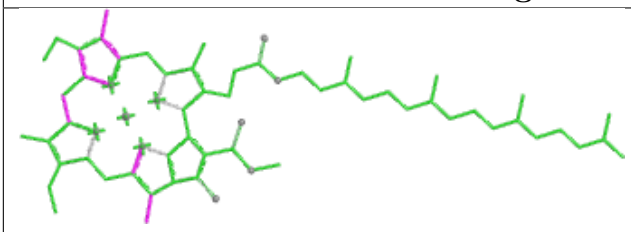


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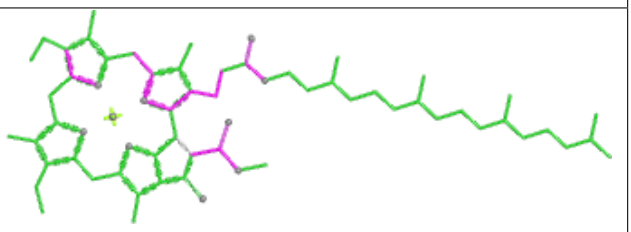


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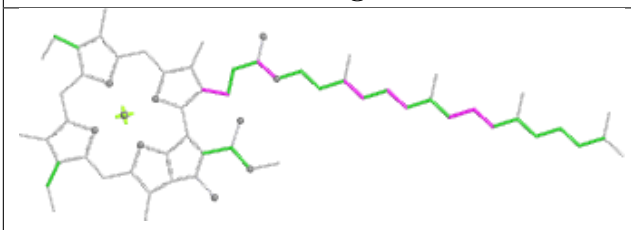
Ligand CLA A2 810



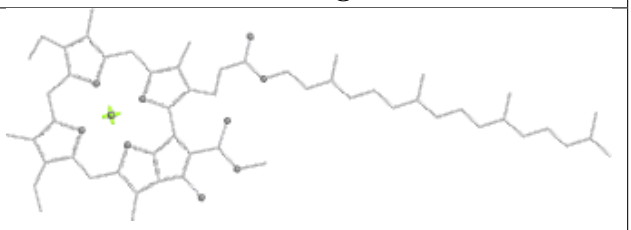
Bond lengths



Bond angles

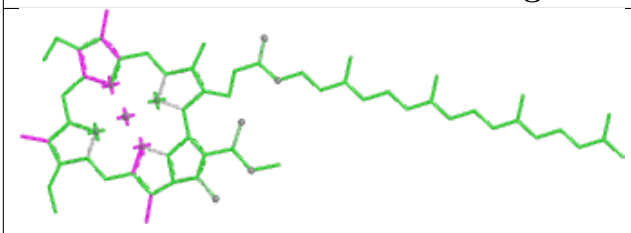


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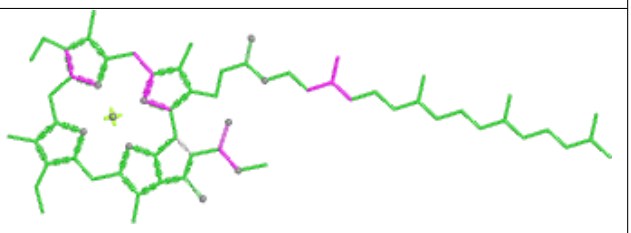


Rings

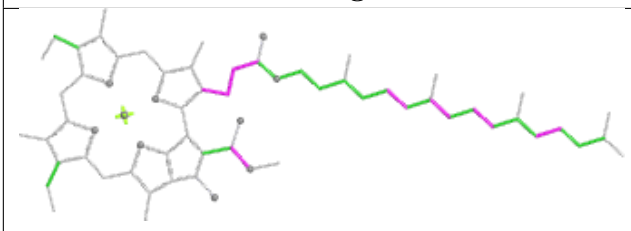
Ligand CLA A 829



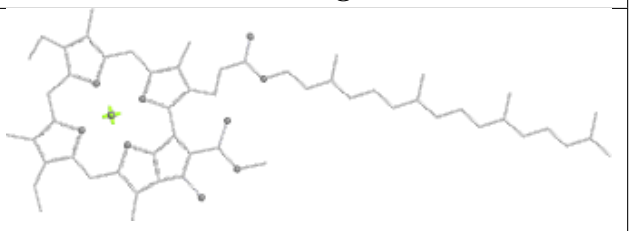
Bond lengths



Bond angles

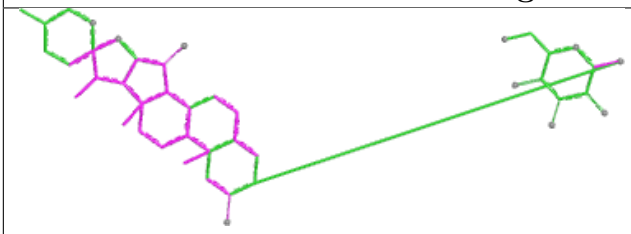


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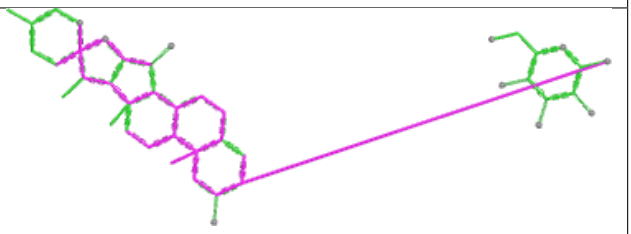


Rings

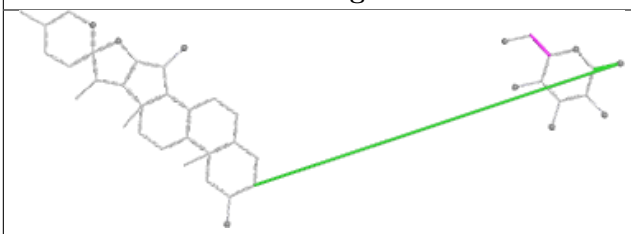
Ligand AJP A1 854



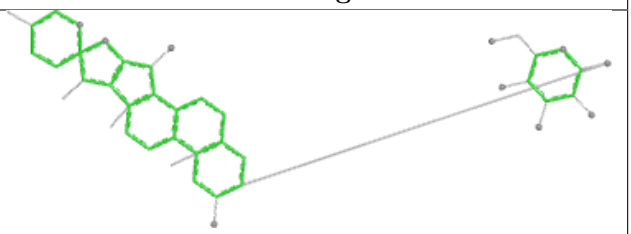
Bond lengths



Bond angles

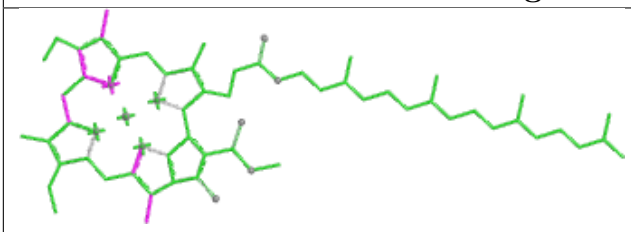


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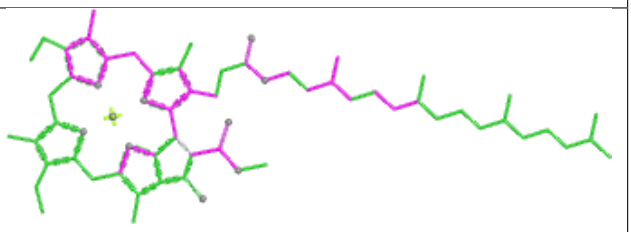


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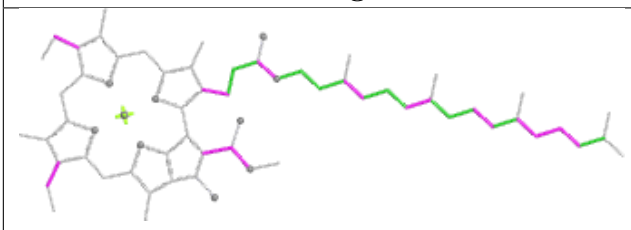
Ligand CLA B 834



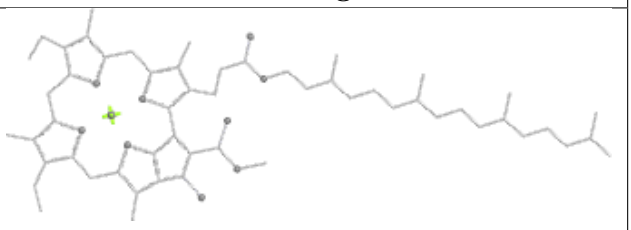
Bond lengths



Bond angles

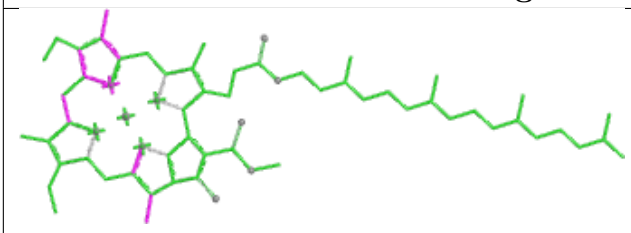


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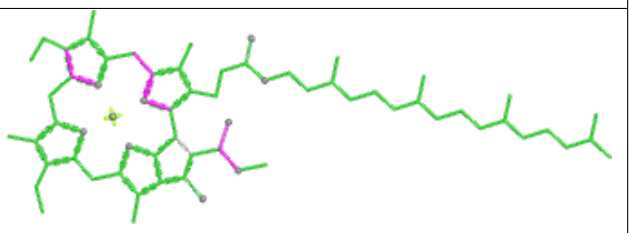


Rings

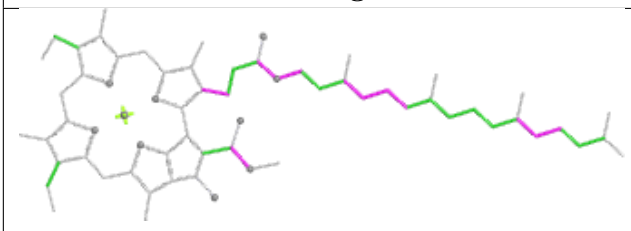
Ligand CLA B2 829



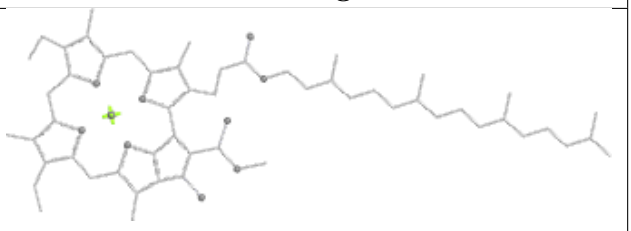
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Bond angles

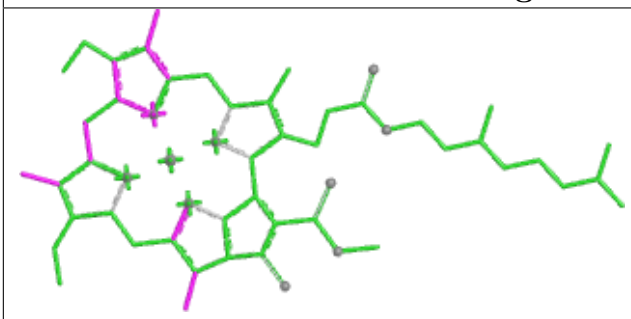


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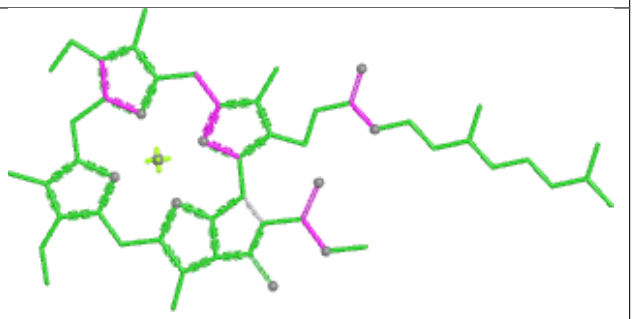


Rings

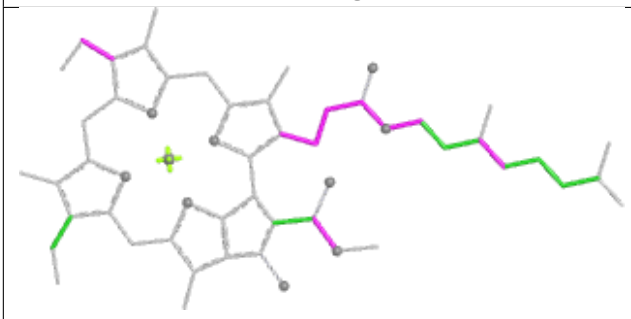
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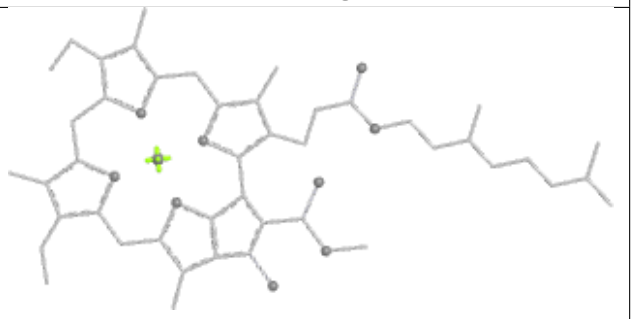
Bond lengths



Bond angles

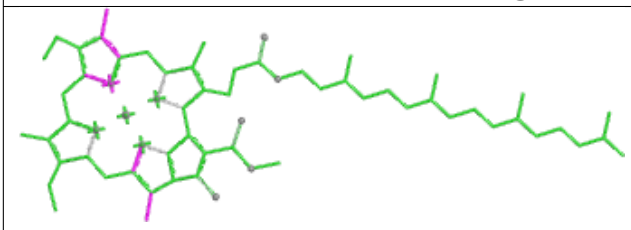


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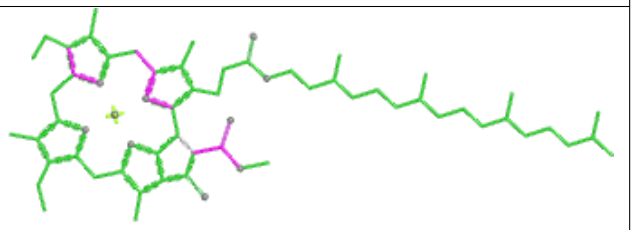


Rings

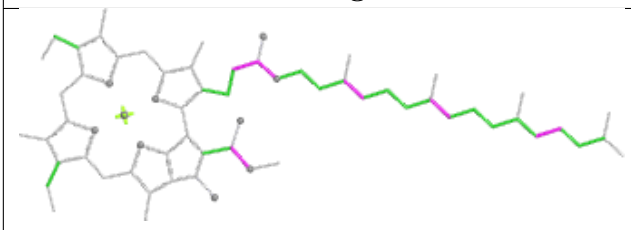
Ligand CLA BB 852



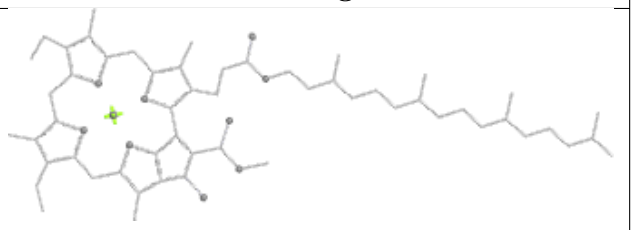
Bond lengths



Bond angles

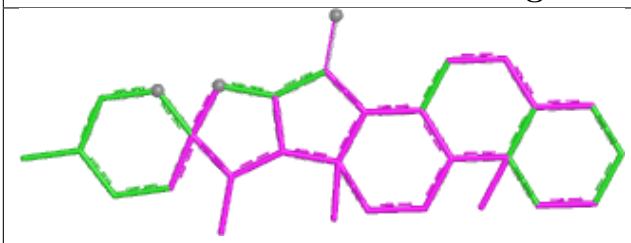


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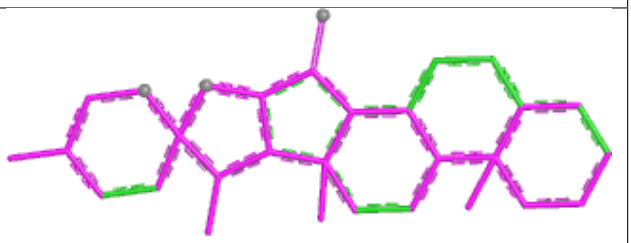


Rings

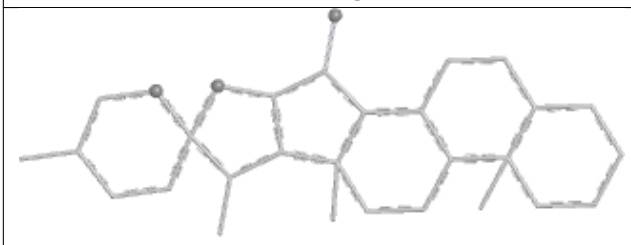
Ligand AJP A 802



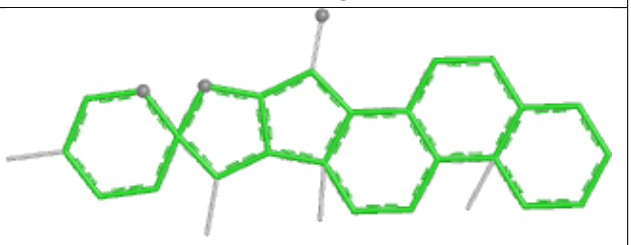
Bond lengths



Bond angles

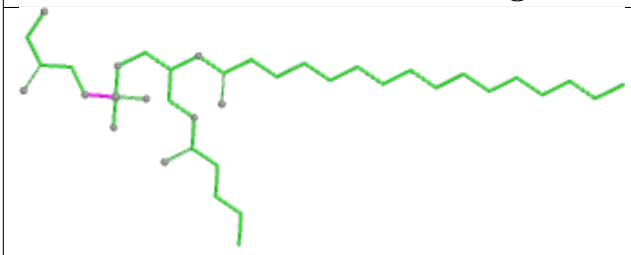


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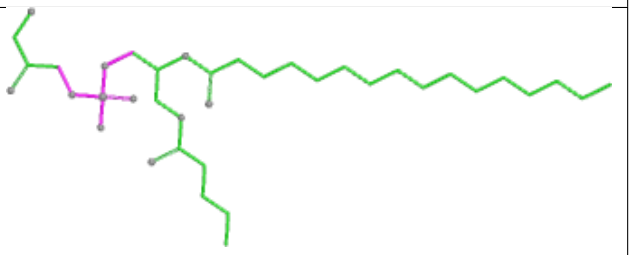


Rings

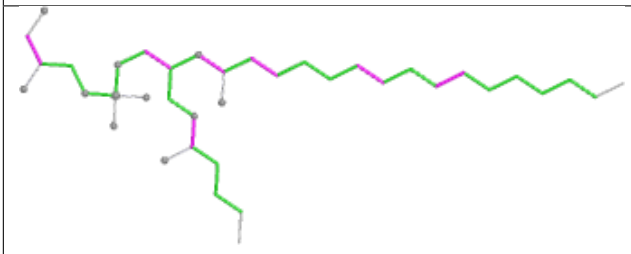
Ligand LHG AA 847



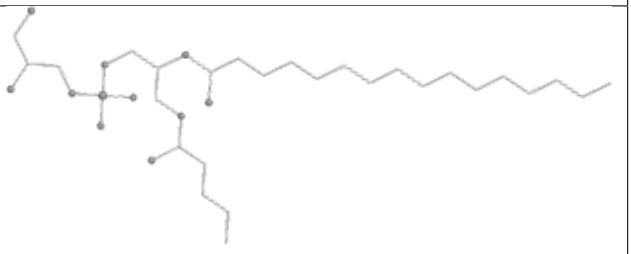
Bond lengths



Bond angles

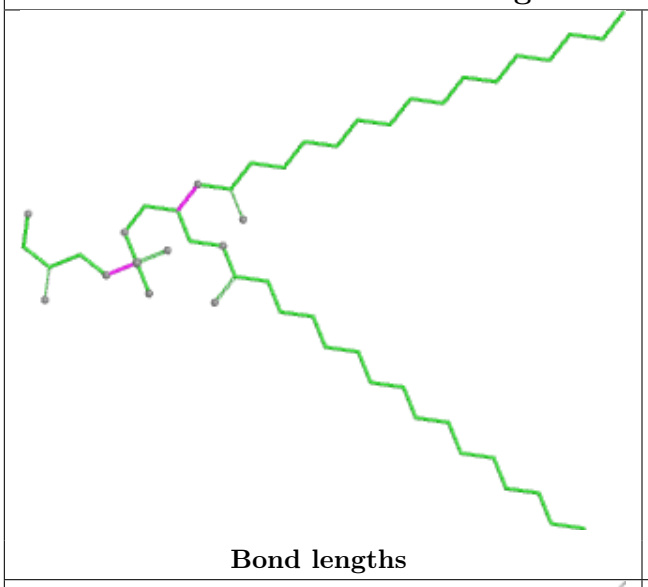


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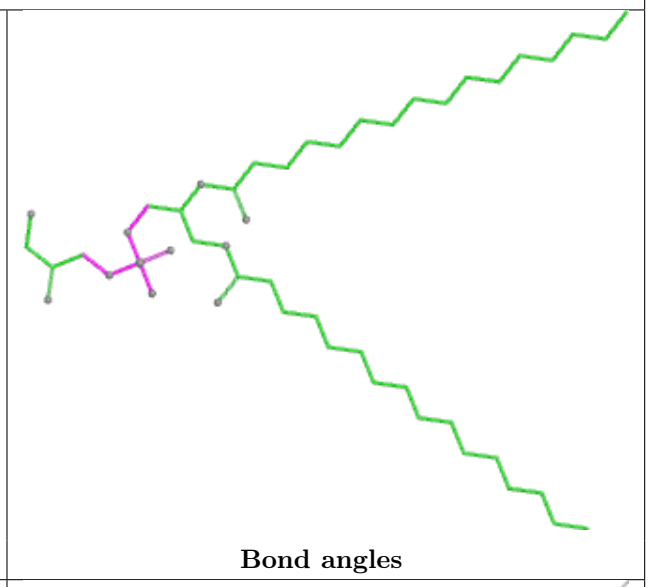


Rings

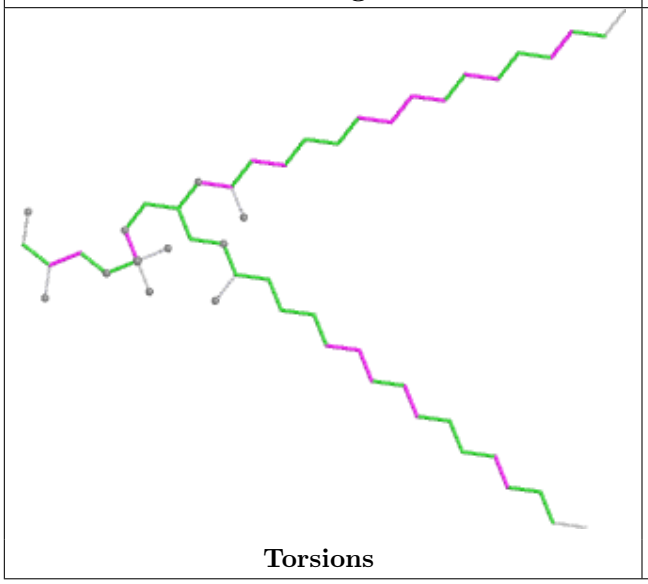
Ligand LHG A2 845



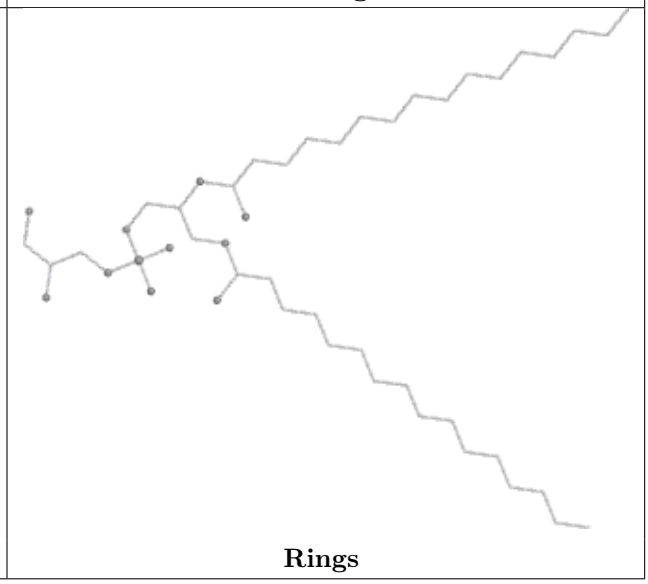
Bond lengths



Bond angles

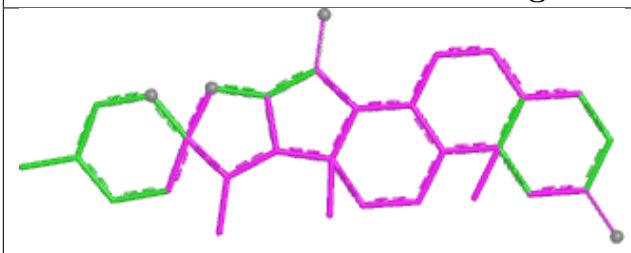


Torsions

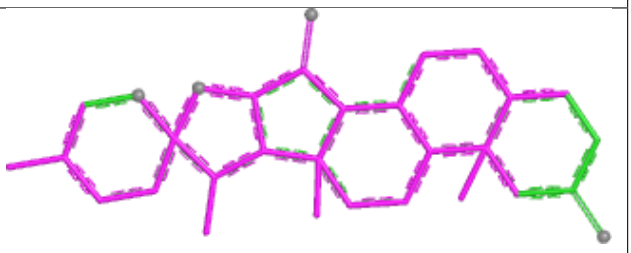


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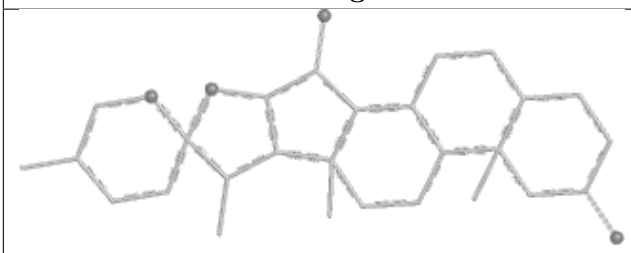
Ligand AJP L 209



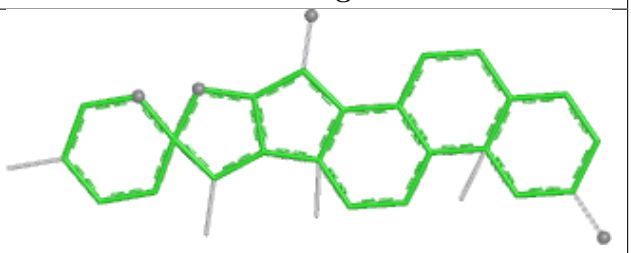
Bond lengths



Bond angles

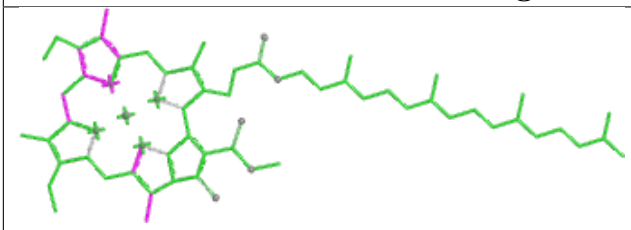


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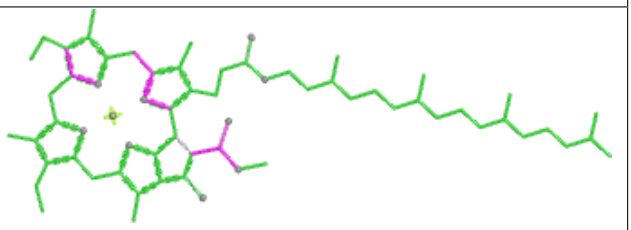


Rings

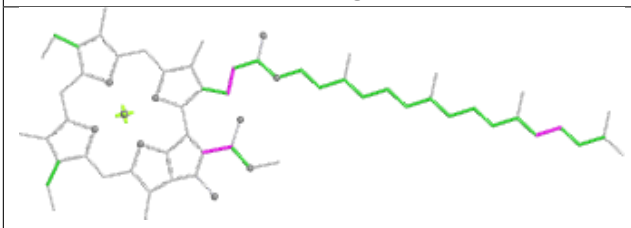
Ligand CLA B1 822



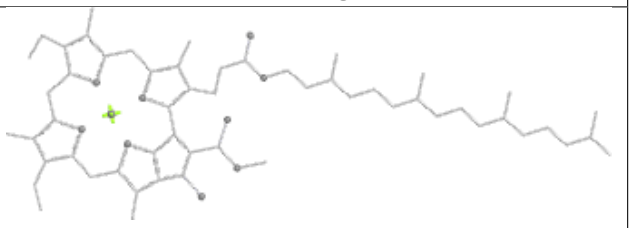
Bond lengths



Bond angles

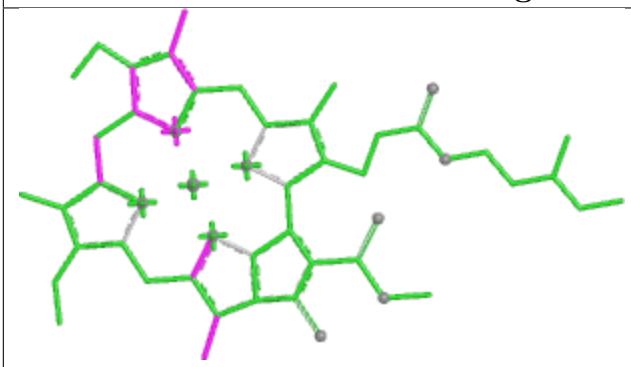


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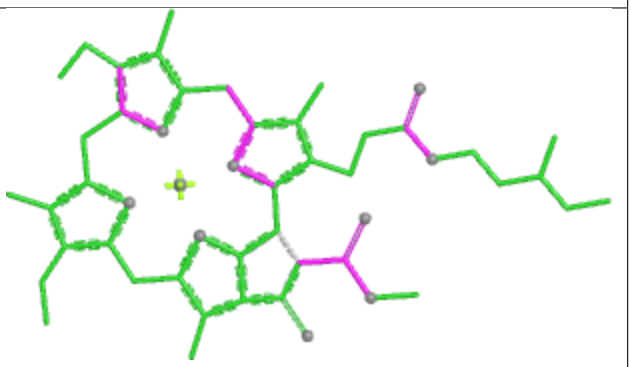


Rings

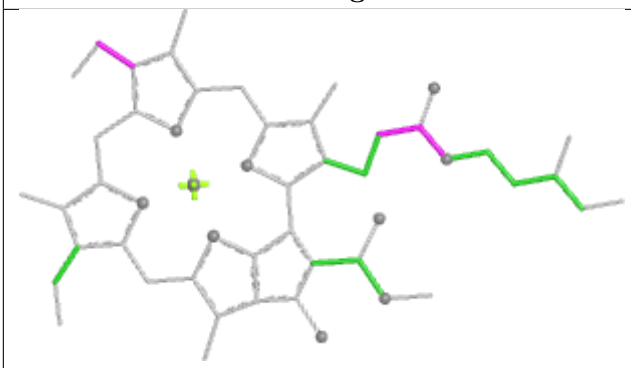
Ligand CLA A2 822



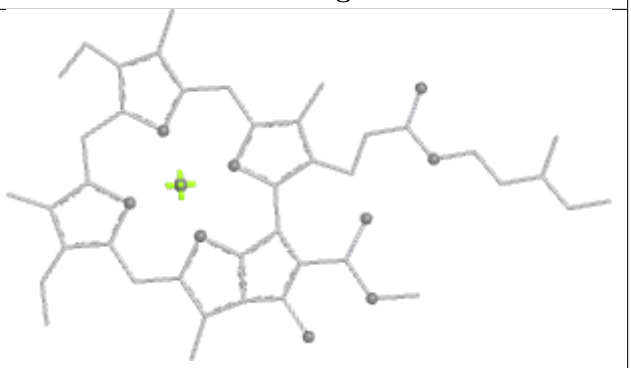
Bond lengths



Bond angles

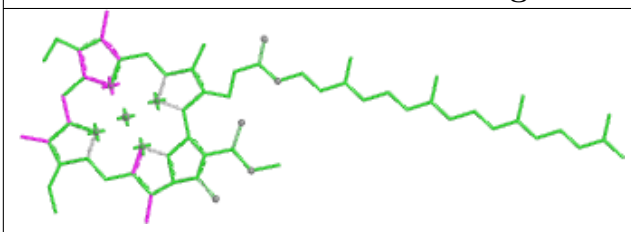


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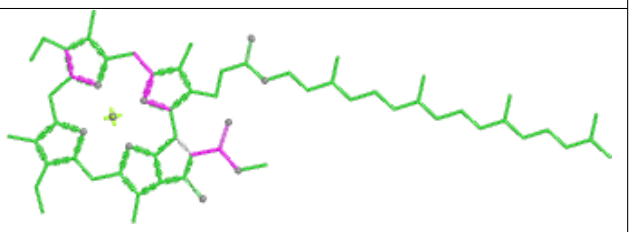


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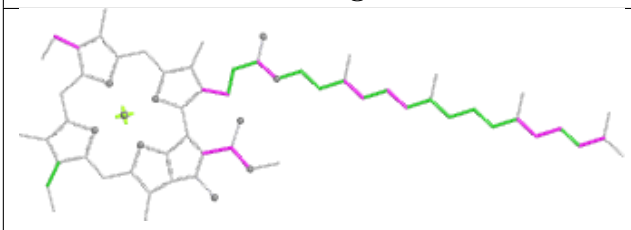
Ligand CLA AA 836



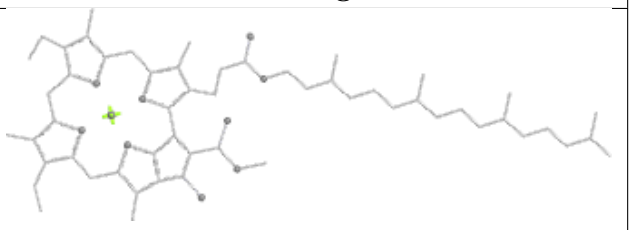
Bond lengths



Bond angles

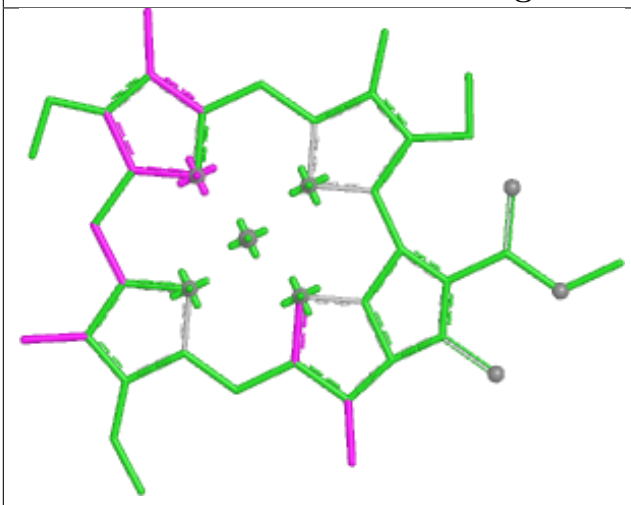


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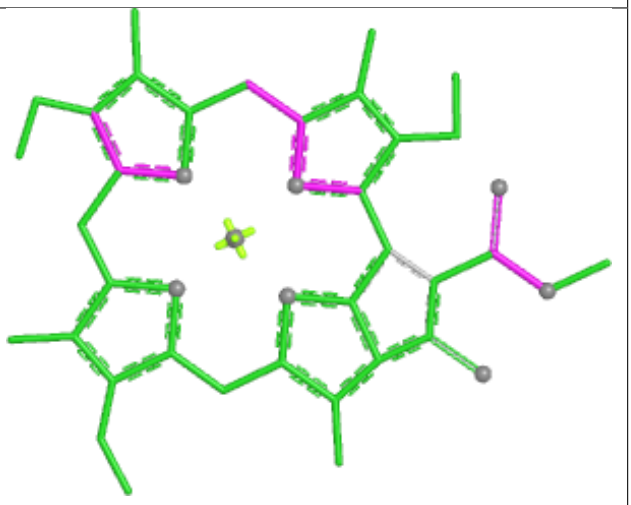


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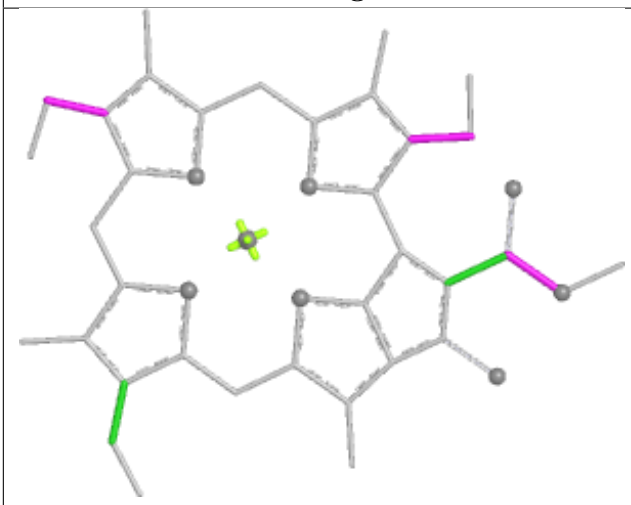
Ligand CLA A2 825



Bond lengths



Bond angles

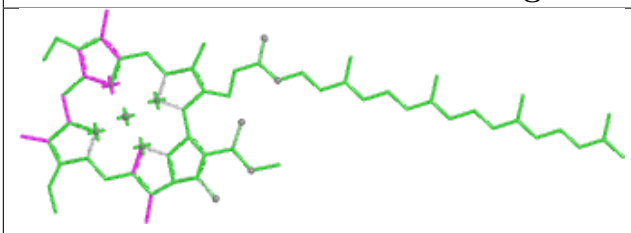


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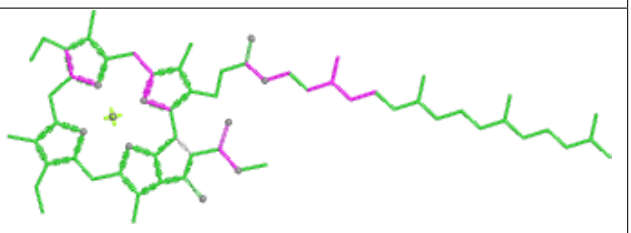


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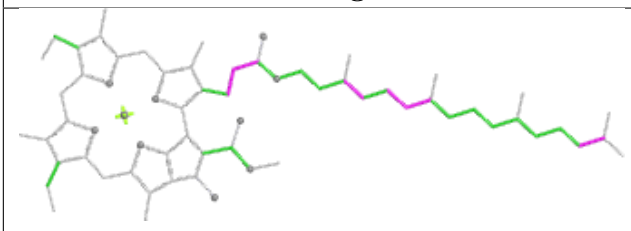
Ligand CLA A 842



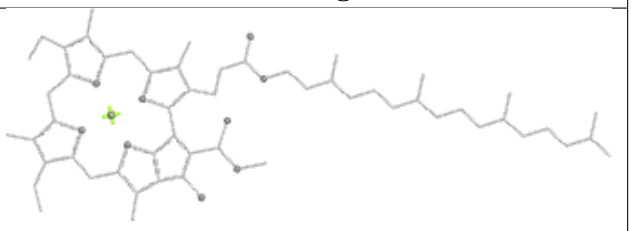
Bond lengths



Bond angles

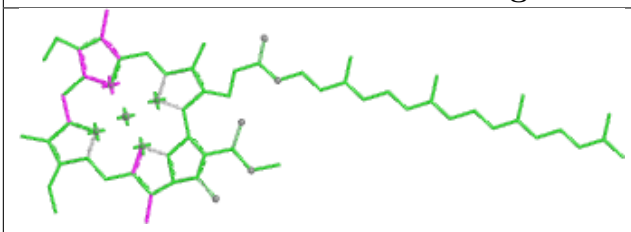


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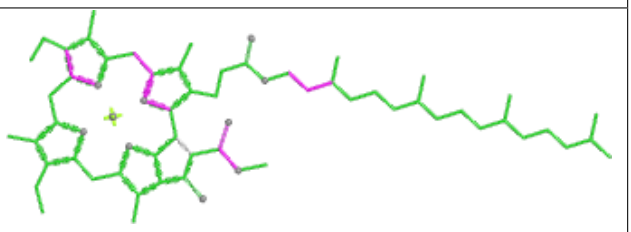


Rings

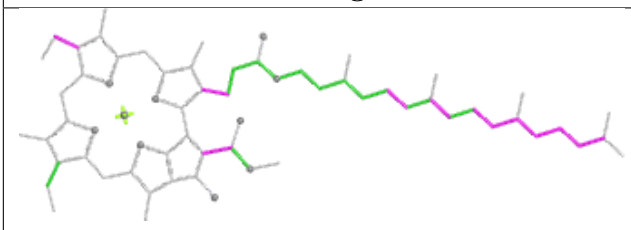
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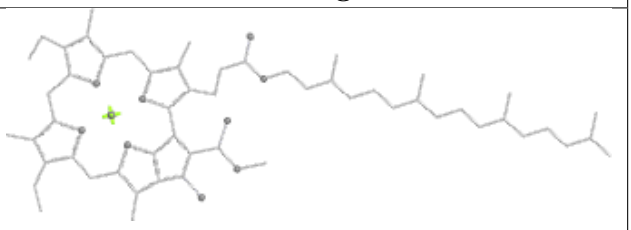
Bond lengths



Bond angles

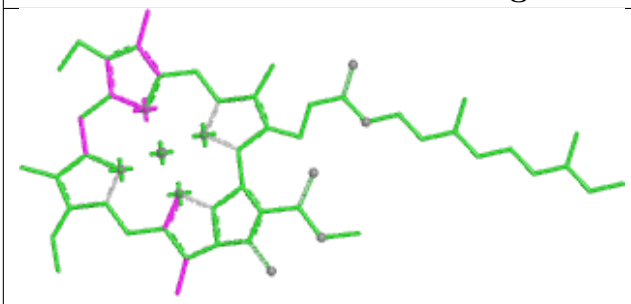


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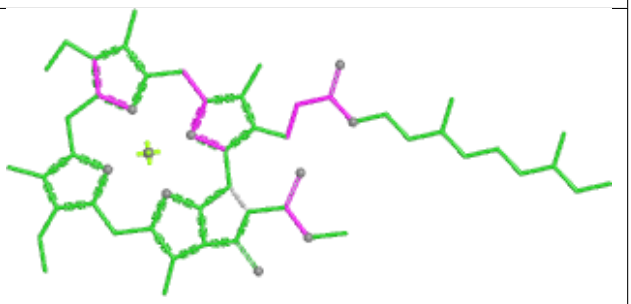


Rings

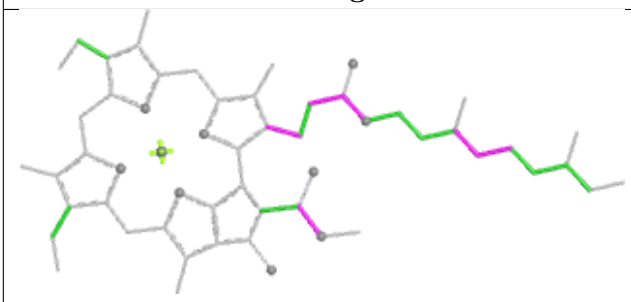
Ligand CLA AA 828



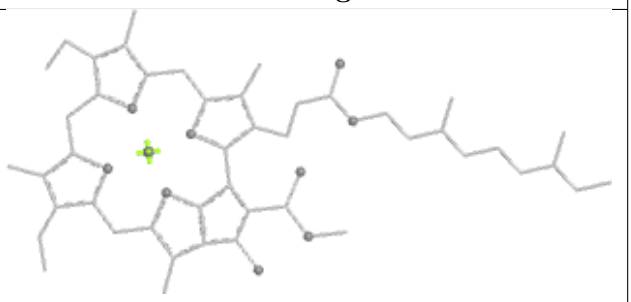
Bond lengths



Bond angles

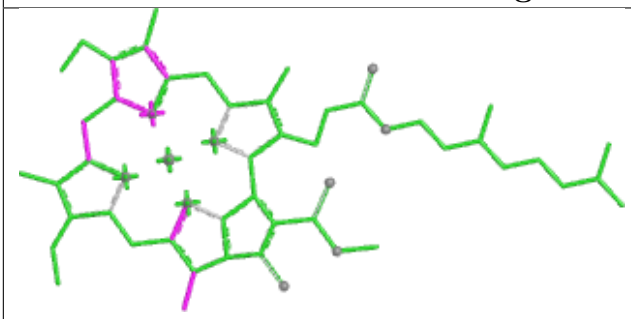


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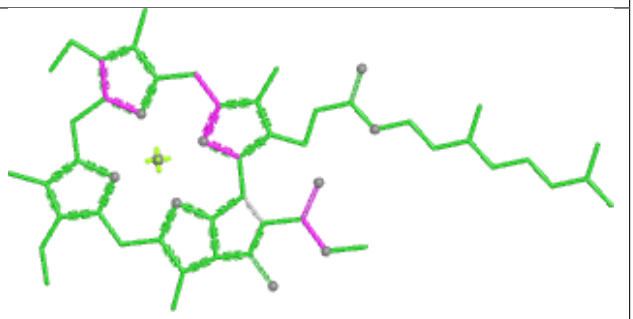


Rings

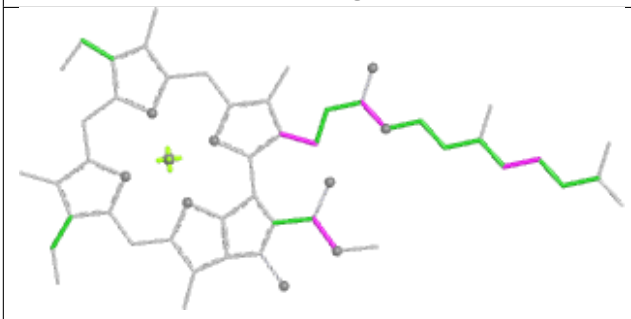
Ligand CLA A1 814



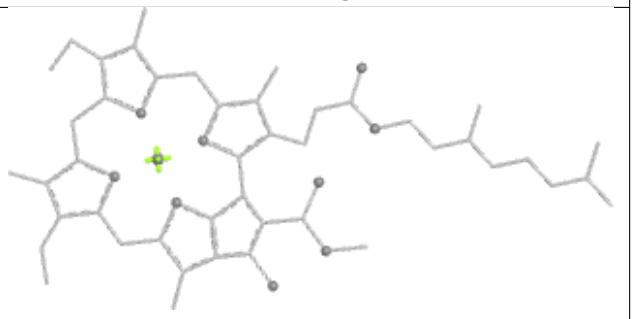
Bond lengths



Bond angles

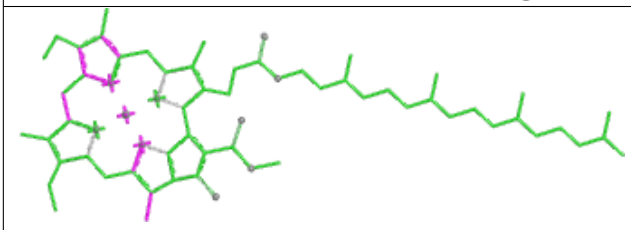


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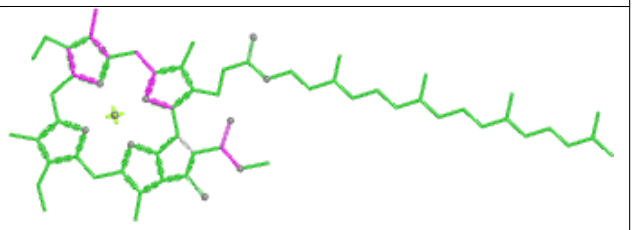


Rings

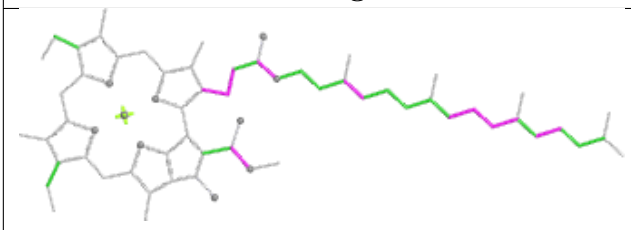
Ligand CLA L2 206



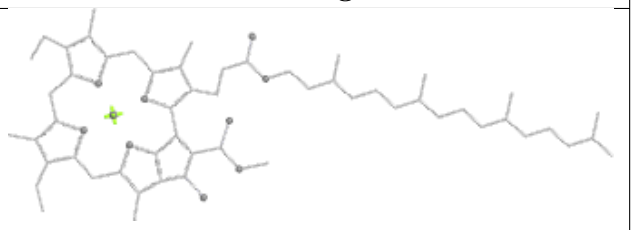
Bond lengths



Bond angles

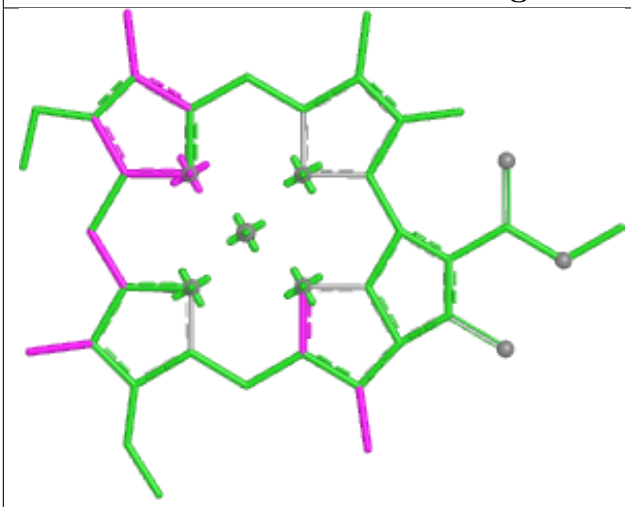


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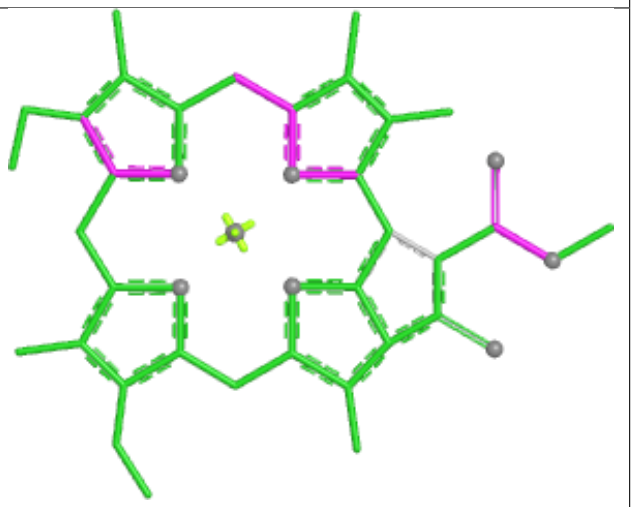


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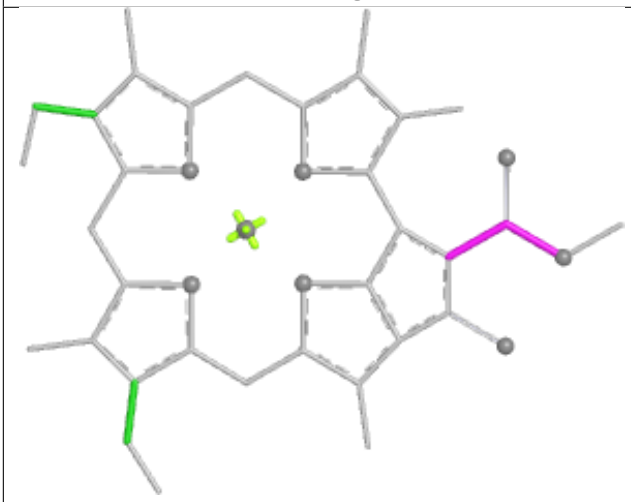
Ligand CLA AA 845



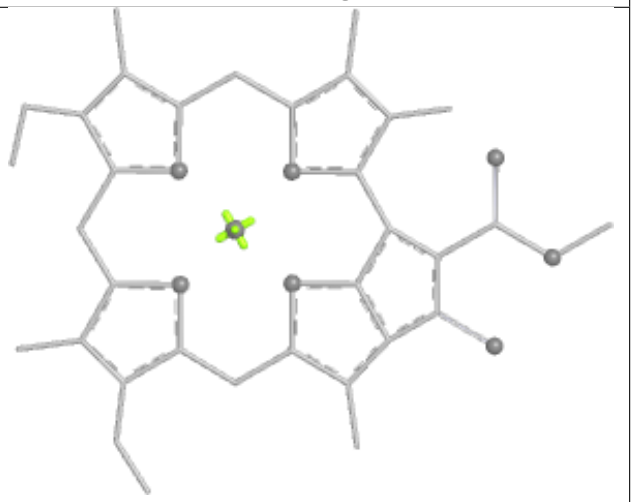
Bond lengths



Bond angles



Torsions

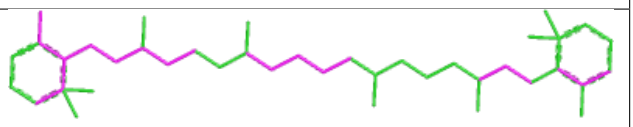


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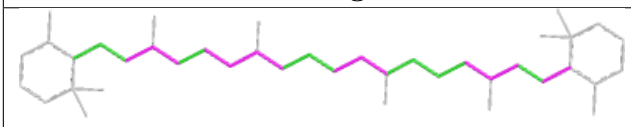
Ligand BCR L1 208



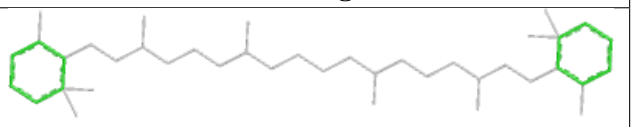
Bond lengths



Bond angles

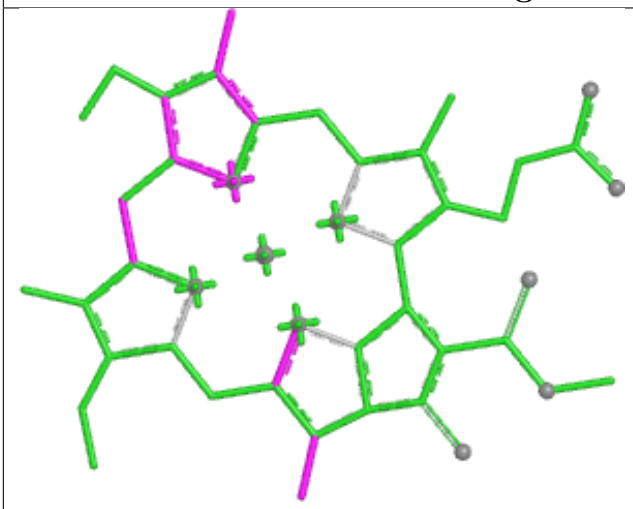


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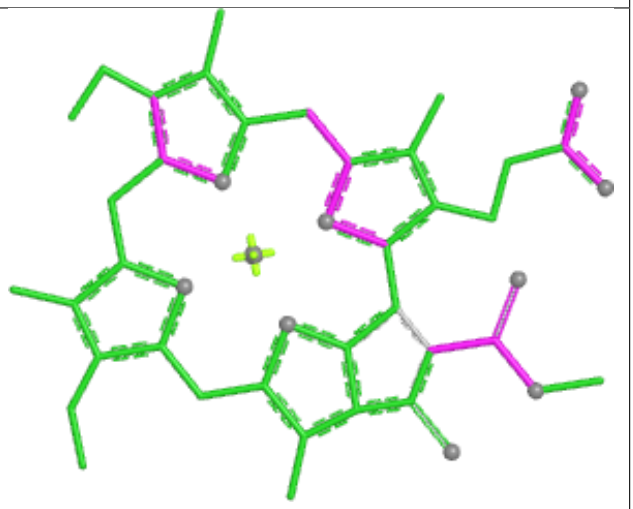


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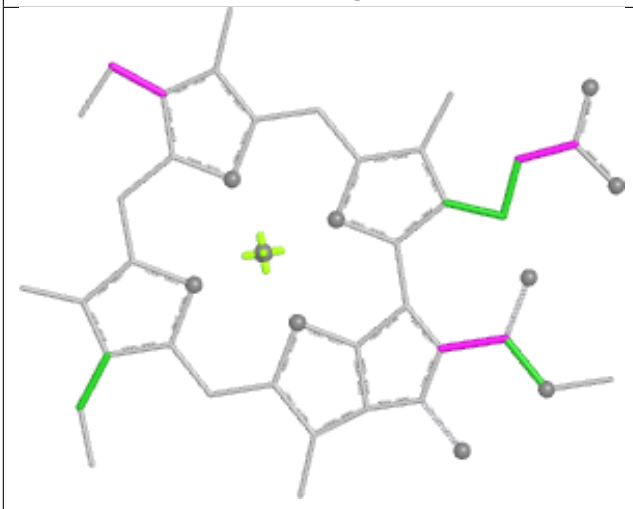
Ligand CLA B2 809



Bond lengths



Bond angles

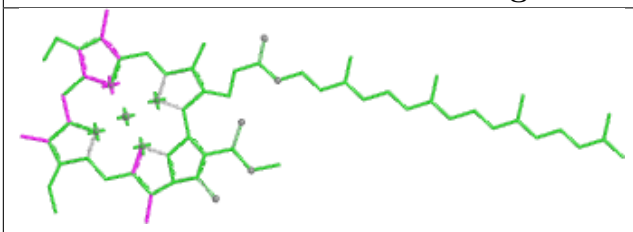


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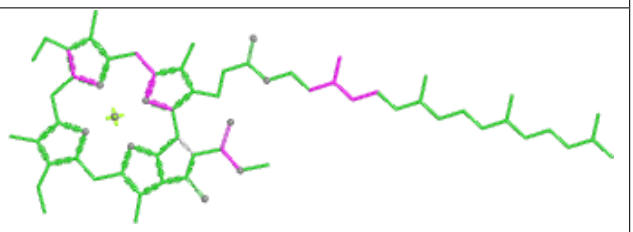


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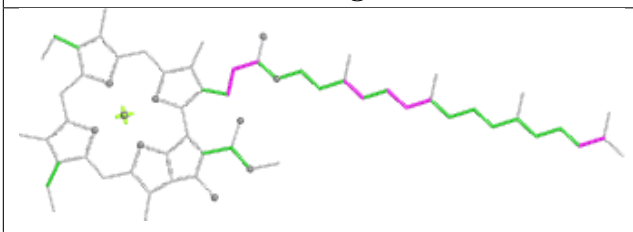
Ligand CLA AA 842



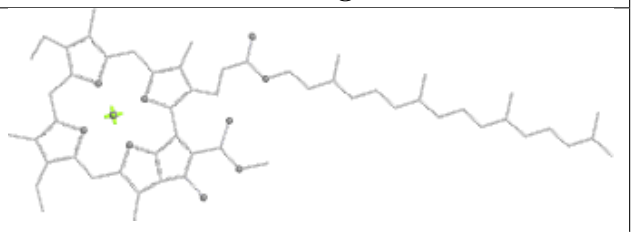
Bond lengths



Bond angles

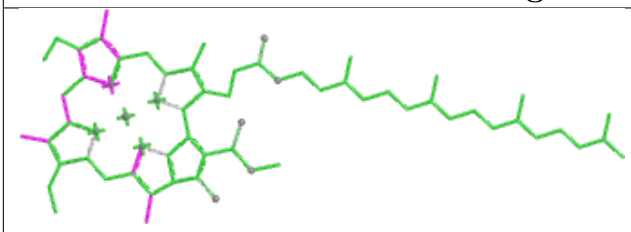


Torsions

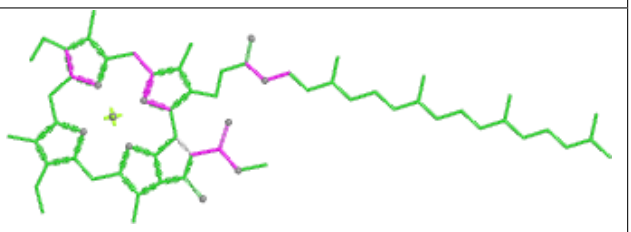


Rings

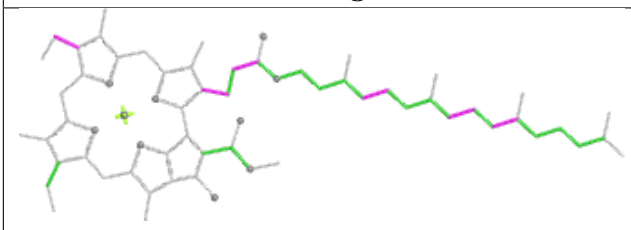
Ligand CLA L 203



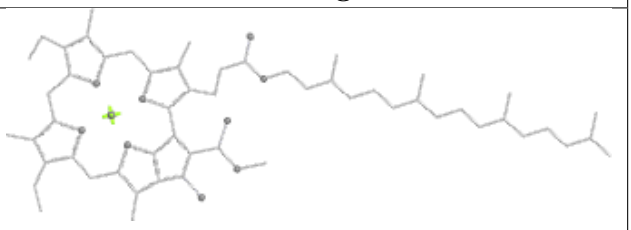
Bond lengths



Bond angles

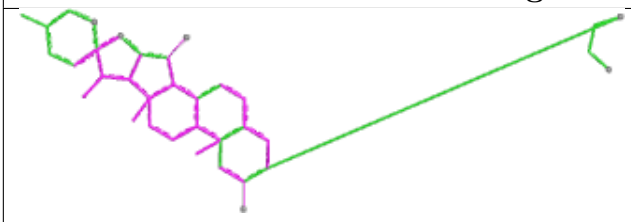


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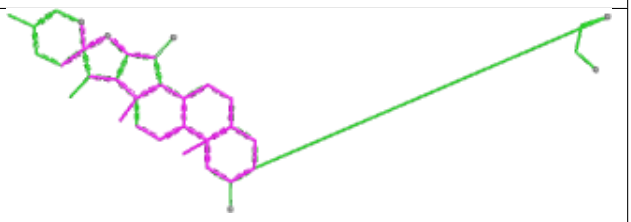


Rings

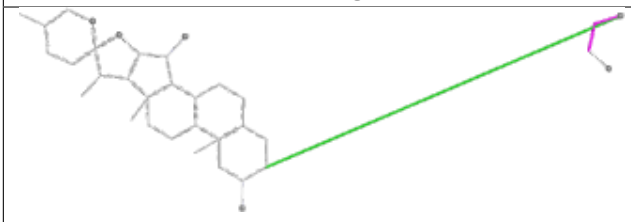
Ligand AJP A 855



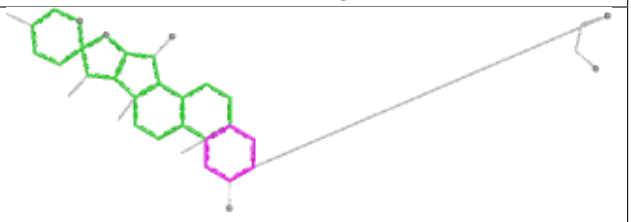
Bond lengths



Bond angles

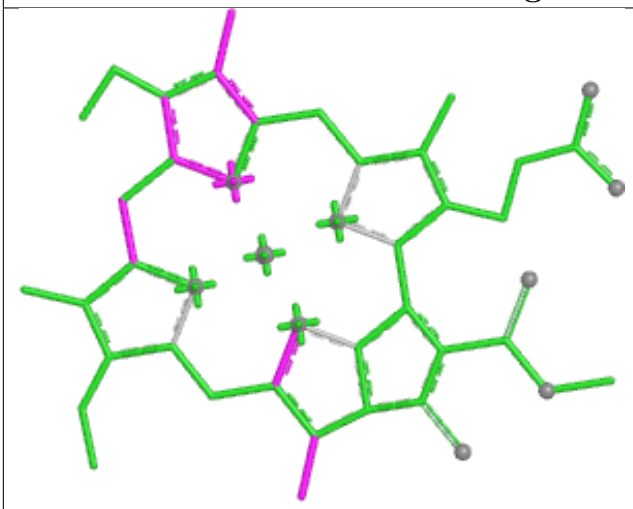


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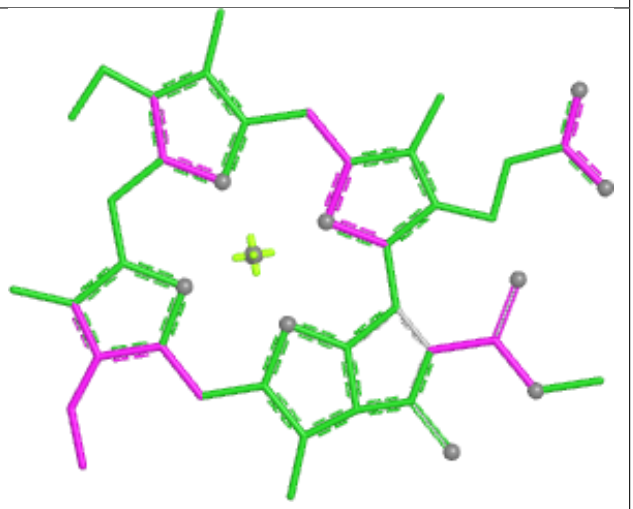


Rings

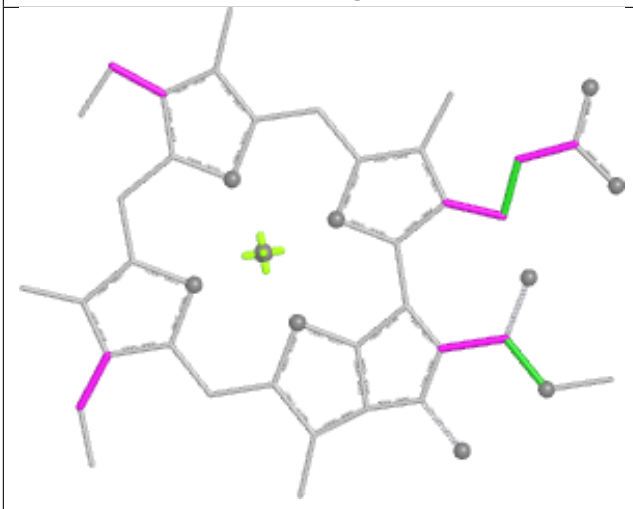
Ligand CLA B 820



Bond lengths



Bond angles

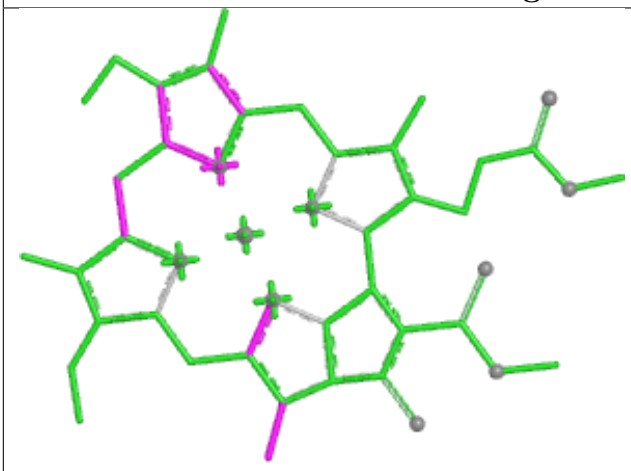


Torsions

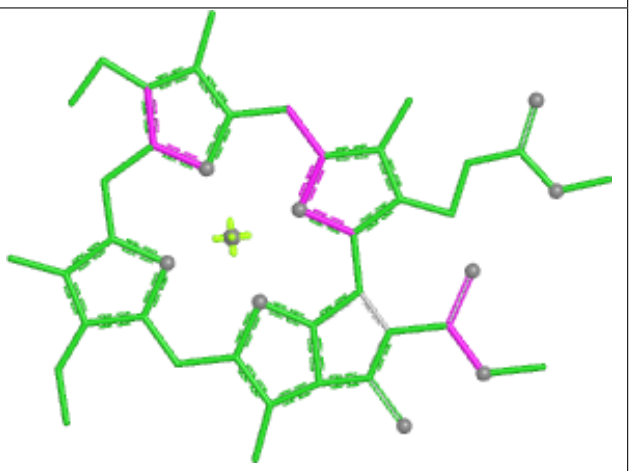


Rings

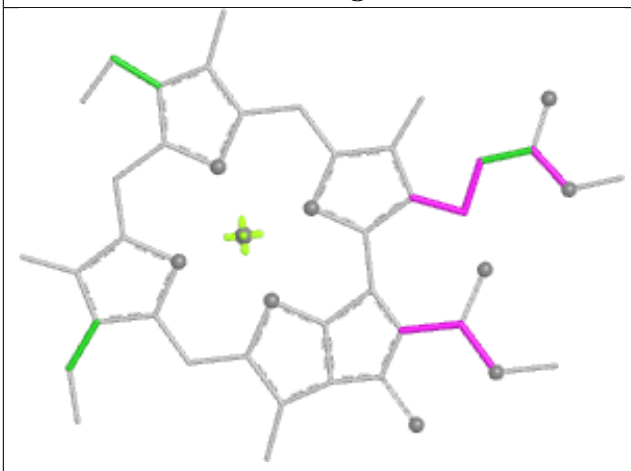
Ligand CLA K 102



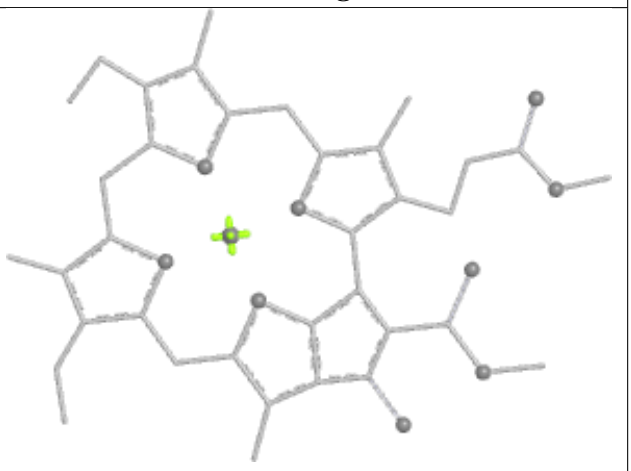
Bond lengths



Bond angles

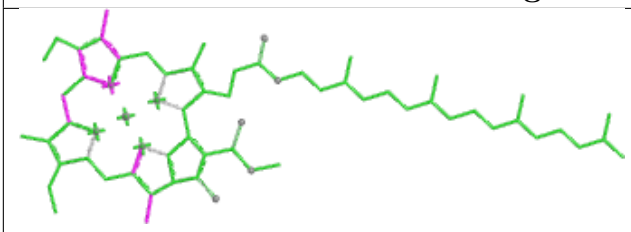


Torsions

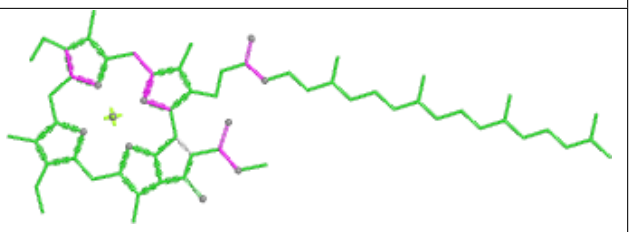


Rings

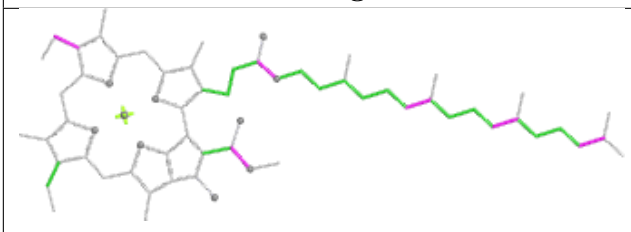
Ligand CLA A 813



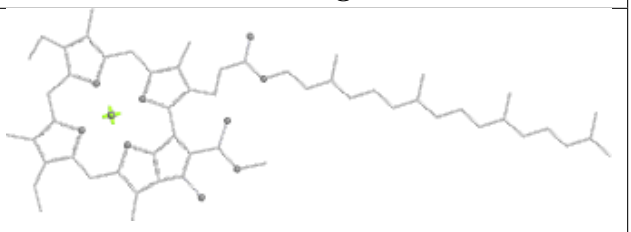
Bond lengths



Bond angles

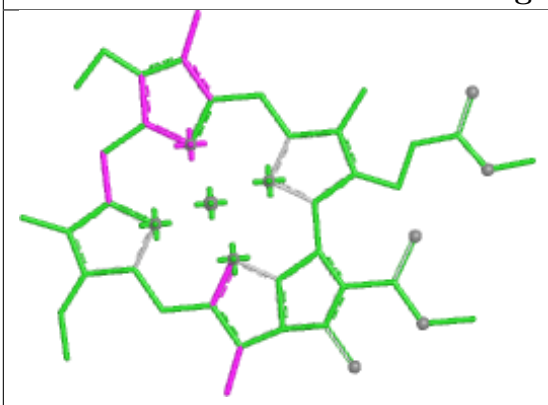


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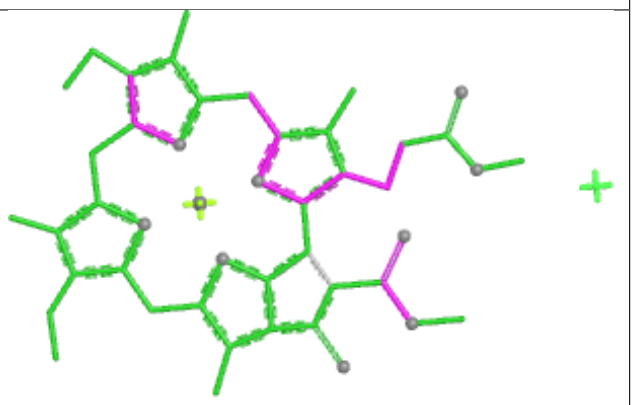


Rings

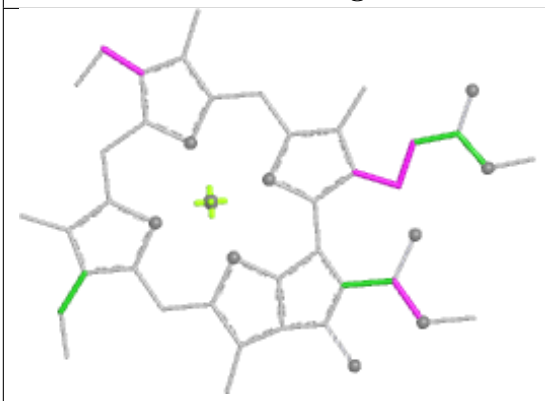
Ligand CLA A2 812



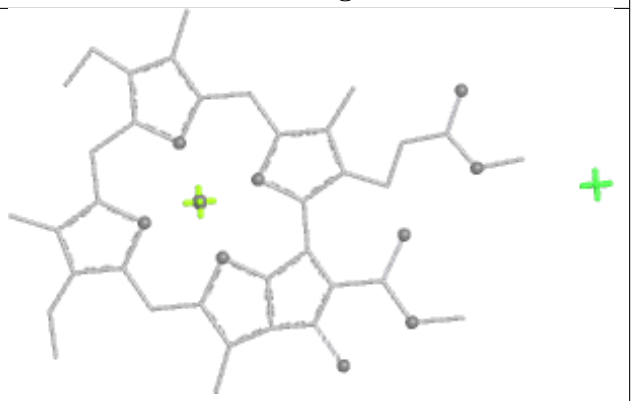
Bond lengths



Bond angles

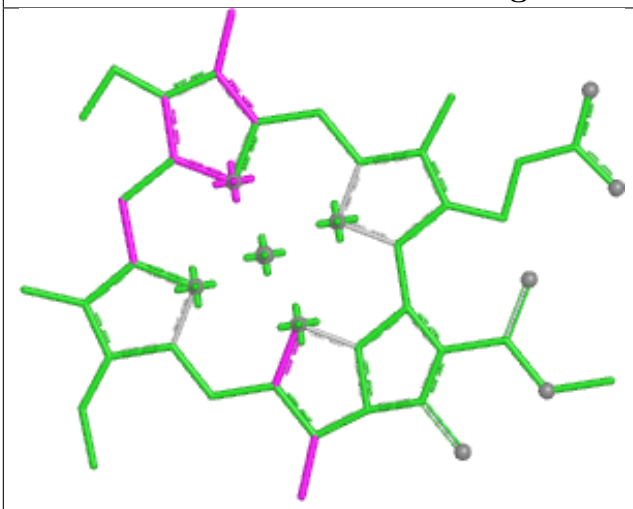


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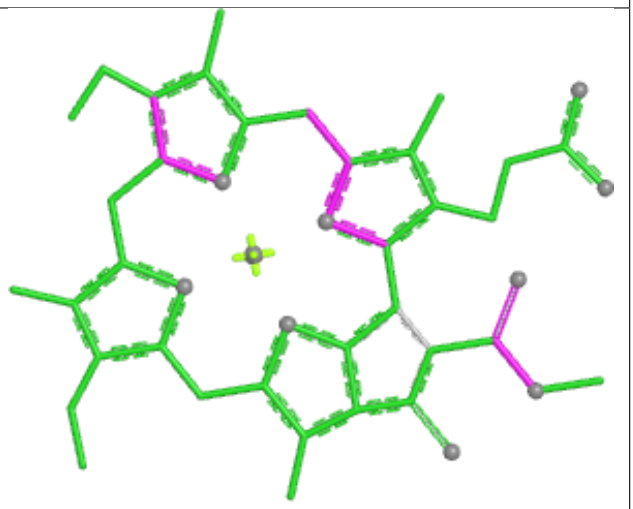


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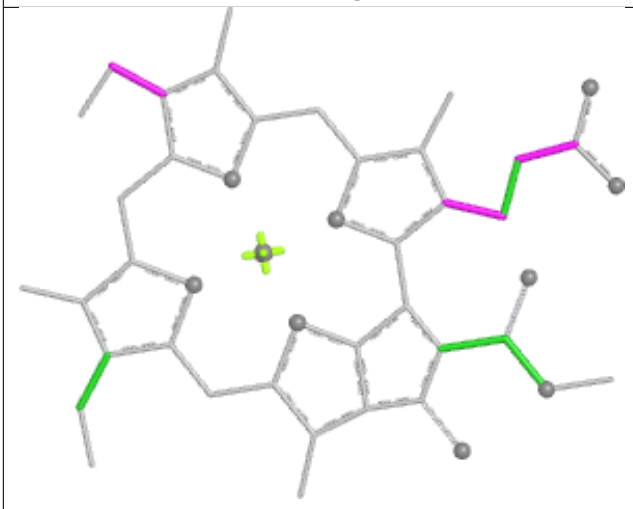
Ligand CLA AA 818



Bond lengths



Bond angles

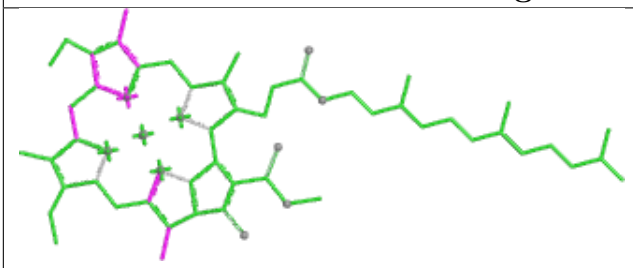


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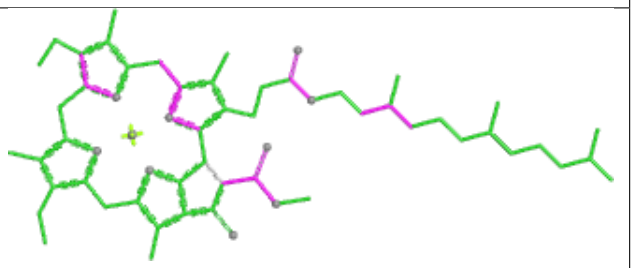


Rings

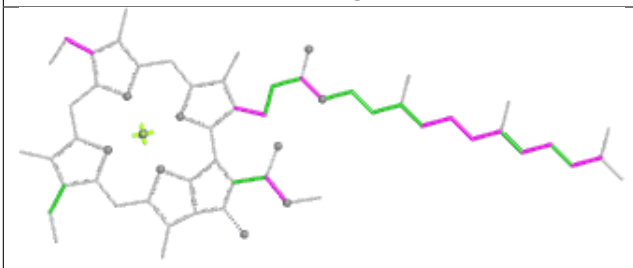
Ligand CLA A2 823



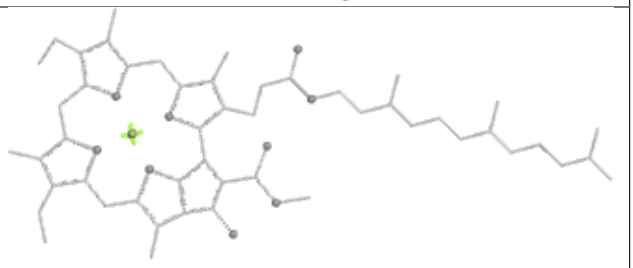
Bond lengths



Bond angles

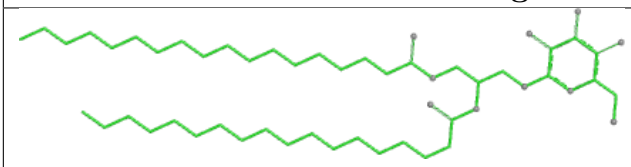


Torsions

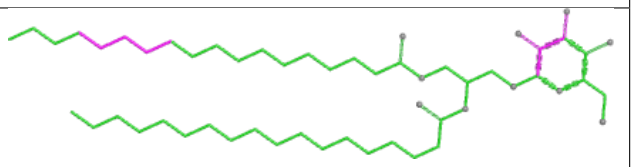


Rings

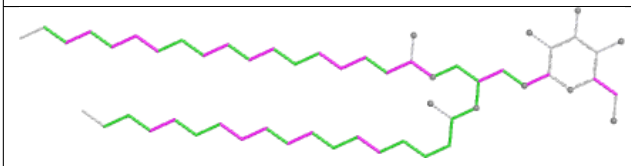
Ligand LMG B2 845



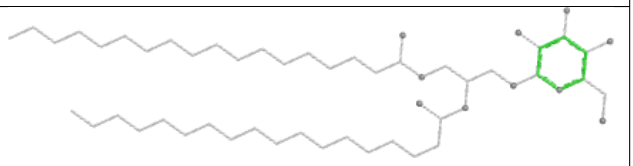
Bond lengths



Bond angles

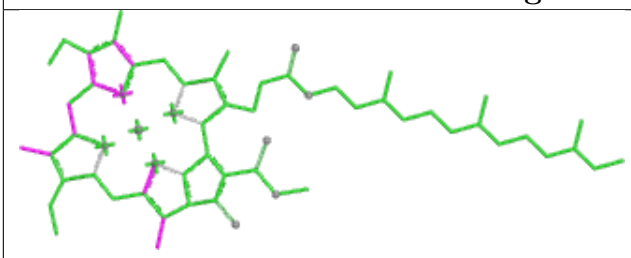


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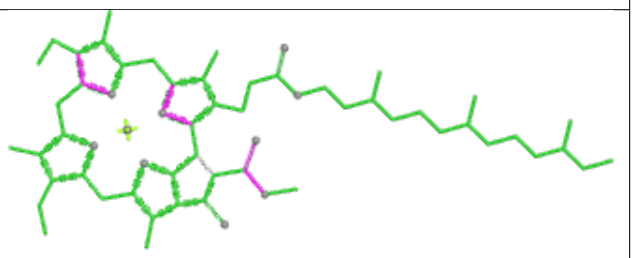


Rings

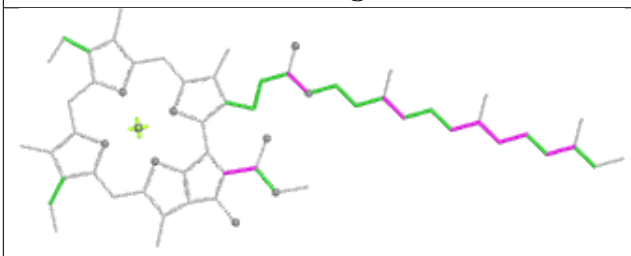
Ligand CLA B 811



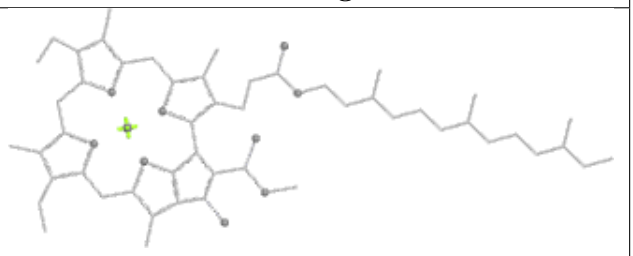
Bond lengths



Bond angles



Torsions



Rings

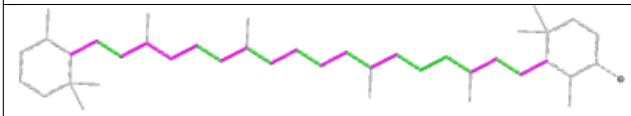
Ligand ECH BB 840



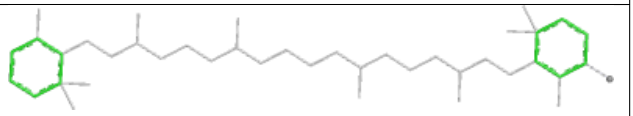
Bond lengths



Bond angles

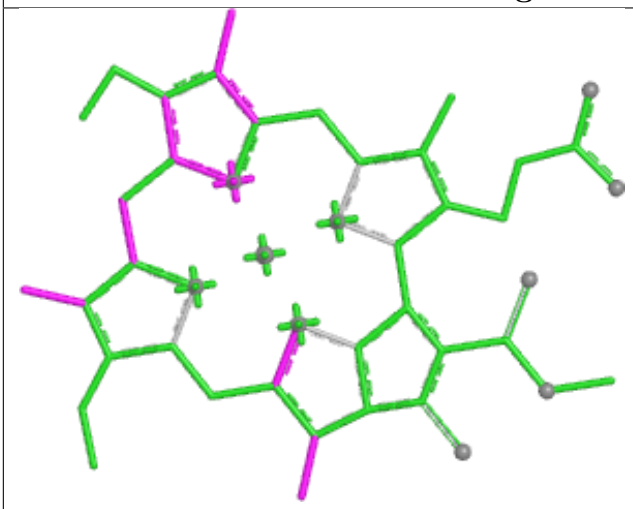


Torsions

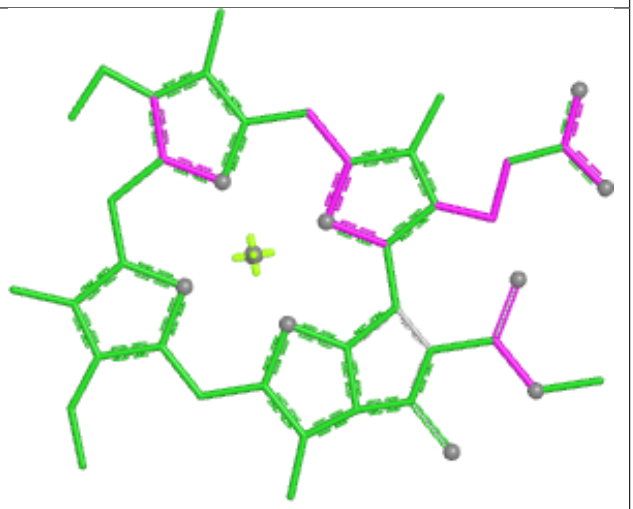


Rings

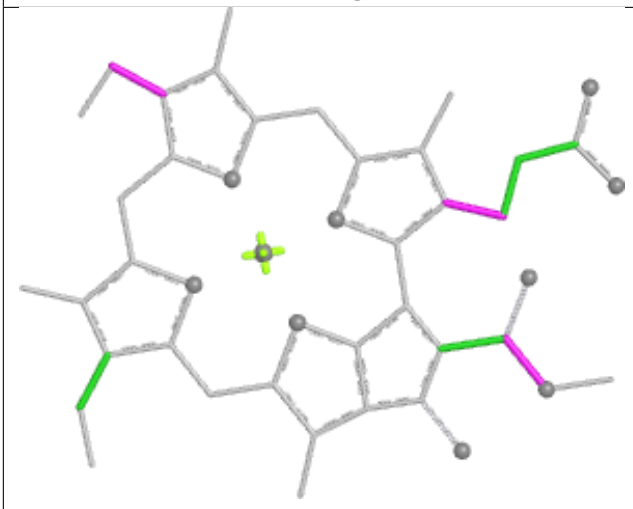
Ligand CLA B2 827



Bond lengths



Bond angles

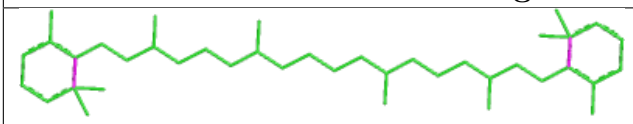


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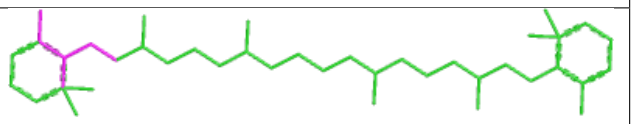


Rings

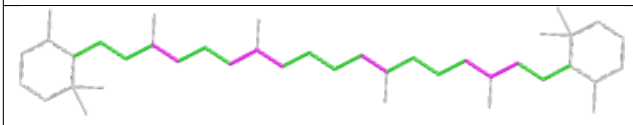
Ligand BCR B1 839



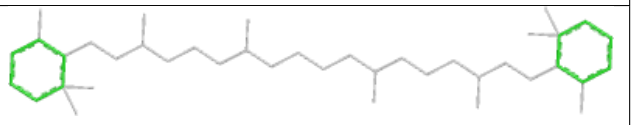
Bond lengths



Bond angles

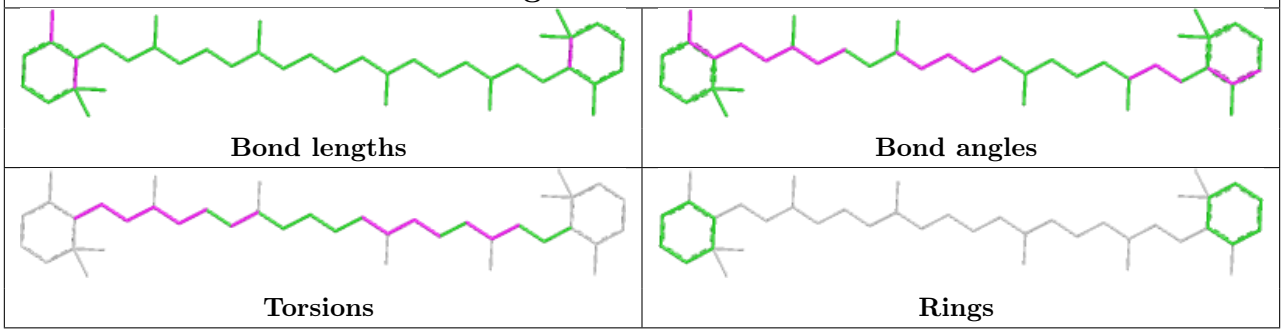


Torsions

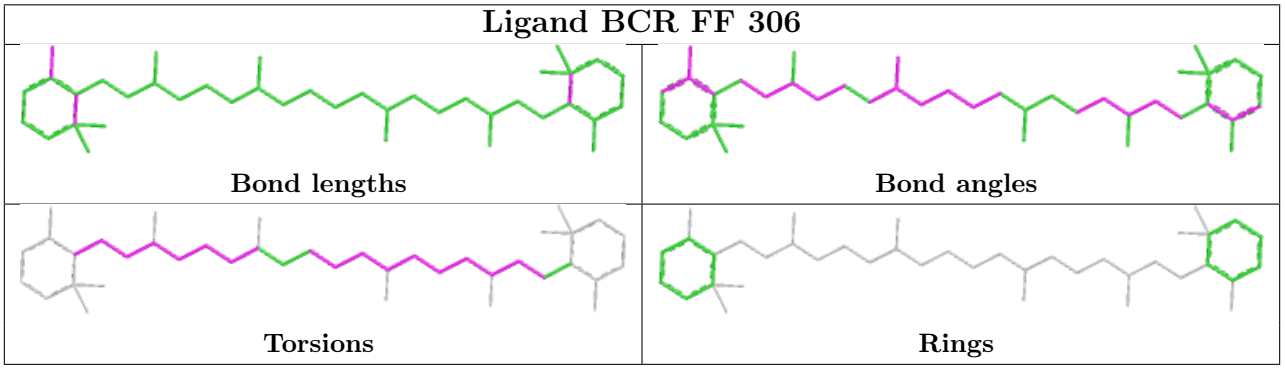


Rings

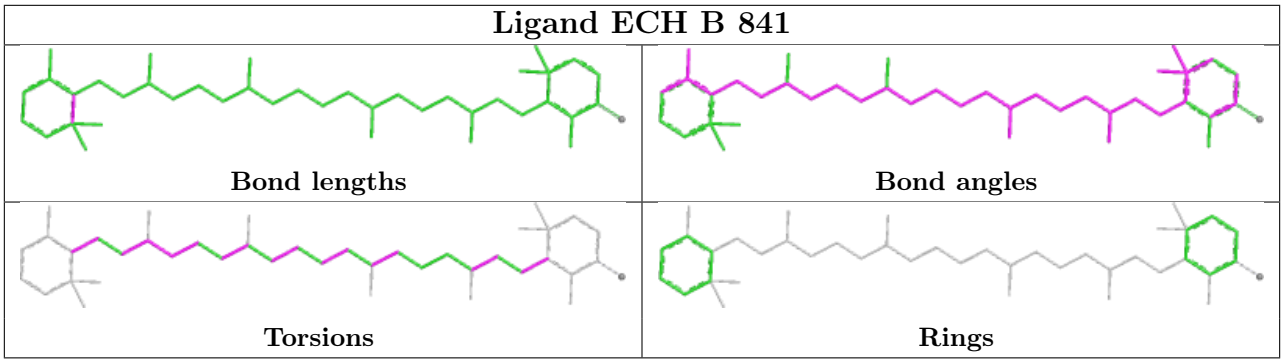
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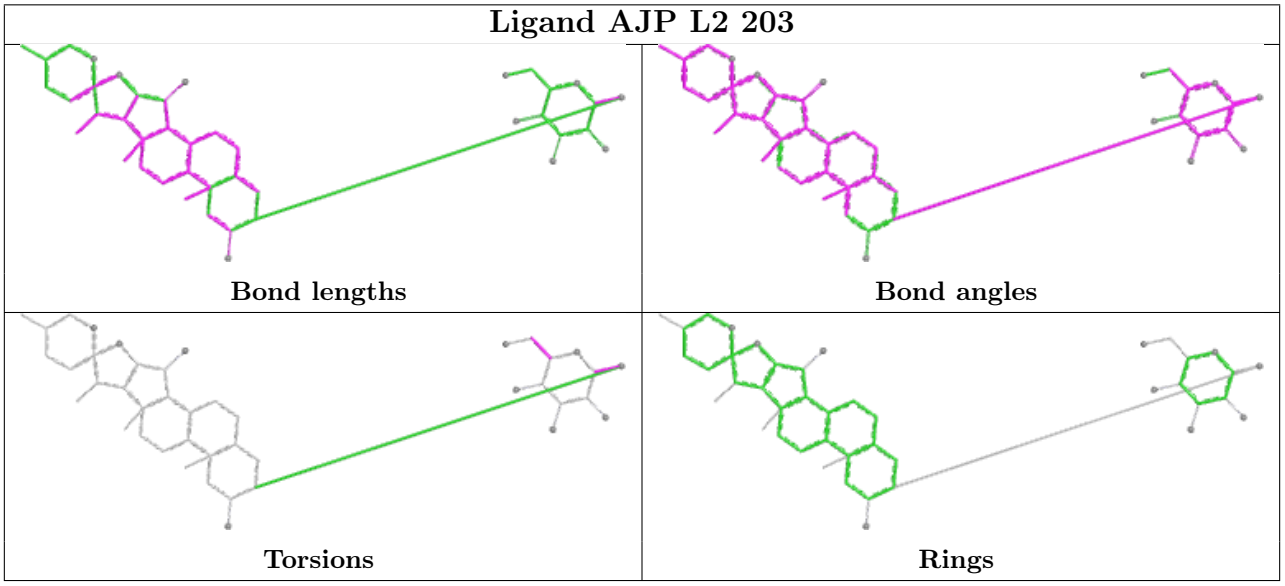
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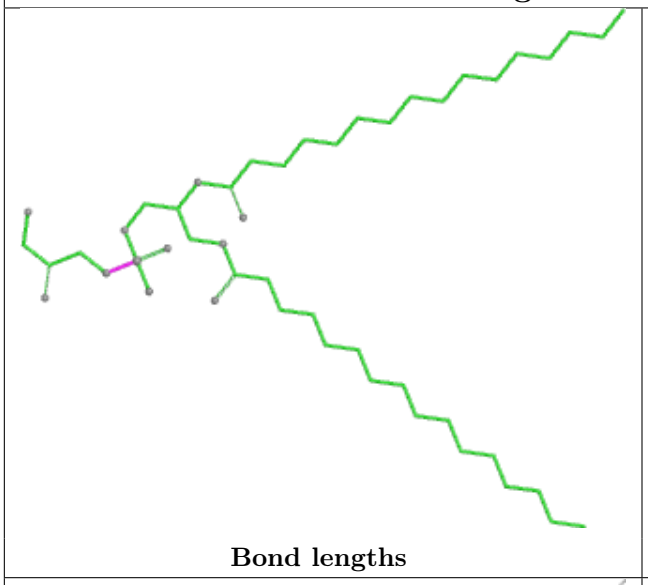
Ligand ECH B 841



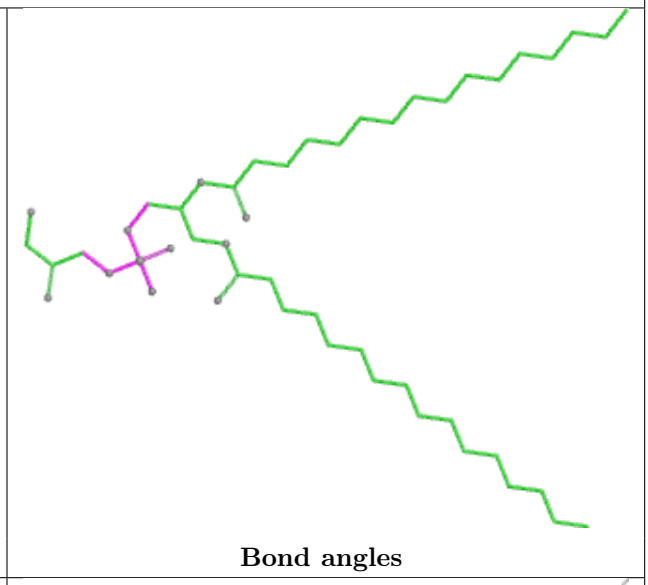
Ligand AJP L2 203



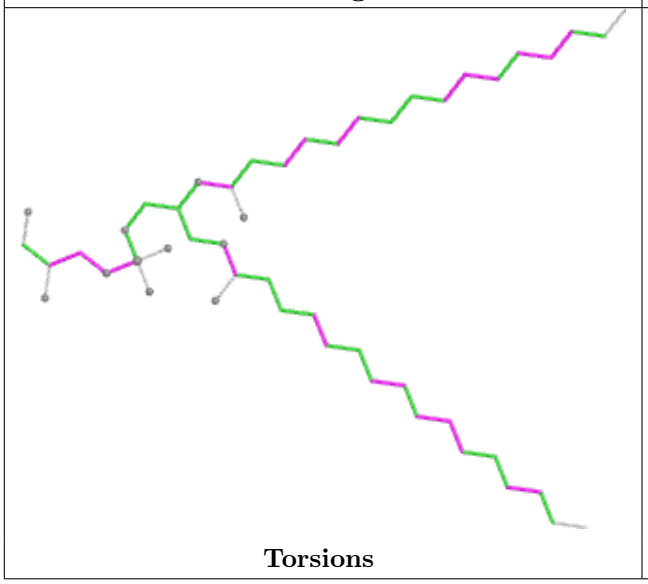
Ligand LHG X1 103



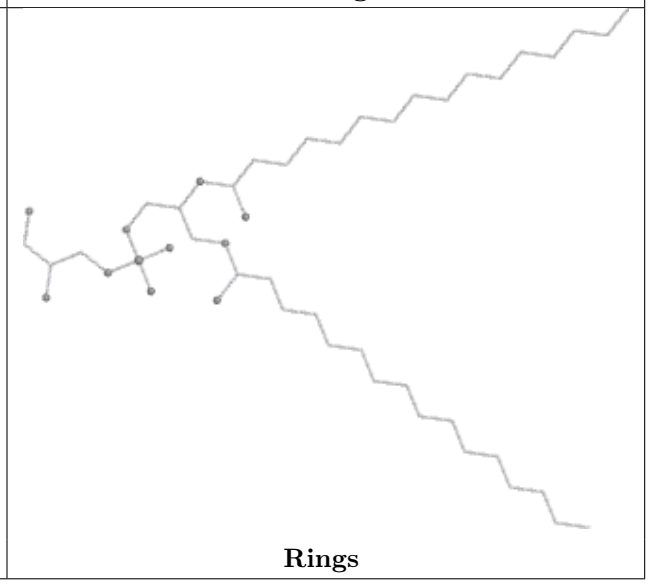
Bond lengths



Bond angles

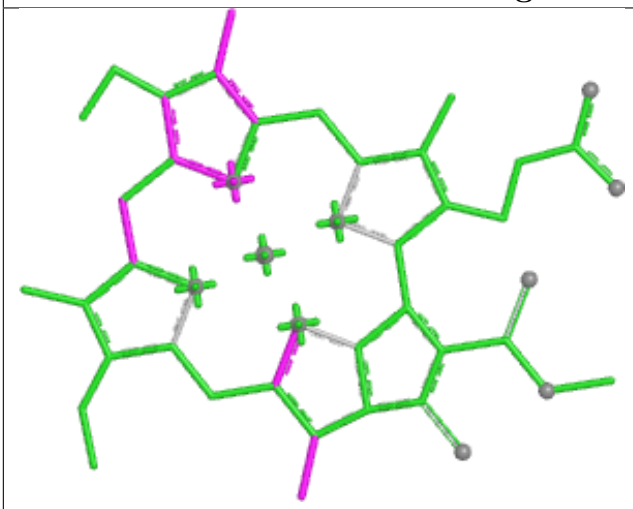


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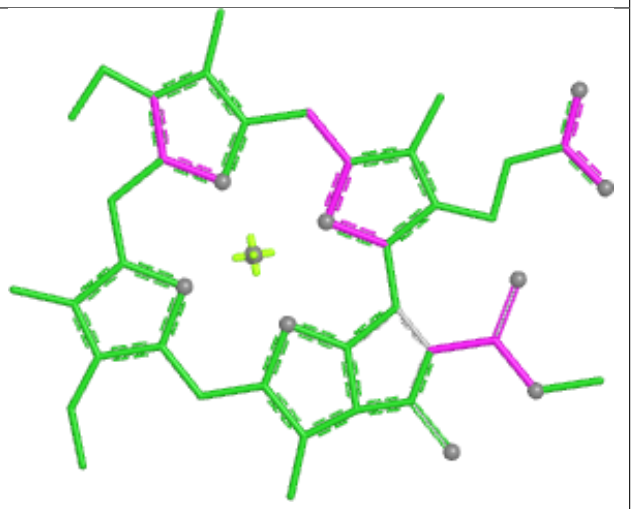


Rings

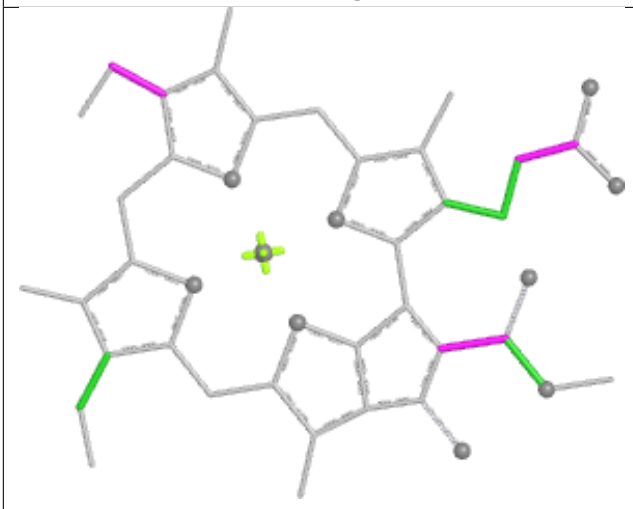
Ligand CLA B1 809



Bond lengths



Bond angles

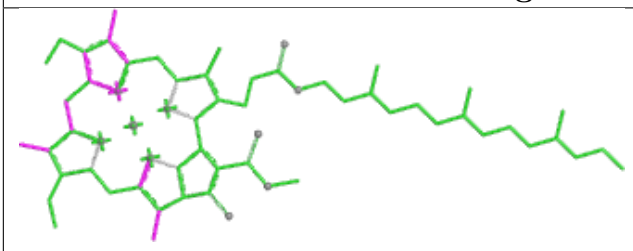


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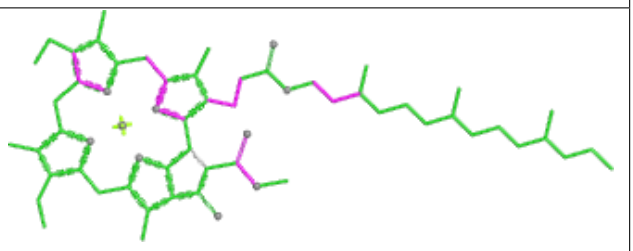


Rings

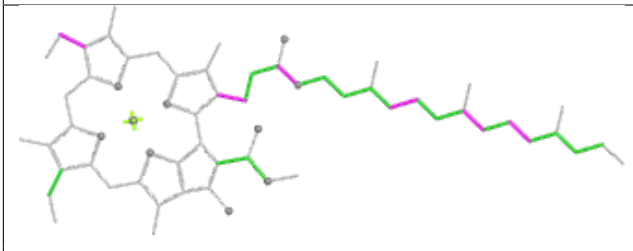
Ligand CLA B1 804



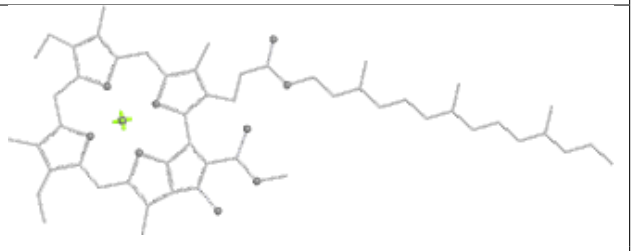
Bond lengths



Bond angles

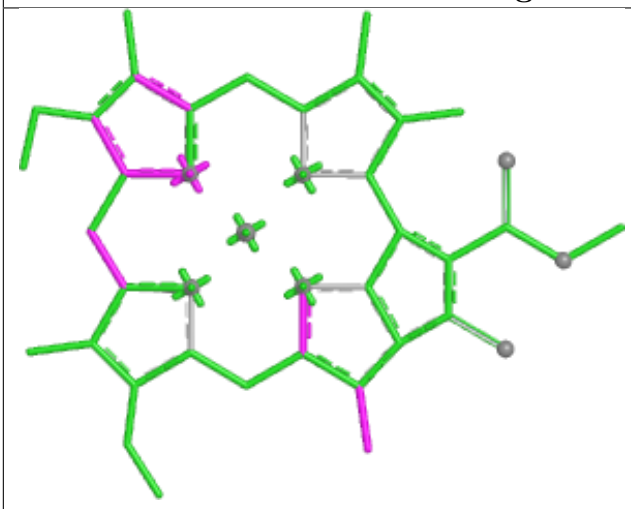


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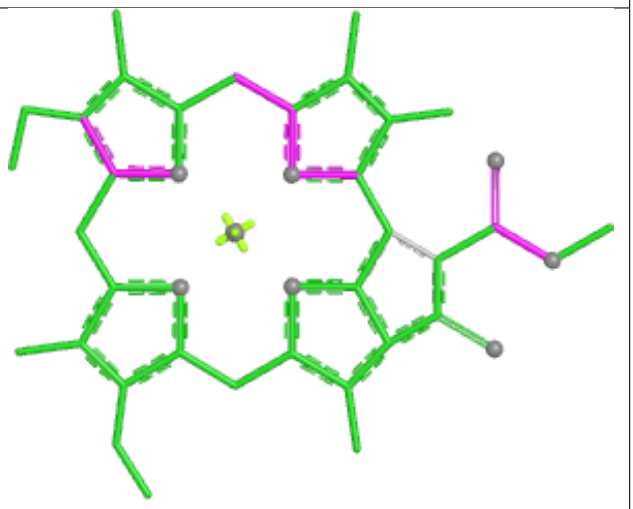


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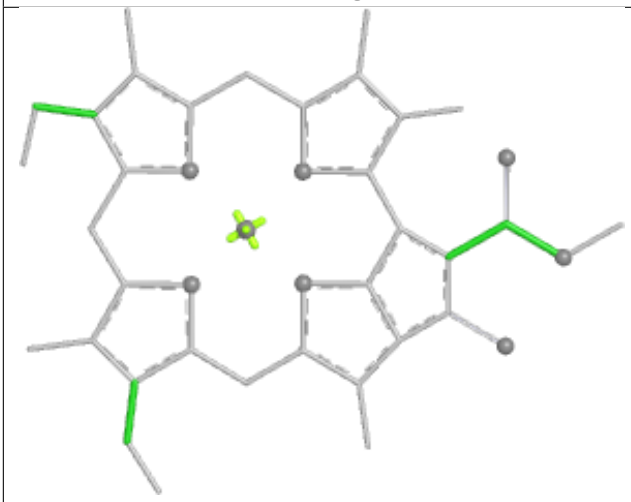
Ligand CLA B1 818



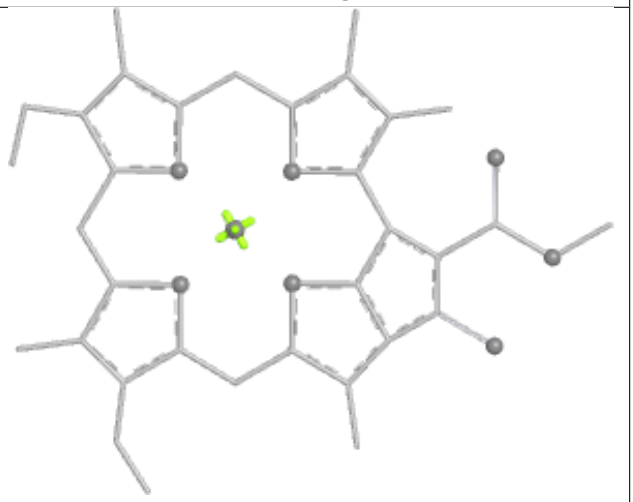
Bond lengths



Bond angles

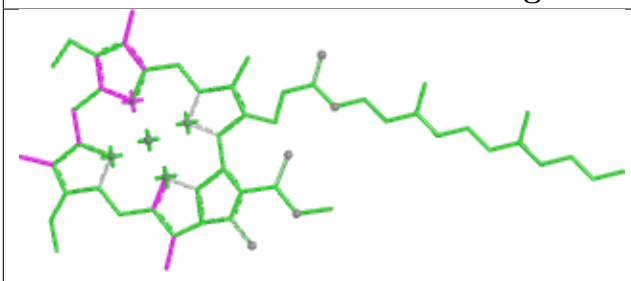


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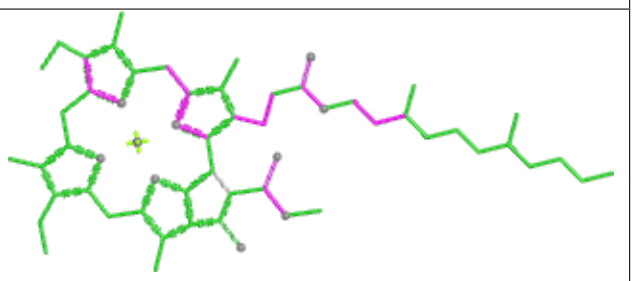


Rings

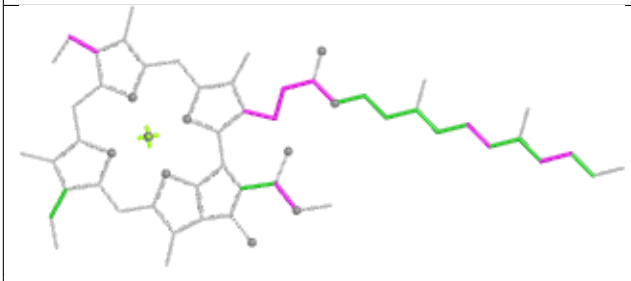
Ligand CLA A 820



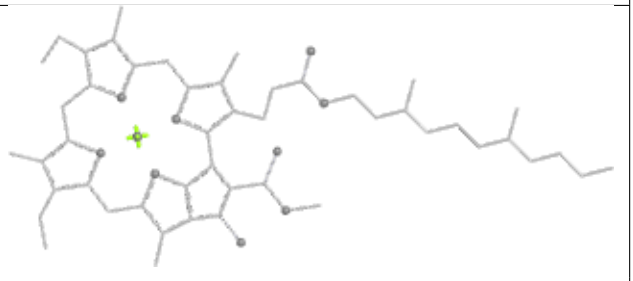
Bond lengths



Bond angles

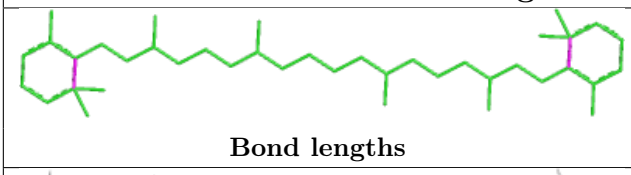


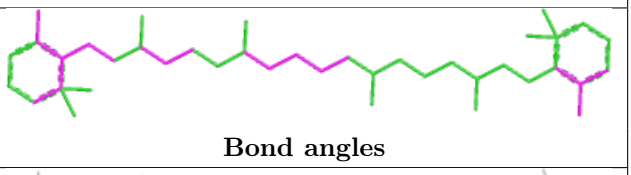
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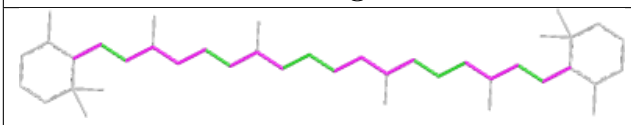


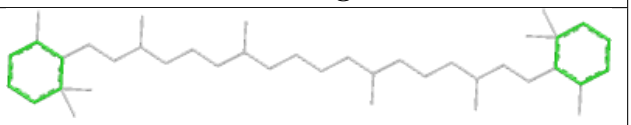
Rings

Ligand BCR JJ 102

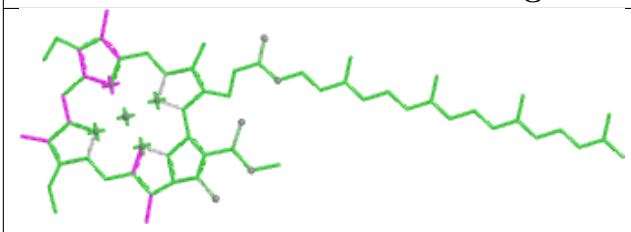

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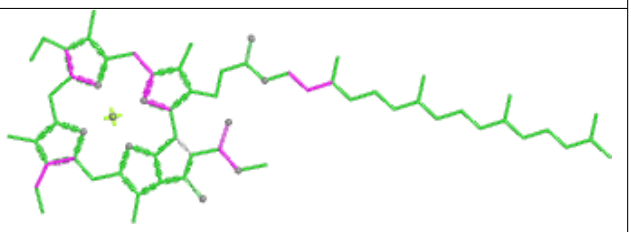

Bond angles

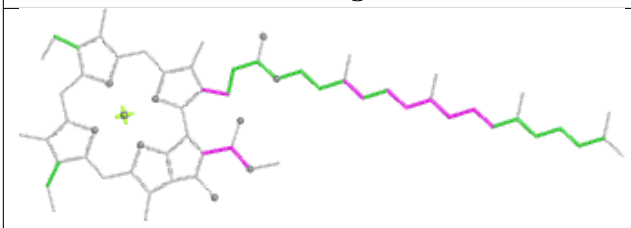

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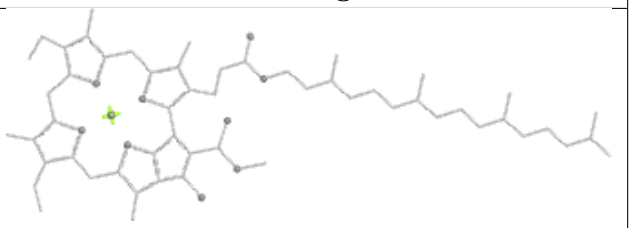

Rings

Ligand CLA B 810

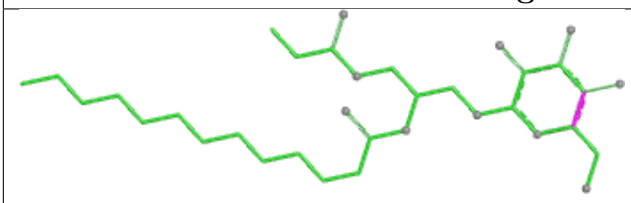

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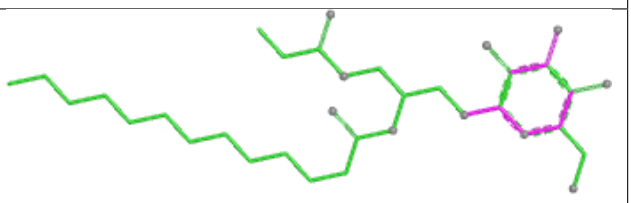

Bond angles

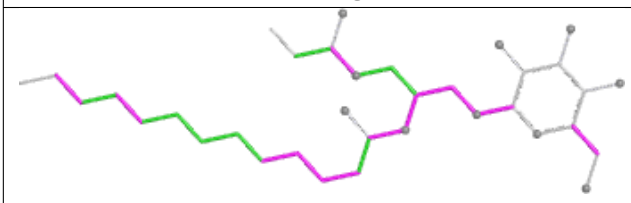

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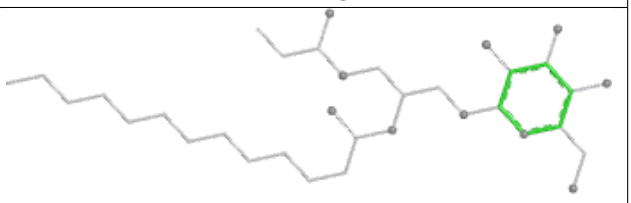

Rings

Ligand LMG I1 102

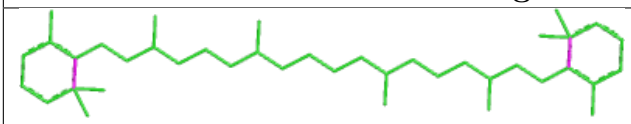

Bond lengths


Bond angles

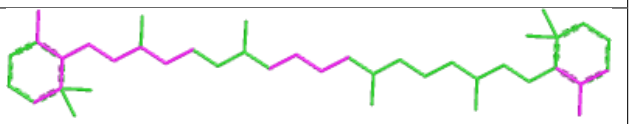

Torsions


Rings

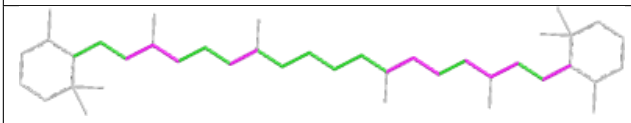
Ligand BCR A1 849



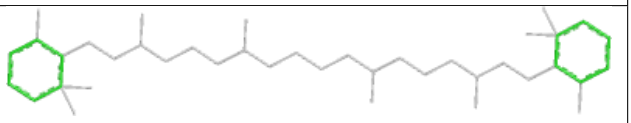
Bond lengths



Bond angles

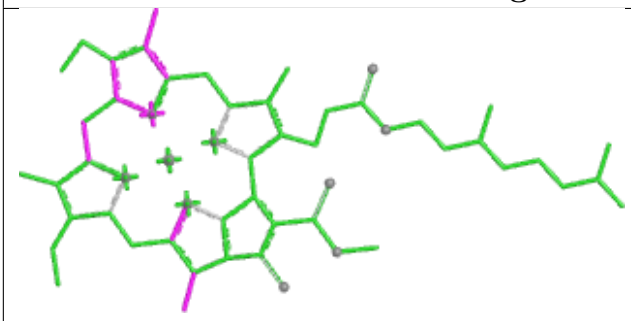


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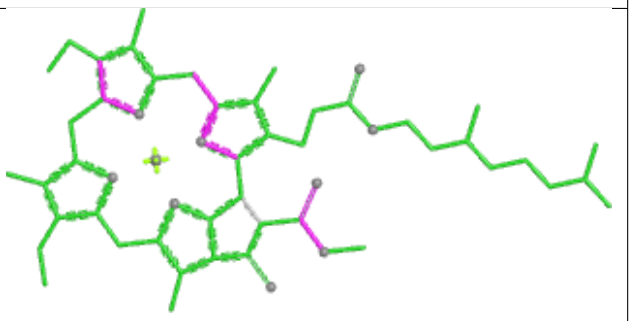


Rings

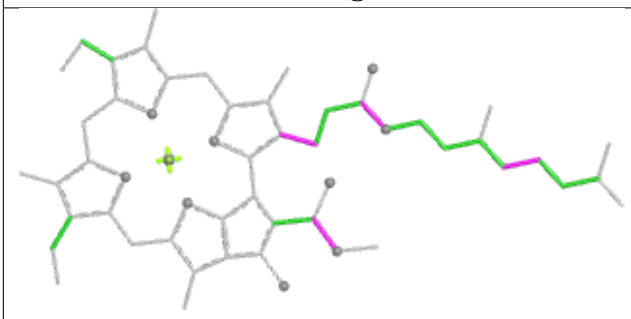
Ligand CLA AA 815



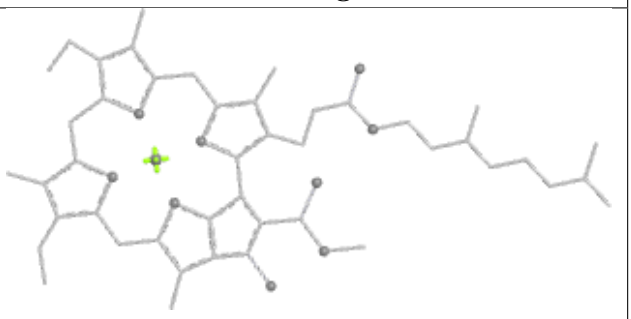
Bond lengths



Bond angles

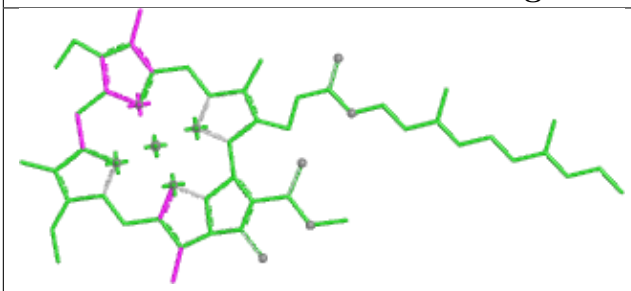


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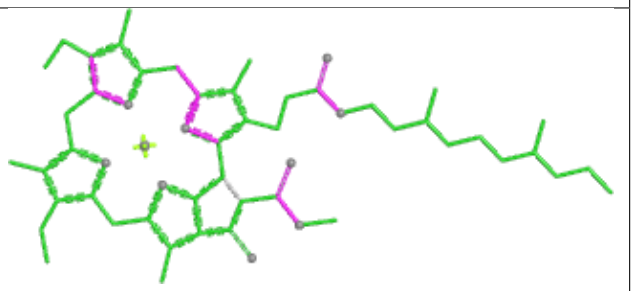


Rings

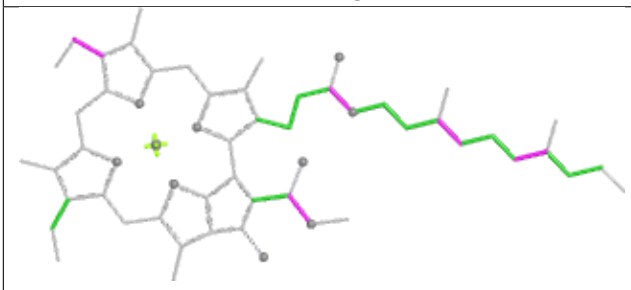
Ligand CLA B 816



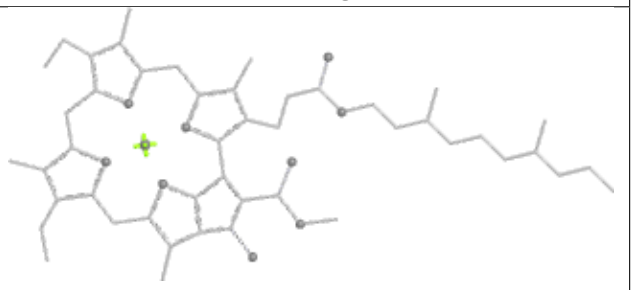
Bond lengths



Bond angles

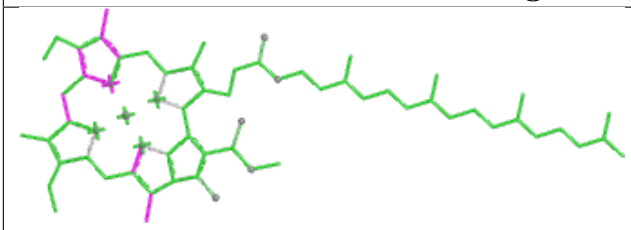


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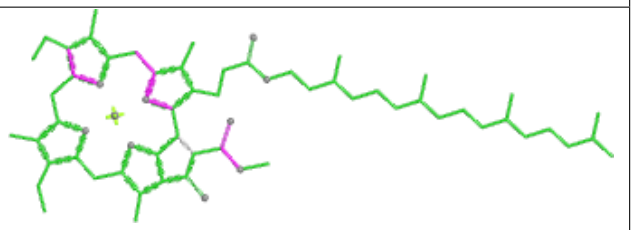


Rings

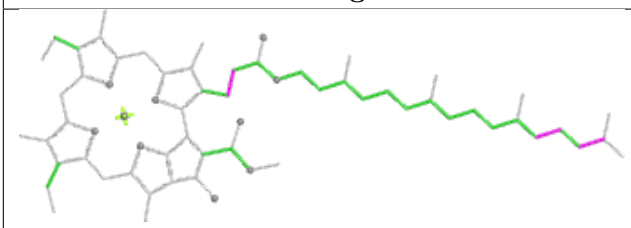
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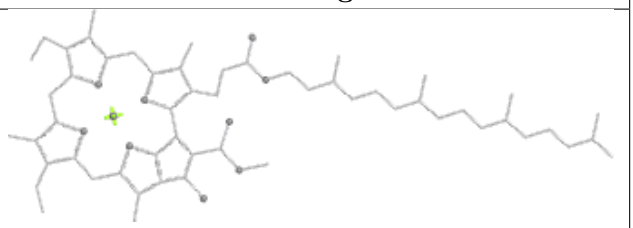
Bond lengths



Bond angles

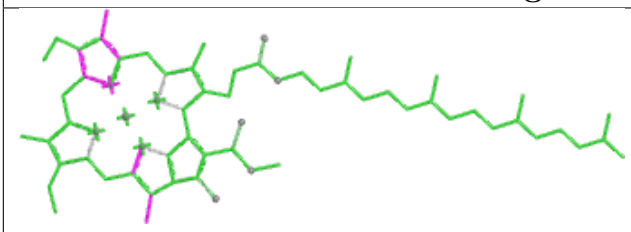


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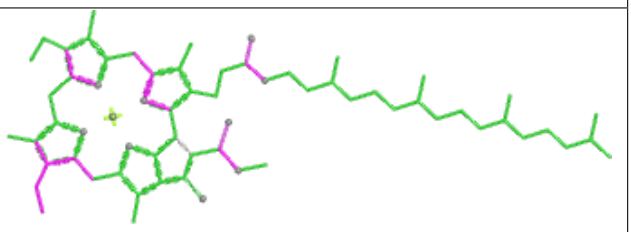


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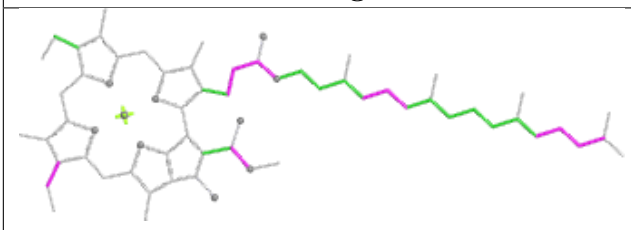
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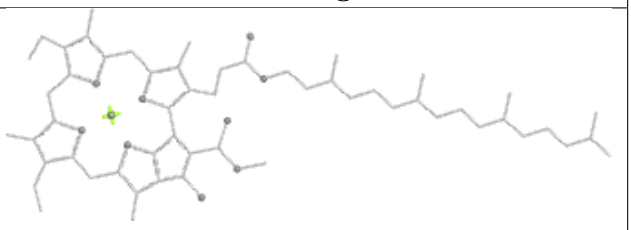
Bond lengths



Bond angles



Torsions

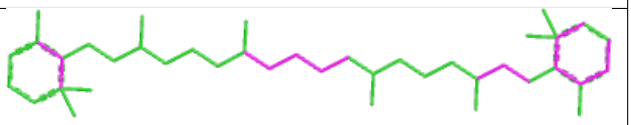


Rings

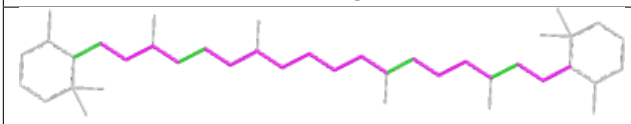
Ligand BCR B2 842



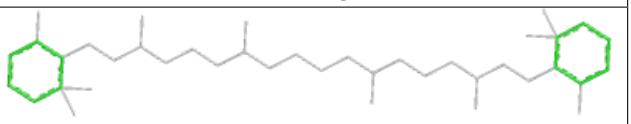
Bond lengths



Bond angles

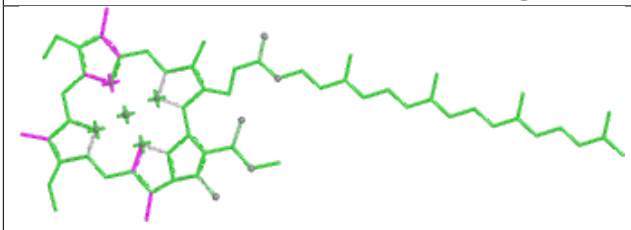


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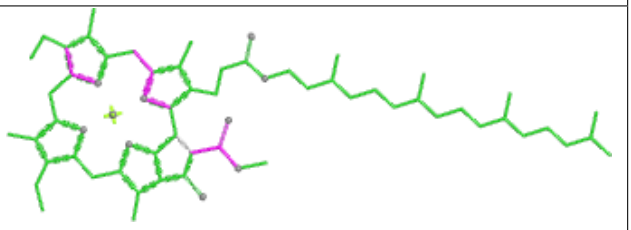


Rings

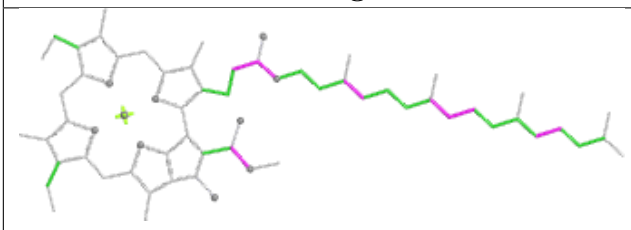
Ligand CLA B1 848



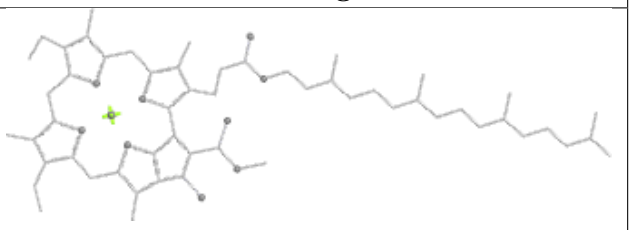
Bond lengths



Bond angles

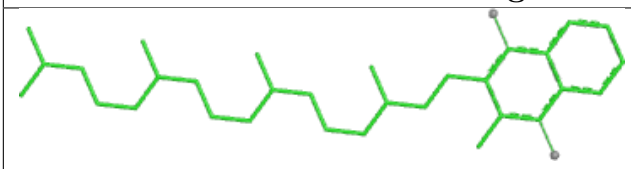


Torsions

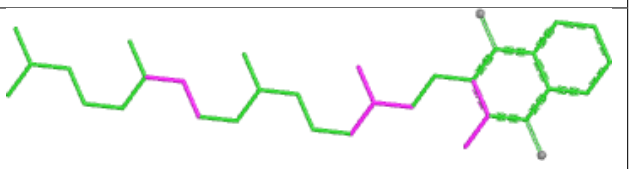


Rings

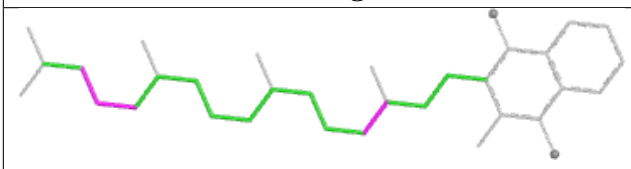
Ligand PQN AA 844



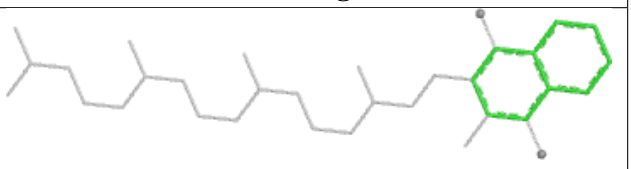
Bond lengths



Bond angles

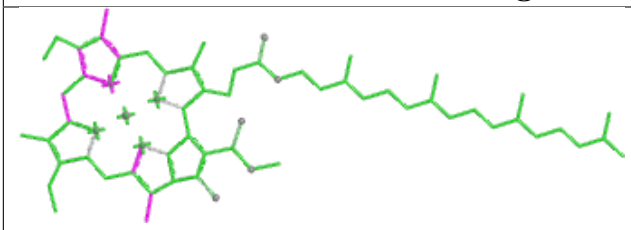


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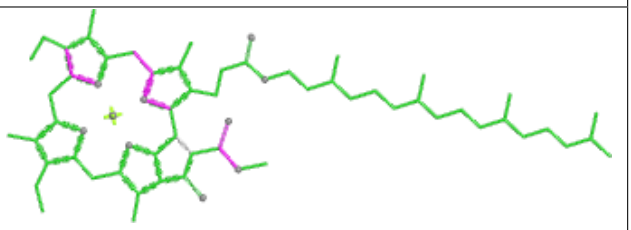


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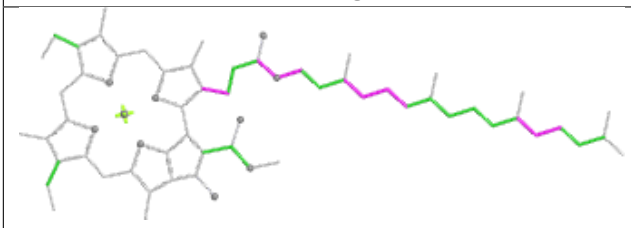
Ligand CLA B1 828



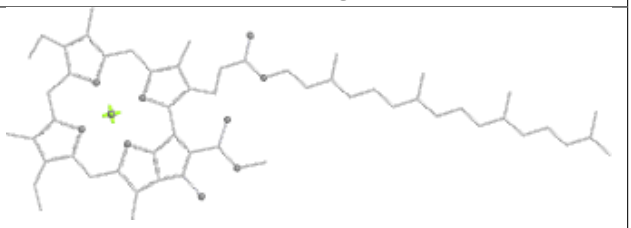
Bond lengths



Bond angles

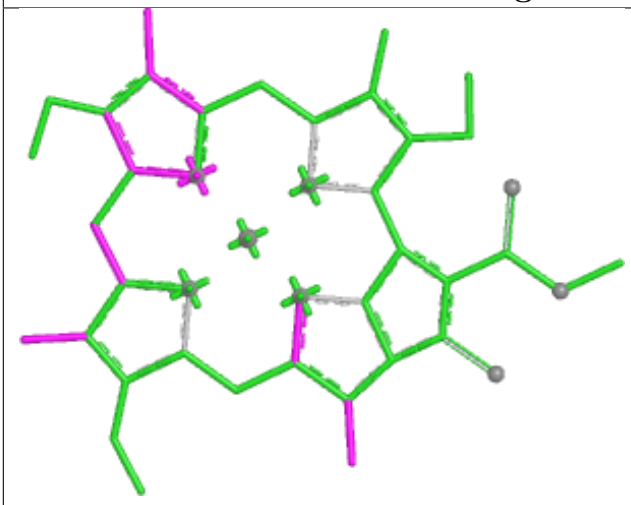


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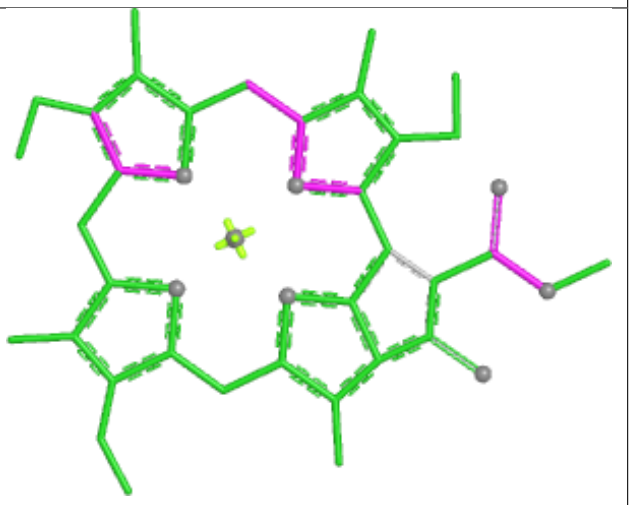


Rings

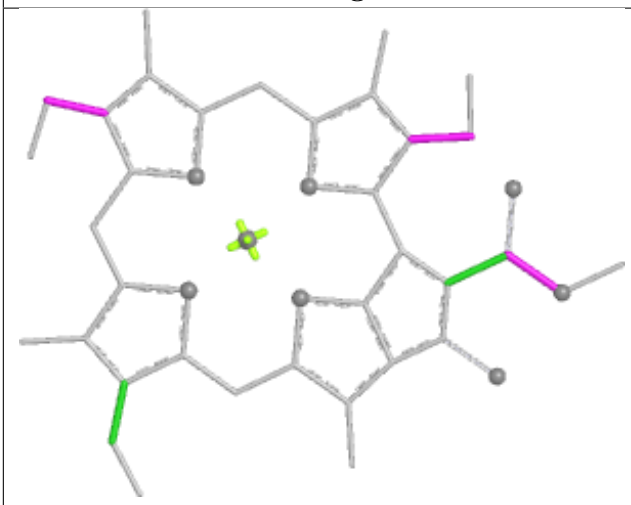
Ligand CLA A2 814



Bond lengths



Bond angles

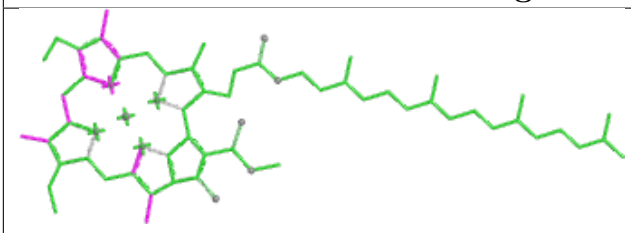


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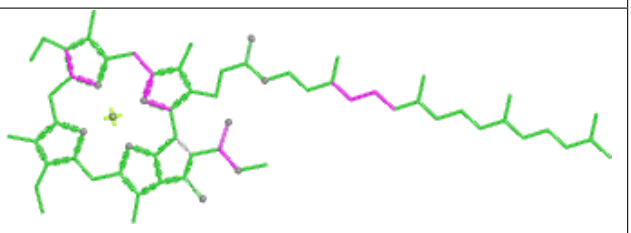


Rings

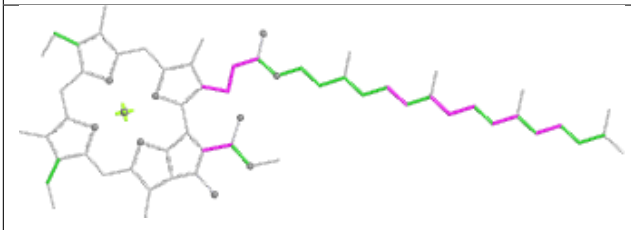
Ligand CLA A2 852



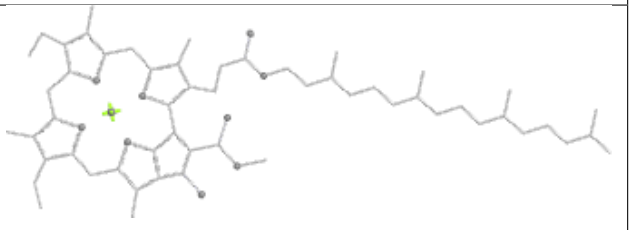
Bond lengths



Bond angles

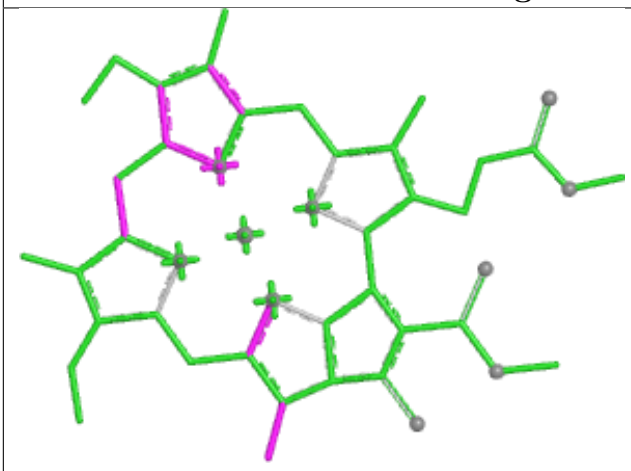


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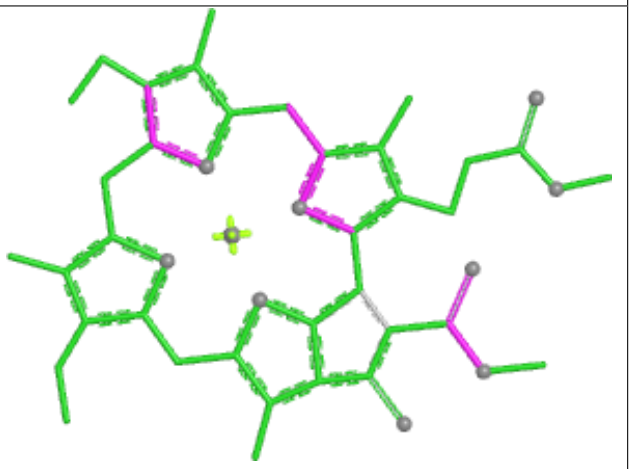


Rings

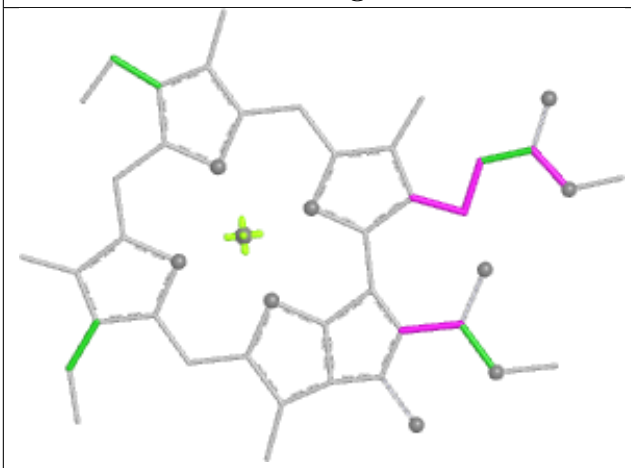
Ligand CLA K1 103



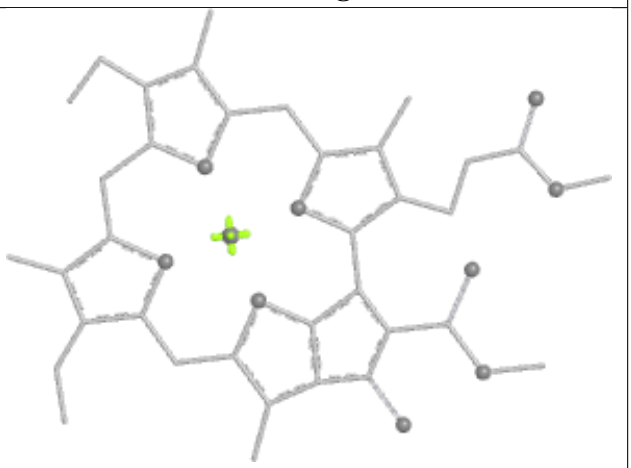
Bond lengths



Bond angles

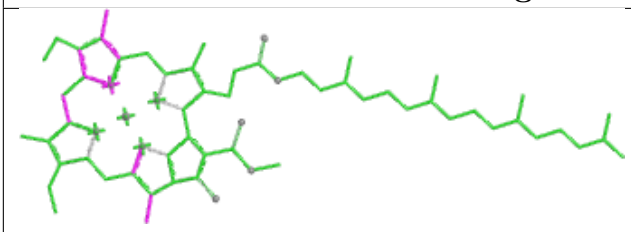


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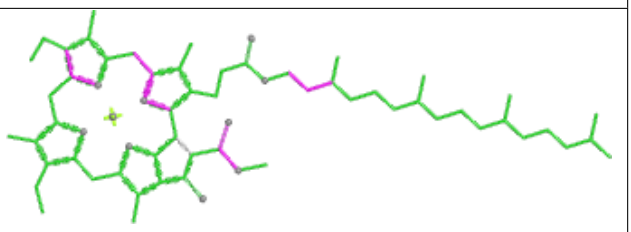


Rings

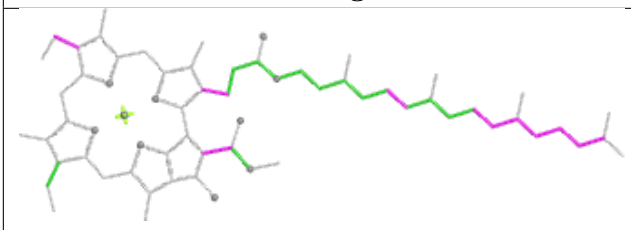
Ligand CLA A1 806



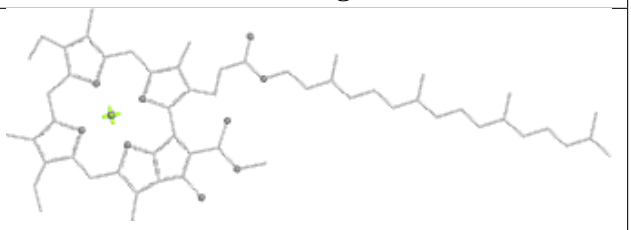
Bond lengths



Bond angles

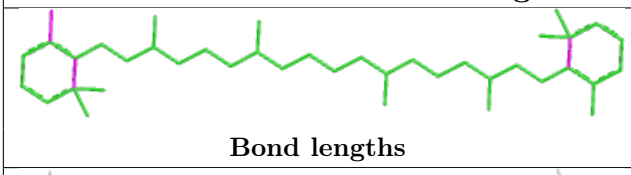


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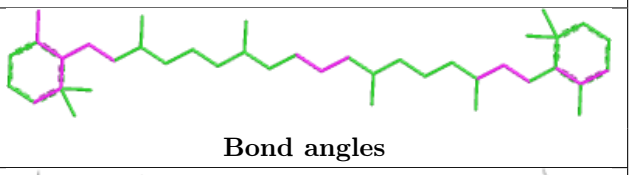


Rings

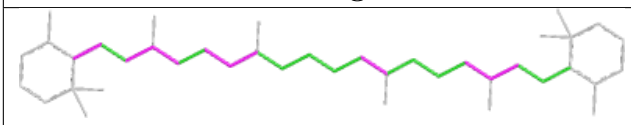
Ligand BCR A2 850



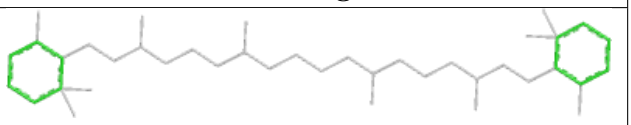
Bond lengths



Bond angles

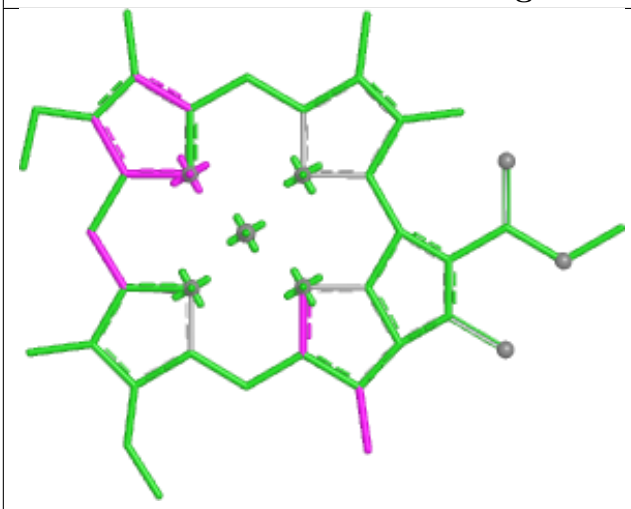


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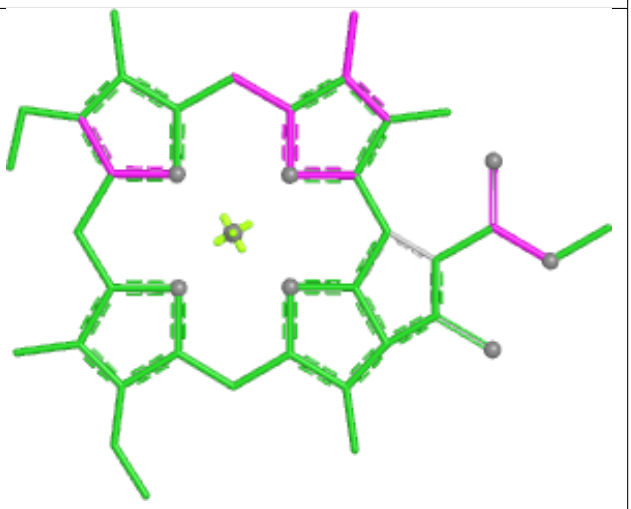


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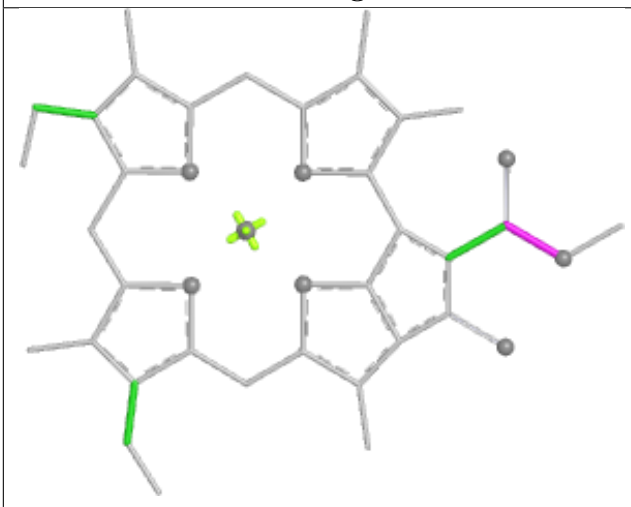
Ligand CLA B1 819



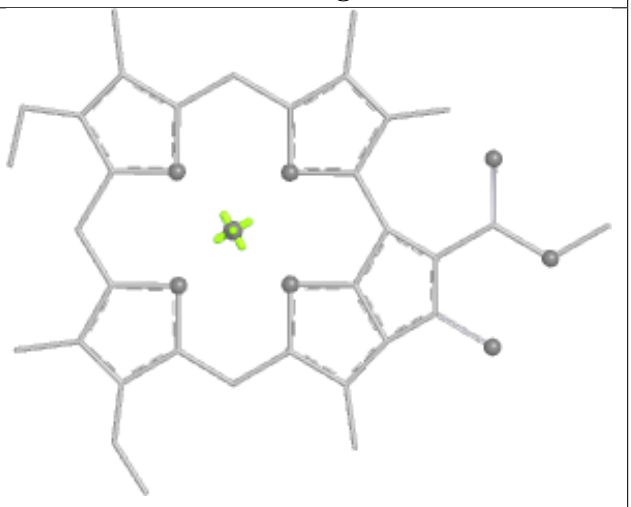
Bond lengths



Bond angles

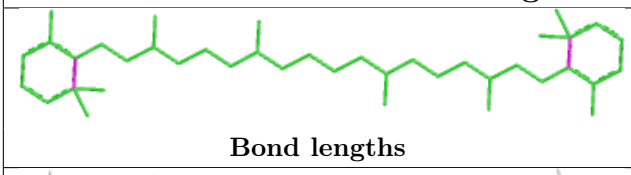


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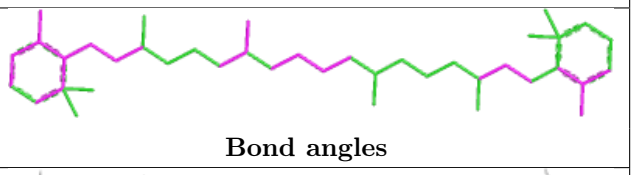


Rings

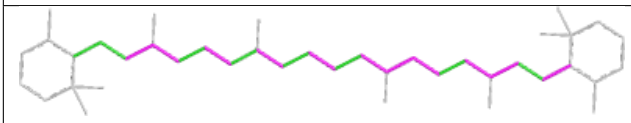
Ligand BCR A 849



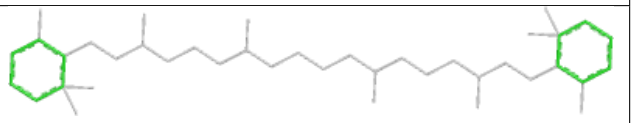
Bond lengths



Bond angles

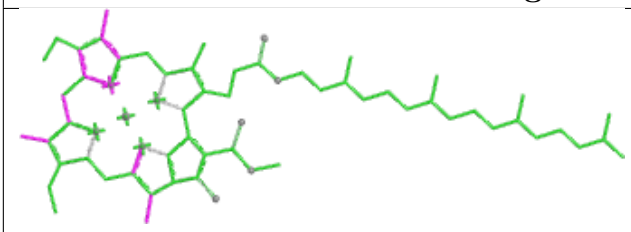


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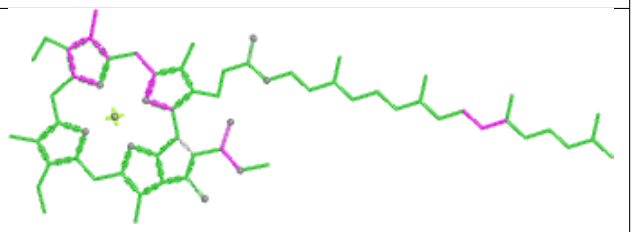


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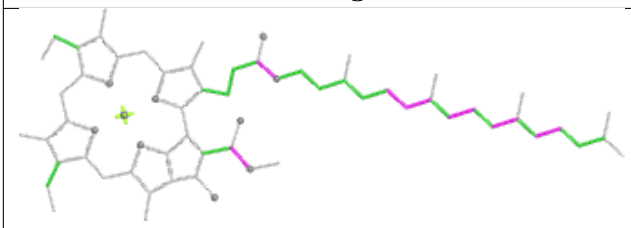
Ligand CLA B 803



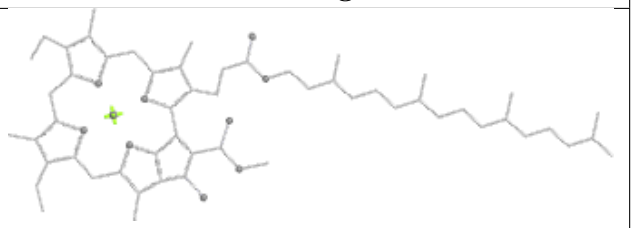
Bond lengths



Bond angles

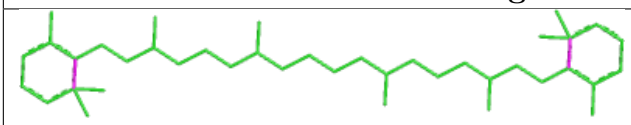


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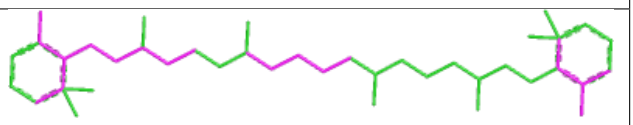


Rings

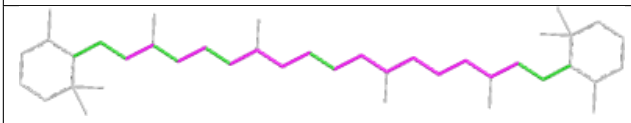
Ligand BCR AA 854



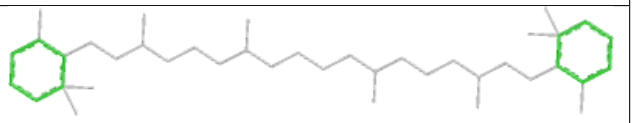
Bond lengths



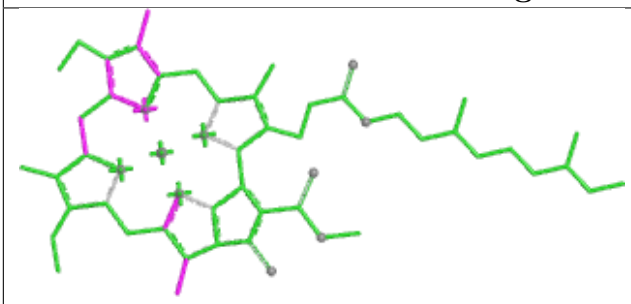
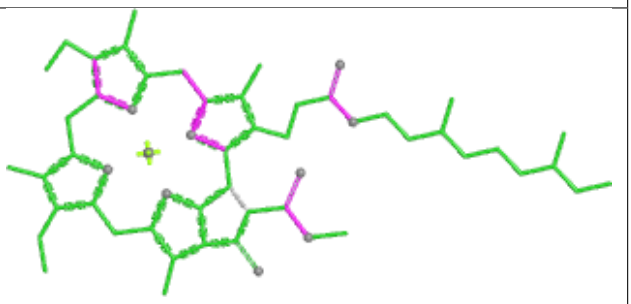
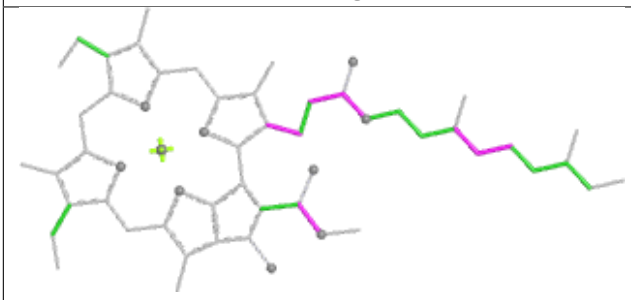
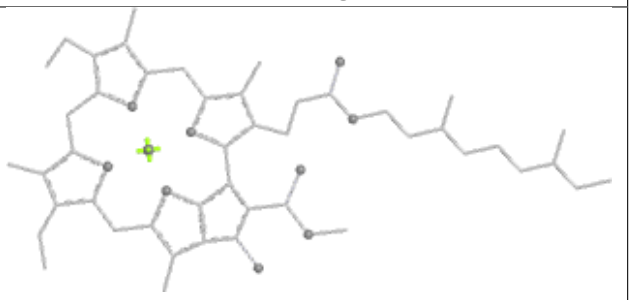
Bond angles

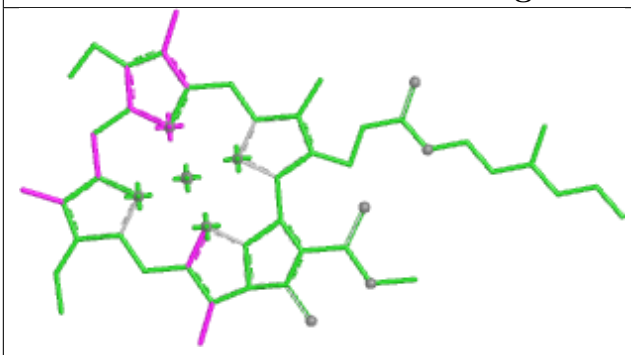
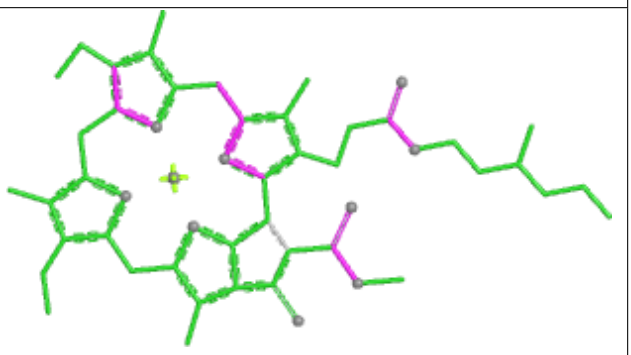
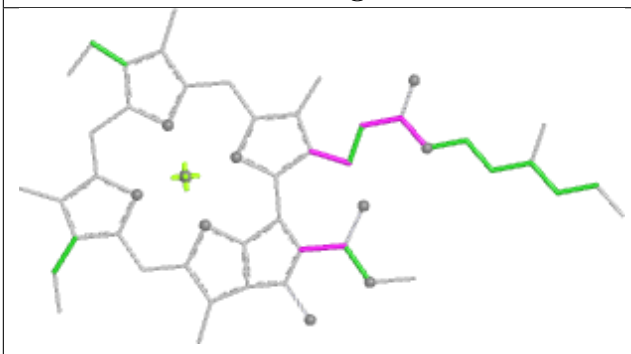
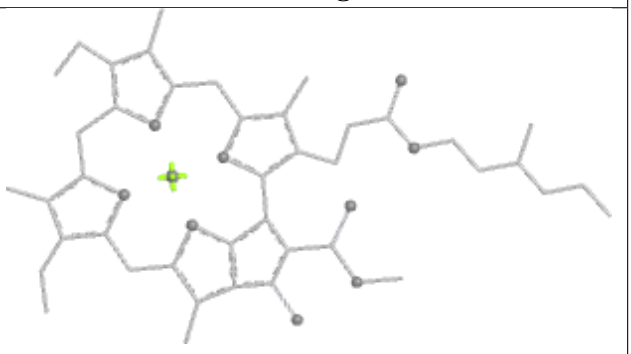


Torsions

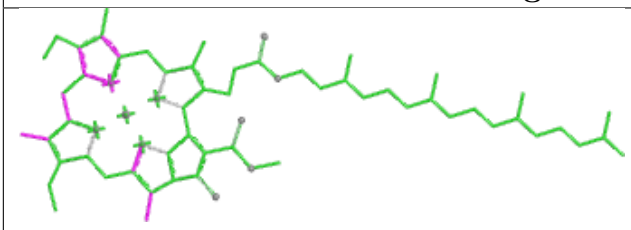


Rings

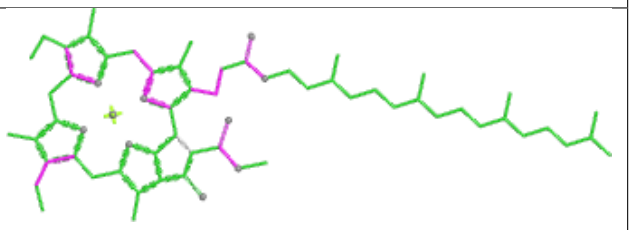
Ligand CLA A1 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

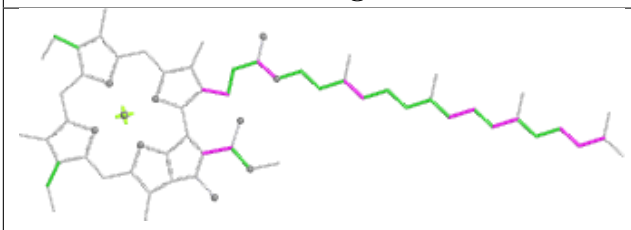
Ligand CLA A 821



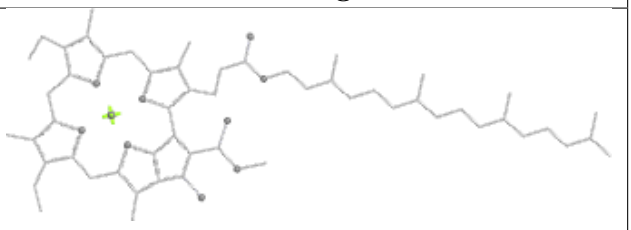
Bond lengths



Bond angles

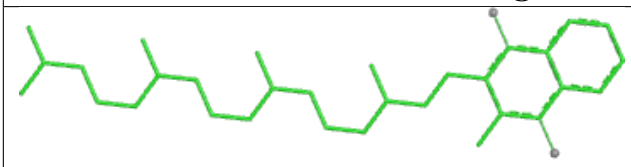


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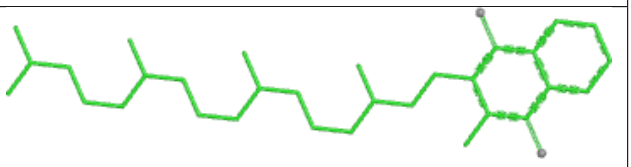


Rings

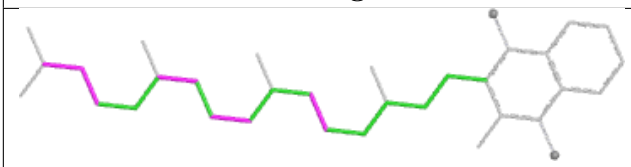
Ligand PQN B2 838



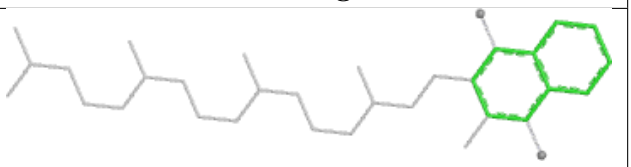
Bond lengths



Bond angles

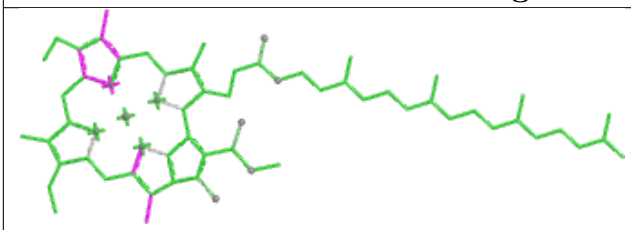


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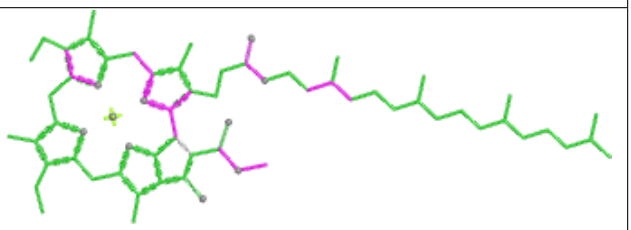


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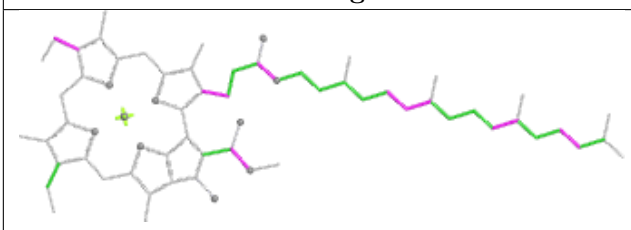
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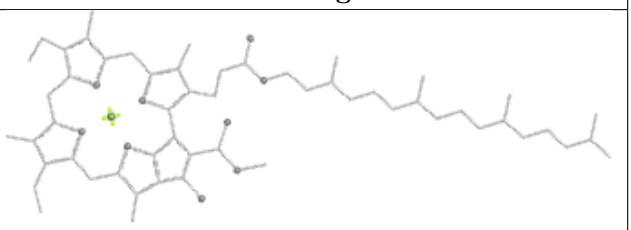
Bond lengths



Bond angles

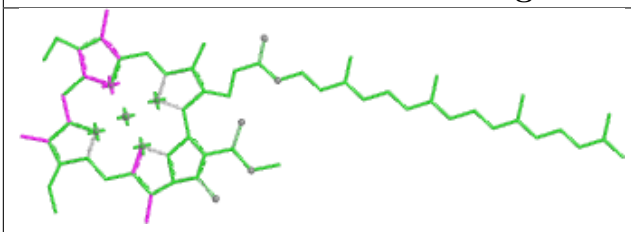


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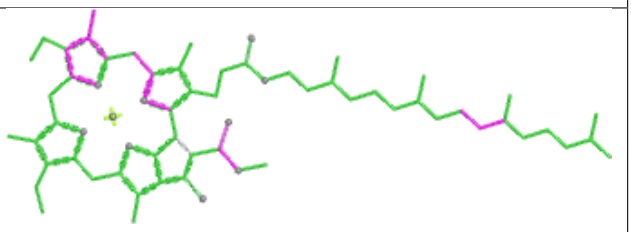


Rings

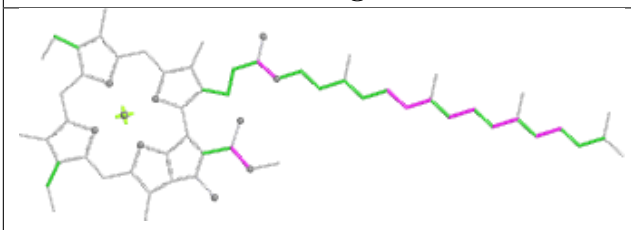
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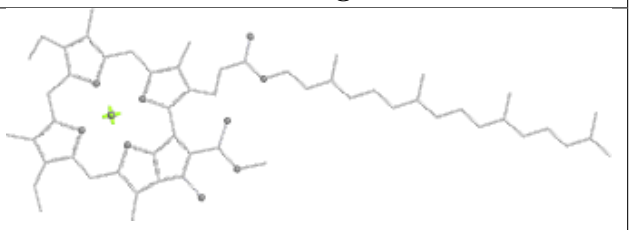
Bond lengths



Bond angles

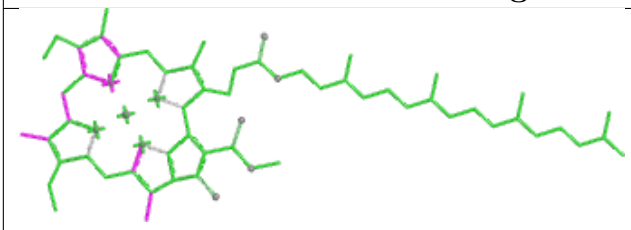


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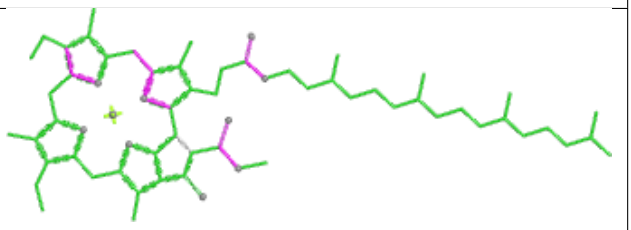


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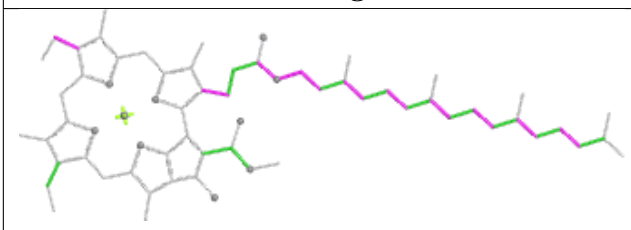
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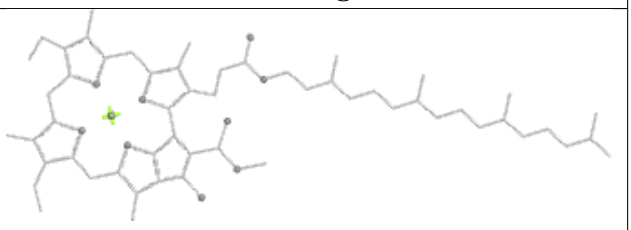
Bond lengths



Bond angles

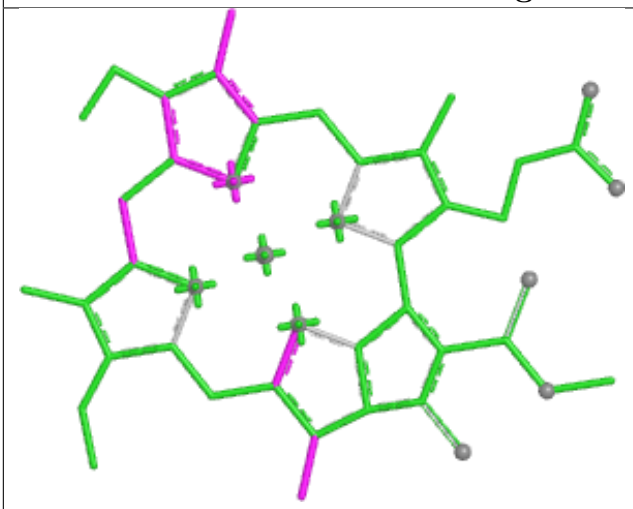


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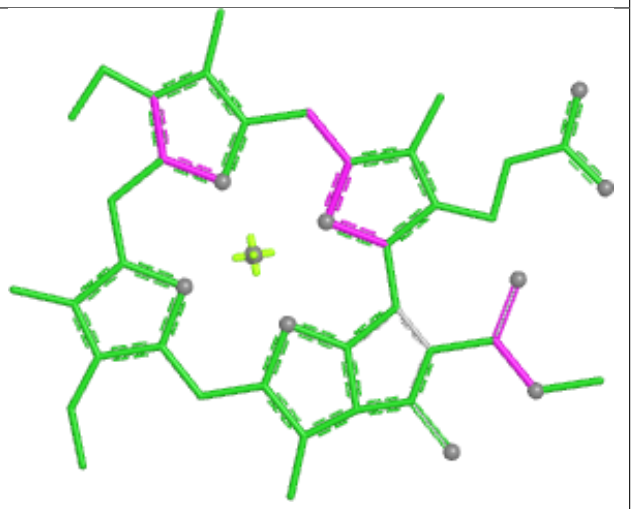


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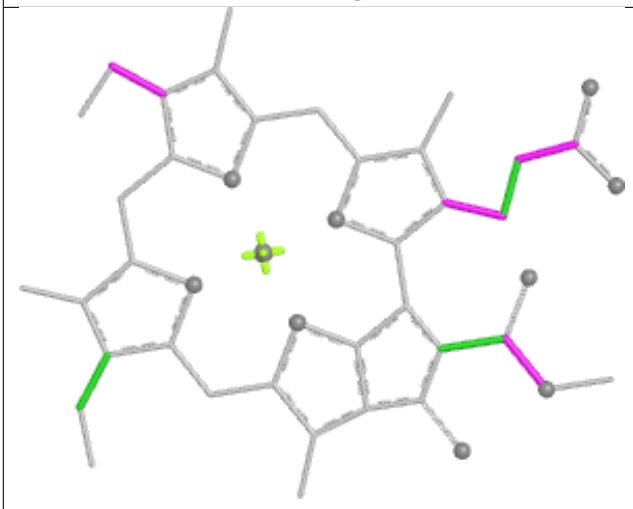
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Bond lengths



Bond angles

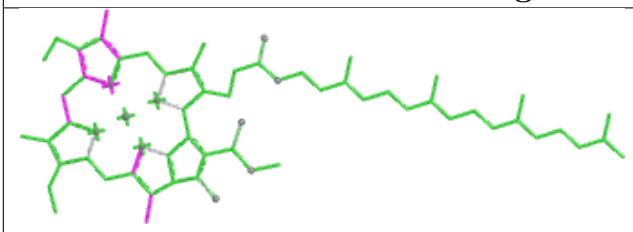


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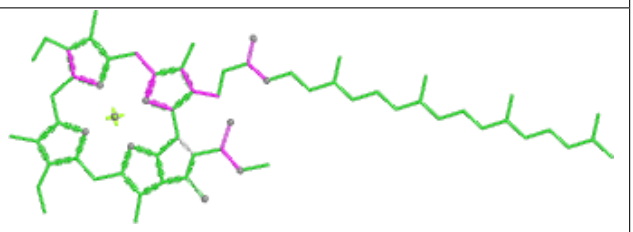


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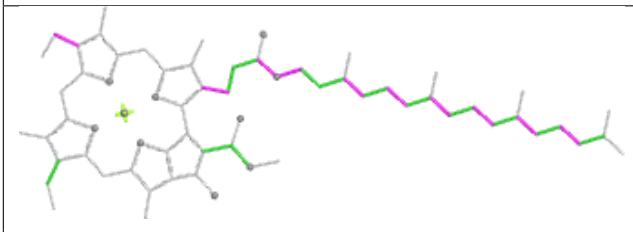
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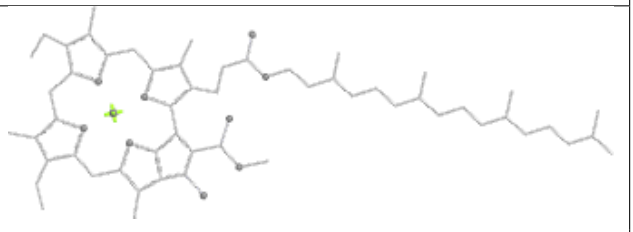
Bond lengths



Bond angles

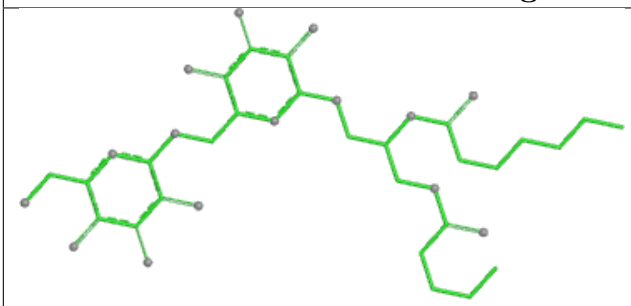


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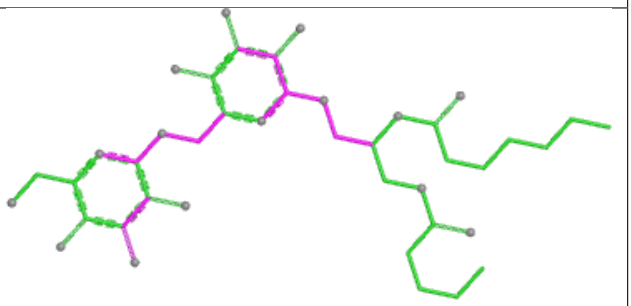


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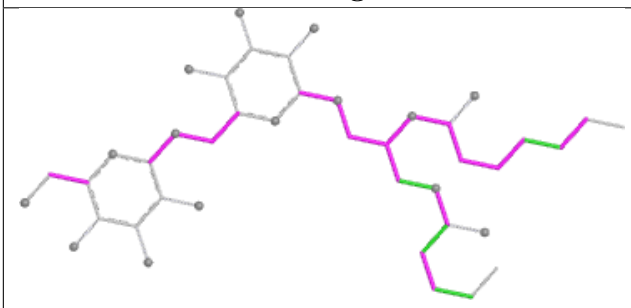
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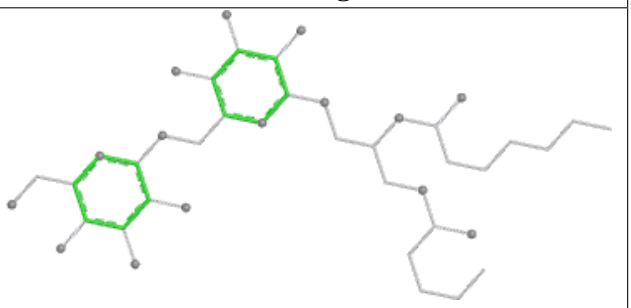
Bond lengths



Bond angles

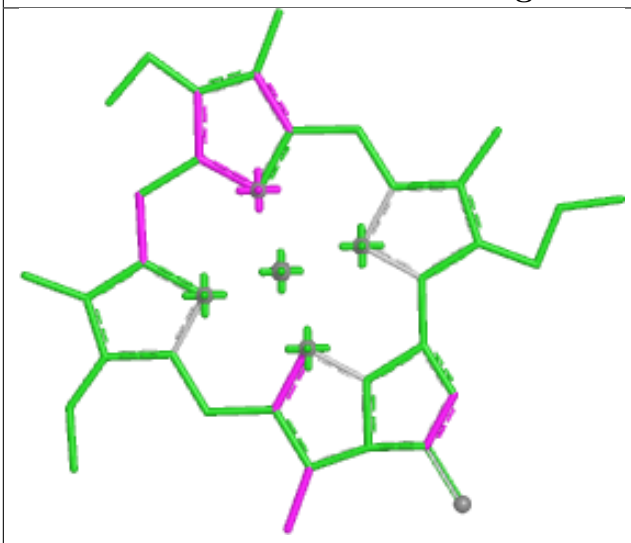


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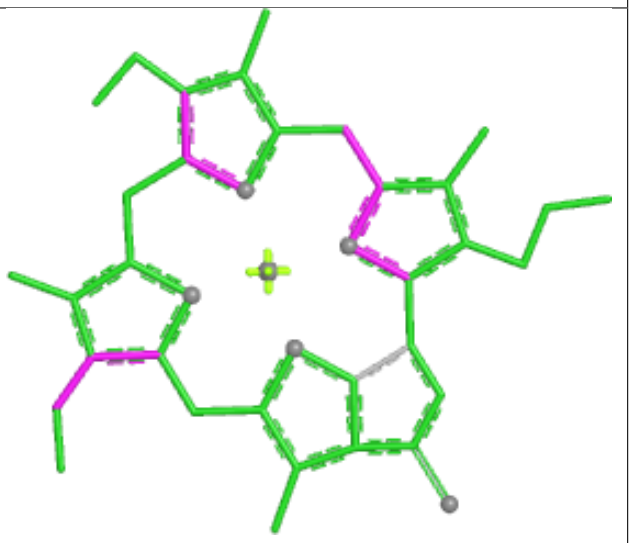


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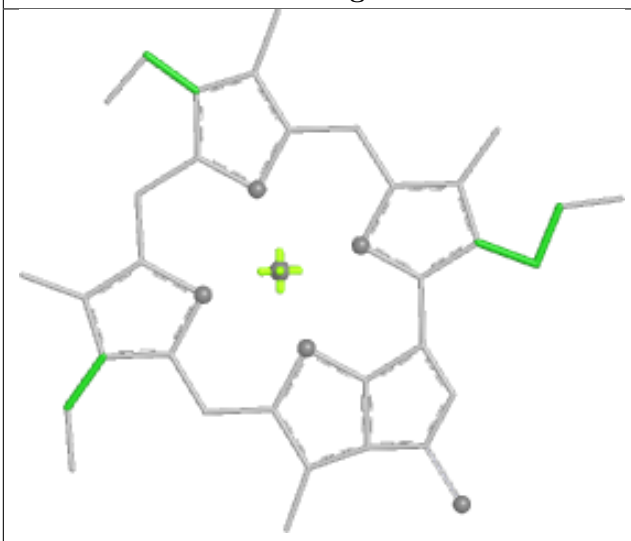
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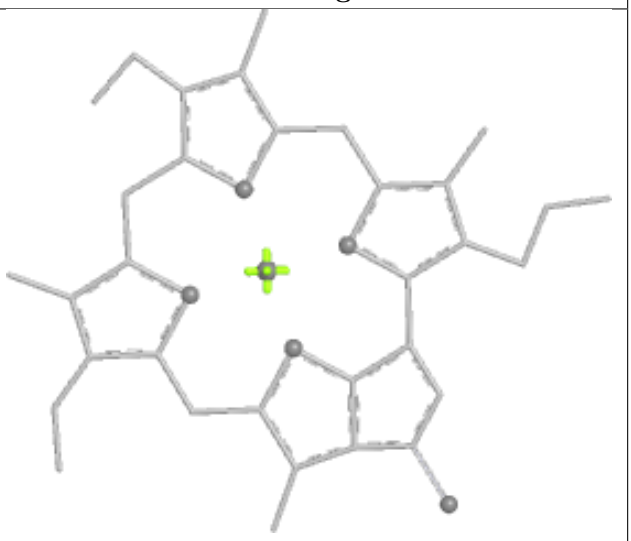
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Bond angles

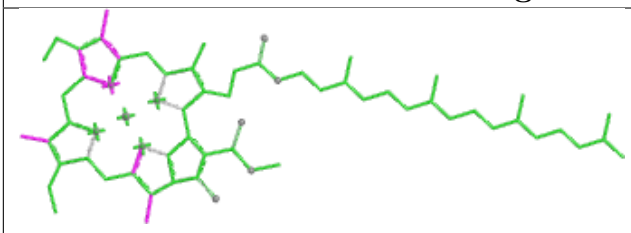


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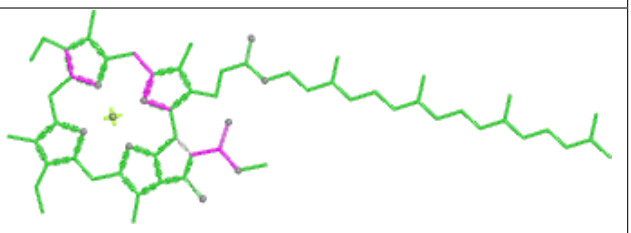


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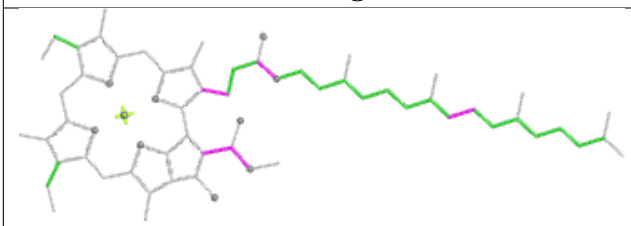
Ligand CLA A1 831



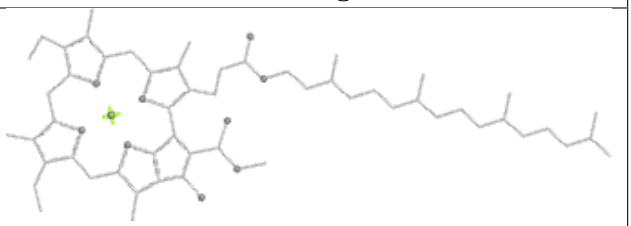
Bond lengths



Bond angles

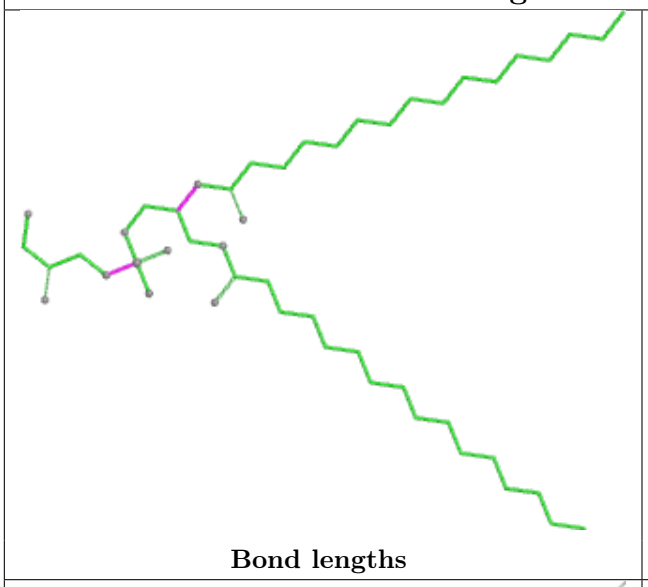


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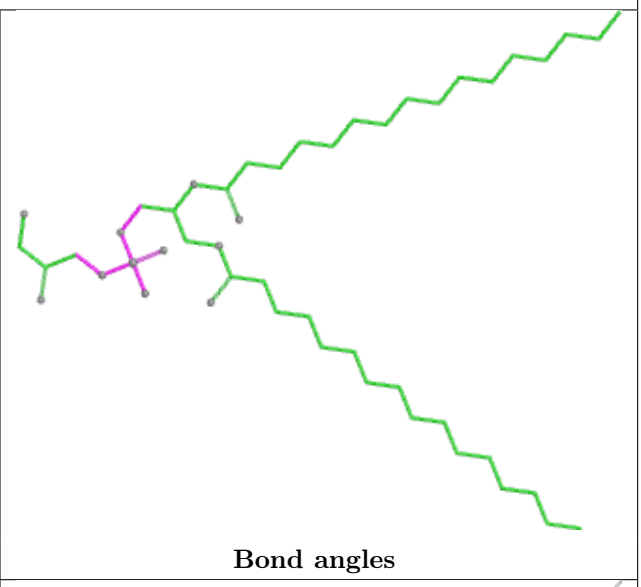


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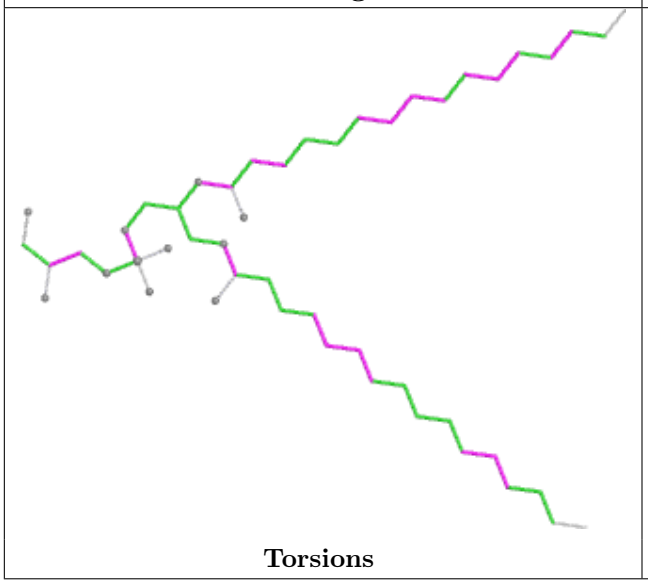
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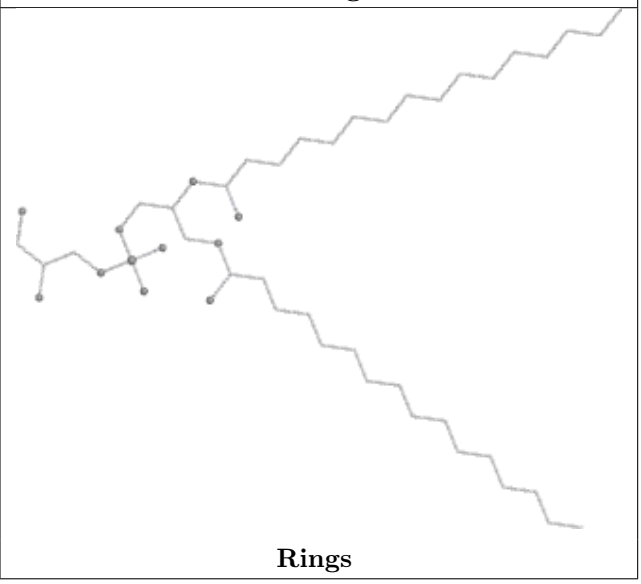
Bond lengths



Bond angles



Torsions



Rings

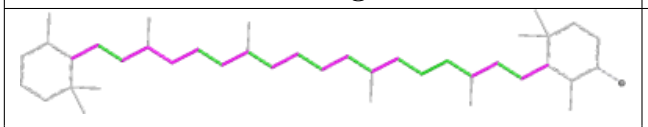
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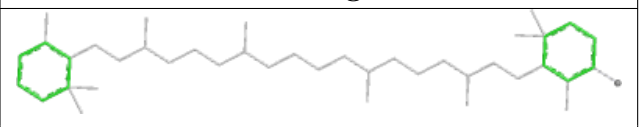
Bond lengths



Bond angles

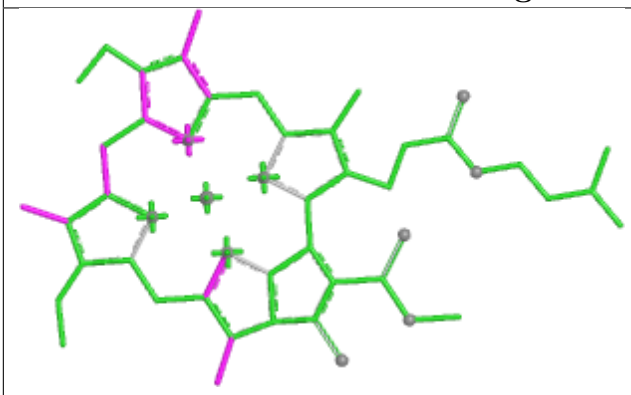


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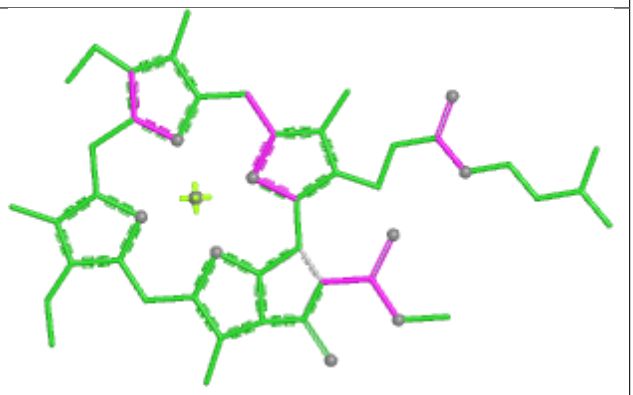


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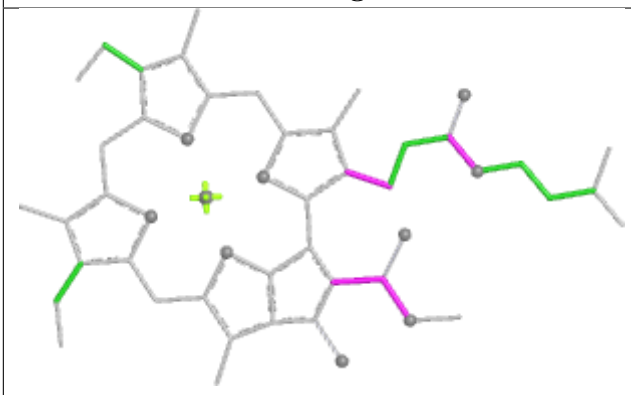
Ligand CLA A1 832



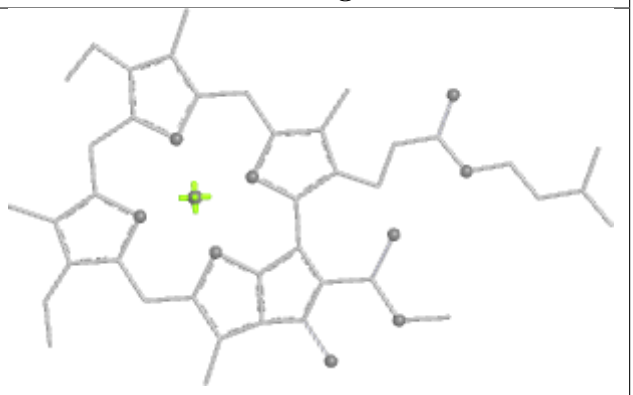
Bond lengths



Bond angles



Torsions

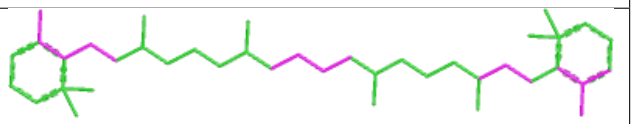


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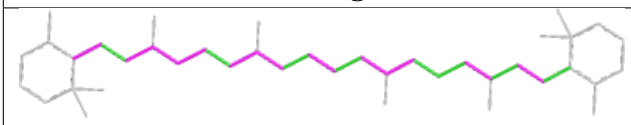
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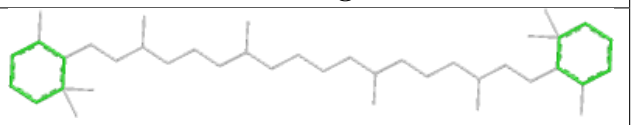
Bond lengths



Bond angles

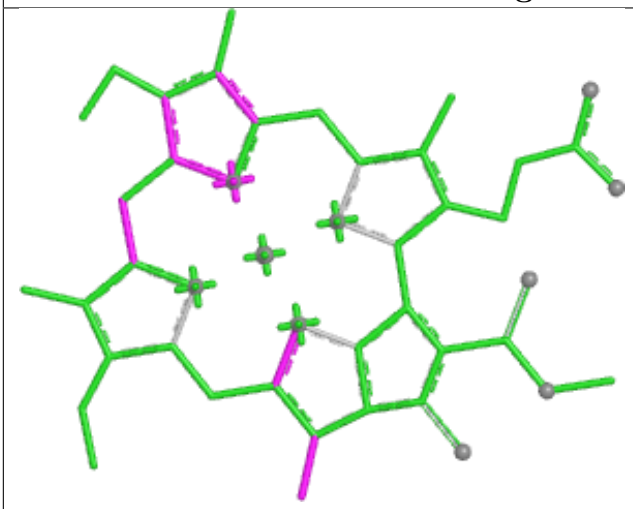


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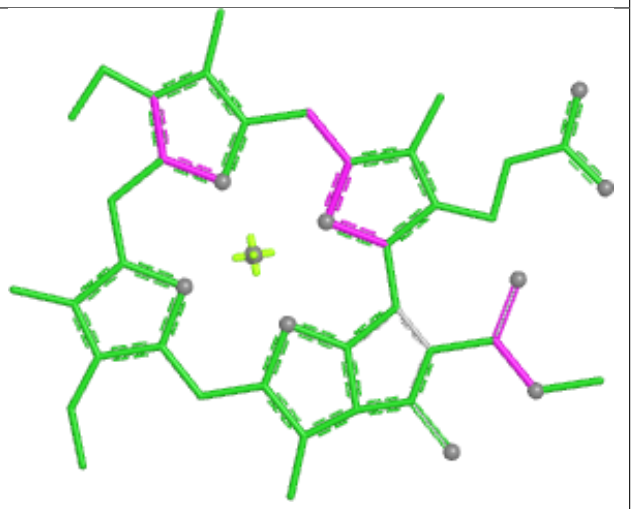


Rings

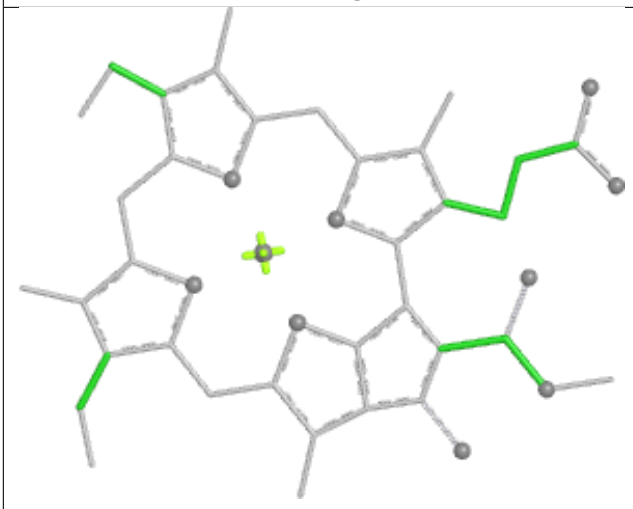
Ligand CLA B2 828



Bond lengths



Bond angles

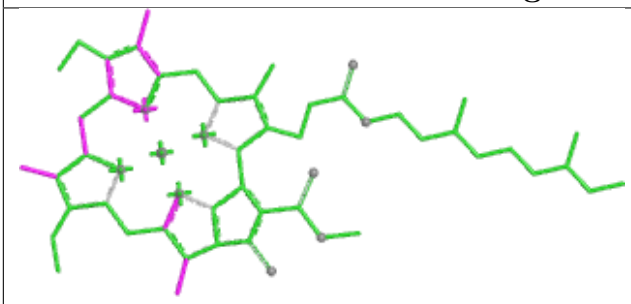


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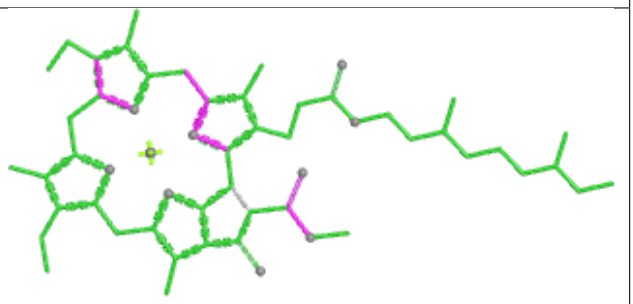


Rings

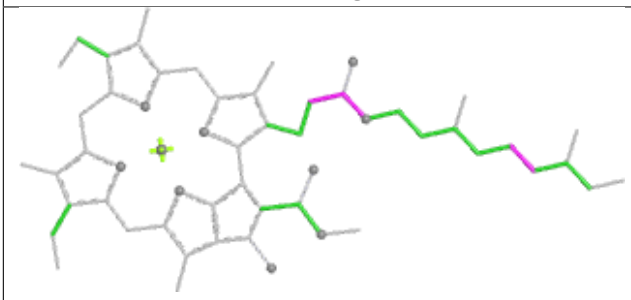
Ligand CLA A 840



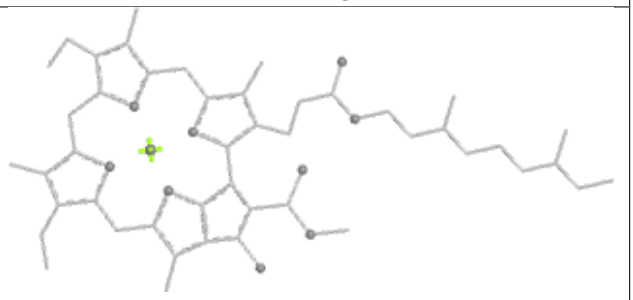
Bond lengths



Bond angles

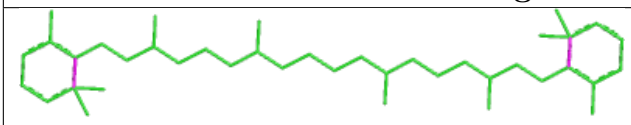


Torsions

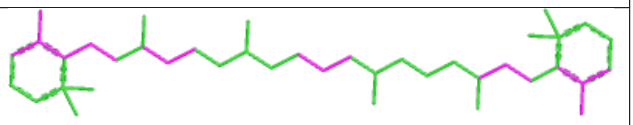


Rings

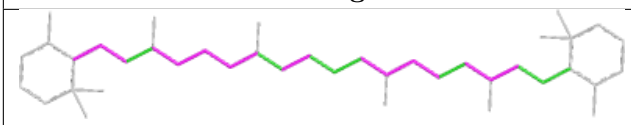
Ligand BCR LL 204



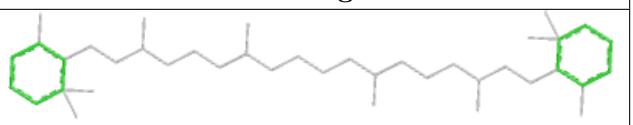
Bond lengths



Bond angles

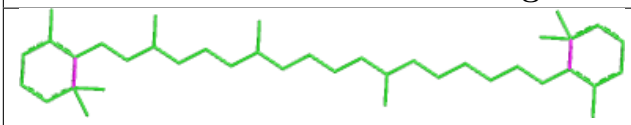


Torsions

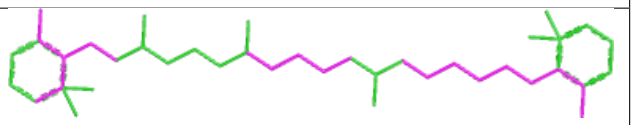


Rings

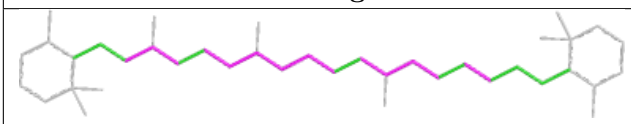
Ligand BCR A 847



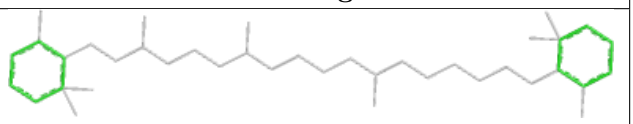
Bond lengths



Bond angles

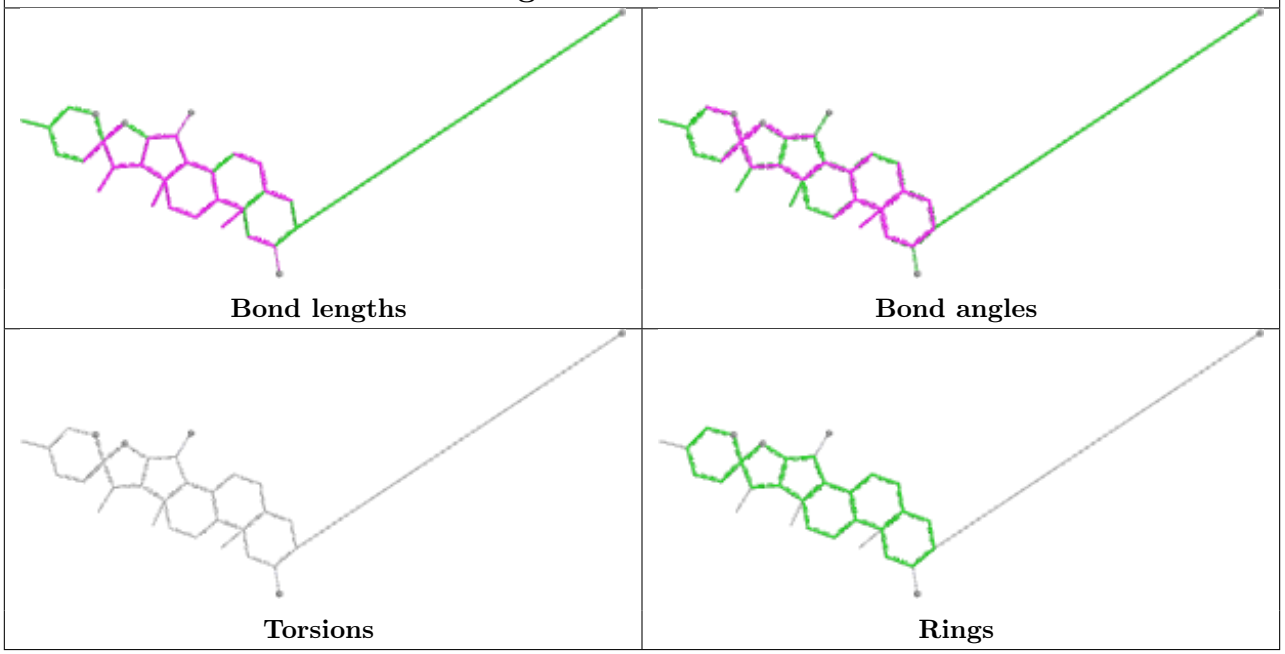


Torsions

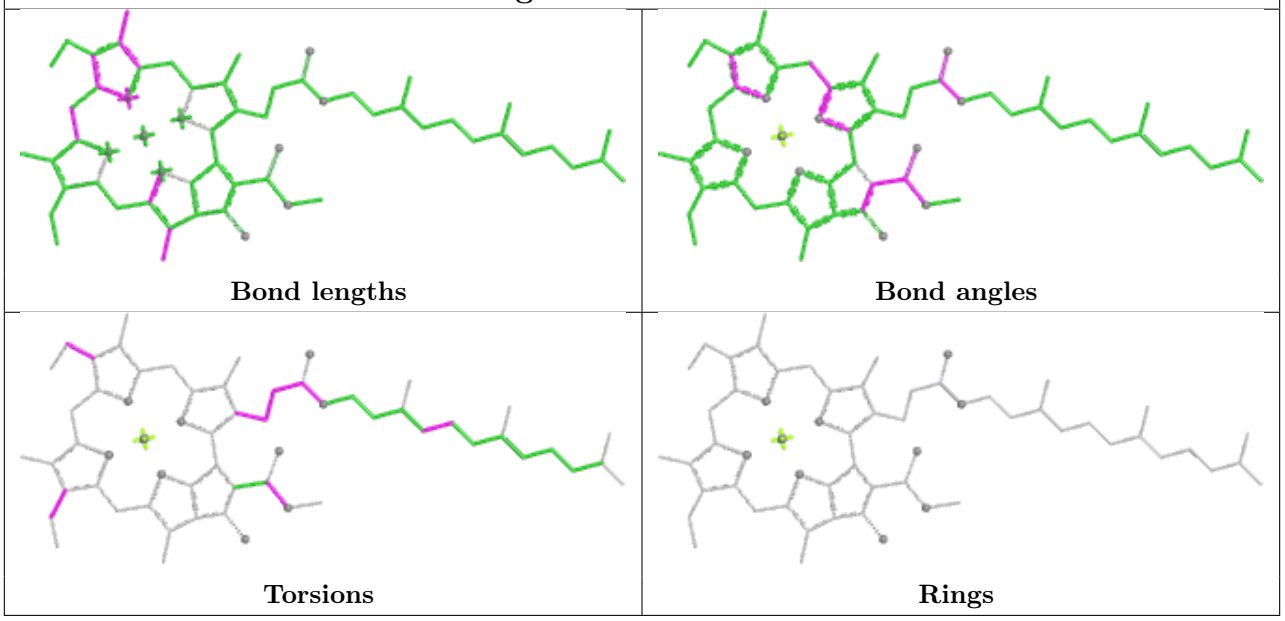


Rings

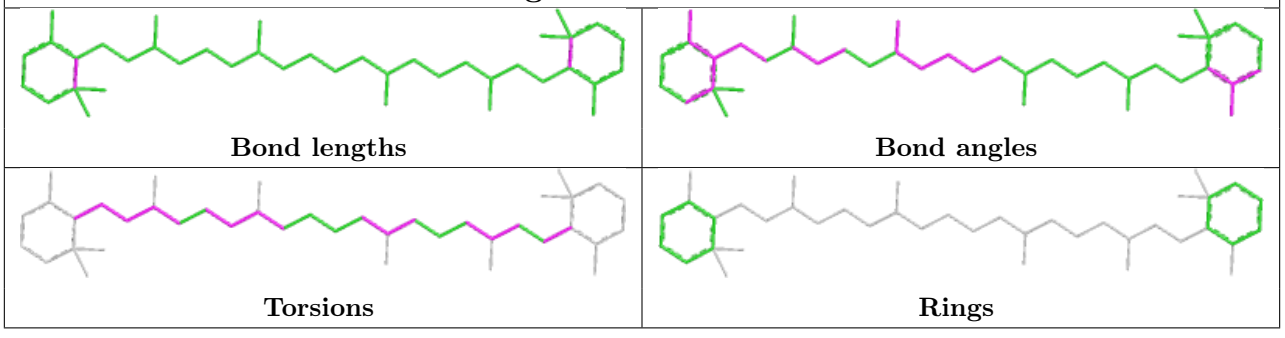
Ligand AJP A1 855



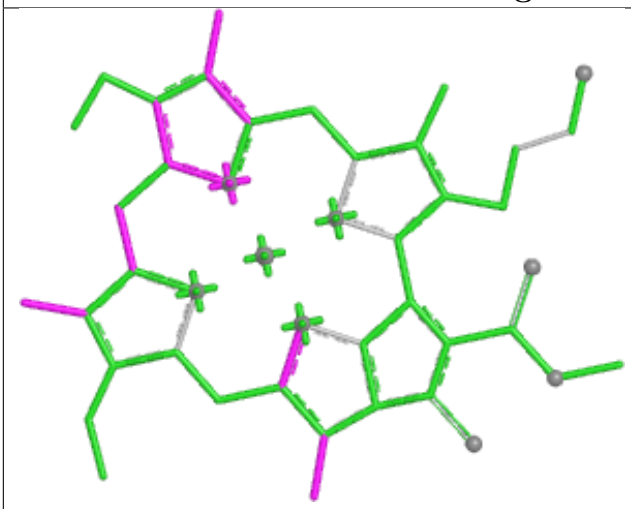
Ligand CLA FF 301



Ligand BCR F 303



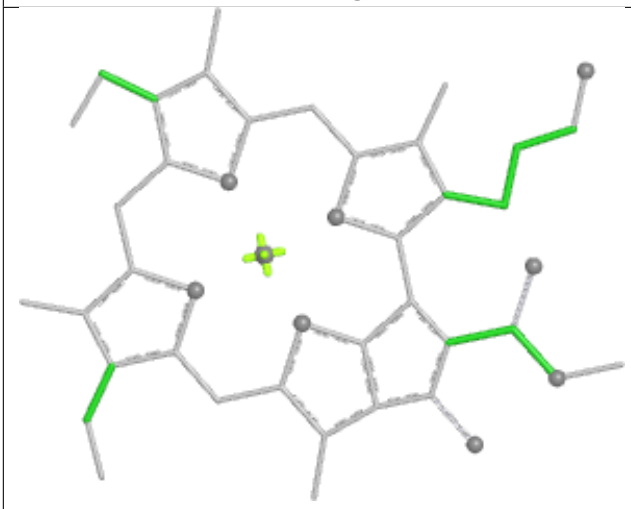
Ligand CLA A1 816



Bond lengths



Bond angles

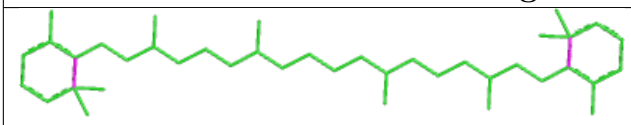


Torsions

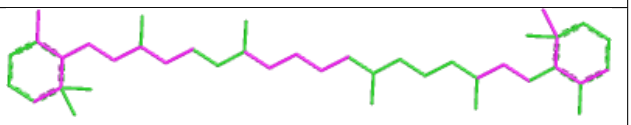


Rings

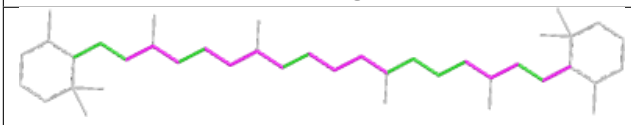
Ligand BCR I2 103



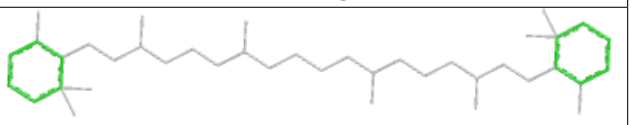
Bond lengths



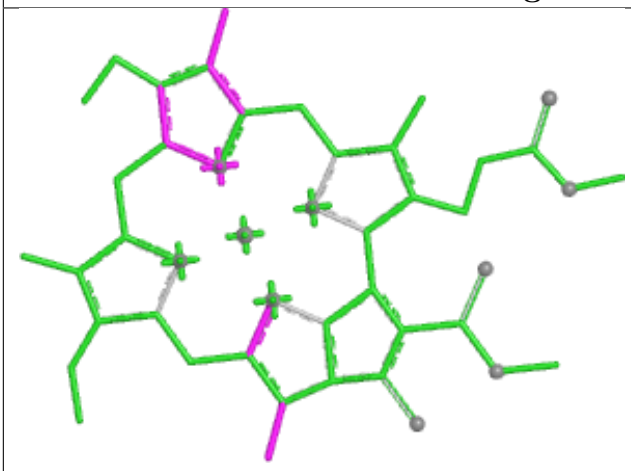
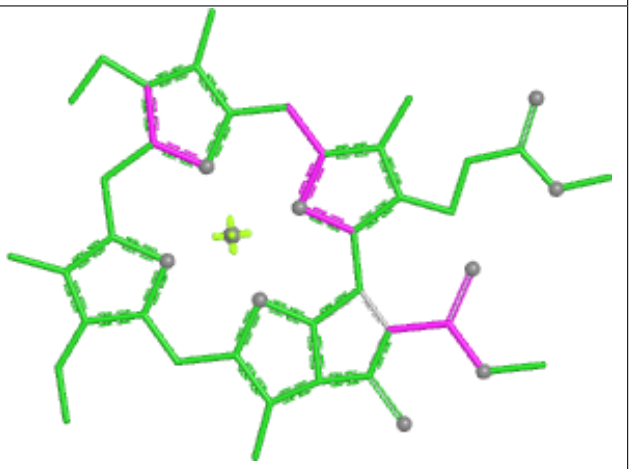
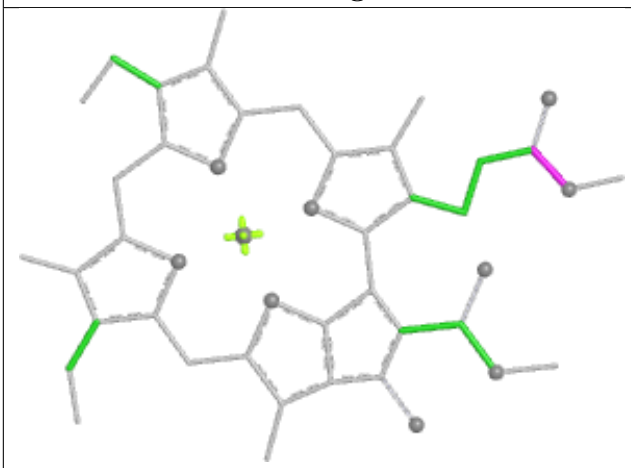
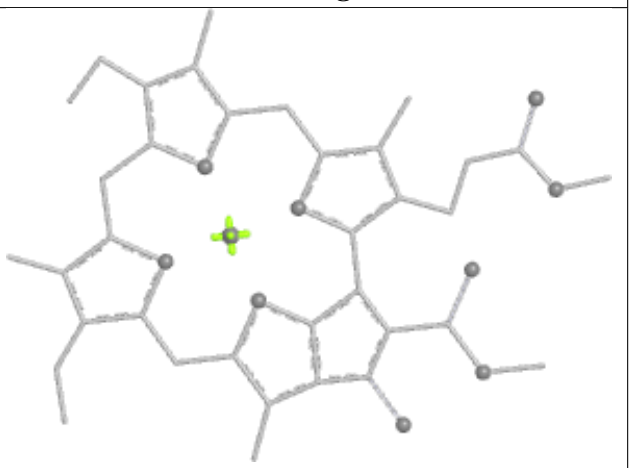
Bond angles



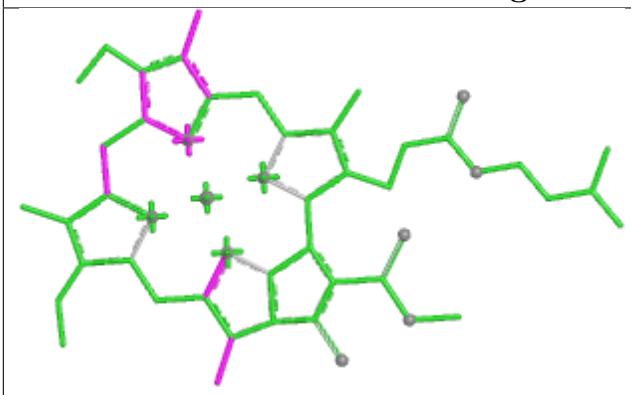
Torsions



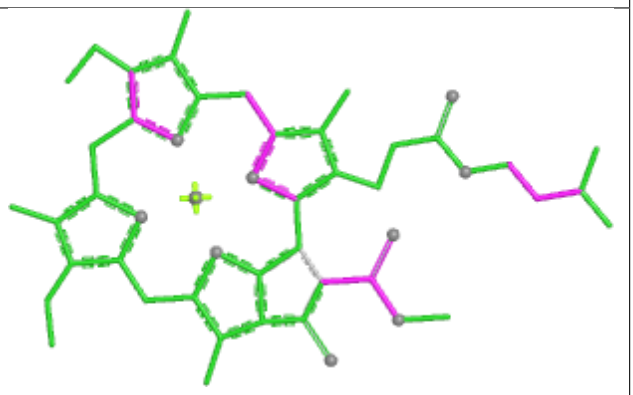
Rings

Ligand CLA A 841	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

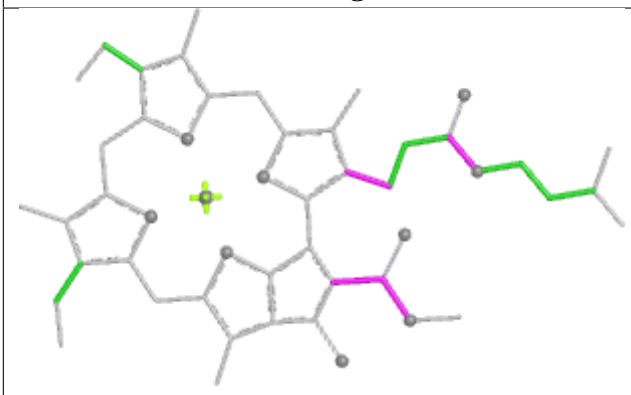
Ligand CLA AA 816



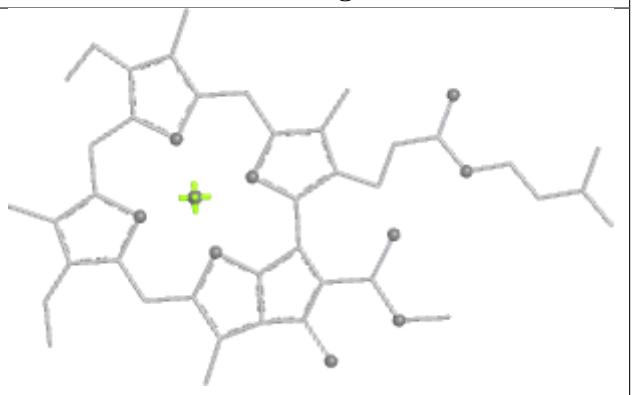
Bond lengths



Bond angles

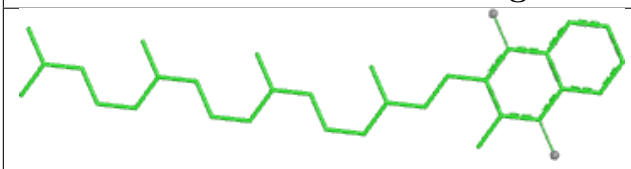


Torsions

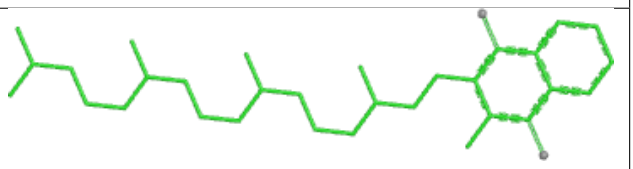


Rings

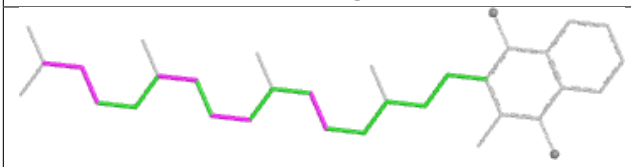
Ligand PQN BB 837



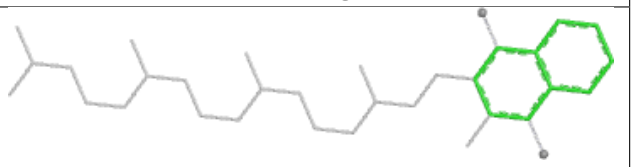
Bond lengths



Bond angles



Torsions

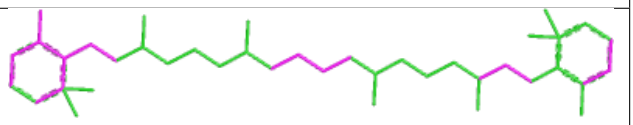


Rings

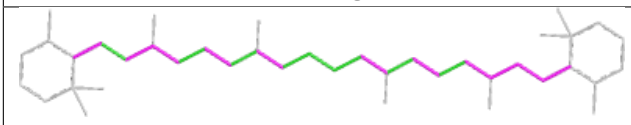
Ligand BCR A2 851



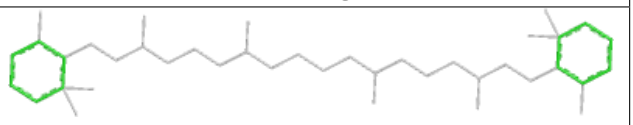
Bond lengths



Bond angles

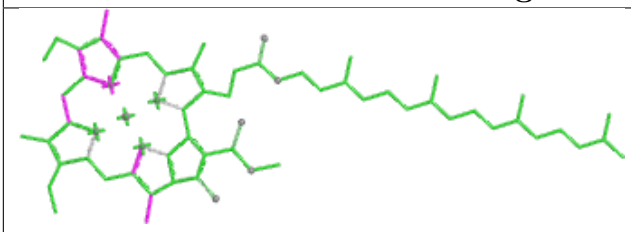


Torsions

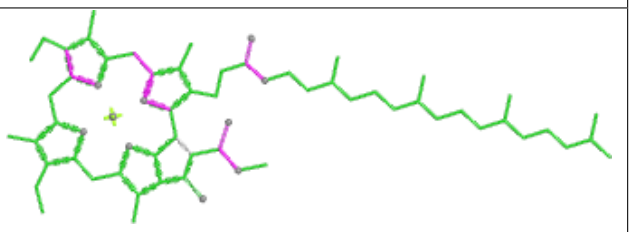


Rings

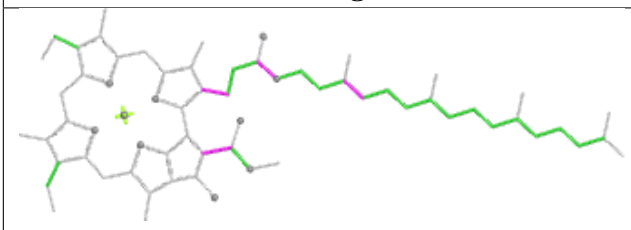
Ligand CLA B2 802



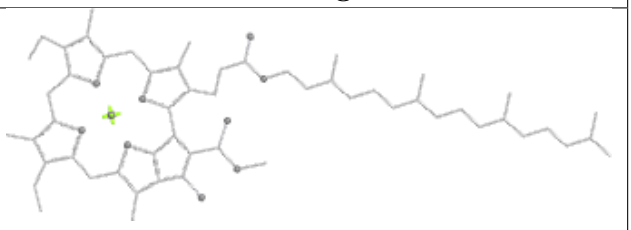
Bond lengths



Bond angles

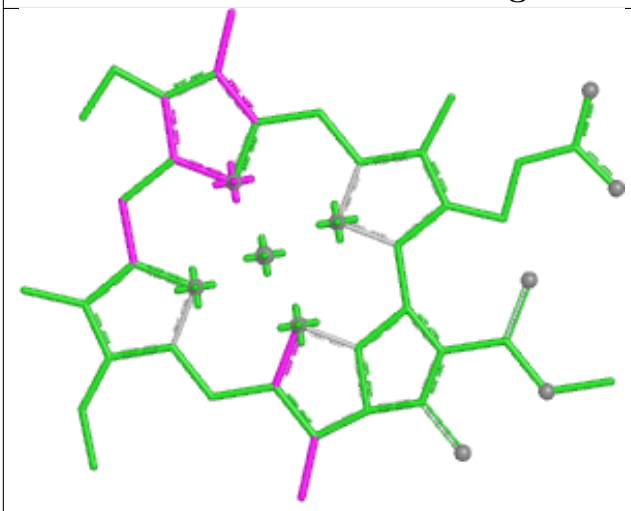


Torsions

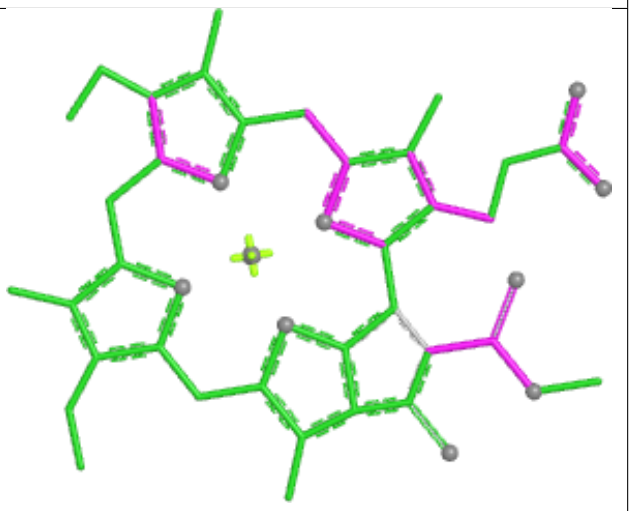


Rings

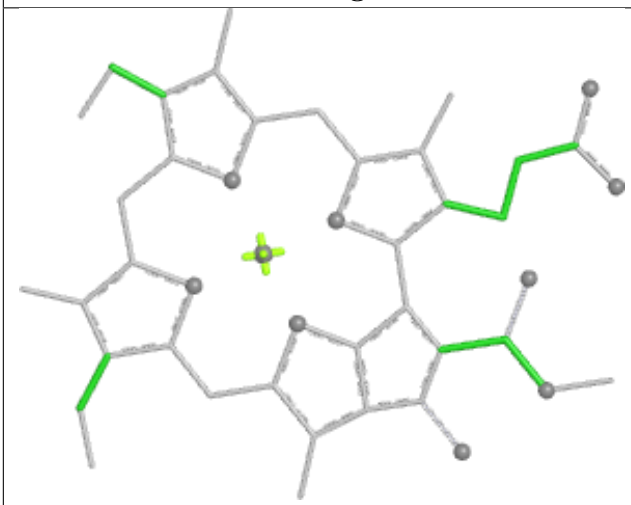
Ligand CLA KK 101



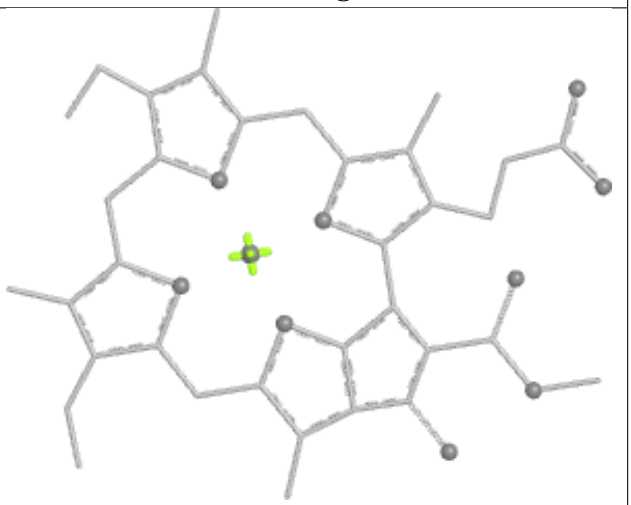
Bond lengths



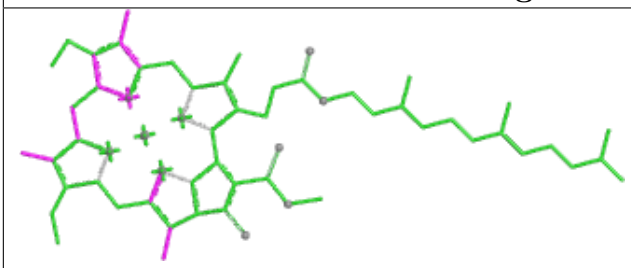
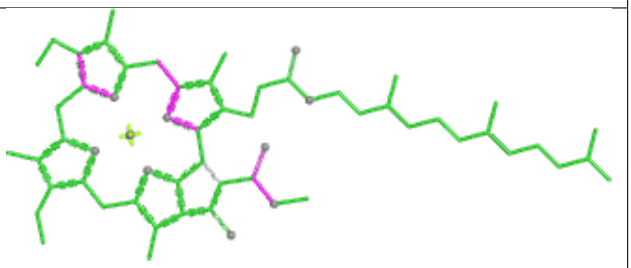
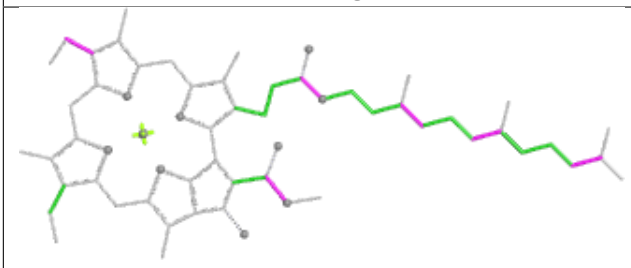
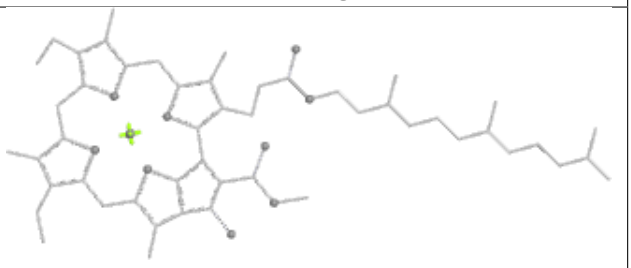
Bond angles

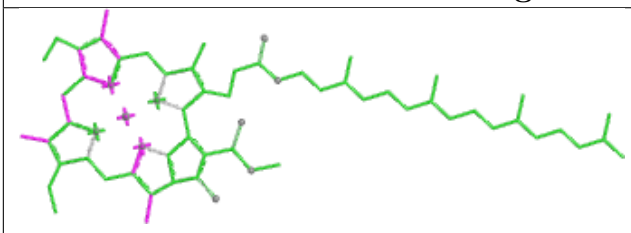
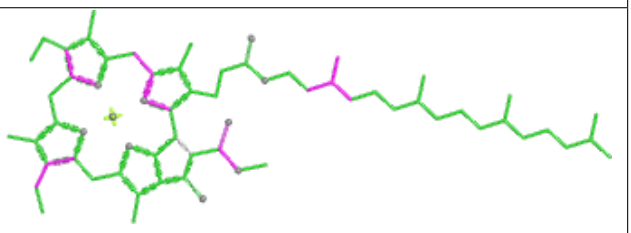
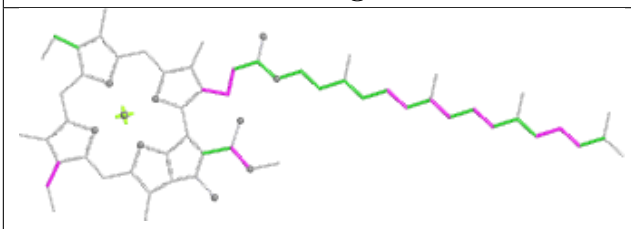
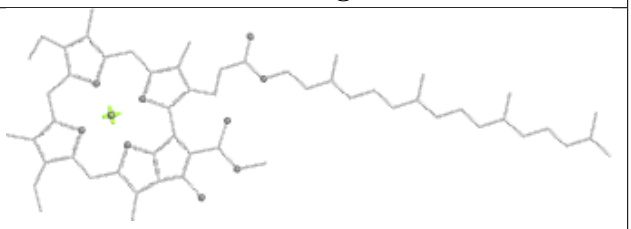


Torsions

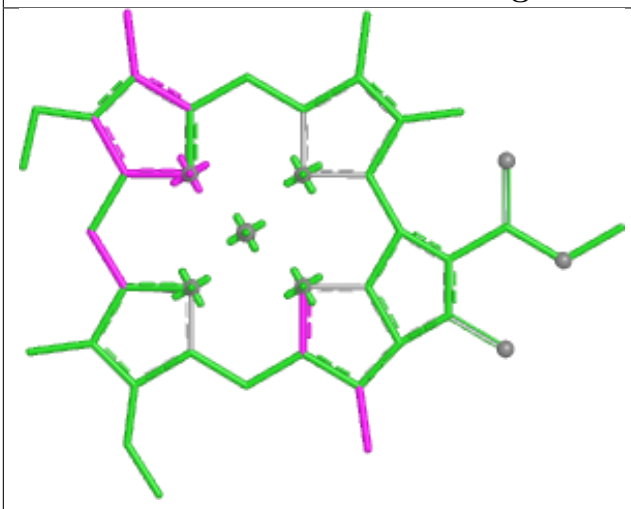


Rings

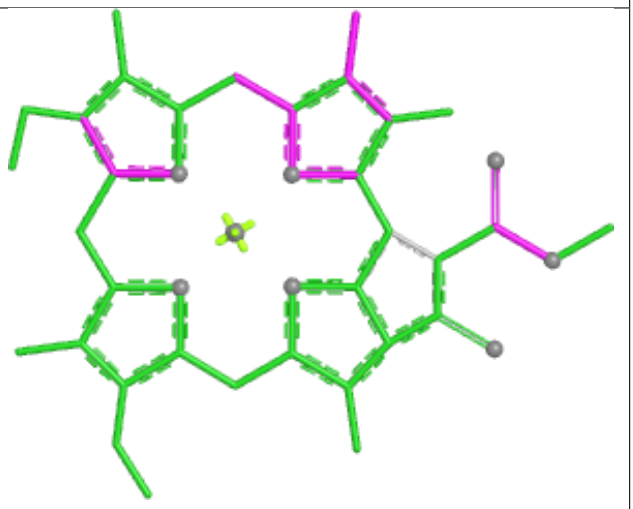
Ligand CLA B1 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A2 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

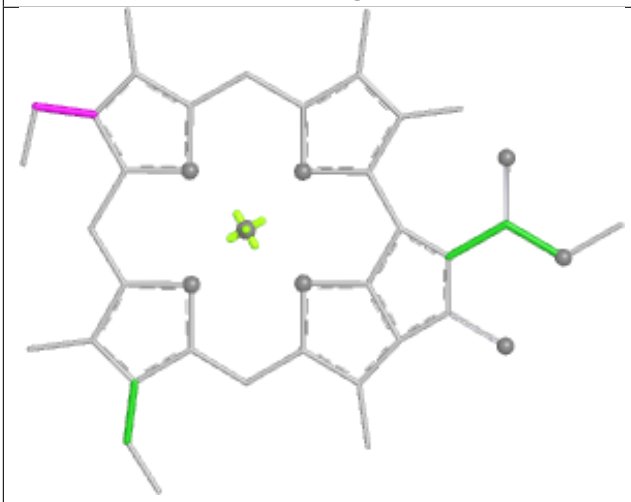
Ligand CLA BB 818



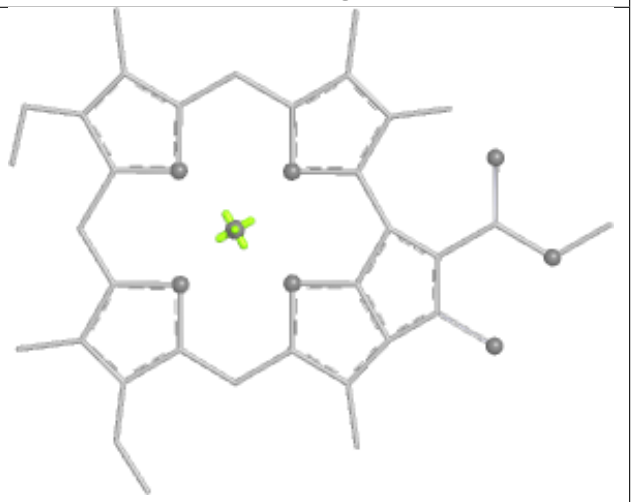
Bond lengths



Bond angles



Torsions

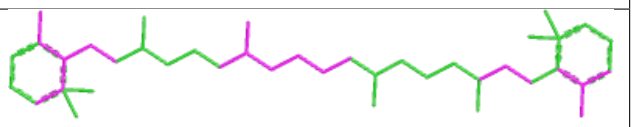


Rings

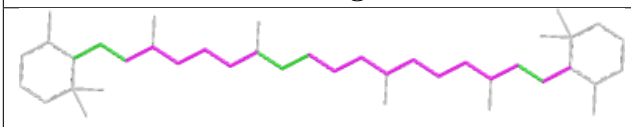
Ligand BCR KK 103



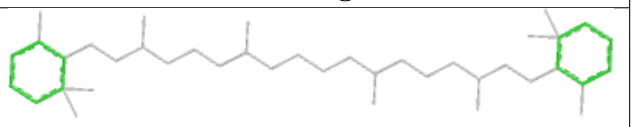
Bond lengths



Bond angles

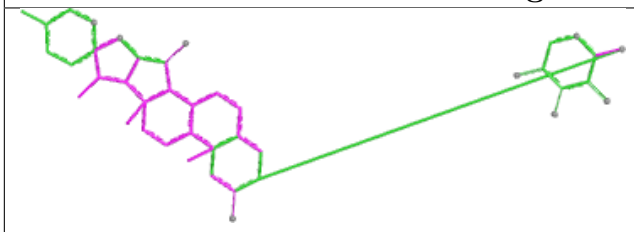


Torsions

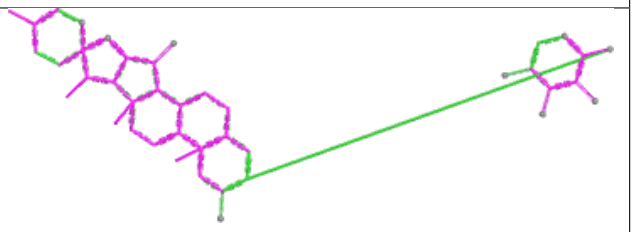


Rings

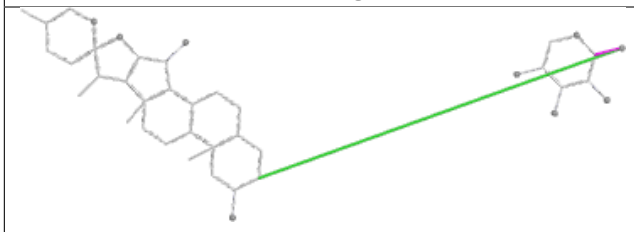
Ligand AJP K 104



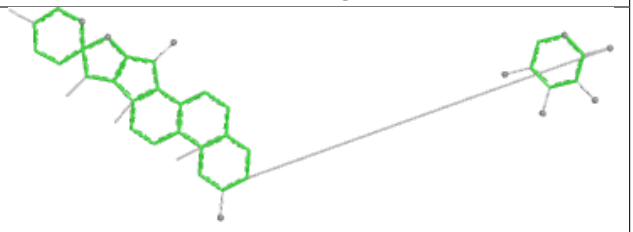
Bond lengths



Bond angles

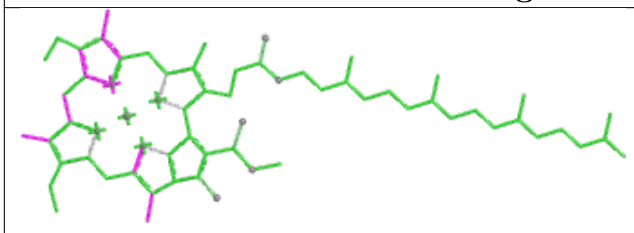


Torsions

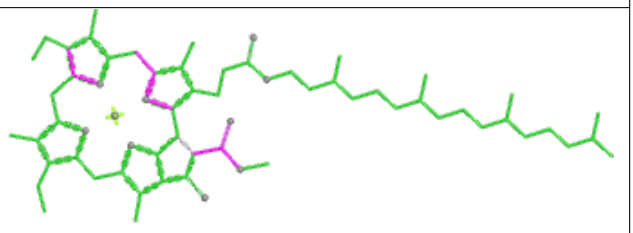


Rings

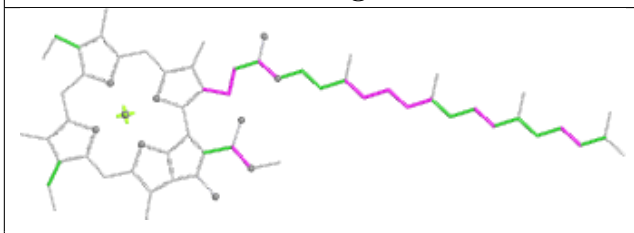
Ligand CLA A2 808



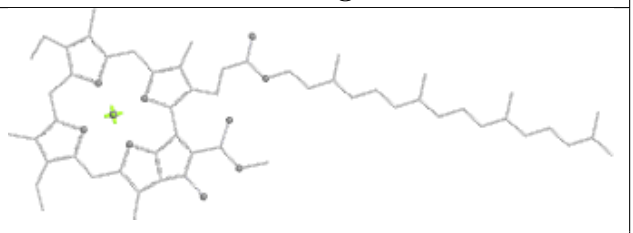
Bond lengths



Bond angles

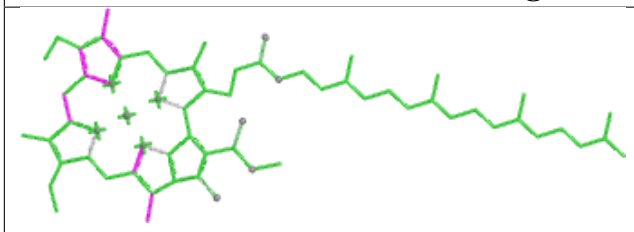


Torsions

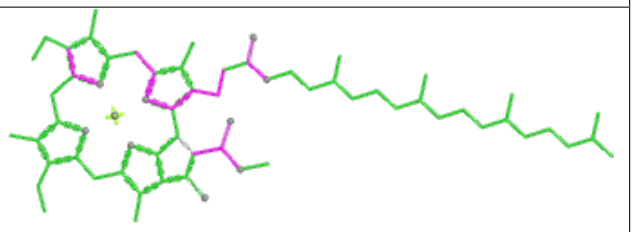


Rings

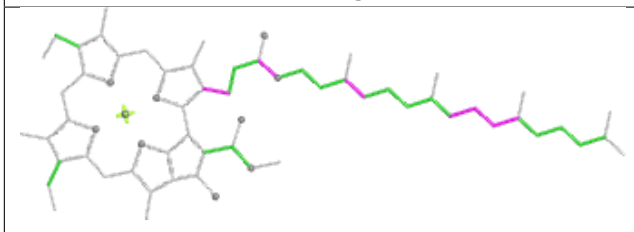
Ligand CLA A 810



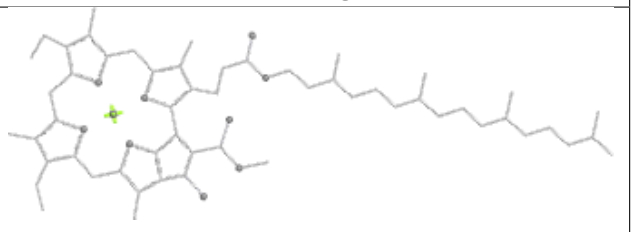
Bond lengths



Bond angles

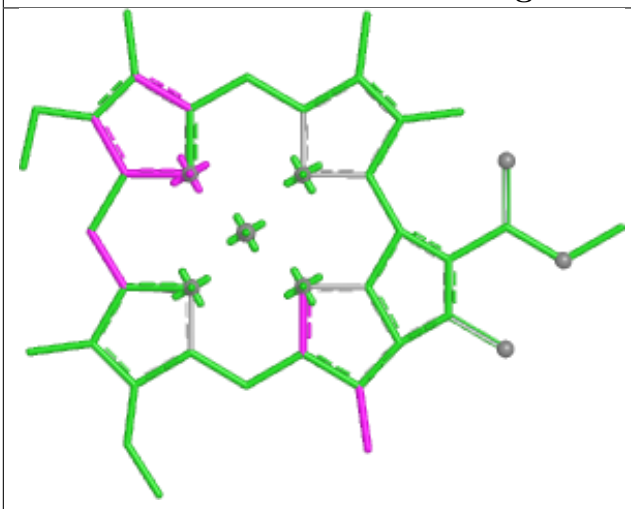


Torsions

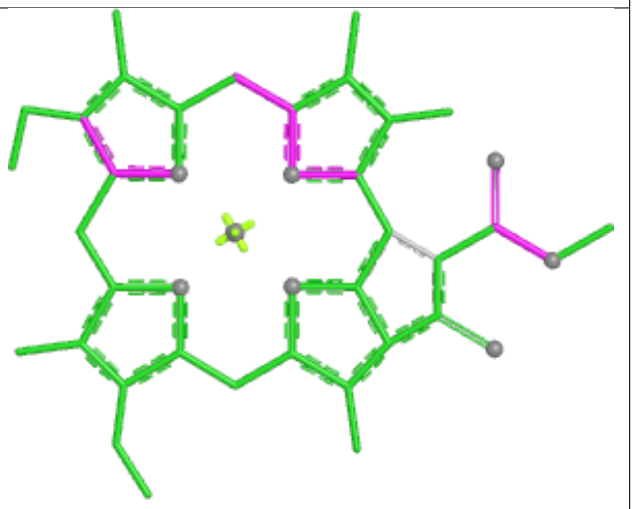


Rings

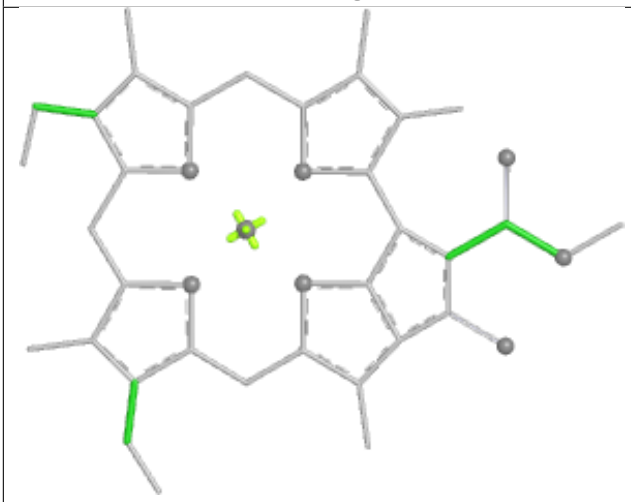
Ligand CLA B2 818



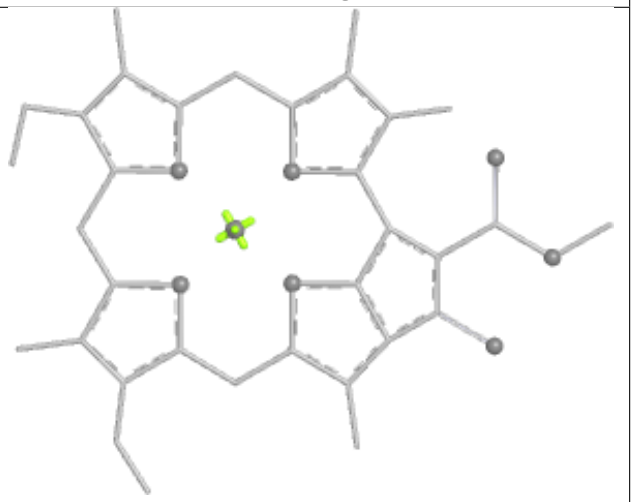
Bond lengths



Bond angles

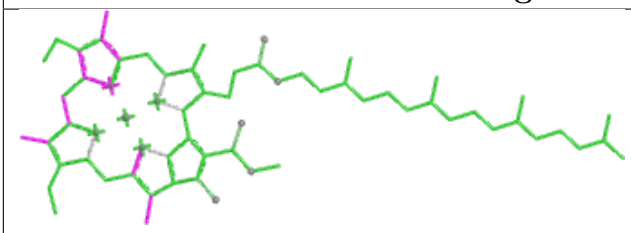


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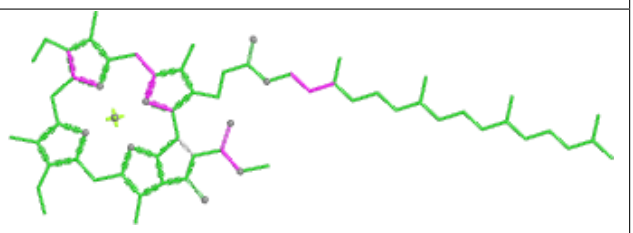


Rings

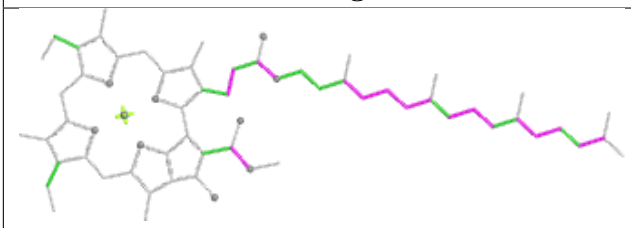
Ligand CLA A1 803



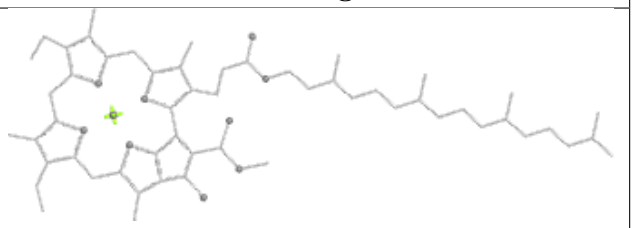
Bond lengths



Bond angles

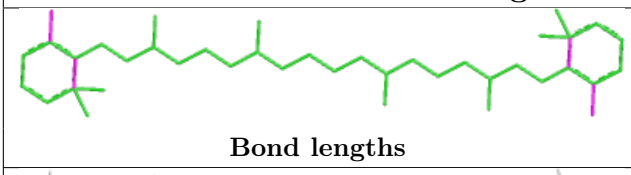


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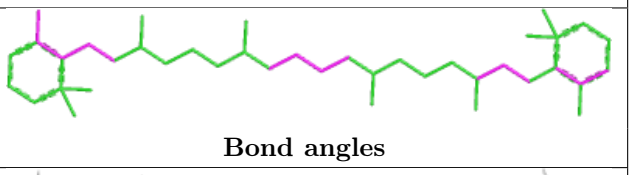


Rings

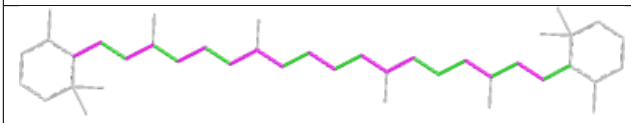
Ligand BCR BB 843



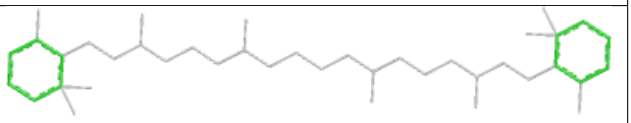
Bond lengths



Bond angles

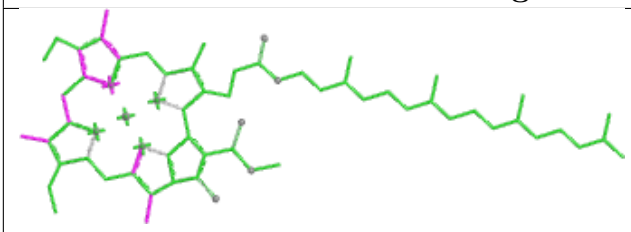


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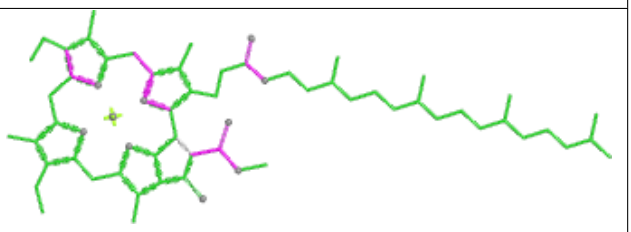


Rings

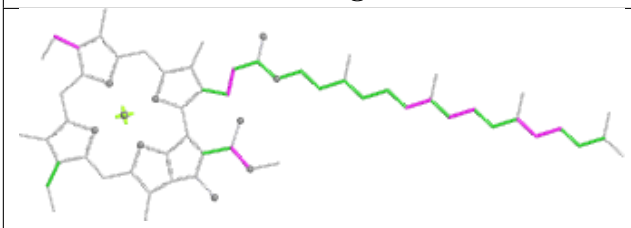
Ligand CLA BB 835



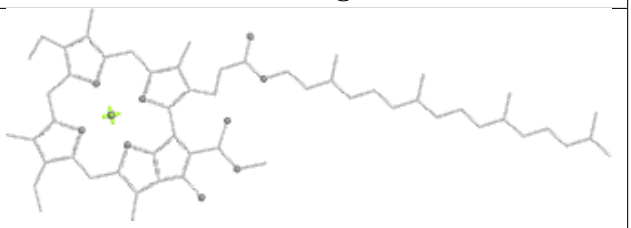
Bond lengths



Bond angles

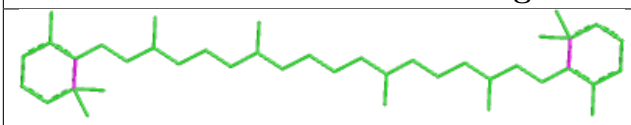


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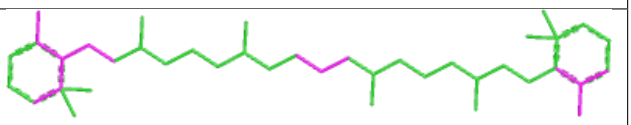


Rings

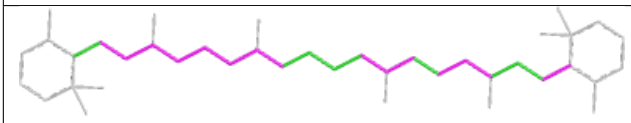
Ligand BCR B2 843



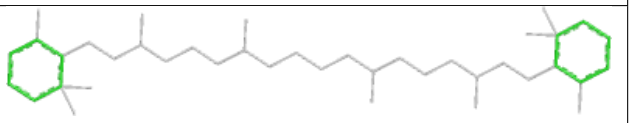
Bond lengths



Bond angles

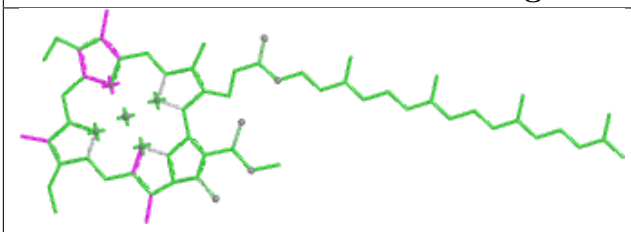


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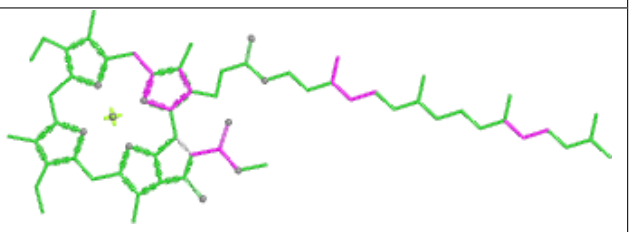


Rings

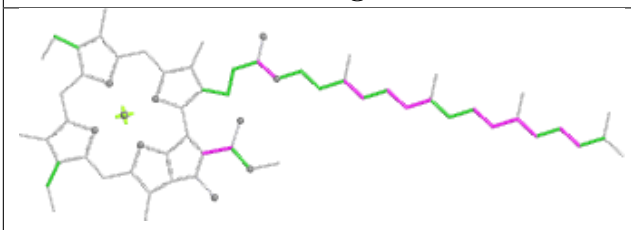
Ligand CLA B 826



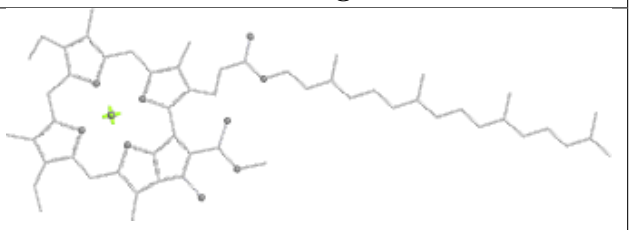
Bond lengths



Bond angles

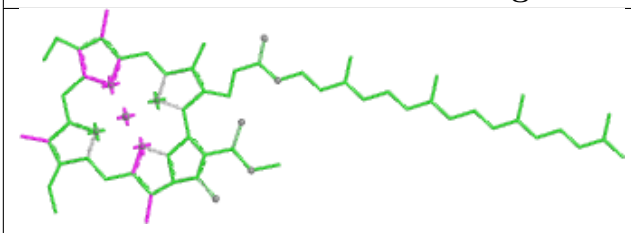


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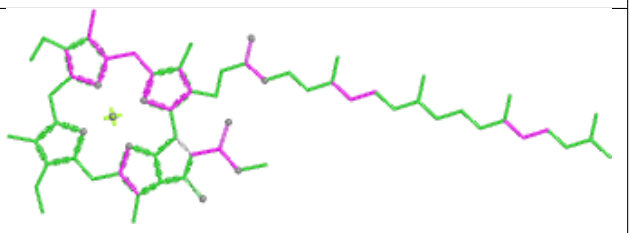


Rings

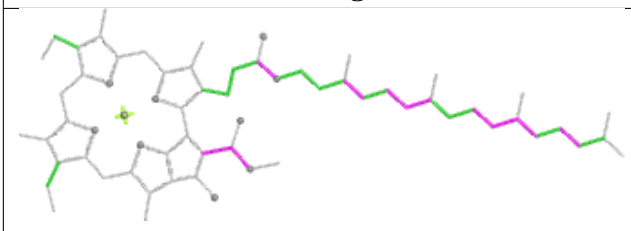
Ligand CLA BB 826



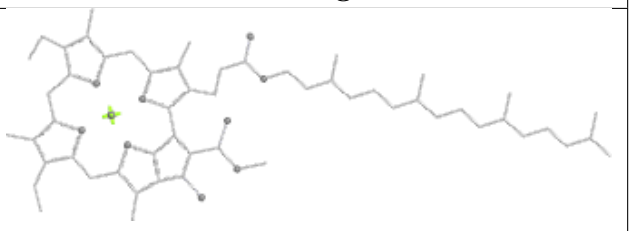
Bond lengths



Bond angles

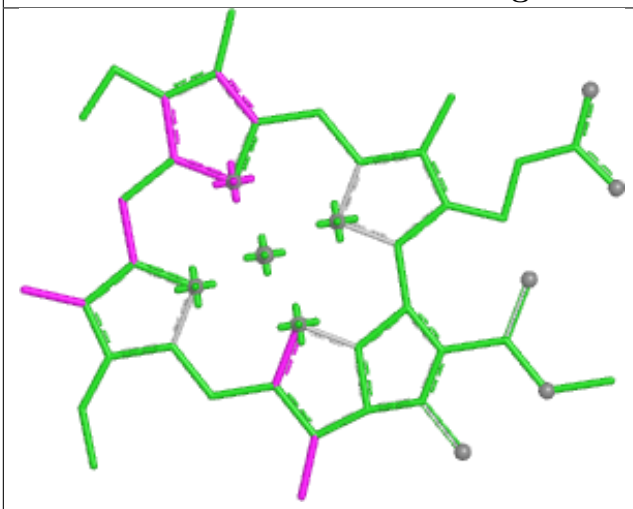


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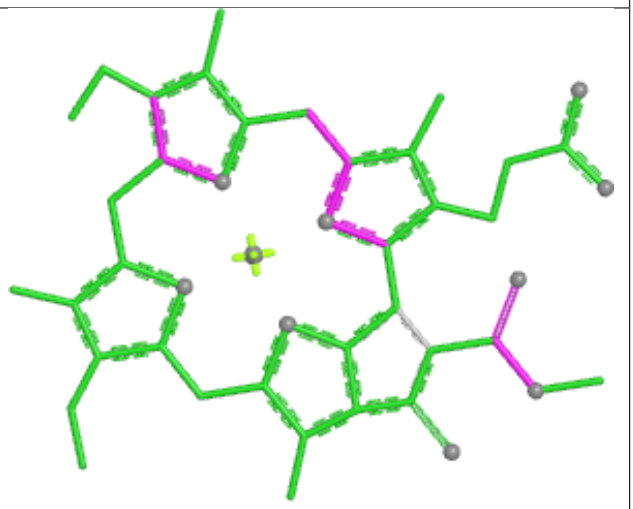


Rings

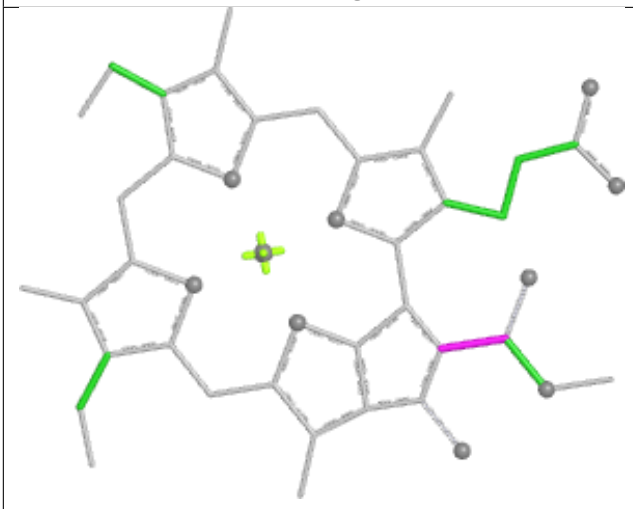
Ligand CLA BB 828



Bond lengths



Bond angles

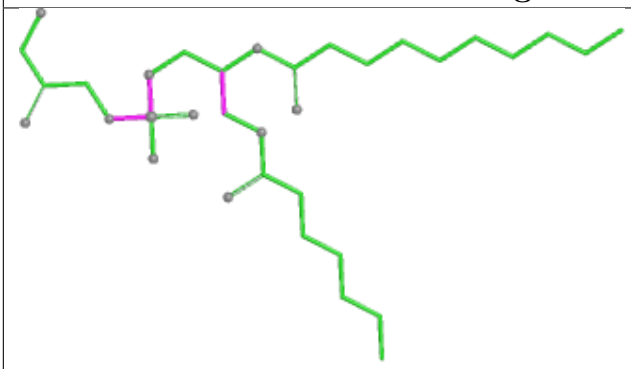


Torsions

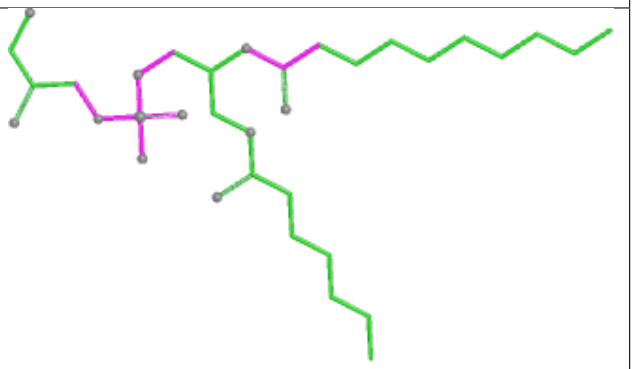


Rings

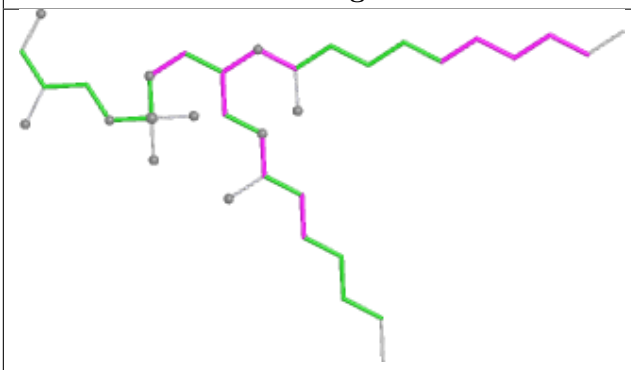
Ligand LHG LL 205



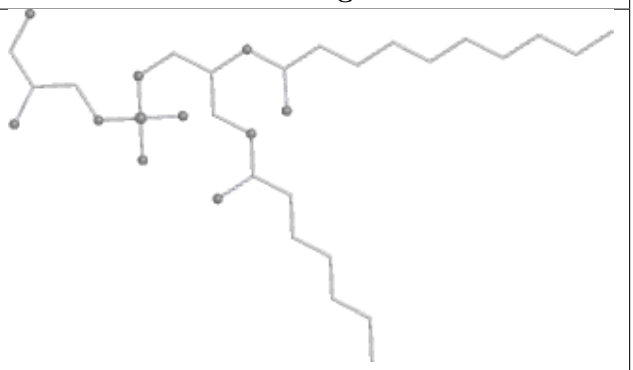
Bond lengths



Bond angles

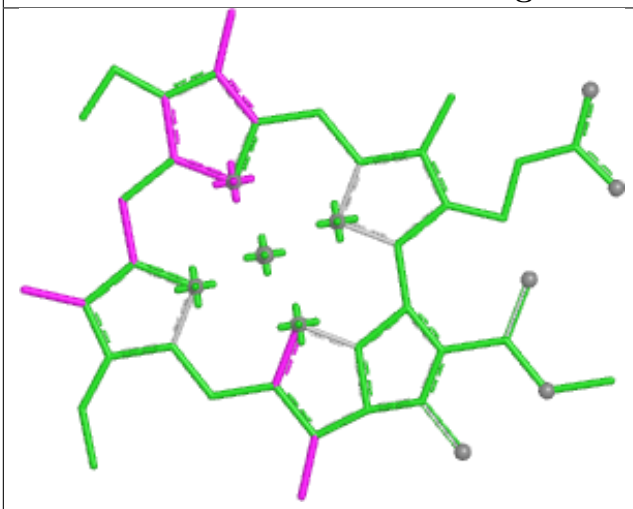


Torsions

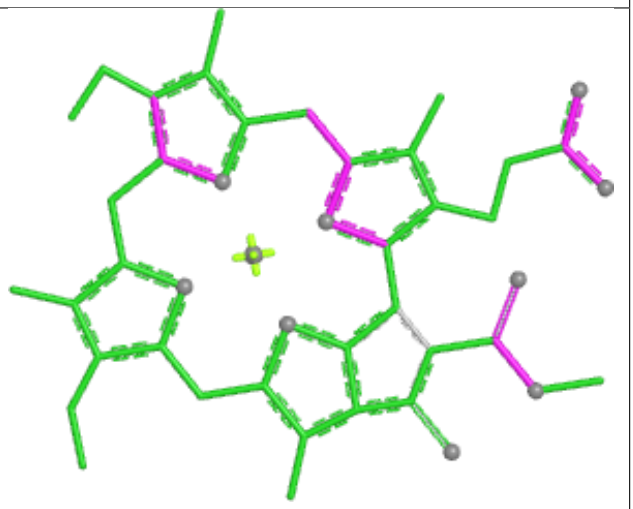


Rings

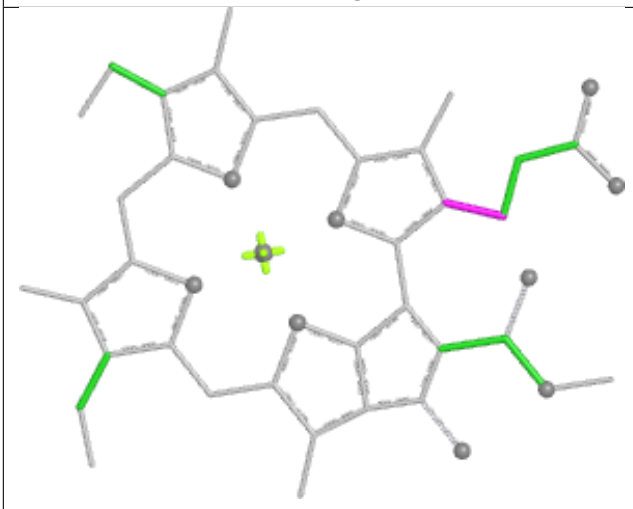
Ligand CLA B2 835



Bond lengths



Bond angles

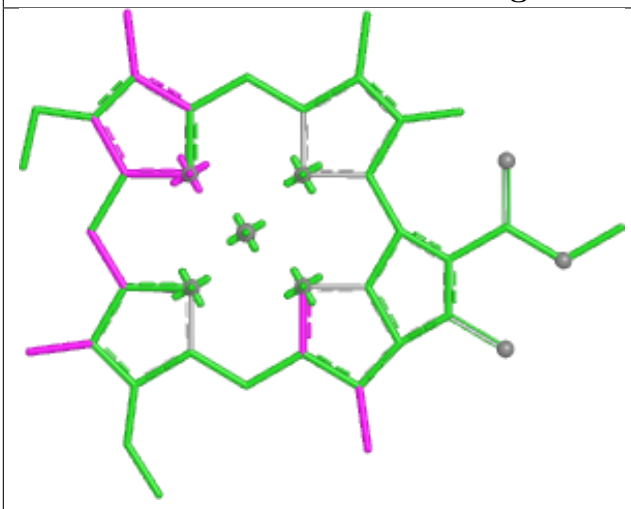


Torsions

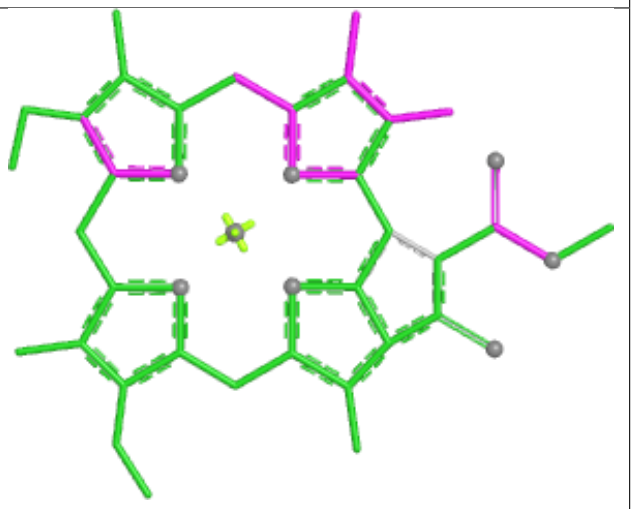


Rings

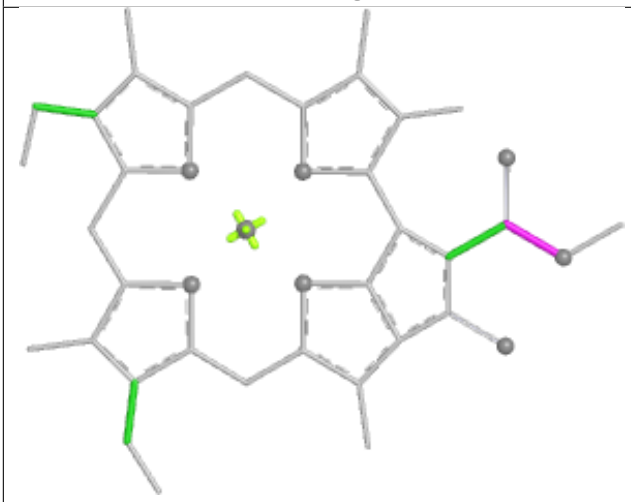
Ligand CLA AA 834



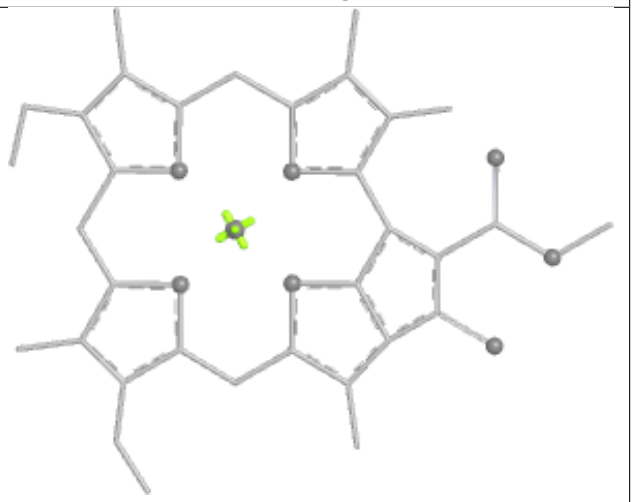
Bond lengths



Bond angles

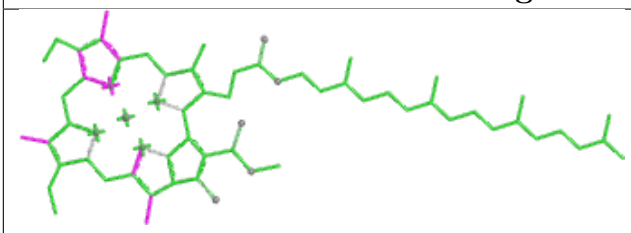


Torsions

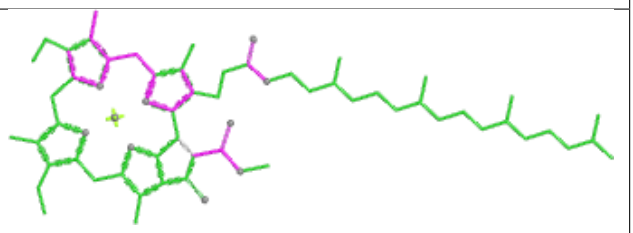


Rings

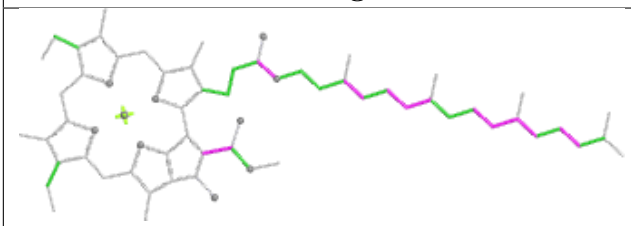
Ligand CLA B1 826



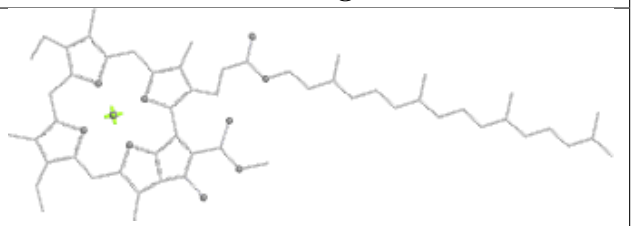
Bond lengths



Bond angles

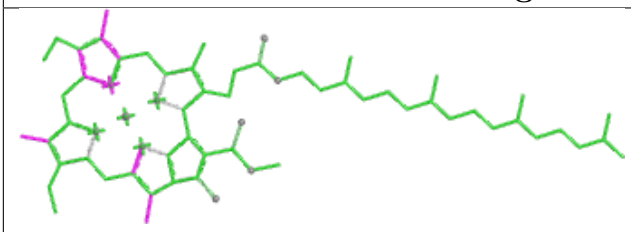


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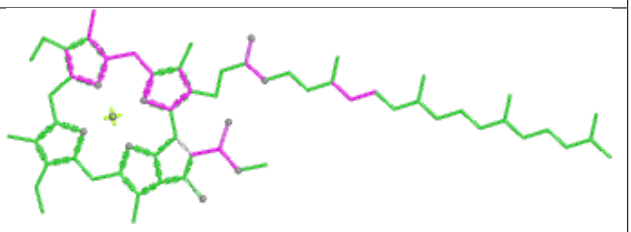


Rings

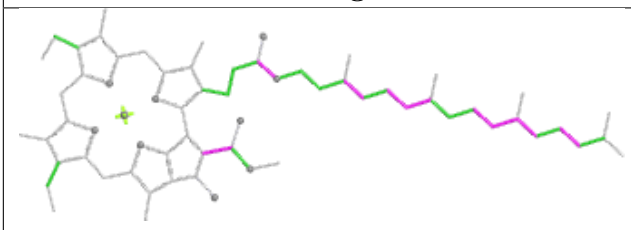
Ligand CLA B2 826



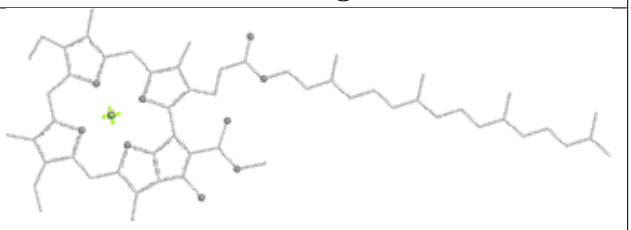
Bond lengths



Bond angles

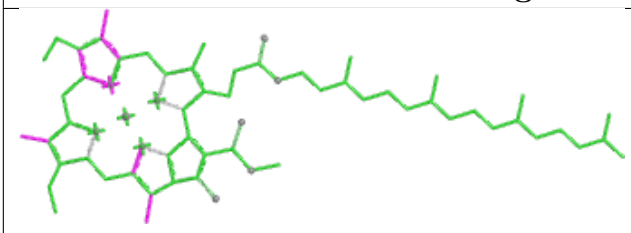


Torsions

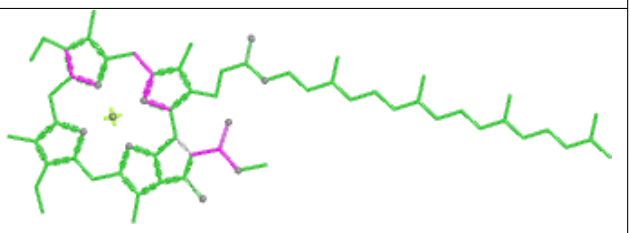


Rings

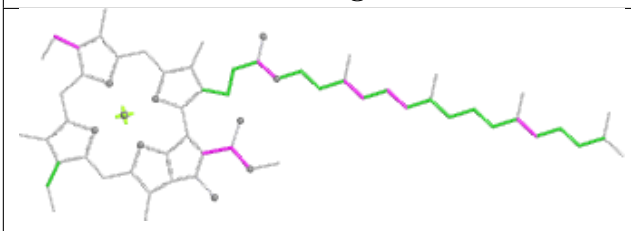
Ligand CLA A1 835



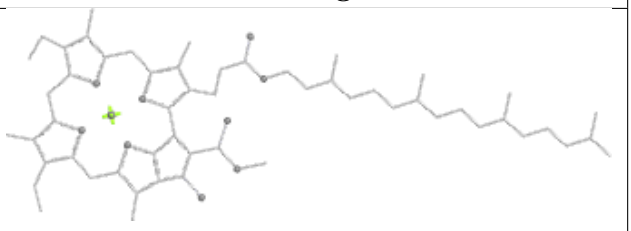
Bond lengths



Bond angles

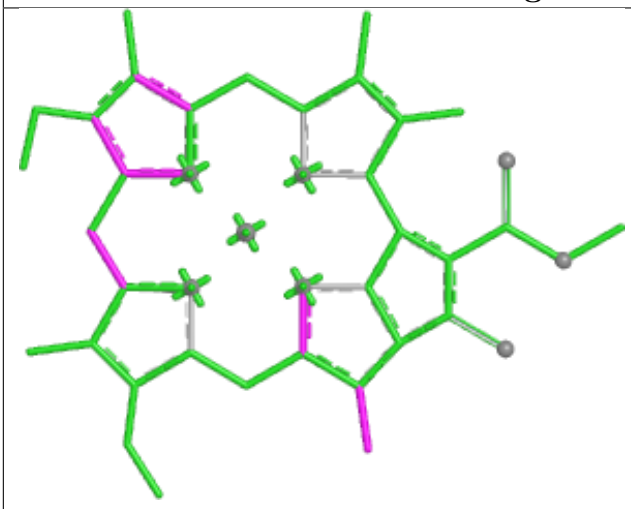


Torsions

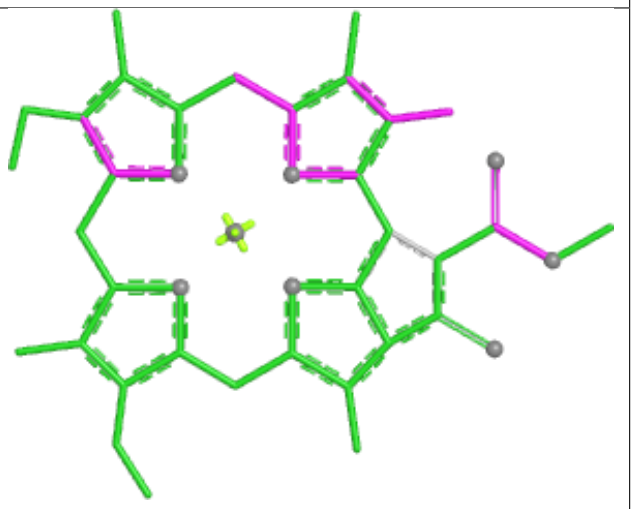


Rings

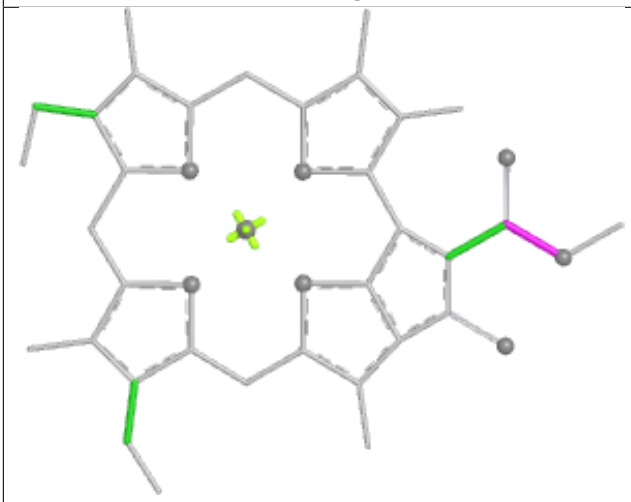
Ligand CLA B 818



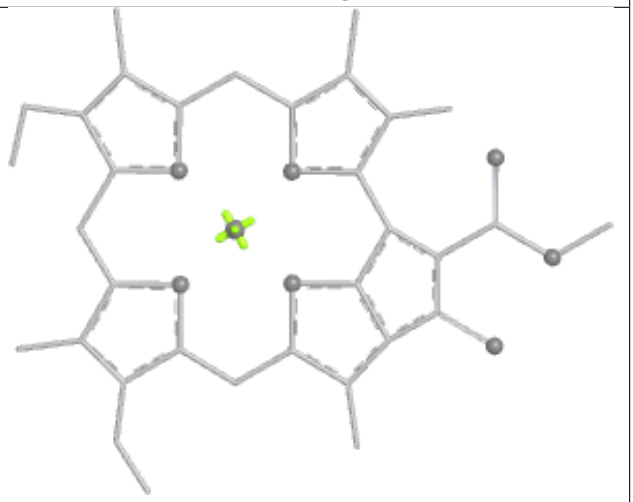
Bond lengths



Bond angles

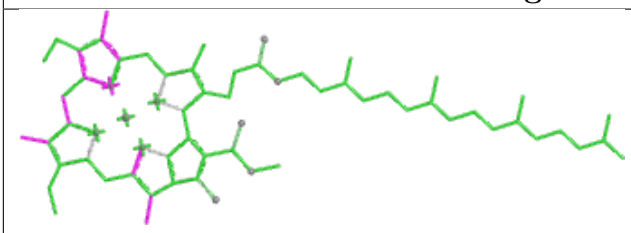


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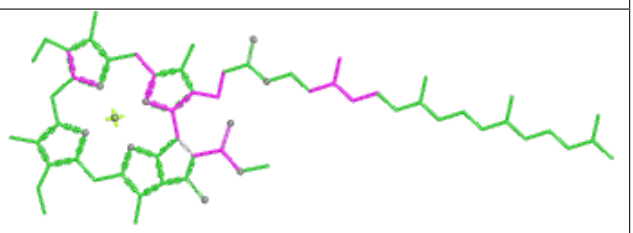


Rings

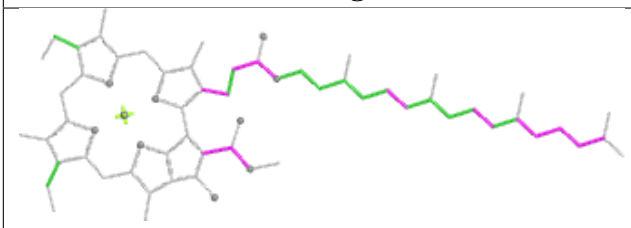
Ligand CLA B 801



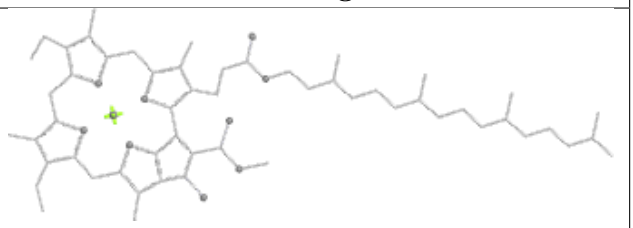
Bond lengths



Bond angles

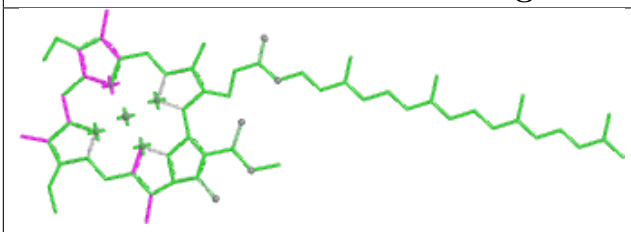


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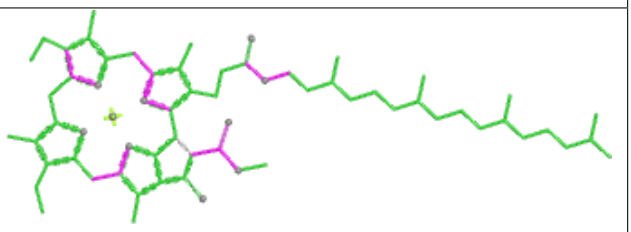


Rings

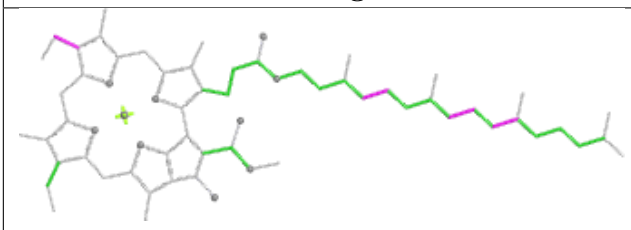
Ligand CLA LL 202



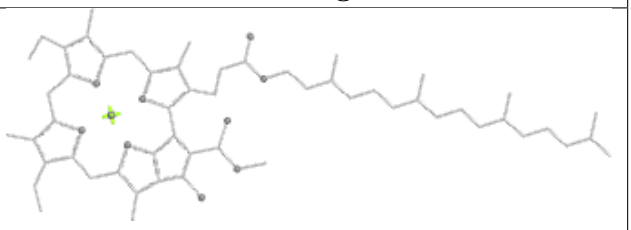
Bond lengths



Bond angles

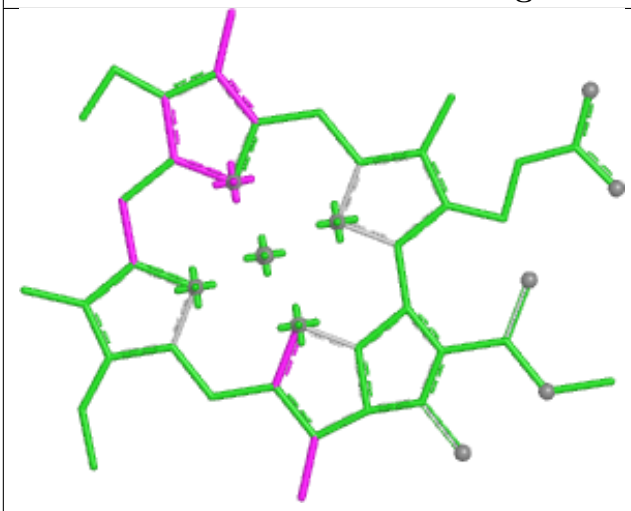


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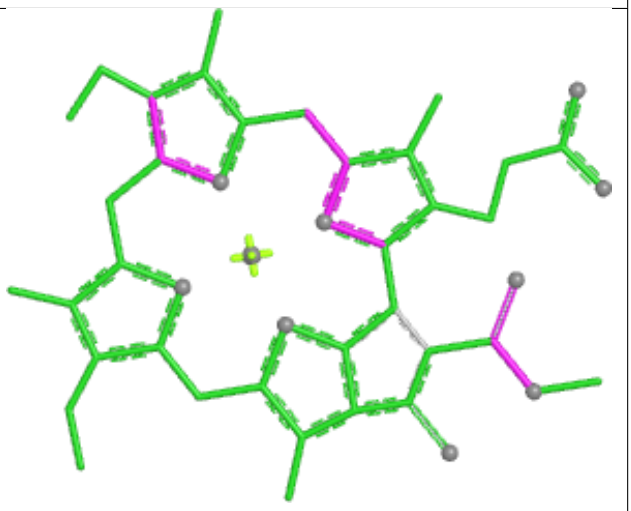


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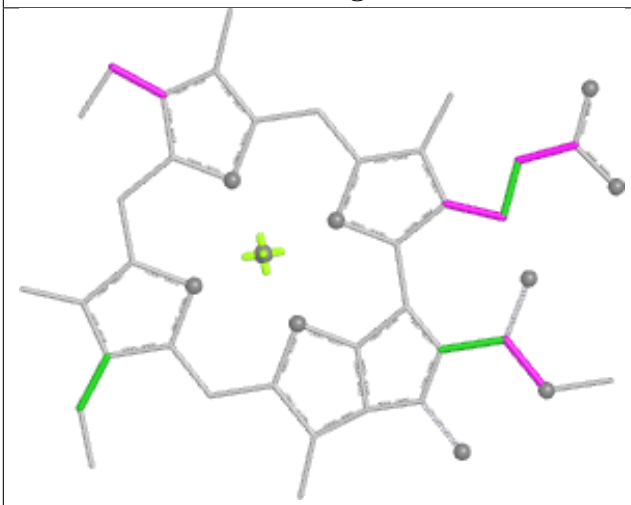
Ligand CLA B1 831



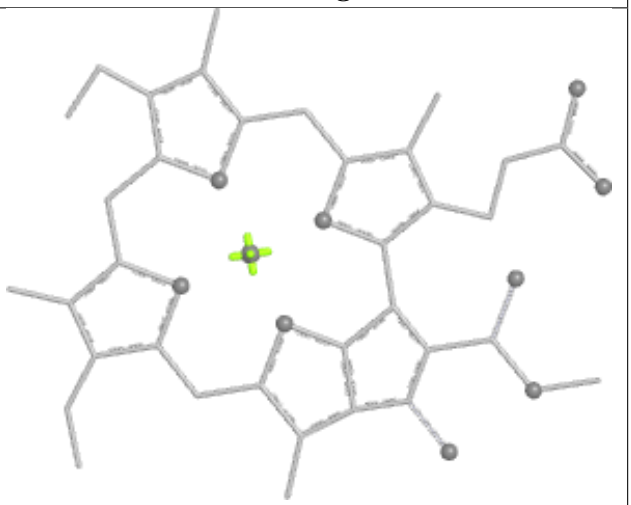
Bond lengths



Bond angles

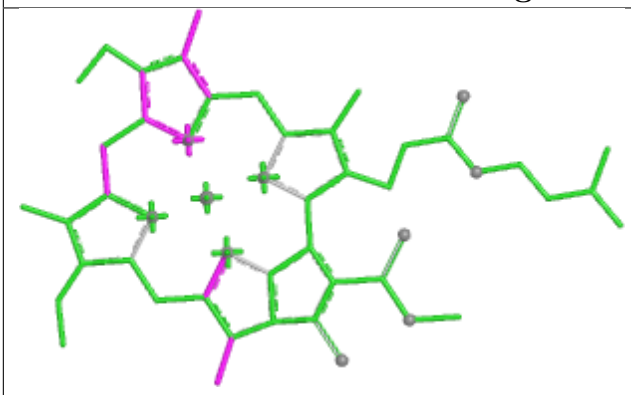


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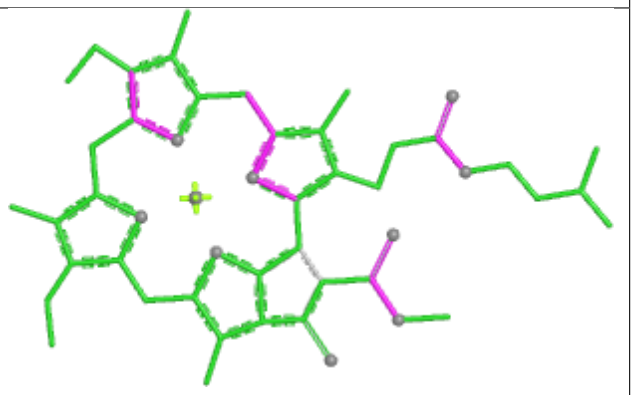


Rings

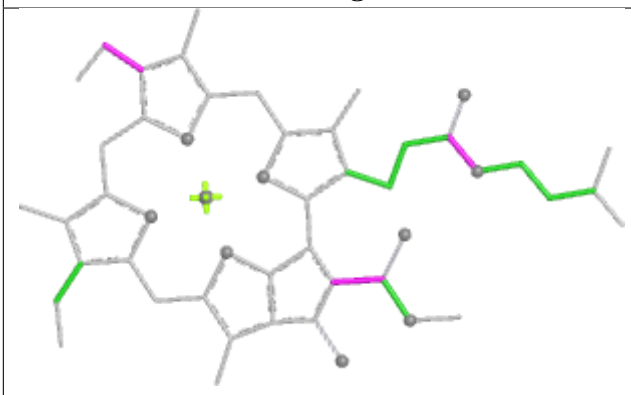
Ligand CLA A2 809



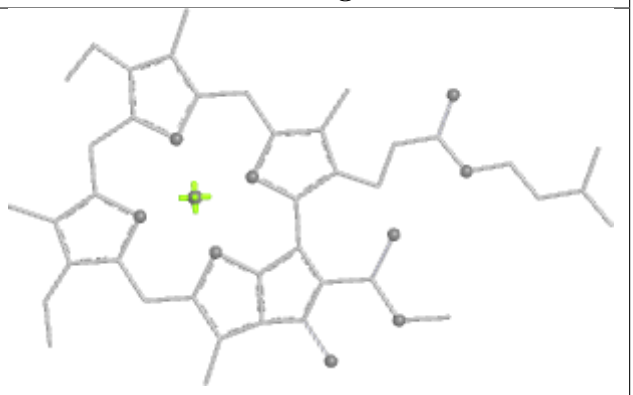
Bond lengths



Bond angles

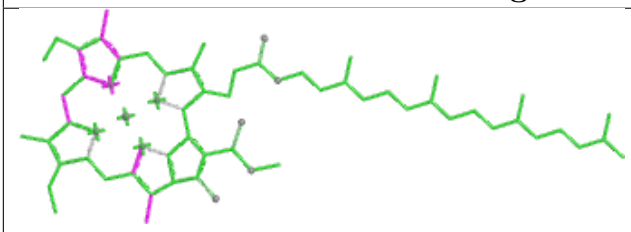


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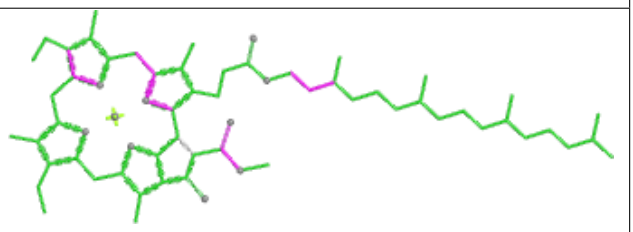


Rings

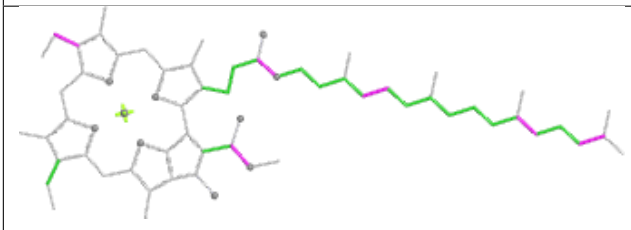
Ligand CLA AA 835



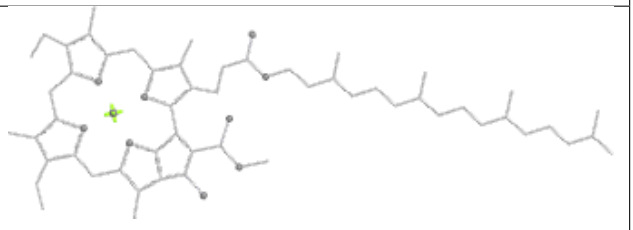
Bond lengths



Bond angles

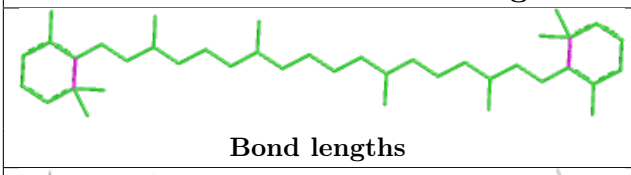


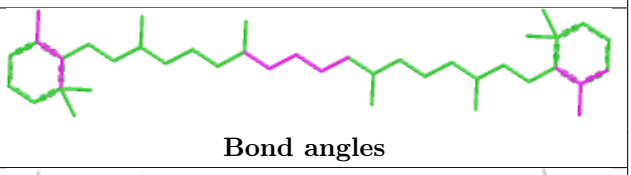
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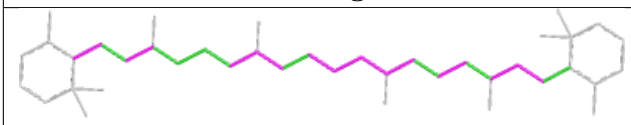


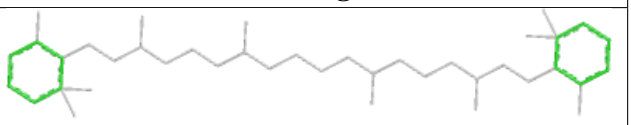
Rings

Ligand BCR BB 847

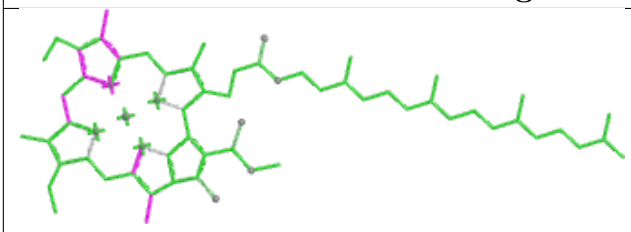

Bond lengths

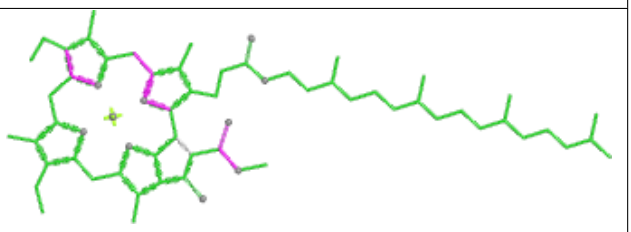

Bond angles

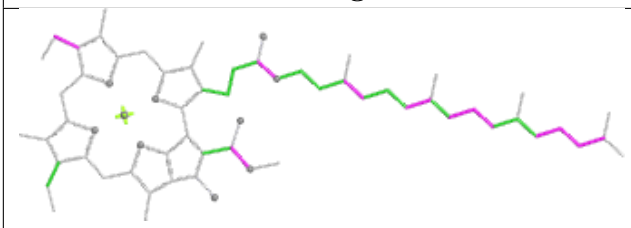

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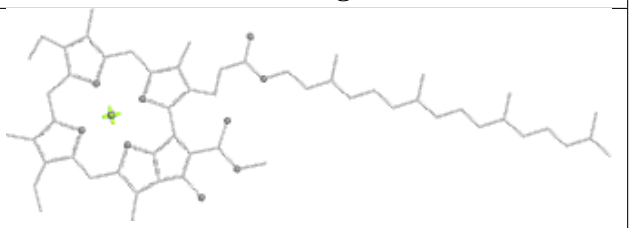

Rings

Ligand CLA B1 823

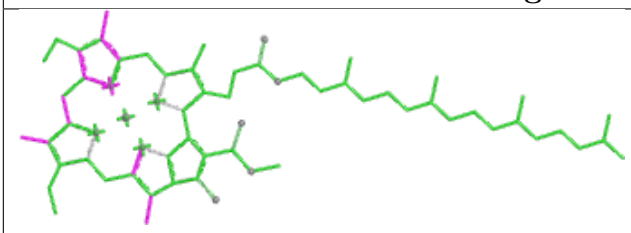

Bond lengths

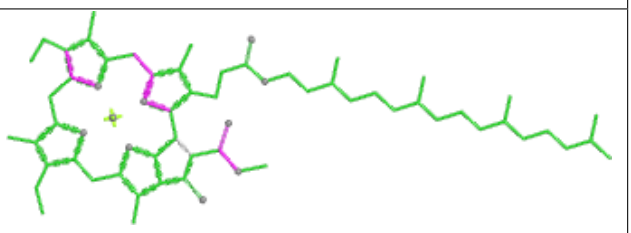

Bond angles

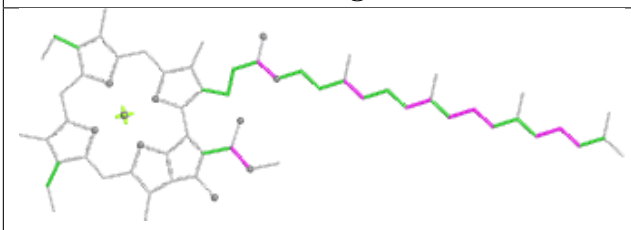

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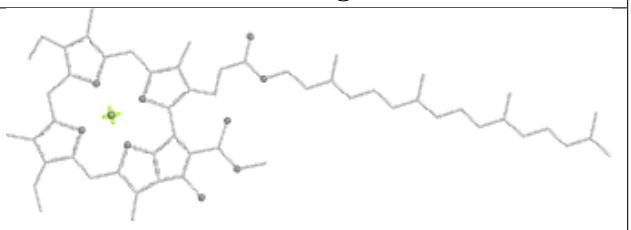

Rings

Ligand CLA B 823

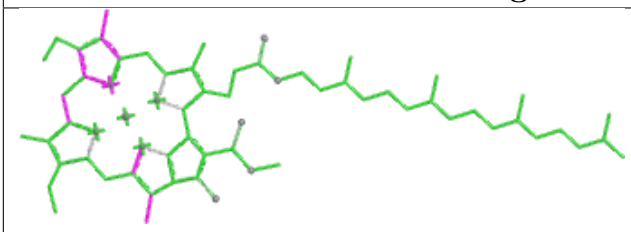

Bond lengths


Bond angles

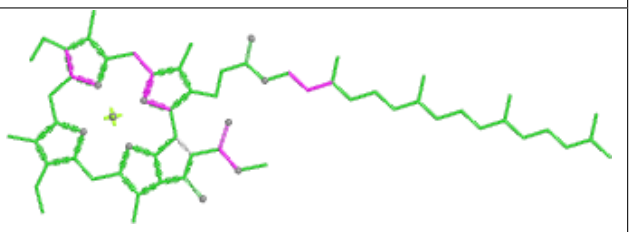

Torsions


Rings

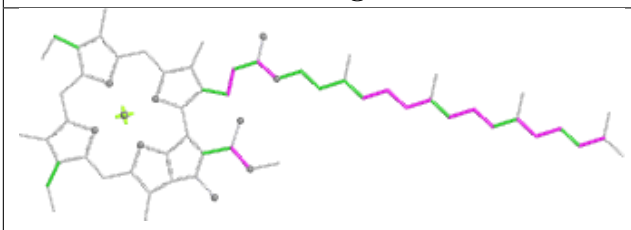
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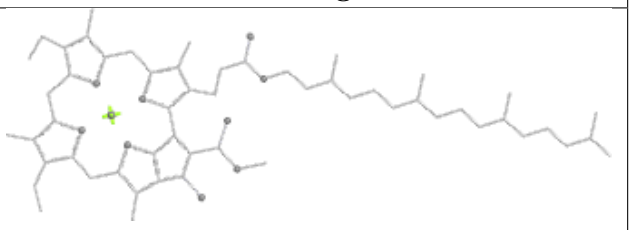
Bond lengths



Bond angles

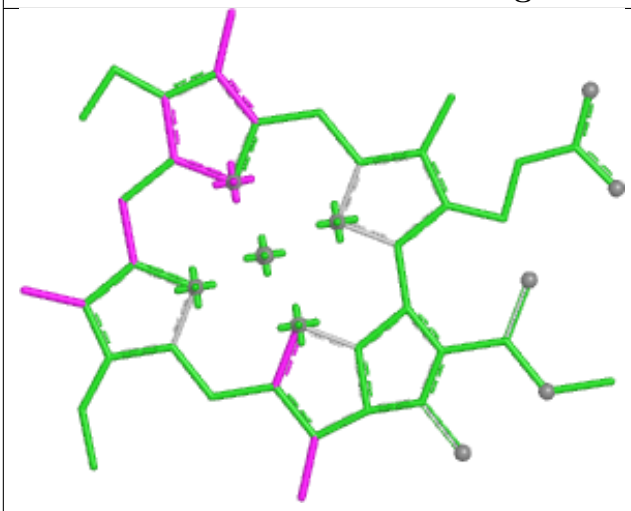


Torsions

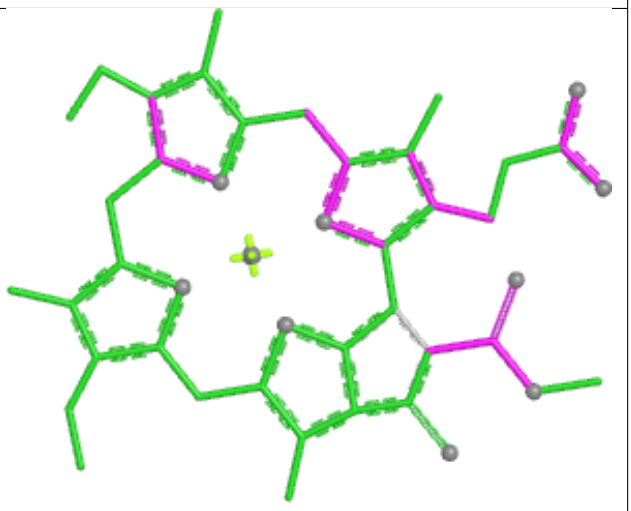


Rings

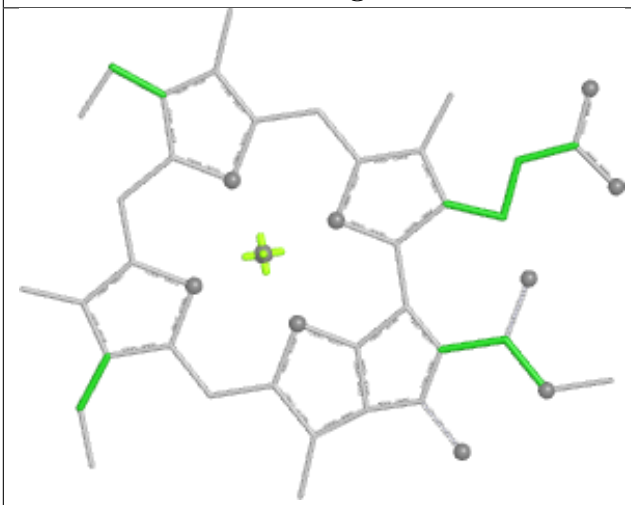
Ligand CLA K2 102



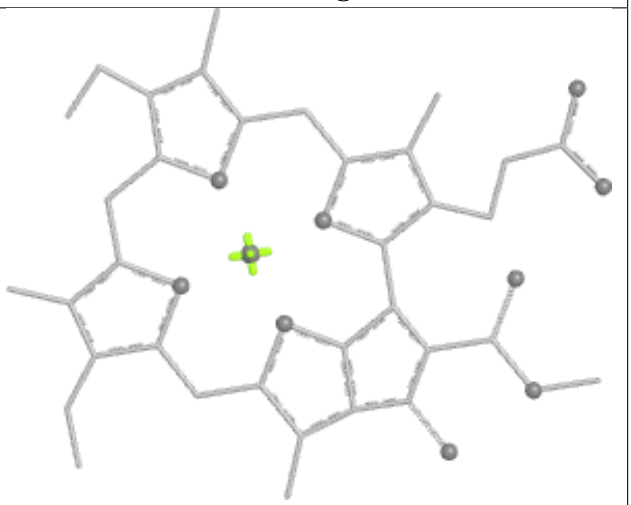
Bond lengths



Bond angles

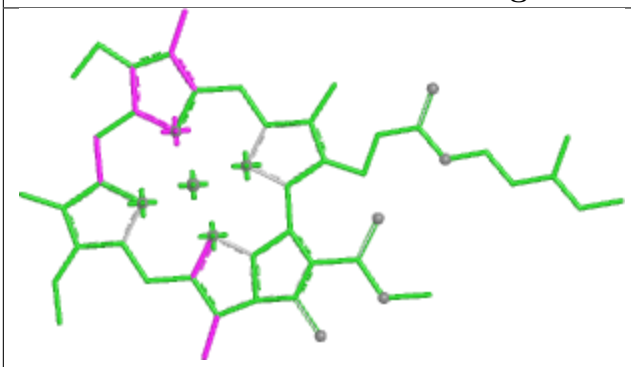


Torsions

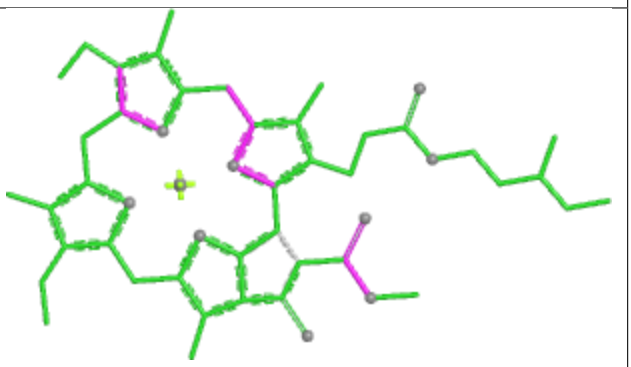


Rings

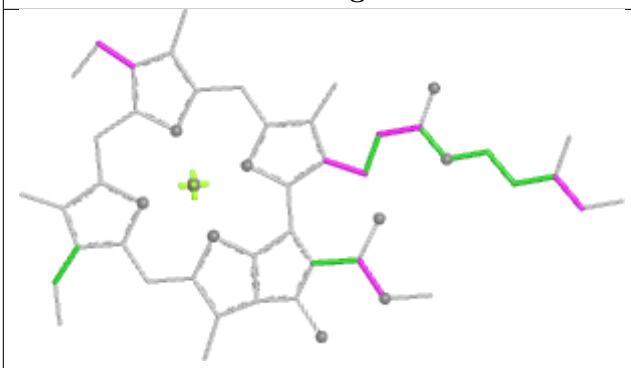
Ligand CLA AA 822



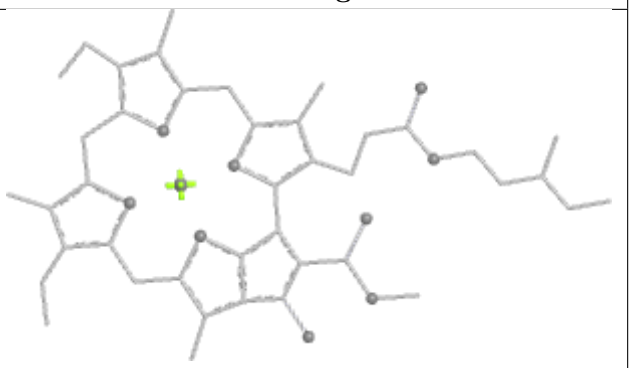
Bond lengths



Bond angles

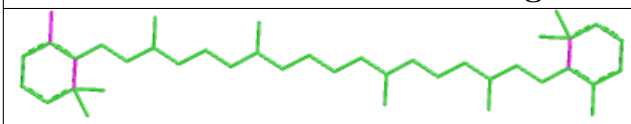


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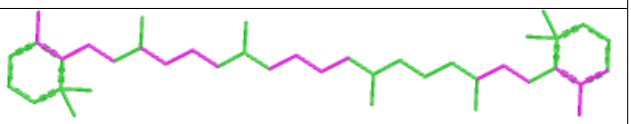


Rings

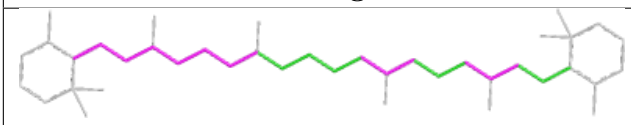
Ligand BCR L 206



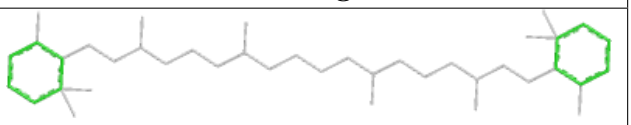
Bond lengths



Bond angles

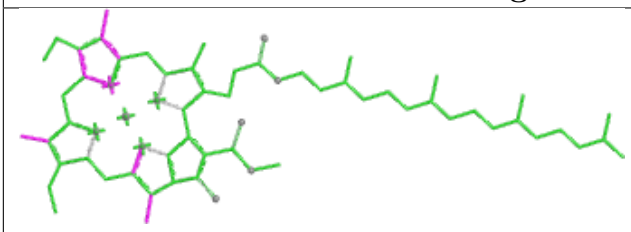


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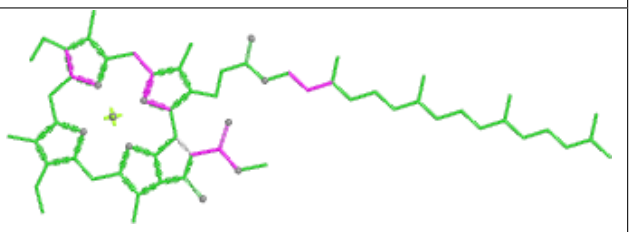


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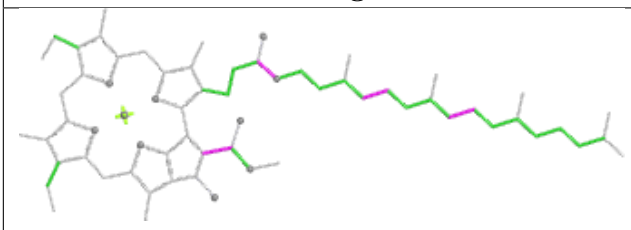
Ligand CLA AA 832



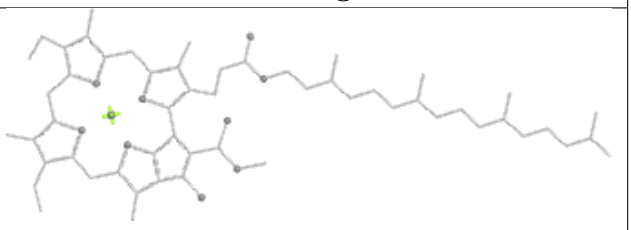
Bond lengths



Bond angles



Torsions

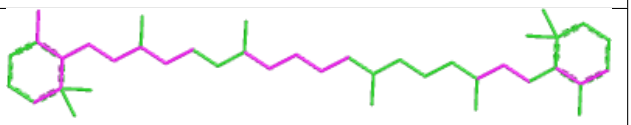


Rings

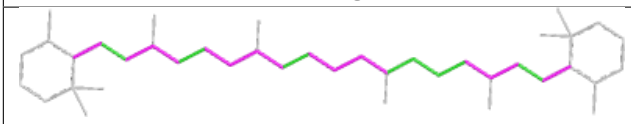
Ligand BCR L 205



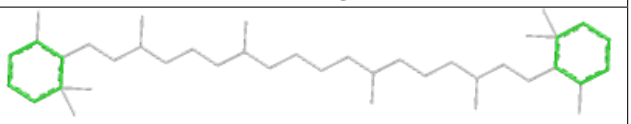
Bond lengths



Bond angles

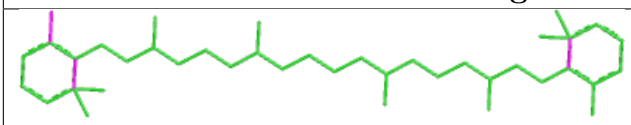


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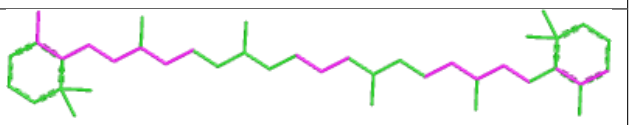


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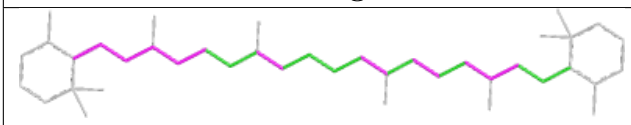
Ligand BCR BB 838



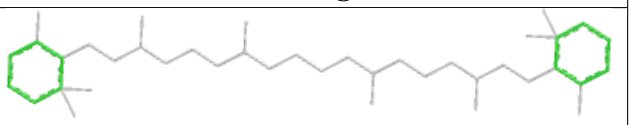
Bond lengths



Bond angles

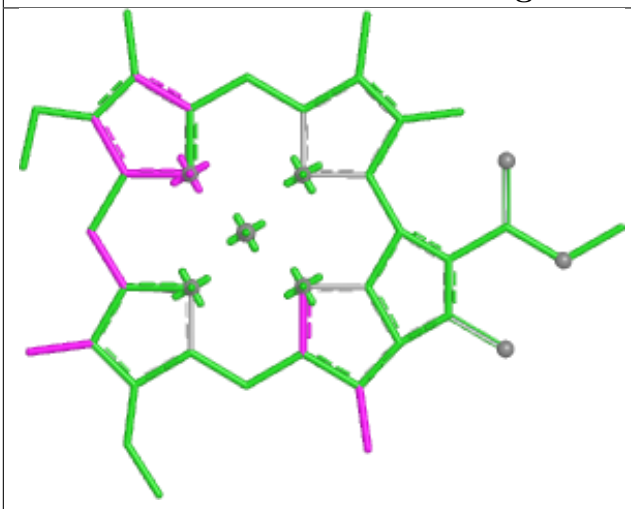


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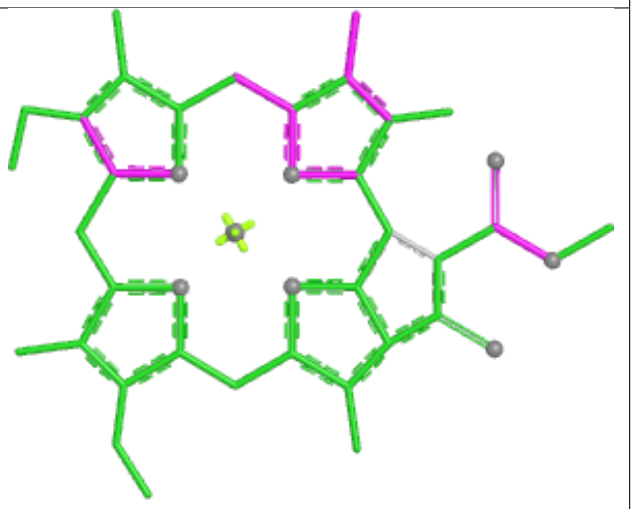


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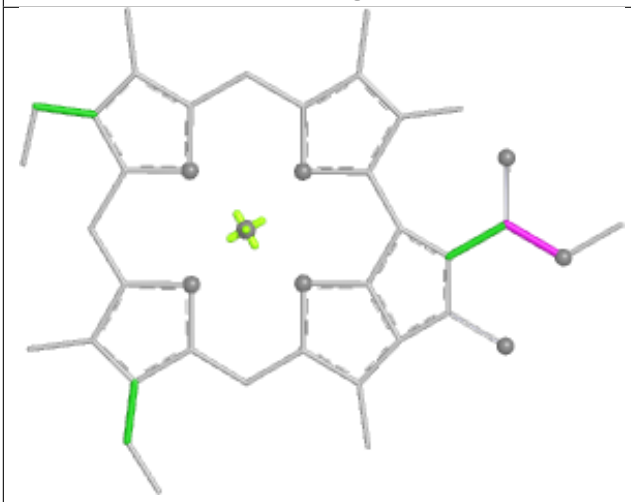
Ligand CLA B2 819



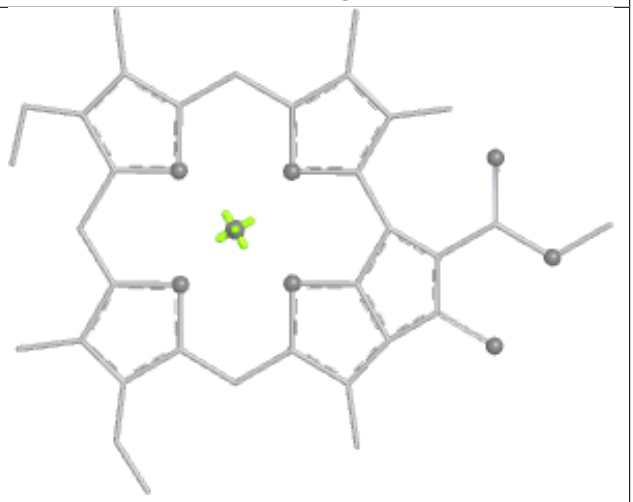
Bond lengths



Bond angles

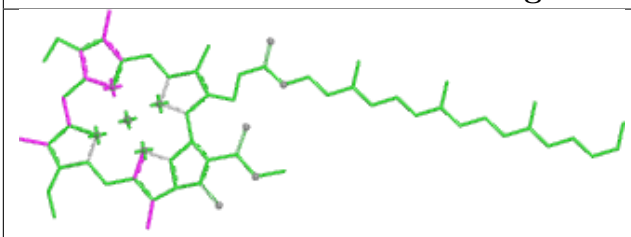


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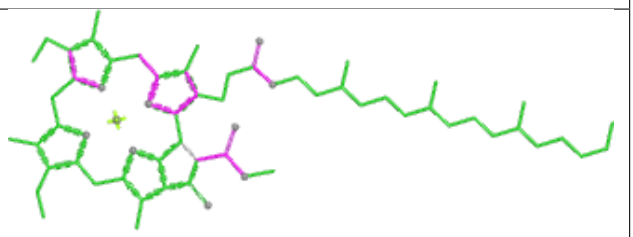


Rings

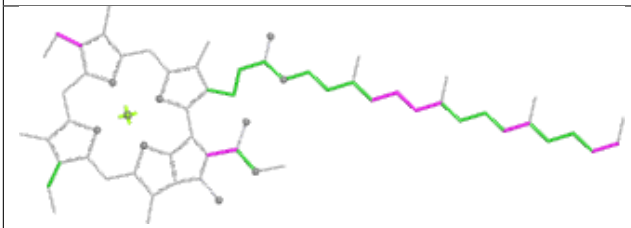
Ligand CLA B 805



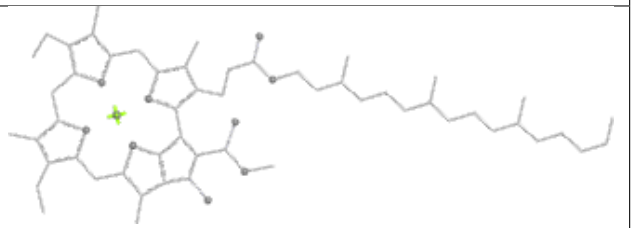
Bond lengths



Bond angles

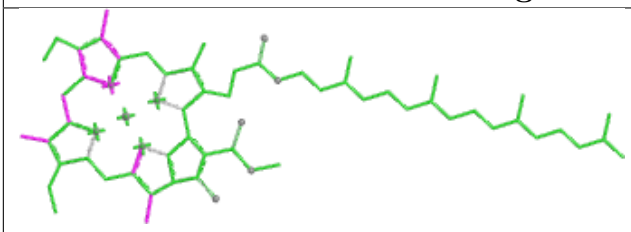


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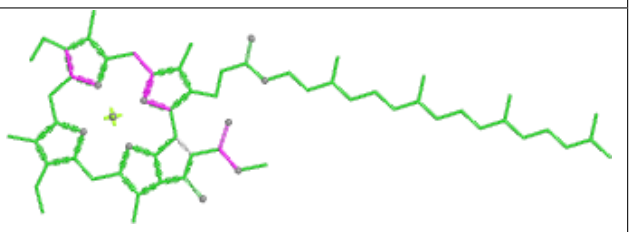


Rings

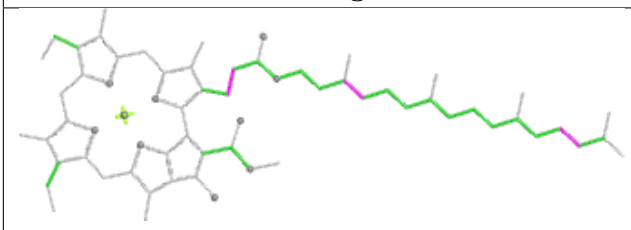
Ligand CLA B1 849



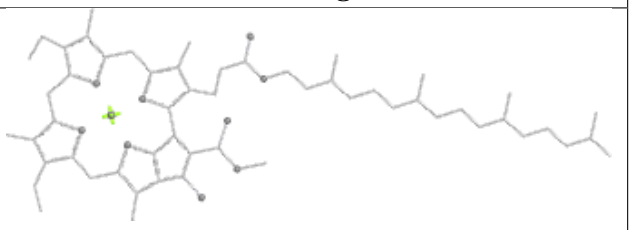
Bond lengths



Bond angles

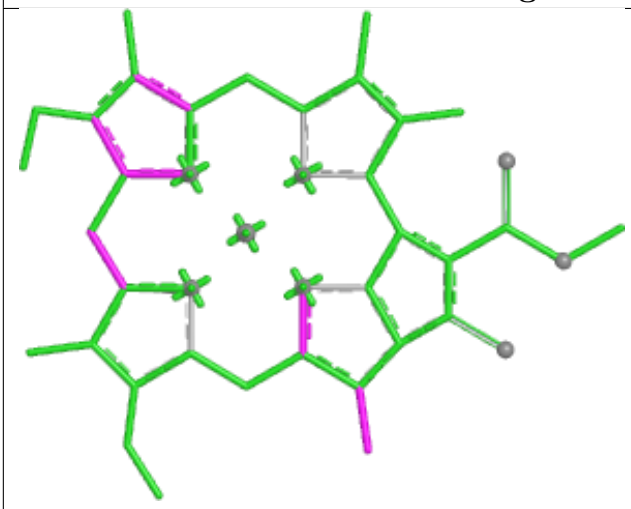


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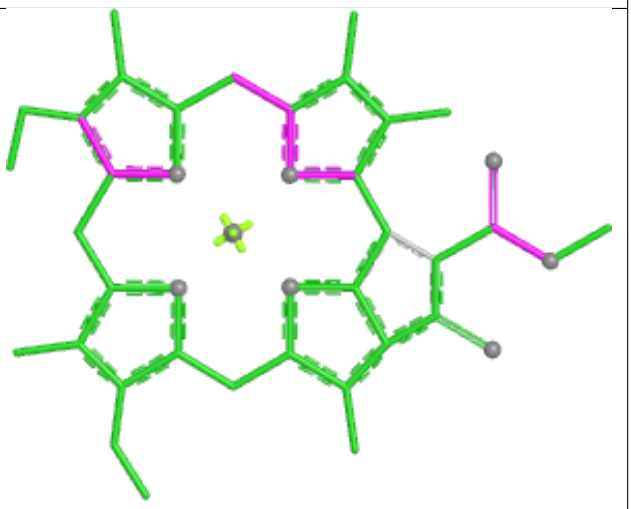


Rings

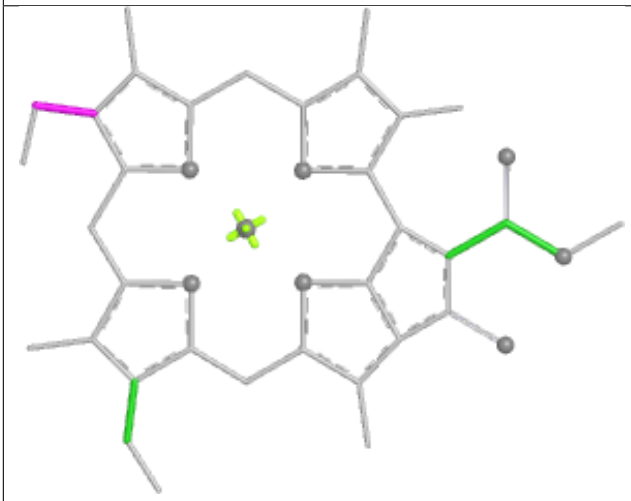
Ligand CLA J1 103



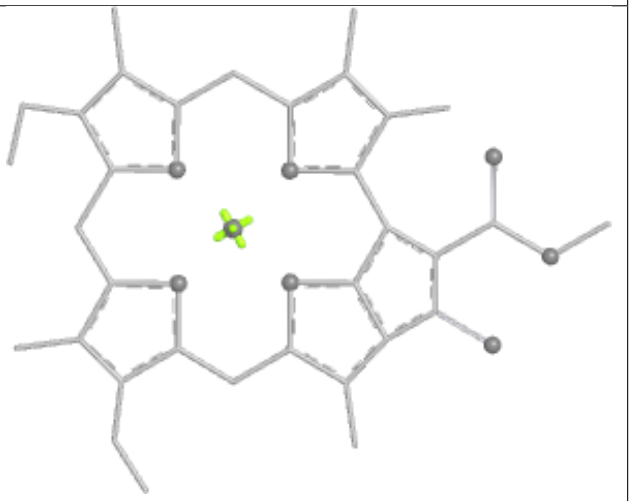
Bond lengths



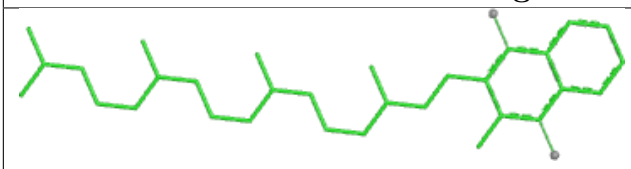
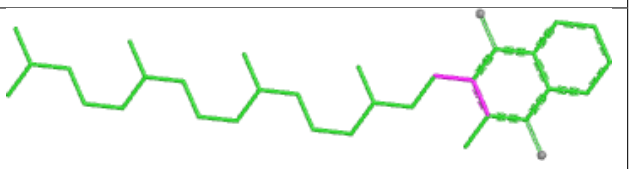
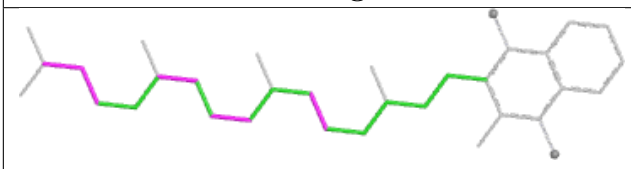
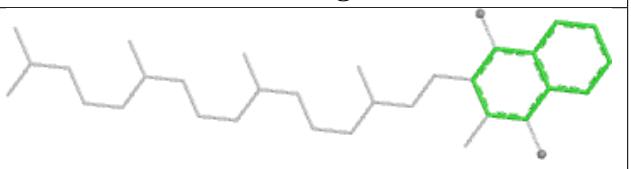
Bond angles

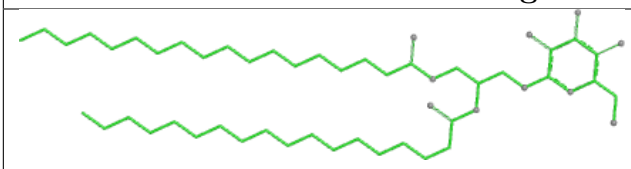
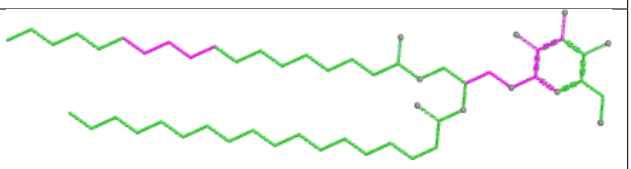
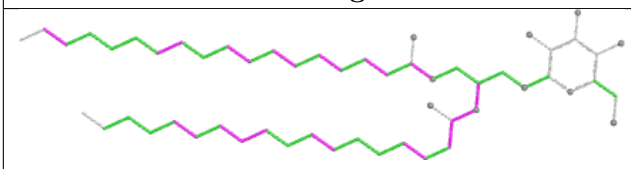
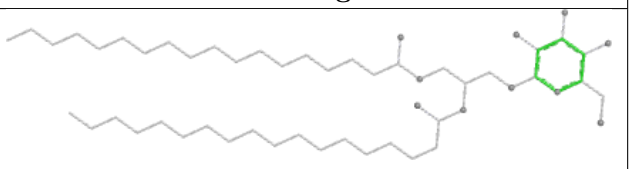


Torsions

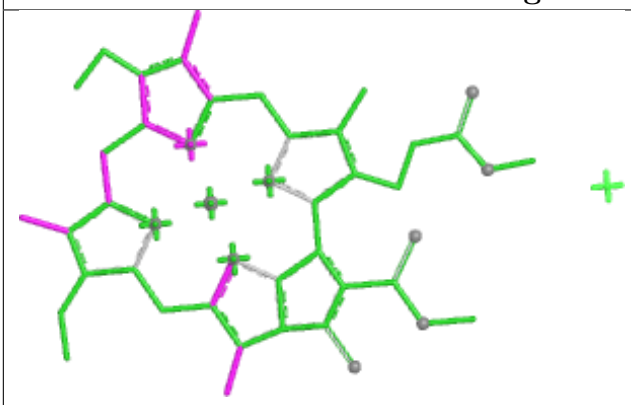


Rings

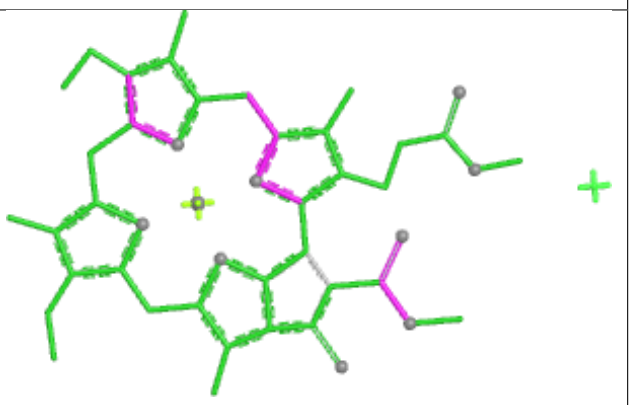
Ligand PQN B1 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

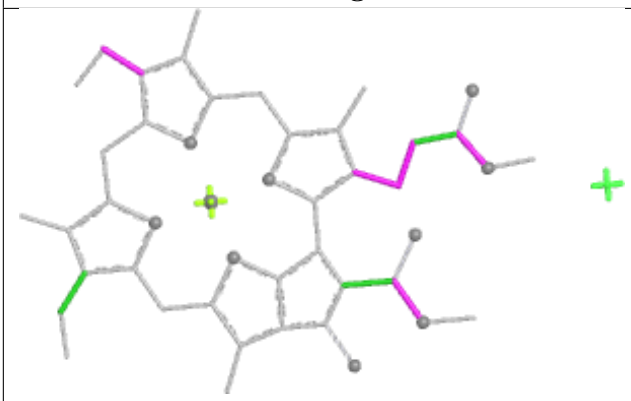
Ligand CLA A 812



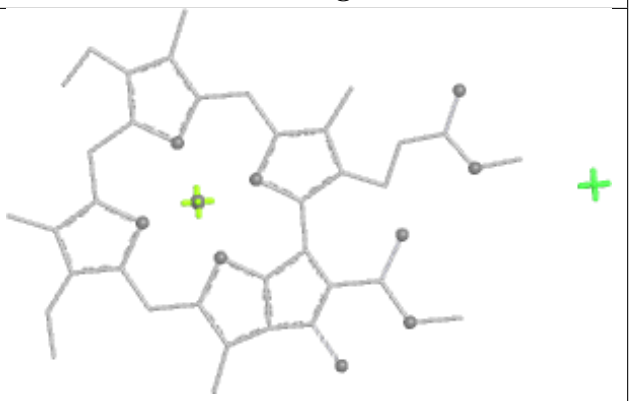
Bond lengths



Bond angles



Torsions

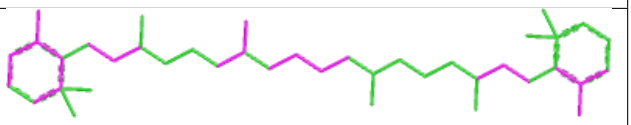


Rings

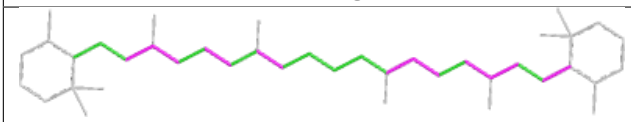
Ligand BCR AA 850



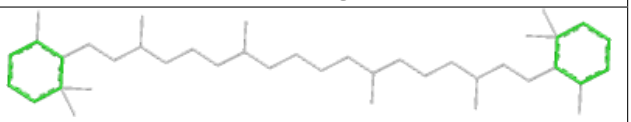
Bond lengths



Bond angles

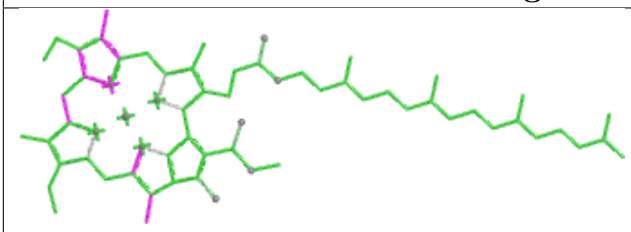


Torsions

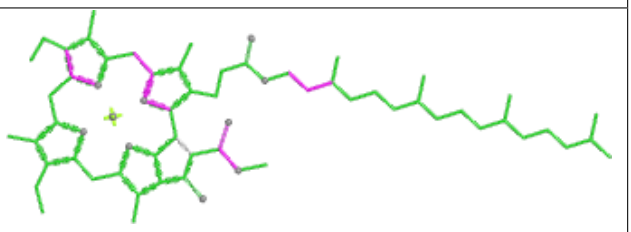


Rings

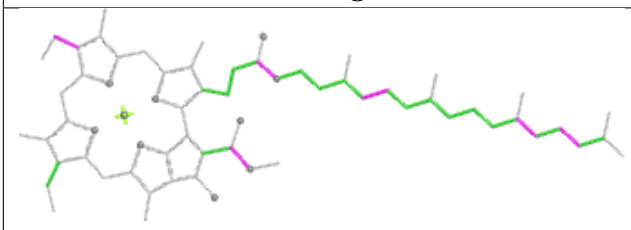
Ligand CLA A 835



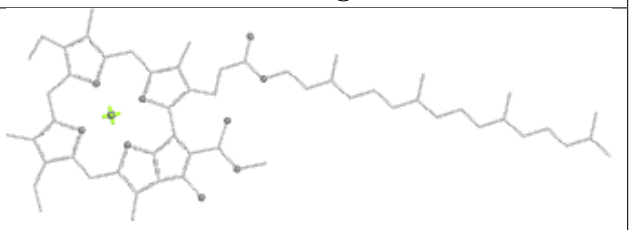
Bond lengths



Bond angles



Torsions

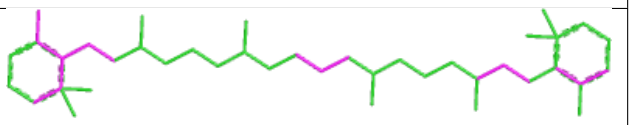


Rings

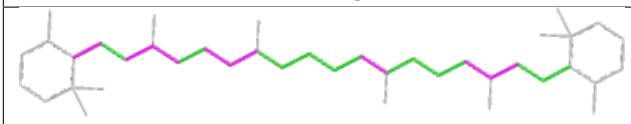
Ligand BCR A1 850



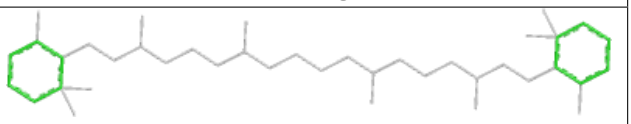
Bond lengths



Bond angles

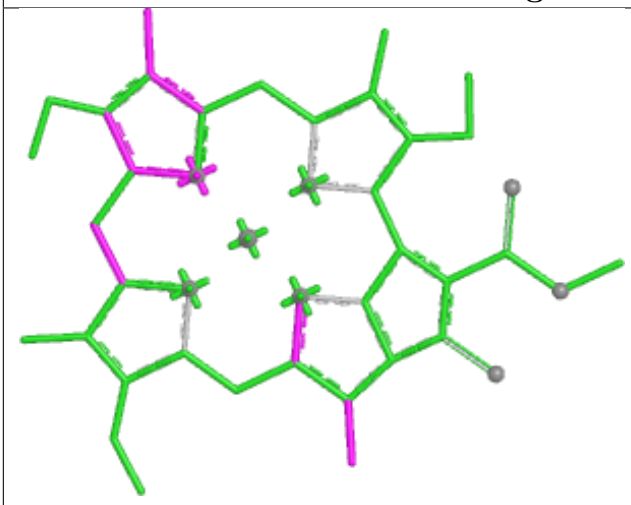


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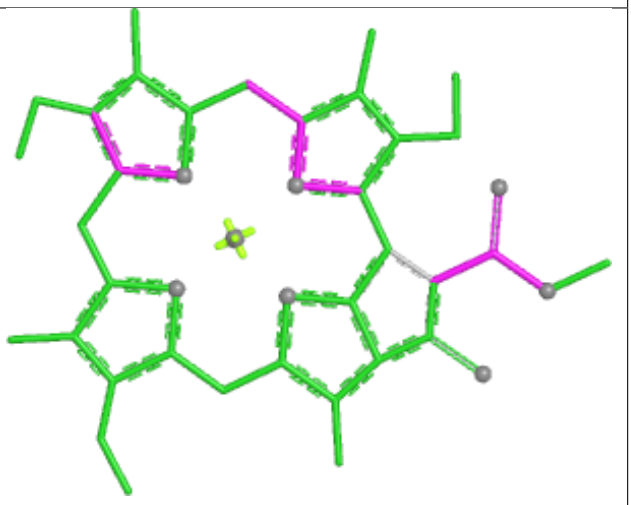


Rings

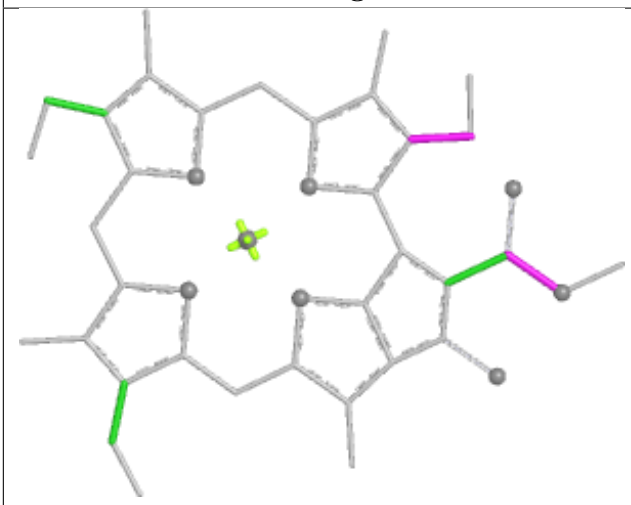
Ligand CLA F 302



Bond lengths



Bond angles

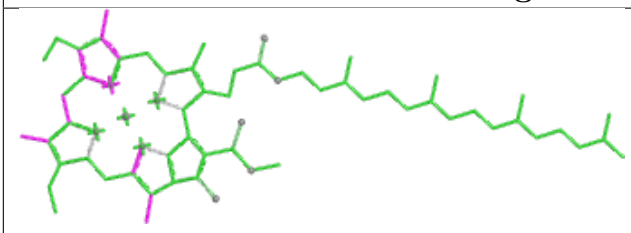


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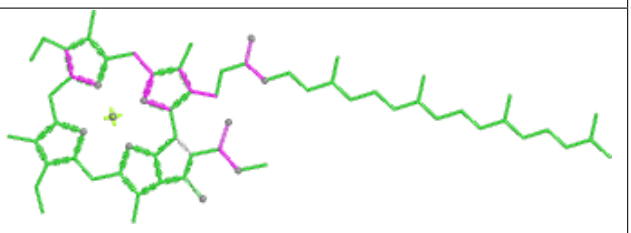


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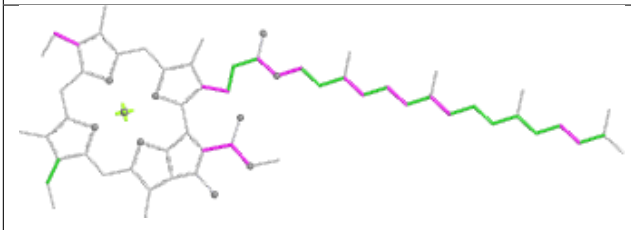
Ligand CLA A1 826



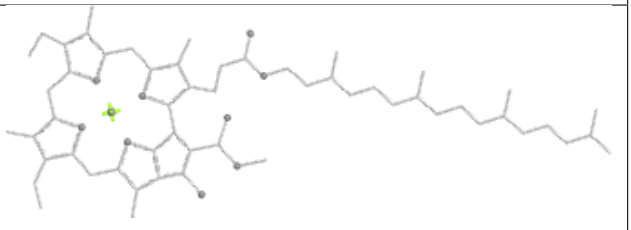
Bond lengths



Bond angles

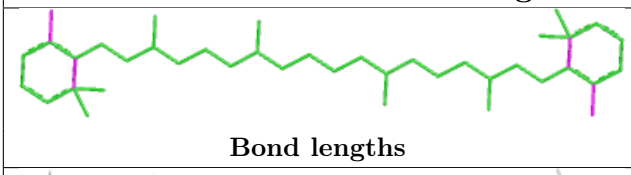


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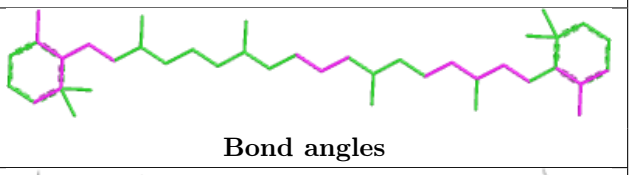


Rings

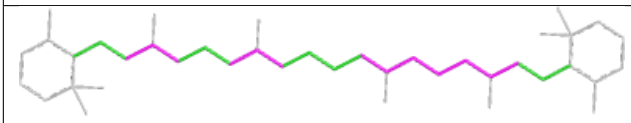
Ligand BCR F1 304



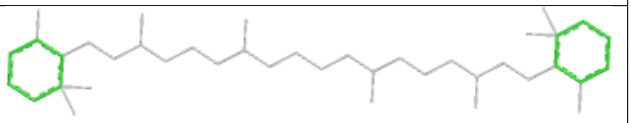
Bond lengths



Bond angles



Torsions

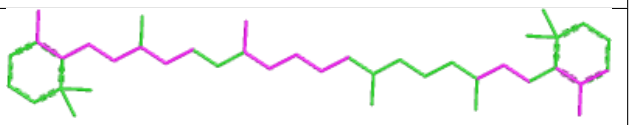


Rings

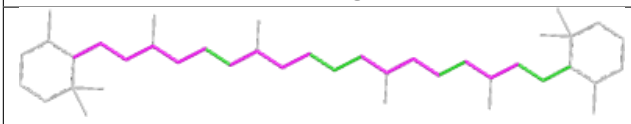
Ligand BCR B1 838



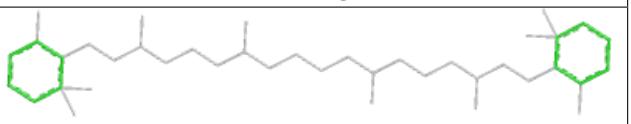
Bond lengths



Bond angles

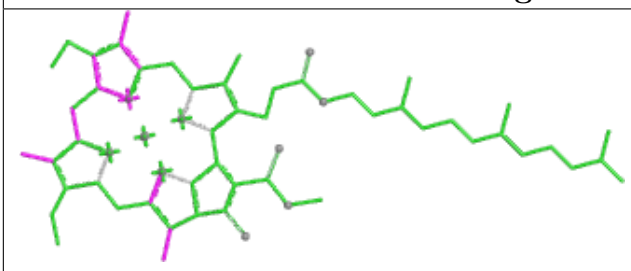


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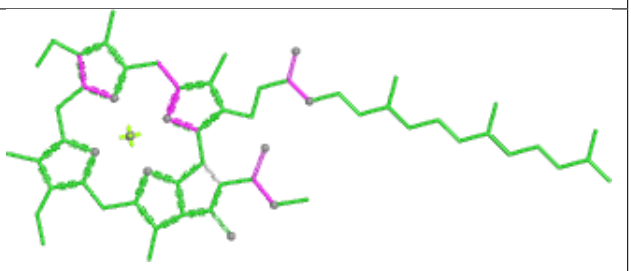


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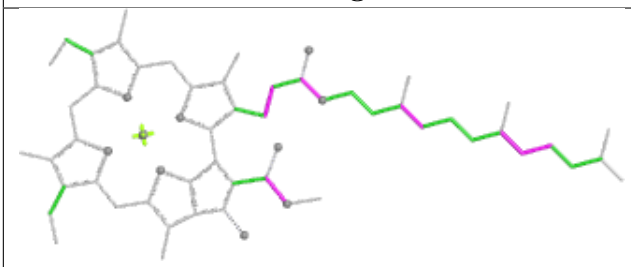
Ligand CLA A1 818



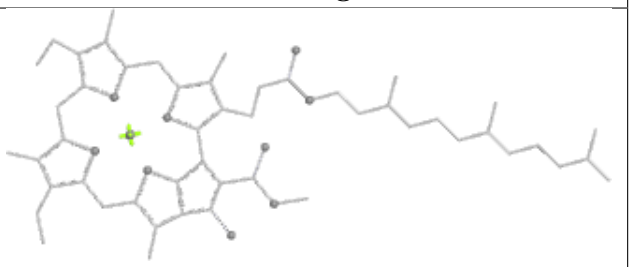
Bond lengths



Bond angles

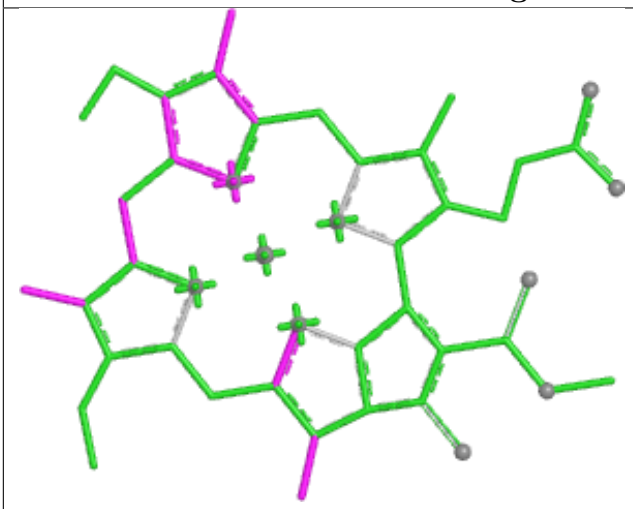


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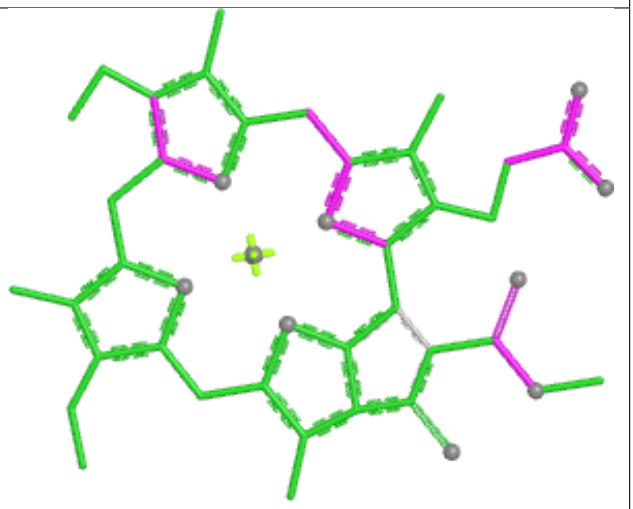


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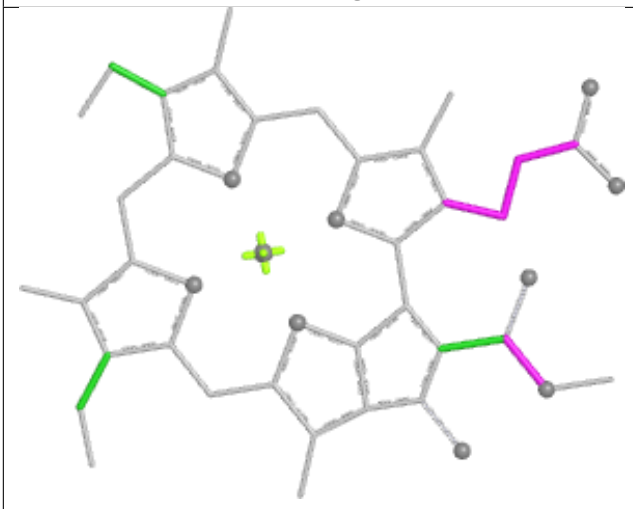
Ligand CLA AA 826



Bond lengths



Bond angles

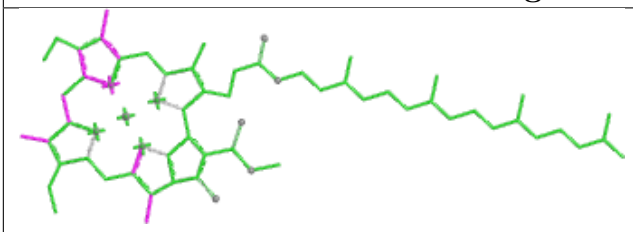


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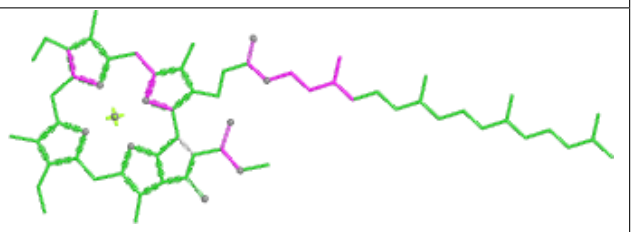


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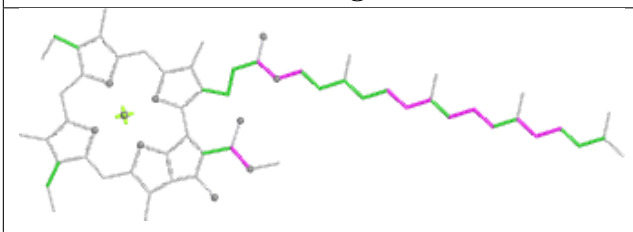
Ligand CLA B 806



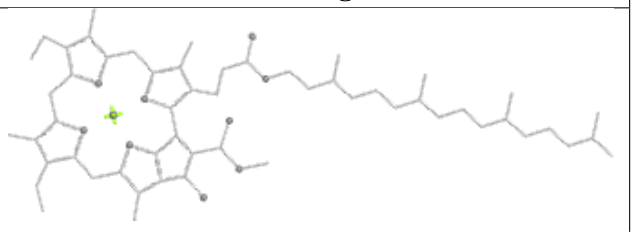
Bond lengths



Bond angles

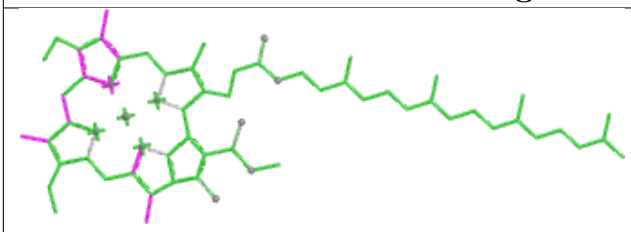


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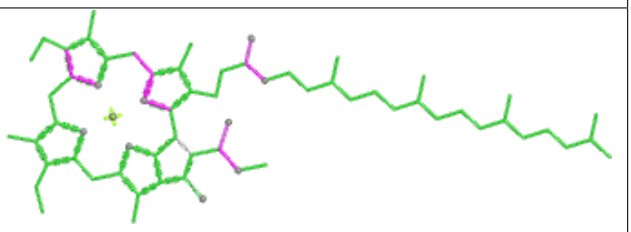


Rings

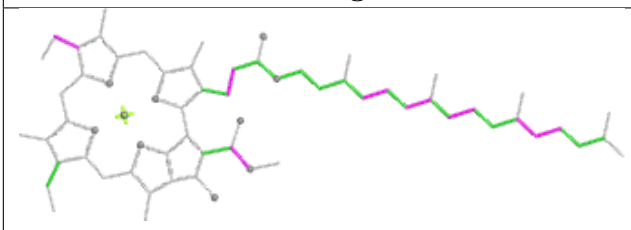
Ligand CLA B1 835



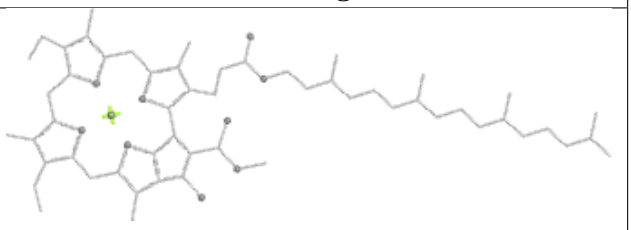
Bond lengths



Bond angles

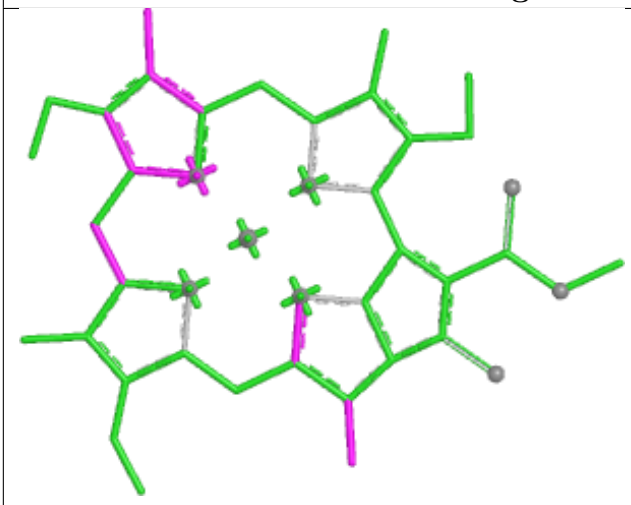


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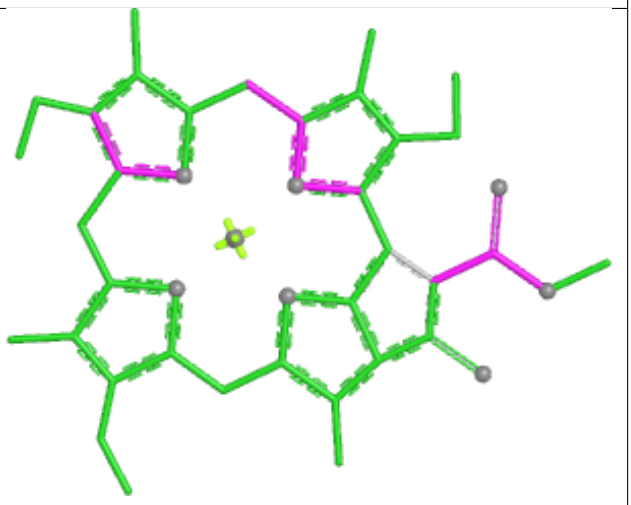


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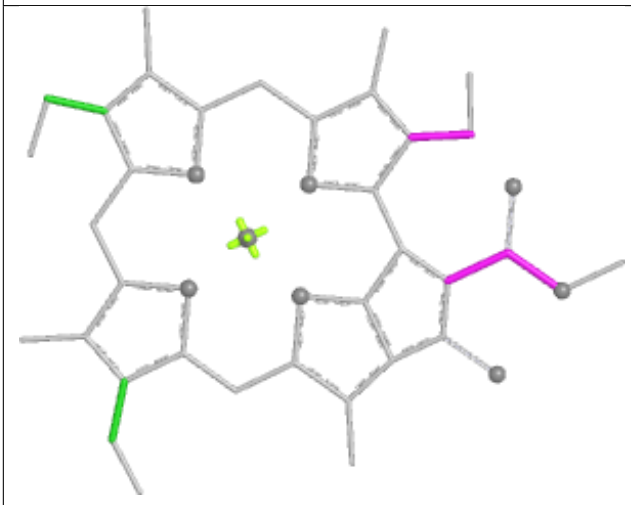
Ligand CLA BB 813



Bond lengths



Bond angles

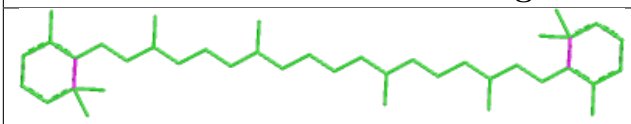


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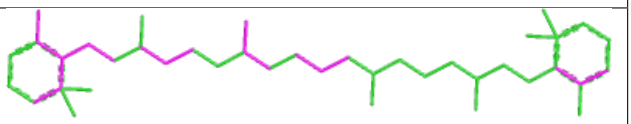


Rings

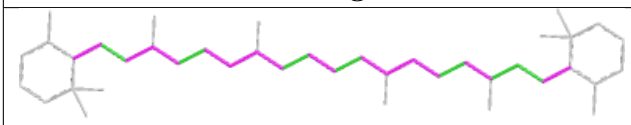
Ligand BCR F1 303



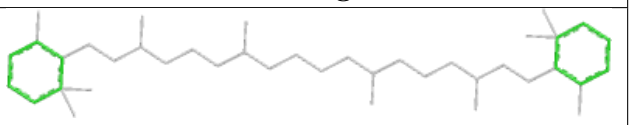
Bond lengths



Bond angles

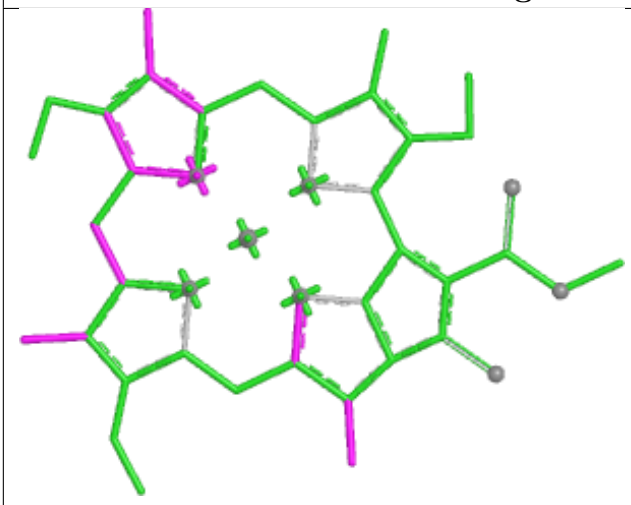


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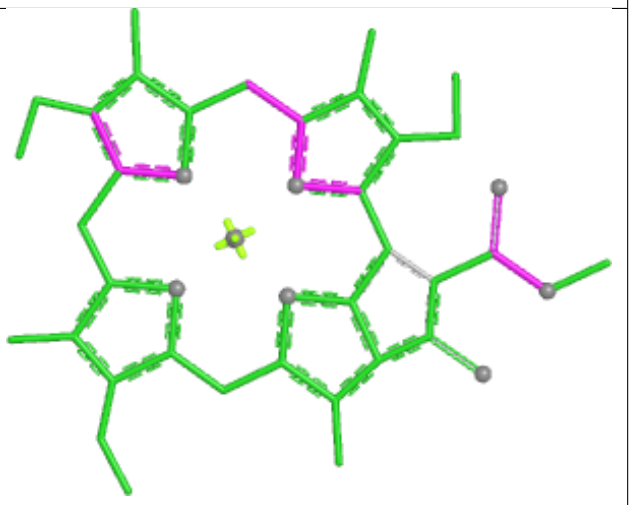


Rings

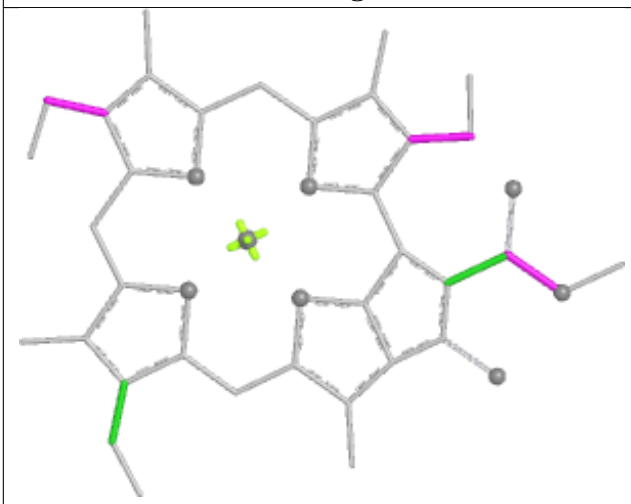
Ligand CLA A1 813



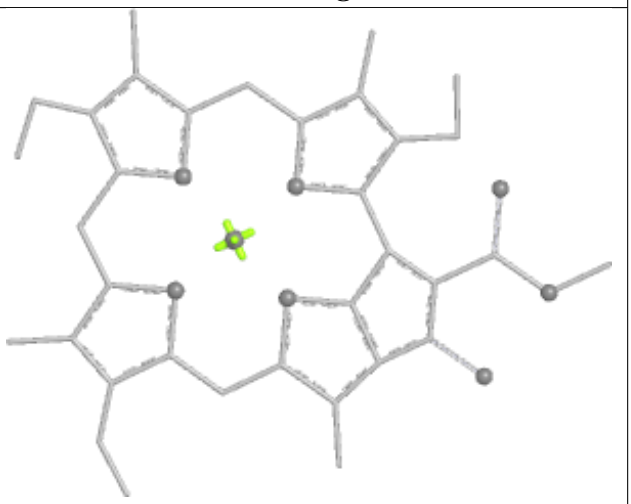
Bond lengths



Bond angles

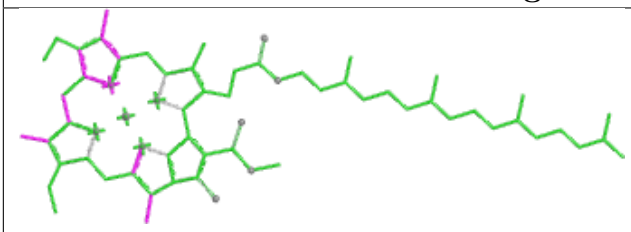


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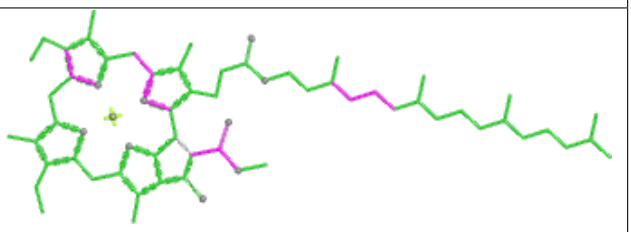


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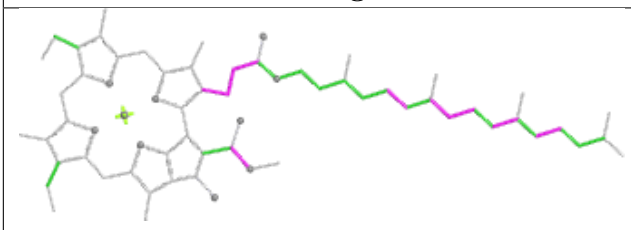
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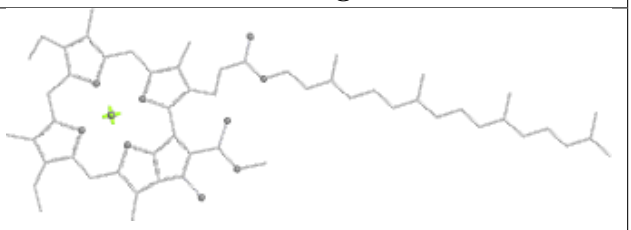
Bond lengths



Bond angles

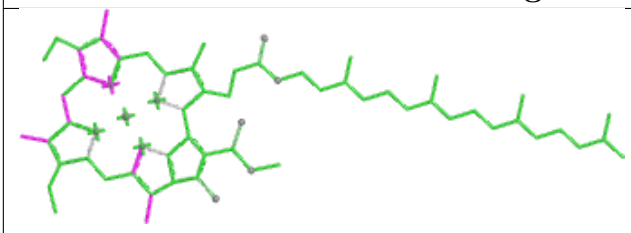


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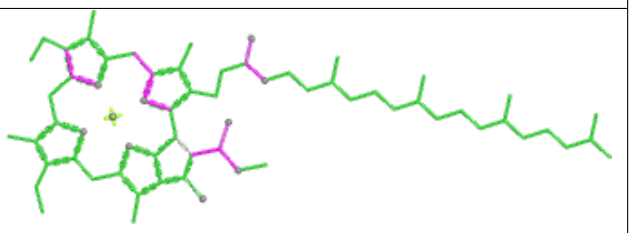


Rings

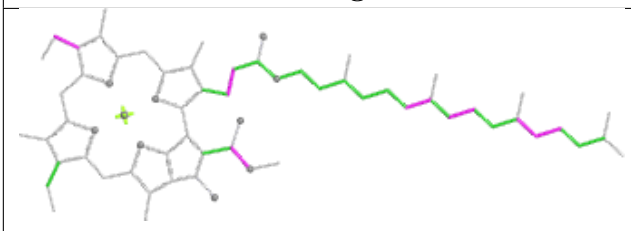
Ligand CLA B 836



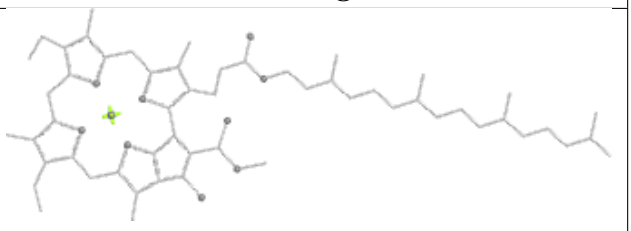
Bond lengths



Bond angles

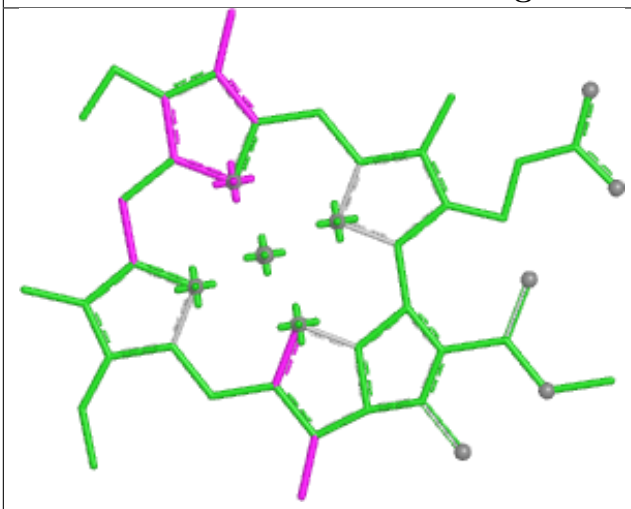


Torsions

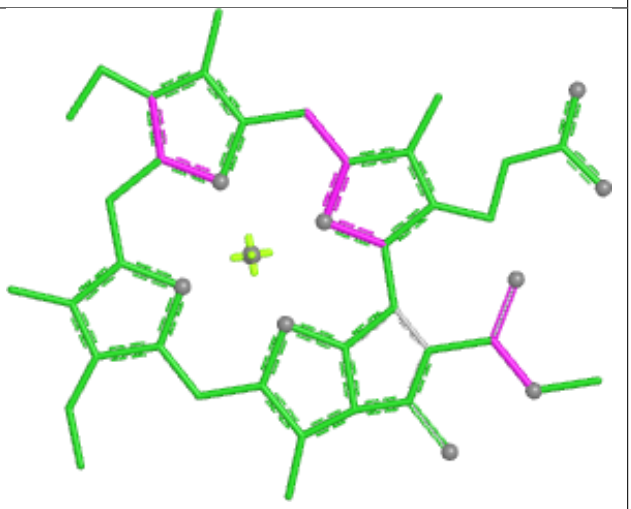


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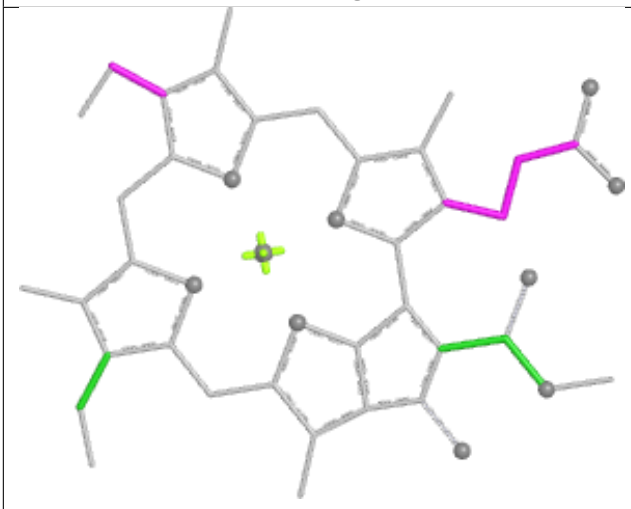
Ligand CLA X1 101



Bond lengths



Bond angles

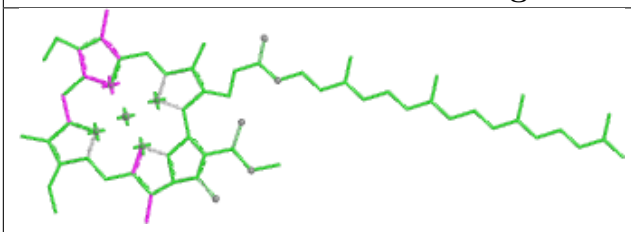


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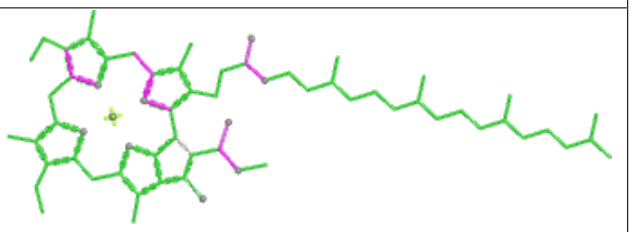


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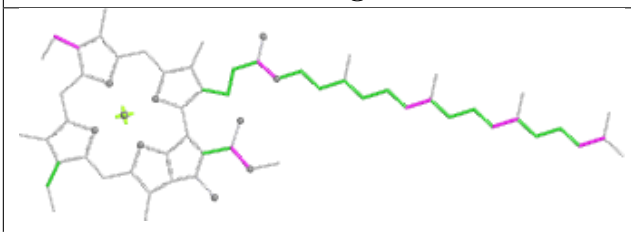
Ligand CLA AA 813



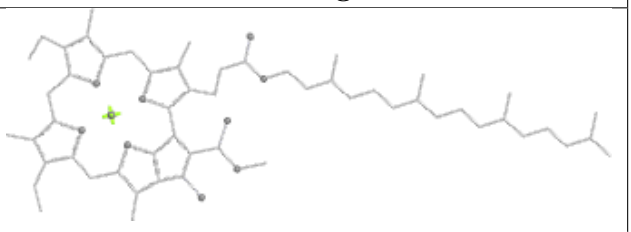
Bond lengths



Bond angles

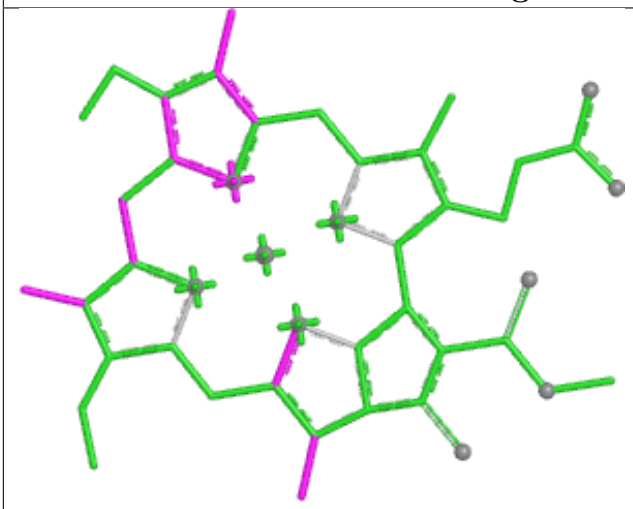


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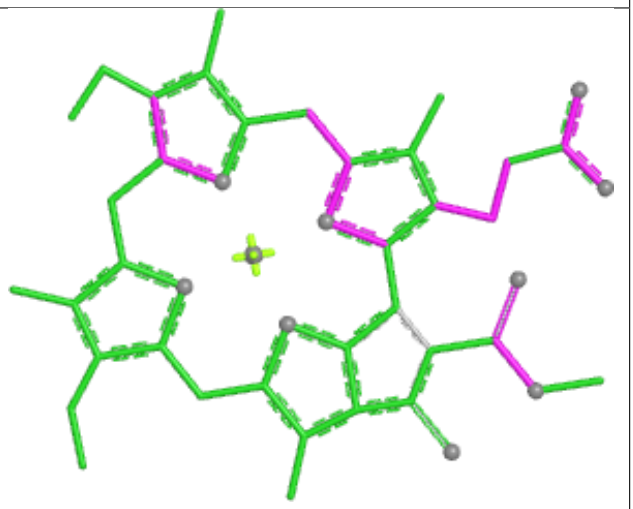


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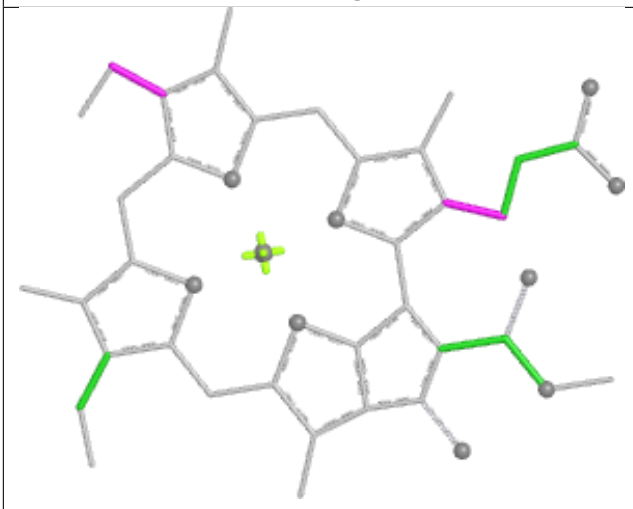
Ligand CLA BB 827



Bond lengths



Bond angles

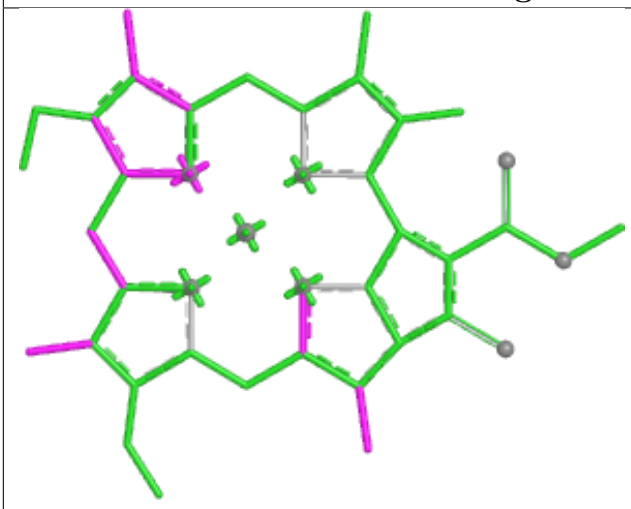


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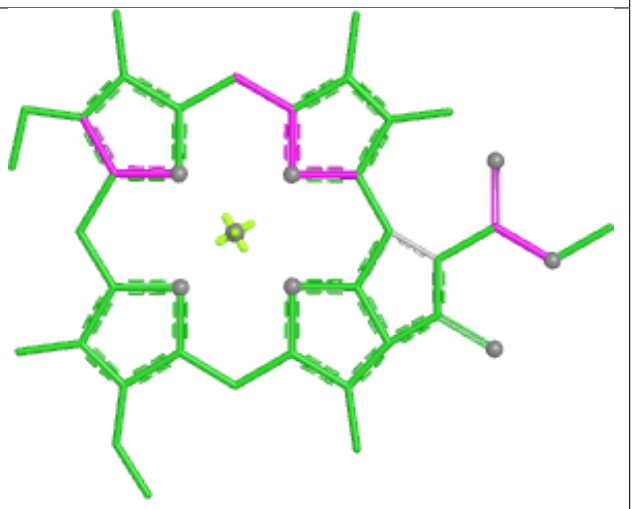


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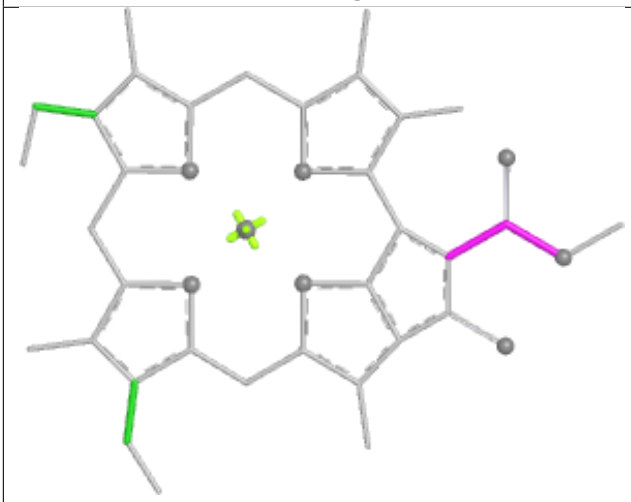
Ligand CLA A1 844



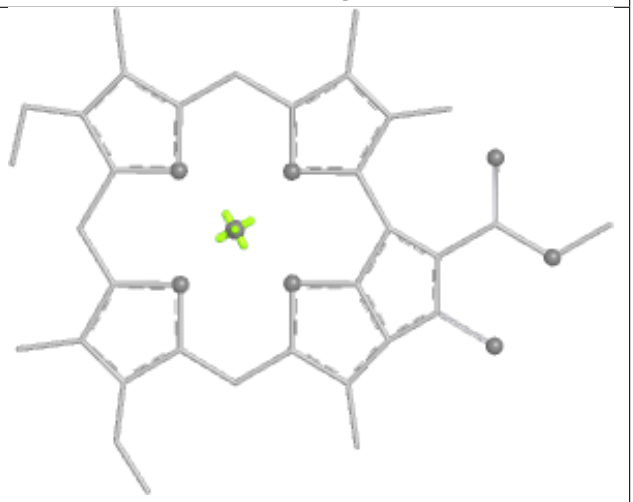
Bond lengths



Bond angles

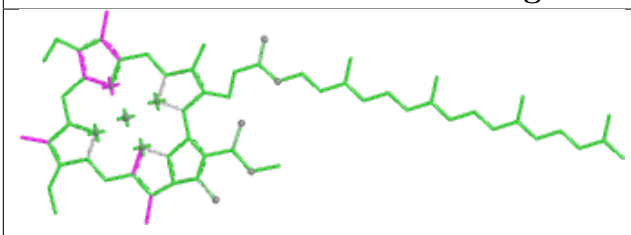


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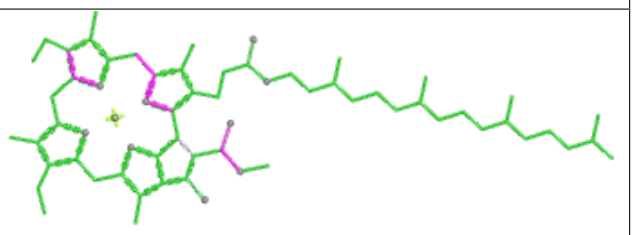


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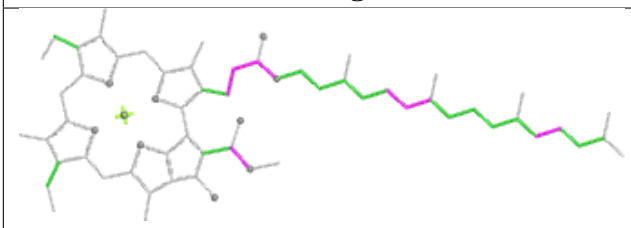
Ligand CLA A 831



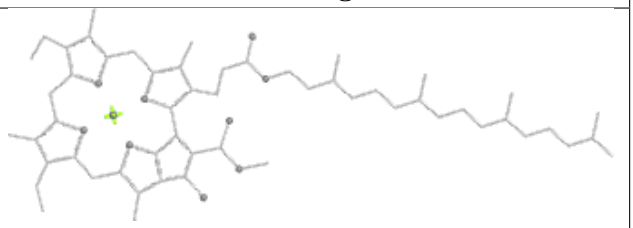
Bond lengths



Bond angles

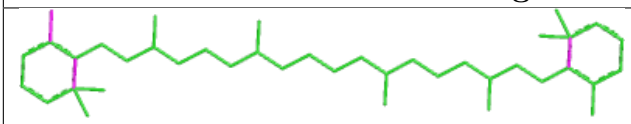


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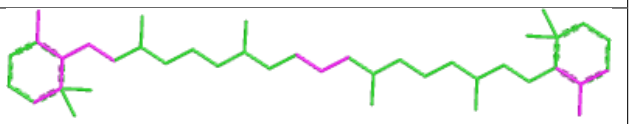


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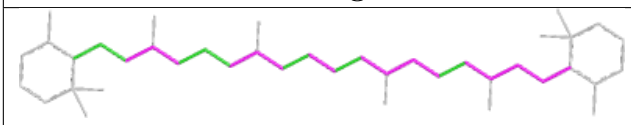
Ligand BCR K1 104



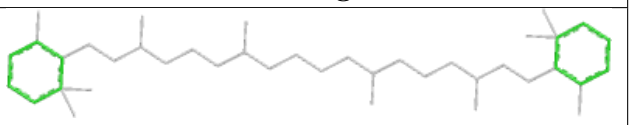
Bond lengths



Bond angles

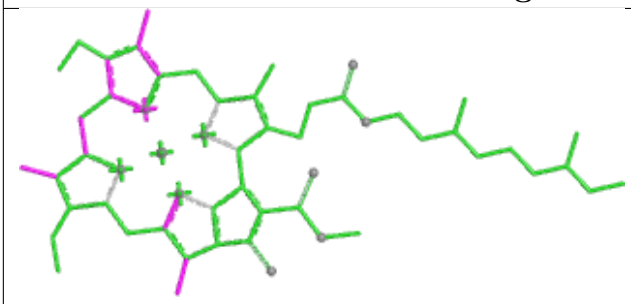


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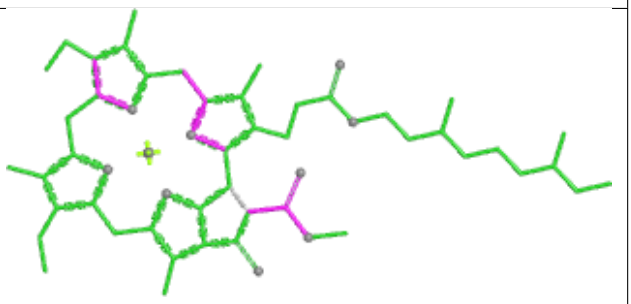


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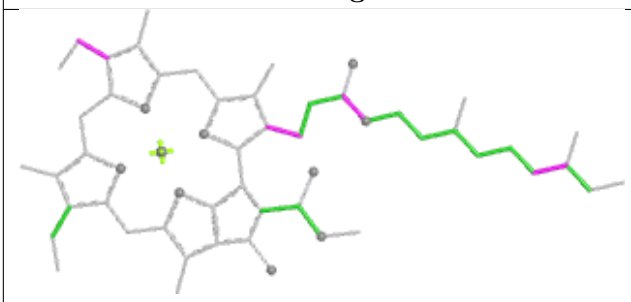
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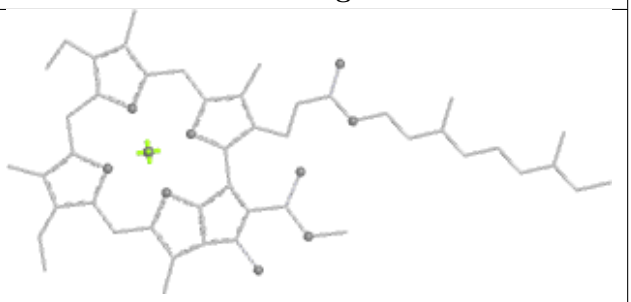
Bond lengths



Bond angles

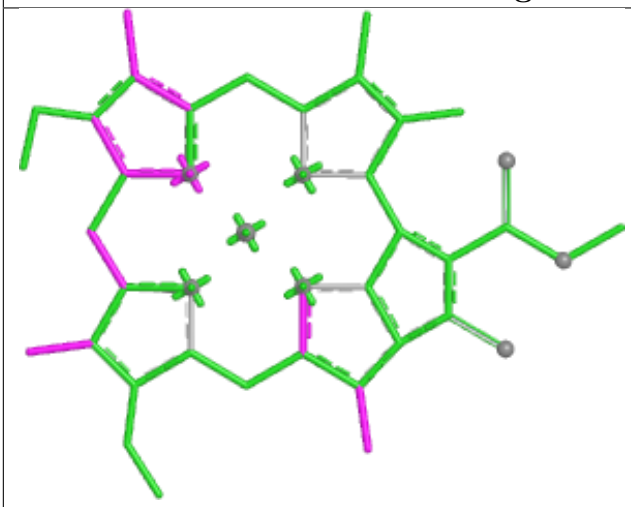


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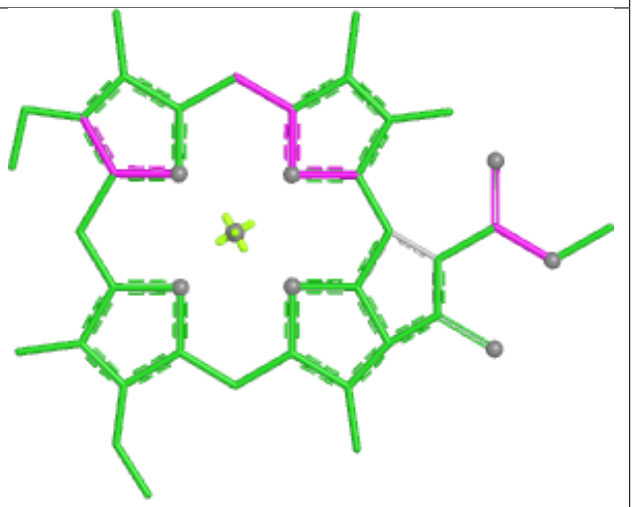


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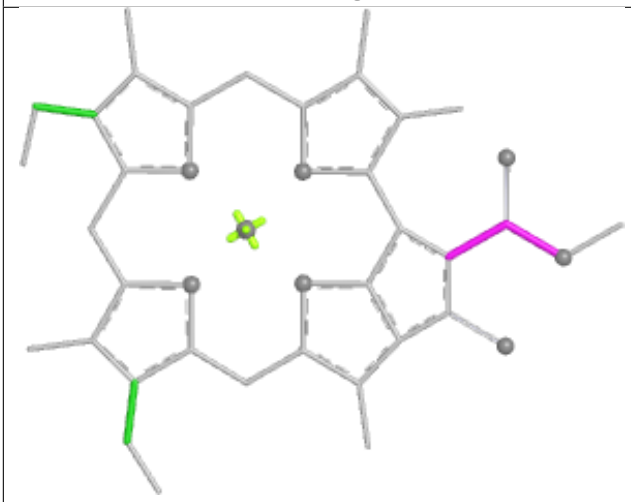
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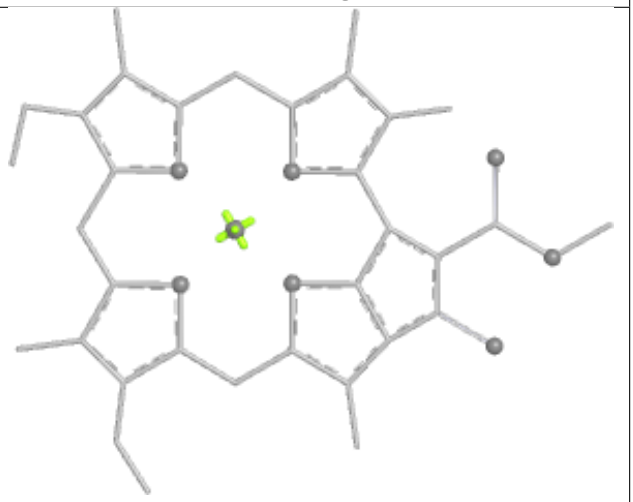
Bond lengths



Bond angles

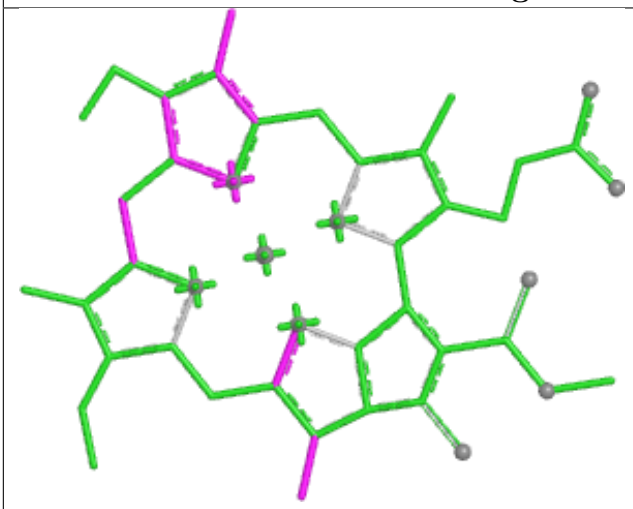


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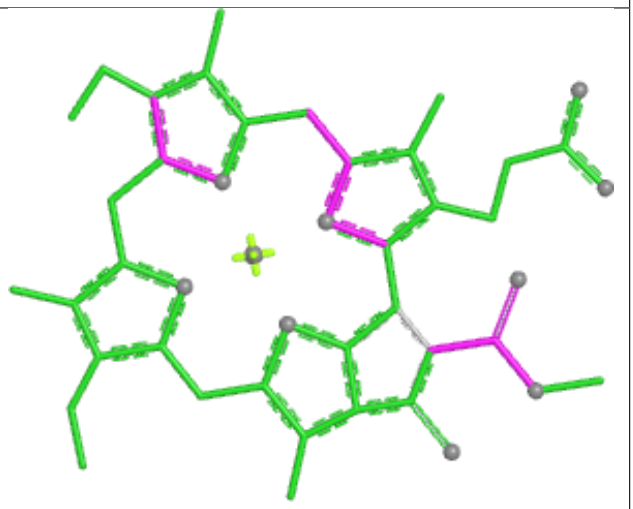


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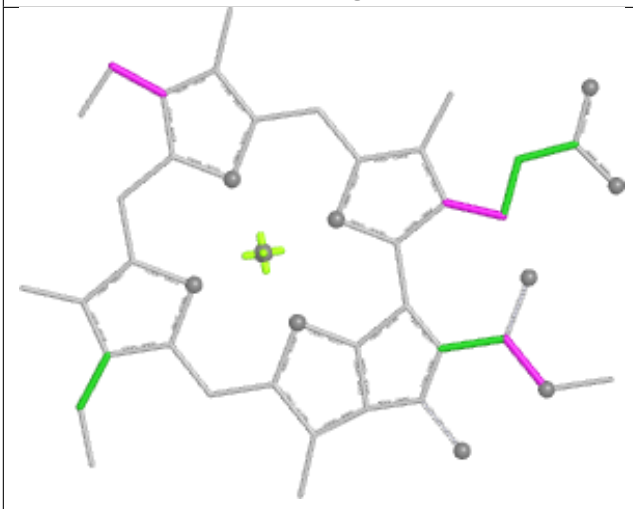
Ligand CLA BB 831



Bond lengths



Bond angles

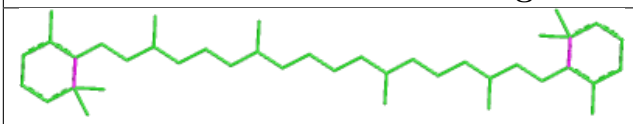


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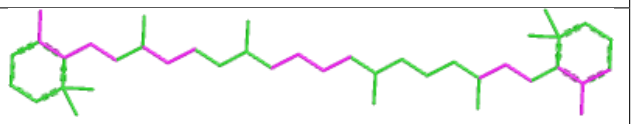


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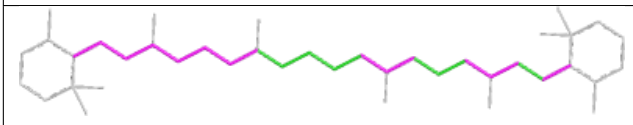
Ligand BCR L1 209



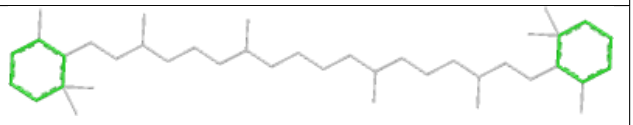
Bond lengths



Bond angles

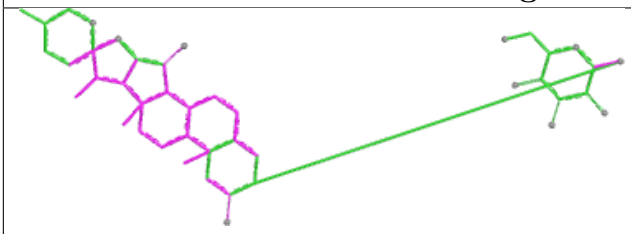


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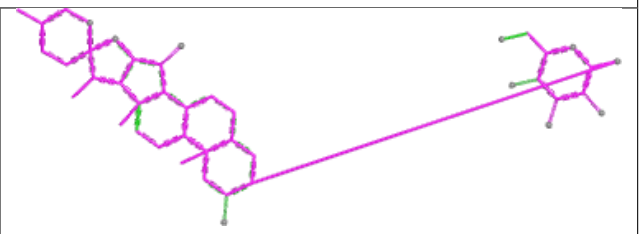


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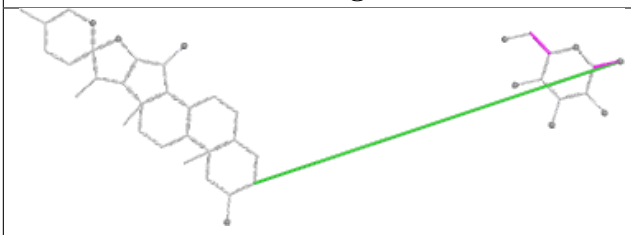
Ligand AJP L1 204



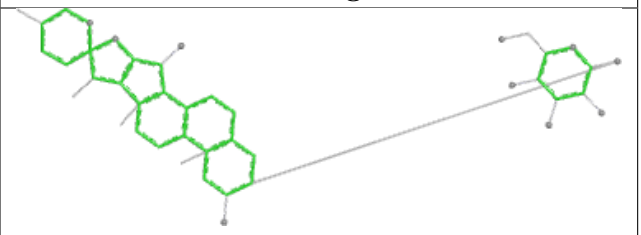
Bond lengths



Bond angles

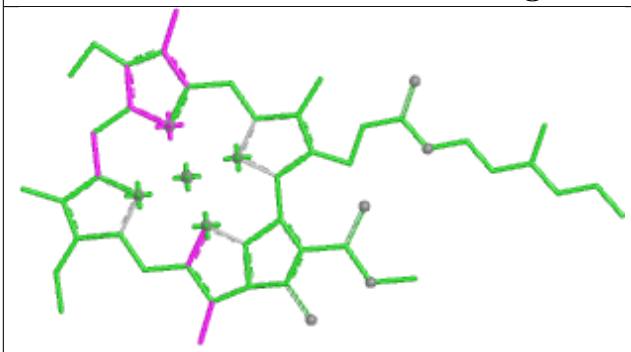


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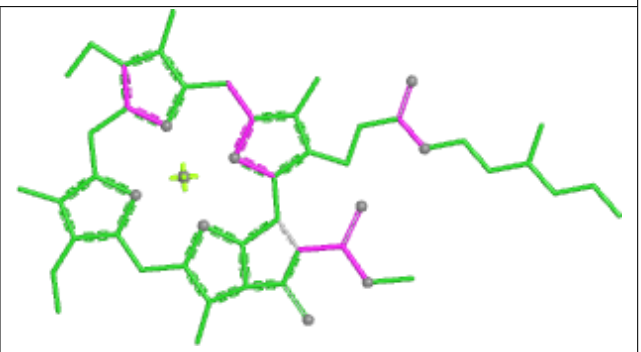


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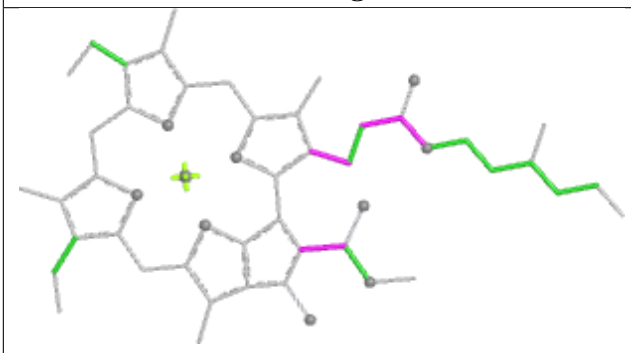
Ligand CLA A 839



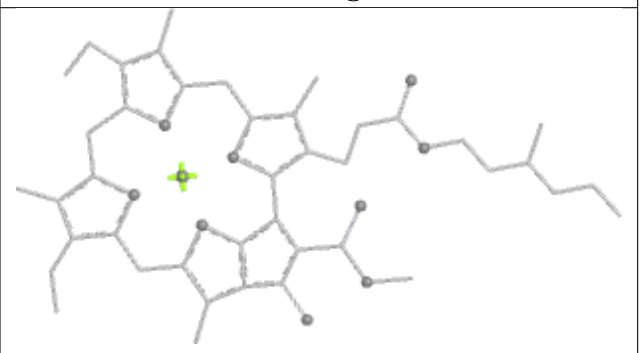
Bond lengths



Bond angles

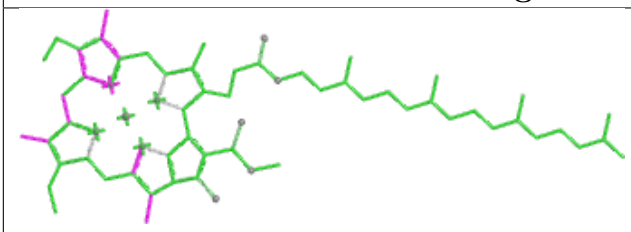


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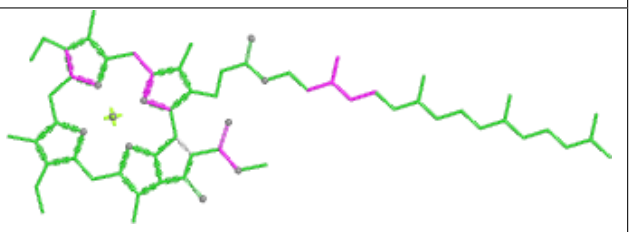


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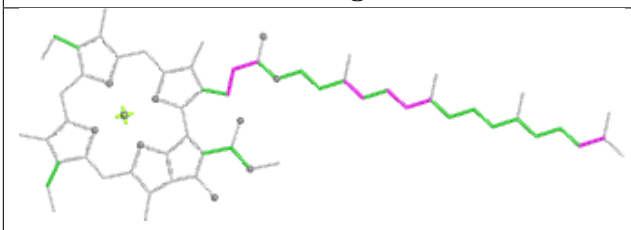
Ligand CLA A1 841



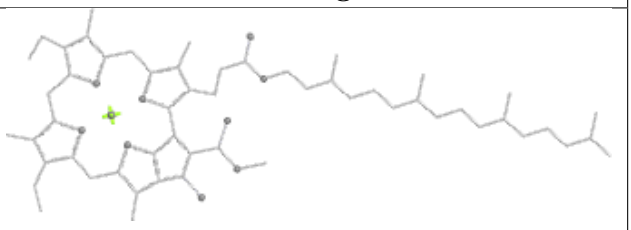
Bond lengths



Bond angles

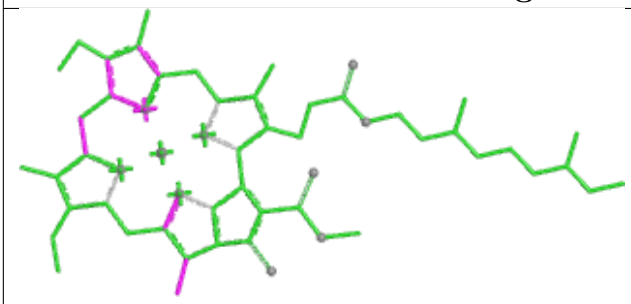


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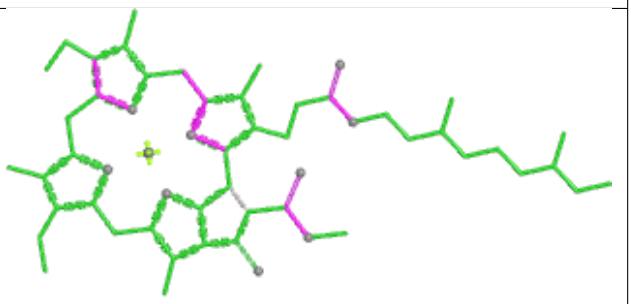


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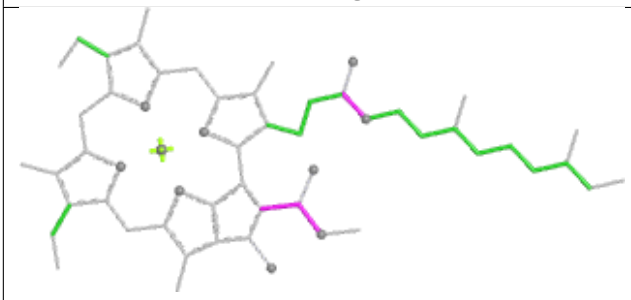
Ligand CLA B2 831



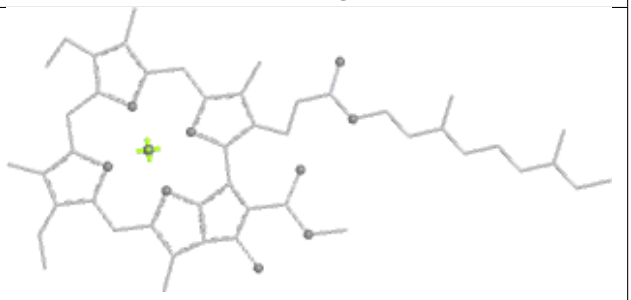
Bond lengths



Bond angles



Torsions

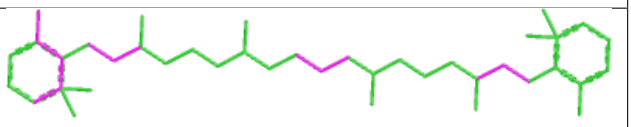


Rings

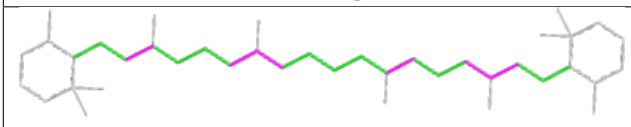
Ligand BCR II 102



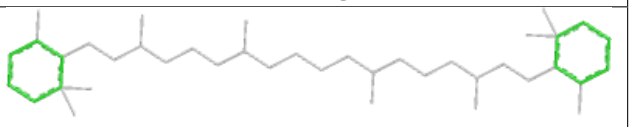
Bond lengths



Bond angles

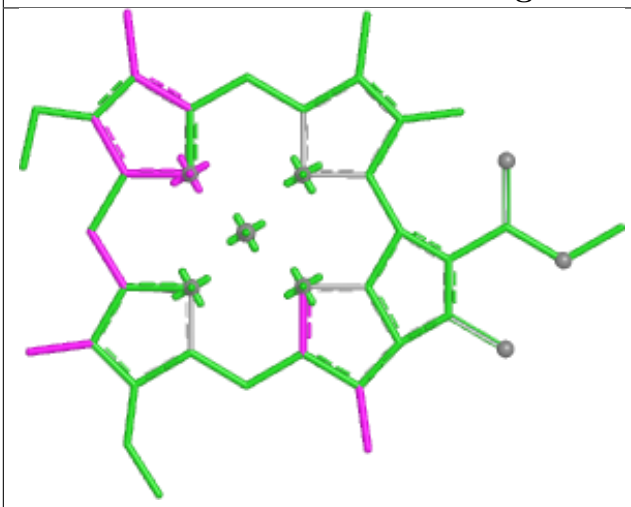


Torsions

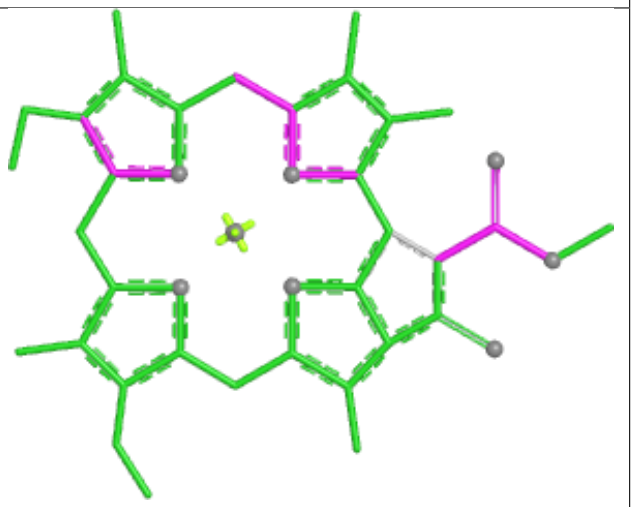


Rings

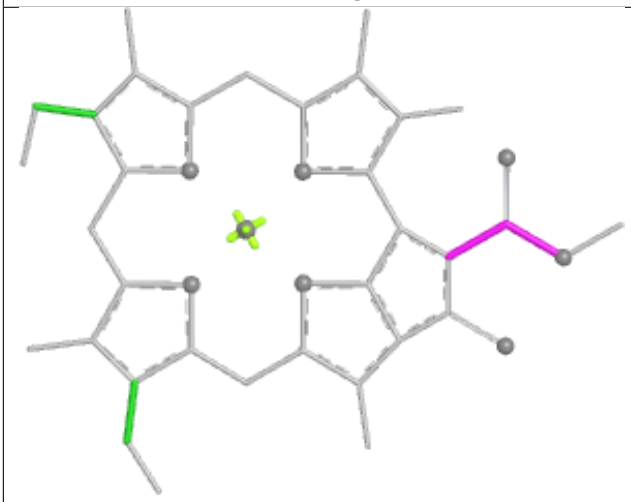
Ligand CLA B2 812



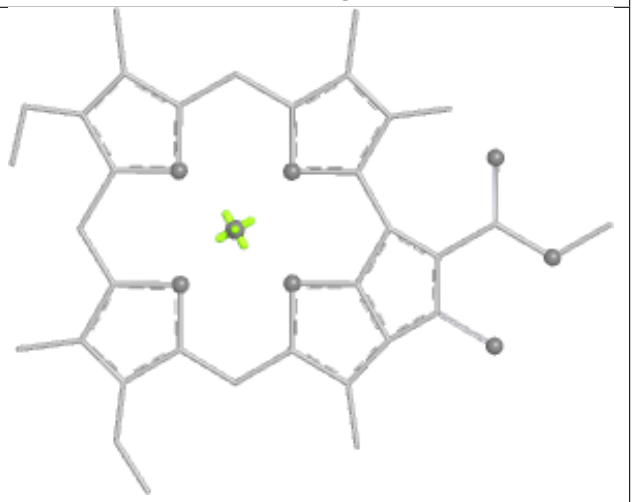
Bond lengths



Bond angles

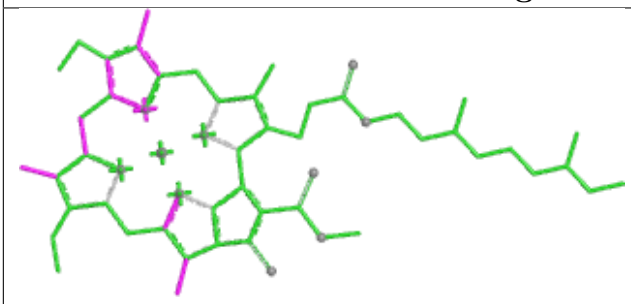


Torsions

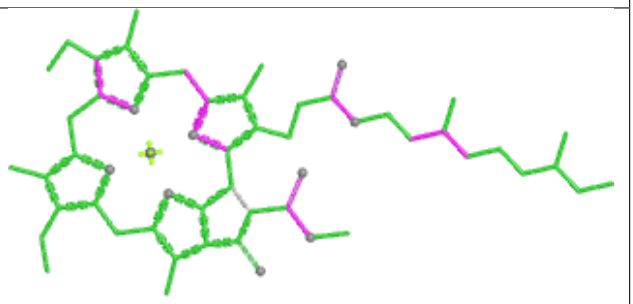


Rings

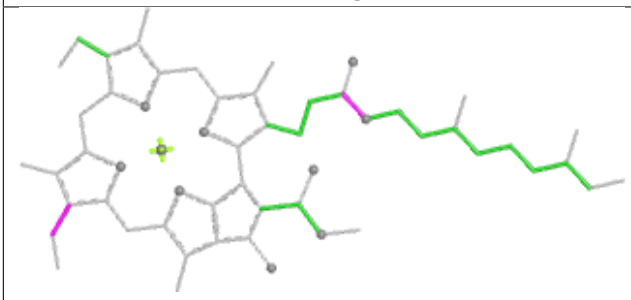
Ligand CLA B2 830



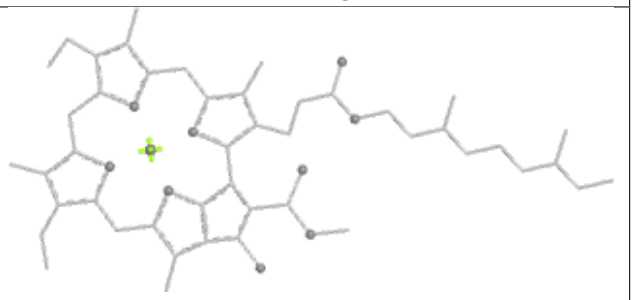
Bond lengths



Bond angles

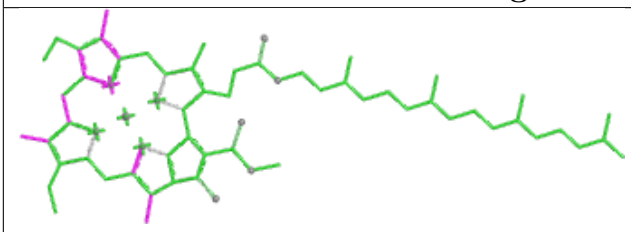


Torsions

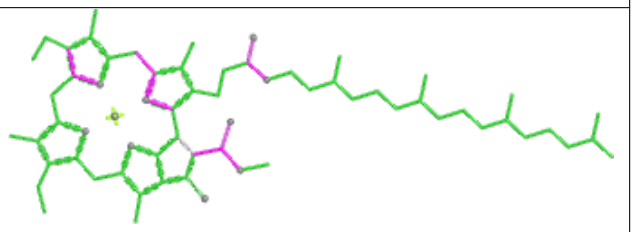


Rings

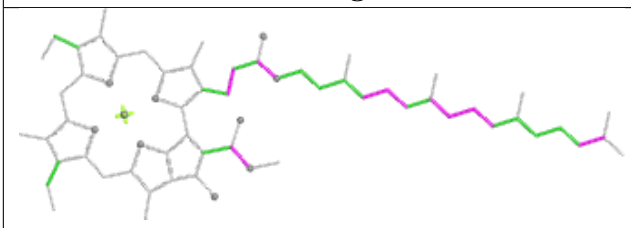
Ligand CLA AA 801



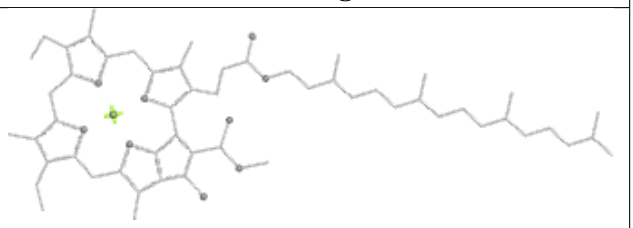
Bond lengths



Bond angles



Torsions

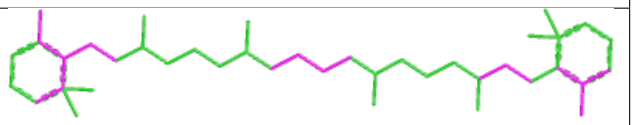


Rings

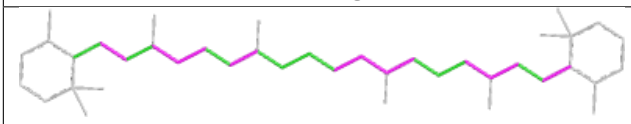
Ligand BCR JJ 104



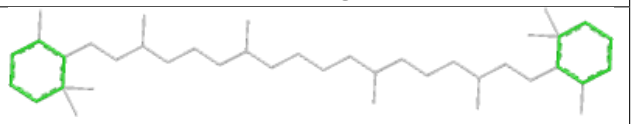
Bond lengths



Bond angles

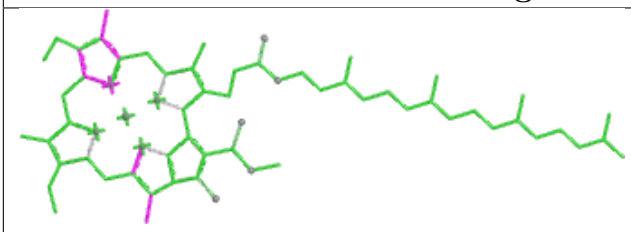


Torsions

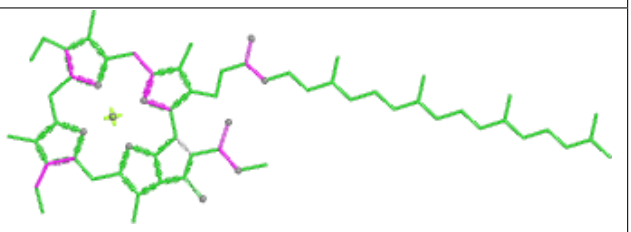


Rings

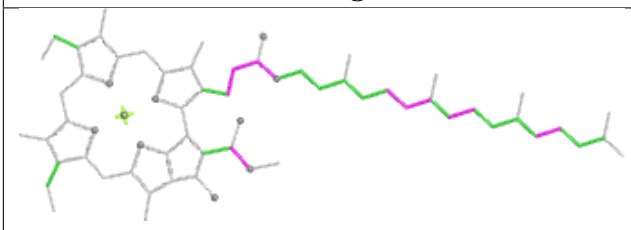
Ligand CLA A1 830



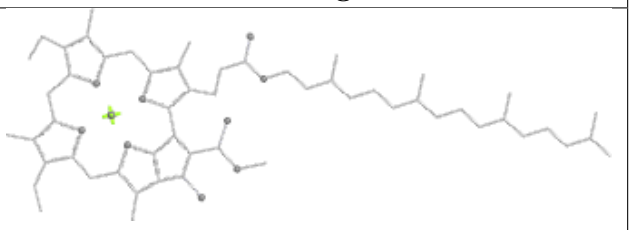
Bond lengths



Bond angles

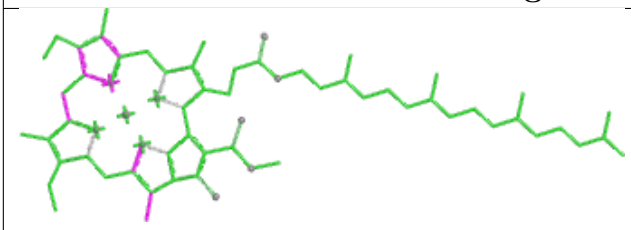


Torsions

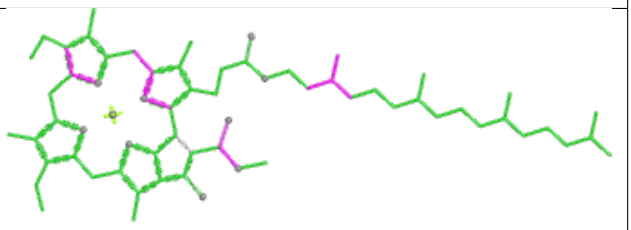


Rings

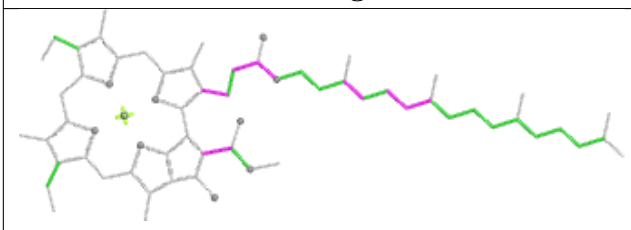
Ligand CLA B 821



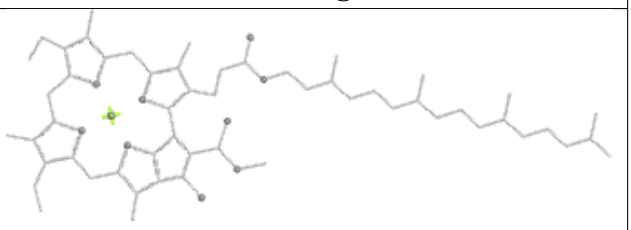
Bond lengths



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.

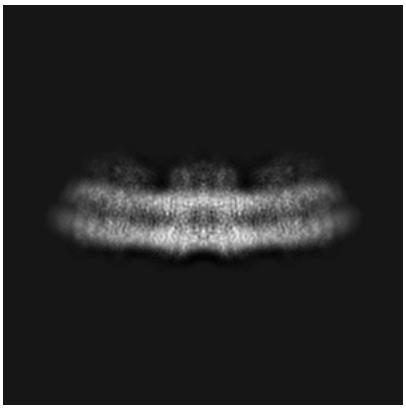
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10461. These allow visual inspection of the internal detail of the map and identification of artifacts.

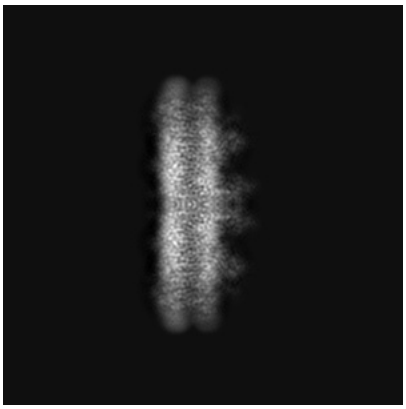
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

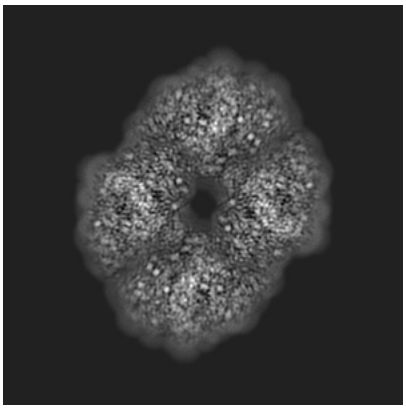
6.1.1 Primary map



X

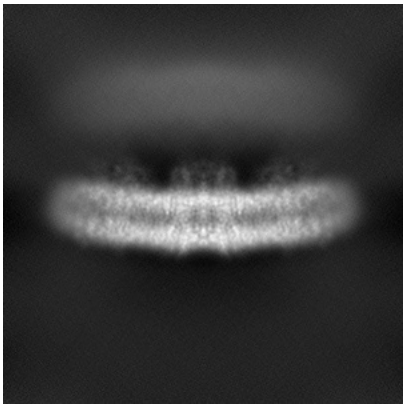


Y

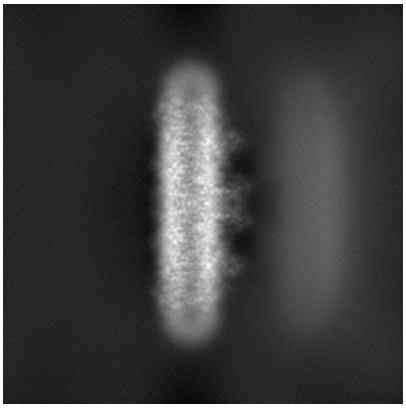


Z

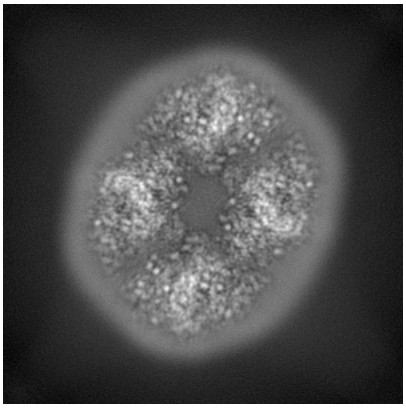
6.1.2 Raw map



X



Y

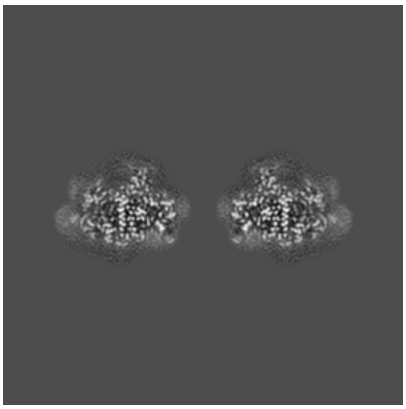


Z

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

6.2 Central slices (i)

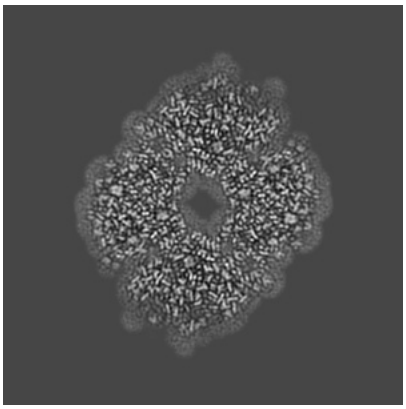
6.2.1 Primary map



X Index: 185

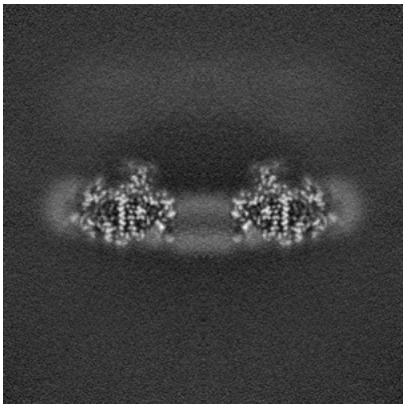


Y Index: 185

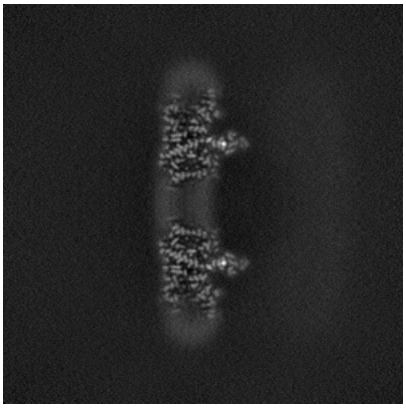


Z Index: 185

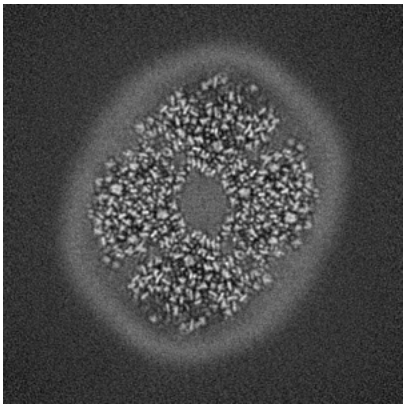
6.2.2 Raw map



X Index: 185



Y Index: 185

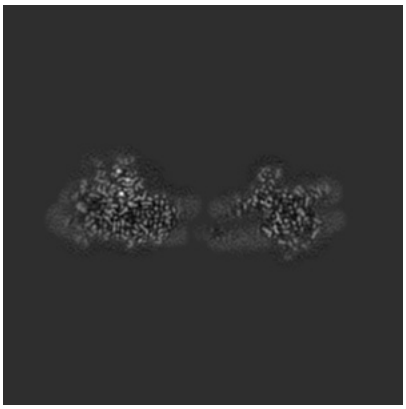


Z Index: 185

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

6.3 Largest variance slices (i)

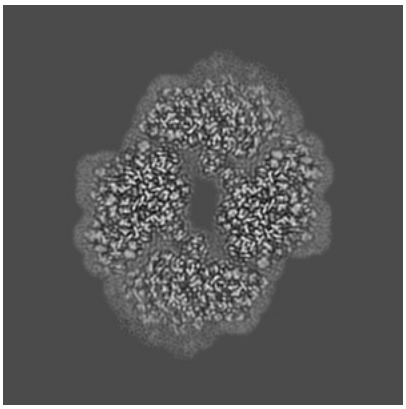
6.3.1 Primary map



X Index: 173

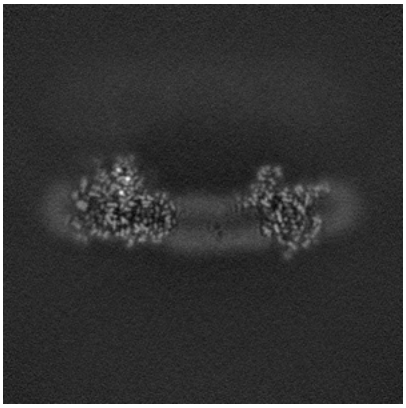


Y Index: 168

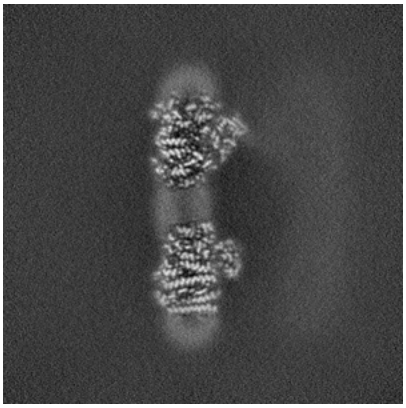


Z Index: 160

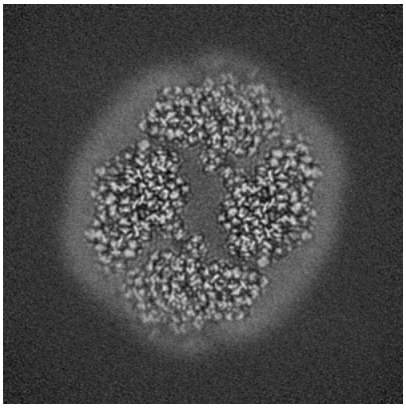
6.3.2 Raw map



X Index: 174



Y Index: 168

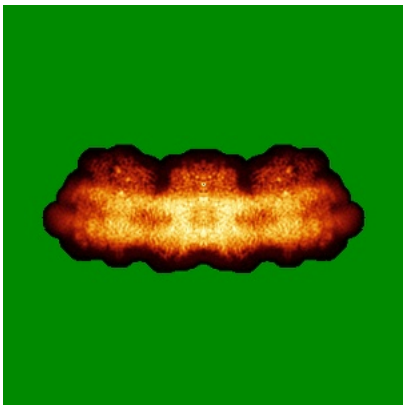


Z Index: 160

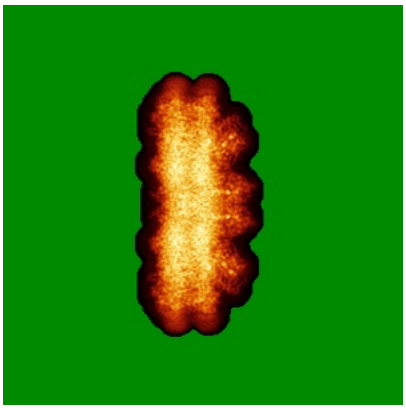
The images above show the largest variance slices of the map in three orthogonal directions.

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

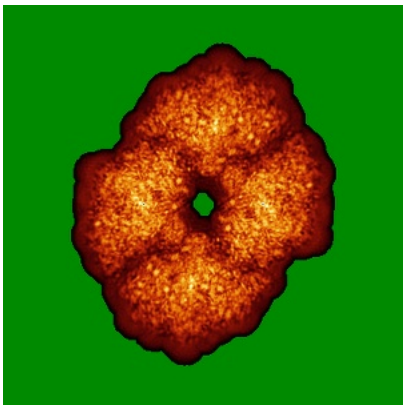
6.4.1 Primary map



X

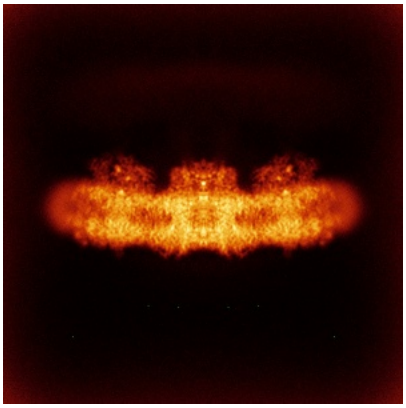


Y

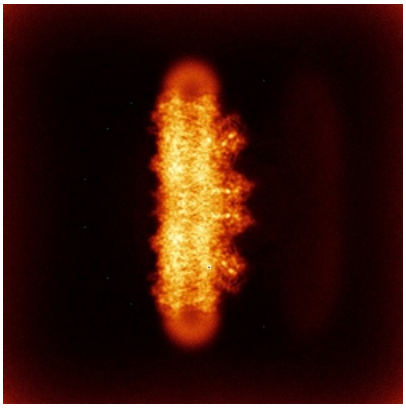


Z

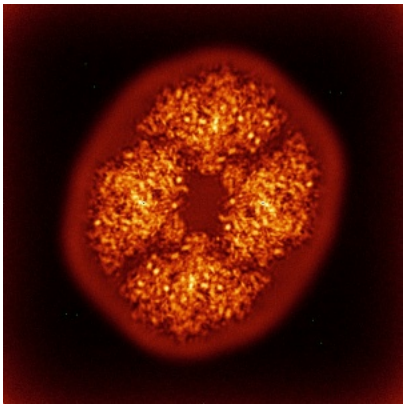
6.4.2 Raw map



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 0.434. 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.

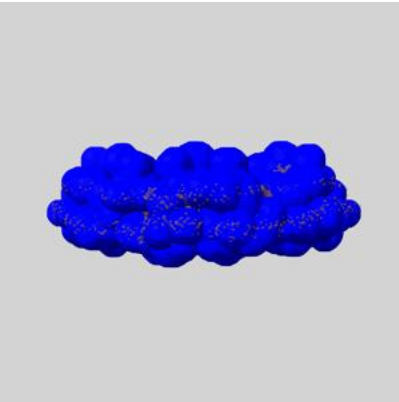
6.6 Mask visualisation

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

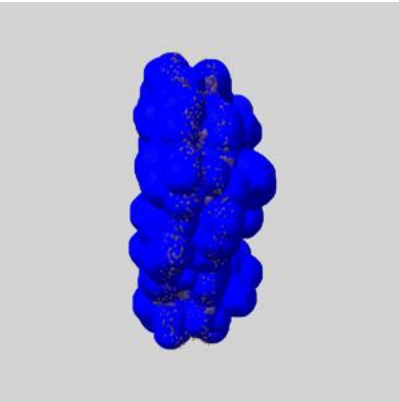
A mask typically either:

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

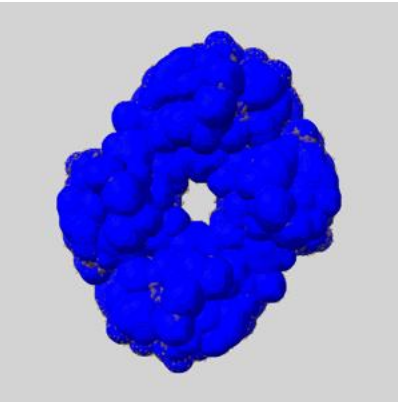
6.6.1 emd_10461_msk_1.map



X



Y

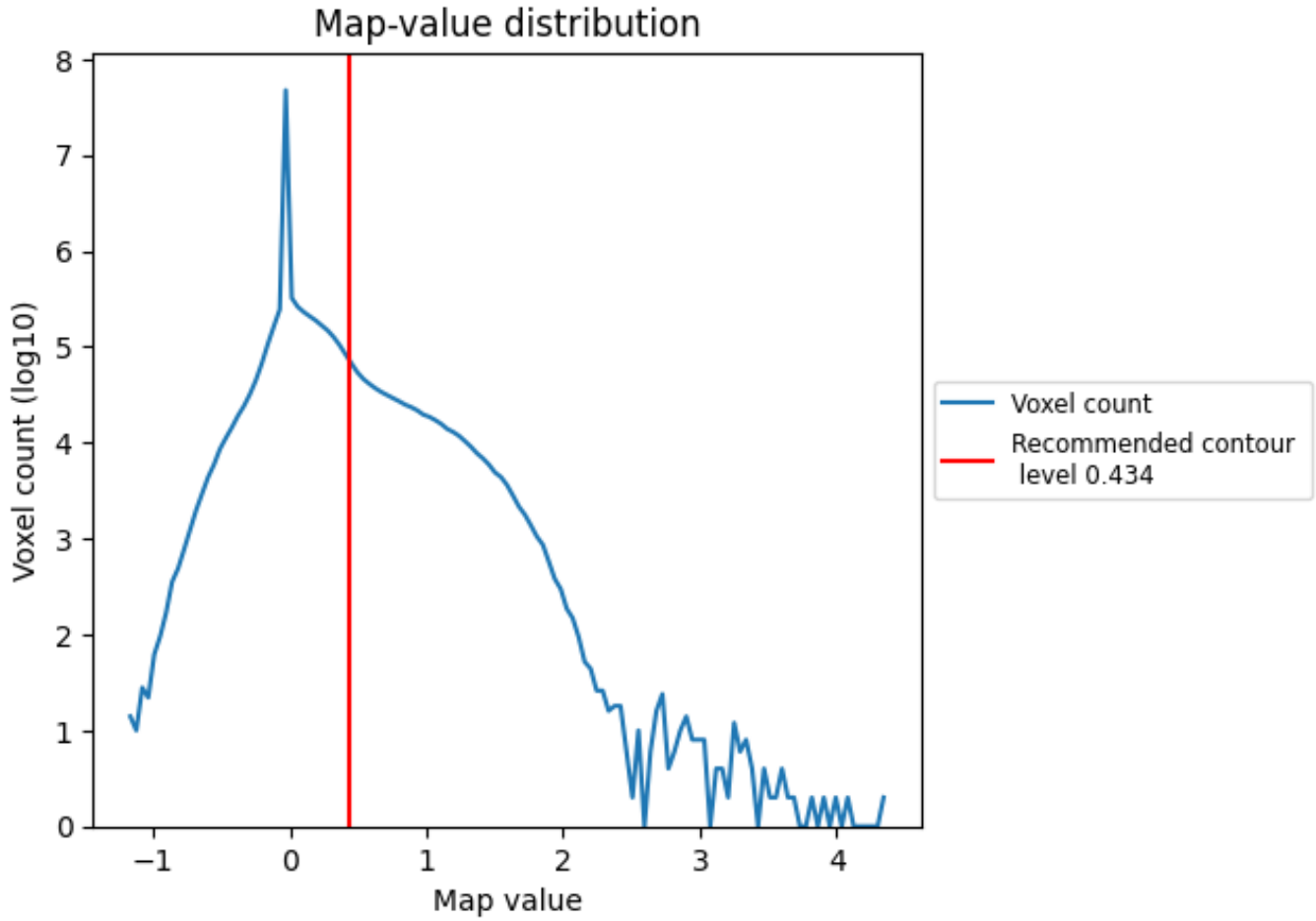


Z

7 Map analysis

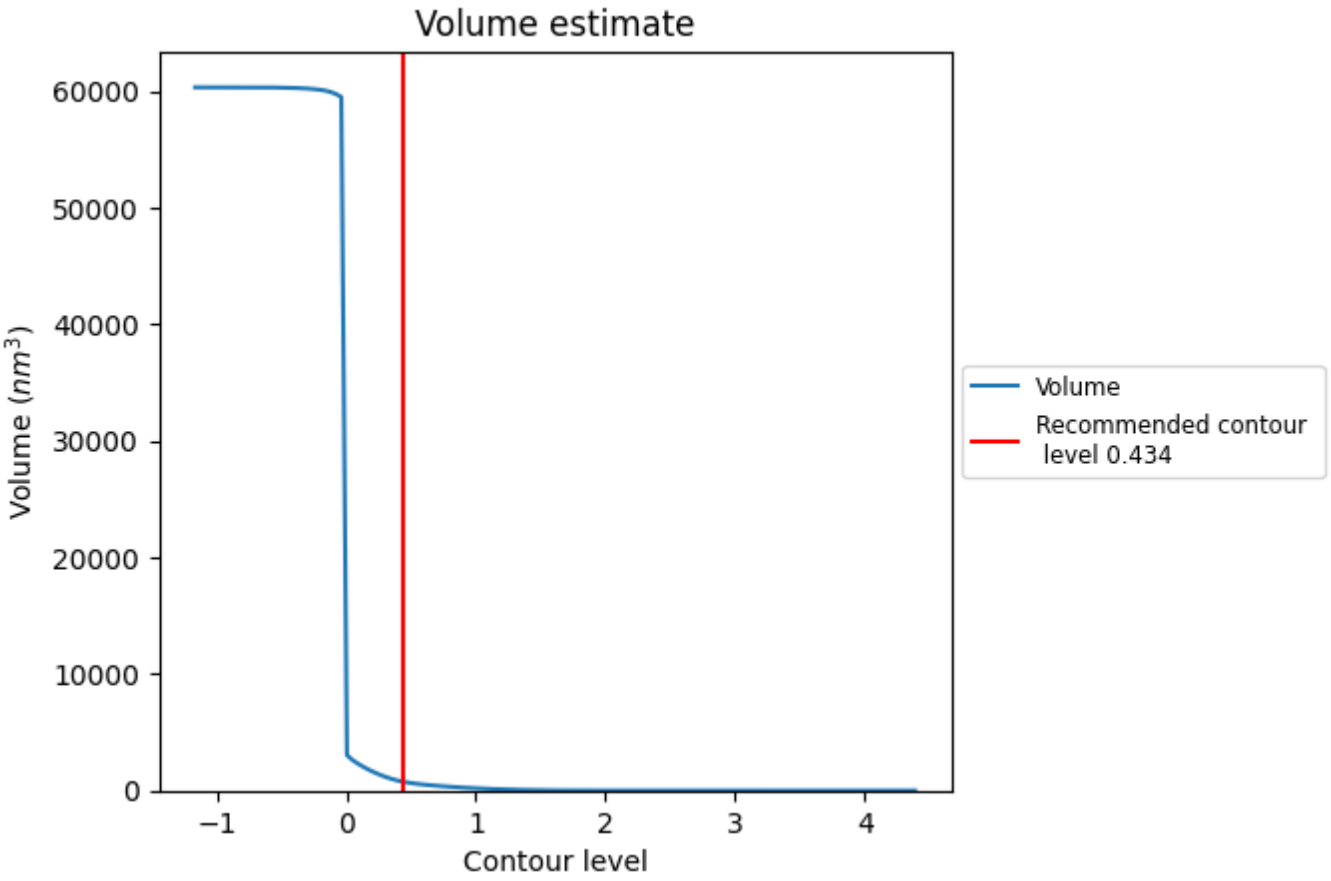
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

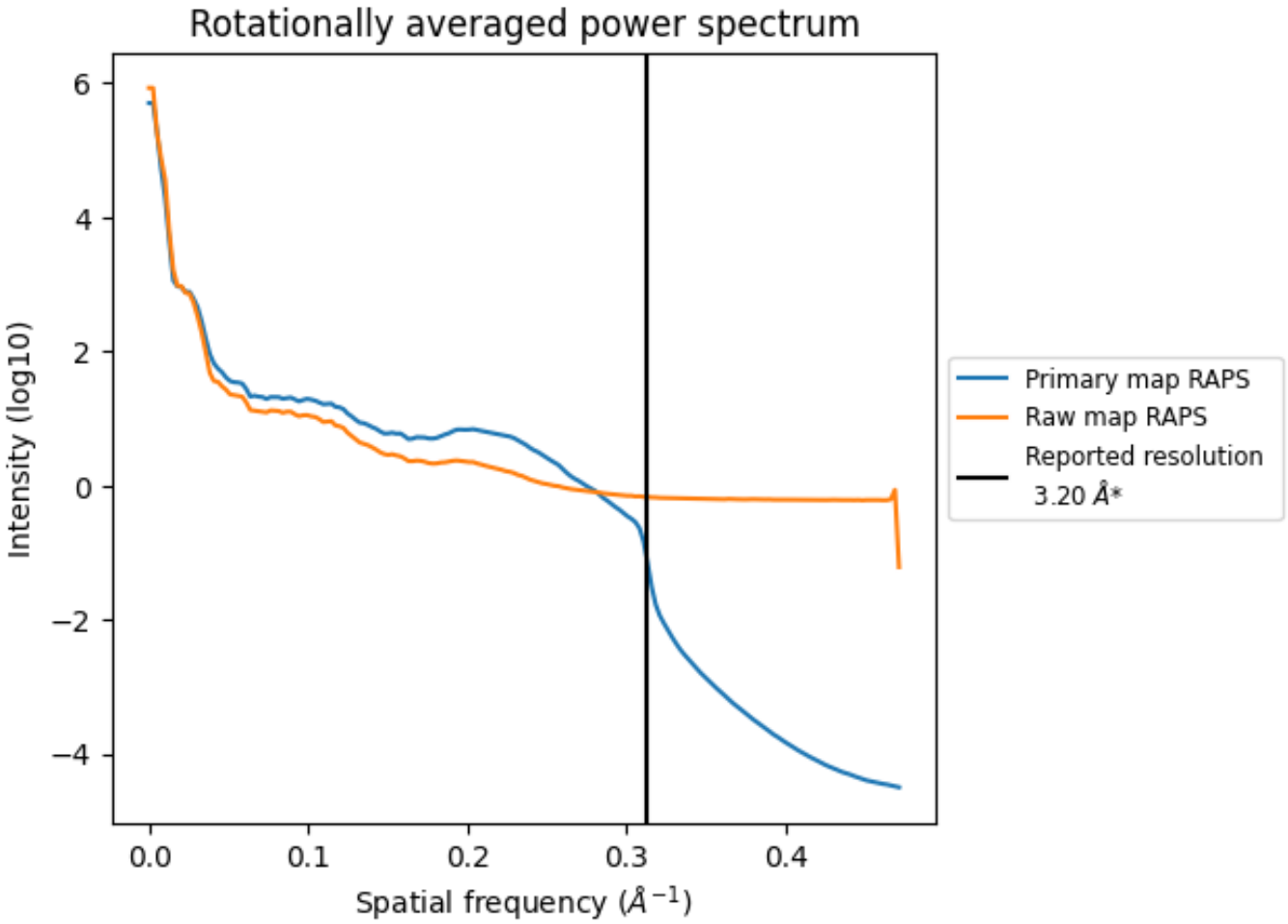
7.2 Volume estimate



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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)

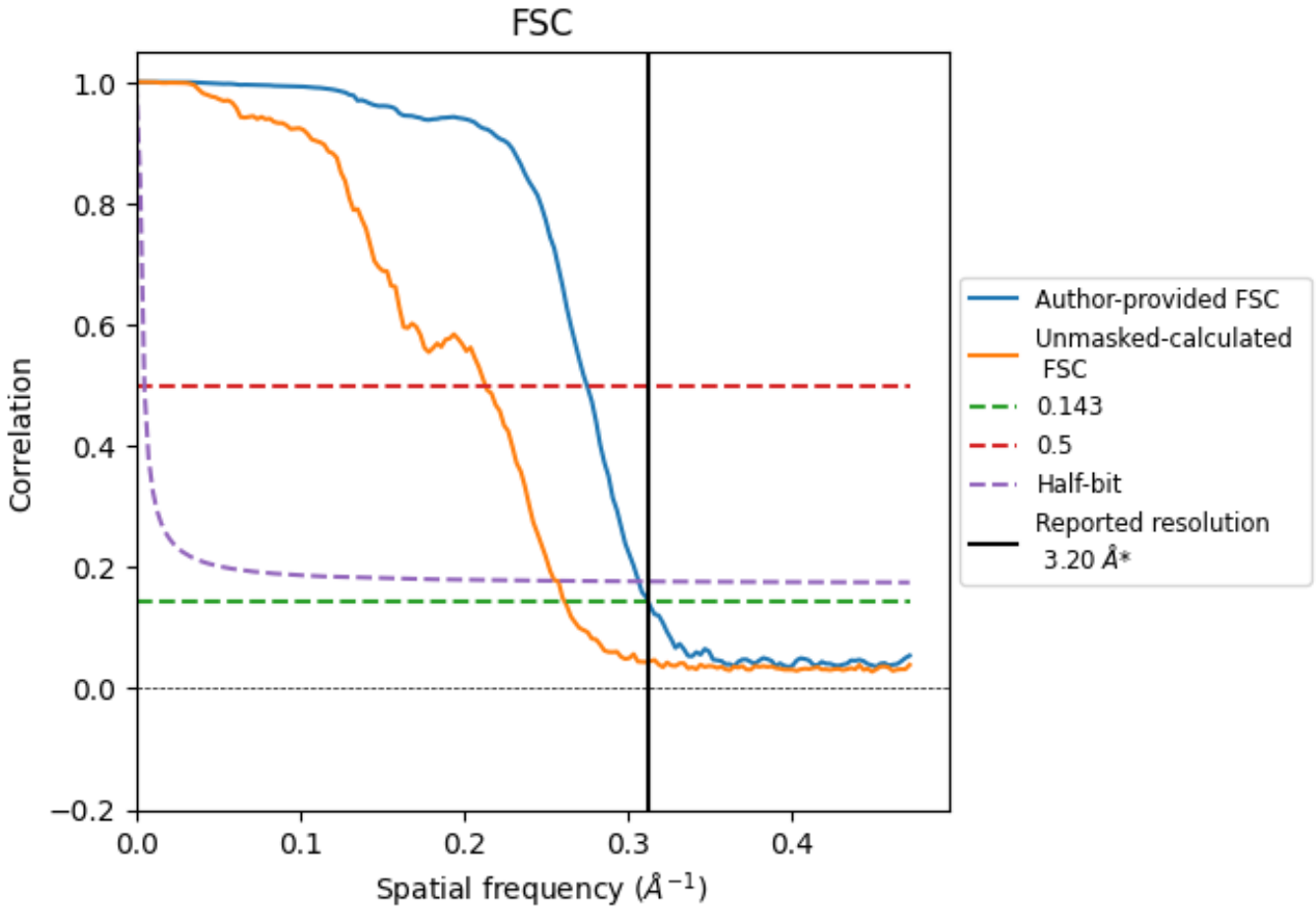


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

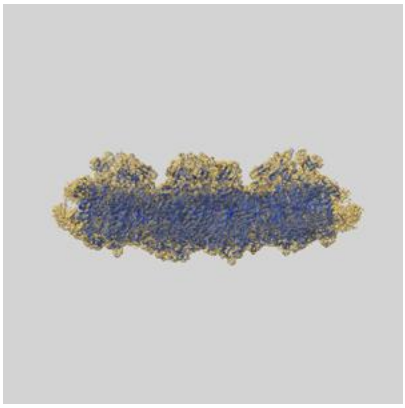
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.64	3.26
Unmasked-calculated*	3.83	4.69	3.89

*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 3.83 differs from the reported value 3.2 by more than 10 %

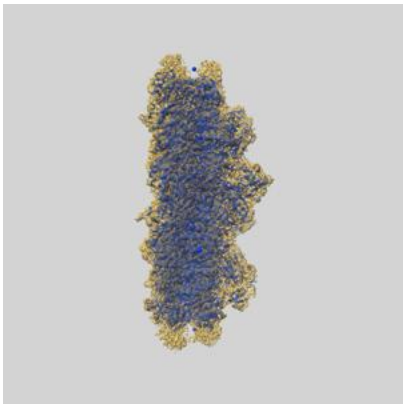
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10461 and PDB model 6TCL. Per-residue inclusion information can be found in section 3 on page 52.

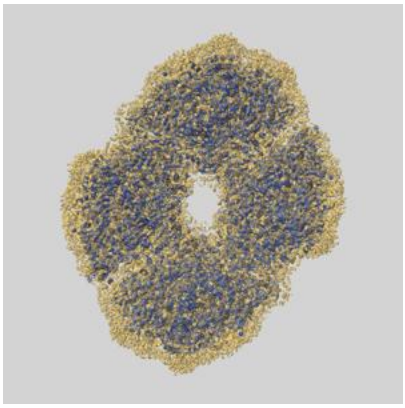
9.1 Map-model overlay



X



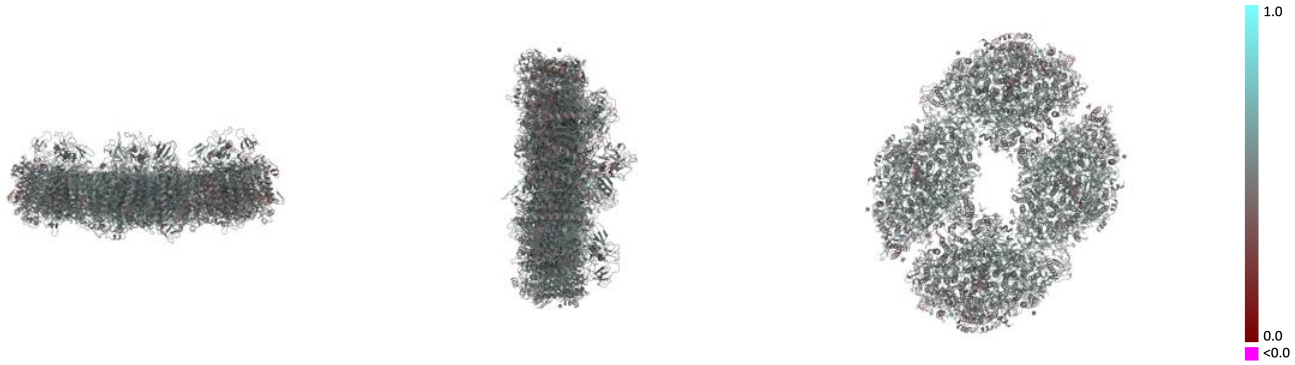
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.434 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

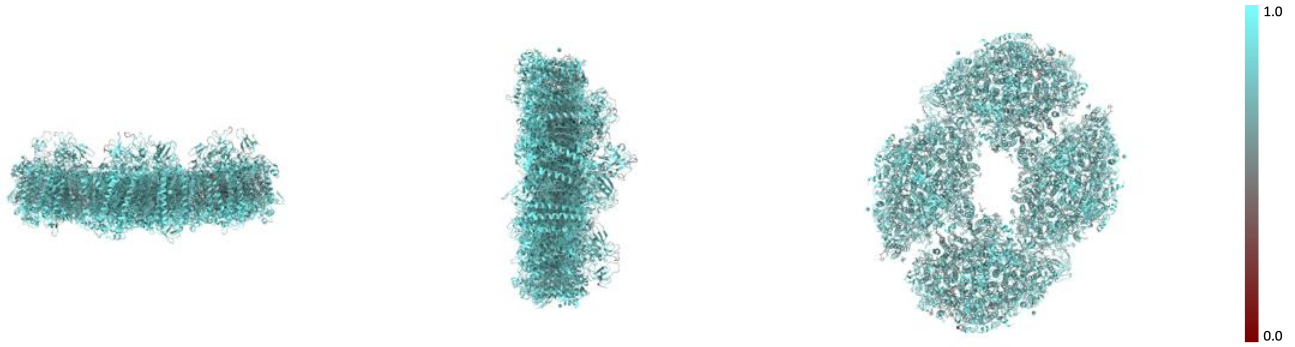
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

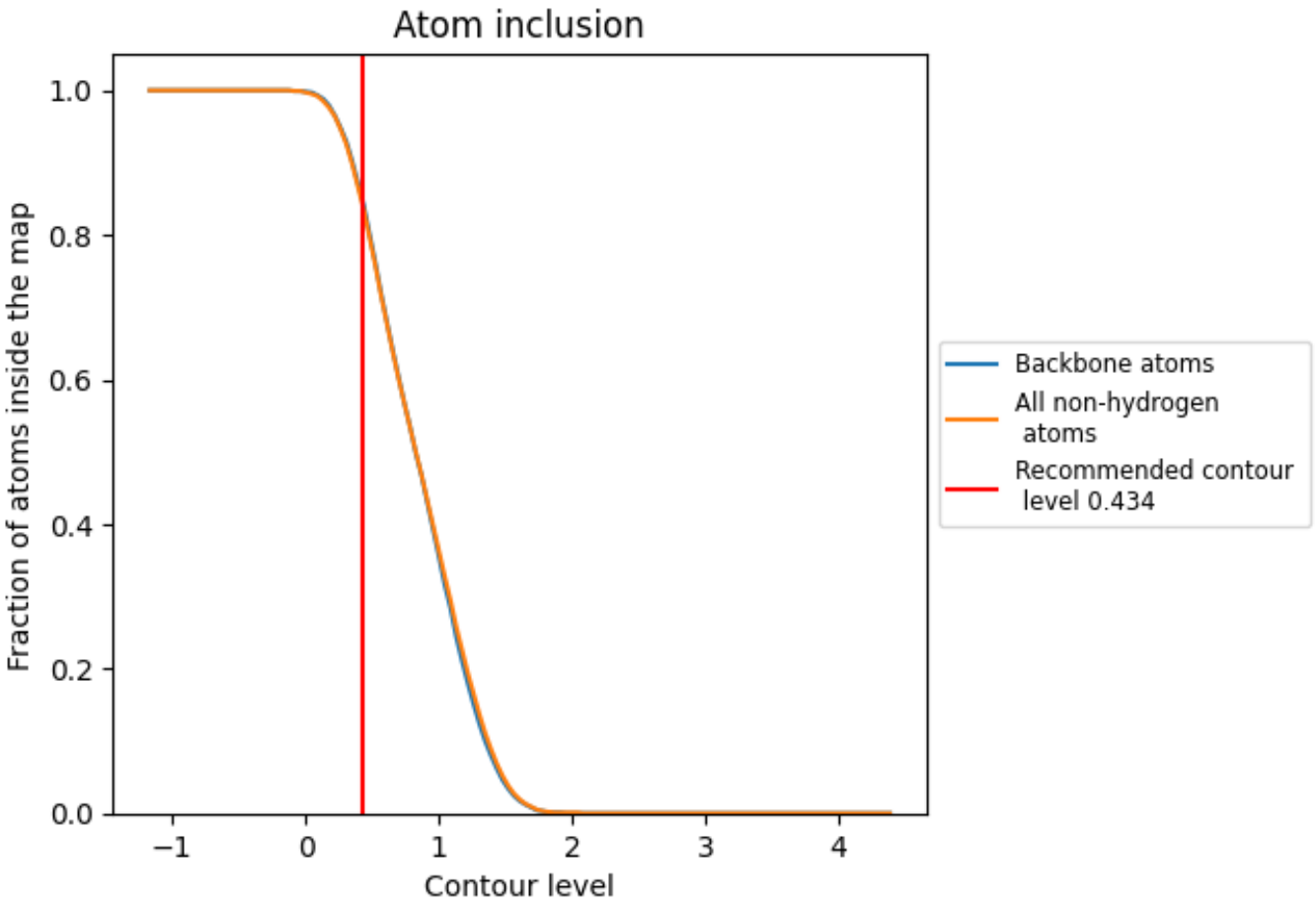
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.434).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.5090
A	0.8610	0.5210
A1	0.8530	0.5190
A2	0.8530	0.5170
AA	0.8600	0.5210
B	0.8670	0.5280
B1	0.8290	0.5000
B2	0.8310	0.5000
BB	0.8730	0.5310
C	0.8500	0.4900
C1	0.8340	0.4840
C2	0.8250	0.5000
CC	0.8340	0.4910
D	0.8260	0.5140
D1	0.7880	0.5010
D2	0.7910	0.5050
DD	0.8140	0.5130
E	0.7800	0.4770
E1	0.7570	0.4530
E2	0.7500	0.4610
EE	0.7840	0.4900
F	0.8440	0.4940
F1	0.7870	0.4560
F2	0.7880	0.4470
FF	0.8380	0.4990
I	0.8570	0.5390
I1	0.8490	0.5220
I2	0.8110	0.5110
II	0.8330	0.5380
J	0.8570	0.4860
J1	0.7840	0.4490
J2	0.8020	0.4530
JJ	0.8510	0.4850
K	0.7080	0.4170
K1	0.8090	0.4850



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Chain	Atom inclusion	Q-score
K2	0.8070	0.4820
KK	0.7200	0.4200
L	0.8190	0.5020
L1	0.8190	0.5050
L2	0.8360	0.5040
LL	0.8360	0.5080
M	0.8100	0.5100
M1	0.7310	0.4640
M2	0.7160	0.4600
MM	0.8260	0.5060
X	0.7890	0.4990
X1	0.6720	0.4540
X2	0.6770	0.4530
XX	0.7840	0.4930