Full wwPDB EM Validation Report (i)

Sep 30, 2025 – 04:25 PM JST

PDB ID	:	9VFJ / pdb_00009vfj
EMDB ID	:	EMD-65026
Title	:	PSI-LHCI of Euglena gracilis strain Z
Authors	:	Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on	:	2025-06-11
Resolution	:	2.83 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

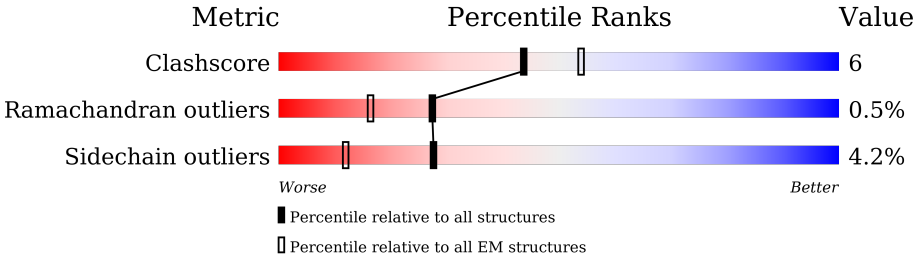
EMDB validation analysis	:	0.0.1.dev129
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive 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)	:	2.46

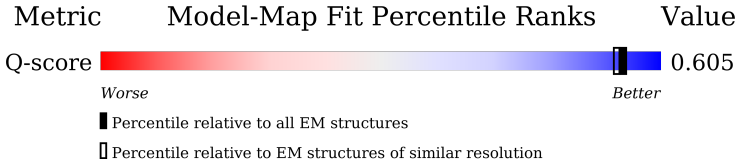
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.83 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	760	89% 9% •
2	B	734	88% 11% •
3	C	81	81% 15% •••
4	D	698	23% • 73%

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Mol	Chain	Length	Quality of chain
5	E	161	36% 61%
6	F	333	45% 5% 50%
7	J	37	5% 86% 14%
8	M	31	10% 94% 6%
9	1	492	5% 33% 7% 60%
10	2	620	30% 5% 65%
11	3	431	6% 45% 6% 48%
12	4	411	14% 35% 6% 59%
13	5	252	6% 58% 6% 35%
14	6	889	16% 81%
15	7	616	25% 71%
16	8	828	5% 19% 79%
17	9	873	8% 18% 80%
18	10	643	16% 18% 78%
19	11	1048	7% 14% 84%
19	12	1048	8% 12% 86%
19	13	1048	7% 6% 93%

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
20	CL0	A	801	X	-	-	-
21	CLA	1	501	X	-	-	-
21	CLA	1	504	X	-	-	-
21	CLA	1	505	X	-	-	-
21	CLA	1	506	X	-	-	-
21	CLA	1	507	X	-	-	-
21	CLA	1	509	X	-	-	-
21	CLA	1	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	511	X	-	-	-
21	CLA	1	512	X	-	-	-
21	CLA	1	514	X	-	-	-
21	CLA	1	515	X	-	-	-
21	CLA	1	516	X	-	-	-
21	CLA	10	703	X	-	-	-
21	CLA	10	704	X	-	-	-
21	CLA	10	705	X	-	-	-
21	CLA	10	706	X	-	-	-
21	CLA	10	707	X	-	-	-
21	CLA	10	708	X	-	-	-
21	CLA	10	709	X	-	-	-
21	CLA	10	710	X	-	-	-
21	CLA	10	711	X	-	-	-
21	CLA	10	712	X	-	-	-
21	CLA	11	701	X	-	-	-
21	CLA	11	702	X	-	-	-
21	CLA	11	703	X	-	-	-
21	CLA	11	704	X	-	-	-
21	CLA	11	705	X	-	-	-
21	CLA	11	706	X	-	-	-
21	CLA	11	707	X	-	-	-
21	CLA	11	708	X	-	-	-
21	CLA	11	709	X	-	-	-
21	CLA	11	711	X	-	-	-
21	CLA	12	501	X	-	-	-
21	CLA	12	502	X	-	-	-
21	CLA	12	503	X	-	-	-
21	CLA	12	504	X	-	-	-
21	CLA	12	505	X	-	-	-
21	CLA	12	506	X	-	-	-
21	CLA	12	507	X	-	-	-
21	CLA	12	508	X	-	-	-
21	CLA	13	501	X	-	-	-
21	CLA	13	502	X	-	-	-
21	CLA	13	503	X	-	-	-
21	CLA	2	503	X	-	-	-
21	CLA	2	504	X	-	-	-
21	CLA	2	505	X	-	-	-
21	CLA	2	506	X	-	-	-
21	CLA	2	508	X	-	-	-
21	CLA	2	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	510	X	-	-	-
21	CLA	2	511	X	-	-	-
21	CLA	2	513	X	-	-	-
21	CLA	2	514	X	-	-	-
21	CLA	2	515	X	-	-	-
21	CLA	2	517	X	-	-	-
21	CLA	3	701	X	-	-	-
21	CLA	3	703	X	-	-	-
21	CLA	3	704	X	-	-	-
21	CLA	3	705	X	-	-	-
21	CLA	3	706	X	-	-	-
21	CLA	3	707	X	-	-	-
21	CLA	3	708	X	-	-	-
21	CLA	3	709	X	-	-	-
21	CLA	3	711	X	-	-	-
21	CLA	3	712	X	-	-	-
21	CLA	3	713	X	-	-	-
21	CLA	3	714	X	-	-	-
21	CLA	3	715	X	-	-	-
21	CLA	4	703	X	-	-	-
21	CLA	4	704	X	-	-	-
21	CLA	4	706	X	-	-	-
21	CLA	4	707	X	-	-	-
21	CLA	4	708	X	-	-	-
21	CLA	4	709	X	-	-	-
21	CLA	4	711	X	-	-	-
21	CLA	5	701	X	-	-	-
21	CLA	5	702	X	-	-	-
21	CLA	5	703	X	-	-	-
21	CLA	5	705	X	-	-	-
21	CLA	5	706	X	-	-	-
21	CLA	5	707	X	-	-	-
21	CLA	5	708	X	-	-	-
21	CLA	5	709	X	-	-	-
21	CLA	5	711	X	-	-	-
21	CLA	6	903	X	-	-	-
21	CLA	6	904	X	-	-	-
21	CLA	6	905	X	-	-	-
21	CLA	6	906	X	-	-	-
21	CLA	6	908	X	-	-	-
21	CLA	6	909	X	-	-	-
21	CLA	6	910	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	911	X	-	-	-
21	CLA	6	912	X	-	-	-
21	CLA	6	913	X	-	-	-
21	CLA	7	702	X	-	-	-
21	CLA	7	704	X	-	-	-
21	CLA	7	705	X	-	-	-
21	CLA	7	707	X	-	-	-
21	CLA	7	708	X	-	-	-
21	CLA	7	709	X	-	-	-
21	CLA	7	710	X	-	-	-
21	CLA	7	711	X	-	-	-
21	CLA	7	712	X	-	-	-
21	CLA	7	713	X	-	-	-
21	CLA	7	714	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	605	X	-	-	-
21	CLA	8	606	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	9	902	X	-	-	-
21	CLA	9	903	X	-	-	-
21	CLA	9	904	X	-	-	-
21	CLA	9	905	X	-	-	-
21	CLA	9	907	X	-	-	-
21	CLA	9	908	X	-	-	-
21	CLA	9	909	X	-	-	-
21	CLA	9	910	X	-	-	-
21	CLA	9	911	X	-	-	-
21	CLA	9	912	X	-	-	-
21	CLA	9	914	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	844	X	-	-	-
21	CLA	A	862	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	F	401	X	-	-	-
21	CLA	F	403	X	-	-	-
21	CLA	F	404	X	-	-	-
21	CLA	J	101	X	-	-	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 48242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5881	3861	994	1005	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5863	3857	984	1007	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	596	363	104	118	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	189	1471	941	250	278	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	62	500	318	84	98	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	166	1266	813	213	238	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	37	304	209	43	51	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	31	242	162	37	42	1	0	0

- Molecule 9 is a protein called LHCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	1	199	1513	976	258	273	6	0	0

- Molecule 10 is a protein called LHCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	2	217	1654	1080	272	298	4	0	0

- Molecule 11 is a protein called LHCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	3	222	1689	1095	284	305	5	0	0

- Molecule 12 is a protein called LHCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	4	169	1308	848	214	242	4	0	0

- Molecule 13 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	5	165	1269	816	219	227	7	0	0

- Molecule 14 is a protein called LHCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	6	171	1327	854	228	240	5	0	0

- Molecule 15 is a protein called LHCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	7	180	1427	929	243	249	6	0	0

- Molecule 16 is a protein called LHCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	8	177	1350	864	239	243	4	0	0

- Molecule 17 is a protein called LHCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	9	174	1350	865	233	247	5	0	0

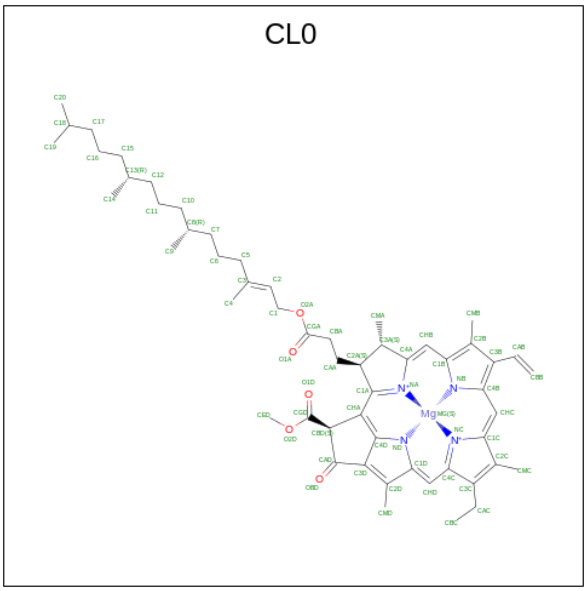
- Molecule 18 is a protein called LHCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	10	142	1102	714	190	192	6	0	0

- Molecule 19 is a protein called LHCI-11.

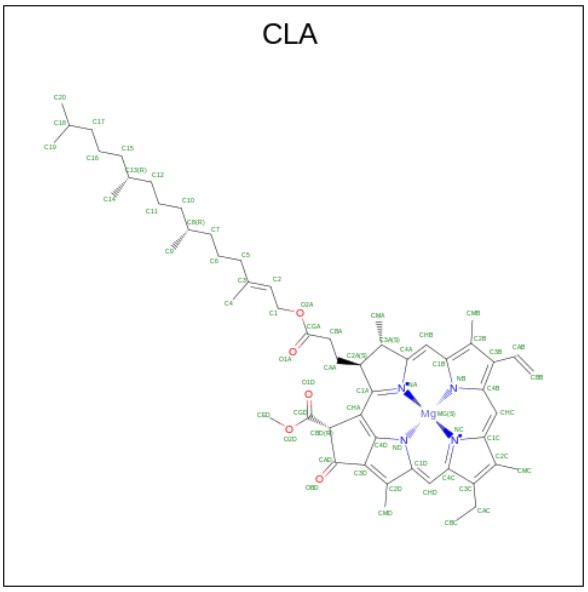
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	11	171	1277	822	219	232	4	0	0
			Total	C	N	O	S		
19	12	150	1127	726	190	207	4	0	0
			Total	C	N	O	S		
19	13	78	594	386	103	101	4	0	0

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	51	41	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	59	49	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	60	50	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	54	44	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	51	41	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	47	37	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	52	42	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	F	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	F	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
21	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	47	37	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	2	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
21	3	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	47	37	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	9	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
21	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	10	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	10	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	10	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	10	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	10	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	11	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	11	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	11	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	12	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	12	1	45	35	1	4	5	0

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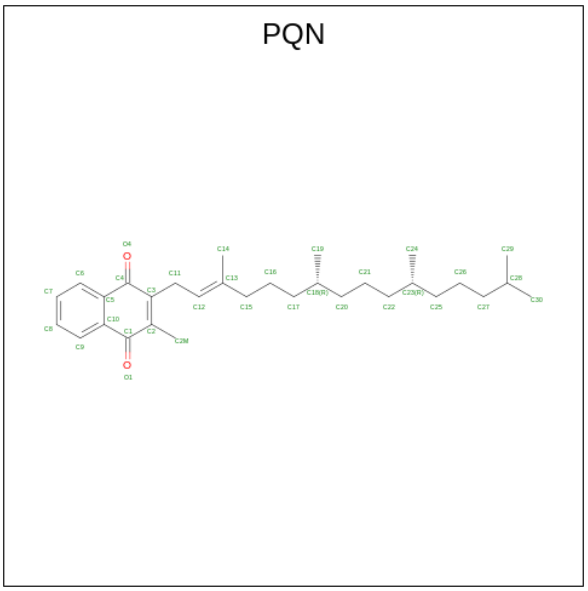
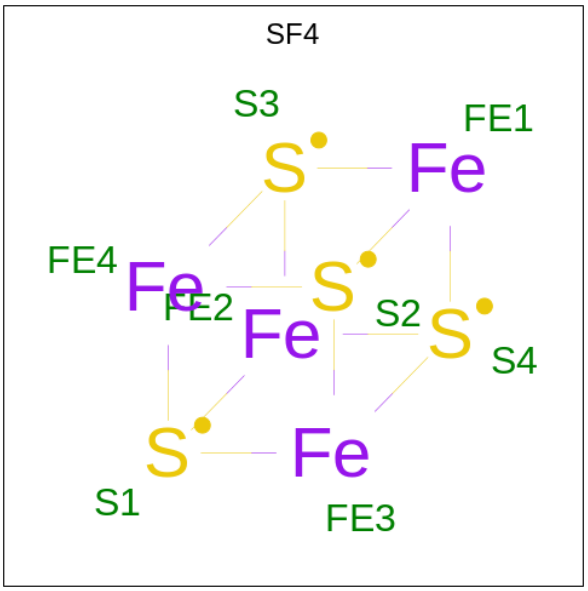
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	13	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	13	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	13	1	47	37	1	4	5	0

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



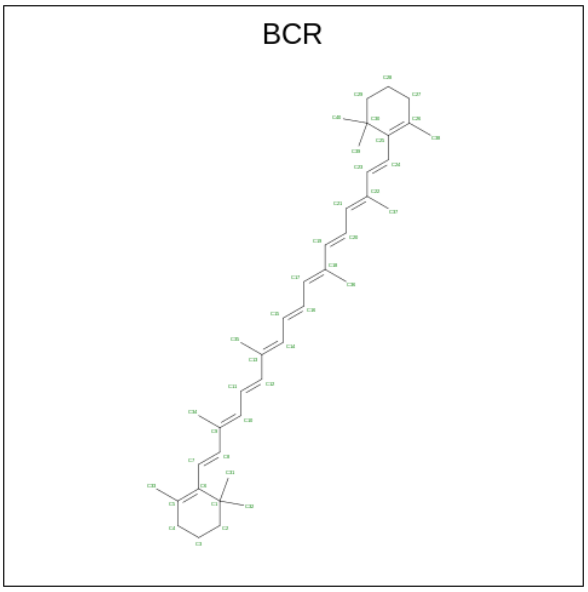
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	A	1	33	31	2	0
			Total	C	O	
22	B	1	31	29	2	0

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

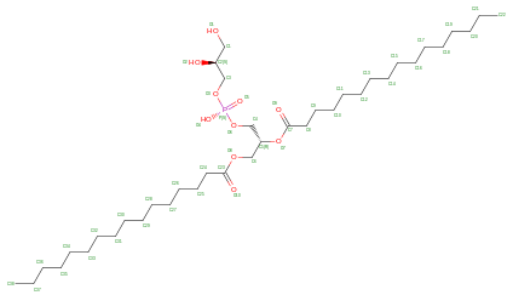
- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
24	A	1	40	40	0
24	A	1	40	40	0
24	A	1	40	40	0
24	A	1	40	40	0
24	A	1	40	40	0
24	A	1	40	40	0
24	B	1	40	40	0
24	B	1	40	40	0
24	B	1	40	40	0
24	B	1	40	40	0
24	B	1	40	40	0
24	B	1	40	40	0
24	F	1	40	40	0
24	F	1	40	40	0
24	J	1	40	40	0
24	J	1	40	40	0
24	M	1	40	40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

LHG

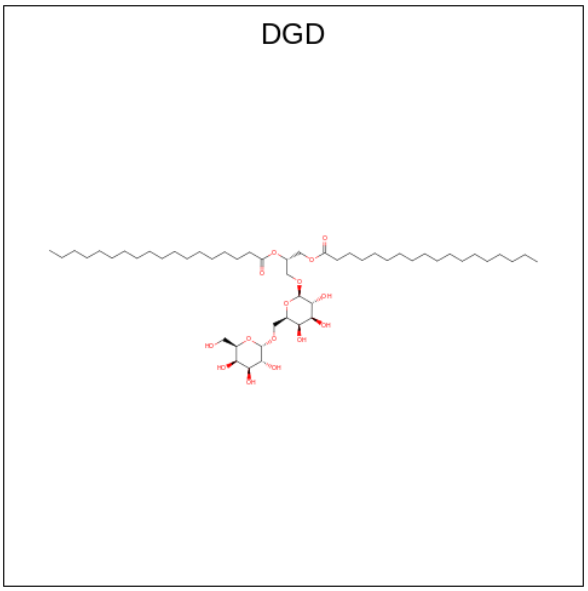


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	A	1	49	38	10	1	0
			Total	C	O	P	
25	A	1	27	16	10	1	0
			Total	C	O	P	
25	B	1	23	12	10	1	0
			Total	C	O	P	
25	1	1	36	25	10	1	0
			Total	C	O	P	
25	2	1	30	19	10	1	0
			Total	C	O	P	
25	3	1	25	14	10	1	0
			Total	C	O	P	
25	4	1	19	10	8	1	0
			Total	C	O	P	
25	5	1	32	21	10	1	0
			Total	C	O	P	
25	6	1	28	17	10	1	0
			Total	C	O	P	
25	7	1	48	37	10	1	0
			Total	C	O	P	
25	8	1	33	22	10	1	0
			Total	C	O	P	
25	9	1	34	23	10	1	0
			Total	C	O	P	
25	10	1	32	21	10	1	0
			Total	C	O	P	
25	11	1	30	19	10	1	0

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

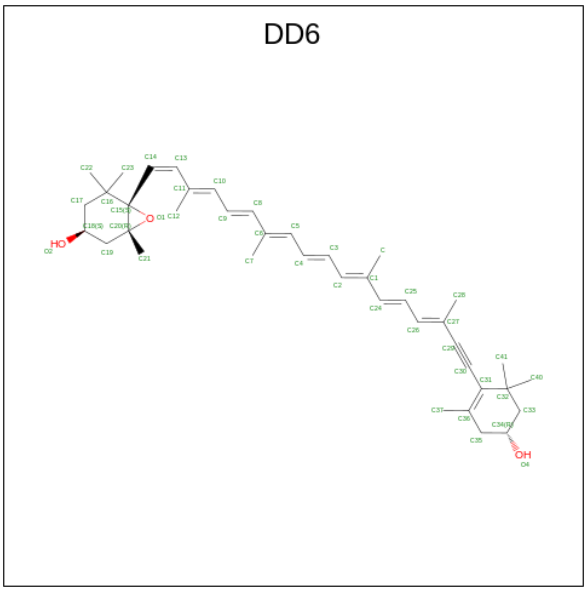
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	A	7	97	97	0
26	B	5	62	62	0
26	D	1	6	6	0
26	F	1	9	9	0
26	M	2	20	20	0
26	1	4	42	42	0
26	2	5	42	42	0
26	6	4	47	47	0
26	7	6	67	67	0
26	8	4	46	46	0
26	9	1	15	15	0
26	10	2	26	26	0

- Molecule 27 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
			Total	C	O	
27	B	1	57	42	15	0

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	J	1	43	40	3	0
			Total	C	O	
28	1	1	43	40	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	1	1	43	40	3	0
			Total	C	O	
28	1	1	43	40	3	0
			Total	C	O	
28	2	1	43	40	3	0
			Total	C	O	
28	2	1	43	40	3	0
			Total	C	O	
28	2	1	43	40	3	0
			Total	C	O	
28	3	1	43	40	3	0
			Total	C	O	
28	3	1	43	40	3	0
			Total	C	O	
28	3	1	43	40	3	0
			Total	C	O	
28	4	1	43	40	3	0
			Total	C	O	
28	4	1	43	40	3	0
			Total	C	O	
28	5	1	43	40	3	0
			Total	C	O	
28	5	1	43	40	3	0
			Total	C	O	
28	6	1	43	40	3	0
			Total	C	O	
28	6	1	43	40	3	0
			Total	C	O	
28	7	1	43	40	3	0
			Total	C	O	
28	7	1	43	40	3	0
			Total	C	O	
28	8	1	43	40	3	0
			Total	C	O	
28	8	1	43	40	3	0
			Total	C	O	
28	9	1	43	40	3	0
			Total	C	O	
28	9	1	43	40	3	0
			Total	C	O	
28	11	1	43	40	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	11	1	43	40	3	0
28	12	1	43	40	3	0
28	12	1	43	40	3	0

- Molecule 29 is water.

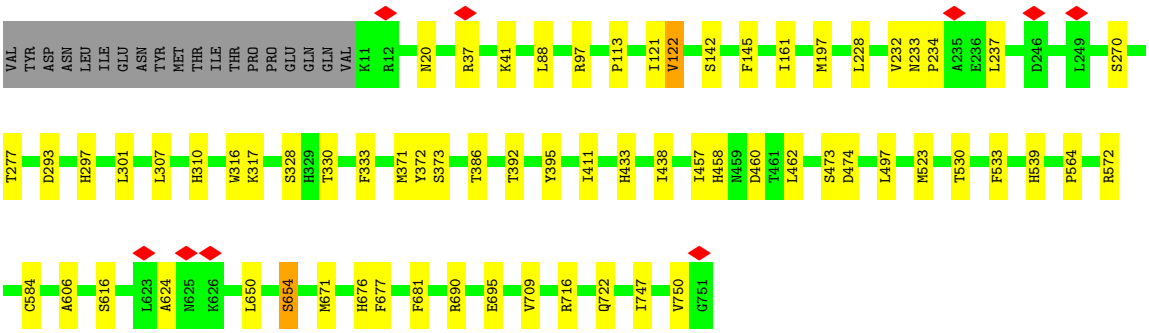
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
29	A	7	7	7	0
29	B	9	9	9	0
29	D	1	1	1	0
29	F	1	1	1	0
29	J	1	1	1	0
29	1	4	4	4	0
29	2	4	4	4	0
29	3	4	4	4	0
29	4	3	3	3	0
29	5	2	2	2	0
29	6	1	1	1	0
29	7	2	2	2	0
29	8	2	2	2	0
29	9	2	2	2	0
29	11	1	1	1	0

3 Residue-property plots (i)

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

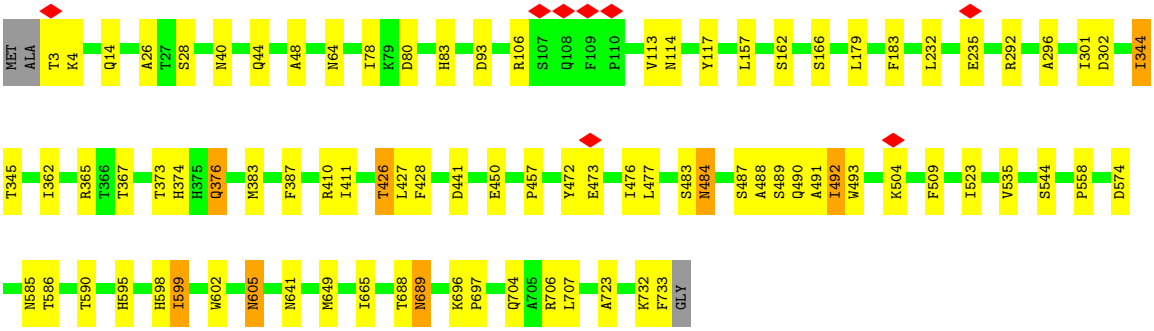
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



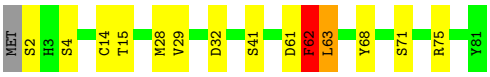
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



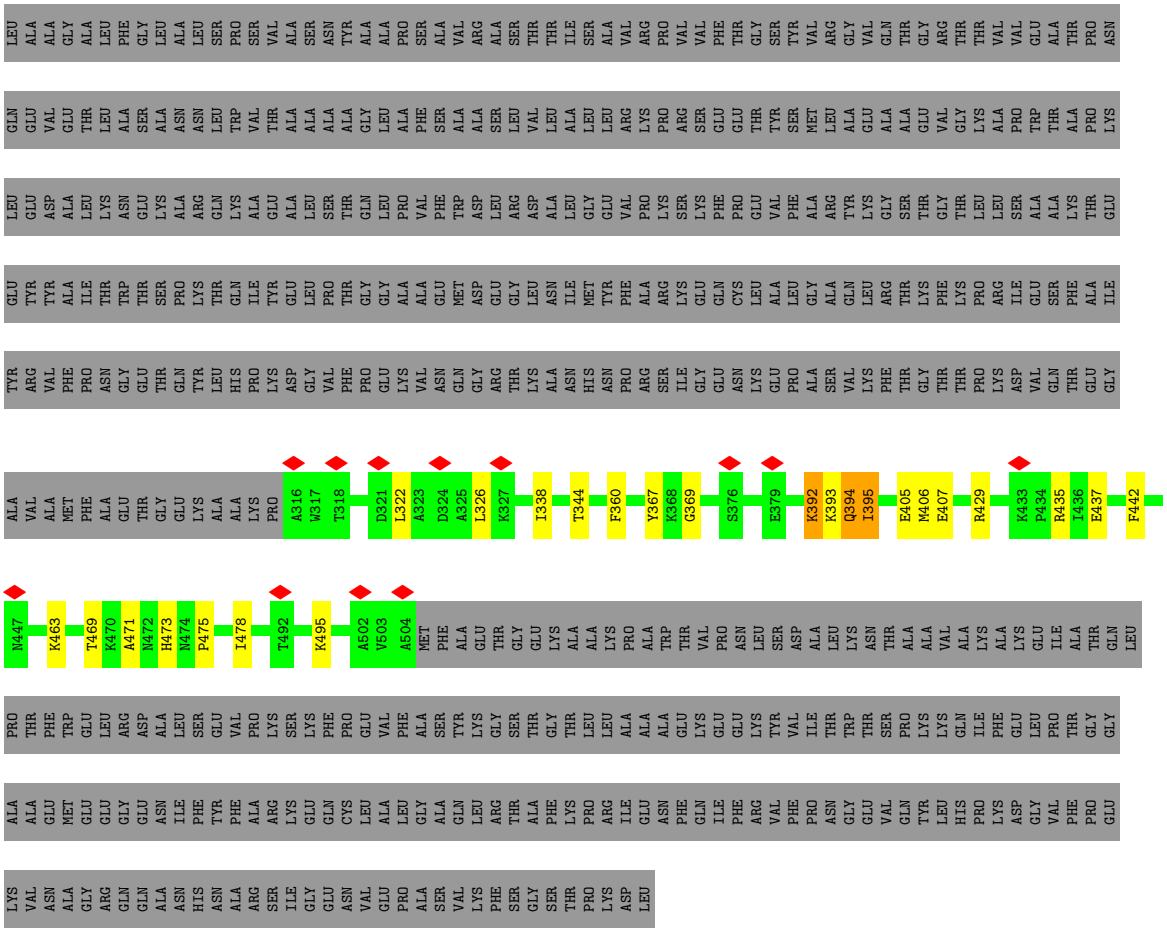
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



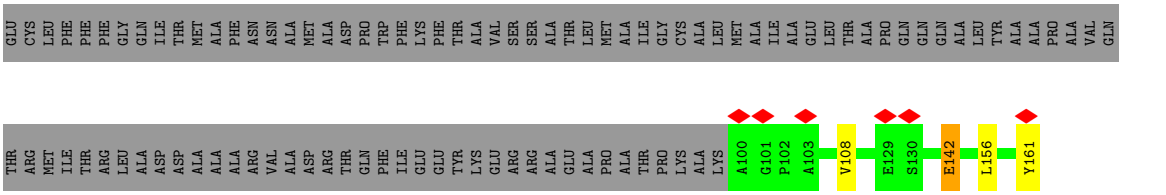
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



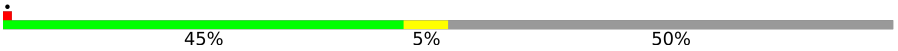
• Molecule 5: Photosystem I reaction center subunit IV

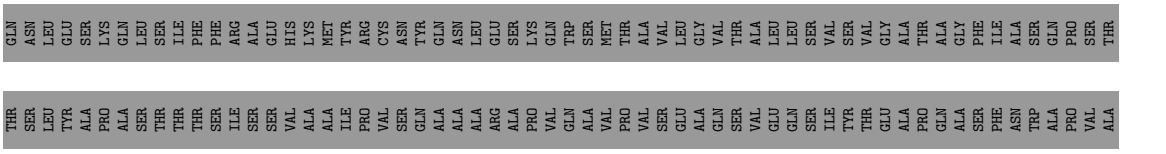
Chain E:

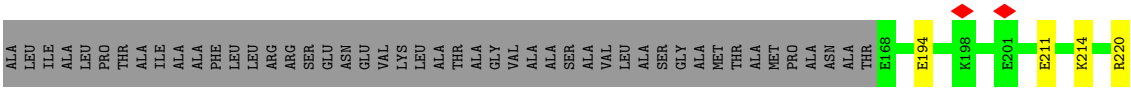


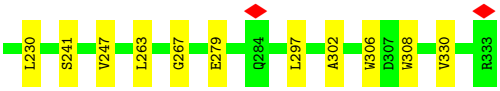
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



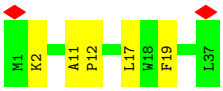






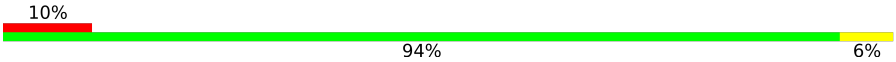
• Molecule 7: Photosystem I reaction center subunit IX

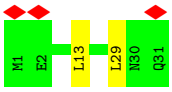
Chain J:



• Molecule 8: Photosystem I reaction center subunit XII

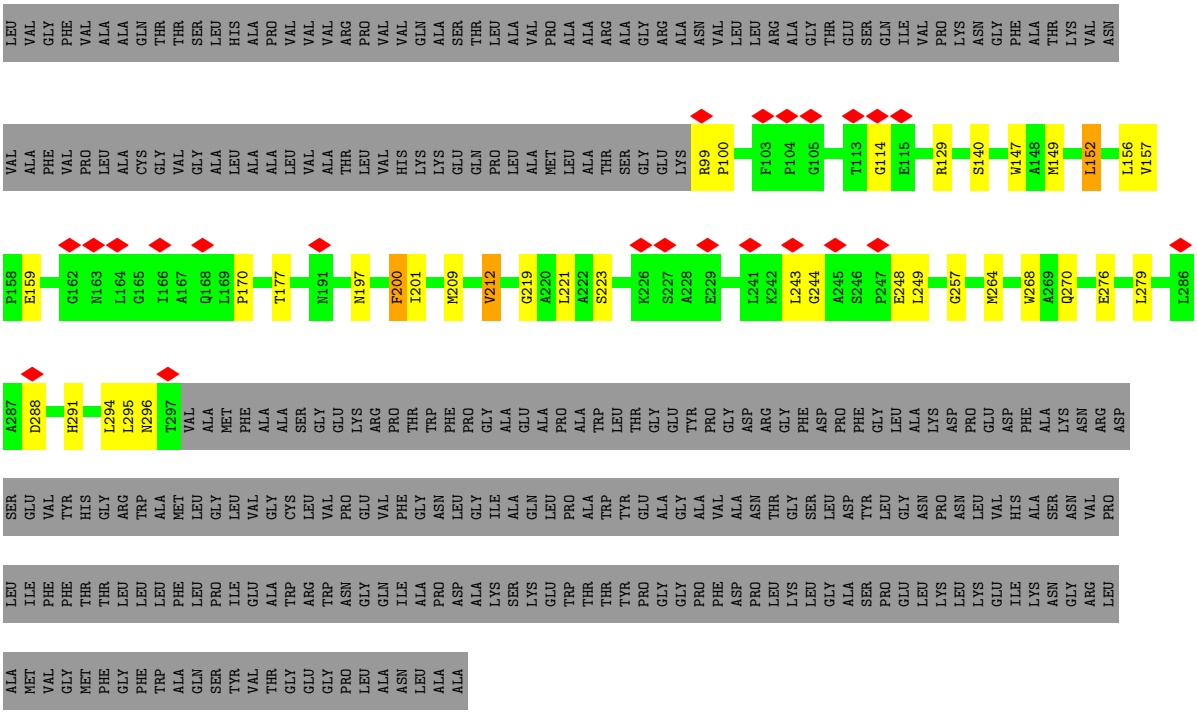
Chain M:





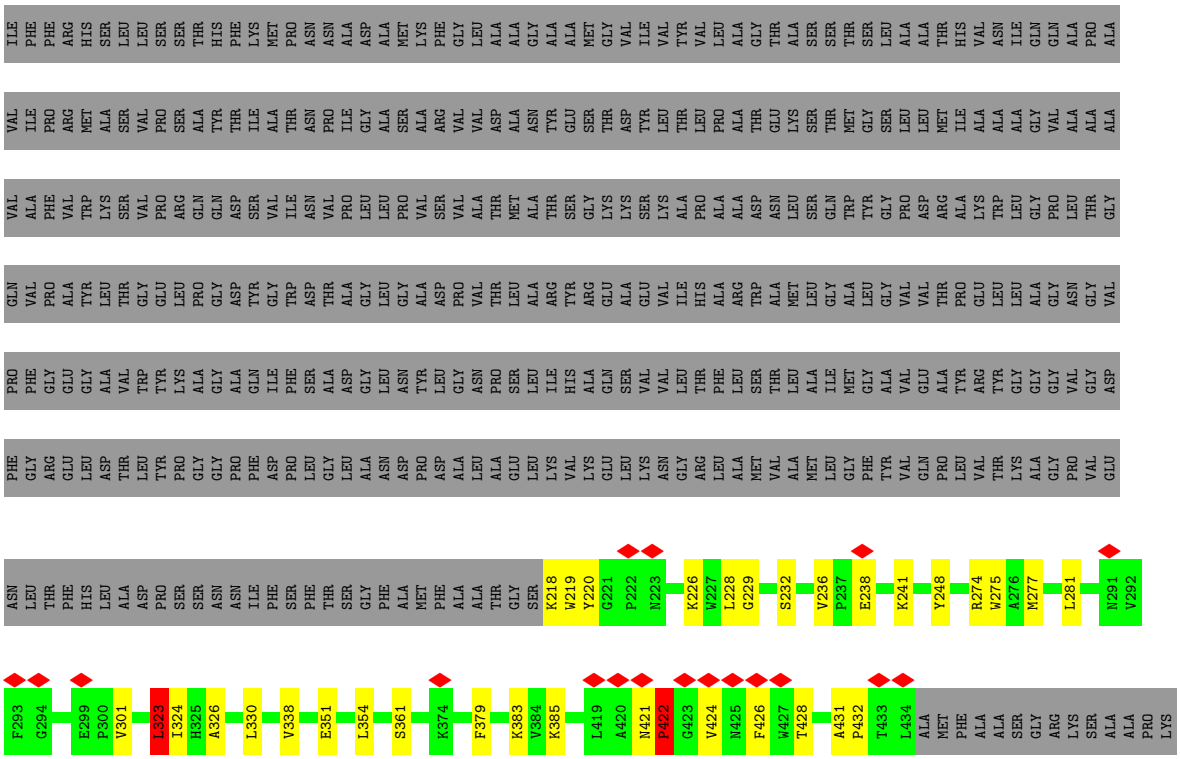
• Molecule 9: LHCI-1

Chain 1:



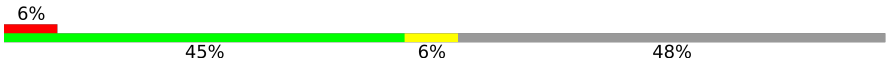
• Molecule 10: LHCI-2

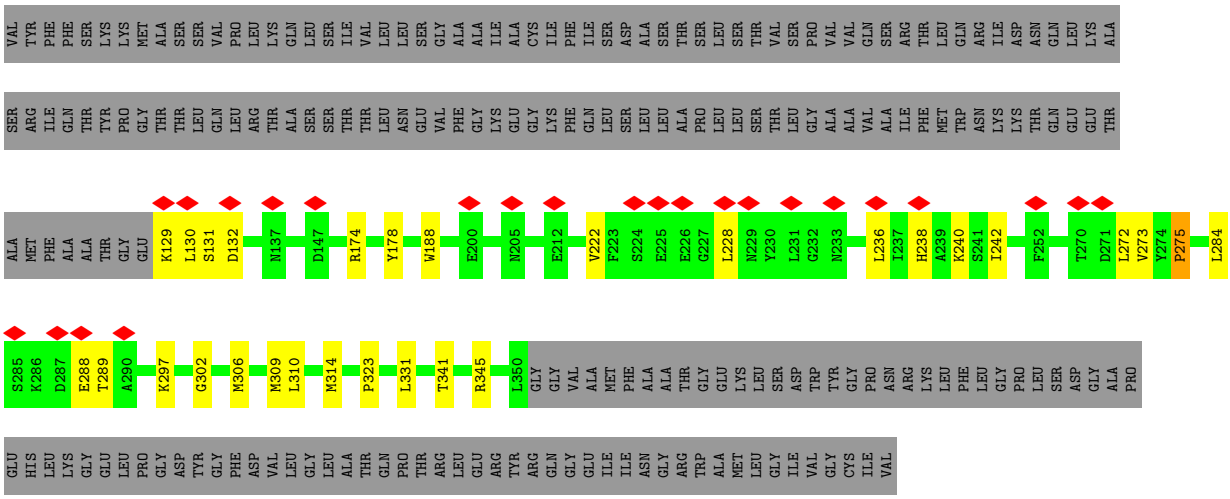
Chain 2:



- Molecule 11: LHCI-3

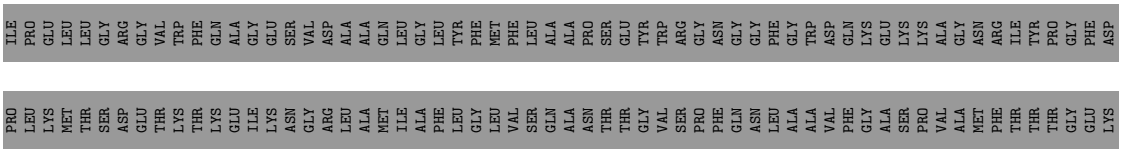
Chain 3:

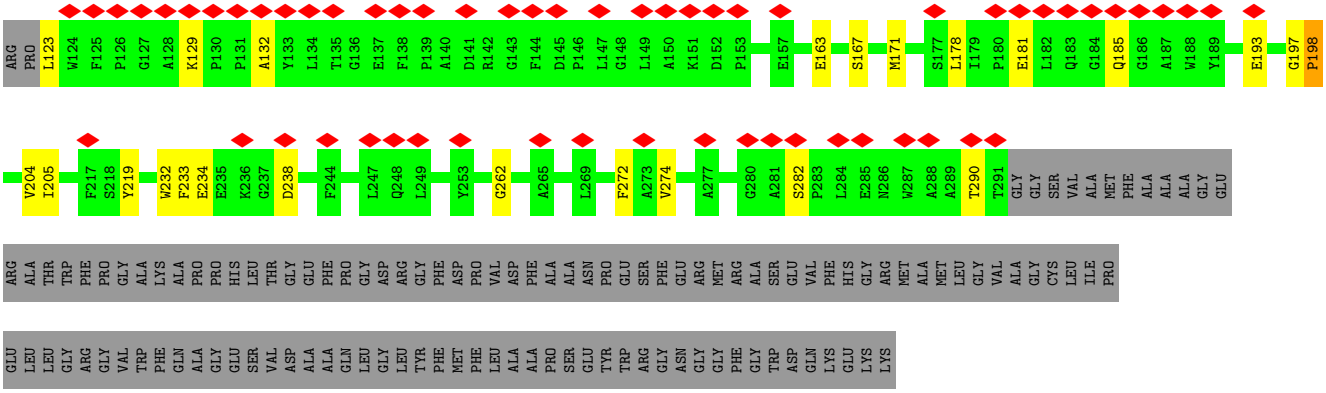




- Molecule 12: LHCI-4

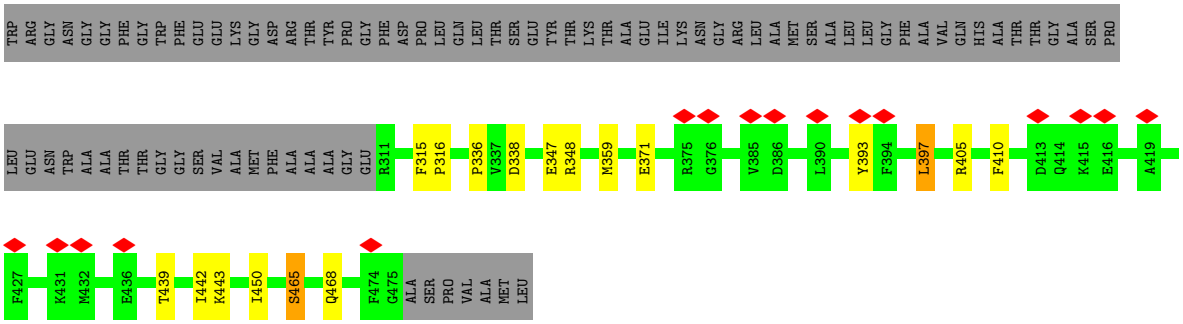
Chain 4:





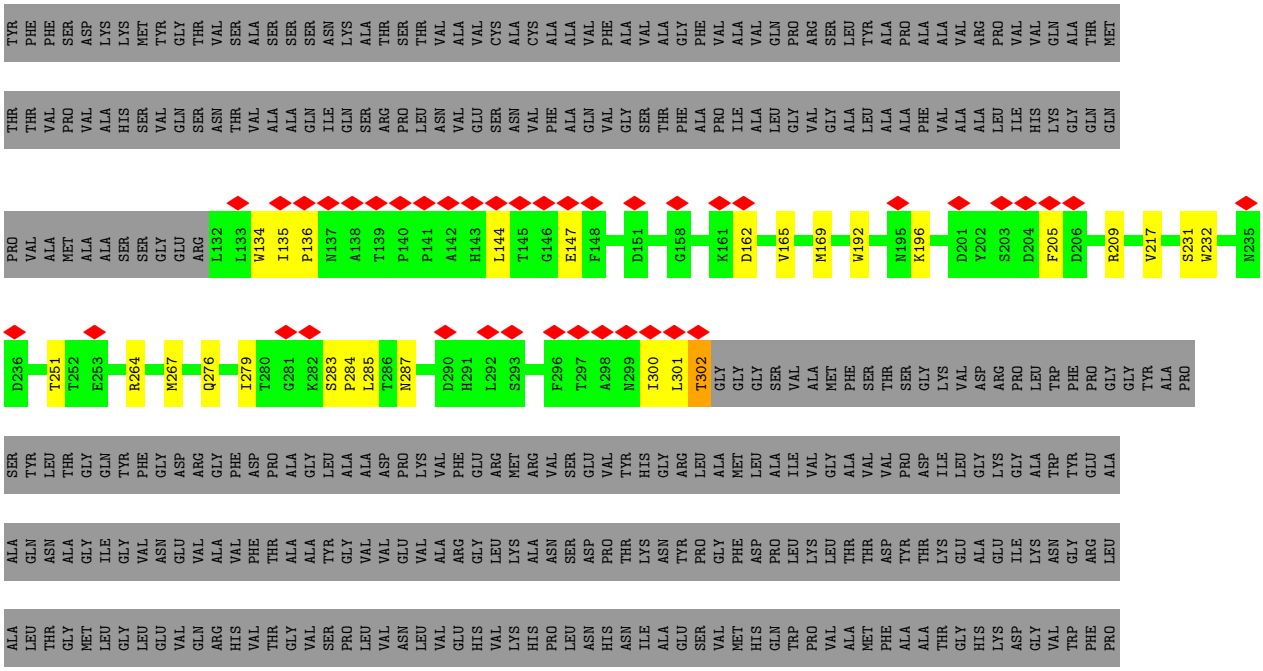
- Molecule 13: Chloroplast light-harvesting complex I protein

Chain 5:



- Molecule 14: LHCI-6

Chain 6:



GLY ALA GLN PRO PRO ALA HIS LEU THR GLY GLU TYR PRO ALA ASP ARG GLY PHE ASP PRO LEU SER LEU ALA ALA ASP PRO THR VAL TYR ALA ARG MET ARG VAL SER GLU VAL PHE HIS ALA ARG LEU SER MET LEU ALA ILE VAL GLY SER ILE VAL PRO GLU LEU LEU GLY LYS GLY

ALA TRP PHE GLU VAL GLY ASN SER VAL ASP GLY GLY ILE LYS LEU GLY PHE ILE LEU MET ALA ILE ALA ALA PRO THR GLU TYR TRP ARG GLY ASN GLY GLY PHE ASN TRP ASP LYS GLY THR ALA ASP ARG SER TYR PRO GLY PHE ASP PRO LEU LYS LEU THR THR ASP TYR THR LYS ALA

ALA GLU ILE LYS ASN GLY ARG LEU ALA MET THR GLY LEU LEU GLY LEU THR PHE GLN TYR LEU ALA THR GLY GLU SER PRO LEU ALA ASN LEU ALA ALA HIS LEU ALA ASN PRO VAL GLY ALA ASN ILE THR THR THR THR LEU ALA MET TYR SER THR SER GLY GLU LYS TYR ARG GLY LEU

TRP PHE PRO ASN ILE THR PRO PRO ALA TYR LEU THR GLY GLU PHE PRO ALA ASP ARG GLY PHE ASP PRO ALA GLY LEU ALA ALA ASP PRO LYS VAL TYR GLU ARG MET ARG VAL ALA GLU VAL PHE ASN GLY ARG LEU ALA ILE VAL GLY CYS VAL TYR PRO GLU GLU LEU LEU

GLY ASN GLY VAL TRP PHE GLU VAL TRP ASN LYS VAL ASP PHE TYR ARG PHE ALA LEU ILE SER LEU GLN VAL VAL ALA PRO LEU GLU GLU TYR TRP ARG GLY ASN GLY GLY PHE GLY TRP ASP GLY VAL GLU GLU LYS TYR ASP ARG SER TYR PRO GLY PHE ASP PRO CYS ASN LEU THR THR GLU

TYR THR LYS ALA ALA GLU ILE LYS ASN GLY ARG LEU ALA MET ILE GLY MET PHE GLY LEU GLU VAL GLN ASN HIS VAL THR ALA GLN GLY PRO VAL ALA ASN LEU ILE GLU HIS LEU ARG HIS PRO LEU ALA ALA ASN ILE GLY ALA SER LEU ALA HIS PRO TRP PRO PRO VAL ALA MET

PHE ALA THR THR GLY HIS LYS ASP GLY VAL TRP PHE PRO GLY ALA GLN PRO PRO ALA HIS LEU

- Molecule 15: LHCI-7

Chain 7:

GLU ILE LYS ASN GLY ARG LEU ALA MET THR ALA MET LEU GLY LEU GLU VAL GLN SER HIS ILE THR GLY LYS SER PRO LEU THR ASN LEU SER GLU HIS LEU SER HIS PRO LEU SER ALA ASN LEU LEU THR GLY GLY GLY SER LEU ALA MET PHE SER THR ALA GLY GLN LYS THR ASP

ARG ARG PRO LEU TRP PHE PRO GLY GLY TYR ALA PRO SER TRP LEU THR GLY GLN HIS PHE GLY ASP ARG GLY PHE ASP PRO ALA GLY LEU ALA ALA ASP PRO LYS VAL PHE GLU ARG MET ARG VAL SER GLU VAL TYR HIS GLY ARG LEU ALA MET LEU LEU ALA ILE VAL GLY ALA VAL VAL

PRO ASP ILE GLN GLY LYS GLY ALA TRP TYR GLU ALA ALA GLN SER ALA GLY ILE GLY VAL ASN GLU VAL ALA VAL PHE THR ALA ALA TYR GLY ILE ALA GLU VAL ALA ARG GLY LEU LYS ALA ASN SER ASP PRO THR SER ARG TYR PRO GLY PHE ASP PRO LEU ASN LEU THR THR ASP

TYR THR LYS GLU ALA GLU ILE LYS ASN GLY ARG LEU ALA LEU THR ALA MET LEU GLY LEU GLU VAL GLN ARG HIS VAL THR GLY VAL SER PRO LEU VAL ASN LEU VAL GLU HIS VAL LYS HIS PRO LEU GLY HIS ASN ILE ALA GLU SER VAL MET HIS GLN TRP PRO VAL ALA MET PHE

ALA ALA THR GLY HIS LYS ASP GLY VAL TRP PHE PRO GLY ALA THR PRO PRO ALA HIS LEU THR GLY GLU TYR PRO ALA ASP ARG GLY PHE ASP PRO LEU SER LEU ALA ALA ASP PRO THR VAL TYR ALA ARG MET ARG VAL SER GLU VAL PHE HIS ALA ARG LEU SER MET LEU ALA ILE

VAL GLY ALA ILE VAL PRO GLU GLU VAL LEU GLY LYS GLY ALA TRP PHE GLU ALA GLY ASN SER VAL ASP GLY ILE LYS LEU GLY PHE ILE ALA MET ALA ILE ALA ALA PRO THR GLU TYR TRP ARG GLY ASN GLY GLY PHE ASN TRP ASP LYS GLY ALA ALA ASP ARG SER TYR PRO GLY PHE

ASP PRO LEU LYS LEU THR THR ASP TYR THR LYS ALA ALA GLU ILE LYS ASN GLY ARG LEU ALA MET ALA GLY LEU LEU GLY LEU THR PHE GLN TYR LEU ALA THR GLY GLU SER PRO LEU ALA ASN LEU ALA ALA HIS LEU ALA ASN PRO VAL GLY ALA ASN ILE THR THR THR LEU ALA

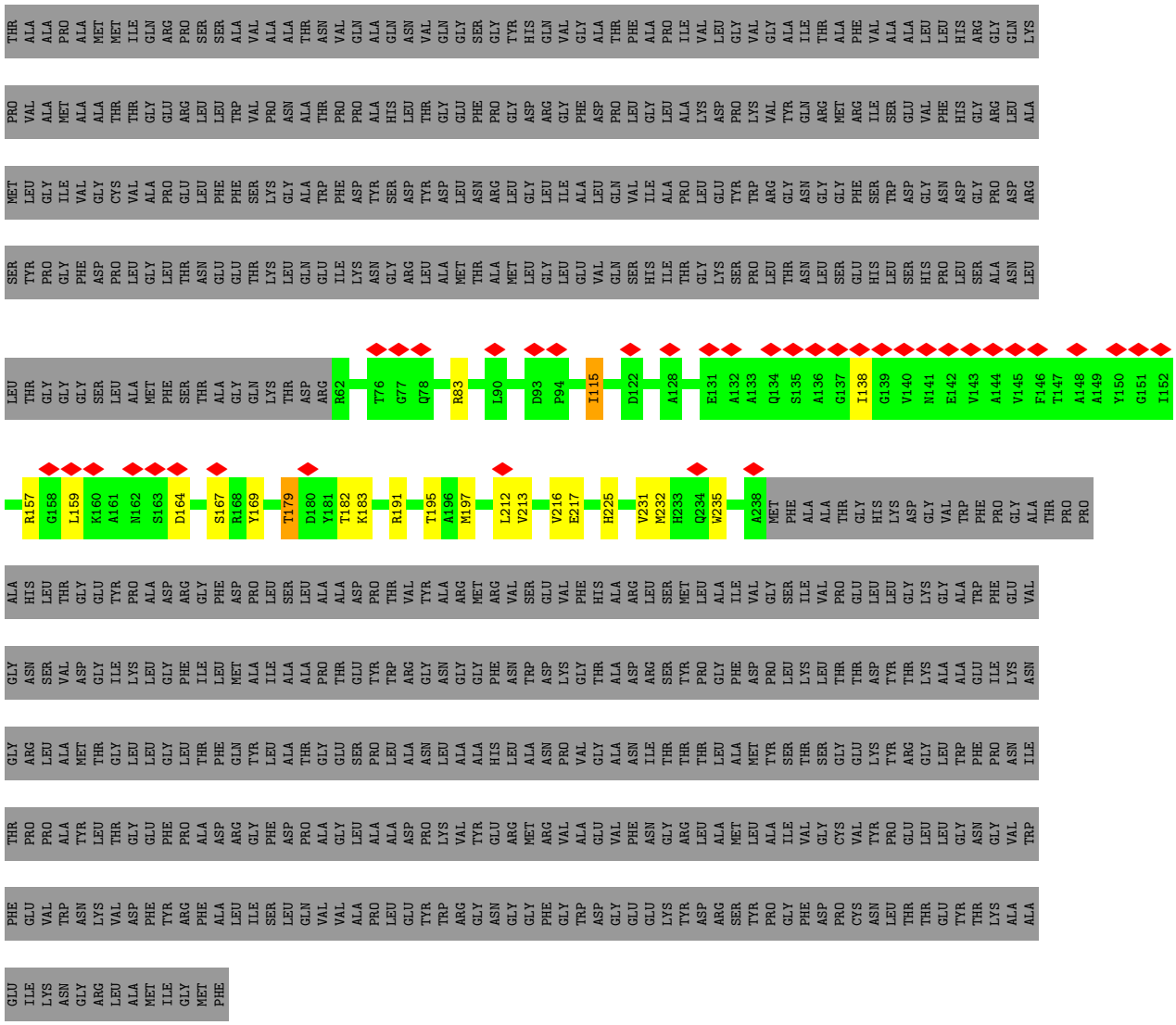
MET TYR SER THR SER GLY GLU K428 Y429 R430 F434 P435 T444 D450 D461 P462 E466 R467 I470 G476 D505 R508 Q515 V516 V517 Y522 W531 D532 G533 E534 E535 S540 K560 M566 L572 P583 L595 H605 P606 W607 PRO

PRO VAL ALA MET PHE ALA THR THR

- Molecule 16: LHCI-8

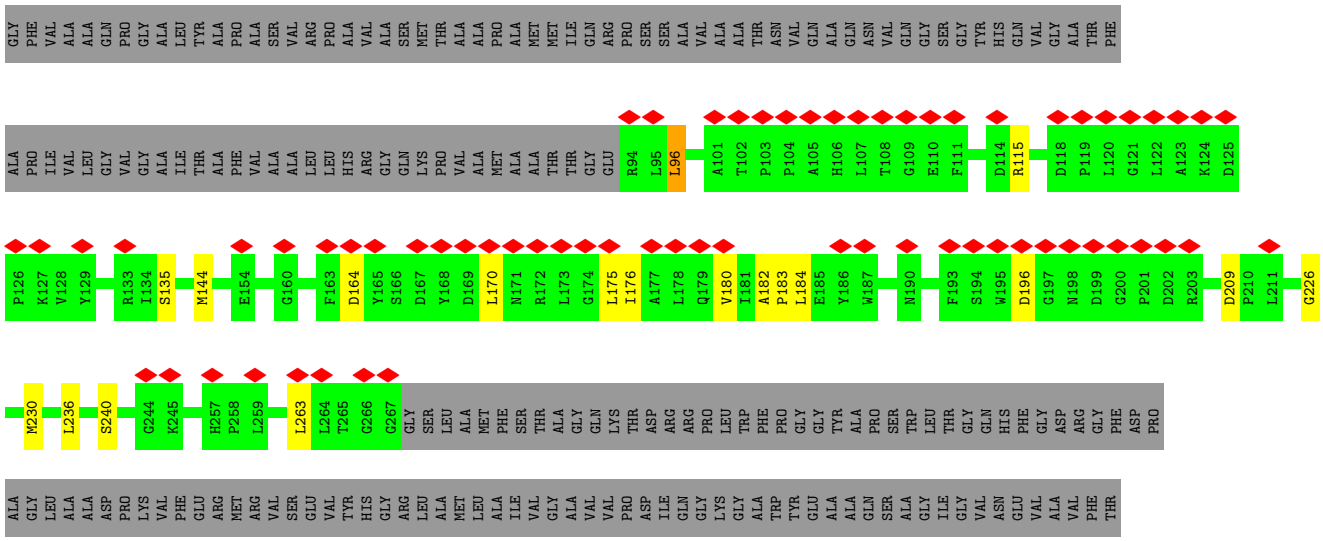
Chain 8:

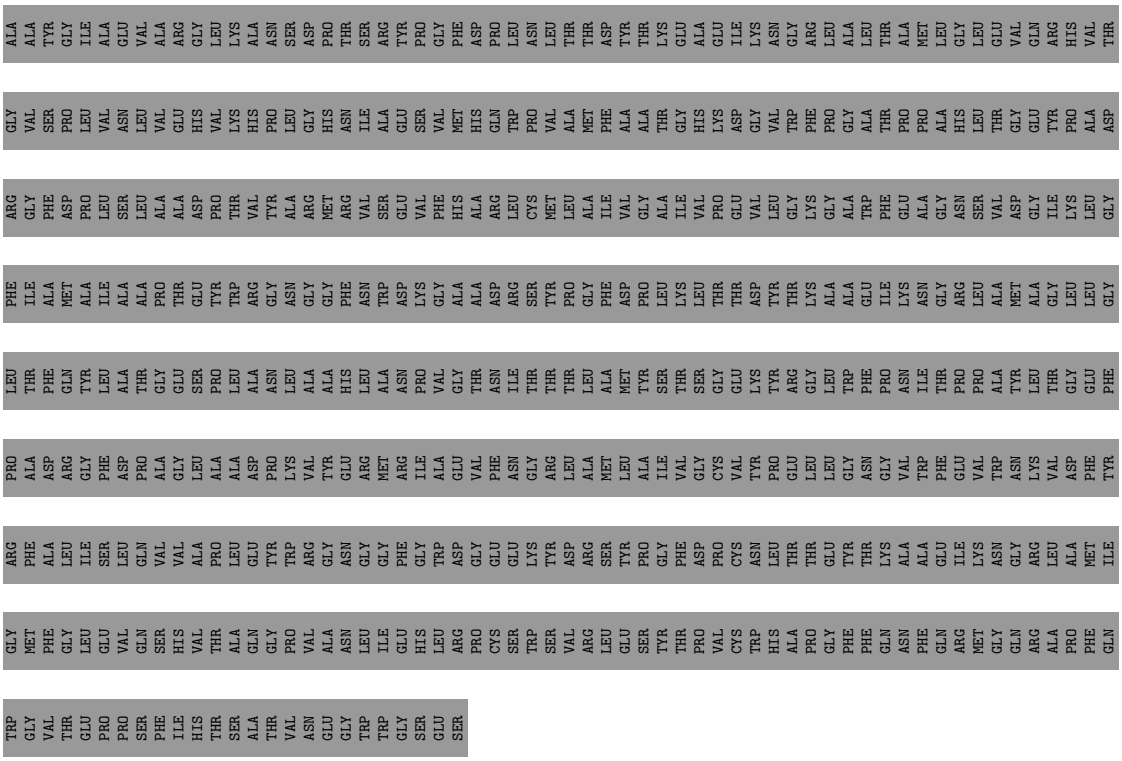
PHE PHE SER ILE GLU LYS LYS MET TYR GLY ALA ALA HIS ASN SER SER SER ASN LYS ASN ALA THR SER ILE VAL ALA PHE PHE GLY CYS ALA ALA VAL PHE ALA VAL ALA GLY PHE VAL ALA ALA GLN PRO GLY ALA LEU TYR ALA PRO ALA SER VAL ARG PRO ALA VAL ALA SER MET



- Molecule 17: LHCI-9

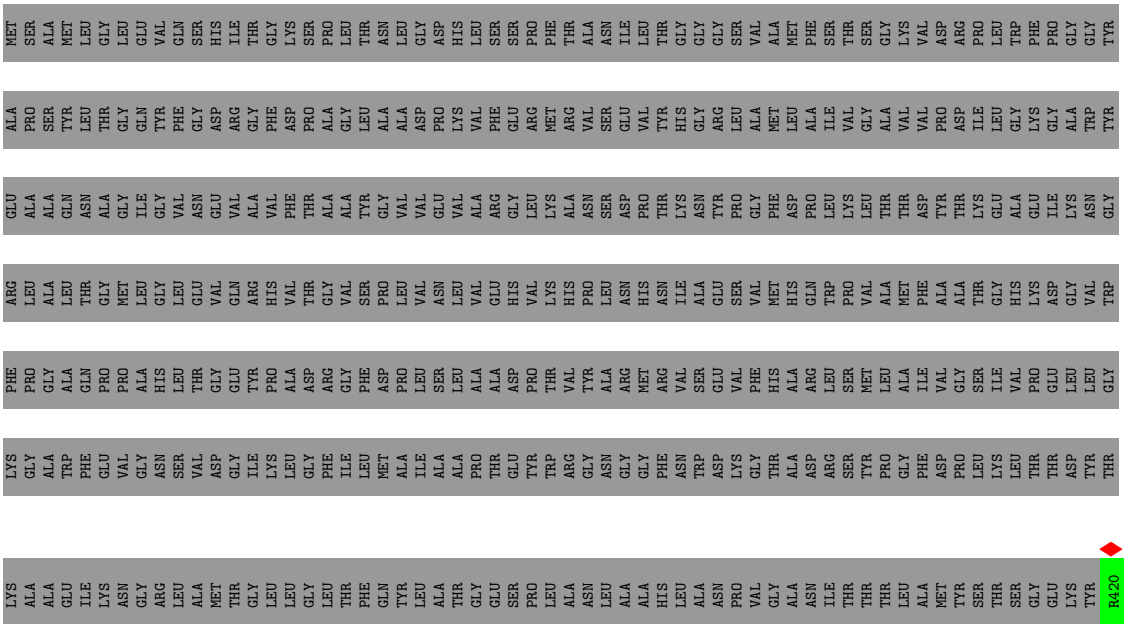
Chain 9:

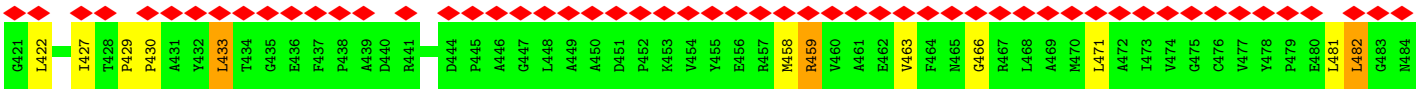


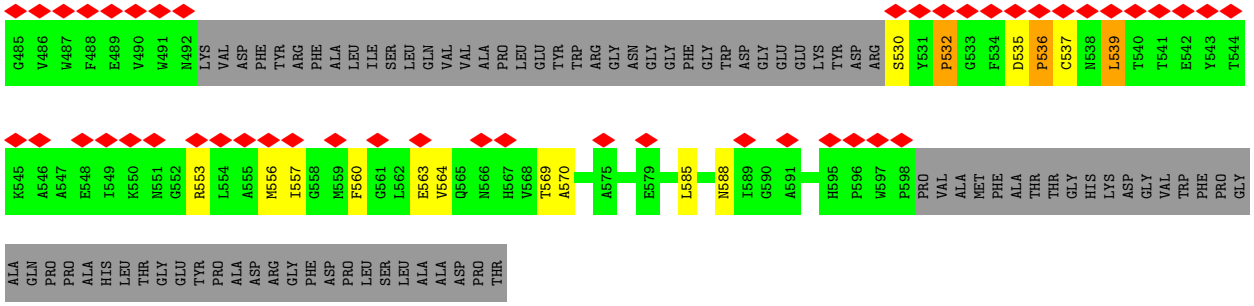


- Molecule 18: LHCI-10

Chain 10:

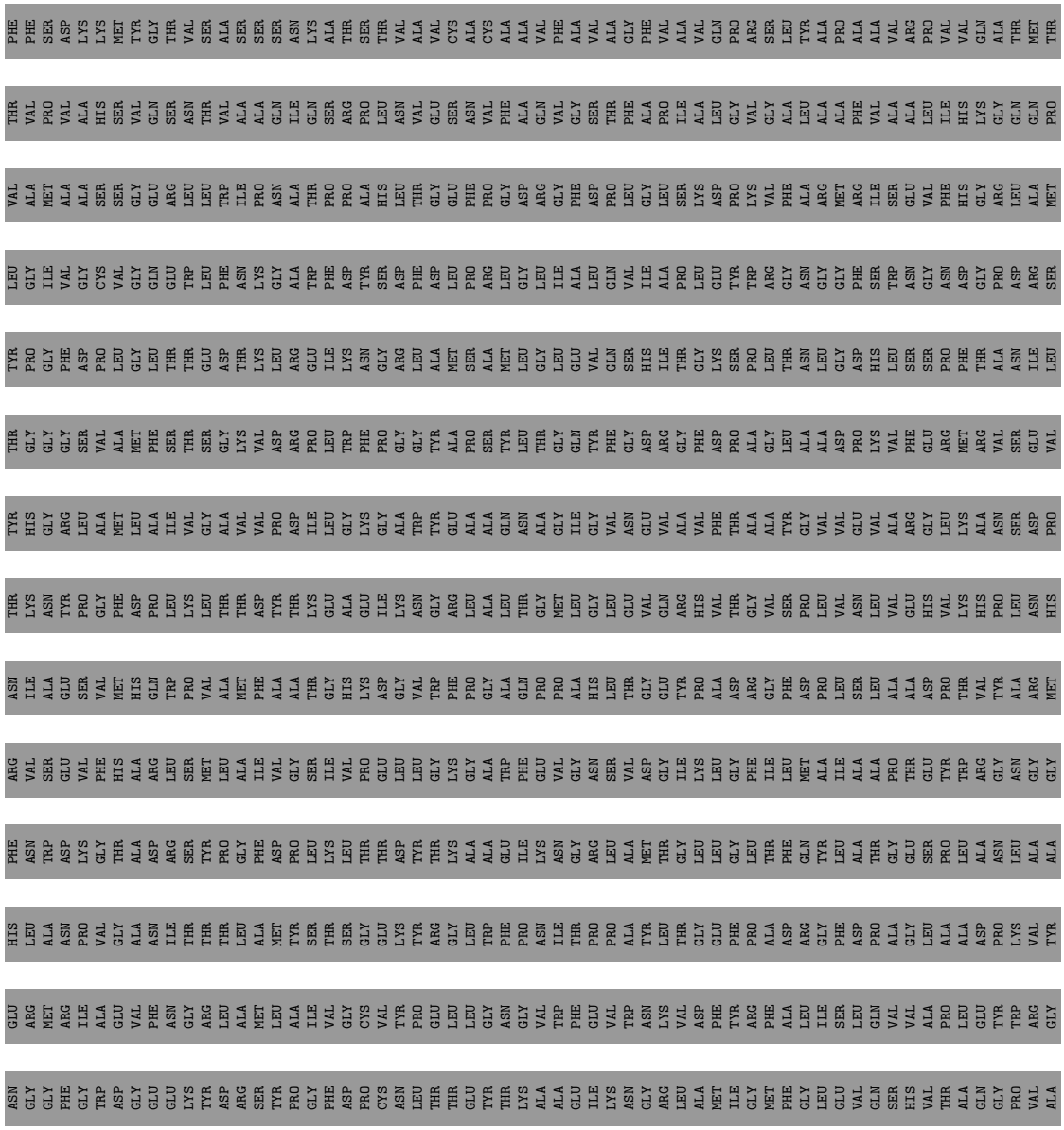


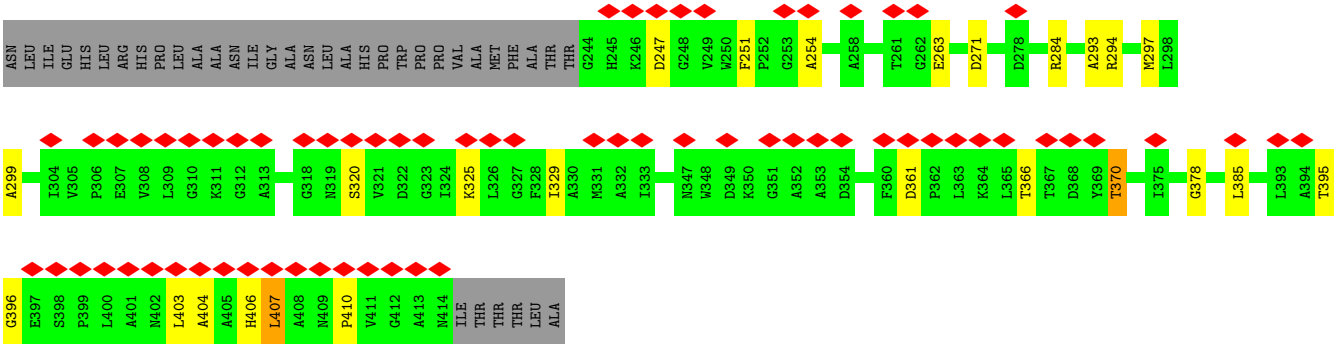




• Molecule 19: LHCI-11

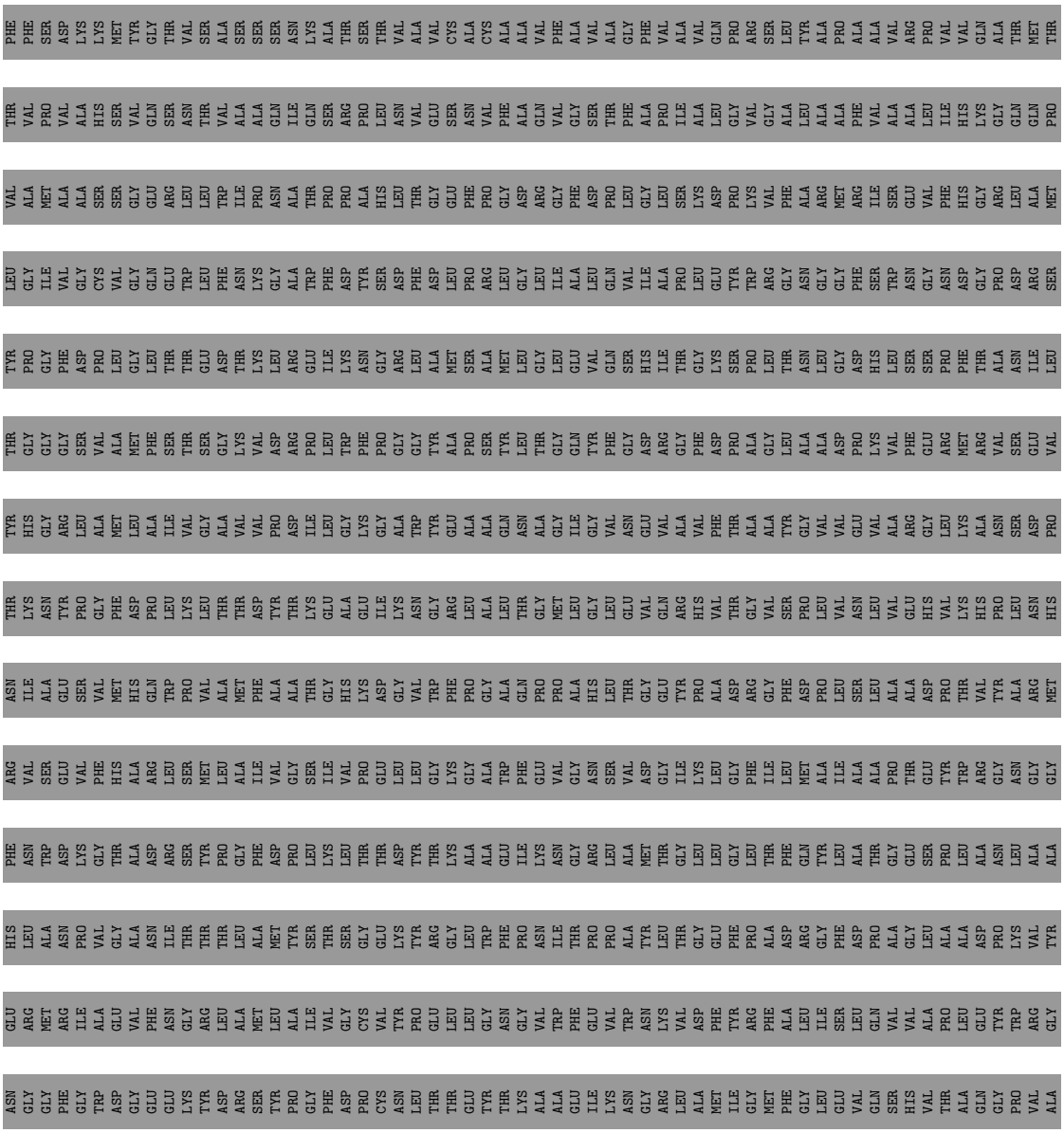
Chain 11:

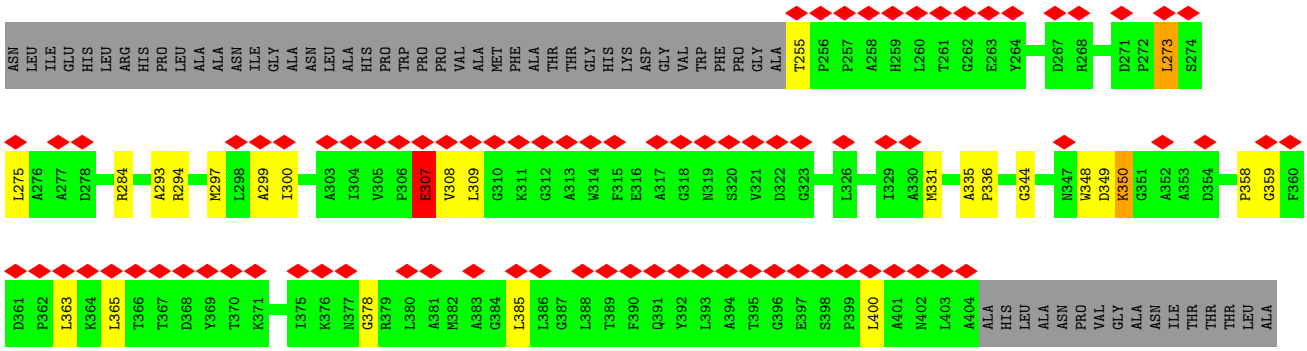




- Molecule 19: LHCI-11

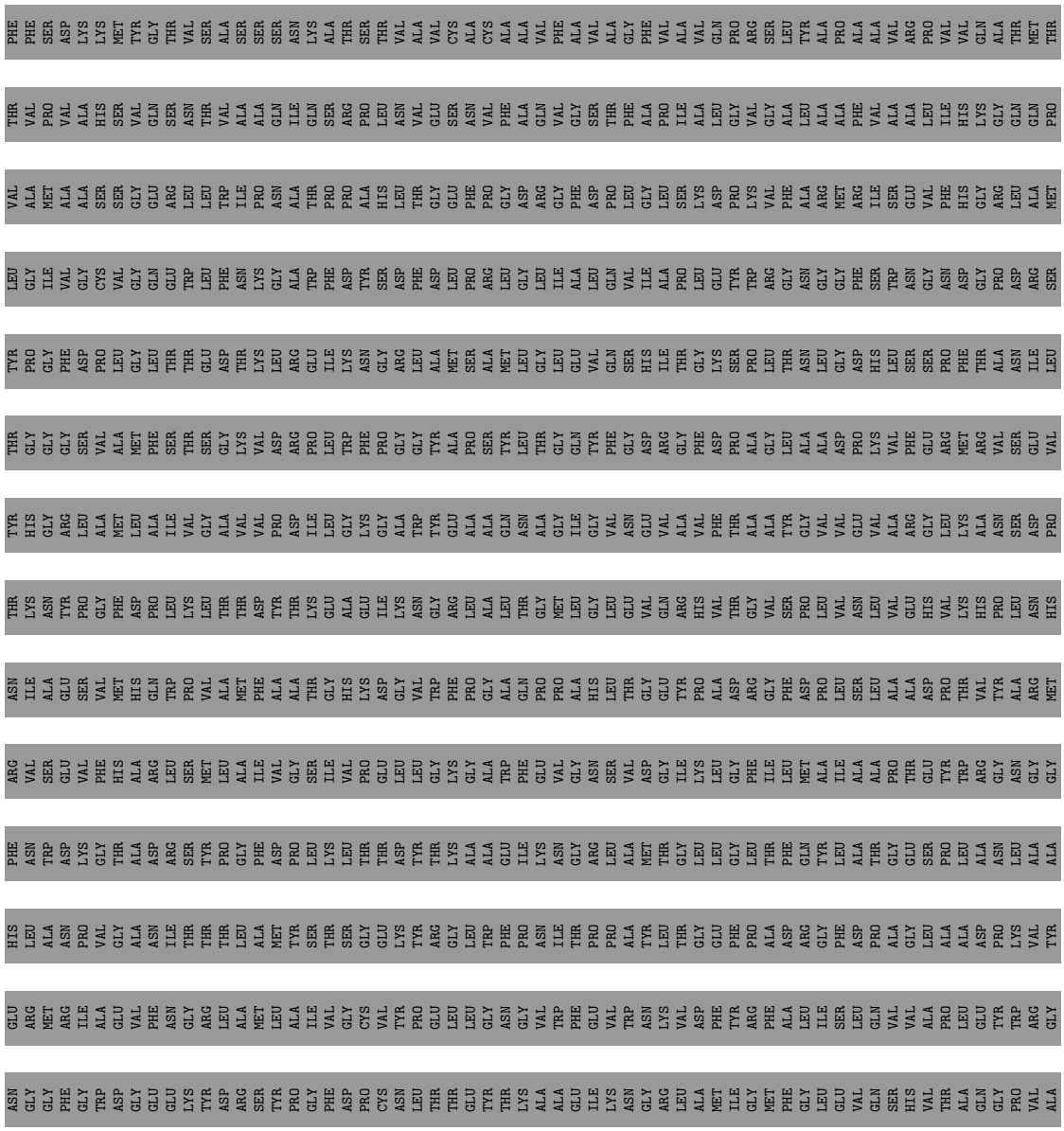
Chain 12:

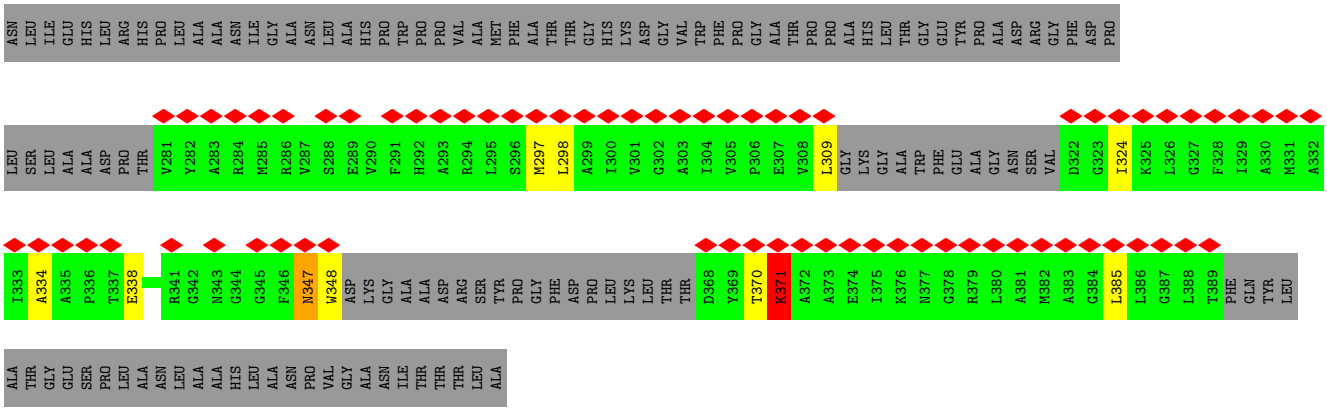




- Molecule 19: LHCI-11

Chain 13: 7% 6% 93%




ASN LEU ILE GLU HIS LEU ARG HIS PRO LEU ALA ALA ASN ILE GLY ALA ASN LEU ALA HIS PRO TRP PRO PRO VAL ALA MET PHE ALA THR THR GLY HIS LYS ASP GLY VAL TRP PHE PRO GLY ALA THR PRO PRO ALA HIS LEU THR GLY GLU TYR PRO ALA ASP ARG GLY PHE ASP PRO
LEU SER LEU ALA ALA ASP PRO THR V281 Y282 A283 R284 M285 R286 V287 S288 E289 V290 F291 H292 A293 R294 L295 S296 M297 L298 A299 I300 V301 G302 A303 I304 V305 P306 E307 V308 L309 GLY LYS GLY ALA TRP PHE GLU ALA GLY ASN SER VAL D322 G323 I324 K325 L326 G327 F328 I329 A330 M331 A332
I333 A334 A335 P336 T337 E338 R341 G342 N343 G344 G345 F346 N347 W348 ASP LYS GLY ALA ALA ASP ARG SER TYR PRO GLY PHE ASP PRO LEU LYS LEU THR THR D368 Y369 T370 K371 A372 A373 E374 I375 K376 N377 G378 R379 L380 A381 M382 A383 G384 L385 L386 G387 L388 T389 PHE GLN TYR LEU
ALA THR GLY GLU SER PRO LEU ALA ASN LEU ALA ALA HIS LEU ALA ASN PRO VAL GLY ALA ASN ILE THR THR THR LEU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	216.57599, 216.57599, 216.57599	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, BCR, PQN, UNL, LHG, DD6, CL0, CLA, SF4

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	0.78	0/6082	1.06	6/8290 (0.1%)
2	B	0.77	1/6073 (0.0%)	1.07	8/8282 (0.1%)
3	C	0.80	0/606	1.16	2/819 (0.2%)
4	D	0.56	0/1507	0.98	1/2042 (0.0%)
5	E	0.51	0/512	0.89	0/696
6	F	0.58	0/1292	0.96	0/1751
7	J	0.66	0/313	0.97	0/429
8	M	0.59	0/246	0.91	0/332
9	1	0.52	0/1561	0.91	2/2134 (0.1%)
10	2	0.57	0/1704	1.11	7/2323 (0.3%)
11	3	0.54	0/1732	0.96	3/2352 (0.1%)
12	4	0.51	0/1350	0.96	1/1836 (0.1%)
13	5	0.56	0/1306	0.95	0/1765
14	6	0.51	0/1366	0.93	0/1857
15	7	0.61	0/1474	1.02	3/2009 (0.1%)
16	8	0.49	0/1388	0.95	0/1893
17	9	0.49	0/1388	0.93	2/1886 (0.1%)
18	10	0.51	0/1137	1.04	3/1554 (0.2%)
19	11	0.54	0/1314	0.96	0/1791
19	12	0.52	0/1157	1.01	1/1575 (0.1%)
19	13	0.51	0/604	0.94	1/813 (0.1%)
All	All	0.64	1/34112 (0.0%)	1.01	40/46429 (0.1%)

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
1	A	0	3
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
10	2	0	1
12	4	0	1
16	8	0	1
19	12	0	2
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	598	HIS	CG-CD2	-5.10	1.30	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	2	422	PRO	N-CA-CB	-18.37	83.96	103.25
10	2	422	PRO	N-CD-CG	-11.53	85.91	103.20
18	10	536	PRO	CB-CG-CD	-10.82	71.49	106.10
18	10	536	PRO	CA-N-CD	-10.76	96.93	112.00
3	C	62	PHE	CA-CB-CG	-9.64	104.16	113.80
10	2	422	PRO	CA-N-CD	-8.73	99.78	112.00
10	2	422	PRO	CB-CG-CD	-8.42	79.16	106.10
17	9	209	ASP	CA-CB-CG	7.55	120.15	112.60
18	10	536	PRO	N-CA-CB	-7.52	95.36	103.25
2	B	558	PRO	CB-CA-C	-7.39	101.31	113.06
2	B	373	THR	CA-CB-OG1	-6.97	99.14	109.60
2	B	345	THR	CA-CB-OG1	-6.97	99.14	109.60
10	2	422	PRO	N-CA-C	6.85	126.58	112.47
12	4	198	PRO	N-CA-CB	-6.48	96.45	103.25
1	A	372	TYR	N-CA-CB	6.43	119.84	110.26
2	B	457	PRO	CB-CA-C	-6.35	104.46	113.09
1	A	392	THR	CA-CB-OG1	-6.19	100.32	109.60
2	B	64	ASN	N-CA-C	-6.12	104.53	111.14
4	D	475	PRO	N-CA-CB	-6.03	98.77	102.81
19	13	371	LYS	N-CA-C	-5.96	105.31	113.30
10	2	323	LEU	CA-C-N	-5.85	116.96	123.16
10	2	323	LEU	C-N-CA	-5.85	116.96	123.16
1	A	676	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	A	564	PRO	N-CA-C	5.60	120.86	113.86
11	3	132	ASP	N-CA-C	-5.44	106.59	113.18
17	9	209	ASP	CB-CA-C	5.40	118.97	110.71
19	12	307	GLU	CB-CA-C	5.26	115.95	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	3	131	SER	N-CA-C	-5.21	107.94	114.56
2	B	93	ASP	CA-CB-CG	5.17	117.77	112.60
15	7	522	TYR	N-CA-C	-5.13	105.58	111.07
15	7	462	PRO	N-CA-C	5.13	120.28	113.57
2	B	605	ASN	CA-CB-CG	5.11	117.71	112.60
3	C	62	PHE	CB-CA-C	5.11	120.58	110.42
11	3	309	MET	N-CA-C	-5.10	105.80	111.36
2	B	689	ASN	CB-CA-C	-5.10	100.28	110.42
1	A	20	ASN	O-C-N	-5.07	119.20	121.53
1	A	386	THR	N-CA-C	-5.07	105.66	111.14
9	1	156	LEU	CA-C-N	5.02	123.40	120.24
9	1	156	LEU	C-N-CA	5.02	123.40	120.24
15	7	606	PRO	N-CA-C	5.02	121.23	113.75

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	12	349	ASP	Peptide
19	12	350	LYS	Peptide
10	2	421	ASN	Peptide
12	4	197	GLY	Peptide
16	8	157	ARG	Sidechain
1	A	572	ARG	Sidechain
1	A	690	ARG	Sidechain
1	A	716	ARG	Sidechain
2	B	410	ARG	Sidechain
3	C	61	ASP	Peptide
3	C	75	ARG	Sidechain

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	5881	0	5748	39	0
2	B	5863	0	5664	50	0
3	C	596	0	571	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1471	0	1460	15	0
5	E	500	0	476	3	0
6	F	1266	0	1299	10	0
7	J	304	0	317	2	0
8	M	242	0	258	2	0
9	1	1513	0	1464	22	0
10	2	1654	0	1635	22	0
11	3	1689	0	1700	13	0
12	4	1308	0	1256	10	0
13	5	1269	0	1228	12	0
14	6	1327	0	1300	13	0
15	7	1427	0	1379	13	0
16	8	1350	0	1326	12	0
17	9	1350	0	1322	8	0
18	10	1102	0	1071	16	0
19	11	1277	0	1248	15	0
19	12	1127	0	1111	20	0
19	13	594	0	608	7	0
20	A	65	0	72	2	0
21	1	727	0	586	21	0
21	10	470	0	369	11	0
21	11	555	0	480	13	0
21	12	383	0	304	12	0
21	13	139	0	103	3	0
21	2	724	0	577	30	0
21	3	712	0	565	22	0
21	4	525	0	415	14	0
21	5	530	0	418	14	0
21	6	581	0	464	13	0
21	7	650	0	540	16	0
21	8	598	0	499	11	0
21	9	635	0	513	11	0
21	A	2561	0	2534	92	0
21	B	2179	0	2080	64	0
21	F	141	0	107	5	0
21	J	45	0	33	1	0
22	A	33	0	46	2	0
22	B	31	0	39	0	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	A	240	0	336	21	0
24	B	240	0	336	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	80	0	112	5	0
24	J	80	0	112	8	0
24	M	40	0	56	2	0
25	1	36	0	42	0	0
25	10	32	0	34	0	0
25	11	30	0	30	0	0
25	2	30	0	30	1	0
25	3	25	0	20	1	0
25	4	19	0	11	3	0
25	5	32	0	34	0	0
25	6	28	0	26	0	0
25	7	48	0	69	0	0
25	8	33	0	36	0	0
25	9	34	0	38	0	0
25	A	76	0	98	1	0
25	B	23	0	16	0	0
26	1	42	0	0	0	0
26	10	26	0	0	0	0
26	2	42	0	0	0	0
26	6	47	0	0	0	0
26	7	67	0	0	0	0
26	8	46	0	0	0	0
26	9	15	0	0	0	0
26	A	97	0	0	0	0
26	B	62	0	0	0	0
26	D	6	0	0	0	0
26	F	9	0	0	0	0
26	M	20	0	0	0	0
27	B	57	0	75	3	0
28	1	129	0	0	1	0
28	11	86	0	0	1	0
28	12	86	0	0	0	0
28	2	129	0	0	0	0
28	3	129	0	0	1	0
28	4	86	0	0	2	0
28	5	86	0	0	0	0
28	6	86	0	0	1	0
28	7	86	0	0	0	0
28	8	86	0	0	0	0
28	9	86	0	0	0	0
28	J	43	0	0	0	0
29	1	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	11	1	0	0	0	0
29	2	4	0	0	0	0
29	3	4	0	0	0	0
29	4	3	0	0	0	0
29	5	2	0	0	0	0
29	6	1	0	0	0	0
29	7	2	0	0	0	0
29	8	2	0	0	0	0
29	9	2	0	0	0	0
29	A	7	0	0	0	0
29	B	9	0	0	0	0
29	D	1	0	0	1	0
29	F	1	0	0	0	0
29	J	1	0	0	0	0
All	All	48242	0	44696	585	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 6.

All (585) 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)
16:8:83:ARG:HD2	21:8:603:CLA:O1D	1.69	0.93
10:2:218:LYS:O	10:2:218:LYS:NZ	2.08	0.85
1:A:197:MET:HE1	21:A:826:CLA:H142	1.60	0.81
21:2:505:CLA:HBB1	21:2:505:CLA:HHC	1.64	0.79
21:B:831:CLA:HBC2	21:B:831:CLA:HHD	1.62	0.79
2:B:387:PHE:CZ	24:B:845:BCR:H373	2.18	0.77
19:13:347:ASN:HD22	19:13:348:TRP:N	1.83	0.76
11:3:130:LEU:HD11	11:3:289:THR:HA	1.69	0.75
2:B:387:PHE:CE2	24:B:845:BCR:H373	2.22	0.74
5:E:142:GLU:CD	5:E:142:GLU:H	1.96	0.73
21:A:804:CLA:HHC	21:A:804:CLA:HBB1	1.69	0.73
4:D:473:HIS:NE2	29:D:801:HOH:O	2.20	0.73
21:B:838:CLA:HHC	21:B:838:CLA:HBB1	1.71	0.72
21:A:817:CLA:HHC	21:A:817:CLA:HBB1	1.72	0.72
12:4:167:SER:OG	12:4:262:GLY:HA3	1.91	0.71
21:F:401:CLA:HHC	21:F:401:CLA:HBB1	1.71	0.70
1:A:671:MET:HE1	24:A:852:BCR:H352	1.74	0.69
24:A:852:BCR:H382	24:A:852:BCR:H23C	1.74	0.69
4:D:395:ILE:HD13	4:D:405:GLU:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:836:CLA:HHC	21:A:836:CLA:HBB1	1.74	0.69
21:1:507:CLA:H2	21:1:517:CLA:HBD	1.75	0.69
21:9:910:CLA:HHC	21:9:910:CLA:HBB1	1.75	0.69
21:B:831:CLA:H191	21:B:835:CLA:H13	1.76	0.68
4:D:435:ARG:HD2	4:D:437:GLU:OE2	1.93	0.68
21:A:821:CLA:O1A	13:5:336:PRO:HB3	1.94	0.67
21:A:819:CLA:HBB1	21:A:819:CLA:HHC	1.76	0.67
21:3:710:CLA:HHC	21:3:710:CLA:HBB1	1.77	0.67
10:2:323:LEU:O	21:2:515:CLA:O1D	2.13	0.66
21:B:823:CLA:H2A	21:B:823:CLA:O1A	1.96	0.66
24:A:847:BCR:HC41	24:A:848:BCR:H23C	1.75	0.66
15:7:516:VAL:HA	21:7:713:CLA:HBC3	1.77	0.66
9:1:147:TRP:CE2	21:1:508:CLA:HED2	2.30	0.66
21:7:708:CLA:CGA	21:7:708:CLA:H3A	2.26	0.66
19:11:403:LEU:O	19:11:407:LEU:HD23	1.96	0.66
21:B:829:CLA:HBC2	24:B:844:BCR:H393	1.78	0.65
21:B:807:CLA:HAA1	21:B:807:CLA:HBD	1.78	0.65
24:A:852:BCR:H362	21:A:862:CLA:C4	2.26	0.65
19:11:325:LYS:O	19:11:329:ILE:HD12	1.97	0.65
21:7:707:CLA:HHC	21:7:707:CLA:HBB1	1.78	0.65
21:A:812:CLA:HHC	21:A:812:CLA:HBB1	1.79	0.64
21:A:828:CLA:HHC	21:A:828:CLA:HBB1	1.79	0.64
21:B:830:CLA:HBC3	24:F:405:BCR:H17C	1.78	0.64
9:1:295:LEU:HD23	21:1:514:CLA:HED1	1.79	0.64
14:6:217:VAL:HA	21:6:914:CLA:HBC3	1.80	0.64
21:2:511:CLA:HHC	21:2:511:CLA:HBB1	1.80	0.63
14:6:135:ILE:HB	14:6:136:PRO:HD2	1.80	0.63
21:2:503:CLA:HBB1	21:2:503:CLA:HHC	1.79	0.63
21:A:803:CLA:HBA1	2:B:426:THR:HG22	1.80	0.63
21:A:840:CLA:HMB1	21:A:840:CLA:HBB1	1.81	0.63
21:3:709:CLA:HHC	21:3:709:CLA:HBB1	1.80	0.63
10:2:229:GLY:O	10:2:232:SER:OG	2.13	0.63
17:9:115:ARG:HG2	21:9:902:CLA:O1D	1.98	0.63
21:F:403:CLA:HHC	21:F:403:CLA:HBB1	1.81	0.63
14:6:232:TRP:HB2	19:11:284:ARG:HG3	1.81	0.63
21:B:828:CLA:HBB1	21:B:828:CLA:HMB1	1.81	0.62
21:B:831:CLA:HHC	21:B:831:CLA:HBB1	1.79	0.62
10:2:238:GLU:O	10:2:241:LYS:HD3	1.99	0.62
21:6:908:CLA:HHC	21:6:908:CLA:HBB1	1.81	0.62
21:B:819:CLA:HHC	21:B:819:CLA:HBB1	1.81	0.62
21:2:514:CLA:HHC	21:2:514:CLA:HBB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:13:503:CLA:HHC	21:13:503:CLA:HBB1	1.82	0.62
21:4:711:CLA:HHC	21:4:711:CLA:HBB1	1.82	0.62
21:8:604:CLA:CGA	21:8:604:CLA:H3A	2.30	0.62
15:7:467:ARG:HG3	19:12:348:TRP:HB2	1.81	0.61
21:A:822:CLA:HBB1	21:A:822:CLA:HMB3	1.83	0.61
1:A:722:GLN:HG3	25:A:853:LHG:O9	2.00	0.61
21:7:714:CLA:HHC	21:7:714:CLA:HBB1	1.82	0.61
21:A:808:CLA:HHC	21:A:808:CLA:HBB1	1.82	0.61
19:12:307:GLU:OE2	19:12:400:LEU:CD2	2.49	0.60
21:B:835:CLA:C1A	21:B:835:CLA:CGA	2.79	0.60
21:8:611:CLA:HHC	21:8:611:CLA:HBB1	1.82	0.60
21:2:517:CLA:HHC	21:2:517:CLA:HBB1	1.84	0.59
19:11:370:THR:HG22	21:11:707:CLA:HHB	1.84	0.59
21:11:705:CLA:HHC	21:11:705:CLA:HBB1	1.85	0.59
21:4:701:CLA:HHC	21:4:701:CLA:HBB1	1.83	0.59
21:7:713:CLA:HHC	21:7:713:CLA:HBB1	1.84	0.59
21:A:839:CLA:HHC	21:A:839:CLA:HBB1	1.83	0.59
12:4:181:GLU:OE2	12:4:282:SER:OG	2.19	0.59
2:B:183:PHE:CE2	21:B:812:CLA:H92	2.38	0.58
21:2:509:CLA:H3A	21:2:509:CLA:CGA	2.33	0.58
21:A:834:CLA:HHC	21:A:834:CLA:HBB1	1.84	0.58
2:B:590:THR:HG21	21:B:834:CLA:HBB2	1.85	0.58
19:11:294:ARG:HD3	21:11:707:CLA:CHD	2.34	0.58
11:3:297:LYS:HG3	21:3:708:CLA:HED3	1.85	0.58
21:7:705:CLA:HHC	21:7:705:CLA:HBB1	1.85	0.58
21:A:806:CLA:H151	24:A:849:BCR:H372	1.85	0.58
21:3:712:CLA:HHC	21:3:712:CLA:HBB1	1.84	0.58
2:B:595:HIS:CD2	2:B:599:ILE:HD13	2.38	0.58
21:B:831:CLA:C19	21:B:835:CLA:H13	2.33	0.58
2:B:491:ALA:O	2:B:492:ILE:HG12	2.03	0.58
21:5:702:CLA:CGA	21:5:702:CLA:H3A	2.33	0.58
2:B:292:ARG:NH1	2:B:296:ALA:O	2.37	0.58
21:5:709:CLA:HHC	21:5:709:CLA:HBB1	1.86	0.58
21:1:512:CLA:HBB1	21:1:512:CLA:HHC	1.85	0.57
19:11:284:ARG:NH1	21:11:703:CLA:O1A	2.37	0.57
19:12:297:MET:HE1	21:12:506:CLA:HHC	1.84	0.57
21:B:827:CLA:HMB3	21:B:827:CLA:HBB1	1.86	0.57
21:5:706:CLA:HHC	21:5:706:CLA:HBB1	1.85	0.57
21:A:820:CLA:CMB	21:A:820:CLA:HBB1	2.34	0.57
9:1:159:GLU:HG2	9:1:279:LEU:HB2	1.85	0.57
21:6:913:CLA:HHC	21:6:913:CLA:HBB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:803:CLA:HAA1	21:B:803:CLA:HBD	1.87	0.57
21:2:509:CLA:CGA	21:2:509:CLA:C3A	2.83	0.57
21:B:821:CLA:HMB1	21:B:821:CLA:HBB1	1.87	0.57
21:9:907:CLA:HHC	21:9:907:CLA:HBB1	1.87	0.57
21:A:842:CLA:C1A	21:A:842:CLA:CGA	2.83	0.56
21:10:709:CLA:HHC	21:10:709:CLA:HBB1	1.87	0.56
21:11:710:CLA:HHC	21:11:710:CLA:HBB1	1.86	0.56
21:2:507:CLA:HHC	21:2:507:CLA:HBB1	1.86	0.56
18:10:553:ARG:HD2	21:10:704:CLA:C4C	2.35	0.56
19:11:294:ARG:HD3	21:11:707:CLA:C4C	2.35	0.56
21:A:821:CLA:HAA2	21:A:821:CLA:HBD	1.86	0.56
21:8:607:CLA:HHC	21:8:607:CLA:HBB1	1.88	0.56
21:11:709:CLA:HHC	21:11:709:CLA:HBB1	1.85	0.56
21:1:517:CLA:HHC	21:1:517:CLA:HBB1	1.87	0.56
21:9:902:CLA:HHC	21:9:902:CLA:HBB1	1.88	0.56
18:10:588:ASN:HD22	21:10:711:CLA:HED3	1.70	0.56
21:A:820:CLA:HBB1	21:A:820:CLA:HMB3	1.87	0.55
1:A:533:PHE:HA	21:A:839:CLA:HED1	1.88	0.55
6:F:306:TRP:CH2	21:2:505:CLA:HED1	2.42	0.55
21:4:709:CLA:HHC	21:4:709:CLA:HBB1	1.88	0.55
18:10:459:ARG:HH21	18:10:463:VAL:HG21	1.70	0.55
10:2:219:TRP:HE3	10:2:220:TYR:H	1.53	0.55
21:11:701:CLA:HHC	21:11:701:CLA:HBB1	1.88	0.55
21:A:802:CLA:OBD	21:B:801:CLA:HMB2	2.07	0.55
19:12:307:GLU:OE2	19:12:400:LEU:HD23	2.06	0.55
15:7:531:TRP:HB2	19:12:284:ARG:HG3	1.90	0.54
1:A:750:VAL:O	1:A:750:VAL:HG23	2.07	0.54
21:1:513:CLA:HHC	21:1:513:CLA:HBB1	1.88	0.54
21:9:914:CLA:HHC	21:9:914:CLA:HBB1	1.88	0.54
1:A:458:HIS:NE2	1:A:462:LEU:HD12	2.22	0.54
9:1:294:LEU:HD13	21:1:513:CLA:HMD3	1.88	0.54
24:A:851:BCR:H382	24:A:851:BCR:H23C	1.88	0.54
21:4:710:CLA:HHC	21:4:710:CLA:HBB1	1.89	0.54
21:A:829:CLA:HBB1	21:A:829:CLA:HMB1	1.88	0.54
5:E:108:VAL:HG12	5:E:161:TYR:HB3	1.89	0.54
21:A:833:CLA:H11	21:A:833:CLA:C4D	2.37	0.54
21:A:839:CLA:CGA	21:A:839:CLA:C1A	2.85	0.53
9:1:201:ILE:HG12	21:1:516:CLA:HBC2	1.90	0.53
19:11:361:ASP:OD1	19:11:366:THR:OG1	2.26	0.53
1:A:277:THR:OG1	1:A:293:ASP:OD1	2.23	0.53
11:3:323:PRO:O	28:3:716:DD6:O2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:704:CLA:HBB1	21:3:704:CLA:HMB1	1.91	0.53
21:8:612:CLA:HHC	21:8:612:CLA:HBB1	1.91	0.53
21:9:911:CLA:HHC	21:9:911:CLA:HBB1	1.90	0.53
21:A:844:CLA:HBA1	21:A:844:CLA:HBD	1.89	0.53
19:12:293:ALA:HB1	19:12:378:GLY:HA3	1.90	0.53
21:4:701:CLA:CAD	25:4:714:LHG:HC5	2.39	0.53
13:5:315:PHE:CD1	13:5:316:PRO:HD2	2.44	0.53
21:5:707:CLA:HBB1	21:5:707:CLA:HMB3	1.89	0.53
21:1:509:CLA:HAA1	21:1:509:CLA:HBD	1.91	0.53
19:12:299:ALA:HB3	19:12:385:LEU:HD11	1.91	0.53
19:12:294:ARG:HD3	21:12:506:CLA:CHD	2.39	0.53
21:2:508:CLA:HAA1	21:2:508:CLA:HBD	1.91	0.53
13:5:405:ARG:NH2	21:5:706:CLA:O1D	2.42	0.53
21:7:708:CLA:CGA	21:7:708:CLA:C3A	2.87	0.53
19:13:347:ASN:ND2	19:13:348:TRP:N	2.54	0.53
21:5:711:CLA:HHC	21:5:711:CLA:HBB1	1.90	0.52
21:A:844:CLA:H93	4:D:360:PHE:CZ	2.45	0.52
21:3:707:CLA:H2A	21:3:707:CLA:O1D	2.09	0.52
12:4:272:PHE:HE2	28:4:712:DD6:O1	1.92	0.52
21:6:909:CLA:CGA	21:6:909:CLA:H3A	2.39	0.52
21:6:911:CLA:HHC	21:6:911:CLA:HBB1	1.90	0.52
21:12:505:CLA:HHC	21:12:505:CLA:HBB1	1.91	0.52
20:A:801:CL0:CGD	20:A:801:CL0:H8	2.38	0.52
21:A:804:CLA:H122	7:J:19:PHE:HB3	1.92	0.52
21:A:817:CLA:HBB1	21:A:817:CLA:CHC	2.39	0.52
12:4:274:VAL:HG21	21:4:710:CLA:HAC2	1.92	0.52
14:6:276:GLN:HE21	14:6:287:ASN:HD22	1.58	0.52
21:A:862:CLA:HBC2	2:B:585:ASN:HB2	1.92	0.52
21:3:705:CLA:HHC	21:3:705:CLA:HBB1	1.90	0.52
1:A:681:PHE:HZ	21:A:842:CLA:HBC2	1.75	0.52
21:A:842:CLA:HHC	21:A:842:CLA:HBB1	1.92	0.52
2:B:665:ILE:HB	21:B:802:CLA:HBC2	1.92	0.52
13:5:393:TYR:O	13:5:397:LEU:HD22	2.09	0.52
21:A:843:CLA:HHC	21:A:843:CLA:HBB1	1.91	0.52
21:5:707:CLA:O1A	21:5:707:CLA:H3A	2.10	0.52
2:B:26:ALA:HB2	27:B:847:DGD:HA32	1.92	0.51
9:1:197:ASN:CG	9:1:200:PHE:CE2	2.88	0.51
21:7:703:CLA:CGA	21:7:703:CLA:H3A	2.40	0.51
21:9:909:CLA:HHC	21:9:909:CLA:HBB1	1.92	0.51
21:10:708:CLA:HHC	21:10:708:CLA:HBB1	1.92	0.51
21:A:807:CLA:HHC	21:A:807:CLA:HBB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2:275:TRP:CE2	21:2:507:CLA:HED2	2.44	0.51
11:3:275:PRO:HD2	21:3:707:CLA:OBD	2.10	0.51
21:5:707:CLA:H3A	21:5:707:CLA:CGA	2.41	0.51
21:3:701:CLA:HHC	21:3:701:CLA:HBB1	1.92	0.51
18:10:563:GLU:HG3	21:10:712:CLA:HMA2	1.91	0.51
1:A:228:LEU:HG	1:A:237:LEU:HD11	1.92	0.51
4:D:429:ARG:O	4:D:435:ARG:HD3	2.09	0.51
9:1:219:GLY:HA2	21:1:508:CLA:HBC1	1.92	0.51
21:A:806:CLA:H161	24:A:848:BCR:H332	1.92	0.51
21:A:807:CLA:HED1	21:A:831:CLA:H2	1.92	0.51
21:6:904:CLA:H3A	21:6:904:CLA:CGA	2.41	0.51
21:7:710:CLA:HHC	21:7:710:CLA:HBB1	1.92	0.51
9:1:152:LEU:HA	9:1:264:MET:HE3	1.93	0.51
21:4:708:CLA:HHC	21:4:708:CLA:HBB1	1.91	0.51
14:6:264:ARG:HA	14:6:267:MET:HE3	1.91	0.51
21:7:713:CLA:CAD	16:8:235:TRP:HE1	2.24	0.51
1:A:316:TRP:O	1:A:317:LYS:HB3	2.11	0.50
21:B:839:CLA:HBB1	21:B:839:CLA:HHC	1.92	0.50
21:7:708:CLA:HBB1	21:7:708:CLA:HMB3	1.94	0.50
21:B:807:CLA:C4A	21:B:807:CLA:HBA2	2.40	0.50
21:A:810:CLA:HBB1	21:A:810:CLA:HMB3	1.93	0.50
21:A:817:CLA:HBA2	21:4:711:CLA:HMB3	1.92	0.50
21:A:824:CLA:HHC	21:A:824:CLA:HBB1	1.93	0.50
6:F:194:GLU:OE1	6:F:214:LYS:HE2	2.11	0.50
10:2:354:LEU:HB2	21:2:507:CLA:HMC2	1.94	0.50
21:B:816:CLA:HBB1	21:B:816:CLA:HHC	1.93	0.50
21:J:101:CLA:HBB1	21:J:101:CLA:HHC	1.94	0.50
21:1:505:CLA:CGA	21:1:505:CLA:H3A	2.41	0.50
21:8:604:CLA:CGA	21:8:604:CLA:C3A	2.90	0.50
21:12:504:CLA:O1D	21:12:504:CLA:H2A	2.10	0.50
2:B:376:GLN:HE21	2:B:376:GLN:HA	1.76	0.50
10:2:274:ARG:HA	10:2:277:MET:HE3	1.93	0.50
21:7:709:CLA:HHC	21:7:709:CLA:HBB1	1.93	0.50
21:10:707:CLA:HHC	21:10:707:CLA:HBB1	1.94	0.50
19:12:363:LEU:HB2	19:12:365:LEU:HD13	1.93	0.50
21:3:702:CLA:CGA	21:3:702:CLA:H3A	2.41	0.50
21:4:702:CLA:CGA	21:4:702:CLA:H3A	2.42	0.50
21:2:510:CLA:HBD	21:2:511:CLA:OBD	2.12	0.50
18:10:422:LEU:HD21	18:10:429:PRO:HB3	1.93	0.50
21:13:501:CLA:HHC	21:13:501:CLA:HBB1	1.93	0.50
21:A:837:CLA:HHC	21:A:837:CLA:HBB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:852:BCR:H362	21:A:862:CLA:H41	1.93	0.49
13:5:371:GLU:OE2	13:5:465:SER:OG	2.27	0.49
1:A:232:VAL:O	1:A:232:VAL:CG1	2.60	0.49
21:A:810:CLA:H192	21:A:812:CLA:H112	1.93	0.49
21:A:821:CLA:HHC	21:A:821:CLA:HBB1	1.94	0.49
21:A:833:CLA:HBB1	21:A:833:CLA:HMB3	1.94	0.49
21:A:862:CLA:HBB1	21:A:862:CLA:HMB3	1.93	0.49
11:3:188:TRP:CE2	21:3:705:CLA:HED2	2.47	0.49
2:B:707:LEU:HD23	27:B:847:DGD:HA21	1.95	0.49
21:2:510:CLA:C4D	21:2:511:CLA:HMD3	2.42	0.49
21:7:703:CLA:H3A	21:7:703:CLA:O1A	2.12	0.49
19:13:347:ASN:ND2	19:13:348:TRP:O	2.46	0.49
24:A:852:BCR:H362	21:A:862:CLA:H42	1.92	0.49
21:3:706:CLA:HAA1	21:3:706:CLA:HBD	1.95	0.49
21:11:703:CLA:HHC	21:11:703:CLA:HBB1	1.94	0.49
16:8:169:TYR:HB3	21:8:609:CLA:HED2	1.94	0.49
17:9:144:MET:HE2	17:9:226:GLY:N	2.27	0.49
2:B:232:LEU:HA	2:B:235:GLU:HG2	1.95	0.49
2:B:523:ILE:HG12	2:B:590:THR:HG22	1.95	0.49
10:2:248:TYR:OH	25:2:521:LHG:O5	2.28	0.49
1:A:411:ILE:HD13	21:A:831:CLA:HED3	1.94	0.49
21:2:510:CLA:HHC	21:2:510:CLA:HBB1	1.95	0.49
14:6:301:LEU:O	14:6:302:THR:C	2.55	0.49
21:B:833:CLA:HHC	21:B:833:CLA:HBB1	1.95	0.49
17:9:226:GLY:O	17:9:230:MET:HG3	2.12	0.49
2:B:3:THR:OG1	2:B:4:LYS:N	2.45	0.48
21:12:508:CLA:HHC	21:12:508:CLA:HBB1	1.95	0.48
14:6:300:ILE:HG23	14:6:301:LEU:HD22	1.95	0.48
21:B:835:CLA:H141	6:F:263:LEU:HD11	1.95	0.48
10:2:385:LYS:HE3	21:2:511:CLA:HBD	1.95	0.48
2:B:40:ASN:OD1	2:B:44:GLN:NE2	2.45	0.48
15:7:476:GLY:CA	15:7:566:MET:HE2	2.44	0.48
21:A:803:CLA:H12	2:B:427:LEU:HD23	1.96	0.48
2:B:450:GLU:OE2	6:F:220:ARG:NE	2.46	0.48
21:3:706:CLA:HHC	21:3:706:CLA:HBB1	1.96	0.48
18:10:532:PRO:HG2	21:10:707:CLA:HMD2	1.94	0.48
21:11:711:CLA:HHC	21:11:711:CLA:HBB1	1.95	0.48
1:A:142:SER:HB3	21:A:829:CLA:HAA2	1.95	0.48
2:B:301:ILE:HG21	21:B:823:CLA:HAC1	1.95	0.48
21:12:507:CLA:HHC	21:12:507:CLA:HBB1	1.96	0.48
21:1:514:CLA:HHC	21:1:514:CLA:HBB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CZ	21:A:844:CLA:HED2	2.48	0.48
21:B:806:CLA:C1A	21:B:806:CLA:CGA	2.92	0.48
11:3:222:VAL:HG11	11:3:242:ILE:HD13	1.95	0.48
13:5:439:THR:HB	21:5:708:CLA:HED1	1.95	0.48
21:A:844:CLA:H62	21:A:844:CLA:H2	1.74	0.48
9:1:197:ASN:CG	9:1:200:PHE:CD2	2.92	0.48
24:F:405:BCR:H383	24:F:405:BCR:H23C	1.95	0.47
21:1:516:CLA:HHC	21:1:516:CLA:HBB1	1.95	0.47
16:8:115:ILE:HG12	16:8:197:MET:SD	2.54	0.47
19:11:251:PHE:HB3	19:11:254:ALA:HB2	1.95	0.47
1:A:330:THR:O	21:A:844:CLA:HBC3	2.14	0.47
21:B:835:CLA:H172	24:F:405:BCR:H381	1.97	0.47
9:1:248:GLU:HG3	9:1:249:LEU:N	2.29	0.47
11:3:341:THR:HG22	11:3:345:ARG:HH21	1.79	0.47
2:B:383:MET:HE1	24:B:845:BCR:H361	1.95	0.47
17:9:180:VAL:HA	21:9:913:CLA:HBC3	1.96	0.47
19:12:297:MET:HA	19:12:300:ILE:HG22	1.95	0.47
19:13:347:ASN:ND2	19:13:348:TRP:H	2.12	0.47
24:A:852:BCR:H23C	24:A:852:BCR:C38	2.44	0.47
2:B:365:ARG:HB3	2:B:602:TRP:CZ3	2.49	0.47
21:B:827:CLA:HBB1	21:B:827:CLA:CMB	2.44	0.47
9:1:99:ARG:HD2	9:1:100:PRO:O	2.14	0.47
21:11:708:CLA:HHC	21:11:708:CLA:HBB1	1.96	0.47
21:13:502:CLA:HHC	21:13:502:CLA:HBB1	1.96	0.47
2:B:106:ARG:NH1	2:B:113:VAL:O	2.48	0.47
2:B:488:ALA:O	2:B:490:GLN:N	2.48	0.47
21:B:831:CLA:HBC2	21:B:831:CLA:CHD	2.39	0.47
9:1:200:PHE:CD2	9:1:200:PHE:N	2.83	0.47
21:2:507:CLA:O1D	21:2:507:CLA:H2A	2.15	0.47
21:5:707:CLA:CGA	21:5:707:CLA:C3A	2.92	0.47
16:8:179:THR:O	16:8:183:LYS:HG2	2.15	0.47
18:10:557:ILE:HD11	21:10:704:CLA:HAC1	1.97	0.47
1:A:310:HIS:CE1	24:A:847:BCR:H363	2.50	0.47
2:B:586:THR:O	2:B:590:THR:HG23	2.15	0.47
10:2:281:LEU:HD23	21:2:506:CLA:HMC1	1.96	0.47
1:A:310:HIS:O	21:A:821:CLA:HED1	2.14	0.47
12:4:233:PHE:HZ	13:5:347:GLU:HG2	1.80	0.47
21:6:912:CLA:HHC	21:6:912:CLA:HBB1	1.97	0.46
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.98	0.46
3:C:2:SER:N	3:C:71:SER:HG	2.13	0.46
10:2:218:LYS:HD2	21:2:510:CLA:CED	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:513:CLA:HHC	21:2:513:CLA:HBB1	1.97	0.46
11:3:238:HIS:NE2	11:3:240:LYS:NZ	2.63	0.46
14:6:165:VAL:O	14:6:169:MET:HG2	2.15	0.46
22:A:845:PQN:H141	21:F:401:CLA:HBB2	1.97	0.46
21:1:504:CLA:HHC	21:1:504:CLA:HBB1	1.97	0.46
21:5:707:CLA:HBB1	21:5:707:CLA:CMB	2.45	0.46
21:B:823:CLA:HAA2	21:B:823:CLA:HBD	1.97	0.46
21:1:515:CLA:HHC	21:1:515:CLA:HBB1	1.98	0.46
10:2:431:ALA:N	10:2:432:PRO:HD2	2.30	0.46
21:6:910:CLA:HHC	21:6:910:CLA:HBB1	1.96	0.46
15:7:560:LYS:HE2	21:7:709:CLA:O2D	2.15	0.46
19:11:406:HIS:O	19:11:410:PRO:HD3	2.16	0.46
21:A:803:CLA:HBB1	21:A:803:CLA:CMB	2.46	0.46
21:A:827:CLA:H52	21:A:838:CLA:H11	1.97	0.46
24:A:850:BCR:H403	24:A:850:BCR:H23C	1.97	0.46
2:B:117:TYR:HA	2:B:367:THR:HG22	1.96	0.46
21:B:815:CLA:HAA1	21:B:815:CLA:HBD	1.98	0.46
21:2:504:CLA:CGA	21:2:504:CLA:H3A	2.46	0.46
21:3:715:CLA:HHC	21:3:715:CLA:HBB1	1.98	0.46
21:7:708:CLA:H3A	21:7:708:CLA:O1A	2.16	0.46
19:12:400:LEU:HD23	19:12:400:LEU:H	1.80	0.46
1:A:677:PHE:CD2	24:A:852:BCR:H363	2.51	0.45
21:A:804:CLA:H93	21:A:809:CLA:H171	1.99	0.45
6:F:279:GLU:HG2	6:F:297:LEU:HD11	1.98	0.45
21:4:706:CLA:HHC	21:4:706:CLA:HBB1	1.98	0.45
19:11:404:ALA:HA	19:11:407:LEU:HD21	1.98	0.45
21:12:504:CLA:HHC	21:12:504:CLA:HBB1	1.98	0.45
1:A:113:PRO:HB3	1:A:145:PHE:CD2	2.51	0.45
1:A:650:LEU:O	1:A:654:SER:HB3	2.16	0.45
2:B:80:ASP:OD2	2:B:83:HIS:HB2	2.16	0.45
21:B:824:CLA:HBB1	21:B:824:CLA:HMB3	1.99	0.45
19:11:293:ALA:HB1	19:11:378:GLY:HA3	1.97	0.45
19:12:297:MET:CE	21:12:506:CLA:HHC	2.45	0.45
1:A:457:ILE:HG22	21:A:835:CLA:HBC2	1.98	0.45
21:B:804:CLA:HMB1	21:B:804:CLA:HBB1	1.98	0.45
21:B:831:CLA:H152	6:F:263:LEU:HD22	1.97	0.45
21:12:502:CLA:HHC	21:12:502:CLA:HBB1	1.98	0.45
1:A:37:ARG:O	1:A:37:ARG:NH1	2.45	0.45
21:A:813:CLA:HHC	21:A:813:CLA:HBB1	1.99	0.45
10:2:379:PHE:CZ	10:2:383:LYS:HE2	2.51	0.45
10:2:385:LYS:HE2	21:2:511:CLA:O1A	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:11:271:ASP:OD1	28:11:713:DD6:O4	2.35	0.45
9:1:209:MET:HB3	9:1:209:MET:HE3	1.82	0.45
21:8:613:CLA:HHC	21:8:613:CLA:HBB1	1.98	0.45
19:13:371:LYS:HA	19:13:371:LYS:HD3	1.63	0.45
1:A:473:SER:OG	1:A:474:ASP:N	2.50	0.45
21:B:827:CLA:H3A	21:B:827:CLA:HBA2	1.52	0.45
21:5:702:CLA:CGA	21:5:702:CLA:C3A	2.94	0.45
19:12:294:ARG:HG2	21:12:506:CLA:C3C	2.47	0.45
21:A:825:CLA:HBB1	21:A:825:CLA:HHC	1.99	0.45
2:B:48:ALA:HB3	8:M:29:LEU:HD21	1.98	0.45
2:B:374:HIS:HE1	21:B:826:CLA:ND	2.14	0.45
21:B:838:CLA:HHC	21:B:838:CLA:CBB	2.43	0.45
6:F:267:GLY:HA3	6:F:308:TRP:CZ2	2.52	0.45
21:1:511:CLA:HHC	21:1:511:CLA:HBB1	1.97	0.45
18:10:430:PRO:HG2	18:10:433:LEU:HB2	1.98	0.45
2:B:504:LYS:HD3	2:B:504:LYS:N	2.32	0.45
9:1:99:ARG:HH12	9:1:114:GLY:CA	2.30	0.45
9:1:212:VAL:HG13	29:1:604:HOH:O	2.15	0.45
21:3:701:CLA:HMD2	25:3:719:LHG:O9	2.17	0.45
18:10:471:LEU:HB3	21:10:706:CLA:HBB2	1.99	0.45
21:A:803:CLA:CGA	21:A:803:CLA:H3A	2.46	0.45
21:A:813:CLA:HAA1	21:A:813:CLA:HBD	1.99	0.45
21:A:818:CLA:C4A	21:A:818:CLA:HBA2	2.44	0.45
21:A:829:CLA:HBA2	21:A:829:CLA:H3A	1.54	0.45
21:B:829:CLA:HAA1	21:B:839:CLA:H41	1.98	0.45
21:B:830:CLA:C4A	21:B:830:CLA:HBA2	2.46	0.45
24:J:102:BCR:H371	24:J:102:BCR:H24C	1.74	0.45
21:1:515:CLA:CBB	21:1:517:CLA:HBB2	2.47	0.45
21:3:711:CLA:HHC	21:3:711:CLA:HBB1	1.99	0.45
21:4:701:CLA:HMD2	25:4:714:LHG:O9	2.17	0.45
1:A:474:ASP:OD2	1:A:530:THR:OG1	2.27	0.45
21:B:803:CLA:C4A	21:B:803:CLA:HBA2	2.47	0.45
21:B:825:CLA:CMB	21:B:825:CLA:HBB1	2.47	0.45
6:F:302:ALA:HB1	21:F:403:CLA:HED3	1.98	0.45
21:B:802:CLA:CGA	21:B:802:CLA:H3A	2.48	0.44
4:D:392:LYS:HG3	4:D:394:GLN:HG2	1.99	0.44
21:6:909:CLA:CGA	21:6:909:CLA:C3A	2.94	0.44
17:9:176:ILE:HG23	21:9:913:CLA:HMD1	1.99	0.44
2:B:491:ALA:O	2:B:493:TRP:CE3	2.71	0.44
21:10:712:CLA:HHC	21:10:712:CLA:HBB1	2.00	0.44
21:A:862:CLA:HHB	21:B:801:CLA:H202	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:804:CLA:H141	21:B:804:CLA:H162	1.82	0.44
21:B:826:CLA:HBA2	21:B:826:CLA:H3A	1.65	0.44
3:C:14:CYS:O	3:C:15:THR:OG1	2.24	0.44
21:4:708:CLA:NC	25:4:714:LHG:HC42	2.32	0.44
19:11:395:THR:OG1	19:11:396:GLY:N	2.47	0.44
1:A:709:VAL:O	1:A:709:VAL:HG22	2.18	0.44
21:A:839:CLA:HAA1	21:A:839:CLA:HBD	1.99	0.44
2:B:732:LYS:HG3	2:B:733:PHE:CE2	2.52	0.44
21:B:817:CLA:CMB	21:B:817:CLA:HBB1	2.48	0.44
12:4:232:TRP:HB2	13:5:348:ARG:HG3	1.99	0.44
21:5:701:CLA:HHC	21:5:701:CLA:HBB1	2.00	0.44
16:8:225:HIS:HB3	21:8:612:CLA:HED1	1.99	0.44
21:A:802:CLA:HAA2	21:A:802:CLA:HBD	1.99	0.44
21:A:826:CLA:HBA1	21:A:830:CLA:H193	2.00	0.44
21:A:833:CLA:H62	21:A:833:CLA:H41	1.83	0.44
2:B:374:HIS:HE2	21:B:827:CLA:C1B	2.30	0.44
21:B:816:CLA:H3A	21:B:816:CLA:HBA2	1.72	0.44
11:3:310:LEU:HD13	21:3:703:CLA:HBB2	1.99	0.44
19:12:344:GLY:HA2	21:12:504:CLA:HBC1	2.00	0.44
1:A:37:ARG:HH12	1:A:41:LYS:HD2	1.82	0.44
21:B:812:CLA:H42	24:B:842:BCR:H19C	2.00	0.44
3:C:62:PHE:HD2	4:D:478:ILE:HG21	1.83	0.44
10:2:275:TRP:CE2	21:2:508:CLA:HBC3	2.53	0.44
2:B:590:THR:HG21	21:B:834:CLA:CBB	2.47	0.44
15:7:434:PHE:O	15:7:435:PRO:C	2.60	0.44
16:8:213:VAL:O	16:8:217:GLU:HG2	2.18	0.44
21:A:820:CLA:HBA2	21:A:820:CLA:H3A	1.80	0.44
24:A:848:BCR:H11C	24:A:848:BCR:H341	1.87	0.44
4:D:367:TYR:O	4:D:369:GLY:N	2.51	0.44
21:6:904:CLA:CGA	21:6:904:CLA:C3A	2.96	0.44
21:10:706:CLA:HHC	21:10:706:CLA:HBB1	1.99	0.44
19:13:334:ALA:O	19:13:338:GLU:HB2	2.18	0.44
1:A:232:VAL:O	1:A:232:VAL:HG12	2.18	0.43
21:A:810:CLA:H11	24:J:102:BCR:C19	2.48	0.43
21:A:811:CLA:HHC	21:A:811:CLA:HBB1	2.00	0.43
21:A:829:CLA:H191	24:J:102:BCR:H14C	1.99	0.43
21:A:803:CLA:HBB1	21:A:803:CLA:HMB1	2.00	0.43
2:B:411:ILE:CD1	21:B:829:CLA:HBC3	2.48	0.43
21:B:829:CLA:HBA2	21:B:829:CLA:H3A	1.74	0.43
4:D:393:LYS:NZ	4:D:407:GLU:OE1	2.51	0.43
9:1:270:GLN:HE22	28:1:518:DD6:C19	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:713:CLA:HHC	21:3:713:CLA:HBB1	2.00	0.43
21:B:835:CLA:CMB	21:B:835:CLA:HBB1	2.48	0.43
24:A:847:BCR:H331	24:A:847:BCR:C8	2.48	0.43
24:A:852:BCR:C38	24:A:852:BCR:C23	2.96	0.43
24:B:845:BCR:H15C	24:B:845:BCR:H351	1.83	0.43
21:3:707:CLA:CGA	21:3:707:CLA:C3A	2.96	0.43
14:6:192:TRP:HB2	14:6:285:LEU:HD11	2.00	0.43
21:11:705:CLA:HBD	21:11:705:CLA:HBA1	2.01	0.43
19:11:299:ALA:HB3	19:11:385:LEU:HD11	2.01	0.43
21:A:823:CLA:CMB	21:A:823:CLA:HBB1	2.48	0.43
21:A:831:CLA:HBB1	21:A:831:CLA:HMB3	2.01	0.43
2:B:483:SER:O	2:B:487:SER:OG	2.33	0.43
21:B:830:CLA:HAA1	21:B:830:CLA:HBD	2.01	0.43
13:5:443:LYS:HE3	21:5:708:CLA:C3D	2.47	0.43
15:7:430:ARG:HD2	15:7:450:ASP:O	2.19	0.43
24:M:102:BCR:H11C	24:M:102:BCR:H341	1.86	0.43
9:1:268:TRP:HZ3	21:1:506:CLA:HBB2	1.84	0.43
14:6:209:ARG:HH22	15:7:606:PRO:HA	1.83	0.43
24:A:849:BCR:H11C	24:A:849:BCR:H341	1.73	0.43
21:B:828:CLA:H161	21:B:828:CLA:H192	1.80	0.43
6:F:247:VAL:HG21	10:2:330:LEU:HD13	2.00	0.43
7:J:11:ALA:N	7:J:12:PRO:HD2	2.34	0.43
24:J:102:BCR:H321	24:J:102:BCR:HC8	2.00	0.43
12:4:163:GLU:O	12:4:167:SER:HB2	2.18	0.43
14:6:284:PRO:O	28:6:915:DD6:O2	2.37	0.43
24:B:841:BCR:H351	24:B:841:BCR:H15C	1.86	0.43
24:B:845:BCR:H403	24:B:845:BCR:H23C	2.01	0.43
21:2:505:CLA:HBB1	21:2:505:CLA:CHC	2.42	0.43
15:7:508:ARG:HB3	16:8:232:MET:HE1	1.99	0.43
18:10:537:CYS:O	18:10:539:LEU:HD22	2.19	0.43
1:A:371:MET:HE1	21:A:830:CLA:O1D	2.19	0.43
21:A:805:CLA:H3A	21:A:805:CLA:HBA2	1.72	0.43
21:B:805:CLA:HMC3	24:B:842:BCR:H401	2.00	0.43
9:1:244:GLY:HA3	21:1:510:CLA:HAA2	1.99	0.43
14:6:134:TRP:CE2	14:6:135:ILE:HG12	2.54	0.43
18:10:560:PHE:O	18:10:564:VAL:HG23	2.19	0.43
21:11:703:CLA:H2	21:11:703:CLA:H62	1.76	0.43
21:A:842:CLA:H92	22:A:845:PQN:H191	2.02	0.42
11:3:302:GLY:O	11:3:306:MET:HG3	2.19	0.42
21:4:704:CLA:HHC	21:4:704:CLA:HBB1	2.00	0.42
18:10:466:GLY:HA2	18:10:556:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:826:CLA:HAA2	21:A:826:CLA:HBD	2.00	0.42
21:A:842:CLA:O2A	21:A:842:CLA:CHA	2.67	0.42
24:B:841:BCR:H23C	24:B:841:BCR:H382	2.00	0.42
3:C:68:TYR:CG	4:D:495:LYS:HD2	2.54	0.42
1:A:671:MET:CE	24:A:852:BCR:H352	2.46	0.42
21:A:829:CLA:HBB1	21:A:829:CLA:CMB	2.50	0.42
24:A:851:BCR:H382	24:A:851:BCR:C23	2.50	0.42
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.93	0.42
2:B:574:ASP:OD1	2:B:706:ARG:NH1	2.52	0.42
3:C:41:SER:HB2	4:D:471:ALA:H	1.85	0.42
12:4:178:LEU:O	12:4:181:GLU:HB3	2.19	0.42
18:10:588:ASN:N	18:10:588:ASN:OD1	2.52	0.42
1:A:297:HIS:HE1	21:A:819:CLA:ND	2.18	0.42
1:A:539:HIS:CE1	1:A:606:ALA:HA	2.54	0.42
8:M:13:LEU:HG	24:M:102:BCR:H402	2.01	0.42
21:1:504:CLA:HMD1	21:1:505:CLA:HMD1	2.01	0.42
11:3:228:LEU:HD11	21:3:714:CLA:HAC1	2.02	0.42
16:8:182:THR:HG22	21:8:609:CLA:HHB	2.02	0.42
19:12:344:GLY:HA2	21:12:504:CLA:CBC	2.49	0.42
21:B:804:CLA:HBA1	21:B:804:CLA:H3A	1.76	0.42
21:2:509:CLA:H3A	21:2:509:CLA:O1A	2.19	0.42
2:B:476:ILE:O	2:B:477:LEU:C	2.60	0.42
2:B:484:ASN:OD1	2:B:484:ASN:N	2.41	0.42
3:C:15:THR:HG22	3:C:28:MET:HG3	2.02	0.42
4:D:393:LYS:HA	4:D:406:MET:O	2.20	0.42
24:J:102:BCR:H11C	24:J:102:BCR:H341	1.84	0.42
20:A:801:CL0:H12	21:A:862:CLA:OBD	2.19	0.42
21:A:823:CLA:HBB1	21:A:823:CLA:HMB3	2.01	0.42
24:B:841:BCR:H403	24:B:841:BCR:H24C	1.80	0.42
14:6:196:LYS:HA	14:6:196:LYS:HD3	1.81	0.42
18:10:433:LEU:HD13	18:10:433:LEU:HA	1.93	0.42
21:A:841:CLA:H112	21:A:841:CLA:HAB	2.02	0.42
2:B:179:LEU:HD21	21:B:818:CLA:C3B	2.49	0.42
2:B:428:PHE:CD2	2:B:428:PHE:C	2.97	0.42
4:D:395:ILE:HD13	4:D:405:GLU:CG	2.47	0.42
10:2:422:PRO:O	21:2:513:CLA:HMA2	2.20	0.42
11:3:174:ARG:HD3	11:3:178:TYR:OH	2.19	0.42
19:12:335:ALA:HB3	19:12:336:PRO:HD3	2.02	0.42
2:B:649:MET:HG2	2:B:723:ALA:HB2	2.02	0.42
21:2:509:CLA:CGA	21:2:509:CLA:C4A	2.98	0.42
21:A:810:CLA:H111	21:A:810:CLA:H72	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:211:GLU:OE2	6:F:211:GLU:HA	2.20	0.41
9:1:288:ASP:OD2	9:1:291:HIS:HB2	2.20	0.41
1:A:228:LEU:HD21	1:A:234:PRO:HG3	2.02	0.41
24:A:851:BCR:C23	24:A:851:BCR:C38	2.98	0.41
2:B:472:TYR:O	2:B:473:GLU:HG3	2.20	0.41
9:1:200:PHE:H	9:1:200:PHE:HD2	1.68	0.41
16:8:191:ARG:O	16:8:195:THR:HG22	2.21	0.41
21:B:835:CLA:H172	24:F:405:BCR:C38	2.50	0.41
24:B:845:BCR:H331	24:B:845:BCR:C8	2.51	0.41
21:F:404:CLA:HHC	21:F:404:CLA:HBB1	2.01	0.41
21:4:702:CLA:CGA	21:4:702:CLA:C3A	2.98	0.41
21:6:910:CLA:C4D	21:6:911:CLA:HMD3	2.50	0.41
1:A:433:HIS:CE1	21:A:832:CLA:ND	2.88	0.41
21:A:829:CLA:H93	24:J:102:BCR:H361	2.01	0.41
2:B:344:ILE:HD13	2:B:344:ILE:HA	1.84	0.41
21:6:907:CLA:HBB1	21:6:907:CLA:CHC	2.50	0.41
21:A:809:CLA:H3A	21:A:809:CLA:HBA2	1.55	0.41
16:8:195:THR:HG23	21:8:612:CLA:HBB2	2.02	0.41
21:A:828:CLA:H161	21:A:828:CLA:H193	1.88	0.41
2:B:704:GLN:HG3	27:B:847:DGD:HA22	2.02	0.41
18:10:482:LEU:HD22	18:10:482:LEU:HA	1.93	0.41
18:10:569:THR:O	18:10:570:ALA:HB3	2.20	0.41
1:A:747:ILE:HD12	1:A:747:ILE:HA	1.94	0.41
5:E:156:LEU:HD12	5:E:161:TYR:OH	2.21	0.41
24:F:402:BCR:H11C	24:F:402:BCR:H341	1.92	0.41
24:J:102:BCR:H383	24:J:102:BCR:H23C	2.03	0.41
9:1:149:MET:HE2	9:1:257:GLY:N	2.35	0.41
10:2:228:LEU:HD23	10:2:228:LEU:HA	1.94	0.41
21:A:823:CLA:HBA2	21:A:823:CLA:H3A	1.65	0.41
3:C:63:LEU:H	3:C:63:LEU:HG	1.47	0.41
21:3:708:CLA:HHC	21:3:708:CLA:HBB1	2.02	0.41
21:A:818:CLA:HAA1	21:A:818:CLA:HBD	2.03	0.41
24:A:849:BCR:H383	24:A:849:BCR:H23C	2.02	0.41
2:B:114:ASN:HD22	2:B:114:ASN:HA	1.73	0.41
3:C:32:ASP:OD2	3:C:32:ASP:N	2.53	0.41
4:D:322:LEU:HD13	4:D:442:PHE:CD1	2.56	0.41
9:1:170:PRO:HD2	21:1:507:CLA:HED3	2.03	0.41
12:4:171:MET:HB3	28:4:712:DD6:C2	2.50	0.41
17:9:175:LEU:HD23	19:13:324:ILE:HG22	2.03	0.41
19:12:308:VAL:HG12	19:12:309:LEU:HD23	2.03	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:825:CLA:HBD	21:B:825:CLA:HAA2	2.03	0.41
21:2:503:CLA:HBB1	21:2:503:CLA:CHC	2.49	0.41
13:5:315:PHE:CG	13:5:316:PRO:HD2	2.56	0.41
16:8:164:ASP:O	16:8:167:SER:OG	2.30	0.41
21:9:910:CLA:HBB1	21:9:910:CLA:CHC	2.47	0.41
19:12:273:LEU:HB3	19:12:275:LEU:HG	2.02	0.41
21:B:811:CLA:HHC	21:B:811:CLA:HBB1	2.03	0.40
10:2:426:PHE:HB3	10:2:428:THR:H	1.86	0.40
13:5:450:ILE:HD13	13:5:450:ILE:HA	1.94	0.40
21:6:903:CLA:HHC	21:6:903:CLA:HBB1	2.03	0.40
17:9:182:ALA:HB3	17:9:183:PRO:HD3	2.02	0.40
2:B:696:LYS:HA	2:B:697:PRO:HD3	1.93	0.40
21:B:815:CLA:CHD	21:B:816:CLA:HBB2	2.52	0.40
24:B:844:BCR:H11C	24:B:844:BCR:H341	1.93	0.40
24:J:103:BCR:H11C	24:J:103:BCR:H341	1.98	0.40
10:2:226:LYS:HE2	10:2:236:VAL:HG21	2.03	0.40
11:3:314:MET:HG3	21:3:710:CLA:HAC2	2.03	0.40
15:7:515:GLN:HG3	19:12:331:MET:HE2	2.03	0.40
15:7:572:LEU:HD22	15:7:583:PRO:HB3	2.03	0.40
1:A:695:GLU:OE2	2:B:544:SER:OG	2.32	0.40
15:7:515:GLN:HG3	19:12:331:MET:CE	2.52	0.40
17:9:96:LEU:HD13	17:9:96:LEU:HA	1.87	0.40
21:9:913:CLA:HHC	21:9:913:CLA:HBB1	2.03	0.40
1:A:297:HIS:NE2	1:A:301:LEU:HD11	2.37	0.40
2:B:411:ILE:HD11	21:B:829:CLA:HBC3	2.03	0.40
21:B:835:CLA:HBB1	21:B:835:CLA:HMB1	2.03	0.40
10:2:324:ILE:HG22	10:2:326:ALA:HB2	2.03	0.40
21:2:511:CLA:HBD	21:2:511:CLA:HAA2	2.02	0.40
12:4:233:PHE:CZ	13:5:347:GLU:HG2	2.56	0.40
21:7:703:CLA:HMB1	21:7:703:CLA:HBB1	2.02	0.40
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.92	0.40
4:D:435:ARG:HB3	4:D:437:GLU:OE2	2.21	0.40
15:7:470:ILE:HG13	15:7:540:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/760 (97%)	706 (96%)	30 (4%)	3 (0%)	30	49
2	B	729/734 (99%)	700 (96%)	26 (4%)	3 (0%)	30	49
3	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	10	20
4	D	187/698 (27%)	177 (95%)	10 (5%)	0	100	100
5	E	60/161 (37%)	60 (100%)	0	0	100	100
6	F	164/333 (49%)	159 (97%)	5 (3%)	0	100	100
7	J	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	1	197/492 (40%)	188 (95%)	9 (5%)	0	100	100
10	2	215/620 (35%)	201 (94%)	13 (6%)	1 (0%)	25	44
11	3	220/431 (51%)	204 (93%)	14 (6%)	2 (1%)	14	28
12	4	167/411 (41%)	152 (91%)	12 (7%)	3 (2%)	7	15
13	5	163/252 (65%)	151 (93%)	12 (7%)	0	100	100
14	6	169/889 (19%)	158 (94%)	11 (6%)	0	100	100
15	7	178/616 (29%)	173 (97%)	3 (2%)	2 (1%)	12	24
16	8	175/828 (21%)	166 (95%)	8 (5%)	1 (1%)	22	40
17	9	172/873 (20%)	164 (95%)	8 (5%)	0	100	100
18	10	138/643 (22%)	125 (91%)	11 (8%)	2 (1%)	9	19
19	11	169/1048 (16%)	157 (93%)	12 (7%)	0	100	100
19	12	148/1048 (14%)	135 (91%)	10 (7%)	3 (2%)	6	13
19	13	72/1048 (7%)	67 (93%)	5 (7%)	0	100	100
All	All	4204/12034 (35%)	3978 (95%)	205 (5%)	21 (0%)	27	44

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
10	2	422	PRO
12	4	132	ALA
12	4	198	PRO
16	8	138	ILE
19	12	350	LYS
2	B	492	ILE
18	10	536	PRO
19	12	358	PRO
1	A	233	ASN
2	B	489	SER
15	7	435	PRO
15	7	534	GLU
11	3	288	GLU
18	10	532	PRO
1	A	624	ALA
11	3	275	PRO
12	4	238	ASP
2	B	509	PHE
19	12	359	GLY
1	A	122	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/641 (97%)	609 (98%)	13 (2%)	48	72
2	B	608/609 (100%)	590 (97%)	18 (3%)	36	61
3	C	69/70 (99%)	65 (94%)	4 (6%)	17	34
4	D	154/557 (28%)	146 (95%)	8 (5%)	19	39
5	E	53/127 (42%)	52 (98%)	1 (2%)	52	75
6	F	132/259 (51%)	129 (98%)	3 (2%)	45	70
7	J	34/34 (100%)	32 (94%)	2 (6%)	16	33
8	M	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1	152/372 (41%)	140 (92%)	12 (8%)	10	21
10	2	166/465 (36%)	160 (96%)	6 (4%)	30	55
11	3	174/343 (51%)	168 (97%)	6 (3%)	32	57
12	4	131/310 (42%)	122 (93%)	9 (7%)	13	26
13	5	125/186 (67%)	118 (94%)	7 (6%)	17	35
14	6	140/688 (20%)	131 (94%)	9 (6%)	14	30
15	7	142/471 (30%)	139 (98%)	3 (2%)	48	72
16	8	136/633 (22%)	130 (96%)	6 (4%)	24	47
17	9	142/672 (21%)	133 (94%)	9 (6%)	15	30
18	10	111/497 (22%)	101 (91%)	10 (9%)	8	16
19	11	123/803 (15%)	117 (95%)	6 (5%)	21	42
19	12	110/803 (14%)	107 (97%)	3 (3%)	40	65
19	13	57/803 (7%)	50 (88%)	7 (12%)	4	7
All	All	3407/9369 (36%)	3265 (96%)	142 (4%)	27	49

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	161	ILE
1	A	270	SER
1	A	307	LEU
1	A	328	SER
1	A	373	SER
1	A	395	TYR
1	A	460	ASP
1	A	497	LEU
1	A	523	MET
1	A	584	CYS
1	A	616	SER
1	A	654	SER
2	B	14	GLN
2	B	28	SER
2	B	78	ILE
2	B	162	SER
2	B	166	SER
2	B	302	ASP

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Mol	Chain	Res	Type
2	B	344	ILE
2	B	362	ILE
2	B	376	GLN
2	B	426	THR
2	B	441	ASP
2	B	484	ASN
2	B	535	VAL
2	B	599	ILE
2	B	605	ASN
2	B	641	ASN
2	B	688	THR
2	B	689	ASN
3	C	4	SER
3	C	29	VAL
3	C	62	PHE
3	C	63	LEU
4	D	326	LEU
4	D	338	ILE
4	D	344	THR
4	D	392	LYS
4	D	394	GLN
4	D	395	ILE
4	D	463	LYS
4	D	469	THR
5	E	142	GLU
6	F	230	LEU
6	F	241	SER
6	F	330	VAL
7	J	2	LYS
7	J	17	LEU
9	1	129	ARG
9	1	140	SER
9	1	152	LEU
9	1	157	VAL
9	1	177	THR
9	1	200	PHE
9	1	212	VAL
9	1	221	LEU
9	1	223	SER
9	1	243	LEU
9	1	276	GLU
9	1	296	ASN

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Mol	Chain	Res	Type
10	2	301	VAL
10	2	323	LEU
10	2	338	VAL
10	2	351	GLU
10	2	361	SER
10	2	424	VAL
11	3	129	LYS
11	3	236	LEU
11	3	272	LEU
11	3	273	VAL
11	3	284	LEU
11	3	331	LEU
12	4	123	LEU
12	4	129	LYS
12	4	185	GLN
12	4	193	GLU
12	4	204	VAL
12	4	205	ILE
12	4	219	TYR
12	4	234	GLU
12	4	290	THR
13	5	338	ASP
13	5	359	MET
13	5	397	LEU
13	5	410	PHE
13	5	442	ILE
13	5	465	SER
13	5	468	GLN
14	6	144	LEU
14	6	147	GLU
14	6	162	ASP
14	6	205	PHE
14	6	231	SER
14	6	251	THR
14	6	279	ILE
14	6	283	SER
14	6	302	THR
15	7	444	THR
15	7	466	GLU
15	7	517	VAL
16	8	115	ILE
16	8	159	LEU

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Mol	Chain	Res	Type
16	8	179	THR
16	8	212	LEU
16	8	216	VAL
16	8	231	VAL
17	9	96	LEU
17	9	135	SER
17	9	164	ASP
17	9	170	LEU
17	9	184	LEU
17	9	196	ASP
17	9	236	LEU
17	9	240	SER
17	9	263	LEU
18	10	427	ILE
18	10	433	LEU
18	10	458	MET
18	10	459	ARG
18	10	481	LEU
18	10	482	LEU
18	10	530	SER
18	10	535	ASP
18	10	539	LEU
18	10	585	LEU
19	11	247	ASP
19	11	263	GLU
19	11	297	MET
19	11	320	SER
19	11	370	THR
19	11	407	LEU
19	12	255	THR
19	12	273	LEU
19	12	307	GLU
19	13	297	MET
19	13	298	LEU
19	13	309	LEU
19	13	347	ASN
19	13	370	THR
19	13	371	LYS
19	13	385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	225	ASN
1	A	478	GLN
1	A	480	GLN
1	A	485	GLN
2	B	14	GLN
2	B	108	GLN
2	B	114	ASN
2	B	218	HIS
2	B	376	GLN
2	B	470	ASN
3	C	16	GLN
5	E	153	ASN
6	F	183	GLN
6	F	288	GLN
6	F	310	ASN
8	M	6	ASN
8	M	30	ASN
9	1	292	ASN
10	2	325	HIS
11	3	171	GLN
11	3	233	ASN
12	4	185	GLN
13	5	460	ASN
14	6	287	ASN
15	7	502	ASN
15	7	602	ASN
16	8	233	HIS
17	9	215	ASN
17	9	262	ASN
19	11	402	ASN
19	13	347	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 342 ligands modelled in this entry, 42 are unknown - leaving 300 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	2	512	10	55,63,73	2.19	17 (30%)	64,101,113	3.02	27 (42%)
21	CLA	B	802	-	65,73,73	1.82	15 (23%)	76,113,113	2.84	32 (42%)
21	CLA	F	404	6	45,53,73	2.28	17 (37%)	52,89,113	3.31	27 (51%)
21	CLA	2	515	10	45,53,73	2.41	17 (37%)	52,89,113	3.21	28 (53%)
21	CLA	2	514	29	45,53,73	2.50	17 (37%)	52,89,113	3.06	26 (50%)
21	CLA	1	513	9	60,68,73	1.98	17 (28%)	69,106,113	2.77	25 (36%)
21	CLA	A	815	1	60,68,73	1.85	17 (28%)	70,107,113	3.27	35 (50%)
21	CLA	3	705	29	47,55,73	2.27	17 (36%)	54,91,113	3.28	25 (46%)
21	CLA	A	841	1	65,73,73	1.75	16 (24%)	76,113,113	2.87	27 (35%)
21	CLA	3	714	29	45,53,73	2.33	18 (40%)	52,89,113	3.05	25 (48%)
21	CLA	6	906	14	50,58,73	2.33	16 (32%)	58,95,113	3.12	28 (48%)
21	CLA	1	507	29	50,58,73	2.37	16 (32%)	58,95,113	2.84	27 (46%)
21	CLA	12	508	19	45,53,73	2.52	17 (37%)	52,89,113	3.20	26 (50%)
21	CLA	B	806	2	65,73,73	1.87	15 (23%)	76,113,113	2.70	33 (43%)
21	CLA	4	708	25	43,51,73	2.40	17 (39%)	49,86,113	3.12	24 (48%)
21	CLA	4	709	12	45,53,73	2.55	17 (37%)	52,89,113	3.31	29 (55%)
21	CLA	12	503	-	45,53,73	2.50	18 (40%)	52,89,113	3.25	26 (50%)
21	CLA	B	832	2	58,66,73	2.07	16 (27%)	67,104,113	3.10	31 (46%)
21	CLA	A	839	1	65,73,73	1.84	20 (30%)	76,113,113	2.90	34 (44%)
21	CLA	2	503	10	45,53,73	2.32	15 (33%)	52,89,113	3.17	25 (48%)
21	CLA	B	812	2	65,73,73	1.81	15 (23%)	76,113,113	2.70	28 (36%)
21	CLA	8	611	16	45,53,73	2.42	16 (35%)	52,89,113	3.17	28 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	12	502	19	45,53,73	2.40	16 (35%)	52,89,113	3.07	28 (53%)
25	LHG	3	719	21	24,24,48	0.38	0	27,30,54	0.58	0
21	CLA	A	823	1	45,53,73	2.23	13 (28%)	52,89,113	3.37	26 (50%)
21	CLA	9	904	17	45,53,73	2.51	17 (37%)	52,89,113	3.11	25 (48%)
24	BCR	J	102	-	41,41,41	1.67	10 (24%)	56,56,56	1.51	7 (12%)
21	CLA	B	808	2	45,53,73	2.33	20 (44%)	52,89,113	3.08	28 (53%)
21	CLA	8	609	16	62,70,73	2.19	15 (24%)	72,109,113	2.61	25 (34%)
21	CLA	A	809	1	65,73,73	1.98	17 (26%)	76,113,113	2.64	34 (44%)
21	CLA	1	508	29	47,55,73	2.30	17 (36%)	54,91,113	3.41	31 (57%)
21	CLA	B	813	2	65,73,73	2.01	21 (32%)	76,113,113	2.54	28 (36%)
21	CLA	A	803	-	65,73,73	1.93	16 (24%)	76,113,113	2.88	30 (39%)
21	CLA	B	838	2	45,53,73	1.95	15 (33%)	52,89,113	3.66	32 (61%)
21	CLA	B	807	2	65,73,73	1.78	20 (30%)	76,113,113	2.65	29 (38%)
21	CLA	7	705	29	50,58,73	2.22	15 (30%)	58,95,113	3.17	28 (48%)
21	CLA	4	705	29	47,55,73	2.24	16 (34%)	54,91,113	3.27	28 (51%)
21	CLA	B	804	2	65,73,73	1.85	19 (29%)	76,113,113	2.90	36 (47%)
21	CLA	7	709	25	43,51,73	2.24	17 (39%)	49,86,113	3.11	31 (63%)
21	CLA	7	713	15	47,55,73	2.32	16 (34%)	54,91,113	3.20	26 (48%)
21	CLA	A	808	1	51,59,73	2.11	19 (37%)	59,96,113	3.01	25 (42%)
21	CLA	11	707	19	54,62,73	2.31	16 (29%)	62,99,113	2.74	26 (41%)
25	LHG	B	848	21	22,22,48	0.37	0	25,28,54	1.07	2 (8%)
21	CLA	9	908	17	62,70,73	2.17	15 (24%)	72,109,113	2.67	27 (37%)
25	LHG	4	714	21	18,18,48	0.56	0	22,23,54	0.84	1 (4%)
21	CLA	8	607	29	47,55,73	2.27	17 (36%)	54,91,113	3.20	28 (51%)
25	LHG	9	917	21	33,33,48	0.38	0	36,39,54	0.83	1 (2%)
21	CLA	A	862	29	65,73,73	1.74	16 (24%)	76,113,113	3.26	37 (48%)
25	LHG	7	717	21	47,47,48	0.50	0	50,53,54	1.02	3 (6%)
21	CLA	A	825	1	59,67,73	1.84	15 (25%)	68,105,113	2.86	27 (39%)
28	DD6	11	712	-	39,45,45	1.64	8 (20%)	52,67,67	1.40	9 (17%)
25	LHG	A	853	-	48,48,48	0.66	1 (2%)	51,54,54	0.67	1 (1%)
28	DD6	4	712	-	39,45,45	1.48	8 (20%)	52,67,67	1.61	11 (21%)
21	CLA	3	702	11	60,68,73	1.91	16 (26%)	70,107,113	3.00	31 (44%)
28	DD6	7	715	-	39,45,45	1.53	8 (20%)	52,67,67	1.52	7 (13%)
21	CLA	5	711	13	45,53,73	2.53	16 (35%)	52,89,113	3.12	24 (46%)
21	CLA	7	702	15	47,55,73	2.28	16 (34%)	54,91,113	3.35	29 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	CLA	13	503	19	47,55,73	2.37	16 (34%)	54,91,113	3.14	26 (48%)
21	CLA	B	822	2	45,53,73	2.31	18 (40%)	52,89,113	3.06	30 (57%)
21	CLA	4	702	12	55,63,73	2.19	17 (30%)	64,101,113	3.02	26 (40%)
28	DD6	2	520	-	39,45,45	1.54	8 (20%)	52,67,67	1.54	8 (15%)
21	CLA	7	712	15	45,53,73	2.30	15 (33%)	52,89,113	3.36	31 (59%)
21	CLA	9	912	17	45,53,73	2.46	18 (40%)	52,89,113	3.24	25 (48%)
24	BCR	A	848	-	41,41,41	1.61	8 (19%)	56,56,56	1.69	12 (21%)
21	CLA	5	705	29	47,55,73	2.37	16 (34%)	54,91,113	3.01	29 (53%)
24	BCR	A	852	-	41,41,41	2.03	7 (17%)	56,56,56	1.40	7 (12%)
21	CLA	12	507	19	45,53,73	2.50	15 (33%)	52,89,113	3.24	27 (51%)
21	CLA	6	903	14	47,55,73	2.43	16 (34%)	54,91,113	3.28	29 (53%)
21	CLA	A	822	29	65,73,73	1.95	19 (29%)	76,113,113	2.57	32 (42%)
21	CLA	2	505	10	45,53,73	2.28	15 (33%)	52,89,113	2.96	25 (48%)
21	CLA	9	902	17	42,50,73	2.38	17 (40%)	48,85,113	3.15	25 (52%)
21	CLA	A	806	1	65,73,73	1.94	16 (24%)	76,113,113	2.63	34 (44%)
28	DD6	1	520	-	39,45,45	1.57	8 (20%)	52,67,67	1.59	10 (19%)
21	CLA	A	836	1	54,62,73	1.91	15 (27%)	62,99,113	2.98	28 (45%)
21	CLA	12	506	19	55,63,73	2.23	14 (25%)	64,101,113	2.87	28 (43%)
21	CLA	11	709	19	45,53,73	2.46	17 (37%)	52,89,113	3.04	26 (50%)
21	CLA	1	512	9	45,53,73	2.43	14 (31%)	52,89,113	3.19	29 (55%)
24	BCR	B	842	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
21	CLA	9	906	29	47,55,73	2.36	17 (36%)	54,91,113	3.19	26 (48%)
21	CLA	7	707	15	47,55,73	2.25	16 (34%)	54,91,113	3.04	25 (46%)
21	CLA	J	101	7	45,53,73	2.45	18 (40%)	52,89,113	3.28	30 (57%)
21	CLA	2	506	29	50,58,73	2.29	16 (32%)	58,95,113	2.95	30 (51%)
21	CLA	4	701	-	41,49,73	2.44	15 (36%)	47,84,113	3.69	25 (53%)
21	CLA	7	708	15	62,70,73	1.97	17 (27%)	72,109,113	2.70	31 (43%)
21	CLA	10	703	18	41,49,73	2.54	15 (36%)	47,84,113	3.10	26 (55%)
21	CLA	11	702	19	60,68,73	2.03	16 (26%)	70,107,113	2.63	29 (41%)
28	DD6	2	518	-	39,45,45	1.58	6 (15%)	52,67,67	1.69	10 (19%)
21	CLA	1	510	9	62,70,73	2.06	16 (25%)	72,109,113	2.65	28 (38%)
21	CLA	9	913	17	47,55,73	2.42	18 (38%)	54,91,113	3.21	26 (48%)
21	CLA	B	827	2	65,73,73	1.85	16 (24%)	76,113,113	2.75	32 (42%)
21	CLA	8	605	16	45,53,73	2.48	16 (35%)	52,89,113	3.09	25 (48%)
21	CLA	B	828	2	65,73,73	1.75	18 (27%)	76,113,113	3.05	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	BCR	A	847	-	41,41,41	1.51	10 (24%)	56,56,56	1.62	9 (16%)
21	CLA	B	821	2	55,63,73	2.13	15 (27%)	64,101,113	3.23	33 (51%)
21	CLA	A	817	29	49,57,73	2.07	16 (32%)	55,93,113	3.17	26 (47%)
21	CLA	5	704	29	50,58,73	2.37	15 (30%)	58,95,113	3.07	27 (46%)
25	LHG	1	521	21	35,35,48	0.38	0	38,41,54	0.90	2 (5%)
28	DD6	12	510	-	39,45,45	1.52	8 (20%)	52,67,67	2.08	14 (26%)
21	CLA	7	714	15	47,55,73	2.26	16 (34%)	54,91,113	3.21	26 (48%)
21	CLA	A	804	1	65,73,73	1.77	14 (21%)	76,113,113	2.84	32 (42%)
21	CLA	2	511	10	45,53,73	2.50	15 (33%)	52,89,113	3.17	27 (51%)
21	CLA	8	603	16	47,55,73	2.24	12 (25%)	54,91,113	3.29	26 (48%)
28	DD6	7	716	-	39,45,45	1.52	8 (20%)	52,67,67	1.52	8 (15%)
21	CLA	B	836	2	47,55,73	2.11	16 (34%)	54,91,113	3.69	35 (64%)
21	CLA	2	508	10	47,55,73	2.27	14 (29%)	54,91,113	3.17	28 (51%)
21	CLA	11	708	25	43,51,73	2.41	17 (39%)	49,86,113	3.28	26 (53%)
21	CLA	A	819	1	54,62,73	2.07	16 (29%)	62,99,113	2.87	30 (48%)
21	CLA	F	401	29	51,59,73	2.05	14 (27%)	59,96,113	3.15	25 (42%)
21	CLA	4	706	12	47,55,73	2.41	15 (31%)	54,91,113	3.03	27 (50%)
21	CLA	1	509	9	47,55,73	2.48	15 (31%)	54,91,113	3.18	26 (48%)
21	CLA	5	702	13	60,68,73	2.00	18 (30%)	70,107,113	2.60	30 (42%)
21	CLA	6	905	14	45,53,73	2.36	16 (35%)	52,89,113	3.05	26 (50%)
21	CLA	11	701	19	41,49,73	2.49	17 (41%)	47,84,113	3.25	26 (55%)
21	CLA	5	701	13	45,53,73	2.34	17 (37%)	52,89,113	2.99	29 (55%)
21	CLA	A	816	1	45,53,73	2.32	15 (33%)	52,89,113	3.31	27 (51%)
21	CLA	7	710	15	45,53,73	2.37	15 (33%)	52,89,113	3.24	26 (50%)
23	SF4	C	101	3	0,12,12	-	-	-		
21	CLA	2	510	25	43,51,73	2.24	14 (32%)	49,86,113	3.49	24 (48%)
28	DD6	1	519	-	39,45,45	1.61	7 (17%)	52,67,67	1.56	11 (21%)
21	CLA	4	710	12	45,53,73	2.44	16 (35%)	52,89,113	3.23	22 (42%)
27	DGD	B	847	-	58,58,67	1.01	4 (6%)	72,72,81	1.34	8 (11%)
21	CLA	B	811	2	45,53,73	2.29	14 (31%)	52,89,113	3.24	25 (48%)
21	CLA	4	703	12	45,53,73	2.35	16 (35%)	52,89,113	3.31	27 (51%)
21	CLA	B	830	2	49,57,73	2.37	17 (34%)	55,93,113	3.25	32 (58%)
21	CLA	B	805	2	65,73,73	1.97	12 (18%)	76,113,113	2.39	27 (35%)
21	CLA	F	403	29	45,53,73	2.25	14 (31%)	52,89,113	3.10	28 (53%)
28	DD6	12	509	-	39,45,45	1.52	8 (20%)	52,67,67	1.52	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	CLA	3	703	11	45,53,73	2.46	16 (35%)	52,89,113	3.08	29 (55%)
21	CLA	B	823	29	54,62,73	2.10	16 (29%)	62,99,113	2.99	28 (45%)
21	CLA	2	516	29	45,53,73	2.37	17 (37%)	52,89,113	2.91	23 (44%)
21	CLA	A	805	1	59,67,73	1.95	18 (30%)	68,105,113	3.10	30 (44%)
21	CLA	8	612	16	65,73,73	1.94	15 (23%)	76,113,113	2.63	27 (35%)
23	SF4	A	846	2,1	0,12,12	-	-	-		
25	LHG	11	714	21	29,29,48	0.36	0	32,35,54	0.72	1 (3%)
28	DD6	11	713	-	39,45,45	1.60	8 (20%)	52,67,67	1.64	9 (17%)
21	CLA	A	842	1	65,73,73	1.86	15 (23%)	76,113,113	2.73	27 (35%)
21	CLA	3	712	29	45,53,73	2.45	16 (35%)	52,89,113	3.04	27 (51%)
21	CLA	6	907	29	47,55,73	2.32	18 (38%)	54,91,113	3.10	30 (55%)
25	LHG	6	917	21	27,27,48	0.36	0	30,33,54	1.21	4 (13%)
28	DD6	2	519	-	39,45,45	1.78	7 (17%)	52,67,67	1.69	14 (26%)
24	BCR	F	405	-	41,41,41	1.65	9 (21%)	56,56,56	1.97	13 (23%)
21	CLA	3	707	11	62,70,73	2.01	14 (22%)	72,109,113	2.77	29 (40%)
21	CLA	4	711	29	45,53,73	2.34	15 (33%)	52,89,113	3.13	28 (53%)
21	CLA	5	708	25	43,51,73	2.43	15 (34%)	49,86,113	3.21	24 (48%)
24	BCR	M	102	-	41,41,41	1.58	11 (26%)	56,56,56	1.49	7 (12%)
28	DD6	3	718	-	39,45,45	1.55	9 (23%)	52,67,67	1.58	10 (19%)
21	CLA	A	807	1	65,73,73	2.02	16 (24%)	76,113,113	2.68	35 (46%)
21	CLA	B	820	2	45,53,73	2.34	16 (35%)	52,89,113	3.34	23 (44%)
21	CLA	B	831	2	65,73,73	1.87	14 (21%)	76,113,113	2.88	27 (35%)
21	CLA	11	710	19	45,53,73	2.35	19 (42%)	52,89,113	3.35	25 (48%)
28	DD6	8	616	-	39,45,45	1.54	8 (20%)	52,67,67	1.56	8 (15%)
28	DD6	3	717	-	39,45,45	1.83	7 (17%)	52,67,67	1.96	11 (21%)
24	BCR	B	843	-	41,41,41	1.68	7 (17%)	56,56,56	1.49	10 (17%)
21	CLA	A	840	1	47,55,73	2.24	16 (34%)	54,91,113	4.00	32 (59%)
21	CLA	9	905	29	50,58,73	2.31	15 (30%)	58,95,113	3.03	28 (48%)
21	CLA	6	904	14	60,68,73	2.10	16 (26%)	70,107,113	2.74	32 (45%)
21	CLA	11	703	19	65,73,73	1.94	16 (24%)	76,113,113	2.69	27 (35%)
21	CLA	9	909	25	43,51,73	2.34	16 (37%)	49,86,113	3.18	23 (46%)
21	CLA	1	505	9	60,68,73	2.09	15 (25%)	70,107,113	2.52	25 (35%)
21	CLA	2	507	29	47,55,73	2.16	17 (36%)	54,91,113	3.21	27 (50%)
21	CLA	8	613	16	45,53,73	2.49	16 (35%)	52,89,113	3.32	30 (57%)
21	CLA	3	701	11	41,49,73	2.46	15 (36%)	47,84,113	3.35	23 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	B	809	2	45,53,73	2.30	16 (35%)	52,89,113	3.09	27 (51%)
21	CLA	B	837	29	45,53,73	2.41	14 (31%)	52,89,113	2.88	23 (44%)
28	DD6	5	713	-	39,45,45	1.85	9 (23%)	52,67,67	1.89	13 (25%)
28	DD6	9	916	-	39,45,45	1.61	7 (17%)	52,67,67	1.67	10 (19%)
21	CLA	B	815	2	55,63,73	2.05	18 (32%)	64,101,113	2.67	25 (39%)
21	CLA	2	504	10	60,68,73	2.00	15 (25%)	70,107,113	2.78	32 (45%)
24	BCR	B	846	-	41,41,41	1.75	12 (29%)	56,56,56	1.39	10 (17%)
21	CLA	6	913	14	45,53,73	2.49	15 (33%)	52,89,113	3.13	27 (51%)
21	CLA	9	911	17	55,63,73	2.18	16 (29%)	64,101,113	2.91	26 (40%)
28	DD6	1	518	-	39,45,45	1.53	8 (20%)	52,67,67	1.49	8 (15%)
21	CLA	8	604	16	60,68,73	1.96	16 (26%)	70,107,113	2.88	28 (40%)
21	CLA	A	837	1	45,53,73	2.42	15 (33%)	52,89,113	3.26	26 (50%)
22	PQN	A	845	-	34,34,34	1.68	4 (11%)	42,45,45	1.42	6 (14%)
21	CLA	13	501	19	45,53,73	2.49	18 (40%)	52,89,113	3.12	26 (50%)
21	CLA	9	907	17	47,55,73	2.44	16 (34%)	54,91,113	3.61	31 (57%)
21	CLA	7	706	29	47,55,73	2.21	17 (36%)	54,91,113	3.10	27 (50%)
21	CLA	B	839	25	65,73,73	1.96	20 (30%)	76,113,113	2.88	33 (43%)
21	CLA	6	911	14	45,53,73	2.45	14 (31%)	52,89,113	3.17	27 (51%)
21	CLA	A	810	1	65,73,73	1.91	17 (26%)	76,113,113	2.86	26 (34%)
21	CLA	2	517	-	45,53,73	2.58	16 (35%)	52,89,113	3.15	24 (46%)
21	CLA	3	706	11	47,55,73	2.34	16 (34%)	54,91,113	3.22	30 (55%)
21	CLA	A	811	1	45,53,73	2.28	13 (28%)	52,89,113	3.37	27 (51%)
21	CLA	A	824	1	51,59,73	2.01	14 (27%)	59,96,113	3.36	30 (50%)
21	CLA	8	608	16	47,55,73	2.39	16 (34%)	54,91,113	3.14	30 (55%)
21	CLA	B	814	2	45,53,73	2.32	18 (40%)	52,89,113	3.23	28 (53%)
24	BCR	A	851	-	41,41,41	1.74	12 (29%)	56,56,56	1.31	7 (12%)
21	CLA	12	505	19	47,55,73	2.32	14 (29%)	54,91,113	3.06	27 (50%)
21	CLA	13	502	-	47,55,73	2.43	17 (36%)	54,91,113	3.06	26 (48%)
24	BCR	J	103	-	41,41,41	1.67	10 (24%)	56,56,56	1.55	7 (12%)
21	CLA	10	709	18	45,53,73	2.36	16 (35%)	52,89,113	3.28	26 (50%)
21	CLA	11	704	29	45,53,73	2.43	17 (37%)	52,89,113	3.21	26 (50%)
21	CLA	8	614	16	47,55,73	2.31	18 (38%)	54,91,113	3.09	24 (44%)
21	CLA	A	829	1	65,73,73	1.69	16 (24%)	76,113,113	2.87	35 (46%)
21	CLA	B	817	2	60,68,73	1.88	16 (26%)	70,107,113	3.06	34 (48%)
21	CLA	9	914	17	47,55,73	2.48	16 (34%)	54,91,113	3.11	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
28	DD6	J	104	-	39,45,45	1.60	8 (20%)	52,67,67	1.63	9 (17%)
21	CLA	4	707	12	62,70,73	2.12	16 (25%)	72,109,113	2.80	33 (45%)
21	CLA	1	504	9	42,50,73	2.48	16 (38%)	48,85,113	3.15	25 (52%)
25	LHG	5	714	21	31,31,48	0.35	0	34,37,54	0.62	0
21	CLA	B	819	2	47,55,73	2.38	17 (36%)	54,91,113	3.19	30 (55%)
21	CLA	6	909	14	62,70,73	2.02	15 (24%)	72,109,113	2.80	28 (38%)
21	CLA	1	506	9	45,53,73	2.34	15 (33%)	52,89,113	2.98	26 (50%)
21	CLA	A	813	1	54,62,73	2.16	19 (35%)	62,99,113	2.76	25 (40%)
21	CLA	6	914	14	47,55,73	2.33	15 (31%)	54,91,113	3.16	27 (50%)
25	LHG	8	617	21	32,32,48	0.40	0	35,38,54	0.98	1 (2%)
23	SF4	C	102	3	0,12,12	-	-	-		
21	CLA	9	910	17	45,53,73	2.37	17 (37%)	52,89,113	3.49	30 (57%)
25	LHG	A	854	21	26,26,48	0.46	0	29,32,54	1.25	5 (17%)
21	CLA	6	908	14	45,53,73	2.23	16 (35%)	52,89,113	3.33	28 (53%)
21	CLA	A	812	1	65,73,73	1.76	15 (23%)	76,113,113	2.80	33 (43%)
21	CLA	7	703	15	60,68,73	2.07	17 (28%)	70,107,113	2.92	26 (37%)
21	CLA	A	821	1	61,69,73	1.74	13 (21%)	71,108,113	3.10	26 (36%)
21	CLA	A	802	29	65,73,73	1.85	20 (30%)	76,113,113	2.79	33 (43%)
21	CLA	11	711	19	45,53,73	2.52	17 (37%)	52,89,113	3.22	26 (50%)
21	CLA	10	712	18	47,55,73	2.41	17 (36%)	54,91,113	3.15	24 (44%)
21	CLA	B	829	2	45,53,73	2.40	16 (35%)	52,89,113	3.55	30 (57%)
21	CLA	B	825	2	65,73,73	1.82	16 (24%)	76,113,113	2.63	34 (44%)
21	CLA	A	827	29	60,68,73	2.01	19 (31%)	70,107,113	2.86	30 (42%)
21	CLA	B	833	2	45,53,73	2.28	15 (33%)	52,89,113	3.42	32 (61%)
21	CLA	A	828	1	65,73,73	1.80	15 (23%)	76,113,113	2.88	29 (38%)
21	CLA	A	838	1	51,59,73	2.14	18 (35%)	59,96,113	2.92	24 (40%)
21	CLA	1	501	29	45,53,73	2.34	18 (40%)	52,89,113	3.24	27 (51%)
21	CLA	1	517	29	45,53,73	2.43	18 (40%)	52,89,113	3.07	24 (46%)
21	CLA	3	715	11	45,53,73	2.46	15 (33%)	52,89,113	3.26	29 (55%)
21	CLA	9	903	17	60,68,73	2.22	14 (23%)	70,107,113	2.95	30 (42%)
21	CLA	2	513	10	45,53,73	2.46	16 (35%)	52,89,113	3.19	25 (48%)
21	CLA	10	704	18	60,68,73	2.19	16 (26%)	70,107,113	2.84	27 (38%)
24	BCR	B	841	-	41,41,41	1.50	8 (19%)	56,56,56	1.53	9 (16%)
24	BCR	F	402	-	41,41,41	1.58	8 (19%)	56,56,56	1.66	10 (17%)
21	CLA	11	705	-	47,55,73	2.33	17 (36%)	54,91,113	2.97	28 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	A	814	1	60,68,73	2.12	18 (30%)	70,107,113	2.61	28 (40%)
21	CLA	B	824	29	46,54,73	2.22	16 (34%)	53,90,113	3.31	31 (58%)
20	CL0	A	801	1	65,73,73	2.11	21 (32%)	76,113,113	2.78	32 (42%)
21	CLA	A	843	29	52,60,73	2.06	15 (28%)	60,97,113	3.10	31 (51%)
21	CLA	8	606	29	45,53,73	2.42	18 (40%)	52,89,113	3.18	23 (44%)
21	CLA	A	833	1	65,73,73	1.86	17 (26%)	76,113,113	2.92	30 (39%)
21	CLA	3	709	11	45,53,73	2.23	16 (35%)	52,89,113	3.14	28 (53%)
21	CLA	B	826	2	65,73,73	1.85	20 (30%)	76,113,113	2.92	30 (39%)
21	CLA	5	706	13	45,53,73	2.43	14 (31%)	52,89,113	3.20	29 (55%)
21	CLA	11	706	19	65,73,73	1.96	16 (24%)	76,113,113	2.74	32 (42%)
28	DD6	9	915	-	39,45,45	1.62	8 (20%)	52,67,67	1.65	9 (17%)
21	CLA	B	818	29	65,73,73	1.92	15 (23%)	76,113,113	2.76	25 (32%)
28	DD6	4	713	-	39,45,45	1.58	7 (17%)	52,67,67	1.61	8 (15%)
21	CLA	B	803	2	54,62,73	2.05	17 (31%)	62,99,113	3.21	28 (45%)
21	CLA	A	830	1	65,73,73	2.03	17 (26%)	76,113,113	2.67	34 (44%)
21	CLA	A	835	1	45,53,73	2.28	18 (40%)	52,89,113	3.23	25 (48%)
21	CLA	B	810	2	45,53,73	2.29	16 (35%)	52,89,113	3.29	29 (55%)
21	CLA	5	710	13	50,58,73	2.36	16 (32%)	58,95,113	3.38	29 (50%)
24	BCR	A	849	-	41,41,41	1.83	10 (24%)	56,56,56	1.61	14 (25%)
24	BCR	A	850	-	41,41,41	1.61	10 (24%)	56,56,56	1.50	13 (23%)
21	CLA	A	818	1	54,62,73	2.10	15 (27%)	62,99,113	2.89	28 (45%)
21	CLA	5	703	13	45,53,73	2.25	13 (28%)	52,89,113	2.97	25 (48%)
21	CLA	8	610	25	43,51,73	2.15	14 (32%)	49,86,113	3.21	28 (57%)
21	CLA	10	711	18	45,53,73	2.44	18 (40%)	52,89,113	3.10	25 (48%)
28	DD6	6	915	-	39,45,45	1.55	8 (20%)	52,67,67	1.58	13 (25%)
21	CLA	A	820	1	65,73,73	1.76	17 (26%)	76,113,113	3.05	32 (42%)
21	CLA	1	511	25	43,51,73	2.35	16 (37%)	49,86,113	3.21	24 (48%)
21	CLA	6	910	25	43,51,73	2.38	15 (34%)	49,86,113	3.37	27 (55%)
21	CLA	12	504	-	41,49,73	2.53	16 (39%)	47,84,113	2.96	24 (51%)
22	PQN	B	840	-	32,32,34	1.75	5 (15%)	39,42,45	1.76	8 (20%)
21	CLA	10	705	18	45,53,73	2.50	15 (33%)	52,89,113	3.42	25 (48%)
24	BCR	B	845	-	41,41,41	1.63	10 (24%)	56,56,56	1.49	9 (16%)
25	LHG	10	713	21	31,31,48	0.32	0	34,37,54	0.94	2 (5%)
28	DD6	5	712	-	39,45,45	1.57	9 (23%)	52,67,67	1.47	8 (15%)
21	CLA	6	912	14	45,53,73	2.46	16 (35%)	52,89,113	3.09	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	BCR	B	844	-	41,41,41	1.72	9 (21%)	56,56,56	1.49	10 (17%)
21	CLA	10	707	18	48,56,73	2.43	17 (35%)	55,92,113	3.07	29 (52%)
21	CLA	3	704	29	42,50,73	2.22	16 (38%)	48,85,113	3.35	26 (54%)
21	CLA	10	710	18	55,63,73	2.19	16 (29%)	64,101,113	2.80	25 (39%)
21	CLA	A	831	1	65,73,73	1.73	16 (24%)	76,113,113	3.01	30 (39%)
28	DD6	3	716	-	39,45,45	1.40	7 (17%)	52,67,67	1.58	9 (17%)
21	CLA	1	515	29	45,53,73	2.43	14 (31%)	52,89,113	3.07	27 (51%)
21	CLA	3	708	25	43,51,73	2.31	15 (34%)	49,86,113	3.07	26 (53%)
21	CLA	B	835	2	65,73,73	1.93	17 (26%)	76,113,113	2.58	33 (43%)
21	CLA	A	834	1	45,53,73	2.21	13 (28%)	52,89,113	3.59	27 (51%)
21	CLA	12	501	19	60,68,73	2.10	16 (26%)	70,107,113	2.85	30 (42%)
21	CLA	A	826	29	65,73,73	1.97	17 (26%)	76,113,113	2.66	32 (42%)
28	DD6	6	916	-	39,45,45	1.41	7 (17%)	52,67,67	1.55	8 (15%)
21	CLA	B	801	2	65,73,73	2.02	20 (30%)	76,113,113	2.49	31 (40%)
21	CLA	5	707	13	55,63,73	2.25	16 (29%)	64,101,113	2.95	28 (43%)
21	CLA	B	834	2	60,68,73	2.22	19 (31%)	70,107,113	2.93	32 (45%)
21	CLA	2	509	10	62,70,73	2.00	17 (27%)	72,109,113	2.78	25 (34%)
21	CLA	1	516	9	45,53,73	2.41	16 (35%)	52,89,113	3.06	27 (51%)
21	CLA	1	514	9	45,53,73	2.48	15 (33%)	52,89,113	3.08	27 (51%)
21	CLA	3	713	11	45,53,73	2.44	16 (35%)	52,89,113	3.24	24 (46%)
21	CLA	A	832	1	50,58,73	2.03	11 (22%)	58,95,113	3.29	35 (60%)
21	CLA	5	709	13	45,53,73	2.50	17 (37%)	52,89,113	3.25	27 (51%)
21	CLA	7	704	15	45,53,73	2.34	16 (35%)	52,89,113	3.00	25 (48%)
21	CLA	3	711	11	45,53,73	2.40	15 (33%)	52,89,113	3.15	24 (46%)
21	CLA	10	706	-	41,49,73	2.52	15 (36%)	47,84,113	3.33	25 (53%)
25	LHG	2	521	21	29,29,48	0.39	0	32,35,54	1.24	4 (12%)
21	CLA	10	708	25	43,51,73	2.43	15 (34%)	49,86,113	3.25	24 (48%)
21	CLA	4	704	29	50,58,73	2.32	16 (32%)	58,95,113	3.00	28 (48%)
21	CLA	7	711	15	65,73,73	1.89	15 (23%)	76,113,113	2.47	24 (31%)
21	CLA	A	844	25	65,73,73	1.95	17 (26%)	76,113,113	2.97	34 (44%)
28	DD6	8	615	-	39,45,45	1.52	8 (20%)	52,67,67	1.46	8 (15%)
21	CLA	3	710	11	55,63,73	2.10	13 (23%)	64,101,113	2.95	26 (40%)
21	CLA	B	816	2	59,67,73	2.04	17 (28%)	68,105,113	3.00	32 (47%)

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
21	CLA	2	512	10	-	15/25/103/115	-
21	CLA	B	802	-	1/1/15/20	10/37/115/115	-
21	CLA	F	404	6	1/1/11/20	5/13/91/115	-
21	CLA	2	515	10	1/1/11/20	3/13/91/115	-
21	CLA	2	514	29	1/1/11/20	4/13/91/115	-
21	CLA	3	705	29	1/1/11/20	3/16/94/115	-
21	CLA	A	815	1	1/1/14/20	16/31/109/115	-
21	CLA	3	714	29	1/1/11/20	2/13/91/115	-
21	CLA	A	841	1	1/1/15/20	10/37/115/115	-
21	CLA	6	906	14	1/1/12/20	5/19/97/115	-
21	CLA	1	513	9	-	9/29/107/115	-
21	CLA	1	507	29	1/1/12/20	3/19/97/115	-
21	CLA	12	508	19	1/1/11/20	6/13/91/115	-
21	CLA	B	806	2	1/1/15/20	10/37/115/115	-
21	CLA	4	708	25	1/1/10/20	0/11/89/115	-
21	CLA	4	709	12	1/1/11/20	5/13/91/115	-
21	CLA	12	503	-	1/1/11/20	2/13/91/115	-
21	CLA	B	832	2	1/1/13/20	11/29/107/115	-
21	CLA	A	839	1	1/1/15/20	13/37/115/115	-
21	CLA	2	503	10	1/1/11/20	4/13/91/115	-
21	CLA	B	812	2	1/1/15/20	18/37/115/115	-
21	CLA	8	611	16	1/1/11/20	3/13/91/115	-
21	CLA	12	502	19	1/1/11/20	5/13/91/115	-
25	LHG	3	719	21	-	9/28/28/53	-
21	CLA	A	823	1	-	4/13/91/115	-
21	CLA	9	904	17	1/1/11/20	4/13/91/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	B	808	2	1/1/11/20	2/13/91/115	-
21	CLA	8	609	16	1/1/14/20	4/34/112/115	-
21	CLA	A	809	1	1/1/15/20	14/37/115/115	-
21	CLA	7	705	29	1/1/12/20	4/19/97/115	-
21	CLA	B	813	2	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	803	-	-	12/37/115/115	-
21	CLA	B	838	2	-	3/13/91/115	-
21	CLA	B	807	2	1/1/15/20	11/37/115/115	-
21	CLA	7	709	25	1/1/10/20	2/11/89/115	-
21	CLA	7	713	15	1/1/11/20	0/16/94/115	-
21	CLA	B	804	2	1/1/15/20	11/37/115/115	-
21	CLA	11	707	19	1/1/12/20	3/24/102/115	-
21	CLA	1	508	29	-	3/16/94/115	-
21	CLA	A	808	1	1/1/12/20	3/21/99/115	-
21	CLA	4	705	29	-	3/16/94/115	-
25	LHG	B	848	21	-	11/26/26/53	-
21	CLA	9	908	17	1/1/14/20	5/34/112/115	-
25	LHG	4	714	21	-	7/19/19/53	-
21	CLA	8	607	29	-	0/16/94/115	-
25	LHG	9	917	21	-	21/38/38/53	-
21	CLA	A	862	29	1/1/15/20	13/37/115/115	-
25	LHG	7	717	21	-	21/52/52/53	-
21	CLA	A	825	1	-	12/30/108/115	-
28	DD6	11	712	-	-	4/26/80/80	0/3/3/3
25	LHG	A	853	-	-	19/53/53/53	-
28	DD6	4	712	-	-	3/26/80/80	0/3/3/3
21	CLA	3	702	11	-	7/31/109/115	-
28	DD6	7	715	-	-	13/26/80/80	0/3/3/3
21	CLA	5	711	13	1/1/11/20	2/13/91/115	-
21	CLA	7	702	15	1/1/11/20	8/16/94/115	-
21	CLA	13	503	19	1/1/11/20	2/16/94/115	-
21	CLA	B	822	2	1/1/11/20	3/13/91/115	-
21	CLA	4	702	12	-	3/25/103/115	-
28	DD6	2	520	-	-	10/26/80/80	0/3/3/3
21	CLA	7	712	15	1/1/11/20	1/13/91/115	-
21	CLA	9	912	17	1/1/11/20	4/13/91/115	-
24	BCR	A	848	-	-	6/29/63/63	0/2/2/2
21	CLA	5	705	29	1/1/11/20	4/16/94/115	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	12	507	19	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	903	14	1/1/11/20	8/16/94/115	-
21	CLA	A	822	29	-	11/37/115/115	-
21	CLA	2	505	10	1/1/11/20	6/13/91/115	-
21	CLA	9	902	17	1/1/10/20	2/10/88/115	-
21	CLA	A	806	1	1/1/15/20	13/37/115/115	-
28	DD6	1	520	-	-	14/26/80/80	0/3/3/3
21	CLA	A	836	1	-	5/24/102/115	-
21	CLA	12	506	19	1/1/13/20	6/25/103/115	-
21	CLA	11	709	19	1/1/11/20	4/13/91/115	-
21	CLA	1	512	9	1/1/11/20	3/13/91/115	-
24	BCR	B	842	-	-	11/29/63/63	0/2/2/2
21	CLA	9	906	29	-	2/16/94/115	-
21	CLA	7	707	15	1/1/11/20	2/16/94/115	-
21	CLA	J	101	7	1/1/11/20	6/13/91/115	-
21	CLA	2	506	29	1/1/12/20	4/19/97/115	-
21	CLA	7	708	15	1/1/14/20	8/34/112/115	-
21	CLA	10	703	18	1/1/10/20	2/8/86/115	-
21	CLA	4	701	-	-	4/8/86/115	-
21	CLA	11	702	19	1/1/14/20	8/31/109/115	-
28	DD6	2	518	-	-	2/26/80/80	0/3/3/3
21	CLA	1	510	9	1/1/14/20	8/34/112/115	-
21	CLA	9	913	17	-	4/16/94/115	-
21	CLA	B	827	2	1/1/15/20	14/37/115/115	-
21	CLA	8	605	16	1/1/11/20	3/13/91/115	-
21	CLA	B	828	2	1/1/15/20	8/37/115/115	-
24	BCR	A	847	-	-	4/29/63/63	0/2/2/2
21	CLA	B	821	2	1/1/13/20	7/25/103/115	-
21	CLA	A	817	29	-	2/18/96/115	-
21	CLA	5	704	29	-	4/19/97/115	-
25	LHG	1	521	21	-	15/40/40/53	-
28	DD6	12	510	-	-	11/26/80/80	0/3/3/3
21	CLA	7	714	15	1/1/11/20	2/16/94/115	-
21	CLA	A	804	1	1/1/15/20	13/37/115/115	-
21	CLA	2	511	10	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	603	16	1/1/11/20	6/16/94/115	-
28	DD6	7	716	-	-	1/26/80/80	0/3/3/3
21	CLA	B	836	2	1/1/11/20	1/16/94/115	-
21	CLA	2	508	10	1/1/11/20	2/16/94/115	-
21	CLA	11	708	25	1/1/10/20	5/11/89/115	-
21	CLA	A	819	1	1/1/12/20	8/24/102/115	-
21	CLA	F	401	29	1/1/12/20	9/21/99/115	-
21	CLA	4	706	12	1/1/11/20	3/16/94/115	-
21	CLA	1	509	9	1/1/11/20	2/16/94/115	-
21	CLA	5	702	13	1/1/14/20	6/31/109/115	-
21	CLA	6	905	14	1/1/11/20	3/13/91/115	-
21	CLA	11	701	19	1/1/10/20	2/8/86/115	-
21	CLA	5	701	13	1/1/11/20	8/13/91/115	-
21	CLA	A	816	1	-	2/13/91/115	-
21	CLA	7	710	15	1/1/11/20	6/13/91/115	-
23	SF4	C	101	3	-	-	0/6/5/5
21	CLA	2	510	25	1/1/10/20	3/11/89/115	-
28	DD6	1	519	-	-	2/26/80/80	0/3/3/3
21	CLA	4	710	12	-	7/13/91/115	-
27	DGD	B	847	-	-	23/46/86/95	0/2/2/2
21	CLA	B	811	2	-	4/13/91/115	-
21	CLA	4	703	12	1/1/11/20	6/13/91/115	-
21	CLA	B	830	2	1/1/11/20	8/18/96/115	-
21	CLA	B	805	2	1/1/15/20	16/37/115/115	-
21	CLA	F	403	29	1/1/11/20	5/13/91/115	-
28	DD6	12	509	-	-	3/26/80/80	0/3/3/3
21	CLA	3	703	11	1/1/11/20	4/13/91/115	-
21	CLA	B	823	29	1/1/12/20	8/24/102/115	-
21	CLA	2	516	29	-	1/13/91/115	-
21	CLA	A	805	1	1/1/13/20	12/30/108/115	-
21	CLA	8	612	16	-	11/37/115/115	-
25	LHG	11	714	21	-	11/34/34/53	-
28	DD6	11	713	-	-	9/26/80/80	0/3/3/3
23	SF4	A	846	2,1	-	-	0/6/5/5
21	CLA	A	842	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	712	29	1/1/11/20	7/13/91/115	-
21	CLA	6	907	29	-	1/16/94/115	-
25	LHG	6	917	21	-	14/32/32/53	-
28	DD6	2	519	-	-	4/26/80/80	0/3/3/3
24	BCR	F	405	-	-	5/29/63/63	0/2/2/2
21	CLA	3	707	11	1/1/14/20	4/34/112/115	-
21	CLA	4	711	29	1/1/11/20	4/13/91/115	-
21	CLA	5	708	25	1/1/10/20	5/11/89/115	-
24	BCR	M	102	-	-	3/29/63/63	0/2/2/2
28	DD6	3	718	-	-	7/26/80/80	0/3/3/3
21	CLA	A	807	1	1/1/15/20	10/37/115/115	-
21	CLA	B	831	2	1/1/15/20	17/37/115/115	-
21	CLA	B	820	2	-	6/13/91/115	-
21	CLA	11	710	19	-	7/13/91/115	-
28	DD6	8	616	-	-	7/26/80/80	0/3/3/3
28	DD6	3	717	-	-	9/26/80/80	0/3/3/3
24	BCR	B	843	-	-	6/29/63/63	0/2/2/2
21	CLA	A	840	1	1/1/11/20	8/16/94/115	-
21	CLA	9	905	29	1/1/12/20	5/19/97/115	-
21	CLA	6	904	14	1/1/14/20	5/31/109/115	-
21	CLA	11	703	19	1/1/15/20	16/37/115/115	-
21	CLA	9	909	25	1/1/10/20	3/11/89/115	-
21	CLA	1	505	9	1/1/14/20	9/31/109/115	-
21	CLA	8	613	16	1/1/11/20	5/13/91/115	-
21	CLA	2	507	29	-	6/16/94/115	-
21	CLA	3	701	11	1/1/10/20	4/8/86/115	-
21	CLA	B	809	2	1/1/11/20	4/13/91/115	-
21	CLA	B	837	29	1/1/11/20	5/13/91/115	-
28	DD6	5	713	-	-	5/26/80/80	0/3/3/3
28	DD6	9	916	-	-	10/26/80/80	0/3/3/3
21	CLA	B	815	2	1/1/13/20	9/25/103/115	-
21	CLA	2	504	10	1/1/14/20	12/31/109/115	-
24	BCR	B	846	-	-	0/29/63/63	0/2/2/2
21	CLA	6	913	14	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	911	17	1/1/13/20	8/25/103/115	-
28	DD6	1	518	-	-	14/26/80/80	0/3/3/3
21	CLA	8	604	16	1/1/14/20	6/31/109/115	-
21	CLA	A	837	1	-	6/13/91/115	-
22	PQN	A	845	-	-	8/23/43/43	0/2/2/2
21	CLA	13	501	19	1/1/11/20	5/13/91/115	-
21	CLA	9	907	17	1/1/11/20	2/16/94/115	-
21	CLA	7	706	29	-	5/16/94/115	-
21	CLA	B	839	25	1/1/15/20	15/37/115/115	-
21	CLA	6	911	14	1/1/11/20	3/13/91/115	-
21	CLA	A	810	1	-	14/37/115/115	-
21	CLA	2	517	-	1/1/11/20	2/13/91/115	-
21	CLA	3	706	11	1/1/11/20	7/16/94/115	-
21	CLA	A	811	1	1/1/11/20	5/13/91/115	-
21	CLA	A	824	1	-	11/21/99/115	-
21	CLA	8	608	16	1/1/11/20	2/16/94/115	-
21	CLA	B	814	2	1/1/11/20	2/13/91/115	-
24	BCR	A	851	-	-	0/29/63/63	0/2/2/2
21	CLA	12	505	19	1/1/11/20	2/16/94/115	-
21	CLA	13	502	-	1/1/11/20	4/16/94/115	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	CLA	10	709	18	1/1/11/20	3/13/91/115	-
21	CLA	11	704	29	1/1/11/20	0/13/91/115	-
21	CLA	8	614	16	-	2/16/94/115	-
21	CLA	A	829	1	1/1/15/20	18/37/115/115	-
21	CLA	B	817	2	1/1/14/20	12/31/109/115	-
21	CLA	9	914	17	1/1/11/20	5/16/94/115	-
28	DD6	J	104	-	-	16/26/80/80	0/3/3/3
21	CLA	4	707	12	1/1/14/20	4/34/112/115	-
21	CLA	1	504	9	1/1/10/20	1/10/88/115	-
25	LHG	5	714	21	-	15/36/36/53	-
21	CLA	6	909	14	1/1/14/20	4/34/112/115	-
21	CLA	B	819	2	-	6/16/94/115	-
21	CLA	1	506	9	1/1/11/20	5/13/91/115	-
21	CLA	A	813	1	1/1/12/20	10/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	914	14	-	7/16/94/115	-
25	LHG	8	617	21	-	15/37/37/53	-
23	SF4	C	102	3	-	-	0/6/5/5
21	CLA	9	910	17	1/1/11/20	5/13/91/115	-
25	LHG	A	854	21	-	13/31/31/53	-
21	CLA	6	908	14	1/1/11/20	1/13/91/115	-
21	CLA	A	812	1	1/1/15/20	5/37/115/115	-
21	CLA	7	703	15	-	8/31/109/115	-
21	CLA	A	821	1	1/1/14/20	12/33/111/115	-
21	CLA	A	802	29	1/1/15/20	3/37/115/115	-
21	CLA	11	711	19	1/1/11/20	4/13/91/115	-
21	CLA	10	712	18	1/1/11/20	4/16/94/115	-
21	CLA	B	829	2	-	4/13/91/115	-
21	CLA	B	825	2	1/1/15/20	4/37/115/115	-
21	CLA	A	827	29	1/1/14/20	9/31/109/115	-
21	CLA	B	833	2	1/1/11/20	9/13/91/115	-
21	CLA	A	828	1	1/1/15/20	13/37/115/115	-
21	CLA	A	838	1	1/1/12/20	4/21/99/115	-
21	CLA	1	501	29	1/1/11/20	2/13/91/115	-
21	CLA	3	715	11	1/1/11/20	5/13/91/115	-
21	CLA	9	903	17	1/1/14/20	6/31/109/115	-
21	CLA	10	704	18	1/1/14/20	6/31/109/115	-
21	CLA	2	513	10	1/1/11/20	7/13/91/115	-
21	CLA	1	517	29	-	2/13/91/115	-
24	BCR	B	841	-	-	2/29/63/63	0/2/2/2
24	BCR	F	402	-	-	1/29/63/63	0/2/2/2
21	CLA	11	705	-	1/1/11/20	6/16/94/115	-
21	CLA	A	814	1	1/1/14/20	7/31/109/115	-
21	CLA	B	824	29	1/1/11/20	4/15/93/115	-
20	CL0	A	801	1	3/3/20/25	5/37/135/135	-
21	CLA	A	843	29	1/1/12/20	4/22/100/115	-
21	CLA	8	606	29	1/1/11/20	0/13/91/115	-
21	CLA	A	833	1	1/1/15/20	5/37/115/115	-
21	CLA	3	709	11	1/1/11/20	5/13/91/115	-
21	CLA	B	826	2	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	706	13	1/1/11/20	3/13/91/115	-
21	CLA	11	706	19	1/1/15/20	12/37/115/115	-
28	DD6	9	915	-	-	12/26/80/80	0/3/3/3
21	CLA	B	818	29	1/1/15/20	4/37/115/115	-
28	DD6	4	713	-	-	14/26/80/80	0/3/3/3
21	CLA	B	803	2	1/1/12/20	13/24/102/115	-
21	CLA	A	830	1	1/1/15/20	13/37/115/115	-
21	CLA	A	835	1	-	5/13/91/115	-
21	CLA	B	810	2	1/1/11/20	4/13/91/115	-
21	CLA	5	710	13	-	8/19/97/115	-
24	BCR	A	849	-	-	4/29/63/63	0/2/2/2
24	BCR	A	850	-	-	6/29/63/63	0/2/2/2
21	CLA	A	818	1	1/1/12/20	12/24/102/115	-
21	CLA	5	703	13	1/1/11/20	5/13/91/115	-
21	CLA	8	610	25	1/1/10/20	2/11/89/115	-
21	CLA	10	711	18	1/1/11/20	1/13/91/115	-
28	DD6	6	915	-	-	3/26/80/80	0/3/3/3
21	CLA	A	820	1	1/1/15/20	15/37/115/115	-
21	CLA	1	511	25	1/1/10/20	2/11/89/115	-
21	CLA	6	910	25	1/1/10/20	3/11/89/115	-
21	CLA	12	504	-	1/1/10/20	1/8/86/115	-
22	PQN	B	840	-	-	4/21/41/43	0/2/2/2
21	CLA	10	705	18	1/1/11/20	3/13/91/115	-
24	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	LHG	10	713	21	-	17/36/36/53	-
28	DD6	5	712	-	-	3/26/80/80	0/3/3/3
21	CLA	6	912	14	1/1/11/20	6/13/91/115	-
24	BCR	B	844	-	-	2/29/63/63	0/2/2/2
21	CLA	10	707	18	1/1/11/20	7/17/95/115	-
21	CLA	3	704	29	1/1/10/20	2/10/88/115	-
21	CLA	10	710	18	1/1/13/20	3/25/103/115	-
21	CLA	A	831	1	1/1/15/20	8/37/115/115	-
28	DD6	3	716	-	-	4/26/80/80	0/3/3/3
21	CLA	1	515	29	1/1/11/20	1/13/91/115	-
21	CLA	3	708	25	1/1/10/20	6/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	835	2	1/1/15/20	15/37/115/115	-
21	CLA	A	834	1	1/1/11/20	4/13/91/115	-
21	CLA	12	501	19	1/1/14/20	7/31/109/115	-
21	CLA	A	826	29	1/1/15/20	14/37/115/115	-
28	DD6	6	916	-	-	6/26/80/80	0/3/3/3
21	CLA	B	801	2	1/1/15/20	3/37/115/115	-
21	CLA	5	707	13	1/1/13/20	6/25/103/115	-
21	CLA	B	834	2	1/1/14/20	9/31/109/115	-
21	CLA	2	509	10	1/1/14/20	5/34/112/115	-
21	CLA	1	516	9	1/1/11/20	1/13/91/115	-
21	CLA	1	514	9	1/1/11/20	1/13/91/115	-
21	CLA	3	713	11	1/1/11/20	5/13/91/115	-
21	CLA	5	709	13	1/1/11/20	3/13/91/115	-
21	CLA	A	832	1	-	4/19/97/115	-
21	CLA	7	704	15	1/1/11/20	3/13/91/115	-
21	CLA	3	711	11	1/1/11/20	4/13/91/115	-
21	CLA	10	706	-	1/1/10/20	2/8/86/115	-
25	LHG	2	521	21	-	16/34/34/53	-
21	CLA	10	708	25	1/1/10/20	2/11/89/115	-
21	CLA	4	704	29	1/1/12/20	0/19/97/115	-
21	CLA	7	711	15	1/1/15/20	7/37/115/115	-
21	CLA	A	844	25	1/1/15/20	13/37/115/115	-
28	DD6	8	615	-	-	12/26/80/80	0/3/3/3
21	CLA	3	710	11	-	11/25/103/115	-
21	CLA	B	816	2	1/1/13/20	5/30/108/115	-

All (4198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	807	CLA	C1B-NB	-8.18	1.27	1.35
21	B	801	CLA	C1B-NB	-8.10	1.28	1.35
21	A	838	CLA	C1B-NB	-6.91	1.29	1.35
21	9	908	CLA	C3B-C2B	6.89	1.49	1.40
21	A	826	CLA	C1B-NB	-6.87	1.29	1.35
21	B	834	CLA	C1B-NB	-6.82	1.29	1.35
21	B	832	CLA	C1B-NB	-6.73	1.29	1.35
21	6	904	CLA	C3B-C2B	6.70	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	510	CLA	C3B-C2B	6.60	1.49	1.40
21	2	512	CLA	C3B-C2B	6.56	1.49	1.40
22	A	845	PQN	C3-C2	6.53	1.47	1.35
21	7	702	CLA	C3B-C2B	6.51	1.49	1.40
21	9	904	CLA	C3B-C2B	6.48	1.49	1.40
21	4	702	CLA	C3B-C2B	6.45	1.49	1.40
21	12	504	CLA	C1D-ND	6.44	1.45	1.37
21	6	911	CLA	C3C-C2C	6.35	1.50	1.36
21	10	704	CLA	C3B-C2B	6.34	1.49	1.40
21	1	509	CLA	C3B-C2B	6.32	1.49	1.40
22	B	840	PQN	C3-C2	6.30	1.46	1.35
21	8	613	CLA	O2D-CGD	6.23	1.48	1.33
21	B	829	CLA	CHC-C1C	6.21	1.50	1.35
21	B	803	CLA	C1B-NB	-6.20	1.29	1.35
24	A	852	BCR	C14-C13	6.19	1.44	1.35
21	A	834	CLA	C1B-NB	-6.18	1.29	1.35
21	8	606	CLA	C3B-C2B	6.17	1.48	1.40
21	6	913	CLA	C3B-C2B	6.17	1.48	1.40
21	2	505	CLA	C1D-ND	6.16	1.45	1.37
21	12	503	CLA	C3B-C2B	6.16	1.48	1.40
21	A	844	CLA	O2D-CGD	6.15	1.48	1.33
21	B	805	CLA	O2A-CGA	6.15	1.51	1.33
21	9	912	CLA	C3B-C2B	6.15	1.48	1.40
21	13	501	CLA	C3B-C2B	6.15	1.48	1.40
21	2	517	CLA	C3B-C2B	6.13	1.48	1.40
21	1	504	CLA	C3B-C2B	6.11	1.48	1.40
21	8	613	CLA	C3B-C2B	6.07	1.48	1.40
21	1	509	CLA	CHC-C1C	6.07	1.50	1.35
21	A	808	CLA	CHC-C1C	6.07	1.50	1.35
21	6	905	CLA	C3B-C2B	6.07	1.48	1.40
21	9	903	CLA	C3C-C2C	6.04	1.49	1.36
21	3	707	CLA	C3B-C2B	6.02	1.48	1.40
28	2	519	DD6	C5-C6	6.02	1.43	1.35
21	9	907	CLA	C3B-C2B	6.01	1.48	1.40
21	A	823	CLA	C3B-C2B	6.00	1.48	1.40
21	4	709	CLA	C3B-C2B	5.99	1.48	1.40
21	2	509	CLA	C3B-C2B	5.98	1.48	1.40
21	1	507	CLA	C3B-C2B	5.95	1.48	1.40
21	10	707	CLA	C3B-C2B	5.95	1.48	1.40
21	1	505	CLA	C3C-C2C	5.95	1.49	1.36
21	4	703	CLA	C3B-C2B	5.94	1.48	1.40
21	9	903	CLA	CHC-C1C	5.94	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	837	CLA	C3C-C2C	5.94	1.49	1.36
21	A	830	CLA	C1B-NB	-5.93	1.29	1.35
21	5	706	CLA	OBD-CAD	5.92	1.32	1.22
21	4	709	CLA	O2D-CGD	5.92	1.47	1.33
21	13	501	CLA	O2D-CGD	5.90	1.47	1.33
21	A	806	CLA	O2A-CGA	5.89	1.50	1.33
21	1	514	CLA	C3B-C2B	5.88	1.48	1.40
21	11	708	CLA	C3B-C2B	5.88	1.48	1.40
21	B	834	CLA	CHC-C1C	5.88	1.50	1.35
20	A	801	CL0	C1B-NB	-5.86	1.30	1.35
21	3	701	CLA	O2D-CGD	5.85	1.47	1.33
21	7	704	CLA	C1B-NB	-5.84	1.30	1.35
21	10	703	CLA	C3C-C2C	5.84	1.49	1.36
24	A	852	BCR	C17-C18	5.84	1.43	1.35
21	B	813	CLA	C4B-NB	-5.84	1.30	1.35
21	5	711	CLA	C3B-C2B	5.84	1.48	1.40
21	7	710	CLA	CHC-C1C	5.83	1.49	1.35
21	10	705	CLA	C3B-C2B	5.83	1.48	1.40
21	5	708	CLA	C1D-ND	5.83	1.44	1.37
21	4	701	CLA	C3B-C2B	5.83	1.48	1.40
21	10	708	CLA	C3B-C2B	5.83	1.48	1.40
21	8	605	CLA	C3B-C2B	5.82	1.48	1.40
21	11	711	CLA	C3B-C2B	5.82	1.48	1.40
21	B	819	CLA	C3B-C2B	5.81	1.48	1.40
21	3	712	CLA	C3C-C2C	5.81	1.49	1.36
21	B	831	CLA	C1B-NB	-5.81	1.30	1.35
21	B	805	CLA	CHC-C1C	5.81	1.49	1.35
21	B	830	CLA	O2A-CGA	5.80	1.50	1.33
21	5	710	CLA	C3B-C2B	5.80	1.48	1.40
21	1	512	CLA	O2D-CGD	5.80	1.47	1.33
21	9	902	CLA	C3B-C2B	5.80	1.48	1.40
21	3	701	CLA	C3C-C2C	5.79	1.49	1.36
21	A	811	CLA	O2A-CGA	5.78	1.50	1.30
21	B	827	CLA	O2A-CGA	5.75	1.50	1.33
21	B	824	CLA	C3B-C2B	5.74	1.48	1.40
21	13	503	CLA	O2D-CGD	5.72	1.47	1.33
21	9	914	CLA	C3B-C2B	5.72	1.48	1.40
21	4	710	CLA	C3B-C2B	5.72	1.48	1.40
21	5	711	CLA	O2D-CGD	5.72	1.47	1.33
21	B	809	CLA	CHC-C1C	5.71	1.49	1.35
21	4	704	CLA	O2A-CGA	5.70	1.50	1.33
21	B	833	CLA	CHC-C1C	5.70	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	810	CLA	O2A-CGA	5.70	1.49	1.30
21	6	906	CLA	O2D-CGD	5.69	1.47	1.33
21	B	821	CLA	CHC-C1C	5.68	1.49	1.35
21	10	710	CLA	CHC-C1C	5.67	1.49	1.35
21	4	707	CLA	C3B-C2B	5.67	1.48	1.40
20	A	801	CL0	C4B-NB	-5.66	1.30	1.35
21	5	703	CLA	C3B-C2B	5.66	1.48	1.40
21	8	609	CLA	CHC-C1C	5.66	1.49	1.35
21	11	702	CLA	CHC-C1C	5.66	1.49	1.35
21	8	607	CLA	C3B-C2B	5.66	1.48	1.40
21	13	502	CLA	C3B-C2B	5.66	1.48	1.40
21	2	504	CLA	C3B-C2B	5.66	1.48	1.40
21	B	806	CLA	CHC-C1C	5.66	1.49	1.35
21	7	711	CLA	CHC-C1C	5.65	1.49	1.35
21	1	509	CLA	C3C-C2C	5.64	1.48	1.36
21	6	906	CLA	C3C-C2C	5.64	1.48	1.36
21	2	517	CLA	O2D-CGD	5.64	1.47	1.33
21	7	714	CLA	O2A-CGA	5.64	1.49	1.33
21	A	821	CLA	CHC-C1C	5.64	1.49	1.35
28	3	717	DD6	C2-C1	5.63	1.43	1.35
21	J	101	CLA	CHC-C1C	5.63	1.49	1.35
21	9	904	CLA	C3C-C2C	5.63	1.48	1.36
21	3	701	CLA	C3B-C2B	5.63	1.48	1.40
21	6	905	CLA	O2D-CGD	5.62	1.46	1.33
21	B	817	CLA	CHC-C1C	5.62	1.49	1.35
21	2	503	CLA	O2D-CGD	5.62	1.46	1.33
21	3	708	CLA	C1D-ND	5.62	1.44	1.37
21	6	911	CLA	O2D-CGD	5.62	1.46	1.33
21	12	502	CLA	O2D-CGD	5.62	1.46	1.33
21	8	605	CLA	O2D-CGD	5.62	1.46	1.33
21	A	825	CLA	CHC-C1C	5.61	1.49	1.35
21	4	707	CLA	C3C-C2C	5.60	1.48	1.36
21	B	828	CLA	O2A-CGA	5.60	1.49	1.33
21	4	706	CLA	C3C-C2C	5.60	1.48	1.36
21	2	515	CLA	C3C-C2C	5.59	1.48	1.36
21	10	711	CLA	C3C-C2C	5.59	1.48	1.36
21	2	503	CLA	C3C-C2C	5.58	1.48	1.36
21	B	821	CLA	O2A-CGA	5.58	1.49	1.33
21	11	709	CLA	O2D-CGD	5.58	1.46	1.33
28	2	519	DD6	C2-C1	5.58	1.43	1.35
21	9	913	CLA	C3B-C2B	5.57	1.48	1.40
21	7	707	CLA	O2A-CGA	5.57	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	507	CLA	O2D-CGD	5.57	1.46	1.33
21	2	516	CLA	CHC-C1C	5.56	1.49	1.35
21	9	903	CLA	O2D-CGD	5.56	1.46	1.33
21	1	515	CLA	CHC-C1C	5.56	1.49	1.35
21	7	714	CLA	CHC-C1C	5.55	1.49	1.35
21	6	914	CLA	O2A-CGA	5.55	1.49	1.33
21	12	501	CLA	C3C-C2C	5.54	1.48	1.36
21	6	903	CLA	C3C-C2C	5.54	1.48	1.36
21	9	909	CLA	C1D-ND	5.54	1.44	1.37
21	1	506	CLA	O2D-CGD	5.53	1.46	1.33
21	4	708	CLA	C3B-C2B	5.53	1.48	1.40
21	13	501	CLA	C3C-C2C	5.52	1.48	1.36
21	3	713	CLA	O2D-CGD	5.52	1.46	1.33
21	1	516	CLA	C3B-C2B	5.52	1.48	1.40
21	4	703	CLA	O2D-CGD	5.52	1.46	1.33
21	2	514	CLA	C3C-C2C	5.51	1.48	1.36
21	11	701	CLA	C3B-C2B	5.51	1.48	1.40
21	3	703	CLA	C1D-ND	5.51	1.44	1.37
24	B	843	BCR	C10-C9	5.51	1.43	1.35
21	B	819	CLA	O2A-CGA	5.51	1.49	1.33
21	6	903	CLA	C3B-C2B	5.51	1.48	1.40
21	5	704	CLA	O2D-CGD	5.51	1.46	1.33
21	12	508	CLA	C3B-C2B	5.50	1.48	1.40
21	5	709	CLA	CHC-C1C	5.50	1.49	1.35
21	5	711	CLA	C3C-C2C	5.49	1.48	1.36
21	10	703	CLA	C3B-C2B	5.49	1.48	1.40
21	A	843	CLA	O2A-CGA	5.49	1.49	1.33
21	12	504	CLA	O2D-CGD	5.48	1.46	1.33
21	9	911	CLA	C3B-C2B	5.48	1.48	1.40
21	A	818	CLA	O2A-CGA	5.48	1.49	1.33
21	10	705	CLA	O2D-CGD	5.48	1.46	1.33
21	8	606	CLA	C3C-C2C	5.47	1.48	1.36
21	9	907	CLA	C3C-C2C	5.47	1.48	1.36
21	B	832	CLA	CHC-C1C	5.47	1.49	1.35
21	13	502	CLA	O2D-CGD	5.46	1.46	1.33
21	6	913	CLA	C3C-C2C	5.46	1.48	1.36
21	12	501	CLA	O2D-CGD	5.46	1.46	1.33
21	8	607	CLA	O2D-CGD	5.46	1.46	1.33
21	1	505	CLA	C3B-C2B	5.46	1.47	1.40
21	10	709	CLA	O2D-CGD	5.46	1.46	1.33
21	A	818	CLA	CHC-C1C	5.46	1.49	1.35
21	12	506	CLA	CHC-C1C	5.46	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	704	CLA	C3C-C2C	5.45	1.48	1.36
21	B	836	CLA	C3B-C2B	5.45	1.47	1.40
21	8	609	CLA	C3C-C2C	5.45	1.48	1.36
21	7	704	CLA	C3B-C2B	5.45	1.47	1.40
21	10	709	CLA	C3B-C2B	5.45	1.47	1.40
21	3	707	CLA	CHC-C1C	5.45	1.48	1.35
21	9	906	CLA	C3C-C2C	5.45	1.48	1.36
21	12	507	CLA	C3B-C2B	5.44	1.47	1.40
21	A	833	CLA	O2A-CGA	5.44	1.49	1.33
21	2	504	CLA	C3C-C2C	5.44	1.48	1.36
21	J	101	CLA	O2A-CGA	5.44	1.49	1.30
21	B	810	CLA	CHC-C1C	5.43	1.48	1.35
21	10	706	CLA	C3B-C2B	5.43	1.47	1.40
21	2	513	CLA	C3B-C2B	5.43	1.47	1.40
28	3	717	DD6	C5-C6	5.43	1.43	1.35
21	4	702	CLA	CHC-C1C	5.43	1.48	1.35
21	3	706	CLA	C1D-ND	5.43	1.44	1.37
21	B	831	CLA	CHC-C1C	5.43	1.48	1.35
21	10	712	CLA	O2D-CGD	5.42	1.46	1.33
21	12	508	CLA	C3C-C2C	5.42	1.48	1.36
21	A	832	CLA	O2A-CGA	5.42	1.49	1.33
21	8	611	CLA	O2D-CGD	5.42	1.46	1.33
21	9	904	CLA	O2D-CGD	5.42	1.46	1.33
21	6	914	CLA	C3B-C2B	5.41	1.47	1.40
21	10	704	CLA	C3C-C2C	5.41	1.48	1.36
21	A	832	CLA	C1B-NB	-5.41	1.30	1.35
21	B	819	CLA	C1D-ND	5.41	1.44	1.37
21	9	911	CLA	CHC-C1C	5.41	1.48	1.35
21	1	517	CLA	C3C-C2C	5.40	1.48	1.36
21	1	510	CLA	CHC-C1C	5.40	1.48	1.35
21	4	701	CLA	O2D-CGD	5.40	1.46	1.33
21	5	709	CLA	O2D-CGD	5.40	1.46	1.33
21	B	814	CLA	C3B-C2B	5.40	1.47	1.40
21	8	608	CLA	C1D-ND	5.40	1.44	1.37
21	2	511	CLA	C1D-ND	5.39	1.44	1.37
21	B	837	CLA	CHC-C1C	5.39	1.48	1.35
21	6	912	CLA	O2D-CGD	5.39	1.46	1.33
21	A	840	CLA	O2A-CGA	5.39	1.49	1.33
21	1	515	CLA	O2D-CGD	5.39	1.46	1.33
21	11	703	CLA	CHC-C1C	5.39	1.48	1.35
21	10	711	CLA	O2D-CGD	5.39	1.46	1.33
21	8	609	CLA	C3B-C2B	5.38	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	912	CLA	C3C-C2C	5.38	1.48	1.36
21	B	820	CLA	O2D-CGD	5.38	1.46	1.33
21	12	507	CLA	C3C-C2C	5.38	1.48	1.36
21	B	821	CLA	C3B-C2B	5.38	1.47	1.40
21	A	813	CLA	CHD-C1D	5.38	1.48	1.38
21	1	512	CLA	C3B-C2B	5.37	1.47	1.40
21	1	501	CLA	O2A-CGA	5.37	1.48	1.30
21	6	913	CLA	O2D-CGD	5.37	1.46	1.33
21	3	709	CLA	O2D-CGD	5.37	1.46	1.33
21	A	803	CLA	O2A-CGA	5.36	1.49	1.33
21	3	713	CLA	C3B-C2B	5.36	1.47	1.40
21	2	506	CLA	C3B-C2B	5.36	1.47	1.40
21	12	506	CLA	C3C-C2C	5.36	1.48	1.36
21	9	912	CLA	O2D-CGD	5.35	1.46	1.33
21	11	701	CLA	C3C-C2C	5.35	1.48	1.36
21	1	511	CLA	C3B-C2B	5.35	1.47	1.40
21	A	828	CLA	CHC-C1C	5.34	1.48	1.35
21	6	910	CLA	C3B-C2B	5.34	1.47	1.40
21	3	706	CLA	O2D-CGD	5.34	1.46	1.33
21	9	905	CLA	O2D-CGD	5.34	1.46	1.33
21	11	711	CLA	O2D-CGD	5.34	1.46	1.33
21	3	715	CLA	C1D-ND	5.34	1.44	1.37
21	A	830	CLA	C3B-C2B	5.34	1.47	1.40
21	7	710	CLA	O2D-CGD	5.33	1.46	1.33
21	B	818	CLA	CHC-C1C	5.33	1.48	1.35
21	11	704	CLA	C3B-C2B	5.33	1.47	1.40
21	11	705	CLA	CHC-C1C	5.33	1.48	1.35
21	12	508	CLA	C1D-ND	5.33	1.44	1.37
21	2	507	CLA	C3C-C2C	5.33	1.48	1.36
21	A	810	CLA	C4B-NB	-5.33	1.30	1.35
21	9	914	CLA	C3C-C2C	5.33	1.48	1.36
21	A	832	CLA	CHC-C1C	5.33	1.48	1.35
21	7	702	CLA	O2A-CGA	5.33	1.48	1.33
21	1	514	CLA	C1D-ND	5.33	1.44	1.37
21	11	707	CLA	C3C-C2C	5.32	1.48	1.36
21	5	707	CLA	C3C-C2C	5.32	1.48	1.36
21	F	404	CLA	O2A-CGA	5.32	1.48	1.30
21	8	604	CLA	CHC-C1C	5.32	1.48	1.35
21	1	508	CLA	O2A-CGA	5.31	1.48	1.33
21	6	907	CLA	O2A-CGA	5.31	1.48	1.33
21	3	715	CLA	CHC-C1C	5.31	1.48	1.35
21	8	611	CLA	C3C-C2C	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	815	CLA	O2A-CGA	5.30	1.48	1.33
21	B	808	CLA	C3B-C2B	5.30	1.47	1.40
21	B	802	CLA	C1B-NB	-5.30	1.30	1.35
21	10	706	CLA	C1D-ND	5.30	1.44	1.37
21	5	706	CLA	C1B-NB	-5.30	1.30	1.35
21	8	611	CLA	C1D-ND	5.30	1.44	1.37
21	10	704	CLA	O2D-CGD	5.29	1.46	1.33
21	4	701	CLA	C3C-C2C	5.29	1.48	1.36
21	7	712	CLA	C3C-C2C	5.29	1.48	1.36
21	10	708	CLA	O2D-CGD	5.29	1.46	1.33
21	4	709	CLA	C3C-C2C	5.29	1.48	1.36
21	A	809	CLA	CHC-C1C	5.29	1.48	1.35
21	2	511	CLA	O2D-CGD	5.29	1.46	1.33
21	11	708	CLA	O2D-CGD	5.29	1.46	1.33
21	A	842	CLA	C1D-ND	5.29	1.44	1.37
21	11	711	CLA	C3C-C2C	5.29	1.48	1.36
21	9	908	CLA	CHC-C1C	5.28	1.48	1.35
21	A	844	CLA	O2A-CGA	5.28	1.48	1.33
21	11	711	CLA	C1D-ND	5.28	1.44	1.37
21	B	837	CLA	C1B-NB	-5.28	1.30	1.35
21	F	403	CLA	CHC-C1C	5.28	1.48	1.35
21	3	715	CLA	O2A-CGA	5.28	1.48	1.30
21	2	508	CLA	O2A-CGA	5.27	1.48	1.33
21	10	710	CLA	O2D-CGD	5.27	1.46	1.33
21	9	914	CLA	C1D-ND	5.27	1.44	1.37
21	9	914	CLA	O2D-CGD	5.27	1.46	1.33
21	9	913	CLA	C3C-C2C	5.27	1.47	1.36
21	8	611	CLA	CHC-C1C	5.27	1.48	1.35
21	11	709	CLA	C3C-C2C	5.26	1.47	1.36
21	1	511	CLA	C3C-C2C	5.26	1.47	1.36
21	10	712	CLA	C3B-C2B	5.26	1.47	1.40
21	10	707	CLA	O2D-CGD	5.26	1.46	1.33
21	12	508	CLA	O2D-CGD	5.26	1.46	1.33
21	B	836	CLA	O2A-CGA	5.25	1.48	1.33
21	A	823	CLA	CHC-C1C	5.25	1.48	1.35
21	9	902	CLA	CHC-C1C	5.25	1.48	1.35
21	12	505	CLA	C3C-C2C	5.24	1.47	1.36
21	3	711	CLA	C3B-C2B	5.24	1.47	1.40
21	5	709	CLA	C3B-C2B	5.24	1.47	1.40
21	B	820	CLA	C1D-ND	5.24	1.44	1.37
21	3	706	CLA	O2A-CGA	5.24	1.48	1.33
21	1	514	CLA	O2D-CGD	5.24	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	10	703	CLA	CHC-C1C	5.24	1.48	1.35
21	12	505	CLA	O2D-CGD	5.24	1.46	1.33
21	6	913	CLA	CHC-C1C	5.24	1.48	1.35
21	B	829	CLA	O2D-CGD	5.24	1.46	1.33
21	4	708	CLA	O2D-CGD	5.24	1.46	1.33
21	3	707	CLA	O2D-CGD	5.24	1.46	1.33
21	1	517	CLA	C1D-ND	5.24	1.44	1.37
21	8	603	CLA	CHC-C1C	5.23	1.48	1.35
21	5	706	CLA	CHC-C1C	5.23	1.48	1.35
28	5	713	DD6	C2-C1	5.23	1.42	1.35
21	7	705	CLA	O2A-CGA	5.23	1.48	1.33
21	B	813	CLA	CHD-C1D	5.23	1.48	1.38
21	7	713	CLA	O2A-CGA	5.23	1.48	1.33
21	4	710	CLA	O2D-CGD	5.23	1.46	1.33
21	4	710	CLA	C3C-C2C	5.23	1.47	1.36
21	10	709	CLA	C3C-C2C	5.23	1.47	1.36
21	11	711	CLA	CHC-C1C	5.22	1.48	1.35
21	A	819	CLA	O2A-CGA	5.22	1.48	1.33
21	10	706	CLA	O2D-CGD	5.22	1.45	1.33
21	1	516	CLA	C3C-C2C	5.22	1.47	1.36
21	10	712	CLA	C3C-C2C	5.22	1.47	1.36
21	10	703	CLA	O2D-CGD	5.22	1.45	1.33
21	2	507	CLA	O2A-CGA	5.21	1.48	1.33
21	4	709	CLA	O2A-CGA	5.21	1.48	1.30
21	3	703	CLA	O2D-CGD	5.21	1.45	1.33
21	A	816	CLA	C3B-C2B	5.21	1.47	1.40
22	A	845	PQN	C10-C5	5.21	1.49	1.40
21	A	816	CLA	O2A-CGA	5.21	1.48	1.30
21	7	706	CLA	O2D-CGD	5.21	1.45	1.33
21	3	704	CLA	O2D-CGD	5.20	1.45	1.33
21	4	704	CLA	CHC-C1C	5.20	1.48	1.35
21	5	706	CLA	O2A-CGA	5.20	1.48	1.30
21	B	819	CLA	CHC-C1C	5.20	1.48	1.35
21	12	503	CLA	O2D-CGD	5.19	1.45	1.33
21	9	905	CLA	CHC-C1C	5.19	1.48	1.35
21	8	613	CLA	C3C-C2C	5.19	1.47	1.36
21	10	706	CLA	C3C-C2C	5.19	1.47	1.36
21	10	708	CLA	C1D-ND	5.19	1.44	1.37
21	1	514	CLA	C3C-C2C	5.19	1.47	1.36
21	1	509	CLA	O2A-CGA	5.19	1.48	1.33
21	B	812	CLA	C3C-C2C	5.19	1.47	1.36
21	5	705	CLA	C3C-C2C	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	903	CLA	C3B-C2B	5.18	1.47	1.40
21	11	707	CLA	C3B-C2B	5.18	1.47	1.40
21	1	504	CLA	C3C-C2C	5.18	1.47	1.36
21	1	507	CLA	O2D-CGD	5.17	1.45	1.33
21	6	903	CLA	O2D-CGD	5.17	1.45	1.33
21	3	704	CLA	C3B-C2B	5.16	1.47	1.40
21	1	508	CLA	OBD-CAD	5.16	1.31	1.22
21	4	706	CLA	C1B-NB	-5.16	1.30	1.35
21	12	506	CLA	C3B-C2B	5.16	1.47	1.40
21	12	501	CLA	C3B-C2B	5.16	1.47	1.40
21	A	824	CLA	CHC-C1C	5.15	1.48	1.35
21	3	713	CLA	C3C-C2C	5.15	1.47	1.36
21	11	707	CLA	CHC-C1C	5.15	1.48	1.35
21	12	501	CLA	CHC-C1C	5.15	1.48	1.35
24	A	849	BCR	C8-C9	-5.15	1.34	1.45
21	8	605	CLA	CHC-C1C	5.15	1.48	1.35
21	2	504	CLA	CHC-C1C	5.14	1.48	1.35
21	B	829	CLA	C3C-C2C	5.14	1.47	1.36
21	8	608	CLA	C3B-C2B	5.14	1.47	1.40
21	4	705	CLA	CHC-C1C	5.14	1.48	1.35
21	6	911	CLA	CHC-C1C	5.14	1.48	1.35
21	10	705	CLA	C3C-C2C	5.14	1.47	1.36
21	6	909	CLA	O2A-CGA	5.14	1.48	1.33
21	3	712	CLA	CHD-C1D	5.14	1.48	1.38
21	3	715	CLA	C3B-C2B	5.14	1.47	1.40
21	10	707	CLA	CHC-C1C	5.14	1.48	1.35
21	6	907	CLA	O2D-CGD	5.13	1.45	1.33
21	2	517	CLA	C3C-C2C	5.13	1.47	1.36
21	F	401	CLA	CHC-C1C	5.13	1.48	1.35
21	1	515	CLA	C3B-C2B	5.13	1.47	1.40
21	B	812	CLA	C3B-C2B	5.13	1.47	1.40
21	11	709	CLA	C3B-C2B	5.13	1.47	1.40
21	10	711	CLA	CHC-C1C	5.13	1.48	1.35
21	5	704	CLA	CHC-C1C	5.12	1.48	1.35
21	9	912	CLA	C3C-C2C	5.12	1.47	1.36
21	8	608	CLA	CHC-C1C	5.12	1.48	1.35
21	B	814	CLA	O2A-CGA	5.12	1.48	1.30
21	12	506	CLA	O2D-CGD	5.12	1.45	1.33
21	7	705	CLA	C3C-C2C	5.12	1.47	1.36
21	8	604	CLA	C3B-C2B	5.12	1.47	1.40
21	7	708	CLA	O2A-CGA	5.12	1.48	1.33
21	7	712	CLA	CHC-C1C	5.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	702	CLA	C3C-C2C	5.11	1.47	1.36
21	10	705	CLA	C1D-ND	5.11	1.44	1.37
21	11	701	CLA	CHC-C1C	5.10	1.48	1.35
21	2	513	CLA	C3C-C2C	5.10	1.47	1.36
21	3	706	CLA	C3C-C2C	5.10	1.47	1.36
21	A	839	CLA	CHC-C1C	5.10	1.48	1.35
21	9	914	CLA	CHC-C1C	5.10	1.48	1.35
21	5	710	CLA	O2A-CGA	5.10	1.48	1.33
21	12	503	CLA	C3C-C2C	5.10	1.47	1.36
21	2	506	CLA	C3C-C2C	5.10	1.47	1.36
21	3	705	CLA	O2A-CGA	5.09	1.48	1.33
21	11	705	CLA	O2A-CGA	5.09	1.48	1.33
21	B	809	CLA	O2A-CGA	5.09	1.47	1.30
21	9	913	CLA	O2D-CGD	5.09	1.45	1.33
21	8	614	CLA	CHC-C1C	5.09	1.48	1.35
21	1	504	CLA	CHC-C1C	5.09	1.48	1.35
21	F	401	CLA	O2A-CGA	5.09	1.48	1.33
21	7	708	CLA	CHC-C1C	5.09	1.48	1.35
21	6	910	CLA	CHC-C1C	5.09	1.48	1.35
21	B	801	CLA	CHC-C1C	5.09	1.48	1.35
21	A	844	CLA	C3C-C2C	5.09	1.47	1.36
21	7	710	CLA	O2A-CGA	5.08	1.47	1.30
21	2	516	CLA	O2D-CGD	5.08	1.45	1.33
21	11	709	CLA	CHC-C1C	5.08	1.48	1.35
21	11	710	CLA	CHC-C1C	5.08	1.48	1.35
21	11	707	CLA	O2D-CGD	5.08	1.45	1.33
21	13	502	CLA	C3C-C2C	5.08	1.47	1.36
21	12	504	CLA	CHC-C1C	5.08	1.48	1.35
21	7	709	CLA	CHC-C1C	5.08	1.48	1.35
28	11	712	DD6	C2-C1	5.08	1.42	1.35
21	9	910	CLA	O2A-CGA	5.08	1.47	1.30
21	A	819	CLA	CHD-C4C	5.08	1.50	1.39
21	8	609	CLA	C1D-ND	5.08	1.44	1.37
21	1	511	CLA	CHC-C1C	5.08	1.48	1.35
21	B	822	CLA	O2D-CGD	5.07	1.45	1.33
21	9	910	CLA	C3C-C2C	5.07	1.47	1.36
21	6	904	CLA	O2D-CGD	5.07	1.45	1.33
21	11	703	CLA	O2D-CGD	5.07	1.45	1.33
21	6	907	CLA	C1D-ND	5.07	1.44	1.37
21	B	823	CLA	C3C-C2C	5.07	1.47	1.36
21	9	908	CLA	O2D-CGD	5.07	1.45	1.33
21	5	709	CLA	C1D-ND	5.07	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	707	CLA	O2D-CGD	5.07	1.45	1.33
21	10	707	CLA	C3C-C2C	5.07	1.47	1.36
21	13	503	CLA	C3B-C2B	5.07	1.47	1.40
21	11	708	CLA	C3C-C2C	5.07	1.47	1.36
21	5	707	CLA	O2D-CGD	5.07	1.45	1.33
21	9	906	CLA	O2D-CGD	5.06	1.45	1.33
21	4	709	CLA	CHC-C1C	5.06	1.48	1.35
21	12	505	CLA	CHC-C1C	5.06	1.48	1.35
21	13	502	CLA	C1D-ND	5.06	1.44	1.37
21	11	706	CLA	C3B-C2B	5.06	1.47	1.40
21	12	508	CLA	CHC-C1C	5.06	1.47	1.35
28	2	518	DD6	C10-C11	5.06	1.42	1.35
21	B	804	CLA	O2A-CGA	5.06	1.48	1.33
21	8	606	CLA	C1D-ND	5.06	1.44	1.37
21	10	708	CLA	C3C-C2C	5.05	1.47	1.36
21	3	712	CLA	O2A-CGA	5.05	1.47	1.30
21	A	804	CLA	C3B-C2B	5.05	1.47	1.40
21	A	825	CLA	O2A-CGA	5.05	1.48	1.33
21	5	705	CLA	CHC-C1C	5.05	1.47	1.35
21	2	513	CLA	O2D-CGD	5.05	1.45	1.33
21	1	501	CLA	C1D-ND	5.04	1.44	1.37
21	A	837	CLA	O2A-CGA	5.04	1.47	1.30
21	B	830	CLA	CHC-C1C	5.04	1.47	1.35
21	2	508	CLA	CHC-C1C	5.04	1.47	1.35
21	1	516	CLA	O2D-CGD	5.04	1.45	1.33
21	2	511	CLA	CHC-C1C	5.04	1.47	1.35
21	1	509	CLA	O2D-CGD	5.04	1.45	1.33
21	10	706	CLA	CHC-C1C	5.03	1.47	1.35
21	3	705	CLA	O2D-CGD	5.03	1.45	1.33
21	2	511	CLA	C1B-NB	-5.03	1.30	1.35
21	8	612	CLA	CHC-C1C	5.03	1.47	1.35
21	7	713	CLA	C3C-C2C	5.03	1.47	1.36
21	4	701	CLA	C1D-ND	5.03	1.44	1.37
21	1	504	CLA	O2D-CGD	5.03	1.45	1.33
21	12	505	CLA	C3B-C2B	5.03	1.47	1.40
21	3	714	CLA	CHC-C1C	5.03	1.47	1.35
21	B	838	CLA	O2A-CGA	5.03	1.47	1.30
21	3	707	CLA	O2A-CGA	5.02	1.48	1.33
21	B	809	CLA	O2D-CGD	5.02	1.45	1.33
21	3	713	CLA	C1D-ND	5.02	1.44	1.37
21	7	710	CLA	C1D-ND	5.02	1.44	1.37
21	5	703	CLA	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	517	CLA	O2A-CGA	5.02	1.47	1.30
21	B	807	CLA	CHC-C1C	5.02	1.47	1.35
28	11	712	DD6	C5-C6	5.02	1.42	1.35
21	5	705	CLA	C1D-ND	5.01	1.43	1.37
21	5	711	CLA	CHC-C1C	5.01	1.47	1.35
21	1	512	CLA	C1D-ND	5.01	1.43	1.37
21	11	704	CLA	O2D-CGD	5.01	1.45	1.33
21	1	506	CLA	C3C-C2C	5.01	1.47	1.36
21	5	702	CLA	O2D-CGD	5.00	1.45	1.33
21	10	704	CLA	CHC-C1C	5.00	1.47	1.35
21	A	835	CLA	O2A-CGA	5.00	1.47	1.30
21	11	708	CLA	CHC-C1C	5.00	1.47	1.35
21	11	710	CLA	O2D-CGD	5.00	1.45	1.33
21	2	514	CLA	CHD-C1D	4.99	1.48	1.38
21	2	515	CLA	O2D-CGD	4.99	1.45	1.33
21	A	813	CLA	O2A-CGA	4.99	1.47	1.33
21	5	702	CLA	C3B-C2B	4.99	1.47	1.40
21	4	706	CLA	O2A-CGA	4.99	1.47	1.33
21	6	906	CLA	CHC-C1C	4.99	1.47	1.35
21	A	836	CLA	O2A-CGA	4.99	1.47	1.33
21	8	605	CLA	C1D-ND	4.99	1.43	1.37
21	A	815	CLA	C3C-C2C	4.99	1.47	1.36
21	11	701	CLA	O2D-CGD	4.99	1.45	1.33
21	9	907	CLA	O2D-CGD	4.99	1.45	1.33
21	7	711	CLA	O2D-CGD	4.98	1.45	1.33
21	3	705	CLA	CHC-C1C	4.98	1.47	1.35
21	4	711	CLA	O2A-CGA	4.98	1.47	1.30
21	10	709	CLA	CHC-C1C	4.98	1.47	1.35
21	10	705	CLA	CHC-C1C	4.98	1.47	1.35
21	B	803	CLA	O2A-CGA	4.98	1.47	1.33
21	A	831	CLA	CHC-C1C	4.98	1.47	1.35
21	2	511	CLA	C3C-C2C	4.97	1.47	1.36
21	3	708	CLA	CHC-C1C	4.97	1.47	1.35
21	B	816	CLA	C1B-NB	-4.97	1.30	1.35
21	7	703	CLA	CHC-C1C	4.97	1.47	1.35
21	7	705	CLA	O2D-CGD	4.97	1.45	1.33
21	A	837	CLA	C3B-C2B	4.97	1.47	1.40
21	A	830	CLA	CHD-C1D	4.97	1.48	1.38
21	3	712	CLA	C1D-ND	4.97	1.43	1.37
21	3	711	CLA	CHC-C1C	4.97	1.47	1.35
21	9	910	CLA	CHC-C1C	4.96	1.47	1.35
21	5	707	CLA	C1D-ND	4.96	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	908	CLA	C3C-C2C	4.96	1.47	1.36
21	5	710	CLA	C1D-ND	4.96	1.43	1.37
21	A	818	CLA	O2D-CGD	4.96	1.45	1.33
21	2	515	CLA	O2A-CGA	4.96	1.47	1.30
21	12	507	CLA	C1D-ND	4.96	1.43	1.37
21	4	703	CLA	C3C-C2C	4.95	1.47	1.36
21	A	811	CLA	C3C-C2C	4.95	1.47	1.36
21	5	707	CLA	CHC-C1C	4.95	1.47	1.35
21	A	813	CLA	CHC-C1C	4.95	1.47	1.35
21	12	504	CLA	CHD-C4C	4.95	1.50	1.39
21	12	503	CLA	CHC-C1C	4.95	1.47	1.35
21	4	708	CLA	C3C-C2C	4.95	1.47	1.36
21	7	705	CLA	C3B-C2B	4.95	1.47	1.40
21	9	907	CLA	CHC-C1C	4.94	1.47	1.35
21	4	707	CLA	CHC-C1C	4.94	1.47	1.35
21	B	815	CLA	CHC-C1C	4.94	1.47	1.35
21	3	703	CLA	C3B-C2B	4.94	1.47	1.40
21	13	501	CLA	CHC-C1C	4.94	1.47	1.35
21	1	512	CLA	C3C-C2C	4.94	1.47	1.36
21	1	508	CLA	CHC-C1C	4.94	1.47	1.35
21	4	708	CLA	CHC-C1C	4.94	1.47	1.35
21	2	509	CLA	CHC-C1C	4.94	1.47	1.35
21	5	711	CLA	O2A-CGA	4.93	1.47	1.30
21	2	516	CLA	C1D-ND	4.93	1.43	1.37
21	11	706	CLA	O2A-CGA	4.93	1.47	1.33
21	6	903	CLA	C1D-ND	4.93	1.43	1.37
21	11	709	CLA	C1D-ND	4.93	1.43	1.37
21	13	503	CLA	C3C-C2C	4.93	1.47	1.36
21	7	706	CLA	O2A-CGA	4.93	1.47	1.33
21	F	404	CLA	O2D-CGD	4.93	1.45	1.33
21	4	705	CLA	C3C-C2C	4.93	1.47	1.36
21	A	824	CLA	O2A-CGA	4.92	1.47	1.33
21	9	908	CLA	O2A-CGA	4.92	1.47	1.33
21	8	613	CLA	CHC-C1C	4.92	1.47	1.35
21	A	827	CLA	C3B-C2B	4.92	1.47	1.40
21	7	703	CLA	C1D-ND	4.92	1.43	1.37
21	A	816	CLA	C3C-C2C	4.92	1.47	1.36
21	6	912	CLA	C1D-ND	4.92	1.43	1.37
21	B	832	CLA	O2A-CGA	4.92	1.47	1.33
21	B	811	CLA	O2A-CGA	4.92	1.47	1.30
21	5	701	CLA	O2A-CGA	4.92	1.47	1.30
21	3	714	CLA	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	914	CLA	CHC-C1C	4.91	1.47	1.35
21	B	834	CLA	C1D-ND	4.91	1.43	1.37
21	2	509	CLA	O2A-CGA	4.91	1.47	1.33
21	9	913	CLA	CHC-C1C	4.91	1.47	1.35
21	4	711	CLA	CHC-C1C	4.91	1.47	1.35
21	5	710	CLA	O2D-CGD	4.91	1.45	1.33
21	4	704	CLA	C3B-C2B	4.90	1.47	1.40
21	2	513	CLA	C1D-ND	4.90	1.43	1.37
21	2	513	CLA	CHC-C1C	4.90	1.47	1.35
21	9	911	CLA	O2D-CGD	4.90	1.45	1.33
21	4	707	CLA	O2A-CGA	4.90	1.47	1.33
21	12	504	CLA	C3C-C2C	4.90	1.47	1.36
21	12	505	CLA	O2A-CGA	4.90	1.47	1.33
21	10	712	CLA	C1D-ND	4.90	1.43	1.37
21	9	907	CLA	C1D-ND	4.90	1.43	1.37
21	F	403	CLA	O2A-CGA	4.90	1.47	1.30
21	13	502	CLA	CHC-C1C	4.90	1.47	1.35
21	4	711	CLA	O2D-CGD	4.90	1.45	1.33
21	8	614	CLA	C3C-C2C	4.90	1.47	1.36
24	J	103	BCR	C10-C9	4.90	1.42	1.35
21	9	905	CLA	C3C-C2C	4.89	1.47	1.36
21	3	703	CLA	CHD-C1D	4.89	1.47	1.38
21	B	822	CLA	C3C-C2C	4.89	1.47	1.36
21	8	603	CLA	O2A-CGA	4.89	1.47	1.33
21	9	910	CLA	C3B-C2B	4.89	1.47	1.40
21	9	909	CLA	CHC-C1C	4.89	1.47	1.35
21	A	822	CLA	C1D-ND	4.89	1.43	1.37
21	A	834	CLA	CHC-C1C	4.89	1.47	1.35
21	B	839	CLA	O2A-CGA	4.89	1.47	1.33
21	10	712	CLA	CHC-C1C	4.89	1.47	1.35
21	B	839	CLA	O2D-CGD	4.88	1.45	1.33
21	7	707	CLA	CHC-C1C	4.88	1.47	1.35
21	1	512	CLA	CHC-C1C	4.88	1.47	1.35
21	11	702	CLA	O2D-CGD	4.88	1.45	1.33
21	1	515	CLA	C3C-C2C	4.88	1.47	1.36
24	B	846	BCR	C14-C13	4.88	1.42	1.35
21	3	709	CLA	C3C-C2C	4.88	1.47	1.36
21	6	905	CLA	C3C-C2C	4.88	1.47	1.36
21	6	914	CLA	C3C-C2C	4.87	1.47	1.36
21	1	515	CLA	O2A-CGA	4.86	1.47	1.30
21	11	706	CLA	CHC-C1C	4.86	1.47	1.35
21	F	401	CLA	C1B-NB	-4.86	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	905	CLA	O2A-CGA	4.86	1.47	1.33
21	4	708	CLA	C1D-ND	4.86	1.43	1.37
21	6	912	CLA	CHC-C1C	4.86	1.47	1.35
24	F	405	BCR	C8-C9	-4.86	1.35	1.45
21	B	839	CLA	C3B-C2B	4.86	1.47	1.40
21	2	508	CLA	O2D-CGD	4.85	1.45	1.33
21	5	704	CLA	O2A-CGA	4.85	1.47	1.33
21	2	517	CLA	C1D-ND	4.85	1.43	1.37
21	8	612	CLA	C1B-NB	-4.85	1.30	1.35
21	6	904	CLA	CHC-C1C	4.85	1.47	1.35
21	2	514	CLA	O2A-CGA	4.85	1.47	1.30
21	A	815	CLA	CHC-C1C	4.85	1.47	1.35
21	B	822	CLA	C3B-C2B	4.84	1.47	1.40
21	A	823	CLA	O2D-CGD	4.84	1.45	1.33
21	7	707	CLA	C3C-C2C	4.84	1.47	1.36
21	10	707	CLA	O2A-CGA	4.84	1.47	1.33
21	12	506	CLA	O2A-CGA	4.84	1.47	1.33
21	6	910	CLA	C3C-C2C	4.84	1.47	1.36
21	6	908	CLA	O2A-CGA	4.84	1.47	1.30
21	3	701	CLA	C1D-ND	4.84	1.43	1.37
21	1	505	CLA	CHC-C1C	4.84	1.47	1.35
21	2	506	CLA	O2D-CGD	4.84	1.45	1.33
21	5	704	CLA	C3B-C2B	4.84	1.47	1.40
21	12	504	CLA	CHD-C1D	4.84	1.47	1.38
21	5	707	CLA	O2A-CGA	4.84	1.47	1.33
21	4	706	CLA	C1D-ND	4.83	1.43	1.37
21	2	516	CLA	O2A-CGA	4.83	1.47	1.30
21	A	842	CLA	CHC-C1C	4.83	1.47	1.35
21	9	903	CLA	C1D-ND	4.83	1.43	1.37
21	11	710	CLA	C3B-C2B	4.83	1.47	1.40
21	8	608	CLA	O2A-CGA	4.83	1.47	1.33
21	6	911	CLA	C3B-C2B	4.82	1.47	1.40
21	1	510	CLA	C3C-C2C	4.82	1.47	1.36
21	2	511	CLA	O2A-CGA	4.82	1.47	1.30
21	B	823	CLA	O2A-CGA	4.82	1.47	1.33
21	6	909	CLA	CHC-C1C	4.82	1.47	1.35
21	3	711	CLA	O2A-CGA	4.82	1.46	1.30
21	A	840	CLA	C4B-NB	-4.82	1.30	1.35
21	1	517	CLA	CHC-C1C	4.82	1.47	1.35
21	5	708	CLA	C3B-C2B	4.81	1.47	1.40
21	6	903	CLA	O2A-CGA	4.81	1.47	1.33
21	12	502	CLA	CHC-C1C	4.81	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	710	CLA	CHC-C1C	4.81	1.47	1.35
21	7	712	CLA	O2A-CGA	4.81	1.46	1.30
28	1	519	DD6	C2-C1	4.81	1.42	1.35
21	6	914	CLA	O2D-CGD	4.81	1.44	1.33
21	9	905	CLA	C3B-C2B	4.81	1.47	1.40
21	12	502	CLA	O2A-CGA	4.80	1.46	1.30
21	13	501	CLA	C1D-ND	4.80	1.43	1.37
21	2	510	CLA	C3B-C2B	4.80	1.47	1.40
21	1	516	CLA	O2A-CGA	4.80	1.46	1.30
21	5	709	CLA	CHD-C4C	4.80	1.50	1.39
21	8	611	CLA	CHD-C4C	4.80	1.50	1.39
21	9	906	CLA	O2A-CGA	4.80	1.47	1.33
21	8	608	CLA	O2D-CGD	4.80	1.44	1.33
21	11	704	CLA	O2A-CGA	4.80	1.46	1.30
21	6	904	CLA	C3C-C2C	4.79	1.46	1.36
21	8	607	CLA	O2A-CGA	4.79	1.47	1.33
21	6	912	CLA	C3B-C2B	4.79	1.47	1.40
21	3	710	CLA	O2D-CGD	4.79	1.44	1.33
21	3	709	CLA	CHC-C1C	4.79	1.47	1.35
21	4	706	CLA	CHC-C1C	4.79	1.47	1.35
21	1	507	CLA	O2A-CGA	4.79	1.47	1.33
21	A	805	CLA	CHD-C4C	4.79	1.50	1.39
21	5	701	CLA	C3B-C2B	4.79	1.47	1.40
21	3	714	CLA	O2A-CGA	4.79	1.46	1.30
21	13	503	CLA	CHC-C1C	4.79	1.47	1.35
20	A	801	CL0	CHD-C1D	4.79	1.47	1.38
21	10	708	CLA	CHC-C1C	4.79	1.47	1.35
21	3	710	CLA	O2A-CGA	4.79	1.47	1.33
21	F	403	CLA	C3C-C2C	4.79	1.46	1.36
21	A	841	CLA	CHC-C1C	4.78	1.47	1.35
21	10	710	CLA	C3B-C2B	4.78	1.47	1.40
21	B	820	CLA	O2A-CGA	4.78	1.46	1.30
21	2	505	CLA	O2A-CGA	4.78	1.46	1.30
21	B	824	CLA	O2A-CGA	4.77	1.48	1.33
21	6	910	CLA	C1D-ND	4.77	1.43	1.37
21	7	713	CLA	O2D-CGD	4.77	1.44	1.33
21	7	702	CLA	C3C-C2C	4.77	1.46	1.36
21	10	707	CLA	C1D-ND	4.77	1.43	1.37
21	5	707	CLA	C1B-NB	-4.77	1.31	1.35
21	4	711	CLA	C3B-C2B	4.77	1.47	1.40
21	A	809	CLA	C3D-C4D	-4.77	1.33	1.44
21	8	613	CLA	O2A-CGA	4.76	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	702	CLA	O2D-CGD	4.76	1.44	1.33
21	8	610	CLA	CHC-C1C	4.76	1.47	1.35
21	1	513	CLA	O2D-CGD	4.76	1.44	1.33
21	9	909	CLA	C3B-C2B	4.76	1.47	1.40
21	6	906	CLA	O2A-CGA	4.76	1.47	1.33
21	11	705	CLA	C3B-C2B	4.76	1.47	1.40
21	6	903	CLA	CHC-C1C	4.76	1.47	1.35
24	B	844	BCR	C17-C18	4.76	1.42	1.35
21	1	514	CLA	CHC-C1C	4.76	1.47	1.35
21	1	512	CLA	O2A-CGA	4.76	1.46	1.30
21	A	807	CLA	O2A-CGA	4.76	1.47	1.33
21	9	912	CLA	O2A-CGA	4.76	1.46	1.30
21	8	614	CLA	O2A-CGA	4.76	1.47	1.33
21	A	830	CLA	OBD-CAD	4.76	1.30	1.22
21	B	833	CLA	O2A-CGA	4.75	1.46	1.30
21	A	824	CLA	O2D-CGD	4.75	1.44	1.33
21	12	507	CLA	CHC-C1C	4.75	1.47	1.35
21	B	824	CLA	CHD-C1D	4.75	1.47	1.38
21	9	911	CLA	C3C-C2C	4.75	1.46	1.36
21	1	513	CLA	CHC-C1C	4.75	1.47	1.35
21	10	712	CLA	O2A-CGA	4.75	1.47	1.33
21	5	701	CLA	O2D-CGD	4.75	1.44	1.33
21	8	614	CLA	O2D-CGD	4.75	1.44	1.33
21	2	517	CLA	CHC-C1C	4.74	1.47	1.35
21	4	710	CLA	O2A-CGA	4.74	1.46	1.30
21	4	705	CLA	O2D-CGD	4.74	1.44	1.33
21	1	506	CLA	O2A-CGA	4.74	1.46	1.30
21	7	712	CLA	C3B-C2B	4.74	1.46	1.40
21	10	710	CLA	C3C-C2C	4.74	1.46	1.36
21	9	911	CLA	C1D-ND	4.74	1.43	1.37
21	8	605	CLA	O2A-CGA	4.74	1.46	1.30
21	B	837	CLA	CHD-C1D	4.74	1.47	1.38
21	1	511	CLA	O2D-CGD	4.74	1.44	1.33
21	2	510	CLA	C3C-C2C	4.74	1.46	1.36
21	7	713	CLA	CHC-C1C	4.73	1.47	1.35
21	9	912	CLA	CHC-C1C	4.73	1.47	1.35
21	B	837	CLA	O2A-CGA	4.73	1.46	1.30
21	A	806	CLA	CHC-C1C	4.73	1.47	1.35
21	10	711	CLA	C1D-ND	4.73	1.43	1.37
21	A	822	CLA	C3C-C2C	4.73	1.46	1.36
21	11	704	CLA	C3C-C2C	4.73	1.46	1.36
21	1	501	CLA	C3C-C2C	4.73	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	710	CLA	C3C-C2C	4.73	1.46	1.36
21	9	910	CLA	O2D-CGD	4.73	1.44	1.33
21	A	816	CLA	CHD-C1D	4.72	1.47	1.38
21	B	805	CLA	C1C-NC	-4.72	1.30	1.37
21	1	507	CLA	C3C-C2C	4.72	1.46	1.36
21	4	704	CLA	O2D-CGD	4.72	1.44	1.33
21	B	811	CLA	CHC-C1C	4.72	1.47	1.35
21	6	906	CLA	C1D-ND	4.72	1.43	1.37
21	9	913	CLA	O2A-CGA	4.71	1.47	1.33
21	7	704	CLA	O2D-CGD	4.71	1.44	1.33
21	2	512	CLA	O2A-CGA	4.71	1.47	1.33
21	3	712	CLA	O2D-CGD	4.71	1.44	1.33
21	A	814	CLA	O2A-CGA	4.71	1.47	1.33
21	3	709	CLA	C1D-ND	4.71	1.43	1.37
21	9	904	CLA	CHC-C1C	4.71	1.47	1.35
21	7	713	CLA	C3B-C2B	4.71	1.46	1.40
21	3	711	CLA	C3C-C2C	4.71	1.46	1.36
21	2	514	CLA	OBD-CAD	4.71	1.30	1.22
21	4	701	CLA	CHC-C1C	4.71	1.47	1.35
21	A	837	CLA	CHC-C1C	4.70	1.47	1.35
21	2	509	CLA	O2D-CGD	4.70	1.44	1.33
21	5	705	CLA	O2A-CGA	4.70	1.47	1.33
21	8	606	CLA	O2A-CGA	4.70	1.46	1.30
21	4	711	CLA	C3C-C2C	4.70	1.46	1.36
21	B	822	CLA	O2A-CGA	4.69	1.46	1.30
21	3	713	CLA	CHC-C1C	4.69	1.47	1.35
21	5	702	CLA	CHC-C1C	4.69	1.47	1.35
21	1	517	CLA	O2D-CGD	4.69	1.44	1.33
21	2	508	CLA	C3C-C2C	4.69	1.46	1.36
21	B	830	CLA	C1B-NB	-4.69	1.31	1.35
21	6	912	CLA	O2A-CGA	4.68	1.46	1.30
21	9	908	CLA	CHD-C1D	4.68	1.47	1.38
21	2	513	CLA	O2A-CGA	4.68	1.46	1.30
21	B	807	CLA	C1D-ND	4.68	1.43	1.37
21	6	910	CLA	CHD-C1D	4.68	1.47	1.38
21	11	709	CLA	O2A-CGA	4.68	1.46	1.30
21	12	502	CLA	C3C-C2C	4.68	1.46	1.36
21	5	703	CLA	O2A-CGA	4.68	1.46	1.30
21	A	817	CLA	O2A-CGA	4.68	1.47	1.33
21	5	708	CLA	O2D-CGD	4.68	1.44	1.33
21	11	704	CLA	CHC-C1C	4.67	1.47	1.35
21	B	808	CLA	O2A-CGA	4.67	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	709	CLA	O2A-CGA	4.67	1.46	1.30
21	3	715	CLA	C3C-C2C	4.67	1.46	1.36
21	A	814	CLA	OBD-CAD	4.67	1.30	1.22
21	B	830	CLA	C3B-C2B	4.67	1.46	1.40
21	A	822	CLA	O2A-CGA	4.67	1.47	1.33
21	10	711	CLA	O2A-CGA	4.67	1.46	1.30
21	1	506	CLA	CHC-C1C	4.67	1.46	1.35
21	A	809	CLA	OBD-CAD	4.67	1.30	1.22
21	2	505	CLA	CHC-C1C	4.67	1.46	1.35
21	1	505	CLA	O2D-CGD	4.67	1.44	1.33
21	6	907	CLA	C3B-C2B	4.67	1.46	1.40
21	A	835	CLA	CHD-C1D	4.66	1.47	1.38
21	1	513	CLA	O2A-CGA	4.66	1.47	1.33
21	9	913	CLA	C1D-ND	4.66	1.43	1.37
21	A	814	CLA	CHC-C1C	4.66	1.46	1.35
21	3	706	CLA	CHC-C1C	4.66	1.46	1.35
21	11	706	CLA	O2D-CGD	4.66	1.44	1.33
21	3	703	CLA	C3C-C2C	4.66	1.46	1.36
21	7	707	CLA	O2D-CGD	4.66	1.44	1.33
21	2	503	CLA	O2A-CGA	4.66	1.46	1.30
21	B	801	CLA	C1D-ND	4.66	1.43	1.37
21	9	914	CLA	O2A-CGA	4.66	1.46	1.33
21	12	503	CLA	O2A-CGA	4.65	1.46	1.30
21	3	714	CLA	C1D-ND	4.65	1.43	1.37
21	2	517	CLA	O2A-CGA	4.65	1.46	1.30
21	8	611	CLA	O2A-CGA	4.65	1.46	1.30
21	10	709	CLA	O2A-CGA	4.65	1.46	1.30
21	10	703	CLA	C1D-ND	4.65	1.43	1.37
21	8	603	CLA	C3B-C2B	4.65	1.46	1.40
21	5	704	CLA	CHD-C1D	4.65	1.47	1.38
21	9	902	CLA	OBD-CAD	4.65	1.30	1.22
21	7	703	CLA	C1C-NC	-4.65	1.30	1.37
21	A	808	CLA	O2D-CGD	4.65	1.44	1.33
21	2	510	CLA	CHC-C1C	4.65	1.46	1.35
21	4	705	CLA	O2A-CGA	4.65	1.46	1.33
21	1	506	CLA	C1D-ND	4.64	1.43	1.37
21	1	501	CLA	CHC-C1C	4.64	1.46	1.35
21	6	913	CLA	O2A-CGA	4.64	1.46	1.30
21	3	713	CLA	O2A-CGA	4.64	1.46	1.30
21	B	813	CLA	O2D-CGD	4.63	1.44	1.33
21	11	703	CLA	C1D-ND	4.63	1.43	1.37
21	12	503	CLA	C1D-ND	4.63	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	502	CLA	C3B-C2B	4.63	1.46	1.40
21	13	503	CLA	C1D-ND	4.63	1.43	1.37
21	1	514	CLA	O2A-CGA	4.63	1.46	1.30
21	3	709	CLA	O2A-CGA	4.63	1.46	1.30
21	8	614	CLA	C3B-C2B	4.63	1.46	1.40
21	A	843	CLA	O2D-CGD	4.62	1.44	1.33
21	7	704	CLA	O2A-CGA	4.62	1.46	1.30
21	3	703	CLA	O2A-CGA	4.62	1.46	1.30
21	9	909	CLA	C3C-C2C	4.62	1.46	1.36
21	5	705	CLA	C3B-C2B	4.62	1.46	1.40
21	5	701	CLA	C3C-C2C	4.62	1.46	1.36
21	3	708	CLA	C3C-C2C	4.62	1.46	1.36
21	8	613	CLA	C1D-ND	4.62	1.43	1.37
21	8	603	CLA	O2D-CGD	4.62	1.44	1.33
21	2	506	CLA	CHC-C1C	4.62	1.46	1.35
21	4	706	CLA	C3B-C2B	4.62	1.46	1.40
21	9	902	CLA	C3C-C2C	4.62	1.46	1.36
21	3	714	CLA	C3C-C2C	4.61	1.46	1.36
21	8	609	CLA	O2A-CGA	4.61	1.46	1.33
21	A	840	CLA	C3B-C2B	4.61	1.46	1.40
21	2	514	CLA	C3B-C2B	4.61	1.46	1.40
21	8	612	CLA	C3B-C2B	4.61	1.46	1.40
21	A	804	CLA	O2A-CGA	4.61	1.46	1.33
21	11	705	CLA	C3C-C2C	4.61	1.46	1.36
21	A	802	CLA	O2A-CGA	4.61	1.46	1.33
21	9	904	CLA	O2A-CGA	4.60	1.46	1.30
21	3	705	CLA	C3C-C2C	4.60	1.46	1.36
21	8	605	CLA	C3C-C2C	4.60	1.46	1.36
21	6	905	CLA	O2A-CGA	4.60	1.46	1.30
21	B	816	CLA	CHC-C1C	4.60	1.46	1.35
21	J	101	CLA	C1B-NB	-4.60	1.31	1.35
21	12	507	CLA	O2A-CGA	4.60	1.46	1.30
21	6	907	CLA	C3C-C2C	4.60	1.46	1.36
21	8	608	CLA	C3C-C2C	4.59	1.46	1.36
21	A	817	CLA	CHC-C1C	4.59	1.46	1.35
21	B	829	CLA	O2A-CGA	4.59	1.46	1.30
24	A	852	BCR	C10-C9	4.59	1.41	1.35
21	13	502	CLA	O2A-CGA	4.59	1.46	1.33
21	10	705	CLA	O2A-CGA	4.59	1.46	1.30
21	11	710	CLA	O2A-CGA	4.59	1.46	1.30
21	B	818	CLA	CHD-C4C	4.58	1.49	1.39
21	2	507	CLA	CHC-C1C	4.58	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	811	CLA	C3B-C2B	4.58	1.46	1.40
21	A	802	CLA	C1B-NB	-4.58	1.31	1.35
21	11	703	CLA	CHD-C1D	4.58	1.47	1.38
21	B	814	CLA	CHC-C1C	4.58	1.46	1.35
21	B	816	CLA	O2A-CGA	4.58	1.46	1.33
21	A	842	CLA	CHD-C1D	4.58	1.47	1.38
21	11	711	CLA	O2A-CGA	4.57	1.46	1.30
21	1	510	CLA	O2A-CGA	4.57	1.46	1.33
21	7	707	CLA	C3B-C2B	4.57	1.46	1.40
21	11	701	CLA	C1D-ND	4.57	1.43	1.37
21	8	607	CLA	CHC-C1C	4.57	1.46	1.35
21	3	703	CLA	CHC-C1C	4.57	1.46	1.35
21	7	706	CLA	CHC-C1C	4.56	1.46	1.35
21	B	837	CLA	C1D-ND	4.56	1.43	1.37
21	A	816	CLA	C1C-NC	-4.56	1.31	1.37
21	B	811	CLA	C3C-C2C	4.56	1.46	1.36
21	4	710	CLA	C1D-ND	4.56	1.43	1.37
21	12	508	CLA	O2A-CGA	4.56	1.46	1.30
21	5	701	CLA	OBD-CAD	4.56	1.30	1.22
21	B	826	CLA	C3C-C2C	4.56	1.46	1.36
21	6	910	CLA	O2D-CGD	4.55	1.44	1.33
21	9	907	CLA	O2A-CGA	4.55	1.46	1.33
21	4	703	CLA	O2A-CGA	4.55	1.46	1.30
21	A	837	CLA	C1D-ND	4.55	1.43	1.37
21	9	908	CLA	C1D-ND	4.55	1.43	1.37
21	7	714	CLA	C1D-ND	4.55	1.43	1.37
21	9	906	CLA	C3B-C2B	4.55	1.46	1.40
21	1	516	CLA	CHC-C1C	4.55	1.46	1.35
21	5	703	CLA	CHC-C1C	4.54	1.46	1.35
21	6	909	CLA	O2D-CGD	4.54	1.44	1.33
21	B	835	CLA	CHC-C1C	4.54	1.46	1.35
21	2	514	CLA	C1D-ND	4.54	1.43	1.37
21	5	711	CLA	C1D-ND	4.54	1.43	1.37
21	F	404	CLA	C3C-C2C	4.54	1.46	1.36
21	F	404	CLA	CHC-C1C	4.54	1.46	1.35
21	A	826	CLA	C4B-NB	-4.54	1.31	1.35
21	3	704	CLA	C3C-C2C	4.54	1.46	1.36
21	7	708	CLA	C3C-C2C	4.54	1.46	1.36
21	A	834	CLA	O2A-CGA	4.54	1.46	1.30
21	8	609	CLA	CHD-C4C	4.54	1.49	1.39
21	8	607	CLA	C3C-C2C	4.54	1.46	1.36
21	11	707	CLA	CHD-C4C	4.54	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	713	DD6	C5-C6	4.54	1.41	1.35
21	11	707	CLA	C1D-ND	4.53	1.43	1.37
21	A	810	CLA	O2D-CGD	4.53	1.44	1.33
21	B	812	CLA	CHC-C1C	4.53	1.46	1.35
21	13	501	CLA	O2A-CGA	4.53	1.46	1.30
21	B	828	CLA	CHC-C1C	4.53	1.46	1.35
21	8	610	CLA	C3C-C2C	4.53	1.46	1.36
21	3	711	CLA	O2D-CGD	4.53	1.44	1.33
21	11	707	CLA	O2A-CGA	4.52	1.46	1.33
21	3	701	CLA	CHC-C1C	4.52	1.46	1.35
21	10	710	CLA	C1D-ND	4.52	1.43	1.37
21	5	705	CLA	O2D-CGD	4.52	1.44	1.33
21	8	604	CLA	O2D-CGD	4.52	1.44	1.33
21	A	840	CLA	C1D-ND	4.52	1.43	1.37
21	A	811	CLA	CHC-C1C	4.52	1.46	1.35
21	2	515	CLA	CHD-C1D	4.51	1.47	1.38
21	A	810	CLA	C3C-C2C	4.51	1.46	1.36
21	A	805	CLA	CHC-C1C	4.51	1.46	1.35
21	9	912	CLA	C1D-ND	4.51	1.43	1.37
21	3	710	CLA	C3B-C2B	4.51	1.46	1.40
21	B	821	CLA	O2D-CGD	4.51	1.44	1.33
21	3	711	CLA	CHD-C1D	4.51	1.47	1.38
21	4	703	CLA	CHC-C1C	4.51	1.46	1.35
21	9	907	CLA	OBD-CAD	4.50	1.30	1.22
21	3	708	CLA	CHD-C1D	4.50	1.47	1.38
21	6	911	CLA	O2A-CGA	4.50	1.45	1.30
21	J	101	CLA	C3C-C2C	4.50	1.46	1.36
21	B	825	CLA	C3C-C2C	4.50	1.46	1.36
21	B	837	CLA	O2D-CGD	4.49	1.44	1.33
21	9	904	CLA	C1D-ND	4.49	1.43	1.37
20	A	801	CL0	C1D-ND	4.49	1.43	1.37
21	1	517	CLA	C3B-C2B	4.49	1.46	1.40
21	12	508	CLA	CHD-C1D	4.49	1.47	1.38
21	A	808	CLA	O2A-CGA	4.49	1.46	1.33
21	4	704	CLA	C3C-C2C	4.49	1.46	1.36
21	A	805	CLA	O2A-CGA	4.49	1.46	1.33
21	8	605	CLA	CHD-C1D	4.48	1.47	1.38
21	2	512	CLA	C1D-ND	4.48	1.43	1.37
21	B	802	CLA	CHC-C1C	4.48	1.46	1.35
21	B	831	CLA	C1D-ND	4.48	1.43	1.37
21	1	507	CLA	CHC-C1C	4.48	1.46	1.35
21	A	806	CLA	CHD-C4C	4.48	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	507	CLA	CHD-C1D	4.48	1.47	1.38
21	9	903	CLA	OBD-CAD	4.47	1.30	1.22
21	13	502	CLA	CHD-C1D	4.47	1.47	1.38
21	J	101	CLA	CHD-C1D	4.47	1.47	1.38
21	12	507	CLA	CHD-C4C	4.47	1.49	1.39
21	5	710	CLA	CHC-C1C	4.47	1.46	1.35
21	B	820	CLA	C3C-C2C	4.47	1.46	1.36
21	11	708	CLA	C1D-ND	4.47	1.43	1.37
21	3	708	CLA	C3B-C2B	4.47	1.46	1.40
21	2	514	CLA	CHC-C1C	4.47	1.46	1.35
21	1	516	CLA	C1D-ND	4.47	1.43	1.37
21	B	830	CLA	CHD-C4C	4.47	1.49	1.39
21	2	517	CLA	CHD-C4C	4.46	1.49	1.39
21	B	827	CLA	C1C-NC	-4.46	1.31	1.37
21	13	503	CLA	O2A-CGA	4.46	1.46	1.33
21	1	513	CLA	C3B-C2B	4.46	1.46	1.40
21	A	815	CLA	C3B-C2B	4.46	1.46	1.40
21	11	707	CLA	C3D-C2D	4.46	1.51	1.39
21	6	909	CLA	C3B-C2B	4.46	1.46	1.40
21	1	505	CLA	CHD-C1D	4.46	1.47	1.38
21	5	708	CLA	C3C-C2C	4.46	1.46	1.36
21	1	508	CLA	O2D-CGD	4.46	1.44	1.33
21	6	913	CLA	C1D-ND	4.45	1.43	1.37
21	4	709	CLA	CHD-C4C	4.45	1.49	1.39
21	A	814	CLA	CHD-C4C	4.45	1.49	1.39
21	A	803	CLA	C1C-NC	-4.45	1.31	1.37
21	B	806	CLA	O2A-CGA	4.45	1.46	1.33
21	9	906	CLA	CHC-C1C	4.44	1.46	1.35
21	8	605	CLA	CHD-C4C	4.44	1.49	1.39
21	B	830	CLA	C3C-C2C	4.44	1.46	1.36
21	J	101	CLA	C3B-C2B	4.44	1.46	1.40
21	A	843	CLA	C3C-C2C	4.44	1.46	1.36
21	6	911	CLA	C1D-ND	4.44	1.43	1.37
21	1	505	CLA	C1D-ND	4.44	1.43	1.37
21	A	812	CLA	CHC-C1C	4.44	1.46	1.35
21	A	827	CLA	CHD-C1D	4.43	1.47	1.38
21	A	843	CLA	CHC-C1C	4.43	1.46	1.35
28	1	519	DD6	C5-C6	4.43	1.41	1.35
21	B	813	CLA	CHC-C1C	4.42	1.46	1.35
21	11	701	CLA	CHD-C1D	4.42	1.47	1.38
21	4	707	CLA	C1D-ND	4.42	1.43	1.37
21	B	808	CLA	CHC-C1C	4.42	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	704	CLA	C1B-NB	-4.42	1.31	1.35
21	7	703	CLA	C3C-C2C	4.42	1.46	1.36
21	A	827	CLA	CHC-C1C	4.41	1.46	1.35
21	A	827	CLA	C3C-C2C	4.41	1.46	1.36
21	A	820	CLA	C1B-NB	-4.41	1.31	1.35
21	6	908	CLA	CHC-C1C	4.41	1.46	1.35
21	6	912	CLA	CHD-C1D	4.41	1.46	1.38
21	B	839	CLA	CHC-C1C	4.41	1.46	1.35
21	1	507	CLA	CHD-C1D	4.41	1.46	1.38
21	4	704	CLA	C1D-ND	4.41	1.43	1.37
21	7	705	CLA	CHC-C1C	4.40	1.46	1.35
21	3	711	CLA	C1D-ND	4.40	1.43	1.37
21	J	101	CLA	C1D-ND	4.40	1.43	1.37
21	1	504	CLA	C1D-ND	4.40	1.43	1.37
21	11	703	CLA	O2A-CGA	4.40	1.46	1.33
21	B	810	CLA	C3B-C2B	4.40	1.46	1.40
21	8	609	CLA	CHD-C1D	4.40	1.46	1.38
21	A	802	CLA	MG-ND	-4.40	1.97	2.05
21	B	806	CLA	C3B-C2B	4.40	1.46	1.40
21	10	706	CLA	CHD-C1D	4.40	1.46	1.38
21	B	809	CLA	C1D-ND	4.39	1.43	1.37
21	9	914	CLA	CHD-C1D	4.39	1.46	1.38
21	12	501	CLA	C1D-ND	4.39	1.43	1.37
21	11	710	CLA	C3C-C2C	4.39	1.46	1.36
21	B	838	CLA	OBD-CAD	4.38	1.30	1.22
21	1	509	CLA	C1D-ND	4.38	1.43	1.37
21	3	705	CLA	OBD-CAD	4.38	1.30	1.22
21	B	804	CLA	CHC-C1C	4.38	1.46	1.35
21	A	819	CLA	CHC-C1C	4.38	1.46	1.35
21	A	831	CLA	O2A-CGA	4.38	1.46	1.33
21	2	511	CLA	CHD-C1D	4.38	1.46	1.38
21	B	829	CLA	OBD-CAD	4.37	1.30	1.22
21	7	708	CLA	C1B-NB	-4.37	1.31	1.35
21	9	902	CLA	O2D-CGD	4.37	1.43	1.33
21	A	804	CLA	O2D-CGD	4.37	1.43	1.33
21	11	709	CLA	CHD-C1D	4.37	1.46	1.38
21	A	816	CLA	O2D-CGD	4.37	1.43	1.33
21	7	710	CLA	CHD-C4C	4.36	1.49	1.39
21	3	710	CLA	CHC-C1C	4.36	1.46	1.35
21	12	502	CLA	CHD-C1D	4.36	1.46	1.38
21	B	810	CLA	O2D-CGD	4.36	1.43	1.33
21	13	503	CLA	CHD-C1D	4.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	819	CLA	C3C-C2C	4.36	1.46	1.36
21	8	604	CLA	C3C-C2C	4.35	1.46	1.36
21	B	834	CLA	O2A-CGA	4.35	1.46	1.33
21	A	809	CLA	O2A-CGA	4.35	1.46	1.33
21	A	826	CLA	CHC-C1C	4.35	1.46	1.35
21	8	608	CLA	CHD-C1D	4.35	1.46	1.38
21	10	708	CLA	CHD-C1D	4.35	1.46	1.38
21	8	606	CLA	O2D-CGD	4.35	1.43	1.33
21	A	803	CLA	C1D-ND	4.35	1.43	1.37
21	11	702	CLA	C3B-C2B	4.35	1.46	1.40
21	6	909	CLA	C3C-C2C	4.35	1.46	1.36
21	11	704	CLA	CHD-C1D	4.34	1.46	1.38
21	B	827	CLA	C4B-NB	-4.34	1.31	1.35
21	B	821	CLA	C1D-ND	4.34	1.43	1.37
21	9	913	CLA	CHD-C1D	4.33	1.46	1.38
21	A	831	CLA	C3C-C2C	4.33	1.45	1.36
21	B	826	CLA	O2A-CGA	4.33	1.46	1.33
21	2	516	CLA	C3C-C2C	4.33	1.45	1.36
21	B	830	CLA	O2D-CGD	4.33	1.43	1.33
21	A	833	CLA	C3B-C2B	4.33	1.46	1.40
21	B	802	CLA	CHD-C4C	4.33	1.49	1.39
21	10	707	CLA	CHD-C1D	4.33	1.46	1.38
21	4	709	CLA	C1D-ND	4.33	1.43	1.37
21	A	819	CLA	C4B-NB	-4.33	1.31	1.35
21	4	708	CLA	CHD-C1D	4.33	1.46	1.38
21	A	833	CLA	C1B-NB	-4.32	1.31	1.35
21	A	835	CLA	O2D-CGD	4.32	1.43	1.33
21	B	823	CLA	C3B-C2B	4.32	1.46	1.40
21	9	911	CLA	O2A-CGA	4.32	1.46	1.33
21	B	826	CLA	C3B-C2B	4.32	1.46	1.40
21	3	702	CLA	O2A-CGA	4.32	1.46	1.33
21	7	714	CLA	O2D-CGD	4.32	1.43	1.33
21	A	828	CLA	CHD-C1D	4.32	1.46	1.38
21	A	837	CLA	O2D-CGD	4.32	1.43	1.33
24	J	103	BCR	C14-C13	4.32	1.41	1.35
21	3	710	CLA	C3C-C2C	4.31	1.45	1.36
21	10	706	CLA	CHD-C4C	4.31	1.49	1.39
21	9	906	CLA	OBD-CAD	4.31	1.29	1.22
21	1	510	CLA	O2D-CGD	4.31	1.43	1.33
21	B	823	CLA	O2D-CGD	4.31	1.43	1.33
21	12	503	CLA	CHD-C1D	4.31	1.46	1.38
21	12	508	CLA	CHD-C4C	4.30	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	715	CLA	CHD-C1D	4.30	1.46	1.38
21	B	835	CLA	C4B-NB	-4.30	1.31	1.35
21	9	910	CLA	C1B-NB	-4.30	1.31	1.35
21	3	707	CLA	C3C-C2C	4.30	1.45	1.36
21	4	708	CLA	CHD-C4C	4.30	1.49	1.39
21	2	514	CLA	O2D-CGD	4.30	1.43	1.33
21	11	705	CLA	C1D-ND	4.30	1.43	1.37
21	6	908	CLA	C3B-C2B	4.29	1.46	1.40
21	B	805	CLA	C1D-ND	4.29	1.43	1.37
21	A	806	CLA	C1D-ND	4.29	1.43	1.37
21	10	710	CLA	O2A-CGA	4.29	1.45	1.33
21	4	704	CLA	CHD-C4C	4.29	1.49	1.39
21	A	841	CLA	C3B-C2B	4.29	1.46	1.40
21	B	818	CLA	C3B-C2B	4.29	1.46	1.40
21	11	710	CLA	C1D-ND	4.29	1.43	1.37
21	B	831	CLA	O2A-CGA	4.29	1.45	1.33
21	11	711	CLA	CHD-C1D	4.29	1.46	1.38
21	4	703	CLA	C1D-ND	4.28	1.43	1.37
21	7	709	CLA	C1D-ND	4.28	1.43	1.37
21	11	707	CLA	CHD-C1D	4.28	1.46	1.38
21	6	909	CLA	C1B-NB	-4.28	1.31	1.35
21	B	839	CLA	CHD-C4C	4.27	1.49	1.39
21	7	706	CLA	CHD-C1D	4.27	1.46	1.38
21	A	818	CLA	C1D-ND	4.27	1.43	1.37
21	B	829	CLA	C3B-C2B	4.27	1.46	1.40
21	2	503	CLA	CHC-C1C	4.27	1.45	1.35
21	B	839	CLA	C3C-C2C	4.27	1.45	1.36
21	5	706	CLA	C3C-C2C	4.26	1.45	1.36
21	A	832	CLA	O2D-CGD	4.26	1.43	1.33
21	5	708	CLA	CHD-C1D	4.26	1.46	1.38
21	B	811	CLA	C1B-NB	-4.26	1.31	1.35
21	9	905	CLA	CHD-C1D	4.26	1.46	1.38
21	3	702	CLA	O2D-CGD	4.26	1.43	1.33
21	5	703	CLA	C3C-C2C	4.26	1.45	1.36
21	3	705	CLA	C3B-C2B	4.26	1.46	1.40
21	A	828	CLA	C1B-NB	-4.25	1.31	1.35
21	3	710	CLA	C1D-ND	4.25	1.43	1.37
21	7	706	CLA	OBD-CAD	4.25	1.29	1.22
21	7	708	CLA	CHD-C1D	4.25	1.46	1.38
21	B	825	CLA	O2A-CGA	4.25	1.45	1.33
21	B	824	CLA	CHC-C1C	4.25	1.45	1.35
21	7	712	CLA	O2D-CGD	4.25	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	507	CLA	C3B-C2B	4.25	1.46	1.40
21	9	909	CLA	CHD-C1D	4.24	1.46	1.38
21	11	705	CLA	O2D-CGD	4.24	1.43	1.33
21	A	843	CLA	C3B-C2B	4.24	1.46	1.40
21	9	905	CLA	C1D-ND	4.24	1.43	1.37
21	A	862	CLA	O2A-CGA	4.24	1.45	1.33
21	7	703	CLA	C1B-NB	-4.24	1.31	1.35
21	12	502	CLA	C1D-ND	4.24	1.43	1.37
21	B	818	CLA	C3C-C2C	4.23	1.45	1.36
21	10	704	CLA	O2A-CGA	4.23	1.45	1.33
21	12	501	CLA	CHD-C1D	4.23	1.46	1.38
21	B	836	CLA	C4B-NB	-4.23	1.31	1.35
21	B	820	CLA	CHC-C1C	4.23	1.45	1.35
21	10	705	CLA	CHD-C1D	4.23	1.46	1.38
21	7	703	CLA	O2D-CGD	4.23	1.43	1.33
21	B	816	CLA	C3C-C2C	4.22	1.45	1.36
21	5	708	CLA	C4B-NB	-4.22	1.31	1.35
21	9	903	CLA	O2A-CGA	4.22	1.45	1.33
21	3	704	CLA	CHC-C1C	4.22	1.45	1.35
21	8	604	CLA	C3D-C2D	4.22	1.50	1.39
21	4	707	CLA	CHD-C1D	4.22	1.46	1.38
21	9	914	CLA	CHD-C4C	4.21	1.48	1.39
21	11	705	CLA	CHD-C1D	4.21	1.46	1.38
21	B	817	CLA	CHD-C4C	4.21	1.48	1.39
21	2	517	CLA	C3D-C2D	4.21	1.50	1.39
21	5	709	CLA	C3C-C2C	4.21	1.45	1.36
21	A	820	CLA	C3C-C2C	4.21	1.45	1.36
21	3	703	CLA	CHD-C4C	4.21	1.48	1.39
21	A	820	CLA	CHC-C1C	4.21	1.45	1.35
21	12	501	CLA	O2A-CGA	4.21	1.45	1.33
21	A	828	CLA	O2A-CGA	4.21	1.45	1.33
21	10	704	CLA	C1D-ND	4.21	1.43	1.37
21	4	706	CLA	O2D-CGD	4.20	1.43	1.33
21	A	804	CLA	CHC-C1C	4.20	1.45	1.35
21	5	702	CLA	OBD-CAD	4.20	1.29	1.22
21	3	706	CLA	C3B-C2B	4.19	1.46	1.40
21	2	510	CLA	CHD-C1D	4.19	1.46	1.38
21	A	827	CLA	C1B-NB	-4.19	1.31	1.35
21	11	704	CLA	C1D-ND	4.19	1.42	1.37
21	1	508	CLA	C3C-C2C	4.19	1.45	1.36
21	B	816	CLA	C3D-C4D	-4.19	1.34	1.44
21	1	510	CLA	C1D-ND	4.19	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	512	CLA	O2D-CGD	4.19	1.43	1.33
21	1	512	CLA	CHD-C4C	4.19	1.48	1.39
21	2	517	CLA	CHD-C1D	4.19	1.46	1.38
21	6	904	CLA	O2A-CGA	4.19	1.45	1.33
21	B	830	CLA	C1D-ND	4.18	1.42	1.37
21	4	711	CLA	CHD-C4C	4.18	1.48	1.39
21	5	708	CLA	CHC-C1C	4.18	1.45	1.35
21	10	703	CLA	CHD-C1D	4.18	1.46	1.38
21	11	703	CLA	CHD-C4C	4.18	1.48	1.39
28	9	915	DD6	C10-C11	4.18	1.41	1.35
21	B	837	CLA	C3B-C2B	4.18	1.46	1.40
21	A	844	CLA	CHC-C1C	4.17	1.45	1.35
21	B	806	CLA	CHD-C1D	4.17	1.46	1.38
21	2	505	CLA	CHD-C1D	4.17	1.46	1.38
21	3	712	CLA	C3B-C2B	4.17	1.46	1.40
21	A	827	CLA	O2A-CGA	4.17	1.45	1.33
21	B	826	CLA	CHC-C1C	4.17	1.45	1.35
21	13	502	CLA	CHD-C4C	4.16	1.48	1.39
21	A	814	CLA	C1D-ND	4.16	1.42	1.37
21	4	709	CLA	CHD-C1D	4.16	1.46	1.38
28	2	518	DD6	C2-C1	4.16	1.41	1.35
21	1	516	CLA	C3D-C2D	4.16	1.50	1.39
21	A	822	CLA	CHC-C1C	4.16	1.45	1.35
21	B	814	CLA	C4B-NB	-4.16	1.31	1.35
21	10	704	CLA	OBD-CAD	4.16	1.29	1.22
21	11	706	CLA	C3D-C2D	4.16	1.50	1.39
21	A	806	CLA	C3D-C4D	-4.16	1.34	1.44
21	A	823	CLA	O2A-CGA	4.15	1.44	1.30
21	B	805	CLA	O2D-CGD	4.15	1.43	1.33
21	A	840	CLA	CHC-C1C	4.15	1.45	1.35
21	B	827	CLA	O2D-CGD	4.15	1.43	1.33
21	A	808	CLA	C3C-C2C	4.15	1.45	1.36
21	B	834	CLA	C3C-C2C	4.15	1.45	1.36
21	A	824	CLA	C3C-C2C	4.15	1.45	1.36
21	9	912	CLA	C3D-C2D	4.15	1.50	1.39
21	A	829	CLA	C3B-C2B	4.14	1.46	1.40
21	1	504	CLA	CHD-C1D	4.14	1.46	1.38
21	B	833	CLA	C3C-C2C	4.14	1.45	1.36
21	B	825	CLA	OBD-CAD	4.14	1.29	1.22
21	8	609	CLA	C3D-C2D	4.14	1.50	1.39
21	10	704	CLA	CHD-C4C	4.14	1.48	1.39
21	B	807	CLA	OBD-CAD	4.14	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	702	CLA	C3C-C2C	4.13	1.45	1.36
21	A	842	CLA	CHD-C4C	4.13	1.48	1.39
21	A	804	CLA	C1C-NC	-4.13	1.31	1.37
21	B	819	CLA	CHD-C1D	4.13	1.46	1.38
21	10	705	CLA	CHD-C4C	4.13	1.48	1.39
21	3	710	CLA	CHD-C1D	4.13	1.46	1.38
21	B	806	CLA	CHD-C4C	4.12	1.48	1.39
21	10	707	CLA	CHD-C4C	4.12	1.48	1.39
21	3	714	CLA	CHD-C1D	4.12	1.46	1.38
21	12	507	CLA	C3D-C2D	4.12	1.50	1.39
21	A	841	CLA	C3C-C2C	4.12	1.45	1.36
24	A	849	BCR	C23-C22	-4.12	1.37	1.45
21	2	513	CLA	CHD-C1D	4.12	1.46	1.38
21	A	810	CLA	O2A-CGA	4.12	1.45	1.33
21	8	611	CLA	CHD-C1D	4.12	1.46	1.38
21	4	703	CLA	CHD-C1D	4.12	1.46	1.38
21	5	711	CLA	OBD-CAD	4.12	1.29	1.22
21	10	710	CLA	CHD-C1D	4.12	1.46	1.38
21	A	837	CLA	CHD-C4C	4.11	1.48	1.39
21	A	830	CLA	O2D-CGD	4.11	1.43	1.33
21	A	807	CLA	C3C-C2C	4.11	1.45	1.36
21	10	712	CLA	CHD-C4C	4.11	1.48	1.39
28	9	916	DD6	C10-C11	4.11	1.41	1.35
21	7	709	CLA	CHD-C1D	4.11	1.46	1.38
21	A	830	CLA	CHC-C1C	4.11	1.45	1.35
21	12	506	CLA	C1D-ND	4.11	1.42	1.37
21	A	812	CLA	C3B-C2B	4.11	1.46	1.40
21	B	820	CLA	CHD-C4C	4.11	1.48	1.39
21	A	843	CLA	CHD-C1D	4.11	1.46	1.38
21	A	815	CLA	O2A-CGA	4.11	1.45	1.33
21	7	711	CLA	C3D-C2D	4.11	1.50	1.39
21	A	818	CLA	CHD-C4C	4.10	1.48	1.39
21	3	702	CLA	C3C-C2C	4.10	1.45	1.36
28	12	509	DD6	C10-C11	4.10	1.41	1.35
21	4	705	CLA	C3B-C2B	4.10	1.46	1.40
28	12	509	DD6	C2-C1	4.10	1.41	1.35
21	12	506	CLA	C3D-C2D	4.10	1.50	1.39
21	9	911	CLA	CHD-C4C	4.10	1.48	1.39
21	A	814	CLA	O2D-CGD	4.10	1.43	1.33
24	B	843	BCR	C21-C22	4.10	1.41	1.35
21	9	909	CLA	O2D-CGD	4.10	1.43	1.33
21	A	805	CLA	C1D-ND	4.09	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	516	CLA	C3B-C2B	4.09	1.46	1.40
21	9	903	CLA	C3D-C2D	4.09	1.50	1.39
21	B	815	CLA	C1D-ND	4.09	1.42	1.37
21	1	511	CLA	C1D-ND	4.09	1.42	1.37
21	B	818	CLA	CHD-C1D	4.09	1.46	1.38
21	5	701	CLA	CHC-C1C	4.09	1.45	1.35
21	1	504	CLA	OBD-CAD	4.09	1.29	1.22
21	10	704	CLA	CHD-C1D	4.09	1.46	1.38
21	7	703	CLA	O2A-CGA	4.09	1.45	1.33
21	1	517	CLA	C1C-C2C	4.08	1.52	1.44
21	7	702	CLA	CHC-C1C	4.08	1.45	1.35
21	11	710	CLA	CHD-C1D	4.08	1.46	1.38
21	7	711	CLA	CHD-C4C	4.08	1.48	1.39
21	9	904	CLA	CHD-C4C	4.08	1.48	1.39
21	13	501	CLA	CHD-C1D	4.08	1.46	1.38
24	A	848	BCR	C14-C13	4.07	1.41	1.35
21	6	903	CLA	CHD-C1D	4.07	1.46	1.38
21	2	515	CLA	CHC-C1C	4.07	1.45	1.35
21	6	908	CLA	CHD-C4C	4.07	1.48	1.39
21	5	709	CLA	CHD-C1D	4.07	1.46	1.38
21	2	506	CLA	O2A-CGA	4.07	1.45	1.33
21	B	835	CLA	OBD-CAD	4.07	1.29	1.22
21	B	820	CLA	C3D-C2D	4.07	1.50	1.39
21	2	504	CLA	O2A-CGA	4.07	1.45	1.33
21	B	819	CLA	CHD-C4C	4.06	1.48	1.39
21	A	817	CLA	C3C-C2C	4.06	1.45	1.36
21	A	802	CLA	C1C-NC	-4.06	1.31	1.37
21	B	803	CLA	CHC-C1C	4.06	1.45	1.35
21	2	512	CLA	CHC-C1C	4.06	1.45	1.35
21	8	609	CLA	O2D-CGD	4.06	1.43	1.33
21	A	810	CLA	C3B-C2B	4.06	1.46	1.40
21	4	705	CLA	C1D-ND	4.06	1.42	1.37
21	1	517	CLA	CHD-C1D	4.06	1.46	1.38
21	7	703	CLA	C3B-C2B	4.06	1.46	1.40
21	9	914	CLA	OBD-CAD	4.06	1.29	1.22
21	11	709	CLA	CHD-C4C	4.06	1.48	1.39
21	5	711	CLA	CHD-C4C	4.06	1.48	1.39
21	1	506	CLA	CHD-C1D	4.05	1.46	1.38
28	9	916	DD6	C2-C1	4.05	1.41	1.35
21	4	710	CLA	CHD-C1D	4.05	1.46	1.38
21	9	902	CLA	CHD-C4C	4.05	1.48	1.39
21	2	506	CLA	CHD-C4C	4.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	512	CLA	CHD-C1D	4.05	1.46	1.38
21	3	713	CLA	CHD-C4C	4.05	1.48	1.39
21	10	712	CLA	CHD-C1D	4.05	1.46	1.38
21	B	811	CLA	C1D-ND	4.05	1.42	1.37
21	8	610	CLA	C3B-C2B	4.05	1.46	1.40
21	A	810	CLA	C1B-NB	-4.04	1.31	1.35
21	8	612	CLA	CHD-C4C	4.04	1.48	1.39
24	A	852	BCR	C12-C13	-4.04	1.37	1.45
21	B	823	CLA	C1D-ND	4.04	1.42	1.37
21	5	707	CLA	C3B-C2B	4.04	1.46	1.40
21	4	706	CLA	CHD-C4C	4.04	1.48	1.39
28	11	713	DD6	C10-C11	4.04	1.41	1.35
21	1	504	CLA	CHD-C4C	4.04	1.48	1.39
21	B	810	CLA	CHD-C1D	4.04	1.46	1.38
21	6	914	CLA	C1D-ND	4.04	1.42	1.37
21	A	812	CLA	CHD-C4C	4.04	1.48	1.39
21	9	904	CLA	CHD-C1D	4.04	1.46	1.38
21	10	707	CLA	C3D-C2D	4.03	1.50	1.39
21	8	611	CLA	C3B-C2B	4.03	1.46	1.40
21	2	511	CLA	C3D-C2D	4.03	1.50	1.39
21	3	706	CLA	CHD-C1D	4.03	1.46	1.38
21	A	835	CLA	C3D-C4D	-4.03	1.35	1.44
21	B	818	CLA	O2A-CGA	4.03	1.45	1.33
20	A	801	CL0	O2A-CGA	4.03	1.45	1.33
21	11	701	CLA	OBD-CAD	4.03	1.29	1.22
21	4	701	CLA	CHD-C4C	4.03	1.48	1.39
21	10	711	CLA	C1B-NB	-4.02	1.31	1.35
28	9	916	DD6	C5-C6	4.02	1.41	1.35
21	2	515	CLA	OBD-CAD	4.02	1.29	1.22
21	12	503	CLA	CHD-C4C	4.02	1.48	1.39
28	J	104	DD6	C2-C1	4.02	1.41	1.35
21	4	706	CLA	CHD-C1D	4.02	1.46	1.38
21	2	513	CLA	CHD-C4C	4.02	1.48	1.39
21	6	905	CLA	C1D-ND	4.02	1.42	1.37
21	11	702	CLA	C1D-ND	4.02	1.42	1.37
21	8	608	CLA	CHD-C4C	4.02	1.48	1.39
21	10	708	CLA	C3D-C2D	4.02	1.50	1.39
21	1	514	CLA	OBD-CAD	4.02	1.29	1.22
21	6	908	CLA	C3C-C2C	4.02	1.45	1.36
21	3	715	CLA	O2D-CGD	4.01	1.43	1.33
21	A	814	CLA	C1C-NC	-4.01	1.31	1.37
21	B	813	CLA	O2A-CGA	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	606	CLA	CHD-C1D	4.01	1.46	1.38
21	6	914	CLA	CHD-C1D	4.01	1.46	1.38
21	3	715	CLA	CHD-C4C	4.01	1.48	1.39
21	B	835	CLA	CAA-C2A	-4.01	1.46	1.54
21	8	614	CLA	C1D-ND	4.01	1.42	1.37
24	B	842	BCR	C10-C9	4.01	1.41	1.35
21	F	403	CLA	CHD-C4C	4.01	1.48	1.39
21	5	704	CLA	OBD-CAD	4.01	1.29	1.22
24	J	102	BCR	C14-C13	4.01	1.41	1.35
21	6	913	CLA	CHD-C1D	4.01	1.46	1.38
21	4	710	CLA	CHD-C4C	4.01	1.48	1.39
21	2	512	CLA	C3C-C2C	4.01	1.45	1.36
21	11	702	CLA	O2A-CGA	4.01	1.45	1.33
21	A	829	CLA	C3C-C2C	4.00	1.45	1.36
21	11	711	CLA	CHD-C4C	4.00	1.48	1.39
21	3	710	CLA	C1B-NB	-4.00	1.31	1.35
21	2	513	CLA	OBD-CAD	4.00	1.29	1.22
21	2	505	CLA	C1B-NB	-4.00	1.31	1.35
21	B	802	CLA	C1D-ND	4.00	1.42	1.37
21	2	506	CLA	C1D-ND	4.00	1.42	1.37
21	2	515	CLA	C1C-NC	-4.00	1.31	1.37
21	A	802	CLA	OBD-CAD	4.00	1.29	1.22
21	11	706	CLA	C3C-C2C	4.00	1.45	1.36
21	4	702	CLA	C3D-C2D	4.00	1.50	1.39
21	5	701	CLA	CHD-C1D	4.00	1.46	1.38
21	9	905	CLA	C3D-C2D	3.99	1.50	1.39
21	B	819	CLA	O2D-CGD	3.99	1.42	1.33
21	8	612	CLA	C3C-C2C	3.99	1.45	1.36
21	A	812	CLA	CHD-C1D	3.99	1.46	1.38
21	6	906	CLA	CHD-C1D	3.99	1.46	1.38
21	A	839	CLA	C3B-C2B	3.99	1.45	1.40
21	8	610	CLA	O2D-CGD	3.99	1.42	1.33
21	3	702	CLA	C1B-NB	-3.99	1.31	1.35
21	11	710	CLA	CHD-C4C	3.99	1.48	1.39
21	3	702	CLA	CHD-C1D	3.98	1.46	1.38
21	3	712	CLA	CHD-C4C	3.98	1.48	1.39
21	2	511	CLA	C3B-C2B	3.98	1.45	1.40
24	B	845	BCR	C8-C9	-3.98	1.37	1.45
21	A	817	CLA	O2D-CGD	3.98	1.42	1.33
21	6	903	CLA	C3D-C2D	3.98	1.50	1.39
28	6	915	DD6	C10-C11	3.98	1.41	1.35
21	3	713	CLA	OBD-CAD	3.98	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	807	CLA	CHD-C1D	3.98	1.46	1.38
21	6	906	CLA	CHD-C4C	3.98	1.48	1.39
21	5	704	CLA	CHD-C4C	3.98	1.48	1.39
21	A	803	CLA	C4B-NB	-3.98	1.31	1.35
21	2	511	CLA	CHD-C4C	3.97	1.48	1.39
21	11	704	CLA	CHD-C4C	3.97	1.48	1.39
21	5	706	CLA	O2D-CGD	3.97	1.42	1.33
21	2	504	CLA	O2D-CGD	3.97	1.42	1.33
21	B	833	CLA	CHD-C1D	3.97	1.46	1.38
21	1	509	CLA	CHD-C4C	3.97	1.48	1.39
21	7	713	CLA	CHD-C1D	3.97	1.46	1.38
21	9	909	CLA	CHD-C4C	3.97	1.48	1.39
21	11	708	CLA	CHD-C1D	3.97	1.46	1.38
21	A	862	CLA	C4B-NB	-3.97	1.31	1.35
21	B	808	CLA	CHD-C4C	3.97	1.48	1.39
21	10	706	CLA	OBD-CAD	3.97	1.29	1.22
21	A	835	CLA	C3C-C2C	3.97	1.45	1.36
21	6	908	CLA	O2D-CGD	3.96	1.42	1.33
21	1	514	CLA	C3D-C2D	3.96	1.49	1.39
21	9	911	CLA	C3D-C2D	3.96	1.49	1.39
21	12	506	CLA	CHD-C4C	3.96	1.48	1.39
21	7	705	CLA	C1D-ND	3.96	1.42	1.37
21	4	702	CLA	OBD-CAD	3.96	1.29	1.22
21	B	833	CLA	C1D-ND	3.96	1.42	1.37
21	B	816	CLA	O2D-CGD	3.96	1.42	1.33
21	10	710	CLA	CHD-C4C	3.96	1.48	1.39
21	1	515	CLA	C1B-NB	-3.96	1.31	1.35
28	9	915	DD6	C5-C6	3.96	1.41	1.35
21	6	914	CLA	CHD-C4C	3.95	1.48	1.39
21	7	702	CLA	O2D-CGD	3.95	1.42	1.33
21	12	508	CLA	C3D-C2D	3.95	1.49	1.39
21	10	706	CLA	C3D-C2D	3.95	1.49	1.39
21	B	811	CLA	CHD-C1D	3.95	1.46	1.38
21	B	814	CLA	C3D-C2D	3.95	1.49	1.39
21	A	841	CLA	C1C-NC	-3.95	1.31	1.37
21	7	713	CLA	C1D-ND	3.95	1.42	1.37
21	B	810	CLA	C3C-C2C	3.94	1.45	1.36
21	6	914	CLA	OBD-CAD	3.94	1.29	1.22
21	6	903	CLA	CHD-C4C	3.94	1.48	1.39
21	2	503	CLA	C1D-ND	3.94	1.42	1.37
21	2	517	CLA	OBD-CAD	3.94	1.29	1.22
21	A	830	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	711	CLA	CHD-C1D	3.94	1.46	1.38
24	A	851	BCR	C23-C22	-3.94	1.37	1.45
21	13	503	CLA	CHD-C4C	3.94	1.48	1.39
21	1	511	CLA	C3D-C2D	3.94	1.49	1.39
21	4	710	CLA	OBD-CAD	3.94	1.29	1.22
21	1	506	CLA	CHD-C4C	3.94	1.48	1.39
21	6	906	CLA	C3B-C2B	3.94	1.45	1.40
21	2	506	CLA	CHD-C1D	3.94	1.46	1.38
21	B	820	CLA	C3B-C2B	3.94	1.45	1.40
21	B	835	CLA	C3D-C4D	-3.93	1.35	1.44
21	10	708	CLA	CHD-C4C	3.93	1.48	1.39
21	6	912	CLA	C3D-C2D	3.93	1.49	1.39
21	9	902	CLA	C3D-C2D	3.93	1.49	1.39
21	4	702	CLA	C1D-ND	3.93	1.42	1.37
21	A	811	CLA	CHD-C4C	3.93	1.48	1.39
28	4	713	DD6	C10-C11	3.93	1.41	1.35
21	7	711	CLA	O2A-CGA	3.93	1.44	1.33
21	5	710	CLA	C3D-C2D	3.93	1.49	1.39
21	7	712	CLA	C1D-ND	3.93	1.42	1.37
21	1	511	CLA	OBD-CAD	3.93	1.29	1.22
21	B	809	CLA	C1B-NB	-3.93	1.31	1.35
21	6	910	CLA	CHD-C4C	3.93	1.48	1.39
21	2	512	CLA	CHD-C1D	3.93	1.46	1.38
21	B	823	CLA	C1B-NB	-3.93	1.31	1.35
21	1	515	CLA	CHD-C4C	3.92	1.48	1.39
21	6	909	CLA	CHD-C1D	3.92	1.46	1.38
21	7	714	CLA	C3B-C2B	3.92	1.45	1.40
21	9	913	CLA	CHD-C4C	3.92	1.48	1.39
21	8	604	CLA	OBD-CAD	3.92	1.29	1.22
21	12	507	CLA	OBD-CAD	3.92	1.29	1.22
24	A	850	BCR	C21-C22	3.91	1.41	1.35
21	5	706	CLA	C3B-C2B	3.91	1.45	1.40
21	11	708	CLA	OBD-CAD	3.91	1.29	1.22
21	10	711	CLA	CHD-C1D	3.91	1.46	1.38
21	9	902	CLA	CHD-C1D	3.91	1.46	1.38
21	5	705	CLA	C1B-NB	-3.91	1.31	1.35
21	A	808	CLA	CHD-C4C	3.91	1.48	1.39
21	1	507	CLA	C1D-ND	3.91	1.42	1.37
21	J	101	CLA	CHD-C4C	3.90	1.48	1.39
21	11	703	CLA	C3B-C2B	3.90	1.45	1.40
21	B	818	CLA	C1B-NB	-3.90	1.31	1.35
28	6	915	DD6	C5-C6	3.90	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	838	CLA	C3D-C2D	3.90	1.49	1.39
21	B	836	CLA	C3C-C2C	3.90	1.45	1.36
28	11	713	DD6	C5-C6	3.90	1.40	1.35
21	2	508	CLA	CHD-C1D	3.90	1.46	1.38
21	B	832	CLA	C3C-C2C	3.90	1.45	1.36
21	2	504	CLA	C1B-NB	-3.89	1.31	1.35
21	B	835	CLA	O2A-CGA	3.89	1.44	1.33
24	B	845	BCR	C12-C13	-3.89	1.37	1.45
21	F	403	CLA	C3D-C2D	3.89	1.49	1.39
21	A	839	CLA	OBD-CAD	3.89	1.29	1.22
21	A	803	CLA	CHC-C1C	3.89	1.44	1.35
21	A	838	CLA	CHC-C1C	3.89	1.44	1.35
21	7	709	CLA	O2D-CGD	3.89	1.42	1.33
21	9	910	CLA	CHD-C4C	3.89	1.48	1.39
21	J	101	CLA	O2D-CGD	3.89	1.42	1.33
21	A	814	CLA	CMD-C2D	-3.89	1.42	1.50
21	12	508	CLA	OBD-CAD	3.89	1.29	1.22
21	4	702	CLA	O2A-CGA	3.89	1.44	1.33
21	A	839	CLA	C3C-C2C	3.89	1.45	1.36
21	B	808	CLA	C3C-C2C	3.89	1.45	1.36
21	8	614	CLA	CHD-C1D	3.89	1.45	1.38
21	8	610	CLA	C1D-ND	3.89	1.42	1.37
21	6	905	CLA	CHC-C1C	3.89	1.44	1.35
28	3	718	DD6	C10-C11	3.89	1.40	1.35
21	11	704	CLA	OBD-CAD	3.89	1.29	1.22
21	5	708	CLA	CHD-C4C	3.88	1.48	1.39
21	3	713	CLA	CHD-C1D	3.88	1.45	1.38
21	10	711	CLA	C3D-C2D	3.88	1.49	1.39
21	9	906	CLA	CHD-C4C	3.88	1.48	1.39
21	8	610	CLA	CHD-C1D	3.88	1.45	1.38
21	3	708	CLA	O2D-CGD	3.88	1.42	1.33
21	1	512	CLA	C3D-C2D	3.88	1.49	1.39
21	7	714	CLA	CHD-C4C	3.88	1.48	1.39
21	3	701	CLA	C3D-C2D	3.88	1.49	1.39
21	B	801	CLA	O2A-CGA	3.88	1.44	1.33
21	2	514	CLA	CHD-C4C	3.88	1.48	1.39
21	5	705	CLA	CHD-C1D	3.88	1.45	1.38
21	B	812	CLA	O2A-CGA	3.88	1.44	1.33
21	B	833	CLA	CHD-C4C	3.88	1.48	1.39
21	A	803	CLA	C3C-C2C	3.88	1.45	1.36
21	B	837	CLA	C3C-C2C	3.88	1.45	1.36
21	8	612	CLA	O2A-CGA	3.88	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	908	CLA	CHD-C4C	3.88	1.48	1.39
21	F	403	CLA	C1D-ND	3.87	1.42	1.37
21	2	503	CLA	CHD-C4C	3.87	1.48	1.39
21	B	805	CLA	C1B-NB	-3.87	1.31	1.35
21	A	834	CLA	OBD-CAD	3.87	1.29	1.22
21	A	829	CLA	CHC-C1C	3.87	1.44	1.35
28	9	915	DD6	C2-C1	3.87	1.40	1.35
21	B	839	CLA	C1D-ND	3.87	1.42	1.37
21	6	911	CLA	CHD-C1D	3.87	1.45	1.38
28	2	518	DD6	C5-C6	3.87	1.40	1.35
21	10	705	CLA	OBD-CAD	3.87	1.29	1.22
21	1	507	CLA	CHD-C4C	3.87	1.48	1.39
21	A	826	CLA	O2A-CGA	3.87	1.44	1.33
28	11	713	DD6	C2-C1	3.86	1.40	1.35
28	J	104	DD6	C10-C11	3.86	1.40	1.35
21	3	705	CLA	CHD-C4C	3.86	1.48	1.39
21	B	827	CLA	C1D-ND	3.86	1.42	1.37
21	B	825	CLA	CHC-C1C	3.86	1.44	1.35
24	A	851	BCR	C10-C9	3.86	1.40	1.35
21	10	704	CLA	C3D-C2D	3.86	1.49	1.39
21	8	606	CLA	CHC-C1C	3.86	1.44	1.35
21	A	834	CLA	O2D-CGD	3.85	1.42	1.33
21	A	844	CLA	C1B-NB	-3.85	1.31	1.35
21	4	704	CLA	C3D-C2D	3.85	1.49	1.39
21	5	710	CLA	OBD-CAD	3.85	1.29	1.22
21	5	706	CLA	C3D-C2D	3.85	1.49	1.39
21	3	702	CLA	C3B-C2B	3.85	1.45	1.40
21	A	829	CLA	CAA-C2A	-3.85	1.47	1.54
21	2	508	CLA	OBD-CAD	3.85	1.29	1.22
21	7	709	CLA	OBD-CAD	3.85	1.29	1.22
21	A	813	CLA	CAA-C2A	-3.85	1.47	1.54
21	6	906	CLA	OBD-CAD	3.85	1.29	1.22
21	F	404	CLA	C1B-NB	-3.85	1.31	1.35
28	4	713	DD6	C2-C1	3.85	1.40	1.35
21	7	711	CLA	CHD-C1D	3.85	1.45	1.38
21	A	830	CLA	C1C-NC	-3.85	1.32	1.37
21	4	707	CLA	OBD-CAD	3.85	1.29	1.22
21	8	606	CLA	C3D-C2D	3.85	1.49	1.39
21	B	833	CLA	C3B-C2B	3.85	1.45	1.40
21	A	822	CLA	C1B-NB	-3.84	1.31	1.35
21	11	711	CLA	OBD-CAD	3.84	1.29	1.22
21	8	614	CLA	CHD-C4C	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	12	510	DD6	C5-C6	3.84	1.40	1.35
21	A	817	CLA	C1B-NB	-3.84	1.31	1.35
21	B	832	CLA	C1C-C2C	3.84	1.52	1.44
21	7	710	CLA	C3D-C2D	3.84	1.49	1.39
21	8	612	CLA	OBD-CAD	3.84	1.29	1.22
21	A	836	CLA	C3B-C2B	3.84	1.45	1.40
21	9	903	CLA	CHD-C4C	3.84	1.48	1.39
24	B	843	BCR	C16-C17	-3.84	1.31	1.43
21	A	806	CLA	O2D-CGD	3.84	1.42	1.33
21	3	711	CLA	C1B-NB	-3.84	1.31	1.35
21	7	705	CLA	C1B-NB	-3.84	1.31	1.35
21	2	510	CLA	C3D-C2D	3.84	1.49	1.39
21	5	708	CLA	C1C-NC	-3.83	1.32	1.37
21	A	842	CLA	O2A-CGA	3.83	1.44	1.33
21	A	826	CLA	C3C-C2C	3.83	1.44	1.36
21	7	714	CLA	C3C-C2C	3.83	1.44	1.36
21	B	830	CLA	CHD-C1D	3.83	1.45	1.38
21	F	404	CLA	C3D-C2D	3.83	1.49	1.39
21	B	810	CLA	C1B-NB	-3.83	1.31	1.35
21	6	913	CLA	C3D-C2D	3.82	1.49	1.39
21	2	508	CLA	C1B-NB	-3.82	1.31	1.35
21	4	707	CLA	CHD-C4C	3.82	1.48	1.39
21	1	510	CLA	C3D-C2D	3.82	1.49	1.39
21	A	822	CLA	CHD-C1D	3.82	1.45	1.38
21	6	907	CLA	CHC-C1C	3.82	1.44	1.35
21	11	704	CLA	C3D-C2D	3.82	1.49	1.39
28	1	520	DD6	C2-C1	3.82	1.40	1.35
21	12	503	CLA	OBD-CAD	3.81	1.29	1.22
21	B	815	CLA	O2D-CGD	3.81	1.42	1.33
21	12	501	CLA	CHD-C4C	3.81	1.47	1.39
21	1	513	CLA	CHD-C1D	3.81	1.45	1.38
27	B	847	DGD	O2G-C1B	3.81	1.45	1.34
21	3	710	CLA	C3D-C2D	3.81	1.49	1.39
21	5	705	CLA	CHD-C4C	3.81	1.47	1.39
21	10	709	CLA	C1D-ND	3.81	1.42	1.37
21	A	829	CLA	CHD-C1D	3.81	1.45	1.38
21	1	514	CLA	CHD-C4C	3.81	1.47	1.39
21	4	701	CLA	CHD-C1D	3.81	1.45	1.38
21	3	712	CLA	C3D-C2D	3.81	1.49	1.39
21	1	511	CLA	CHD-C1D	3.81	1.45	1.38
28	4	713	DD6	C5-C6	3.81	1.40	1.35
21	13	502	CLA	C3D-C2D	3.80	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	705	CLA	C3D-C2D	3.80	1.49	1.39
21	7	713	CLA	CHD-C4C	3.80	1.47	1.39
21	A	839	CLA	CHD-C1D	3.80	1.45	1.38
21	A	815	CLA	O2D-CGD	3.80	1.42	1.33
21	5	711	CLA	C3D-C2D	3.80	1.49	1.39
21	A	822	CLA	C3B-C2B	3.80	1.45	1.40
21	6	905	CLA	CHD-C1D	3.80	1.45	1.38
21	6	904	CLA	C1D-ND	3.80	1.42	1.37
21	B	825	CLA	MG-ND	-3.80	1.98	2.05
21	A	807	CLA	CHC-C1C	3.80	1.44	1.35
24	B	842	BCR	C14-C13	3.79	1.40	1.35
21	9	914	CLA	C3D-C2D	3.79	1.49	1.39
21	A	818	CLA	C3B-C2B	3.79	1.45	1.40
21	3	712	CLA	CHC-C1C	3.79	1.44	1.35
21	5	707	CLA	CHD-C1D	3.79	1.45	1.38
21	A	835	CLA	CHC-C1C	3.79	1.44	1.35
21	1	508	CLA	C1D-ND	3.79	1.42	1.37
21	2	507	CLA	C1B-NB	-3.79	1.31	1.35
21	12	505	CLA	C3D-C2D	3.79	1.49	1.39
21	J	101	CLA	OBD-CAD	3.79	1.29	1.22
21	2	513	CLA	C3D-C2D	3.79	1.49	1.39
21	8	613	CLA	CHD-C1D	3.79	1.45	1.38
21	A	805	CLA	C3B-C2B	3.78	1.45	1.40
21	11	702	CLA	CHD-C1D	3.78	1.45	1.38
21	6	913	CLA	OBD-CAD	3.78	1.29	1.22
21	6	907	CLA	CHD-C4C	3.78	1.47	1.39
21	8	609	CLA	C1B-NB	-3.78	1.31	1.35
21	7	707	CLA	OBD-CAD	3.77	1.29	1.22
21	2	510	CLA	O2D-CGD	3.77	1.42	1.33
21	8	612	CLA	O2D-CGD	3.77	1.42	1.33
21	A	811	CLA	C3B-C2B	3.77	1.45	1.40
21	5	703	CLA	CHD-C1D	3.77	1.45	1.38
21	A	841	CLA	CHD-C4C	3.77	1.47	1.39
21	10	703	CLA	CHD-C4C	3.77	1.47	1.39
21	3	707	CLA	C3D-C2D	3.77	1.49	1.39
21	B	812	CLA	CHD-C1D	3.76	1.45	1.38
28	J	104	DD6	C5-C6	3.76	1.40	1.35
21	6	911	CLA	C1B-NB	-3.76	1.31	1.35
21	10	712	CLA	OBD-CAD	3.76	1.29	1.22
21	B	815	CLA	OBD-CAD	3.76	1.29	1.22
21	7	704	CLA	CHC-C1C	3.76	1.44	1.35
21	A	837	CLA	CHD-C1D	3.76	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	912	CLA	OBD-CAD	3.76	1.29	1.22
21	6	913	CLA	CHD-C4C	3.76	1.47	1.39
21	1	501	CLA	CHD-C1D	3.76	1.45	1.38
21	1	505	CLA	O2A-CGA	3.75	1.44	1.33
21	3	708	CLA	OBD-CAD	3.75	1.28	1.22
21	9	909	CLA	C3D-C2D	3.75	1.49	1.39
21	7	711	CLA	C3B-C2B	3.75	1.45	1.40
21	5	702	CLA	O2A-CGA	3.75	1.44	1.33
21	F	403	CLA	OBD-CAD	3.75	1.28	1.22
21	3	701	CLA	OBD-CAD	3.75	1.28	1.22
21	2	512	CLA	CHD-C4C	3.75	1.47	1.39
21	7	709	CLA	C3D-C4D	-3.75	1.35	1.44
21	A	833	CLA	C1D-ND	3.75	1.42	1.37
21	B	806	CLA	C1D-ND	3.75	1.42	1.37
21	4	701	CLA	OBD-CAD	3.75	1.28	1.22
21	B	829	CLA	C3D-C2D	3.74	1.49	1.39
21	B	822	CLA	CHC-C1C	3.74	1.44	1.35
21	6	912	CLA	CHD-C4C	3.74	1.47	1.39
21	B	809	CLA	OBD-CAD	3.74	1.28	1.22
21	A	833	CLA	C3C-C2C	3.74	1.44	1.36
21	3	709	CLA	CHD-C1D	3.74	1.45	1.38
28	12	510	DD6	C2-C1	3.74	1.40	1.35
21	A	809	CLA	CHD-C4C	3.74	1.47	1.39
21	2	503	CLA	C3B-C2B	3.74	1.45	1.40
21	12	503	CLA	C3D-C2D	3.74	1.49	1.39
21	9	911	CLA	CHD-C1D	3.74	1.45	1.38
21	1	513	CLA	C3C-C2C	3.74	1.44	1.36
21	3	708	CLA	CHD-C4C	3.73	1.47	1.39
21	4	704	CLA	CHD-C1D	3.73	1.45	1.38
21	A	838	CLA	C3B-C2B	3.73	1.45	1.40
21	5	710	CLA	CHD-C1D	3.73	1.45	1.38
21	12	506	CLA	OBD-CAD	3.73	1.28	1.22
21	10	710	CLA	C3D-C2D	3.73	1.49	1.39
24	B	841	BCR	C10-C9	3.73	1.40	1.35
21	A	803	CLA	O2D-CGD	3.73	1.42	1.33
21	1	505	CLA	CHD-C4C	3.73	1.47	1.39
21	B	817	CLA	MG-ND	-3.73	1.98	2.05
21	6	911	CLA	C3D-C2D	3.73	1.49	1.39
21	A	832	CLA	C3C-C2C	3.72	1.44	1.36
21	7	704	CLA	C1D-ND	3.72	1.42	1.37
21	2	505	CLA	C3D-C2D	3.72	1.49	1.39
21	A	804	CLA	C1C-C2C	3.72	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	712	DD6	C5-C6	3.72	1.40	1.35
21	B	823	CLA	C3D-C2D	3.72	1.49	1.39
21	1	516	CLA	CHD-C1D	3.72	1.45	1.38
21	B	823	CLA	CHC-C1C	3.72	1.44	1.35
21	1	513	CLA	OBD-CAD	3.72	1.28	1.22
21	10	709	CLA	CHD-C1D	3.72	1.45	1.38
28	5	713	DD6	C10-C11	3.71	1.40	1.35
21	2	504	CLA	OBD-CAD	3.71	1.28	1.22
21	8	612	CLA	C3D-C2D	3.71	1.49	1.39
21	11	701	CLA	CHD-C4C	3.71	1.47	1.39
21	9	912	CLA	CHD-C1D	3.71	1.45	1.38
21	1	505	CLA	C3D-C2D	3.71	1.49	1.39
21	3	701	CLA	CHD-C4C	3.71	1.47	1.39
21	8	613	CLA	OBD-CAD	3.71	1.28	1.22
21	7	704	CLA	C3C-C2C	3.71	1.44	1.36
21	7	706	CLA	C3C-C2C	3.71	1.44	1.36
21	7	711	CLA	C3C-C2C	3.71	1.44	1.36
21	4	711	CLA	CHD-C1D	3.71	1.45	1.38
21	A	822	CLA	CHD-C4C	3.71	1.47	1.39
21	A	836	CLA	O2D-CGD	3.71	1.42	1.33
21	12	506	CLA	CHD-C1D	3.71	1.45	1.38
21	A	811	CLA	C1D-ND	3.70	1.42	1.37
21	1	507	CLA	C3D-C2D	3.70	1.49	1.39
21	A	841	CLA	O2A-CGA	3.70	1.44	1.33
21	3	708	CLA	C3D-C2D	3.70	1.49	1.39
21	10	703	CLA	C3D-C2D	3.70	1.49	1.39
21	11	707	CLA	OBD-CAD	3.70	1.28	1.22
21	1	501	CLA	O2D-CGD	3.70	1.42	1.33
21	A	826	CLA	CHD-C1D	3.70	1.45	1.38
21	2	508	CLA	C3D-C4D	-3.70	1.35	1.44
21	A	812	CLA	C1B-NB	-3.69	1.31	1.35
21	2	515	CLA	C4B-NB	-3.69	1.31	1.35
21	2	509	CLA	OBD-CAD	3.69	1.28	1.22
21	7	702	CLA	OBD-CAD	3.69	1.28	1.22
21	B	803	CLA	C3C-C2C	3.69	1.44	1.36
21	B	834	CLA	C4B-NB	-3.69	1.31	1.35
21	A	807	CLA	O2D-CGD	3.69	1.42	1.33
21	6	903	CLA	OBD-CAD	3.69	1.28	1.22
21	10	703	CLA	OBD-CAD	3.69	1.28	1.22
21	A	819	CLA	C1C-NC	-3.69	1.32	1.37
24	B	842	BCR	C17-C18	3.69	1.40	1.35
21	A	819	CLA	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	614	CLA	OBD-CAD	3.69	1.28	1.22
21	11	711	CLA	C3D-C2D	3.68	1.49	1.39
21	4	711	CLA	OBD-CAD	3.68	1.28	1.22
21	13	501	CLA	C3D-C2D	3.68	1.49	1.39
21	A	809	CLA	CHD-C1D	3.68	1.45	1.38
21	1	501	CLA	OBD-CAD	3.68	1.28	1.22
21	5	702	CLA	CHD-C4C	3.68	1.47	1.39
21	B	815	CLA	CHD-C1D	3.68	1.45	1.38
21	3	714	CLA	C3B-C2B	3.68	1.45	1.40
21	A	812	CLA	O2A-CGA	3.68	1.44	1.33
21	10	711	CLA	C3B-C2B	3.68	1.45	1.40
21	7	704	CLA	CHD-C1D	3.68	1.45	1.38
21	3	702	CLA	OBD-CAD	3.67	1.28	1.22
21	3	714	CLA	C3D-C2D	3.67	1.49	1.39
21	10	705	CLA	C3D-C2D	3.67	1.49	1.39
21	9	906	CLA	CHD-C1D	3.67	1.45	1.38
21	9	905	CLA	CHD-C4C	3.67	1.47	1.39
21	9	907	CLA	CHD-C4C	3.67	1.47	1.39
21	7	712	CLA	C3D-C2D	3.67	1.49	1.39
21	3	705	CLA	CHD-C1D	3.67	1.45	1.38
20	A	801	CL0	CHD-C4C	3.67	1.47	1.39
21	9	913	CLA	C3D-C2D	3.66	1.49	1.39
22	B	840	PQN	C5-C4	-3.66	1.41	1.48
21	5	709	CLA	OBD-CAD	3.66	1.28	1.22
21	13	501	CLA	CHD-C4C	3.66	1.47	1.39
21	2	506	CLA	C4B-NB	-3.66	1.31	1.35
21	1	514	CLA	CHD-C1D	3.66	1.45	1.38
21	6	904	CLA	C3D-C4D	-3.66	1.35	1.44
21	9	905	CLA	OBD-CAD	3.66	1.28	1.22
21	1	504	CLA	C3D-C2D	3.66	1.49	1.39
21	10	709	CLA	OBD-CAD	3.66	1.28	1.22
21	10	709	CLA	CHD-C4C	3.66	1.47	1.39
21	9	906	CLA	C1D-ND	3.66	1.42	1.37
21	8	603	CLA	C1D-ND	3.65	1.42	1.37
21	A	823	CLA	C1D-ND	3.65	1.42	1.37
21	6	904	CLA	OBD-CAD	3.65	1.28	1.22
21	2	512	CLA	C3D-C2D	3.65	1.49	1.39
21	A	820	CLA	CHD-C4C	3.65	1.47	1.39
21	B	833	CLA	C3D-C4D	-3.65	1.35	1.44
21	4	705	CLA	CHD-C1D	3.65	1.45	1.38
21	2	510	CLA	OBD-CAD	3.65	1.28	1.22
21	2	516	CLA	CHD-C4C	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	852	BCR	C8-C9	-3.65	1.38	1.45
21	B	805	CLA	CHD-C1D	3.65	1.45	1.38
21	2	516	CLA	CHD-C1D	3.65	1.45	1.38
21	B	834	CLA	CHD-C4C	3.65	1.47	1.39
21	11	705	CLA	CHD-C4C	3.64	1.47	1.39
21	5	709	CLA	C3D-C2D	3.64	1.49	1.39
21	B	820	CLA	OBD-CAD	3.64	1.28	1.22
21	11	710	CLA	OBD-CAD	3.64	1.28	1.22
21	5	701	CLA	C1D-ND	3.64	1.42	1.37
21	B	807	CLA	O2A-CGA	3.64	1.44	1.33
21	6	908	CLA	C1D-ND	3.64	1.42	1.37
21	3	710	CLA	CHD-C4C	3.64	1.47	1.39
21	8	607	CLA	CHD-C4C	3.64	1.47	1.39
21	7	711	CLA	OBD-CAD	3.64	1.28	1.22
21	10	712	CLA	C3D-C2D	3.63	1.49	1.39
21	F	401	CLA	CHD-C4C	3.63	1.47	1.39
21	B	824	CLA	C3C-C2C	3.63	1.44	1.36
21	9	912	CLA	OBD-CAD	3.63	1.28	1.22
21	B	827	CLA	C1B-NB	-3.63	1.32	1.35
21	9	906	CLA	C3D-C2D	3.63	1.49	1.39
21	8	603	CLA	C3C-C2C	3.63	1.44	1.36
21	4	703	CLA	CHD-C4C	3.63	1.47	1.39
21	10	711	CLA	CHD-C4C	3.63	1.47	1.39
21	10	708	CLA	OBD-CAD	3.63	1.28	1.22
21	1	511	CLA	CHD-C4C	3.63	1.47	1.39
21	A	828	CLA	C3B-C2B	3.63	1.45	1.40
21	A	822	CLA	O2D-CGD	3.63	1.42	1.33
21	B	832	CLA	MG-ND	-3.62	1.98	2.05
21	10	709	CLA	C3D-C2D	3.62	1.49	1.39
21	A	821	CLA	CHD-C4C	3.62	1.47	1.39
21	A	821	CLA	C3D-C2D	3.62	1.49	1.39
21	2	508	CLA	C1D-ND	3.62	1.42	1.37
21	A	840	CLA	C1C-NC	-3.62	1.32	1.37
21	8	604	CLA	O2A-CGA	3.62	1.43	1.33
21	A	838	CLA	O2A-CGA	3.62	1.43	1.33
21	A	817	CLA	C1C-NC	-3.61	1.32	1.37
21	5	702	CLA	C3D-C4D	-3.61	1.36	1.44
21	1	513	CLA	C3D-C2D	3.61	1.49	1.39
21	7	710	CLA	CHD-C1D	3.61	1.45	1.38
21	A	862	CLA	C3C-C2C	3.61	1.44	1.36
21	2	506	CLA	C3D-C2D	3.61	1.49	1.39
21	A	808	CLA	C1D-ND	3.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	603	CLA	C1B-NB	-3.61	1.32	1.35
21	A	821	CLA	C3B-C2B	3.61	1.45	1.40
21	B	825	CLA	C3D-C2D	3.61	1.49	1.39
21	B	818	CLA	OBD-CAD	3.61	1.28	1.22
21	F	403	CLA	O2D-CGD	3.61	1.42	1.33
24	A	851	BCR	C8-C9	-3.61	1.38	1.45
21	12	504	CLA	C3B-C2B	3.61	1.45	1.40
21	12	505	CLA	CHD-C4C	3.61	1.47	1.39
21	4	709	CLA	C3D-C2D	3.61	1.49	1.39
21	1	516	CLA	OBD-CAD	3.61	1.28	1.22
21	B	835	CLA	CHD-C1D	3.61	1.45	1.38
21	5	707	CLA	CHD-C4C	3.60	1.47	1.39
21	3	704	CLA	C3D-C4D	-3.60	1.36	1.44
21	A	813	CLA	C3B-C2B	3.60	1.45	1.40
21	11	709	CLA	OBD-CAD	3.60	1.28	1.22
21	A	811	CLA	O2D-CGD	3.60	1.42	1.33
21	5	706	CLA	CHD-C1D	3.60	1.45	1.38
21	B	821	CLA	C3D-C2D	3.60	1.48	1.39
21	11	708	CLA	C3D-C2D	3.60	1.48	1.39
21	1	515	CLA	C3D-C2D	3.60	1.48	1.39
21	B	812	CLA	O2D-CGD	3.60	1.42	1.33
21	7	710	CLA	C3B-C2B	3.60	1.45	1.40
21	1	509	CLA	C3D-C2D	3.59	1.48	1.39
21	A	803	CLA	CHD-C1D	3.59	1.45	1.38
21	4	706	CLA	C3D-C2D	3.59	1.48	1.39
21	3	710	CLA	OBD-CAD	3.59	1.28	1.22
21	1	507	CLA	OBD-CAD	3.59	1.28	1.22
21	F	401	CLA	O2D-CGD	3.59	1.42	1.33
21	B	825	CLA	C3D-C4D	-3.59	1.36	1.44
21	11	706	CLA	CHD-C4C	3.59	1.47	1.39
21	A	819	CLA	O2D-CGD	3.59	1.42	1.33
21	4	704	CLA	OBD-CAD	3.59	1.28	1.22
24	B	844	BCR	C21-C22	3.59	1.40	1.35
21	A	816	CLA	CHD-C4C	3.59	1.47	1.39
21	B	811	CLA	O2D-CGD	3.58	1.41	1.33
21	B	826	CLA	O2D-CGD	3.58	1.41	1.33
21	B	821	CLA	CHD-C4C	3.58	1.47	1.39
21	B	802	CLA	C3C-C2C	3.58	1.44	1.36
21	2	504	CLA	CHD-C1D	3.58	1.45	1.38
21	3	715	CLA	C3D-C2D	3.58	1.48	1.39
21	1	515	CLA	OBD-CAD	3.58	1.28	1.22
24	A	849	BCR	C19-C18	-3.58	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	613	CLA	CHD-C4C	3.58	1.47	1.39
21	4	710	CLA	C3D-C2D	3.58	1.48	1.39
21	B	809	CLA	CHD-C4C	3.58	1.47	1.39
21	7	703	CLA	CHD-C4C	3.57	1.47	1.39
21	F	401	CLA	OBD-CAD	3.57	1.28	1.22
21	F	404	CLA	CHD-C4C	3.57	1.47	1.39
21	4	711	CLA	C1D-ND	3.57	1.42	1.37
21	7	706	CLA	CHD-C4C	3.57	1.47	1.39
21	A	844	CLA	CHD-C4C	3.57	1.47	1.39
21	2	510	CLA	CHD-C4C	3.57	1.47	1.39
21	B	834	CLA	C1C-NC	-3.57	1.32	1.37
28	2	520	DD6	C10-C11	3.56	1.40	1.35
21	13	503	CLA	OBD-CAD	3.56	1.28	1.22
28	1	520	DD6	C10-C11	3.56	1.40	1.35
21	F	404	CLA	C3B-C2B	3.56	1.45	1.40
21	11	705	CLA	OBD-CAD	3.56	1.28	1.22
21	3	711	CLA	CHD-C4C	3.56	1.47	1.39
21	5	708	CLA	OBD-CAD	3.56	1.28	1.22
21	B	808	CLA	C4B-NB	-3.56	1.32	1.35
21	B	811	CLA	OBD-CAD	3.56	1.28	1.22
21	B	808	CLA	C3D-C4D	-3.56	1.36	1.44
21	2	508	CLA	CHD-C4C	3.56	1.47	1.39
21	1	509	CLA	CHD-C1D	3.56	1.45	1.38
21	B	818	CLA	C1D-ND	3.56	1.42	1.37
21	11	706	CLA	C1D-ND	3.56	1.42	1.37
21	6	907	CLA	C4C-C3C	3.56	1.51	1.45
28	3	717	DD6	C13-C14	3.55	1.40	1.32
21	8	607	CLA	C1D-ND	3.55	1.42	1.37
28	2	520	DD6	C5-C6	3.55	1.40	1.35
28	7	715	DD6	C10-C11	3.55	1.40	1.35
21	1	509	CLA	OBD-CAD	3.55	1.28	1.22
21	2	510	CLA	C1D-ND	3.55	1.42	1.37
21	A	835	CLA	CHD-C4C	3.55	1.47	1.39
21	A	824	CLA	CHD-C1D	3.55	1.45	1.38
28	8	616	DD6	C2-C1	3.55	1.40	1.35
21	A	843	CLA	OBD-CAD	3.55	1.28	1.22
21	3	702	CLA	C3D-C4D	-3.55	1.36	1.44
21	A	826	CLA	C3B-C2B	3.55	1.45	1.40
21	A	813	CLA	O2D-CGD	3.55	1.41	1.33
21	B	802	CLA	O2D-CGD	3.54	1.41	1.33
21	7	709	CLA	C3C-C2C	3.54	1.44	1.36
21	3	713	CLA	C3D-C2D	3.54	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	849	BCR	C17-C18	3.54	1.40	1.35
21	8	607	CLA	CHD-C1D	3.54	1.45	1.38
21	9	903	CLA	CHD-C1D	3.54	1.45	1.38
21	1	510	CLA	OBD-CAD	3.54	1.28	1.22
24	J	102	BCR	C12-C13	-3.54	1.38	1.45
21	F	403	CLA	CHD-C1D	3.54	1.45	1.38
21	B	814	CLA	C3C-C2C	3.54	1.44	1.36
21	A	817	CLA	C3B-C2B	3.54	1.45	1.40
21	A	862	CLA	C1C-NC	-3.54	1.32	1.37
21	1	513	CLA	CHD-C4C	3.54	1.47	1.39
21	7	708	CLA	CHD-C4C	3.54	1.47	1.39
21	6	909	CLA	C3D-C2D	3.54	1.48	1.39
21	B	806	CLA	C3C-C2C	3.54	1.44	1.36
21	5	706	CLA	C3D-C4D	-3.53	1.36	1.44
21	2	509	CLA	C3D-C2D	3.53	1.48	1.39
21	4	708	CLA	OBD-CAD	3.53	1.28	1.22
21	A	814	CLA	C3B-C2B	3.53	1.45	1.40
20	A	801	CL0	CHC-C1C	3.53	1.44	1.35
21	3	701	CLA	CHD-C1D	3.53	1.45	1.38
28	5	712	DD6	C24-C1	-3.53	1.38	1.45
21	8	610	CLA	C3D-C2D	3.53	1.48	1.39
21	B	836	CLA	O2D-CGD	3.53	1.41	1.33
21	7	706	CLA	C1D-ND	3.53	1.42	1.37
21	6	906	CLA	C1B-NB	-3.53	1.32	1.35
21	B	821	CLA	C3C-C2C	3.52	1.44	1.36
21	6	911	CLA	CHD-C4C	3.52	1.47	1.39
21	9	910	CLA	C3D-C2D	3.52	1.48	1.39
21	B	834	CLA	C3D-C4D	-3.52	1.36	1.44
21	F	404	CLA	C1D-ND	3.52	1.42	1.37
21	A	834	CLA	C3D-C4D	-3.52	1.36	1.44
21	2	505	CLA	C3C-C2C	3.52	1.44	1.36
21	B	824	CLA	C1C-NC	-3.52	1.32	1.37
21	3	702	CLA	CHC-C1C	3.52	1.44	1.35
21	1	513	CLA	C1D-ND	3.51	1.42	1.37
21	8	613	CLA	C3D-C2D	3.51	1.48	1.39
21	A	807	CLA	C3D-C2D	3.51	1.48	1.39
21	3	711	CLA	OBD-CAD	3.51	1.28	1.22
21	B	802	CLA	CBD-CGD	-3.51	1.41	1.52
21	12	505	CLA	C1B-NB	-3.51	1.32	1.35
21	A	839	CLA	C1D-ND	3.51	1.42	1.37
21	A	831	CLA	OBD-CAD	3.51	1.28	1.22
21	8	606	CLA	OBD-CAD	3.51	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	708	CLA	C3D-C2D	3.51	1.48	1.39
21	A	834	CLA	C3C-C2C	3.51	1.44	1.36
21	1	516	CLA	CHD-C4C	3.51	1.47	1.39
21	A	837	CLA	OBD-CAD	3.51	1.28	1.22
21	B	816	CLA	C2A-C1A	-3.50	1.44	1.52
21	7	710	CLA	C3C-C2C	3.50	1.44	1.36
21	B	826	CLA	C1B-NB	-3.50	1.32	1.35
21	A	823	CLA	C3C-C2C	3.50	1.44	1.36
21	9	904	CLA	C3D-C2D	3.50	1.48	1.39
24	B	842	BCR	C21-C22	3.50	1.40	1.35
21	6	908	CLA	C3D-C2D	3.50	1.48	1.39
21	1	508	CLA	CHD-C4C	3.50	1.47	1.39
21	B	837	CLA	C3D-C2D	3.50	1.48	1.39
21	1	501	CLA	CHD-C4C	3.49	1.47	1.39
21	11	702	CLA	CHD-C4C	3.49	1.47	1.39
24	B	846	BCR	C19-C18	-3.49	1.38	1.45
21	A	842	CLA	C3D-C2D	3.49	1.48	1.39
21	A	819	CLA	C3C-C2C	3.49	1.44	1.36
21	3	704	CLA	C4B-NB	-3.49	1.32	1.35
21	2	503	CLA	OBD-CAD	3.49	1.28	1.22
21	A	805	CLA	C1B-NB	-3.48	1.32	1.35
28	8	616	DD6	C5-C6	3.48	1.40	1.35
21	A	810	CLA	C1C-NC	-3.48	1.32	1.37
21	5	705	CLA	OBD-CAD	3.48	1.28	1.22
24	M	102	BCR	C19-C18	-3.48	1.38	1.45
21	A	826	CLA	CHD-C4C	3.48	1.47	1.39
21	11	710	CLA	C3D-C2D	3.48	1.48	1.39
21	10	710	CLA	OBD-CAD	3.48	1.28	1.22
21	9	912	CLA	CHD-C4C	3.48	1.47	1.39
21	A	811	CLA	C1B-NB	-3.48	1.32	1.35
21	11	709	CLA	C3D-C2D	3.47	1.48	1.39
21	11	708	CLA	CHD-C4C	3.47	1.47	1.39
21	3	709	CLA	C3B-C2B	3.47	1.45	1.40
21	8	608	CLA	C3D-C2D	3.47	1.48	1.39
21	B	804	CLA	CHD-C4C	3.47	1.47	1.39
21	A	826	CLA	O2D-CGD	3.47	1.41	1.33
21	B	837	CLA	CHD-C4C	3.47	1.47	1.39
21	A	838	CLA	C1D-ND	3.47	1.42	1.37
21	2	509	CLA	CHD-C4C	3.47	1.47	1.39
21	B	826	CLA	CHD-C1D	3.47	1.45	1.38
21	A	805	CLA	C1C-NC	-3.47	1.32	1.37
21	A	828	CLA	C3C-C2C	3.47	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	803	CLA	C3D-C4D	-3.47	1.36	1.44
21	A	836	CLA	C3C-C2C	3.47	1.44	1.36
21	2	509	CLA	CHD-C1D	3.46	1.45	1.38
24	F	405	BCR	C21-C22	3.46	1.40	1.35
21	A	835	CLA	OBD-CAD	3.46	1.28	1.22
21	6	910	CLA	OBD-CAD	3.46	1.28	1.22
24	A	849	BCR	C12-C13	-3.46	1.38	1.45
21	A	810	CLA	CHD-C4C	3.46	1.47	1.39
21	B	814	CLA	CHD-C4C	3.46	1.47	1.39
21	B	838	CLA	O2D-CGD	3.46	1.41	1.33
28	1	518	DD6	C5-C6	3.46	1.40	1.35
21	6	904	CLA	CHD-C4C	3.46	1.47	1.39
21	A	809	CLA	C3B-C2B	3.45	1.45	1.40
21	5	703	CLA	C1D-ND	3.45	1.42	1.37
21	6	908	CLA	CHD-C1D	3.45	1.45	1.38
21	5	701	CLA	CHD-C4C	3.45	1.47	1.39
21	A	817	CLA	CHD-C4C	3.45	1.47	1.39
21	4	709	CLA	OBD-CAD	3.45	1.28	1.22
21	A	838	CLA	O2D-CGD	3.45	1.41	1.33
21	B	816	CLA	CHD-C4C	3.45	1.47	1.39
21	B	818	CLA	O2D-CGD	3.45	1.41	1.33
21	B	815	CLA	C3D-C2D	3.45	1.48	1.39
24	A	848	BCR	C23-C22	-3.44	1.38	1.45
28	1	518	DD6	C10-C11	3.44	1.40	1.35
21	B	831	CLA	C3C-C2C	3.44	1.44	1.36
21	A	833	CLA	CHC-C1C	3.44	1.43	1.35
21	A	803	CLA	CHD-C4C	3.44	1.47	1.39
21	9	913	CLA	OBD-CAD	3.44	1.28	1.22
21	B	816	CLA	OBD-CAD	3.44	1.28	1.22
21	B	806	CLA	O2D-CGD	3.44	1.41	1.33
21	5	710	CLA	CHD-C4C	3.43	1.47	1.39
21	B	813	CLA	C3C-C2C	3.43	1.44	1.36
21	10	707	CLA	OBD-CAD	3.43	1.28	1.22
21	A	836	CLA	CHD-C1D	3.43	1.45	1.38
21	A	829	CLA	C3D-C4D	-3.43	1.36	1.44
21	A	813	CLA	CHD-C4C	3.43	1.47	1.39
21	A	811	CLA	C3D-C2D	3.43	1.48	1.39
24	M	102	BCR	C23-C22	-3.43	1.38	1.45
21	A	823	CLA	CHD-C4C	3.43	1.47	1.39
21	2	505	CLA	O2D-CGD	3.43	1.41	1.33
21	B	837	CLA	C3D-C4D	-3.43	1.36	1.44
21	6	905	CLA	CHD-C4C	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	706	CLA	CHD-C4C	3.43	1.47	1.39
21	10	711	CLA	OBD-CAD	3.42	1.28	1.22
21	B	834	CLA	O2D-CGD	3.42	1.41	1.33
24	J	102	BCR	C17-C18	3.42	1.40	1.35
21	7	707	CLA	CHD-C4C	3.42	1.47	1.39
21	8	609	CLA	OBD-CAD	3.42	1.28	1.22
21	B	808	CLA	CHD-C1D	3.42	1.45	1.38
21	2	503	CLA	C1B-NB	-3.42	1.32	1.35
21	2	509	CLA	C3D-C4D	-3.42	1.36	1.44
21	12	501	CLA	C3D-C2D	3.42	1.48	1.39
21	A	833	CLA	O2D-CGD	3.42	1.41	1.33
28	1	518	DD6	C2-C1	3.42	1.40	1.35
21	A	827	CLA	CHD-C4C	3.41	1.47	1.39
21	7	705	CLA	CHD-C1D	3.41	1.45	1.38
21	B	816	CLA	C3D-C2D	3.41	1.48	1.39
21	5	704	CLA	C3D-C2D	3.41	1.48	1.39
21	1	506	CLA	C3D-C4D	-3.41	1.36	1.44
21	B	822	CLA	C1C-C2C	3.41	1.51	1.44
24	B	845	BCR	C19-C18	-3.41	1.38	1.45
21	12	502	CLA	C3D-C2D	3.41	1.48	1.39
21	12	505	CLA	C1D-ND	3.41	1.42	1.37
21	A	827	CLA	OBD-CAD	3.41	1.28	1.22
21	2	503	CLA	C3D-C2D	3.41	1.48	1.39
21	4	702	CLA	CHD-C4C	3.41	1.47	1.39
21	B	808	CLA	OBD-CAD	3.40	1.28	1.22
28	2	520	DD6	C2-C1	3.40	1.40	1.35
21	1	517	CLA	CHD-C4C	3.40	1.47	1.39
21	8	607	CLA	C3D-C2D	3.40	1.48	1.39
21	B	833	CLA	C3D-C2D	3.40	1.48	1.39
28	7	716	DD6	C10-C11	3.40	1.40	1.35
21	B	832	CLA	CHD-C1D	3.40	1.45	1.38
21	A	805	CLA	CHD-C1D	3.40	1.45	1.38
21	A	811	CLA	OBD-CAD	3.40	1.28	1.22
24	F	402	BCR	C12-C13	-3.40	1.38	1.45
24	F	402	BCR	C21-C22	3.40	1.40	1.35
21	4	705	CLA	C3D-C2D	3.40	1.48	1.39
21	4	708	CLA	C3D-C2D	3.40	1.48	1.39
28	6	916	DD6	C8-C6	-3.39	1.38	1.45
21	B	815	CLA	CHD-C4C	3.39	1.47	1.39
21	B	805	CLA	C4B-NB	-3.39	1.32	1.35
21	13	503	CLA	C3D-C2D	3.39	1.48	1.39
21	6	908	CLA	OBD-CAD	3.39	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	904	CLA	C3D-C2D	3.39	1.48	1.39
21	8	603	CLA	C3D-C2D	3.39	1.48	1.39
21	5	701	CLA	C3D-C2D	3.39	1.48	1.39
21	B	838	CLA	C3B-C2B	3.38	1.45	1.40
21	A	838	CLA	CHD-C4C	3.38	1.47	1.39
21	8	603	CLA	CHD-C4C	3.38	1.46	1.39
21	5	702	CLA	CHD-C1D	3.38	1.44	1.38
21	A	837	CLA	C1C-NC	-3.38	1.32	1.37
24	F	402	BCR	C23-C22	-3.38	1.38	1.45
21	7	714	CLA	CHD-C1D	3.38	1.44	1.38
24	M	102	BCR	C14-C13	3.38	1.40	1.35
21	A	821	CLA	O2D-CGD	3.38	1.41	1.33
21	A	836	CLA	CHC-C1C	3.37	1.43	1.35
21	A	803	CLA	C3B-C2B	3.37	1.45	1.40
21	B	835	CLA	O2D-CGD	3.37	1.41	1.33
21	B	829	CLA	C1B-NB	-3.37	1.32	1.35
21	A	818	CLA	C3D-C2D	3.37	1.48	1.39
21	A	820	CLA	C1C-NC	-3.37	1.32	1.37
21	9	907	CLA	CHD-C1D	3.37	1.44	1.38
28	1	520	DD6	C5-C6	3.37	1.40	1.35
21	7	702	CLA	CHD-C1D	3.36	1.44	1.38
20	A	801	CL0	C2A-C1A	-3.36	1.44	1.52
21	11	701	CLA	C3D-C2D	3.36	1.48	1.39
21	A	831	CLA	C3B-C2B	3.36	1.45	1.40
21	7	703	CLA	C3D-C2D	3.36	1.48	1.39
21	B	824	CLA	CMB-C2B	-3.36	1.44	1.51
21	1	508	CLA	CHD-C1D	3.36	1.44	1.38
21	11	702	CLA	C3D-C2D	3.36	1.48	1.39
21	A	839	CLA	O2A-CGA	3.36	1.43	1.33
21	1	515	CLA	CHD-C1D	3.35	1.44	1.38
21	A	833	CLA	C3D-C2D	3.35	1.48	1.39
21	12	504	CLA	C3D-C2D	3.35	1.48	1.39
21	B	814	CLA	C1D-ND	3.35	1.41	1.37
21	B	833	CLA	C1C-NC	-3.35	1.32	1.37
28	5	712	DD6	C2-C1	3.35	1.40	1.35
21	A	812	CLA	C3C-C2C	3.35	1.43	1.36
21	1	515	CLA	C3D-C4D	-3.35	1.36	1.44
21	13	502	CLA	OBD-CAD	3.35	1.28	1.22
21	9	902	CLA	C1D-ND	3.35	1.41	1.37
21	7	707	CLA	CHD-C1D	3.35	1.44	1.38
21	7	712	CLA	CHD-C1D	3.35	1.44	1.38
28	8	616	DD6	C10-C11	3.35	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	905	CLA	C3D-C2D	3.34	1.48	1.39
21	A	822	CLA	C4B-NB	-3.34	1.32	1.35
21	12	502	CLA	C1B-NB	-3.34	1.32	1.35
20	A	801	CL0	CMB-C2B	-3.34	1.44	1.51
21	9	911	CLA	OBD-CAD	3.34	1.28	1.22
21	A	862	CLA	CHC-C1C	3.34	1.43	1.35
21	A	828	CLA	O2D-CGD	3.34	1.41	1.33
21	1	506	CLA	C1B-NB	-3.34	1.32	1.35
21	8	611	CLA	C3D-C2D	3.34	1.48	1.39
21	B	806	CLA	MG-ND	-3.33	1.99	2.05
21	6	909	CLA	C1D-ND	3.33	1.41	1.37
21	A	837	CLA	C3D-C2D	3.33	1.48	1.39
21	A	824	CLA	C1C-NC	-3.33	1.32	1.37
24	B	846	BCR	C12-C13	-3.33	1.38	1.45
21	2	503	CLA	C3D-C4D	-3.33	1.36	1.44
28	3	718	DD6	C26-C27	3.33	1.44	1.37
21	B	824	CLA	CHD-C4C	3.33	1.46	1.39
21	4	709	CLA	C1B-NB	-3.33	1.32	1.35
21	B	813	CLA	C3D-C4D	-3.33	1.36	1.44
21	A	802	CLA	CHC-C1C	3.33	1.43	1.35
21	2	515	CLA	C3D-C2D	3.32	1.48	1.39
21	4	705	CLA	CHD-C4C	3.32	1.46	1.39
21	1	501	CLA	C4B-NB	-3.31	1.32	1.35
21	A	830	CLA	C3D-C4D	-3.31	1.36	1.44
28	8	615	DD6	C10-C11	3.31	1.40	1.35
21	7	711	CLA	C1D-ND	3.31	1.41	1.37
21	3	704	CLA	CHD-C1D	3.31	1.44	1.38
21	6	907	CLA	CHD-C1D	3.31	1.44	1.38
21	A	815	CLA	C4B-NB	-3.31	1.32	1.35
21	3	715	CLA	C1B-NB	-3.31	1.32	1.35
21	A	836	CLA	C1B-NB	-3.31	1.32	1.35
21	A	815	CLA	CHD-C1D	3.31	1.44	1.38
21	12	504	CLA	OBD-CAD	3.31	1.28	1.22
21	B	825	CLA	O2D-CGD	3.30	1.41	1.33
21	B	813	CLA	C1C-NC	-3.30	1.32	1.37
28	6	916	DD6	C5-C6	3.30	1.40	1.35
21	8	610	CLA	CHD-C4C	3.30	1.46	1.39
21	12	502	CLA	CHD-C4C	3.30	1.46	1.39
21	B	829	CLA	CHD-C4C	3.30	1.46	1.39
21	7	713	CLA	OBD-CAD	3.30	1.28	1.22
21	7	708	CLA	C3B-C2B	3.30	1.44	1.40
21	7	707	CLA	C3D-C2D	3.30	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	907	CLA	C1B-NB	-3.30	1.32	1.35
21	8	607	CLA	OBD-CAD	3.29	1.28	1.22
21	A	862	CLA	C3B-C2B	3.29	1.44	1.40
21	5	709	CLA	C1C-C2C	3.29	1.50	1.44
21	3	707	CLA	OBD-CAD	3.29	1.28	1.22
21	5	702	CLA	C3C-C2C	3.29	1.43	1.36
21	1	517	CLA	C3D-C2D	3.29	1.48	1.39
21	A	842	CLA	C3C-C2C	3.29	1.43	1.36
21	A	814	CLA	C3D-C2D	3.29	1.48	1.39
21	2	517	CLA	C4C-C3C	3.29	1.50	1.45
21	8	603	CLA	OBD-CAD	3.29	1.28	1.22
21	7	702	CLA	C1C-NC	-3.28	1.32	1.37
21	B	814	CLA	C1C-NC	-3.28	1.32	1.37
21	2	504	CLA	C3D-C4D	-3.28	1.36	1.44
21	B	835	CLA	C1B-NB	-3.28	1.32	1.35
27	B	847	DGD	O1G-C1A	3.28	1.42	1.33
21	B	804	CLA	O2D-CGD	3.28	1.41	1.33
21	A	811	CLA	C3D-C4D	-3.28	1.36	1.44
21	B	815	CLA	C1B-NB	-3.28	1.32	1.35
21	A	814	CLA	C3C-C2C	3.28	1.43	1.36
21	8	611	CLA	C3D-C4D	-3.27	1.36	1.44
21	B	826	CLA	C1C-NC	-3.27	1.32	1.37
21	6	910	CLA	C3D-C2D	3.27	1.48	1.39
21	8	612	CLA	C1D-ND	3.27	1.41	1.37
21	7	704	CLA	C3D-C4D	-3.27	1.36	1.44
21	8	612	CLA	CHD-C1D	3.27	1.44	1.38
21	B	809	CLA	C3B-C2B	3.27	1.44	1.40
24	A	851	BCR	C19-C18	-3.26	1.38	1.45
21	8	614	CLA	C3D-C2D	3.26	1.48	1.39
21	A	820	CLA	C1D-ND	3.26	1.41	1.37
28	12	509	DD6	C5-C6	3.26	1.40	1.35
21	B	810	CLA	CHD-C4C	3.26	1.46	1.39
24	A	847	BCR	C12-C13	-3.26	1.38	1.45
21	4	701	CLA	C3D-C2D	3.26	1.48	1.39
21	B	838	CLA	CHC-C1C	3.26	1.43	1.35
21	A	802	CLA	CHD-C1D	3.26	1.44	1.38
21	B	835	CLA	C1D-ND	3.26	1.41	1.37
28	7	715	DD6	C5-C6	3.26	1.40	1.35
21	12	501	CLA	OBD-CAD	3.25	1.28	1.22
21	B	823	CLA	CHD-C4C	3.25	1.46	1.39
21	2	507	CLA	O2D-CGD	3.25	1.41	1.33
21	A	844	CLA	C1C-NC	-3.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	702	CLA	C1D-ND	3.25	1.41	1.37
21	A	804	CLA	C3C-C2C	3.25	1.43	1.36
21	B	831	CLA	CHD-C4C	3.25	1.46	1.39
21	A	823	CLA	OBD-CAD	3.25	1.28	1.22
21	A	838	CLA	OBD-CAD	3.25	1.28	1.22
21	11	705	CLA	C3D-C2D	3.24	1.48	1.39
21	A	832	CLA	CHD-C4C	3.24	1.46	1.39
21	B	822	CLA	C4B-NB	-3.24	1.32	1.35
21	3	703	CLA	C3D-C4D	-3.24	1.36	1.44
21	2	506	CLA	C1B-NB	-3.24	1.32	1.35
21	7	709	CLA	CHD-C4C	3.24	1.46	1.39
21	7	708	CLA	O2D-CGD	3.23	1.41	1.33
21	12	505	CLA	CHD-C1D	3.23	1.44	1.38
21	6	909	CLA	CHD-C4C	3.23	1.46	1.39
21	A	833	CLA	OBD-CAD	3.23	1.28	1.22
20	A	801	CL0	CBD-CGD	-3.23	1.42	1.52
21	F	403	CLA	C1B-CHB	3.23	1.50	1.41
21	7	704	CLA	CHD-C4C	3.23	1.46	1.39
22	B	840	PQN	C11-C3	-3.23	1.46	1.51
21	6	906	CLA	C3D-C2D	3.22	1.47	1.39
21	2	506	CLA	C1C-NC	-3.22	1.33	1.37
28	12	510	DD6	C8-C6	-3.22	1.39	1.45
21	B	803	CLA	C3B-C2B	3.22	1.44	1.40
21	3	709	CLA	C3D-C2D	3.22	1.47	1.39
21	B	801	CLA	CHD-C1D	3.22	1.44	1.38
21	A	822	CLA	C3D-C2D	3.22	1.47	1.39
21	3	712	CLA	OBD-CAD	3.22	1.28	1.22
28	3	718	DD6	C5-C6	3.22	1.40	1.35
21	1	515	CLA	C1D-ND	3.22	1.41	1.37
21	A	809	CLA	O2D-CGD	3.22	1.41	1.33
21	8	603	CLA	CHD-C1D	3.21	1.44	1.38
21	A	844	CLA	C3D-C2D	3.21	1.47	1.39
21	7	703	CLA	CHD-C1D	3.21	1.44	1.38
21	6	904	CLA	CHD-C1D	3.21	1.44	1.38
21	3	714	CLA	CHD-C4C	3.21	1.46	1.39
21	B	828	CLA	MG-ND	-3.21	1.99	2.05
21	A	832	CLA	CHD-C1D	3.21	1.44	1.38
21	A	808	CLA	C3D-C4D	-3.21	1.36	1.44
21	8	610	CLA	C1B-NB	-3.20	1.32	1.35
21	8	605	CLA	C3D-C2D	3.20	1.47	1.39
21	6	908	CLA	C3D-C4D	-3.20	1.36	1.44
21	1	508	CLA	C3B-C2B	3.20	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	505	CLA	CHD-C4C	3.20	1.46	1.39
21	A	803	CLA	C3D-C2D	3.20	1.47	1.39
21	9	904	CLA	OBD-CAD	3.20	1.28	1.22
21	3	705	CLA	C3D-C2D	3.20	1.47	1.39
21	A	840	CLA	CHD-C1D	3.20	1.44	1.38
21	3	711	CLA	C3D-C2D	3.19	1.47	1.39
21	A	835	CLA	C1D-ND	3.19	1.41	1.37
21	B	839	CLA	CHD-C1D	3.19	1.44	1.38
21	1	507	CLA	C1B-NB	-3.19	1.32	1.35
24	A	852	BCR	C21-C22	3.19	1.40	1.35
21	B	804	CLA	C1D-ND	3.19	1.41	1.37
21	B	804	CLA	C3D-C4D	-3.19	1.37	1.44
21	2	507	CLA	CHD-C4C	3.19	1.46	1.39
21	A	825	CLA	O2D-CGD	3.19	1.41	1.33
24	B	844	BCR	C8-C9	-3.19	1.39	1.45
21	B	825	CLA	C3B-C2B	3.19	1.44	1.40
24	A	848	BCR	C21-C22	3.18	1.40	1.35
24	B	841	BCR	C8-C9	-3.18	1.39	1.45
21	7	709	CLA	C3D-C2D	3.18	1.47	1.39
21	B	804	CLA	OBD-CAD	3.18	1.28	1.22
21	B	804	CLA	CMB-C2B	-3.18	1.45	1.51
21	B	818	CLA	C3D-C2D	3.18	1.47	1.39
24	A	851	BCR	C15-C14	-3.18	1.33	1.43
21	B	819	CLA	OBD-CAD	3.17	1.27	1.22
21	5	707	CLA	C3D-C2D	3.17	1.47	1.39
21	B	813	CLA	C3B-C2B	3.17	1.44	1.40
21	7	702	CLA	C1D-ND	3.17	1.41	1.37
21	B	806	CLA	C3D-C4D	-3.17	1.37	1.44
21	10	710	CLA	C1B-NB	-3.17	1.32	1.35
21	A	813	CLA	OBD-CAD	3.17	1.27	1.22
24	J	102	BCR	C21-C22	3.17	1.40	1.35
24	J	102	BCR	C23-C22	-3.17	1.39	1.45
21	7	706	CLA	C1B-NB	-3.17	1.32	1.35
21	9	908	CLA	OBD-CAD	3.17	1.27	1.22
21	B	805	CLA	C3D-C2D	3.17	1.47	1.39
21	3	702	CLA	CHD-C4C	3.17	1.46	1.39
24	A	850	BCR	C23-C22	-3.17	1.39	1.45
21	A	811	CLA	CHD-C1D	3.17	1.44	1.38
21	B	801	CLA	CAA-C2A	-3.17	1.48	1.54
21	8	608	CLA	OBD-CAD	3.17	1.27	1.22
21	3	704	CLA	C3D-C2D	3.17	1.47	1.39
28	6	915	DD6	C2-C1	3.16	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	828	CLA	OBD-CAD	3.16	1.27	1.22
27	B	847	DGD	O1G-C1G	-3.16	1.37	1.45
21	2	510	CLA	C1B-NB	-3.16	1.32	1.35
21	A	806	CLA	CMB-C2B	-3.16	1.45	1.51
21	B	835	CLA	CMC-C2C	-3.16	1.44	1.50
21	3	715	CLA	C3D-C4D	-3.16	1.37	1.44
21	7	713	CLA	C3D-C2D	3.16	1.47	1.39
28	7	715	DD6	C2-C1	3.15	1.40	1.35
21	1	505	CLA	OBD-CAD	3.15	1.27	1.22
21	B	804	CLA	C3C-C2C	3.15	1.43	1.36
21	7	714	CLA	OBD-CAD	3.15	1.27	1.22
21	B	831	CLA	CMD-C2D	-3.15	1.44	1.50
21	5	707	CLA	OBD-CAD	3.15	1.27	1.22
24	J	103	BCR	C19-C18	-3.15	1.39	1.45
21	B	801	CLA	O2D-CGD	3.15	1.40	1.33
21	A	862	CLA	C1D-ND	3.15	1.41	1.37
21	4	707	CLA	C3D-C2D	3.15	1.47	1.39
21	6	905	CLA	OBD-CAD	3.15	1.27	1.22
21	B	831	CLA	OBD-CAD	3.14	1.27	1.22
21	B	813	CLA	C1C-C2C	3.14	1.50	1.44
21	1	510	CLA	CHD-C1D	3.14	1.44	1.38
21	B	835	CLA	CHD-C4C	3.14	1.46	1.39
21	B	813	CLA	C4D-CHA	3.14	1.49	1.38
21	B	823	CLA	OBD-CAD	3.14	1.27	1.22
21	9	903	CLA	C4B-CHC	3.14	1.49	1.41
21	2	512	CLA	C1C-NC	-3.14	1.33	1.37
28	9	916	DD6	C26-C27	3.14	1.43	1.37
21	A	838	CLA	C3D-C4D	-3.14	1.37	1.44
21	1	505	CLA	C1B-NB	-3.14	1.32	1.35
21	A	806	CLA	CBD-CGD	-3.14	1.42	1.52
21	9	908	CLA	C3D-C2D	3.14	1.47	1.39
21	B	824	CLA	OBD-CAD	3.13	1.27	1.22
28	3	716	DD6	C8-C6	-3.13	1.39	1.45
21	A	809	CLA	CMC-C2C	-3.13	1.44	1.50
21	3	707	CLA	C1D-ND	3.13	1.41	1.37
21	2	510	CLA	C3D-C4D	-3.13	1.37	1.44
21	B	814	CLA	CHD-C1D	3.13	1.44	1.38
24	A	847	BCR	C21-C22	3.13	1.39	1.35
21	2	515	CLA	C3D-C4D	-3.13	1.37	1.44
21	A	802	CLA	C3D-C2D	3.13	1.47	1.39
21	A	843	CLA	C3D-C4D	-3.12	1.37	1.44
21	A	840	CLA	CMB-C2B	-3.12	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	824	CLA	C2A-C1A	-3.12	1.45	1.52
21	B	834	CLA	CHD-C1D	3.12	1.44	1.38
20	A	801	CL0	CMD-C2D	-3.12	1.44	1.50
21	A	825	CLA	C3D-C2D	3.12	1.47	1.39
28	4	712	DD6	C2-C1	3.12	1.39	1.35
21	B	839	CLA	C3D-C2D	3.12	1.47	1.39
21	A	836	CLA	C3D-C4D	-3.12	1.37	1.44
21	B	811	CLA	C3D-C2D	3.12	1.47	1.39
21	A	827	CLA	CBD-CGD	-3.12	1.42	1.52
21	3	714	CLA	OBD-CAD	3.11	1.27	1.22
21	A	813	CLA	MG-ND	-3.11	1.99	2.05
21	4	703	CLA	C3D-C2D	3.11	1.47	1.39
21	A	812	CLA	C3D-C4D	-3.11	1.37	1.44
21	1	515	CLA	C4B-CHC	3.11	1.49	1.41
24	B	844	BCR	C12-C13	-3.11	1.39	1.45
28	3	718	DD6	C2-C1	3.11	1.39	1.35
21	5	710	CLA	C1B-NB	-3.11	1.32	1.35
28	8	615	DD6	C5-C6	3.11	1.39	1.35
21	B	827	CLA	CHC-C1C	3.11	1.42	1.35
21	A	810	CLA	CHC-C1C	3.11	1.42	1.35
21	A	808	CLA	C3D-C2D	3.11	1.47	1.39
24	B	844	BCR	C19-C18	-3.11	1.39	1.45
21	A	844	CLA	C3D-C4D	-3.11	1.37	1.44
21	6	914	CLA	C3D-C2D	3.11	1.47	1.39
21	9	906	CLA	C4C-C3C	3.11	1.50	1.45
21	4	702	CLA	CHD-C1D	3.11	1.44	1.38
21	B	816	CLA	C3B-C2B	3.10	1.44	1.40
21	A	833	CLA	CHD-C4C	3.10	1.46	1.39
21	3	707	CLA	C1B-NB	-3.10	1.32	1.35
21	A	816	CLA	C4B-NB	-3.10	1.32	1.35
24	M	102	BCR	C15-C14	-3.10	1.33	1.43
21	B	828	CLA	CHD-C4C	3.10	1.46	1.39
21	4	705	CLA	OBD-CAD	3.10	1.27	1.22
21	B	828	CLA	C3D-C2D	3.10	1.47	1.39
21	5	710	CLA	CBA-CGA	3.10	1.59	1.50
28	4	713	DD6	C26-C27	3.10	1.43	1.37
21	B	823	CLA	CHD-C1D	3.10	1.44	1.38
21	B	805	CLA	C3B-C2B	3.10	1.44	1.40
21	1	516	CLA	C1C-NC	-3.10	1.33	1.37
21	A	805	CLA	O2D-CGD	3.09	1.40	1.33
21	A	840	CLA	O2D-CGD	3.09	1.40	1.33
21	B	817	CLA	CHD-C1D	3.09	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	842	CLA	O2D-CGD	3.09	1.40	1.33
21	4	711	CLA	C3D-C2D	3.09	1.47	1.39
21	5	706	CLA	CHD-C4C	3.09	1.46	1.39
21	A	807	CLA	C1D-ND	3.09	1.41	1.37
21	A	813	CLA	C3C-C2C	3.09	1.43	1.36
24	F	402	BCR	C16-C17	-3.09	1.33	1.43
21	2	514	CLA	C1C-NC	-3.09	1.33	1.37
21	B	803	CLA	O2D-CGD	3.09	1.40	1.33
21	1	501	CLA	C3D-C2D	3.09	1.47	1.39
21	7	714	CLA	C3D-C2D	3.09	1.47	1.39
21	7	712	CLA	CHD-C4C	3.08	1.46	1.39
21	8	605	CLA	OBD-CAD	3.08	1.27	1.22
21	A	812	CLA	C4D-CHA	3.08	1.49	1.38
21	B	812	CLA	CHD-C4C	3.08	1.46	1.39
21	1	507	CLA	C3D-C4D	-3.08	1.37	1.44
28	8	615	DD6	C2-C1	3.08	1.39	1.35
21	A	803	CLA	OBD-CAD	3.08	1.27	1.22
21	2	515	CLA	CHD-C4C	3.08	1.46	1.39
21	7	713	CLA	C1B-NB	-3.08	1.32	1.35
21	B	835	CLA	C1C-NC	-3.08	1.33	1.37
21	A	862	CLA	MG-ND	-3.08	1.99	2.05
21	B	817	CLA	C3B-C2B	3.08	1.44	1.40
24	B	846	BCR	C10-C9	3.07	1.39	1.35
21	B	817	CLA	O2A-CGA	3.07	1.42	1.33
21	A	815	CLA	C1C-NC	-3.07	1.33	1.37
21	A	807	CLA	C3D-C4D	-3.07	1.37	1.44
21	3	705	CLA	C1D-ND	3.07	1.41	1.37
22	B	840	PQN	C10-C5	3.07	1.45	1.40
21	4	711	CLA	C3D-C4D	-3.07	1.37	1.44
21	B	824	CLA	C4D-CHA	3.07	1.49	1.38
21	8	606	CLA	CHD-C4C	3.07	1.46	1.39
21	7	708	CLA	C1D-ND	3.07	1.41	1.37
21	A	828	CLA	MG-ND	-3.07	1.99	2.05
21	2	504	CLA	CHD-C4C	3.07	1.46	1.39
24	B	844	BCR	C23-C22	-3.06	1.39	1.45
24	B	845	BCR	C21-C22	3.06	1.39	1.35
21	B	808	CLA	O2D-CGD	3.06	1.40	1.33
28	4	712	DD6	C10-C11	3.06	1.39	1.35
21	B	803	CLA	C3D-C2D	3.06	1.47	1.39
21	7	713	CLA	C3D-C4D	-3.06	1.37	1.44
21	9	910	CLA	C1C-C2C	3.06	1.50	1.44
21	A	810	CLA	C3D-C2D	3.06	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	836	CLA	C1C-NC	-3.06	1.33	1.37
21	B	830	CLA	OBD-CAD	3.06	1.27	1.22
21	A	825	CLA	CHD-C1D	3.06	1.44	1.38
21	2	516	CLA	C3D-C2D	3.06	1.47	1.39
21	A	839	CLA	C1B-NB	-3.06	1.32	1.35
24	B	842	BCR	C8-C9	-3.06	1.39	1.45
21	B	821	CLA	OBD-CAD	3.05	1.27	1.22
21	B	831	CLA	O2D-CGD	3.05	1.40	1.33
21	B	805	CLA	CHD-C4C	3.05	1.46	1.39
21	F	401	CLA	C3D-C2D	3.05	1.47	1.39
21	2	516	CLA	C1C-C2C	3.05	1.50	1.44
21	B	822	CLA	C3D-C2D	3.05	1.47	1.39
21	7	707	CLA	C3D-C4D	-3.05	1.37	1.44
21	A	807	CLA	C4D-CHA	3.05	1.49	1.38
21	B	838	CLA	C3C-C2C	3.04	1.43	1.36
21	B	817	CLA	C1D-ND	3.04	1.41	1.37
21	9	910	CLA	OBD-CAD	3.04	1.27	1.22
21	B	813	CLA	C1D-ND	3.04	1.41	1.37
21	11	702	CLA	OBD-CAD	3.04	1.27	1.22
21	11	706	CLA	C3D-C4D	-3.04	1.37	1.44
21	4	703	CLA	OBD-CAD	3.04	1.27	1.22
21	7	712	CLA	OBD-CAD	3.04	1.27	1.22
24	A	850	BCR	C12-C13	-3.04	1.39	1.45
21	2	509	CLA	C3C-C2C	3.04	1.43	1.36
21	A	821	CLA	O2A-C1	-3.04	1.37	1.46
21	4	711	CLA	C1B-NB	-3.04	1.32	1.35
21	A	835	CLA	MG-ND	-3.04	1.99	2.05
24	A	850	BCR	C10-C9	3.04	1.39	1.35
21	B	825	CLA	CHD-C1D	3.03	1.44	1.38
21	A	805	CLA	C4B-NB	-3.03	1.32	1.35
21	13	501	CLA	OBD-CAD	3.03	1.27	1.22
21	8	604	CLA	CHD-C4C	3.03	1.46	1.39
21	12	506	CLA	C4B-CHC	3.03	1.49	1.41
21	A	813	CLA	C1B-NB	-3.03	1.32	1.35
21	7	710	CLA	C3D-C4D	-3.03	1.37	1.44
21	9	904	CLA	C3D-C4D	-3.03	1.37	1.44
28	3	716	DD6	C5-C6	3.03	1.39	1.35
21	5	702	CLA	C3D-C2D	3.03	1.47	1.39
21	B	836	CLA	C3D-C4D	-3.03	1.37	1.44
28	3	717	DD6	C9-C10	-3.02	1.34	1.43
21	A	809	CLA	C4B-NB	-3.02	1.32	1.35
21	5	703	CLA	C1B-NB	-3.02	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	908	CLA	C1C-NC	-3.02	1.33	1.37
28	3	717	DD6	C24-C1	-3.02	1.39	1.45
21	A	805	CLA	C3D-C2D	3.02	1.47	1.39
21	9	907	CLA	C3D-C2D	3.02	1.47	1.39
21	11	706	CLA	C1B-NB	-3.02	1.32	1.35
21	A	818	CLA	CHD-C1D	3.02	1.44	1.38
21	B	814	CLA	O2D-CGD	3.02	1.40	1.33
21	5	703	CLA	MG-ND	-3.02	1.99	2.05
21	B	819	CLA	C3D-C2D	3.02	1.47	1.39
21	A	828	CLA	C4D-ND	-3.01	1.33	1.37
21	A	814	CLA	C1B-NB	-3.01	1.32	1.35
21	6	911	CLA	OBD-CAD	3.01	1.27	1.22
21	3	703	CLA	C4D-CHA	3.01	1.49	1.38
21	A	834	CLA	C3B-C2B	3.01	1.44	1.40
21	3	714	CLA	C4B-NB	-3.00	1.32	1.35
21	3	712	CLA	C1C-C2C	3.00	1.50	1.44
21	1	506	CLA	C3D-C2D	3.00	1.47	1.39
21	2	504	CLA	C3D-C2D	3.00	1.47	1.39
21	2	509	CLA	C1C-NC	-3.00	1.33	1.37
21	1	506	CLA	C3B-C2B	3.00	1.44	1.40
21	A	805	CLA	C3C-C2C	3.00	1.43	1.36
21	3	707	CLA	CHD-C1D	3.00	1.44	1.38
24	B	841	BCR	C21-C22	3.00	1.39	1.35
21	9	910	CLA	CHD-C1D	3.00	1.44	1.38
24	A	849	BCR	C21-C22	3.00	1.39	1.35
21	3	704	CLA	OBD-CAD	3.00	1.27	1.22
21	A	841	CLA	O2D-CGD	2.99	1.40	1.33
21	A	821	CLA	C3C-C2C	2.99	1.43	1.36
21	B	837	CLA	C1C-NC	-2.99	1.33	1.37
21	5	704	CLA	C1D-ND	2.99	1.41	1.37
21	A	826	CLA	C1D-ND	2.99	1.41	1.37
21	9	909	CLA	C1B-NB	-2.99	1.32	1.35
21	A	818	CLA	OBD-CAD	2.99	1.27	1.22
21	11	706	CLA	OBD-CAD	2.99	1.27	1.22
21	9	909	CLA	OBD-CAD	2.98	1.27	1.22
21	1	508	CLA	C4C-C3C	2.98	1.50	1.45
21	B	806	CLA	OBD-CAD	2.98	1.27	1.22
28	4	712	DD6	C5-C6	2.98	1.39	1.35
21	4	702	CLA	C1B-NB	-2.98	1.32	1.35
21	1	513	CLA	C1B-NB	-2.98	1.32	1.35
21	B	804	CLA	CHD-C1D	2.98	1.44	1.38
28	1	519	DD6	C10-C11	2.98	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	704	CLA	C4D-CHA	2.98	1.49	1.38
21	A	830	CLA	C3D-C2D	2.98	1.47	1.39
21	10	703	CLA	C3D-C4D	-2.98	1.37	1.44
28	8	615	DD6	C8-C6	-2.98	1.39	1.45
21	A	812	CLA	OBD-CAD	2.97	1.27	1.22
21	A	828	CLA	OBD-CAD	2.97	1.27	1.22
21	7	706	CLA	C3B-C2B	2.97	1.44	1.40
21	B	810	CLA	C3D-C4D	-2.97	1.37	1.44
21	A	825	CLA	C1D-ND	2.97	1.41	1.37
21	B	833	CLA	OBD-CAD	2.97	1.27	1.22
21	A	831	CLA	MG-ND	-2.97	1.99	2.05
21	6	909	CLA	OBD-CAD	2.96	1.27	1.22
28	7	716	DD6	C26-C27	2.96	1.43	1.37
21	A	839	CLA	C3D-C2D	2.96	1.47	1.39
21	B	822	CLA	C4C-C3C	2.96	1.50	1.45
21	11	703	CLA	C3C-C2C	2.96	1.43	1.36
21	B	812	CLA	OBD-CAD	2.96	1.27	1.22
21	B	809	CLA	CHD-C1D	2.96	1.44	1.38
21	6	911	CLA	C3D-C4D	-2.96	1.37	1.44
21	7	705	CLA	OBD-CAD	2.96	1.27	1.22
24	J	102	BCR	C19-C18	-2.96	1.39	1.45
28	1	520	DD6	C26-C27	2.96	1.43	1.37
21	11	702	CLA	C1B-NB	-2.96	1.32	1.35
28	1	519	DD6	C26-C27	2.95	1.43	1.37
21	A	818	CLA	C3C-C2C	2.95	1.43	1.36
21	B	817	CLA	C1B-CHB	2.95	1.49	1.41
21	A	827	CLA	C3D-C4D	-2.95	1.37	1.44
21	7	706	CLA	C4C-C3C	2.95	1.50	1.45
21	A	836	CLA	CBD-CGD	-2.95	1.43	1.52
21	8	604	CLA	C4B-CHC	2.95	1.49	1.41
24	F	402	BCR	C8-C9	-2.95	1.39	1.45
21	9	910	CLA	C4C-C3C	2.95	1.50	1.45
21	11	705	CLA	C4C-C3C	2.95	1.50	1.45
28	8	616	DD6	C26-C27	2.95	1.43	1.37
21	3	714	CLA	C1C-C2C	2.95	1.50	1.44
28	7	716	DD6	C5-C6	2.95	1.39	1.35
21	7	711	CLA	C3D-C4D	-2.95	1.37	1.44
24	A	850	BCR	C8-C9	-2.94	1.39	1.45
21	B	809	CLA	C1C-C2C	2.94	1.50	1.44
21	A	824	CLA	C1B-NB	-2.94	1.32	1.35
28	12	510	DD6	C26-C27	2.94	1.43	1.37
21	A	825	CLA	C3C-C2C	2.94	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	911	CLA	C3D-C4D	-2.94	1.37	1.44
21	B	801	CLA	CHD-C4C	2.94	1.45	1.39
28	3	717	DD6	C10-C11	2.94	1.39	1.35
24	B	842	BCR	C23-C22	-2.94	1.39	1.45
21	5	703	CLA	C3D-C2D	2.93	1.47	1.39
21	A	803	CLA	CBD-CGD	-2.93	1.43	1.52
21	2	511	CLA	OBD-CAD	2.93	1.27	1.22
21	B	836	CLA	CHC-C1C	2.93	1.42	1.35
21	A	842	CLA	C3D-C4D	-2.93	1.37	1.44
21	B	816	CLA	C1C-NC	-2.93	1.33	1.37
21	7	708	CLA	C3D-C2D	2.93	1.47	1.39
21	B	828	CLA	C1C-NC	-2.93	1.33	1.37
21	A	840	CLA	CHD-C4C	2.92	1.45	1.39
21	A	822	CLA	C1C-NC	-2.92	1.33	1.37
21	A	820	CLA	C4C-C3C	2.92	1.50	1.45
21	7	702	CLA	C3D-C2D	2.92	1.47	1.39
21	A	833	CLA	CHD-C1D	2.92	1.44	1.38
21	B	814	CLA	OBD-CAD	2.92	1.27	1.22
21	1	508	CLA	C3D-C4D	-2.92	1.37	1.44
24	A	847	BCR	C19-C18	-2.92	1.39	1.45
21	A	817	CLA	C3D-C4D	-2.92	1.37	1.44
21	A	825	CLA	C1B-NB	-2.92	1.32	1.35
28	3	716	DD6	C2-C1	2.92	1.39	1.35
21	5	705	CLA	C3D-C4D	-2.92	1.37	1.44
20	A	801	CL0	C3C-C2C	2.92	1.42	1.36
21	A	820	CLA	O2A-CGA	2.92	1.41	1.33
21	A	834	CLA	C1C-C2C	2.92	1.50	1.44
21	A	841	CLA	C1D-ND	2.92	1.41	1.37
21	7	703	CLA	OBD-CAD	2.91	1.27	1.22
28	7	716	DD6	C8-C6	-2.91	1.39	1.45
24	B	844	BCR	C10-C9	2.91	1.39	1.35
21	B	815	CLA	C3D-C4D	-2.91	1.37	1.44
21	3	709	CLA	CHD-C4C	2.91	1.45	1.39
24	A	852	BCR	C23-C22	-2.91	1.39	1.45
21	A	838	CLA	CBD-CGD	-2.91	1.43	1.52
28	J	104	DD6	C26-C27	2.91	1.43	1.37
28	12	509	DD6	C26-C27	2.91	1.43	1.37
21	3	715	CLA	OBD-CAD	2.91	1.27	1.22
21	3	702	CLA	C4B-CHC	2.90	1.49	1.41
28	12	510	DD6	C24-C1	-2.90	1.39	1.45
28	7	716	DD6	C36-C31	-2.90	1.31	1.34
21	2	507	CLA	CHD-C1D	2.90	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	845	BCR	C10-C9	2.90	1.39	1.35
21	7	705	CLA	C3D-C4D	-2.90	1.37	1.44
21	A	809	CLA	C1C-NC	-2.90	1.33	1.37
21	B	828	CLA	C3B-C2B	2.90	1.44	1.40
21	A	829	CLA	C3D-C2D	2.90	1.47	1.39
21	B	837	CLA	OBD-CAD	2.90	1.27	1.22
21	7	712	CLA	C3D-C4D	-2.89	1.37	1.44
24	M	102	BCR	C11-C10	-2.89	1.34	1.43
21	9	906	CLA	C3D-C4D	-2.89	1.37	1.44
21	B	825	CLA	C2A-C1A	-2.89	1.45	1.52
28	2	519	DD6	C10-C11	2.89	1.39	1.35
21	12	502	CLA	OBD-CAD	2.89	1.27	1.22
21	2	516	CLA	CAA-C2A	-2.89	1.48	1.54
21	2	510	CLA	C1C-NC	-2.89	1.33	1.37
24	F	405	BCR	C12-C13	-2.89	1.39	1.45
21	F	404	CLA	OBD-CAD	2.89	1.27	1.22
21	2	512	CLA	OBD-CAD	2.89	1.27	1.22
21	B	838	CLA	C1C-NC	-2.88	1.33	1.37
21	1	512	CLA	OBD-CAD	2.88	1.27	1.22
21	B	829	CLA	C3D-C4D	-2.88	1.37	1.44
21	B	807	CLA	O2D-CGD	2.88	1.40	1.33
24	A	848	BCR	C19-C18	-2.88	1.39	1.45
21	B	801	CLA	C1C-NC	-2.88	1.33	1.37
21	A	806	CLA	C3D-C2D	2.88	1.47	1.39
24	A	848	BCR	C8-C9	-2.88	1.39	1.45
21	6	910	CLA	C1B-NB	-2.88	1.32	1.35
28	6	916	DD6	C10-C11	2.87	1.39	1.35
21	10	703	CLA	C1B-NB	-2.87	1.32	1.35
21	F	401	CLA	C1C-NC	-2.87	1.33	1.37
21	2	512	CLA	C4B-NB	-2.87	1.32	1.35
21	2	507	CLA	C3D-C2D	2.87	1.46	1.39
21	A	810	CLA	C3D-C4D	-2.87	1.37	1.44
21	8	604	CLA	C3D-C4D	-2.87	1.37	1.44
21	B	827	CLA	C2-C3	2.87	1.39	1.33
21	A	824	CLA	C3D-C4D	-2.87	1.37	1.44
21	7	708	CLA	C4B-CHC	2.86	1.49	1.41
28	1	519	DD6	C8-C6	-2.86	1.39	1.45
21	A	820	CLA	CHD-C1D	2.86	1.43	1.38
21	12	505	CLA	OBD-CAD	2.86	1.27	1.22
21	B	813	CLA	C1B-NB	-2.86	1.32	1.35
21	B	832	CLA	OBD-CAD	2.86	1.27	1.22
21	3	702	CLA	C1C-NC	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	11	712	DD6	C26-C27	2.86	1.43	1.37
21	A	813	CLA	C3D-C4D	-2.85	1.37	1.44
24	A	850	BCR	C19-C18	-2.85	1.39	1.45
21	B	804	CLA	C2A-C1A	-2.85	1.45	1.52
21	B	822	CLA	MG-ND	-2.85	2.00	2.05
21	A	841	CLA	C3D-C4D	-2.85	1.37	1.44
21	11	706	CLA	CHD-C1D	2.85	1.43	1.38
21	6	907	CLA	C1C-C2C	2.85	1.50	1.44
21	7	708	CLA	OBD-CAD	2.85	1.27	1.22
21	1	505	CLA	C3D-C4D	-2.85	1.37	1.44
21	B	807	CLA	CHD-C4C	2.85	1.45	1.39
21	6	910	CLA	C3D-C4D	-2.85	1.37	1.44
24	B	846	BCR	C8-C9	-2.85	1.39	1.45
28	5	713	DD6	C9-C10	-2.85	1.34	1.43
21	B	802	CLA	O2A-CGA	2.85	1.41	1.33
21	B	803	CLA	OBD-CAD	2.85	1.27	1.22
21	11	708	CLA	C1B-NB	-2.84	1.32	1.35
21	A	830	CLA	C4D-CHA	2.84	1.48	1.38
21	2	516	CLA	MG-ND	-2.84	2.00	2.05
21	2	515	CLA	C3B-C2B	2.84	1.44	1.40
28	5	712	DD6	C10-C11	2.84	1.39	1.35
21	7	705	CLA	C3D-C2D	2.84	1.46	1.39
24	J	103	BCR	C12-C13	-2.84	1.39	1.45
21	4	702	CLA	C3D-C4D	-2.84	1.37	1.44
21	2	506	CLA	C3D-C4D	-2.84	1.37	1.44
21	8	610	CLA	OBD-CAD	2.84	1.27	1.22
21	7	712	CLA	C4B-CHC	2.84	1.48	1.41
21	6	905	CLA	MG-ND	-2.84	2.00	2.05
21	B	801	CLA	C4B-NB	-2.84	1.32	1.35
21	5	702	CLA	C4B-CHC	2.84	1.48	1.41
21	7	707	CLA	C1B-NB	-2.84	1.32	1.35
21	A	862	CLA	CHD-C1D	2.84	1.43	1.38
21	B	826	CLA	C1D-ND	2.84	1.41	1.37
21	8	606	CLA	C1C-C2C	2.83	1.50	1.44
28	5	713	DD6	C26-C27	2.83	1.42	1.37
21	3	708	CLA	C1B-NB	-2.83	1.32	1.35
21	B	802	CLA	C4B-CHC	2.83	1.48	1.41
21	A	816	CLA	C4D-CHA	2.83	1.48	1.38
21	8	604	CLA	C1D-ND	2.83	1.41	1.37
21	B	814	CLA	C1C-C2C	2.83	1.50	1.44
21	B	819	CLA	C1C-C2C	2.83	1.50	1.44
21	7	714	CLA	C1B-NB	-2.83	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	707	CLA	C1B-NB	-2.83	1.32	1.35
24	F	402	BCR	C10-C9	2.83	1.39	1.35
21	7	709	CLA	C3B-C2B	2.83	1.44	1.40
21	A	823	CLA	CHD-C1D	2.83	1.43	1.38
21	2	506	CLA	OBD-CAD	2.83	1.27	1.22
21	6	906	CLA	C3D-C4D	-2.83	1.37	1.44
21	3	710	CLA	C1C-NC	-2.83	1.33	1.37
21	A	831	CLA	C3D-C4D	-2.82	1.37	1.44
21	B	812	CLA	C1B-NB	-2.82	1.32	1.35
21	13	502	CLA	C4C-C3C	2.82	1.49	1.45
24	B	844	BCR	C16-C17	-2.82	1.34	1.43
21	A	833	CLA	C3D-C4D	-2.82	1.37	1.44
28	5	712	DD6	C8-C6	-2.82	1.39	1.45
21	A	839	CLA	C3D-C4D	-2.82	1.37	1.44
21	A	839	CLA	CHD-C4C	2.82	1.45	1.39
21	A	819	CLA	CHD-C1D	2.82	1.43	1.38
21	4	706	CLA	C3D-C4D	-2.82	1.37	1.44
20	A	801	CL0	C1C-NC	-2.81	1.33	1.37
24	B	841	BCR	C23-C22	-2.81	1.39	1.45
21	A	836	CLA	CHD-C4C	2.81	1.45	1.39
28	3	718	DD6	C13-C11	-2.81	1.39	1.45
21	A	827	CLA	C1C-NC	-2.81	1.33	1.37
21	A	802	CLA	C1D-ND	2.81	1.41	1.37
21	8	614	CLA	C4C-C3C	2.81	1.49	1.45
21	2	509	CLA	C1B-NB	-2.81	1.32	1.35
21	A	807	CLA	CHD-C4C	2.81	1.45	1.39
21	A	824	CLA	C3B-C2B	2.81	1.44	1.40
21	A	808	CLA	C4B-CHC	2.81	1.48	1.41
21	B	807	CLA	CHD-C1D	2.80	1.43	1.38
21	B	839	CLA	OBD-CAD	2.80	1.27	1.22
21	1	513	CLA	C1B-CHB	2.80	1.48	1.41
21	B	812	CLA	C3D-C4D	-2.80	1.37	1.44
21	A	809	CLA	C3D-C2D	2.80	1.46	1.39
21	2	512	CLA	C1B-CHB	2.80	1.48	1.41
21	A	819	CLA	C3D-C4D	-2.80	1.37	1.44
21	B	801	CLA	MG-NA	-2.80	1.99	2.06
21	B	832	CLA	C3D-C4D	-2.80	1.37	1.44
28	2	519	DD6	C13-C11	-2.80	1.39	1.45
28	2	520	DD6	C26-C27	2.80	1.42	1.37
21	1	510	CLA	CHD-C4C	2.79	1.45	1.39
21	6	907	CLA	C3D-C2D	2.79	1.46	1.39
21	4	706	CLA	OBD-CAD	2.79	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	706	CLA	C4C-C3C	2.79	1.49	1.45
21	A	827	CLA	C4B-CHC	2.79	1.48	1.41
21	7	705	CLA	CHD-C4C	2.79	1.45	1.39
21	B	822	CLA	C1D-ND	2.79	1.41	1.37
21	B	807	CLA	C3B-C2B	2.79	1.44	1.40
21	7	703	CLA	C4B-CHC	2.79	1.48	1.41
28	4	712	DD6	C24-C1	-2.79	1.40	1.45
21	B	836	CLA	C4C-C3C	2.79	1.49	1.45
21	J	101	CLA	C3D-C4D	-2.79	1.37	1.44
21	2	507	CLA	C3D-C4D	-2.79	1.37	1.44
21	A	809	CLA	C1D-ND	2.79	1.41	1.37
24	A	851	BCR	C11-C10	-2.79	1.34	1.43
21	A	828	CLA	C1C-NC	-2.79	1.33	1.37
21	3	711	CLA	C3D-C4D	-2.78	1.37	1.44
28	8	615	DD6	C24-C1	-2.78	1.40	1.45
24	B	846	BCR	C21-C22	2.78	1.39	1.35
21	A	825	CLA	CMB-C2B	-2.78	1.45	1.51
28	5	712	DD6	C25-C26	-2.78	1.34	1.43
21	12	502	CLA	C3D-C4D	-2.78	1.37	1.44
21	A	820	CLA	OBD-CAD	2.78	1.27	1.22
21	A	822	CLA	OBD-CAD	2.78	1.27	1.22
21	A	832	CLA	C3D-C2D	2.78	1.46	1.39
21	12	502	CLA	C4D-CHA	2.78	1.48	1.38
21	3	704	CLA	CHD-C4C	2.78	1.45	1.39
21	B	839	CLA	C1B-CHB	2.78	1.48	1.41
21	A	841	CLA	CBD-CGD	-2.78	1.43	1.52
21	A	808	CLA	C1B-NB	-2.78	1.32	1.35
21	A	844	CLA	C1D-ND	2.78	1.41	1.37
21	B	835	CLA	C3C-C2C	2.77	1.42	1.36
24	F	405	BCR	C14-C13	2.77	1.39	1.35
21	F	403	CLA	C4D-CHA	2.77	1.48	1.38
21	A	814	CLA	C1D-C2D	-2.77	1.39	1.45
28	9	915	DD6	C26-C27	2.77	1.42	1.37
21	A	837	CLA	C3D-C4D	-2.77	1.37	1.44
21	A	817	CLA	C1D-ND	2.77	1.41	1.37
28	11	712	DD6	C10-C11	2.77	1.39	1.35
21	A	826	CLA	C1B-CHB	2.77	1.48	1.41
21	B	826	CLA	C4B-NB	-2.77	1.32	1.35
21	8	612	CLA	C3D-C4D	-2.77	1.37	1.44
21	9	908	CLA	C1B-NB	-2.77	1.32	1.35
21	A	827	CLA	C2A-C1A	-2.77	1.46	1.52
28	1	519	DD6	C24-C1	-2.76	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	822	CLA	CHD-C4C	2.76	1.45	1.39
24	M	102	BCR	C12-C13	-2.76	1.40	1.45
28	7	715	DD6	C24-C1	-2.76	1.40	1.45
21	A	831	CLA	C4B-NB	-2.76	1.32	1.35
21	2	517	CLA	C1C-C2C	2.76	1.49	1.44
21	2	508	CLA	C3B-C2B	2.76	1.44	1.40
21	B	821	CLA	C3D-C4D	-2.76	1.37	1.44
21	8	610	CLA	C3D-C4D	-2.76	1.37	1.44
21	B	832	CLA	O2D-CGD	2.76	1.39	1.33
21	A	843	CLA	C1C-NC	-2.76	1.33	1.37
24	B	846	BCR	C23-C22	-2.76	1.40	1.45
21	11	703	CLA	C3D-C4D	-2.76	1.38	1.44
21	B	809	CLA	C3D-C2D	2.76	1.46	1.39
21	A	813	CLA	C4D-CHA	2.76	1.48	1.38
24	A	848	BCR	C12-C13	-2.75	1.40	1.45
21	1	514	CLA	C4D-CHA	2.75	1.48	1.38
21	A	816	CLA	C1D-ND	2.75	1.41	1.37
21	A	813	CLA	CMC-C2C	-2.75	1.45	1.50
21	7	702	CLA	CHD-C4C	2.75	1.45	1.39
21	A	821	CLA	O2A-CGA	2.75	1.41	1.33
28	11	713	DD6	C26-C27	2.75	1.42	1.37
21	B	824	CLA	O2D-CGD	2.75	1.39	1.33
21	1	512	CLA	C4D-CHA	2.75	1.48	1.38
21	B	832	CLA	C3B-C2B	2.75	1.44	1.40
21	J	101	CLA	C1C-NC	-2.75	1.33	1.37
21	B	802	CLA	C3B-C2B	2.75	1.44	1.40
21	12	507	CLA	C4C-C3C	2.75	1.49	1.45
21	1	510	CLA	C3D-C4D	-2.75	1.38	1.44
21	B	820	CLA	C1B-CHB	2.75	1.48	1.41
21	B	802	CLA	C3D-C2D	2.74	1.46	1.39
21	8	609	CLA	C3D-C4D	-2.74	1.38	1.44
21	A	862	CLA	C3D-C2D	2.74	1.46	1.39
21	B	830	CLA	C3D-C2D	2.74	1.46	1.39
24	J	103	BCR	C21-C22	2.74	1.39	1.35
21	5	703	CLA	CHD-C4C	2.74	1.45	1.39
21	B	820	CLA	C1C-NC	-2.74	1.33	1.37
21	3	703	CLA	C3D-C2D	2.74	1.46	1.39
21	11	709	CLA	C4C-C3C	2.74	1.49	1.45
21	11	711	CLA	C4B-CHC	2.74	1.48	1.41
24	B	846	BCR	C17-C18	2.74	1.39	1.35
21	2	514	CLA	C4B-NB	-2.74	1.32	1.35
21	B	811	CLA	CHD-C4C	2.74	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	101	CLA	CMD-C2D	-2.74	1.45	1.50
28	7	715	DD6	C26-C27	2.74	1.42	1.37
21	1	504	CLA	C3D-C4D	-2.74	1.38	1.44
21	8	605	CLA	C4D-CHA	2.74	1.48	1.38
28	11	713	DD6	C24-C1	-2.74	1.40	1.45
21	A	816	CLA	CHC-C1C	2.74	1.42	1.35
21	1	508	CLA	C3D-C2D	2.74	1.46	1.39
21	11	707	CLA	C4C-C3C	2.74	1.49	1.45
21	9	905	CLA	C1C-C2C	2.73	1.49	1.44
21	1	507	CLA	C4B-NB	-2.73	1.32	1.35
21	11	704	CLA	C1B-NB	-2.73	1.32	1.35
24	B	841	BCR	C16-C17	-2.73	1.35	1.43
21	11	707	CLA	C3D-C4D	-2.73	1.38	1.44
21	4	707	CLA	C4B-CHC	2.73	1.48	1.41
21	B	818	CLA	C4B-CHC	2.73	1.48	1.41
21	B	804	CLA	C3D-C2D	2.73	1.46	1.39
21	B	807	CLA	C4B-NB	-2.73	1.32	1.35
21	6	912	CLA	C3D-C4D	-2.72	1.38	1.44
21	A	821	CLA	C3D-C4D	-2.72	1.38	1.44
21	B	820	CLA	CHD-C1D	2.72	1.43	1.38
21	5	704	CLA	C3D-C4D	-2.72	1.38	1.44
28	8	616	DD6	C13-C11	-2.72	1.40	1.45
21	A	817	CLA	CHD-C1D	2.72	1.43	1.38
21	6	912	CLA	C1B-NB	-2.72	1.32	1.35
28	1	518	DD6	C26-C27	2.72	1.42	1.37
21	A	830	CLA	C4B-NB	-2.72	1.32	1.35
21	A	825	CLA	C4D-CHA	2.71	1.48	1.38
21	2	514	CLA	C4D-CHA	2.71	1.48	1.38
21	11	706	CLA	C1B-CHB	2.71	1.48	1.41
21	7	707	CLA	C1B-CHB	2.71	1.48	1.41
21	10	707	CLA	C4B-CHC	2.71	1.48	1.41
21	8	608	CLA	C1B-NB	-2.71	1.32	1.35
21	A	802	CLA	O2D-CGD	2.71	1.39	1.33
24	J	102	BCR	C2-C3	-2.71	1.45	1.52
21	A	826	CLA	C4D-CHA	2.71	1.48	1.38
21	2	514	CLA	C1C-C2C	2.71	1.49	1.44
21	A	802	CLA	C4B-NB	-2.71	1.32	1.35
21	8	603	CLA	C3D-C4D	-2.71	1.38	1.44
21	B	827	CLA	C3C-C2C	2.71	1.42	1.36
21	2	511	CLA	C4B-CHC	2.71	1.48	1.41
21	F	404	CLA	C4C-C3C	2.71	1.49	1.45
21	7	703	CLA	CBD-CGD	-2.71	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	706	CLA	C1C-NC	-2.70	1.33	1.37
21	B	836	CLA	C3D-C2D	2.70	1.46	1.39
21	B	830	CLA	C4B-CHC	2.70	1.48	1.41
21	A	836	CLA	C3D-C2D	2.70	1.46	1.39
21	5	710	CLA	C1C-NC	-2.70	1.33	1.37
21	8	610	CLA	C1C-NC	-2.70	1.33	1.37
21	A	817	CLA	OBD-CAD	2.70	1.27	1.22
21	1	507	CLA	C1B-CHB	2.70	1.48	1.41
21	A	817	CLA	CBD-CGD	-2.70	1.44	1.52
21	A	832	CLA	C3B-C2B	2.70	1.44	1.40
21	B	810	CLA	C1D-ND	2.70	1.41	1.37
21	2	516	CLA	C4D-CHA	2.70	1.48	1.38
21	12	501	CLA	C4B-CHC	2.70	1.48	1.41
28	8	616	DD6	C8-C6	-2.70	1.40	1.45
21	A	842	CLA	C3B-C2B	2.69	1.44	1.40
21	9	902	CLA	C1C-C2C	2.69	1.49	1.44
21	8	614	CLA	C1B-NB	-2.69	1.32	1.35
21	B	803	CLA	C1C-NC	-2.69	1.33	1.37
21	8	614	CLA	C3D-C4D	-2.69	1.38	1.44
21	12	501	CLA	C3D-C4D	-2.69	1.38	1.44
22	B	840	PQN	C2-C1	-2.69	1.42	1.48
21	A	834	CLA	CHD-C4C	2.69	1.45	1.39
21	B	820	CLA	C4B-CHC	2.69	1.48	1.41
21	3	712	CLA	C4B-NB	-2.69	1.32	1.35
21	B	822	CLA	OBD-CAD	2.69	1.27	1.22
21	A	835	CLA	C1B-NB	-2.69	1.32	1.35
21	B	807	CLA	C4B-CHC	2.69	1.48	1.41
21	11	705	CLA	C1B-NB	-2.68	1.32	1.35
21	12	508	CLA	C4C-C3C	2.68	1.49	1.45
21	A	825	CLA	C3B-C2B	2.68	1.44	1.40
21	A	842	CLA	C1C-NC	-2.68	1.33	1.37
21	2	508	CLA	C3D-C2D	2.68	1.46	1.39
28	9	915	DD6	C24-C1	-2.68	1.40	1.45
28	2	520	DD6	C8-C6	-2.68	1.40	1.45
21	A	823	CLA	C3D-C2D	2.67	1.46	1.39
21	B	817	CLA	C1B-NB	-2.67	1.32	1.35
21	A	820	CLA	C1C-C2C	2.67	1.49	1.44
28	7	715	DD6	C8-C6	-2.67	1.40	1.45
21	2	517	CLA	C4D-CHA	2.67	1.47	1.38
21	7	709	CLA	C4D-CHA	2.67	1.47	1.38
21	A	830	CLA	CAA-C2A	-2.67	1.49	1.54
21	A	832	CLA	C4D-CHA	2.67	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	10	710	CLA	C4B-CHC	2.67	1.48	1.41
21	A	816	CLA	CMB-C2B	-2.67	1.46	1.51
21	7	713	CLA	C1C-NC	-2.66	1.33	1.37
21	2	503	CLA	C4B-CHC	2.66	1.48	1.41
21	8	614	CLA	C4D-CHA	2.66	1.47	1.38
21	B	836	CLA	CHD-C1D	2.66	1.43	1.38
21	3	705	CLA	C3D-C4D	-2.66	1.38	1.44
21	12	504	CLA	C4D-CHA	2.66	1.47	1.38
21	F	403	CLA	C4B-CHC	2.66	1.48	1.41
21	7	709	CLA	C4C-C3C	2.66	1.49	1.45
21	3	704	CLA	C1C-NC	-2.66	1.33	1.37
21	A	813	CLA	C1D-ND	2.66	1.41	1.37
24	A	851	BCR	C21-C22	2.66	1.39	1.35
21	A	804	CLA	C3D-C2D	2.66	1.46	1.39
21	3	704	CLA	C1B-NB	-2.66	1.32	1.35
21	A	841	CLA	C3D-C2D	2.66	1.46	1.39
21	F	404	CLA	C3D-C4D	-2.66	1.38	1.44
21	B	809	CLA	C4B-CHC	2.66	1.48	1.41
21	A	821	CLA	C1B-CHB	2.66	1.48	1.41
21	12	507	CLA	C4D-CHA	2.65	1.47	1.38
21	A	822	CLA	CBD-CGD	-2.65	1.44	1.52
21	9	912	CLA	C4D-CHA	2.65	1.47	1.38
21	A	806	CLA	C1B-CHB	2.65	1.48	1.41
21	1	504	CLA	C4D-CHA	2.65	1.47	1.38
21	B	815	CLA	MG-ND	-2.65	2.00	2.05
21	A	834	CLA	C4D-CHA	2.65	1.47	1.38
21	6	909	CLA	C4B-CHC	2.65	1.48	1.41
21	8	613	CLA	C4D-CHA	2.65	1.47	1.38
21	13	503	CLA	C1B-NB	-2.65	1.32	1.35
21	11	704	CLA	C3D-C4D	-2.65	1.38	1.44
21	A	862	CLA	CHD-C4C	2.65	1.45	1.39
21	B	817	CLA	O2D-CGD	2.65	1.39	1.33
21	4	705	CLA	C1B-CHB	2.64	1.48	1.41
21	7	710	CLA	C4D-CHA	2.64	1.47	1.38
28	5	713	DD6	C8-C6	-2.64	1.40	1.45
21	A	812	CLA	C1C-NC	-2.64	1.33	1.37
24	M	102	BCR	C21-C22	2.64	1.39	1.35
24	A	850	BCR	C17-C18	2.64	1.39	1.35
21	7	711	CLA	C1C-NC	-2.64	1.33	1.37
21	A	831	CLA	CHD-C4C	2.64	1.45	1.39
21	9	903	CLA	C1C-C2C	2.64	1.49	1.44
21	13	503	CLA	C4C-C3C	2.64	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	821	CLA	CHD-C1D	2.64	1.43	1.38
21	4	707	CLA	C3D-C4D	-2.64	1.38	1.44
28	3	716	DD6	C10-C11	2.64	1.39	1.35
21	F	401	CLA	C3C-C2C	2.64	1.42	1.36
21	8	611	CLA	OBD-CAD	2.64	1.27	1.22
21	6	913	CLA	C3D-C4D	-2.64	1.38	1.44
21	B	819	CLA	C1B-NB	-2.64	1.32	1.35
21	A	838	CLA	CMB-C2B	-2.64	1.46	1.51
21	6	911	CLA	C4B-CHC	2.64	1.48	1.41
28	4	712	DD6	C36-C31	-2.64	1.32	1.34
21	3	712	CLA	C1C-NC	-2.64	1.33	1.37
21	A	841	CLA	C4D-CHA	2.63	1.47	1.38
21	2	505	CLA	C1B-CHB	2.63	1.48	1.41
21	1	513	CLA	C1C-NC	-2.63	1.33	1.37
21	5	711	CLA	C4C-C3C	2.63	1.49	1.45
21	A	862	CLA	C1B-NB	-2.63	1.32	1.35
21	B	820	CLA	C4B-NB	-2.63	1.32	1.35
21	B	829	CLA	C4D-CHA	2.63	1.47	1.38
28	3	716	DD6	C26-C27	2.63	1.42	1.37
21	12	505	CLA	C4C-C3C	2.63	1.49	1.45
21	A	829	CLA	C4B-CHC	2.63	1.48	1.41
21	11	705	CLA	C4B-CHC	2.63	1.48	1.41
21	B	827	CLA	CMD-C2D	-2.63	1.45	1.50
21	A	803	CLA	MG-ND	-2.63	2.00	2.05
21	3	701	CLA	C4D-CHA	2.63	1.47	1.38
21	B	838	CLA	CHD-C4C	2.63	1.45	1.39
21	B	807	CLA	MG-ND	-2.63	2.00	2.05
21	9	904	CLA	C1B-CHB	2.63	1.48	1.41
21	9	914	CLA	C4B-CHC	2.63	1.48	1.41
21	2	515	CLA	C1D-ND	2.63	1.41	1.37
20	A	801	CL0	MG-ND	-2.63	2.00	2.05
24	A	847	BCR	C11-C10	-2.62	1.35	1.43
21	4	709	CLA	C3D-C4D	-2.62	1.38	1.44
21	2	507	CLA	CBD-CGD	-2.62	1.44	1.52
21	1	509	CLA	C3D-C4D	-2.62	1.38	1.44
21	8	613	CLA	C3D-C4D	-2.62	1.38	1.44
21	2	505	CLA	C3B-C2B	2.62	1.44	1.40
21	B	816	CLA	CHD-C1D	2.62	1.43	1.38
21	3	710	CLA	C4D-CHA	2.62	1.47	1.38
21	3	707	CLA	CHD-C4C	2.62	1.45	1.39
21	A	829	CLA	C1B-NB	-2.62	1.32	1.35
21	11	710	CLA	C1B-NB	-2.62	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	801	CLA	C3C-C2C	2.62	1.42	1.36
24	A	847	BCR	C8-C9	-2.62	1.40	1.45
21	A	802	CLA	C3D-C4D	-2.62	1.38	1.44
21	A	835	CLA	CMD-C2D	-2.62	1.45	1.50
21	10	704	CLA	C4B-CHC	2.62	1.48	1.41
28	1	520	DD6	C13-C11	-2.62	1.40	1.45
28	1	518	DD6	C24-C1	-2.61	1.40	1.45
21	A	842	CLA	C1C-C2C	2.61	1.49	1.44
21	8	612	CLA	C4C-C3C	2.61	1.49	1.45
27	B	847	DGD	O5D-C1E	2.61	1.44	1.40
21	B	811	CLA	C1C-NC	-2.61	1.33	1.37
21	13	503	CLA	C3D-C4D	-2.61	1.38	1.44
21	5	709	CLA	C4D-CHA	2.61	1.47	1.38
21	5	704	CLA	C4D-CHA	2.61	1.47	1.38
21	A	862	CLA	CBD-CGD	-2.61	1.44	1.52
21	B	833	CLA	CAA-C2A	-2.61	1.49	1.54
21	11	701	CLA	C1B-NB	-2.61	1.32	1.35
21	B	807	CLA	C3C-C2C	2.61	1.42	1.36
21	A	809	CLA	C3C-C2C	2.60	1.42	1.36
21	12	505	CLA	C3D-C4D	-2.60	1.38	1.44
21	10	708	CLA	C1B-NB	-2.60	1.32	1.35
21	8	607	CLA	C3D-C4D	-2.60	1.38	1.44
21	A	839	CLA	C4D-CHA	2.60	1.47	1.38
21	B	827	CLA	C3B-C2B	2.60	1.44	1.40
21	5	711	CLA	C4B-CHC	2.60	1.48	1.41
21	13	501	CLA	C3D-C4D	-2.60	1.38	1.44
21	B	819	CLA	C1C-NC	-2.60	1.33	1.37
21	A	829	CLA	CHD-C4C	2.60	1.45	1.39
21	8	609	CLA	C4C-C3C	2.60	1.49	1.45
28	6	915	DD6	C24-C1	-2.60	1.40	1.45
21	6	905	CLA	C1C-NC	-2.60	1.33	1.37
21	4	705	CLA	C4B-CHC	2.60	1.48	1.41
21	B	818	CLA	C4D-CHA	2.60	1.47	1.38
21	B	808	CLA	C1D-ND	2.59	1.41	1.37
21	1	501	CLA	C1B-CHB	2.59	1.48	1.41
21	9	905	CLA	C4D-CHA	2.59	1.47	1.38
20	A	801	CL0	C4D-CHA	2.59	1.47	1.38
21	B	835	CLA	C3B-C2B	2.59	1.44	1.40
21	A	831	CLA	CAA-C2A	-2.59	1.49	1.54
21	B	832	CLA	CHD-C4C	2.59	1.45	1.39
21	B	839	CLA	C1C-NC	-2.59	1.33	1.37
21	F	403	CLA	C3B-C2B	2.59	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	904	CLA	C4C-C3C	2.59	1.49	1.45
21	12	508	CLA	C4D-CHA	2.59	1.47	1.38
21	9	914	CLA	C4D-CHA	2.59	1.47	1.38
21	2	513	CLA	C4D-CHA	2.59	1.47	1.38
21	11	702	CLA	C3D-C4D	-2.59	1.38	1.44
28	2	520	DD6	C13-C11	-2.59	1.40	1.45
21	B	834	CLA	C3B-C2B	2.59	1.44	1.40
21	A	841	CLA	C4B-NB	-2.59	1.32	1.35
21	1	501	CLA	CBD-CGD	-2.59	1.44	1.52
21	3	709	CLA	C4D-CHA	2.58	1.47	1.38
21	5	706	CLA	C1D-ND	2.58	1.41	1.37
21	B	822	CLA	CHD-C1D	2.58	1.43	1.38
21	3	712	CLA	C1B-CHB	2.58	1.48	1.41
21	7	706	CLA	C1C-C2C	2.58	1.49	1.44
21	F	403	CLA	C3D-C4D	-2.58	1.38	1.44
21	B	826	CLA	C3D-C2D	2.58	1.46	1.39
21	11	703	CLA	C4D-CHA	2.58	1.47	1.38
21	10	712	CLA	C1B-CHB	2.58	1.48	1.41
21	11	709	CLA	C4D-CHA	2.58	1.47	1.38
21	3	706	CLA	OBD-CAD	2.58	1.26	1.22
28	2	519	DD6	C24-C1	-2.58	1.40	1.45
21	B	823	CLA	C4B-CHC	2.58	1.48	1.41
21	1	508	CLA	C4B-CHC	2.58	1.48	1.41
21	2	516	CLA	OBD-CAD	2.58	1.26	1.22
21	10	705	CLA	C4C-C3C	2.58	1.49	1.45
21	11	711	CLA	C4D-CHA	2.58	1.47	1.38
28	2	518	DD6	C24-C1	-2.58	1.40	1.45
21	B	808	CLA	C2A-C1A	-2.58	1.46	1.52
21	3	712	CLA	C3D-C4D	-2.58	1.38	1.44
21	2	507	CLA	C4B-NB	-2.58	1.32	1.35
21	9	911	CLA	C1B-NB	-2.58	1.32	1.35
21	11	701	CLA	C3A-C2A	-2.58	1.52	1.54
21	A	824	CLA	MG-ND	-2.58	2.00	2.05
28	3	718	DD6	C8-C6	-2.58	1.40	1.45
28	8	615	DD6	C13-C11	-2.58	1.40	1.45
21	B	803	CLA	C4B-CHC	2.58	1.48	1.41
21	2	513	CLA	C1C-C2C	2.58	1.49	1.44
21	A	802	CLA	CHD-C4C	2.58	1.45	1.39
28	2	519	DD6	C26-C27	2.57	1.42	1.37
21	B	804	CLA	C1C-NC	-2.57	1.34	1.37
21	6	904	CLA	C4D-CHA	2.57	1.47	1.38
21	8	608	CLA	C4B-CHC	2.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	705	CLA	C1B-CHB	2.57	1.48	1.41
21	A	826	CLA	C3D-C2D	2.57	1.46	1.39
20	A	801	CL0	C4D-ND	2.57	1.41	1.37
21	2	512	CLA	C1C-C2C	2.57	1.49	1.44
21	B	836	CLA	MG-ND	-2.57	2.00	2.05
21	B	804	CLA	C1B-NB	-2.57	1.32	1.35
21	10	707	CLA	C4D-CHA	2.57	1.47	1.38
21	3	706	CLA	C4D-CHA	2.57	1.47	1.38
21	7	704	CLA	OBD-CAD	2.57	1.26	1.22
21	4	706	CLA	C4D-CHA	2.57	1.47	1.38
28	1	520	DD6	C8-C6	-2.57	1.40	1.45
28	1	518	DD6	C8-C6	-2.57	1.40	1.45
21	6	909	CLA	C1D-C2D	2.57	1.50	1.45
21	7	706	CLA	C3D-C4D	-2.57	1.38	1.44
21	A	831	CLA	C3D-C2D	2.57	1.46	1.39
21	12	504	CLA	C1B-NB	-2.57	1.32	1.35
21	10	709	CLA	C4D-CHA	2.57	1.47	1.38
21	1	507	CLA	C4D-CHA	2.56	1.47	1.38
21	B	826	CLA	CBD-CGD	-2.56	1.44	1.52
21	11	703	CLA	C1C-C2C	2.56	1.49	1.44
21	A	843	CLA	CHD-C4C	2.56	1.45	1.39
24	F	405	BCR	C16-C17	-2.56	1.35	1.43
20	A	801	CL0	C3A-C2A	-2.56	1.47	1.54
21	5	701	CLA	C1C-NC	-2.56	1.34	1.37
21	8	606	CLA	C1B-CHB	2.56	1.48	1.41
21	11	709	CLA	C1B-NB	-2.56	1.32	1.35
21	2	511	CLA	C1C-C2C	2.56	1.49	1.44
21	2	514	CLA	C3D-C4D	-2.56	1.38	1.44
21	6	908	CLA	MG-ND	-2.56	2.00	2.05
21	B	815	CLA	C1B-CHB	2.56	1.48	1.41
21	1	506	CLA	C4D-CHA	2.56	1.47	1.38
21	2	514	CLA	C3D-C2D	2.56	1.46	1.39
21	B	817	CLA	CMD-C2D	-2.56	1.45	1.50
21	3	714	CLA	C4D-CHA	2.56	1.47	1.38
28	6	916	DD6	C26-C27	2.56	1.42	1.37
21	A	862	CLA	CMB-C2B	-2.56	1.46	1.51
21	B	813	CLA	C2A-C1A	-2.56	1.46	1.52
21	B	830	CLA	C3D-C4D	-2.56	1.38	1.44
21	A	829	CLA	C1C-NC	-2.56	1.34	1.37
21	3	713	CLA	C4C-C3C	2.56	1.49	1.45
21	B	839	CLA	C4C-C3C	2.56	1.49	1.45
24	B	846	BCR	C36-C18	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	819	CLA	C3D-C2D	2.55	1.46	1.39
21	9	914	CLA	C4C-C3C	2.55	1.49	1.45
21	B	808	CLA	C4D-CHA	2.55	1.47	1.38
21	B	812	CLA	C1C-NC	-2.55	1.34	1.37
21	B	803	CLA	CHD-C4C	2.55	1.45	1.39
21	B	821	CLA	C1B-CHB	2.55	1.48	1.41
21	3	709	CLA	C1B-NB	-2.55	1.32	1.35
21	3	707	CLA	C4D-CHA	2.55	1.47	1.38
21	2	507	CLA	C4D-CHA	2.55	1.47	1.38
21	9	910	CLA	C3D-C4D	-2.55	1.38	1.44
21	A	805	CLA	C4B-CHC	2.55	1.48	1.41
21	2	517	CLA	C4B-CHC	2.55	1.48	1.41
21	7	705	CLA	C1C-NC	-2.55	1.34	1.37
21	4	710	CLA	C4D-CHA	2.55	1.47	1.38
21	A	807	CLA	MG-ND	-2.55	2.00	2.05
21	9	910	CLA	C4D-CHA	2.55	1.47	1.38
21	B	825	CLA	C1B-CHB	2.55	1.48	1.41
21	A	806	CLA	C2A-C1A	-2.55	1.46	1.52
21	7	713	CLA	C4D-CHA	2.54	1.47	1.38
24	B	843	BCR	C8-C9	-2.54	1.40	1.45
21	B	827	CLA	C1C-C2C	2.54	1.49	1.44
21	6	913	CLA	C4B-CHC	2.54	1.48	1.41
21	A	835	CLA	C4C-C3C	2.54	1.49	1.45
21	10	706	CLA	C4C-C3C	2.54	1.49	1.45
21	12	504	CLA	C4C-C3C	2.54	1.49	1.45
21	A	836	CLA	OBD-CAD	2.54	1.26	1.22
21	3	706	CLA	C3D-C4D	-2.54	1.38	1.44
28	J	104	DD6	C24-C1	-2.54	1.40	1.45
21	2	503	CLA	CHD-C1D	2.54	1.43	1.38
21	2	505	CLA	C3D-C4D	-2.54	1.38	1.44
21	5	709	CLA	C3D-C4D	-2.54	1.38	1.44
21	11	705	CLA	C1C-C2C	2.54	1.49	1.44
21	6	910	CLA	C1C-NC	-2.54	1.34	1.37
24	B	841	BCR	C12-C13	-2.54	1.40	1.45
21	6	903	CLA	C4C-C3C	2.54	1.49	1.45
21	B	812	CLA	MG-ND	-2.54	2.00	2.05
28	2	520	DD6	C24-C1	-2.53	1.40	1.45
21	7	704	CLA	C3D-C2D	2.53	1.46	1.39
21	10	706	CLA	C1C-C2C	2.53	1.49	1.44
21	A	802	CLA	C3C-C2C	2.53	1.42	1.36
21	1	517	CLA	CAA-C2A	-2.53	1.49	1.54
21	5	709	CLA	C4C-C3C	2.53	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	520	DD6	C24-C1	-2.53	1.40	1.45
21	A	823	CLA	C3D-C4D	-2.53	1.38	1.44
21	A	805	CLA	CBD-CGD	-2.53	1.44	1.52
21	3	703	CLA	C1B-NB	-2.53	1.33	1.35
21	9	904	CLA	C4D-CHA	2.53	1.47	1.38
21	10	711	CLA	C4B-CHC	2.53	1.48	1.41
24	F	405	BCR	C19-C18	-2.53	1.40	1.45
21	10	711	CLA	C3D-C4D	-2.53	1.38	1.44
21	A	823	CLA	C2A-C1A	-2.52	1.46	1.52
21	12	503	CLA	C3D-C4D	-2.52	1.38	1.44
21	8	605	CLA	C1B-CHB	2.52	1.48	1.41
21	3	701	CLA	C3D-C4D	-2.52	1.38	1.44
21	A	813	CLA	C4B-NB	2.52	1.37	1.35
21	B	804	CLA	C1C-C2C	2.52	1.49	1.44
21	B	803	CLA	CBD-CGD	-2.52	1.44	1.52
21	7	708	CLA	C4D-CHA	2.52	1.47	1.38
21	4	708	CLA	C4D-CHA	2.52	1.47	1.38
21	9	907	CLA	C3D-C4D	-2.52	1.38	1.44
21	A	817	CLA	CMB-C2B	-2.52	1.46	1.51
24	J	102	BCR	C8-C9	-2.52	1.40	1.45
21	4	704	CLA	C3D-C4D	-2.52	1.38	1.44
28	5	712	DD6	C13-C11	-2.52	1.40	1.45
21	11	711	CLA	C1C-C2C	2.52	1.49	1.44
21	B	825	CLA	C4B-NB	-2.52	1.33	1.35
21	A	812	CLA	O2D-CGD	2.52	1.39	1.33
28	8	615	DD6	C26-C27	2.52	1.42	1.37
21	A	840	CLA	C3C-C2C	2.52	1.42	1.36
21	9	909	CLA	C4B-CHC	2.52	1.48	1.41
21	7	712	CLA	C1B-CHB	2.52	1.48	1.41
21	10	703	CLA	C3A-C2A	-2.51	1.52	1.54
21	A	844	CLA	CHD-C1D	2.51	1.43	1.38
21	A	820	CLA	C3D-C4D	-2.51	1.38	1.44
21	3	714	CLA	C1C-NC	-2.51	1.34	1.37
21	A	836	CLA	C1D-ND	2.51	1.40	1.37
21	1	511	CLA	C3D-C4D	-2.51	1.38	1.44
21	2	510	CLA	C4B-CHC	2.51	1.48	1.41
21	B	831	CLA	C3B-C2B	2.51	1.43	1.40
21	A	829	CLA	O2D-CGD	2.51	1.39	1.33
21	B	809	CLA	C3C-C2C	2.51	1.42	1.36
21	13	502	CLA	C4D-CHA	2.51	1.47	1.38
21	6	904	CLA	C1B-NB	-2.51	1.33	1.35
21	B	807	CLA	C2A-C1A	-2.51	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	843	CLA	MG-ND	-2.51	2.00	2.05
21	10	709	CLA	C3D-C4D	-2.50	1.38	1.44
21	B	829	CLA	C2A-C1A	-2.50	1.46	1.52
21	B	808	CLA	C3D-C2D	2.50	1.45	1.39
21	B	820	CLA	C3D-C4D	-2.50	1.38	1.44
21	B	823	CLA	C4C-C3C	2.50	1.49	1.45
21	2	509	CLA	C4B-NB	-2.50	1.33	1.35
21	B	827	CLA	CAA-C2A	-2.50	1.49	1.54
21	1	516	CLA	C3D-C4D	-2.50	1.38	1.44
21	9	911	CLA	C4D-CHA	2.50	1.47	1.38
21	B	829	CLA	CHD-C1D	2.50	1.43	1.38
24	B	842	BCR	C19-C18	-2.50	1.40	1.45
21	B	839	CLA	C3D-C4D	-2.50	1.38	1.44
21	1	510	CLA	C4B-CHC	2.49	1.47	1.41
21	A	820	CLA	CBD-CGD	-2.49	1.44	1.52
21	9	905	CLA	C1B-CHB	2.49	1.47	1.41
21	1	508	CLA	C4D-CHA	2.49	1.47	1.38
21	6	905	CLA	C1B-NB	-2.49	1.33	1.35
28	4	712	DD6	C26-C27	2.49	1.42	1.37
21	A	840	CLA	MG-ND	-2.49	2.00	2.05
21	A	838	CLA	C1C-NC	-2.49	1.34	1.37
21	7	714	CLA	C1C-C2C	2.49	1.49	1.44
21	B	834	CLA	CBD-CGD	-2.49	1.44	1.52
21	2	517	CLA	C1B-CHB	2.49	1.47	1.41
21	4	703	CLA	C3D-C4D	-2.49	1.38	1.44
21	5	711	CLA	C4D-CHA	2.49	1.47	1.38
24	A	849	BCR	C16-C17	-2.49	1.35	1.43
21	A	806	CLA	C1C-NC	-2.49	1.34	1.37
21	A	810	CLA	C2A-C1A	-2.49	1.46	1.52
21	6	913	CLA	C4D-CHA	2.49	1.47	1.38
21	7	708	CLA	C3D-C4D	-2.49	1.38	1.44
21	A	806	CLA	OBD-CAD	2.49	1.26	1.22
21	A	836	CLA	C4D-CHA	2.48	1.47	1.38
21	10	712	CLA	C4C-C3C	2.48	1.49	1.45
21	12	501	CLA	C1B-NB	-2.48	1.33	1.35
21	8	608	CLA	C4D-CHA	2.48	1.47	1.38
21	A	810	CLA	C1D-ND	2.48	1.40	1.37
21	A	829	CLA	C4D-CHA	2.48	1.47	1.38
21	1	517	CLA	OBD-CAD	2.48	1.26	1.22
28	8	616	DD6	C24-C1	-2.48	1.40	1.45
21	B	822	CLA	C2A-C1A	-2.48	1.46	1.52
21	10	704	CLA	C3D-C4D	-2.48	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	611	CLA	C1C-C2C	2.48	1.49	1.44
28	3	718	DD6	C24-C1	-2.48	1.40	1.45
21	B	823	CLA	C3D-C4D	-2.48	1.38	1.44
21	2	515	CLA	C1C-C2C	2.48	1.49	1.44
21	8	611	CLA	C4D-CHA	2.48	1.47	1.38
21	A	817	CLA	C3D-C2D	2.48	1.45	1.39
21	F	401	CLA	C4D-CHA	2.48	1.47	1.38
21	B	838	CLA	MG-ND	-2.48	2.00	2.05
21	B	817	CLA	C4D-CHA	2.48	1.47	1.38
24	A	850	BCR	C16-C17	-2.47	1.35	1.43
21	8	605	CLA	C3D-C4D	-2.47	1.38	1.44
21	4	702	CLA	C4B-CHC	2.47	1.47	1.41
21	10	705	CLA	C4D-CHA	2.47	1.47	1.38
24	A	849	BCR	C29-C28	-2.47	1.46	1.52
21	B	818	CLA	C3D-C4D	-2.47	1.38	1.44
21	B	810	CLA	OBD-CAD	2.47	1.26	1.22
21	B	817	CLA	C2-C3	2.47	1.38	1.33
21	10	711	CLA	C4D-CHA	2.47	1.47	1.38
21	2	503	CLA	C1B-CHB	2.47	1.47	1.41
21	10	707	CLA	C3D-C4D	-2.47	1.38	1.44
21	6	908	CLA	C4D-CHA	2.47	1.47	1.38
21	B	802	CLA	CHD-C1D	2.47	1.43	1.38
21	B	834	CLA	C1B-CHB	2.47	1.47	1.41
28	7	716	DD6	C24-C1	-2.47	1.40	1.45
21	B	835	CLA	C3D-C2D	2.47	1.45	1.39
28	6	915	DD6	C25-C26	-2.47	1.35	1.43
21	A	819	CLA	C1B-CHB	2.47	1.47	1.41
21	3	713	CLA	C3D-C4D	-2.47	1.38	1.44
21	A	804	CLA	MG-ND	-2.46	2.00	2.05
21	2	507	CLA	C4C-C3C	2.46	1.49	1.45
21	B	838	CLA	C3D-C2D	2.46	1.45	1.39
21	10	712	CLA	C4D-CHA	2.46	1.47	1.38
21	B	828	CLA	CAA-C2A	-2.46	1.49	1.54
21	6	911	CLA	C4D-CHA	2.46	1.47	1.38
21	A	824	CLA	C1D-ND	2.46	1.40	1.37
21	A	840	CLA	C1C-C2C	2.46	1.49	1.44
24	J	103	BCR	C11-C10	-2.46	1.35	1.43
21	8	607	CLA	C1C-C2C	2.46	1.49	1.44
21	4	701	CLA	C1B-CHB	2.46	1.47	1.41
21	4	709	CLA	C4D-CHA	2.46	1.47	1.38
21	A	805	CLA	OBD-CAD	2.46	1.26	1.22
21	A	824	CLA	C4D-CHA	2.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	804	CLA	OBD-CAD	2.45	1.26	1.22
21	A	827	CLA	C1D-ND	2.45	1.40	1.37
21	8	614	CLA	C4B-CHC	2.45	1.47	1.41
21	B	830	CLA	C4C-C3C	2.45	1.49	1.45
21	B	825	CLA	C4B-CHC	2.45	1.47	1.41
21	2	508	CLA	C4B-CHC	2.45	1.47	1.41
24	J	103	BCR	C8-C9	-2.45	1.40	1.45
21	11	703	CLA	C1C-NC	-2.45	1.34	1.37
21	10	708	CLA	C1C-NC	-2.45	1.34	1.37
21	B	834	CLA	C2A-C1A	-2.45	1.46	1.52
21	B	829	CLA	C4B-CHC	2.45	1.47	1.41
21	B	823	CLA	C1B-CHB	2.45	1.47	1.41
21	9	911	CLA	C1B-CHB	2.45	1.47	1.41
21	B	808	CLA	MG-ND	-2.45	2.00	2.05
21	A	837	CLA	C4D-CHA	2.45	1.47	1.38
21	1	504	CLA	C4B-CHC	2.45	1.47	1.41
21	5	707	CLA	C1C-NC	-2.45	1.34	1.37
21	A	826	CLA	C3D-C4D	-2.45	1.38	1.44
21	2	504	CLA	C4D-CHA	2.45	1.47	1.38
21	11	703	CLA	C3D-C2D	2.45	1.45	1.39
21	A	833	CLA	C1C-NC	-2.45	1.34	1.37
21	10	703	CLA	C4B-CHC	2.45	1.47	1.41
21	A	828	CLA	C1D-ND	2.45	1.40	1.37
24	A	847	BCR	C23-C22	-2.45	1.40	1.45
28	1	518	DD6	C13-C11	-2.45	1.40	1.45
24	B	846	BCR	C15-C14	-2.44	1.35	1.43
21	A	805	CLA	C3D-C4D	-2.44	1.38	1.44
24	A	849	BCR	C10-C9	2.44	1.39	1.35
21	5	705	CLA	C4B-CHC	2.44	1.47	1.41
21	B	815	CLA	C3C-C2C	2.44	1.41	1.36
21	12	503	CLA	C4C-C3C	2.44	1.49	1.45
21	5	707	CLA	C4B-CHC	2.44	1.47	1.41
21	A	816	CLA	C3D-C4D	-2.44	1.38	1.44
21	B	830	CLA	CBD-CGD	-2.44	1.44	1.52
21	A	826	CLA	CAA-C2A	-2.44	1.49	1.54
21	6	907	CLA	C1C-NC	-2.44	1.34	1.37
21	4	701	CLA	C4D-CHA	2.44	1.47	1.38
21	A	814	CLA	C4B-NB	-2.44	1.33	1.35
24	A	848	BCR	C16-C17	-2.44	1.35	1.43
28	7	715	DD6	C13-C11	-2.44	1.40	1.45
21	4	707	CLA	C4D-CHA	2.44	1.47	1.38
21	4	708	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	514	CLA	C1B-CHB	2.44	1.47	1.41
21	11	702	CLA	C4B-CHC	2.44	1.47	1.41
28	6	916	DD6	C25-C26	-2.44	1.35	1.43
21	9	906	CLA	C1B-CHB	2.44	1.47	1.41
21	5	710	CLA	C3D-C4D	-2.44	1.38	1.44
21	7	706	CLA	C3D-C2D	2.44	1.45	1.39
21	12	505	CLA	C4D-CHA	2.44	1.47	1.38
21	B	831	CLA	C3D-C4D	-2.43	1.38	1.44
21	A	838	CLA	CHD-C1D	2.43	1.43	1.38
21	3	715	CLA	C4B-CHC	2.43	1.47	1.41
21	10	712	CLA	C3D-C4D	-2.43	1.38	1.44
21	A	844	CLA	CBA-CGA	2.43	1.57	1.50
21	6	912	CLA	C4D-CHA	2.43	1.47	1.38
21	B	808	CLA	CAA-C2A	-2.43	1.49	1.54
21	10	704	CLA	C4D-CHA	2.43	1.47	1.38
21	9	902	CLA	C4B-CHC	2.43	1.47	1.41
21	3	714	CLA	C1B-NB	-2.43	1.33	1.35
21	8	607	CLA	C4D-CHA	2.43	1.47	1.38
21	10	712	CLA	C4B-CHC	2.43	1.47	1.41
21	B	832	CLA	O2D-CED	-2.43	1.39	1.45
21	7	704	CLA	C1C-NC	-2.43	1.34	1.37
28	3	717	DD6	C26-C27	2.43	1.42	1.37
21	2	512	CLA	C4D-CHA	2.43	1.47	1.38
21	9	913	CLA	C1C-NC	-2.43	1.34	1.37
21	F	404	CLA	C4D-CHA	2.43	1.47	1.38
21	9	904	CLA	C1B-NB	-2.43	1.33	1.35
21	2	515	CLA	C4D-CHA	2.42	1.47	1.38
21	4	703	CLA	C1B-CHB	2.42	1.47	1.41
21	F	401	CLA	C3B-C2B	2.42	1.43	1.40
21	3	708	CLA	C4B-CHC	2.42	1.47	1.41
24	A	847	BCR	C16-C17	-2.42	1.35	1.43
21	10	706	CLA	C4B-CHC	2.42	1.47	1.41
24	B	845	BCR	C17-C18	2.42	1.39	1.35
21	6	914	CLA	C1C-NC	-2.42	1.34	1.37
21	B	803	CLA	CAA-C2A	-2.42	1.49	1.54
24	J	102	BCR	C16-C17	-2.42	1.35	1.43
21	B	838	CLA	C1C-C2C	2.42	1.49	1.44
21	A	822	CLA	C1B-CHB	2.42	1.47	1.41
21	B	833	CLA	CMA-C3A	2.42	1.58	1.53
21	10	708	CLA	C4D-CHA	2.42	1.47	1.38
21	7	711	CLA	C1B-NB	-2.42	1.33	1.35
21	12	508	CLA	C4B-CHC	2.42	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	834	CLA	C4D-CHA	2.42	1.47	1.38
21	8	606	CLA	C4D-CHA	2.42	1.47	1.38
24	A	851	BCR	C12-C13	-2.42	1.40	1.45
21	A	813	CLA	C3D-C2D	2.42	1.45	1.39
21	B	814	CLA	C1B-NB	-2.42	1.33	1.35
21	13	501	CLA	C4B-CHC	2.42	1.47	1.41
28	J	104	DD6	C8-C6	-2.41	1.40	1.45
21	A	822	CLA	MG-ND	-2.41	2.01	2.05
21	B	807	CLA	CMD-C2D	-2.41	1.45	1.50
21	5	701	CLA	C1B-CHB	2.41	1.47	1.41
21	A	818	CLA	MG-ND	-2.41	2.01	2.05
21	11	705	CLA	MG-ND	-2.41	2.01	2.05
21	A	829	CLA	C1D-ND	2.41	1.40	1.37
21	9	907	CLA	C4B-CHC	2.41	1.47	1.41
24	B	845	BCR	C15-C14	-2.41	1.36	1.43
21	B	809	CLA	CMD-C2D	-2.41	1.45	1.50
21	A	807	CLA	C3B-C2B	2.41	1.43	1.40
21	5	702	CLA	C4D-CHA	2.41	1.47	1.38
21	A	831	CLA	CHD-C1D	2.41	1.43	1.38
21	4	711	CLA	C4C-C3C	2.41	1.49	1.45
21	12	506	CLA	C4D-CHA	2.41	1.47	1.38
21	3	705	CLA	C1B-CHB	2.41	1.47	1.41
21	4	706	CLA	C4B-CHC	2.41	1.47	1.41
21	F	401	CLA	C3D-C4D	-2.41	1.38	1.44
21	A	819	CLA	CMB-C2B	-2.41	1.46	1.51
21	1	512	CLA	C4B-CHC	2.41	1.47	1.41
21	3	714	CLA	C4B-CHC	2.41	1.47	1.41
21	2	509	CLA	C1D-ND	2.40	1.40	1.37
21	A	804	CLA	C3D-C4D	-2.40	1.38	1.44
28	4	713	DD6	C8-C6	-2.40	1.40	1.45
21	A	840	CLA	C1B-CHB	2.40	1.47	1.41
24	B	845	BCR	C16-C17	-2.40	1.36	1.43
21	12	504	CLA	C1B-CHB	2.40	1.47	1.41
24	M	102	BCR	C8-C9	-2.40	1.40	1.45
21	4	709	CLA	C1C-C2C	2.40	1.49	1.44
21	A	830	CLA	CHD-C4C	2.40	1.44	1.39
28	J	104	DD6	C13-C11	-2.40	1.40	1.45
21	9	903	CLA	C1B-CHB	2.40	1.47	1.41
21	4	705	CLA	C4D-CHA	2.40	1.46	1.38
21	3	714	CLA	C3D-C4D	-2.40	1.38	1.44
21	11	710	CLA	C4D-CHA	2.40	1.46	1.38
21	13	502	CLA	C4B-CHC	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	843	BCR	C12-C13	-2.40	1.40	1.45
21	B	815	CLA	C4B-NB	-2.40	1.33	1.35
21	8	604	CLA	CHD-C1D	2.40	1.43	1.38
21	12	506	CLA	C1C-C2C	2.40	1.49	1.44
21	1	505	CLA	C4B-CHC	2.40	1.47	1.41
21	3	706	CLA	C1B-CHB	2.40	1.47	1.41
21	1	501	CLA	C1B-NB	-2.40	1.33	1.35
21	A	828	CLA	C3D-C4D	-2.40	1.38	1.44
21	A	812	CLA	C4B-NB	-2.39	1.33	1.35
21	11	701	CLA	C1C-NC	-2.39	1.34	1.37
21	B	801	CLA	C3D-C4D	-2.39	1.38	1.44
21	12	508	CLA	C1C-C2C	2.39	1.49	1.44
24	A	851	BCR	C2-C3	-2.39	1.46	1.52
21	6	906	CLA	C4D-CHA	2.39	1.46	1.38
24	B	842	BCR	C12-C13	-2.39	1.40	1.45
21	A	844	CLA	OBD-CAD	2.39	1.26	1.22
21	3	709	CLA	C3D-C4D	-2.39	1.38	1.44
21	4	704	CLA	C1B-CHB	2.39	1.47	1.41
21	4	707	CLA	C1B-CHB	2.39	1.47	1.41
21	1	508	CLA	C1C-C2C	2.39	1.49	1.44
21	1	513	CLA	C4B-NB	-2.39	1.33	1.35
21	A	821	CLA	C1C-NC	-2.39	1.34	1.37
21	8	605	CLA	C1C-C2C	2.39	1.49	1.44
21	3	706	CLA	C1C-C2C	2.39	1.49	1.44
21	10	705	CLA	C1C-C2C	2.39	1.49	1.44
21	8	607	CLA	C1B-CHB	2.39	1.47	1.41
21	9	913	CLA	C4D-CHA	2.39	1.46	1.38
21	B	807	CLA	C3A-C2A	-2.38	1.47	1.54
21	A	807	CLA	O1D-CGD	2.38	1.27	1.21
21	3	709	CLA	C1B-CHB	2.38	1.47	1.41
21	4	703	CLA	C4D-CHA	2.38	1.46	1.38
21	8	605	CLA	C4C-C3C	2.38	1.49	1.45
21	A	833	CLA	C4B-CHC	2.38	1.47	1.41
21	3	709	CLA	C4B-CHC	2.38	1.47	1.41
28	2	518	DD6	C26-C27	2.38	1.42	1.37
21	1	511	CLA	C1B-NB	-2.38	1.33	1.35
21	8	610	CLA	C4B-CHC	2.38	1.47	1.41
21	3	702	CLA	C4C-C3C	2.38	1.49	1.45
21	2	509	CLA	C4B-CHC	2.38	1.47	1.41
21	B	814	CLA	C3A-C2A	-2.38	1.47	1.54
21	B	838	CLA	C3D-C4D	-2.38	1.38	1.44
21	12	501	CLA	C4D-CHA	2.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	850	BCR	C14-C13	2.37	1.38	1.35
21	11	711	CLA	C4C-C3C	2.37	1.49	1.45
24	J	103	BCR	C15-C14	-2.37	1.36	1.43
21	1	516	CLA	C4C-C3C	2.37	1.49	1.45
21	1	501	CLA	CMB-C2B	-2.37	1.46	1.51
21	9	906	CLA	C4B-CHC	2.37	1.47	1.41
21	2	511	CLA	C3D-C4D	-2.37	1.38	1.44
21	A	817	CLA	C4B-CHC	2.37	1.47	1.41
21	5	703	CLA	C4D-CHA	2.37	1.46	1.38
21	5	710	CLA	C4B-CHC	2.37	1.47	1.41
21	A	820	CLA	C4D-CHA	2.37	1.46	1.38
21	2	515	CLA	CBA-CGA	2.37	1.56	1.50
21	B	814	CLA	CBD-CGD	-2.37	1.45	1.52
21	B	839	CLA	C4D-CHA	2.37	1.46	1.38
21	3	703	CLA	C1B-CHB	2.37	1.47	1.41
21	9	908	CLA	C4B-CHC	2.37	1.47	1.41
21	11	710	CLA	C3D-C4D	-2.37	1.38	1.44
21	13	503	CLA	C4D-CHA	2.37	1.46	1.38
21	A	808	CLA	C2A-C1A	-2.37	1.46	1.52
21	13	501	CLA	C4D-CHA	2.37	1.46	1.38
28	6	916	DD6	C2-C1	2.37	1.38	1.35
21	6	906	CLA	C1C-C2C	2.37	1.49	1.44
24	A	848	BCR	C15-C14	-2.37	1.36	1.43
21	A	827	CLA	C4D-CHA	2.37	1.46	1.38
21	12	503	CLA	C4B-CHC	2.36	1.47	1.41
21	9	912	CLA	C1B-NB	-2.36	1.33	1.35
21	9	913	CLA	C1B-NB	-2.36	1.33	1.35
21	B	804	CLA	C4B-CHC	2.36	1.47	1.41
21	6	910	CLA	C4D-CHA	2.36	1.46	1.38
21	7	702	CLA	MG-ND	-2.36	2.01	2.05
21	7	712	CLA	C4D-CHA	2.36	1.46	1.38
21	4	705	CLA	C3D-C4D	-2.36	1.38	1.44
21	A	811	CLA	C4D-CHA	2.36	1.46	1.38
21	9	909	CLA	C4B-NB	-2.36	1.33	1.35
21	B	809	CLA	C1B-CHB	2.36	1.47	1.41
21	A	862	CLA	C1B-CHB	2.36	1.47	1.41
28	6	915	DD6	C36-C31	-2.36	1.32	1.34
21	A	813	CLA	C4B-CHC	2.36	1.47	1.41
21	B	837	CLA	C4B-CHC	2.36	1.47	1.41
21	9	902	CLA	C1C-NC	-2.35	1.34	1.37
21	A	824	CLA	OBD-CAD	2.35	1.26	1.22
21	9	902	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	801	CL0	C3D-C2D	2.35	1.45	1.39
21	10	704	CLA	C1B-CHB	2.35	1.47	1.41
28	8	615	DD6	C25-C26	-2.35	1.36	1.43
21	6	903	CLA	C4D-CHA	2.35	1.46	1.38
21	11	701	CLA	C3D-C4D	-2.35	1.38	1.44
21	A	819	CLA	C4D-CHA	2.35	1.46	1.38
21	3	711	CLA	C1C-NC	-2.35	1.34	1.37
21	9	913	CLA	C3D-C4D	-2.35	1.38	1.44
21	5	709	CLA	C1B-CHB	2.35	1.47	1.41
21	A	812	CLA	C1D-ND	2.35	1.40	1.37
21	10	707	CLA	C4C-C3C	2.35	1.49	1.45
21	1	511	CLA	C1C-NC	-2.35	1.34	1.37
21	A	833	CLA	C4B-NB	-2.35	1.33	1.35
21	3	711	CLA	C4B-CHC	2.35	1.47	1.41
21	B	805	CLA	MG-ND	-2.35	2.01	2.05
21	A	818	CLA	C1B-NB	-2.35	1.33	1.35
21	7	704	CLA	C1C-C2C	2.35	1.49	1.44
21	B	828	CLA	C3C-C2C	2.35	1.41	1.36
21	B	819	CLA	MG-ND	-2.35	2.01	2.05
21	A	815	CLA	OBD-CAD	2.35	1.26	1.22
21	11	704	CLA	C4D-CHA	2.35	1.46	1.38
21	13	502	CLA	C3D-C4D	-2.35	1.38	1.44
21	7	714	CLA	C3D-C4D	-2.34	1.38	1.44
21	3	702	CLA	C4D-CHA	2.34	1.46	1.38
21	11	701	CLA	C4B-CHC	2.34	1.47	1.41
21	10	703	CLA	C4C-C3C	2.34	1.49	1.45
21	8	607	CLA	C4C-C3C	2.34	1.49	1.45
21	6	910	CLA	C1C-C2C	2.34	1.49	1.44
21	B	836	CLA	CHD-C4C	2.34	1.44	1.39
21	2	513	CLA	C4B-CHC	2.34	1.47	1.41
21	A	829	CLA	O2A-CGA	2.34	1.40	1.33
21	A	831	CLA	C4D-CHA	2.34	1.46	1.38
21	1	511	CLA	C4D-CHA	2.34	1.46	1.38
21	9	912	CLA	C1B-CHB	2.34	1.47	1.41
28	11	713	DD6	C8-C6	-2.34	1.40	1.45
21	A	808	CLA	C3B-C2B	2.34	1.43	1.40
21	4	710	CLA	C1B-CHB	2.34	1.47	1.41
21	A	815	CLA	C4B-CHC	2.34	1.47	1.41
21	8	613	CLA	C1C-C2C	2.34	1.49	1.44
21	8	613	CLA	C4B-CHC	2.34	1.47	1.41
21	9	906	CLA	C4D-CHA	2.34	1.46	1.38
21	A	814	CLA	MG-ND	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	504	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	850	BCR	C11-C10	-2.34	1.36	1.43
21	11	704	CLA	C4B-CHC	2.33	1.47	1.41
21	A	815	CLA	CHD-C4C	2.33	1.44	1.39
24	B	845	BCR	C11-C10	-2.33	1.36	1.43
21	10	709	CLA	C4B-CHC	2.33	1.47	1.41
21	B	828	CLA	C4B-CHC	2.33	1.47	1.41
21	11	703	CLA	OBD-CAD	2.33	1.26	1.22
21	B	826	CLA	CMD-C2D	-2.33	1.45	1.50
21	10	706	CLA	C4D-CHA	2.33	1.46	1.38
21	8	606	CLA	C3D-C4D	-2.33	1.38	1.44
21	B	832	CLA	C3D-C2D	2.33	1.45	1.39
21	1	511	CLA	C1B-CHB	2.33	1.47	1.41
21	3	705	CLA	MG-ND	-2.33	2.01	2.05
21	3	712	CLA	C4D-CHA	2.33	1.46	1.38
21	9	908	CLA	C4D-CHA	2.33	1.46	1.38
28	12	509	DD6	C24-C1	-2.33	1.40	1.45
21	8	608	CLA	C3D-C4D	-2.33	1.38	1.44
21	A	805	CLA	MG-ND	-2.33	2.01	2.05
21	11	710	CLA	C4C-C3C	2.33	1.49	1.45
21	5	708	CLA	C4D-CHA	2.32	1.46	1.38
21	A	829	CLA	CBD-CGD	-2.32	1.45	1.52
28	6	915	DD6	C8-C6	-2.32	1.41	1.45
21	A	820	CLA	C2-C3	2.32	1.38	1.33
21	12	506	CLA	C3D-C4D	-2.32	1.38	1.44
21	4	708	CLA	C4B-CHC	2.32	1.47	1.41
21	B	812	CLA	C4D-CHA	2.32	1.46	1.38
21	A	809	CLA	C1B-NB	-2.32	1.33	1.35
21	3	705	CLA	C1B-NB	-2.32	1.33	1.35
21	4	702	CLA	C4D-CHA	2.32	1.46	1.38
21	B	806	CLA	C3D-C2D	2.32	1.45	1.39
21	1	508	CLA	C1B-CHB	2.32	1.47	1.41
28	7	716	DD6	C-C1	-2.32	1.46	1.50
21	6	914	CLA	C4D-CHA	2.32	1.46	1.38
21	5	704	CLA	C4B-CHC	2.32	1.47	1.41
21	6	903	CLA	C4B-CHC	2.32	1.47	1.41
28	2	518	DD6	C25-C26	-2.32	1.36	1.43
21	B	827	CLA	C2A-C1A	-2.32	1.47	1.52
21	A	808	CLA	OBD-CAD	2.32	1.26	1.22
21	7	702	CLA	CBD-CGD	-2.32	1.45	1.52
21	3	701	CLA	C1B-CHB	2.32	1.47	1.41
28	3	718	DD6	C25-C26	-2.32	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	826	CLA	CAA-C2A	-2.32	1.49	1.54
21	3	706	CLA	C3D-C2D	2.32	1.45	1.39
21	6	906	CLA	C4C-C3C	2.32	1.49	1.45
21	6	907	CLA	C1B-CHB	2.32	1.47	1.41
28	4	713	DD6	C24-C1	-2.31	1.41	1.45
21	5	702	CLA	C1B-CHB	2.31	1.47	1.41
21	4	710	CLA	C4C-C3C	2.31	1.49	1.45
21	B	839	CLA	C4B-NB	-2.31	1.33	1.35
21	5	711	CLA	C3D-C4D	-2.31	1.39	1.44
21	1	504	CLA	C4C-C3C	2.31	1.49	1.45
21	A	839	CLA	C2A-C1A	-2.31	1.47	1.52
21	2	505	CLA	MG-ND	-2.31	2.01	2.05
21	5	702	CLA	C2A-C1A	-2.31	1.47	1.52
21	12	503	CLA	C4D-CHA	2.31	1.46	1.38
28	5	713	DD6	C36-C31	-2.31	1.32	1.34
21	B	816	CLA	C1D-ND	2.31	1.40	1.37
21	B	836	CLA	CBA-CGA	2.31	1.57	1.50
21	4	708	CLA	C1B-CHB	2.31	1.47	1.41
21	B	834	CLA	C3D-C2D	2.31	1.45	1.39
21	1	501	CLA	C4B-CHC	2.31	1.47	1.41
21	3	715	CLA	C4D-CHA	2.30	1.46	1.38
21	B	830	CLA	C4D-CHA	2.30	1.46	1.38
21	6	905	CLA	C3D-C4D	-2.30	1.39	1.44
21	A	816	CLA	C1B-CHB	2.30	1.47	1.41
21	3	713	CLA	C4B-CHC	2.30	1.47	1.41
21	4	702	CLA	C1B-CHB	2.30	1.47	1.41
21	A	804	CLA	C4B-NB	-2.30	1.33	1.35
21	A	831	CLA	C1B-CHB	2.30	1.47	1.41
21	B	826	CLA	C3D-C4D	-2.30	1.39	1.44
21	7	702	CLA	C1B-CHB	2.30	1.47	1.41
21	2	503	CLA	C1C-NC	-2.30	1.34	1.37
21	9	902	CLA	C4D-CHA	2.30	1.46	1.38
21	8	606	CLA	C4B-CHC	2.30	1.47	1.41
21	B	810	CLA	CBD-CGD	-2.30	1.45	1.52
21	7	705	CLA	C4D-CHA	2.30	1.46	1.38
21	A	819	CLA	OBD-CAD	2.30	1.26	1.22
21	9	906	CLA	C1C-C2C	2.30	1.49	1.44
21	A	809	CLA	C4C-C3C	2.30	1.49	1.45
21	8	606	CLA	C1C-NC	-2.30	1.34	1.37
21	6	907	CLA	CMD-C2D	-2.30	1.45	1.50
21	13	502	CLA	C1C-C2C	2.30	1.49	1.44
21	11	708	CLA	C4B-CHC	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	708	CLA	C1C-NC	-2.30	1.34	1.37
21	11	707	CLA	C4D-CHA	2.29	1.46	1.38
21	9	905	CLA	C4B-CHC	2.29	1.47	1.41
21	9	909	CLA	C4C-C3C	2.29	1.49	1.45
21	5	705	CLA	C4D-CHA	2.29	1.46	1.38
21	B	838	CLA	C4D-CHA	2.29	1.46	1.38
21	11	708	CLA	C1D-C2D	2.29	1.49	1.45
21	A	821	CLA	CHD-C1D	2.29	1.42	1.38
21	A	803	CLA	C3D-C4D	-2.29	1.39	1.44
21	A	838	CLA	C3C-C2C	2.29	1.41	1.36
21	B	810	CLA	CBA-CGA	2.29	1.55	1.50
21	B	839	CLA	CAA-C2A	-2.29	1.49	1.54
21	9	913	CLA	C4B-CHC	2.29	1.47	1.41
21	A	840	CLA	C3D-C4D	-2.29	1.39	1.44
21	3	704	CLA	C4D-CHA	2.29	1.46	1.38
21	A	837	CLA	C2A-C1A	-2.29	1.47	1.52
21	3	706	CLA	C4B-CHC	2.29	1.47	1.41
21	4	701	CLA	C4C-C3C	2.29	1.49	1.45
21	1	511	CLA	C1C-C2C	2.29	1.49	1.44
21	7	707	CLA	C1D-ND	2.29	1.40	1.37
21	A	806	CLA	MG-NA	-2.29	2.00	2.06
21	13	501	CLA	C1C-C2C	2.29	1.49	1.44
21	3	714	CLA	C1B-CHB	2.29	1.47	1.41
21	7	708	CLA	C2A-C1A	-2.29	1.47	1.52
21	B	831	CLA	CHD-C1D	2.29	1.42	1.38
21	A	814	CLA	C1B-CHB	2.29	1.47	1.41
21	4	701	CLA	C3D-C4D	-2.29	1.39	1.44
21	3	708	CLA	C4D-CHA	2.29	1.46	1.38
21	A	818	CLA	C2A-C1A	-2.29	1.47	1.52
21	B	812	CLA	C3D-C2D	2.29	1.45	1.39
21	A	814	CLA	C3D-C4D	-2.29	1.39	1.44
21	4	708	CLA	C1C-NC	-2.29	1.34	1.37
21	1	511	CLA	C4B-CHC	2.28	1.47	1.41
21	A	818	CLA	C4B-CHC	2.28	1.47	1.41
21	10	704	CLA	C4C-C3C	2.28	1.49	1.45
21	A	841	CLA	CMB-C2B	-2.28	1.46	1.51
21	A	843	CLA	C3D-C2D	2.28	1.45	1.39
21	A	824	CLA	C3D-C2D	2.28	1.45	1.39
24	B	846	BCR	C11-C10	-2.28	1.36	1.43
21	3	713	CLA	C4D-CHA	2.28	1.46	1.38
21	J	101	CLA	C4D-CHA	2.28	1.46	1.38
21	A	838	CLA	C4D-CHA	2.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	913	CLA	C1C-C2C	2.28	1.49	1.44
21	11	708	CLA	C1C-C2C	2.28	1.49	1.44
21	11	709	CLA	C4B-CHC	2.28	1.47	1.41
28	5	713	DD6	C13-C11	-2.28	1.41	1.45
21	12	504	CLA	C4B-CHC	2.28	1.47	1.41
21	3	705	CLA	C4B-CHC	2.28	1.47	1.41
21	A	825	CLA	CBD-CGD	-2.28	1.45	1.52
28	9	915	DD6	C13-C11	-2.28	1.41	1.45
21	A	844	CLA	C1C-C2C	2.28	1.49	1.44
21	A	828	CLA	C2A-C1A	-2.28	1.47	1.52
21	A	835	CLA	C3D-C2D	2.28	1.45	1.39
21	6	905	CLA	C4D-CHA	2.28	1.46	1.38
21	6	909	CLA	C1B-CHB	2.28	1.47	1.41
21	A	827	CLA	O2D-CED	-2.28	1.40	1.45
21	B	831	CLA	C4C-C3C	2.28	1.49	1.45
21	6	903	CLA	C1C-C2C	2.28	1.49	1.44
21	A	835	CLA	C3B-C2B	2.28	1.43	1.40
21	11	704	CLA	C1C-NC	-2.28	1.34	1.37
21	3	713	CLA	C1B-NB	-2.28	1.33	1.35
21	B	826	CLA	MG-ND	-2.28	2.01	2.05
21	F	404	CLA	CHD-C1D	2.27	1.42	1.38
21	B	832	CLA	CBD-CGD	-2.27	1.45	1.52
21	11	707	CLA	C4B-CHC	2.27	1.47	1.41
21	5	711	CLA	C1C-C2C	2.27	1.49	1.44
21	7	702	CLA	C3D-C4D	-2.27	1.39	1.44
21	8	614	CLA	C1C-C2C	2.27	1.49	1.44
21	11	710	CLA	C1B-CHB	2.27	1.47	1.41
28	6	915	DD6	C26-C27	2.27	1.41	1.37
21	B	819	CLA	C4C-C3C	2.27	1.49	1.45
21	5	707	CLA	C4D-CHA	2.27	1.46	1.38
21	A	839	CLA	C1B-CHB	2.27	1.47	1.41
21	1	514	CLA	C4B-CHC	2.27	1.47	1.41
21	A	802	CLA	C4B-CHC	2.27	1.47	1.41
21	4	702	CLA	C4C-C3C	2.27	1.48	1.45
21	9	912	CLA	C3D-C4D	-2.27	1.39	1.44
21	4	704	CLA	C4D-CHA	2.27	1.46	1.38
21	2	516	CLA	CMD-C2D	-2.27	1.46	1.50
24	A	851	BCR	C16-C17	-2.27	1.36	1.43
21	4	710	CLA	C3D-C4D	-2.27	1.39	1.44
21	1	517	CLA	C4B-CHC	2.27	1.47	1.41
21	1	501	CLA	C4D-CHA	2.27	1.46	1.38
21	9	913	CLA	C1C-C2C	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	102	BCR	C16-C17	-2.27	1.36	1.43
21	8	604	CLA	C4D-CHA	2.27	1.46	1.38
21	9	906	CLA	C1B-NB	-2.27	1.33	1.35
21	B	803	CLA	C2A-C1A	-2.27	1.47	1.52
21	7	711	CLA	C4D-CHA	2.26	1.46	1.38
21	1	501	CLA	C3B-C2B	2.26	1.43	1.40
28	2	519	DD6	C8-C6	-2.26	1.41	1.45
21	2	505	CLA	OBD-CAD	2.26	1.26	1.22
21	11	711	CLA	C3D-C4D	-2.26	1.39	1.44
21	A	810	CLA	C1B-CHB	2.26	1.47	1.41
21	1	512	CLA	C4C-C3C	2.26	1.48	1.45
21	B	822	CLA	C4D-CHA	2.26	1.46	1.38
21	9	913	CLA	C1B-CHB	2.26	1.47	1.41
21	A	843	CLA	C1C-C2C	2.26	1.48	1.44
21	3	709	CLA	C1C-C2C	2.26	1.48	1.44
21	11	703	CLA	C1B-CHB	2.26	1.47	1.41
21	6	907	CLA	C4D-CHA	2.26	1.46	1.38
21	6	914	CLA	C3D-C4D	-2.26	1.39	1.44
21	3	703	CLA	OBD-CAD	2.26	1.26	1.22
28	9	916	DD6	C24-C1	-2.26	1.41	1.45
21	A	839	CLA	MG-ND	-2.26	2.01	2.05
21	11	701	CLA	C4D-CHA	2.26	1.46	1.38
21	B	826	CLA	CHD-C4C	2.26	1.44	1.39
21	A	842	CLA	OBD-CAD	2.26	1.26	1.22
21	A	827	CLA	O2D-CGD	2.26	1.38	1.33
21	B	824	CLA	CBD-CGD	-2.26	1.45	1.52
21	B	836	CLA	OBD-CAD	2.26	1.26	1.22
21	1	514	CLA	C1C-C2C	2.26	1.48	1.44
21	B	802	CLA	MG-ND	-2.26	2.01	2.05
21	4	710	CLA	C4B-CHC	2.26	1.47	1.41
21	10	710	CLA	C1C-C2C	2.26	1.48	1.44
28	11	712	DD6	C13-C11	-2.26	1.41	1.45
21	9	912	CLA	C1C-C2C	2.26	1.48	1.44
21	B	802	CLA	CMC-C2C	-2.26	1.46	1.50
24	B	843	BCR	C1-C6	-2.25	1.50	1.53
21	4	705	CLA	C4C-C3C	2.25	1.48	1.45
21	5	705	CLA	C4C-C3C	2.25	1.48	1.45
21	8	604	CLA	C1B-NB	-2.25	1.33	1.35
21	B	813	CLA	C3D-C2D	2.25	1.45	1.39
21	1	513	CLA	C3D-C4D	-2.25	1.39	1.44
21	4	704	CLA	C4C-C3C	2.25	1.48	1.45
21	B	824	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	507	CLA	C3D-C4D	-2.25	1.39	1.44
21	B	802	CLA	C1C-NC	-2.25	1.34	1.37
21	A	827	CLA	CMB-C2B	-2.25	1.47	1.51
21	12	502	CLA	C1C-NC	-2.25	1.34	1.37
21	1	512	CLA	C3D-C4D	-2.25	1.39	1.44
21	1	508	CLA	C2A-C1A	-2.25	1.47	1.52
21	7	706	CLA	C4D-CHA	2.25	1.46	1.38
21	9	908	CLA	C1D-C2D	2.25	1.49	1.45
21	A	831	CLA	CMB-C2B	-2.25	1.47	1.51
21	6	903	CLA	C1B-CHB	2.25	1.47	1.41
28	3	716	DD6	C24-C1	-2.25	1.41	1.45
21	A	831	CLA	C1D-ND	2.25	1.40	1.37
25	A	853	LHG	C8-C7	-2.25	1.44	1.50
21	7	711	CLA	CMB-C2B	-2.25	1.47	1.51
21	A	821	CLA	C4B-CHC	2.25	1.47	1.41
21	1	517	CLA	C1C-NC	-2.25	1.34	1.37
21	4	711	CLA	C1C-NC	-2.25	1.34	1.37
24	F	402	BCR	C14-C13	2.24	1.38	1.35
21	B	813	CLA	C2-C3	2.24	1.38	1.33
21	A	815	CLA	C4D-CHA	2.24	1.46	1.38
21	4	701	CLA	C1C-C2C	2.24	1.48	1.44
21	B	828	CLA	C1B-CHB	2.24	1.47	1.41
21	B	825	CLA	CAA-C2A	-2.24	1.49	1.54
21	B	823	CLA	C4D-CHA	2.24	1.46	1.38
21	3	704	CLA	C1B-CHB	2.24	1.47	1.41
21	B	838	CLA	CMD-C2D	-2.24	1.46	1.50
21	A	862	CLA	CBA-CGA	2.24	1.57	1.50
21	9	910	CLA	C1D-ND	2.24	1.40	1.37
21	A	806	CLA	CBD-CHA	-2.24	1.41	1.52
21	12	501	CLA	C1B-CHB	2.24	1.47	1.41
28	11	712	DD6	C8-C6	-2.24	1.41	1.45
21	5	702	CLA	CBD-CGD	-2.24	1.45	1.52
21	10	706	CLA	C1B-CHB	2.24	1.47	1.41
21	5	708	CLA	C1B-NB	-2.24	1.33	1.35
21	3	702	CLA	CBD-CGD	-2.24	1.45	1.52
21	7	709	CLA	C1B-NB	-2.24	1.33	1.35
21	9	908	CLA	C3D-C4D	-2.24	1.39	1.44
21	7	714	CLA	MG-ND	-2.24	2.01	2.05
21	B	826	CLA	OBD-CAD	2.24	1.26	1.22
28	4	713	DD6	C13-C11	-2.23	1.41	1.45
21	9	913	CLA	C4C-C3C	2.23	1.48	1.45
20	A	801	CL0	OBD-CAD	2.23	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	847	BCR	C29-C28	-2.23	1.47	1.52
21	A	835	CLA	CMC-C2C	-2.23	1.46	1.50
21	B	810	CLA	C3D-C2D	2.23	1.45	1.39
21	7	709	CLA	MG-ND	-2.23	2.01	2.05
28	7	715	DD6	C25-C26	-2.23	1.36	1.43
21	1	517	CLA	C4D-CHA	2.23	1.46	1.38
21	5	706	CLA	C1B-CHB	2.23	1.47	1.41
21	8	609	CLA	C4B-CHC	2.23	1.47	1.41
21	2	507	CLA	C1D-ND	2.23	1.40	1.37
21	B	812	CLA	C1C-C2C	2.23	1.48	1.44
21	A	810	CLA	OBD-CAD	2.23	1.26	1.22
21	6	904	CLA	C4B-CHC	2.23	1.47	1.41
21	A	841	CLA	OBD-CAD	2.23	1.26	1.22
21	6	906	CLA	C4B-CHC	2.23	1.47	1.41
21	9	909	CLA	C4D-CHA	2.23	1.46	1.38
21	A	839	CLA	C4B-NB	-2.23	1.33	1.35
21	1	504	CLA	C1B-CHB	2.23	1.47	1.41
24	B	841	BCR	C19-C18	-2.23	1.41	1.45
21	5	707	CLA	C1D-C2D	2.23	1.49	1.45
21	4	709	CLA	C4B-CHC	2.23	1.47	1.41
21	2	512	CLA	C3D-C4D	-2.23	1.39	1.44
21	5	702	CLA	C4C-C3C	2.23	1.48	1.45
21	7	703	CLA	CMB-C2B	-2.23	1.47	1.51
21	F	404	CLA	C4B-CHC	2.23	1.47	1.41
21	10	710	CLA	C3D-C4D	-2.22	1.39	1.44
21	3	707	CLA	C3D-C4D	-2.22	1.39	1.44
21	B	806	CLA	C3A-C2A	-2.22	1.48	1.54
21	3	713	CLA	C1C-NC	-2.22	1.34	1.37
21	B	814	CLA	MG-ND	-2.22	2.01	2.05
24	B	843	BCR	C20-C21	-2.22	1.36	1.43
21	10	707	CLA	C1B-CHB	2.22	1.47	1.41
21	11	705	CLA	C1B-CHB	2.22	1.47	1.41
21	B	834	CLA	CMD-C2D	-2.22	1.46	1.50
21	2	507	CLA	C1B-CHB	2.22	1.47	1.41
21	B	815	CLA	CAA-C2A	-2.22	1.50	1.54
24	A	851	BCR	C20-C21	-2.22	1.36	1.43
21	A	825	CLA	CHD-C4C	2.22	1.44	1.39
21	B	816	CLA	C4D-CHA	2.22	1.46	1.38
21	13	502	CLA	C1B-CHB	2.22	1.47	1.41
21	1	510	CLA	C1C-C2C	2.22	1.48	1.44
21	3	703	CLA	C1C-C2C	2.22	1.48	1.44
28	5	713	DD6	C13-C14	2.22	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	10	703	CLA	C4D-CHA	2.22	1.46	1.38
21	8	607	CLA	C4B-CHC	2.22	1.47	1.41
21	2	513	CLA	C1B-NB	-2.22	1.33	1.35
21	A	818	CLA	C4D-CHA	2.22	1.46	1.38
21	4	705	CLA	C1C-C2C	2.22	1.48	1.44
21	11	702	CLA	C1C-C2C	2.22	1.48	1.44
28	4	712	DD6	C8-C6	-2.22	1.41	1.45
21	11	708	CLA	C4D-CHA	2.22	1.46	1.38
21	B	813	CLA	CHD-C4C	2.22	1.44	1.39
21	B	832	CLA	C4B-CHC	2.21	1.47	1.41
28	9	915	DD6	C25-C26	-2.21	1.36	1.43
21	A	807	CLA	C4D-ND	2.21	1.40	1.37
28	1	518	DD6	C25-C26	-2.21	1.36	1.43
21	B	821	CLA	C1C-C2C	2.21	1.48	1.44
21	A	826	CLA	O2A-C1	-2.21	1.39	1.46
28	9	916	DD6	C13-C11	-2.21	1.41	1.45
21	6	907	CLA	OBD-CAD	2.21	1.26	1.22
21	B	833	CLA	C3A-C2A	-2.21	1.48	1.54
28	9	916	DD6	C8-C6	-2.21	1.41	1.45
21	4	703	CLA	C1C-NC	-2.21	1.34	1.37
21	7	714	CLA	C4B-CHC	2.21	1.47	1.41
21	B	821	CLA	C1C-NC	-2.21	1.34	1.37
21	10	712	CLA	C1C-NC	-2.21	1.34	1.37
21	B	828	CLA	CMC-C2C	-2.21	1.46	1.50
24	F	405	BCR	C29-C28	-2.21	1.47	1.52
21	B	828	CLA	C4C-C3C	2.21	1.48	1.45
21	4	707	CLA	C1B-NB	-2.21	1.33	1.35
21	11	708	CLA	C4C-C3C	2.21	1.48	1.45
21	B	811	CLA	C1D-C2D	2.20	1.49	1.45
21	8	608	CLA	C1D-C2D	2.20	1.49	1.45
21	A	830	CLA	C2A-C1A	-2.20	1.47	1.52
21	A	815	CLA	C1B-CHB	2.20	1.47	1.41
21	A	837	CLA	C1B-CHB	2.20	1.47	1.41
21	3	709	CLA	OBD-CAD	2.20	1.26	1.22
21	B	828	CLA	O2D-CGD	2.20	1.38	1.33
21	7	713	CLA	C1B-CHB	2.20	1.47	1.41
24	B	845	BCR	C20-C21	-2.20	1.36	1.43
21	A	815	CLA	C3D-C2D	2.20	1.45	1.39
21	B	801	CLA	C3D-C2D	2.20	1.45	1.39
21	A	815	CLA	C3D-C4D	-2.20	1.39	1.44
24	M	102	BCR	C1-C6	-2.20	1.50	1.53
21	11	710	CLA	C1C-C2C	2.20	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	505	CLA	C4D-CHA	2.20	1.46	1.38
21	4	709	CLA	C4C-C3C	2.20	1.48	1.45
21	11	704	CLA	C4B-NB	-2.20	1.33	1.35
21	B	838	CLA	CAA-C2A	-2.20	1.50	1.54
21	B	813	CLA	MG-ND	-2.20	2.01	2.05
21	4	703	CLA	C1C-C2C	2.20	1.48	1.44
21	10	712	CLA	C1C-C2C	2.20	1.48	1.44
21	A	810	CLA	C4B-CHC	2.20	1.47	1.41
21	7	714	CLA	C1B-CHB	2.20	1.47	1.41
21	7	707	CLA	C4B-CHC	2.20	1.47	1.41
21	2	510	CLA	C4D-CHA	2.20	1.46	1.38
21	4	704	CLA	C1B-NB	-2.19	1.33	1.35
21	B	819	CLA	C1B-CHB	2.19	1.47	1.41
21	10	705	CLA	C4B-CHC	2.19	1.47	1.41
21	7	706	CLA	C1C-NC	-2.19	1.34	1.37
21	A	816	CLA	C3D-C2D	2.19	1.45	1.39
21	A	822	CLA	C4B-CHC	2.19	1.47	1.41
21	F	401	CLA	C1B-CHB	2.19	1.47	1.41
21	2	505	CLA	C4B-CHC	2.19	1.47	1.41
28	7	716	DD6	C2-C1	2.19	1.38	1.35
28	9	915	DD6	C8-C6	-2.19	1.41	1.45
21	B	824	CLA	MG-ND	-2.19	2.01	2.05
21	12	504	CLA	C1C-NC	-2.19	1.34	1.37
21	A	825	CLA	C3D-C4D	-2.19	1.39	1.44
21	12	503	CLA	C1B-NB	-2.19	1.33	1.35
21	5	709	CLA	C4B-CHC	2.19	1.47	1.41
21	7	707	CLA	C1C-NC	-2.19	1.34	1.37
21	A	844	CLA	C4D-CHA	2.19	1.46	1.38
21	B	831	CLA	C3D-C2D	2.19	1.45	1.39
21	5	710	CLA	C1B-CHB	2.19	1.47	1.41
21	6	903	CLA	C3D-C4D	-2.19	1.39	1.44
21	7	708	CLA	C1B-CHB	2.19	1.47	1.41
21	A	815	CLA	C3A-C2A	-2.19	1.48	1.54
21	A	830	CLA	C1B-CHB	2.19	1.47	1.41
21	B	817	CLA	C3D-C2D	2.19	1.45	1.39
21	7	704	CLA	C4B-CHC	2.19	1.47	1.41
21	7	707	CLA	MG-ND	-2.19	2.01	2.05
21	B	801	CLA	C3B-C2B	2.18	1.43	1.40
28	11	713	DD6	C13-C11	-2.18	1.41	1.45
21	11	703	CLA	C4B-CHC	2.18	1.47	1.41
28	2	520	DD6	C25-C26	-2.18	1.36	1.43
21	10	710	CLA	C4D-CHA	2.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	914	CLA	C1B-CHB	2.18	1.47	1.41
21	5	708	CLA	C3D-C4D	-2.18	1.39	1.44
21	5	709	CLA	MG-NA	2.18	2.11	2.06
21	5	704	CLA	C1B-CHB	2.18	1.47	1.41
21	2	512	CLA	C1B-NB	-2.18	1.33	1.35
21	2	516	CLA	C3D-C4D	-2.18	1.39	1.44
21	1	504	CLA	C1B-NB	-2.18	1.33	1.35
21	11	708	CLA	C3D-C4D	-2.18	1.39	1.44
21	B	813	CLA	C4B-CHC	2.18	1.47	1.41
21	8	606	CLA	C4B-NB	-2.18	1.33	1.35
21	8	612	CLA	C1C-C2C	2.18	1.48	1.44
21	A	840	CLA	CBA-CGA	2.18	1.57	1.50
21	9	914	CLA	C3D-C4D	-2.18	1.39	1.44
21	10	704	CLA	C1C-C2C	2.17	1.48	1.44
21	9	909	CLA	C3D-C4D	-2.17	1.39	1.44
21	A	844	CLA	C1B-CHB	2.17	1.47	1.41
21	1	514	CLA	C1B-CHB	2.17	1.47	1.41
21	5	703	CLA	C3D-C4D	-2.17	1.39	1.44
21	A	827	CLA	C3A-C2A	-2.17	1.48	1.54
21	A	808	CLA	CMD-C2D	-2.17	1.46	1.50
21	7	710	CLA	C1C-C2C	2.17	1.48	1.44
21	10	705	CLA	C3D-C4D	-2.17	1.39	1.44
21	B	827	CLA	CHD-C4C	2.17	1.44	1.39
21	8	604	CLA	C2A-C1A	-2.17	1.47	1.52
21	9	911	CLA	C1C-C2C	2.17	1.48	1.44
21	2	513	CLA	C3D-C4D	-2.17	1.39	1.44
21	1	509	CLA	C1B-CHB	2.17	1.47	1.41
28	12	509	DD6	C25-C26	-2.16	1.36	1.43
21	8	611	CLA	C4B-CHC	2.16	1.47	1.41
21	8	611	CLA	C1C-NC	-2.16	1.34	1.37
28	11	712	DD6	C24-C1	-2.16	1.41	1.45
28	11	713	DD6	C25-C26	-2.16	1.36	1.43
21	11	709	CLA	C1B-CHB	2.16	1.47	1.41
21	1	506	CLA	C4B-CHC	2.16	1.47	1.41
21	4	709	CLA	C1C-NC	-2.16	1.34	1.37
21	8	613	CLA	C1C-NC	-2.16	1.34	1.37
21	B	817	CLA	C4C-C3C	2.16	1.48	1.45
28	5	712	DD6	C9-C10	-2.16	1.36	1.43
28	J	104	DD6	C25-C26	-2.16	1.36	1.43
21	B	808	CLA	C1C-NC	-2.16	1.34	1.37
21	A	814	CLA	CBD-CGD	-2.16	1.45	1.52
28	12	509	DD6	C8-C6	-2.16	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	801	CLA	CMD-C2D	-2.16	1.46	1.50
21	B	810	CLA	C1C-C2C	2.16	1.48	1.44
21	1	510	CLA	MG-ND	-2.16	2.01	2.05
21	B	813	CLA	C1B-CHB	2.16	1.47	1.41
21	5	701	CLA	C4B-NB	-2.16	1.33	1.35
21	8	608	CLA	C1B-CHB	2.16	1.47	1.41
21	B	813	CLA	OBD-CAD	2.16	1.26	1.22
21	12	503	CLA	C1C-C2C	2.16	1.48	1.44
28	11	712	DD6	C25-C26	-2.16	1.36	1.43
21	13	501	CLA	C4C-C3C	2.16	1.48	1.45
21	1	517	CLA	C3D-C4D	-2.16	1.39	1.44
21	3	705	CLA	C4D-CHA	2.16	1.46	1.38
21	12	507	CLA	C4B-CHC	2.16	1.47	1.41
21	12	508	CLA	C1B-CHB	2.16	1.47	1.41
21	B	825	CLA	CMB-C2B	-2.16	1.47	1.51
21	6	909	CLA	C4D-CHA	2.16	1.46	1.38
21	2	509	CLA	C1B-CHB	2.16	1.47	1.41
24	B	844	BCR	C14-C13	2.15	1.38	1.35
21	A	823	CLA	CMC-C2C	-2.15	1.46	1.50
21	B	804	CLA	C1B-CHB	2.15	1.47	1.41
21	A	803	CLA	C3A-C2A	-2.15	1.48	1.54
21	11	706	CLA	C4B-NB	-2.15	1.33	1.35
21	B	806	CLA	C1C-C2C	2.15	1.48	1.44
21	5	705	CLA	C1C-C2C	2.15	1.48	1.44
21	B	839	CLA	C1B-NB	-2.15	1.33	1.35
21	B	814	CLA	C3D-C4D	-2.15	1.39	1.44
21	8	611	CLA	C1B-CHB	2.15	1.47	1.41
21	B	818	CLA	CBD-CGD	-2.15	1.45	1.52
21	3	701	CLA	C4B-CHC	2.15	1.47	1.41
21	9	909	CLA	C1C-NC	-2.15	1.34	1.37
21	1	506	CLA	C1C-NC	-2.15	1.34	1.37
21	11	704	CLA	C4C-C3C	2.15	1.48	1.45
21	A	808	CLA	C1C-C2C	2.15	1.48	1.44
21	6	912	CLA	C1C-NC	-2.15	1.34	1.37
21	11	709	CLA	C3D-C4D	-2.15	1.39	1.44
21	1	513	CLA	C4D-CHA	2.15	1.46	1.38
28	12	510	DD6	C10-C11	2.15	1.38	1.35
28	1	519	DD6	C25-C26	-2.15	1.36	1.43
21	9	912	CLA	C4B-NB	-2.15	1.33	1.35
21	5	702	CLA	C1C-C2C	2.15	1.48	1.44
21	7	709	CLA	O1D-CGD	2.15	1.26	1.21
21	F	404	CLA	C1B-CHB	2.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	841	CLA	MG-ND	-2.15	2.01	2.05
20	A	801	CL0	C1D-C2D	2.15	1.49	1.45
21	B	809	CLA	C3D-C4D	-2.14	1.39	1.44
21	5	711	CLA	C1B-CHB	2.14	1.47	1.41
21	13	501	CLA	C1B-NB	-2.14	1.33	1.35
21	B	828	CLA	C4D-CHA	2.14	1.46	1.38
21	6	913	CLA	C1B-CHB	2.14	1.47	1.41
21	2	517	CLA	C3D-C4D	-2.14	1.39	1.44
28	1	520	DD6	C25-C26	-2.14	1.36	1.43
21	7	709	CLA	CMC-C2C	-2.14	1.46	1.50
21	B	801	CLA	OBD-CAD	2.14	1.26	1.22
21	A	833	CLA	MG-ND	-2.14	2.01	2.05
21	4	710	CLA	C1C-NC	-2.14	1.34	1.37
21	7	710	CLA	CAA-C2A	-2.14	1.50	1.54
21	6	907	CLA	MG-ND	-2.14	2.01	2.05
21	B	810	CLA	C4D-CHA	2.14	1.46	1.38
21	8	614	CLA	C1B-CHB	2.14	1.46	1.41
21	13	501	CLA	C1B-CHB	2.14	1.46	1.41
21	A	843	CLA	CMB-C2B	-2.14	1.47	1.51
21	11	709	CLA	C1C-C2C	2.14	1.48	1.44
21	A	825	CLA	CAA-C2A	-2.14	1.50	1.54
21	A	822	CLA	C3D-C4D	-2.14	1.39	1.44
21	A	802	CLA	C3B-C2B	2.14	1.43	1.40
21	3	708	CLA	C3D-C4D	-2.14	1.39	1.44
24	F	405	BCR	C15-C14	-2.14	1.36	1.43
21	10	709	CLA	C1C-NC	-2.14	1.34	1.37
21	11	708	CLA	C1C-NC	-2.14	1.34	1.37
21	B	828	CLA	CAA-CBA	-2.13	1.46	1.52
21	A	820	CLA	C3D-C2D	2.13	1.44	1.39
21	A	819	CLA	MG-ND	-2.13	2.01	2.05
21	B	807	CLA	CMB-C2B	-2.13	1.47	1.51
21	A	807	CLA	OBD-CAD	2.13	1.26	1.22
21	B	807	CLA	C1B-CHB	2.13	1.46	1.41
21	8	609	CLA	C4D-CHA	2.13	1.46	1.38
21	A	826	CLA	OBD-CAD	2.13	1.26	1.22
21	B	826	CLA	C1C-C2C	2.13	1.48	1.44
21	B	834	CLA	C3B-CAB	2.13	1.52	1.47
21	B	829	CLA	C1D-ND	2.13	1.40	1.37
21	J	101	CLA	CBA-CGA	2.13	1.55	1.50
21	10	706	CLA	C3D-C4D	-2.13	1.39	1.44
21	6	912	CLA	C4B-CHC	2.13	1.46	1.41
21	1	510	CLA	C4D-CHA	2.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	820	CLA	C2A-C1A	-2.13	1.47	1.52
21	A	838	CLA	C1B-CHB	2.13	1.46	1.41
21	8	606	CLA	MG-ND	-2.13	2.01	2.05
21	10	708	CLA	C3D-C4D	-2.13	1.39	1.44
21	12	507	CLA	C1C-C2C	2.13	1.48	1.44
21	A	802	CLA	C1B-CHB	2.13	1.46	1.41
21	A	842	CLA	CAA-C2A	-2.13	1.50	1.54
21	A	844	CLA	C3B-C2B	2.13	1.43	1.40
21	6	910	CLA	C4B-CHC	2.12	1.46	1.41
21	3	704	CLA	C1C-C2C	2.12	1.48	1.44
21	B	830	CLA	MG-ND	-2.12	2.01	2.05
24	F	402	BCR	C15-C14	-2.12	1.36	1.43
21	1	515	CLA	C1C-C2C	2.12	1.48	1.44
21	13	502	CLA	C1B-NB	-2.12	1.33	1.35
21	2	508	CLA	C1C-NC	-2.12	1.34	1.37
21	6	907	CLA	C4B-CHC	2.12	1.46	1.41
21	9	902	CLA	C4C-C3C	2.12	1.48	1.45
21	2	507	CLA	C1C-C2C	2.12	1.48	1.44
21	B	808	CLA	CMD-C2D	-2.12	1.46	1.50
21	1	509	CLA	C1C-C2C	2.12	1.48	1.44
21	11	706	CLA	C4B-CHC	2.12	1.46	1.41
21	A	842	CLA	C3A-C2A	-2.12	1.48	1.54
28	3	716	DD6	C25-C26	-2.12	1.36	1.43
28	12	510	DD6	C13-C11	-2.12	1.41	1.45
21	5	707	CLA	MG-ND	-2.12	2.01	2.05
21	7	706	CLA	CMB-C2B	-2.11	1.47	1.51
21	4	704	CLA	C5-C3	2.11	1.56	1.50
21	7	709	CLA	C4B-CHC	2.11	1.46	1.41
21	B	807	CLA	C3D-C4D	-2.11	1.39	1.44
21	10	709	CLA	C1B-CHB	2.11	1.46	1.41
24	F	405	BCR	C20-C21	-2.11	1.36	1.43
21	1	516	CLA	C4B-CHC	2.11	1.46	1.41
21	A	802	CLA	C4D-CHA	2.11	1.45	1.38
21	A	815	CLA	C1B-NB	-2.11	1.33	1.35
21	8	607	CLA	C1C-NC	-2.11	1.34	1.37
21	2	515	CLA	CMB-C2B	-2.11	1.47	1.51
21	B	827	CLA	C3D-C2D	2.11	1.44	1.39
21	F	401	CLA	O2D-CED	-2.11	1.40	1.45
21	12	508	CLA	C1D-C2D	2.11	1.49	1.45
21	7	702	CLA	C1C-C2C	2.11	1.48	1.44
21	9	902	CLA	C1B-CHB	2.11	1.46	1.41
21	4	703	CLA	C4B-CHC	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	810	CLA	C4D-CHA	2.11	1.45	1.38
21	A	802	CLA	CMA-C3A	-2.10	1.48	1.53
21	1	507	CLA	C4B-CHC	2.10	1.46	1.41
21	11	702	CLA	C4D-CHA	2.10	1.45	1.38
21	A	832	CLA	C4C-C3C	2.10	1.48	1.45
21	3	708	CLA	C4B-NB	-2.10	1.33	1.35
21	9	910	CLA	MG-NA	2.10	2.11	2.06
21	B	815	CLA	C1C-C2C	2.10	1.48	1.44
21	1	516	CLA	C4D-CHA	2.10	1.45	1.38
21	B	806	CLA	C4C-C3C	2.10	1.48	1.45
21	B	817	CLA	CMA-C3A	-2.10	1.48	1.53
21	A	809	CLA	C3B-CAB	-2.10	1.43	1.47
21	A	806	CLA	CHD-C1D	2.10	1.42	1.38
21	A	812	CLA	C3D-C2D	2.10	1.44	1.39
21	A	839	CLA	O2D-CED	-2.10	1.40	1.45
21	3	711	CLA	C4D-CHA	2.10	1.45	1.38
21	A	808	CLA	C4C-C3C	2.10	1.48	1.45
21	B	826	CLA	C2A-C1A	-2.10	1.47	1.52
21	8	605	CLA	C4B-CHC	2.10	1.46	1.41
21	B	836	CLA	C4D-CHA	2.10	1.45	1.38
21	12	502	CLA	C1B-CHB	2.10	1.46	1.41
21	9	912	CLA	C1C-NC	-2.10	1.34	1.37
21	11	711	CLA	C1B-CHB	2.09	1.46	1.41
21	5	701	CLA	MG-ND	-2.09	2.01	2.05
21	B	828	CLA	C2A-C1A	-2.09	1.47	1.52
28	4	712	DD6	C25-C26	-2.09	1.37	1.43
21	2	506	CLA	C1B-CHB	2.09	1.46	1.41
21	9	912	CLA	C4B-CHC	2.09	1.46	1.41
21	10	708	CLA	C4B-CHC	2.09	1.46	1.41
21	B	807	CLA	C3D-C2D	2.09	1.44	1.39
21	A	839	CLA	O2D-CGD	2.09	1.38	1.33
21	7	708	CLA	C4B-NB	-2.09	1.33	1.35
21	1	509	CLA	MG-ND	-2.09	2.01	2.05
21	4	702	CLA	C4B-NB	-2.09	1.33	1.35
21	B	803	CLA	C4D-CHA	2.09	1.45	1.38
21	5	706	CLA	C1C-C2C	2.09	1.48	1.44
21	B	824	CLA	C3A-C2A	-2.09	1.48	1.54
21	11	701	CLA	C1B-CHB	2.09	1.46	1.41
24	J	102	BCR	C11-C10	-2.09	1.37	1.43
21	12	503	CLA	C1B-CHB	2.09	1.46	1.41
21	5	708	CLA	C1B-CHB	2.09	1.46	1.41
21	9	907	CLA	C4D-CHA	2.09	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	904	CLA	C4B-NB	-2.09	1.33	1.35
21	12	508	CLA	C3D-C4D	-2.08	1.39	1.44
24	A	847	BCR	C15-C14	-2.08	1.37	1.43
21	2	504	CLA	C4B-CHC	2.08	1.46	1.41
21	5	701	CLA	C3D-C4D	-2.08	1.39	1.44
21	1	505	CLA	C1B-CHB	2.08	1.46	1.41
21	A	834	CLA	C4C-C3C	2.08	1.48	1.45
21	B	839	CLA	C4B-CHC	2.08	1.46	1.41
21	7	713	CLA	C4B-CHC	2.08	1.46	1.41
21	J	101	CLA	C1C-C2C	2.08	1.48	1.44
21	A	808	CLA	CMC-C2C	-2.08	1.46	1.50
21	A	834	CLA	CHD-C1D	2.08	1.42	1.38
21	11	701	CLA	C1C-C2C	2.08	1.48	1.44
21	3	702	CLA	C4B-NB	-2.08	1.33	1.35
21	A	813	CLA	C2A-C1A	-2.08	1.47	1.52
21	A	833	CLA	C1B-CHB	2.08	1.46	1.41
21	9	911	CLA	C4B-CHC	2.08	1.46	1.41
21	1	504	CLA	C1C-C2C	2.07	1.48	1.44
21	6	914	CLA	C4C-C3C	2.07	1.48	1.45
21	A	808	CLA	CHD-C1D	2.07	1.42	1.38
22	A	845	PQN	C8-C7	2.07	1.43	1.38
21	10	707	CLA	C1C-C2C	2.07	1.48	1.44
21	4	708	CLA	C4C-C3C	2.07	1.48	1.45
21	B	815	CLA	C3B-C2B	2.07	1.43	1.40
21	A	805	CLA	C4D-CHA	2.07	1.45	1.38
21	6	904	CLA	C1B-CHB	2.07	1.46	1.41
21	B	833	CLA	O2D-CED	-2.07	1.40	1.45
21	11	707	CLA	C1C-NC	-2.07	1.34	1.37
21	3	707	CLA	C4B-CHC	2.07	1.46	1.41
21	7	712	CLA	C1C-NC	-2.07	1.34	1.37
21	1	514	CLA	C4C-C3C	2.07	1.48	1.45
21	3	703	CLA	C4B-NB	-2.06	1.33	1.35
28	3	718	DD6	C3-C2	-2.06	1.37	1.43
21	2	511	CLA	C4D-CHA	2.06	1.45	1.38
21	A	804	CLA	C4D-CHA	2.06	1.45	1.38
21	11	711	CLA	C1D-C2D	2.06	1.49	1.45
21	B	808	CLA	CBD-CGD	-2.06	1.46	1.52
21	A	835	CLA	C4D-CHA	2.06	1.45	1.38
21	13	501	CLA	C1C-NC	-2.06	1.34	1.37
21	6	905	CLA	C4B-CHC	2.06	1.46	1.41
21	A	830	CLA	CBD-CGD	-2.06	1.46	1.52
21	A	828	CLA	CBD-CGD	-2.06	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	801	CLA	C4D-CHA	2.06	1.45	1.38
21	B	820	CLA	C4D-CHA	2.06	1.45	1.38
21	A	822	CLA	C4D-CHA	2.06	1.45	1.38
22	A	845	PQN	C2-C1	-2.06	1.43	1.48
21	9	907	CLA	C1C-NC	-2.06	1.34	1.37
24	A	847	BCR	C2-C3	-2.06	1.47	1.52
21	3	705	CLA	C4C-C3C	2.05	1.48	1.45
21	B	804	CLA	C3B-CAB	-2.05	1.43	1.47
21	3	701	CLA	C1A-CHA	2.05	1.51	1.43
21	6	914	CLA	C1B-NB	-2.05	1.33	1.35
21	1	509	CLA	C4C-C3C	2.05	1.48	1.45
21	10	711	CLA	C4C-C3C	2.05	1.48	1.45
21	6	908	CLA	C1B-NB	-2.05	1.33	1.35
28	8	616	DD6	C25-C26	-2.05	1.37	1.43
21	B	811	CLA	C3D-C4D	-2.05	1.39	1.44
21	J	101	CLA	C3D-C2D	2.05	1.44	1.39
21	9	914	CLA	C1C-C2C	2.05	1.48	1.44
21	7	710	CLA	C1B-CHB	2.05	1.46	1.41
21	A	804	CLA	C1B-CHB	2.05	1.46	1.41
21	4	711	CLA	CBA-CGA	2.05	1.55	1.50
21	2	504	CLA	C1B-CHB	2.05	1.46	1.41
28	12	510	DD6	C25-C26	-2.05	1.37	1.43
21	2	513	CLA	C1B-CHB	2.05	1.46	1.41
21	3	701	CLA	C3A-C2A	-2.05	1.52	1.54
21	10	711	CLA	C1B-CHB	2.05	1.46	1.41
21	8	612	CLA	C2A-C1A	-2.05	1.47	1.52
21	A	839	CLA	C1C-C2C	2.05	1.48	1.44
21	1	513	CLA	C4C-C3C	2.04	1.48	1.45
21	F	404	CLA	C2A-C1A	-2.04	1.47	1.52
24	B	846	BCR	C20-C21	-2.04	1.37	1.43
21	2	509	CLA	C4D-CHA	2.04	1.45	1.38
21	8	614	CLA	MG-ND	-2.04	2.01	2.05
21	6	912	CLA	C1B-CHB	2.04	1.46	1.41
21	8	610	CLA	C4D-CHA	2.04	1.45	1.38
24	J	103	BCR	C20-C21	-2.04	1.37	1.43
21	8	613	CLA	C4B-NB	-2.04	1.33	1.35
21	1	517	CLA	C1B-CHB	2.04	1.46	1.41
20	A	801	CL0	CAC-C3C	-2.04	1.45	1.51
21	B	804	CLA	C4C-C3C	2.04	1.48	1.45
24	B	841	BCR	C15-C14	-2.04	1.37	1.43
21	B	816	CLA	C4B-CHC	2.04	1.46	1.41
21	B	801	CLA	CMA-C3A	2.04	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	902	CLA	C3D-CAD	2.04	1.52	1.45
21	1	510	CLA	C1B-NB	-2.04	1.33	1.35
21	11	705	CLA	C4D-CHA	2.04	1.45	1.38
21	10	710	CLA	C1B-CHB	2.03	1.46	1.41
21	5	701	CLA	C4D-CHA	2.03	1.45	1.38
21	9	903	CLA	C4D-CHA	2.03	1.45	1.38
21	A	802	CLA	CBD-CGD	-2.03	1.46	1.52
21	11	710	CLA	C4B-CHC	2.03	1.46	1.41
21	4	706	CLA	C1C-NC	-2.03	1.34	1.37
21	1	506	CLA	C1B-CHB	2.03	1.46	1.41
21	B	816	CLA	C4C-C3C	2.03	1.48	1.45
21	3	704	CLA	C4C-C3C	2.03	1.48	1.45
21	B	807	CLA	CBD-CGD	-2.03	1.46	1.52
21	B	839	CLA	C2A-C1A	-2.03	1.47	1.52
21	B	801	CLA	C4B-CHC	2.03	1.46	1.41
21	12	501	CLA	C1C-C2C	2.03	1.48	1.44
21	B	829	CLA	C4B-NB	2.03	1.37	1.35
21	A	838	CLA	C2A-C1A	-2.03	1.47	1.52
21	12	502	CLA	C4B-CHC	2.03	1.46	1.41
21	2	514	CLA	MG-NA	2.03	2.11	2.06
21	5	701	CLA	C4C-C3C	2.03	1.48	1.45
21	B	822	CLA	C1B-CHB	2.03	1.46	1.41
21	B	815	CLA	C4D-CHA	2.02	1.45	1.38
21	9	910	CLA	C4B-CHC	2.02	1.46	1.41
21	B	819	CLA	C3D-C4D	-2.02	1.39	1.44
21	4	701	CLA	C4B-CHC	2.02	1.46	1.41
28	6	916	DD6	C24-C1	-2.02	1.41	1.45
28	12	509	DD6	C13-C11	-2.02	1.41	1.45
21	9	904	CLA	C4B-CHC	2.02	1.46	1.41
21	1	501	CLA	C3D-C4D	-2.02	1.39	1.44
21	10	711	CLA	C1C-C2C	2.02	1.48	1.44
21	11	702	CLA	C2A-C1A	-2.02	1.47	1.52
21	1	517	CLA	C1B-NB	-2.02	1.33	1.35
24	A	849	BCR	C11-C10	-2.02	1.37	1.43
21	B	835	CLA	C1B-CHB	2.02	1.46	1.41
21	4	708	CLA	C1C-C2C	2.02	1.48	1.44
21	2	516	CLA	C1B-CHB	2.02	1.46	1.41
21	B	836	CLA	C1B-NB	-2.02	1.33	1.35
21	11	710	CLA	C1C-NC	-2.02	1.34	1.37
28	5	712	DD6	C4-C5	-2.01	1.37	1.43
24	M	102	BCR	C17-C18	2.01	1.38	1.35
21	10	708	CLA	C1B-CHB	2.01	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	821	CLA	C4D-CHA	2.01	1.45	1.38
21	7	710	CLA	C4B-CHC	2.01	1.46	1.41
24	A	851	BCR	C1-C6	-2.01	1.51	1.53
21	2	504	CLA	C1D-ND	2.01	1.40	1.37
21	A	843	CLA	C4D-CHA	2.01	1.45	1.38
21	A	835	CLA	C2A-C1A	-2.01	1.47	1.52
21	B	808	CLA	C1B-CHB	2.01	1.46	1.41
21	B	822	CLA	CBA-CGA	2.01	1.55	1.50
21	7	703	CLA	C3D-C4D	-2.01	1.39	1.44
21	13	503	CLA	C4B-CHC	2.01	1.46	1.41
21	9	905	CLA	C3D-C4D	-2.01	1.39	1.44
21	4	707	CLA	C1A-CHA	2.01	1.51	1.43
21	10	707	CLA	C1C-NC	-2.01	1.34	1.37
21	6	908	CLA	C1C-C2C	2.01	1.48	1.44
21	13	503	CLA	C1C-NC	-2.01	1.34	1.37
21	3	715	CLA	C2A-C1A	-2.00	1.47	1.52
21	10	709	CLA	C1C-C2C	2.00	1.48	1.44
21	2	506	CLA	C4D-CHA	2.00	1.45	1.38
21	J	101	CLA	C3A-C2A	-2.00	1.48	1.54
21	9	907	CLA	C1C-C2C	2.00	1.48	1.44
21	10	711	CLA	C4B-NB	-2.00	1.33	1.35
24	J	103	BCR	C1-C6	-2.00	1.51	1.53
21	12	503	CLA	C1C-NC	-2.00	1.34	1.37
21	11	710	CLA	C1D-C2D	2.00	1.49	1.45
21	B	803	CLA	C4B-NB	-2.00	1.33	1.35
21	8	604	CLA	CMB-C2B	-2.00	1.47	1.51
21	9	904	CLA	C1C-C2C	2.00	1.48	1.44
21	1	516	CLA	C1B-CHB	2.00	1.46	1.41
21	7	703	CLA	C4D-CHA	2.00	1.45	1.38
21	4	708	CLA	C1A-CHA	2.00	1.51	1.43
21	A	808	CLA	C1B-CHB	2.00	1.46	1.41
21	A	839	CLA	O1D-CGD	2.00	1.26	1.21

All (7093) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	829	CLA	C2D-C1D-ND	12.22	119.11	110.10
21	A	834	CLA	C1D-ND-C4D	-11.90	97.88	106.33
21	A	827	CLA	C1D-ND-C4D	-11.77	97.98	106.33
21	9	907	CLA	C1D-ND-C4D	-11.63	98.07	106.33
21	A	823	CLA	C1D-ND-C4D	-11.38	98.25	106.33
21	4	701	CLA	C1D-ND-C4D	-11.30	98.31	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	815	CLA	C1D-ND-C4D	-11.27	98.33	106.33
21	B	829	CLA	C1D-ND-C4D	-11.15	98.41	106.33
21	B	838	CLA	C2D-C1D-ND	10.93	118.16	110.10
21	A	828	CLA	C2D-C1D-ND	10.89	118.13	110.10
21	5	710	CLA	C1D-ND-C4D	-10.81	98.66	106.33
21	B	821	CLA	C1D-ND-C4D	-10.77	98.69	106.33
21	2	507	CLA	C1D-ND-C4D	-10.75	98.70	106.33
21	B	810	CLA	C1D-ND-C4D	-10.74	98.71	106.33
21	B	818	CLA	C1D-ND-C4D	-10.72	98.72	106.33
21	B	820	CLA	C1D-ND-C4D	-10.67	98.76	106.33
21	A	824	CLA	C1D-ND-C4D	-10.56	98.83	106.33
21	3	702	CLA	C1D-ND-C4D	-10.53	98.85	106.33
21	10	705	CLA	C1D-ND-C4D	-10.52	98.86	106.33
21	B	820	CLA	C2D-C1D-ND	10.50	117.84	110.10
21	1	508	CLA	C1D-ND-C4D	-10.39	98.95	106.33
21	9	910	CLA	C1D-ND-C4D	-10.38	98.96	106.33
21	8	603	CLA	C1D-ND-C4D	-10.37	98.97	106.33
21	4	705	CLA	C1D-ND-C4D	-10.35	98.98	106.33
21	A	805	CLA	C1D-ND-C4D	-10.34	98.99	106.33
21	B	802	CLA	C2D-C1D-ND	10.30	117.69	110.10
21	9	903	CLA	C1D-ND-C4D	-10.29	99.02	106.33
21	3	705	CLA	C1D-ND-C4D	-10.28	99.03	106.33
21	A	817	CLA	C1D-ND-C4D	-10.27	99.04	106.33
21	B	832	CLA	C1D-ND-C4D	-10.26	99.04	106.33
21	B	802	CLA	C1D-ND-C4D	-10.23	99.07	106.33
21	B	826	CLA	C1D-ND-C4D	-10.23	99.07	106.33
21	11	710	CLA	C1D-ND-C4D	-10.23	99.07	106.33
21	8	604	CLA	C1D-ND-C4D	-10.22	99.07	106.33
21	B	803	CLA	C2D-C1D-ND	10.22	117.64	110.10
21	3	710	CLA	C1D-ND-C4D	-10.17	99.11	106.33
21	A	816	CLA	C1D-ND-C4D	-10.16	99.12	106.33
21	B	821	CLA	C2D-C1D-ND	10.15	117.58	110.10
21	A	821	CLA	C1D-ND-C4D	-10.14	99.13	106.33
21	4	702	CLA	C1D-ND-C4D	-10.13	99.14	106.33
21	B	831	CLA	C1D-ND-C4D	-10.12	99.15	106.33
21	B	828	CLA	C1D-ND-C4D	-10.11	99.16	106.33
21	A	834	CLA	C2D-C1D-ND	10.10	117.55	110.10
21	F	404	CLA	C1D-ND-C4D	-10.09	99.16	106.33
21	A	831	CLA	C1D-ND-C4D	-10.09	99.17	106.33
21	4	703	CLA	C1D-ND-C4D	-10.06	99.19	106.33
21	F	401	CLA	C2D-C1D-ND	10.06	117.51	110.10
21	B	824	CLA	C1D-ND-C4D	-10.05	99.20	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	704	CLA	C1D-ND-C4D	-10.05	99.20	106.33
21	A	824	CLA	C2D-C1D-ND	10.05	117.51	110.10
21	1	513	CLA	C1D-ND-C4D	-10.00	99.23	106.33
21	9	913	CLA	C1D-ND-C4D	-9.99	99.24	106.33
21	4	710	CLA	C1D-ND-C4D	-9.98	99.25	106.33
21	B	804	CLA	C1D-ND-C4D	-9.98	99.25	106.33
21	2	510	CLA	C1D-ND-C4D	-9.95	99.27	106.33
21	2	508	CLA	C1D-ND-C4D	-9.94	99.27	106.33
21	A	832	CLA	C1D-ND-C4D	-9.94	99.27	106.33
21	A	837	CLA	C1D-ND-C4D	-9.92	99.29	106.33
21	A	832	CLA	C2D-C1D-ND	9.89	117.39	110.10
21	B	803	CLA	C1D-ND-C4D	-9.89	99.31	106.33
21	B	828	CLA	C2D-C1D-ND	9.85	117.36	110.10
21	6	903	CLA	C1D-ND-C4D	-9.82	99.36	106.33
21	B	812	CLA	C1D-ND-C4D	-9.80	99.37	106.33
21	3	706	CLA	C1D-ND-C4D	-9.78	99.39	106.33
21	B	817	CLA	C1D-ND-C4D	-9.77	99.39	106.33
21	9	907	CLA	C2D-C1D-ND	9.77	117.30	110.10
21	2	512	CLA	C1D-ND-C4D	-9.73	99.42	106.33
21	3	710	CLA	C2D-C1D-ND	9.73	117.27	110.10
21	B	811	CLA	C1D-ND-C4D	-9.69	99.45	106.33
21	A	836	CLA	C1D-ND-C4D	-9.69	99.45	106.33
21	A	815	CLA	C2D-C1D-ND	9.69	117.24	110.10
21	12	501	CLA	C1D-ND-C4D	-9.69	99.45	106.33
21	A	828	CLA	C1D-ND-C4D	-9.69	99.45	106.33
21	A	862	CLA	O2D-CGD-CBD	9.68	128.46	111.27
21	1	509	CLA	C1D-ND-C4D	-9.66	99.47	106.33
21	A	844	CLA	C1D-ND-C4D	-9.66	99.48	106.33
21	12	506	CLA	C1D-ND-C4D	-9.65	99.48	106.33
21	2	513	CLA	C1D-ND-C4D	-9.65	99.48	106.33
21	10	704	CLA	C1D-ND-C4D	-9.65	99.48	106.33
21	4	709	CLA	C1D-ND-C4D	-9.64	99.49	106.33
21	A	835	CLA	C1D-ND-C4D	-9.64	99.49	106.33
21	7	703	CLA	C1D-ND-C4D	-9.63	99.50	106.33
21	9	902	CLA	C1D-ND-C4D	-9.61	99.51	106.33
21	8	607	CLA	C1D-ND-C4D	-9.61	99.51	106.33
21	9	911	CLA	C1D-ND-C4D	-9.60	99.51	106.33
21	10	712	CLA	C1D-ND-C4D	-9.60	99.52	106.33
21	A	840	CLA	O2D-CGD-CBD	9.59	128.31	111.27
21	2	509	CLA	C1D-ND-C4D	-9.58	99.53	106.33
21	6	914	CLA	C1D-ND-C4D	-9.58	99.53	106.33
21	A	808	CLA	C1D-ND-C4D	-9.57	99.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	839	CLA	C1D-ND-C4D	-9.57	99.54	106.33
21	9	906	CLA	C1D-ND-C4D	-9.56	99.54	106.33
21	10	709	CLA	C1D-ND-C4D	-9.56	99.55	106.33
21	5	710	CLA	C2D-C1D-ND	9.56	117.15	110.10
21	B	828	CLA	O2D-CGD-CBD	9.52	128.19	111.27
21	8	607	CLA	C2D-C1D-ND	9.52	117.12	110.10
21	12	508	CLA	C1D-ND-C4D	-9.51	99.58	106.33
21	A	812	CLA	C1D-ND-C4D	-9.50	99.59	106.33
21	8	604	CLA	C2D-C1D-ND	9.49	117.10	110.10
21	F	401	CLA	C1D-ND-C4D	-9.49	99.59	106.33
21	B	839	CLA	O2D-CGD-CBD	9.48	128.12	111.27
21	11	711	CLA	C1D-ND-C4D	-9.48	99.60	106.33
21	3	715	CLA	C1D-ND-C4D	-9.48	99.60	106.33
21	B	816	CLA	C1D-ND-C4D	-9.47	99.61	106.33
21	7	713	CLA	C1D-ND-C4D	-9.47	99.61	106.33
21	B	807	CLA	C1D-ND-C4D	-9.46	99.61	106.33
21	11	701	CLA	C1D-ND-C4D	-9.46	99.62	106.33
21	4	711	CLA	C1D-ND-C4D	-9.44	99.63	106.33
21	7	706	CLA	C1D-ND-C4D	-9.44	99.63	106.33
21	9	910	CLA	C2D-C1D-ND	9.43	117.06	110.10
21	5	711	CLA	C1D-ND-C4D	-9.43	99.63	106.33
21	10	703	CLA	C1D-ND-C4D	-9.42	99.64	106.33
21	1	504	CLA	C1D-ND-C4D	-9.42	99.64	106.33
21	12	503	CLA	C1D-ND-C4D	-9.40	99.66	106.33
21	1	501	CLA	C1D-ND-C4D	-9.38	99.67	106.33
21	7	702	CLA	C1D-ND-C4D	-9.38	99.67	106.33
21	2	504	CLA	C1D-ND-C4D	-9.38	99.67	106.33
21	6	909	CLA	C1D-ND-C4D	-9.38	99.67	106.33
21	A	821	CLA	C2D-C1D-ND	9.38	117.02	110.10
21	B	838	CLA	C1D-ND-C4D	-9.38	99.67	106.33
21	10	706	CLA	C1D-ND-C4D	-9.37	99.68	106.33
21	8	612	CLA	C1D-ND-C4D	-9.37	99.68	106.33
21	A	803	CLA	C1D-ND-C4D	-9.36	99.69	106.33
21	F	404	CLA	C2D-C1D-ND	9.34	116.99	110.10
21	A	862	CLA	C1D-ND-C4D	-9.31	99.72	106.33
21	B	822	CLA	C1D-ND-C4D	-9.31	99.72	106.33
21	10	707	CLA	C1D-ND-C4D	-9.30	99.73	106.33
21	9	908	CLA	C1D-ND-C4D	-9.29	99.74	106.33
21	11	704	CLA	C1D-ND-C4D	-9.27	99.75	106.33
21	B	832	CLA	C2D-C1D-ND	9.26	116.93	110.10
21	7	705	CLA	C2D-C1D-ND	9.26	116.93	110.10
21	6	913	CLA	C1D-ND-C4D	-9.25	99.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	914	CLA	C1D-ND-C4D	-9.25	99.76	106.33
21	A	839	CLA	O2D-CGD-O1D	-9.25	105.76	123.84
21	1	515	CLA	C1D-ND-C4D	-9.23	99.77	106.33
21	11	708	CLA	C1D-ND-C4D	-9.23	99.78	106.33
21	5	709	CLA	C1D-ND-C4D	-9.22	99.78	106.33
21	4	708	CLA	C1D-ND-C4D	-9.22	99.78	106.33
21	3	713	CLA	C1D-ND-C4D	-9.21	99.79	106.33
21	A	811	CLA	O2D-CGD-CBD	9.21	127.64	111.27
21	4	707	CLA	C1D-ND-C4D	-9.20	99.80	106.33
21	B	836	CLA	C1D-ND-C4D	-9.18	99.81	106.33
21	1	511	CLA	C1D-ND-C4D	-9.18	99.81	106.33
21	B	834	CLA	C1D-ND-C4D	-9.18	99.82	106.33
21	3	701	CLA	C1D-ND-C4D	-9.17	99.82	106.33
21	A	823	CLA	C2D-C1D-ND	9.17	116.86	110.10
21	9	905	CLA	C1D-ND-C4D	-9.17	99.82	106.33
21	7	712	CLA	C1D-ND-C4D	-9.16	99.83	106.33
21	A	862	CLA	C2D-C1D-ND	9.16	116.85	110.10
21	J	101	CLA	C1D-ND-C4D	-9.15	99.84	106.33
21	3	709	CLA	C1D-ND-C4D	-9.15	99.84	106.33
21	A	840	CLA	C1D-ND-C4D	-9.14	99.84	106.33
21	9	903	CLA	C2D-C1D-ND	9.14	116.84	110.10
21	8	605	CLA	C1D-ND-C4D	-9.14	99.85	106.33
21	A	825	CLA	C2D-C1D-ND	9.13	116.83	110.10
21	7	714	CLA	C2D-C1D-ND	9.13	116.83	110.10
21	8	614	CLA	C1D-ND-C4D	-9.12	99.86	106.33
21	2	517	CLA	C1D-ND-C4D	-9.12	99.86	106.33
21	9	912	CLA	C1D-ND-C4D	-9.12	99.86	106.33
21	A	831	CLA	C2D-C1D-ND	9.11	116.82	110.10
21	A	841	CLA	C2D-C1D-ND	9.11	116.81	110.10
21	3	704	CLA	C1D-ND-C4D	-9.10	99.87	106.33
21	B	809	CLA	C1D-ND-C4D	-9.10	99.87	106.33
21	4	706	CLA	C1D-ND-C4D	-9.09	99.88	106.33
21	10	710	CLA	C1D-ND-C4D	-9.08	99.88	106.33
21	A	818	CLA	C1D-ND-C4D	-9.08	99.89	106.33
21	A	843	CLA	C1D-ND-C4D	-9.06	99.90	106.33
21	7	708	CLA	C1D-ND-C4D	-9.05	99.91	106.33
21	B	814	CLA	C1D-ND-C4D	-9.05	99.91	106.33
21	1	506	CLA	C1D-ND-C4D	-9.01	99.93	106.33
21	11	702	CLA	C1D-ND-C4D	-9.00	99.94	106.33
21	A	826	CLA	C1D-ND-C4D	-9.00	99.94	106.33
21	8	608	CLA	C1D-ND-C4D	-9.00	99.94	106.33
21	2	503	CLA	C1D-ND-C4D	-8.99	99.95	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	714	CLA	C1D-ND-C4D	-8.99	99.95	106.33
21	1	512	CLA	C1D-ND-C4D	-8.99	99.95	106.33
21	B	823	CLA	C1D-ND-C4D	-8.98	99.95	106.33
21	4	701	CLA	C2D-C1D-ND	8.96	116.71	110.10
21	2	511	CLA	C1D-ND-C4D	-8.95	99.98	106.33
21	A	810	CLA	C2D-C1D-ND	8.94	116.69	110.10
21	8	611	CLA	C1D-ND-C4D	-8.93	99.99	106.33
21	B	814	CLA	C2D-C1D-ND	8.93	116.68	110.10
21	A	819	CLA	C1D-ND-C4D	-8.93	99.99	106.33
21	7	705	CLA	C1D-ND-C4D	-8.93	99.99	106.33
20	A	801	CL0	C1D-ND-C4D	-8.92	100.00	106.33
21	6	910	CLA	C1D-ND-C4D	-8.92	100.00	106.33
21	11	709	CLA	C1D-ND-C4D	-8.90	100.01	106.33
21	B	836	CLA	C2D-C1D-ND	8.90	116.66	110.10
21	4	702	CLA	C2D-C1D-ND	8.90	116.66	110.10
21	3	711	CLA	C1D-ND-C4D	-8.88	100.03	106.33
21	10	705	CLA	C2D-C1D-ND	8.86	116.63	110.10
21	B	818	CLA	C2D-C1D-ND	8.85	116.62	110.10
21	13	502	CLA	C1D-ND-C4D	-8.84	100.05	106.33
21	6	911	CLA	C1D-ND-C4D	-8.83	100.06	106.33
21	5	708	CLA	C1D-ND-C4D	-8.83	100.06	106.33
21	B	813	CLA	C1D-ND-C4D	-8.82	100.07	106.33
21	8	613	CLA	C1D-ND-C4D	-8.82	100.07	106.33
21	12	505	CLA	C1D-ND-C4D	-8.81	100.07	106.33
21	A	838	CLA	C2D-C1D-ND	8.81	116.60	110.10
21	5	706	CLA	C1D-ND-C4D	-8.77	100.11	106.33
21	4	704	CLA	C1D-ND-C4D	-8.74	100.12	106.33
21	7	702	CLA	C2D-C1D-ND	8.74	116.54	110.10
21	A	839	CLA	C1D-ND-C4D	-8.74	100.13	106.33
21	10	711	CLA	C1D-ND-C4D	-8.73	100.13	106.33
21	9	912	CLA	C2D-C1D-ND	8.72	116.53	110.10
21	A	811	CLA	C1D-ND-C4D	-8.71	100.15	106.33
21	A	805	CLA	C2D-C1D-ND	8.70	116.52	110.10
21	B	831	CLA	C2D-C1D-ND	8.68	116.50	110.10
21	F	403	CLA	C1D-ND-C4D	-8.68	100.17	106.33
21	8	606	CLA	C1D-ND-C4D	-8.68	100.17	106.33
21	A	844	CLA	C2D-C1D-ND	8.67	116.49	110.10
21	11	705	CLA	C1D-ND-C4D	-8.66	100.18	106.33
21	8	614	CLA	C2D-C1D-ND	8.66	116.48	110.10
21	2	509	CLA	C2D-C1D-ND	8.65	116.47	110.10
21	A	810	CLA	C1D-ND-C4D	-8.64	100.20	106.33
21	A	816	CLA	C2D-C1D-ND	8.64	116.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	707	CLA	C2D-C1D-ND	8.63	116.46	110.10
21	6	912	CLA	C1D-ND-C4D	-8.63	100.21	106.33
21	A	804	CLA	C2D-C1D-ND	8.63	116.46	110.10
21	2	510	CLA	C2D-C1D-ND	8.61	116.45	110.10
21	1	513	CLA	C2D-C1D-ND	8.60	116.44	110.10
21	5	701	CLA	C1D-ND-C4D	-8.60	100.22	106.33
21	4	710	CLA	C2D-C1D-ND	8.60	116.44	110.10
21	6	905	CLA	C1D-ND-C4D	-8.59	100.23	106.33
21	7	710	CLA	O2D-CGD-CBD	8.58	126.51	111.27
21	A	813	CLA	C1D-ND-C4D	-8.58	100.24	106.33
21	5	703	CLA	C1D-ND-C4D	-8.57	100.24	106.33
21	2	513	CLA	C2D-C1D-ND	8.57	116.42	110.10
21	A	838	CLA	C1D-ND-C4D	-8.57	100.25	106.33
21	9	904	CLA	C1D-ND-C4D	-8.55	100.26	106.33
21	13	501	CLA	C1D-ND-C4D	-8.55	100.26	106.33
21	A	842	CLA	C1D-ND-C4D	-8.54	100.27	106.33
21	A	811	CLA	C2D-C1D-ND	8.53	116.39	110.10
21	B	833	CLA	O2D-CGD-O1D	-8.52	107.17	123.84
21	A	804	CLA	C1D-ND-C4D	-8.52	100.28	106.33
21	10	709	CLA	C2D-C1D-ND	8.52	116.38	110.10
21	1	510	CLA	C1D-ND-C4D	-8.52	100.28	106.33
21	9	907	CLA	CMD-C2D-C1D	8.51	139.72	124.71
21	A	829	CLA	C1D-ND-C4D	-8.51	100.29	106.33
21	4	705	CLA	C2D-C1D-ND	8.50	116.37	110.10
21	5	707	CLA	C1D-ND-C4D	-8.50	100.30	106.33
21	1	509	CLA	C2D-C1D-ND	8.49	116.36	110.10
21	A	803	CLA	C2D-C1D-ND	8.49	116.36	110.10
21	10	712	CLA	C2D-C1D-ND	8.49	116.36	110.10
21	3	707	CLA	C1D-ND-C4D	-8.49	100.30	106.33
21	8	613	CLA	C2D-C1D-ND	8.48	116.35	110.10
21	B	827	CLA	C1D-ND-C4D	-8.47	100.32	106.33
21	B	812	CLA	C2D-C1D-ND	8.44	116.32	110.10
21	B	831	CLA	CAC-C3C-C4C	8.44	135.76	124.81
21	A	825	CLA	C1D-ND-C4D	-8.42	100.35	106.33
21	B	819	CLA	C1D-ND-C4D	-8.41	100.36	106.33
21	11	703	CLA	C1D-ND-C4D	-8.39	100.37	106.33
21	3	712	CLA	C1D-ND-C4D	-8.39	100.38	106.33
21	A	820	CLA	C1D-ND-C4D	-8.39	100.38	106.33
21	6	906	CLA	C1D-ND-C4D	-8.38	100.38	106.33
21	12	506	CLA	C2D-C1D-ND	8.37	116.27	110.10
21	2	506	CLA	C1D-ND-C4D	-8.37	100.39	106.33
21	B	817	CLA	C2D-C1D-ND	8.37	116.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	809	CLA	C1D-ND-C4D	-8.36	100.39	106.33
21	B	801	CLA	C1D-ND-C4D	-8.35	100.41	106.33
21	B	830	CLA	C1D-ND-C4D	-8.35	100.41	106.33
21	B	808	CLA	C1D-ND-C4D	-8.34	100.41	106.33
21	6	907	CLA	C1D-ND-C4D	-8.34	100.41	106.33
21	A	836	CLA	C2D-C1D-ND	8.33	116.25	110.10
21	A	814	CLA	C1D-ND-C4D	-8.33	100.42	106.33
21	9	909	CLA	C1D-ND-C4D	-8.32	100.42	106.33
21	A	833	CLA	O2A-C1-C2	8.32	130.49	108.64
21	A	833	CLA	C1D-ND-C4D	-8.31	100.43	106.33
21	A	817	CLA	C2D-C1D-ND	8.31	116.23	110.10
21	A	841	CLA	C1D-ND-C4D	-8.30	100.44	106.33
21	6	903	CLA	C2D-C1D-ND	8.29	116.22	110.10
21	A	822	CLA	C1D-ND-C4D	-8.28	100.45	106.33
21	10	708	CLA	C1D-ND-C4D	-8.27	100.46	106.33
21	8	606	CLA	C2D-C1D-ND	8.25	116.18	110.10
21	8	610	CLA	C1D-ND-C4D	-8.23	100.49	106.33
21	2	503	CLA	C2D-C1D-ND	8.23	116.17	110.10
21	B	811	CLA	C2D-C1D-ND	8.22	116.16	110.10
21	B	835	CLA	C1D-ND-C4D	-8.21	100.50	106.33
21	1	505	CLA	C1D-ND-C4D	-8.21	100.50	106.33
21	4	703	CLA	C2D-C1D-ND	8.21	116.15	110.10
21	A	808	CLA	C2D-C1D-ND	8.20	116.15	110.10
21	12	507	CLA	C1D-ND-C4D	-8.20	100.51	106.33
21	B	806	CLA	C1D-ND-C4D	-8.18	100.52	106.33
21	B	824	CLA	C2D-C1D-ND	8.18	116.14	110.10
21	1	514	CLA	C1D-ND-C4D	-8.18	100.52	106.33
21	3	702	CLA	C2D-C1D-ND	8.18	116.13	110.10
21	2	514	CLA	C1D-ND-C4D	-8.18	100.53	106.33
21	3	701	CLA	C2D-C1D-ND	8.17	116.13	110.10
21	6	909	CLA	C2D-C1D-ND	8.17	116.12	110.10
21	9	911	CLA	C2D-C1D-ND	8.17	116.12	110.10
21	A	806	CLA	C1D-ND-C4D	-8.17	100.53	106.33
21	2	512	CLA	C2D-C1D-ND	8.16	116.12	110.10
21	3	705	CLA	C2D-C1D-ND	8.16	116.11	110.10
21	7	711	CLA	C1D-ND-C4D	-8.15	100.54	106.33
21	2	516	CLA	C1D-ND-C4D	-8.13	100.56	106.33
20	A	801	CL0	O2D-CGD-CBD	8.13	125.72	111.27
21	6	910	CLA	O2D-CGD-CBD	8.13	125.71	111.27
21	A	831	CLA	O2D-CGD-CBD	8.11	125.68	111.27
21	B	822	CLA	C2D-C1D-ND	8.11	116.08	110.10
21	9	905	CLA	C2D-C1D-ND	8.09	116.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	515	CLA	C1D-ND-C4D	-8.09	100.59	106.33
21	2	517	CLA	C2D-C1D-ND	8.08	116.06	110.10
21	7	712	CLA	C2D-C1D-ND	8.08	116.06	110.10
21	10	707	CLA	C2D-C1D-ND	8.08	116.06	110.10
21	7	707	CLA	C2D-C1D-ND	8.07	116.05	110.10
21	A	827	CLA	C2D-C1D-ND	8.06	116.05	110.10
21	1	514	CLA	C2D-C1D-ND	8.06	116.05	110.10
21	6	904	CLA	C1D-ND-C4D	-8.05	100.62	106.33
21	3	704	CLA	C2D-C1D-ND	8.04	116.03	110.10
21	5	711	CLA	C2D-C1D-ND	8.04	116.03	110.10
21	9	906	CLA	C2D-C1D-ND	8.02	116.02	110.10
21	6	913	CLA	C2D-C1D-ND	8.01	116.01	110.10
21	5	706	CLA	C2D-C1D-ND	8.01	116.00	110.10
21	10	706	CLA	C2D-C1D-ND	8.00	116.00	110.10
21	7	708	CLA	C2D-C1D-ND	7.99	115.99	110.10
21	A	843	CLA	C2D-C1D-ND	7.98	115.99	110.10
21	12	502	CLA	C1D-ND-C4D	-7.98	100.67	106.33
21	9	913	CLA	C2D-C1D-ND	7.98	115.98	110.10
21	3	706	CLA	CMD-C2D-C1D	7.97	138.76	124.71
21	B	837	CLA	C1D-ND-C4D	-7.97	100.67	106.33
21	F	403	CLA	C2D-C1D-ND	7.96	115.97	110.10
21	1	511	CLA	C2D-C1D-ND	7.96	115.97	110.10
21	B	823	CLA	C2D-C1D-ND	7.96	115.97	110.10
21	B	830	CLA	CMD-C2D-C1D	7.96	138.73	124.71
21	2	504	CLA	C2D-C1D-ND	7.94	115.96	110.10
21	3	714	CLA	C1D-ND-C4D	-7.94	100.69	106.33
21	A	829	CLA	C2D-C1D-ND	7.94	115.96	110.10
21	A	842	CLA	O2D-CGD-CBD	7.94	125.37	111.27
21	12	508	CLA	C2D-C1D-ND	7.92	115.94	110.10
21	7	710	CLA	C1D-ND-C4D	-7.91	100.72	106.33
21	5	705	CLA	C1D-ND-C4D	-7.91	100.72	106.33
21	11	711	CLA	C2D-C1D-ND	7.90	115.92	110.10
21	13	502	CLA	C2D-C1D-ND	7.89	115.92	110.10
21	12	504	CLA	C1D-ND-C4D	-7.89	100.73	106.33
21	3	708	CLA	C1D-ND-C4D	-7.89	100.73	106.33
21	9	914	CLA	C2D-C1D-ND	7.89	115.92	110.10
21	1	517	CLA	C1D-ND-C4D	-7.88	100.74	106.33
21	13	503	CLA	C1D-ND-C4D	-7.87	100.75	106.33
21	7	703	CLA	C2D-C1D-ND	7.86	115.90	110.10
21	10	708	CLA	C2D-C1D-ND	7.86	115.90	110.10
21	11	710	CLA	C2D-C1D-ND	7.86	115.90	110.10
21	2	507	CLA	C2D-C1D-ND	7.86	115.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	824	CLA	CHD-C4C-C3C	-7.84	113.31	124.84
21	5	704	CLA	C2D-C1D-ND	7.84	115.88	110.10
21	A	840	CLA	CMD-C2D-C1D	7.84	138.52	124.71
21	1	508	CLA	CMD-C2D-C1D	7.84	138.52	124.71
21	3	713	CLA	C2D-C1D-ND	7.82	115.87	110.10
21	12	505	CLA	C2D-C1D-ND	7.82	115.86	110.10
21	7	704	CLA	C1D-ND-C4D	-7.81	100.78	106.33
21	1	516	CLA	C1D-ND-C4D	-7.81	100.79	106.33
21	1	507	CLA	C1D-ND-C4D	-7.80	100.80	106.33
21	B	838	CLA	O2D-CGD-CBD	7.80	125.12	111.27
21	B	826	CLA	C2D-C1D-ND	7.79	115.85	110.10
21	B	816	CLA	C2D-C1D-ND	7.79	115.84	110.10
21	11	706	CLA	C2D-C1D-ND	7.79	115.84	110.10
21	11	707	CLA	C1D-ND-C4D	-7.78	100.81	106.33
21	1	512	CLA	C2D-C1D-ND	7.78	115.83	110.10
21	B	832	CLA	CHD-C4C-C3C	-7.77	113.42	124.84
21	7	707	CLA	C1D-ND-C4D	-7.76	100.82	106.33
21	A	821	CLA	O2D-CGD-CBD	7.76	125.06	111.27
21	B	815	CLA	C1D-ND-C4D	-7.75	100.83	106.33
21	7	709	CLA	C1D-ND-C4D	-7.75	100.83	106.33
21	8	603	CLA	C2D-C1D-ND	7.73	115.80	110.10
21	1	510	CLA	C2D-C1D-ND	7.73	115.80	110.10
21	9	902	CLA	C2D-C1D-ND	7.72	115.79	110.10
21	12	503	CLA	C2D-C1D-ND	7.71	115.78	110.10
21	A	831	CLA	O2D-CGD-O1D	-7.69	108.80	123.84
21	1	516	CLA	C2D-C1D-ND	7.67	115.75	110.10
21	A	819	CLA	C2D-C1D-ND	7.66	115.75	110.10
21	11	704	CLA	C2D-C1D-ND	7.65	115.74	110.10
21	10	711	CLA	C2D-C1D-ND	7.65	115.74	110.10
21	10	710	CLA	C2D-C1D-ND	7.65	115.74	110.10
21	2	510	CLA	O2D-CGD-CBD	7.64	124.85	111.27
21	3	703	CLA	CMD-C2D-C1D	7.64	138.18	124.71
21	11	706	CLA	C1D-ND-C4D	-7.64	100.91	106.33
21	1	508	CLA	C2D-C1D-ND	7.64	115.73	110.10
21	A	802	CLA	O2D-CGD-CBD	7.63	124.83	111.27
21	6	914	CLA	C2D-C1D-ND	7.63	115.73	110.10
21	A	837	CLA	C2D-C1D-ND	7.61	115.72	110.10
21	B	837	CLA	C2D-C1D-ND	7.61	115.71	110.10
21	5	702	CLA	C1D-ND-C4D	-7.59	100.94	106.33
21	A	818	CLA	C2D-C1D-ND	7.59	115.69	110.10
21	B	824	CLA	O2D-CGD-CBD	7.58	124.74	111.27
21	A	839	CLA	O1D-CGD-CBD	7.58	140.00	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	507	CLA	C2D-C1D-ND	7.58	115.69	110.10
21	B	806	CLA	CMD-C2D-C1D	7.58	138.07	124.71
21	4	706	CLA	C2D-C1D-ND	7.58	115.69	110.10
21	A	830	CLA	C1D-ND-C4D	-7.57	100.96	106.33
21	A	840	CLA	C2D-C1D-ND	7.56	115.68	110.10
21	3	714	CLA	C2D-C1D-ND	7.54	115.66	110.10
21	4	704	CLA	C2D-C1D-ND	7.53	115.66	110.10
21	8	608	CLA	CMD-C2D-C1D	7.53	137.98	124.71
21	A	820	CLA	O2D-CGD-CBD	7.51	124.61	111.27
21	11	701	CLA	C2D-C1D-ND	7.48	115.62	110.10
21	4	709	CLA	C2D-C1D-ND	7.47	115.61	110.10
21	12	501	CLA	C2D-C1D-ND	7.46	115.60	110.10
21	A	805	CLA	O2D-CGD-CBD	7.46	124.53	111.27
21	3	709	CLA	C2D-C1D-ND	7.46	115.60	110.10
21	5	709	CLA	C4A-NA-C1A	-7.44	103.36	106.71
21	9	908	CLA	CMD-C2D-C1D	7.44	137.83	124.71
21	1	515	CLA	C2D-C1D-ND	7.44	115.59	110.10
21	B	810	CLA	C2D-C1D-ND	7.44	115.58	110.10
21	A	815	CLA	CHD-C4C-C3C	-7.40	113.97	124.84
21	3	711	CLA	C2D-C1D-ND	7.38	115.55	110.10
21	B	836	CLA	O2D-CGD-CBD	7.38	124.39	111.27
21	B	809	CLA	C2D-C1D-ND	7.38	115.54	110.10
21	B	804	CLA	C2D-C1D-ND	7.38	115.54	110.10
21	8	608	CLA	C2D-C1D-ND	7.38	115.54	110.10
21	8	610	CLA	C2D-C1D-ND	7.38	115.54	110.10
21	10	704	CLA	C2D-C1D-ND	7.37	115.54	110.10
21	2	511	CLA	C4A-NA-C1A	-7.36	103.40	106.71
21	8	609	CLA	C1D-ND-C4D	-7.35	101.11	106.33
21	B	817	CLA	O2D-CGD-CBD	7.35	124.33	111.27
21	A	826	CLA	C2D-C1D-ND	7.35	115.52	110.10
21	6	905	CLA	C2D-C1D-ND	7.33	115.50	110.10
21	5	707	CLA	C2D-C1D-ND	7.31	115.49	110.10
21	1	501	CLA	C2D-C1D-ND	7.31	115.49	110.10
21	4	701	CLA	CMD-C2D-C1D	7.31	137.59	124.71
21	7	706	CLA	C2D-C1D-ND	7.31	115.49	110.10
21	4	711	CLA	C2D-C1D-ND	7.30	115.49	110.10
21	4	708	CLA	C2D-C1D-ND	7.30	115.48	110.10
21	2	514	CLA	C2C-C1C-NC	7.30	116.81	109.97
21	2	515	CLA	C2D-C1D-ND	7.30	115.48	110.10
21	11	711	CLA	CMD-C2D-C1D	7.28	137.55	124.71
21	A	840	CLA	C3C-C4C-NC	7.28	118.74	110.57
21	6	908	CLA	C4A-NA-C1A	-7.28	103.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	713	CLA	C2D-C1D-ND	7.26	115.46	110.10
21	B	829	CLA	CHD-C4C-C3C	-7.26	114.17	124.84
21	3	703	CLA	C1D-ND-C4D	-7.24	101.19	106.33
21	6	910	CLA	C2D-C1D-ND	7.24	115.44	110.10
21	B	825	CLA	C2D-C1D-ND	7.24	115.44	110.10
21	A	814	CLA	C2D-C1D-ND	7.23	115.43	110.10
21	6	906	CLA	C2D-C1D-ND	7.22	115.42	110.10
21	11	708	CLA	C2D-C1D-ND	7.22	115.42	110.10
21	B	831	CLA	O2D-CGD-CBD	7.21	124.08	111.27
21	5	709	CLA	C2D-C1D-ND	7.20	115.41	110.10
21	8	612	CLA	C2D-C1D-ND	7.20	115.41	110.10
21	A	807	CLA	C1D-ND-C4D	-7.17	101.24	106.33
21	6	908	CLA	CMD-C2D-C1D	7.17	137.36	124.71
21	9	903	CLA	CHD-C1D-ND	-7.16	117.87	124.45
21	5	708	CLA	C2D-C1D-ND	7.16	115.38	110.10
21	13	501	CLA	C2D-C1D-ND	7.15	115.37	110.10
21	F	401	CLA	C4-C3-C5	7.13	124.13	115.98
21	A	802	CLA	C2D-C1D-ND	7.12	115.35	110.10
21	A	812	CLA	C2D-C1D-ND	7.12	115.35	110.10
21	11	710	CLA	CMD-C2D-C1D	7.11	137.25	124.71
21	B	819	CLA	CMD-C2D-C1D	7.10	137.23	124.71
21	8	606	CLA	CHD-C4C-C3C	-7.10	114.41	124.84
21	B	834	CLA	C2D-C1D-ND	7.10	115.33	110.10
21	13	503	CLA	CMD-C2D-C1D	7.10	137.22	124.71
21	6	912	CLA	C2D-C1D-ND	7.09	115.33	110.10
21	8	610	CLA	O2D-CGD-CBD	7.08	123.86	111.27
21	9	908	CLA	C2D-C1D-ND	7.08	115.32	110.10
21	1	504	CLA	C2D-C1D-ND	7.07	115.32	110.10
21	B	819	CLA	C2D-C1D-ND	7.07	115.31	110.10
21	11	708	CLA	CMD-C2D-C1D	7.06	137.16	124.71
21	5	701	CLA	C2D-C1D-ND	7.05	115.30	110.10
21	7	711	CLA	C2D-C1D-ND	7.05	115.30	110.10
21	3	713	CLA	CMD-C2D-C1D	7.03	137.10	124.71
21	8	603	CLA	O2D-CGD-CBD	7.03	123.76	111.27
21	B	805	CLA	C1D-ND-C4D	-7.03	101.34	106.33
21	11	702	CLA	C2D-C1D-ND	7.02	115.28	110.10
21	11	707	CLA	C2D-C1D-ND	7.02	115.28	110.10
24	F	405	BCR	C8-C9-C10	7.02	129.71	118.94
21	A	835	CLA	C2D-C1D-ND	7.01	115.27	110.10
21	6	906	CLA	CMD-C2D-C1D	7.01	137.07	124.71
21	2	505	CLA	C1D-ND-C4D	-7.01	101.35	106.33
21	6	904	CLA	CMD-C2D-C1D	7.01	137.07	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	808	CLA	C2D-C1D-ND	7.00	115.27	110.10
21	6	908	CLA	C1D-ND-C4D	-6.98	101.37	106.33
21	4	707	CLA	C2D-C1D-ND	6.97	115.24	110.10
21	7	713	CLA	CMD-C2D-C1D	6.96	136.98	124.71
21	3	715	CLA	C2D-C1D-ND	6.95	115.23	110.10
21	A	833	CLA	C2C-C1C-NC	6.95	116.48	109.97
21	3	706	CLA	CHD-C4C-C3C	-6.94	114.64	124.84
21	A	823	CLA	CHD-C4C-C3C	-6.93	114.65	124.84
21	9	910	CLA	O2D-CGD-CBD	6.93	123.59	111.27
21	11	710	CLA	CHD-C1D-ND	-6.93	118.08	124.45
21	1	506	CLA	C2D-C1D-ND	6.92	115.21	110.10
21	6	908	CLA	C2D-C1D-ND	6.92	115.20	110.10
21	9	904	CLA	CMD-C2D-C1D	6.91	136.89	124.71
21	A	840	CLA	CAC-C3C-C4C	6.91	133.77	124.81
21	4	703	CLA	CMD-C2D-C1D	6.91	136.89	124.71
21	B	833	CLA	C2D-C1D-ND	6.91	115.19	110.10
21	A	840	CLA	CBC-CAC-C3C	-6.89	93.44	112.43
21	A	815	CLA	O2D-CGD-CBD	6.89	123.51	111.27
21	A	842	CLA	C2D-C1D-ND	6.89	115.18	110.10
21	A	810	CLA	CMD-C2D-C1D	6.88	136.83	124.71
21	A	820	CLA	CMD-C2D-C1D	6.87	136.82	124.71
21	1	512	CLA	C4A-NA-C1A	-6.87	103.62	106.71
21	5	706	CLA	O2D-CGD-CBD	6.86	123.46	111.27
21	7	702	CLA	CHD-C4C-C3C	-6.86	114.76	124.84
21	B	838	CLA	O2D-CGD-O1D	-6.86	110.43	123.84
21	8	614	CLA	CMD-C2D-C1D	6.85	136.79	124.71
21	6	904	CLA	C2D-C1D-ND	6.85	115.15	110.10
21	13	503	CLA	C2D-C1D-ND	6.84	115.15	110.10
21	A	830	CLA	C2D-C1D-ND	6.83	115.14	110.10
21	B	835	CLA	O2D-CGD-CBD	6.83	123.40	111.27
21	A	804	CLA	CHD-C4C-C3C	-6.83	114.81	124.84
21	B	833	CLA	C1D-ND-C4D	-6.82	101.49	106.33
21	B	839	CLA	C2D-C1D-ND	6.81	115.13	110.10
21	A	810	CLA	CBC-CAC-C3C	-6.81	93.65	112.43
21	B	807	CLA	C2D-C1D-ND	6.79	115.11	110.10
21	9	904	CLA	C2D-C1D-ND	6.79	115.11	110.10
21	A	839	CLA	C2D-C1D-ND	6.77	115.09	110.10
21	7	706	CLA	CAC-C3C-C4C	6.77	133.59	124.81
21	B	825	CLA	C1D-ND-C4D	-6.77	101.53	106.33
21	B	834	CLA	CHD-C4C-C3C	-6.77	114.89	124.84
21	11	703	CLA	CMD-C2D-C1D	6.76	136.63	124.71
21	6	909	CLA	CMD-C2D-C1D	6.76	136.63	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	705	CLA	CHD-C4C-C3C	-6.76	114.90	124.84
21	9	903	CLA	CMD-C2D-C1D	6.76	136.63	124.71
21	2	508	CLA	C2D-C1D-ND	6.75	115.08	110.10
21	1	515	CLA	CMD-C2D-C1D	6.74	136.59	124.71
21	1	510	CLA	CMD-C2D-C1D	6.74	136.59	124.71
21	6	911	CLA	C2D-C1D-ND	6.73	115.06	110.10
21	A	811	CLA	O2D-CGD-O1D	-6.72	110.69	123.84
21	4	711	CLA	CMD-C2D-C1D	6.72	136.56	124.71
21	2	515	CLA	C2C-C1C-NC	6.72	116.27	109.97
21	3	712	CLA	C2D-C1D-ND	6.71	115.05	110.10
21	8	611	CLA	C4A-NA-C1A	-6.69	103.70	106.71
21	9	909	CLA	C2D-C1D-ND	6.69	115.03	110.10
21	A	834	CLA	CHD-C1D-ND	-6.69	118.31	124.45
21	2	511	CLA	C2D-C1D-ND	6.69	115.03	110.10
21	12	503	CLA	CMD-C2D-C1D	6.67	136.47	124.71
21	3	715	CLA	CMD-C2D-C1D	6.67	136.47	124.71
21	4	704	CLA	C4A-NA-C1A	-6.67	103.71	106.71
21	A	835	CLA	O2D-CGD-CBD	6.67	123.12	111.27
21	11	711	CLA	CHD-C1D-ND	-6.67	118.33	124.45
21	2	505	CLA	O2D-CGD-CBD	6.66	123.11	111.27
21	4	707	CLA	CMD-C2D-C1D	6.66	136.46	124.71
21	1	509	CLA	CHD-C4C-C3C	-6.66	115.05	124.84
21	J	101	CLA	C4A-NA-C1A	-6.66	103.71	106.71
21	10	708	CLA	O2D-CGD-CBD	6.66	123.10	111.27
21	6	906	CLA	C2C-C1C-NC	6.65	116.20	109.97
21	5	704	CLA	C4A-NA-C1A	-6.65	103.72	106.71
21	12	507	CLA	C4A-NA-C1A	-6.64	103.72	106.71
21	10	704	CLA	CHD-C1D-ND	-6.64	118.35	124.45
21	B	826	CLA	C3C-C4C-NC	6.64	118.02	110.57
21	A	841	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
21	A	828	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
21	10	705	CLA	CMD-C2D-C1D	6.63	136.39	124.71
21	A	821	CLA	C1-C2-C3	-6.62	114.59	126.04
21	11	705	CLA	C2D-C1D-ND	6.61	114.97	110.10
21	10	704	CLA	CMD-C2D-C1D	6.61	136.36	124.71
21	12	503	CLA	CHD-C1D-ND	-6.60	118.39	124.45
21	5	704	CLA	CHD-C1D-ND	-6.60	118.39	124.45
21	10	703	CLA	C2D-C1D-ND	6.60	114.97	110.10
21	3	708	CLA	O2D-CGD-CBD	6.59	122.99	111.27
21	A	828	CLA	C3D-C2D-C1D	-6.59	96.83	105.83
21	A	809	CLA	C2D-C1D-ND	6.59	114.96	110.10
21	3	704	CLA	C2C-C1C-NC	6.59	116.15	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	909	CLA	CMD-C2D-C1D	6.58	136.31	124.71
21	2	506	CLA	C2D-C1D-ND	6.58	114.95	110.10
21	A	815	CLA	C4A-NA-C1A	-6.58	103.75	106.71
21	B	818	CLA	CHD-C1D-ND	-6.58	118.41	124.45
21	3	705	CLA	CMD-C2D-C1D	6.57	136.30	124.71
21	9	910	CLA	C4A-NA-C1A	-6.57	103.75	106.71
21	B	832	CLA	C3C-C4C-NC	6.57	117.94	110.57
21	6	911	CLA	CHD-C4C-C3C	-6.57	115.19	124.84
21	2	516	CLA	CMC-C2C-C1C	6.56	135.04	125.04
21	1	505	CLA	C2D-C1D-ND	6.56	114.94	110.10
21	A	820	CLA	CHD-C1D-ND	-6.56	118.43	124.45
21	B	815	CLA	C2D-C1D-ND	6.55	114.93	110.10
21	2	505	CLA	CHD-C4C-C3C	-6.55	115.21	124.84
21	6	909	CLA	CHD-C1D-ND	-6.55	118.44	124.45
21	A	844	CLA	CMD-C2D-C1D	6.54	136.24	124.71
21	B	836	CLA	C2C-C1C-NC	6.54	116.10	109.97
21	A	808	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
21	2	508	CLA	CHD-C1D-ND	-6.54	118.45	124.45
21	6	910	CLA	CMD-C2D-C1D	6.54	136.23	124.71
21	10	706	CLA	CMD-C2D-C1D	6.53	136.23	124.71
21	9	914	CLA	CMD-C2D-C1D	6.53	136.22	124.71
21	11	709	CLA	C2D-C1D-ND	6.53	114.92	110.10
28	3	717	DD6	C12-C11-C10	-6.53	113.78	122.92
21	3	711	CLA	CMD-C2D-C1D	6.51	136.18	124.71
21	A	804	CLA	O2D-CGD-CBD	6.51	122.83	111.27
21	8	613	CLA	O2D-CGD-CBD	6.51	122.83	111.27
21	5	711	CLA	CMD-C2D-C1D	6.51	136.18	124.71
21	13	503	CLA	C2C-C1C-NC	6.50	116.07	109.97
21	7	714	CLA	CMD-C2D-C1D	6.50	136.18	124.71
21	4	705	CLA	CMD-C2D-C1D	6.50	136.18	124.71
21	7	709	CLA	C2D-C1D-ND	6.50	114.89	110.10
21	4	710	CLA	CMD-C2D-C1D	6.50	136.17	124.71
21	2	503	CLA	CMD-C2D-C1D	6.50	136.16	124.71
21	5	707	CLA	CMD-C2D-C1D	6.49	136.15	124.71
21	B	839	CLA	CMD-C2D-C1D	6.49	136.15	124.71
21	A	823	CLA	CHD-C1D-ND	-6.48	118.50	124.45
21	7	712	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
21	1	509	CLA	CMD-C2D-C1D	6.48	136.13	124.71
21	10	705	CLA	CHD-C1D-ND	-6.48	118.50	124.45
21	6	911	CLA	C4A-NA-C1A	-6.47	103.80	106.71
21	11	704	CLA	CHD-C1D-ND	-6.47	118.50	124.45
21	B	808	CLA	C2C-C1C-NC	6.47	116.03	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	820	CLA	O2A-C1-C2	6.47	125.64	108.64
21	7	707	CLA	CMD-C2D-C1D	6.45	136.08	124.71
21	B	830	CLA	O2D-CGD-CBD	6.44	122.70	111.27
21	A	829	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
21	1	511	CLA	O2D-CGD-CBD	6.43	122.70	111.27
21	9	910	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
21	12	508	CLA	CMD-C2D-C1D	6.43	136.05	124.71
21	B	809	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
21	10	712	CLA	CMD-C2D-C1D	6.42	136.03	124.71
21	A	862	CLA	CHD-C4C-C3C	-6.41	115.41	124.84
21	6	914	CLA	CMD-C2D-C1D	6.41	136.01	124.71
21	11	706	CLA	C2C-C1C-NC	6.41	115.97	109.97
21	A	805	CLA	CMD-C2D-C1D	6.40	136.00	124.71
21	11	703	CLA	C2D-C1D-ND	6.40	114.82	110.10
21	A	807	CLA	CAA-C2A-C3A	-6.40	95.25	112.78
21	8	611	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
21	12	501	CLA	CMD-C2D-C1D	6.40	135.99	124.71
21	13	502	CLA	CMD-C2D-C1D	6.40	135.99	124.71
21	7	703	CLA	CHD-C4C-C3C	-6.39	115.45	124.84
21	A	822	CLA	C2D-C1D-ND	6.39	114.81	110.10
21	B	828	CLA	O2D-CGD-O1D	-6.39	111.35	123.84
21	7	712	CLA	CMD-C2D-C1D	6.38	135.96	124.71
21	12	507	CLA	CHD-C1D-ND	-6.38	118.59	124.45
21	A	810	CLA	C2C-C1C-NC	6.38	115.94	109.97
21	A	834	CLA	O2D-CGD-CBD	6.37	122.59	111.27
21	4	708	CLA	CMD-C2D-C1D	6.37	135.95	124.71
21	3	702	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
21	1	514	CLA	CMD-C2D-C1D	6.37	135.94	124.71
21	B	805	CLA	C2D-C1D-ND	6.37	114.80	110.10
21	9	913	CLA	CHD-C1D-ND	-6.36	118.61	124.45
21	A	838	CLA	C2C-C1C-NC	6.36	115.93	109.97
21	9	906	CLA	CMD-C2D-C1D	6.36	135.93	124.71
21	3	706	CLA	C2D-C1D-ND	6.36	114.79	110.10
21	11	706	CLA	CMD-C2D-C1D	6.36	135.93	124.71
21	1	517	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
21	J	101	CLA	CMD-C2D-C1D	6.35	135.91	124.71
21	8	608	CLA	CHD-C1D-ND	-6.35	118.62	124.45
21	5	710	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
21	8	612	CLA	CMD-C2D-C1D	6.35	135.90	124.71
21	4	710	CLA	CHD-C1D-ND	-6.34	118.63	124.45
21	5	705	CLA	C2D-C1D-ND	6.34	114.77	110.10
21	2	517	CLA	C2C-C1C-NC	6.34	115.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	909	CLA	O2D-CGD-CBD	6.32	122.50	111.27
21	7	704	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
21	B	837	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
21	A	830	CLA	CAC-C3C-C4C	6.31	133.00	124.81
21	2	508	CLA	CMD-C2D-C1D	6.31	135.83	124.71
21	A	820	CLA	CAC-C3C-C4C	6.31	132.99	124.81
21	7	710	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
21	B	830	CLA	C2D-C1D-ND	6.30	114.75	110.10
21	3	714	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
21	2	506	CLA	C2C-C1C-NC	6.30	115.87	109.97
21	B	826	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
21	8	603	CLA	CHD-C1D-ND	-6.29	118.67	124.45
21	B	807	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
21	2	512	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
21	4	707	CLA	O2D-CGD-CBD	6.29	122.44	111.27
21	B	836	CLA	C4A-NA-C1A	-6.29	103.88	106.71
21	1	506	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
21	2	506	CLA	CMD-C2D-C1D	6.28	135.79	124.71
21	8	611	CLA	C2D-C1D-ND	6.28	114.73	110.10
21	13	501	CLA	CMD-C2D-C1D	6.28	135.78	124.71
21	B	810	CLA	CHD-C4C-C3C	-6.28	115.62	124.84
21	A	805	CLA	CHD-C1D-ND	-6.27	118.69	124.45
21	6	914	CLA	CHD-C1D-ND	-6.27	118.69	124.45
21	B	815	CLA	O2D-CGD-CBD	6.27	122.40	111.27
21	12	508	CLA	CHD-C1D-ND	-6.26	118.70	124.45
21	A	843	CLA	CMD-C2D-C1D	6.26	135.75	124.71
21	A	843	CLA	O2D-CGD-CBD	6.25	122.38	111.27
21	B	821	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
21	12	501	CLA	CHD-C1D-ND	-6.24	118.72	124.45
21	2	507	CLA	C2C-C1C-NC	6.24	115.82	109.97
21	3	705	CLA	CHD-C1D-ND	-6.24	118.72	124.45
21	B	826	CLA	O2D-CGD-CBD	6.24	122.35	111.27
21	B	801	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
21	9	903	CLA	O2D-CGD-CBD	6.23	122.34	111.27
21	A	836	CLA	CHD-C1D-ND	-6.23	118.73	124.45
21	3	701	CLA	CMD-C2D-C1D	6.23	135.68	124.71
21	9	912	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
21	5	705	CLA	O2D-CGD-CBD	6.21	122.30	111.27
21	1	517	CLA	C2D-C1D-ND	6.21	114.68	110.10
21	8	609	CLA	CMD-C2D-C1D	6.20	135.64	124.71
21	12	507	CLA	CMD-C2D-C1D	6.20	135.63	124.71
21	A	820	CLA	C2D-C1D-ND	6.19	114.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	613	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
21	2	513	CLA	CMD-C2D-C1D	6.19	135.62	124.71
21	7	713	CLA	CHD-C1D-ND	-6.19	118.77	124.45
21	11	708	CLA	CHD-C1D-ND	-6.18	118.77	124.45
21	3	707	CLA	CHD-C1D-ND	-6.18	118.77	124.45
21	7	712	CLA	C4A-NA-C1A	-6.18	103.93	106.71
21	2	513	CLA	CHD-C1D-ND	-6.17	118.78	124.45
21	5	708	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
21	11	703	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
21	4	709	CLA	O2D-CGD-CBD	6.17	122.23	111.27
21	B	803	CLA	CHD-C4C-C3C	-6.17	115.78	124.84
21	B	834	CLA	C4A-NA-C1A	-6.17	103.93	106.71
21	2	517	CLA	CHD-C1D-ND	-6.16	118.79	124.45
21	A	834	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
21	4	706	CLA	CHD-C1D-ND	-6.16	118.79	124.45
21	9	913	CLA	CMD-C2D-C1D	6.16	135.56	124.71
21	A	821	CLA	CHD-C1D-ND	-6.15	118.80	124.45
21	A	842	CLA	CAC-C3C-C4C	6.15	132.79	124.81
21	6	908	CLA	C2C-C1C-NC	6.14	115.73	109.97
21	B	804	CLA	CHD-C1D-ND	-6.14	118.81	124.45
21	B	817	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
21	8	612	CLA	CHD-C1D-ND	-6.14	118.81	124.45
21	7	702	CLA	CMD-C2D-C1D	6.14	135.53	124.71
21	A	833	CLA	C2D-C1D-ND	6.13	114.62	110.10
21	A	844	CLA	CHD-C4C-C3C	-6.13	115.82	124.84
21	2	507	CLA	O2D-CGD-CBD	6.13	122.17	111.27
21	6	912	CLA	CMD-C2D-C1D	6.13	135.52	124.71
21	10	706	CLA	CHD-C1D-ND	-6.13	118.82	124.45
21	A	813	CLA	CHD-C4C-C3C	-6.13	115.84	124.84
21	J	101	CLA	O2D-CGD-O1D	-6.12	111.86	123.84
21	7	704	CLA	CMD-C2D-C1D	6.12	135.50	124.71
21	11	704	CLA	CMD-C2D-C1D	6.12	135.50	124.71
21	B	825	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
21	B	823	CLA	C2C-C1C-NC	6.11	115.70	109.97
21	2	509	CLA	CHD-C1D-ND	-6.10	118.85	124.45
21	B	827	CLA	C2D-C1D-ND	6.10	114.60	110.10
21	A	837	CLA	CMD-C2D-C1D	6.10	135.47	124.71
21	6	907	CLA	C2C-C1C-NC	6.10	115.69	109.97
21	B	814	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
21	11	704	CLA	C2C-C1C-NC	6.10	115.69	109.97
21	4	708	CLA	CHD-C1D-ND	-6.10	118.85	124.45
21	B	827	CLA	CHD-C4C-C3C	-6.10	115.88	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	715	CLA	C4A-NA-C1A	-6.10	103.96	106.71
21	A	838	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
21	6	913	CLA	CMD-C2D-C1D	6.10	135.46	124.71
21	A	821	CLA	O2D-CGD-O1D	-6.09	111.94	123.84
21	2	510	CLA	C4A-NA-C1A	-6.09	103.97	106.71
21	9	907	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
21	2	504	CLA	CMD-C2D-C1D	6.08	135.44	124.71
21	2	509	CLA	C2C-C1C-NC	6.08	115.67	109.97
28	12	510	DD6	C12-C11-C10	-6.08	114.40	122.92
21	7	711	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
21	5	711	CLA	CHD-C1D-ND	-6.08	118.87	124.45
21	A	824	CLA	C3C-C4C-NC	6.08	117.39	110.57
21	12	505	CLA	CHD-C1D-ND	-6.08	118.87	124.45
21	10	709	CLA	CMD-C2D-C1D	6.07	135.42	124.71
21	5	709	CLA	CMD-C2D-C1D	6.07	135.41	124.71
21	B	811	CLA	CHD-C1D-ND	-6.07	118.88	124.45
21	10	704	CLA	O2D-CGD-CBD	6.07	122.05	111.27
21	A	842	CLA	O2D-CGD-O1D	-6.06	111.99	123.84
21	12	502	CLA	C2D-C1D-ND	6.06	114.57	110.10
21	2	504	CLA	CHD-C1D-ND	-6.06	118.89	124.45
21	3	707	CLA	CMD-C2D-C1D	6.05	135.38	124.71
21	4	709	CLA	CMD-C2D-C1D	6.05	135.38	124.71
21	1	512	CLA	CMD-C2D-C1D	6.05	135.37	124.71
21	2	514	CLA	CMD-C2D-C1D	6.04	135.36	124.71
21	B	803	CLA	O2D-CGD-CBD	6.04	122.00	111.27
21	B	823	CLA	C4A-NA-C1A	-6.04	103.99	106.71
21	A	802	CLA	C1D-ND-C4D	-6.04	102.05	106.33
21	3	709	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
21	2	506	CLA	CHD-C1D-ND	-6.03	118.91	124.45
21	3	704	CLA	CHD-C1D-ND	-6.02	118.92	124.45
21	4	701	CLA	C2C-C1C-NC	6.02	115.61	109.97
21	3	708	CLA	C2D-C1D-ND	6.02	114.54	110.10
21	6	911	CLA	O2D-CGD-CBD	6.02	121.96	111.27
21	B	820	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
21	A	840	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
21	7	709	CLA	CMD-C2D-C1D	6.01	135.31	124.71
21	9	909	CLA	CHD-C1D-ND	-6.01	118.93	124.45
21	8	609	CLA	C4A-NA-C1A	-6.01	104.00	106.71
21	B	836	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
21	5	706	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
21	8	604	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
21	9	906	CLA	C2C-C1C-NC	6.00	115.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	828	CLA	CMD-C2D-C1D	6.00	135.29	124.71
21	2	516	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
21	4	703	CLA	CHD-C1D-ND	-6.00	118.94	124.45
21	9	911	CLA	C4A-NA-C1A	-6.00	104.01	106.71
21	10	710	CLA	CMD-C2D-C1D	6.00	135.28	124.71
21	A	827	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
21	10	709	CLA	CHD-C1D-ND	-5.99	118.95	124.45
21	A	833	CLA	CMD-C2D-C1D	5.99	135.27	124.71
21	6	903	CLA	CMD-C2D-C1D	5.99	135.27	124.71
21	A	862	CLA	C1-C2-C3	-5.99	115.69	126.04
21	5	703	CLA	C2D-C1D-ND	5.99	114.52	110.10
21	1	517	CLA	C4A-NA-C1A	-5.98	104.02	106.71
21	9	906	CLA	C4A-NA-C1A	-5.98	104.02	106.71
21	2	505	CLA	CMD-C2D-C1D	5.98	135.25	124.71
21	B	819	CLA	O2D-CGD-CBD	5.98	121.89	111.27
21	A	837	CLA	CBC-CAC-C3C	-5.98	95.95	112.43
21	3	706	CLA	CHD-C1D-ND	-5.97	118.96	124.45
21	5	707	CLA	CHD-C1D-ND	-5.96	118.97	124.45
21	A	840	CLA	CHD-C1D-ND	-5.96	118.98	124.45
21	12	507	CLA	C2C-C1C-NC	5.95	115.55	109.97
21	B	834	CLA	O2D-CGD-CBD	5.95	121.85	111.27
21	7	704	CLA	C2C-C1C-NC	5.95	115.55	109.97
21	4	705	CLA	CHD-C1D-ND	-5.95	118.99	124.45
21	B	806	CLA	C4A-NA-C1A	-5.95	104.03	106.71
21	6	908	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
21	11	702	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
21	1	517	CLA	CMC-C2C-C1C	5.95	134.09	125.04
21	B	805	CLA	CAC-C3C-C4C	5.94	132.52	124.81
21	4	706	CLA	CMD-C2D-C1D	5.94	135.18	124.71
21	6	906	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
21	12	502	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
21	A	830	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
21	13	503	CLA	CHD-C1D-ND	-5.93	119.00	124.45
21	B	830	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
21	A	836	CLA	C2C-C1C-NC	5.93	115.53	109.97
21	3	708	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
21	1	508	CLA	CHD-C1D-ND	-5.93	119.01	124.45
21	6	907	CLA	CAC-C3C-C4C	5.92	132.50	124.81
21	1	516	CLA	C2C-C1C-NC	5.92	115.52	109.97
21	B	829	CLA	C3D-C2D-C1D	-5.92	97.75	105.83
21	9	914	CLA	CHD-C1D-ND	-5.92	119.02	124.45
21	B	813	CLA	CHD-C4C-C3C	-5.92	116.14	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	702	CLA	C2C-C1C-NC	5.92	115.51	109.97
21	13	502	CLA	CHD-C1D-ND	-5.91	119.02	124.45
21	A	806	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
21	5	707	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
21	4	705	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
21	2	505	CLA	C2D-C1D-ND	5.89	114.44	110.10
21	1	507	CLA	C2C-C1C-NC	5.89	115.49	109.97
21	2	517	CLA	CMD-C2D-C1D	5.89	135.09	124.71
21	10	707	CLA	CHD-C1D-ND	-5.89	119.05	124.45
21	B	811	CLA	CMD-C2D-C1D	5.88	135.08	124.71
21	7	712	CLA	O2D-CGD-CBD	5.88	121.71	111.27
21	A	816	CLA	C2C-C1C-NC	5.86	115.47	109.97
21	2	511	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
21	10	710	CLA	CHD-C1D-ND	-5.86	119.07	124.45
21	A	824	CLA	CHD-C1D-ND	-5.86	119.07	124.45
21	10	708	CLA	CMD-C2D-C1D	5.86	135.04	124.71
21	7	703	CLA	CMD-C2D-C1D	5.86	135.04	124.71
21	3	707	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
21	1	507	CLA	CMD-C2D-C1D	5.86	135.03	124.71
21	J	101	CLA	C2D-C1D-ND	5.85	114.41	110.10
21	8	610	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
21	B	818	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
20	A	801	CL0	CHD-C4C-C3C	-5.84	116.26	124.84
21	5	705	CLA	CMD-C2D-C1D	5.83	134.99	124.71
21	A	807	CLA	C2D-C1D-ND	5.83	114.40	110.10
21	A	814	CLA	CAC-C3C-C4C	5.83	132.38	124.81
21	6	907	CLA	C2D-C1D-ND	5.83	114.40	110.10
21	6	905	CLA	C2C-C1C-NC	5.83	115.43	109.97
21	9	903	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
21	A	804	CLA	CMD-C2D-C1D	5.83	134.98	124.71
21	3	712	CLA	CMD-C2D-C1D	5.82	134.97	124.71
21	2	514	CLA	C1C-C2C-C3C	-5.82	100.84	106.96
21	A	803	CLA	C1-O2A-CGA	5.82	131.71	116.44
21	3	713	CLA	CHD-C1D-ND	-5.82	119.11	124.45
21	3	702	CLA	CHD-C1D-ND	-5.81	119.11	124.45
21	8	603	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
21	5	709	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
21	7	710	CLA	C2D-C1D-ND	5.81	114.38	110.10
21	9	912	CLA	O2D-CGD-CBD	5.81	121.58	111.27
21	A	844	CLA	CHD-C1D-ND	-5.80	119.12	124.45
21	12	502	CLA	C4A-NA-C1A	-5.80	104.10	106.71
21	12	501	CLA	O2D-CGD-CBD	5.80	121.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	709	CLA	O2D-CGD-CBD	5.80	121.57	111.27
21	B	838	CLA	C2C-C1C-NC	5.79	115.40	109.97
21	7	714	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
21	A	862	CLA	CAC-C3C-C4C	5.79	132.32	124.81
21	7	702	CLA	C2C-C1C-NC	5.79	115.39	109.97
21	6	913	CLA	CHD-C1D-ND	-5.79	119.14	124.45
21	F	403	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
21	1	504	CLA	CMD-C2D-C1D	5.78	134.91	124.71
28	2	518	DD6	C12-C11-C10	-5.78	114.82	122.92
21	4	703	CLA	C2C-C1C-NC	5.78	115.39	109.97
20	A	801	CL0	O2D-CGD-O1D	-5.78	112.54	123.84
21	4	709	CLA	CHD-C1D-ND	-5.78	119.14	124.45
21	2	510	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
21	4	707	CLA	CHD-C1D-ND	-5.77	119.15	124.45
21	A	844	CLA	O2D-CGD-CBD	5.77	121.53	111.27
21	A	816	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
21	B	821	CLA	O2D-CGD-CBD	5.77	121.52	111.27
21	3	711	CLA	O2D-CGD-CBD	5.77	121.52	111.27
21	3	704	CLA	CMD-C2D-C1D	5.75	134.85	124.71
21	A	826	CLA	C2C-C1C-NC	5.74	115.35	109.97
21	2	514	CLA	C2D-C1D-ND	5.74	114.33	110.10
21	2	503	CLA	CHD-C1D-ND	-5.74	119.18	124.45
21	2	503	CLA	C2C-C1C-NC	5.74	115.35	109.97
21	7	713	CLA	O2D-CGD-CBD	5.73	121.46	111.27
21	A	820	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
21	A	823	CLA	CMD-C2D-C1D	5.73	134.81	124.71
21	B	810	CLA	CHD-C1D-ND	-5.73	119.19	124.45
21	A	840	CLA	C2C-C1C-NC	5.73	115.34	109.97
21	B	817	CLA	CHD-C1D-ND	-5.73	119.19	124.45
21	A	825	CLA	CHD-C1D-ND	-5.72	119.20	124.45
21	9	904	CLA	CHD-C1D-ND	-5.72	119.20	124.45
21	8	611	CLA	CMD-C2D-C1D	5.71	134.78	124.71
21	7	707	CLA	CHD-C1D-ND	-5.71	119.20	124.45
21	10	710	CLA	C4A-NA-C1A	-5.71	104.14	106.71
21	11	703	CLA	O2D-CGD-CBD	5.70	121.40	111.27
21	7	711	CLA	CMD-C2D-C1D	5.70	134.76	124.71
21	4	702	CLA	O2D-CGD-CBD	5.70	121.40	111.27
21	9	906	CLA	CHD-C1D-ND	-5.70	119.22	124.45
21	B	839	CLA	C2C-C1C-NC	5.70	115.31	109.97
21	3	701	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
21	1	515	CLA	CHD-C1D-ND	-5.69	119.23	124.45
21	8	605	CLA	C2D-C1D-ND	5.68	114.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	819	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
21	A	841	CLA	CMD-C2D-C1D	5.68	134.73	124.71
21	8	613	CLA	CMD-C2D-C1D	5.68	134.72	124.71
21	B	803	CLA	CMD-C2D-C1D	5.68	134.72	124.71
21	A	831	CLA	CMD-C2D-C1D	5.67	134.71	124.71
21	3	713	CLA	C2C-C1C-NC	5.67	115.29	109.97
21	11	709	CLA	CMD-C2D-C1D	5.67	134.70	124.71
21	F	401	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
21	A	817	CLA	CMD-C2D-C1D	5.66	134.70	124.71
21	4	704	CLA	CHD-C1D-ND	-5.66	119.25	124.45
21	6	905	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
21	2	516	CLA	C2D-C1D-ND	5.66	114.28	110.10
21	12	506	CLA	CHD-C1D-ND	-5.66	119.25	124.45
21	6	910	CLA	CHD-C1D-ND	-5.66	119.25	124.45
21	A	831	CLA	CHD-C4C-C3C	-5.66	116.53	124.84
21	10	709	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
21	1	511	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
21	10	703	CLA	CMD-C2D-C1D	5.65	134.66	124.71
21	5	704	CLA	CMD-C2D-C1D	5.65	134.66	124.71
21	A	811	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
21	A	819	CLA	C2C-C1C-NC	5.64	115.25	109.97
21	7	713	CLA	C2C-C1C-NC	5.64	115.25	109.97
21	B	839	CLA	CHD-C1D-ND	-5.64	119.28	124.45
21	6	907	CLA	CMD-C2D-C1D	5.63	134.64	124.71
21	7	710	CLA	CMD-C2D-C1D	5.63	134.64	124.71
21	12	504	CLA	CMD-C2D-C1D	5.63	134.64	124.71
21	7	709	CLA	CAC-C3C-C4C	5.63	132.12	124.81
21	A	843	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
21	6	905	CLA	CMD-C2D-C1D	5.63	134.63	124.71
21	2	512	CLA	O2D-CGD-CBD	5.63	121.27	111.27
21	10	705	CLA	C2C-C1C-NC	5.63	115.24	109.97
21	B	804	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
21	B	804	CLA	CMD-C2D-C1D	5.62	134.62	124.71
21	A	822	CLA	CMD-C2D-C1D	5.62	134.62	124.71
21	10	707	CLA	CMD-C2D-C1D	5.62	134.61	124.71
21	13	503	CLA	C4A-NA-C1A	-5.61	104.18	106.71
21	B	824	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
21	A	833	CLA	CHD-C1D-ND	-5.61	119.30	124.45
21	2	512	CLA	C2C-C1C-NC	5.61	115.23	109.97
21	2	509	CLA	CMD-C2D-C1D	5.60	134.59	124.71
21	B	818	CLA	CMD-C2D-C1D	5.60	134.59	124.71
21	B	821	CLA	CHD-C1D-ND	-5.60	119.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	603	CLA	CMD-C2D-C1D	5.60	134.58	124.71
21	8	607	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
21	7	704	CLA	C2D-C1D-ND	5.60	114.23	110.10
21	9	911	CLA	CMD-C2D-C1D	5.59	134.57	124.71
21	9	905	CLA	CHD-C1D-ND	-5.59	119.31	124.45
21	J	101	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
21	5	702	CLA	CMD-C2D-C1D	5.59	134.56	124.71
21	10	711	CLA	CMD-C2D-C1D	5.59	134.56	124.71
21	12	503	CLA	C2C-C1C-NC	5.58	115.20	109.97
21	1	505	CLA	CMD-C2D-C1D	5.58	134.55	124.71
21	3	709	CLA	CMD-C2D-C1D	5.58	134.55	124.71
21	10	712	CLA	C2C-C1C-NC	5.58	115.20	109.97
21	4	701	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
21	B	836	CLA	CBC-CAC-C3C	-5.58	97.06	112.43
21	4	711	CLA	CHD-C1D-ND	-5.57	119.33	124.45
21	8	611	CLA	O2D-CGD-CBD	5.57	121.17	111.27
21	A	818	CLA	CHD-C1D-ND	-5.57	119.33	124.45
21	A	803	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
21	1	501	CLA	O2D-CGD-CBD	5.56	121.15	111.27
21	6	903	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
21	11	701	CLA	CMD-C2D-C1D	5.56	134.51	124.71
21	2	510	CLA	CHD-C1D-ND	-5.56	119.35	124.45
21	5	702	CLA	C2D-C1D-ND	5.56	114.20	110.10
21	F	403	CLA	O2D-CGD-O1D	-5.56	112.97	123.84
21	4	701	CLA	CHD-C1D-ND	-5.55	119.35	124.45
21	2	503	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
21	A	834	CLA	CMD-C2D-C1D	5.55	134.50	124.71
21	B	828	CLA	C2C-C1C-NC	5.55	115.17	109.97
21	4	702	CLA	CHD-C1D-ND	-5.55	119.36	124.45
21	1	517	CLA	C2C-C1C-NC	5.55	115.17	109.97
21	3	711	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
21	3	715	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
21	B	806	CLA	CHD-C1D-ND	-5.54	119.36	124.45
21	B	801	CLA	C2D-C1D-ND	5.54	114.19	110.10
21	9	907	CLA	CHD-C1D-ND	-5.54	119.36	124.45
21	3	713	CLA	C4A-NA-C1A	-5.54	104.22	106.71
21	A	818	CLA	CMD-C2D-C1D	5.54	134.47	124.71
21	A	809	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
21	9	913	CLA	C2C-C1C-NC	5.53	115.16	109.97
21	4	703	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
21	8	610	CLA	CMD-C2D-C1D	5.53	134.46	124.71
21	3	702	CLA	CMD-C2D-C1D	5.53	134.46	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	512	CLA	CHD-C1D-ND	-5.53	119.37	124.45
21	7	705	CLA	C3D-C2D-C1D	-5.53	98.29	105.83
21	7	702	CLA	C3C-C4C-NC	5.53	116.77	110.57
21	13	501	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
21	2	516	CLA	C1D-CHD-C4C	-5.53	114.13	126.06
21	A	814	CLA	C3C-C4C-NC	5.52	116.77	110.57
21	5	709	CLA	CHD-C1D-ND	-5.52	119.38	124.45
21	A	817	CLA	C2C-C1C-NC	5.52	115.15	109.97
21	7	703	CLA	C2C-C1C-NC	5.52	115.15	109.97
21	10	708	CLA	C2C-C1C-NC	5.52	115.15	109.97
21	1	508	CLA	CAC-C3C-C4C	5.52	131.97	124.81
21	6	903	CLA	C2C-C1C-NC	5.52	115.14	109.97
21	1	507	CLA	C2D-C1D-ND	5.52	114.17	110.10
21	5	703	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
21	8	608	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
21	9	905	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
21	9	908	CLA	CHD-C1D-ND	-5.51	119.39	124.45
21	A	836	CLA	CMD-C2D-C1D	5.51	134.43	124.71
21	11	708	CLA	C2C-C1C-NC	5.51	115.14	109.97
21	13	502	CLA	C2C-C1C-NC	5.51	115.13	109.97
21	5	710	CLA	O2A-CGA-O1A	-5.50	109.70	123.59
21	B	812	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
21	4	701	CLA	O2D-CGD-CBD	5.50	121.04	111.27
21	10	712	CLA	CHD-C1D-ND	-5.50	119.40	124.45
21	7	711	CLA	CHD-C1D-ND	-5.49	119.41	124.45
21	A	844	CLA	CAA-C2A-C3A	-5.49	97.75	112.78
21	A	810	CLA	CHD-C1D-ND	-5.49	119.41	124.45
21	10	706	CLA	C2C-C1C-NC	5.49	115.11	109.97
21	A	821	CLA	CMD-C2D-C1D	5.49	134.38	124.71
21	5	707	CLA	C4A-NA-C1A	-5.49	104.24	106.71
21	7	703	CLA	C4A-NA-C1A	-5.48	104.24	106.71
21	B	813	CLA	C2D-C1D-ND	5.48	114.14	110.10
21	13	501	CLA	O2D-CGD-CBD	5.48	121.01	111.27
21	1	501	CLA	CMD-C2D-C1D	5.48	134.36	124.71
21	7	714	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
21	B	816	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
21	A	830	CLA	O2D-CGD-CBD	5.47	120.99	111.27
21	1	511	CLA	CMD-C2D-C1D	5.47	134.35	124.71
21	3	710	CLA	CHD-C1D-ND	-5.47	119.43	124.45
21	1	501	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
21	8	605	CLA	CMD-C2D-C1D	5.46	134.34	124.71
21	A	837	CLA	CHD-C4C-C3C	-5.46	116.81	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	705	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
21	A	828	CLA	C3C-C4C-NC	5.46	116.69	110.57
21	10	711	CLA	CHD-C1D-ND	-5.46	119.44	124.45
21	A	825	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
21	7	712	CLA	CHD-C1D-ND	-5.46	119.44	124.45
28	12	510	DD6	C8-C6-C5	5.45	127.30	118.94
21	5	708	CLA	CMD-C2D-C1D	5.45	134.31	124.71
21	7	707	CLA	C2C-C1C-NC	5.44	115.07	109.97
21	6	910	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
21	A	843	CLA	CHD-C1D-ND	-5.44	119.45	124.45
21	A	821	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
21	1	509	CLA	CHD-C1D-ND	-5.44	119.46	124.45
21	7	710	CLA	C1D-CHD-C4C	-5.44	114.33	126.06
24	A	847	BCR	C34-C9-C8	5.44	126.64	118.08
21	11	710	CLA	C2C-C1C-NC	5.43	115.06	109.97
21	4	702	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
21	A	824	CLA	CMD-C2D-C1D	5.43	134.28	124.71
21	A	862	CLA	O2D-CGD-O1D	-5.43	113.23	123.84
21	12	506	CLA	CMD-C2D-C1D	5.42	134.27	124.71
21	12	502	CLA	CMD-C2D-C1D	5.42	134.27	124.71
21	6	904	CLA	CHD-C1D-ND	-5.42	119.47	124.45
21	1	517	CLA	CMD-C2D-C1D	5.42	134.27	124.71
21	B	827	CLA	C2C-C1C-NC	5.42	115.05	109.97
21	A	832	CLA	CBC-CAC-C3C	-5.42	97.49	112.43
21	A	831	CLA	C3C-C4C-NC	5.42	116.65	110.57
21	4	710	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
21	3	712	CLA	C2C-C1C-NC	5.41	115.04	109.97
21	6	908	CLA	O2D-CGD-CBD	5.41	120.88	111.27
21	1	513	CLA	CMD-C2D-C1D	5.41	134.25	124.71
21	A	805	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
21	A	817	CLA	O2D-CGD-CBD	5.41	120.88	111.27
28	5	713	DD6	C12-C11-C10	-5.41	115.35	122.92
21	B	825	CLA	O2D-CGD-O1D	-5.41	113.27	123.84
21	A	817	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
21	A	817	CLA	CHD-C1D-ND	-5.40	119.49	124.45
21	1	514	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
21	B	829	CLA	C3C-C4C-NC	5.40	116.63	110.57
21	12	505	CLA	CMD-C2D-C1D	5.40	134.23	124.71
21	A	815	CLA	C3C-C4C-NC	5.40	116.62	110.57
21	B	806	CLA	C2D-C1D-ND	5.40	114.08	110.10
21	A	814	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
21	6	912	CLA	O2D-CGD-CBD	5.39	120.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	501	CLA	CHD-C1D-ND	-5.39	119.50	124.45
21	1	515	CLA	C4A-NA-C1A	-5.39	104.28	106.71
21	10	711	CLA	C2C-C1C-NC	5.39	115.02	109.97
21	3	708	CLA	CMD-C2D-C1D	5.39	134.21	124.71
21	3	714	CLA	O2D-CGD-CBD	5.39	120.84	111.27
21	B	836	CLA	O2D-CGD-O1D	-5.39	113.31	123.84
21	A	822	CLA	CBC-CAC-C3C	-5.38	97.59	112.43
21	A	822	CLA	CHD-C4C-C3C	-5.38	116.92	124.84
21	12	504	CLA	C2D-C1D-ND	5.38	114.07	110.10
21	A	838	CLA	C3C-C4C-NC	5.38	116.61	110.57
21	8	614	CLA	CHD-C1D-ND	-5.38	119.51	124.45
21	12	501	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
21	11	709	CLA	CHD-C1D-ND	-5.38	119.51	124.45
21	8	607	CLA	CMD-C2D-C1D	5.38	134.19	124.71
21	6	913	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
21	F	404	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
21	B	838	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
21	B	827	CLA	CAC-C3C-C4C	5.37	131.77	124.81
21	8	605	CLA	C2C-C1C-NC	5.36	115.00	109.97
21	1	510	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
21	3	705	CLA	O2D-CGD-CBD	5.36	120.80	111.27
21	3	715	CLA	O2D-CGD-CBD	5.36	120.80	111.27
21	A	841	CLA	OBD-CAD-C3D	-5.36	115.62	128.52
21	9	904	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
21	10	709	CLA	C2C-C1C-NC	5.35	114.99	109.97
21	8	606	CLA	C2C-C1C-NC	5.35	114.98	109.97
24	A	849	BCR	C8-C9-C10	5.35	127.15	118.94
21	12	506	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
21	2	507	CLA	C3D-C4D-ND	5.35	118.89	110.24
21	B	813	CLA	C3C-C4C-NC	5.34	116.56	110.57
21	3	712	CLA	CHD-C1D-ND	-5.34	119.54	124.45
21	2	516	CLA	C4A-NA-C1A	-5.34	104.31	106.71
21	B	832	CLA	O2D-CGD-CBD	5.34	120.75	111.27
21	9	904	CLA	C2C-C1C-NC	5.34	114.97	109.97
21	B	807	CLA	O2D-CGD-CBD	5.34	120.75	111.27
21	B	815	CLA	CAC-C3C-C4C	5.34	131.73	124.81
21	5	708	CLA	C2C-C1C-NC	5.34	114.97	109.97
21	11	703	CLA	C4A-NA-C1A	-5.33	104.31	106.71
21	7	706	CLA	CMD-C2D-C1D	5.33	134.11	124.71
21	B	802	CLA	C4-C3-C5	5.33	124.24	115.27
21	B	805	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
21	B	817	CLA	CAC-C3C-C4C	5.33	131.73	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	710	CLA	CMD-C2D-C1D	5.33	134.10	124.71
21	10	711	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
21	5	711	CLA	C2C-C1C-NC	5.32	114.96	109.97
21	A	819	CLA	CMD-C2D-C1D	5.32	134.09	124.71
21	B	821	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
21	9	902	CLA	CHD-C1D-ND	-5.31	119.57	124.45
21	A	805	CLA	C2C-C1C-NC	5.31	114.95	109.97
21	6	903	CLA	CHD-C1D-ND	-5.31	119.57	124.45
21	1	508	CLA	C2C-C1C-NC	5.31	114.95	109.97
21	1	507	CLA	C4A-NA-C1A	-5.31	104.32	106.71
21	9	907	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
21	B	833	CLA	O1D-CGD-CBD	5.31	135.34	124.48
21	B	828	CLA	C1-O2A-CGA	5.30	130.35	116.44
21	11	707	CLA	CHD-C1D-ND	-5.30	119.58	124.45
21	4	709	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
21	B	820	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
21	11	701	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
21	7	703	CLA	O2D-CGD-CBD	5.29	120.68	111.27
21	3	703	CLA	C2C-C1C-NC	5.29	114.93	109.97
21	11	708	CLA	O2D-CGD-CBD	5.29	120.67	111.27
21	1	504	CLA	CHD-C1D-ND	-5.29	119.59	124.45
21	1	516	CLA	CMD-C2D-C1D	5.29	134.03	124.71
21	B	813	CLA	CAC-C3C-C4C	5.29	131.67	124.81
21	3	701	CLA	CHD-C1D-ND	-5.29	119.60	124.45
21	6	903	CLA	O2D-CGD-CBD	5.29	120.66	111.27
21	9	914	CLA	C2C-C1C-NC	5.28	114.92	109.97
21	1	513	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
21	B	833	CLA	OBD-CAD-C3D	-5.28	115.81	128.52
21	6	904	CLA	C2C-C1C-NC	5.28	114.92	109.97
21	B	805	CLA	CMD-C2D-C1D	5.28	134.01	124.71
21	9	913	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
22	B	840	PQN	O4-C4-C5	-5.28	113.02	121.56
21	9	907	CLA	C4A-NA-C1A	-5.28	104.33	106.71
21	11	711	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
21	2	507	CLA	CMD-C2D-C1D	5.28	134.01	124.71
21	10	712	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
21	10	710	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
21	A	862	CLA	C2C-C1C-NC	5.27	114.91	109.97
21	11	705	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
21	8	605	CLA	CHD-C1D-ND	-5.27	119.61	124.45
21	F	404	CLA	O2D-CGD-CBD	5.27	120.63	111.27
21	2	508	CLA	C2C-C1C-NC	5.27	114.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	839	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
21	A	832	CLA	O2D-CGD-CBD	5.26	120.62	111.27
21	A	821	CLA	C3D-C4D-ND	5.26	118.74	110.24
21	A	824	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
21	11	702	CLA	O2D-CGD-CBD	5.25	120.61	111.27
21	B	836	CLA	CMD-C2D-C1D	5.25	133.97	124.71
21	3	715	CLA	CHD-C1D-ND	-5.25	119.63	124.45
21	B	835	CLA	O2D-CGD-O1D	-5.25	113.57	123.84
21	9	909	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
21	F	404	CLA	CAC-C3C-C4C	5.24	131.62	124.81
21	B	804	CLA	O2A-CGA-CBA	5.24	128.37	111.91
21	B	810	CLA	C3D-C4D-ND	5.24	118.72	110.24
21	9	902	CLA	C3D-C4D-ND	5.24	118.71	110.24
21	A	836	CLA	C4A-NA-C1A	-5.24	104.35	106.71
21	B	807	CLA	CMC-C2C-C1C	5.24	133.01	125.04
21	B	809	CLA	CMD-C2D-C1D	5.23	133.94	124.71
21	10	708	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
28	12	510	DD6	C13-C11-C10	5.23	126.97	118.94
21	1	514	CLA	C2C-C1C-NC	5.23	114.87	109.97
21	8	609	CLA	C2D-C1D-ND	5.23	113.96	110.10
21	3	713	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
21	9	911	CLA	O2D-CGD-CBD	5.23	120.56	111.27
21	13	501	CLA	CHD-C1D-ND	-5.23	119.65	124.45
21	7	702	CLA	CHD-C1D-ND	-5.22	119.65	124.45
21	B	815	CLA	C4A-NA-C1A	-5.22	104.36	106.71
21	11	702	CLA	CMD-C2D-C1D	5.21	133.90	124.71
21	A	827	CLA	C3D-C4D-ND	5.21	118.67	110.24
21	3	701	CLA	O2D-CGD-CBD	5.21	120.53	111.27
21	6	908	CLA	C1D-CHD-C4C	-5.21	114.82	126.06
21	4	706	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
20	A	801	CL0	C3D-C4D-ND	5.21	118.66	110.24
21	B	837	CLA	CMD-C2D-C1D	5.21	133.89	124.71
21	B	819	CLA	CHD-C1D-ND	-5.21	119.67	124.45
21	1	511	CLA	CHD-C1D-ND	-5.21	119.67	124.45
21	8	607	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
21	A	831	CLA	C4A-NA-C1A	-5.20	104.37	106.71
21	2	513	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
21	B	813	CLA	O2D-CGD-CBD	5.20	120.51	111.27
21	A	862	CLA	CED-O2D-CGD	-5.20	104.18	115.94
21	6	907	CLA	C4A-NA-C1A	-5.20	104.37	106.71
21	12	503	CLA	O2D-CGD-CBD	5.20	120.50	111.27
21	11	709	CLA	C2C-C1C-NC	5.20	114.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	819	CLA	O2D-CGD-CBD	5.20	120.50	111.27
21	8	613	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
21	3	709	CLA	O2D-CGD-CBD	5.19	120.50	111.27
21	10	708	CLA	CHD-C1D-ND	-5.19	119.68	124.45
21	5	710	CLA	C3D-C4D-ND	5.19	118.63	110.24
21	A	841	CLA	O2D-CGD-CBD	5.19	120.49	111.27
21	7	705	CLA	C3C-C4C-NC	5.19	116.39	110.57
21	A	827	CLA	CHD-C1D-ND	-5.19	119.69	124.45
21	B	820	CLA	C2C-C1C-NC	5.19	114.83	109.97
21	A	802	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
21	A	806	CLA	CAA-C2A-C3A	-5.18	98.58	112.78
21	A	837	CLA	CHD-C1D-ND	-5.18	119.69	124.45
21	10	705	CLA	O2D-CGD-CBD	5.18	120.48	111.27
21	A	806	CLA	C2D-C1D-ND	5.18	113.92	110.10
21	A	829	CLA	C4-C3-C5	5.18	123.98	115.27
21	5	704	CLA	C3D-C4D-ND	5.18	118.62	110.24
21	6	914	CLA	C2C-C1C-NC	5.18	114.82	109.97
21	8	609	CLA	CHD-C1D-ND	-5.18	119.70	124.45
21	8	614	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
21	B	802	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
21	11	707	CLA	C4A-NA-C1A	-5.17	104.38	106.71
21	12	501	CLA	C4A-NA-C1A	-5.17	104.38	106.71
21	B	822	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
21	8	614	CLA	C2C-C1C-NC	5.17	114.82	109.97
21	9	905	CLA	CMD-C2D-C1D	5.17	133.82	124.71
21	4	704	CLA	CMD-C2D-C1D	5.17	133.82	124.71
21	B	833	CLA	CBC-CAC-C3C	-5.16	98.19	112.43
21	B	808	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
21	A	812	CLA	CMD-C2D-C1D	5.16	133.81	124.71
20	A	801	CL0	C1D-CHD-C4C	-5.15	114.94	126.06
21	B	808	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
21	5	708	CLA	O2D-CGD-CBD	5.15	120.41	111.27
21	10	707	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
21	B	821	CLA	CMD-C2D-C1D	5.14	133.78	124.71
21	A	829	CLA	C3C-C4C-NC	5.14	116.34	110.57
21	2	512	CLA	CHD-C1D-ND	-5.14	119.73	124.45
28	3	716	DD6	C12-C11-C13	5.14	126.17	118.08
21	7	706	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
21	8	604	CLA	C3D-C4D-ND	5.14	118.55	110.24
21	B	833	CLA	CAC-C3C-C4C	5.14	131.47	124.81
21	11	709	CLA	C4A-NA-C1A	-5.13	104.40	106.71
21	A	835	CLA	CAC-C3C-C4C	5.13	131.47	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	803	CLA	C3C-C4C-NC	5.13	116.32	110.57
21	A	862	CLA	C1D-CHD-C4C	-5.13	115.00	126.06
21	3	705	CLA	C3D-C4D-ND	5.12	118.53	110.24
21	11	710	CLA	C4A-NA-C1A	-5.12	104.40	106.71
21	A	829	CLA	CHD-C1D-ND	-5.12	119.75	124.45
21	B	838	CLA	CMC-C2C-C1C	5.12	132.83	125.04
21	5	701	CLA	C2C-C1C-NC	5.12	114.77	109.97
21	B	823	CLA	O2D-CGD-CBD	5.12	120.36	111.27
21	3	702	CLA	O2D-CGD-CBD	5.12	120.36	111.27
21	A	830	CLA	C3C-C4C-NC	5.12	116.31	110.57
21	F	404	CLA	C2C-C1C-NC	5.11	114.76	109.97
21	B	826	CLA	CMD-C2D-C1D	5.11	133.72	124.71
21	B	828	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
21	10	704	CLA	C2C-C1C-NC	5.11	114.76	109.97
21	B	823	CLA	CHD-C1D-ND	-5.11	119.76	124.45
21	1	510	CLA	CHD-C1D-ND	-5.11	119.76	124.45
21	A	862	CLA	C3C-C4C-NC	5.10	116.30	110.57
21	1	505	CLA	CHD-C1D-ND	-5.10	119.76	124.45
21	6	912	CLA	CHD-C1D-ND	-5.10	119.76	124.45
21	12	508	CLA	O2D-CGD-CBD	5.10	120.34	111.27
21	A	833	CLA	O2D-CGD-CBD	5.10	120.33	111.27
21	11	710	CLA	C3D-C4D-ND	5.10	118.49	110.24
21	3	709	CLA	C4A-NA-C1A	-5.10	104.41	106.71
21	2	512	CLA	CMD-C2D-C1D	5.10	133.70	124.71
21	4	705	CLA	C4A-NA-C1A	-5.10	104.42	106.71
21	2	510	CLA	CMD-C2D-C1D	5.09	133.69	124.71
21	5	703	CLA	CMD-C2D-C1D	5.09	133.69	124.71
21	12	508	CLA	C2C-C1C-NC	5.09	114.74	109.97
21	10	705	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
21	5	710	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
21	9	902	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
21	B	829	CLA	CMD-C2D-C1D	5.09	133.68	124.71
21	4	708	CLA	C2C-C1C-NC	5.09	114.74	109.97
21	B	816	CLA	CHD-C1D-ND	-5.09	119.78	124.45
21	A	842	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
21	A	840	CLA	CED-O2D-CGD	-5.09	104.44	115.94
21	1	513	CLA	CHD-C1D-ND	-5.08	119.78	124.45
21	B	804	CLA	O2D-CGD-CBD	5.08	120.30	111.27
21	12	505	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
21	7	708	CLA	CMD-C2D-C1D	5.08	133.67	124.71
21	3	711	CLA	C4A-NA-C1A	-5.08	104.42	106.71
21	12	502	CLA	C2C-C1C-NC	5.08	114.73	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	810	CLA	CHD-C4C-C3C	-5.07	117.38	124.84
21	A	843	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
21	4	707	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
21	10	703	CLA	C3D-C4D-ND	5.07	118.44	110.24
21	B	828	CLA	CAC-C3C-C4C	5.07	131.39	124.81
21	B	812	CLA	CMD-C2D-C1D	5.07	133.65	124.71
21	5	704	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
21	3	704	CLA	CBC-CAC-C3C	-5.07	98.45	112.43
21	11	707	CLA	CMD-C2D-C1D	5.07	133.64	124.71
21	8	613	CLA	C4A-NA-C1A	-5.07	104.43	106.71
21	B	803	CLA	CHD-C1D-ND	-5.07	119.80	124.45
21	2	515	CLA	C1C-C2C-C3C	-5.07	101.63	106.96
21	A	818	CLA	C4A-NA-C1A	-5.06	104.43	106.71
21	9	903	CLA	C4A-NA-C1A	-5.06	104.43	106.71
21	9	911	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
21	4	702	CLA	C2C-C1C-NC	5.05	114.71	109.97
21	B	816	CLA	CMD-C2D-C1D	5.05	133.62	124.71
21	10	704	CLA	C3D-C4D-ND	5.05	118.41	110.24
21	10	703	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
21	3	710	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
21	B	833	CLA	CMD-C2D-C1D	5.05	133.61	124.71
21	8	603	CLA	C3D-C4D-ND	5.05	118.41	110.24
21	12	504	CLA	C2C-C1C-NC	5.05	114.70	109.97
21	1	513	CLA	C3D-C4D-ND	5.05	118.40	110.24
21	B	823	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
21	11	710	CLA	CHD-C4C-C3C	-5.04	117.42	124.84
21	B	826	CLA	CHD-C1D-ND	-5.04	119.82	124.45
21	1	508	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
21	A	802	CLA	CAC-C3C-C4C	5.04	131.35	124.81
21	A	802	CLA	C2C-C1C-NC	5.04	114.69	109.97
21	11	704	CLA	C4A-NA-C1A	-5.04	104.44	106.71
21	12	508	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
21	A	818	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
21	12	508	CLA	C4A-NA-C1A	-5.04	104.44	106.71
21	B	816	CLA	O2D-CGD-CBD	5.04	120.22	111.27
21	4	704	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
21	1	501	CLA	C2C-C1C-NC	5.03	114.69	109.97
21	7	703	CLA	CHD-C1D-ND	-5.03	119.83	124.45
21	A	822	CLA	C2C-C1C-NC	5.03	114.69	109.97
21	7	702	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
21	1	516	CLA	C4A-NA-C1A	-5.03	104.44	106.71
21	12	504	CLA	CAC-C3C-C4C	5.03	131.34	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	820	CLA	CMD-C2D-C1D	5.03	133.58	124.71
21	9	905	CLA	C2C-C1C-NC	5.03	114.68	109.97
21	8	606	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
21	3	704	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
21	B	838	CLA	CHB-C4A-NA	5.02	131.45	124.51
21	8	611	CLA	C1D-CHD-C4C	-5.02	115.23	126.06
21	8	612	CLA	C3D-C4D-ND	5.02	118.36	110.24
21	B	836	CLA	C3C-C4C-NC	5.02	116.20	110.57
21	B	830	CLA	C2C-C1C-NC	5.01	114.67	109.97
21	11	710	CLA	O2D-CGD-CBD	5.01	120.18	111.27
21	8	607	CLA	CHD-C1D-ND	-5.01	119.85	124.45
21	B	803	CLA	CAC-C3C-C4C	5.01	131.31	124.81
24	B	843	BCR	C37-C22-C21	-5.01	115.90	122.92
21	B	814	CLA	O2D-CGD-CBD	5.01	120.17	111.27
21	8	612	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
21	B	811	CLA	O2D-CGD-CBD	5.01	120.17	111.27
21	2	504	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
21	12	503	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
21	B	815	CLA	O2D-CGD-O1D	-5.01	114.05	123.84
21	10	706	CLA	CHD-C4C-C3C	-5.00	117.48	124.84
21	B	823	CLA	CMD-C2D-C1D	5.00	133.53	124.71
21	2	510	CLA	C3D-C4D-ND	5.00	118.33	110.24
21	B	838	CLA	CAC-C3C-C4C	5.00	131.30	124.81
21	7	713	CLA	C4A-NA-C1A	-5.00	104.46	106.71
21	5	701	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
21	6	909	CLA	C2C-C1C-NC	5.00	114.66	109.97
21	B	826	CLA	C3D-C4D-ND	5.00	118.33	110.24
21	1	515	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
21	1	507	CLA	CHD-C1D-ND	-5.00	119.86	124.45
21	11	701	CLA	CHD-C1D-ND	-5.00	119.86	124.45
21	B	824	CLA	CHB-C4A-NA	4.99	131.41	124.51
21	5	702	CLA	CHD-C1D-ND	-4.99	119.87	124.45
21	B	815	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
21	11	706	CLA	CHD-C1D-ND	-4.99	119.87	124.45
21	A	812	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
21	13	503	CLA	CAC-C3C-C4C	4.99	131.28	124.81
21	B	801	CLA	CMD-C2D-C1D	4.98	133.50	124.71
28	6	916	DD6	C12-C11-C13	4.98	125.93	118.08
21	A	840	CLA	O2A-CGA-O1A	-4.98	111.02	123.59
21	A	813	CLA	CMD-C2D-C1D	4.98	133.49	124.71
21	A	834	CLA	C3D-C4D-ND	4.98	118.29	110.24
21	1	516	CLA	CHD-C4C-C3C	-4.98	117.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	807	CLA	O2D-CGD-O1D	-4.98	114.11	123.84
21	B	826	CLA	C3B-C4B-NB	4.97	115.64	109.21
21	1	512	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
21	9	914	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
21	A	842	CLA	CMD-C2D-C1D	4.97	133.47	124.71
21	A	835	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
21	10	705	CLA	C4A-NA-C1A	-4.97	104.47	106.71
21	A	803	CLA	CMD-C2D-C1D	4.97	133.47	124.71
21	11	708	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
21	B	820	CLA	CHD-C1D-ND	-4.97	119.89	124.45
21	2	511	CLA	O2D-CGD-CBD	4.97	120.09	111.27
21	A	844	CLA	C2C-C1C-NC	4.96	114.62	109.97
21	B	818	CLA	C4A-NA-C1A	-4.96	104.47	106.71
21	B	818	CLA	C3D-C4D-ND	4.96	118.27	110.24
21	3	714	CLA	C4A-NA-C1A	-4.96	104.47	106.71
21	2	514	CLA	C4A-NA-C1A	-4.96	104.48	106.71
21	2	508	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
21	A	841	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
21	11	709	CLA	CHD-C4C-C3C	-4.96	117.56	124.84
21	11	702	CLA	CHD-C1D-ND	-4.96	119.90	124.45
21	3	714	CLA	CMD-C2D-C1D	4.95	133.44	124.71
21	7	708	CLA	O2D-CGD-O1D	-4.95	114.15	123.84
21	13	502	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
21	11	703	CLA	CHD-C1D-ND	-4.95	119.91	124.45
21	8	610	CLA	O2D-CGD-O1D	-4.95	114.16	123.84
21	A	802	CLA	C4A-NA-C1A	-4.95	104.48	106.71
21	A	813	CLA	C2D-C1D-ND	4.95	113.75	110.10
21	10	704	CLA	CHD-C4C-C3C	-4.94	117.57	124.84
21	3	701	CLA	C2C-C1C-NC	4.94	114.60	109.97
21	6	911	CLA	CMD-C2D-C1D	4.94	133.42	124.71
21	6	909	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
21	B	825	CLA	CMD-C2D-C1D	4.94	133.42	124.71
21	1	516	CLA	CHD-C1D-ND	-4.94	119.92	124.45
21	8	607	CLA	C2C-C1C-NC	4.94	114.60	109.97
21	1	517	CLA	O2D-CGD-CBD	4.94	120.04	111.27
21	4	709	CLA	C4A-NA-C1A	-4.94	104.49	106.71
21	6	912	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
21	11	703	CLA	CAC-C3C-C4C	4.94	131.22	124.81
21	B	826	CLA	C2C-C1C-NC	4.94	114.60	109.97
21	9	911	CLA	CHD-C1D-ND	-4.94	119.92	124.45
21	11	706	CLA	C3D-C2D-C1D	-4.94	99.10	105.83
21	5	710	CLA	CHD-C1D-ND	-4.93	119.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	803	CLA	CHD-C1D-ND	-4.93	119.92	124.45
21	9	906	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
21	B	830	CLA	CHD-C1D-ND	-4.93	119.92	124.45
21	A	812	CLA	C1D-CHD-C4C	-4.93	115.42	126.06
21	B	822	CLA	CMD-C2D-C1D	4.93	133.40	124.71
21	7	705	CLA	C2C-C1C-NC	4.93	114.59	109.97
21	A	832	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
21	8	610	CLA	CHD-C1D-ND	-4.92	119.93	124.45
21	10	712	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
21	A	821	CLA	CAA-CBA-CGA	-4.92	98.87	113.25
21	A	834	CLA	C4A-NA-C1A	-4.92	104.49	106.71
21	13	501	CLA	C4A-NA-C1A	-4.92	104.49	106.71
21	3	706	CLA	O2D-CGD-CBD	4.92	120.01	111.27
21	1	504	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
21	2	517	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
21	10	707	CLA	C2C-C1C-NC	4.92	114.58	109.97
21	6	904	CLA	O2D-CGD-CBD	4.92	120.00	111.27
21	2	513	CLA	C2C-C1C-NC	4.91	114.58	109.97
21	13	501	CLA	C2C-C1C-NC	4.91	114.57	109.97
21	A	825	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
21	B	821	CLA	C3C-C4C-NC	4.91	116.08	110.57
28	2	519	DD6	C14-C13-C11	4.91	133.14	125.53
21	3	711	CLA	CHD-C1D-ND	-4.90	119.95	124.45
21	12	504	CLA	C1D-CHD-C4C	-4.90	115.48	126.06
21	12	506	CLA	C3D-C4D-ND	4.90	118.17	110.24
21	B	811	CLA	CHD-C4C-C3C	-4.90	117.64	124.84
21	4	701	CLA	C3D-C4D-ND	4.90	118.16	110.24
21	9	903	CLA	C3D-C4D-ND	4.90	118.16	110.24
21	6	912	CLA	C4A-NA-C1A	-4.90	104.50	106.71
21	2	509	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
21	B	812	CLA	C3D-C4D-ND	4.89	118.16	110.24
21	A	812	CLA	CBC-CAC-C3C	-4.89	98.94	112.43
21	8	612	CLA	C4A-NA-C1A	-4.89	104.51	106.71
21	1	510	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
21	9	905	CLA	C4A-NA-C1A	-4.89	104.51	106.71
21	11	704	CLA	CHD-C4C-C3C	-4.89	117.66	124.84
21	8	609	CLA	CMB-C2B-C3B	4.89	133.82	124.68
21	7	705	CLA	CMD-C2D-C1D	4.89	133.32	124.71
21	B	832	CLA	C4C-C3C-C2C	-4.89	99.78	106.90
21	7	707	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
21	1	510	CLA	CMB-C2B-C3B	4.89	133.82	124.68
21	A	804	CLA	C3C-C4C-NC	4.88	116.05	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	826	CLA	CAC-C3C-C4C	4.88	131.15	124.81
21	5	710	CLA	C2C-C1C-NC	4.88	114.55	109.97
21	A	808	CLA	CAC-C3C-C4C	4.88	131.15	124.81
21	B	837	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
21	1	514	CLA	CHD-C1D-ND	-4.88	119.97	124.45
21	B	834	CLA	C3C-C4C-NC	4.88	116.04	110.57
21	6	906	CLA	C3C-C4C-NC	4.88	116.04	110.57
21	3	709	CLA	CHD-C1D-ND	-4.88	119.97	124.45
21	9	912	CLA	CHD-C1D-ND	-4.88	119.97	124.45
21	A	827	CLA	CMD-C2D-C1D	4.87	133.30	124.71
21	9	913	CLA	C3D-C4D-ND	4.87	118.12	110.24
21	F	403	CLA	CMD-C2D-C1D	4.87	133.30	124.71
21	11	705	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	2	511	CLA	C1D-CHD-C4C	-4.87	115.56	126.06
21	8	606	CLA	CMD-C2D-C1D	4.87	133.29	124.71
21	1	514	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
21	5	702	CLA	CAC-C3C-C4C	4.86	131.12	124.81
21	A	833	CLA	O2A-CGA-CBA	4.86	127.17	111.91
21	7	706	CLA	C3C-C4C-NC	4.86	116.02	110.57
21	6	907	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
21	A	818	CLA	C4-C3-C5	4.86	123.44	115.27
21	B	809	CLA	CAC-C3C-C4C	4.86	131.11	124.81
21	13	502	CLA	C4A-NA-C1A	-4.86	104.52	106.71
21	2	515	CLA	CHD-C1D-ND	-4.86	119.99	124.45
21	8	605	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
21	7	713	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
21	10	708	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
21	2	515	CLA	C3C-C4C-NC	4.85	116.01	110.57
21	6	903	CLA	C3D-C4D-ND	4.85	118.08	110.24
21	A	815	CLA	C3D-C4D-ND	4.85	118.08	110.24
21	6	904	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
21	12	507	CLA	O2D-CGD-CBD	4.85	119.89	111.27
21	8	604	CLA	O2D-CGD-CBD	4.85	119.88	111.27
21	2	509	CLA	CAC-C3C-C4C	4.85	131.10	124.81
21	B	827	CLA	O2A-C1-C2	4.85	121.37	108.64
21	11	711	CLA	C4A-NA-C1A	-4.84	104.53	106.71
21	A	823	CLA	C3D-C4D-ND	4.84	118.07	110.24
21	B	806	CLA	O2D-CGD-CBD	4.84	119.87	111.27
21	9	912	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
21	B	832	CLA	CMD-C2D-C1D	4.84	133.25	124.71
21	A	834	CLA	C3C-C4C-NC	4.84	116.00	110.57
21	B	811	CLA	C2C-C1C-NC	4.84	114.51	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	912	CLA	C2C-C1C-NC	4.84	114.50	109.97
21	6	913	CLA	C4A-NA-C1A	-4.84	104.53	106.71
21	7	707	CLA	C4A-NA-C1A	-4.84	104.53	106.71
21	B	837	CLA	CHD-C1D-ND	-4.84	120.01	124.45
21	11	707	CLA	C2C-C1C-NC	4.83	114.50	109.97
21	9	910	CLA	C3D-C4D-ND	4.83	118.05	110.24
21	13	502	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
21	5	707	CLA	O2D-CGD-CBD	4.83	119.84	111.27
21	5	702	CLA	CHD-C4C-C3C	-4.83	117.75	124.84
21	9	905	CLA	O2D-CGD-CBD	4.82	119.84	111.27
21	3	714	CLA	CMC-C2C-C1C	4.82	132.38	125.04
21	6	903	CLA	C4A-NA-C1A	-4.82	104.54	106.71
28	3	717	DD6	C13-C11-C10	4.82	126.34	118.94
21	B	825	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
21	8	605	CLA	C3D-C4D-ND	4.82	118.04	110.24
21	12	501	CLA	C3D-C4D-ND	4.82	118.03	110.24
21	2	510	CLA	C2C-C1C-NC	4.82	114.49	109.97
21	6	914	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
21	3	708	CLA	C1D-CHD-C4C	-4.82	115.67	126.06
21	F	403	CLA	O2D-CGD-CBD	4.82	119.83	111.27
21	5	708	CLA	C3B-C4B-NB	4.81	115.43	109.21
21	4	702	CLA	CMD-C2D-C1D	4.81	133.20	124.71
21	A	822	CLA	CHD-C1D-ND	-4.81	120.03	124.45
28	5	713	DD6	C10-C9-C8	4.81	138.23	123.22
21	4	708	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
21	B	816	CLA	C6-C5-C3	-4.81	100.85	113.45
21	2	503	CLA	CBC-CAC-C3C	-4.80	99.19	112.43
21	4	711	CLA	C3D-C4D-ND	4.80	118.01	110.24
21	3	710	CLA	CAC-C3C-C4C	4.80	131.04	124.81
21	8	614	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
28	12	510	DD6	C3-C4-C5	4.80	133.30	123.47
21	B	809	CLA	C4A-NA-C1A	-4.80	104.55	106.71
21	9	902	CLA	CMD-C2D-C1D	4.79	133.16	124.71
21	B	808	CLA	C1D-CHD-C4C	-4.79	115.72	126.06
21	5	711	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
21	B	810	CLA	CMD-C2D-C1D	4.79	133.16	124.71
21	1	504	CLA	C4A-NA-C1A	-4.79	104.55	106.71
21	B	820	CLA	O2D-CGD-CBD	4.79	119.77	111.27
21	B	833	CLA	CHB-C4A-NA	4.78	131.13	124.51
21	7	714	CLA	CHD-C1D-ND	-4.78	120.06	124.45
21	4	705	CLA	C3D-C4D-ND	4.78	117.98	110.24
21	9	914	CLA	C4A-NA-C1A	-4.78	104.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	711	CLA	C2C-C1C-NC	4.78	114.45	109.97
21	B	834	CLA	CAC-C3C-C4C	4.78	131.01	124.81
21	A	802	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
21	B	827	CLA	CMC-C2C-C1C	4.78	132.32	125.04
21	1	509	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
21	2	505	CLA	C1D-CHD-C4C	-4.78	115.75	126.06
21	3	705	CLA	C4A-NA-C1A	-4.78	104.56	106.71
21	A	826	CLA	CHD-C4C-C3C	-4.78	117.82	124.84
21	3	704	CLA	CHD-C4C-C3C	-4.78	117.82	124.84
21	1	504	CLA	C3D-C4D-ND	4.77	117.96	110.24
21	4	703	CLA	C3D-C4D-ND	4.77	117.96	110.24
21	5	705	CLA	CHD-C1D-ND	-4.77	120.07	124.45
21	11	704	CLA	C3D-C4D-ND	4.77	117.96	110.24
21	B	836	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
21	6	909	CLA	C3D-C4D-ND	4.77	117.96	110.24
21	A	829	CLA	O2D-CGD-CBD	4.77	119.75	111.27
21	A	829	CLA	C2C-C1C-NC	4.77	114.44	109.97
21	3	711	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
21	B	836	CLA	CMC-C2C-C1C	4.77	132.30	125.04
21	A	837	CLA	C2C-C1C-NC	4.77	114.44	109.97
21	3	707	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
21	10	705	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
21	B	821	CLA	C1-O2A-CGA	4.77	128.95	116.44
21	5	701	CLA	CMD-C2D-C1D	4.76	133.11	124.71
21	4	703	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
21	8	613	CLA	C1D-CHD-C4C	-4.76	115.79	126.06
28	5	713	DD6	C13-C11-C10	4.76	126.25	118.94
21	1	516	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
21	1	506	CLA	C4A-NA-C1A	-4.76	104.57	106.71
21	B	831	CLA	CMD-C2D-C1D	4.76	133.10	124.71
21	A	813	CLA	C3D-C4D-ND	4.76	117.93	110.24
21	9	908	CLA	C3D-C4D-ND	4.76	117.93	110.24
21	2	513	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
21	12	507	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
21	1	508	CLA	O2D-CGD-CBD	4.75	119.71	111.27
21	B	814	CLA	C3C-C4C-NC	4.75	115.90	110.57
21	4	709	CLA	C2C-C1C-NC	4.75	114.42	109.97
21	1	515	CLA	C3D-C4D-ND	4.75	117.92	110.24
21	A	812	CLA	O2D-CGD-O1D	-4.75	114.56	123.84
21	2	515	CLA	O2D-CGD-CBD	4.75	119.70	111.27
21	8	604	CLA	C3C-C4C-NC	4.75	115.89	110.57
21	1	504	CLA	C2C-C1C-NC	4.74	114.42	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	512	CLA	C2C-C1C-NC	4.74	114.42	109.97
21	A	803	CLA	C4C-C3C-C2C	-4.74	99.99	106.90
21	A	825	CLA	CMD-C2D-C1D	4.74	133.07	124.71
21	11	708	CLA	C3D-C4D-ND	4.74	117.90	110.24
21	B	834	CLA	C4C-C3C-C2C	-4.73	100.00	106.90
21	1	506	CLA	CMD-C2D-C1D	4.73	133.06	124.71
21	A	840	CLA	C4C-C3C-C2C	-4.73	100.00	106.90
21	8	605	CLA	C4A-NA-C1A	-4.73	104.58	106.71
21	4	709	CLA	C3D-C4D-ND	4.73	117.89	110.24
21	11	706	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
21	1	517	CLA	C3C-C4C-NC	4.73	115.88	110.57
21	5	705	CLA	C4A-NA-C1A	-4.73	104.58	106.71
21	7	706	CLA	O2D-CGD-CBD	4.73	119.67	111.27
21	A	810	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
21	A	833	CLA	CAC-C3C-C4C	4.73	130.95	124.81
21	A	840	CLA	O2A-CGA-CBA	4.73	126.75	111.91
21	A	826	CLA	C3B-C4B-NB	4.73	115.32	109.21
21	B	835	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
21	10	709	CLA	C4A-NA-C1A	-4.73	104.58	106.71
21	2	515	CLA	CMD-C2D-C1D	4.73	133.04	124.71
21	4	702	CLA	C3D-C4D-ND	4.72	117.88	110.24
21	3	703	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
21	9	906	CLA	C3D-C4D-ND	4.72	117.88	110.24
21	2	517	CLA	O2D-CGD-CBD	4.72	119.66	111.27
21	8	604	CLA	C2C-C1C-NC	4.72	114.39	109.97
21	9	912	CLA	CMD-C2D-C1D	4.72	133.03	124.71
21	4	711	CLA	C2C-C1C-NC	4.72	114.39	109.97
21	10	705	CLA	C3D-C4D-ND	4.72	117.87	110.24
21	2	511	CLA	C3D-C4D-ND	4.72	117.87	110.24
21	B	827	CLA	O2D-CGD-CBD	4.72	119.65	111.27
21	9	903	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
21	5	705	CLA	O2D-CGD-O1D	-4.72	114.61	123.84
21	4	710	CLA	C2C-C1C-NC	4.72	114.39	109.97
21	B	809	CLA	C3C-C4C-NC	4.72	115.86	110.57
21	2	515	CLA	CHD-C4C-C3C	-4.72	117.91	124.84
21	8	608	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
21	8	613	CLA	CHD-C1D-ND	-4.71	120.12	124.45
21	7	709	CLA	CHD-C4C-C3C	-4.71	117.91	124.84
21	3	703	CLA	C1D-CHD-C4C	-4.71	115.89	126.06
21	6	911	CLA	C1D-CHD-C4C	-4.71	115.89	126.06
21	B	807	CLA	C3C-C4C-NC	4.71	115.86	110.57
21	11	711	CLA	C3D-C2D-C1D	-4.71	99.40	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	706	CLA	C2C-C1C-NC	4.71	114.39	109.97
21	7	714	CLA	C2C-C1C-NC	4.71	114.39	109.97
21	12	503	CLA	C3D-C4D-ND	4.71	117.86	110.24
21	7	711	CLA	O2D-CGD-CBD	4.71	119.63	111.27
21	5	708	CLA	C1D-CHD-C4C	-4.71	115.90	126.06
21	2	513	CLA	O2D-CGD-CBD	4.70	119.63	111.27
21	B	811	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
21	6	910	CLA	C4A-NA-C1A	-4.70	104.59	106.71
21	5	705	CLA	C2C-C1C-NC	4.70	114.38	109.97
21	7	704	CLA	C1D-CHD-C4C	-4.70	115.92	126.06
21	9	913	CLA	C4A-NA-C1A	-4.70	104.59	106.71
21	B	833	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
21	11	705	CLA	CAC-C3C-C4C	4.70	130.90	124.81
21	B	804	CLA	C2C-C1C-NC	4.70	114.37	109.97
21	1	505	CLA	C2C-C1C-NC	4.70	114.37	109.97
21	2	510	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
21	8	608	CLA	C4A-NA-C1A	-4.70	104.59	106.71
21	A	836	CLA	C3D-C4D-ND	4.70	117.83	110.24
21	1	511	CLA	C2C-C1C-NC	4.69	114.37	109.97
21	11	705	CLA	C2C-C1C-NC	4.69	114.37	109.97
21	A	802	CLA	C3C-C4C-NC	4.69	115.83	110.57
21	B	833	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
21	J	101	CLA	CHD-C1D-ND	-4.69	120.14	124.45
21	6	906	CLA	CHD-C1D-ND	-4.69	120.15	124.45
21	2	508	CLA	C3D-C4D-ND	4.68	117.81	110.24
21	11	701	CLA	C2C-C1C-NC	4.68	114.36	109.97
21	B	835	CLA	C2D-C1D-ND	4.68	113.55	110.10
21	3	713	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
21	A	829	CLA	O2D-CGD-O1D	-4.68	114.69	123.84
21	B	812	CLA	CAC-C3C-C4C	4.68	130.88	124.81
28	1	519	DD6	C12-C11-C13	4.68	125.45	118.08
21	3	705	CLA	CHD-C4C-C3C	-4.68	117.97	124.84
21	3	713	CLA	O2D-CGD-CBD	4.67	119.57	111.27
21	4	708	CLA	O2D-CGD-CBD	4.67	119.57	111.27
21	A	815	CLA	CHD-C1D-ND	-4.67	120.16	124.45
21	A	810	CLA	O2A-CGA-CBA	4.67	126.57	111.91
21	B	803	CLA	C3C-C4C-NC	4.67	115.81	110.57
21	7	703	CLA	C3D-C4D-ND	4.67	117.79	110.24
21	4	701	CLA	C4A-NA-C1A	-4.67	104.61	106.71
21	1	517	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
21	7	712	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
21	3	712	CLA	CHD-C4C-C3C	-4.66	117.98	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	506	CLA	C1D-CHD-C4C	-4.66	116.00	126.06
21	1	513	CLA	C4A-NA-C1A	-4.66	104.61	106.71
21	A	835	CLA	CHC-C1C-NC	4.66	131.28	124.20
21	10	706	CLA	O2D-CGD-CBD	4.66	119.55	111.27
21	10	706	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	A	848	BCR	C16-C15-C14	4.66	133.02	123.47
21	13	502	CLA	O2D-CGD-CBD	4.66	119.55	111.27
21	A	844	CLA	C3C-C4C-NC	4.66	115.80	110.57
21	A	820	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
21	B	835	CLA	C1D-CHD-C4C	-4.66	116.01	126.06
21	6	906	CLA	C4A-NA-C1A	-4.66	104.61	106.71
21	11	706	CLA	O2D-CGD-CBD	4.65	119.54	111.27
21	11	705	CLA	CMD-C2D-C1D	4.65	132.91	124.71
21	A	807	CLA	C4A-NA-C1A	-4.65	104.61	106.71
21	A	840	CLA	O2D-CGD-O1D	-4.65	114.74	123.84
21	4	702	CLA	CAC-C3C-C4C	4.65	130.84	124.81
21	3	710	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
21	A	832	CLA	C2C-C1C-NC	4.65	114.33	109.97
21	3	705	CLA	C2C-C1C-NC	4.65	114.33	109.97
21	3	701	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
21	A	839	CLA	C4D-CHA-C1A	-4.65	115.59	121.25
21	A	809	CLA	C1D-CHD-C4C	-4.65	116.03	126.06
21	12	506	CLA	C4A-NA-C1A	-4.65	104.62	106.71
21	B	826	CLA	C4C-C3C-C2C	-4.65	100.13	106.90
21	5	702	CLA	CMC-C2C-C1C	4.64	132.11	125.04
21	3	710	CLA	C3D-C4D-ND	4.64	117.75	110.24
21	11	701	CLA	C3D-C4D-ND	4.64	117.75	110.24
21	2	512	CLA	C3D-C4D-ND	4.64	117.75	110.24
21	3	710	CLA	C2C-C1C-NC	4.64	114.32	109.97
21	B	819	CLA	C3C-C4C-NC	4.64	115.78	110.57
21	B	839	CLA	C3D-C4D-ND	4.64	117.74	110.24
21	9	914	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
21	10	707	CLA	O2D-CGD-CBD	4.64	119.51	111.27
21	3	702	CLA	C3D-C4D-ND	4.64	117.74	110.24
21	9	905	CLA	C3C-C4C-NC	4.63	115.77	110.57
21	A	816	CLA	CHD-C1D-ND	-4.63	120.20	124.45
21	8	604	CLA	CMD-C2D-C1D	4.63	132.87	124.71
21	4	710	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
21	7	708	CLA	CHD-C4C-C3C	-4.62	118.04	124.84
21	7	704	CLA	C3C-C4C-NC	4.62	115.75	110.57
24	J	102	BCR	C34-C9-C10	-4.62	116.45	122.92
21	9	911	CLA	C3D-C2D-C1D	-4.62	99.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	803	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
21	5	711	CLA	O2D-CGD-CBD	4.62	119.47	111.27
21	10	707	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
21	8	606	CLA	O2D-CGD-CBD	4.61	119.47	111.27
21	B	801	CLA	C1D-CHD-C4C	-4.61	116.11	126.06
21	A	812	CLA	C1-O2A-CGA	4.61	128.54	116.44
21	B	828	CLA	C3D-C4D-ND	4.61	117.69	110.24
21	3	715	CLA	C3D-C4D-ND	4.61	117.69	110.24
21	10	711	CLA	C4A-NA-C1A	-4.61	104.63	106.71
21	7	711	CLA	CBC-CAC-C3C	-4.61	99.73	112.43
21	7	712	CLA	C2C-C1C-NC	4.61	114.29	109.97
21	2	503	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
21	4	711	CLA	CHD-C4C-C3C	-4.61	118.07	124.84
21	A	820	CLA	CBC-CAC-C3C	-4.61	99.73	112.43
21	A	817	CLA	C3D-C4D-ND	4.60	117.69	110.24
21	8	606	CLA	C1D-CHD-C4C	-4.60	116.12	126.06
21	A	838	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
21	6	910	CLA	O2D-CGD-O1D	-4.60	114.84	123.84
21	2	514	CLA	CHD-C4C-C3C	-4.60	118.07	124.84
21	3	703	CLA	C2D-C1D-ND	4.60	113.50	110.10
21	7	710	CLA	C4A-NA-C1A	-4.60	104.64	106.71
21	9	910	CLA	CMD-C2D-C1D	4.60	132.82	124.71
21	7	714	CLA	C4A-NA-C1A	-4.60	104.64	106.71
21	A	840	CLA	CMC-C2C-C1C	4.60	132.04	125.04
21	5	711	CLA	C3D-C4D-ND	4.60	117.68	110.24
21	3	702	CLA	C3C-C4C-NC	4.60	115.73	110.57
21	9	902	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	10	704	CLA	O2D-CGD-O1D	-4.60	114.85	123.84
21	4	703	CLA	O2D-CGD-CBD	4.60	119.43	111.27
21	5	708	CLA	CHD-C1D-ND	-4.59	120.23	124.45
21	A	827	CLA	O2D-CGD-CBD	4.59	119.43	111.27
21	6	913	CLA	O2D-CGD-CBD	4.59	119.43	111.27
21	12	508	CLA	C3D-C4D-ND	4.59	117.67	110.24
21	12	503	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
21	6	905	CLA	CHD-C1D-ND	-4.59	120.24	124.45
21	B	834	CLA	CMD-C2D-C1D	4.59	132.80	124.71
21	B	839	CLA	O2D-CGD-O1D	-4.59	114.87	123.84
21	5	706	CLA	CHD-C1D-ND	-4.59	120.24	124.45
21	11	701	CLA	O2D-CGD-CBD	4.59	119.42	111.27
21	B	804	CLA	C3D-C4D-ND	4.59	117.66	110.24
21	1	508	CLA	C3D-C4D-ND	4.59	117.66	110.24
21	11	711	CLA	O2D-CGD-CBD	4.59	119.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	509	CLA	C3D-C4D-ND	4.59	117.66	110.24
21	A	813	CLA	C4A-NA-C1A	-4.58	104.64	106.71
21	6	906	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
21	6	913	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
21	A	802	CLA	CBC-CAC-C3C	-4.58	99.80	112.43
24	B	841	BCR	C24-C23-C22	-4.58	119.31	126.23
21	F	401	CLA	CMC-C2C-C1C	4.58	132.01	125.04
21	1	505	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
21	9	907	CLA	C3D-C4D-ND	4.58	117.64	110.24
21	B	804	CLA	CAC-C3C-C4C	4.57	130.75	124.81
21	A	825	CLA	CAC-C3C-C4C	4.57	130.74	124.81
21	6	911	CLA	C3D-C4D-ND	4.57	117.63	110.24
21	2	510	CLA	O2D-CGD-O1D	-4.57	114.90	123.84
21	B	832	CLA	C3D-C4D-ND	4.57	117.63	110.24
21	3	711	CLA	C3C-C4C-NC	4.57	115.70	110.57
21	B	819	CLA	C2C-C1C-NC	4.57	114.25	109.97
21	B	829	CLA	C3D-C4D-ND	4.57	117.63	110.24
21	B	806	CLA	CAC-C3C-C4C	4.57	130.74	124.81
21	A	814	CLA	C4C-C3C-C2C	-4.57	100.24	106.90
21	11	706	CLA	CAC-C3C-C4C	4.57	130.74	124.81
21	1	511	CLA	C3D-C4D-ND	4.57	117.63	110.24
21	13	503	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
21	9	910	CLA	C1D-CHD-C4C	-4.57	116.21	126.06
21	12	507	CLA	CHD-C4C-C3C	-4.56	118.13	124.84
21	A	820	CLA	C3C-C4C-NC	4.56	115.69	110.57
21	9	911	CLA	C3D-C4D-ND	4.56	117.61	110.24
21	8	609	CLA	C1D-CHD-C4C	-4.56	116.22	126.06
21	11	709	CLA	O2D-CGD-CBD	4.56	119.37	111.27
21	A	829	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
21	10	710	CLA	C3D-C4D-ND	4.56	117.61	110.24
21	6	908	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
21	B	812	CLA	C3C-C4C-NC	4.55	115.68	110.57
21	5	709	CLA	C1D-CHD-C4C	-4.55	116.24	126.06
21	B	824	CLA	C3D-C4D-ND	4.55	117.60	110.24
20	A	801	CL0	C3B-C4B-NB	4.55	115.09	109.21
21	B	814	CLA	CAC-C3C-C4C	4.55	130.71	124.81
21	B	802	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
21	7	713	CLA	C3D-C4D-ND	4.55	117.59	110.24
21	A	807	CLA	CHD-C4C-C3C	-4.55	118.16	124.84
21	10	706	CLA	C3D-C4D-ND	4.55	117.59	110.24
21	A	832	CLA	CMD-C2D-C1D	4.54	132.72	124.71
21	A	837	CLA	C3D-C4D-ND	4.54	117.58	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	710	CLA	C3C-C4C-NC	4.54	115.66	110.57
21	A	833	CLA	CHD-C4C-C3C	-4.54	118.17	124.84
21	10	709	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
21	B	832	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
21	10	706	CLA	C4A-NA-C1A	-4.54	104.67	106.71
21	A	841	CLA	CHD-C1D-ND	-4.54	120.28	124.45
21	B	817	CLA	CMC-C2C-C1C	4.54	131.95	125.04
21	B	824	CLA	O2D-CGD-O1D	-4.53	114.97	123.84
21	B	814	CLA	C1D-CHD-C4C	-4.53	116.28	126.06
21	A	862	CLA	O2A-CGA-O1A	-4.53	112.15	123.59
21	A	812	CLA	O2D-CGD-CBD	4.53	119.32	111.27
21	A	833	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
21	8	603	CLA	C3B-C4B-NB	4.53	115.07	109.21
21	B	813	CLA	C1D-CHD-C4C	-4.53	116.29	126.06
21	B	833	CLA	C2C-C1C-NC	4.53	114.22	109.97
21	9	907	CLA	O2D-CGD-CBD	4.53	119.32	111.27
21	4	710	CLA	C3D-C4D-ND	4.53	117.56	110.24
21	7	711	CLA	C3D-C4D-ND	4.53	117.56	110.24
21	7	707	CLA	C3C-C4C-NC	4.53	115.65	110.57
21	3	708	CLA	CHD-C1D-ND	-4.53	120.29	124.45
21	B	826	CLA	CAC-C3C-C4C	4.53	130.68	124.81
21	A	813	CLA	CAC-C3C-C4C	4.53	130.68	124.81
21	B	816	CLA	C3D-C4D-ND	4.53	117.56	110.24
21	7	710	CLA	O2D-CGD-O1D	-4.52	114.99	123.84
21	11	702	CLA	C3D-C4D-ND	4.52	117.56	110.24
21	3	712	CLA	C3D-C4D-ND	4.52	117.56	110.24
21	12	508	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
21	10	707	CLA	C3D-C4D-ND	4.52	117.55	110.24
21	B	827	CLA	CHD-C1D-ND	-4.52	120.30	124.45
21	1	516	CLA	CAC-C3C-C4C	4.52	130.68	124.81
20	A	801	CL0	C2A-C1A-CHA	-4.52	115.96	123.86
21	B	832	CLA	C1D-CHD-C4C	-4.52	116.31	126.06
21	1	514	CLA	C1D-CHD-C4C	-4.52	116.32	126.06
21	10	711	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
21	9	910	CLA	CHD-C1D-ND	-4.51	120.31	124.45
21	A	836	CLA	CBC-CAC-C3C	-4.51	100.00	112.43
21	6	907	CLA	CHD-C1D-ND	-4.51	120.31	124.45
21	6	910	CLA	C2C-C1C-NC	4.51	114.19	109.97
21	A	805	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
21	11	709	CLA	C3D-C4D-ND	4.51	117.53	110.24
21	A	835	CLA	C1D-CHD-C4C	-4.50	116.34	126.06
21	A	821	CLA	C3C-C4C-NC	4.50	115.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	703	CLA	C3D-C4D-ND	4.50	117.52	110.24
21	2	506	CLA	C3D-C4D-ND	4.50	117.52	110.24
21	A	842	CLA	C1D-CHD-C4C	-4.50	116.36	126.06
21	7	709	CLA	C2C-C1C-NC	4.50	114.19	109.97
21	4	702	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
21	4	704	CLA	C2C-C1C-NC	4.49	114.18	109.97
21	B	816	CLA	CHB-C4A-NA	4.49	130.73	124.51
21	8	608	CLA	C2C-C1C-NC	4.49	114.18	109.97
21	2	504	CLA	O2D-CGD-CBD	4.49	119.25	111.27
21	6	903	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
21	A	830	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
21	A	835	CLA	C4A-NA-C1A	-4.49	104.69	106.71
21	10	707	CLA	C4A-NA-C1A	-4.49	104.69	106.71
21	2	517	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
21	A	835	CLA	C2C-C1C-NC	4.49	114.17	109.97
21	7	714	CLA	C3C-C4C-NC	4.49	115.60	110.57
21	A	808	CLA	O2A-CGA-CBA	4.49	125.98	111.91
21	B	820	CLA	C3D-C4D-ND	4.48	117.49	110.24
21	A	809	CLA	CAC-C3C-C4C	4.48	130.63	124.81
21	7	708	CLA	O2D-CGD-CBD	4.48	119.24	111.27
21	B	816	CLA	C2C-C1C-NC	4.48	114.17	109.97
21	4	705	CLA	C3C-C4C-NC	4.48	115.60	110.57
21	A	811	CLA	CMD-C2D-C1D	4.48	132.62	124.71
21	5	711	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
24	A	848	BCR	C37-C22-C23	4.48	125.14	118.08
21	6	913	CLA	C3D-C4D-ND	4.48	117.49	110.24
21	6	909	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
21	12	504	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
21	B	835	CLA	C3D-C4D-ND	4.48	117.49	110.24
21	4	701	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
21	A	805	CLA	C3D-C4D-ND	4.48	117.48	110.24
21	A	831	CLA	C1D-CHD-C4C	-4.48	116.40	126.06
21	A	802	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
21	B	828	CLA	C3C-C4C-NC	4.48	115.59	110.57
21	6	908	CLA	C3B-C4B-NB	4.48	115.00	109.21
24	J	103	BCR	C34-C9-C8	4.48	125.13	118.08
21	3	714	CLA	CHD-C1D-ND	-4.47	120.34	124.45
21	6	912	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
21	2	507	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
28	12	509	DD6	C4-C3-C2	4.47	132.64	123.47
21	1	513	CLA	O2D-CGD-CBD	4.47	119.22	111.27
21	B	836	CLA	C3D-C4D-ND	4.47	117.47	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	826	CLA	O2D-CGD-CBD	4.47	119.22	111.27
21	5	708	CLA	C3C-C4C-NC	4.47	115.58	110.57
21	B	817	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
21	A	832	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
21	6	914	CLA	C3D-C4D-ND	4.47	117.47	110.24
21	8	607	CLA	C3C-C4C-NC	4.47	115.58	110.57
21	B	816	CLA	CAC-C3C-C4C	4.47	130.61	124.81
21	A	835	CLA	CHC-C1C-C2C	-4.47	114.36	126.72
21	7	702	CLA	C3D-C4D-ND	4.47	117.46	110.24
21	7	706	CLA	C2C-C1C-NC	4.46	114.15	109.97
21	4	706	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
21	B	830	CLA	C1D-CHD-C4C	-4.46	116.43	126.06
21	5	706	CLA	CMD-C2D-C1D	4.46	132.57	124.71
21	A	820	CLA	C4A-NA-C1A	-4.46	104.70	106.71
21	12	502	CLA	O2D-CGD-CBD	4.46	119.19	111.27
21	F	404	CLA	CAA-C2A-C3A	-4.46	100.57	112.78
21	B	825	CLA	C2A-C1A-CHA	-4.46	116.06	123.86
21	6	910	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
21	A	807	CLA	C2C-C1C-NC	4.46	114.15	109.97
21	A	837	CLA	C1D-CHD-C4C	-4.46	116.45	126.06
21	8	606	CLA	C3C-C4C-NC	4.45	115.57	110.57
21	A	841	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	B	812	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	12	501	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	13	503	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
21	3	705	CLA	CAC-C3C-C4C	4.45	130.59	124.81
21	3	701	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
21	7	712	CLA	C3D-C4D-ND	4.45	117.44	110.24
21	A	830	CLA	CMB-C2B-C3B	4.45	133.00	124.68
21	B	838	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
21	11	707	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
21	6	906	CLA	O2D-CGD-CBD	4.45	119.17	111.27
21	2	511	CLA	CMD-C2D-C1D	4.45	132.55	124.71
21	6	909	CLA	CAC-C3C-C4C	4.44	130.57	124.81
21	10	709	CLA	C3D-C4D-ND	4.44	117.42	110.24
21	13	501	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
21	11	711	CLA	C3D-C4D-ND	4.44	117.42	110.24
21	2	505	CLA	C3C-C4C-NC	4.44	115.55	110.57
21	7	710	CLA	CAC-C3C-C4C	4.44	130.57	124.81
21	3	701	CLA	C1D-CHD-C4C	-4.44	116.48	126.06
21	F	404	CLA	CHD-C1D-ND	-4.44	120.38	124.45
21	A	839	CLA	C2C-C1C-NC	4.44	114.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	701	CLA	C3D-C4D-ND	4.44	117.41	110.24
21	B	807	CLA	CMD-C2D-C1D	4.44	132.53	124.71
21	1	501	CLA	C1D-CHD-C4C	-4.44	116.49	126.06
21	B	804	CLA	O2D-CGD-O1D	-4.43	115.17	123.84
21	5	703	CLA	C2C-C1C-NC	4.43	114.12	109.97
21	11	705	CLA	C3D-C4D-ND	4.43	117.41	110.24
21	B	830	CLA	C4A-NA-C1A	-4.43	104.71	106.71
21	1	509	CLA	C4A-NA-C1A	-4.43	104.71	106.71
21	4	710	CLA	O2D-CGD-CBD	4.43	119.14	111.27
22	B	840	PQN	C17-C16-C15	-4.43	101.34	113.36
21	5	710	CLA	O2D-CGD-CBD	4.43	119.14	111.27
21	B	807	CLA	CAA-C2A-C3A	-4.43	100.66	112.78
21	5	709	CLA	C3D-C4D-ND	4.43	117.40	110.24
21	12	505	CLA	C2C-C1C-NC	4.43	114.12	109.97
24	M	102	BCR	C34-C9-C10	-4.43	116.72	122.92
21	7	712	CLA	C3C-C4C-NC	4.43	115.53	110.57
21	A	862	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
21	9	912	CLA	C2C-C1C-NC	4.42	114.12	109.97
21	9	905	CLA	C3D-C4D-ND	4.42	117.39	110.24
21	A	808	CLA	CMD-C2D-C1D	4.42	132.51	124.71
21	A	841	CLA	C1D-CHD-C4C	-4.42	116.52	126.06
21	A	813	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
21	12	502	CLA	C1D-CHD-C4C	-4.42	116.52	126.06
21	B	818	CLA	C4-C3-C5	4.42	122.70	115.27
21	B	812	CLA	CHD-C1D-ND	-4.42	120.39	124.45
21	A	840	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
21	2	504	CLA	C3D-C4D-ND	4.42	117.38	110.24
21	B	827	CLA	CBC-CAC-C3C	-4.42	100.26	112.43
21	5	709	CLA	CAC-C3C-C4C	4.42	130.54	124.81
21	F	404	CLA	C3D-C4D-ND	4.42	117.38	110.24
21	3	712	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	3	711	CLA	C2C-C1C-NC	4.41	114.10	109.97
21	7	705	CLA	C4A-NA-C1A	-4.41	104.72	106.71
21	B	817	CLA	C2C-C1C-NC	4.41	114.10	109.97
21	A	816	CLA	C1D-CHD-C4C	-4.40	116.56	126.06
21	12	503	CLA	C4A-NA-C1A	-4.40	104.73	106.71
21	B	811	CLA	C3D-C4D-ND	4.40	117.36	110.24
21	7	707	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
24	F	405	BCR	C37-C22-C23	4.40	125.01	118.08
21	5	706	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
21	2	517	CLA	C3D-C4D-ND	4.40	117.35	110.24
21	B	824	CLA	C3C-C4C-NC	4.40	115.50	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	910	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
21	9	907	CLA	C2C-C1C-NC	4.39	114.09	109.97
21	B	834	CLA	C1D-CHD-C4C	-4.39	116.58	126.06
21	3	711	CLA	C3D-C4D-ND	4.39	117.34	110.24
21	A	829	CLA	OBD-CAD-C3D	-4.39	117.95	128.52
21	A	838	CLA	O2D-CGD-CBD	4.39	119.07	111.27
21	4	707	CLA	C2C-C1C-NC	4.39	114.08	109.97
21	B	810	CLA	CMC-C2C-C1C	4.39	131.72	125.04
21	A	837	CLA	O2D-CGD-CBD	4.39	119.07	111.27
28	11	713	DD6	C3-C4-C5	4.39	132.46	123.47
21	A	806	CLA	CMD-C2D-C1D	4.39	132.45	124.71
21	6	904	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
21	A	832	CLA	CHD-C1D-ND	-4.39	120.42	124.45
21	1	506	CLA	O2D-CGD-CBD	4.39	119.06	111.27
21	2	513	CLA	C3D-C4D-ND	4.39	117.33	110.24
21	A	807	CLA	O2A-CGA-CBA	4.38	125.67	111.91
21	A	817	CLA	CAC-C3C-C4C	4.38	130.50	124.81
21	3	704	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
21	6	912	CLA	C3D-C4D-ND	4.38	117.33	110.24
21	A	804	CLA	C1D-CHD-C4C	-4.38	116.61	126.06
28	7	716	DD6	C12-C11-C13	4.38	124.98	118.08
21	2	512	CLA	C3B-C4B-NB	4.38	114.87	109.21
28	7	716	DD6	C12-C11-C10	-4.38	116.79	122.92
21	A	820	CLA	C4C-C3C-C2C	-4.38	100.52	106.90
21	8	611	CLA	CHD-C1D-ND	-4.38	120.43	124.45
21	5	706	CLA	C3C-C4C-NC	4.38	115.48	110.57
21	B	822	CLA	C3D-C4D-ND	4.37	117.31	110.24
21	1	507	CLA	C3D-C4D-ND	4.37	117.31	110.24
21	4	708	CLA	C3D-C4D-ND	4.37	117.31	110.24
21	A	825	CLA	C2C-C1C-NC	4.37	114.07	109.97
21	A	809	CLA	CMD-C2D-C1D	4.37	132.42	124.71
21	8	612	CLA	C2C-C1C-NC	4.37	114.07	109.97
21	B	819	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
21	2	510	CLA	C3C-C4C-NC	4.37	115.47	110.57
21	8	605	CLA	C1D-CHD-C4C	-4.37	116.63	126.06
21	2	517	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
20	A	801	CL0	C2C-C1C-NC	4.37	114.06	109.97
21	3	714	CLA	C3C-C4C-NC	4.37	115.47	110.57
21	A	807	CLA	C1-C2-C3	-4.36	118.50	126.04
21	B	810	CLA	O2D-CGD-CBD	4.36	119.02	111.27
21	2	509	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
21	9	906	CLA	C3D-C2D-C1D	-4.36	99.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	913	CLA	C2C-C1C-NC	4.36	114.06	109.97
21	2	516	CLA	CAC-C3C-C4C	4.36	130.47	124.81
21	3	712	CLA	O2D-CGD-CBD	4.36	119.02	111.27
21	J	101	CLA	C3C-C4C-NC	4.36	115.46	110.57
21	12	505	CLA	C4A-NA-C1A	-4.36	104.75	106.71
21	3	715	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
21	3	707	CLA	CAC-C3C-C4C	4.36	130.46	124.81
21	A	833	CLA	C3D-C4D-ND	4.36	117.28	110.24
21	A	841	CLA	C3C-C4C-NC	4.36	115.46	110.57
21	A	803	CLA	C2C-C1C-NC	4.36	114.05	109.97
21	A	813	CLA	C3C-C4C-NC	4.35	115.45	110.57
21	A	821	CLA	CAA-C2A-C1A	-4.35	97.71	111.97
21	9	909	CLA	C2C-C1C-NC	4.35	114.05	109.97
21	8	604	CLA	CHD-C1D-ND	-4.35	120.45	124.45
21	A	802	CLA	C1D-CHD-C4C	-4.35	116.67	126.06
21	B	821	CLA	C3D-C4D-ND	4.35	117.27	110.24
21	B	806	CLA	CHD-C4C-C3C	-4.35	118.45	124.84
21	9	908	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
21	5	701	CLA	CHD-C1D-ND	-4.35	120.46	124.45
21	A	810	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	F	402	BCR	C34-C9-C10	-4.35	116.83	122.92
21	B	835	CLA	CAC-C3C-C4C	4.34	130.45	124.81
21	A	841	CLA	C4C-C3C-C2C	-4.34	100.57	106.90
21	A	803	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
21	B	817	CLA	C1D-CHD-C4C	-4.34	116.69	126.06
21	2	509	CLA	CMC-C2C-C1C	4.34	131.65	125.04
21	A	810	CLA	CAC-C3C-C4C	4.34	130.44	124.81
21	9	914	CLA	C3D-C4D-ND	4.34	117.26	110.24
21	9	914	CLA	O2D-CGD-CBD	4.34	118.98	111.27
21	8	610	CLA	C2C-C1C-NC	4.34	114.03	109.97
21	4	705	CLA	O2D-CGD-CBD	4.33	118.97	111.27
21	A	816	CLA	O2D-CGD-CBD	4.33	118.97	111.27
21	11	704	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
21	A	843	CLA	C3C-C4C-NC	4.33	115.43	110.57
21	1	512	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
21	F	403	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
21	7	712	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
21	1	509	CLA	C3D-C4D-ND	4.33	117.24	110.24
21	B	804	CLA	CHB-C4A-NA	4.33	130.50	124.51
21	B	833	CLA	CAA-C2A-C1A	4.33	126.16	111.97
21	11	703	CLA	C1D-CHD-C4C	-4.33	116.73	126.06
21	8	614	CLA	CAC-C3C-C4C	4.33	130.42	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	703	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
21	B	814	CLA	C3D-C4D-ND	4.32	117.23	110.24
21	10	712	CLA	C3D-C4D-ND	4.32	117.23	110.24
21	A	806	CLA	C1D-CHD-C4C	-4.32	116.74	126.06
21	9	909	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
21	2	507	CLA	CHD-C4C-C3C	-4.32	118.49	124.84
21	B	824	CLA	OBD-CAD-C3D	-4.32	118.12	128.52
21	A	841	CLA	C1-C2-C3	-4.32	118.58	126.04
21	A	862	CLA	CMC-C2C-C1C	4.32	131.61	125.04
21	A	843	CLA	C3D-C4D-ND	4.32	117.22	110.24
21	A	832	CLA	CHB-C4A-NA	4.32	130.48	124.51
21	8	607	CLA	C4A-NA-C1A	-4.32	104.77	106.71
21	B	825	CLA	O2D-CGD-CBD	4.31	118.94	111.27
24	A	848	BCR	C34-C9-C10	-4.31	116.88	122.92
21	5	706	CLA	C4A-NA-C1A	-4.31	104.77	106.71
21	4	705	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
21	F	403	CLA	C2C-C1C-NC	4.31	114.01	109.97
21	A	819	CLA	C1D-CHD-C4C	-4.31	116.76	126.06
21	A	844	CLA	C3D-C4D-ND	4.31	117.21	110.24
21	6	908	CLA	C3C-C4C-NC	4.31	115.40	110.57
21	1	508	CLA	CMC-C2C-C1C	4.31	131.60	125.04
21	1	505	CLA	O2D-CGD-CBD	4.31	118.92	111.27
21	9	912	CLA	C3D-C4D-ND	4.31	117.21	110.24
21	4	701	CLA	CHC-C1C-C2C	-4.31	114.81	126.72
21	F	401	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
21	3	714	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
21	A	825	CLA	O2D-CGD-CBD	4.30	118.92	111.27
21	A	809	CLA	O2A-CGA-CBA	4.30	125.41	111.91
21	10	703	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
28	11	713	DD6	C12-C11-C10	-4.30	116.90	122.92
21	4	703	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
24	F	405	BCR	C36-C18-C17	-4.30	116.90	122.92
21	1	501	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
21	B	807	CLA	CAC-C3C-C4C	4.29	130.38	124.81
21	A	818	CLA	C1-O2A-CGA	4.29	127.71	116.44
21	B	838	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
21	6	911	CLA	CHD-C1D-ND	-4.29	120.51	124.45
21	8	610	CLA	C3C-C4C-NC	4.29	115.39	110.57
21	B	812	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
21	B	831	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
21	4	705	CLA	CAC-C3C-C4C	4.29	130.38	124.81
24	A	852	BCR	C37-C22-C21	-4.29	116.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	2	518	DD6	C13-C11-C10	4.29	125.53	118.94
21	7	704	CLA	C3B-C4B-NB	4.29	114.76	109.21
21	A	831	CLA	C2C-C1C-NC	4.29	113.99	109.97
21	1	501	CLA	C3D-C4D-ND	4.29	117.18	110.24
21	6	906	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
21	A	809	CLA	O2D-CGD-CBD	4.29	118.89	111.27
21	B	839	CLA	CHD-C4C-C3C	-4.29	118.54	124.84
21	12	506	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
21	B	802	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
21	2	506	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
21	B	823	CLA	C3D-C4D-ND	4.28	117.17	110.24
21	9	913	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
21	6	914	CLA	CAC-C3C-C4C	4.28	130.37	124.81
21	A	806	CLA	CAC-C3C-C4C	4.28	130.37	124.81
21	9	907	CLA	C1D-CHD-C4C	-4.28	116.82	126.06
21	A	821	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	F	402	BCR	C37-C22-C21	-4.28	116.93	122.92
21	B	819	CLA	C4A-NA-C1A	-4.28	104.78	106.71
21	8	609	CLA	C3D-C4D-ND	4.28	117.16	110.24
24	B	842	BCR	C37-C22-C21	-4.28	116.93	122.92
21	A	826	CLA	CMD-C2D-C1D	4.28	132.25	124.71
21	A	844	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
21	9	912	CLA	C1D-CHD-C4C	-4.27	116.84	126.06
21	7	705	CLA	O2A-CGA-CBA	4.27	125.32	111.91
21	B	834	CLA	CHD-C1D-ND	-4.27	120.53	124.45
21	A	804	CLA	CMC-C2C-C1C	4.27	131.55	125.04
21	9	912	CLA	CMB-C2B-C3B	4.27	132.67	124.68
21	A	808	CLA	CHD-C1D-ND	-4.27	120.53	124.45
28	5	712	DD6	C12-C11-C13	4.27	124.81	118.08
21	3	712	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
21	1	505	CLA	C3D-C4D-ND	4.27	117.14	110.24
21	6	914	CLA	C4A-NA-C1A	-4.27	104.79	106.71
21	1	516	CLA	C3C-C4C-NC	4.26	115.35	110.57
21	A	838	CLA	C3B-C4B-NB	4.26	114.72	109.21
21	8	606	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
21	A	812	CLA	CHD-C1D-ND	-4.26	120.54	124.45
21	3	706	CLA	C1D-CHD-C4C	-4.26	116.87	126.06
21	4	707	CLA	C3D-C4D-ND	4.26	117.13	110.24
21	1	513	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
21	10	712	CLA	C4A-NA-C1A	-4.26	104.79	106.71
21	5	702	CLA	C2C-C1C-NC	4.26	113.96	109.97
21	1	513	CLA	C2C-C1C-NC	4.26	113.96	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	806	CLA	CHD-C1D-ND	-4.25	120.54	124.45
21	1	511	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
21	8	609	CLA	O2D-CGD-CBD	4.25	118.83	111.27
21	A	832	CLA	CAA-C2A-C3A	-4.25	101.13	112.78
21	A	836	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
21	4	704	CLA	C3D-C4D-ND	4.25	117.12	110.24
21	B	831	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
21	6	907	CLA	O2D-CGD-CBD	4.25	118.82	111.27
21	A	803	CLA	O2A-CGA-CBA	4.25	125.24	111.91
21	2	505	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
21	B	829	CLA	CHD-C1D-ND	-4.25	120.55	124.45
21	10	711	CLA	C3D-C4D-ND	4.25	117.11	110.24
21	A	804	CLA	CAC-C3C-C4C	4.25	130.32	124.81
21	9	910	CLA	C2C-C1C-NC	4.25	113.95	109.97
21	6	904	CLA	C4A-NA-C1A	-4.25	104.80	106.71
21	1	507	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
21	8	605	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	J	103	BCR	C37-C22-C23	4.24	124.77	118.08
21	A	820	CLA	C2C-C1C-NC	4.24	113.95	109.97
24	A	847	BCR	C34-C9-C10	-4.24	116.98	122.92
28	4	713	DD6	C12-C11-C10	-4.24	116.98	122.92
21	A	817	CLA	C4A-NA-C1A	-4.24	104.80	106.71
21	11	708	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
28	5	713	DD6	C4-C5-C6	4.24	133.36	127.31
21	A	812	CLA	C3D-C4D-ND	4.24	117.10	110.24
21	A	841	CLA	CHB-C4A-NA	4.24	130.37	124.51
21	2	509	CLA	CHD-C4C-C3C	-4.24	118.61	124.84
21	12	501	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
21	B	809	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
21	8	611	CLA	C3D-C4D-ND	4.24	117.09	110.24
28	9	915	DD6	C12-C11-C10	-4.23	116.99	122.92
21	2	512	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
21	B	803	CLA	C2C-C1C-NC	4.23	113.94	109.97
21	A	842	CLA	C3D-C4D-ND	4.23	117.09	110.24
21	B	811	CLA	C3C-C4C-NC	4.23	115.32	110.57
21	3	713	CLA	C3D-C4D-ND	4.23	117.08	110.24
21	B	824	CLA	C1-O2A-CGA	4.23	130.05	116.11
21	B	813	CLA	C4A-NA-C1A	-4.23	104.81	106.71
21	B	835	CLA	CMD-C2D-C1D	4.23	132.16	124.71
21	5	701	CLA	O2D-CGD-CBD	4.23	118.78	111.27
21	7	706	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	B	845	BCR	C16-C15-C14	4.23	132.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	713	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
21	A	818	CLA	C3D-C4D-ND	4.22	117.07	110.24
21	F	404	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
21	5	706	CLA	C3D-C4D-ND	4.22	117.07	110.24
21	4	705	CLA	C2C-C1C-NC	4.22	113.93	109.97
21	A	828	CLA	OBD-CAD-C3D	-4.22	118.36	128.52
21	B	838	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
21	A	825	CLA	C3C-C4C-NC	4.22	115.30	110.57
21	9	904	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
21	A	825	CLA	O2A-CGA-CBA	4.22	125.14	111.91
21	A	807	CLA	O1D-CGD-CBD	4.22	133.11	124.48
21	B	814	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
21	12	505	CLA	C3D-C4D-ND	4.22	117.06	110.24
21	A	815	CLA	C4C-C3C-C2C	-4.22	100.75	106.90
21	1	509	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
21	12	504	CLA	C4A-NA-C1A	-4.22	104.81	106.71
21	A	804	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
21	1	512	CLA	C3D-C4D-ND	4.21	117.06	110.24
21	A	807	CLA	C4-C3-C5	4.21	122.36	115.27
21	A	825	CLA	CBC-CAC-C3C	-4.21	100.81	112.43
21	10	703	CLA	C2C-C1C-NC	4.21	113.92	109.97
21	2	503	CLA	O2D-CGD-CBD	4.21	118.75	111.27
21	A	808	CLA	C3D-C4D-ND	4.21	117.05	110.24
21	3	702	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
21	3	701	CLA	C3D-C4D-ND	4.21	117.05	110.24
28	6	916	DD6	C12-C11-C10	-4.21	117.03	122.92
21	13	503	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
21	B	833	CLA	C3C-C4C-NC	4.20	115.28	110.57
21	A	802	CLA	C4C-C3C-C2C	-4.20	100.77	106.90
21	5	708	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
21	B	831	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
21	B	835	CLA	C2A-C1A-CHA	-4.20	116.52	123.86
21	B	801	CLA	C3C-C4C-NC	4.20	115.28	110.57
21	7	709	CLA	O2D-CGD-O1D	-4.20	115.63	123.84
21	B	805	CLA	C1D-CHD-C4C	-4.20	117.00	126.06
21	8	609	CLA	C2C-C1C-NC	4.20	113.90	109.97
21	10	710	CLA	C2C-C1C-NC	4.20	113.90	109.97
21	2	506	CLA	CHD-C4C-C3C	-4.20	118.67	124.84
21	3	704	CLA	C3D-C4D-ND	4.20	117.03	110.24
21	3	709	CLA	C3C-C4C-NC	4.20	115.28	110.57
21	5	707	CLA	C1D-CHD-C4C	-4.20	117.01	126.06
21	A	806	CLA	C2C-C1C-NC	4.20	113.90	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	831	CLA	O1D-CGD-CBD	-4.19	115.91	124.48
21	A	816	CLA	CAC-C3C-C4C	4.19	130.25	124.81
21	5	703	CLA	C3B-C4B-NB	4.19	114.63	109.21
21	10	705	CLA	C3B-C4B-NB	4.19	114.63	109.21
21	A	811	CLA	C4A-NA-C1A	-4.19	104.82	106.71
21	A	808	CLA	C3C-C4C-NC	4.19	115.27	110.57
24	J	102	BCR	C7-C8-C9	-4.19	119.91	126.23
21	A	816	CLA	C3B-C4B-NB	4.19	114.62	109.21
21	6	911	CLA	C2C-C1C-NC	4.19	113.89	109.97
21	B	806	CLA	C3D-C4D-ND	4.19	117.01	110.24
21	A	839	CLA	CBC-CAC-C3C	-4.18	100.90	112.43
21	1	516	CLA	O2D-CGD-CBD	4.18	118.70	111.27
21	2	507	CLA	CHD-C1D-ND	-4.18	120.61	124.45
21	3	708	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
21	12	507	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
21	B	836	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
21	A	839	CLA	C2A-C1A-CHA	-4.18	116.55	123.86
21	8	604	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
28	1	519	DD6	C12-C11-C10	-4.18	117.07	122.92
21	11	704	CLA	C1C-C2C-C3C	-4.18	102.57	106.96
21	B	802	CLA	CHD-C1D-ND	-4.18	120.62	124.45
28	3	718	DD6	C13-C11-C10	4.17	125.35	118.94
21	11	706	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
21	5	703	CLA	CHD-C1D-ND	-4.17	120.62	124.45
24	B	845	BCR	C37-C22-C23	4.17	124.65	118.08
21	6	912	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
21	13	501	CLA	C3D-C4D-ND	4.17	116.99	110.24
21	10	710	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
21	3	705	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
21	F	401	CLA	CAC-C3C-C4C	4.17	130.22	124.81
21	5	710	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
21	3	703	CLA	CAC-C3C-C4C	4.17	130.22	124.81
21	B	829	CLA	C4C-C3C-C2C	-4.17	100.83	106.90
21	5	703	CLA	C1D-CHD-C4C	-4.17	117.07	126.06
28	4	712	DD6	C12-C11-C13	4.17	124.64	118.08
21	12	504	CLA	CHC-C1C-C2C	-4.16	115.20	126.72
21	B	834	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
21	12	507	CLA	C3B-C4B-NB	4.16	114.59	109.21
21	3	703	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
21	5	703	CLA	O2D-CGD-CBD	4.16	118.66	111.27
28	4	712	DD6	C12-C11-C10	-4.16	117.09	122.92
21	4	704	CLA	O2D-CGD-CBD	4.16	118.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	611	CLA	C2C-C1C-NC	4.16	113.87	109.97
21	A	814	CLA	CMD-C2D-C1D	4.16	132.04	124.71
21	7	709	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
21	A	819	CLA	O2A-CGA-CBA	4.16	124.96	111.91
21	A	810	CLA	C4C-C3C-C2C	-4.16	100.84	106.90
21	A	819	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
21	11	705	CLA	C4A-NA-C1A	-4.16	104.84	106.71
21	9	908	CLA	CHD-C4C-C3C	-4.16	118.73	124.84
21	A	817	CLA	C3C-C4C-NC	4.16	115.23	110.57
21	8	610	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
21	11	707	CLA	C3D-C4D-ND	4.15	116.96	110.24
21	9	911	CLA	C2C-C1C-NC	4.15	113.86	109.97
21	2	514	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
21	7	710	CLA	C3D-C4D-ND	4.15	116.95	110.24
21	2	512	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
21	3	703	CLA	CHC-C1C-C2C	-4.15	115.24	126.72
21	11	703	CLA	C3C-C4C-NC	4.15	115.22	110.57
28	1	518	DD6	C12-C11-C10	-4.15	117.11	122.92
21	3	704	CLA	CAC-C3C-C4C	4.15	130.19	124.81
21	B	831	CLA	CHC-C1C-NC	4.15	130.50	124.20
21	4	711	CLA	CAC-C3C-C4C	4.15	130.19	124.81
21	10	711	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
21	A	822	CLA	C3C-C4C-NC	4.15	115.22	110.57
21	7	708	CLA	C2C-C1C-NC	4.14	113.86	109.97
21	3	709	CLA	C2C-C1C-NC	4.14	113.85	109.97
21	11	710	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
21	A	807	CLA	CMD-C2D-C1D	4.14	132.01	124.71
21	6	905	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
21	3	706	CLA	C3D-C4D-ND	4.14	116.93	110.24
21	10	711	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
21	B	836	CLA	CAC-C3C-C4C	4.14	130.18	124.81
28	12	510	DD6	C7-C6-C5	-4.13	117.13	122.92
21	A	824	CLA	CHB-C4A-NA	4.13	130.23	124.51
21	13	501	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
21	4	706	CLA	C4A-NA-C1A	-4.13	104.85	106.71
21	1	504	CLA	O2D-CGD-CBD	4.13	118.61	111.27
21	A	807	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
28	J	104	DD6	C12-C11-C10	-4.13	117.14	122.92
21	5	704	CLA	O2D-CGD-CBD	4.13	118.61	111.27
21	A	826	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
21	9	905	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
21	1	510	CLA	C3D-C4D-ND	4.13	116.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	816	CLA	C3D-C4D-ND	4.13	116.91	110.24
21	1	514	CLA	C4A-NA-C1A	-4.13	104.85	106.71
21	A	808	CLA	C1D-CHD-C4C	-4.13	117.16	126.06
21	7	703	CLA	C4C-C3C-C2C	-4.13	100.89	106.90
21	7	714	CLA	CAC-C3C-C4C	4.12	130.16	124.81
28	7	715	DD6	C12-C11-C10	-4.12	117.14	122.92
21	A	844	CLA	O1D-CGD-CBD	-4.12	116.05	124.48
21	2	512	CLA	CMC-C2C-C1C	4.12	131.32	125.04
21	3	709	CLA	O2D-CGD-O1D	-4.12	115.78	123.84
21	B	818	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
21	9	912	CLA	C3C-C4C-NC	4.12	115.19	110.57
21	9	909	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
21	A	803	CLA	C3D-C4D-ND	4.12	116.91	110.24
21	A	823	CLA	CAA-C2A-C1A	-4.12	98.47	111.97
21	7	708	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
21	6	905	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
21	F	401	CLA	C2C-C1C-NC	4.12	113.83	109.97
21	4	707	CLA	CMB-C2B-C3B	4.12	132.38	124.68
21	2	504	CLA	C2C-C1C-NC	4.12	113.83	109.97
24	F	402	BCR	C34-C9-C8	4.12	124.56	118.08
21	9	904	CLA	C3D-C4D-ND	4.12	116.90	110.24
21	A	804	CLA	CMA-C3A-C4A	-4.12	100.71	111.77
21	1	501	CLA	C4A-NA-C1A	-4.11	104.86	106.71
21	B	838	CLA	C3C-C4C-NC	4.11	115.19	110.57
21	3	710	CLA	CMD-C2D-C1D	4.11	131.96	124.71
21	B	832	CLA	C4A-NA-C1A	-4.11	104.86	106.71
28	2	520	DD6	C12-C11-C10	-4.11	117.16	122.92
21	8	606	CLA	CMC-C2C-C1C	4.11	131.30	125.04
21	8	604	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
21	5	709	CLA	C2C-C1C-NC	4.11	113.82	109.97
21	8	605	CLA	CAC-C3C-C4C	4.11	130.14	124.81
21	11	706	CLA	O2A-CGA-CBA	4.11	124.79	111.91
21	7	704	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
21	11	701	CLA	C4A-NA-C1A	-4.10	104.86	106.71
21	4	708	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
21	10	709	CLA	C3C-C4C-NC	4.10	115.17	110.57
21	A	804	CLA	CBC-CAC-C3C	-4.10	101.12	112.43
21	B	810	CLA	CHB-C4A-NA	4.10	130.19	124.51
21	11	708	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
21	A	811	CLA	CHD-C1D-ND	-4.10	120.69	124.45
21	A	812	CLA	CMC-C2C-C1C	4.10	131.28	125.04
21	9	910	CLA	C3C-C4C-NC	4.10	115.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	608	CLA	C3D-C4D-ND	4.10	116.87	110.24
28	9	916	DD6	C3-C4-C5	4.10	131.87	123.47
21	9	908	CLA	CMB-C2B-C3B	4.10	132.35	124.68
21	A	862	CLA	C4C-C3C-C2C	-4.10	100.92	106.90
21	A	811	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
21	A	806	CLA	C1-C2-C3	-4.10	118.95	126.04
21	6	914	CLA	CHC-C1C-C2C	-4.10	115.38	126.72
21	11	705	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
21	B	821	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	10	711	CLA	O2D-CGD-CBD	4.10	118.55	111.27
21	A	814	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	8	613	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	5	709	CLA	CMC-C2C-C1C	4.10	131.28	125.04
21	J	101	CLA	C4C-C3C-C2C	-4.10	100.93	106.90
21	A	816	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
21	B	820	CLA	C3C-C4C-NC	4.10	115.16	110.57
21	F	403	CLA	C3D-C2D-C1D	-4.09	100.24	105.83
28	6	915	DD6	C12-C11-C10	-4.09	117.19	122.92
21	4	706	CLA	C3D-C4D-ND	4.09	116.86	110.24
21	F	404	CLA	C3C-C4C-NC	4.09	115.16	110.57
21	A	830	CLA	C4C-C3C-C2C	-4.09	100.94	106.90
21	7	709	CLA	CHD-C1D-ND	-4.09	120.70	124.45
21	6	910	CLA	C3D-C4D-ND	4.09	116.85	110.24
21	12	505	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
21	12	507	CLA	C3D-C4D-ND	4.09	116.85	110.24
21	A	832	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
21	A	819	CLA	CHD-C1D-ND	-4.09	120.70	124.45
21	13	502	CLA	C3D-C4D-ND	4.09	116.85	110.24
21	8	614	CLA	C3C-C4C-NC	4.09	115.15	110.57
21	A	831	CLA	C3B-C4B-NB	4.09	114.49	109.21
28	9	916	DD6	C12-C11-C10	-4.09	117.20	122.92
21	11	707	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
28	3	717	DD6	C4-C3-C2	4.09	131.84	123.47
21	4	701	CLA	C3B-C4B-NB	4.08	114.49	109.21
21	3	712	CLA	C4A-NA-C1A	-4.08	104.87	106.71
21	8	614	CLA	C4A-NA-C1A	-4.08	104.87	106.71
21	3	701	CLA	CBC-CAC-C3C	-4.08	101.17	112.43
21	8	607	CLA	CED-O2D-CGD	4.08	125.17	115.94
21	2	512	CLA	C3C-C4C-NC	4.08	115.15	110.57
28	8	615	DD6	C12-C11-C10	-4.08	117.20	122.92
21	5	709	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
21	2	515	CLA	C4A-NA-C1A	-4.08	104.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	827	CLA	O2A-CGA-CBA	4.08	124.71	111.91
21	7	705	CLA	C1-O2A-CGA	4.08	127.15	116.44
21	B	813	CLA	C3D-C4D-ND	4.08	116.83	110.24
21	A	833	CLA	O2D-CGD-O1D	-4.08	115.87	123.84
21	6	906	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
21	1	513	CLA	C3C-C4C-NC	4.08	115.14	110.57
21	8	609	CLA	CHD-C4C-C3C	-4.08	118.85	124.84
21	2	506	CLA	CBC-CAC-C3C	-4.08	101.19	112.43
21	3	702	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
21	2	505	CLA	CMC-C2C-C1C	4.08	131.25	125.04
21	B	819	CLA	CAC-C3C-C4C	4.08	130.10	124.81
21	A	818	CLA	O2D-CGD-CBD	4.08	118.51	111.27
21	A	832	CLA	C3D-C4D-ND	4.08	116.83	110.24
21	6	905	CLA	C3D-C4D-ND	4.08	116.83	110.24
21	7	702	CLA	C4A-NA-C1A	-4.07	104.87	106.71
21	10	705	CLA	CAC-C3C-C4C	4.07	130.10	124.81
21	5	706	CLA	C2C-C1C-NC	4.07	113.79	109.97
24	A	847	BCR	C37-C22-C21	-4.07	117.22	122.92
21	3	704	CLA	C3C-C4C-NC	4.07	115.14	110.57
21	J	101	CLA	O2A-CGA-CBA	4.07	127.12	114.03
21	6	907	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
21	A	835	CLA	C3D-C4D-ND	4.07	116.83	110.24
21	10	712	CLA	C3C-C4C-NC	4.07	115.14	110.57
21	A	839	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
21	F	401	CLA	CMD-C2D-C1D	4.07	131.89	124.71
21	A	840	CLA	C3B-C4B-NB	4.07	114.47	109.21
21	9	912	CLA	CBC-CAC-C3C	-4.07	101.21	112.43
21	3	702	CLA	C4A-NA-C1A	-4.07	104.88	106.71
21	9	904	CLA	C4A-NA-C1A	-4.07	104.88	106.71
21	8	603	CLA	CBC-CAC-C3C	-4.07	101.22	112.43
21	A	810	CLA	C3B-C4B-NB	4.07	114.47	109.21
21	3	703	CLA	C3B-C4B-NB	4.07	114.47	109.21
21	8	612	CLA	CAC-C3C-C4C	4.07	130.09	124.81
21	A	808	CLA	C4C-C3C-C2C	-4.07	100.97	106.90
21	B	837	CLA	C1D-CHD-C4C	-4.07	117.29	126.06
21	A	812	CLA	C4A-NA-C1A	-4.06	104.88	106.71
21	4	710	CLA	CAC-C3C-C4C	4.06	130.08	124.81
21	B	823	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
21	3	708	CLA	C4A-NA-C1A	-4.06	104.88	106.71
21	B	822	CLA	CHD-C1D-ND	-4.06	120.72	124.45
21	B	834	CLA	C3B-C4B-NB	4.06	114.46	109.21
21	B	833	CLA	CAA-C2A-C3A	-4.06	101.66	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	705	CLA	C3C-C4C-NC	4.06	115.12	110.57
21	A	828	CLA	O2D-CGD-CBD	4.06	118.48	111.27
21	1	506	CLA	C3D-C4D-ND	4.06	116.80	110.24
21	J	101	CLA	CAC-C3C-C4C	4.06	130.07	124.81
21	A	842	CLA	CHC-C1C-NC	4.06	130.36	124.20
21	4	711	CLA	C4A-NA-C1A	-4.05	104.88	106.71
21	A	828	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
21	7	708	CLA	C3D-C4D-ND	4.05	116.80	110.24
21	8	607	CLA	C3D-C4D-ND	4.05	116.79	110.24
21	B	839	CLA	CAC-C3C-C4C	4.05	130.07	124.81
21	B	825	CLA	C1-C2-C3	-4.05	119.03	126.04
21	4	704	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
21	11	701	CLA	C3D-C2D-C1D	-4.05	100.30	105.83
21	A	813	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
21	2	513	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
28	9	915	DD6	C3-C4-C5	4.05	131.77	123.47
21	2	506	CLA	CHC-C1C-C2C	-4.05	115.52	126.72
21	A	815	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
21	1	509	CLA	O2D-CGD-CBD	4.05	118.46	111.27
21	6	907	CLA	C3D-C4D-ND	4.05	116.78	110.24
21	6	903	CLA	C3C-C4C-NC	4.04	115.11	110.57
21	6	906	CLA	C3B-C4B-NB	4.04	114.44	109.21
21	B	814	CLA	CMC-C2C-C1C	4.04	131.20	125.04
21	9	909	CLA	C3D-C4D-ND	4.04	116.78	110.24
21	F	401	CLA	O2A-CGA-CBA	4.04	124.59	111.91
21	7	704	CLA	OBD-CAD-C3D	-4.04	118.80	128.52
21	2	511	CLA	C2C-C1C-NC	4.04	113.76	109.97
21	2	515	CLA	CAC-C3C-C4C	4.04	130.05	124.81
21	7	712	CLA	CAC-C3C-C4C	4.04	130.05	124.81
21	B	817	CLA	C3D-C4D-ND	4.04	116.77	110.24
21	A	862	CLA	C3D-C4D-ND	4.04	116.77	110.24
21	10	703	CLA	CHD-C1D-ND	-4.04	120.74	124.45
21	6	908	CLA	CHD-C1D-ND	-4.04	120.75	124.45
21	A	811	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
21	1	512	CLA	O2D-CGD-CBD	4.03	118.43	111.27
21	5	705	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
21	B	824	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
21	B	803	CLA	C3D-C4D-ND	4.03	116.76	110.24
21	A	816	CLA	CHC-C1C-C2C	-4.03	115.57	126.72
21	A	831	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
28	9	916	DD6	C24-C1-C2	4.03	125.12	118.94
21	7	708	CLA	C1D-CHD-C4C	-4.03	117.37	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	714	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
21	A	834	CLA	C2C-C1C-NC	4.03	113.74	109.97
21	A	814	CLA	CHD-C1D-ND	-4.02	120.76	124.45
21	B	830	CLA	C3C-C4C-NC	4.02	115.08	110.57
21	11	702	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
21	11	706	CLA	C3B-C4B-NB	4.02	114.41	109.21
24	J	103	BCR	C37-C22-C21	-4.02	117.29	122.92
21	B	811	CLA	CAC-C3C-C4C	4.02	130.03	124.81
21	3	708	CLA	C3D-C4D-ND	4.02	116.74	110.24
21	4	701	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
21	6	904	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
21	B	828	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
21	7	706	CLA	C4C-C3C-C2C	-4.02	101.04	106.90
21	9	912	CLA	C3B-C4B-NB	4.02	114.40	109.21
21	A	828	CLA	C4C-C3C-C2C	-4.02	101.04	106.90
21	B	806	CLA	CAA-C2A-C3A	-4.02	101.78	112.78
21	7	703	CLA	C3C-C4C-NC	4.02	115.07	110.57
21	A	823	CLA	CHD-C4C-NC	4.01	130.53	124.20
21	F	401	CLA	O2D-CGD-CBD	4.01	118.40	111.27
21	8	605	CLA	O2D-CGD-CBD	4.01	118.40	111.27
21	B	805	CLA	CHD-C1D-ND	-4.01	120.77	124.45
21	3	703	CLA	CHD-C1D-ND	-4.01	120.77	124.45
21	9	913	CLA	C3C-C4C-NC	4.01	115.07	110.57
21	7	709	CLA	CHB-C4A-NA	4.01	130.06	124.51
21	1	506	CLA	CHD-C1D-ND	-4.01	120.77	124.45
21	B	803	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
21	2	508	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
21	6	908	CLA	CHC-C1C-C2C	-4.01	115.63	126.72
21	13	503	CLA	CHC-C1C-C2C	-4.01	115.63	126.72
21	5	703	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
21	3	705	CLA	CHC-C1C-C2C	-4.01	115.63	126.72
21	B	822	CLA	C2C-C1C-NC	4.01	113.73	109.97
21	B	803	CLA	C4-C3-C5	4.01	122.01	115.27
21	5	701	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
21	4	711	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
21	3	715	CLA	CBC-CAC-C3C	-4.01	101.39	112.43
21	A	824	CLA	C4C-C3C-C2C	-4.01	101.06	106.90
21	B	807	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
21	A	813	CLA	CMC-C2C-C1C	4.01	131.14	125.04
21	A	813	CLA	C4C-C3C-C2C	-4.00	101.06	106.90
21	B	838	CLA	C1B-CHB-C4A	-4.00	122.19	130.12
21	11	710	CLA	CAC-C3C-C4C	4.00	130.00	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	824	CLA	CMC-C2C-C1C	4.00	131.14	125.04
21	A	805	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
21	6	905	CLA	C3C-C4C-NC	4.00	115.06	110.57
21	12	506	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	1	516	CLA	C3D-C4D-ND	4.00	116.71	110.24
21	B	816	CLA	CAA-C2A-C3A	-4.00	101.83	112.78
21	6	909	CLA	C1C-C2C-C3C	-4.00	102.76	106.96
24	F	405	BCR	C19-C18-C17	3.99	125.07	118.94
21	B	809	CLA	O2D-CGD-CBD	3.99	118.37	111.27
21	1	515	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
21	A	820	CLA	O2A-CGA-CBA	3.99	124.44	111.91
21	B	827	CLA	C3C-C4C-NC	3.99	115.05	110.57
21	B	836	CLA	O2A-CGA-O1A	-3.99	113.52	123.59
21	A	807	CLA	C11-C12-C13	-3.99	103.01	115.92
28	8	616	DD6	C12-C11-C10	-3.99	117.33	122.92
21	B	814	CLA	C2C-C1C-NC	3.99	113.71	109.97
21	1	511	CLA	C3C-C4C-NC	3.99	115.04	110.57
21	2	504	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
21	J	101	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
21	12	502	CLA	C3D-C4D-ND	3.99	116.69	110.24
21	F	403	CLA	CHD-C1D-ND	-3.99	120.79	124.45
21	A	823	CLA	C3D-C2D-C1D	-3.98	100.39	105.83
21	A	805	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
21	B	808	CLA	CMC-C2C-C1C	3.98	131.10	125.04
21	6	905	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
21	B	802	CLA	CMD-C2D-C1D	3.98	131.73	124.71
21	1	517	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
21	4	710	CLA	C4A-NA-C1A	-3.98	104.92	106.71
21	4	701	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
21	A	822	CLA	C3D-C4D-ND	3.98	116.67	110.24
21	B	833	CLA	C4C-C3C-C2C	-3.98	101.10	106.90
21	6	907	CLA	CHC-C1C-C2C	-3.98	115.72	126.72
21	7	710	CLA	CHC-C1C-NC	3.98	130.24	124.20
21	11	709	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
21	2	514	CLA	C3D-C4D-ND	3.98	116.67	110.24
21	B	808	CLA	CHB-C4A-NA	3.98	130.01	124.51
21	A	818	CLA	C1D-CHD-C4C	-3.97	117.48	126.06
28	8	616	DD6	C4-C3-C2	3.97	131.62	123.47
21	11	708	CLA	CAC-C3C-C4C	3.97	129.97	124.81
21	2	516	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
21	A	825	CLA	CAA-C2A-C3A	-3.97	101.89	112.78
21	A	833	CLA	C3C-C4C-NC	3.97	115.03	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	101	CLA	C3D-C4D-ND	3.97	116.66	110.24
21	11	705	CLA	CHD-C1D-ND	-3.97	120.81	124.45
21	6	904	CLA	CMB-C2B-C3B	3.97	132.10	124.68
21	B	836	CLA	CMB-C2B-C3B	3.97	132.10	124.68
21	6	903	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
21	A	838	CLA	CHD-C1D-ND	-3.97	120.81	124.45
28	3	716	DD6	C12-C11-C10	-3.96	117.37	122.92
21	9	913	CLA	O2D-CGD-CBD	3.96	118.31	111.27
28	6	915	DD6	C12-C11-C13	3.96	124.32	118.08
21	3	709	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
28	3	717	DD6	C9-C8-C6	3.96	137.55	126.42
21	1	509	CLA	C3C-C4C-NC	3.96	115.02	110.57
21	2	504	CLA	CBC-CAC-C3C	-3.96	101.51	112.43
21	9	914	CLA	CAC-C3C-C4C	3.96	129.95	124.81
21	B	831	CLA	CAC-C3C-C2C	-3.96	120.75	127.53
21	2	505	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
21	A	832	CLA	C4A-NA-C1A	-3.96	104.92	106.71
21	9	906	CLA	O2D-CGD-CBD	3.96	118.31	111.27
21	1	501	CLA	CHC-C1C-C2C	-3.96	115.77	126.72
21	9	902	CLA	O2D-CGD-CBD	3.96	118.31	111.27
28	J	104	DD6	C3-C4-C5	3.96	131.59	123.47
21	3	702	CLA	CAC-C3C-C4C	3.96	129.95	124.81
28	1	520	DD6	C12-C11-C10	-3.96	117.38	122.92
24	B	841	BCR	C37-C22-C21	-3.96	117.38	122.92
21	2	514	CLA	CHD-C1D-ND	-3.96	120.82	124.45
21	A	815	CLA	CAA-C2A-C3A	-3.96	101.94	112.78
21	5	705	CLA	C3D-C4D-ND	3.96	116.64	110.24
21	9	911	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
21	5	708	CLA	C3D-C4D-ND	3.96	116.64	110.24
21	3	715	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
21	A	815	CLA	C3D-C2D-C1D	-3.95	100.43	105.83
21	8	614	CLA	C3D-C4D-ND	3.95	116.64	110.24
21	8	606	CLA	CHD-C1D-ND	-3.95	120.82	124.45
21	A	842	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
21	F	401	CLA	C3C-C4C-NC	3.95	115.00	110.57
21	B	808	CLA	CBA-CAA-C2A	-3.95	102.19	113.86
21	9	908	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
21	8	613	CLA	C3C-C4C-NC	3.95	115.00	110.57
21	A	824	CLA	C4A-NA-C1A	-3.95	104.93	106.71
28	3	717	DD6	C4-C5-C6	3.95	132.95	127.31
21	A	835	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
21	A	809	CLA	C4C-C3C-C2C	-3.95	101.14	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	845	BCR	C34-C9-C8	3.95	124.30	118.08
21	1	514	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
21	1	505	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
21	F	403	CLA	C4A-NA-C1A	-3.95	104.93	106.71
21	A	808	CLA	O2A-CGA-O1A	-3.95	113.64	123.59
21	11	709	CLA	CAC-C3C-C4C	3.94	129.93	124.81
21	B	818	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	A	822	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
21	B	838	CLA	CMD-C2D-C1D	3.94	131.66	124.71
21	7	703	CLA	O1D-CGD-CBD	-3.94	116.42	124.48
21	B	814	CLA	CHD-C1D-ND	-3.94	120.83	124.45
28	12	509	DD6	C12-C11-C10	-3.94	117.41	122.92
21	3	709	CLA	C3D-C4D-ND	3.94	116.61	110.24
21	7	708	CLA	CAA-C2A-C3A	-3.94	102.00	112.78
21	B	824	CLA	CAC-C3C-C4C	3.94	129.92	124.81
21	2	511	CLA	CAC-C3C-C4C	3.94	129.92	124.81
21	B	816	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
24	B	846	BCR	C34-C9-C8	3.94	124.28	118.08
21	2	515	CLA	C3D-C4D-ND	3.94	116.60	110.24
21	7	712	CLA	C4C-C3C-C2C	-3.94	101.16	106.90
21	A	824	CLA	C4-C3-C5	3.94	120.48	115.98
21	B	819	CLA	C3D-C4D-ND	3.93	116.60	110.24
21	2	503	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
21	8	606	CLA	CBC-CAC-C3C	-3.93	101.59	112.43
21	1	507	CLA	C1-O2A-CGA	3.93	126.75	116.44
21	B	804	CLA	C3C-C4C-NC	3.93	114.98	110.57
21	B	830	CLA	C3D-C4D-ND	3.93	116.59	110.24
21	8	608	CLA	O2D-CGD-CBD	3.93	118.25	111.27
21	J	101	CLA	CBC-CAC-C3C	-3.93	101.61	112.43
24	B	842	BCR	C34-C9-C10	-3.92	117.43	122.92
21	7	709	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
21	5	711	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
21	B	802	CLA	O2A-C1-C2	-3.92	98.33	108.64
21	3	707	CLA	CMB-C2B-C3B	3.92	132.01	124.68
21	A	820	CLA	C1-C2-C3	-3.92	119.26	126.04
21	A	817	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
21	B	814	CLA	CMD-C2D-C1D	3.92	131.62	124.71
21	11	706	CLA	C3C-C4C-NC	3.92	114.97	110.57
21	10	706	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
21	B	802	CLA	C4A-NA-C1A	-3.92	104.94	106.71
21	B	807	CLA	C4A-NA-C1A	-3.92	104.94	106.71
21	A	836	CLA	C1C-C2C-C3C	-3.92	102.84	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	703	CLA	CHC-C1C-C2C	-3.92	115.89	126.72
21	B	817	CLA	O2A-CGA-CBA	3.92	124.20	111.91
21	B	801	CLA	CAA-C2A-C3A	-3.92	102.06	112.78
21	2	511	CLA	CHD-C1D-ND	-3.92	120.86	124.45
21	A	804	CLA	CHB-C4A-NA	3.91	129.93	124.51
21	5	705	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
21	11	701	CLA	C3C-C4C-NC	3.91	114.96	110.57
21	B	809	CLA	CHD-C1D-ND	-3.91	120.86	124.45
21	A	830	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
21	A	829	CLA	CHB-C4A-NA	3.91	129.92	124.51
21	11	707	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
21	B	805	CLA	C1-O2A-CGA	3.91	126.70	116.44
21	A	839	CLA	C3D-C4D-ND	3.91	116.56	110.24
21	A	805	CLA	O1D-CGD-CBD	-3.91	116.49	124.48
21	3	707	CLA	C2C-C1C-NC	3.90	113.63	109.97
21	A	837	CLA	C3B-C4B-NB	3.90	114.26	109.21
21	9	906	CLA	C3C-C4C-NC	3.90	114.95	110.57
21	A	814	CLA	C3D-C4D-ND	3.90	116.55	110.24
21	A	824	CLA	C3D-C4D-ND	3.90	116.55	110.24
21	3	714	CLA	C2C-C1C-NC	3.90	113.62	109.97
21	1	510	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
21	5	710	CLA	O2A-CGA-CBA	3.90	124.14	111.91
21	A	803	CLA	CAC-C3C-C4C	3.90	129.87	124.81
21	10	704	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
21	1	507	CLA	CMB-C2B-C3B	3.90	131.97	124.68
21	A	835	CLA	C2A-C1A-CHA	-3.90	117.05	123.86
21	A	829	CLA	C4C-C3C-C2C	-3.90	101.22	106.90
21	B	807	CLA	C3D-C4D-ND	3.90	116.54	110.24
21	A	803	CLA	CMA-C3A-C2A	-3.89	98.13	113.83
21	2	516	CLA	C3D-C4D-ND	3.89	116.53	110.24
21	7	709	CLA	CBC-CAC-C3C	-3.89	101.70	112.43
21	10	708	CLA	CAC-C3C-C4C	3.89	129.86	124.81
21	A	839	CLA	C3C-C4C-NC	3.89	114.94	110.57
21	5	704	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
28	2	519	DD6	C13-C11-C10	3.89	124.91	118.94
21	13	503	CLA	C3B-C4B-NB	3.89	114.24	109.21
21	6	910	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
24	F	405	BCR	C34-C9-C8	-3.89	111.95	118.08
21	F	403	CLA	C3D-C4D-ND	3.89	116.53	110.24
21	B	806	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
21	A	843	CLA	CBC-CAC-C3C	-3.89	101.72	112.43
21	A	809	CLA	CHB-C4A-NA	3.89	129.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	825	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
21	7	711	CLA	C4A-NA-C1A	-3.89	104.96	106.71
25	2	521	LHG	O7-C7-C8	3.89	119.87	111.50
21	7	702	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
21	A	838	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
21	B	814	CLA	C4A-NA-C1A	-3.88	104.96	106.71
21	10	703	CLA	O2D-CGD-CBD	3.88	118.17	111.27
21	F	401	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
21	7	705	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
21	8	605	CLA	CHC-C1C-C2C	-3.88	115.98	126.72
21	9	911	CLA	CBC-CAC-C3C	-3.88	101.73	112.43
21	6	908	CLA	CAC-C3C-C4C	3.88	129.84	124.81
28	11	712	DD6	C12-C11-C10	-3.88	117.49	122.92
21	A	826	CLA	C3D-C4D-ND	3.88	116.51	110.24
21	A	822	CLA	CMB-C2B-C3B	3.88	131.94	124.68
21	A	815	CLA	CAA-C2A-C1A	-3.87	99.28	111.97
21	11	703	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
21	9	907	CLA	C3C-C4C-NC	3.87	114.92	110.57
21	B	823	CLA	C3B-C4B-NB	3.87	114.22	109.21
21	F	404	CLA	CMD-C2D-C1D	3.87	131.53	124.71
21	1	513	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
24	F	402	BCR	C2-C1-C6	3.87	116.44	110.48
21	10	705	CLA	C3C-C4C-NC	3.87	114.91	110.57
21	B	815	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
21	B	808	CLA	C3D-C4D-ND	3.87	116.50	110.24
21	2	506	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
21	1	501	CLA	CBC-CAC-C3C	-3.87	101.77	112.43
21	A	834	CLA	CAC-C3C-C4C	3.87	129.83	124.81
21	B	804	CLA	C3D-C2D-C1D	-3.87	100.56	105.83
21	7	706	CLA	C4A-NA-C1A	-3.86	104.97	106.71
21	12	503	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
21	A	809	CLA	C2C-C1C-NC	3.86	113.59	109.97
21	2	516	CLA	CMD-C2D-C1D	3.86	131.52	124.71
21	B	827	CLA	CMD-C2D-C1D	3.86	131.52	124.71
21	3	706	CLA	CHD-C4C-NC	3.86	130.29	124.20
21	8	611	CLA	CHD-C4C-NC	3.86	130.28	124.20
21	12	504	CLA	CHC-C1C-NC	3.86	130.06	124.20
21	B	836	CLA	CHD-C1D-ND	-3.86	120.91	124.45
21	3	710	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
21	7	709	CLA	C3C-C4C-NC	3.86	114.89	110.57
21	B	826	CLA	CBC-CAC-C3C	-3.85	101.81	112.43
21	1	501	CLA	O1D-CGD-CBD	-3.85	116.60	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	507	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
21	A	823	CLA	CBC-CAC-C3C	-3.85	101.81	112.43
21	B	822	CLA	CHB-C4A-NA	3.85	129.84	124.51
21	1	508	CLA	C3D-C2D-C1D	-3.85	100.58	105.83
21	B	816	CLA	O2A-CGA-CBA	3.85	123.99	111.91
21	A	806	CLA	O2D-CGD-CBD	3.85	118.11	111.27
21	5	710	CLA	C4A-NA-C1A	-3.85	104.98	106.71
21	10	703	CLA	C4A-NA-C1A	-3.85	104.98	106.71
21	13	502	CLA	C3C-C4C-NC	3.85	114.88	110.57
20	A	801	CL0	CHB-C4A-NA	3.85	129.83	124.51
21	6	910	CLA	C3C-C4C-NC	3.84	114.88	110.57
21	4	709	CLA	C1D-CHD-C4C	-3.84	117.76	126.06
21	8	603	CLA	C3D-C2D-C1D	-3.84	100.58	105.83
21	A	820	CLA	C3D-C4D-ND	3.84	116.46	110.24
21	2	512	CLA	C4A-NA-C1A	-3.84	104.98	106.71
21	B	808	CLA	C1B-CHB-C4A	-3.84	122.51	130.12
21	A	828	CLA	CAC-C3C-C4C	3.84	129.80	124.81
21	2	515	CLA	CMA-C3A-C4A	-3.84	101.45	111.77
21	B	815	CLA	C3C-C4C-NC	3.84	114.88	110.57
21	4	701	CLA	C3C-C4C-NC	3.84	114.88	110.57
21	5	703	CLA	CMB-C2B-C3B	3.84	131.86	124.68
21	F	401	CLA	CHD-C1D-ND	-3.84	120.93	124.45
21	2	515	CLA	C3D-C2D-C1D	-3.84	100.60	105.83
21	A	832	CLA	C3C-C4C-NC	3.83	114.87	110.57
21	2	508	CLA	O2D-CGD-CBD	3.83	118.08	111.27
21	A	837	CLA	CHC-C1C-C2C	-3.83	116.12	126.72
21	4	708	CLA	C4A-NA-C1A	-3.83	104.98	106.71
21	9	908	CLA	C2C-C1C-NC	3.83	113.56	109.97
21	1	515	CLA	CAC-C3C-C4C	3.83	129.78	124.81
21	A	829	CLA	CMD-C2D-C1D	3.83	131.47	124.71
21	2	514	CLA	C3C-C4C-NC	3.83	114.87	110.57
21	5	710	CLA	C5-C3-C4	3.83	123.06	114.60
21	8	610	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
21	8	606	CLA	C3D-C4D-ND	3.83	116.43	110.24
21	7	703	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
21	6	914	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
21	9	904	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
21	A	832	CLA	CAC-C3C-C4C	3.83	129.78	124.81
21	B	822	CLA	CMA-C3A-C4A	-3.83	101.49	111.77
21	8	613	CLA	C3D-C4D-ND	3.82	116.42	110.24
21	1	505	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
24	A	850	BCR	C7-C8-C9	-3.82	120.46	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	818	CLA	CHC-C1C-NC	3.82	130.00	124.20
21	6	912	CLA	CAC-C3C-C4C	3.82	129.77	124.81
21	B	806	CLA	CHC-C1C-NC	3.82	130.00	124.20
21	5	702	CLA	C3D-C4D-ND	3.82	116.42	110.24
21	3	703	CLA	O2D-CGD-CBD	3.82	118.06	111.27
21	11	710	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
21	1	506	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
21	4	710	CLA	C3C-C4C-NC	3.82	114.86	110.57
21	3	715	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
28	3	718	DD6	C-C1-C2	-3.82	117.57	122.92
21	B	809	CLA	C3D-C4D-ND	3.82	116.42	110.24
21	6	906	CLA	CHC-C1C-C2C	-3.82	116.16	126.72
21	3	701	CLA	CHD-C4C-NC	3.82	130.22	124.20
21	4	707	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
21	B	817	CLA	C3C-C4C-NC	3.82	114.85	110.57
21	3	706	CLA	C3C-C4C-NC	3.82	114.85	110.57
21	10	708	CLA	C3C-C4C-NC	3.81	114.85	110.57
21	1	512	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
28	7	715	DD6	C-C1-C2	-3.81	117.58	122.92
21	7	705	CLA	CBC-CAC-C3C	-3.81	101.92	112.43
21	A	806	CLA	C2A-C1A-CHA	-3.81	117.19	123.86
21	B	820	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
21	4	703	CLA	C3C-C4C-NC	3.81	114.85	110.57
21	10	708	CLA	C3D-C4D-ND	3.81	116.40	110.24
21	10	704	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
28	4	713	DD6	C3-C4-C5	3.81	131.28	123.47
21	B	806	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
21	5	702	CLA	C2A-C1A-CHA	-3.81	117.20	123.86
21	11	707	CLA	CAC-C3C-C4C	3.81	129.75	124.81
21	A	819	CLA	CAC-C3C-C4C	3.81	129.75	124.81
21	2	508	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
21	8	613	CLA	CAC-C3C-C4C	3.81	129.75	124.81
21	5	702	CLA	C4A-NA-C1A	-3.81	105.00	106.71
21	B	812	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
24	B	844	BCR	C16-C17-C18	3.81	132.74	127.31
21	A	819	CLA	C3D-C2D-C1D	-3.80	100.64	105.83
21	A	806	CLA	CHB-C4A-NA	3.80	129.77	124.51
21	A	819	CLA	C3D-C4D-ND	3.80	116.39	110.24
21	A	825	CLA	OBD-CAD-C3D	-3.80	119.37	128.52
21	A	827	CLA	C4-C3-C5	3.80	121.67	115.27
21	1	507	CLA	C3B-C4B-NB	3.80	114.13	109.21
21	3	714	CLA	CAC-C3C-C4C	3.80	129.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	9	916	DD6	C-C1-C2	-3.80	117.60	122.92
21	A	809	CLA	CMA-C3A-C4A	-3.80	101.56	111.77
21	A	822	CLA	O2D-CGD-CBD	3.80	118.02	111.27
21	9	904	CLA	CHC-C1C-C2C	-3.80	116.21	126.72
21	8	607	CLA	CAC-C3C-C4C	3.80	129.74	124.81
21	A	835	CLA	OBD-CAD-C3D	-3.80	119.38	128.52
28	4	713	DD6	C4-C3-C2	3.80	131.25	123.47
21	A	816	CLA	CHB-C4A-NA	3.80	129.76	124.51
21	11	706	CLA	C3D-C4D-ND	3.80	116.38	110.24
21	12	502	CLA	C3C-C4C-NC	3.80	114.83	110.57
21	3	707	CLA	C4A-NA-C1A	-3.79	105.00	106.71
21	7	708	CLA	C1-O2A-CGA	3.79	126.40	116.44
21	5	710	CLA	C4C-C3C-C2C	-3.79	101.37	106.90
21	B	828	CLA	CED-O2D-CGD	-3.79	107.36	115.94
21	A	841	CLA	C3B-C4B-NB	3.79	114.11	109.21
21	9	905	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
21	A	823	CLA	C3C-C4C-NC	3.79	114.82	110.57
21	9	902	CLA	C3C-C4C-NC	3.79	114.82	110.57
21	10	707	CLA	C3C-C4C-NC	3.79	114.82	110.57
21	B	811	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
21	3	715	CLA	C2C-C1C-NC	3.79	113.52	109.97
21	4	706	CLA	O2D-CGD-CBD	3.79	118.00	111.27
21	4	707	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
21	4	702	CLA	CMC-C2C-C1C	3.79	130.81	125.04
21	2	504	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
21	3	703	CLA	CMB-C2B-C3B	3.79	131.76	124.68
21	B	801	CLA	CBA-CAA-C2A	-3.79	102.69	113.86
21	7	713	CLA	C3C-C4C-NC	3.79	114.82	110.57
21	F	403	CLA	C3C-C4C-NC	3.79	114.82	110.57
21	11	704	CLA	O2D-CGD-CBD	3.79	117.99	111.27
21	A	819	CLA	CHC-C1C-C2C	-3.78	116.25	126.72
21	3	707	CLA	C3D-C4D-ND	3.78	116.36	110.24
21	A	821	CLA	C4A-NA-C1A	-3.78	105.01	106.71
21	A	830	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
21	7	707	CLA	CHC-C1C-C2C	-3.78	116.26	126.72
21	A	826	CLA	CHD-C1D-ND	-3.78	120.98	124.45
28	3	718	DD6	C12-C11-C10	-3.78	117.63	122.92
21	4	709	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
21	7	702	CLA	C3B-C4B-NB	3.78	114.09	109.21
21	7	702	CLA	O2A-CGA-CBA	3.78	123.76	111.91
21	10	703	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
21	6	906	CLA	C3D-C4D-ND	3.77	116.34	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	612	CLA	O2D-CGD-CBD	3.77	117.97	111.27
21	A	806	CLA	CMC-C2C-C1C	3.77	130.79	125.04
21	11	704	CLA	CAC-C3C-C4C	3.77	129.71	124.81
24	B	842	BCR	C16-C15-C14	3.77	131.20	123.47
21	6	905	CLA	C3B-C4B-NB	3.77	114.09	109.21
21	13	503	CLA	C3D-C4D-ND	3.77	116.34	110.24
21	2	508	CLA	O2A-CGA-CBA	3.77	123.74	111.91
21	11	707	CLA	CMB-C2B-C3B	3.77	131.73	124.68
21	B	809	CLA	CMC-C2C-C1C	3.77	130.78	125.04
21	A	809	CLA	C6-C5-C3	-3.77	103.57	113.45
21	13	501	CLA	C3C-C4C-NC	3.77	114.80	110.57
21	A	823	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
21	B	805	CLA	C3D-C4D-ND	3.77	116.33	110.24
21	10	710	CLA	O2D-CGD-CBD	3.77	117.96	111.27
21	B	823	CLA	CAC-C3C-C4C	3.77	129.70	124.81
21	B	812	CLA	C4C-C3C-C2C	-3.77	101.41	106.90
21	2	505	CLA	C2C-C1C-NC	3.77	113.50	109.97
21	B	822	CLA	CMC-C2C-C1C	3.77	130.78	125.04
21	9	909	CLA	CAC-C3C-C4C	3.77	129.70	124.81
21	6	903	CLA	C3B-C4B-NB	3.77	114.08	109.21
21	9	906	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
21	8	610	CLA	C3D-C4D-ND	3.77	116.33	110.24
21	7	707	CLA	C4C-C3C-C2C	-3.77	101.41	106.90
28	8	616	DD6	C-C1-C2	-3.76	117.65	122.92
21	6	910	CLA	CAC-C3C-C4C	3.76	129.69	124.81
21	7	714	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
21	9	904	CLA	CMB-C2B-C3B	3.76	131.72	124.68
21	B	808	CLA	CHC-C1C-C2C	-3.76	116.31	126.72
21	5	708	CLA	C4C-C3C-C2C	-3.76	101.41	106.90
21	2	515	CLA	O2A-CGA-O1A	-3.76	113.92	123.30
21	1	511	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
21	B	835	CLA	CMB-C2B-C3B	3.76	131.71	124.68
21	9	906	CLA	CAC-C3C-C4C	3.76	129.69	124.81
21	B	831	CLA	C3D-C4D-ND	3.76	116.32	110.24
21	6	904	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
21	10	708	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
21	11	701	CLA	CAA-C2A-C3A	-3.76	107.33	116.10
28	7	715	DD6	C24-C1-C2	3.76	124.71	118.94
21	9	904	CLA	C3B-C4B-NB	3.76	114.07	109.21
21	5	707	CLA	CHD-C4C-NC	3.76	130.12	124.20
21	A	827	CLA	CBC-CAC-C3C	-3.76	102.08	112.43
21	A	831	CLA	CAC-C3C-C4C	3.75	129.68	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	703	CLA	CMC-C2C-C1C	3.75	130.76	125.04
21	11	710	CLA	C3B-C4B-NB	3.75	114.06	109.21
21	10	711	CLA	CED-O2D-CGD	3.75	124.43	115.94
21	2	509	CLA	C3C-C4C-NC	3.75	114.78	110.57
21	B	817	CLA	CHC-C1C-C2C	-3.75	116.34	126.72
21	5	710	CLA	CMB-C2B-C3B	3.75	131.70	124.68
21	11	701	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
21	A	812	CLA	C2C-C1C-NC	3.75	113.49	109.97
21	7	706	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
21	B	834	CLA	C3D-C4D-ND	3.75	116.30	110.24
21	A	833	CLA	CMB-C2B-C3B	3.75	131.69	124.68
21	A	816	CLA	CAA-C2A-C1A	3.75	124.26	111.97
21	A	830	CLA	C3D-C4D-ND	3.75	116.30	110.24
21	A	836	CLA	C4-C3-C5	3.75	121.58	115.27
21	B	822	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
21	1	513	CLA	CAC-C3C-C4C	3.75	129.67	124.81
21	9	909	CLA	C3C-C4C-NC	3.75	114.77	110.57
21	3	709	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
21	12	507	CLA	CHC-C1C-C2C	-3.75	116.36	126.72
28	4	712	DD6	C4-C3-C2	3.75	131.15	123.47
21	1	516	CLA	C4C-C3C-C2C	-3.75	101.44	106.90
21	B	816	CLA	C1-C2-C3	-3.75	119.56	126.04
21	A	838	CLA	CAC-C3C-C4C	3.74	129.67	124.81
21	5	707	CLA	CBC-CAC-C3C	-3.74	102.11	112.43
21	2	507	CLA	CHC-C1C-C2C	-3.74	116.37	126.72
21	1	506	CLA	CHD-C4C-NC	3.74	130.10	124.20
25	8	617	LHG	O7-C5-C4	-3.74	94.85	108.40
24	A	852	BCR	C37-C22-C23	3.74	123.97	118.08
21	9	913	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
28	1	520	DD6	C24-C1-C2	3.74	124.68	118.94
21	5	707	CLA	O2A-CGA-CBA	3.74	123.65	111.91
21	5	703	CLA	CHC-C1C-NC	3.74	129.87	124.20
21	A	837	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
21	8	610	CLA	C4C-C3C-C2C	-3.74	101.45	106.90
21	A	830	CLA	C2C-C1C-NC	3.74	113.47	109.97
21	A	831	CLA	C4C-C3C-C2C	-3.74	101.45	106.90
21	A	804	CLA	O1D-CGD-CBD	-3.74	116.84	124.48
21	12	503	CLA	CAC-C3C-C4C	3.74	129.66	124.81
21	A	828	CLA	O2A-CGA-CBA	3.74	123.63	111.91
21	12	502	CLA	CHD-C1D-ND	-3.73	121.02	124.45
21	B	823	CLA	CBC-CAC-C3C	-3.73	102.14	112.43
21	7	714	CLA	C3D-C4D-ND	3.73	116.28	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	703	CLA	C3B-C4B-NB	3.73	114.04	109.21
21	7	703	CLA	C3B-C4B-NB	3.73	114.04	109.21
24	M	102	BCR	C34-C9-C8	3.73	123.96	118.08
21	B	825	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
21	A	803	CLA	C4A-NA-C1A	-3.73	105.03	106.71
21	B	830	CLA	CMB-C2B-C3B	3.73	131.66	124.68
21	5	707	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
21	12	505	CLA	C3C-C4C-NC	3.73	114.76	110.57
21	3	705	CLA	CHC-C1C-NC	3.73	129.86	124.20
21	A	831	CLA	C3D-C4D-ND	3.73	116.27	110.24
21	6	911	CLA	CHD-C4C-NC	3.73	130.08	124.20
28	1	520	DD6	C4-C3-C2	3.73	131.11	123.47
21	10	710	CLA	C3C-C4C-NC	3.73	114.75	110.57
21	B	811	CLA	C3B-C4B-NB	3.73	114.03	109.21
21	5	706	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
21	A	835	CLA	C3C-C4C-NC	3.73	114.75	110.57
21	7	705	CLA	C4C-C3C-C2C	-3.73	101.47	106.90
21	5	707	CLA	CAA-C2A-C3A	-3.73	102.58	112.78
21	B	817	CLA	CMD-C2D-C1D	3.73	131.28	124.71
21	F	404	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
21	13	503	CLA	C1D-CHD-C4C	-3.72	118.02	126.06
28	8	615	DD6	C3-C4-C5	3.72	131.10	123.47
21	3	713	CLA	C3C-C4C-NC	3.72	114.75	110.57
21	11	706	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
21	10	712	CLA	O2D-CGD-CBD	3.72	117.88	111.27
21	A	810	CLA	CMC-C2C-C1C	3.72	130.71	125.04
21	B	825	CLA	C3C-C4C-NC	3.72	114.75	110.57
21	B	826	CLA	CMA-C3A-C4A	-3.72	101.77	111.77
21	A	826	CLA	C4A-NA-C1A	-3.72	105.03	106.71
21	5	705	CLA	CAC-C3C-C4C	3.72	129.64	124.81
21	5	707	CLA	CMB-C2B-C3B	3.72	131.64	124.68
21	6	907	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
21	7	708	CLA	C2A-C1A-CHA	-3.72	117.36	123.86
21	A	829	CLA	C3D-C4D-ND	3.72	116.25	110.24
21	B	813	CLA	CMC-C2C-C1C	3.72	130.70	125.04
21	B	827	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
21	3	713	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
21	4	702	CLA	C3C-C4C-NC	3.71	114.74	110.57
21	8	603	CLA	C2C-C1C-NC	3.71	113.45	109.97
21	A	835	CLA	C3D-C2D-C1D	-3.71	100.76	105.83
21	1	504	CLA	C3D-C2D-C1D	-3.71	100.76	105.83
28	4	713	DD6	C-C1-C2	-3.71	117.72	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	807	CLA	CHD-C1D-ND	-3.71	121.04	124.45
21	12	505	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
21	B	807	CLA	O2A-CGA-O1A	-3.71	114.22	123.59
21	3	701	CLA	CHC-C1C-C2C	-3.71	116.46	126.72
21	B	801	CLA	O2D-CGD-CBD	3.71	117.86	111.27
21	5	704	CLA	C3C-C4C-NC	3.71	114.73	110.57
21	7	707	CLA	O2A-CGA-CBA	3.71	123.55	111.91
21	4	706	CLA	C3C-C4C-NC	3.71	114.73	110.57
21	B	828	CLA	C3D-C2D-C1D	-3.71	100.77	105.83
21	A	827	CLA	C3C-C4C-NC	3.71	114.73	110.57
21	7	704	CLA	O2D-CGD-CBD	3.71	117.86	111.27
21	A	842	CLA	CHD-C1D-ND	-3.71	121.05	124.45
21	B	815	CLA	C3D-C4D-ND	3.71	116.23	110.24
21	7	705	CLA	CHD-C1D-ND	-3.71	121.05	124.45
21	12	508	CLA	CAC-C3C-C4C	3.70	129.62	124.81
21	8	603	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
21	2	514	CLA	O2D-CGD-CBD	3.70	117.85	111.27
21	B	830	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
21	1	507	CLA	CHC-C1C-C2C	-3.70	116.47	126.72
21	3	711	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
20	A	801	CL0	C1-O2A-CGA	3.70	126.16	116.44
21	12	505	CLA	C4C-C3C-C2C	-3.70	101.50	106.90
21	1	504	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
28	2	520	DD6	C-C1-C2	-3.70	117.74	122.92
21	A	809	CLA	C3C-C4C-NC	3.70	114.72	110.57
21	7	710	CLA	C3C-C4C-NC	3.70	114.72	110.57
21	12	506	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
21	6	909	CLA	C4A-NA-C1A	-3.70	105.04	106.71
21	1	514	CLA	C3D-C4D-ND	3.70	116.22	110.24
21	A	836	CLA	CHC-C1C-C2C	-3.70	116.49	126.72
21	4	711	CLA	CHC-C1C-C2C	-3.70	116.50	126.72
21	6	905	CLA	O2D-CGD-CBD	3.70	117.83	111.27
21	B	801	CLA	CHB-C4A-NA	3.69	129.62	124.51
21	A	841	CLA	C4-C3-C5	3.69	121.48	115.27
21	B	808	CLA	CMB-C2B-C3B	3.69	131.59	124.68
21	A	809	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
21	1	512	CLA	CAC-C3C-C4C	3.69	129.60	124.81
21	3	713	CLA	CAC-C3C-C4C	3.69	129.60	124.81
21	12	505	CLA	CAC-C3C-C4C	3.69	129.60	124.81
21	1	514	CLA	O2D-CGD-CBD	3.69	117.83	111.27
21	A	812	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
21	7	711	CLA	C3D-C2D-C1D	-3.69	100.80	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	709	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
21	5	708	CLA	CHB-C4A-NA	3.69	129.61	124.51
21	9	904	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
21	A	808	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
21	8	612	CLA	CBC-CAC-C3C	-3.69	102.27	112.43
21	B	802	CLA	C3B-C4B-NB	3.69	113.98	109.21
21	3	707	CLA	CMC-C2C-C1C	3.69	130.65	125.04
21	5	706	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
21	A	840	CLA	O1D-CGD-CBD	-3.68	116.94	124.48
21	9	910	CLA	CMC-C2C-C1C	3.68	130.65	125.04
21	A	841	CLA	CAC-C3C-C4C	3.68	129.59	124.81
21	11	704	CLA	C3B-C4B-NB	3.68	113.97	109.21
21	B	803	CLA	CMC-C2C-C1C	3.68	130.64	125.04
21	B	802	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
21	11	702	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
21	11	703	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
21	2	510	CLA	C4C-C3C-C2C	-3.68	101.54	106.90
21	1	517	CLA	C3D-C4D-ND	3.67	116.18	110.24
21	8	606	CLA	CHD-C4C-NC	3.67	129.99	124.20
21	A	826	CLA	CHC-C1C-C2C	-3.67	116.56	126.72
21	3	704	CLA	C3B-C4B-NB	3.67	113.96	109.21
21	9	913	CLA	CAC-C3C-C4C	3.67	129.58	124.81
21	B	818	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
21	A	802	CLA	CAA-C2A-C3A	-3.67	102.72	112.78
21	12	502	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
21	2	511	CLA	C3C-C4C-NC	3.67	114.69	110.57
21	12	504	CLA	CHD-C1D-ND	-3.67	121.08	124.45
21	8	609	CLA	CHC-C1C-C2C	-3.67	116.57	126.72
21	5	701	CLA	CHC-C1C-C2C	-3.67	116.57	126.72
21	8	609	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
21	B	810	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
21	B	839	CLA	O1D-CGD-CBD	-3.67	116.98	124.48
21	4	707	CLA	C4A-NA-C1A	-3.67	105.06	106.71
21	1	509	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
21	8	608	CLA	C3C-C4C-NC	3.67	114.68	110.57
21	A	844	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
21	1	517	CLA	C3D-C2D-C1D	-3.67	100.83	105.83
21	6	903	CLA	CHC-C1C-C2C	-3.67	116.58	126.72
21	11	706	CLA	CHC-C1C-C2C	-3.66	116.58	126.72
21	4	703	CLA	C1D-CHD-C4C	-3.66	118.15	126.06
21	3	703	CLA	CHC-C1C-NC	3.66	129.76	124.20
21	2	503	CLA	C3D-C4D-ND	3.66	116.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	504	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
21	A	803	CLA	C2A-C1A-CHA	-3.66	117.46	123.86
21	6	905	CLA	CHC-C1C-C2C	-3.66	116.59	126.72
21	B	832	CLA	CAC-C3C-C4C	3.66	129.56	124.81
21	A	833	CLA	CHC-C1C-C2C	-3.66	116.60	126.72
21	7	705	CLA	OBD-CAD-C3D	-3.66	119.71	128.52
21	10	705	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
21	8	604	CLA	C2A-C1A-CHA	-3.66	117.47	123.86
28	2	519	DD6	C12-C11-C10	-3.66	117.80	122.92
21	A	815	CLA	CMB-C2B-C3B	3.66	131.52	124.68
21	A	802	CLA	CMD-C2D-C1D	3.65	131.15	124.71
21	A	805	CLA	CMC-C2C-C1C	3.65	130.60	125.04
21	7	711	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
21	2	510	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
21	A	804	CLA	C3D-C4D-ND	3.65	116.14	110.24
21	5	707	CLA	C3D-C4D-ND	3.65	116.14	110.24
21	B	831	CLA	CGD-CBD-CAD	-3.65	98.91	110.73
21	1	509	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
21	B	838	CLA	OBD-CAD-C3D	-3.65	119.74	128.52
21	A	818	CLA	C3D-C2D-C1D	-3.65	100.85	105.83
21	B	822	CLA	C3C-C4C-NC	3.65	114.66	110.57
21	12	505	CLA	CHC-C1C-C2C	-3.65	116.63	126.72
21	B	814	CLA	CMB-C2B-C3B	3.65	131.50	124.68
21	5	702	CLA	CBC-CAC-C3C	-3.64	102.39	112.43
21	7	702	CLA	C4C-C3C-C2C	-3.64	101.59	106.90
21	A	838	CLA	CHC-C1C-C2C	-3.64	116.64	126.72
21	B	802	CLA	C2C-C1C-NC	3.64	113.39	109.97
21	7	707	CLA	C3D-C4D-ND	3.64	116.13	110.24
21	B	835	CLA	CHB-C4A-NA	3.64	129.55	124.51
21	A	828	CLA	CMC-C2C-C1C	3.64	130.59	125.04
21	B	829	CLA	CHB-C4A-NA	3.64	129.55	124.51
21	B	824	CLA	C4C-C3C-C2C	-3.64	101.59	106.90
21	A	829	CLA	C11-C12-C13	-3.64	104.15	115.92
21	3	712	CLA	C3C-C4C-NC	3.64	114.65	110.57
21	B	816	CLA	C4C-C3C-C2C	-3.64	101.59	106.90
21	A	806	CLA	C3D-C4D-ND	3.64	116.12	110.24
21	10	708	CLA	CHC-C1C-C2C	-3.64	116.66	126.72
21	A	844	CLA	CHB-C4A-NA	3.63	129.54	124.51
21	B	808	CLA	C3D-C2D-C1D	-3.63	100.87	105.83
21	6	914	CLA	CHC-C1C-NC	3.63	129.72	124.20
21	3	703	CLA	C3D-C2D-C1D	-3.63	100.87	105.83
21	13	503	CLA	C3C-C4C-NC	3.63	114.64	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	504	CLA	CAC-C3C-C4C	3.63	129.52	124.81
21	6	908	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	M	102	BCR	C7-C8-C9	-3.63	120.75	126.23
28	12	510	DD6	C9-C10-C11	3.63	132.49	127.31
21	7	705	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	A	803	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	J	101	CLA	O2D-CGD-CBD	3.63	117.72	111.27
21	5	706	CLA	CAA-C2A-C3A	-3.63	102.84	112.78
21	A	825	CLA	CHC-C1C-C2C	-3.63	116.68	126.72
21	12	504	CLA	C3D-C4D-ND	3.63	116.11	110.24
21	B	820	CLA	CHB-C4A-NA	3.63	129.53	124.51
21	6	913	CLA	C3C-C4C-NC	3.63	114.64	110.57
21	3	703	CLA	OBD-CAD-C3D	-3.63	119.80	128.52
21	A	840	CLA	C3D-C4D-ND	3.63	116.10	110.24
21	A	835	CLA	CHD-C1D-ND	-3.62	121.12	124.45
21	11	710	CLA	C3C-C4C-NC	3.62	114.64	110.57
21	A	815	CLA	CMD-C2D-C1D	3.62	131.10	124.71
21	2	513	CLA	CBC-CAC-C3C	-3.62	102.44	112.43
21	A	836	CLA	CHD-C4C-C3C	-3.62	119.52	124.84
21	6	913	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
21	2	516	CLA	CHD-C4C-NC	3.62	129.91	124.20
21	A	827	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
21	B	802	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
21	B	803	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
21	B	809	CLA	OBD-CAD-C3D	-3.62	119.81	128.52
21	4	707	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
21	5	701	CLA	C4A-NA-C1A	-3.62	105.08	106.71
24	A	851	BCR	C37-C22-C21	-3.62	117.86	122.92
24	B	845	BCR	C37-C22-C21	-3.62	117.86	122.92
21	12	505	CLA	CAA-C2A-C3A	-3.62	102.87	112.78
21	10	712	CLA	CAC-C3C-C4C	3.62	129.50	124.81
21	B	818	CLA	C4C-C3C-C2C	-3.62	101.63	106.90
21	6	909	CLA	C1-O2A-CGA	3.62	125.93	116.44
28	5	713	DD6	C9-C8-C6	3.61	136.57	126.42
21	11	709	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
21	2	513	CLA	C4A-NA-C1A	-3.61	105.08	106.71
21	7	703	CLA	CHC-C1C-C2C	-3.61	116.72	126.72
21	9	910	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
28	2	519	DD6	C3-C4-C5	3.61	130.88	123.47
21	A	820	CLA	C3B-C4B-NB	3.61	113.88	109.21
21	11	709	CLA	CHC-C1C-C2C	-3.61	116.73	126.72
21	A	840	CLA	C1B-CHB-C4A	-3.61	122.96	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	515	CLA	CHC-C1C-C2C	-3.61	116.73	126.72
21	B	833	CLA	C4D-CHA-C1A	-3.61	116.85	121.25
21	B	813	CLA	C2C-C1C-NC	3.61	113.36	109.97
21	A	833	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
21	1	513	CLA	C3B-C4B-NB	3.61	113.88	109.21
21	5	701	CLA	C3D-C2D-C1D	-3.61	100.91	105.83
21	4	707	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
21	B	810	CLA	CBC-CAC-C3C	-3.61	102.48	112.43
21	A	842	CLA	O2A-CGA-CBA	3.61	123.23	111.91
21	2	511	CLA	O1D-CGD-CBD	-3.61	117.11	124.48
21	2	517	CLA	C4A-NA-C1A	-3.61	105.08	106.71
21	6	911	CLA	C3C-C4C-NC	3.61	114.61	110.57
21	8	611	CLA	C3D-C2D-C1D	-3.60	100.91	105.83
21	10	709	CLA	CHC-C1C-C2C	-3.60	116.75	126.72
24	A	849	BCR	C34-C9-C10	-3.60	117.88	122.92
28	1	520	DD6	C-C1-C2	-3.60	117.88	122.92
21	A	802	CLA	CMB-C2B-C3B	3.60	131.41	124.68
21	A	815	CLA	C4-C3-C5	3.60	121.33	115.27
21	8	609	CLA	CAA-C2A-C3A	-3.60	102.92	112.78
21	2	507	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
21	A	813	CLA	CHD-C1D-ND	-3.60	121.15	124.45
21	A	803	CLA	CBA-CAA-C2A	-3.60	103.24	113.86
21	4	704	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
21	8	604	CLA	CMB-C2B-C3B	3.60	131.41	124.68
21	B	811	CLA	C4C-C3C-C2C	-3.60	101.66	106.90
21	8	608	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
21	11	702	CLA	C3C-C4C-NC	3.60	114.60	110.57
21	A	808	CLA	CHB-C4A-NA	3.59	129.48	124.51
21	A	844	CLA	CHC-C1C-C2C	-3.59	116.78	126.72
21	A	843	CLA	CMC-C2C-C1C	3.59	130.51	125.04
21	1	509	CLA	CHD-C4C-NC	3.59	129.86	124.20
21	B	837	CLA	C4A-NA-C1A	-3.59	105.09	106.71
21	3	710	CLA	C4A-NA-C1A	-3.59	105.09	106.71
21	11	704	CLA	C3C-C4C-NC	3.59	114.60	110.57
21	A	802	CLA	C4-C3-C5	3.59	121.31	115.27
21	B	825	CLA	C3D-C4D-ND	3.59	116.05	110.24
21	A	812	CLA	C3D-C2D-C1D	-3.59	100.93	105.83
21	B	822	CLA	CAA-C2A-C1A	-3.59	100.21	111.97
21	8	612	CLA	C3D-C2D-C1D	-3.59	100.93	105.83
21	3	714	CLA	C3D-C4D-ND	3.59	116.04	110.24
21	2	505	CLA	CAC-C3C-C4C	3.59	129.46	124.81
21	B	823	CLA	C3C-C4C-NC	3.59	114.59	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	902	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
21	B	837	CLA	CHD-C4C-NC	3.59	129.85	124.20
21	B	816	CLA	CHC-C1C-C2C	-3.59	116.80	126.72
21	12	504	CLA	O2D-CGD-CBD	3.59	117.64	111.27
21	6	914	CLA	O2D-CGD-CBD	3.58	117.64	111.27
21	B	833	CLA	CHD-C1D-ND	-3.58	121.16	124.45
21	A	809	CLA	C3D-C4D-ND	3.58	116.03	110.24
21	A	834	CLA	C3D-C2D-C1D	-3.58	100.94	105.83
21	11	711	CLA	CAC-C3C-C4C	3.58	129.46	124.81
21	B	820	CLA	C3B-C4B-NB	3.58	113.84	109.21
21	1	510	CLA	C2C-C1C-NC	3.58	113.33	109.97
21	A	811	CLA	C3C-C4C-NC	3.58	114.59	110.57
21	12	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
21	12	506	CLA	C2C-C1C-NC	3.58	113.33	109.97
21	7	704	CLA	CHC-C1C-C2C	-3.58	116.82	126.72
21	5	703	CLA	CAC-C3C-C4C	3.58	129.46	124.81
21	8	605	CLA	C3B-C4B-NB	3.58	113.84	109.21
21	A	815	CLA	O2A-CGA-CBA	3.58	123.14	111.91
21	7	713	CLA	CHC-C1C-C2C	-3.58	116.82	126.72
21	5	702	CLA	O2D-CGD-CBD	3.58	117.62	111.27
21	3	708	CLA	CBC-CAC-C3C	-3.58	102.57	112.43
21	3	710	CLA	CBC-CAC-C3C	-3.58	102.57	112.43
21	10	712	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
21	A	832	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
21	2	508	CLA	CHB-C4A-NA	3.57	129.46	124.51
21	A	807	CLA	C3D-C4D-ND	3.57	116.02	110.24
21	A	837	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
20	A	801	CL0	CMC-C2C-C1C	3.57	130.48	125.04
21	6	914	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
21	12	501	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
21	B	837	CLA	C3D-C4D-ND	3.57	116.02	110.24
21	2	511	CLA	C3D-C2D-C1D	-3.57	100.95	105.83
21	A	812	CLA	CHD-C4C-NC	3.57	129.83	124.20
21	2	503	CLA	CHC-C1C-C2C	-3.57	116.84	126.72
21	B	802	CLA	C3D-C4D-ND	3.57	116.02	110.24
21	B	816	CLA	C3C-C4C-NC	3.57	114.58	110.57
20	A	801	CL0	CMD-C2D-C1D	3.57	131.01	124.71
21	1	509	CLA	CHC-C1C-NC	3.57	129.62	124.20
21	B	812	CLA	CHC-C1C-C2C	-3.57	116.84	126.72
21	12	503	CLA	C3C-C4C-NC	3.57	114.58	110.57
21	A	817	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
21	A	802	CLA	OBD-CAD-C3D	-3.57	119.93	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	819	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
21	A	813	CLA	O2D-CGD-CBD	3.57	117.61	111.27
21	3	707	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
21	1	517	CLA	CHD-C1D-ND	-3.57	121.17	124.45
21	7	708	CLA	CHD-C1D-ND	-3.57	121.17	124.45
21	B	837	CLA	C3C-C4C-NC	3.56	114.57	110.57
21	1	508	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
21	9	909	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
28	2	520	DD6	C24-C1-C2	3.56	124.41	118.94
21	7	708	CLA	C4A-NA-C1A	-3.56	105.10	106.71
21	1	508	CLA	C3C-C4C-NC	3.56	114.57	110.57
21	A	805	CLA	CHB-C4A-NA	3.56	129.44	124.51
21	A	803	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
21	3	707	CLA	CBC-CAC-C3C	-3.56	102.61	112.43
24	F	405	BCR	C34-C9-C10	-3.56	117.94	122.92
21	1	501	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
21	8	606	CLA	C4A-NA-C1A	-3.56	105.11	106.71
21	8	609	CLA	C3D-C2D-C1D	-3.56	100.98	105.83
21	B	828	CLA	CHD-C1D-ND	-3.56	121.19	124.45
21	8	610	CLA	CAC-C3C-C4C	3.55	129.42	124.81
21	9	902	CLA	C4A-NA-C1A	-3.55	105.11	106.71
21	A	826	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
21	5	709	CLA	O2D-CGD-CBD	3.55	117.58	111.27
21	A	821	CLA	C4-C3-C5	3.55	121.25	115.27
21	7	709	CLA	C3D-C4D-ND	3.55	115.99	110.24
21	5	707	CLA	CHC-C1C-NC	3.55	129.59	124.20
21	A	862	CLA	CHA-C1A-NA	-3.55	118.26	126.40
21	12	503	CLA	C3B-C4B-NB	3.55	113.80	109.21
21	2	511	CLA	CBC-CAC-C3C	-3.55	102.64	112.43
21	B	836	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
24	B	844	BCR	C34-C9-C10	-3.55	117.95	122.92
21	B	832	CLA	C4-C3-C5	3.55	121.24	115.27
21	A	805	CLA	C3C-C4C-NC	3.55	114.55	110.57
21	B	817	CLA	O2A-C1-C2	3.55	117.97	108.64
21	2	512	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
21	12	501	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
21	B	829	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
21	9	914	CLA	C3C-C4C-NC	3.55	114.55	110.57
21	B	832	CLA	CMC-C2C-C1C	3.55	130.44	125.04
21	10	707	CLA	CAC-C3C-C4C	3.55	129.41	124.81
21	13	502	CLA	CAC-C3C-C4C	3.55	129.41	124.81
21	5	703	CLA	CHB-C4A-NA	3.55	129.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	704	CLA	CAC-C3C-C4C	3.55	129.41	124.81
21	A	802	CLA	CHD-C1D-ND	-3.55	121.19	124.45
21	9	908	CLA	C3B-C4B-NB	3.55	113.79	109.21
21	B	810	CLA	CHD-C4C-NC	3.54	129.79	124.20
21	B	828	CLA	C4C-C3C-C2C	-3.54	101.73	106.90
21	2	508	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
21	A	805	CLA	C1B-CHB-C4A	-3.54	123.10	130.12
28	9	916	DD6	C4-C3-C2	3.54	130.73	123.47
21	4	709	CLA	C2A-C1A-CHA	-3.54	117.66	123.86
21	3	707	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
21	B	815	CLA	CMC-C2C-C1C	3.54	130.43	125.04
21	B	806	CLA	CHC-C1C-C2C	-3.54	116.92	126.72
21	B	826	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
21	2	517	CLA	CHC-C1C-C2C	-3.54	116.93	126.72
21	A	835	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
21	4	708	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
21	5	701	CLA	CAC-C3C-C4C	3.54	129.40	124.81
21	A	816	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
21	F	403	CLA	CAC-C3C-C4C	3.54	129.40	124.81
21	2	508	CLA	CHC-C1C-C2C	-3.54	116.93	126.72
21	A	816	CLA	C3C-C4C-NC	3.54	114.54	110.57
21	11	707	CLA	O2A-CGA-CBA	3.54	123.01	111.91
21	11	707	CLA	C3B-C4B-NB	3.54	113.78	109.21
21	F	404	CLA	CHC-C1C-C2C	-3.54	116.94	126.72
21	9	904	CLA	O2D-CGD-CBD	3.54	117.55	111.27
28	3	718	DD6	C24-C1-C2	3.54	124.37	118.94
21	A	862	CLA	CMD-C2D-C1D	3.54	130.94	124.71
21	9	914	CLA	C1D-CHD-C4C	-3.53	118.43	126.06
21	10	705	CLA	CMB-C2B-C3B	3.53	131.29	124.68
21	B	838	CLA	CHC-C1C-C2C	-3.53	116.95	126.72
21	8	603	CLA	CHD-C4C-NC	3.53	129.77	124.20
21	11	702	CLA	C4A-NA-C1A	-3.53	105.12	106.71
21	B	801	CLA	C3D-C4D-ND	3.53	115.95	110.24
21	6	904	CLA	C3D-C4D-ND	3.53	115.95	110.24
21	3	708	CLA	C2C-C1C-NC	3.53	113.28	109.97
21	6	907	CLA	CMC-C2C-C1C	3.53	130.42	125.04
21	B	811	CLA	CHB-C4A-NA	3.53	129.39	124.51
21	B	817	CLA	CHC-C1C-NC	3.53	129.56	124.20
21	B	827	CLA	C3D-C4D-ND	3.53	115.95	110.24
21	3	702	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
21	A	818	CLA	CHD-C4C-NC	3.53	129.76	124.20
21	12	502	CLA	CBC-CAC-C3C	-3.53	102.71	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	802	CLA	C5-C3-C2	-3.53	113.98	121.12
21	2	514	CLA	C3D-C2D-C1D	-3.53	101.02	105.83
21	A	811	CLA	C2A-C1A-CHA	-3.53	117.69	123.86
28	J	104	DD6	C24-C1-C2	3.52	124.35	118.94
21	10	709	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
21	12	507	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
21	1	508	CLA	CHB-C4A-NA	3.52	129.38	124.51
21	B	818	CLA	CHC-C1C-NC	3.52	129.55	124.20
21	4	702	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
21	3	705	CLA	O2A-CGA-CBA	3.52	122.96	111.91
21	B	818	CLA	C2C-C1C-NC	3.52	113.27	109.97
21	B	815	CLA	CHD-C1D-ND	-3.52	121.22	124.45
21	1	501	CLA	CHC-C1C-NC	3.52	129.54	124.20
21	3	706	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
21	4	705	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
21	12	507	CLA	CAC-C3C-C4C	3.52	129.38	124.81
21	A	816	CLA	CMD-C2D-C1D	3.52	130.91	124.71
21	A	809	CLA	C1-O2A-CGA	3.52	125.67	116.44
21	6	911	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
21	1	505	CLA	CHC-C1C-C2C	-3.52	116.99	126.72
21	B	810	CLA	CMA-C3A-C4A	-3.52	102.32	111.77
21	B	821	CLA	CHB-C4A-NA	3.52	129.37	124.51
21	11	711	CLA	C3C-C4C-NC	3.52	114.51	110.57
28	11	713	DD6	C7-C6-C5	-3.52	118.00	122.92
21	B	813	CLA	C3B-C4B-NB	3.51	113.75	109.21
28	2	520	DD6	C4-C3-C2	3.51	130.67	123.47
21	12	505	CLA	O2D-CGD-CBD	3.51	117.51	111.27
21	11	708	CLA	C3B-C4B-NB	3.51	113.75	109.21
21	7	706	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
21	3	710	CLA	CHC-C1C-C2C	-3.51	117.00	126.72
21	B	804	CLA	C3B-C4B-NB	3.51	113.75	109.21
21	3	711	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
21	6	909	CLA	C3B-C4B-NB	3.51	113.75	109.21
21	7	711	CLA	CHD-C4C-NC	3.51	129.74	124.20
21	A	843	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
21	8	609	CLA	CHC-C1C-NC	3.51	129.53	124.20
21	1	513	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
21	7	702	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
21	4	709	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
21	3	708	CLA	CHD-C4C-NC	3.51	129.73	124.20
21	A	817	CLA	CHC-C1C-C2C	-3.51	117.02	126.72
21	8	607	CLA	O2A-CGA-CBA	3.51	122.91	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	508	CLA	O2A-CGA-CBA	3.50	122.91	111.91
21	B	823	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
21	3	710	CLA	C3B-C4B-NB	3.50	113.74	109.21
21	10	708	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
28	2	520	DD6	C3-C4-C5	3.50	130.65	123.47
21	7	703	CLA	CAC-C3C-C4C	3.50	129.35	124.81
21	1	514	CLA	CBC-CAC-C3C	-3.50	102.78	112.43
21	A	827	CLA	C2A-C1A-CHA	-3.50	117.74	123.86
21	B	819	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
28	8	616	DD6	C24-C1-C2	3.50	124.31	118.94
21	1	511	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	F	405	BCR	C15-C14-C13	3.50	132.30	127.31
21	9	908	CLA	C4A-NA-C1A	-3.50	105.13	106.71
21	A	825	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
21	B	837	CLA	CAC-C3C-C4C	3.50	129.35	124.81
21	10	703	CLA	CAC-C3C-C4C	3.50	129.35	124.81
21	6	911	CLA	CHC-C1C-C2C	-3.50	117.05	126.72
21	6	914	CLA	C3C-C4C-NC	3.50	114.49	110.57
21	A	806	CLA	C3C-C4C-NC	3.49	114.49	110.57
21	10	711	CLA	C3C-C4C-NC	3.49	114.49	110.57
21	3	704	CLA	C4A-NA-C1A	-3.49	105.14	106.71
28	9	916	DD6	C7-C6-C5	-3.49	118.03	122.92
21	7	710	CLA	CHD-C4C-NC	3.49	129.71	124.20
21	A	814	CLA	O1D-CGD-CBD	-3.49	117.34	124.48
21	1	504	CLA	CAC-C3C-C4C	3.49	129.34	124.81
21	A	843	CLA	CHB-C4A-NA	3.49	129.34	124.51
21	B	826	CLA	O1D-CGD-CBD	-3.49	117.34	124.48
21	B	828	CLA	CMD-C2D-C1D	3.49	130.87	124.71
21	3	711	CLA	CAC-C3C-C4C	3.49	129.34	124.81
21	4	702	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
21	A	826	CLA	C7-C6-C5	-3.49	103.88	113.36
21	1	501	CLA	CHD-C4C-NC	3.49	129.70	124.20
21	8	613	CLA	CMB-C2B-C3B	3.49	131.21	124.68
21	A	824	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
21	11	706	CLA	CBC-CAC-C3C	-3.49	102.81	112.43
28	4	713	DD6	C7-C6-C5	-3.49	118.04	122.92
21	11	711	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
21	11	703	CLA	C2C-C1C-NC	3.49	113.24	109.97
21	10	706	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
21	A	808	CLA	CBC-CAC-C3C	-3.49	102.82	112.43
21	4	702	CLA	C3B-C4B-NB	3.49	113.72	109.21
21	A	810	CLA	O2A-CGA-O1A	-3.49	114.79	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	F	405	BCR	C37-C22-C21	-3.49	118.04	122.92
28	4	713	DD6	C24-C1-C2	3.49	124.29	118.94
21	6	909	CLA	CMC-C2C-C1C	3.49	130.35	125.04
21	B	812	CLA	CBC-CAC-C3C	-3.49	102.82	112.43
21	12	501	CLA	C1-O2A-CGA	3.48	125.59	116.44
21	8	608	CLA	CAC-C3C-C4C	3.48	129.33	124.81
22	B	840	PQN	C11-C12-C13	-3.48	120.99	126.79
21	2	517	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
21	7	713	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
21	3	702	CLA	CHC-C1C-C2C	-3.48	117.09	126.72
21	A	826	CLA	C3C-C4C-NC	3.48	114.47	110.57
21	A	841	CLA	CHC-C1C-C2C	-3.48	117.09	126.72
21	9	903	CLA	C3C-C4C-NC	3.48	114.47	110.57
21	3	707	CLA	O2A-CGA-CBA	3.48	122.82	111.91
21	5	711	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
21	4	711	CLA	CHB-C4A-NA	3.47	129.31	124.51
28	9	915	DD6	C7-C6-C5	-3.47	118.06	122.92
21	8	609	CLA	CAC-C3C-C4C	3.47	129.31	124.81
21	11	703	CLA	C1-O2A-CGA	3.47	125.55	116.44
21	2	506	CLA	C4A-NA-C1A	-3.47	105.15	106.71
21	4	704	CLA	CHC-C1C-C2C	-3.47	117.12	126.72
21	B	821	CLA	C3B-C4B-NB	3.47	113.69	109.21
21	7	703	CLA	C2A-C1A-CHA	-3.47	117.79	123.86
21	B	816	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
21	9	907	CLA	O2A-CGA-CBA	3.47	122.79	111.91
21	10	710	CLA	C1-O2A-CGA	3.47	125.54	116.44
21	B	824	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
21	A	807	CLA	CHC-C1C-C2C	-3.47	117.13	126.72
21	3	713	CLA	CHC-C1C-C2C	-3.47	117.13	126.72
21	1	512	CLA	CHC-C1C-C2C	-3.47	117.13	126.72
21	B	821	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
21	B	833	CLA	O2D-CGD-CBD	3.47	117.43	111.27
21	A	844	CLA	O2A-CGA-O1A	-3.47	114.85	123.59
21	B	818	CLA	CHD-C4C-NC	3.47	129.66	124.20
21	2	513	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
21	B	810	CLA	C3C-C4C-NC	3.46	114.46	110.57
21	B	807	CLA	O2A-CGA-CBA	3.46	122.78	111.91
21	B	830	CLA	CHC-C1C-C2C	-3.46	117.14	126.72
21	3	703	CLA	C3D-C4D-ND	3.46	115.84	110.24
21	10	708	CLA	CBC-CAC-C3C	-3.46	102.88	112.43
21	A	813	CLA	CAA-CBA-CGA	-3.46	103.13	113.25
21	B	819	CLA	O2D-CGD-O1D	-3.46	117.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	502	CLA	CHC-C1C-C2C	-3.46	117.14	126.72
28	J	104	DD6	C7-C6-C5	-3.46	118.07	122.92
21	8	605	CLA	CMB-C2B-C3B	3.46	131.15	124.68
21	A	829	CLA	C6-C7-C8	-3.46	104.73	115.92
21	A	811	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
28	3	717	DD6	C7-C6-C8	3.46	123.53	118.08
21	B	809	CLA	C3D-C2D-C1D	-3.46	101.11	105.83
21	1	516	CLA	CHC-C1C-C2C	-3.46	117.15	126.72
21	B	823	CLA	CHC-C1C-C2C	-3.46	117.16	126.72
21	3	706	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
21	A	810	CLA	CAA-CBA-CGA	-3.46	103.15	113.25
21	B	818	CLA	CHC-C1C-C2C	-3.46	117.16	126.72
21	4	703	CLA	CHC-C1C-C2C	-3.46	117.16	126.72
21	9	913	CLA	CHC-C1C-C2C	-3.46	117.16	126.72
21	B	821	CLA	CBC-CAC-C3C	-3.46	102.91	112.43
21	9	908	CLA	CBC-CAC-C3C	-3.46	102.91	112.43
21	4	708	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
21	10	708	CLA	C3B-C4B-NB	3.45	113.68	109.21
21	4	704	CLA	O2A-CGA-CBA	3.45	122.75	111.91
21	7	710	CLA	CHC-C1C-C2C	-3.45	117.17	126.72
21	12	508	CLA	C3C-C4C-NC	3.45	114.44	110.57
21	7	706	CLA	CMC-C2C-C1C	3.45	130.29	125.04
21	5	707	CLA	C2C-C1C-NC	3.45	113.20	109.97
21	6	903	CLA	CAC-C3C-C4C	3.45	129.29	124.81
24	F	402	BCR	C37-C22-C23	3.45	123.51	118.08
21	A	823	CLA	CHB-C4A-NA	3.45	129.28	124.51
21	A	807	CLA	CAC-C3C-C4C	3.45	129.28	124.81
21	A	804	CLA	C2C-C1C-NC	3.45	113.20	109.97
21	5	707	CLA	CHC-C1C-C2C	-3.45	117.19	126.72
21	B	827	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
21	3	714	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
21	A	803	CLA	C1D-CHD-C4C	-3.45	118.63	126.06
21	12	508	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
21	8	603	CLA	O1D-CGD-CBD	-3.44	117.44	124.48
21	6	905	CLA	CAC-C3C-C4C	3.44	129.28	124.81
21	B	839	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
21	B	829	CLA	O2D-CGD-CBD	3.44	117.39	111.27
21	12	503	CLA	CMB-C2B-C3B	3.44	131.12	124.68
21	2	505	CLA	C4A-NA-C1A	-3.44	105.16	106.71
21	6	909	CLA	C3C-C4C-NC	3.44	114.43	110.57
21	A	824	CLA	CBC-CAC-C3C	-3.44	102.95	112.43
21	11	703	CLA	C3D-C4D-ND	3.44	115.80	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	824	CLA	C2A-C1A-CHA	-3.44	117.85	123.86
24	A	850	BCR	C29-C30-C25	3.44	115.77	110.48
21	11	711	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
21	12	502	CLA	CAC-C3C-C4C	3.44	129.27	124.81
21	4	706	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
21	8	610	CLA	CHB-C4A-NA	3.44	129.26	124.51
21	B	827	CLA	CHC-C1C-C2C	-3.44	117.22	126.72
25	7	717	LHG	O7-C5-C4	-3.44	95.96	108.40
21	8	613	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
21	B	803	CLA	C3B-C4B-NB	3.44	113.65	109.21
21	2	514	CLA	CHC-C1C-C2C	-3.43	117.22	126.72
21	3	707	CLA	C3C-C4C-NC	3.43	114.42	110.57
21	3	710	CLA	C3C-C4C-NC	3.43	114.42	110.57
21	7	714	CLA	C1-O2A-CGA	3.43	126.71	116.73
21	10	712	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
21	9	914	CLA	CHC-C1C-C2C	-3.43	117.22	126.72
21	13	501	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
21	B	836	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
21	F	404	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
21	4	711	CLA	C2A-C1A-CHA	-3.43	117.86	123.86
28	3	717	DD6	O1-C20-C19	-3.43	110.81	113.38
21	4	710	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
21	3	705	CLA	C3B-C4B-NB	3.43	113.64	109.21
28	J	104	DD6	C-C1-C2	-3.43	118.12	122.92
21	B	804	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
21	10	711	CLA	CHC-C1C-C2C	-3.43	117.24	126.72
21	12	506	CLA	CMC-C2C-C1C	3.43	130.26	125.04
21	B	829	CLA	CMA-C3A-C4A	-3.43	102.56	111.77
21	4	707	CLA	CAA-C2A-C3A	-3.43	103.40	112.78
21	7	714	CLA	CMC-C2C-C1C	3.43	130.26	125.04
28	5	712	DD6	C4-C3-C2	3.43	130.49	123.47
21	10	710	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
21	A	828	CLA	CHD-C1D-ND	-3.42	121.31	124.45
21	13	501	CLA	CHC-C1C-C2C	-3.42	117.25	126.72
21	B	819	CLA	O2A-CGA-CBA	3.42	122.65	111.91
22	A	845	PQN	C17-C16-C15	-3.42	104.06	113.36
21	7	708	CLA	CAC-C3C-C4C	3.42	129.25	124.81
21	4	710	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
28	11	712	DD6	C4-C3-C2	3.42	130.48	123.47
21	12	506	CLA	O2A-CGA-CBA	3.42	122.64	111.91
21	3	713	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
21	8	611	CLA	CHC-C1C-C2C	-3.42	117.27	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	503	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
21	9	913	CLA	O2A-CGA-CBA	3.42	122.63	111.91
21	10	706	CLA	C3C-C4C-NC	3.41	114.40	110.57
22	B	840	PQN	O4-C4-C3	3.41	126.05	120.56
21	11	701	CLA	CHC-C1C-C2C	-3.41	117.28	126.72
21	B	824	CLA	C4D-CHA-C1A	-3.41	117.09	121.25
21	A	805	CLA	C3B-C4B-NB	3.41	113.62	109.21
21	7	706	CLA	CHD-C1D-ND	-3.41	121.32	124.45
21	F	401	CLA	C4-C3-C2	-3.41	114.92	123.68
24	A	851	BCR	C37-C22-C23	3.41	123.45	118.08
21	B	837	CLA	CMC-C2C-C1C	3.41	130.23	125.04
21	8	612	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
21	A	837	CLA	C3C-C4C-NC	3.41	114.39	110.57
21	2	507	CLA	O2A-CGA-CBA	3.41	122.61	111.91
21	4	711	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
21	9	902	CLA	CHB-C4A-NA	3.41	129.22	124.51
24	B	842	BCR	C15-C16-C17	3.40	130.45	123.47
21	A	811	CLA	C3D-C4D-ND	3.40	115.75	110.24
21	1	510	CLA	C3C-C4C-NC	3.40	114.39	110.57
21	A	830	CLA	CHC-C1C-C2C	-3.40	117.31	126.72
21	9	909	CLA	CHB-C4A-NA	3.40	129.22	124.51
21	F	403	CLA	CHC-C1C-C2C	-3.40	117.31	126.72
28	9	915	DD6	C24-C1-C2	3.40	124.16	118.94
21	6	912	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
21	B	839	CLA	C3B-C4B-NB	3.40	113.61	109.21
21	A	803	CLA	CED-O2D-CGD	-3.40	108.25	115.94
21	10	704	CLA	CMB-C2B-C3B	3.40	131.04	124.68
21	10	709	CLA	CAC-C3C-C4C	3.40	129.22	124.81
21	1	515	CLA	O2D-CGD-CBD	3.40	117.31	111.27
21	5	705	CLA	C3C-C4C-NC	3.40	114.38	110.57
21	11	708	CLA	C3C-C4C-NC	3.40	114.38	110.57
21	B	826	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
21	B	809	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
21	10	707	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
21	B	833	CLA	CHC-C1C-C2C	-3.40	117.33	126.72
28	1	518	DD6	C-C1-C2	-3.40	118.17	122.92
21	A	814	CLA	C3B-C4B-NB	3.39	113.60	109.21
21	11	710	CLA	CHC-C1C-C2C	-3.39	117.34	126.72
21	A	829	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
21	11	708	CLA	CHC-C1C-C2C	-3.39	117.34	126.72
21	6	904	CLA	C3B-C4B-NB	3.39	113.59	109.21
21	A	837	CLA	CHC-C1C-NC	3.39	129.35	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	822	CLA	C3D-C2D-C1D	-3.39	101.21	105.83
21	11	707	CLA	CHC-C1C-C2C	-3.39	117.35	126.72
21	1	516	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	J	102	BCR	C15-C16-C17	3.39	130.41	123.47
21	9	908	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
21	4	710	CLA	CHC-C1C-C2C	-3.39	117.35	126.72
21	12	508	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
21	A	816	CLA	CBC-CAC-C3C	-3.39	103.10	112.43
21	4	709	CLA	O2A-CGA-CBA	3.39	124.91	114.03
21	A	804	CLA	C1-O2A-CGA	3.39	125.33	116.44
21	A	807	CLA	CHD-C1D-ND	-3.39	121.34	124.45
24	M	102	BCR	C37-C22-C21	-3.39	118.18	122.92
21	5	702	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
21	A	842	CLA	O2A-C1-C2	3.38	117.53	108.64
21	8	603	CLA	CHC-C1C-C2C	-3.38	117.36	126.72
21	5	711	CLA	CAC-C3C-C4C	3.38	129.20	124.81
21	5	705	CLA	O2A-CGA-CBA	3.38	122.52	111.91
21	12	508	CLA	CHC-C1C-C2C	-3.38	117.36	126.72
21	4	704	CLA	C3B-C4B-NB	3.38	113.58	109.21
21	A	814	CLA	O2D-CGD-CBD	3.38	117.28	111.27
21	1	508	CLA	C2A-C1A-CHA	-3.38	117.95	123.86
21	2	511	CLA	CHC-C1C-C2C	-3.38	117.37	126.72
21	3	712	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
21	11	709	CLA	C3D-C2D-C1D	-3.38	101.22	105.83
21	B	830	CLA	CGD-CBD-CAD	-3.38	99.79	110.73
24	A	847	BCR	C29-C30-C25	3.38	115.68	110.48
21	B	810	CLA	C3D-C2D-C1D	-3.38	101.22	105.83
28	7	715	DD6	C3-C4-C5	3.38	130.39	123.47
24	B	842	BCR	C1-C6-C5	-3.38	117.86	122.61
21	1	508	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
21	8	614	CLA	C1D-CHD-C4C	-3.38	118.78	126.06
21	A	802	CLA	CHC-C1C-C2C	-3.38	117.38	126.72
21	5	701	CLA	C3C-C4C-NC	3.37	114.36	110.57
21	4	704	CLA	O2A-C1-C2	3.37	117.50	108.64
21	10	706	CLA	CAC-C3C-C4C	3.37	129.19	124.81
24	B	844	BCR	C37-C22-C23	3.37	123.39	118.08
28	J	104	DD6	C4-C3-C2	3.37	130.38	123.47
21	5	704	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
21	A	838	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
21	B	816	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
21	10	703	CLA	CHC-C1C-C2C	-3.37	117.40	126.72
21	3	705	CLA	C1D-CHD-C4C	-3.37	118.79	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	803	CLA	CHB-C4A-NA	3.37	129.17	124.51
25	7	717	LHG	O7-C7-C8	3.37	118.76	111.50
21	13	502	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
21	A	822	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
21	7	709	CLA	CHC-C1C-C2C	-3.37	117.40	126.72
21	B	839	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
21	6	914	CLA	C3B-C4B-NB	3.37	113.56	109.21
21	8	613	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
21	9	913	CLA	C3B-C4B-NB	3.36	113.56	109.21
21	A	803	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
21	A	808	CLA	CHD-C4C-NC	3.36	129.50	124.20
21	7	708	CLA	C3C-C4C-NC	3.36	114.34	110.57
21	7	704	CLA	C3D-C2D-C1D	-3.36	101.24	105.83
21	B	821	CLA	CAC-C3C-C4C	3.36	129.17	124.81
21	9	910	CLA	CHC-C1C-C2C	-3.36	117.42	126.72
21	6	914	CLA	C1-O2A-CGA	3.36	126.50	116.73
21	7	711	CLA	C3C-C4C-NC	3.36	114.34	110.57
21	2	516	CLA	O2D-CGD-CBD	3.36	117.24	111.27
21	10	710	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
21	7	704	CLA	CAC-C3C-C4C	3.36	129.17	124.81
21	A	806	CLA	C3B-C4B-NB	3.36	113.55	109.21
21	6	909	CLA	CHC-C1C-C2C	-3.36	117.44	126.72
21	2	503	CLA	C3C-C4C-NC	3.36	114.33	110.57
21	A	826	CLA	C3D-C2D-C1D	-3.36	101.25	105.83
21	9	911	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
21	5	711	CLA	CHC-C1C-C2C	-3.35	117.44	126.72
21	7	710	CLA	CHB-C4A-NA	3.35	129.15	124.51
21	B	802	CLA	C2A-C1A-CHA	-3.35	117.99	123.86
21	A	839	CLA	CMB-C2B-C1B	3.35	133.62	128.46
21	3	708	CLA	CAC-C3C-C4C	3.35	129.16	124.81
28	7	715	DD6	C4-C3-C2	3.35	130.34	123.47
21	8	612	CLA	CHC-C1C-C2C	-3.35	117.45	126.72
21	7	709	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
21	5	707	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
21	3	707	CLA	O2D-CGD-CBD	3.35	117.22	111.27
28	2	520	DD6	C7-C6-C5	-3.35	118.23	122.92
21	5	701	CLA	CHB-C4A-NA	3.35	129.15	124.51
21	5	702	CLA	CHB-C4A-NA	3.35	129.15	124.51
21	B	834	CLA	C1-O2A-CGA	3.35	125.24	116.44
21	A	834	CLA	CMC-C2C-C1C	3.35	130.14	125.04
28	8	615	DD6	C-C1-C2	-3.35	118.23	122.92
21	1	514	CLA	CHC-C1C-C2C	-3.35	117.46	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	517	CLA	C3C-C4C-NC	3.35	114.33	110.57
21	A	814	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
21	3	704	CLA	CHC-C1C-C2C	-3.35	117.46	126.72
21	B	815	CLA	C1-O2A-CGA	3.35	125.23	116.44
21	1	504	CLA	CHC-C1C-C2C	-3.35	117.46	126.72
21	7	714	CLA	O2D-CGD-CBD	3.35	117.22	111.27
21	A	829	CLA	C5-C3-C2	-3.35	114.34	121.12
21	8	604	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
21	9	902	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
21	11	709	CLA	C3B-C4B-NB	3.35	113.53	109.21
21	2	509	CLA	C2A-C1A-CHA	-3.34	118.01	123.86
21	A	830	CLA	C3B-C4B-NB	3.34	113.53	109.21
21	7	703	CLA	CHD-C4C-NC	3.34	129.47	124.20
21	A	809	CLA	C11-C10-C8	-3.34	105.11	115.92
21	A	812	CLA	CAC-C3C-C4C	3.34	129.15	124.81
21	7	702	CLA	CMB-C2B-C3B	3.34	130.93	124.68
21	2	504	CLA	C3C-C4C-NC	3.34	114.32	110.57
21	A	809	CLA	OBD-CAD-C3D	-3.34	120.48	128.52
21	7	704	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	2	512	CLA	CMB-C2B-C3B	3.34	130.93	124.68
21	12	502	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	F	402	BCR	C36-C18-C17	-3.34	118.25	122.92
21	9	912	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
21	11	708	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
21	1	508	CLA	C4A-NA-C1A	-3.34	105.20	106.71
21	1	504	CLA	C3C-C4C-NC	3.34	114.31	110.57
21	8	607	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
21	7	702	CLA	CHC-C1C-C2C	-3.34	117.49	126.72
21	8	607	CLA	CMC-C2C-C1C	3.34	130.12	125.04
21	12	505	CLA	C3B-C4B-NB	3.34	113.52	109.21
21	9	904	CLA	CAC-C3C-C4C	3.34	129.14	124.81
21	A	843	CLA	O2A-CGA-CBA	3.34	122.38	111.91
21	7	706	CLA	O1D-CGD-CBD	-3.34	117.66	124.48
21	12	506	CLA	C3C-C4C-NC	3.33	114.31	110.57
28	1	520	DD6	C3-C4-C5	3.33	130.31	123.47
21	B	805	CLA	CHB-C4A-NA	3.33	129.12	124.51
21	B	806	CLA	CMC-C2C-C1C	3.33	130.12	125.04
21	4	705	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
21	11	704	CLA	CHC-C1C-C2C	-3.33	117.50	126.72
21	11	703	CLA	CHC-C1C-C2C	-3.33	117.50	126.72
21	A	823	CLA	C2A-C1A-CHA	-3.33	118.03	123.86
21	B	831	CLA	C4C-C3C-C2C	-3.33	102.04	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	706	CLA	O2A-CGA-CBA	3.33	122.36	111.91
28	1	518	DD6	C3-C4-C5	3.33	130.30	123.47
21	13	502	CLA	CHC-C1C-C2C	-3.33	117.51	126.72
21	A	841	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
21	4	702	CLA	C2A-C1A-CHA	-3.33	118.04	123.86
21	3	708	CLA	C3D-C2D-C1D	-3.33	101.29	105.83
21	B	835	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
21	9	909	CLA	C4A-NA-C1A	-3.33	105.21	106.71
21	A	809	CLA	C1-C2-C3	-3.33	120.29	126.04
21	7	706	CLA	O2A-CGA-CBA	3.33	122.35	111.91
21	2	510	CLA	CAC-C3C-C4C	3.33	129.13	124.81
21	3	715	CLA	CHD-C4C-NC	3.33	129.44	124.20
21	9	913	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
21	6	912	CLA	CHC-C1C-C2C	-3.32	117.53	126.72
21	9	910	CLA	CHD-C4C-NC	3.32	129.44	124.20
21	A	812	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
21	6	904	CLA	CHC-C1C-C2C	-3.32	117.53	126.72
20	A	801	CL0	CMB-C2B-C3B	3.32	130.89	124.68
21	8	604	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
21	6	903	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
21	1	506	CLA	C3C-C4C-NC	3.32	114.30	110.57
28	9	915	DD6	C13-C11-C10	3.32	124.04	118.94
21	A	811	CLA	CHB-C4A-NA	3.32	129.10	124.51
21	B	822	CLA	C2A-C1A-CHA	-3.32	118.06	123.86
21	2	517	CLA	CAC-C3C-C4C	3.32	129.12	124.81
21	1	508	CLA	OBD-CAD-C3D	-3.32	120.53	128.52
21	9	902	CLA	C3D-C2D-C1D	-3.32	101.30	105.83
21	7	704	CLA	C3D-C4D-ND	3.32	115.61	110.24
21	A	841	CLA	CHD-C4C-NC	3.32	129.43	124.20
21	9	902	CLA	CAC-C3C-C4C	3.32	129.11	124.81
28	8	616	DD6	C7-C6-C5	-3.32	118.28	122.92
21	9	908	CLA	CAC-C3C-C4C	3.32	129.11	124.81
21	B	821	CLA	CHC-C1C-C2C	-3.31	117.55	126.72
21	6	912	CLA	CBC-CAC-C3C	-3.31	103.29	112.43
21	10	711	CLA	C3B-C4B-NB	3.31	113.50	109.21
21	8	611	CLA	C3C-C4C-NC	3.31	114.29	110.57
21	F	401	CLA	C3D-C4D-ND	3.31	115.60	110.24
21	12	505	CLA	CHC-C1C-NC	3.31	129.23	124.20
21	1	506	CLA	C2C-C1C-NC	3.31	113.08	109.97
21	9	914	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
21	11	704	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
21	B	806	CLA	C1C-C2C-C3C	-3.31	103.47	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	805	CLA	CMC-C2C-C1C	3.31	130.08	125.04
21	B	834	CLA	O2A-CGA-CBA	3.31	122.30	111.91
21	A	834	CLA	CBC-CAC-C3C	-3.31	103.30	112.43
21	5	709	CLA	CHD-C4C-NC	3.31	129.42	124.20
21	B	802	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
21	9	906	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
21	1	510	CLA	CAC-C3C-C4C	3.31	129.10	124.81
24	B	842	BCR	C36-C18-C17	-3.31	118.29	122.92
21	8	613	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
21	1	501	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
21	6	910	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
21	11	705	CLA	CAA-CBA-CGA	3.31	122.92	113.25
21	A	842	CLA	CHB-C4A-NA	3.31	129.09	124.51
25	6	917	LHG	O7-C5-C4	-3.31	96.42	108.40
21	7	705	CLA	O2A-CGA-O1A	-3.31	115.25	123.59
21	A	823	CLA	O2D-CGD-CBD	3.31	117.14	111.27
21	6	907	CLA	C3C-C4C-NC	3.30	114.28	110.57
21	11	708	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
21	A	844	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
21	12	503	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
21	11	707	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
21	10	712	CLA	CHC-C1C-C2C	-3.30	117.59	126.72
21	A	830	CLA	C4-C3-C5	3.30	120.83	115.27
21	A	817	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	B	844	BCR	C37-C22-C21	-3.30	118.30	122.92
20	A	801	CL0	C3C-C4C-NC	3.30	114.27	110.57
21	A	815	CLA	CHD-C4C-NC	3.30	129.40	124.20
21	3	713	CLA	C3B-C4B-NB	3.30	113.48	109.21
21	B	828	CLA	CHC-C1C-C2C	-3.30	117.59	126.72
21	A	829	CLA	CAC-C3C-C4C	3.30	129.09	124.81
21	10	705	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
21	2	507	CLA	C3C-C4C-NC	3.30	114.27	110.57
21	A	833	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
21	9	906	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
21	B	820	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
21	A	843	CLA	OBD-CAD-C3D	-3.30	120.59	128.52
21	2	505	CLA	C3D-C4D-ND	3.30	115.57	110.24
21	7	710	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
21	B	839	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
21	6	909	CLA	C2A-C1A-CHA	-3.29	118.10	123.86
25	6	917	LHG	O7-C5-C6	3.29	120.33	108.40
21	7	704	CLA	CBC-CAC-C3C	-3.29	103.35	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	512	CLA	C3C-C4C-NC	3.29	114.27	110.57
21	B	821	CLA	O2A-CGA-CBA	3.29	122.24	111.91
21	2	506	CLA	C3B-C4B-NB	3.29	113.47	109.21
21	4	704	CLA	C3C-C4C-NC	3.29	114.26	110.57
21	11	702	CLA	C2C-C1C-NC	3.29	113.06	109.97
21	1	504	CLA	C3B-C4B-NB	3.29	113.46	109.21
21	11	701	CLA	CAC-C3C-C4C	3.29	129.08	124.81
21	3	712	CLA	C3B-C4B-NB	3.29	113.46	109.21
21	B	827	CLA	CHB-C4A-NA	3.29	129.06	124.51
21	5	709	CLA	C3C-C4C-NC	3.29	114.26	110.57
21	A	814	CLA	O2A-CGA-CBA	3.29	122.23	111.91
21	A	815	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
21	3	711	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
21	6	903	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
28	12	509	DD6	C-C1-C2	-3.29	118.32	122.92
21	1	507	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
21	11	705	CLA	C3D-C2D-C1D	-3.29	101.34	105.83
21	A	808	CLA	CHC-C1C-NC	3.29	129.19	124.20
21	6	914	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
21	B	807	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
21	A	844	CLA	C1-O2A-CGA	3.29	125.07	116.44
21	A	804	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
21	1	504	CLA	CAA-C2A-C3A	-3.29	106.05	114.26
21	B	823	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
21	9	909	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
21	4	711	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
21	4	708	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
21	2	508	CLA	CMA-C3A-C4A	-3.28	102.95	111.77
21	9	911	CLA	CAC-C3C-C4C	3.28	129.07	124.81
21	10	706	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
21	J	101	CLA	OBD-CAD-C3D	-3.28	120.63	128.52
24	B	841	BCR	C34-C9-C10	-3.28	118.33	122.92
21	A	811	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
21	A	862	CLA	C1-O2A-CGA	3.28	125.04	116.44
21	B	839	CLA	CHB-C4A-NA	3.28	129.04	124.51
21	A	825	CLA	CHC-C1C-NC	3.28	129.17	124.20
21	12	503	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
21	A	815	CLA	C2C-C1C-NC	3.28	113.04	109.97
21	B	811	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
21	3	715	CLA	C2A-C1A-CHA	-3.28	118.13	123.86
21	5	706	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
21	A	807	CLA	C3D-C2D-C1D	-3.27	101.36	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	704	CLA	CED-O2D-CGD	3.27	123.34	115.94
21	7	709	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
21	12	506	CLA	CAC-C3C-C4C	3.27	129.06	124.81
21	3	708	CLA	C3B-C4B-NB	3.27	113.44	109.21
28	1	520	DD6	C7-C6-C5	-3.27	118.34	122.92
21	1	515	CLA	CMC-C2C-C1C	3.27	130.02	125.04
21	B	813	CLA	CHB-C4A-NA	3.27	129.03	124.51
21	A	832	CLA	CMB-C2B-C1B	3.27	133.49	128.46
21	1	512	CLA	CED-O2D-CGD	3.27	123.33	115.94
21	5	711	CLA	C3C-C4C-NC	3.27	114.24	110.57
21	5	709	CLA	CHC-C1C-C2C	-3.27	117.68	126.72
21	11	703	CLA	CHC-C1C-NC	3.27	129.16	124.20
21	5	702	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
21	4	702	CLA	CMB-C2B-C3B	3.27	130.79	124.68
21	3	707	CLA	CHD-C4C-NC	3.27	129.35	124.20
21	2	506	CLA	O2A-CGA-CBA	3.26	122.15	111.91
24	B	842	BCR	C35-C13-C14	-3.26	118.35	122.92
21	10	704	CLA	C3C-C4C-NC	3.26	114.23	110.57
21	A	830	CLA	C2A-C1A-CHA	-3.26	118.15	123.86
21	A	839	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
21	7	707	CLA	CAC-C3C-C4C	3.26	129.04	124.81
21	A	810	CLA	C3D-C4D-ND	3.26	115.52	110.24
21	A	838	CLA	C3D-C4D-ND	3.26	115.52	110.24
21	J	101	CLA	O2A-CGA-O1A	-3.26	115.17	123.30
21	B	801	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
21	9	910	CLA	CBC-CAC-C3C	-3.26	103.44	112.43
24	J	103	BCR	C34-C9-C10	-3.26	118.36	122.92
21	1	505	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
21	A	843	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
21	4	703	CLA	CAC-C3C-C4C	3.26	129.04	124.81
21	A	814	CLA	C1-O2A-CGA	3.26	125.00	116.44
21	B	804	CLA	C1-O2A-CGA	3.26	125.00	116.44
21	4	706	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
21	B	808	CLA	C3C-C4C-NC	3.26	114.23	110.57
21	A	804	CLA	CHD-C1D-ND	-3.26	121.46	124.45
21	B	806	CLA	C2C-C1C-NC	3.26	113.03	109.97
21	B	801	CLA	C3B-C4B-NB	3.26	113.42	109.21
21	6	910	CLA	C3B-C4B-NB	3.26	113.42	109.21
21	A	827	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
21	4	711	CLA	O2D-CGD-CBD	3.26	117.06	111.27
21	2	503	CLA	OBD-CAD-C3D	-3.26	120.68	128.52
21	B	827	CLA	O1A-CGA-CBA	-3.26	111.02	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	911	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
21	9	905	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
21	1	516	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
21	1	510	CLA	O2A-CGA-CBA	3.26	122.13	111.91
21	8	603	CLA	C4A-NA-C1A	-3.26	105.24	106.71
21	5	708	CLA	CAC-C3C-C4C	3.26	129.03	124.81
21	1	507	CLA	CBC-CAC-C3C	-3.26	103.46	112.43
21	B	803	CLA	C2A-C1A-CHA	-3.25	118.17	123.86
21	B	821	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
21	B	817	CLA	C3D-C2D-C1D	-3.25	101.39	105.83
21	6	903	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
21	9	910	CLA	CAC-C3C-C4C	3.25	129.03	124.81
21	7	714	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
21	1	515	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
21	3	712	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
21	A	844	CLA	C4A-NA-C1A	-3.25	105.25	106.71
21	10	712	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
21	A	811	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
21	2	513	CLA	CMC-C2C-C1C	3.25	129.99	125.04
21	A	811	CLA	OBD-CAD-C3D	-3.25	120.70	128.52
28	7	716	DD6	C-C1-C2	-3.25	118.37	122.92
21	5	705	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
21	A	830	CLA	CHC-C1C-NC	3.25	129.13	124.20
21	B	837	CLA	CHC-C1C-NC	3.25	129.13	124.20
21	2	513	CLA	C3C-C4C-NC	3.25	114.21	110.57
21	7	704	CLA	CMC-C2C-C1C	3.25	129.98	125.04
21	B	838	CLA	CHD-C1D-ND	-3.25	121.47	124.45
21	11	701	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
21	B	812	CLA	O2D-CGD-CBD	3.25	117.04	111.27
21	F	403	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
25	10	713	LHG	O7-C7-C8	3.25	118.50	111.50
21	9	907	CLA	CMB-C2B-C3B	3.24	130.75	124.68
21	B	805	CLA	C3D-C2D-C1D	-3.24	101.40	105.83
21	9	902	CLA	CAA-C2A-C3A	-3.24	106.15	114.26
21	11	710	CLA	CMC-C2C-C1C	3.24	129.98	125.04
21	2	507	CLA	C4A-NA-C1A	-3.24	105.25	106.71
21	12	501	CLA	C3C-C4C-NC	3.24	114.21	110.57
21	8	603	CLA	CHC-C1C-NC	3.24	129.12	124.20
28	7	715	DD6	C7-C6-C5	-3.24	118.38	122.92
21	3	706	CLA	CMD-C2D-C3D	-3.24	120.16	127.61
21	7	709	CLA	CMA-C3A-C4A	-3.24	103.06	111.77
21	5	708	CLA	CHC-C1C-C2C	-3.24	117.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	708	CLA	C4A-NA-C1A	-3.24	105.25	106.71
21	2	506	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
21	10	705	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
21	4	711	CLA	C3C-C4C-NC	3.24	114.20	110.57
21	1	507	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
21	3	703	CLA	C2A-C1A-CHA	-3.24	118.19	123.86
21	A	862	CLA	CHB-C4A-NA	3.24	128.99	124.51
21	A	813	CLA	CHC-C1C-NC	3.24	129.12	124.20
28	3	717	DD6	C10-C9-C8	3.24	133.32	123.22
21	1	514	CLA	C3B-C4B-NB	3.24	113.40	109.21
21	B	831	CLA	CAA-CBA-CGA	-3.24	103.79	113.25
21	7	713	CLA	C3B-C4B-NB	3.24	113.39	109.21
21	B	810	CLA	CAC-C3C-C4C	3.24	129.01	124.81
21	A	836	CLA	C3C-C4C-NC	3.24	114.20	110.57
21	2	507	CLA	C2A-C1A-CHA	-3.24	118.20	123.86
21	B	817	CLA	C4-C3-C5	3.24	120.71	115.27
21	10	703	CLA	C3C-C4C-NC	3.23	114.20	110.57
21	7	705	CLA	CMC-C2C-C1C	3.23	129.97	125.04
21	11	705	CLA	CMC-C2C-C1C	3.23	129.97	125.04
21	4	701	CLA	CHC-C1C-NC	3.23	129.11	124.20
21	4	708	CLA	CAC-C3C-C4C	3.23	129.01	124.81
21	7	703	CLA	O2A-CGA-O1A	-3.23	115.43	123.59
21	10	710	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
21	11	702	CLA	CHD-C4C-NC	3.23	129.30	124.20
21	2	515	CLA	CHB-C4A-NA	3.23	128.98	124.51
20	A	801	CL0	CAA-C2A-C3A	-3.23	103.93	112.78
21	A	839	CLA	O2A-CGA-CBA	3.23	122.05	111.91
21	A	842	CLA	CMC-C2C-C1C	3.23	129.96	125.04
21	A	824	CLA	CHD-C4C-NC	3.23	129.30	124.20
21	9	912	CLA	C4A-NA-C1A	-3.23	105.25	106.71
21	A	822	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
21	B	810	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
21	6	904	CLA	C2A-C1A-CHA	-3.23	118.21	123.86
21	5	703	CLA	C3C-C4C-NC	3.23	114.19	110.57
21	J	101	CLA	CAA-C2A-C3A	-3.23	103.94	112.78
21	8	606	CLA	C3B-C4B-NB	3.23	113.38	109.21
21	7	710	CLA	C2A-C1A-CHA	-3.23	118.22	123.86
21	A	822	CLA	CHB-C4A-NA	3.23	128.97	124.51
21	3	705	CLA	C2A-C1A-CHA	-3.23	118.22	123.86
21	2	508	CLA	C1-O2A-CGA	3.23	126.10	116.73
21	2	510	CLA	C3B-C4B-NB	3.23	113.38	109.21
21	B	831	CLA	CHC-C1C-C2C	-3.22	117.80	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	614	CLA	CHC-C1C-C2C	-3.22	117.80	126.72
21	B	808	CLA	CAC-C3C-C4C	3.22	128.99	124.81
21	B	836	CLA	C1-O2A-CGA	3.22	126.09	116.73
21	10	703	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
21	2	511	CLA	C2A-C1A-CHA	-3.22	118.22	123.86
21	4	709	CLA	C3C-C4C-NC	3.22	114.19	110.57
21	6	908	CLA	CMC-C2C-C1C	3.22	129.95	125.04
21	B	822	CLA	O2D-CGD-CBD	3.22	116.99	111.27
21	1	510	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
28	1	519	DD6	C4-C3-C2	3.22	130.07	123.47
21	9	911	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
21	B	815	CLA	C3D-C2D-C1D	-3.22	101.44	105.83
21	3	703	CLA	CBC-CAC-C3C	-3.22	103.56	112.43
21	6	911	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
21	10	704	CLA	C3B-C4B-NB	3.22	113.37	109.21
21	2	506	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	9	916	DD6	C8-C6-C5	3.22	123.88	118.94
21	7	713	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
28	9	915	DD6	C-C1-C2	-3.22	118.42	122.92
21	5	707	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
21	9	909	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
21	A	815	CLA	C3B-C4B-NB	3.21	113.37	109.21
21	5	705	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
21	2	509	CLA	CMB-C2B-C3B	3.21	130.69	124.68
21	4	711	CLA	CHC-C1C-NC	3.21	129.08	124.20
28	4	713	DD6	C8-C6-C5	3.21	123.87	118.94
21	4	705	CLA	O2A-CGA-CBA	3.21	121.99	111.91
21	7	713	CLA	CGD-CBD-CAD	-3.21	100.33	110.73
28	11	713	DD6	C8-C6-C5	3.21	123.87	118.94
21	B	826	CLA	CAA-CBA-CGA	-3.21	103.87	113.25
21	B	807	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
28	J	104	DD6	C8-C6-C5	3.21	123.87	118.94
21	6	908	CLA	C3D-C4D-ND	3.21	115.43	110.24
21	B	831	CLA	C3C-C4C-NC	3.21	114.17	110.57
21	A	818	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
21	A	818	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
21	A	832	CLA	CMA-C3A-C4A	-3.21	103.16	111.77
28	5	712	DD6	C12-C11-C10	-3.21	118.43	122.92
21	13	502	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
21	B	804	CLA	C11-C12-C13	-3.21	105.56	115.92
21	A	841	CLA	O2A-CGA-O1A	-3.21	115.50	123.59
21	3	702	CLA	C1C-C2C-C3C	-3.20	103.59	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	511	CLA	C3B-C4B-NB	3.20	113.35	109.21
21	B	816	CLA	CMA-C3A-C4A	-3.20	103.16	111.77
21	9	903	CLA	CHD-C4C-NC	3.20	129.25	124.20
21	7	703	CLA	O2A-CGA-CBA	3.20	121.96	111.91
21	2	512	CLA	CHD-C4C-NC	3.20	129.25	124.20
21	B	827	CLA	C2A-C1A-CHA	-3.20	118.26	123.86
21	B	833	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
21	A	839	CLA	CMD-C2D-C1D	3.20	130.36	124.71
21	A	839	CLA	CED-O2D-CGD	-3.20	108.69	115.94
21	A	829	CLA	C9-C8-C10	3.20	122.89	111.29
21	12	502	CLA	CED-O2D-CGD	3.20	123.18	115.94
21	A	833	CLA	C4-C3-C5	3.20	120.66	115.27
21	A	821	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
21	B	825	CLA	CHD-C4C-NC	3.20	129.25	124.20
25	A	854	LHG	O4-P-O3	-3.20	92.88	107.75
21	B	826	CLA	CHB-C4A-NA	3.20	128.94	124.51
28	6	916	DD6	C-C1-C2	-3.20	118.44	122.92
21	B	811	CLA	OBD-CAD-C3D	-3.20	120.82	128.52
21	8	610	CLA	C4A-NA-C1A	-3.20	105.27	106.71
21	8	607	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
21	7	714	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
21	1	514	CLA	CHD-C4C-NC	3.20	129.24	124.20
21	A	831	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	A	824	CLA	CAA-C2A-C3A	-3.20	104.03	112.78
21	B	830	CLA	CMD-C2D-C3D	-3.20	120.26	127.61
21	B	836	CLA	CHA-C1A-NA	-3.20	119.08	126.40
21	11	701	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
21	B	814	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
20	A	801	CL0	CHD-C4C-NC	3.19	129.24	124.20
21	A	827	CLA	CHD-C4C-NC	3.19	129.24	124.20
21	A	820	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
21	3	702	CLA	CHB-C4A-NA	3.19	128.93	124.51
21	7	710	CLA	C3D-C2D-C1D	-3.19	101.47	105.83
21	A	807	CLA	C3B-C4B-NB	3.19	113.34	109.21
21	13	501	CLA	CED-O2D-CGD	3.19	123.16	115.94
21	3	702	CLA	CMB-C2B-C3B	3.19	130.65	124.68
21	A	836	CLA	C3B-C4B-NB	3.19	113.33	109.21
21	6	912	CLA	C3B-C4B-NB	3.19	113.33	109.21
21	6	908	CLA	CBC-CAC-C3C	-3.19	103.64	112.43
21	A	827	CLA	C4A-NA-C1A	-3.19	105.27	106.71
20	A	801	CL0	CGD-CBD-CAD	-3.19	100.41	110.73
21	7	705	CLA	C3D-C4D-ND	3.19	115.39	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	518	DD6	C24-C1-C2	3.19	123.83	118.94
21	6	907	CLA	O2A-CGA-CBA	3.19	121.91	111.91
21	B	805	CLA	C3C-C4C-NC	3.19	114.15	110.57
21	3	702	CLA	C1-C2-C3	-3.19	120.53	126.04
21	B	817	CLA	CHD-C4C-NC	3.19	129.22	124.20
21	4	706	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
21	9	902	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
21	10	704	CLA	C2A-C1A-CHA	-3.19	118.29	123.86
21	1	506	CLA	CBC-CAC-C3C	-3.19	103.65	112.43
21	2	507	CLA	CAC-C3C-C4C	3.19	128.94	124.81
21	7	710	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
21	4	706	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
21	1	511	CLA	CAC-C3C-C4C	3.18	128.94	124.81
21	2	514	CLA	C3B-C4B-NB	3.18	113.32	109.21
21	7	714	CLA	CBC-CAC-C3C	-3.18	103.66	112.43
28	8	615	DD6	C7-C6-C5	-3.18	118.47	122.92
25	B	848	LHG	O7-C7-C8	3.18	118.36	111.50
28	1	518	DD6	C7-C6-C5	-3.18	118.47	122.92
21	1	511	CLA	C3B-C4B-NB	3.18	113.32	109.21
21	A	806	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
21	12	504	CLA	C3B-C4B-NB	3.18	113.32	109.21
21	B	804	CLA	CMB-C2B-C3B	3.18	130.63	124.68
21	4	709	CLA	CED-O2D-CGD	3.18	123.13	115.94
21	2	515	CLA	C3B-C4B-NB	3.18	113.32	109.21
21	4	708	CLA	C3B-C4B-NB	3.18	113.32	109.21
21	9	907	CLA	CMA-C3A-C4A	-3.18	103.23	111.77
21	B	816	CLA	CHC-C1C-NC	3.18	129.02	124.20
21	B	820	CLA	CMB-C2B-C3B	3.18	130.62	124.68
21	1	515	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
21	1	510	CLA	CMC-C2C-C1C	3.18	129.88	125.04
21	8	613	CLA	CHD-C4C-NC	3.18	129.21	124.20
21	6	911	CLA	CHC-C1C-NC	3.18	129.02	124.20
28	3	718	DD6	C7-C6-C5	-3.17	118.48	122.92
21	B	825	CLA	C2C-C1C-NC	3.17	112.94	109.97
21	2	515	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
21	6	913	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
24	A	848	BCR	C37-C22-C21	-3.17	118.48	122.92
21	B	804	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
21	A	820	CLA	C3D-C2D-C1D	-3.17	101.50	105.83
21	A	806	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
21	A	833	CLA	C3B-C4B-NB	3.17	113.31	109.21
21	8	604	CLA	CAC-C3C-C4C	3.17	128.92	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	835	CLA	C4A-NA-C1A	-3.17	105.28	106.71
21	7	705	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
21	A	835	CLA	CMD-C2D-C1D	3.17	130.30	124.71
21	B	818	CLA	CAC-C3C-C4C	3.17	128.92	124.81
21	5	706	CLA	C3B-C4B-NB	3.17	113.31	109.21
21	3	705	CLA	C3C-C4C-NC	3.17	114.12	110.57
21	A	834	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
21	9	905	CLA	CAC-C3C-C4C	3.17	128.92	124.81
21	5	710	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
21	5	702	CLA	CMB-C2B-C3B	3.17	130.60	124.68
21	5	706	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
21	10	707	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
21	B	802	CLA	CHC-C1C-NC	3.17	129.01	124.20
21	2	505	CLA	CHD-C1D-ND	-3.17	121.55	124.45
21	6	912	CLA	C3C-C4C-NC	3.17	114.12	110.57
21	8	614	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
21	2	514	CLA	CHB-C4A-NA	3.16	128.89	124.51
21	A	820	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
21	B	808	CLA	CMD-C2D-C1D	3.16	130.29	124.71
21	8	611	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
21	J	101	CLA	C3B-C4B-NB	3.16	113.30	109.21
21	B	832	CLA	CHC-C1C-NC	3.16	129.00	124.20
21	A	831	CLA	CMC-C2C-C1C	3.16	129.86	125.04
21	B	811	CLA	C4A-NA-C1A	-3.16	105.28	106.71
21	2	505	CLA	CHD-C4C-NC	3.16	129.19	124.20
21	6	906	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
21	9	907	CLA	CHD-C4C-NC	3.16	129.18	124.20
21	A	819	CLA	C3B-C4B-NB	3.16	113.30	109.21
21	10	712	CLA	C3B-C4B-NB	3.16	113.30	109.21
21	4	708	CLA	C3C-C4C-NC	3.16	114.11	110.57
21	3	709	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
21	B	825	CLA	C4D-CHA-C1A	-3.16	117.41	121.25
21	A	839	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
21	11	705	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
21	8	603	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
28	11	713	DD6	C-C1-C2	-3.15	118.51	122.92
21	7	712	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
21	F	401	CLA	C6-C5-C3	3.15	128.96	113.58
21	A	838	CLA	CMD-C2D-C1D	3.15	130.27	124.71
21	A	826	CLA	C14-C13-C15	-3.15	99.88	111.29
21	2	514	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
21	A	807	CLA	C1C-C2C-C3C	-3.15	103.64	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	907	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
21	10	707	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
21	2	513	CLA	CAC-C3C-C4C	3.15	128.90	124.81
21	5	704	CLA	C2A-C1A-CHA	-3.15	118.35	123.86
21	7	713	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
21	B	827	CLA	C3B-C4B-NB	3.15	113.28	109.21
21	11	701	CLA	C3B-C4B-NB	3.15	113.28	109.21
21	A	837	CLA	CHB-C4A-NA	3.15	128.87	124.51
21	B	825	CLA	CMA-C3A-C2A	-3.15	101.13	113.83
25	1	521	LHG	O7-C7-C8	3.15	118.28	111.50
21	6	910	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
21	10	707	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
21	9	914	CLA	C3B-C4B-NB	3.15	113.28	109.21
21	9	912	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
21	1	507	CLA	CAC-C3C-C4C	3.15	128.89	124.81
21	6	909	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
21	3	715	CLA	CHC-C1C-C2C	-3.14	118.02	126.72
21	A	843	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
28	1	518	DD6	C4-C3-C2	3.14	129.92	123.47
28	1	519	DD6	C3-C4-C5	3.14	129.91	123.47
21	A	862	CLA	CBC-CAC-C3C	-3.14	103.76	112.43
20	A	801	CL0	C1-C2-C3	-3.14	120.61	126.04
21	4	701	CLA	CAC-C3C-C4C	3.14	128.89	124.81
21	A	814	CLA	C4A-NA-C1A	-3.14	105.29	106.71
21	8	614	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
21	F	404	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
21	B	830	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
21	7	704	CLA	CMB-C2B-C3B	3.14	130.56	124.68
21	2	509	CLA	CBC-CAC-C3C	-3.14	103.77	112.43
21	1	504	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
24	A	852	BCR	C36-C18-C17	-3.14	118.52	122.92
21	3	708	CLA	C3C-C4C-NC	3.14	114.09	110.57
21	B	813	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	13	501	CLA	CAC-C3C-C4C	3.14	128.88	124.81
24	B	845	BCR	C34-C9-C10	-3.14	118.53	122.92
21	2	508	CLA	C3C-C4C-NC	3.14	114.09	110.57
21	A	827	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
28	11	713	DD6	C24-C1-C2	3.14	123.76	118.94
21	9	906	CLA	O2A-CGA-CBA	3.14	121.76	111.91
24	B	846	BCR	C37-C22-C23	3.14	123.02	118.08
21	B	810	CLA	O2A-CGA-CBA	3.14	124.11	114.03
21	5	704	CLA	CHC-C1C-NC	3.14	128.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	517	CLA	CMC-C2C-C1C	3.13	129.81	125.04
21	1	507	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
21	11	710	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
21	3	713	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
21	7	708	CLA	CBC-CAC-C3C	-3.13	103.80	112.43
21	A	834	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
21	A	827	CLA	CHC-C1C-NC	3.13	128.95	124.20
28	8	616	DD6	C3-C4-C5	3.13	129.88	123.47
21	A	839	CLA	C6-C7-C8	-3.13	105.81	115.92
21	2	504	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	B	826	CLA	C4-C3-C5	3.13	120.53	115.27
21	4	709	CLA	C3B-C4B-NB	3.13	113.25	109.21
21	9	904	CLA	C3C-C4C-NC	3.13	114.08	110.57
21	B	831	CLA	C2A-C3A-C4A	-3.13	96.82	101.87
21	B	828	CLA	C4-C3-C5	3.13	120.53	115.27
21	3	704	CLA	CMC-C2C-C1C	3.13	129.80	125.04
21	A	812	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
21	B	808	CLA	CHD-C1D-ND	-3.13	121.58	124.45
21	1	509	CLA	CHC-C1C-C2C	-3.13	118.08	126.72
24	B	843	BCR	C36-C18-C17	-3.12	118.55	122.92
21	4	707	CLA	C1-O2A-CGA	3.12	124.64	116.44
21	A	816	CLA	CHC-C1C-NC	3.12	128.94	124.20
21	B	812	CLA	O2A-CGA-CBA	3.12	121.71	111.91
21	5	708	CLA	CMB-C2B-C3B	3.12	130.52	124.68
21	B	834	CLA	CHC-C1C-NC	3.12	128.94	124.20
21	A	804	CLA	CHD-C4C-NC	3.12	129.12	124.20
21	5	704	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
21	1	501	CLA	CHB-C4A-NA	3.12	128.83	124.51
21	2	509	CLA	CHB-C4A-NA	3.12	128.83	124.51
21	5	707	CLA	C3B-C4B-NB	3.12	113.24	109.21
21	B	810	CLA	C2C-C1C-NC	3.12	112.89	109.97
21	A	811	CLA	CHC-C1C-NC	3.12	128.94	124.20
21	10	707	CLA	C1-O2A-CGA	3.12	124.63	116.44
21	A	809	CLA	C2A-C1A-CHA	-3.12	118.41	123.86
21	9	905	CLA	CMC-C2C-C1C	3.12	129.79	125.04
21	2	516	CLA	C2C-C1C-NC	3.12	112.89	109.97
21	5	704	CLA	C2C-C1C-NC	3.12	112.89	109.97
21	3	707	CLA	C2A-C1A-CHA	-3.12	118.41	123.86
21	9	913	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
21	B	832	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	B	821	CLA	CMA-C3A-C4A	-3.12	103.40	111.77
21	B	837	CLA	CHC-C1C-C2C	-3.12	118.10	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	6	916	DD6	C3-C4-C5	3.11	129.85	123.47
21	B	801	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
21	A	842	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
21	B	831	CLA	C4A-NA-C1A	-3.11	105.31	106.71
21	B	839	CLA	C4A-NA-C1A	-3.11	105.31	106.71
21	6	907	CLA	CHB-C4A-NA	3.11	128.82	124.51
21	3	707	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
28	8	616	DD6	C8-C6-C5	3.11	123.72	118.94
21	9	907	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
21	8	605	CLA	CHC-C1C-NC	3.11	128.93	124.20
21	B	822	CLA	O2A-CGA-O1A	-3.11	115.54	123.30
21	6	906	CLA	CED-O2D-CGD	3.11	122.97	115.94
21	B	837	CLA	O2D-CGD-CBD	3.11	116.80	111.27
21	6	913	CLA	CAC-C3C-C4C	3.11	128.85	124.81
21	B	833	CLA	CMA-C3A-C4A	-3.11	103.42	111.77
21	7	712	CLA	CHD-C4C-NC	3.11	129.10	124.20
21	3	701	CLA	CHC-C1C-NC	3.11	128.92	124.20
21	11	707	CLA	O2D-CGD-CBD	3.11	116.79	111.27
21	A	836	CLA	CAC-C3C-C4C	3.11	128.84	124.81
21	12	501	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
21	2	513	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
21	A	812	CLA	OBD-CAD-C3D	-3.10	121.05	128.52
21	B	808	CLA	CMA-C3A-C4A	-3.10	103.43	111.77
21	4	705	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
21	9	912	CLA	CHD-C4C-NC	3.10	129.09	124.20
21	1	506	CLA	OBD-CAD-C3D	-3.10	121.05	128.52
21	B	818	CLA	C3C-C4C-NC	3.10	114.05	110.57
21	F	401	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
21	A	834	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
21	B	812	CLA	CHC-C1C-NC	3.10	128.91	124.20
21	3	706	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
21	B	810	CLA	CMB-C2B-C3B	3.10	130.48	124.68
21	A	844	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
21	12	508	CLA	C3B-C4B-NB	3.10	113.22	109.21
28	3	718	DD6	C4-C3-C2	3.10	129.82	123.47
21	9	908	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
21	B	834	CLA	C2C-C1C-NC	3.10	112.87	109.97
21	B	835	CLA	C3B-C4B-NB	3.10	113.21	109.21
21	10	703	CLA	C3B-C4B-NB	3.10	113.21	109.21
21	B	834	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
21	A	830	CLA	OBD-CAD-C3D	-3.10	121.07	128.52
21	8	612	CLA	C3C-C4C-NC	3.10	114.04	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	711	CLA	C2A-C1A-CHA	-3.10	118.45	123.86
21	B	803	CLA	O2A-CGA-CBA	3.09	121.62	111.91
21	2	507	CLA	C3B-C4B-NB	3.09	113.21	109.21
21	B	824	CLA	CMA-C3A-C2A	-3.09	101.34	113.83
21	B	834	CLA	C2A-C1A-CHA	-3.09	118.45	123.86
21	12	504	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
21	3	703	CLA	CHB-C4A-NA	3.09	128.79	124.51
21	3	706	CLA	CHB-C4A-NA	3.09	128.79	124.51
24	B	841	BCR	C35-C13-C14	-3.09	118.59	122.92
21	8	607	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
21	6	910	CLA	CBC-CAC-C3C	-3.09	103.90	112.43
21	B	813	CLA	CMD-C2D-C1D	3.09	130.16	124.71
21	7	705	CLA	CAC-C3C-C4C	3.09	128.82	124.81
21	10	709	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
21	A	843	CLA	C1-O2A-CGA	3.09	124.55	116.44
21	A	822	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
21	A	824	CLA	O2D-CGD-CBD	3.09	116.76	111.27
21	12	507	CLA	C3C-C4C-NC	3.09	114.04	110.57
21	B	830	CLA	O1D-CGD-CBD	-3.09	118.16	124.48
21	B	825	CLA	CHB-C4A-NA	3.09	128.78	124.51
21	B	839	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
21	B	819	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
21	10	708	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
21	B	827	CLA	CMA-C3A-C2A	-3.09	101.37	113.83
21	A	803	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
21	2	507	CLA	C3D-C2D-C1D	-3.09	101.62	105.83
21	A	862	CLA	C4-C3-C5	3.09	120.46	115.27
21	9	904	CLA	CED-O2D-CGD	3.09	122.92	115.94
21	A	842	CLA	CMA-C3A-C2A	-3.09	101.38	113.83
21	F	404	CLA	C4A-NA-C1A	-3.09	105.32	106.71
21	6	911	CLA	C1C-C2C-C3C	-3.08	103.71	106.96
21	5	703	CLA	CHD-C4C-NC	3.08	129.06	124.20
21	A	844	CLA	O2A-CGA-CBA	3.08	121.59	111.91
21	2	516	CLA	C3C-C4C-NC	3.08	114.03	110.57
21	A	826	CLA	CMB-C2B-C3B	3.08	130.45	124.68
21	11	710	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
21	6	907	CLA	C1-O2A-CGA	3.08	125.68	116.73
21	B	825	CLA	CHD-C1D-ND	-3.08	121.62	124.45
21	B	826	CLA	CMC-C2C-C1C	3.08	129.73	125.04
21	2	511	CLA	CHD-C4C-NC	3.08	129.06	124.20
21	7	710	CLA	CHD-C1D-ND	-3.08	121.62	124.45
21	1	515	CLA	CMB-C2B-C3B	3.08	130.44	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	906	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
21	13	501	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
21	3	707	CLA	C3B-C4B-NB	3.08	113.19	109.21
21	B	834	CLA	CHD-C4C-NC	3.08	129.05	124.20
21	11	709	CLA	CED-O2D-CGD	3.08	122.90	115.94
21	B	823	CLA	O2A-CGA-CBA	3.08	121.56	111.91
21	10	703	CLA	CAA-C2A-C3A	-3.08	108.92	116.10
21	3	710	CLA	C1-O2A-CGA	3.08	124.51	116.44
21	10	709	CLA	C3B-C4B-NB	3.07	113.19	109.21
21	B	825	CLA	CMB-C2B-C3B	3.07	130.43	124.68
21	10	704	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
21	6	904	CLA	OBD-CAD-C3D	-3.07	121.13	128.52
21	B	827	CLA	CHD-C4C-NC	3.07	129.04	124.20
21	6	904	CLA	CBC-CAC-C3C	-3.07	103.96	112.43
21	1	511	CLA	C4A-NA-C1A	-3.07	105.33	106.71
21	7	708	CLA	C3B-C4B-NB	3.07	113.18	109.21
21	9	911	CLA	CMC-C2C-C1C	3.07	129.71	125.04
21	2	509	CLA	O2D-CGD-CBD	3.07	116.72	111.27
21	11	709	CLA	C3C-C4C-NC	3.07	114.01	110.57
21	B	822	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
21	B	815	CLA	CHC-C1C-NC	3.07	128.86	124.20
21	8	608	CLA	CMC-C2C-C1C	3.07	129.71	125.04
21	A	840	CLA	CHB-C4A-NA	3.07	128.75	124.51
21	F	404	CLA	CBC-CAC-C3C	-3.07	103.97	112.43
21	1	511	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
21	B	814	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
21	7	708	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
21	11	703	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
21	A	818	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
21	B	830	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
21	A	817	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
21	B	835	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
21	8	611	CLA	CHC-C1C-NC	3.07	128.85	124.20
21	5	701	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
21	2	511	CLA	CHC-C1C-NC	3.06	128.85	124.20
21	A	804	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
21	3	715	CLA	CAC-C3C-C4C	3.06	128.79	124.81
21	7	702	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
28	9	915	DD6	C8-C6-C5	3.06	123.64	118.94
28	12	509	DD6	C24-C1-C2	3.06	123.64	118.94
21	6	911	CLA	O2A-CGA-O1A	-3.06	115.66	123.30
21	9	903	CLA	O2A-CGA-CBA	3.06	121.52	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	703	CLA	OBD-CAD-C3D	-3.06	121.15	128.52
21	A	822	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
21	A	841	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
21	A	809	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	1	508	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
21	A	831	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
21	6	913	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
21	A	837	CLA	O2A-CGA-CBA	3.06	123.86	114.03
21	A	839	CLA	CHD-C1D-ND	-3.06	121.64	124.45
21	B	838	CLA	C3D-C4D-ND	3.06	115.18	110.24
21	A	862	CLA	C3B-C4B-NB	3.06	113.16	109.21
21	A	829	CLA	C7-C6-C5	-3.06	105.06	113.36
21	10	710	CLA	CAC-C3C-C4C	3.06	128.78	124.81
21	B	835	CLA	C2C-C1C-NC	3.06	112.83	109.97
21	B	832	CLA	C2A-C1A-CHA	-3.05	118.52	123.86
21	4	704	CLA	CAC-C3C-C4C	3.05	128.77	124.81
21	3	701	CLA	C3B-C4B-NB	3.05	113.16	109.21
21	3	702	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
21	A	825	CLA	CHB-C4A-NA	3.05	128.73	124.51
21	A	804	CLA	C1-C2-C3	-3.05	120.77	126.04
21	A	812	CLA	C2A-C1A-CHA	-3.05	118.52	123.86
21	A	802	CLA	C3B-C4B-NB	3.05	113.16	109.21
21	B	823	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
21	B	808	CLA	O2D-CGD-CBD	3.05	116.69	111.27
21	5	710	CLA	C3B-C4B-NB	3.05	113.15	109.21
21	A	843	CLA	C4A-NA-C1A	-3.05	105.33	106.71
21	B	832	CLA	CAA-C2A-C3A	-3.05	104.43	112.78
28	2	520	DD6	C8-C6-C5	3.05	123.62	118.94
21	9	907	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
21	11	703	CLA	CHD-C4C-NC	3.05	129.00	124.20
21	B	802	CLA	C3C-C4C-NC	3.05	113.99	110.57
21	9	914	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
21	1	516	CLA	C3B-C4B-NB	3.05	113.15	109.21
21	A	834	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
21	9	910	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
21	9	908	CLA	O2D-CGD-CBD	3.04	116.68	111.27
21	A	834	CLA	C3B-C4B-NB	3.04	113.14	109.21
21	4	710	CLA	C3B-C4B-NB	3.04	113.14	109.21
21	2	512	CLA	CAC-C3C-C4C	3.04	128.76	124.81
21	4	709	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
21	B	801	CLA	CAC-C3C-C4C	3.04	128.76	124.81
21	9	904	CLA	CHC-C1C-NC	3.04	128.82	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	702	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
21	11	705	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
21	2	509	CLA	C3B-C4B-NB	3.04	113.14	109.21
21	4	702	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	J	102	BCR	C24-C23-C22	-3.04	121.64	126.23
21	2	503	CLA	CHD-C4C-NC	3.04	128.99	124.20
21	5	709	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
21	A	805	CLA	O2A-CGA-CBA	3.04	121.44	111.91
21	6	909	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
21	2	504	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
24	B	846	BCR	C34-C9-C10	-3.04	118.67	122.92
21	9	908	CLA	O2A-CGA-CBA	3.04	121.43	111.91
21	8	606	CLA	CMB-C2B-C3B	3.03	130.36	124.68
21	A	820	CLA	CAA-C2A-C1A	-3.03	102.03	111.97
21	2	515	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
21	A	862	CLA	O1D-CGD-CBD	-3.03	118.28	124.48
21	6	911	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
21	4	705	CLA	CMC-C2C-C1C	3.03	129.66	125.04
21	B	808	CLA	C3B-C4B-NB	3.03	113.13	109.21
21	B	820	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
21	B	803	CLA	CED-O2D-CGD	-3.03	109.08	115.94
21	B	801	CLA	CHD-C4C-NC	3.03	128.98	124.20
21	7	706	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
21	A	838	CLA	C1-O2A-CGA	3.03	124.39	116.44
21	1	511	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
21	A	806	CLA	CHD-C4C-NC	3.03	128.98	124.20
21	A	816	CLA	CHD-C4C-NC	3.03	128.98	124.20
21	B	829	CLA	CHD-C4C-NC	3.03	128.98	124.20
21	A	832	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
21	5	706	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
21	B	813	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
21	8	607	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
21	7	713	CLA	CAC-C3C-C4C	3.03	128.74	124.81
21	A	819	CLA	CHB-C4A-NA	3.03	128.70	124.51
21	A	824	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
22	A	845	PQN	C7-C8-C9	3.03	124.80	120.19
21	5	707	CLA	C2A-C1A-CHA	-3.03	118.57	123.86
28	2	518	DD6	C23-C16-C22	3.03	111.83	107.37
21	11	706	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
21	8	612	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
21	B	805	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
21	9	903	CLA	C4C-C3C-C2C	-3.02	102.49	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	844	BCR	C34-C9-C8	3.02	122.84	118.08
20	A	801	CL0	CMA-C3A-C2A	-3.02	101.64	113.83
21	F	403	CLA	CHB-C4A-NA	3.02	128.69	124.51
21	5	703	CLA	CBC-CAC-C3C	-3.02	104.10	112.43
21	1	505	CLA	C4A-NA-C1A	-3.02	105.35	106.71
21	B	835	CLA	C1-C2-C3	-3.02	120.83	126.04
21	2	510	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
21	9	910	CLA	C3B-C4B-NB	3.02	113.11	109.21
21	B	833	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
21	3	708	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
21	4	707	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
21	9	904	CLA	CHD-C4C-NC	3.01	128.95	124.20
21	A	823	CLA	C3B-C4B-NB	3.01	113.11	109.21
21	B	801	CLA	CMA-C3A-C4A	-3.01	103.67	111.77
21	6	908	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
21	1	505	CLA	CAC-C3C-C4C	3.01	128.72	124.81
21	A	820	CLA	CMC-C2C-C1C	3.01	129.63	125.04
20	A	801	CL0	C1C-C2C-C3C	-3.01	103.79	106.96
21	5	702	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
21	2	507	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	1	517	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	A	850	BCR	C37-C22-C21	-3.01	118.71	122.92
21	1	506	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
21	B	831	CLA	O2A-C1-C2	3.01	116.54	108.64
21	B	824	CLA	C3D-C2D-C1D	-3.01	101.72	105.83
21	5	702	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
21	8	610	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
21	6	904	CLA	CAC-C3C-C4C	3.01	128.71	124.81
21	5	701	CLA	CAA-C2A-C3A	-3.01	104.54	112.78
21	A	816	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
21	3	703	CLA	C4A-NA-C1A	-3.01	105.35	106.71
21	8	614	CLA	O2D-CGD-CBD	3.01	116.61	111.27
21	2	504	CLA	C3B-C4B-NB	3.01	113.10	109.21
21	2	504	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
21	A	810	CLA	O2D-CGD-CBD	3.01	116.61	111.27
28	4	712	DD6	C-C1-C2	-3.00	118.71	122.92
25	6	917	LHG	O7-C7-C8	3.00	117.97	111.50
21	B	807	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
21	A	812	CLA	CHB-C4A-NA	3.00	128.66	124.51
21	B	806	CLA	CHD-C4C-NC	3.00	128.93	124.20
21	12	507	CLA	CED-O2D-CGD	3.00	122.72	115.94
21	B	825	CLA	CHC-C1C-C2C	-3.00	118.43	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	705	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
21	B	813	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
21	B	838	CLA	C2A-C1A-CHA	-3.00	118.62	123.86
21	3	714	CLA	CHD-C4C-NC	3.00	128.93	124.20
21	10	708	CLA	O1D-CGD-CBD	-3.00	118.35	124.48
21	A	817	CLA	O1D-CGD-CBD	-3.00	118.35	124.48
21	A	841	CLA	CHC-C1C-NC	3.00	128.75	124.20
21	B	814	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
21	A	819	CLA	C1-O2A-CGA	3.00	124.30	116.44
21	A	833	CLA	CHB-C4A-NA	3.00	128.65	124.51
21	A	828	CLA	C3D-C4D-ND	3.00	115.08	110.24
21	B	825	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
21	5	706	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
21	5	710	CLA	CAC-C3C-C4C	3.00	128.70	124.81
21	B	819	CLA	C2A-C1A-CHA	-3.00	118.62	123.86
21	8	603	CLA	C3C-C4C-NC	2.99	113.93	110.57
21	11	706	CLA	CHB-C4A-NA	2.99	128.65	124.51
28	11	713	DD6	C4-C3-C2	2.99	129.61	123.47
21	A	830	CLA	C7-C6-C5	-2.99	105.23	113.36
21	A	802	CLA	C1-O2A-CGA	2.99	124.30	116.44
21	B	823	CLA	C4-C3-C5	2.99	120.31	115.27
20	A	801	CL0	O2A-C1-C2	-2.99	100.77	108.64
21	11	706	CLA	C1-O2A-CGA	2.99	124.29	116.44
24	A	852	BCR	C16-C15-C14	2.99	129.60	123.47
21	A	862	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
21	B	831	CLA	CHD-C1D-ND	-2.99	121.71	124.45
21	2	505	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
21	4	701	CLA	C2A-C1A-CHA	-2.99	118.64	123.85
28	8	615	DD6	C24-C1-C2	2.99	123.53	118.94
21	3	710	CLA	C1C-C2C-C3C	-2.99	103.82	106.96
21	A	814	CLA	CHB-C4A-NA	2.99	128.64	124.51
21	A	822	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	A	845	PQN	C21-C20-C18	-2.98	106.27	115.92
21	A	812	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	7	711	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	5	709	CLA	C2A-C1A-CHA	-2.98	118.64	123.86
21	4	706	CLA	O2A-CGA-CBA	2.98	121.27	111.91
21	9	910	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
21	B	830	CLA	C1-O2A-CGA	2.98	124.27	116.44
21	8	611	CLA	C2A-C1A-CHA	-2.98	118.65	123.86
21	B	814	CLA	O1D-CGD-CBD	-2.98	118.38	124.48
21	4	706	CLA	CAC-C3C-C4C	2.98	128.68	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	512	CLA	CBC-CAC-C3C	-2.98	104.21	112.43
21	1	510	CLA	C4A-NA-C1A	-2.98	105.37	106.71
21	13	502	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
21	B	820	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
21	11	702	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
21	4	702	CLA	CGD-CBD-CAD	-2.98	101.08	110.73
21	11	703	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
21	B	812	CLA	C4A-NA-C1A	-2.98	105.37	106.71
21	2	512	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
21	B	804	CLA	CMC-C2C-C1C	2.98	129.57	125.04
28	6	916	DD6	C14-C13-C11	2.98	130.15	125.53
21	6	906	CLA	CAC-C3C-C4C	2.98	128.67	124.81
20	A	801	CL0	CBC-CAC-C3C	-2.98	104.23	112.43
21	B	808	CLA	CBC-CAC-C3C	-2.98	104.23	112.43
21	11	711	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
21	11	705	CLA	CHB-C4A-NA	2.97	128.62	124.51
21	A	844	CLA	CAC-C3C-C4C	2.97	128.67	124.81
21	11	707	CLA	CAA-C2A-C3A	-2.97	104.63	112.78
21	A	823	CLA	CHC-C1C-NC	2.97	128.71	124.20
21	B	832	CLA	CAA-C2A-C1A	-2.97	102.23	111.97
24	B	846	BCR	C36-C18-C17	-2.97	118.76	122.92
21	5	710	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
21	B	818	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
21	8	608	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
21	2	503	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
21	2	506	CLA	C3C-C4C-NC	2.97	113.90	110.57
21	1	509	CLA	C1-O2A-CGA	2.97	125.36	116.73
21	6	913	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
21	6	914	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
21	3	706	CLA	C1-O2A-CGA	2.97	125.36	116.73
28	5	713	DD6	C-C1-C2	-2.97	118.76	122.92
21	5	701	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
21	A	811	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
21	9	903	CLA	C1D-CHD-C4C	-2.97	119.66	126.06
21	8	605	CLA	CED-O2D-CGD	2.97	122.65	115.94
21	9	908	CLA	CHB-C4A-NA	2.97	128.62	124.51
21	B	830	CLA	O2A-C1-C2	2.97	115.91	108.97
21	1	517	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
21	9	911	CLA	CHD-C4C-NC	2.97	128.88	124.20
21	5	711	CLA	CHB-C4A-NA	2.97	128.62	124.51
21	4	711	CLA	C3B-C4B-NB	2.97	113.05	109.21
21	4	707	CLA	C3C-C4C-NC	2.97	113.90	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	501	CLA	C3B-C4B-NB	2.97	113.04	109.21
21	B	828	CLA	C3B-C4B-NB	2.96	113.04	109.21
21	3	714	CLA	CAA-C2A-C3A	-2.96	104.66	112.78
21	A	826	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
21	4	701	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
21	3	709	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
28	2	519	DD6	C22-C16-C15	2.96	118.04	110.05
21	3	701	CLA	CMA-C3A-C2A	-2.96	109.19	116.10
21	B	819	CLA	CMC-C2C-C1C	2.96	129.55	125.04
21	F	401	CLA	OBD-CAD-C3D	-2.96	121.40	128.52
21	B	801	CLA	CHD-C1D-ND	-2.96	121.73	124.45
21	4	707	CLA	C3B-C4B-NB	2.96	113.03	109.21
21	10	706	CLA	CMC-C2C-C1C	2.96	129.54	125.04
21	A	830	CLA	O2A-CGA-CBA	2.96	121.19	111.91
21	A	843	CLA	C1D-CHD-C4C	-2.96	119.68	126.06
21	11	701	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
21	B	820	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
21	A	817	CLA	CBC-CAC-C3C	-2.96	104.28	112.43
21	3	708	CLA	CHB-C4A-NA	2.96	128.60	124.51
21	4	704	CLA	CHC-C1C-NC	2.96	128.69	124.20
21	2	509	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
21	1	514	CLA	CAC-C3C-C4C	2.96	128.65	124.81
20	A	801	CL0	C2D-C1D-ND	2.96	112.28	110.10
21	7	708	CLA	CAA-CBA-CGA	2.95	121.89	113.25
21	A	813	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
21	10	704	CLA	C1D-CHD-C4C	-2.95	119.69	126.06
21	8	611	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
21	A	805	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
21	4	702	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
21	B	815	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
21	A	837	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
21	8	608	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
21	12	501	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
21	B	830	CLA	O2A-CGA-CBA	2.95	121.17	111.91
21	3	703	CLA	CED-O2D-CGD	2.95	122.61	115.94
21	7	712	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
21	A	806	CLA	CAA-C2A-C1A	-2.95	102.31	111.97
21	8	605	CLA	C3D-C2D-C1D	-2.95	101.81	105.83
21	A	862	CLA	CHD-C1D-ND	-2.95	121.75	124.45
21	8	608	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
21	B	805	CLA	CHD-C4C-NC	2.95	128.84	124.20
21	6	909	CLA	O2D-CGD-CBD	2.94	116.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	905	CLA	O2A-CGA-CBA	2.94	121.14	111.91
21	11	704	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	A	824	CLA	CAC-C3C-C4C	2.94	128.63	124.81
21	5	701	CLA	C3B-C4B-NB	2.94	113.01	109.21
21	5	701	CLA	CHC-C1C-NC	2.94	128.66	124.20
21	A	806	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	A	809	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
21	B	820	CLA	CHD-C4C-NC	2.94	128.83	124.20
21	2	515	CLA	CBC-CAC-C3C	-2.94	104.33	112.43
21	B	830	CLA	CAC-C3C-C4C	2.94	128.62	124.81
21	A	815	CLA	CAA-CBA-CGA	-2.94	104.67	113.25
21	7	710	CLA	O1D-CGD-CBD	-2.94	118.48	124.48
21	2	517	CLA	C3B-C4B-NB	2.94	113.00	109.21
21	B	804	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
21	3	701	CLA	CED-O2D-CGD	2.93	122.57	115.94
21	12	501	CLA	CHD-C4C-NC	2.93	128.83	124.20
21	8	606	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
21	A	837	CLA	C4A-NA-C1A	-2.93	105.39	106.71
21	A	811	CLA	CAC-C3C-C4C	2.93	128.62	124.81
21	A	839	CLA	C3D-C2D-C1D	-2.93	101.83	105.83
28	J	104	DD6	C13-C11-C10	2.93	123.44	118.94
21	A	835	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	1	510	CLA	C3B-C4B-NB	2.93	113.00	109.21
21	8	609	CLA	C3B-C4B-NB	2.93	113.00	109.21
21	A	808	CLA	CMC-C2C-C1C	2.93	129.50	125.04
21	4	707	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
21	A	819	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
21	7	714	CLA	O2A-CGA-CBA	2.93	121.10	111.91
21	B	807	CLA	C3D-C2D-C1D	-2.93	101.83	105.83
21	3	711	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
21	1	514	CLA	C3C-C4C-NC	2.93	113.85	110.57
21	2	516	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	6	908	CLA	CHC-C1C-NC	2.93	128.64	124.20
21	1	511	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	10	706	CLA	C3B-C4B-NB	2.93	112.99	109.21
21	1	508	CLA	CMD-C2D-C3D	-2.93	120.88	127.61
21	5	710	CLA	CHD-C4C-NC	2.93	128.81	124.20
28	3	716	DD6	C9-C10-C11	2.93	131.49	127.31
21	5	703	CLA	C3D-C2D-C1D	-2.93	101.84	105.83
21	3	715	CLA	C3C-C4C-NC	2.93	113.85	110.57
21	3	715	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
21	A	841	CLA	O2A-CGA-CBA	2.93	121.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	825	CLA	O2A-CGA-O1A	-2.92	116.21	123.59
21	2	506	CLA	CAC-C3C-C4C	2.92	128.60	124.81
21	F	403	CLA	CHC-C1C-NC	2.92	128.64	124.20
21	4	706	CLA	C3B-C4B-NB	2.92	112.99	109.21
21	7	710	CLA	CAA-CBA-CGA	-2.92	104.75	112.51
21	B	829	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
21	7	708	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
21	2	512	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
21	6	904	CLA	C3C-C4C-NC	2.92	113.85	110.57
21	9	909	CLA	C3B-C4B-NB	2.92	112.99	109.21
21	B	829	CLA	CMB-C2B-C1B	2.92	132.96	128.46
21	B	824	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	7	704	CLA	CHB-C4A-NA	2.92	128.55	124.51
21	B	804	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
21	B	827	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
21	B	821	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
21	8	607	CLA	O2D-CGD-CBD	2.92	116.45	111.27
21	10	703	CLA	CHC-C1C-NC	2.92	128.63	124.20
21	7	710	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
21	5	709	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
21	B	830	CLA	CHD-C4C-NC	2.92	128.80	124.20
21	3	710	CLA	CHC-C1C-NC	2.92	128.63	124.20
21	B	814	CLA	CMA-C3A-C2A	-2.92	102.06	113.83
21	8	605	CLA	CHD-C4C-NC	2.92	128.80	124.20
21	B	835	CLA	C3C-C4C-NC	2.92	113.84	110.57
21	12	502	CLA	CHD-C4C-NC	2.92	128.80	124.20
21	B	807	CLA	C2C-C1C-NC	2.92	112.70	109.97
21	4	709	CLA	CAC-C3C-C4C	2.91	128.59	124.81
21	B	817	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
21	A	827	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
21	B	810	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
21	B	825	CLA	CHC-C1C-NC	2.91	128.62	124.20
21	B	828	CLA	C4A-NA-C1A	-2.91	105.40	106.71
21	8	612	CLA	CMC-C2C-C1C	2.91	129.48	125.04
21	9	910	CLA	CHC-C1C-NC	2.91	128.62	124.20
21	A	825	CLA	C3D-C4D-ND	2.91	114.95	110.24
21	10	705	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
21	11	708	CLA	C4A-NA-C1A	-2.91	105.40	106.71
21	6	912	CLA	O2A-CGA-CBA	2.91	123.38	114.03
21	A	834	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
21	A	808	CLA	O2D-CGD-CBD	2.91	116.44	111.27
21	9	908	CLA	O2A-CGA-O1A	-2.91	116.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	801	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
21	B	839	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
21	6	913	CLA	CMB-C2B-C3B	2.91	130.12	124.68
21	A	842	CLA	CMA-C3A-C4A	-2.91	103.95	111.77
21	1	508	CLA	C3B-C4B-NB	2.91	112.97	109.21
21	6	911	CLA	CBC-CAC-C3C	-2.91	104.41	112.43
21	B	806	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	B	827	CLA	C6-C7-C8	-2.91	106.52	115.92
21	4	703	CLA	CMB-C2B-C3B	2.91	130.12	124.68
21	1	513	CLA	C1-O2A-CGA	2.91	124.07	116.44
21	6	910	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	A	849	BCR	C15-C16-C17	2.91	129.43	123.47
21	9	905	CLA	C3B-C4B-NB	2.91	112.97	109.21
21	1	505	CLA	CBC-CAC-C3C	-2.90	104.42	112.43
28	12	510	DD6	C22-C16-C17	-2.90	103.94	108.98
21	A	806	CLA	CAA-CBA-CGA	-2.90	104.77	113.25
21	7	707	CLA	O2D-CGD-CBD	2.90	116.43	111.27
21	B	804	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
21	3	702	CLA	CHD-C4C-NC	2.90	128.78	124.20
21	B	832	CLA	C1-C2-C3	-2.90	121.03	126.04
21	A	842	CLA	CHD-C4C-NC	2.90	128.77	124.20
21	1	505	CLA	CHC-C1C-NC	2.90	128.60	124.20
21	B	820	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
21	J	101	CLA	O1D-CGD-CBD	2.90	130.42	124.48
21	6	909	CLA	CMA-C3A-C2A	-2.90	102.13	113.83
24	B	842	BCR	C19-C18-C17	2.90	123.39	118.94
21	A	843	CLA	C2C-C1C-NC	2.90	112.69	109.97
21	2	503	CLA	C3B-C4B-NB	2.90	112.96	109.21
21	3	703	CLA	CMD-C2D-C3D	-2.90	120.95	127.61
21	2	512	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
21	5	710	CLA	C1-O2A-CGA	2.90	124.05	116.44
21	2	515	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	A	829	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
21	A	839	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
21	1	505	CLA	CMB-C2B-C3B	2.90	130.10	124.68
21	1	507	CLA	CED-O2D-CGD	2.90	122.49	115.94
21	2	515	CLA	O2A-CGA-CBA	2.90	123.33	114.03
21	1	513	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
28	11	712	DD6	C3-C4-C5	2.89	129.40	123.47
21	7	707	CLA	CHC-C1C-NC	2.89	128.59	124.20
21	3	706	CLA	C4A-NA-C1A	-2.89	105.41	106.71
21	A	812	CLA	C11-C12-C13	-2.89	106.57	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	504	CLA	O2A-CGA-CBA	2.89	120.98	111.91
21	9	903	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
21	1	512	CLA	C3B-C4B-NB	2.89	112.95	109.21
21	9	903	CLA	CED-O2D-CGD	2.89	122.48	115.94
21	9	907	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
21	11	708	CLA	CMC-C2C-C1C	2.89	129.44	125.04
21	A	838	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
21	8	612	CLA	C1-C2-C3	-2.89	121.04	126.04
21	3	709	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
21	11	708	CLA	CHB-C4A-NA	2.89	128.51	124.51
21	4	709	CLA	CMC-C2C-C1C	2.89	129.44	125.04
21	5	705	CLA	CHD-C4C-NC	2.89	128.76	124.20
21	B	802	CLA	O2A-CGA-CBA	2.89	120.98	111.91
21	9	902	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
21	B	803	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
21	11	702	CLA	CMC-C2C-C1C	2.89	129.44	125.04
21	2	505	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
21	A	813	CLA	C1-O2A-CGA	2.89	124.02	116.44
21	2	504	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
21	1	504	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
21	A	823	CLA	CMC-C2C-C1C	2.89	129.44	125.04
21	12	508	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
21	4	709	CLA	CBC-CAC-C3C	-2.89	104.47	112.43
21	11	705	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
21	13	501	CLA	O1D-CGD-CBD	-2.89	118.58	124.48
21	A	830	CLA	C11-C10-C8	-2.89	106.59	115.92
21	F	403	CLA	C3B-C4B-NB	2.89	112.94	109.21
21	A	819	CLA	C3C-C4C-NC	2.89	113.81	110.57
21	9	902	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
21	5	705	CLA	CMC-C2C-C1C	2.89	129.43	125.04
21	1	512	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
21	6	909	CLA	CMB-C2B-C3B	2.89	130.08	124.68
28	12	510	DD6	C24-C1-C2	2.88	123.37	118.94
21	11	702	CLA	CHB-C4A-NA	2.88	128.50	124.51
21	12	506	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
21	5	704	CLA	C1D-CHD-C4C	-2.88	119.83	126.06
21	A	844	CLA	CHC-C1C-NC	2.88	128.58	124.20
24	B	842	BCR	C12-C13-C14	2.88	123.37	118.94
21	8	604	CLA	CHB-C4A-NA	2.88	128.50	124.51
21	B	831	CLA	C11-C10-C8	-2.88	106.60	115.92
21	6	903	CLA	O2A-CGA-CBA	2.88	120.95	111.91
21	12	501	CLA	CAC-C3C-C4C	2.88	128.55	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	809	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	A	837	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	B	810	CLA	O2A-CGA-O1A	-2.88	116.12	123.30
21	8	607	CLA	O2A-CGA-O1A	-2.88	116.32	123.59
21	11	702	CLA	CAC-C3C-C4C	2.88	128.55	124.81
21	A	807	CLA	CHC-C1C-NC	2.88	128.57	124.20
21	4	703	CLA	CMC-C2C-C1C	2.88	129.42	125.04
21	B	830	CLA	C3B-C4B-NB	2.88	112.93	109.21
21	9	912	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
21	1	505	CLA	CHB-C4A-NA	2.88	128.49	124.51
21	3	710	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
21	13	503	CLA	O2A-CGA-CBA	2.88	120.93	111.91
21	8	609	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	3	709	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
21	A	826	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
21	9	912	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
21	3	706	CLA	CAA-CBA-CGA	2.88	121.66	113.25
21	2	513	CLA	C3B-C4B-NB	2.88	112.93	109.21
21	A	808	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
21	B	802	CLA	CHD-C4C-NC	2.87	128.73	124.20
21	F	403	CLA	CHD-C4C-NC	2.87	128.73	124.20
21	B	809	CLA	C2A-C1A-CHA	-2.87	118.83	123.86
21	B	837	CLA	C2A-C1A-CHA	-2.87	118.83	123.86
21	9	905	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
21	5	706	CLA	CMB-C2B-C3B	2.87	130.05	124.68
21	A	840	CLA	CMB-C2B-C3B	2.87	130.05	124.68
21	5	708	CLA	C4A-NA-C1A	-2.87	105.42	106.71
21	9	909	CLA	CMB-C2B-C3B	2.87	130.05	124.68
21	6	907	CLA	CHC-C1C-NC	2.87	128.56	124.20
21	B	835	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
21	F	404	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
21	A	831	CLA	CMA-C3A-C2A	-2.87	102.26	113.83
21	A	807	CLA	CHB-C4A-NA	2.87	128.48	124.51
21	6	914	CLA	CHB-C4A-NA	2.87	128.48	124.51
21	8	605	CLA	CHB-C4A-NA	2.87	128.48	124.51
21	A	815	CLA	CMC-C2C-C1C	2.87	129.40	125.04
21	A	824	CLA	OBD-CAD-C3D	-2.87	121.62	128.52
21	3	711	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
21	B	828	CLA	CMC-C2C-C1C	2.86	129.40	125.04
21	A	819	CLA	C4A-NA-C1A	-2.86	105.42	106.71
21	7	704	CLA	C4A-NA-C1A	-2.86	105.42	106.71
21	A	814	CLA	CHC-C1C-C2C	-2.86	118.80	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	905	CLA	CHB-C4A-NA	2.86	128.47	124.51
21	B	816	CLA	C9-C8-C7	-2.86	100.92	111.29
21	B	819	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
21	1	514	CLA	CMC-C2C-C1C	2.86	129.40	125.04
21	B	812	CLA	C6-C7-C8	-2.86	106.67	115.92
21	A	804	CLA	C4-C3-C5	2.86	120.09	115.27
21	2	508	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
21	A	819	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
21	B	810	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
24	A	848	BCR	C20-C21-C22	2.86	131.39	127.31
21	2	511	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
21	8	604	CLA	C4A-NA-C1A	-2.86	105.42	106.71
21	3	705	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	2	512	CLA	O2A-CGA-CBA	2.86	120.88	111.91
21	11	703	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
21	5	705	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
21	B	839	CLA	C3C-C4C-NC	2.86	113.78	110.57
21	1	515	CLA	C3C-C4C-NC	2.86	113.78	110.57
21	A	808	CLA	C4-C3-C5	2.86	119.25	115.98
21	8	608	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
21	7	714	CLA	CAA-C2A-C1A	2.86	121.34	111.97
25	A	854	LHG	O6-P-O5	-2.86	97.90	109.07
21	4	709	CLA	CHD-C4C-NC	2.86	128.70	124.20
21	A	802	CLA	CMA-C3A-C2A	-2.86	102.31	113.83
21	3	702	CLA	C2A-C1A-CHA	-2.86	118.87	123.86
21	5	706	CLA	CHC-C1C-NC	2.86	128.53	124.20
21	A	836	CLA	O2A-CGA-CBA	2.85	120.87	111.91
21	B	837	CLA	C2C-C1C-NC	2.85	112.65	109.97
21	3	709	CLA	CHD-C4C-NC	2.85	128.70	124.20
21	12	506	CLA	CHD-C4C-NC	2.85	128.70	124.20
21	12	504	CLA	CHD-C4C-NC	2.85	128.70	124.20
21	7	711	CLA	CHC-C1C-NC	2.85	128.53	124.20
21	B	802	CLA	O2D-CGD-CBD	2.85	116.34	111.27
21	A	802	CLA	CHA-C1A-NA	-2.85	119.87	126.40
21	7	712	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
21	12	505	CLA	C1-O2A-CGA	2.85	125.02	116.73
21	8	603	CLA	CHB-C4A-NA	2.85	128.45	124.51
21	2	509	CLA	O2A-CGA-CBA	2.85	120.85	111.91
21	8	613	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
21	6	903	CLA	CED-O2D-CGD	2.85	122.38	115.94
21	1	506	CLA	CHC-C1C-NC	2.85	128.53	124.20
21	B	806	CLA	CHB-C4A-NA	2.85	128.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	515	CLA	CHD-C4C-NC	2.85	128.69	124.20
21	8	605	CLA	CMC-C2C-C1C	2.85	129.38	125.04
21	1	510	CLA	CHB-C4A-NA	2.85	128.45	124.51
21	11	711	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
21	4	707	CLA	CHD-C4C-NC	2.85	128.69	124.20
21	9	907	CLA	C3B-C4B-NB	2.85	112.89	109.21
21	8	613	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
21	A	842	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
21	B	817	CLA	C4A-NA-C1A	-2.84	105.43	106.71
21	B	825	CLA	O2A-CGA-CBA	2.84	120.83	111.91
21	B	804	CLA	C1D-CHD-C4C	-2.84	119.92	126.06
21	12	506	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
21	A	840	CLA	CAA-C2A-C1A	2.84	121.29	111.97
21	B	813	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
21	A	842	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
21	11	706	CLA	C4-C3-C5	2.84	120.05	115.27
21	B	807	CLA	CMA-C3A-C2A	-2.84	102.36	113.83
21	2	506	CLA	CHC-C1C-NC	2.84	128.52	124.20
21	7	706	CLA	CHB-C4A-NA	2.84	128.44	124.51
28	12	510	DD6	C-C1-C2	-2.84	118.94	122.92
21	B	805	CLA	C4A-NA-C1A	-2.84	105.43	106.71
21	6	905	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
21	F	404	CLA	CHB-C4A-NA	2.84	128.44	124.51
21	11	711	CLA	CMC-C2C-C1C	2.84	129.37	125.04
21	11	704	CLA	CMC-C2C-C1C	2.84	129.37	125.04
21	A	833	CLA	C7-C6-C5	-2.84	105.65	113.36
21	A	833	CLA	O1A-CGA-CBA	-2.84	112.66	123.73
21	A	833	CLA	C1D-CHD-C4C	-2.84	119.93	126.06
21	A	810	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
21	12	507	CLA	CHB-C4A-NA	2.84	128.44	124.51
21	10	711	CLA	O1D-CGD-CBD	-2.84	118.68	124.48
21	A	815	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
21	A	822	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
21	B	836	CLA	O2A-CGA-CBA	2.84	120.81	111.91
21	B	810	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
21	A	803	CLA	C3B-C4B-NB	2.84	112.88	109.21
21	1	506	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
21	A	827	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	A	811	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
28	9	915	DD6	C4-C3-C2	2.83	129.28	123.47
21	2	508	CLA	CAC-C3C-C4C	2.83	128.49	124.81
21	5	705	CLA	C3B-C4B-NB	2.83	112.87	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	712	DD6	C23-C16-C17	2.83	113.90	108.98
21	9	906	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
21	4	704	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
21	B	819	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	1	505	CLA	C3C-C4C-NC	2.83	113.75	110.57
24	B	844	BCR	C27-C26-C25	-2.83	118.62	122.73
21	A	840	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
21	A	844	CLA	C3B-C4B-NB	2.83	112.87	109.21
21	7	702	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	3	704	CLA	CMB-C2B-C3B	2.83	129.97	124.68
21	B	832	CLA	CHB-C4A-NA	2.83	128.42	124.51
21	A	840	CLA	C1D-CHD-C4C	-2.83	119.96	126.06
21	B	802	CLA	CAC-C3C-C4C	2.83	128.48	124.81
21	7	713	CLA	C1-O2A-CGA	2.83	124.94	116.73
21	5	709	CLA	CHC-C1C-NC	2.83	128.49	124.20
21	B	813	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
21	5	711	CLA	CED-O2D-CGD	2.83	122.33	115.94
21	2	504	CLA	CMC-C2C-C1C	2.83	129.34	125.04
21	B	806	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
21	A	842	CLA	C3C-C4C-NC	2.82	113.74	110.57
21	A	839	CLA	CHB-C4A-NA	2.82	128.42	124.51
21	13	503	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
21	9	906	CLA	CMC-C2C-C1C	2.82	129.34	125.04
21	1	515	CLA	C2C-C1C-NC	2.82	112.62	109.97
21	6	907	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
21	B	834	CLA	C3A-C2A-C1A	-2.82	97.11	101.34
21	B	813	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
21	B	832	CLA	OBD-CAD-C3D	-2.82	121.74	128.52
21	11	705	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
21	1	507	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
21	A	805	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
21	A	819	CLA	CHA-C1A-NA	-2.82	119.95	126.40
21	7	705	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
21	9	902	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
21	B	832	CLA	CHD-C4C-NC	2.82	128.64	124.20
21	8	605	CLA	C2A-C1A-CHA	-2.82	118.94	123.86
21	2	506	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
28	2	518	DD6	C4-C3-C2	2.82	129.24	123.47
21	A	810	CLA	OBD-CAD-C3D	-2.82	121.75	128.52
21	4	703	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
21	6	907	CLA	CBC-CAC-C3C	-2.81	104.67	112.43
21	A	807	CLA	C4-C3-C2	-2.81	116.46	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	818	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
21	B	839	CLA	O2A-CGA-CBA	2.81	120.74	111.91
21	B	806	CLA	O2A-CGA-CBA	2.81	120.74	111.91
21	1	512	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	A	804	CLA	OBD-CAD-C3D	-2.81	121.75	128.52
28	8	615	DD6	C8-C6-C5	2.81	123.26	118.94
21	5	708	CLA	CHD-C4C-NC	2.81	128.63	124.20
21	7	705	CLA	CHD-C4C-NC	2.81	128.63	124.20
21	7	707	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
21	7	714	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
21	A	809	CLA	CMA-C3A-C2A	-2.81	102.49	113.83
21	8	609	CLA	O2A-CGA-CBA	2.81	120.73	111.91
21	1	501	CLA	CAC-C3C-C4C	2.81	128.46	124.81
21	A	836	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
21	3	709	CLA	C3B-C4B-NB	2.81	112.84	109.21
21	2	506	CLA	O2D-CGD-CBD	2.81	116.25	111.27
25	9	917	LHG	O7-C7-C8	2.81	117.55	111.50
24	A	850	BCR	C34-C9-C10	-2.81	118.99	122.92
21	1	510	CLA	CHD-C4C-NC	2.81	128.62	124.20
21	8	606	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	B	833	CLA	CHC-C1C-NC	2.81	128.46	124.20
21	A	811	CLA	CMA-C3A-C2A	-2.80	102.51	113.83
21	8	603	CLA	C2A-C1A-CHA	-2.80	118.95	123.86
21	5	702	CLA	CHD-C4C-NC	2.80	128.62	124.20
21	9	905	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
21	A	843	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
21	11	702	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
21	3	712	CLA	CGD-CBD-CAD	-2.80	101.67	110.73
21	A	810	CLA	C1D-CHD-C4C	-2.80	120.02	126.06
21	B	815	CLA	CMD-C2D-C1D	2.80	129.65	124.71
21	4	703	CLA	CHB-C4A-NA	2.80	128.38	124.51
28	12	509	DD6	C7-C6-C5	-2.80	119.00	122.92
21	A	836	CLA	C1-O2A-CGA	2.80	123.79	116.44
21	2	517	CLA	CED-O2D-CGD	2.80	122.27	115.94
21	1	512	CLA	CHC-C1C-NC	2.80	128.45	124.20
21	8	609	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
21	2	510	CLA	CED-O2D-CGD	-2.80	109.61	115.94
21	2	512	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
21	F	404	CLA	C3B-C4B-NB	2.80	112.83	109.21
21	2	512	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	B	841	BCR	C36-C18-C17	-2.80	119.01	122.92
21	8	603	CLA	C1-O2A-CGA	2.80	124.85	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	832	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
21	A	806	CLA	C3D-C2D-C1D	-2.80	102.02	105.83
21	A	821	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
21	7	708	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
21	A	819	CLA	CHC-C1C-NC	2.79	128.44	124.20
21	A	808	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
21	2	505	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
21	B	806	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
21	A	813	CLA	CHD-C4C-NC	2.79	128.61	124.20
21	5	711	CLA	C4A-NA-C1A	-2.79	105.45	106.71
21	A	812	CLA	CHC-C1C-NC	2.79	128.44	124.20
21	B	811	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
21	8	612	CLA	CHC-C1C-NC	2.79	128.44	124.20
21	1	517	CLA	CHD-C4C-NC	2.79	128.60	124.20
21	7	702	CLA	O2D-CGD-CBD	2.79	116.23	111.27
21	B	816	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
24	A	849	BCR	C10-C11-C12	2.79	131.93	123.22
21	12	505	CLA	O2A-CGA-CBA	2.79	120.66	111.91
21	5	707	CLA	C3C-C4C-NC	2.79	113.70	110.57
21	3	715	CLA	CHC-C1C-NC	2.79	128.44	124.20
21	7	702	CLA	CAA-C2A-C1A	-2.79	102.83	111.97
21	A	841	CLA	C3D-C4D-ND	2.79	114.75	110.24
21	B	821	CLA	CHC-C1C-NC	2.79	128.43	124.20
21	8	611	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
21	13	503	CLA	CMB-C2B-C3B	2.79	129.89	124.68
21	6	907	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
21	12	502	CLA	CHB-C4A-NA	2.79	128.37	124.51
21	A	827	CLA	CAA-C2A-C1A	-2.79	102.84	111.97
21	F	401	CLA	CMB-C2B-C1B	2.79	132.75	128.46
24	B	846	BCR	C37-C22-C21	-2.79	119.02	122.92
21	A	839	CLA	CAC-C3C-C4C	2.79	128.43	124.81
21	2	513	CLA	CHD-C4C-NC	2.79	128.59	124.20
28	11	712	DD6	C-C1-C2	-2.79	119.02	122.92
21	B	811	CLA	C1D-CHD-C4C	-2.79	120.05	126.06
21	A	816	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
21	1	508	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
21	B	815	CLA	C4-C3-C5	2.79	119.96	115.27
21	A	804	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
21	B	803	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
28	1	520	DD6	C8-C6-C5	2.79	123.22	118.94
21	A	821	CLA	CMC-C2C-C1C	2.78	129.28	125.04
21	A	812	CLA	O2A-CGA-O1A	-2.78	116.56	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	511	CLA	CED-O2D-CGD	2.78	122.23	115.94
21	A	844	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
21	1	515	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
21	A	841	CLA	O1D-CGD-CBD	-2.78	118.79	124.48
21	3	702	CLA	CMC-C2C-C1C	2.78	129.28	125.04
21	4	707	CLA	CMA-C3A-C2A	-2.78	102.61	113.83
21	3	703	CLA	CHD-C4C-NC	2.78	128.59	124.20
21	A	839	CLA	C4A-NA-C1A	-2.78	105.46	106.71
28	6	915	DD6	C3-C4-C5	2.78	129.17	123.47
21	10	709	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	5	702	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
21	A	822	CLA	CMA-C3A-C2A	-2.78	102.62	113.83
21	11	702	CLA	C4-C3-C5	2.78	119.94	115.27
21	1	507	CLA	O2D-CGD-CBD	2.77	116.20	111.27
21	4	710	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
21	4	704	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
21	7	709	CLA	CHC-C1C-NC	2.77	128.41	124.20
21	8	608	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
21	A	809	CLA	CHD-C4C-NC	2.77	128.57	124.20
21	3	704	CLA	C1D-CHD-C4C	-2.77	120.08	126.06
21	8	610	CLA	C3B-C4B-NB	2.77	112.80	109.21
21	8	612	CLA	C3B-C4B-NB	2.77	112.80	109.21
21	A	834	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
21	11	709	CLA	CHC-C1C-NC	2.77	128.41	124.20
21	11	710	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
21	5	706	CLA	CAC-C3C-C4C	2.77	128.41	124.81
21	A	819	CLA	CMA-C3A-C4A	-2.77	104.32	111.77
21	B	819	CLA	C1-O2A-CGA	2.77	124.78	116.73
21	6	907	CLA	O1D-CGD-CBD	-2.77	118.82	124.48
21	2	508	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
21	8	604	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
21	B	817	CLA	C5-C3-C2	-2.77	115.52	121.12
21	B	836	CLA	C3B-C4B-NB	2.77	112.79	109.21
21	12	505	CLA	CBC-CAC-C3C	-2.77	104.80	112.43
21	1	506	CLA	O2A-CGA-O1A	-2.77	116.40	123.30
21	B	824	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
21	8	608	CLA	CHD-C4C-NC	2.77	128.56	124.20
21	B	829	CLA	OBD-CAD-C3D	-2.77	121.86	128.52
21	1	510	CLA	O2D-CGD-CBD	2.77	116.18	111.27
21	A	821	CLA	C2C-C1C-NC	2.77	112.56	109.97
24	A	851	BCR	C31-C1-C6	-2.77	105.81	110.30
21	6	908	CLA	C1B-CHB-C4A	-2.77	124.64	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	503	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
21	3	702	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
21	12	502	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
28	1	520	DD6	C13-C11-C10	2.76	123.18	118.94
21	A	805	CLA	CHD-C4C-NC	2.76	128.56	124.20
21	9	911	CLA	C3B-C4B-NB	2.76	112.78	109.21
21	B	822	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
21	12	502	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
21	1	504	CLA	CMB-C2B-C3B	2.76	129.84	124.68
21	A	805	CLA	CAC-C3C-C4C	2.76	128.39	124.81
21	A	804	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
21	A	806	CLA	C4A-NA-C1A	-2.76	105.47	106.71
21	A	822	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
21	7	709	CLA	C4D-CHA-C1A	-2.76	117.89	121.25
21	6	908	CLA	CHB-C4A-NA	2.76	128.33	124.51
21	B	805	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
21	A	829	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
22	B	840	PQN	C7-C8-C9	2.76	124.39	120.19
21	B	809	CLA	CHB-C4A-NA	2.76	128.33	124.51
21	1	505	CLA	C3B-C4B-NB	2.76	112.77	109.21
24	J	103	BCR	C16-C15-C14	2.76	129.12	123.47
21	B	835	CLA	CMA-C3A-C2A	-2.76	102.71	113.83
21	1	513	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
21	10	711	CLA	CAC-C3C-C4C	2.76	128.38	124.81
21	B	814	CLA	C3B-C4B-NB	2.75	112.77	109.21
21	J	101	CLA	C2C-C1C-NC	2.75	112.55	109.97
21	B	807	CLA	CHD-C4C-NC	2.75	128.54	124.20
21	3	705	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
20	A	801	CL0	C1B-CHB-C4A	-2.75	124.66	130.12
21	B	809	CLA	CED-O2D-CGD	2.75	122.17	115.94
21	B	837	CLA	OBD-CAD-C3D	-2.75	121.89	128.52
21	5	707	CLA	CMA-C3A-C2A	-2.75	102.72	113.83
21	A	833	CLA	CMC-C2C-C1C	2.75	129.23	125.04
21	3	702	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
21	4	709	CLA	CMB-C2B-C3B	2.75	129.83	124.68
21	3	709	CLA	CHB-C4A-NA	2.75	128.32	124.51
21	8	613	CLA	CHB-C4A-NA	2.75	128.32	124.51
21	3	710	CLA	CMC-C2C-C1C	2.75	129.23	125.04
21	B	805	CLA	C2C-C1C-NC	2.75	112.55	109.97
21	A	809	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
21	4	707	CLA	CED-O2D-CGD	2.75	122.15	115.94
21	B	810	CLA	CHC-C1C-NC	2.75	128.37	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	817	CLA	CAA-C2A-C1A	-2.75	102.97	111.97
21	B	834	CLA	CHA-C1A-NA	-2.75	120.11	126.40
21	7	711	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
27	B	847	DGD	O2G-C1B-C2B	2.75	117.42	111.50
21	A	808	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
21	10	704	CLA	C4A-NA-C1A	-2.74	105.47	106.71
21	B	820	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
21	4	705	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
21	5	708	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
21	B	812	CLA	CAA-C2A-C3A	-2.74	105.26	112.78
21	1	508	CLA	C1-O2A-CGA	2.74	124.70	116.73
21	8	608	CLA	C3B-C4B-NB	2.74	112.76	109.21
21	A	807	CLA	O1A-CGA-CBA	-2.74	113.03	123.73
21	10	710	CLA	C3B-C4B-NB	2.74	112.76	109.21
21	2	510	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
21	B	834	CLA	O1D-CGD-CBD	-2.74	118.87	124.48
21	A	809	CLA	C3B-C4B-NB	2.74	112.75	109.21
21	F	403	CLA	CED-O2D-CGD	-2.74	109.74	115.94
21	B	808	CLA	CHD-C4C-NC	2.74	128.52	124.20
21	4	709	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
21	B	825	CLA	CBA-CAA-C2A	-2.74	105.78	113.86
21	3	708	CLA	CMB-C2B-C3B	2.74	129.80	124.68
21	1	511	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
21	A	831	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
21	10	705	CLA	CHB-C4A-NA	2.74	128.30	124.51
21	B	815	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
21	5	707	CLA	OBD-CAD-C3D	-2.74	121.93	128.52
21	11	703	CLA	C3B-C4B-NB	2.74	112.75	109.21
21	A	811	CLA	C2C-C1C-NC	2.74	112.53	109.97
21	A	824	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
21	7	704	CLA	CHD-C4C-NC	2.74	128.51	124.20
21	B	808	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
21	6	907	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
21	1	507	CLA	C3C-C4C-NC	2.73	113.64	110.57
21	4	702	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
21	4	706	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
21	4	706	CLA	C1-O2A-CGA	2.73	124.67	116.73
21	B	821	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
21	B	806	CLA	CMD-C2D-C3D	-2.73	121.33	127.61
21	11	701	CLA	CHB-C4A-NA	2.73	128.29	124.51
21	A	811	CLA	CHD-C4C-NC	2.73	128.51	124.20
21	B	813	CLA	C1C-C2C-C3C	-2.73	104.09	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	710	CLA	O2D-CGD-CBD	2.73	116.12	111.27
21	J	101	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
21	10	711	CLA	CHD-C4C-NC	2.73	128.50	124.20
21	B	826	CLA	C1-C2-C3	-2.73	121.33	126.04
21	8	608	CLA	C1-O2A-CGA	2.73	124.65	116.73
21	A	806	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
21	11	707	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
21	4	709	CLA	O1D-CGD-CBD	-2.72	118.91	124.48
21	A	816	CLA	O2A-CGA-CBA	2.72	122.78	114.03
21	B	835	CLA	O2A-CGA-CBA	2.72	120.45	111.91
21	6	908	CLA	CHD-C4C-NC	2.72	128.50	124.20
21	1	509	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
21	12	501	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
21	13	503	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
21	B	805	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
21	B	803	CLA	C1-O2A-CGA	2.72	123.58	116.44
21	2	508	CLA	C4A-NA-C1A	-2.72	105.48	106.71
21	3	708	CLA	CHC-C1C-NC	2.72	128.33	124.20
21	6	912	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
21	1	501	CLA	C3B-C4B-NB	2.72	112.73	109.21
21	7	708	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
21	B	819	CLA	C3B-C4B-NB	2.72	112.72	109.21
24	B	844	BCR	C35-C13-C14	-2.72	119.11	122.92
21	B	839	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
21	A	862	CLA	C7-C6-C5	-2.72	105.98	113.36
24	B	843	BCR	C35-C13-C14	-2.72	119.12	122.92
21	F	401	CLA	CHD-C4C-NC	2.72	128.48	124.20
21	7	712	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
21	3	706	CLA	O1D-CGD-CBD	-2.72	118.93	124.48
21	10	705	CLA	CMC-C2C-C1C	2.71	129.17	125.04
21	B	816	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
21	4	703	CLA	C4A-NA-C1A	-2.71	105.49	106.71
21	B	811	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
21	8	605	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
21	A	832	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
21	8	612	CLA	CHD-C4C-NC	2.71	128.48	124.20
21	A	833	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
21	B	801	CLA	O2A-CGA-CBA	2.71	120.42	111.91
21	5	702	CLA	C3C-C4C-NC	2.71	113.61	110.57
21	A	830	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
21	9	906	CLA	C3B-C4B-NB	2.71	112.71	109.21
21	B	826	CLA	O2A-CGA-CBA	2.71	120.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	101	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
21	5	711	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
21	11	711	CLA	C3B-C4B-NB	2.71	112.71	109.21
21	A	828	CLA	C2C-C1C-NC	2.71	112.51	109.97
21	7	709	CLA	C3B-C4B-NB	2.71	112.71	109.21
21	11	707	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
21	10	708	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
21	B	839	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
28	9	916	DD6	C26-C25-C24	2.71	131.66	123.22
21	7	710	CLA	C2C-C1C-NC	2.71	112.51	109.97
21	B	834	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
21	F	401	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
21	13	503	CLA	CHB-C4A-NA	2.71	128.25	124.51
21	1	515	CLA	CBC-CAC-C3C	-2.71	104.97	112.43
21	B	814	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
21	A	809	CLA	C3A-C2A-C1A	-2.70	97.29	101.34
21	9	911	CLA	O2A-CGA-CBA	2.70	120.39	111.91
21	3	708	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
21	11	705	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
21	A	807	CLA	CHD-C4C-NC	2.70	128.46	124.20
21	4	705	CLA	O1D-CGD-CBD	-2.70	118.95	124.48
21	7	710	CLA	CMA-C3A-C4A	-2.70	104.51	111.77
21	1	512	CLA	CHB-C4A-NA	2.70	128.25	124.51
21	5	710	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
21	12	504	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
21	1	506	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
21	10	710	CLA	CHC-C1C-NC	2.70	128.30	124.20
24	B	844	BCR	C29-C30-C25	2.70	114.64	110.48
21	13	503	CLA	CHC-C1C-NC	2.70	128.30	124.20
21	9	911	CLA	C3C-C4C-NC	2.70	113.60	110.57
21	B	803	CLA	CMB-C2B-C1B	2.70	132.61	128.46
21	2	503	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	B	812	CLA	CHA-C1A-NA	-2.70	120.22	126.40
21	A	826	CLA	C1-C2-C3	-2.70	121.38	126.04
21	8	611	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	1	505	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
21	A	817	CLA	OBD-CAD-C3D	-2.69	122.04	128.52
21	13	501	CLA	CHD-C4C-NC	2.69	128.45	124.20
21	A	815	CLA	CMA-C3A-C4A	-2.69	104.53	111.77
21	A	815	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
21	11	701	CLA	CMB-C2B-C3B	2.69	129.72	124.68
21	A	834	CLA	CHC-C1C-NC	2.69	128.29	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	703	CLA	CHD-C4C-NC	2.69	128.44	124.20
21	B	806	CLA	CBC-CAC-C3C	-2.69	105.01	112.43
21	A	824	CLA	C2C-C1C-NC	2.69	112.49	109.97
21	1	516	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	1	517	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
21	B	816	CLA	C7-C6-C5	-2.69	106.05	113.36
21	A	832	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
21	6	911	CLA	CMB-C2B-C3B	2.69	129.71	124.68
21	4	710	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
21	8	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
21	4	707	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	A	804	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
21	3	704	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
21	7	707	CLA	C3B-C4B-NB	2.69	112.68	109.21
21	B	837	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
21	A	834	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	11	702	CLA	C1-O2A-CGA	2.69	123.49	116.44
21	A	819	CLA	CBA-CAA-C2A	2.69	121.79	113.86
21	12	504	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
21	6	908	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
21	9	908	CLA	CHC-C1C-NC	2.69	128.28	124.20
21	1	516	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
21	B	825	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
21	2	512	CLA	C1-O2A-CGA	2.68	123.49	116.44
28	2	518	DD6	C4-C5-C6	2.68	131.14	127.31
21	A	816	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
21	B	834	CLA	OBD-CAD-C3D	-2.68	122.06	128.52
21	A	805	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
21	A	828	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
21	B	833	CLA	C3D-C4D-ND	2.68	114.58	110.24
21	B	827	CLA	OBD-CAD-C3D	-2.68	122.06	128.52
21	5	704	CLA	C3B-C4B-NB	2.68	112.68	109.21
21	B	811	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
24	A	851	BCR	C36-C18-C17	-2.68	119.17	122.92
21	A	837	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
21	A	839	CLA	OBD-CAD-C3D	-2.68	122.07	128.52
21	F	404	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
21	B	816	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
21	B	822	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
21	6	904	CLA	CHD-C4C-NC	2.68	128.43	124.20
21	A	802	CLA	C6-C7-C8	-2.68	107.26	115.92
21	1	508	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	816	CLA	CHD-C4C-NC	2.68	128.42	124.20
21	8	614	CLA	CHB-C4A-NA	2.68	128.21	124.51
21	6	913	CLA	CHD-C4C-NC	2.68	128.42	124.20
21	1	511	CLA	CMC-C2C-C1C	2.68	129.11	125.04
21	4	709	CLA	CHB-C4A-NA	2.68	128.21	124.51
21	6	903	CLA	CHB-C4A-NA	2.68	128.21	124.51
28	3	716	DD6	C-C1-C2	-2.67	119.18	122.92
21	A	815	CLA	O1D-CGD-CBD	-2.67	119.01	124.48
21	A	823	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
21	12	503	CLA	CMC-C2C-C1C	2.67	129.11	125.04
21	7	712	CLA	C3B-C4B-NB	2.67	112.67	109.21
21	8	606	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
28	4	712	DD6	C37-C36-C31	-2.67	120.72	124.35
24	B	846	BCR	C19-C18-C17	2.67	123.04	118.94
21	4	701	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
21	B	804	CLA	CHD-C4C-NC	2.67	128.41	124.20
21	7	702	CLA	CHD-C4C-NC	2.67	128.41	124.20
21	B	805	CLA	C3B-C4B-NB	2.67	112.66	109.21
21	3	708	CLA	CMC-C2C-C1C	2.67	129.10	125.04
21	B	815	CLA	C2C-C1C-NC	2.67	112.47	109.97
21	B	807	CLA	C1-C2-C3	-2.67	121.43	126.04
21	1	511	CLA	CHD-C4C-NC	2.67	128.40	124.20
21	10	711	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
28	2	518	DD6	C7-C6-C5	-2.67	119.19	122.92
28	1	518	DD6	C8-C6-C5	2.66	123.03	118.94
24	A	848	BCR	C24-C23-C22	2.66	130.26	126.23
21	A	807	CLA	CHA-C1A-NA	-2.66	120.30	126.40
21	3	707	CLA	CHC-C1C-NC	2.66	128.24	124.20
21	A	810	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
21	2	508	CLA	O2A-C1-C2	2.66	118.21	108.42
21	6	905	CLA	CHD-C4C-NC	2.66	128.40	124.20
21	5	701	CLA	O2A-CGA-O1A	-2.66	116.66	123.30
21	A	831	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
21	12	506	CLA	O2A-C1-C2	2.66	115.63	108.64
21	B	805	CLA	CHC-C1C-NC	2.66	128.24	124.20
21	A	843	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
21	2	507	CLA	CHB-C4A-NA	2.66	128.19	124.51
21	B	822	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
21	11	705	CLA	C3B-C4B-NB	2.66	112.65	109.21
21	A	839	CLA	CMA-C3A-C2A	-2.66	103.09	113.83
21	8	614	CLA	CHA-C1A-NA	-2.66	120.31	126.40
22	B	840	PQN	C14-C13-C15	2.66	119.75	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	708	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
21	A	815	CLA	CAC-C3C-C4C	2.66	128.26	124.81
21	11	711	CLA	CHD-C4C-NC	2.66	128.39	124.20
21	5	708	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
21	2	506	CLA	CHB-C4A-NA	2.66	128.19	124.51
21	12	502	CLA	CMC-C2C-C1C	2.66	129.09	125.04
21	1	504	CLA	CHB-C4A-NA	2.66	128.19	124.51
21	3	709	CLA	CAC-C3C-C4C	2.66	128.26	124.81
21	9	903	CLA	CMC-C2C-C1C	2.66	129.09	125.04
21	A	823	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
21	11	706	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
21	A	835	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
21	4	708	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
21	9	911	CLA	CHC-C1C-NC	2.66	128.23	124.20
21	9	903	CLA	CAA-C2A-C3A	-2.66	105.51	112.78
21	1	512	CLA	C2A-C1A-CHA	-2.66	119.22	123.86
21	11	703	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	11	701	CLA	CHC-C1C-NC	2.65	128.23	124.20
21	J	101	CLA	C4D-CHA-C1A	-2.65	118.02	121.25
21	4	702	CLA	CHD-C4C-NC	2.65	128.38	124.20
21	10	703	CLA	CHD-C4C-NC	2.65	128.38	124.20
21	3	711	CLA	C3B-C4B-NB	2.65	112.64	109.21
21	9	910	CLA	CHA-C1A-NA	-2.65	120.32	126.40
21	B	814	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
21	10	709	CLA	CHC-C1C-NC	2.65	128.23	124.20
24	B	845	BCR	C20-C21-C22	2.65	131.09	127.31
21	B	809	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
21	A	812	CLA	C4-C3-C5	2.65	119.73	115.27
24	A	852	BCR	C2-C1-C6	2.65	114.56	110.48
21	B	801	CLA	CMA-C3A-C2A	-2.65	103.14	113.83
21	9	912	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	4	710	CLA	CHC-C1C-NC	2.65	128.22	124.20
21	1	505	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
21	11	709	CLA	CHD-C4C-NC	2.65	128.38	124.20
21	A	813	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
24	F	405	BCR	C7-C8-C9	2.65	130.24	126.23
21	3	714	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
21	6	913	CLA	C3B-C4B-NB	2.65	112.63	109.21
21	A	808	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
21	8	604	CLA	CMA-C3A-C2A	-2.65	103.15	113.83
21	A	805	CLA	C1-O2A-CGA	2.65	123.39	116.44
21	A	837	CLA	CAC-C3C-C4C	2.65	128.24	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	702	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
21	B	812	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
21	5	706	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
21	4	711	CLA	O2A-CGA-O1A	-2.64	116.71	123.30
21	3	701	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
21	3	702	CLA	C3B-C4B-NB	2.64	112.63	109.21
21	B	822	CLA	CAC-C3C-C4C	2.64	128.24	124.81
28	6	915	DD6	C-C1-C2	-2.64	119.22	122.92
21	10	704	CLA	CHB-C4A-NA	2.64	128.17	124.51
20	A	801	CL0	CBA-CAA-C2A	-2.64	106.06	113.86
21	B	839	CLA	CMC-C2C-C1C	2.64	129.06	125.04
21	1	510	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
21	8	612	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
21	3	701	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	A	832	CLA	O2A-CGA-CBA	2.64	120.19	111.91
21	3	702	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
21	3	712	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	4	704	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
21	1	506	CLA	C3B-C4B-NB	2.64	112.62	109.21
21	3	715	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
21	5	710	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	5	702	CLA	CMA-C3A-C2A	-2.64	103.18	113.83
21	3	715	CLA	CHB-C4A-NA	2.64	128.16	124.51
28	3	716	DD6	C3-C4-C5	2.64	128.88	123.47
21	B	813	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
21	A	810	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	9	908	CLA	CHD-C4C-NC	2.64	128.36	124.20
21	B	806	CLA	C4-C3-C5	2.64	119.71	115.27
21	B	826	CLA	CMA-C3A-C2A	-2.64	103.19	113.83
21	8	610	CLA	CHD-C4C-NC	2.64	128.36	124.20
21	10	708	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	B	828	CLA	C6-C7-C8	-2.63	107.40	115.92
21	13	502	CLA	C3B-C4B-NB	2.63	112.62	109.21
21	A	803	CLA	O1A-CGA-CBA	-2.63	113.45	123.73
21	3	712	CLA	O2A-CGA-CBA	2.63	122.49	114.03
21	3	711	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	4	712	DD6	C7-C6-C5	-2.63	119.23	122.92
21	6	912	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
21	B	803	CLA	CHD-C4C-NC	2.63	128.35	124.20
21	2	508	CLA	CHD-C4C-NC	2.63	128.35	124.20
21	5	706	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	A	831	CLA	CED-O2D-CGD	-2.63	109.98	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	704	CLA	C1-O2A-CGA	2.63	123.35	116.44
28	3	716	DD6	C4-C3-C2	2.63	128.86	123.47
21	B	801	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
21	A	828	CLA	C11-C10-C8	-2.63	107.42	115.92
21	2	510	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
21	B	801	CLA	C2C-C1C-NC	2.63	112.44	109.97
21	B	812	CLA	C3B-C4B-NB	2.63	112.61	109.21
21	9	904	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
21	3	704	CLA	CED-O2D-CGD	2.63	121.88	115.94
21	A	821	CLA	C6-C5-C3	-2.63	106.56	113.45
21	10	708	CLA	CHC-C1C-NC	2.63	128.19	124.20
21	A	862	CLA	C4-C3-C2	-2.63	116.94	123.68
21	A	822	CLA	C3B-C4B-NB	2.63	112.61	109.21
21	A	832	CLA	CMA-C3A-C2A	-2.63	103.23	113.83
21	4	702	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	2	521	LHG	O9-C7-C8	-2.63	113.48	123.73
21	10	710	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
21	A	830	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
21	1	501	CLA	O2A-CGA-CBA	2.63	122.46	114.03
24	B	842	BCR	C23-C22-C21	2.62	122.97	118.94
21	10	704	CLA	O2A-CGA-CBA	2.62	120.14	111.91
21	B	824	CLA	CMD-C2D-C1D	2.62	129.34	124.71
21	J	101	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
21	12	502	CLA	CMB-C2B-C3B	2.62	129.59	124.68
21	13	502	CLA	O2A-CGA-CBA	2.62	120.14	111.91
21	A	844	CLA	CHD-C4C-NC	2.62	128.33	124.20
21	B	836	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
21	A	806	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
21	3	706	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
28	6	916	DD6	C4-C3-C2	2.62	128.84	123.47
21	B	824	CLA	CHC-C1C-NC	2.62	128.18	124.20
21	6	905	CLA	CMC-C2C-C1C	2.62	129.03	125.04
21	A	844	CLA	CBA-CAA-C2A	2.62	121.59	113.86
21	A	820	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	1	508	CLA	CMB-C2B-C1B	2.62	132.49	128.46
21	F	401	CLA	C4A-NA-C1A	-2.62	105.53	106.71
21	A	833	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
21	B	816	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
21	6	909	CLA	O2A-CGA-CBA	2.62	120.12	111.91
21	7	713	CLA	C2A-C1A-CHA	-2.62	119.29	123.86
24	A	849	BCR	C37-C22-C21	-2.61	119.26	122.92
21	A	827	CLA	O2A-CGA-CBA	2.61	120.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	706	CLA	CHD-C4C-NC	2.61	128.32	124.20
21	F	404	CLA	CHC-C1C-NC	2.61	128.17	124.20
21	12	508	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
21	A	806	CLA	O1A-CGA-CBA	-2.61	113.54	123.73
21	9	909	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	A	806	CLA	CHC-C1C-NC	2.61	128.17	124.20
21	A	827	CLA	CMB-C2B-C3B	2.61	129.56	124.68
21	B	825	CLA	C4-C3-C5	2.61	119.66	115.27
21	3	712	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
21	6	903	CLA	CHC-C1C-NC	2.61	128.16	124.20
24	F	402	BCR	C3-C4-C5	-2.61	109.42	114.08
21	10	703	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	A	862	CLA	O2A-CGA-CBA	2.61	120.09	111.91
21	8	612	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	M	102	BCR	C37-C22-C23	2.61	122.19	118.08
28	2	518	DD6	C-C1-C2	-2.61	119.27	122.92
21	B	839	CLA	C16-C15-C13	-2.61	107.50	115.92
21	B	809	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
21	A	828	CLA	C4-C3-C5	2.60	119.65	115.27
21	A	839	CLA	C4-C3-C5	2.60	119.65	115.27
21	F	401	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
21	6	906	CLA	OBD-CAD-C3D	-2.60	122.25	128.52
21	B	814	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	4	712	DD6	O1-C20-C19	-2.60	111.43	113.38
21	B	802	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
21	10	703	CLA	CMB-C2B-C3B	2.60	129.55	124.68
21	2	516	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
21	A	823	CLA	CMA-C3A-C4A	-2.60	104.78	111.77
21	11	704	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
21	1	515	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
21	A	829	CLA	CAA-CBA-CGA	-2.60	105.65	113.25
21	B	831	CLA	CMC-C2C-C1C	2.60	129.00	125.04
28	1	520	DD6	C14-C13-C11	-2.60	121.50	125.53
21	11	702	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
21	B	836	CLA	C3A-C2A-C1A	-2.60	97.45	101.34
21	1	506	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
21	A	818	CLA	C4D-CHA-C1A	-2.60	118.09	121.25
21	1	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	8	611	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
21	11	710	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
21	B	829	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
21	12	501	CLA	CMC-C2C-C1C	2.60	129.00	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	516	CLA	C3D-C2D-C1D	-2.60	102.29	105.83
21	9	904	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
21	A	822	CLA	C4A-NA-C1A	-2.60	105.54	106.71
21	B	828	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
21	8	610	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
21	12	501	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	B	828	CLA	CMA-C3A-C2A	-2.59	103.36	113.83
21	1	511	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
21	11	707	CLA	CHC-C1C-NC	2.59	128.14	124.20
21	B	829	CLA	C4A-NA-C1A	-2.59	105.54	106.71
21	9	907	CLA	CMD-C2D-C3D	-2.59	121.65	127.61
24	A	847	BCR	C37-C22-C23	2.59	122.16	118.08
21	8	609	CLA	CMA-C3A-C2A	-2.59	103.37	113.83
24	B	841	BCR	C16-C15-C14	2.59	128.78	123.47
21	5	711	CLA	CMB-C2B-C3B	2.59	129.53	124.68
21	11	708	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
21	1	510	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
21	12	507	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
21	2	515	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
21	12	506	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
21	A	862	CLA	CHD-C4C-NC	2.59	128.28	124.20
21	4	701	CLA	CHD-C4C-NC	2.59	128.28	124.20
21	A	834	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
27	B	847	DGD	CDB-CCB-CBB	-2.59	101.28	114.42
21	B	802	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	1	510	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
21	7	711	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
21	B	801	CLA	C1-C2-C3	-2.59	121.57	126.04
21	2	507	CLA	C1-O2A-CGA	2.59	124.25	116.73
21	7	714	CLA	C3B-C4B-NB	2.59	112.56	109.21
21	7	703	CLA	CHC-C1C-NC	2.59	128.13	124.20
21	A	818	CLA	CAC-C3C-C4C	2.59	128.16	124.81
21	A	844	CLA	CED-O2D-CGD	2.59	121.78	115.94
21	3	710	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
28	7	715	DD6	C8-C6-C5	2.58	122.91	118.94
21	4	704	CLA	CHD-C4C-NC	2.58	128.28	124.20
21	8	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
21	6	910	CLA	CHD-C4C-NC	2.58	128.28	124.20
21	1	501	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
21	7	708	CLA	O2A-CGA-CBA	2.58	120.02	111.91
21	9	909	CLA	CHC-C1C-NC	2.58	128.12	124.20
21	A	820	CLA	CMD-C2D-C3D	-2.58	121.67	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	712	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
21	7	705	CLA	C3B-C4B-NB	2.58	112.55	109.21
21	B	830	CLA	CHC-C1C-NC	2.58	128.12	124.20
21	A	802	CLA	O2A-CGA-CBA	2.58	120.01	111.91
21	8	609	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
21	5	709	CLA	C3B-C4B-NB	2.58	112.54	109.21
21	1	511	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	1	501	CLA	C3C-C4C-NC	2.58	113.46	110.57
21	A	822	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
21	2	513	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	8	611	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
21	7	705	CLA	C1-C2-C3	-2.58	122.58	126.75
21	3	713	CLA	CED-O2D-CGD	2.58	121.77	115.94
21	6	912	CLA	O2A-CGA-O1A	-2.58	116.88	123.30
21	A	827	CLA	C2C-C1C-NC	2.58	112.39	109.97
21	B	825	CLA	CMC-C2C-C1C	2.58	128.96	125.04
28	2	519	DD6	C4-C3-C2	2.58	128.75	123.47
21	B	801	CLA	CHC-C1C-NC	2.58	128.11	124.20
21	9	914	CLA	O2A-CGA-CBA	2.58	119.99	111.91
21	B	817	CLA	C1-O2A-CGA	2.57	123.20	116.44
21	4	707	CLA	O2A-CGA-CBA	2.57	119.99	111.91
21	2	508	CLA	C3B-C4B-NB	2.57	112.54	109.21
21	B	802	CLA	C1-C2-C3	-2.57	121.59	126.04
21	8	613	CLA	CMC-C2C-C1C	2.57	128.96	125.04
21	6	908	CLA	OBD-CAD-C3D	-2.57	122.33	128.52
21	2	506	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
21	12	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	5	709	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
21	A	805	CLA	C4-C3-C5	2.57	119.60	115.27
21	8	608	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	4	711	CLA	O2A-CGA-CBA	2.57	122.30	114.03
21	B	812	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	12	508	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
21	2	508	CLA	CHC-C1C-NC	2.57	128.10	124.20
21	3	709	CLA	CHC-C1C-NC	2.57	128.10	124.20
21	10	712	CLA	O2A-CGA-CBA	2.57	119.98	111.91
21	3	712	CLA	CAA-CBA-CGA	2.57	119.33	112.51
21	6	905	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
21	A	805	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
21	8	611	CLA	CAC-C3C-C4C	2.57	128.14	124.81
21	B	835	CLA	CHD-C4C-NC	2.57	128.25	124.20
21	9	905	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	704	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
21	A	832	CLA	C3B-C4B-NB	2.57	112.53	109.21
21	A	839	CLA	C3B-C4B-NB	2.57	112.53	109.21
21	B	812	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
21	A	815	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
21	7	708	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
21	A	806	CLA	C4D-C3D-CAD	-2.57	105.07	108.10
21	2	504	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	A	826	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
21	B	827	CLA	C16-C15-C13	-2.57	107.62	115.92
21	5	711	CLA	CMC-C2C-C1C	2.57	128.95	125.04
21	3	708	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
21	B	802	CLA	C11-C10-C8	-2.57	107.62	115.92
21	6	912	CLA	CHD-C4C-NC	2.57	128.25	124.20
21	9	911	CLA	CMB-C2B-C3B	2.57	129.48	124.68
21	2	504	CLA	C1D-CHD-C4C	-2.56	120.53	126.06
21	B	837	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
21	10	709	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	B	843	BCR	C34-C9-C8	2.56	122.12	118.08
21	B	818	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
21	B	820	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
21	A	837	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
21	1	507	CLA	O2A-CGA-CBA	2.56	119.95	111.91
21	B	829	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
21	B	801	CLA	CED-O2D-CGD	2.56	121.73	115.94
21	6	910	CLA	CMC-C2C-C1C	2.56	128.94	125.04
21	B	829	CLA	CHC-C1C-NC	2.56	128.09	124.20
21	1	515	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
21	7	711	CLA	C4-C3-C5	2.56	119.58	115.27
21	B	829	CLA	CAC-C3C-C2C	2.56	131.91	127.53
28	3	718	DD6	C33-C32-C31	2.56	114.81	109.62
21	9	907	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
21	4	710	CLA	CHD-C4C-NC	2.56	128.24	124.20
21	3	703	CLA	C3C-C4C-NC	2.56	113.44	110.57
21	5	704	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
21	2	514	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
21	12	507	CLA	CHC-C1C-NC	2.56	128.08	124.20
21	11	706	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
21	11	710	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
21	4	705	CLA	C3A-C2A-C1A	-2.56	97.51	101.34
21	B	833	CLA	C4A-NA-C1A	-2.56	105.56	106.71
21	7	702	CLA	CMA-C3A-C4A	-2.55	104.91	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	517	CLA	C4C-C3C-C2C	-2.55	103.17	106.90
21	A	815	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	1	510	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
21	B	817	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
21	9	907	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	13	501	CLA	CHC-C1C-NC	2.55	128.08	124.20
21	12	507	CLA	CMC-C2C-C1C	2.55	128.93	125.04
25	A	854	LHG	O4-P-O6	2.55	119.60	107.75
21	B	837	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
21	4	709	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
21	8	614	CLA	C3B-C4B-NB	2.55	112.50	109.21
21	A	836	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
21	3	715	CLA	CMC-C2C-C1C	2.55	128.92	125.04
24	A	847	BCR	C35-C13-C14	-2.55	119.35	122.92
21	A	834	CLA	CHD-C4C-NC	2.55	128.22	124.20
21	7	708	CLA	C4C-C3C-C2C	-2.55	103.19	106.90
21	4	702	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
24	A	849	BCR	C4-C5-C6	-2.54	119.04	122.73
21	9	904	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
21	A	820	CLA	CHC-C1C-NC	2.54	128.06	124.20
21	2	507	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
21	6	914	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
21	B	804	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
21	4	711	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
21	A	829	CLA	CHD-C4C-NC	2.54	128.21	124.20
21	10	704	CLA	C4-C3-C5	2.54	119.55	115.27
21	A	826	CLA	CHC-C1C-NC	2.54	128.06	124.20
21	A	835	CLA	CBC-CAC-C3C	-2.54	105.42	112.43
21	A	828	CLA	CHD-C4C-NC	2.54	128.21	124.20
21	1	513	CLA	O2A-CGA-CBA	2.54	119.88	111.91
21	B	821	CLA	CHD-C4C-NC	2.54	128.21	124.20
21	8	608	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
21	B	818	CLA	C5-C3-C2	-2.54	115.98	121.12
21	B	824	CLA	CMB-C2B-C3B	2.54	129.43	124.68
21	6	903	CLA	C1-O2A-CGA	2.54	124.11	116.73
21	5	701	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
21	A	829	CLA	C3B-C4B-NB	2.54	112.49	109.21
21	6	913	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
21	10	712	CLA	CED-O2D-CGD	2.54	121.68	115.94
21	A	825	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
21	11	706	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
28	12	510	DD6	C10-C9-C8	-2.54	115.31	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	903	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
21	A	822	CLA	C7-C6-C5	-2.53	106.48	113.36
21	A	824	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
21	A	832	CLA	C1-O2A-CGA	2.53	123.09	116.44
21	B	833	CLA	CMA-C3A-C2A	-2.53	103.61	113.83
21	8	605	CLA	C3C-C4C-NC	2.53	113.41	110.57
21	A	819	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
21	B	829	CLA	C2C-C1C-NC	2.53	112.34	109.97
21	11	711	CLA	CMB-C2B-C3B	2.53	129.41	124.68
21	3	712	CLA	CBA-CAA-C2A	2.53	121.33	113.86
21	B	810	CLA	C3B-C4B-NB	2.53	112.48	109.21
21	1	512	CLA	CHD-C4C-NC	2.53	128.19	124.20
21	4	711	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
21	A	862	CLA	C11-C12-C13	-2.53	107.75	115.92
28	11	713	DD6	C13-C11-C10	2.53	122.82	118.94
27	B	847	DGD	O1G-C1G-C2G	-2.53	101.08	108.43
21	6	906	CLA	C5-C3-C4	2.53	120.19	114.60
21	B	830	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
21	4	702	CLA	C1-C2-C3	-2.53	121.67	126.04
21	10	706	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
21	B	825	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
21	9	903	CLA	C2C-C1C-NC	2.53	112.34	109.97
21	2	504	CLA	CHD-C4C-NC	2.53	128.18	124.20
21	6	903	CLA	CHD-C4C-NC	2.53	128.18	124.20
21	B	823	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
21	F	404	CLA	CMC-C2C-C1C	2.52	128.88	125.04
21	A	833	CLA	C2A-C1A-CHA	-2.52	119.44	123.86
21	11	707	CLA	C3C-C4C-NC	2.52	113.40	110.57
21	1	509	CLA	CED-O2D-CGD	2.52	121.65	115.94
21	12	501	CLA	C3B-C4B-NB	2.52	112.47	109.21
21	A	842	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
21	3	710	CLA	O2A-CGA-CBA	2.52	119.83	111.91
21	9	911	CLA	C4-C3-C5	2.52	119.52	115.27
21	6	913	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
21	B	813	CLA	CHD-C1D-ND	-2.52	122.14	124.45
21	B	830	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
21	B	831	CLA	C6-C7-C8	-2.52	107.77	115.92
21	B	814	CLA	CHD-C4C-NC	2.52	128.18	124.20
21	3	706	CLA	CMC-C2C-C1C	2.52	128.88	125.04
21	1	504	CLA	CHC-C1C-NC	2.52	128.03	124.20
21	2	510	CLA	CHD-C4C-NC	2.52	128.18	124.20
21	A	823	CLA	C1B-CHB-C4A	-2.52	125.12	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	908	CLA	CHA-C1A-NA	-2.52	120.63	126.40
21	3	709	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
21	7	707	CLA	CHB-C4A-NA	2.52	127.99	124.51
21	1	504	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
21	B	838	CLA	CMB-C2B-C1B	2.52	132.33	128.46
21	10	704	CLA	CHD-C4C-NC	2.52	128.17	124.20
21	A	802	CLA	C3D-C4D-ND	2.52	114.31	110.24
21	11	707	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
21	12	502	CLA	CHC-C1C-NC	2.52	128.02	124.20
24	J	103	BCR	C36-C18-C17	-2.51	119.40	122.92
21	1	513	CLA	CMC-C2C-C1C	2.51	128.87	125.04
21	12	506	CLA	CMB-C2B-C3B	2.51	129.38	124.68
21	2	512	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	1	507	CLA	CHC-C1C-NC	2.51	128.02	124.20
21	7	707	CLA	C1D-CHD-C4C	-2.51	120.64	126.06
21	11	704	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
21	12	503	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	6	914	CLA	O2A-CGA-CBA	2.51	119.79	111.91
21	4	711	CLA	CAA-CBA-CGA	2.51	119.17	112.51
21	B	824	CLA	O2A-CGA-CBA	2.51	122.16	112.23
21	B	810	CLA	CGD-CBD-CAD	-2.51	102.60	110.73
21	B	835	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
21	3	710	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
21	A	818	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	2	508	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
21	11	709	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
21	7	707	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
21	5	704	CLA	O2A-CGA-CBA	2.51	119.78	111.91
21	7	714	CLA	CHA-C1A-NA	-2.51	120.65	126.40
21	7	702	CLA	CAC-C3C-C2C	2.51	131.82	127.53
21	A	831	CLA	CMB-C2B-C3B	2.51	129.37	124.68
21	2	505	CLA	CHC-C1C-NC	2.51	128.01	124.20
21	A	827	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	A	801	CL0	C4D-CHA-C1A	-2.51	118.20	121.25
21	9	907	CLA	C4D-CHA-C1A	-2.51	118.20	121.25
21	5	704	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
21	B	817	CLA	C4C-C3C-C2C	-2.51	103.25	106.90
21	10	706	CLA	CAA-C2A-C3A	-2.51	110.25	116.10
21	9	910	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
21	A	809	CLA	CMB-C2B-C3B	2.50	129.36	124.68
21	A	826	CLA	CMC-C2C-C1C	2.50	128.85	125.04
21	A	831	CLA	CHC-C1C-C2C	-2.50	119.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	703	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
21	A	828	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	8	614	CLA	CMC-C2C-C1C	2.50	128.85	125.04
21	B	805	CLA	O2D-CGD-CBD	2.50	115.72	111.27
24	B	843	BCR	C34-C9-C10	-2.50	119.42	122.92
21	B	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	2	508	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
21	9	905	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	A	850	BCR	C30-C25-C24	2.50	122.86	115.78
21	A	839	CLA	CMC-C2C-C1C	2.50	128.85	125.04
21	3	704	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
21	2	506	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
21	B	829	CLA	CED-O2D-CGD	2.50	121.59	115.94
21	7	713	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
21	A	805	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
21	B	817	CLA	C3B-C4B-NB	2.50	112.44	109.21
21	F	401	CLA	C4C-C3C-C2C	-2.50	103.26	106.90
21	10	707	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	3	709	CLA	CAA-CBA-CGA	-2.50	105.88	112.51
24	B	844	BCR	C24-C23-C22	-2.50	122.46	126.23
21	5	701	CLA	CHD-C4C-NC	2.50	128.14	124.20
21	B	831	CLA	O2A-CGA-CBA	2.50	119.74	111.91
21	8	610	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
21	11	708	CLA	C4C-C3C-C2C	-2.50	103.26	106.90
21	3	709	CLA	CMB-C2B-C3B	2.49	129.35	124.68
21	A	807	CLA	C3C-C4C-NC	2.49	113.37	110.57
24	A	851	BCR	C34-C9-C8	2.49	122.01	118.08
21	11	708	CLA	CED-O2D-CGD	2.49	121.58	115.94
21	2	505	CLA	C3B-C4B-NB	2.49	112.43	109.21
21	9	913	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	B	841	BCR	C34-C9-C8	2.49	122.00	118.08
21	A	840	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
21	B	814	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
28	7	716	DD6	C23-C16-C22	2.49	111.05	107.37
21	A	840	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
21	10	705	CLA	CED-O2D-CGD	2.49	121.57	115.94
28	2	519	DD6	C4-C5-C6	2.49	130.87	127.31
21	J	101	CLA	CHC-C1C-NC	2.49	127.98	124.20
21	2	506	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
21	1	516	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	B	842	BCR	C8-C9-C10	2.49	122.76	118.94
21	2	511	CLA	C1C-C2C-C3C	-2.49	104.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	836	CLA	CHC-C1C-NC	2.49	127.98	124.20
21	10	712	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	A	810	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
24	A	849	BCR	C16-C17-C18	2.49	130.86	127.31
21	A	820	CLA	CMB-C2B-C3B	2.49	129.33	124.68
21	2	515	CLA	CED-O2D-CGD	2.49	121.56	115.94
21	3	710	CLA	CHD-C4C-NC	2.48	128.12	124.20
21	A	838	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
27	B	847	DGD	O6D-C1D-O3G	-2.48	104.09	109.97
21	A	829	CLA	C16-C15-C13	-2.48	107.89	115.92
21	7	706	CLA	OBD-CAD-C3D	-2.48	122.54	128.52
21	8	613	CLA	C3B-C4B-NB	2.48	112.42	109.21
21	4	708	CLA	CHD-C4C-NC	2.48	128.12	124.20
21	1	509	CLA	C2C-C1C-NC	2.48	112.30	109.97
21	10	707	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
21	6	912	CLA	CHC-C1C-NC	2.48	127.97	124.20
21	10	706	CLA	CHD-C4C-NC	2.48	128.12	124.20
21	3	712	CLA	CAC-C3C-C4C	2.48	128.03	124.81
21	6	911	CLA	C3B-C4B-NB	2.48	112.42	109.21
21	A	824	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
21	11	704	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
24	A	848	BCR	C36-C18-C17	-2.48	119.45	122.92
21	B	805	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	F	403	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
21	A	817	CLA	C1-O2A-CGA	2.48	122.95	116.44
21	B	838	CLA	CHD-C1D-C2D	-2.48	120.28	125.48
21	3	712	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
21	B	836	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
24	M	102	BCR	C1-C6-C7	-2.48	108.77	115.78
21	9	905	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
21	10	704	CLA	CAC-C3C-C4C	2.48	128.03	124.81
21	B	826	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
21	1	505	CLA	CHD-C4C-NC	2.48	128.11	124.20
21	7	706	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
21	12	505	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
21	12	503	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
21	A	814	CLA	CMB-C2B-C3B	2.48	129.31	124.68
21	A	830	CLA	C1-C2-C3	-2.48	121.76	126.04
21	7	704	CLA	CHA-C1A-NA	-2.48	120.73	126.40
21	A	815	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
22	A	845	PQN	C11-C12-C13	-2.47	122.67	126.79
21	A	813	CLA	O2A-CGA-CBA	2.47	119.67	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	829	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
21	8	614	CLA	O2A-CGA-CBA	2.47	119.67	111.91
21	B	822	CLA	CHD-C4C-NC	2.47	128.10	124.20
21	1	513	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
21	A	828	CLA	C4A-NA-C1A	-2.47	105.59	106.71
21	8	611	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	3	703	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
21	11	706	CLA	C4A-NA-C1A	-2.47	105.60	106.71
21	5	710	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
21	6	914	CLA	CBA-CAA-C2A	2.47	121.15	113.86
21	8	608	CLA	O2A-CGA-CBA	2.47	119.65	111.91
21	8	604	CLA	CHD-C4C-NC	2.47	128.09	124.20
21	B	834	CLA	C4-C3-C5	2.47	119.42	115.27
21	12	505	CLA	CHA-C1A-NA	-2.47	120.75	126.40
21	B	830	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
21	3	713	CLA	CHD-C4C-NC	2.47	128.09	124.20
21	9	902	CLA	CMC-C2C-C1C	2.47	128.79	125.04
21	B	803	CLA	CHB-C4A-NA	2.47	127.92	124.51
21	9	903	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
21	A	824	CLA	CMA-C3A-C2A	-2.46	103.89	113.83
21	B	821	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
21	A	862	CLA	C4D-CHA-C1A	2.46	124.25	121.25
21	9	911	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
21	7	702	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
28	7	716	DD6	C3-C4-C5	2.46	128.52	123.47
21	9	902	CLA	C3B-C4B-NB	2.46	112.39	109.21
21	A	814	CLA	CHA-C1A-NA	-2.46	120.76	126.40
21	2	511	CLA	CMB-C2B-C3B	2.46	129.28	124.68
21	6	910	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
21	1	510	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
21	12	506	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
21	11	708	CLA	CHD-C4C-NC	2.46	128.08	124.20
21	B	826	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
21	B	812	CLA	C16-C15-C13	-2.46	107.97	115.92
21	2	511	CLA	CMC-C2C-C1C	2.46	128.78	125.04
21	B	828	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
21	4	705	CLA	CHD-C4C-NC	2.46	128.08	124.20
21	6	905	CLA	CHC-C1C-NC	2.46	127.93	124.20
21	B	835	CLA	C3D-C2D-C1D	-2.46	102.48	105.83
21	B	806	CLA	C6-C7-C8	-2.46	107.97	115.92
21	B	823	CLA	CHA-C1A-NA	-2.46	120.77	126.40
21	4	706	CLA	CHD-C4C-NC	2.46	128.08	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	821	CLA	O1D-CGD-CBD	-2.46	119.46	124.48
21	12	508	CLA	CHD-C4C-NC	2.46	128.07	124.20
24	A	850	BCR	C36-C18-C17	-2.46	119.48	122.92
21	7	712	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
28	4	712	DD6	C24-C1-C2	2.46	122.71	118.94
21	J	101	CLA	CMD-C2D-C3D	-2.46	121.97	127.61
21	B	828	CLA	CBC-CAC-C3C	-2.45	105.66	112.43
25	2	521	LHG	O7-C5-C4	-2.45	99.51	108.40
21	A	821	CLA	CBC-CAC-C3C	-2.45	105.66	112.43
21	B	839	CLA	C1-C2-C3	-2.45	121.80	126.04
21	A	813	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
21	A	818	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
21	B	822	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
21	1	504	CLA	CHD-C4C-NC	2.45	128.07	124.20
21	B	829	CLA	CHD-C1D-C2D	-2.45	120.33	125.48
21	8	607	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	A	802	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
21	7	703	CLA	CMB-C2B-C3B	2.45	129.27	124.68
28	8	615	DD6	C4-C3-C2	2.45	128.50	123.47
21	11	709	CLA	CHB-C4A-NA	2.45	127.90	124.51
21	11	702	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
21	2	516	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	A	803	CLA	CMB-C2B-C3B	2.45	129.26	124.68
21	B	803	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
21	9	908	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
21	7	704	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
21	B	830	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	A	834	CLA	CGD-CBD-CAD	-2.45	102.81	110.73
22	B	840	PQN	C8-C7-C6	-2.45	116.46	120.19
21	7	703	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
21	4	704	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
21	B	817	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
24	J	102	BCR	C8-C9-C10	2.45	122.69	118.94
21	3	706	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
21	4	703	CLA	C4C-C3C-C2C	-2.44	103.33	106.90
24	A	851	BCR	C35-C13-C14	-2.44	119.50	122.92
28	3	718	DD6	C3-C4-C5	2.44	128.48	123.47
21	2	509	CLA	C1D-CHD-C4C	-2.44	120.79	126.06
21	B	815	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
28	2	518	DD6	O1-C20-C19	-2.44	111.55	113.38
21	8	608	CLA	CMB-C2B-C3B	2.44	129.25	124.68
21	A	802	CLA	CHC-C1C-NC	2.44	127.91	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	706	CLA	C2C-C1C-NC	2.44	112.26	109.97
21	8	604	CLA	C4-C3-C5	2.44	119.37	115.27
20	A	801	CL0	CHD-C1D-ND	-2.44	122.21	124.45
21	6	905	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
21	3	713	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	12	504	CLA	CED-O2D-CGD	2.44	121.45	115.94
21	6	909	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	A	849	BCR	C11-C10-C9	-2.44	123.83	127.31
21	10	710	CLA	CHD-C4C-NC	2.44	128.04	124.20
21	B	815	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	3	701	CLA	C3C-C4C-NC	2.44	113.30	110.57
21	B	832	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
21	7	714	CLA	CHD-C4C-NC	2.44	128.04	124.20
21	2	504	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
21	5	705	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	B	832	CLA	CAA-CBA-CGA	-2.43	106.14	113.25
24	B	841	BCR	C37-C22-C23	2.43	121.91	118.08
21	4	705	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
21	7	708	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	4	706	CLA	CHC-C1C-NC	2.43	127.89	124.20
21	1	517	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
21	6	908	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
21	7	711	CLA	CMC-C2C-C1C	2.43	128.74	125.04
21	B	824	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
21	6	910	CLA	CMB-C2B-C3B	2.43	129.22	124.68
21	8	607	CLA	C3B-C4B-NB	2.43	112.35	109.21
21	12	504	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	B	843	BCR	C37-C22-C23	2.43	121.90	118.08
21	9	903	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
21	B	835	CLA	C11-C12-C13	-2.43	108.07	115.92
21	5	709	CLA	CED-O2D-CGD	2.43	121.43	115.94
21	6	909	CLA	CHC-C1C-NC	2.43	127.89	124.20
21	A	802	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
21	6	907	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
21	11	711	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
25	1	521	LHG	O7-C5-C4	-2.43	99.62	108.40
21	7	706	CLA	C1-O2A-CGA	2.43	123.78	116.73
21	4	708	CLA	CMB-C2B-C3B	2.43	129.22	124.68
21	A	833	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
21	B	823	CLA	CMC-C2C-C1C	2.43	128.73	125.04
21	10	707	CLA	C3B-C4B-NB	2.42	112.34	109.21
21	B	804	CLA	C4-C3-C5	2.42	119.35	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	806	CLA	O2A-CGA-CBA	2.42	119.51	111.91
21	3	707	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
21	6	906	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
21	2	514	CLA	CMA-C3A-C4A	-2.42	105.27	111.77
21	13	503	CLA	CHA-C1A-NA	-2.42	120.85	126.40
21	7	709	CLA	CBA-CAA-C2A	2.42	119.13	114.02
21	11	709	CLA	CMC-C2C-C1C	2.42	128.73	125.04
21	A	843	CLA	CHC-C1C-C2C	-2.42	120.03	126.72
21	10	710	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
21	8	607	CLA	CAA-C2A-C1A	2.42	119.91	111.97
21	7	713	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
21	12	501	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
21	5	705	CLA	CHC-C1C-NC	2.42	127.87	124.20
24	A	847	BCR	C32-C1-C6	-2.42	106.38	110.30
21	11	704	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	1	508	CLA	CMA-C3A-C4A	-2.42	105.27	111.77
28	12	510	DD6	C14-C13-C11	-2.42	121.78	125.53
21	8	604	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
21	4	708	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
21	10	703	CLA	C2A-C1A-CHA	-2.42	119.63	123.85
21	B	826	CLA	C6-C7-C8	-2.42	108.10	115.92
21	7	702	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
21	5	702	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
21	12	501	CLA	C4-C3-C5	2.42	119.34	115.27
21	2	517	CLA	CHD-C4C-NC	2.42	128.01	124.20
21	6	913	CLA	CED-O2D-CGD	2.42	121.40	115.94
21	8	611	CLA	CED-O2D-CGD	2.42	121.40	115.94
21	8	612	CLA	C4-C3-C5	2.42	119.33	115.27
21	A	830	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
21	9	903	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
21	A	830	CLA	CMC-C2C-C1C	2.42	128.72	125.04
21	A	809	CLA	O1A-CGA-CBA	-2.41	114.31	123.73
21	7	709	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	1	515	CLA	O2A-CGA-O1A	-2.41	117.29	123.30
21	A	829	CLA	O2A-CGA-CBA	2.41	119.47	111.91
21	B	823	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
21	13	501	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
21	1	508	CLA	CHD-C4C-NC	2.41	128.00	124.20
21	7	711	CLA	C1-O2A-CGA	2.41	122.77	116.44
21	F	403	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
21	A	843	CLA	CHD-C4C-NC	2.41	128.00	124.20
21	6	906	CLA	O2A-CGA-CBA	2.41	119.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	708	CLA	CHD-C4C-NC	2.41	128.00	124.20
21	8	613	CLA	CED-O2D-CGD	2.41	121.39	115.94
21	A	838	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
21	B	826	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
21	5	711	CLA	C3B-C4B-NB	2.41	112.32	109.21
21	A	829	CLA	C1-O2A-CGA	-2.41	110.13	116.44
21	B	807	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	6	909	CLA	CHD-C4C-NC	2.41	128.00	124.20
21	B	803	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	B	822	CLA	C3B-C4B-NB	2.41	112.32	109.21
21	A	843	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
21	B	834	CLA	CMC-C2C-C1C	2.41	128.70	125.04
21	B	827	CLA	C4-C3-C5	-2.40	111.23	115.27
21	1	517	CLA	O2A-CGA-CBA	2.40	121.75	114.03
21	B	828	CLA	CMB-C2B-C3B	2.40	129.17	124.68
21	7	707	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
21	B	836	CLA	CGD-CBD-CAD	-2.40	102.95	110.73
21	12	507	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
21	B	813	CLA	C6-C7-C8	-2.40	108.16	115.92
21	A	840	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
21	3	704	CLA	CAA-C2A-C3A	-2.40	108.26	114.26
21	2	505	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
21	B	823	CLA	CHD-C4C-NC	2.40	127.98	124.20
21	9	909	CLA	CHD-C4C-NC	2.40	127.98	124.20
21	1	514	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	A	809	CLA	C4A-NA-C1A	-2.40	105.63	106.71
21	B	838	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
21	A	839	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
21	11	706	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
21	5	708	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
28	12	509	DD6	C34-C35-C36	2.40	116.63	111.85
21	B	828	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
21	A	832	CLA	C1-C2-C3	-2.40	122.88	126.75
21	A	822	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	A	817	CLA	CMC-C2C-C1C	2.39	128.69	125.04
21	A	826	CLA	CHA-C1A-NA	-2.39	120.91	126.40
21	7	713	CLA	CHC-C1C-NC	2.39	127.84	124.20
28	11	712	DD6	C13-C11-C10	2.39	122.61	118.94
21	5	701	CLA	CAA-CBA-CGA	2.39	118.86	112.51
21	5	701	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
21	8	603	CLA	O2A-CGA-CBA	2.39	119.42	111.91
21	5	705	CLA	C2A-C1A-CHA	-2.39	119.67	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	612	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
21	A	828	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
21	B	809	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
21	A	825	CLA	C3B-C4B-NB	2.39	112.30	109.21
21	A	817	CLA	CHC-C1C-NC	2.39	127.83	124.20
21	11	711	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
21	11	708	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	A	824	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
21	4	707	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
21	1	509	CLA	C3B-C4B-NB	2.39	112.30	109.21
21	9	914	CLA	CHC-C1C-NC	2.39	127.83	124.20
21	A	826	CLA	C1-O2A-CGA	2.39	122.71	116.44
21	5	711	CLA	CHD-C4C-NC	2.39	127.97	124.20
21	A	836	CLA	C1D-CHD-C4C	-2.39	120.91	126.06
21	A	803	CLA	C5-C3-C2	-2.39	116.29	121.12
21	1	506	CLA	CED-O2D-CGD	2.39	121.33	115.94
21	13	503	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
21	A	830	CLA	CMD-C2D-C1D	2.39	128.92	124.71
21	A	839	CLA	CHD-C4C-NC	2.39	127.96	124.20
21	A	828	CLA	C3A-C2A-C1A	-2.39	97.77	101.34
21	4	704	CLA	CMB-C2B-C3B	2.38	129.14	124.68
21	A	826	CLA	C16-C15-C13	-2.38	108.21	115.92
21	3	706	CLA	OBD-CAD-C3D	-2.38	122.78	128.52
21	B	806	CLA	C4-C3-C2	-2.38	117.56	123.68
21	9	910	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
21	B	806	CLA	C1-C2-C3	-2.38	121.92	126.04
21	A	809	CLA	CHC-C1C-NC	2.38	127.82	124.20
21	B	824	CLA	CAA-C2A-C1A	-2.38	104.17	111.97
21	1	510	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
21	A	822	CLA	O2A-CGA-CBA	2.38	119.38	111.91
21	3	707	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	2	515	CLA	C3A-C2A-C1A	-2.38	97.78	101.34
21	5	704	CLA	C1-O2A-CGA	2.38	122.68	116.44
21	12	508	CLA	CHC-C1C-NC	2.38	127.81	124.20
21	3	702	CLA	O2A-CGA-CBA	2.38	119.36	111.91
21	B	801	CLA	C4D-CHA-C1A	-2.38	118.36	121.25
21	B	811	CLA	CHC-C1C-NC	2.38	127.81	124.20
21	12	501	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
21	10	712	CLA	C2A-C1A-CHA	-2.38	119.71	123.86
24	F	402	BCR	C29-C30-C25	2.37	114.14	110.48
21	B	831	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
21	9	903	CLA	C1C-C2C-C3C	-2.37	104.46	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	506	CLA	CMA-C3A-C2A	-2.37	104.25	113.83
21	11	702	CLA	C3B-C4B-NB	2.37	112.28	109.21
21	B	817	CLA	CHA-C1A-NA	-2.37	120.96	126.40
21	12	503	CLA	CHD-C4C-NC	2.37	127.94	124.20
21	3	714	CLA	CHA-C1A-NA	-2.37	120.97	126.40
21	2	503	CLA	CHC-C1C-NC	2.37	127.80	124.20
21	2	513	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
28	6	915	DD6	C22-C16-C17	-2.37	104.86	108.98
21	8	613	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
21	A	862	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
21	4	710	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	5	713	DD6	C3-C2-C1	2.37	130.69	127.31
28	4	713	DD6	C13-C11-C10	2.37	122.58	118.94
21	A	814	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
21	8	607	CLA	CMB-C2B-C3B	2.37	129.11	124.68
21	12	506	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
21	7	707	CLA	C1-O2A-CGA	2.37	123.61	116.73
21	5	709	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
21	9	903	CLA	CHB-C4A-NA	2.37	127.78	124.51
21	11	709	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
21	13	501	CLA	CMB-C2B-C3B	2.37	129.10	124.68
21	6	906	CLA	C1-C2-C3	-2.37	122.92	126.75
21	10	707	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
21	2	514	CLA	O2A-CGA-O1A	-2.37	117.40	123.30
21	10	709	CLA	C2A-C1A-CHA	-2.36	119.72	123.86
24	A	849	BCR	C2-C1-C6	2.36	114.12	110.48
28	1	519	DD6	C9-C10-C11	2.36	130.68	127.31
21	6	910	CLA	CHC-C1C-NC	2.36	127.79	124.20
28	8	616	DD6	C13-C11-C10	2.36	122.57	118.94
21	6	904	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
24	A	850	BCR	C35-C13-C14	-2.36	119.61	122.92
21	A	814	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
21	12	507	CLA	CMB-C2B-C3B	2.36	129.10	124.68
21	7	709	CLA	CMC-C2C-C1C	2.36	128.64	125.04
21	A	842	CLA	CED-O2D-CGD	-2.36	110.60	115.94
28	6	915	DD6	C33-C32-C31	2.36	114.41	109.62
21	8	610	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
21	B	804	CLA	C1-C2-C3	-2.36	121.96	126.04
21	A	826	CLA	C4-C3-C5	2.36	119.24	115.27
21	3	706	CLA	CHC-C1C-NC	2.36	127.78	124.20
21	B	834	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
21	A	815	CLA	C1-C2-C3	-2.36	121.96	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	805	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
21	2	506	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
21	B	809	CLA	C2C-C1C-NC	2.36	112.18	109.97
21	3	707	CLA	C4C-C3C-C2C	-2.36	103.46	106.90
21	1	514	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	11	701	CLA	CHD-C4C-NC	2.36	127.92	124.20
21	3	706	CLA	CED-O2D-CGD	2.36	121.27	115.94
21	6	910	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	10	703	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	7	702	CLA	O2A-C1-C2	2.35	117.07	108.42
21	J	101	CLA	CHD-C4C-NC	2.35	127.91	124.20
21	4	706	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	8	611	CLA	C3B-C4B-NB	2.35	112.25	109.21
21	6	913	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	12	501	CLA	CMB-C2B-C3B	2.35	129.08	124.68
21	F	404	CLA	CMB-C2B-C3B	2.35	129.08	124.68
21	3	714	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
28	5	713	DD6	O1-C20-C19	-2.35	111.62	113.38
21	A	821	CLA	C1D-CHD-C4C	-2.35	120.99	126.06
21	A	831	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
21	2	517	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
21	B	825	CLA	C3A-C2A-C1A	-2.35	97.82	101.34
21	B	839	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
21	5	707	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
27	B	847	DGD	O6E-C5E-C4E	-2.35	105.43	109.69
21	1	501	CLA	O2A-CGA-O1A	-2.35	117.45	123.30
21	A	803	CLA	CHC-C1C-NC	2.35	127.77	124.20
21	B	823	CLA	C1-C2-C3	-2.35	121.98	126.04
21	A	815	CLA	CBA-CAA-C2A	2.35	120.79	113.86
21	9	914	CLA	CHD-C4C-NC	2.35	127.90	124.20
24	F	405	BCR	C2-C1-C6	2.35	114.09	110.48
24	B	843	BCR	C24-C23-C22	-2.35	122.69	126.23
21	A	839	CLA	C5-C3-C2	-2.35	116.37	121.12
21	8	606	CLA	OBD-CAD-C3D	-2.35	122.88	128.52
21	6	907	CLA	CHD-C4C-NC	2.35	127.90	124.20
21	A	828	CLA	CHD-C1D-C2D	-2.34	120.56	125.48
21	9	913	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
21	6	903	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
21	6	907	CLA	CED-O2D-CGD	2.34	121.24	115.94
28	12	509	DD6	C22-C16-C17	-2.34	104.92	108.98
21	9	913	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	F	404	CLA	CHD-C4C-NC	2.34	127.89	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	708	CLA	CMC-C2C-C1C	2.34	128.60	125.04
21	10	709	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	2	507	CLA	CHC-C1C-NC	2.34	127.75	124.20
21	9	902	CLA	CHC-C1C-NC	2.34	127.75	124.20
21	5	709	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	7	708	CLA	CHC-C1C-NC	2.34	127.75	124.20
21	B	834	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
22	A	845	PQN	C8-C9-C10	-2.34	115.39	119.81
21	12	506	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
21	1	516	CLA	O2A-CGA-O1A	-2.34	117.47	123.30
21	B	809	CLA	CHC-C1C-C2C	-2.34	120.26	126.72
21	10	707	CLA	CHD-C4C-NC	2.33	127.88	124.20
21	2	506	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
21	9	903	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
21	2	507	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
21	10	711	CLA	CHC-C1C-NC	2.33	127.74	124.20
21	12	502	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
21	2	506	CLA	CMC-C2C-C3C	2.33	132.45	126.12
21	3	705	CLA	CHB-C4A-NA	2.33	127.74	124.51
21	10	705	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
21	7	711	CLA	C2C-C1C-NC	2.33	112.16	109.97
21	2	509	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
21	5	704	CLA	CHD-C4C-NC	2.33	127.88	124.20
21	2	504	CLA	CHC-C1C-NC	2.33	127.74	124.20
21	13	503	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
21	B	839	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
21	B	813	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
21	A	839	CLA	C4D-C3D-CAD	-2.33	105.35	108.10
21	6	904	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
21	6	913	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
21	A	829	CLA	CMC-C2C-C1C	2.33	128.59	125.04
21	8	605	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	6	911	CLA	O2A-CGA-CBA	2.33	121.51	114.03
24	A	848	BCR	C8-C9-C10	2.33	122.52	118.94
21	10	712	CLA	C1-O2A-CGA	2.33	123.50	116.73
21	1	512	CLA	CMB-C2B-C3B	2.33	129.03	124.68
21	1	515	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
21	4	707	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
21	B	806	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
21	B	834	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
24	A	848	BCR	C35-C13-C14	-2.32	119.67	122.92
21	A	818	CLA	C4-C3-C2	-2.32	117.72	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	908	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
21	A	812	CLA	CMA-C3A-C2A	-2.32	104.46	113.83
21	7	714	CLA	CHC-C1C-NC	2.32	127.73	124.20
21	6	904	CLA	CHB-C4A-NA	2.32	127.72	124.51
21	B	806	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
21	1	505	CLA	C1-C2-C3	-2.32	122.03	126.04
21	A	814	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
21	1	501	CLA	CED-O2D-CGD	-2.32	110.69	115.94
21	A	813	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
28	5	713	DD6	C4-C3-C2	2.32	128.23	123.47
21	B	827	CLA	CHC-C1C-NC	2.32	127.72	124.20
21	5	702	CLA	CHC-C1C-NC	2.32	127.72	124.20
21	11	706	CLA	CMC-C2C-C1C	2.32	128.57	125.04
21	5	702	CLA	C1-C2-C3	-2.32	122.03	126.04
27	B	847	DGD	CFB-CEB-CDB	-2.32	102.65	114.42
24	J	103	BCR	C20-C21-C22	2.32	130.62	127.31
21	A	817	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
21	9	912	CLA	CMC-C2C-C1C	2.32	128.57	125.04
24	B	843	BCR	C36-C18-C19	2.32	121.73	118.08
21	A	808	CLA	C4A-NA-C1A	-2.32	105.66	106.71
21	3	704	CLA	O2D-CGD-CBD	2.32	115.39	111.27
21	12	505	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
21	10	707	CLA	CMB-C2B-C3B	2.32	129.01	124.68
22	A	845	PQN	C10-C5-C4	-2.32	118.17	120.68
21	1	512	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	A	830	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
21	4	705	CLA	CHB-C4A-NA	2.32	127.71	124.51
21	A	841	CLA	CED-O2D-CGD	2.31	121.16	115.94
21	11	710	CLA	CHD-C4C-NC	2.31	127.84	124.20
21	4	704	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
21	A	820	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	B	828	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
21	12	501	CLA	CHC-C1C-NC	2.31	127.71	124.20
21	5	701	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
21	A	822	CLA	CHD-C4C-NC	2.31	127.84	124.20
21	7	712	CLA	CHC-C1C-NC	2.31	127.71	124.20
21	1	508	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	A	833	CLA	CGD-CBD-CAD	-2.31	103.26	110.73
21	2	517	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
21	B	838	CLA	CHD-C4C-NC	2.31	127.84	124.20
21	3	705	CLA	CED-O2D-CGD	2.31	121.15	115.94
21	A	804	CLA	CHC-C1C-NC	2.31	127.70	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	607	CLA	OBD-CAD-C3D	-2.31	122.97	128.52
21	2	514	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
28	5	713	DD6	C3-C4-C5	2.31	128.20	123.47
22	B	840	PQN	C6-C5-C10	2.30	121.82	119.26
24	F	402	BCR	C4-C5-C6	-2.30	119.39	122.73
21	6	906	CLA	CHD-C4C-NC	2.30	127.83	124.20
21	3	707	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
21	9	903	CLA	CAC-C3C-C4C	2.30	127.80	124.81
21	2	510	CLA	CMC-C2C-C1C	2.30	128.55	125.04
21	B	824	CLA	C3B-C4B-NB	2.30	112.19	109.21
28	6	915	DD6	C14-C13-C11	2.30	129.10	125.53
21	13	503	CLA	CED-O2D-CGD	2.30	121.15	115.94
21	3	715	CLA	C3B-C4B-NB	2.30	112.19	109.21
21	3	706	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	A	821	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
21	A	817	CLA	CHD-C4C-NC	2.30	127.83	124.20
21	B	801	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
24	J	102	BCR	C1-C6-C7	2.30	122.29	115.78
21	A	820	CLA	CHD-C4C-NC	2.30	127.83	124.20
21	A	806	CLA	C6-C5-C3	-2.30	107.43	113.45
21	2	513	CLA	C4C-C3C-C2C	-2.30	103.55	106.90
21	12	502	CLA	C4D-CHA-C1A	-2.30	118.45	121.25
28	5	713	DD6	C7-C6-C8	2.30	121.70	118.08
25	4	714	LHG	O4-P-O5	2.30	119.68	110.68
21	1	515	CLA	CHC-C1C-NC	2.30	127.69	124.20
21	A	823	CLA	CAC-C3C-C4C	2.30	127.79	124.81
21	B	824	CLA	CMC-C2C-C1C	2.30	128.54	125.04
21	6	905	CLA	CED-O2D-CGD	2.30	121.13	115.94
21	6	907	CLA	C3B-C4B-NB	2.30	112.18	109.21
25	7	717	LHG	O7-C5-C6	2.30	116.72	108.40
24	A	850	BCR	C28-C27-C26	-2.30	109.98	114.08
21	B	817	CLA	CHB-C4A-NA	2.30	127.69	124.51
21	9	907	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
21	9	908	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
21	A	862	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
21	9	914	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
28	3	718	DD6	C8-C6-C5	2.29	122.46	118.94
21	9	906	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
28	2	519	DD6	C23-C16-C15	-2.29	103.85	110.05
21	9	906	CLA	CED-O2D-CGD	2.29	121.12	115.94
21	6	913	CLA	CHC-C1C-NC	2.29	127.68	124.20
21	10	708	CLA	CMB-C2B-C3B	2.29	128.97	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	519	DD6	C7-C6-C5	-2.29	119.71	122.92
21	9	902	CLA	CHD-C4C-NC	2.29	127.81	124.20
21	12	505	CLA	CHD-C4C-NC	2.29	127.81	124.20
21	1	506	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
21	5	702	CLA	OBD-CAD-C3D	-2.29	123.01	128.52
21	A	807	CLA	CMA-C3A-C2A	-2.29	104.59	113.83
21	B	808	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
21	A	813	CLA	CHB-C4A-NA	2.29	127.68	124.51
21	6	903	CLA	CGD-CBD-CAD	-2.29	103.31	110.73
21	2	514	CLA	CMC-C2C-C1C	2.29	128.53	125.04
21	A	812	CLA	C6-C7-C8	-2.29	108.52	115.92
21	8	613	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
21	9	913	CLA	CMC-C2C-C1C	2.29	128.53	125.04
21	3	707	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
21	B	827	CLA	C7-C6-C5	-2.29	107.14	113.36
28	12	510	DD6	C4-C3-C2	2.29	128.16	123.47
21	5	703	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
25	10	713	LHG	O7-C5-C4	-2.29	100.12	108.40
28	7	716	DD6	C24-C1-C2	2.29	122.45	118.94
21	4	708	CLA	CHB-C4A-NA	2.29	127.67	124.51
21	3	714	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
21	12	507	CLA	CHD-C4C-NC	2.29	127.81	124.20
21	7	703	CLA	CHB-C4A-NA	2.29	127.67	124.51
21	2	504	CLA	C4A-NA-C1A	-2.29	105.68	106.71
21	6	909	CLA	C4C-C3C-C2C	-2.29	103.57	106.90
21	5	710	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	B	802	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
21	1	514	CLA	CHC-C1C-NC	2.28	127.67	124.20
21	A	817	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	F	405	BCR	C4-C5-C6	-2.28	119.42	122.73
21	A	820	CLA	C2A-C3A-C4A	-2.28	98.18	101.87
21	A	814	CLA	CMC-C2C-C1C	2.28	128.51	125.04
21	13	503	CLA	CMC-C2C-C1C	2.28	128.51	125.04
21	12	504	CLA	C2A-C1A-CHA	-2.28	119.87	123.85
28	2	518	DD6	C24-C1-C2	2.28	122.44	118.94
21	A	805	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
21	2	516	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
21	A	830	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	A	826	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	A	827	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	5	707	CLA	CHB-C4A-NA	2.28	127.66	124.51
21	1	505	CLA	C4C-C3C-C2C	-2.28	103.58	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	811	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
21	B	838	CLA	CED-O2D-CGD	-2.28	110.78	115.94
24	F	402	BCR	C15-C16-C17	2.28	128.14	123.47
21	B	816	CLA	CAA-C2A-C1A	-2.28	104.52	111.97
21	9	914	CLA	CHB-C4A-NA	2.28	127.66	124.51
21	B	813	CLA	O2A-CGA-CBA	2.27	119.04	111.91
21	11	704	CLA	O2A-CGA-O1A	-2.27	117.63	123.30
21	9	908	CLA	CMC-C2C-C1C	2.27	128.50	125.04
21	3	715	CLA	CMB-C2B-C3B	2.27	128.93	124.68
21	F	403	CLA	O2A-CGA-O1A	-2.27	117.63	123.30
21	9	913	CLA	CHD-C4C-NC	2.27	127.78	124.20
21	8	614	CLA	C1-O2A-CGA	2.27	123.33	116.73
21	4	710	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
21	A	830	CLA	CHB-C4A-NA	2.27	127.65	124.51
21	A	805	CLA	C4A-NA-C1A	-2.27	105.69	106.71
21	9	910	CLA	O2A-CGA-CBA	2.27	121.32	114.03
21	B	814	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
21	6	905	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
21	B	832	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
21	11	706	CLA	CMB-C2B-C3B	2.27	128.92	124.68
28	11	712	DD6	C33-C32-C31	2.27	114.22	109.62
28	6	915	DD6	C9-C8-C6	2.27	132.79	126.42
21	1	512	CLA	O2A-CGA-CBA	2.27	121.31	114.03
21	1	513	CLA	CHD-C4C-NC	2.27	127.78	124.20
28	2	519	DD6	O1-C20-C19	-2.27	111.68	113.38
28	12	510	DD6	C33-C32-C31	2.27	114.21	109.62
20	A	801	CL0	C11-C10-C8	-2.27	108.59	115.92
21	B	838	CLA	CHC-C1C-NC	2.27	127.64	124.20
21	6	913	CLA	CMC-C2C-C1C	2.27	128.49	125.04
21	7	709	CLA	O1D-CGD-CBD	2.27	129.12	124.48
21	3	715	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
21	A	816	CLA	O2A-CGA-O1A	-2.27	117.65	123.30
24	B	845	BCR	C36-C18-C17	-2.27	119.75	122.92
21	10	711	CLA	CBC-CAC-C3C	-2.27	106.19	112.43
21	10	712	CLA	CHD-C4C-NC	2.27	127.77	124.20
21	11	706	CLA	CHA-C1A-NA	-2.26	121.21	126.40
21	9	907	CLA	CGD-CBD-CAD	-2.26	103.40	110.73
24	A	848	BCR	C23-C22-C21	-2.26	115.47	118.94
21	11	705	CLA	CHD-C4C-NC	2.26	127.77	124.20
21	B	810	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	4	705	CLA	CHC-C1C-NC	2.26	127.64	124.20
21	B	829	CLA	O2A-CGA-O1A	-2.26	117.66	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	7	716	DD6	C4-C5-C6	2.26	130.54	127.31
21	2	509	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
21	2	517	CLA	CMB-C2B-C3B	2.26	128.91	124.68
21	B	808	CLA	CHC-C1C-NC	2.26	127.63	124.20
24	M	102	BCR	C16-C15-C14	2.26	128.10	123.47
21	6	911	CLA	CHA-C1A-NA	-2.26	121.22	126.40
21	10	706	CLA	C2A-C1A-CHA	-2.26	119.91	123.85
21	8	607	CLA	CHD-C4C-NC	2.26	127.77	124.20
21	10	710	CLA	C4-C3-C5	2.26	119.07	115.27
21	B	838	CLA	CGD-CBD-CAD	-2.26	103.42	110.73
21	6	906	CLA	CHB-C4A-NA	2.26	127.64	124.51
21	A	807	CLA	OBD-CAD-C3D	-2.26	123.09	128.52
21	B	821	CLA	OBD-CAD-C3D	-2.26	123.09	128.52
21	B	839	CLA	CMB-C2B-C3B	2.26	128.90	124.68
21	9	912	CLA	CAC-C3C-C4C	2.26	127.74	124.81
21	9	913	CLA	CHB-C4A-NA	2.26	127.63	124.51
21	4	703	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
21	A	827	CLA	CMA-C3A-C2A	-2.26	104.73	113.83
21	A	843	CLA	CMA-C3A-C2A	-2.26	104.73	113.83
21	7	706	CLA	CHA-C1A-NA	-2.25	121.23	126.40
21	6	907	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
21	A	825	CLA	C4D-C3D-CAD	-2.25	105.44	108.10
21	B	804	CLA	CBA-CAA-C2A	2.25	120.52	113.86
21	B	827	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
21	A	804	CLA	C3B-C4B-NB	2.25	112.12	109.21
28	7	716	DD6	C4-C3-C2	2.25	128.09	123.47
21	6	906	CLA	CHC-C1C-NC	2.25	127.62	124.20
21	B	801	CLA	CMB-C2B-C3B	2.25	128.89	124.68
28	5	712	DD6	C28-C27-C29	2.25	121.30	116.84
21	13	501	CLA	CHB-C4A-NA	2.25	127.63	124.51
21	11	707	CLA	CHD-C4C-NC	2.25	127.75	124.20
21	B	817	CLA	O1A-CGA-CBA	-2.25	114.95	123.73
24	B	846	BCR	C11-C10-C9	2.25	130.52	127.31
21	B	813	CLA	C4D-C3D-CAD	-2.25	105.44	108.10
21	4	704	CLA	CHB-C4A-NA	2.25	127.62	124.51
21	12	508	CLA	CHB-C4A-NA	2.25	127.62	124.51
21	1	514	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
21	B	820	CLA	CAC-C3C-C2C	2.25	131.38	127.53
21	A	836	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
21	11	702	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	2	507	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
21	3	712	CLA	CAA-C2A-C3A	-2.25	106.62	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	708	CLA	CHC-C1C-NC	2.25	127.61	124.20
21	1	509	CLA	CMA-C3A-C4A	-2.25	105.73	111.77
21	8	604	CLA	C3B-C4B-NB	2.25	112.12	109.21
21	3	715	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
24	A	850	BCR	C37-C22-C23	2.25	121.62	118.08
21	9	905	CLA	C1-C2-C3	-2.25	123.11	126.75
24	A	852	BCR	C34-C9-C10	-2.25	119.78	122.92
21	B	832	CLA	C1-O2A-CGA	2.25	122.34	116.44
21	2	504	CLA	C7-C6-C5	-2.25	107.26	113.36
21	A	815	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
21	A	814	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
21	7	712	CLA	O2A-CGA-O1A	-2.25	117.70	123.30
28	5	712	DD6	C34-C35-C36	-2.24	107.38	111.85
24	A	850	BCR	C24-C25-C26	-2.24	116.02	121.46
21	B	819	CLA	CMB-C2B-C3B	2.24	128.88	124.68
21	A	802	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
21	B	807	CLA	CHB-C4A-NA	2.24	127.62	124.51
25	B	848	LHG	O4-P-O5	2.24	123.33	112.24
21	B	832	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
21	A	822	CLA	C1-O2A-CGA	2.24	122.33	116.44
21	12	505	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
21	3	706	CLA	CAC-C3C-C4C	2.24	127.72	124.81
21	9	906	CLA	CMB-C2B-C3B	2.24	128.88	124.68
21	B	819	CLA	CHD-C4C-NC	2.24	127.74	124.20
21	B	827	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
21	7	709	CLA	OBD-CAD-C3D	-2.24	123.12	128.52
21	3	715	CLA	C4D-CHA-C1A	-2.24	118.52	121.25
21	4	704	CLA	C1-C2-C3	-2.24	123.12	126.75
21	9	914	CLA	C1-O2A-CGA	2.24	123.24	116.73
21	11	705	CLA	C3A-C2A-C1A	-2.24	97.98	101.34
21	1	509	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	9	914	CLA	CED-O2D-CGD	2.24	121.00	115.94
21	3	704	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
21	5	711	CLA	CHC-C1C-NC	2.24	127.60	124.20
21	A	840	CLA	CGD-CBD-CAD	-2.24	103.48	110.73
21	9	902	CLA	CMB-C2B-C3B	2.24	128.87	124.68
21	12	508	CLA	CMC-C2C-C1C	2.24	128.45	125.04
21	A	830	CLA	CHD-C1D-ND	-2.24	122.40	124.45
21	A	818	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
21	B	835	CLA	C1-O2A-CGA	2.24	122.32	116.44
21	B	833	CLA	CED-O2D-CGD	-2.24	110.88	115.94
24	A	850	BCR	C15-C14-C13	2.24	130.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	10	712	CLA	CMC-C2C-C1C	2.24	128.45	125.04
21	B	810	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
21	7	709	CLA	O2D-CGD-CBD	2.24	115.24	111.27
21	A	807	CLA	C1-O2A-CGA	2.24	122.31	116.44
21	12	503	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
21	A	831	CLA	OBD-CAD-C3D	-2.24	123.14	128.52
21	B	829	CLA	CBA-CAA-C2A	2.24	120.46	113.86
21	9	903	CLA	CHC-C1C-NC	2.24	127.59	124.20
21	B	823	CLA	C4-C3-C2	-2.23	117.94	123.68
21	13	502	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
21	10	706	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
21	B	816	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
21	2	516	CLA	CHD-C1D-ND	-2.23	122.40	124.45
21	1	517	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
21	B	825	CLA	CAC-C3C-C4C	2.23	127.71	124.81
21	10	709	CLA	CED-O2D-CGD	2.23	120.99	115.94
21	4	706	CLA	CMB-C2B-C3B	2.23	128.85	124.68
21	6	914	CLA	CHD-C4C-NC	2.23	127.72	124.20
21	A	836	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
21	A	812	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	A	836	CLA	CHB-C4A-NA	2.23	127.60	124.51
21	B	828	CLA	CHB-C4A-NA	2.23	127.60	124.51
21	A	830	CLA	CMA-C3A-C2A	-2.23	104.83	113.83
21	B	829	CLA	CAA-C2A-C1A	-2.23	104.66	111.97
21	1	513	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
21	A	844	CLA	C11-C10-C8	-2.23	108.71	115.92
21	9	909	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
28	4	712	DD6	C9-C10-C11	2.23	130.49	127.31
21	B	808	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
21	3	701	CLA	CAA-C2A-C3A	-2.23	110.90	116.10
21	A	823	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
21	2	503	CLA	CAC-C3C-C4C	2.23	127.70	124.81
21	B	812	CLA	CMB-C2B-C3B	2.23	128.85	124.68
21	10	711	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
21	12	507	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
21	A	862	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
21	3	714	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
21	F	404	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
21	B	838	CLA	O2A-CGA-CBA	2.23	121.18	114.03
24	B	846	BCR	C15-C16-C17	2.23	128.03	123.47
21	2	516	CLA	CHC-C1C-NC	2.22	127.58	124.20
28	5	713	DD6	C40-C32-C31	-2.22	106.93	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	822	CLA	O2A-CGA-CBA	2.22	121.17	114.03
21	B	801	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
21	A	844	CLA	OBD-CAD-C3D	-2.22	123.17	128.52
21	3	713	CLA	CHC-C1C-NC	2.22	127.57	124.20
21	B	805	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
25	A	853	LHG	O4-P-O5	2.22	123.22	112.24
21	5	706	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
21	7	709	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
21	10	706	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
21	5	702	CLA	O2A-CGA-CBA	2.22	118.87	111.91
21	11	709	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
21	B	819	CLA	CHC-C1C-NC	2.22	127.57	124.20
21	13	502	CLA	CED-O2D-CGD	2.22	120.95	115.94
28	9	916	DD6	C13-C11-C10	2.22	122.34	118.94
21	11	705	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
21	1	512	CLA	O2A-CGA-O1A	-2.22	117.77	123.30
21	6	904	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
21	5	703	CLA	CMC-C2C-C1C	2.22	128.41	125.04
21	B	822	CLA	C4D-CHA-C1A	-2.22	118.55	121.25
21	B	821	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
21	12	507	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
21	2	503	CLA	CED-O2D-CGD	2.21	120.94	115.94
21	B	809	CLA	CHC-C1C-NC	2.21	127.56	124.20
21	A	838	CLA	C1-C2-C3	-2.21	122.22	126.04
21	A	832	CLA	CAA-C2A-C1A	2.21	119.23	111.97
21	11	704	CLA	CHD-C4C-NC	2.21	127.69	124.20
21	B	809	CLA	O2A-CGA-CBA	2.21	121.14	114.03
21	3	711	CLA	CMC-C2C-C1C	2.21	128.41	125.04
21	A	840	CLA	C4A-NA-C1A	-2.21	105.71	106.71
21	10	705	CLA	CHD-C4C-NC	2.21	127.69	124.20
28	11	712	DD6	C24-C1-C2	2.21	122.33	118.94
21	1	515	CLA	CED-O2D-CGD	2.21	120.94	115.94
21	3	704	CLA	CHB-C4A-NA	2.21	127.57	124.51
21	A	807	CLA	CAA-C2A-C1A	2.21	119.22	111.97
21	8	610	CLA	CHC-C1C-NC	2.21	127.56	124.20
21	9	913	CLA	CHC-C1C-NC	2.21	127.56	124.20
21	13	501	CLA	O2A-CGA-CBA	2.21	121.13	114.03
21	7	711	CLA	CAC-C3C-C4C	2.21	127.67	124.81
21	12	501	CLA	CHB-C4A-NA	2.21	127.56	124.51
21	B	825	CLA	CMA-C3A-C4A	-2.21	105.84	111.77
21	B	801	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
21	5	703	CLA	C2A-C1A-CHA	-2.21	120.00	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	904	CLA	CHC-C1C-NC	2.21	127.55	124.20
21	B	824	CLA	CHD-C4C-NC	2.21	127.68	124.20
21	6	904	CLA	C1-C2-C3	-2.20	122.23	126.04
21	9	905	CLA	CGD-CBD-CAD	-2.20	103.60	110.73
21	10	704	CLA	CMC-C2C-C1C	2.20	128.40	125.04
21	11	711	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	B	845	BCR	C35-C13-C14	-2.20	119.84	122.92
21	12	506	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
20	A	801	CL0	CHC-C1C-C2C	-2.20	120.63	126.72
21	A	826	CLA	CHD-C4C-NC	2.20	127.67	124.20
21	A	807	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
21	A	835	CLA	O2A-CGA-O1A	-2.20	117.82	123.30
21	B	807	CLA	C11-C10-C8	-2.20	108.81	115.92
21	9	913	CLA	C1-O2A-CGA	2.20	123.12	116.73
21	A	805	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
21	1	514	CLA	CMB-C2B-C3B	2.20	128.79	124.68
21	1	512	CLA	OBD-CAD-C3D	-2.20	123.23	128.52
21	12	504	CLA	C3C-C4C-NC	2.20	113.04	110.57
21	B	839	CLA	CHD-C4C-NC	2.20	127.67	124.20
21	A	843	CLA	O2A-C1-C2	2.20	114.41	108.64
21	7	705	CLA	O2A-C1-C2	2.20	114.41	108.64
21	3	713	CLA	CMC-C2C-C1C	2.20	128.38	125.04
28	1	519	DD6	C23-C16-C15	2.20	115.97	110.05
21	9	905	CLA	CED-O2D-CGD	2.19	120.90	115.94
21	12	501	CLA	CMA-C3A-C2A	-2.19	104.97	113.83
21	A	809	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
21	10	704	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
21	4	707	CLA	CHC-C1C-NC	2.19	127.53	124.20
21	6	910	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
21	A	844	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
28	6	915	DD6	C7-C6-C5	-2.19	119.85	122.92
21	8	613	CLA	O2A-CGA-O1A	-2.19	117.83	123.30
21	5	705	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
21	6	914	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
21	7	702	CLA	CMA-C3A-C2A	-2.19	104.99	113.83
21	B	807	CLA	CBA-CAA-C2A	2.19	120.33	113.86
21	8	603	CLA	CAA-CBA-CGA	2.19	119.65	113.25
21	11	710	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
21	2	505	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
21	B	816	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
21	B	829	CLA	CMA-C3A-C2A	-2.19	105.00	113.83
21	4	711	CLA	CBC-CAC-C3C	-2.19	106.39	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	905	CLA	C4A-NA-C1A	-2.19	105.72	106.71
21	8	614	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
21	1	514	CLA	CHA-C1A-NA	-2.19	121.39	126.40
21	A	825	CLA	C1-O2A-CGA	2.19	122.18	116.44
21	11	708	CLA	CHC-C1C-NC	2.19	127.52	124.20
21	B	807	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
21	6	911	CLA	CHB-C4A-NA	2.19	127.54	124.51
21	A	835	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
21	3	714	CLA	CHB-C4A-NA	2.19	127.53	124.51
21	A	832	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
21	8	612	CLA	CMB-C2B-C3B	2.18	128.77	124.68
21	4	707	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
21	B	806	CLA	CHA-C1A-NA	-2.18	121.40	126.40
24	A	852	BCR	C15-C14-C13	2.18	130.43	127.31
21	B	835	CLA	CGD-CBD-CAD	-2.18	103.67	110.73
21	10	707	CLA	CBA-CAA-C2A	2.18	120.30	113.86
21	3	705	CLA	CHD-C4C-NC	2.18	127.64	124.20
21	13	502	CLA	CHB-C4A-NA	2.18	127.53	124.51
21	8	604	CLA	C6-C5-C3	-2.18	107.73	113.45
21	10	709	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
21	B	838	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
21	7	706	CLA	CED-O2D-CGD	2.18	120.87	115.94
21	9	910	CLA	CHB-C4A-NA	2.18	127.53	124.51
21	8	610	CLA	CMA-C3A-C2A	-2.18	105.04	113.83
21	7	712	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
21	11	708	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
28	6	916	DD6	O1-C20-C19	-2.18	111.75	113.38
24	A	851	BCR	C11-C10-C9	2.18	130.42	127.31
21	12	504	CLA	CMA-C3A-C2A	-2.18	111.01	116.10
21	6	907	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	A	850	BCR	C34-C9-C8	2.18	121.51	118.08
21	2	505	CLA	CHB-C4A-NA	2.18	127.52	124.51
21	7	712	CLA	CHA-C1A-NA	-2.18	121.41	126.40
21	3	709	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
21	11	710	CLA	CHC-C1C-NC	2.18	127.51	124.20
21	11	706	CLA	C6-C7-C8	-2.18	108.88	115.92
21	B	811	CLA	CMB-C2B-C3B	2.18	128.75	124.68
21	A	824	CLA	C3B-C4B-NB	2.18	112.03	109.21
21	2	514	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
21	A	822	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
21	B	835	CLA	C4D-CHA-C1A	-2.18	118.60	121.25
21	A	829	CLA	CAA-C2A-C3A	-2.18	106.82	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	836	CLA	CHB-C4A-NA	2.18	127.52	124.51
21	4	711	CLA	CHD-C4C-NC	2.18	127.63	124.20
21	A	831	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
21	10	705	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
21	3	701	CLA	C4A-NA-C1A	-2.18	105.73	106.71
28	2	520	DD6	C13-C11-C10	2.18	122.28	118.94
21	12	503	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
21	A	813	CLA	C6-C5-C3	2.17	119.16	113.45
21	11	711	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
24	A	849	BCR	C35-C13-C14	-2.17	119.88	122.92
21	7	711	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
21	10	711	CLA	CHB-C4A-NA	2.17	127.52	124.51
25	A	854	LHG	O4-P-O5	2.17	122.98	112.24
21	7	708	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
28	6	915	DD6	C4-C3-C2	2.17	127.92	123.47
21	A	831	CLA	C4D-CHA-C1A	-2.17	118.61	121.25
21	9	905	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
21	A	827	CLA	C1-C2-C3	-2.17	122.29	126.04
21	B	833	CLA	C3B-C4B-NB	2.17	112.02	109.21
21	B	833	CLA	CAA-CBA-CGA	-2.17	106.74	112.51
21	12	503	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
21	3	706	CLA	CMB-C2B-C3B	2.17	128.74	124.68
21	2	505	CLA	C4D-CHA-C1A	-2.17	118.61	121.25
21	8	608	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
21	A	838	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
21	B	825	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
21	11	704	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
21	B	804	CLA	C16-C17-C18	-2.17	105.76	115.98
21	A	828	CLA	C11-C12-C13	-2.17	108.91	115.92
21	6	903	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	2	514	CLA	O2A-CGA-CBA	2.17	120.99	114.03
21	7	706	CLA	CHC-C1C-NC	2.17	127.49	124.20
21	12	507	CLA	CHA-C1A-NA	-2.17	121.44	126.40
21	B	805	CLA	C4-C3-C5	2.17	118.92	115.27
21	6	904	CLA	C4C-C3C-C2C	-2.17	103.74	106.90
21	6	913	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
21	13	501	CLA	O2A-CGA-O1A	-2.17	117.90	123.30
28	3	717	DD6	C3-C4-C5	2.17	127.91	123.47
21	A	804	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	B	828	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
21	5	701	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
21	B	804	CLA	CHC-C1C-NC	2.17	127.49	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	516	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
21	8	610	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
21	B	836	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
21	A	807	CLA	CMC-C2C-C1C	2.16	128.34	125.04
21	B	833	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
21	8	611	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
21	7	709	CLA	CMA-C3A-C2A	-2.16	105.10	113.83
28	6	915	DD6	C37-C36-C35	2.16	118.36	114.36
21	5	709	CLA	O2A-CGA-CBA	2.16	120.98	114.03
21	A	811	CLA	CMA-C3A-C4A	-2.16	105.96	111.77
21	4	706	CLA	CMA-C3A-C2A	-2.16	105.10	113.83
28	6	916	DD6	C24-C1-C2	2.16	122.26	118.94
24	B	846	BCR	C20-C21-C22	2.16	130.40	127.31
21	B	804	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
21	5	710	CLA	CHC-C1C-NC	2.16	127.48	124.20
21	A	826	CLA	C6-C5-C3	2.16	119.12	113.45
21	5	705	CLA	CMB-C2B-C3B	2.16	128.72	124.68
21	2	514	CLA	CBA-CAA-C2A	2.16	120.24	113.86
21	A	822	CLA	CHC-C1C-NC	2.16	127.48	124.20
21	9	910	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
21	A	844	CLA	CMB-C2B-C1B	2.16	131.78	128.46
21	A	819	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
21	2	509	CLA	O2A-C1-C2	2.16	114.31	108.64
21	A	810	CLA	CMB-C2B-C3B	2.16	128.72	124.68
21	6	906	CLA	CHA-C1A-NA	-2.16	121.45	126.40
21	4	706	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
21	8	609	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	8	604	CLA	O2A-CGA-CBA	2.16	118.68	111.91
21	B	807	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
21	B	815	CLA	O2A-CGA-CBA	2.16	118.68	111.91
21	7	706	CLA	C3B-C4B-NB	2.16	112.00	109.21
21	1	516	CLA	CMB-C2B-C3B	2.16	128.71	124.68
21	B	804	CLA	C14-C13-C12	-2.16	103.48	111.29
21	B	817	CLA	CBA-CAA-C2A	2.16	120.23	113.86
21	4	705	CLA	CHA-C1A-NA	-2.16	121.46	126.40
21	7	712	CLA	CHB-C4A-NA	2.16	127.49	124.51
21	12	501	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
21	3	708	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
21	A	818	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
21	1	513	CLA	C4-C3-C5	2.15	118.89	115.27
21	B	838	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
21	F	403	CLA	O2A-CGA-CBA	2.15	120.95	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	521	LHG	O7-C5-C6	2.15	116.20	108.40
21	A	814	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
21	11	709	CLA	CMB-C2B-C3B	2.15	128.71	124.68
21	3	711	CLA	CHD-C4C-NC	2.15	127.59	124.20
21	10	703	CLA	CHB-C4A-NA	2.15	127.49	124.51
21	4	703	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
21	A	822	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
21	A	843	CLA	CAC-C3C-C4C	2.15	127.60	124.81
21	B	804	CLA	O1A-CGA-CBA	-2.15	115.34	123.73
21	9	906	CLA	CHB-C4A-NA	2.15	127.49	124.51
21	5	702	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	5	704	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
21	B	824	CLA	CHD-C1D-ND	-2.15	122.48	124.45
24	A	849	BCR	C29-C30-C25	2.15	113.79	110.48
24	A	847	BCR	C16-C15-C14	2.15	127.87	123.47
28	11	712	DD6	C4-C5-C6	2.15	130.37	127.31
21	3	713	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
21	4	711	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
21	A	843	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
28	2	518	DD6	C10-C9-C8	2.15	129.91	123.22
21	12	504	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
21	1	516	CLA	O2A-CGA-CBA	2.14	120.92	114.03
21	B	835	CLA	O1A-CGA-CBA	-2.14	115.37	123.73
28	3	718	DD6	C26-C25-C24	2.14	129.90	123.22
24	B	843	BCR	C29-C30-C25	2.14	113.78	110.48
21	4	701	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
21	9	907	CLA	CMC-C2C-C1C	2.14	128.30	125.04
21	A	806	CLA	CMA-C3A-C2A	-2.14	105.19	113.83
21	A	820	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
21	B	819	CLA	CGD-CBD-CAD	-2.14	103.80	110.73
21	5	706	CLA	CMC-C2C-C1C	2.14	128.30	125.04
28	3	717	DD6	C9-C10-C11	2.14	130.36	127.31
28	1	519	DD6	O1-C20-C19	-2.14	111.78	113.38
28	J	104	DD6	C37-C36-C31	-2.14	121.44	124.35
21	7	709	CLA	C4A-NA-C1A	-2.14	105.75	106.71
21	5	703	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
21	4	702	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
28	9	915	DD6	C20-C19-C18	-2.14	108.52	112.75
21	4	706	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
21	B	802	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
21	4	711	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
21	6	904	CLA	CGD-CBD-CAD	-2.14	103.82	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	715	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
28	1	519	DD6	C-C1-C2	-2.13	119.93	122.92
21	10	707	CLA	CMC-C2C-C1C	2.13	128.29	125.04
21	B	802	CLA	CMB-C2B-C3B	2.13	128.67	124.68
21	11	706	CLA	CHC-C1C-NC	2.13	127.44	124.20
21	2	510	CLA	CHB-C4A-NA	2.13	127.46	124.51
28	12	509	DD6	C13-C11-C10	2.13	122.21	118.94
21	6	909	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
21	10	710	CLA	CMC-C2C-C1C	2.13	128.29	125.04
21	A	816	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	A	862	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
21	2	513	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
21	B	815	CLA	CHD-C4C-NC	2.13	127.56	124.20
21	A	829	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
21	B	812	CLA	CHD-C4C-NC	2.13	127.56	124.20
21	7	708	CLA	CHD-C4C-NC	2.13	127.56	124.20
28	11	712	DD6	C7-C6-C5	-2.13	119.94	122.92
27	B	847	DGD	C2G-O2G-C1B	-2.13	112.55	117.79
28	5	713	DD6	C24-C1-C2	2.13	122.21	118.94
21	3	714	CLA	O2A-CGA-CBA	2.13	120.87	114.03
24	A	850	BCR	C1-C6-C7	2.13	121.80	115.78
28	8	615	DD6	C12-C11-C13	2.13	121.43	118.08
21	9	904	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
21	6	906	CLA	CMC-C2C-C1C	2.13	128.28	125.04
24	A	848	BCR	C2-C1-C6	2.13	113.75	110.48
21	A	843	CLA	C1-C2-C3	-2.13	122.36	126.04
21	2	504	CLA	CMA-C3A-C2A	-2.13	105.25	113.83
21	A	809	CLA	CMC-C2C-C1C	2.13	128.28	125.04
21	B	835	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
21	B	837	CLA	C3B-C4B-NB	2.12	111.96	109.21
25	11	714	LHG	O7-C7-C8	-2.12	106.92	111.50
21	5	701	CLA	O2A-CGA-CBA	2.12	120.86	114.03
21	11	707	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
21	2	511	CLA	CHB-C4A-NA	2.12	127.45	124.51
21	1	501	CLA	CHA-C1A-NA	-2.12	121.53	126.40
21	A	821	CLA	CAC-C3C-C4C	2.12	127.56	124.81
21	B	802	CLA	C11-C12-C13	-2.12	109.06	115.92
24	F	405	BCR	C16-C17-C18	2.12	130.34	127.31
21	B	830	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
21	6	904	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
21	13	502	CLA	CHD-C4C-NC	2.12	127.55	124.20
21	9	907	CLA	C1B-CHB-C4A	-2.12	125.91	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	818	CLA	C1-C2-C3	-2.12	122.37	126.04
21	10	707	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
21	1	506	CLA	CMC-C2C-C1C	2.12	128.27	125.04
21	13	502	CLA	CMC-C2C-C1C	2.12	128.27	125.04
28	2	519	DD6	C15-C14-C13	-2.12	121.51	125.99
21	B	821	CLA	C1-C2-C3	-2.12	122.38	126.04
21	A	804	CLA	CMA-C3A-C2A	-2.12	105.27	113.83
21	A	824	CLA	O2A-CGA-CBA	2.12	118.56	111.91
21	A	831	CLA	CHB-C4A-NA	2.12	127.44	124.51
21	A	823	CLA	C2C-C1C-NC	2.12	111.96	109.97
21	8	610	CLA	CMC-C2C-C1C	2.12	128.27	125.04
24	B	843	BCR	C23-C22-C21	2.12	122.19	118.94
21	A	828	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	A	847	BCR	C36-C18-C17	-2.12	119.95	122.92
21	B	832	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
21	B	838	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
21	A	862	CLA	CMB-C2B-C3B	2.12	128.64	124.68
28	5	712	DD6	C9-C10-C11	2.12	130.33	127.31
21	7	703	CLA	C1-C2-C3	-2.12	122.38	126.04
21	5	704	CLA	C5-C3-C4	2.12	119.28	114.60
25	6	917	LHG	O4-P-O5	2.12	122.70	112.24
28	6	915	DD6	C24-C1-C2	2.12	122.19	118.94
21	10	706	CLA	CHB-C4A-NA	2.12	127.44	124.51
21	7	706	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
21	A	831	CLA	O2A-CGA-CBA	2.11	118.54	111.91
21	B	814	CLA	O2A-CGA-CBA	2.11	120.82	114.03
21	A	821	CLA	CHD-C4C-NC	2.11	127.54	124.20
21	A	802	CLA	CHB-C4A-NA	2.11	127.44	124.51
21	A	818	CLA	CAA-C2A-C1A	-2.11	105.05	111.97
21	11	702	CLA	CHC-C1C-NC	2.11	127.41	124.20
28	5	712	DD6	C15-C14-C13	-2.11	121.53	125.99
21	B	836	CLA	CHD-C4C-NC	2.11	127.53	124.20
21	9	907	CLA	CAC-C3C-C4C	2.11	127.55	124.81
21	A	838	CLA	CHC-C1C-NC	2.11	127.41	124.20
21	2	509	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
21	A	818	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
21	4	705	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	9	903	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
21	10	703	CLA	CAA-C2A-C1A	-2.11	106.59	111.81
21	B	835	CLA	CMC-C2C-C1C	2.11	128.25	125.04
21	B	803	CLA	C5-C3-C2	-2.11	116.84	121.12
21	12	506	CLA	C1-C2-C3	-2.11	122.39	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	705	CLA	C1-O2A-CGA	2.11	122.86	116.73
21	A	835	CLA	CHD-C4C-NC	2.11	127.53	124.20
21	A	828	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
21	7	709	CLA	CMB-C2B-C3B	2.11	128.63	124.68
21	8	603	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
28	3	716	DD6	C7-C6-C5	-2.11	119.97	122.92
21	3	709	CLA	CGD-CBD-CAD	-2.11	103.90	110.73
21	12	508	CLA	CMB-C2B-C3B	2.11	128.62	124.68
21	A	806	CLA	C1-O2A-CGA	2.11	121.98	116.44
21	A	825	CLA	CHD-C4C-NC	2.11	127.53	124.20
21	1	507	CLA	C4C-C3C-C2C	-2.11	103.83	106.90
21	B	839	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
21	2	503	CLA	C4A-NA-C1A	-2.11	105.76	106.71
21	9	914	CLA	CMB-C2B-C3B	2.11	128.62	124.68
21	10	707	CLA	CHC-C1C-NC	2.10	127.40	124.20
21	A	840	CLA	C1-O2A-CGA	2.10	122.84	116.73
21	2	513	CLA	CMB-C2B-C3B	2.10	128.62	124.68
21	4	703	CLA	CHC-C1C-NC	2.10	127.39	124.20
21	11	710	CLA	CHB-C4A-NA	2.10	127.42	124.51
21	3	702	CLA	CHC-C1C-NC	2.10	127.39	124.20
21	A	825	CLA	C4C-C3C-C2C	-2.10	103.83	106.90
21	2	508	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
21	A	817	CLA	CMB-C2B-C3B	2.10	128.61	124.68
21	A	838	CLA	CHD-C4C-NC	2.10	127.52	124.20
24	A	849	BCR	C24-C23-C22	-2.10	123.06	126.23
21	4	707	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
21	1	517	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
24	A	849	BCR	C34-C9-C8	-2.10	114.77	118.08
21	3	709	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
21	3	705	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
21	B	835	CLA	CHC-C1C-NC	2.10	127.39	124.20
21	1	508	CLA	CED-O2D-CGD	2.10	120.69	115.94
21	2	514	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
21	9	905	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
21	1	509	CLA	CAC-C3C-C4C	2.10	127.53	124.81
28	1	519	DD6	C3-C2-C1	2.10	130.30	127.31
21	11	703	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
21	1	507	CLA	C5-C3-C4	2.10	119.23	114.60
21	A	824	CLA	CHC-C1C-NC	2.10	127.38	124.20
21	3	703	CLA	C4D-CHA-C1A	-2.10	118.70	121.25
21	10	707	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
21	7	702	CLA	CHA-C1A-NA	-2.10	121.60	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	818	CLA	C2C-C1C-NC	2.10	111.94	109.97
21	A	819	CLA	CBC-CAC-C3C	-2.10	106.66	112.43
21	6	904	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
21	6	905	CLA	CMB-C2B-C3B	2.09	128.60	124.68
21	B	819	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
21	A	832	CLA	C3A-C2A-C1A	-2.09	98.20	101.34
21	A	814	CLA	CHC-C1C-NC	2.09	127.38	124.20
21	7	712	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
21	7	710	CLA	CMA-C3A-C2A	-2.09	105.38	113.83
21	7	707	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
21	A	842	CLA	C3B-C4B-NB	2.09	111.92	109.21
21	9	906	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	F	403	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
24	F	405	BCR	C11-C10-C9	-2.09	124.33	127.31
21	A	828	CLA	CHC-C1C-NC	2.09	127.38	124.20
21	5	705	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
21	3	703	CLA	CMC-C2C-C1C	2.09	128.22	125.04
21	A	837	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
21	A	812	CLA	C3B-C4B-NB	2.09	111.91	109.21
21	B	821	CLA	C3A-C2A-C1A	-2.09	98.21	101.34
21	13	502	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
21	8	614	CLA	CHC-C1C-NC	2.09	127.37	124.20
21	4	701	CLA	CAA-C2A-C3A	-2.09	111.22	116.10
20	A	801	CL0	CAC-C3C-C2C	2.09	131.10	127.53
21	B	819	CLA	C3A-C2A-C1A	-2.09	98.21	101.34
21	6	903	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
21	9	911	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
21	4	705	CLA	C3B-C4B-NB	2.09	111.91	109.21
21	2	510	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
21	5	710	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
21	A	827	CLA	CAC-C3C-C2C	2.09	131.10	127.53
21	7	712	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
21	7	704	CLA	CHC-C1C-NC	2.09	127.37	124.20
27	B	847	DGD	C1E-O6E-C5E	-2.09	109.59	113.69
21	9	905	CLA	CHD-C4C-NC	2.09	127.49	124.20
21	B	834	CLA	O2A-C1-C2	-2.09	103.15	108.64
21	11	706	CLA	CMA-C3A-C2A	-2.09	105.41	113.83
21	B	833	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
21	8	612	CLA	O2A-CGA-CBA	2.09	118.45	111.91
21	11	703	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
21	7	714	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
21	3	712	CLA	CMC-C2C-C1C	2.08	128.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	705	CLA	CHA-C1A-NA	-2.08	121.62	126.40
21	9	912	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
21	A	836	CLA	O2D-CGD-CBD	2.08	114.97	111.27
28	12	510	DD6	C9-C8-C6	2.08	132.27	126.42
21	5	706	CLA	CHA-C1A-NA	-2.08	121.63	126.40
21	3	707	CLA	C1-C2-C3	-2.08	122.44	126.04
21	2	507	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
21	A	810	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
21	7	712	CLA	CMB-C2B-C3B	2.08	128.57	124.68
24	J	102	BCR	C20-C21-C22	2.08	130.28	127.31
21	8	604	CLA	C1-C2-C3	-2.08	122.45	126.04
21	11	704	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
21	A	836	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	12	502	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
21	B	829	CLA	O2A-CGA-CBA	2.08	120.70	114.03
24	A	848	BCR	C33-C5-C6	2.08	126.86	124.53
21	A	832	CLA	CMC-C2C-C1C	2.08	128.20	125.04
21	10	709	CLA	CMC-C2C-C1C	2.08	128.20	125.04
24	A	849	BCR	C12-C13-C14	2.08	122.13	118.94
21	11	701	CLA	C2A-C1A-CHA	-2.08	120.23	123.85
21	2	516	CLA	CHA-C1A-NA	-2.07	121.65	126.40
21	9	908	CLA	C3C-C4C-NC	2.07	112.90	110.57
21	B	836	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
21	6	911	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
21	12	508	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
21	10	705	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
21	B	804	CLA	C4A-NA-C1A	-2.07	105.77	106.71
21	6	912	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
21	5	701	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
21	7	705	CLA	CHA-C1A-NA	-2.07	121.65	126.40
21	A	823	CLA	O2A-CGA-CBA	2.07	120.69	114.03
21	1	504	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
21	1	516	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	6	903	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	3	708	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
21	11	702	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
21	1	509	CLA	CMB-C2B-C3B	2.07	128.55	124.68
21	A	829	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
21	B	822	CLA	CMB-C2B-C3B	2.07	128.55	124.68
21	A	832	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
21	A	836	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
21	11	705	CLA	O2A-CGA-CBA	2.07	118.40	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	518	DD6	C12-C11-C13	2.07	121.34	118.08
21	B	825	CLA	C2A-C3A-C4A	2.07	105.21	101.87
21	B	818	CLA	C6-C7-C8	-2.07	109.23	115.92
21	A	802	CLA	CED-O2D-CGD	-2.07	111.26	115.94
21	2	511	CLA	CHA-C1A-NA	-2.07	121.66	126.40
21	B	815	CLA	C3B-C4B-NB	2.07	111.88	109.21
21	1	504	CLA	CMC-C2C-C1C	2.07	128.19	125.04
21	3	703	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
21	6	910	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
21	A	812	CLA	C11-C10-C8	-2.07	109.24	115.92
21	8	608	CLA	OBD-CAD-C3D	-2.07	123.55	128.52
28	2	519	DD6	C21-C20-C15	-2.07	118.80	122.26
24	B	846	BCR	C16-C15-C14	2.06	127.70	123.47
21	11	702	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
21	J	101	CLA	CMA-C3A-C2A	-2.06	105.50	113.83
21	13	502	CLA	CHC-C1C-NC	2.06	127.33	124.20
21	A	819	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
21	B	821	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
28	2	519	DD6	C3-C2-C1	2.06	130.26	127.31
21	3	713	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
21	1	507	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
21	J	101	CLA	CHB-C4A-NA	2.06	127.36	124.51
21	9	912	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
21	3	711	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
21	4	707	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
21	12	506	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
21	1	513	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
21	A	842	CLA	O1A-CGA-CBA	-2.06	115.69	123.73
28	11	713	DD6	C20-C19-C18	-2.06	108.67	112.75
21	A	837	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
21	4	707	CLA	CGD-CBD-CAD	-2.06	104.06	110.73
21	12	503	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
21	4	701	CLA	CMC-C2C-C1C	2.06	128.18	125.04
21	B	824	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
21	9	906	CLA	CHD-C4C-NC	2.06	127.45	124.20
21	A	819	CLA	CHD-C4C-NC	2.06	127.45	124.20
21	11	702	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
21	B	826	CLA	CED-O2D-CGD	-2.06	111.28	115.94
21	B	808	CLA	O2A-CGA-CBA	2.06	120.64	114.03
28	4	712	DD6	C33-C32-C31	2.06	113.79	109.62
21	1	515	CLA	CHB-C4A-NA	2.06	127.36	124.51
21	A	803	CLA	C4D-CHA-C1A	-2.06	118.75	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	708	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
21	5	707	CLA	CAC-C3C-C4C	2.05	127.48	124.81
28	1	519	DD6	C14-C13-C11	2.05	128.72	125.53
21	B	823	CLA	CMB-C2B-C3B	2.05	128.52	124.68
21	3	704	CLA	CBA-CAA-C2A	2.05	118.04	113.47
21	A	830	CLA	CHD-C4C-NC	2.05	127.44	124.20
21	F	403	CLA	C3A-C2A-C1A	-2.05	98.26	101.34
28	1	520	DD6	C32-C31-C36	-2.05	119.73	122.63
21	12	505	CLA	CHB-C4A-NA	2.05	127.35	124.51
21	11	701	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
21	3	711	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	5	709	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	11	705	CLA	C1-O2A-CGA	2.05	122.69	116.73
21	9	907	CLA	CED-O2D-CGD	2.05	120.58	115.94
21	B	819	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
21	A	819	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
24	B	841	BCR	C30-C25-C24	-2.05	109.98	115.78
28	3	716	DD6	O1-C20-C21	-2.05	112.60	115.06
21	2	504	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
21	B	813	CLA	C1-O2A-CGA	2.05	121.82	116.44
21	6	911	CLA	CAC-C3C-C2C	2.05	131.03	127.53
21	B	805	CLA	CHA-C1A-NA	-2.05	121.71	126.40
21	1	516	CLA	CHC-C1C-NC	2.05	127.31	124.20
21	B	839	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
21	B	821	CLA	CMB-C2B-C3B	2.05	128.51	124.68
21	A	804	CLA	C3A-C2A-C1A	-2.05	98.27	101.34
21	3	702	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
21	9	910	CLA	CAA-CBA-CGA	2.05	117.94	112.51
21	A	821	CLA	C9-C8-C10	2.05	118.70	111.29
21	8	613	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
21	B	822	CLA	CMA-C3A-C2A	-2.04	105.58	113.83
21	A	827	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
21	5	703	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
21	9	904	CLA	CHB-C4A-NA	2.04	127.34	124.51
21	6	914	CLA	O2A-C1-C2	2.04	115.93	108.42
21	9	914	CLA	CMC-C2C-C1C	2.04	128.15	125.04
21	2	504	CLA	C1-O2A-CGA	2.04	121.81	116.44
21	8	613	CLA	CHC-C1C-NC	2.04	127.30	124.20
28	4	712	DD6	C3-C4-C5	2.04	127.66	123.47
21	11	705	CLA	CHC-C1C-NC	2.04	127.30	124.20
21	2	504	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
21	2	515	CLA	CHA-C1A-NA	-2.04	121.72	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	825	CLA	C1-O2A-CGA	2.04	121.80	116.44
21	3	714	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
21	B	822	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
21	A	811	CLA	C4D-CHA-C1A	-2.04	118.77	121.25
21	B	826	CLA	C5-C3-C2	-2.04	116.99	121.12
21	A	838	CLA	CHA-C1A-NA	-2.04	121.73	126.40
21	6	914	CLA	CMA-C3A-C2A	-2.04	105.61	113.83
28	2	519	DD6	C-C1-C2	-2.04	120.07	122.92
21	5	711	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
21	B	838	CLA	C3B-C4B-NB	2.04	111.84	109.21
21	2	506	CLA	CHD-C4C-NC	2.04	127.41	124.20
21	8	609	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
21	4	709	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
21	2	507	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
21	11	709	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
21	A	807	CLA	C11-C10-C8	-2.04	109.34	115.92
21	6	904	CLA	C4-C3-C5	2.03	118.69	115.27
21	4	701	CLA	CHB-C4A-NA	2.03	127.33	124.51
21	1	511	CLA	CHC-C1C-NC	2.03	127.29	124.20
24	B	844	BCR	C38-C26-C25	2.03	126.81	124.53
21	A	832	CLA	CHA-C1A-NA	-2.03	121.74	126.40
25	A	854	LHG	O7-C7-C8	2.03	115.88	111.50
21	7	705	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
21	1	517	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
21	11	711	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
21	3	711	CLA	CAA-CBA-CGA	-2.03	107.12	112.51
28	6	915	DD6	C9-C10-C11	2.03	130.21	127.31
21	8	606	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
21	8	613	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
21	1	512	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
21	3	710	CLA	CHB-C4A-NA	2.03	127.32	124.51
21	1	510	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
21	B	818	CLA	CHB-C4A-NA	2.03	127.32	124.51
21	10	710	CLA	CHB-C4A-NA	2.03	127.32	124.51
21	B	809	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
28	9	916	DD6	C37-C36-C31	-2.03	121.59	124.35
21	5	706	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
21	2	513	CLA	CHC-C1C-NC	2.03	127.28	124.20
21	10	703	CLA	CED-O2D-CGD	2.03	120.52	115.94
21	10	707	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
21	B	831	CLA	OBD-CAD-C3D	-2.03	123.65	128.52
21	A	832	CLA	CHD-C4C-NC	2.03	127.39	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	516	CLA	O2A-CGA-CBA	2.03	120.54	114.03
21	A	834	CLA	CAA-CBA-CGA	-2.02	107.13	112.51
21	2	517	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
21	7	713	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
21	13	502	CLA	C1-O2A-CGA	2.02	122.61	116.73
21	5	704	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
21	2	515	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
21	2	503	CLA	CMB-C2B-C3B	2.02	128.46	124.68
21	A	816	CLA	CAA-CBA-CGA	-2.02	107.14	112.51
21	1	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	B	836	CLA	CED-O2D-CGD	-2.02	111.36	115.94
21	A	820	CLA	C5-C3-C2	2.02	125.21	121.12
21	B	836	CLA	C4D-CHA-C1A	2.02	123.71	121.25
21	8	607	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
20	A	801	CL0	C4C-C3C-C2C	-2.02	103.95	106.90
21	4	707	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
21	5	708	CLA	CHC-C1C-NC	2.02	127.27	124.20
21	B	832	CLA	O2A-CGA-CBA	2.02	118.24	111.91
21	8	607	CLA	CHA-C1A-NA	-2.02	121.78	126.40
21	3	712	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
21	11	711	CLA	O2A-CGA-CBA	2.02	120.51	114.03
21	8	608	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
21	F	403	CLA	CMB-C2B-C1B	2.02	131.56	128.46
21	B	818	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
21	11	701	CLA	CMA-C3A-C2A	-2.02	111.39	116.10
28	2	519	DD6	C37-C36-C31	-2.02	121.61	124.35
21	7	712	CLA	CMC-C2C-C1C	2.02	128.11	125.04
21	A	815	CLA	CAC-C3C-C2C	2.02	130.98	127.53
21	B	821	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
21	8	610	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
21	A	827	CLA	CGD-CBD-CAD	-2.02	104.20	110.73
21	7	712	CLA	O2A-CGA-CBA	2.01	120.50	114.03
21	9	903	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
21	10	709	CLA	O2A-CGA-CBA	2.01	120.50	114.03
21	7	713	CLA	CHD-C4C-NC	2.01	127.38	124.20
21	1	509	CLA	OBD-CAD-C3D	-2.01	123.67	128.52
21	8	610	CLA	CMB-C2B-C3B	2.01	128.44	124.68
21	7	713	CLA	CHB-C4A-NA	2.01	127.30	124.51
21	2	512	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
21	12	508	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
21	B	836	CLA	CAA-C2A-C1A	2.01	118.57	111.97
21	4	703	CLA	O2A-CGA-CBA	2.01	120.49	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	844	CLA	CMC-C2C-C1C	2.01	128.10	125.04
21	10	710	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
21	B	806	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
21	1	516	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
21	1	510	CLA	CHC-C1C-NC	2.01	127.25	124.20
21	5	705	CLA	C3A-C2A-C1A	-2.01	98.33	101.34
21	11	707	CLA	CMC-C2C-C1C	2.01	128.10	125.04
28	3	716	DD6	C23-C16-C17	2.01	112.47	108.98
21	1	514	CLA	CED-O2D-CGD	2.01	120.48	115.94
21	8	608	CLA	CHC-C1C-NC	2.01	127.25	124.20
21	2	517	CLA	CHB-C4A-NA	2.01	127.28	124.51
21	4	709	CLA	CHC-C1C-NC	2.01	127.25	124.20
24	B	845	BCR	C7-C8-C9	2.00	129.26	126.23
21	9	910	CLA	CMB-C2B-C1B	2.00	131.54	128.46
21	3	702	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
21	A	844	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
21	6	912	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
21	1	514	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
21	6	908	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
21	B	817	CLA	C9-C8-C10	2.00	118.54	111.29
21	8	611	CLA	O2A-CGA-CBA	2.00	120.46	114.03
21	B	839	CLA	C6-C7-C8	-2.00	109.45	115.92
21	10	704	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
28	3	717	DD6	C8-C6-C5	-2.00	115.87	118.94
21	10	711	CLA	CHA-C1A-NA	-2.00	121.81	126.40
21	10	706	CLA	CHC-C1C-NC	2.00	127.24	124.20
21	B	832	CLA	C4D-CHA-C1A	-2.00	118.81	121.25
21	6	912	CLA	CMC-C2C-C1C	2.00	128.09	125.04
21	7	707	CLA	CMA-C3A-C2A	-2.00	105.76	113.83
21	1	515	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
21	2	503	CLA	O2D-CGD-O1D	-2.00	119.93	123.84

All (198) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CL0	NA
20	A	801	CL0	NC
20	A	801	CL0	ND
21	A	802	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	807	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	811	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND
21	A	814	CLA	ND
21	A	815	CLA	ND
21	A	818	CLA	ND
21	A	819	CLA	ND
21	A	820	CLA	ND
21	A	821	CLA	ND
21	A	826	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND
21	A	831	CLA	ND
21	A	833	CLA	ND
21	A	834	CLA	ND
21	A	838	CLA	ND
21	A	839	CLA	ND
21	A	840	CLA	ND
21	A	841	CLA	ND
21	A	842	CLA	ND
21	A	843	CLA	ND
21	A	844	CLA	ND
21	A	862	CLA	ND
21	B	801	CLA	ND
21	B	802	CLA	ND
21	B	803	CLA	ND
21	B	804	CLA	ND
21	B	805	CLA	ND
21	B	806	CLA	ND
21	B	807	CLA	ND
21	B	808	CLA	ND
21	B	809	CLA	ND
21	B	810	CLA	ND
21	B	812	CLA	ND
21	B	813	CLA	ND
21	B	814	CLA	ND
21	B	815	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	816	CLA	ND
21	B	817	CLA	ND
21	B	818	CLA	ND
21	B	821	CLA	ND
21	B	822	CLA	ND
21	B	823	CLA	ND
21	B	824	CLA	ND
21	B	825	CLA	ND
21	B	826	CLA	ND
21	B	827	CLA	ND
21	B	828	CLA	ND
21	B	830	CLA	ND
21	B	831	CLA	ND
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	834	CLA	ND
21	B	835	CLA	ND
21	B	836	CLA	ND
21	B	837	CLA	ND
21	B	839	CLA	ND
21	F	401	CLA	ND
21	F	403	CLA	ND
21	F	404	CLA	ND
21	J	101	CLA	ND
21	1	501	CLA	ND
21	1	504	CLA	ND
21	1	505	CLA	ND
21	1	506	CLA	ND
21	1	507	CLA	ND
21	1	509	CLA	ND
21	1	510	CLA	ND
21	1	511	CLA	ND
21	1	512	CLA	ND
21	1	514	CLA	ND
21	1	515	CLA	ND
21	1	516	CLA	ND
21	2	503	CLA	ND
21	2	504	CLA	ND
21	2	505	CLA	ND
21	2	506	CLA	ND
21	2	508	CLA	ND
21	2	509	CLA	ND

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Mol	Chain	Res	Type	Atom
21	2	510	CLA	ND
21	2	511	CLA	ND
21	2	513	CLA	ND
21	2	514	CLA	ND
21	2	515	CLA	ND
21	2	517	CLA	ND
21	3	701	CLA	ND
21	3	703	CLA	ND
21	3	704	CLA	ND
21	3	705	CLA	ND
21	3	706	CLA	ND
21	3	707	CLA	ND
21	3	708	CLA	ND
21	3	709	CLA	ND
21	3	711	CLA	ND
21	3	712	CLA	ND
21	3	713	CLA	ND
21	3	714	CLA	ND
21	3	715	CLA	ND
21	4	703	CLA	ND
21	4	704	CLA	ND
21	4	706	CLA	ND
21	4	707	CLA	ND
21	4	708	CLA	ND
21	4	709	CLA	ND
21	4	711	CLA	ND
21	5	701	CLA	ND
21	5	702	CLA	ND
21	5	703	CLA	ND
21	5	705	CLA	ND
21	5	706	CLA	ND
21	5	707	CLA	ND
21	5	708	CLA	ND
21	5	709	CLA	ND
21	5	711	CLA	ND
21	6	903	CLA	ND
21	6	904	CLA	ND
21	6	905	CLA	ND
21	6	906	CLA	ND
21	6	908	CLA	ND
21	6	909	CLA	ND
21	6	910	CLA	ND

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Mol	Chain	Res	Type	Atom
21	6	911	CLA	ND
21	6	912	CLA	ND
21	6	913	CLA	ND
21	7	702	CLA	ND
21	7	704	CLA	ND
21	7	705	CLA	ND
21	7	707	CLA	ND
21	7	708	CLA	ND
21	7	709	CLA	ND
21	7	710	CLA	ND
21	7	711	CLA	ND
21	7	712	CLA	ND
21	7	713	CLA	ND
21	7	714	CLA	ND
21	8	603	CLA	ND
21	8	604	CLA	ND
21	8	605	CLA	ND
21	8	606	CLA	ND
21	8	608	CLA	ND
21	8	609	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	613	CLA	ND
21	9	902	CLA	ND
21	9	903	CLA	ND
21	9	904	CLA	ND
21	9	905	CLA	ND
21	9	907	CLA	ND
21	9	908	CLA	ND
21	9	909	CLA	ND
21	9	910	CLA	ND
21	9	911	CLA	ND
21	9	912	CLA	ND
21	9	914	CLA	ND
21	10	703	CLA	ND
21	10	704	CLA	ND
21	10	705	CLA	ND
21	10	706	CLA	ND
21	10	707	CLA	ND
21	10	708	CLA	ND
21	10	709	CLA	ND
21	10	710	CLA	ND

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Mol	Chain	Res	Type	Atom
21	10	711	CLA	ND
21	10	712	CLA	ND
21	11	701	CLA	ND
21	11	702	CLA	ND
21	11	703	CLA	ND
21	11	704	CLA	ND
21	11	705	CLA	ND
21	11	706	CLA	ND
21	11	707	CLA	ND
21	11	708	CLA	ND
21	11	709	CLA	ND
21	11	711	CLA	ND
21	12	501	CLA	ND
21	12	502	CLA	ND
21	12	503	CLA	ND
21	12	504	CLA	ND
21	12	505	CLA	ND
21	12	506	CLA	ND
21	12	507	CLA	ND
21	12	508	CLA	ND
21	13	501	CLA	ND
21	13	502	CLA	ND
21	13	503	CLA	ND

All (1907) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	803	CLA	CBA-CGA-O2A-C1
21	A	803	CLA	O1A-CGA-O2A-C1
21	A	803	CLA	O2A-C1-C2-C3
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CBA-CGA-O2A-C1
21	A	807	CLA	C1A-C2A-CAA-CBA
21	A	807	CLA	CBD-CGD-O2D-CED
21	A	809	CLA	C3A-C2A-CAA-CBA
21	A	813	CLA	C2-C3-C5-C6
21	A	813	CLA	C4-C3-C5-C6
21	A	818	CLA	C1A-C2A-CAA-CBA
21	A	818	CLA	C3A-C2A-CAA-CBA
21	A	818	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	818	CLA	C4-C3-C5-C6
21	A	819	CLA	C3A-C2A-CAA-CBA
21	A	820	CLA	C3A-C2A-CAA-CBA
21	A	820	CLA	CAD-CBD-CGD-O2D
21	A	820	CLA	CBD-CGD-O2D-CED
21	A	821	CLA	C11-C10-C8-C9
21	A	823	CLA	C1A-C2A-CAA-CBA
21	A	824	CLA	CHA-CBD-CGD-O1D
21	A	824	CLA	CHA-CBD-CGD-O2D
21	A	824	CLA	C2-C3-C5-C6
21	A	824	CLA	C4-C3-C5-C6
21	A	825	CLA	CHA-CBD-CGD-O1D
21	A	825	CLA	CHA-CBD-CGD-O2D
21	A	828	CLA	CHA-CBD-CGD-O1D
21	A	828	CLA	CHA-CBD-CGD-O2D
21	A	829	CLA	C1A-C2A-CAA-CBA
21	A	829	CLA	C2-C3-C5-C6
21	A	829	CLA	C4-C3-C5-C6
21	A	833	CLA	O2A-C1-C2-C3
21	A	835	CLA	CHA-CBD-CGD-O1D
21	A	835	CLA	CHA-CBD-CGD-O2D
21	A	837	CLA	CHA-CBD-CGD-O1D
21	A	837	CLA	CHA-CBD-CGD-O2D
21	A	839	CLA	CBD-CGD-O2D-CED
21	A	841	CLA	CHA-CBD-CGD-O1D
21	A	841	CLA	CHA-CBD-CGD-O2D
21	A	842	CLA	C2-C3-C5-C6
21	A	842	CLA	C4-C3-C5-C6
21	A	843	CLA	CHA-CBD-CGD-O1D
21	A	843	CLA	CHA-CBD-CGD-O2D
21	A	844	CLA	C1A-C2A-CAA-CBA
21	B	803	CLA	C2-C3-C5-C6
21	B	803	CLA	C4-C3-C5-C6
21	B	804	CLA	C3A-C2A-CAA-CBA
21	B	807	CLA	CHA-CBD-CGD-O1D
21	B	807	CLA	CHA-CBD-CGD-O2D
21	B	815	CLA	C1A-C2A-CAA-CBA
21	B	815	CLA	C3A-C2A-CAA-CBA
21	B	817	CLA	C3A-C2A-CAA-CBA
21	B	819	CLA	C1A-C2A-CAA-CBA
21	B	819	CLA	C3A-C2A-CAA-CBA
21	B	824	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	826	CLA	C3A-C2A-CAA-CBA
21	B	827	CLA	C1A-C2A-CAA-CBA
21	B	827	CLA	C3A-C2A-CAA-CBA
21	B	829	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C1A-C2A-CAA-CBA
21	B	833	CLA	C1A-C2A-CAA-CBA
21	B	833	CLA	CHA-CBD-CGD-O1D
21	B	833	CLA	CHA-CBD-CGD-O2D
21	B	833	CLA	CBD-CGD-O2D-CED
21	B	837	CLA	CBD-CGD-O2D-CED
21	F	401	CLA	CHA-CBD-CGD-O1D
21	F	401	CLA	CHA-CBD-CGD-O2D
21	F	404	CLA	C1A-C2A-CAA-CBA
21	J	101	CLA	CHA-CBD-CGD-O1D
21	J	101	CLA	CHA-CBD-CGD-O2D
21	J	101	CLA	CAD-CBD-CGD-O1D
21	1	507	CLA	CBD-CGD-O2D-CED
21	1	516	CLA	C2A-CAA-CBA-CGA
21	2	512	CLA	CHA-CBD-CGD-O1D
21	2	512	CLA	CHA-CBD-CGD-O2D
21	2	513	CLA	CHA-CBD-CGD-O1D
21	2	513	CLA	CHA-CBD-CGD-O2D
21	2	513	CLA	CAD-CBD-CGD-O1D
21	2	513	CLA	CBD-CGD-O2D-CED
21	2	514	CLA	C1A-C2A-CAA-CBA
21	2	517	CLA	C2A-CAA-CBA-CGA
21	3	703	CLA	CHA-CBD-CGD-O1D
21	3	703	CLA	CHA-CBD-CGD-O2D
21	3	705	CLA	CBD-CGD-O2D-CED
21	3	706	CLA	C1A-C2A-CAA-CBA
21	3	706	CLA	C3A-C2A-CAA-CBA
21	3	708	CLA	CHA-CBD-CGD-O1D
21	3	708	CLA	CHA-CBD-CGD-O2D
21	3	710	CLA	CHA-CBD-CGD-O1D
21	3	710	CLA	CHA-CBD-CGD-O2D
21	3	712	CLA	C1A-C2A-CAA-CBA
21	3	715	CLA	CHA-CBD-CGD-O1D
21	3	715	CLA	CHA-CBD-CGD-O2D
21	4	707	CLA	CBD-CGD-O2D-CED
21	4	707	CLA	O1D-CGD-O2D-CED
21	4	710	CLA	CHA-CBD-CGD-O1D
21	4	710	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	5	706	CLA	CHA-CBD-CGD-O1D
21	5	706	CLA	CHA-CBD-CGD-O2D
21	5	707	CLA	CAD-CBD-CGD-O1D
21	5	707	CLA	CAD-CBD-CGD-O2D
21	5	708	CLA	CAD-CBD-CGD-O1D
21	5	708	CLA	CAD-CBD-CGD-O2D
21	6	903	CLA	C1A-C2A-CAA-CBA
21	6	903	CLA	C3A-C2A-CAA-CBA
21	6	914	CLA	C1A-C2A-CAA-CBA
21	6	914	CLA	C3A-C2A-CAA-CBA
21	6	914	CLA	CHA-CBD-CGD-O1D
21	6	914	CLA	CHA-CBD-CGD-O2D
21	7	702	CLA	CHA-CBD-CGD-O1D
21	7	702	CLA	CHA-CBD-CGD-O2D
21	7	705	CLA	CBA-CGA-O2A-C1
21	7	705	CLA	O1A-CGA-O2A-C1
21	7	706	CLA	CBD-CGD-O2D-CED
21	8	603	CLA	C1A-C2A-CAA-CBA
21	8	603	CLA	C3A-C2A-CAA-CBA
21	8	603	CLA	CBD-CGD-O2D-CED
21	9	902	CLA	CBD-CGD-O2D-CED
21	10	707	CLA	C1A-C2A-CAA-CBA
21	11	703	CLA	CBD-CGD-O2D-CED
21	11	705	CLA	C1A-C2A-CAA-CBA
21	11	708	CLA	CAD-CBD-CGD-O1D
24	A	847	BCR	C23-C24-C25-C26
24	A	848	BCR	C7-C8-C9-C34
24	A	850	BCR	C1-C6-C7-C8
24	A	850	BCR	C5-C6-C7-C8
24	A	850	BCR	C7-C8-C9-C10
24	A	850	BCR	C7-C8-C9-C34
24	A	850	BCR	C23-C24-C25-C30
24	B	841	BCR	C21-C22-C23-C24
24	B	841	BCR	C37-C22-C23-C24
24	B	842	BCR	C6-C7-C8-C9
24	B	842	BCR	C11-C10-C9-C8
24	B	842	BCR	C11-C10-C9-C34
24	B	842	BCR	C12-C13-C14-C15
24	B	842	BCR	C35-C13-C14-C15
24	B	842	BCR	C14-C15-C16-C17
24	B	844	BCR	C21-C22-C23-C24
24	B	844	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	B	845	BCR	C6-C7-C8-C9
24	B	845	BCR	C23-C24-C25-C26
24	B	845	BCR	C23-C24-C25-C30
24	J	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C5-C6-C7-C8
24	J	103	BCR	C23-C24-C25-C26
24	J	103	BCR	C23-C24-C25-C30
25	A	853	LHG	C3-O3-P-O4
25	A	854	LHG	C3-O3-P-O4
25	A	854	LHG	C3-O3-P-O5
25	A	854	LHG	C4-O6-P-O4
25	A	854	LHG	C4-O6-P-O5
25	B	848	LHG	O1-C1-C2-O2
25	B	848	LHG	O1-C1-C2-C3
25	B	848	LHG	C1-C2-C3-O3
25	B	848	LHG	C3-O3-P-O4
25	B	848	LHG	C3-O3-P-O6
25	B	848	LHG	O9-C7-O7-C5
25	B	848	LHG	C8-C7-O7-C5
25	1	521	LHG	O9-C7-O7-C5
25	2	521	LHG	O1-C1-C2-C3
25	2	521	LHG	C4-O6-P-O3
25	2	521	LHG	C4-O6-P-O4
25	2	521	LHG	C4-O6-P-O5
25	2	521	LHG	O9-C7-O7-C5
25	2	521	LHG	C8-C7-O7-C5
25	4	714	LHG	C4-O6-P-O3
25	4	714	LHG	C4-O6-P-O4
25	4	714	LHG	C4-O6-P-O5
25	4	714	LHG	O7-C5-C6-O8
25	5	714	LHG	C4-O6-P-O3
25	5	714	LHG	C4-O6-P-O4
25	5	714	LHG	C4-O6-P-O5
25	6	917	LHG	C4-O6-P-O4
25	6	917	LHG	O9-C7-O7-C5
25	7	717	LHG	O9-C7-O7-C5
25	7	717	LHG	C8-C7-O7-C5
25	8	617	LHG	C3-O3-P-O6
25	8	617	LHG	O9-C7-O7-C5
25	9	917	LHG	C3-O3-P-O5
25	9	917	LHG	C4-O6-P-O4
25	10	713	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	10	713	LHG	O9-C7-O7-C5
25	10	713	LHG	C8-C7-O7-C5
25	11	714	LHG	O1-C1-C2-C3
25	11	714	LHG	O2-C2-C3-O3
27	B	847	DGD	O1B-C1B-O2G-C2G
28	J	104	DD6	C-C1-C2-C3
28	J	104	DD6	C24-C1-C2-C3
28	J	104	DD6	C9-C10-C11-C12
28	J	104	DD6	C9-C10-C11-C13
28	J	104	DD6	C13-C14-C15-O1
28	J	104	DD6	C1-C2-C3-C4
28	J	104	DD6	C24-C25-C26-C27
28	J	104	DD6	C25-C26-C27-C29
28	J	104	DD6	C5-C6-C8-C9
28	J	104	DD6	C7-C6-C8-C9
28	J	104	DD6	C6-C8-C9-C10
28	1	518	DD6	C9-C10-C11-C12
28	1	518	DD6	C9-C10-C11-C13
28	1	518	DD6	C12-C11-C13-C14
28	1	518	DD6	C25-C26-C27-C29
28	1	518	DD6	C4-C5-C6-C7
28	1	518	DD6	C4-C5-C6-C8
28	1	520	DD6	C1-C24-C25-C26
28	1	520	DD6	C25-C26-C27-C28
28	1	520	DD6	C25-C26-C27-C29
28	1	520	DD6	C2-C3-C4-C5
28	1	520	DD6	C4-C5-C6-C7
28	1	520	DD6	C4-C5-C6-C8
28	2	518	DD6	C10-C11-C13-C14
28	2	518	DD6	C12-C11-C13-C14
28	2	520	DD6	C10-C11-C13-C14
28	2	520	DD6	C12-C11-C13-C14
28	2	520	DD6	C5-C6-C8-C9
28	2	520	DD6	C7-C6-C8-C9
28	3	717	DD6	C9-C10-C11-C12
28	3	717	DD6	C9-C10-C11-C13
28	3	717	DD6	C27-C29-C30-C31
28	3	717	DD6	C4-C5-C6-C7
28	3	717	DD6	C4-C5-C6-C8
28	3	718	DD6	C11-C13-C14-C15
28	3	718	DD6	C5-C6-C8-C9
28	3	718	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
28	4	713	DD6	C-C1-C24-C25
28	4	713	DD6	C2-C1-C24-C25
28	4	713	DD6	C5-C6-C8-C9
28	4	713	DD6	C7-C6-C8-C9
28	4	713	DD6	C6-C8-C9-C10
28	5	713	DD6	C12-C11-C13-C14
28	6	916	DD6	C12-C11-C13-C14
28	6	916	DD6	C7-C6-C8-C9
28	7	715	DD6	C9-C10-C11-C12
28	7	715	DD6	C9-C10-C11-C13
28	7	715	DD6	C10-C11-C13-C14
28	7	715	DD6	C12-C11-C13-C14
28	7	715	DD6	C4-C5-C6-C7
28	7	715	DD6	C4-C5-C6-C8
28	7	715	DD6	C5-C6-C8-C9
28	7	715	DD6	C7-C6-C8-C9
28	8	615	DD6	C11-C10-C9-C8
28	8	615	DD6	C10-C11-C13-C14
28	8	615	DD6	C12-C11-C13-C14
28	8	615	DD6	C13-C14-C15-O1
28	8	615	DD6	C1-C24-C25-C26
28	8	615	DD6	C25-C26-C27-C29
28	8	615	DD6	C4-C5-C6-C7
28	8	615	DD6	C4-C5-C6-C8
28	8	616	DD6	C11-C13-C14-C15
28	8	616	DD6	C1-C24-C25-C26
28	8	616	DD6	C25-C26-C27-C28
28	8	616	DD6	C25-C26-C27-C29
28	9	915	DD6	C25-C26-C27-C29
28	9	915	DD6	C4-C5-C6-C7
28	9	915	DD6	C4-C5-C6-C8
28	9	915	DD6	C5-C6-C8-C9
28	9	915	DD6	C7-C6-C8-C9
28	9	916	DD6	C9-C10-C11-C12
28	9	916	DD6	C9-C10-C11-C13
28	9	916	DD6	C1-C24-C25-C26
28	9	916	DD6	C24-C25-C26-C27
28	9	916	DD6	C2-C3-C4-C5
28	11	712	DD6	C9-C10-C11-C12
28	11	713	DD6	C6-C8-C9-C10
28	12	509	DD6	C13-C14-C15-O1
28	12	510	DD6	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	12	510	DD6	C9-C10-C11-C13
28	12	510	DD6	C10-C11-C13-C14
28	12	510	DD6	C12-C11-C13-C14
28	12	510	DD6	C13-C14-C15-O1
28	12	510	DD6	C5-C6-C8-C9
28	12	510	DD6	C7-C6-C8-C9
21	B	831	CLA	C2C-C3C-CAC-CBC
21	B	833	CLA	O1D-CGD-O2D-CED
21	11	703	CLA	O1D-CGD-O2D-CED
21	A	807	CLA	O1D-CGD-O2D-CED
21	A	839	CLA	O1D-CGD-O2D-CED
21	A	811	CLA	CBD-CGD-O2D-CED
21	A	819	CLA	CBD-CGD-O2D-CED
21	A	835	CLA	CBD-CGD-O2D-CED
21	B	823	CLA	CBD-CGD-O2D-CED
21	B	828	CLA	CBD-CGD-O2D-CED
21	B	834	CLA	CBD-CGD-O2D-CED
21	F	401	CLA	CBD-CGD-O2D-CED
21	J	101	CLA	CBD-CGD-O2D-CED
21	1	510	CLA	CBD-CGD-O2D-CED
21	2	507	CLA	CBD-CGD-O2D-CED
21	2	515	CLA	CBD-CGD-O2D-CED
21	3	709	CLA	CBD-CGD-O2D-CED
21	3	712	CLA	CBD-CGD-O2D-CED
21	4	710	CLA	CBD-CGD-O2D-CED
21	5	705	CLA	CBD-CGD-O2D-CED
21	5	710	CLA	CBD-CGD-O2D-CED
21	6	914	CLA	CBD-CGD-O2D-CED
21	10	703	CLA	CBD-CGD-O2D-CED
21	10	706	CLA	CBD-CGD-O2D-CED
21	11	708	CLA	CBD-CGD-O2D-CED
21	A	806	CLA	O1A-CGA-O2A-C1
21	B	815	CLA	O1A-CGA-O2A-C1
21	12	505	CLA	O1A-CGA-O2A-C1
21	A	811	CLA	O1D-CGD-O2D-CED
21	F	401	CLA	O1D-CGD-O2D-CED
21	3	705	CLA	O1D-CGD-O2D-CED
21	A	820	CLA	O1D-CGD-O2D-CED
21	1	507	CLA	O1D-CGD-O2D-CED
21	6	914	CLA	O1D-CGD-O2D-CED
21	7	706	CLA	O1D-CGD-O2D-CED
21	8	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	9	902	CLA	O1D-CGD-O2D-CED
21	A	834	CLA	CBD-CGD-O2D-CED
21	A	840	CLA	CBD-CGD-O2D-CED
21	A	842	CLA	CBD-CGD-O2D-CED
21	A	862	CLA	CBD-CGD-O2D-CED
21	B	802	CLA	CBD-CGD-O2D-CED
21	B	821	CLA	CBD-CGD-O2D-CED
21	F	403	CLA	CBD-CGD-O2D-CED
21	F	404	CLA	CBD-CGD-O2D-CED
21	2	510	CLA	CBD-CGD-O2D-CED
21	3	702	CLA	CBD-CGD-O2D-CED
21	3	708	CLA	CBD-CGD-O2D-CED
21	4	705	CLA	CBD-CGD-O2D-CED
21	5	701	CLA	CBD-CGD-O2D-CED
21	6	903	CLA	CBD-CGD-O2D-CED
21	6	904	CLA	CBD-CGD-O2D-CED
21	6	912	CLA	CBD-CGD-O2D-CED
21	6	913	CLA	CBD-CGD-O2D-CED
21	8	613	CLA	CBD-CGD-O2D-CED
21	9	907	CLA	CBD-CGD-O2D-CED
21	9	910	CLA	CBD-CGD-O2D-CED
21	9	912	CLA	CBD-CGD-O2D-CED
21	9	914	CLA	CBD-CGD-O2D-CED
21	10	704	CLA	CBD-CGD-O2D-CED
21	10	707	CLA	CBD-CGD-O2D-CED
21	11	701	CLA	CBD-CGD-O2D-CED
21	11	710	CLA	CBD-CGD-O2D-CED
21	12	506	CLA	CBD-CGD-O2D-CED
21	A	844	CLA	O1A-CGA-O2A-C1
21	1	509	CLA	O1A-CGA-O2A-C1
21	5	710	CLA	O1A-CGA-O2A-C1
21	6	906	CLA	O1A-CGA-O2A-C1
21	11	706	CLA	O1A-CGA-O2A-C1
21	B	837	CLA	O1D-CGD-O2D-CED
21	B	814	CLA	CBD-CGD-O2D-CED
21	B	820	CLA	CBD-CGD-O2D-CED
21	B	822	CLA	CBD-CGD-O2D-CED
21	B	838	CLA	CBD-CGD-O2D-CED
21	2	509	CLA	CBD-CGD-O2D-CED
21	4	702	CLA	CBD-CGD-O2D-CED
21	B	834	CLA	O1D-CGD-O2D-CED
21	3	712	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A	807	CLA	C3-C5-C6-C7
21	A	809	CLA	C3-C5-C6-C7
21	A	826	CLA	C3-C5-C6-C7
21	A	836	CLA	C3-C5-C6-C7
21	A	844	CLA	C3-C5-C6-C7
21	B	803	CLA	C3-C5-C6-C7
21	B	805	CLA	C3-C5-C6-C7
21	B	807	CLA	C3-C5-C6-C7
21	B	823	CLA	C3-C5-C6-C7
21	1	505	CLA	C3-C5-C6-C7
21	1	513	CLA	C3-C5-C6-C7
21	2	512	CLA	C3-C5-C6-C7
21	3	710	CLA	C3-C5-C6-C7
21	5	702	CLA	C3-C5-C6-C7
21	7	703	CLA	C3-C5-C6-C7
21	9	903	CLA	C3-C5-C6-C7
21	10	704	CLA	C3-C5-C6-C7
21	11	702	CLA	C3-C5-C6-C7
21	12	501	CLA	C3-C5-C6-C7
21	A	809	CLA	CBA-CGA-O2A-C1
21	A	812	CLA	CBA-CGA-O2A-C1
21	A	844	CLA	CBA-CGA-O2A-C1
21	B	815	CLA	CBA-CGA-O2A-C1
21	9	905	CLA	CBA-CGA-O2A-C1
21	12	505	CLA	CBA-CGA-O2A-C1
25	1	521	LHG	C8-C7-O7-C5
25	6	917	LHG	C8-C7-O7-C5
25	8	617	LHG	C8-C7-O7-C5
27	B	847	DGD	C2B-C1B-O2G-C2G
21	J	101	CLA	O1D-CGD-O2D-CED
21	2	513	CLA	O1D-CGD-O2D-CED
21	B	826	CLA	CBD-CGD-O2D-CED
21	2	512	CLA	CBD-CGD-O2D-CED
21	A	833	CLA	C4-C3-C5-C6
21	B	823	CLA	C4-C3-C5-C6
21	8	609	CLA	CBD-CGD-O2D-CED
21	A	803	CLA	C2A-CAA-CBA-CGA
21	A	818	CLA	C2A-CAA-CBA-CGA
21	A	821	CLA	C2A-CAA-CBA-CGA
21	A	830	CLA	C2A-CAA-CBA-CGA
21	B	803	CLA	C2A-CAA-CBA-CGA
21	B	823	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	B	829	CLA	C2A-CAA-CBA-CGA
21	B	837	CLA	C2A-CAA-CBA-CGA
21	3	715	CLA	C2A-CAA-CBA-CGA
21	6	914	CLA	C2A-CAA-CBA-CGA
21	12	508	CLA	C2A-CAA-CBA-CGA
21	1	510	CLA	O1D-CGD-O2D-CED
21	A	803	CLA	C3-C5-C6-C7
21	A	815	CLA	C3-C5-C6-C7
21	A	841	CLA	C3-C5-C6-C7
21	B	835	CLA	C3-C5-C6-C7
21	3	702	CLA	C3-C5-C6-C7
21	1	509	CLA	CBA-CGA-O2A-C1
21	5	704	CLA	CBA-CGA-O2A-C1
21	5	710	CLA	CBA-CGA-O2A-C1
21	6	906	CLA	CBA-CGA-O2A-C1
21	11	706	CLA	CBA-CGA-O2A-C1
21	A	835	CLA	O1D-CGD-O2D-CED
21	10	706	CLA	O1D-CGD-O2D-CED
21	3	710	CLA	CBD-CGD-O2D-CED
21	B	823	CLA	O1D-CGD-O2D-CED
21	2	515	CLA	O1D-CGD-O2D-CED
21	5	710	CLA	O1D-CGD-O2D-CED
21	A	809	CLA	O1A-CGA-O2A-C1
21	A	812	CLA	O1A-CGA-O2A-C1
21	A	836	CLA	O1A-CGA-O2A-C1
21	4	706	CLA	O1A-CGA-O2A-C1
21	9	905	CLA	O1A-CGA-O2A-C1
24	B	842	BCR	C19-C20-C21-C22
28	J	104	DD6	C3-C4-C5-C6
28	1	520	DD6	C3-C4-C5-C6
28	2	520	DD6	C11-C10-C9-C8
28	4	713	DD6	C11-C10-C9-C8
28	11	713	DD6	C24-C25-C26-C27
21	B	817	CLA	CBD-CGD-O2D-CED
21	B	839	CLA	CBD-CGD-O2D-CED
21	2	504	CLA	CBD-CGD-O2D-CED
21	5	707	CLA	CBD-CGD-O2D-CED
21	6	910	CLA	CBD-CGD-O2D-CED
21	13	503	CLA	CBD-CGD-O2D-CED
21	10	703	CLA	O1D-CGD-O2D-CED
25	A	854	LHG	O2-C2-C3-O3
25	B	848	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
21	B	815	CLA	C3-C5-C6-C7
21	A	805	CLA	CBA-CGA-O2A-C1
21	A	836	CLA	CBA-CGA-O2A-C1
21	2	512	CLA	CBA-CGA-O2A-C1
21	3	709	CLA	O1D-CGD-O2D-CED
21	5	705	CLA	O1D-CGD-O2D-CED
21	A	843	CLA	CBD-CGD-O2D-CED
21	2	505	CLA	CBD-CGD-O2D-CED
21	3	713	CLA	CBD-CGD-O2D-CED
21	4	701	CLA	CBD-CGD-O2D-CED
21	5	703	CLA	CBD-CGD-O2D-CED
21	11	706	CLA	CBD-CGD-O2D-CED
21	12	502	CLA	CBD-CGD-O2D-CED
21	13	502	CLA	CBD-CGD-O2D-CED
21	11	708	CLA	O1D-CGD-O2D-CED
21	A	828	CLA	C3-C5-C6-C7
21	10	710	CLA	C3-C5-C6-C7
21	4	706	CLA	CBA-CGA-O2A-C1
21	A	819	CLA	O1D-CGD-O2D-CED
21	A	805	CLA	O1A-CGA-O2A-C1
21	5	704	CLA	O1A-CGA-O2A-C1
21	B	817	CLA	C4-C3-C5-C6
21	B	817	CLA	C2-C3-C5-C6
21	3	711	CLA	CBD-CGD-O2D-CED
21	B	827	CLA	C2A-CAA-CBA-CGA
21	B	830	CLA	C2A-CAA-CBA-CGA
21	1	515	CLA	C2A-CAA-CBA-CGA
21	2	507	CLA	O1D-CGD-O2D-CED
21	2	512	CLA	O1A-CGA-O2A-C1
21	B	830	CLA	CBA-CGA-O2A-C1
21	4	705	CLA	O1D-CGD-O2D-CED
21	4	710	CLA	O1D-CGD-O2D-CED
21	6	904	CLA	O1D-CGD-O2D-CED
21	6	913	CLA	O1D-CGD-O2D-CED
21	8	613	CLA	O1D-CGD-O2D-CED
21	9	907	CLA	O1D-CGD-O2D-CED
21	11	701	CLA	O1D-CGD-O2D-CED
21	10	707	CLA	O1D-CGD-O2D-CED
21	A	840	CLA	O1D-CGD-O2D-CED
21	9	910	CLA	O1D-CGD-O2D-CED
21	11	710	CLA	O1D-CGD-O2D-CED
25	A	854	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	2	521	LHG	C1-C2-C3-O3
21	11	706	CLA	C3-C5-C6-C7
21	A	862	CLA	O1D-CGD-O2D-CED
21	B	802	CLA	O1D-CGD-O2D-CED
21	A	808	CLA	CBA-CGA-O2A-C1
21	A	813	CLA	CBA-CGA-O2A-C1
21	A	825	CLA	CBA-CGA-O2A-C1
21	B	804	CLA	CBA-CGA-O2A-C1
21	B	812	CLA	CBA-CGA-O2A-C1
21	B	813	CLA	CBA-CGA-O2A-C1
21	B	817	CLA	CBA-CGA-O2A-C1
21	1	513	CLA	CBA-CGA-O2A-C1
21	2	506	CLA	CBA-CGA-O2A-C1
21	2	508	CLA	CBA-CGA-O2A-C1
21	8	612	CLA	CBA-CGA-O2A-C1
21	10	707	CLA	CBA-CGA-O2A-C1
21	B	825	CLA	C13-C15-C16-C17
21	A	829	CLA	CBD-CGD-O2D-CED
21	A	837	CLA	CBD-CGD-O2D-CED
21	1	501	CLA	CBD-CGD-O2D-CED
21	1	511	CLA	CBD-CGD-O2D-CED
21	B	821	CLA	O1D-CGD-O2D-CED
28	1	520	DD6	C24-C25-C26-C27
25	5	714	LHG	C23-C24-C25-C26
21	A	820	CLA	C13-C15-C16-C17
21	11	706	CLA	C10-C11-C12-C13
22	B	840	PQN	C20-C21-C22-C23
21	10	707	CLA	O2A-C1-C2-C3
21	A	824	CLA	CBA-CGA-O2A-C1
21	B	812	CLA	O1A-CGA-O2A-C1
21	A	833	CLA	C2-C3-C5-C6
21	A	806	CLA	C14-C13-C15-C16
21	A	828	CLA	C6-C7-C8-C9
21	B	806	CLA	C11-C10-C8-C9
21	B	817	CLA	C6-C7-C8-C9
21	B	818	CLA	C11-C12-C13-C14
21	11	702	CLA	C6-C7-C8-C9
21	4	702	CLA	O1D-CGD-O2D-CED
21	9	912	CLA	O1D-CGD-O2D-CED
21	10	704	CLA	O1D-CGD-O2D-CED
21	12	506	CLA	O1D-CGD-O2D-CED
21	1	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	7	710	CLA	C2A-CAA-CBA-CGA
24	A	847	BCR	C37-C22-C23-C24
24	A	848	BCR	C37-C22-C23-C24
28	1	518	DD6	C7-C6-C8-C9
28	4	713	DD6	C12-C11-C13-C14
28	8	615	DD6	C7-C6-C8-C9
28	8	616	DD6	C7-C6-C8-C9
28	9	915	DD6	C12-C11-C13-C14
28	9	916	DD6	C-C1-C24-C25
28	11	712	DD6	C12-C11-C13-C14
28	11	713	DD6	C-C1-C24-C25
28	11	713	DD6	C12-C11-C13-C14
28	11	713	DD6	C7-C6-C8-C9
24	A	847	BCR	C21-C22-C23-C24
24	A	848	BCR	C21-C22-C23-C24
28	1	518	DD6	C10-C11-C13-C14
28	4	713	DD6	C10-C11-C13-C14
28	8	615	DD6	C5-C6-C8-C9
28	8	616	DD6	C5-C6-C8-C9
28	9	915	DD6	C10-C11-C13-C14
28	11	713	DD6	C2-C1-C24-C25
28	11	713	DD6	C5-C6-C8-C9
21	A	808	CLA	O1A-CGA-O2A-C1
21	A	813	CLA	O1A-CGA-O2A-C1
21	2	506	CLA	O1A-CGA-O2A-C1
21	2	508	CLA	O1A-CGA-O2A-C1
21	A	827	CLA	C8-C10-C11-C12
21	B	804	CLA	C15-C16-C17-C18
21	B	818	CLA	C10-C11-C12-C13
21	B	826	CLA	C8-C10-C11-C12
21	B	826	CLA	C10-C11-C12-C13
21	B	827	CLA	C5-C6-C7-C8
21	8	612	CLA	C10-C11-C12-C13
21	5	701	CLA	O1D-CGD-O2D-CED
21	A	820	CLA	CBA-CGA-O2A-C1
21	A	810	CLA	C13-C15-C16-C17
21	A	814	CLA	C10-C11-C12-C13
21	A	828	CLA	C10-C11-C12-C13
21	B	817	CLA	C5-C6-C7-C8
21	1	505	CLA	C8-C10-C11-C12
25	5	714	LHG	C7-C8-C9-C10
21	6	903	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	6	912	CLA	O1D-CGD-O2D-CED
21	4	709	CLA	CBD-CGD-O2D-CED
21	A	806	CLA	C8-C10-C11-C12
21	A	821	CLA	C8-C10-C11-C12
21	A	827	CLA	C5-C6-C7-C8
21	B	806	CLA	C13-C15-C16-C17
21	B	812	CLA	C10-C11-C12-C13
21	7	703	CLA	C10-C11-C12-C13
21	7	711	CLA	C15-C16-C17-C18
21	8	612	CLA	C8-C10-C11-C12
21	9	914	CLA	O1D-CGD-O2D-CED
25	2	521	LHG	O1-C1-C2-O2
21	A	834	CLA	O1D-CGD-O2D-CED
21	B	828	CLA	O1D-CGD-O2D-CED
21	A	804	CLA	C15-C16-C17-C18
21	A	821	CLA	C10-C11-C12-C13
21	A	839	CLA	C10-C11-C12-C13
21	B	828	CLA	C10-C11-C12-C13
21	11	702	CLA	C10-C11-C12-C13
25	4	714	LHG	C24-C23-O8-C6
21	B	803	CLA	C2-C1-O2A-CGA
21	5	711	CLA	CBD-CGD-O2D-CED
21	8	611	CLA	CBD-CGD-O2D-CED
21	12	501	CLA	CBD-CGD-O2D-CED
21	9	909	CLA	C2A-CAA-CBA-CGA
21	B	820	CLA	O1D-CGD-O2D-CED
21	2	510	CLA	O1D-CGD-O2D-CED
20	A	801	CL0	C12-C13-C15-C16
21	A	822	CLA	C12-C13-C15-C16
21	B	802	CLA	C11-C10-C8-C7
21	8	604	CLA	C11-C10-C8-C7
21	11	703	CLA	C12-C13-C15-C16
21	B	813	CLA	O1A-CGA-O2A-C1
21	1	513	CLA	O1A-CGA-O2A-C1
28	J	104	DD6	C11-C10-C9-C8
28	1	520	DD6	C1-C2-C3-C4
28	8	616	DD6	C11-C10-C9-C8
28	11	713	DD6	C11-C10-C9-C8
21	A	844	CLA	C2A-CAA-CBA-CGA
21	B	833	CLA	C2A-CAA-CBA-CGA
21	6	906	CLA	C2A-CAA-CBA-CGA
21	F	404	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	8	609	CLA	O1D-CGD-O2D-CED
21	A	815	CLA	C8-C10-C11-C12
21	A	830	CLA	C5-C6-C7-C8
21	B	807	CLA	C13-C15-C16-C17
22	A	845	PQN	C23-C25-C26-C27
21	B	831	CLA	C4C-C3C-CAC-CBC
21	8	612	CLA	O1A-CGA-O2A-C1
21	10	707	CLA	O1A-CGA-O2A-C1
21	4	711	CLA	CBD-CGD-O2D-CED
21	A	833	CLA	C5-C6-C7-C8
21	B	812	CLA	C13-C15-C16-C17
21	3	702	CLA	O1D-CGD-O2D-CED
24	B	842	BCR	C18-C19-C20-C21
28	1	518	DD6	C1-C24-C25-C26
28	1	518	DD6	C6-C8-C9-C10
28	1	520	DD6	C6-C8-C9-C10
28	2	520	DD6	C6-C8-C9-C10
28	4	713	DD6	C1-C24-C25-C26
28	8	615	DD6	C6-C8-C9-C10
28	9	915	DD6	C1-C24-C25-C26
28	12	510	DD6	C1-C24-C25-C26
21	A	827	CLA	C3-C5-C6-C7
21	B	812	CLA	C3-C5-C6-C7
21	A	804	CLA	C10-C11-C12-C13
21	A	829	CLA	C10-C11-C12-C13
21	B	831	CLA	C15-C16-C17-C18
21	B	839	CLA	C15-C16-C17-C18
21	5	702	CLA	C8-C10-C11-C12
21	6	909	CLA	C5-C6-C7-C8
21	A	824	CLA	O1A-CGA-O2A-C1
21	B	804	CLA	O1A-CGA-O2A-C1
21	B	817	CLA	O1A-CGA-O2A-C1
21	B	830	CLA	O1A-CGA-O2A-C1
21	A	822	CLA	C8-C10-C11-C12
21	1	505	CLA	C10-C11-C12-C13
21	2	504	CLA	C10-C11-C12-C13
21	2	509	CLA	C8-C10-C11-C12
21	7	711	CLA	C10-C11-C12-C13
21	12	506	CLA	C5-C6-C7-C8
21	B	810	CLA	CBD-CGD-O2D-CED
21	A	825	CLA	O1A-CGA-O2A-C1
21	2	512	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	828	CLA	C15-C16-C17-C18
25	A	853	LHG	C3-O3-P-O6
25	A	854	LHG	C3-O3-P-O6
25	A	854	LHG	C4-O6-P-O3
25	3	719	LHG	C3-O3-P-O6
25	6	917	LHG	C4-O6-P-O3
25	9	917	LHG	C3-O3-P-O6
21	B	806	CLA	CBA-CGA-O2A-C1
21	9	911	CLA	CBA-CGA-O2A-C1
21	A	824	CLA	CBD-CGD-O2D-CED
21	A	829	CLA	C15-C16-C17-C18
21	B	806	CLA	C15-C16-C17-C18
21	B	827	CLA	C10-C11-C12-C13
25	11	714	LHG	C1-C2-C3-O3
21	A	815	CLA	C4-C3-C5-C6
21	A	844	CLA	C8-C10-C11-C12
21	B	807	CLA	C8-C10-C11-C12
21	A	825	CLA	C2A-CAA-CBA-CGA
21	B	820	CLA	C2A-CAA-CBA-CGA
21	5	710	CLA	C2A-CAA-CBA-CGA
21	A	862	CLA	C3-C5-C6-C7
21	A	821	CLA	CBA-CGA-O2A-C1
21	A	839	CLA	CBA-CGA-O2A-C1
21	A	840	CLA	CBA-CGA-O2A-C1
21	B	803	CLA	CBA-CGA-O2A-C1
25	4	714	LHG	O10-C23-O8-C6
28	1	518	DD6	C25-C26-C27-C28
28	9	915	DD6	C25-C26-C27-C28
28	1	520	DD6	C11-C10-C9-C8
27	B	847	DGD	C2A-C3A-C4A-C5A
27	B	847	DGD	C5A-C6A-C7A-C8A
21	A	831	CLA	CBD-CGD-O2D-CED
21	11	702	CLA	CBD-CGD-O2D-CED
24	B	842	BCR	C20-C21-C22-C37
28	2	520	DD6	C9-C10-C11-C12
28	3	716	DD6	C4-C5-C6-C7
28	5	712	DD6	C4-C5-C6-C7
28	5	713	DD6	C9-C10-C11-C12
28	6	915	DD6	C9-C10-C11-C12
25	A	853	LHG	C27-C28-C29-C30
27	B	847	DGD	C4A-C5A-C6A-C7A
21	A	842	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	814	CLA	O1D-CGD-O2D-CED
21	B	826	CLA	O1D-CGD-O2D-CED
21	A	839	CLA	C16-C17-C18-C20
25	A	853	LHG	C11-C10-C9-C8
25	5	714	LHG	C11-C10-C9-C8
25	7	717	LHG	C10-C11-C12-C13
21	13	503	CLA	O1D-CGD-O2D-CED
25	7	717	LHG	C23-C24-C25-C26
25	9	917	LHG	C12-C13-C14-C15
21	B	822	CLA	O1D-CGD-O2D-CED
21	A	821	CLA	O1A-CGA-O2A-C1
25	A	853	LHG	C26-C27-C28-C29
25	1	521	LHG	O2-C2-C3-O3
25	2	521	LHG	O2-C2-C3-O3
27	B	847	DGD	C4B-C5B-C6B-C7B
21	9	909	CLA	CBD-CGD-O2D-CED
25	1	521	LHG	C7-C8-C9-C10
25	8	617	LHG	C7-C8-C9-C10
21	F	403	CLA	O1D-CGD-O2D-CED
21	3	708	CLA	O1D-CGD-O2D-CED
21	12	502	CLA	O1D-CGD-O2D-CED
24	B	842	BCR	C20-C21-C22-C23
28	2	519	DD6	C9-C10-C11-C13
28	3	716	DD6	C4-C5-C6-C8
28	5	712	DD6	C4-C5-C6-C8
28	5	713	DD6	C9-C10-C11-C13
28	11	712	DD6	C9-C10-C11-C13
25	8	617	LHG	C10-C11-C12-C13
21	B	804	CLA	C16-C17-C18-C20
21	B	827	CLA	C16-C17-C18-C19
21	6	910	CLA	O1D-CGD-O2D-CED
21	A	820	CLA	C4-C3-C5-C6
21	B	806	CLA	C4-C3-C5-C6
21	11	707	CLA	C5-C6-C7-C8
21	A	829	CLA	C6-C7-C8-C9
25	3	719	LHG	C7-C8-C9-C10
25	8	617	LHG	C11-C12-C13-C14
21	A	813	CLA	C2A-CAA-CBA-CGA
21	B	811	CLA	C2A-CAA-CBA-CGA
21	2	516	CLA	C2A-CAA-CBA-CGA
21	A	820	CLA	O1A-CGA-O2A-C1
21	A	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	B	806	CLA	O1A-CGA-O2A-C1
21	9	911	CLA	O1A-CGA-O2A-C1
25	A	853	LHG	O1-C1-C2-C3
25	9	917	LHG	O1-C1-C2-C3
28	6	916	DD6	C10-C11-C13-C14
28	6	916	DD6	C5-C6-C8-C9
21	A	818	CLA	C3-C5-C6-C7
21	A	844	CLA	C5-C6-C7-C8
25	1	521	LHG	C24-C25-C26-C27
25	9	917	LHG	C11-C10-C9-C8
21	5	703	CLA	O1D-CGD-O2D-CED
25	A	853	LHG	C17-C18-C19-C20
25	7	717	LHG	C33-C34-C35-C36
27	B	847	DGD	C7B-C8B-C9B-CAB
21	A	826	CLA	C16-C17-C18-C19
21	A	839	CLA	C16-C17-C18-C19
21	B	827	CLA	C16-C17-C18-C20
21	A	820	CLA	C8-C10-C11-C12
21	A	826	CLA	C8-C10-C11-C12
21	13	502	CLA	O1D-CGD-O2D-CED
21	11	703	CLA	C10-C11-C12-C13
21	A	836	CLA	C5-C6-C7-C8
21	A	832	CLA	CBA-CGA-O2A-C1
21	A	838	CLA	CBA-CGA-O2A-C1
21	A	804	CLA	C3A-C2A-CAA-CBA
21	B	812	CLA	C3A-C2A-CAA-CBA
21	B	832	CLA	C3A-C2A-CAA-CBA
21	B	833	CLA	C3A-C2A-CAA-CBA
21	F	404	CLA	C3A-C2A-CAA-CBA
21	3	712	CLA	C3A-C2A-CAA-CBA
21	10	707	CLA	C3A-C2A-CAA-CBA
21	11	705	CLA	C3A-C2A-CAA-CBA
21	B	805	CLA	C5-C6-C7-C8
25	A	853	LHG	C32-C33-C34-C35
25	1	521	LHG	C23-C24-C25-C26
21	2	509	CLA	O1D-CGD-O2D-CED
21	3	713	CLA	O1D-CGD-O2D-CED
21	3	706	CLA	CBD-CGD-O2D-CED
28	J	104	DD6	C2-C3-C4-C5
28	1	518	DD6	C2-C3-C4-C5
28	7	715	DD6	C2-C3-C4-C5
21	A	839	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	826	CLA	C4-C3-C5-C6
21	B	813	CLA	C4-C3-C5-C6
21	A	831	CLA	CBA-CGA-O2A-C1
21	A	820	CLA	C2-C3-C5-C6
21	B	806	CLA	C2-C3-C5-C6
21	B	813	CLA	C2-C3-C5-C6
25	11	714	LHG	C8-C7-O7-C5
21	7	702	CLA	C2A-CAA-CBA-CGA
25	11	714	LHG	O1-C1-C2-O2
25	7	717	LHG	C30-C31-C32-C33
25	9	917	LHG	C11-C12-C13-C14
25	6	917	LHG	C23-C24-C25-C26
21	B	803	CLA	O1A-CGA-O2A-C1
21	B	805	CLA	C10-C11-C12-C13
21	12	508	CLA	CBD-CGD-O2D-CED
21	A	818	CLA	C2-C1-O2A-CGA
21	A	842	CLA	C2-C1-O2A-CGA
21	B	831	CLA	C2-C1-O2A-CGA
21	A	803	CLA	C15-C16-C17-C18
21	A	810	CLA	C5-C6-C7-C8
21	B	802	CLA	C8-C10-C11-C12
21	8	604	CLA	C10-C11-C12-C13
25	5	714	LHG	C9-C10-C11-C12
21	A	842	CLA	C3-C5-C6-C7
24	A	847	BCR	C23-C24-C25-C30
24	A	848	BCR	C23-C24-C25-C26
24	A	848	BCR	C23-C24-C25-C30
24	A	850	BCR	C23-C24-C25-C26
27	B	847	DGD	O6E-C5E-C6E-O5E
21	3	702	CLA	C8-C10-C11-C12
21	8	609	CLA	C5-C6-C7-C8
21	A	810	CLA	CBD-CGD-O2D-CED
25	1	521	LHG	C12-C13-C14-C15
21	A	842	CLA	C10-C11-C12-C13
21	2	512	CLA	C5-C6-C7-C8
21	7	711	CLA	C13-C15-C16-C17
20	A	801	CL0	C11-C12-C13-C15
21	A	862	CLA	C11-C12-C13-C15
21	B	805	CLA	C11-C10-C8-C7
21	B	818	CLA	C11-C12-C13-C15
21	B	826	CLA	C11-C12-C13-C15
21	B	831	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	A	832	CLA	O1A-CGA-O2A-C1
21	A	840	CLA	O1A-CGA-O2A-C1
21	A	810	CLA	C8-C10-C11-C12
21	A	842	CLA	C8-C10-C11-C12
21	7	708	CLA	C5-C6-C7-C8
21	A	815	CLA	CBD-CGD-O2D-CED
21	A	829	CLA	O1D-CGD-O2D-CED
21	2	504	CLA	CBA-CGA-O2A-C1
25	7	717	LHG	C26-C27-C28-C29
21	A	802	CLA	C2A-CAA-CBA-CGA
21	A	809	CLA	C2A-CAA-CBA-CGA
21	4	710	CLA	C2A-CAA-CBA-CGA
21	A	803	CLA	C5-C6-C7-C8
21	B	828	CLA	C13-C15-C16-C17
21	1	511	CLA	O1D-CGD-O2D-CED
21	3	710	CLA	O1D-CGD-O2D-CED
21	5	702	CLA	CBD-CGD-O2D-CED
25	7	717	LHG	C7-C8-C9-C10
21	A	831	CLA	O1D-CGD-O2D-CED
21	11	706	CLA	O1D-CGD-O2D-CED
25	7	717	LHG	C28-C29-C30-C31
21	B	817	CLA	O1D-CGD-O2D-CED
21	B	839	CLA	O1D-CGD-O2D-CED
21	2	504	CLA	O1D-CGD-O2D-CED
25	7	717	LHG	C12-C13-C14-C15
28	7	715	DD6	C1-C24-C25-C26
25	8	617	LHG	C9-C10-C11-C12
25	9	917	LHG	C15-C16-C17-C18
21	A	844	CLA	C13-C15-C16-C17
25	9	917	LHG	C7-C8-C9-C10
21	B	827	CLA	C15-C16-C17-C18
25	A	853	LHG	O7-C5-C6-O8
21	B	804	CLA	C16-C17-C18-C19
25	A	853	LHG	C18-C19-C20-C21
27	B	847	DGD	C2B-C3B-C4B-C5B
21	B	807	CLA	C5-C6-C7-C8
21	B	805	CLA	C4-C3-C5-C6
21	9	903	CLA	C4-C3-C5-C6
21	A	815	CLA	C2-C3-C5-C6
21	B	823	CLA	C2-C3-C5-C6
21	9	903	CLA	C2-C3-C5-C6
28	2	520	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	6	915	DD6	C27-C29-C30-C31
28	7	715	DD6	C27-C29-C30-C31
20	A	801	CL0	C14-C13-C15-C16
21	A	822	CLA	C14-C13-C15-C16
21	B	802	CLA	C11-C10-C8-C9
21	B	826	CLA	C11-C12-C13-C14
21	B	827	CLA	C11-C12-C13-C14
21	B	831	CLA	C14-C13-C15-C16
21	8	604	CLA	C11-C10-C8-C9
21	11	703	CLA	C14-C13-C15-C16
22	A	845	PQN	C24-C23-C25-C26
21	4	702	CLA	C3-C5-C6-C7
21	A	815	CLA	O1D-CGD-O2D-CED
21	A	862	CLA	C2A-CAA-CBA-CGA
21	2	513	CLA	C2A-CAA-CBA-CGA
28	2	519	DD6	C12-C11-C13-C14
21	B	810	CLA	O1D-CGD-O2D-CED
21	B	838	CLA	O1D-CGD-O2D-CED
28	5	713	DD6	C10-C11-C13-C14
28	11	712	DD6	C10-C11-C13-C14
21	A	831	CLA	O1A-CGA-O2A-C1
21	2	504	CLA	O1A-CGA-O2A-C1
21	A	805	CLA	C1A-C2A-CAA-CBA
21	A	809	CLA	C1A-C2A-CAA-CBA
21	A	811	CLA	C1A-C2A-CAA-CBA
21	A	812	CLA	C1A-C2A-CAA-CBA
21	A	816	CLA	C1A-C2A-CAA-CBA
21	A	819	CLA	C1A-C2A-CAA-CBA
21	A	820	CLA	C1A-C2A-CAA-CBA
21	A	825	CLA	C1A-C2A-CAA-CBA
21	A	832	CLA	C1A-C2A-CAA-CBA
21	B	804	CLA	C1A-C2A-CAA-CBA
21	B	810	CLA	C1A-C2A-CAA-CBA
21	B	817	CLA	C1A-C2A-CAA-CBA
21	B	821	CLA	C1A-C2A-CAA-CBA
21	B	826	CLA	C1A-C2A-CAA-CBA
21	B	828	CLA	C1A-C2A-CAA-CBA
21	B	829	CLA	C1A-C2A-CAA-CBA
21	B	836	CLA	C1A-C2A-CAA-CBA
21	B	839	CLA	C1A-C2A-CAA-CBA
21	5	701	CLA	C1A-C2A-CAA-CBA
21	5	704	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	5	710	CLA	C1A-C2A-CAA-CBA
21	9	903	CLA	C1A-C2A-CAA-CBA
21	10	711	CLA	C1A-C2A-CAA-CBA
21	11	707	CLA	C1A-C2A-CAA-CBA
21	12	506	CLA	C1A-C2A-CAA-CBA
21	B	815	CLA	C6-C7-C8-C10
28	3	718	DD6	C1-C2-C3-C4
28	12	510	DD6	C3-C4-C5-C6
21	4	709	CLA	O1D-CGD-O2D-CED
21	8	611	CLA	O1D-CGD-O2D-CED
25	9	917	LHG	C13-C14-C15-C16
25	10	713	LHG	C7-C8-C9-C10
25	7	717	LHG	C32-C33-C34-C35
21	A	822	CLA	C13-C15-C16-C17
21	B	821	CLA	C5-C6-C7-C8
21	B	834	CLA	C8-C10-C11-C12
21	3	707	CLA	C5-C6-C7-C8
25	6	917	LHG	O6-C4-C5-C6
25	10	713	LHG	C24-C25-C26-C27
25	9	917	LHG	C10-C11-C12-C13
21	B	828	CLA	C8-C10-C11-C12
21	B	813	CLA	C15-C16-C17-C18
25	8	617	LHG	C12-C13-C14-C15
25	1	521	LHG	C1-C2-C3-O3
25	11	714	LHG	O9-C7-O7-C5
21	A	830	CLA	C15-C16-C17-C18
21	B	839	CLA	C13-C15-C16-C17
21	7	703	CLA	C8-C10-C11-C12
25	4	714	LHG	C4-C5-C6-O8
25	7	717	LHG	C4-C5-C6-O8
25	8	617	LHG	C4-C5-C6-O8
25	8	617	LHG	C24-C25-C26-C27
27	B	847	DGD	O1G-C1G-C2G-C3G
21	A	814	CLA	C8-C10-C11-C12
25	10	713	LHG	C27-C28-C29-C30
25	11	714	LHG	C11-C12-C13-C14
21	3	711	CLA	O1D-CGD-O2D-CED
21	3	707	CLA	C13-C15-C16-C17
21	B	813	CLA	C13-C15-C16-C17
25	5	714	LHG	C13-C14-C15-C16
21	7	702	CLA	CAA-CBA-CGA-O2A
25	3	719	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	A	853	LHG	C19-C20-C21-C22
21	5	706	CLA	CBD-CGD-O2D-CED
21	A	836	CLA	C6-C7-C8-C9
21	A	805	CLA	C8-C10-C11-C12
21	A	825	CLA	C8-C10-C11-C12
21	A	830	CLA	C13-C15-C16-C17
28	4	713	DD6	C9-C10-C11-C12
28	6	916	DD6	C4-C5-C6-C7
21	A	822	CLA	C4-C3-C5-C6
21	B	812	CLA	C4-C3-C5-C6
21	A	822	CLA	C2-C3-C5-C6
21	A	826	CLA	C16-C17-C18-C20
21	B	831	CLA	CBA-CGA-O2A-C1
21	B	832	CLA	CBA-CGA-O2A-C1
21	B	834	CLA	CBA-CGA-O2A-C1
21	4	703	CLA	CBD-CGD-O2D-CED
21	11	703	CLA	C13-C15-C16-C17
21	9	912	CLA	C2A-CAA-CBA-CGA
21	A	806	CLA	C10-C11-C12-C13
21	A	844	CLA	C15-C16-C17-C18
21	2	505	CLA	O1D-CGD-O2D-CED
21	3	706	CLA	O1D-CGD-O2D-CED
21	4	701	CLA	O1D-CGD-O2D-CED
25	A	853	LHG	C24-C25-C26-C27
25	3	719	LHG	C11-C10-C9-C8
21	A	818	CLA	CBA-CGA-O2A-C1
21	A	827	CLA	CBA-CGA-O2A-C1
21	B	831	CLA	O1A-CGA-O2A-C1
21	A	809	CLA	C16-C17-C18-C19
21	B	834	CLA	O1A-CGA-O2A-C1
21	B	835	CLA	C8-C10-C11-C12
28	2	520	DD6	C9-C10-C11-C13
28	4	713	DD6	C9-C10-C11-C13
28	6	916	DD6	C4-C5-C6-C8
27	B	847	DGD	O2G-C2G-C3G-O3G
21	A	827	CLA	O1A-CGA-O2A-C1
21	3	710	CLA	O1A-CGA-O2A-C1
21	A	810	CLA	C4-C3-C5-C6
21	3	710	CLA	C4-C3-C5-C6
21	A	804	CLA	C11-C10-C8-C7
21	A	806	CLA	C11-C12-C13-C15
21	A	810	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	A	810	CLA	C11-C10-C8-C7
21	A	812	CLA	C11-C12-C13-C15
21	A	822	CLA	C11-C10-C8-C7
21	A	825	CLA	C11-C10-C8-C7
21	A	826	CLA	C12-C13-C15-C16
21	A	830	CLA	C12-C13-C15-C16
21	B	806	CLA	C11-C10-C8-C7
21	B	817	CLA	C6-C7-C8-C10
21	B	832	CLA	C11-C10-C8-C7
21	B	835	CLA	C11-C12-C13-C15
21	B	839	CLA	C6-C7-C8-C10
21	11	702	CLA	C6-C7-C8-C10
22	A	845	PQN	C22-C23-C25-C26
21	A	806	CLA	C3-C5-C6-C7
21	6	904	CLA	C3-C5-C6-C7
21	A	812	CLA	C11-C12-C13-C14
21	A	826	CLA	C14-C13-C15-C16
21	A	830	CLA	C14-C13-C15-C16
21	A	839	CLA	C6-C7-C8-C9
21	A	842	CLA	C11-C12-C13-C14
21	A	862	CLA	C11-C12-C13-C14
21	B	805	CLA	C6-C7-C8-C9
21	B	812	CLA	C11-C10-C8-C9
21	B	826	CLA	C14-C13-C15-C16
21	B	835	CLA	C11-C12-C13-C14
21	7	708	CLA	C14-C13-C15-C16
21	11	706	CLA	C14-C13-C15-C16
27	B	847	DGD	C1B-C2B-C3B-C4B
21	3	710	CLA	CBA-CGA-O2A-C1
21	B	824	CLA	CBA-CGA-O2A-C1
24	F	405	BCR	C7-C8-C9-C34
24	M	102	BCR	C37-C22-C23-C24
28	12	509	DD6	C12-C11-C13-C14
24	A	849	BCR	C7-C8-C9-C10
24	F	405	BCR	C7-C8-C9-C10
28	11	713	DD6	C10-C11-C13-C14
28	12	509	DD6	C10-C11-C13-C14
21	B	839	CLA	CBA-CGA-O2A-C1
21	F	401	CLA	CBA-CGA-O2A-C1
21	B	806	CLA	C8-C10-C11-C12
21	6	909	CLA	C8-C10-C11-C12
25	2	521	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
25	3	719	LHG	O6-C4-C5-C6
25	7	717	LHG	O6-C4-C5-C6
21	2	504	CLA	C8-C10-C11-C12
21	7	708	CLA	C8-C10-C11-C12
21	11	706	CLA	C8-C10-C11-C12
21	5	702	CLA	O1D-CGD-O2D-CED
21	B	835	CLA	C4-C3-C5-C6
21	B	839	CLA	C4-C3-C5-C6
21	A	810	CLA	C2-C3-C5-C6
21	A	826	CLA	C2-C3-C5-C6
21	3	710	CLA	C2-C3-C5-C6
21	2	509	CLA	C13-C15-C16-C17
21	1	501	CLA	O1D-CGD-O2D-CED
25	10	713	LHG	C24-C23-O8-C6
21	A	819	CLA	CAA-CBA-CGA-O2A
21	A	823	CLA	C3A-C2A-CAA-CBA
21	A	829	CLA	C3A-C2A-CAA-CBA
21	B	803	CLA	C3A-C2A-CAA-CBA
21	B	830	CLA	C3A-C2A-CAA-CBA
21	A	822	CLA	C3-C5-C6-C7
21	A	809	CLA	C16-C17-C18-C20
21	2	512	CLA	C6-C7-C8-C10
21	11	705	CLA	CBA-CGA-O2A-C1
25	A	853	LHG	C4-C5-C6-O8
25	3	719	LHG	C4-C5-C6-O8
25	11	714	LHG	C4-C5-C6-O8
21	B	831	CLA	CBD-CGD-O2D-CED
21	1	505	CLA	O1D-CGD-O2D-CED
21	8	604	CLA	C3-C5-C6-C7
21	B	812	CLA	C2-C3-C5-C6
21	5	707	CLA	O1D-CGD-O2D-CED
25	9	917	LHG	C16-C17-C18-C19
25	7	717	LHG	C3-O3-P-O6
21	5	711	CLA	O1D-CGD-O2D-CED
21	12	508	CLA	O1D-CGD-O2D-CED
25	10	713	LHG	O1-C1-C2-O2
21	A	803	CLA	C8-C10-C11-C12
25	2	521	LHG	O6-C4-C5-O7
21	A	821	CLA	CBD-CGD-O2D-CED
21	A	818	CLA	O1A-CGA-O2A-C1
21	B	832	CLA	O1A-CGA-O2A-C1
25	3	719	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	7	717	LHG	O7-C5-C6-O8
25	10	713	LHG	O7-C5-C6-O8
25	11	714	LHG	O7-C5-C6-O8
21	B	835	CLA	C16-C17-C18-C20
21	A	819	CLA	C6-C7-C8-C9
21	A	827	CLA	C2-C1-O2A-CGA
21	B	839	CLA	C2-C3-C5-C6
21	A	804	CLA	C11-C10-C8-C9
21	A	810	CLA	C6-C7-C8-C9
21	A	825	CLA	C11-C10-C8-C9
21	A	829	CLA	C11-C10-C8-C9
25	5	714	LHG	C24-C25-C26-C27
21	A	839	CLA	C8-C10-C11-C12
21	4	707	CLA	C8-C10-C11-C12
21	A	807	CLA	C10-C11-C12-C13
21	A	818	CLA	C5-C6-C7-C8
28	1	518	DD6	C5-C6-C8-C9
28	3	717	DD6	C5-C6-C8-C9
28	9	916	DD6	C2-C1-C24-C25
21	A	804	CLA	C8-C10-C11-C12
25	7	717	LHG	C11-C12-C13-C14
25	10	713	LHG	C10-C11-C12-C13
28	8	615	DD6	C25-C26-C27-C28
25	5	714	LHG	C12-C13-C14-C15
27	B	847	DGD	C8B-C9B-CAB-CBB
25	8	617	LHG	O6-C4-C5-C6
21	A	837	CLA	O1D-CGD-O2D-CED
21	A	821	CLA	C11-C10-C8-C7
21	A	828	CLA	C6-C7-C8-C10
21	A	839	CLA	C6-C7-C8-C10
21	B	802	CLA	C11-C12-C13-C15
21	B	805	CLA	C6-C7-C8-C10
21	1	510	CLA	C12-C13-C15-C16
21	7	708	CLA	C12-C13-C15-C16
21	8	612	CLA	C12-C13-C15-C16
21	9	908	CLA	C12-C13-C15-C16
21	F	401	CLA	O1A-CGA-O2A-C1
25	9	917	LHG	C14-C15-C16-C17
21	A	831	CLA	C15-C16-C17-C18
21	2	509	CLA	C5-C6-C7-C8
21	B	839	CLA	O1A-CGA-O2A-C1
21	9	905	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	A	849	BCR	C16-C17-C18-C36
24	F	402	BCR	C35-C13-C14-C15
24	F	405	BCR	C20-C21-C22-C37
24	J	103	BCR	C35-C13-C14-C15
28	2	519	DD6	C9-C10-C11-C12
28	3	716	DD6	C9-C10-C11-C12
28	4	713	DD6	C4-C5-C6-C7
28	7	716	DD6	C4-C5-C6-C7
28	9	915	DD6	C9-C10-C11-C12
21	11	703	CLA	C3-C5-C6-C7
21	B	815	CLA	C6-C7-C8-C9
21	1	510	CLA	C5-C6-C7-C8
21	B	821	CLA	CBA-CGA-O2A-C1
21	1	505	CLA	CBA-CGA-O2A-C1
21	A	825	CLA	C11-C12-C13-C14
27	B	847	DGD	C3A-C4A-C5A-C6A
21	A	811	CLA	CAD-CBD-CGD-O2D
21	A	813	CLA	CAD-CBD-CGD-O2D
21	A	818	CLA	CAD-CBD-CGD-O2D
21	A	826	CLA	CAD-CBD-CGD-O2D
21	A	827	CLA	CAD-CBD-CGD-O2D
21	B	810	CLA	CAD-CBD-CGD-O2D
21	B	828	CLA	CAD-CBD-CGD-O2D
21	J	101	CLA	CAD-CBD-CGD-O2D
21	1	508	CLA	CAD-CBD-CGD-O2D
21	1	510	CLA	CAD-CBD-CGD-O2D
21	1	512	CLA	CAD-CBD-CGD-O2D
21	2	504	CLA	CAD-CBD-CGD-O2D
21	2	513	CLA	CAD-CBD-CGD-O2D
21	3	705	CLA	CAD-CBD-CGD-O2D
21	3	712	CLA	CAD-CBD-CGD-O2D
21	4	709	CLA	CAD-CBD-CGD-O2D
21	5	705	CLA	CAD-CBD-CGD-O2D
21	6	905	CLA	CAD-CBD-CGD-O2D
21	6	908	CLA	CAD-CBD-CGD-O2D
21	6	909	CLA	CAD-CBD-CGD-O2D
21	6	910	CLA	CAD-CBD-CGD-O2D
21	6	911	CLA	CAD-CBD-CGD-O2D
21	9	903	CLA	CAD-CBD-CGD-O2D
21	9	912	CLA	CAD-CBD-CGD-O2D
21	9	914	CLA	CAD-CBD-CGD-O2D
21	10	705	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	10	709	CLA	CAD-CBD-CGD-O2D
21	11	702	CLA	CAD-CBD-CGD-O2D
21	11	705	CLA	CAD-CBD-CGD-O2D
21	11	706	CLA	CAD-CBD-CGD-O2D
21	11	711	CLA	CAD-CBD-CGD-O2D
21	12	501	CLA	CAD-CBD-CGD-O2D
21	12	502	CLA	CAD-CBD-CGD-O2D
21	12	506	CLA	CAD-CBD-CGD-O2D
21	13	502	CLA	CAD-CBD-CGD-O2D
21	B	830	CLA	O1D-CGD-O2D-CED
21	4	711	CLA	O1D-CGD-O2D-CED
21	A	813	CLA	C3-C5-C6-C7
25	2	521	LHG	C24-C25-C26-C27
24	M	102	BCR	C6-C7-C8-C9
21	A	843	CLA	O1D-CGD-O2D-CED
21	A	805	CLA	C11-C12-C13-C14
25	10	713	LHG	C4-C5-C6-O8
21	B	804	CLA	CBD-CGD-O2D-CED
25	A	854	LHG	O6-C4-C5-O7
25	1	521	LHG	O6-C4-C5-O7
25	6	917	LHG	O6-C4-C5-O7
21	B	835	CLA	C13-C15-C16-C17
21	9	908	CLA	C5-C6-C7-C8
21	B	816	CLA	CAA-CBA-CGA-O2A
21	B	839	CLA	CAA-CBA-CGA-O2A
21	A	809	CLA	C8-C10-C11-C12
21	7	706	CLA	O1A-CGA-O2A-C1
21	2	512	CLA	C6-C7-C8-C9
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	804	CLA	CHA-CBD-CGD-O2D
21	A	805	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O2D
21	A	862	CLA	CHA-CBD-CGD-O1D
21	A	862	CLA	CHA-CBD-CGD-O2D
21	B	809	CLA	CHA-CBD-CGD-O1D
21	B	824	CLA	CHA-CBD-CGD-O1D
21	B	832	CLA	CHA-CBD-CGD-O1D
21	B	832	CLA	CHA-CBD-CGD-O2D
21	B	834	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	CHA-CBD-CGD-O1D
21	1	506	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	2	505	CLA	CHA-CBD-CGD-O2D
21	2	506	CLA	CHA-CBD-CGD-O1D
21	2	506	CLA	CHA-CBD-CGD-O2D
21	3	702	CLA	CHA-CBD-CGD-O1D
21	3	702	CLA	CHA-CBD-CGD-O2D
21	4	701	CLA	CHA-CBD-CGD-O1D
21	4	701	CLA	CHA-CBD-CGD-O2D
21	5	701	CLA	CHA-CBD-CGD-O1D
21	5	701	CLA	CHA-CBD-CGD-O2D
21	6	906	CLA	CHA-CBD-CGD-O1D
21	6	906	CLA	CHA-CBD-CGD-O2D
21	7	710	CLA	CHA-CBD-CGD-O1D
21	7	710	CLA	CHA-CBD-CGD-O2D
21	8	603	CLA	CHA-CBD-CGD-O1D
21	8	603	CLA	CHA-CBD-CGD-O2D
21	9	904	CLA	CHA-CBD-CGD-O1D
21	10	708	CLA	CHA-CBD-CGD-O1D
21	10	708	CLA	CHA-CBD-CGD-O2D
21	11	705	CLA	O1A-CGA-O2A-C1
28	9	915	DD6	C9-C10-C11-C13
22	A	845	PQN	C25-C26-C27-C28
22	B	840	PQN	C25-C26-C27-C28
25	8	617	LHG	O7-C5-C6-O8
27	B	847	DGD	O1G-C1G-C2G-O2G
21	7	708	CLA	O1D-CGD-O2D-CED
21	12	501	CLA	O1D-CGD-O2D-CED
27	B	847	DGD	C9B-CAB-CBB-CCB
21	2	512	CLA	C4-C3-C5-C6
21	11	703	CLA	C2-C3-C5-C6
21	1	508	CLA	O1D-CGD-O2D-CED
28	1	519	DD6	C27-C29-C30-C31
20	A	801	CL0	C11-C12-C13-C14
21	B	802	CLA	C11-C12-C13-C14
21	B	832	CLA	C11-C10-C8-C9
22	B	840	PQN	C21-C22-C23-C24
21	B	821	CLA	O1A-CGA-O2A-C1
21	1	505	CLA	O1A-CGA-O2A-C1
21	9	909	CLA	O1D-CGD-O2D-CED
21	A	815	CLA	C5-C6-C7-C8
24	A	849	BCR	C7-C8-C9-C34
24	J	103	BCR	C7-C8-C9-C34
28	3	717	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
28	3	718	DD6	C12-C11-C13-C14
28	2	519	DD6	C10-C11-C13-C14
28	3	718	DD6	C10-C11-C13-C14
21	A	806	CLA	C1A-C2A-CAA-CBA
21	A	835	CLA	C1A-C2A-CAA-CBA
21	1	510	CLA	C1A-C2A-CAA-CBA
21	7	712	CLA	C1A-C2A-CAA-CBA
21	8	609	CLA	C1A-C2A-CAA-CBA
21	12	501	CLA	C1A-C2A-CAA-CBA
22	A	845	PQN	C26-C27-C28-C29
21	7	706	CLA	CBA-CGA-O2A-C1
21	7	702	CLA	O1A-CGA-O2A-C1
25	6	917	LHG	C3-O3-P-O6
25	9	917	LHG	C4-O6-P-O3
21	4	703	CLA	O1D-CGD-O2D-CED
21	A	822	CLA	CBD-CGD-O2D-CED
21	A	862	CLA	C4-C3-C5-C6
21	7	711	CLA	C3-C5-C6-C7
21	B	805	CLA	C2-C3-C5-C6
25	B	848	LHG	C3-O3-P-O5
25	3	719	LHG	C3-O3-P-O4
25	6	917	LHG	C4-O6-P-O5
25	8	617	LHG	C3-O3-P-O4
25	9	917	LHG	C3-O3-P-O4
25	9	917	LHG	C4-O6-P-O5
25	10	713	LHG	C3-O3-P-O4
21	7	711	CLA	C16-C17-C18-C20
21	7	702	CLA	CBA-CGA-O2A-C1
25	A	854	LHG	O6-C4-C5-C6
25	1	521	LHG	O6-C4-C5-C6
21	A	826	CLA	C5-C6-C7-C8
21	1	513	CLA	C2A-CAA-CBA-CGA
21	B	831	CLA	C3-C5-C6-C7
21	B	834	CLA	C3-C5-C6-C7
21	A	826	CLA	C15-C16-C17-C18
21	A	815	CLA	C11-C12-C13-C15
21	A	808	CLA	C2-C3-C5-C6
21	A	828	CLA	CAD-CBD-CGD-O1D
21	A	839	CLA	CAD-CBD-CGD-O1D
21	A	862	CLA	CAD-CBD-CGD-O1D
21	B	809	CLA	CAD-CBD-CGD-O1D
21	B	834	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	B	839	CLA	CAD-CBD-CGD-O1D
21	F	401	CLA	C2-C3-C5-C6
21	1	506	CLA	CAD-CBD-CGD-O1D
21	3	708	CLA	CAD-CBD-CGD-O1D
21	7	710	CLA	CAD-CBD-CGD-O1D
21	10	704	CLA	CAD-CBD-CGD-O1D
21	A	809	CLA	O1D-CGD-O2D-CED
21	7	703	CLA	CBA-CGA-O2A-C1
21	B	807	CLA	C4-C3-C5-C6
21	A	805	CLA	C11-C10-C8-C7
21	A	806	CLA	C12-C13-C15-C16
21	A	807	CLA	C3A-C2A-CAA-CBA
21	A	815	CLA	C6-C7-C8-C10
21	A	828	CLA	C11-C10-C8-C7
21	A	829	CLA	C11-C12-C13-C15
21	A	829	CLA	C12-C13-C15-C16
21	A	839	CLA	C12-C13-C15-C16
21	B	813	CLA	C12-C13-C15-C16
21	B	825	CLA	C12-C13-C15-C16
21	B	835	CLA	C6-C7-C8-C10
22	A	845	PQN	C17-C18-C20-C21
22	B	840	PQN	C21-C22-C23-C25
25	3	719	LHG	O6-C4-C5-O7
25	5	714	LHG	O6-C4-C5-O7
25	7	717	LHG	O6-C4-C5-O7
25	11	714	LHG	O6-C4-C5-O7
21	3	701	CLA	CBD-CGD-O2D-CED
21	A	824	CLA	O1D-CGD-O2D-CED
25	A	853	LHG	C29-C30-C31-C32
21	A	810	CLA	C15-C16-C17-C18
21	11	703	CLA	C4-C3-C5-C6
21	A	829	CLA	C11-C12-C13-C14
21	A	842	CLA	C6-C7-C8-C9
21	B	835	CLA	C6-C7-C8-C9
21	B	839	CLA	C6-C7-C8-C9
21	7	703	CLA	C6-C7-C8-C9
21	8	612	CLA	C14-C13-C15-C16
21	B	824	CLA	O1A-CGA-O2A-C1
21	13	501	CLA	C2A-CAA-CBA-CGA
21	B	803	CLA	C6-C7-C8-C9
28	3	717	DD6	C6-C8-C9-C10
28	5	713	DD6	C6-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	4	712	DD6	C7-C6-C8-C9
25	6	917	LHG	C9-C10-C11-C12
21	A	829	CLA	C5-C6-C7-C8
21	9	908	CLA	C8-C10-C11-C12
21	8	612	CLA	CBD-CGD-O2D-CED
21	B	830	CLA	C1-C2-C3-C4
21	B	835	CLA	O1A-CGA-O2A-C1
27	B	847	DGD	CEB-CFB-CGB-CHB
25	11	714	LHG	O6-C4-C5-C6
21	B	802	CLA	C2A-CAA-CBA-CGA
21	F	403	CLA	C2A-CAA-CBA-CGA
21	9	911	CLA	C2-C1-O2A-CGA
22	A	845	PQN	C26-C27-C28-C30
21	10	712	CLA	O1A-CGA-O2A-C1
25	A	853	LHG	C16-C17-C18-C19
21	B	827	CLA	O1A-CGA-O2A-C1
21	11	703	CLA	O1A-CGA-O2A-C1
21	A	826	CLA	C13-C15-C16-C17
21	B	826	CLA	C4-C3-C5-C6
21	B	835	CLA	C2-C3-C5-C6
21	2	512	CLA	C2-C3-C5-C6
21	B	801	CLA	C8-C10-C11-C12
21	A	821	CLA	O1D-CGD-O2D-CED
21	10	712	CLA	CBA-CGA-O2A-C1
21	A	809	CLA	C15-C16-C17-C18
21	A	810	CLA	C2A-CAA-CBA-CGA
21	B	831	CLA	C2A-CAA-CBA-CGA
21	1	514	CLA	C2A-CAA-CBA-CGA
21	4	703	CLA	C2A-CAA-CBA-CGA
28	1	519	DD6	C4-C5-C6-C8
28	4	713	DD6	C4-C5-C6-C8
21	B	807	CLA	CBA-CGA-O2A-C1
25	1	521	LHG	C3-O3-P-O6
25	1	521	LHG	C4-O6-P-O3
25	2	521	LHG	C3-O3-P-O6
25	5	714	LHG	C3-O3-P-O6
21	B	832	CLA	C10-C11-C12-C13
21	A	828	CLA	C4-C3-C5-C6
21	10	704	CLA	C4-C3-C5-C6
27	B	847	DGD	C4E-C5E-C6E-O5E
21	A	820	CLA	C11-C12-C13-C15
21	1	505	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	B	816	CLA	O1A-CGA-O2A-C1
21	A	806	CLA	C11-C12-C13-C14
21	A	815	CLA	C6-C7-C8-C9
21	A	820	CLA	C11-C12-C13-C14
21	A	822	CLA	C11-C10-C8-C9
21	A	829	CLA	C14-C13-C15-C16
21	B	813	CLA	C14-C13-C15-C16
21	1	510	CLA	C14-C13-C15-C16
21	9	908	CLA	C14-C13-C15-C16
28	9	915	DD6	C11-C10-C9-C8
24	B	843	BCR	C37-C22-C23-C24
25	A	854	LHG	C10-C11-C12-C13
21	4	703	CLA	CAA-CBA-CGA-O1A
21	13	501	CLA	CAA-CBA-CGA-O1A
21	A	810	CLA	C3-C5-C6-C7
21	7	706	CLA	C2C-C3C-CAC-CBC
21	A	804	CLA	C5-C6-C7-C8
25	2	521	LHG	C23-C24-C25-C26
25	9	917	LHG	O1-C1-C2-O2
25	6	917	LHG	C24-C23-O8-C6
21	7	703	CLA	O1A-CGA-O2A-C1
21	A	822	CLA	C2A-CAA-CBA-CGA
21	2	512	CLA	C2A-CAA-CBA-CGA
21	8	612	CLA	C2A-CAA-CBA-CGA
21	10	705	CLA	CAA-CBA-CGA-O2A
28	4	713	DD6	C1-C2-C3-C4
28	3	717	DD6	C2-C3-C4-C5
21	1	508	CLA	CBD-CGD-O2D-CED
21	1	513	CLA	O1D-CGD-O2D-CED
21	B	807	CLA	O1A-CGA-O2A-C1
21	B	813	CLA	C2-C1-O2A-CGA
21	F	401	CLA	C2-C1-O2A-CGA
21	2	512	CLA	C2-C1-O2A-CGA
21	A	844	CLA	C4C-C3C-CAC-CBC
21	7	708	CLA	CBD-CGD-O2D-CED
21	3	703	CLA	CAA-CBA-CGA-O1A
21	3	703	CLA	CAA-CBA-CGA-O2A
21	2	503	CLA	C2A-CAA-CBA-CGA
21	B	827	CLA	CBA-CGA-O2A-C1
21	A	804	CLA	O1A-CGA-O2A-C1
21	A	838	CLA	C3A-C2A-CAA-CBA
21	1	506	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	6	905	CLA	CAA-CBA-CGA-O1A
21	A	817	CLA	O2A-C1-C2-C3
25	1	521	LHG	C24-C23-O8-C6
21	A	826	CLA	C11-C12-C13-C14
21	A	831	CLA	C16-C17-C18-C19
21	A	837	CLA	CAA-CBA-CGA-O1A
21	6	905	CLA	CAA-CBA-CGA-O2A
21	9	904	CLA	CAA-CBA-CGA-O1A
25	10	713	LHG	C23-C24-C25-C26
24	A	852	BCR	C11-C10-C9-C34
24	A	852	BCR	C16-C17-C18-C36
24	B	843	BCR	C11-C10-C9-C34
24	B	843	BCR	C20-C21-C22-C37
24	F	405	BCR	C16-C17-C18-C36
28	1	520	DD6	C9-C10-C11-C12
21	7	702	CLA	CAA-CBA-CGA-O1A
27	B	847	DGD	O6E-C1E-O5D-C6D
21	1	506	CLA	CAA-CBA-CGA-O1A
21	2	505	CLA	CAA-CBA-CGA-O1A
21	8	605	CLA	CAA-CBA-CGA-O1A
28	12	510	DD6	C2-C3-C4-C5
21	A	830	CLA	CBD-CGD-O2D-CED
21	B	808	CLA	CAA-CBA-CGA-O1A
21	5	703	CLA	CAA-CBA-CGA-O2A
21	A	819	CLA	CAA-CBA-CGA-O1A
21	A	821	CLA	C1A-C2A-CAA-CBA
21	A	838	CLA	C1A-C2A-CAA-CBA
21	B	818	CLA	C1A-C2A-CAA-CBA
21	2	510	CLA	C1A-C2A-CAA-CBA
21	3	707	CLA	C1A-C2A-CAA-CBA
21	3	708	CLA	C1A-C2A-CAA-CBA
21	5	705	CLA	C1A-C2A-CAA-CBA
21	5	708	CLA	C1A-C2A-CAA-CBA
21	6	904	CLA	C1A-C2A-CAA-CBA
21	6	913	CLA	C1A-C2A-CAA-CBA
21	9	913	CLA	C1A-C2A-CAA-CBA
21	11	708	CLA	C1A-C2A-CAA-CBA
21	12	503	CLA	C1A-C2A-CAA-CBA
21	7	711	CLA	C16-C17-C18-C19
21	A	807	CLA	C11-C10-C8-C7
21	B	805	CLA	C11-C12-C13-C15
21	B	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	826	CLA	C12-C13-C15-C16
21	B	831	CLA	C2-C3-C5-C6
21	2	504	CLA	C6-C7-C8-C10
21	7	703	CLA	C11-C10-C8-C7
21	4	707	CLA	C13-C15-C16-C17
25	A	853	LHG	C8-C7-O7-C5
21	B	805	CLA	C15-C16-C17-C18
21	B	808	CLA	CAA-CBA-CGA-O2A
21	4	710	CLA	CAA-CBA-CGA-O1A
21	8	613	CLA	CAA-CBA-CGA-O1A
21	3	709	CLA	CAA-CBA-CGA-O2A
21	3	712	CLA	CAA-CBA-CGA-O2A
21	3	713	CLA	CAA-CBA-CGA-O1A
21	6	911	CLA	CAA-CBA-CGA-O1A
21	6	911	CLA	CAA-CBA-CGA-O2A
21	8	612	CLA	O1D-CGD-O2D-CED
21	8	613	CLA	C2A-CAA-CBA-CGA
21	9	913	CLA	C2A-CAA-CBA-CGA
21	3	711	CLA	CAA-CBA-CGA-O1A
21	5	703	CLA	CAA-CBA-CGA-O1A
25	9	917	LHG	O6-C4-C5-C6
21	2	505	CLA	CAA-CBA-CGA-O2A
21	4	703	CLA	CAA-CBA-CGA-O2A
21	A	827	CLA	C4-C3-C5-C6
21	11	703	CLA	C15-C16-C17-C18
21	A	828	CLA	C2-C3-C5-C6
25	8	617	LHG	C24-C23-O8-C6
21	B	820	CLA	CAA-CBA-CGA-O2A
21	10	705	CLA	CAA-CBA-CGA-O1A
21	B	802	CLA	C10-C11-C12-C13
24	A	852	BCR	C11-C10-C9-C8
24	A	852	BCR	C16-C17-C18-C19
24	B	843	BCR	C11-C10-C9-C8
24	B	843	BCR	C20-C21-C22-C23
27	B	847	DGD	C2E-C1E-O5D-C6D
28	1	520	DD6	C9-C10-C11-C13
21	B	809	CLA	CAA-CBA-CGA-O2A
21	2	511	CLA	CAA-CBA-CGA-O2A
21	3	709	CLA	CAA-CBA-CGA-O1A
21	3	711	CLA	CAA-CBA-CGA-O2A
21	13	501	CLA	CAA-CBA-CGA-O2A
28	1	518	DD6	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	B	820	CLA	CAA-CBA-CGA-O1A
21	3	715	CLA	CAA-CBA-CGA-O1A
21	9	904	CLA	CAA-CBA-CGA-O2A
21	A	815	CLA	C11-C12-C13-C14
21	11	703	CLA	CBA-CGA-O2A-C1
20	A	801	CL0	CAA-CBA-CGA-O2A
21	3	715	CLA	CAA-CBA-CGA-O2A
21	A	841	CLA	C4-C3-C5-C6
21	6	907	CLA	C2-C1-O2A-CGA
21	A	815	CLA	C2-C1-O2A-CGA
21	A	817	CLA	C2-C1-O2A-CGA
21	A	825	CLA	C2-C1-O2A-CGA
21	A	829	CLA	C2-C1-O2A-CGA
21	A	841	CLA	C2-C1-O2A-CGA
21	1	513	CLA	C2-C1-O2A-CGA
21	A	837	CLA	CAA-CBA-CGA-O2A
21	8	605	CLA	CAA-CBA-CGA-O2A
21	8	613	CLA	CAA-CBA-CGA-O2A
21	10	709	CLA	CAA-CBA-CGA-O1A
21	10	709	CLA	CAA-CBA-CGA-O2A
25	1	521	LHG	C11-C10-C9-C8
21	B	805	CLA	C11-C12-C13-C14
21	4	710	CLA	CAA-CBA-CGA-O2A
21	B	801	CLA	C15-C16-C17-C18
21	F	401	CLA	C4-C3-C5-C6
21	9	913	CLA	CAA-CBA-CGA-O2A
21	B	815	CLA	C2A-CAA-CBA-CGA
21	5	701	CLA	C2A-CAA-CBA-CGA
21	2	504	CLA	C11-C12-C13-C14
27	B	847	DGD	C1G-C2G-C3G-O3G
21	8	604	CLA	C8-C10-C11-C12
21	A	803	CLA	C4-C3-C5-C6
21	9	911	CLA	C4-C3-C5-C6
21	3	704	CLA	C1A-C2A-CAA-CBA
21	B	807	CLA	C2-C3-C5-C6
21	B	826	CLA	C2-C3-C5-C6
21	6	912	CLA	CAA-CBA-CGA-O2A
21	11	709	CLA	CAA-CBA-CGA-O2A
21	9	913	CLA	C2-C1-O2A-CGA
21	10	712	CLA	C2-C1-O2A-CGA
21	B	829	CLA	C4C-C3C-CAC-CBC
21	4	711	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	A	825	CLA	C3-C5-C6-C7
21	A	829	CLA	C3-C5-C6-C7
21	A	831	CLA	C5-C6-C7-C8
25	8	617	LHG	O6-C4-C5-O7
21	3	701	CLA	O1D-CGD-O2D-CED
21	5	709	CLA	CAA-CBA-CGA-O2A
28	J	104	DD6	C25-C26-C27-C28
25	10	713	LHG	C9-C10-C11-C12
21	B	804	CLA	CAA-CBA-CGA-O2A
21	B	833	CLA	CAA-CBA-CGA-O1A
21	3	713	CLA	CAA-CBA-CGA-O2A
21	4	709	CLA	CAA-CBA-CGA-O2A
25	5	714	LHG	O6-C4-C5-C6
21	B	827	CLA	C4-C3-C5-C6
21	11	702	CLA	C4-C3-C5-C6
21	A	809	CLA	C6-C7-C8-C10
21	A	830	CLA	C11-C12-C13-C15
21	A	842	CLA	C11-C10-C8-C7
21	B	812	CLA	C11-C10-C8-C7
21	9	903	CLA	C11-C10-C8-C7
21	11	706	CLA	C12-C13-C15-C16
21	A	834	CLA	CAA-CBA-CGA-O1A
21	12	502	CLA	CAA-CBA-CGA-O1A
21	2	507	CLA	CBA-CGA-O2A-C1
21	7	707	CLA	CBA-CGA-O2A-C1
25	A	853	LHG	O1-C1-C2-O2
21	B	813	CLA	C8-C10-C11-C12
28	3	718	DD6	C24-C25-C26-C27
25	7	717	LHG	O7-C7-C8-C9
25	B	848	LHG	O7-C5-C6-O8
21	A	834	CLA	CAA-CBA-CGA-O2A
21	B	809	CLA	CAA-CBA-CGA-O1A
21	3	712	CLA	CAA-CBA-CGA-O1A
25	A	854	LHG	O7-C7-C8-C9
21	B	835	CLA	C16-C17-C18-C19
21	2	511	CLA	CAA-CBA-CGA-O1A
21	2	514	CLA	CAA-CBA-CGA-O2A
21	11	710	CLA	CAA-CBA-CGA-O2A
21	12	502	CLA	CAA-CBA-CGA-O2A
21	12	508	CLA	CAA-CBA-CGA-O2A
21	A	842	CLA	CBA-CGA-O2A-C1
21	B	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	819	CLA	C5-C6-C7-C8
28	2	520	DD6	C-C1-C2-C3
28	4	712	DD6	C4-C5-C6-C7
28	9	916	DD6	C-C1-C2-C3
28	12	510	DD6	C4-C5-C6-C7
21	B	812	CLA	CAA-CBA-CGA-O2A
21	B	819	CLA	CAA-CBA-CGA-O2A
21	A	802	CLA	C4-C3-C5-C6
21	A	830	CLA	C4-C3-C5-C6
21	11	706	CLA	C4-C3-C5-C6
21	12	506	CLA	C4-C3-C5-C6
21	B	811	CLA	CAA-CBA-CGA-O2A
21	9	910	CLA	CAA-CBA-CGA-O2A
21	A	803	CLA	C2-C3-C5-C6
21	4	705	CLA	C2-C1-O2A-CGA
21	B	826	CLA	CBA-CGA-O2A-C1
21	7	714	CLA	CBA-CGA-O2A-C1
21	8	614	CLA	CAA-CBA-CGA-O2A
21	A	803	CLA	C11-C10-C8-C9
21	A	805	CLA	C11-C10-C8-C9
21	A	839	CLA	C14-C13-C15-C16
21	A	841	CLA	C6-C7-C8-C9
21	A	842	CLA	C11-C10-C8-C9
21	B	805	CLA	C14-C13-C15-C16
21	B	825	CLA	C14-C13-C15-C16
21	2	504	CLA	C6-C7-C8-C9
22	A	845	PQN	C19-C18-C20-C21
21	4	711	CLA	CAA-CBA-CGA-O1A
21	5	709	CLA	CAA-CBA-CGA-O1A
21	7	704	CLA	CAA-CBA-CGA-O1A
21	2	514	CLA	C3A-C2A-CAA-CBA
21	A	842	CLA	O1A-CGA-O2A-C1
21	9	911	CLA	CAA-CBA-CGA-O2A
21	1	512	CLA	CAA-CBA-CGA-O2A
21	4	709	CLA	CAA-CBA-CGA-O1A
21	6	913	CLA	CAA-CBA-CGA-O2A
21	A	815	CLA	CAD-CBD-CGD-O2D
21	A	816	CLA	CAD-CBD-CGD-O2D
21	A	832	CLA	CAD-CBD-CGD-O2D
21	B	811	CLA	CAD-CBD-CGD-O2D
21	B	812	CLA	CAD-CBD-CGD-O2D
21	B	813	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	820	CLA	CAD-CBD-CGD-O2D
21	B	825	CLA	CAD-CBD-CGD-O2D
21	1	507	CLA	CAD-CBD-CGD-O2D
21	2	507	CLA	CAD-CBD-CGD-O2D
21	2	515	CLA	CAD-CBD-CGD-O2D
21	2	517	CLA	CAD-CBD-CGD-O2D
21	3	704	CLA	CAD-CBD-CGD-O2D
21	3	706	CLA	CAD-CBD-CGD-O2D
21	3	709	CLA	CAD-CBD-CGD-O2D
21	5	702	CLA	CAD-CBD-CGD-O2D
21	5	703	CLA	CAD-CBD-CGD-O2D
21	5	709	CLA	CAD-CBD-CGD-O2D
21	6	904	CLA	CAD-CBD-CGD-O2D
21	7	704	CLA	CAD-CBD-CGD-O2D
21	8	604	CLA	CAD-CBD-CGD-O2D
21	8	605	CLA	CAD-CBD-CGD-O2D
21	8	611	CLA	CAD-CBD-CGD-O2D
21	9	904	CLA	CAD-CBD-CGD-O2D
21	9	905	CLA	CAD-CBD-CGD-O2D
21	10	712	CLA	CAD-CBD-CGD-O2D
21	11	703	CLA	CAD-CBD-CGD-O2D
21	11	707	CLA	CAD-CBD-CGD-O2D
21	11	708	CLA	CAD-CBD-CGD-O2D
21	12	503	CLA	CAD-CBD-CGD-O2D
21	12	507	CLA	CAD-CBD-CGD-O2D
21	9	908	CLA	C13-C15-C16-C17
21	B	817	CLA	C10-C11-C12-C13
21	5	707	CLA	C3-C5-C6-C7
21	A	824	CLA	C2-C1-O2A-CGA
21	B	837	CLA	CAA-CBA-CGA-O2A
21	1	512	CLA	CAA-CBA-CGA-O1A
21	1	517	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	CBA-CGA-O2A-C1
21	A	813	CLA	C6-C7-C8-C9
21	B	816	CLA	C4-C3-C5-C6
21	1	513	CLA	C4-C3-C5-C6
21	11	709	CLA	CAA-CBA-CGA-O1A
21	12	507	CLA	CAA-CBA-CGA-O2A
21	A	818	CLA	C6-C7-C8-C9
21	A	827	CLA	C2-C3-C5-C6
21	A	841	CLA	C2-C3-C5-C6
21	9	911	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	805	CLA	CAA-CBA-CGA-O2A
21	8	612	CLA	CAA-CBA-CGA-O2A
25	5	714	LHG	O7-C7-C8-C9
25	6	917	LHG	O7-C7-C8-C9
21	2	507	CLA	O1A-CGA-O2A-C1
24	A	848	BCR	C7-C8-C9-C10
24	B	843	BCR	C21-C22-C23-C24
21	A	821	CLA	C14-C13-C15-C16
28	1	520	DD6	C13-C14-C15-O1
21	7	710	CLA	CAA-CBA-CGA-O2A
21	9	914	CLA	CAA-CBA-CGA-O2A
21	B	830	CLA	O2A-C1-C2-C3
21	F	403	CLA	CAA-CBA-CGA-O1A
21	6	912	CLA	CAA-CBA-CGA-O1A
21	7	704	CLA	CAA-CBA-CGA-O2A
21	11	711	CLA	CAA-CBA-CGA-O2A
21	A	862	CLA	O2A-C1-C2-C3
21	B	821	CLA	O2A-C1-C2-C3
21	B	831	CLA	O2A-C1-C2-C3
21	11	703	CLA	O2A-C1-C2-C3
25	7	717	LHG	C17-C18-C19-C20
21	5	702	CLA	C10-C11-C12-C13
21	1	513	CLA	CAA-CBA-CGA-O2A
25	9	917	LHG	O7-C7-C8-C9
21	B	811	CLA	CAA-CBA-CGA-O1A
21	2	514	CLA	CAA-CBA-CGA-O1A
21	6	913	CLA	CAA-CBA-CGA-O1A
21	9	910	CLA	CAA-CBA-CGA-O1A
21	12	508	CLA	CAA-CBA-CGA-O1A
21	A	805	CLA	CHA-CBD-CGD-O2D
21	A	807	CLA	CHA-CBD-CGD-O1D
21	A	814	CLA	CHA-CBD-CGD-O1D
21	A	814	CLA	CHA-CBD-CGD-O2D
21	A	830	CLA	CHA-CBD-CGD-O1D
21	A	830	CLA	CHA-CBD-CGD-O2D
21	A	840	CLA	CHA-CBD-CGD-O1D
21	A	840	CLA	CHA-CBD-CGD-O2D
21	B	803	CLA	CHA-CBD-CGD-O1D
21	B	803	CLA	CHA-CBD-CGD-O2D
21	B	804	CLA	CHA-CBD-CGD-O1D
21	B	819	CLA	CHA-CBD-CGD-O1D
21	B	819	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	822	CLA	CHA-CBD-CGD-O2D
21	B	823	CLA	CHA-CBD-CGD-O1D
21	B	823	CLA	CHA-CBD-CGD-O2D
21	B	827	CLA	CHA-CBD-CGD-O1D
21	B	827	CLA	CHA-CBD-CGD-O2D
21	B	834	CLA	CHA-CBD-CGD-O2D
21	B	835	CLA	CHA-CBD-CGD-O1D
21	B	835	CLA	CHA-CBD-CGD-O2D
21	B	838	CLA	CHA-CBD-CGD-O1D
21	B	839	CLA	CHA-CBD-CGD-O2D
21	1	506	CLA	CHA-CBD-CGD-O2D
21	2	503	CLA	CHA-CBD-CGD-O1D
21	2	503	CLA	CHA-CBD-CGD-O2D
21	2	505	CLA	CHA-CBD-CGD-O1D
21	2	511	CLA	CHA-CBD-CGD-O1D
21	2	511	CLA	CHA-CBD-CGD-O2D
21	3	701	CLA	CHA-CBD-CGD-O1D
21	3	701	CLA	CHA-CBD-CGD-O2D
21	4	703	CLA	CHA-CBD-CGD-O2D
21	5	708	CLA	CHA-CBD-CGD-O1D
21	5	708	CLA	CHA-CBD-CGD-O2D
21	5	710	CLA	CHA-CBD-CGD-O1D
21	5	710	CLA	CHA-CBD-CGD-O2D
21	6	903	CLA	CHA-CBD-CGD-O1D
21	6	903	CLA	CHA-CBD-CGD-O2D
21	6	912	CLA	CHA-CBD-CGD-O1D
21	6	912	CLA	CHA-CBD-CGD-O2D
21	7	709	CLA	CHA-CBD-CGD-O1D
21	7	709	CLA	CHA-CBD-CGD-O2D
21	8	610	CLA	CHA-CBD-CGD-O1D
21	8	610	CLA	CHA-CBD-CGD-O2D
21	9	905	CLA	CHA-CBD-CGD-O2D
21	11	710	CLA	CHA-CBD-CGD-O1D
21	11	710	CLA	CHA-CBD-CGD-O2D
21	12	508	CLA	CHA-CBD-CGD-O2D
21	13	501	CLA	CHA-CBD-CGD-O1D
21	13	501	CLA	CHA-CBD-CGD-O2D
21	7	710	CLA	CAA-CBA-CGA-O1A
21	11	710	CLA	CAA-CBA-CGA-O1A
21	11	711	CLA	CAA-CBA-CGA-O1A
25	1	521	LHG	O7-C7-C8-C9
24	F	405	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	3	716	DD6	C9-C10-C11-C13
28	6	915	DD6	C9-C10-C11-C13
28	9	916	DD6	C24-C1-C2-C3
21	B	837	CLA	CAA-CBA-CGA-O1A
21	B	812	CLA	C15-C16-C17-C18
21	A	840	CLA	CAA-CBA-CGA-O2A
21	3	710	CLA	CAA-CBA-CGA-O2A
21	9	906	CLA	CAA-CBA-CGA-O2A
25	A	853	LHG	O8-C23-C24-C25
21	A	823	CLA	CAA-CBA-CGA-O1A
21	F	403	CLA	CAA-CBA-CGA-O2A
21	12	507	CLA	CAA-CBA-CGA-O1A
21	A	813	CLA	CAA-CBA-CGA-O2A
21	B	801	CLA	CAA-CBA-CGA-O2A
21	B	831	CLA	CAA-CBA-CGA-O2A
21	B	832	CLA	CAA-CBA-CGA-O2A
21	3	706	CLA	CAA-CBA-CGA-O2A
25	2	521	LHG	O7-C7-C8-C9
25	10	713	LHG	O7-C7-C8-C9
21	5	701	CLA	CAA-CBA-CGA-O2A
21	11	706	CLA	C13-C15-C16-C17
21	A	815	CLA	CAA-CBA-CGA-O2A
21	6	903	CLA	CAA-CBA-CGA-O2A
25	9	917	LHG	O8-C23-C24-C25
21	A	829	CLA	C11-C10-C8-C7
21	6	909	CLA	C12-C13-C15-C16
21	10	704	CLA	C2-C3-C5-C6
21	5	701	CLA	CAA-CBA-CGA-O1A
21	A	810	CLA	C11-C10-C8-C9
21	A	828	CLA	C11-C10-C8-C9
21	A	830	CLA	C11-C12-C13-C14
21	1	505	CLA	C11-C10-C8-C9
21	7	703	CLA	C11-C10-C8-C9
21	8	614	CLA	CAA-CBA-CGA-O1A
24	B	842	BCR	C9-C10-C11-C12
28	5	712	DD6	C24-C25-C26-C27
21	2	507	CLA	C2-C1-O2A-CGA
21	A	806	CLA	C2A-CAA-CBA-CGA
21	B	812	CLA	C2A-CAA-CBA-CGA
28	7	715	DD6	C25-C26-C27-C28
25	10	713	LHG	O1-C1-C2-C3
21	B	816	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	B	812	CLA	CAA-CBA-CGA-O1A
21	A	831	CLA	C1A-C2A-CAA-CBA
21	B	812	CLA	C1A-C2A-CAA-CBA
21	B	830	CLA	C1A-C2A-CAA-CBA
21	5	707	CLA	C1A-C2A-CAA-CBA
21	11	711	CLA	C1A-C2A-CAA-CBA
21	13	502	CLA	C1A-C2A-CAA-CBA
21	2	504	CLA	C11-C12-C13-C15
21	9	914	CLA	CAA-CBA-CGA-O1A
21	A	862	CLA	C2-C1-O2A-CGA
21	4	706	CLA	C2-C1-O2A-CGA
21	A	841	CLA	C15-C16-C17-C18
21	B	833	CLA	CAA-CBA-CGA-O2A
21	3	714	CLA	CAA-CBA-CGA-O2A
25	B	848	LHG	C4-C5-C6-O8
21	2	504	CLA	C2A-CAA-CBA-CGA
21	9	911	CLA	C2A-CAA-CBA-CGA
27	B	847	DGD	C6A-C7A-C8A-C9A
25	A	854	LHG	O9-C7-C8-C9
25	5	714	LHG	O9-C7-C8-C9
21	8	608	CLA	O1A-CGA-O2A-C1
21	B	831	CLA	C4-C3-C5-C6
21	9	911	CLA	CAA-CBA-CGA-O1A
21	7	707	CLA	O1A-CGA-O2A-C1
25	6	917	LHG	C3-O3-P-O4
21	9	906	CLA	CAA-CBA-CGA-O1A
21	A	814	CLA	CAA-CBA-CGA-O2A
21	10	710	CLA	O1A-CGA-O2A-C1
27	B	847	DGD	O6D-C5D-C6D-O5D
24	A	849	BCR	C5-C6-C7-C8
21	1	504	CLA	O1D-CGD-O2D-CED
21	11	709	CLA	O1D-CGD-O2D-CED
28	J	104	DD6	C11-C13-C14-C15
21	A	840	CLA	CAA-CBA-CGA-O1A
21	B	819	CLA	CAA-CBA-CGA-O1A
21	1	513	CLA	CAA-CBA-CGA-O1A
21	8	612	CLA	CAA-CBA-CGA-O1A
21	7	708	CLA	C13-C15-C16-C17
21	B	803	CLA	CAA-CBA-CGA-O2A
21	A	815	CLA	C2C-C3C-CAC-CBC
21	B	807	CLA	C2A-CAA-CBA-CGA
21	3	706	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	A	853	LHG	O10-C23-C24-C25
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	811	CLA	CAD-CBD-CGD-O1D
21	A	814	CLA	CAD-CBD-CGD-O1D
21	A	844	CLA	CAD-CBD-CGD-O1D
21	B	806	CLA	CAD-CBD-CGD-O1D
21	B	812	CLA	CAD-CBD-CGD-O1D
21	B	815	CLA	CAD-CBD-CGD-O1D
21	F	404	CLA	CAD-CBD-CGD-O1D
21	2	503	CLA	CAD-CBD-CGD-O1D
21	3	713	CLA	CAD-CBD-CGD-O1D
21	5	704	CLA	CAD-CBD-CGD-O1D
21	7	705	CLA	CAD-CBD-CGD-O1D
21	9	910	CLA	CAD-CBD-CGD-O1D
21	11	709	CLA	CAD-CBD-CGD-O1D
21	11	710	CLA	CAD-CBD-CGD-O1D
21	12	504	CLA	CAD-CBD-CGD-O1D
28	7	715	DD6	C25-C26-C27-C29
21	B	826	CLA	O1A-CGA-O2A-C1
21	3	702	CLA	O1A-CGA-O2A-C1
21	7	714	CLA	O1A-CGA-O2A-C1
25	10	713	LHG	O10-C23-O8-C6
21	A	813	CLA	CAA-CBA-CGA-O1A
21	B	805	CLA	CAA-CBA-CGA-O1A
25	2	521	LHG	O9-C7-C8-C9
25	7	717	LHG	O9-C7-C8-C9
21	A	830	CLA	C10-C11-C12-C13
21	A	820	CLA	C11-C10-C8-C9
21	A	841	CLA	C11-C10-C8-C9
21	B	805	CLA	C11-C10-C8-C9
21	B	804	CLA	O1D-CGD-O2D-CED
21	12	501	CLA	C10-C11-C12-C13
21	A	815	CLA	CAA-CBA-CGA-O1A
21	B	835	CLA	CBA-CGA-O2A-C1
21	A	805	CLA	CAA-CBA-CGA-O2A
21	10	710	CLA	CAA-CBA-CGA-O2A
21	B	812	CLA	C5-C6-C7-C8
21	A	823	CLA	CAA-CBA-CGA-O2A
21	7	702	CLA	C2-C1-O2A-CGA
21	A	828	CLA	O1A-CGA-O2A-C1
21	7	705	CLA	O1D-CGD-O2D-CED
21	A	824	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	A	826	CLA	CAA-CBA-CGA-O2A
21	2	512	CLA	CAA-CBA-CGA-O2A
21	A	833	CLA	C3-C5-C6-C7
21	7	711	CLA	C8-C10-C11-C12
21	B	831	CLA	O1D-CGD-O2D-CED
21	A	802	CLA	C3A-C2A-CAA-CBA
21	A	820	CLA	C11-C10-C8-C7
21	A	841	CLA	C11-C10-C8-C7
21	A	844	CLA	C3A-C2A-CAA-CBA
21	A	862	CLA	C2-C3-C5-C6
21	3	707	CLA	C12-C13-C15-C16
21	7	708	CLA	C11-C12-C13-C15
21	11	703	CLA	C6-C7-C8-C10
21	B	832	CLA	CAA-CBA-CGA-O1A
21	3	710	CLA	CAA-CBA-CGA-O1A
25	9	917	LHG	O10-C23-C24-C25
21	3	714	CLA	CAA-CBA-CGA-O1A
21	A	821	CLA	CAA-CBA-CGA-O2A
21	12	501	CLA	CAA-CBA-CGA-O2A
21	11	705	CLA	C2-C1-O2A-CGA
24	M	102	BCR	C21-C22-C23-C24
28	4	712	DD6	C5-C6-C8-C9
21	A	805	CLA	CAA-CBA-CGA-O1A
28	9	916	DD6	C3-C4-C5-C6
21	A	844	CLA	C2C-C3C-CAC-CBC
25	7	717	LHG	C34-C35-C36-C37
21	A	828	CLA	CAA-CBA-CGA-O2A
21	B	802	CLA	CAA-CBA-CGA-O2A
21	11	702	CLA	O1D-CGD-O2D-CED
21	A	803	CLA	C13-C15-C16-C17
21	A	807	CLA	O1A-CGA-O2A-C1
21	A	824	CLA	CAA-CBA-CGA-O1A
21	B	831	CLA	CAA-CBA-CGA-O1A
25	6	917	LHG	O9-C7-C8-C9
21	8	608	CLA	CBA-CGA-O2A-C1
21	A	804	CLA	C13-C15-C16-C17
21	A	807	CLA	C15-C16-C17-C18
21	A	810	CLA	C10-C11-C12-C13
21	11	703	CLA	CAA-CBA-CGA-O2A
21	A	814	CLA	CAA-CBA-CGA-O1A
21	B	803	CLA	CAA-CBA-CGA-O1A
21	6	903	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	1	510	CLA	C8-C10-C11-C12
21	1	517	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

214 monomers are involved in 397 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	802	CLA	2	0
21	F	404	CLA	1	0
21	2	515	CLA	1	0
21	2	514	CLA	1	0
21	1	513	CLA	2	0
21	3	705	CLA	2	0
21	A	841	CLA	1	0
21	3	714	CLA	1	0
21	1	507	CLA	2	0
21	12	508	CLA	1	0
21	B	806	CLA	1	0
21	4	708	CLA	2	0
21	4	709	CLA	1	0
21	A	839	CLA	4	0
21	2	503	CLA	2	0
21	B	812	CLA	2	0
21	8	611	CLA	1	0
21	12	502	CLA	1	0
25	3	719	LHG	1	0
21	A	823	CLA	3	0
24	J	102	BCR	7	0
21	8	609	CLA	2	0
21	A	809	CLA	2	0
21	1	508	CLA	2	0
21	A	803	CLA	5	0
21	B	838	CLA	2	0
21	B	807	CLA	2	0
21	7	705	CLA	1	0
21	B	804	CLA	3	0
21	7	709	CLA	2	0
21	7	713	CLA	3	0
21	A	808	CLA	1	0
21	11	707	CLA	3	0
25	4	714	LHG	3	0
21	8	607	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	862	CLA	7	0
21	A	825	CLA	1	0
25	A	853	LHG	1	0
28	4	712	DD6	2	0
21	3	702	CLA	1	0
21	5	711	CLA	1	0
21	13	503	CLA	1	0
21	4	702	CLA	2	0
24	A	848	BCR	3	0
24	A	852	BCR	9	0
21	12	507	CLA	1	0
21	6	903	CLA	1	0
21	A	822	CLA	1	0
21	2	505	CLA	3	0
21	9	902	CLA	2	0
21	A	806	CLA	2	0
21	A	836	CLA	1	0
21	12	506	CLA	4	0
21	11	709	CLA	1	0
21	1	512	CLA	1	0
24	B	842	BCR	2	0
21	7	707	CLA	1	0
21	J	101	CLA	1	0
21	2	506	CLA	1	0
21	4	701	CLA	3	0
21	7	708	CLA	4	0
21	1	510	CLA	1	0
21	9	913	CLA	3	0
21	B	827	CLA	4	0
21	B	828	CLA	2	0
24	A	847	BCR	3	0
21	B	821	CLA	1	0
21	A	817	CLA	3	0
21	7	714	CLA	1	0
21	A	804	CLA	3	0
21	2	511	CLA	6	0
21	8	603	CLA	1	0
21	2	508	CLA	2	0
21	11	708	CLA	1	0
21	A	819	CLA	2	0
21	F	401	CLA	2	0
21	4	706	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	509	CLA	1	0
21	5	702	CLA	2	0
21	11	701	CLA	1	0
21	5	701	CLA	1	0
21	7	710	CLA	1	0
21	2	510	CLA	4	0
21	4	710	CLA	2	0
27	B	847	DGD	3	0
21	B	811	CLA	1	0
21	B	830	CLA	3	0
21	B	805	CLA	1	0
21	F	403	CLA	2	0
21	3	703	CLA	1	0
21	B	823	CLA	3	0
21	A	805	CLA	1	0
21	8	612	CLA	3	0
28	11	713	DD6	1	0
21	A	842	CLA	5	0
21	3	712	CLA	1	0
21	6	907	CLA	1	0
24	F	405	BCR	4	0
21	3	707	CLA	3	0
21	4	711	CLA	2	0
21	5	708	CLA	2	0
24	M	102	BCR	2	0
21	A	807	CLA	2	0
21	B	831	CLA	6	0
21	11	710	CLA	1	0
21	A	840	CLA	1	0
21	6	904	CLA	2	0
21	11	703	CLA	3	0
21	9	909	CLA	1	0
21	1	505	CLA	2	0
21	2	507	CLA	4	0
21	8	613	CLA	1	0
21	3	701	CLA	2	0
21	B	815	CLA	2	0
21	2	504	CLA	1	0
21	6	913	CLA	1	0
21	9	911	CLA	1	0
28	1	518	DD6	1	0
21	8	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	837	CLA	1	0
22	A	845	PQN	2	0
21	13	501	CLA	1	0
21	9	907	CLA	1	0
21	B	839	CLA	2	0
21	6	911	CLA	2	0
21	A	810	CLA	4	0
21	2	517	CLA	1	0
21	3	706	CLA	2	0
21	A	811	CLA	1	0
21	A	824	CLA	1	0
24	A	851	BCR	3	0
21	12	505	CLA	1	0
21	13	502	CLA	1	0
24	J	103	BCR	1	0
21	10	709	CLA	1	0
21	A	829	CLA	6	0
21	B	817	CLA	1	0
21	9	914	CLA	1	0
21	1	504	CLA	2	0
21	B	819	CLA	1	0
21	6	909	CLA	2	0
21	1	506	CLA	1	0
21	A	813	CLA	2	0
21	6	914	CLA	1	0
21	9	910	CLA	2	0
21	6	908	CLA	1	0
21	A	812	CLA	2	0
21	7	703	CLA	3	0
21	A	821	CLA	4	0
21	A	802	CLA	2	0
21	11	711	CLA	1	0
21	10	712	CLA	2	0
21	B	829	CLA	5	0
21	B	825	CLA	2	0
21	A	827	CLA	1	0
21	B	833	CLA	1	0
21	A	828	CLA	2	0
21	A	838	CLA	1	0
21	1	517	CLA	3	0
21	3	715	CLA	1	0
21	2	513	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	10	704	CLA	2	0
24	B	841	BCR	3	0
24	F	402	BCR	1	0
21	11	705	CLA	2	0
21	B	824	CLA	1	0
20	A	801	CL0	2	0
21	A	843	CLA	1	0
21	A	833	CLA	3	0
21	3	709	CLA	1	0
21	B	826	CLA	2	0
21	5	706	CLA	2	0
21	B	818	CLA	1	0
21	B	803	CLA	2	0
21	A	830	CLA	2	0
21	A	835	CLA	1	0
24	A	849	BCR	3	0
24	A	850	BCR	1	0
21	A	818	CLA	2	0
21	10	711	CLA	1	0
28	6	915	DD6	1	0
21	A	820	CLA	3	0
21	1	511	CLA	1	0
21	6	910	CLA	2	0
21	12	504	CLA	4	0
24	B	845	BCR	6	0
21	6	912	CLA	1	0
24	B	844	BCR	2	0
21	10	707	CLA	2	0
21	3	704	CLA	1	0
21	A	831	CLA	3	0
28	3	716	DD6	1	0
21	1	515	CLA	2	0
21	3	708	CLA	2	0
21	B	835	CLA	8	0
21	A	834	CLA	1	0
21	A	826	CLA	3	0
21	B	801	CLA	2	0
21	5	707	CLA	5	0
21	B	834	CLA	2	0
21	2	509	CLA	4	0
21	1	516	CLA	2	0
21	1	514	CLA	2	0

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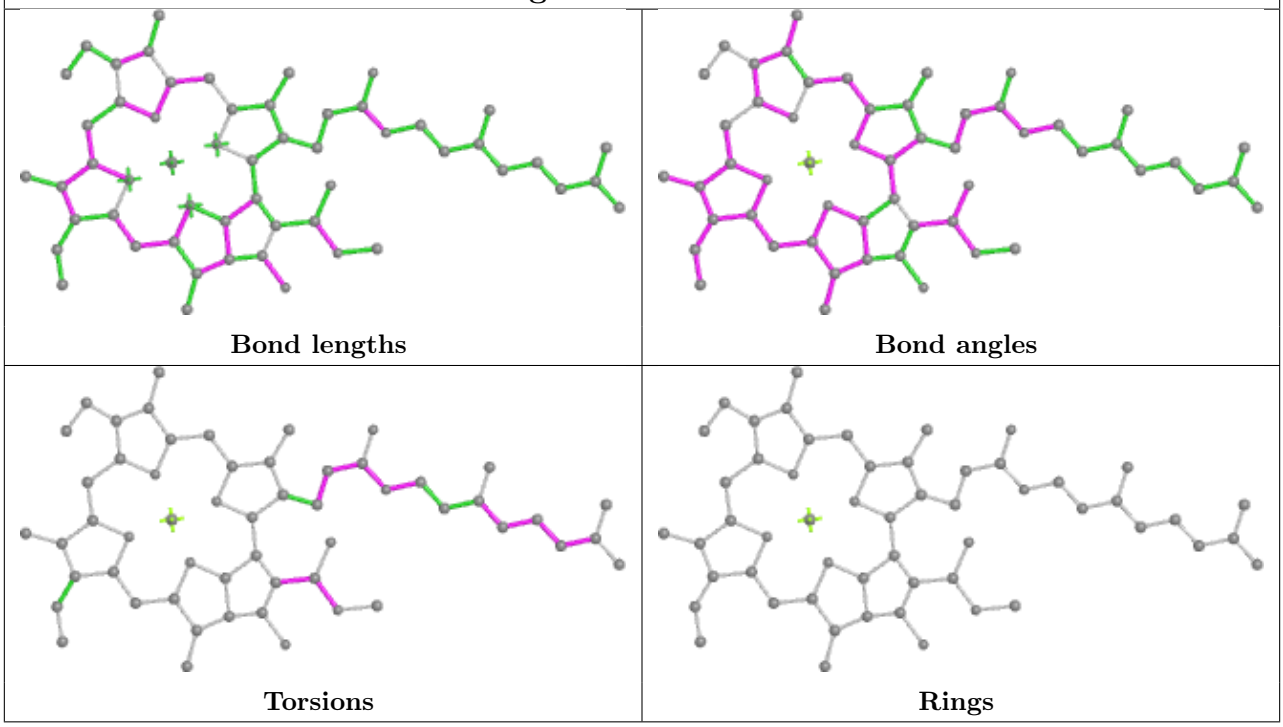
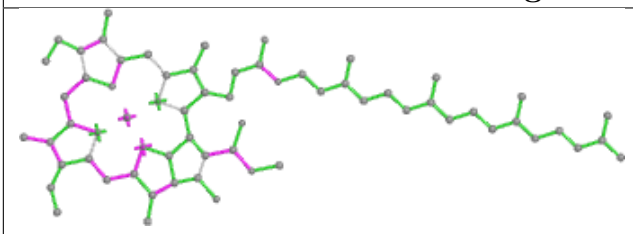
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	713	CLA	1	0
21	A	832	CLA	1	0
21	5	709	CLA	1	0
21	3	711	CLA	1	0
21	10	706	CLA	2	0
25	2	521	LHG	1	0
21	10	708	CLA	1	0
21	4	704	CLA	1	0
21	A	844	CLA	5	0
21	3	710	CLA	2	0
21	B	816	CLA	3	0

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.

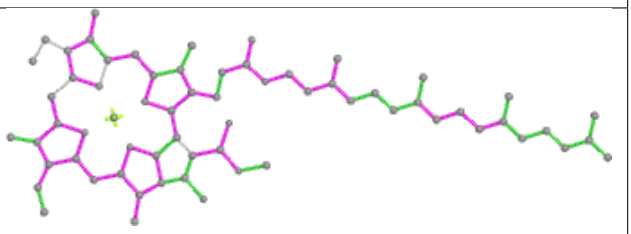
Ligand CLA 2 512



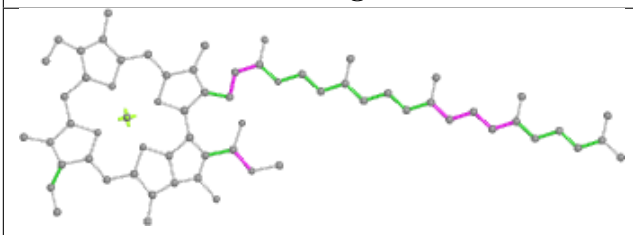
Ligand CLA B 802



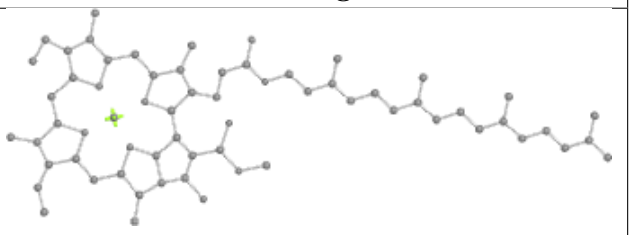
Bond lengths



Bond angles

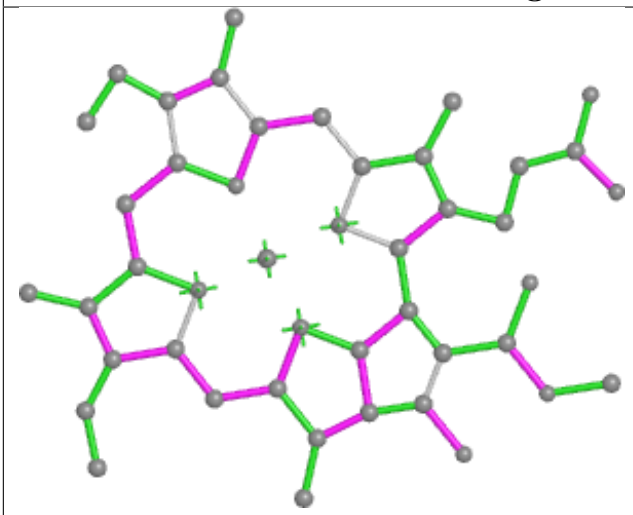


Torsions



Rings

Ligand CLA F 404



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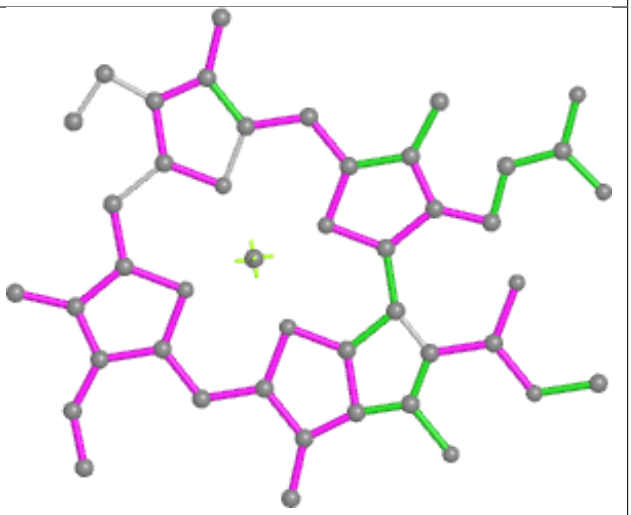
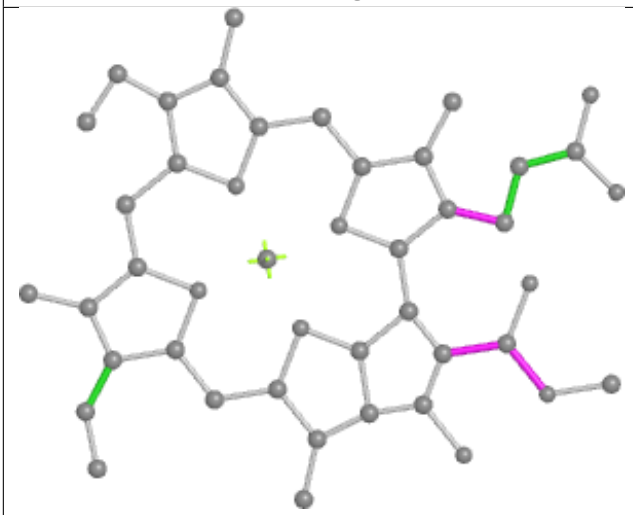


Bond angles



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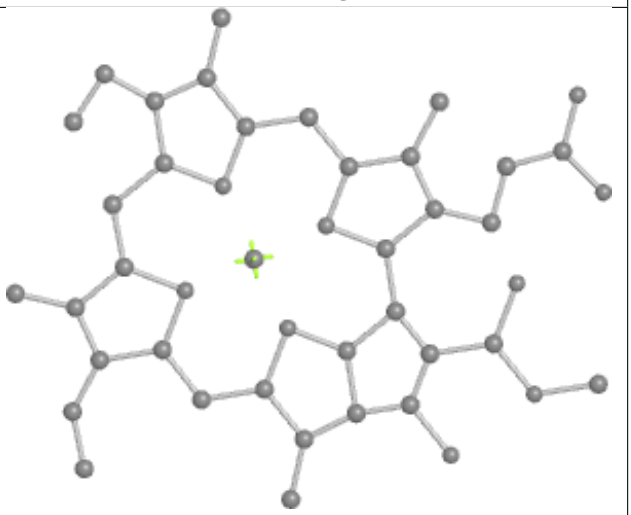

Rings

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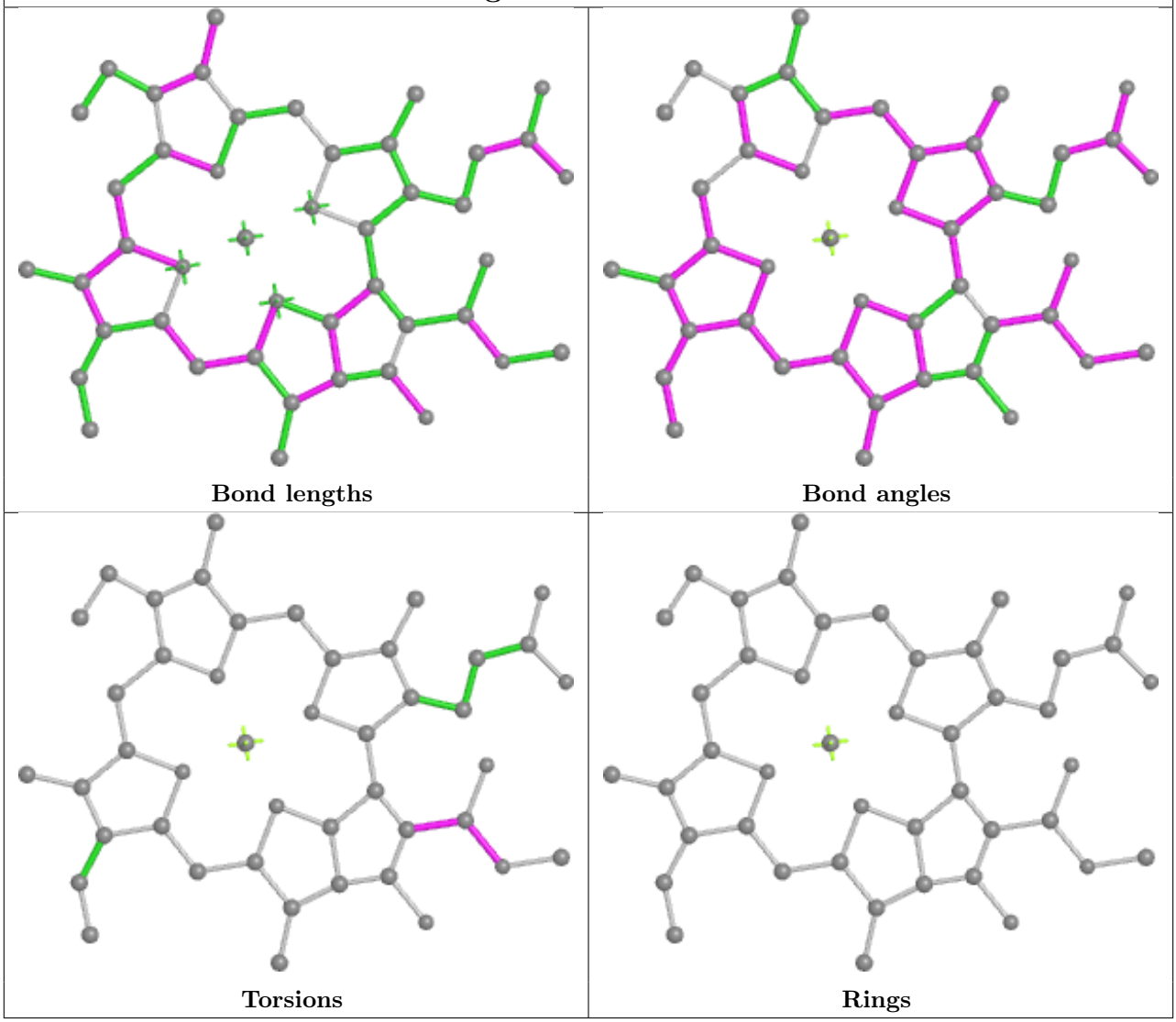

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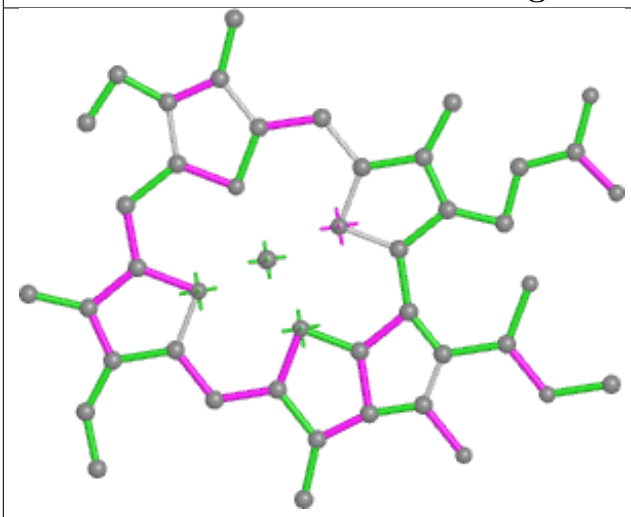
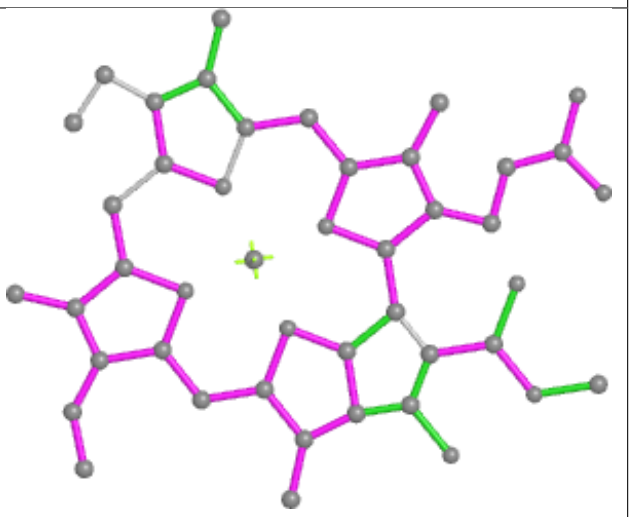
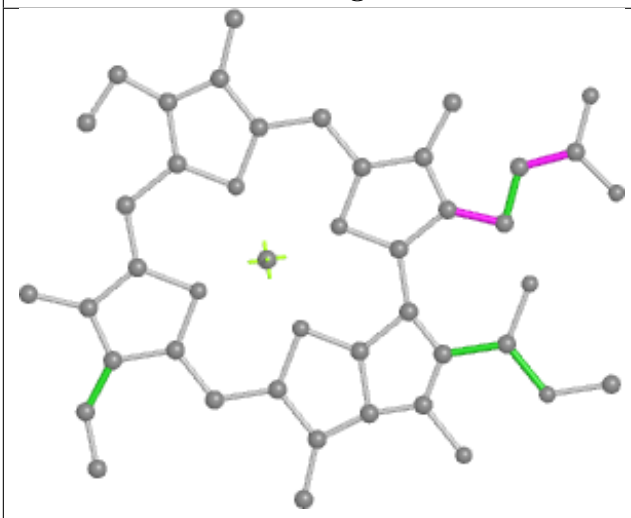


Bond lengths



Bond angles



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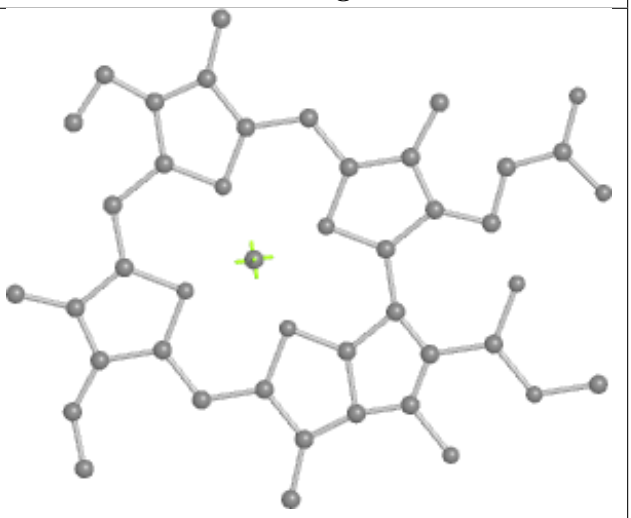

Rings

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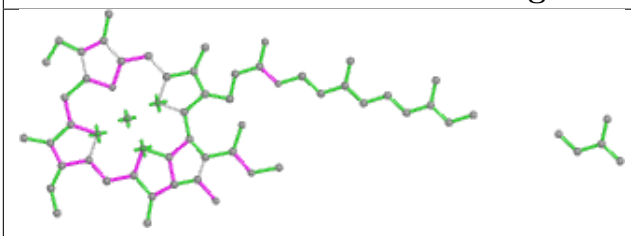
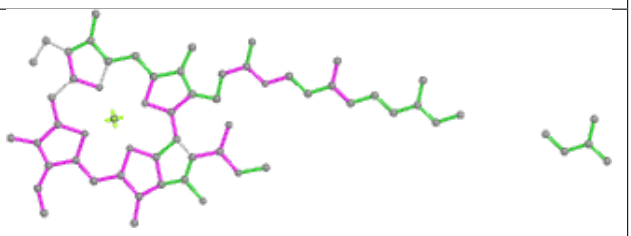
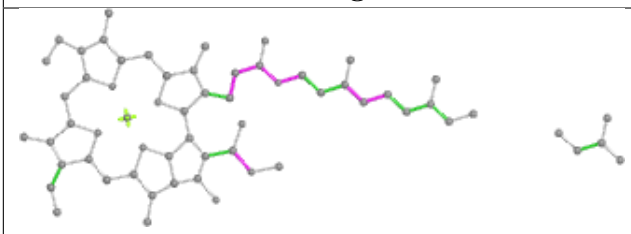


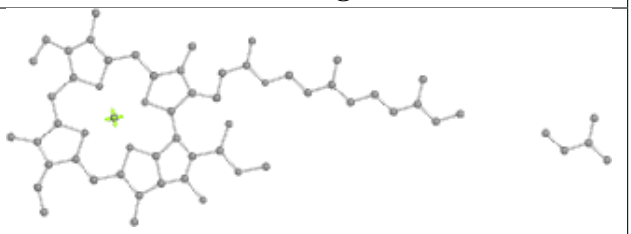
Bond lengths



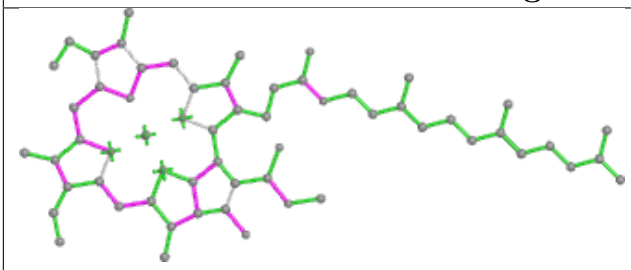
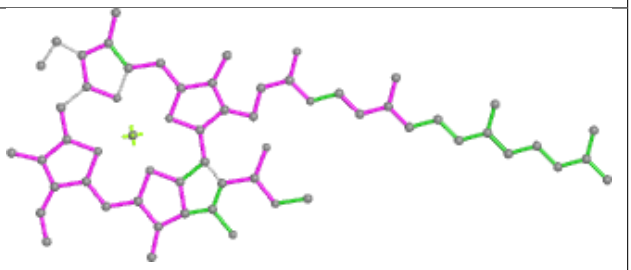
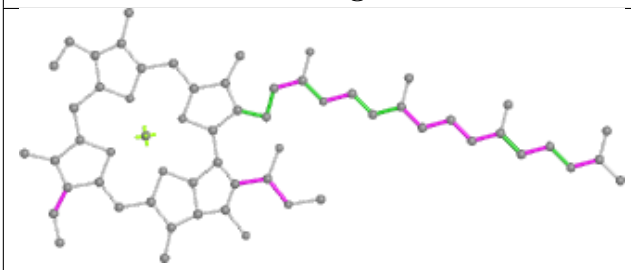
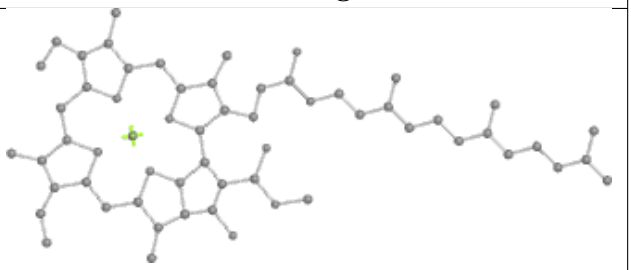
Bond angles



Torsions



Rings

Ligand CLA A 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

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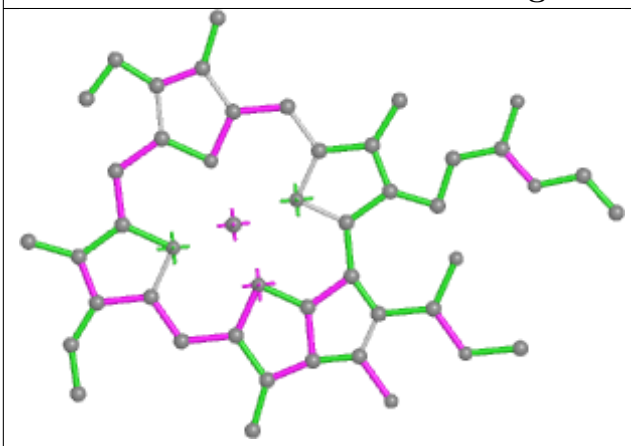
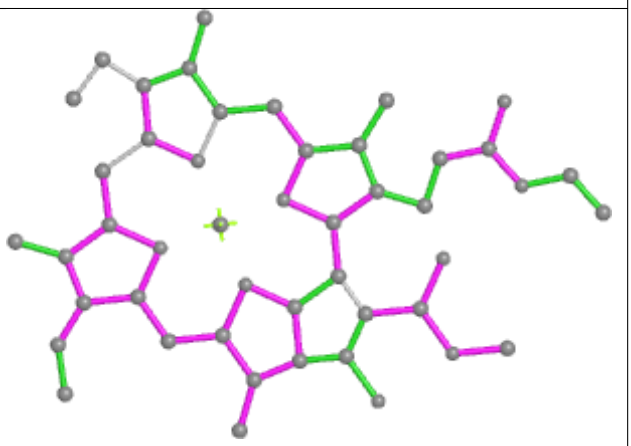
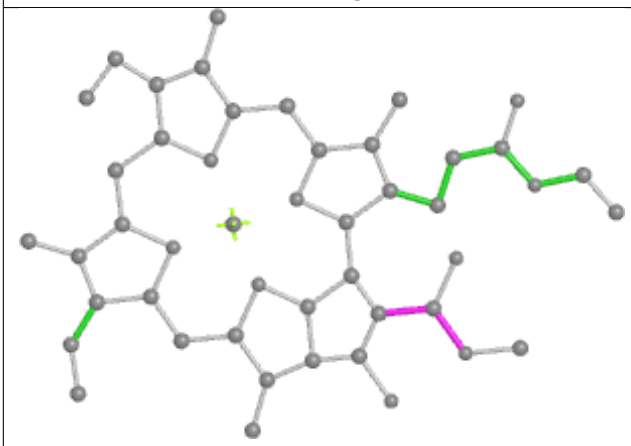
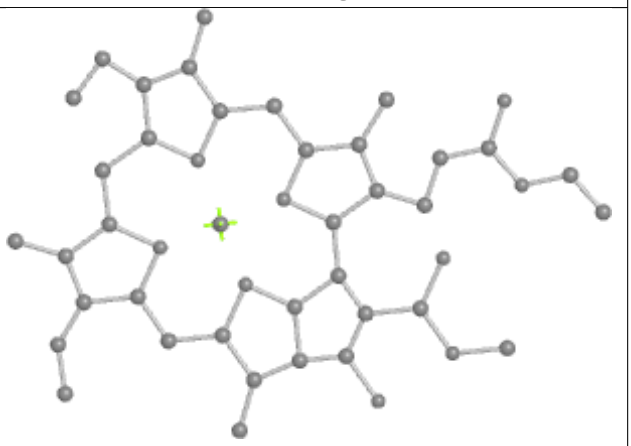
 Bond lengths	 Bond angles
 Torsions	 Rings

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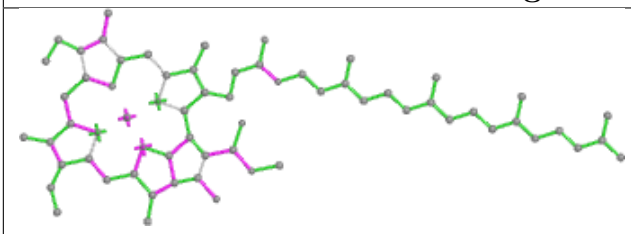
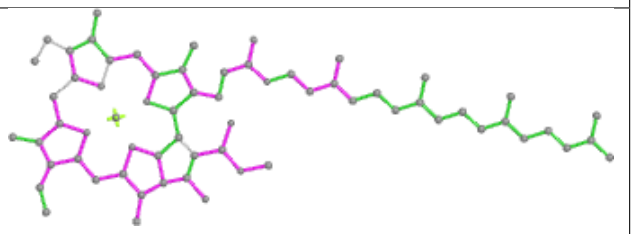
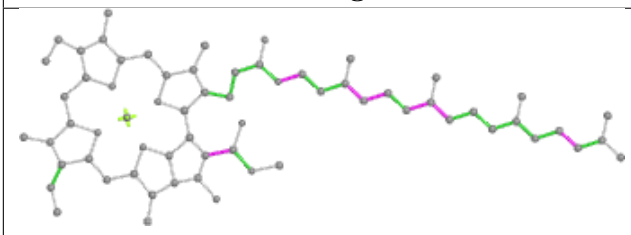
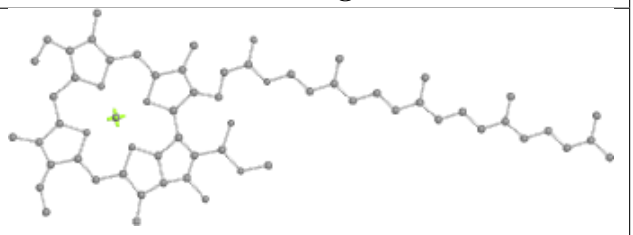
 Bond lengths	 Bond angles
 Torsions	 Rings

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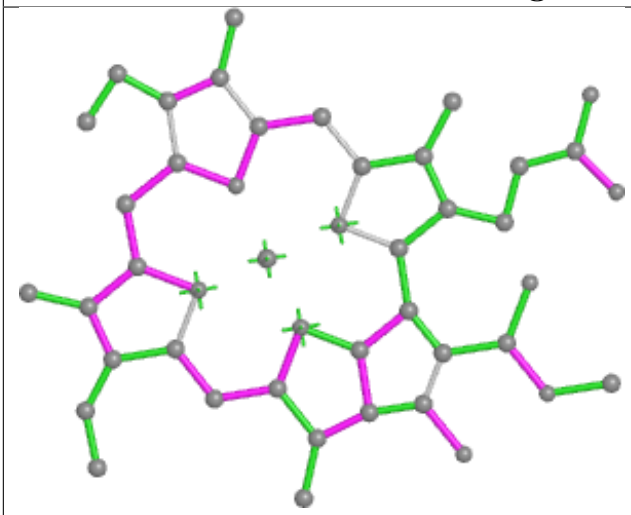
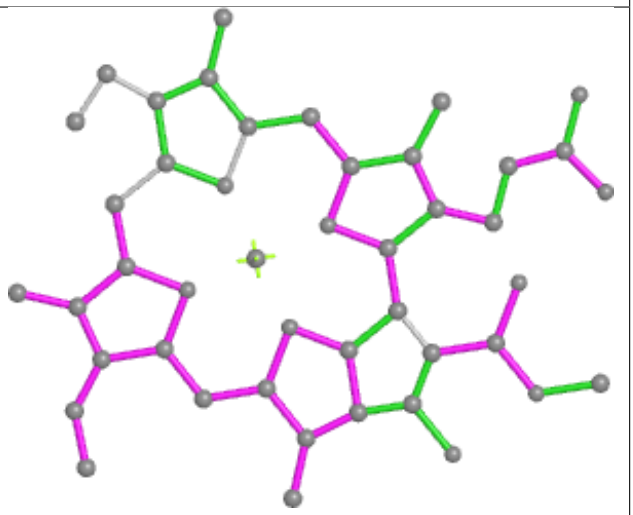
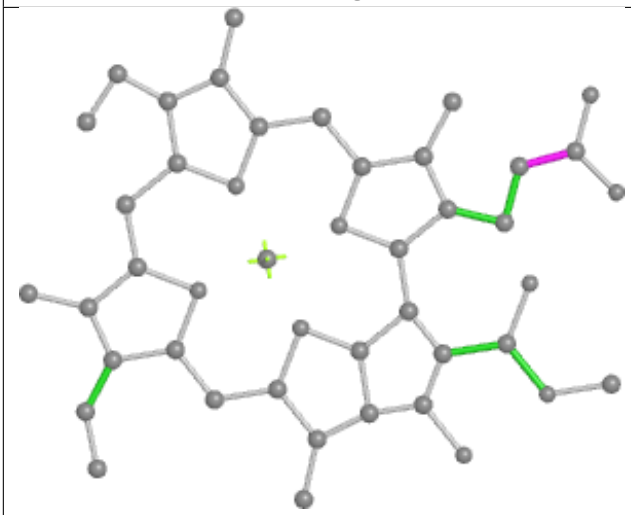
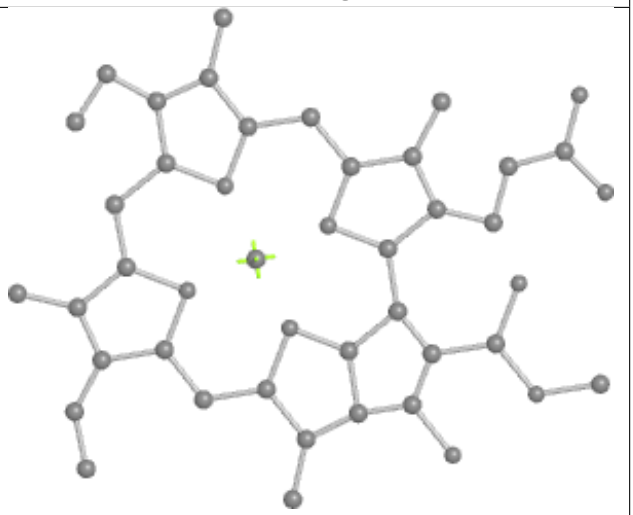
 Bond lengths	 Bond angles
 Torsions	 Rings

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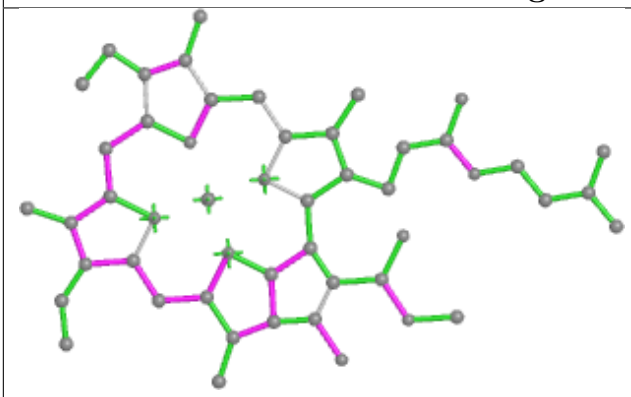
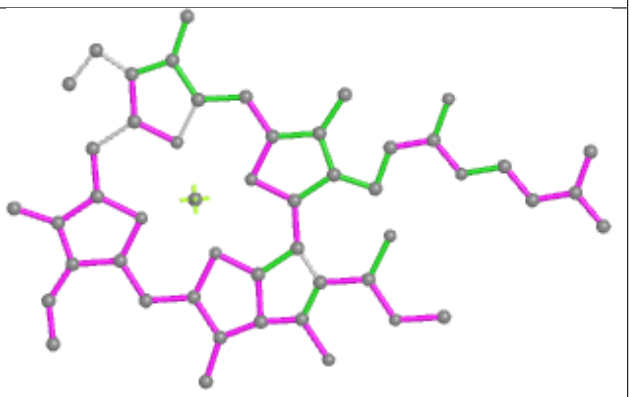
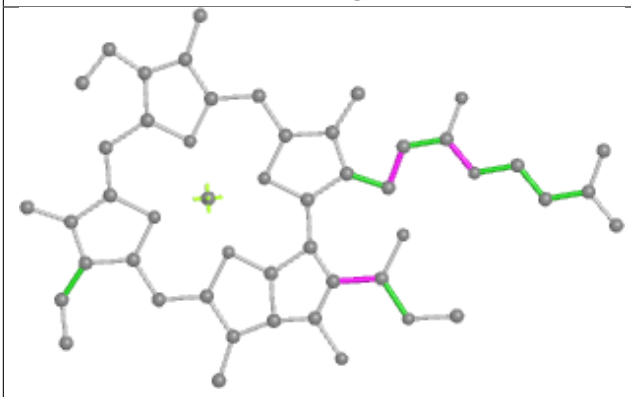
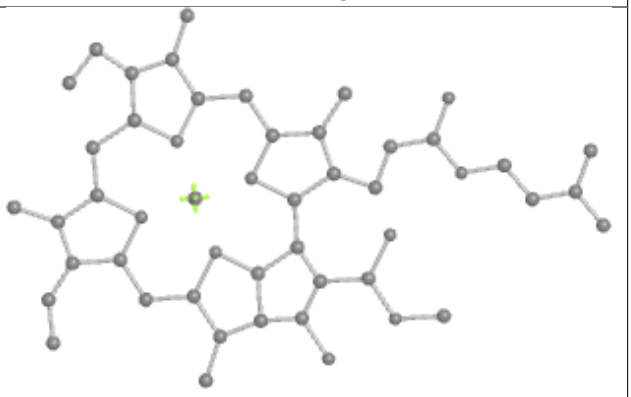
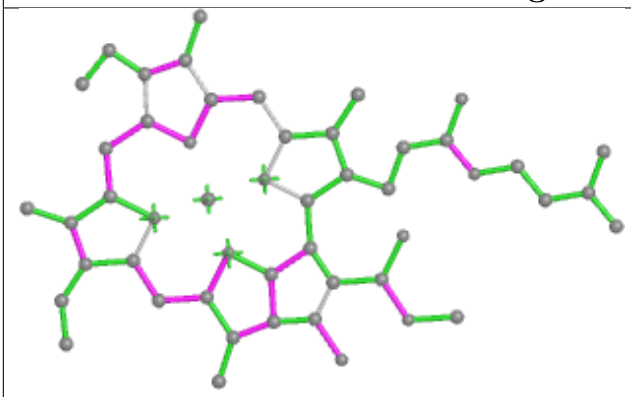
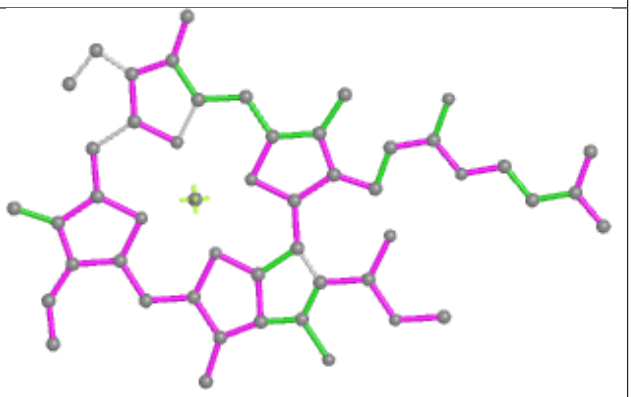
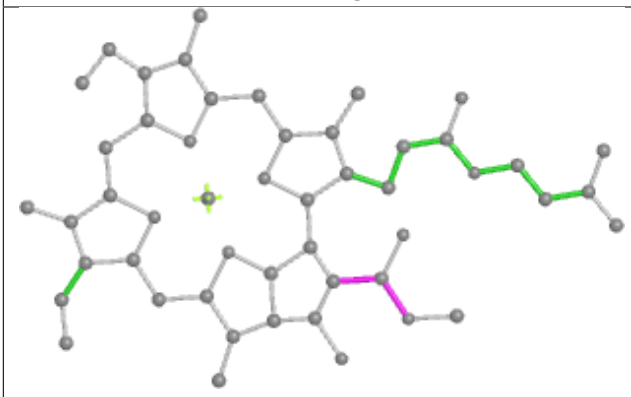
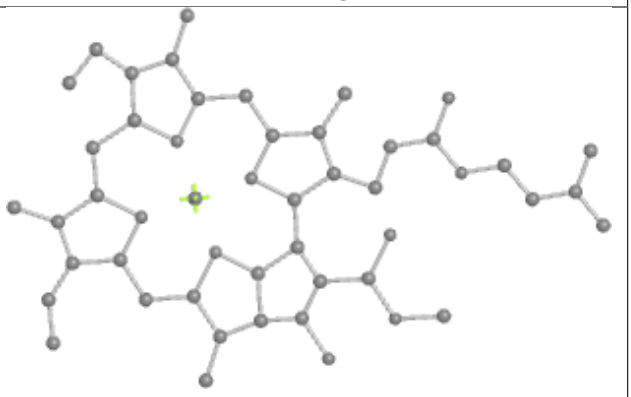
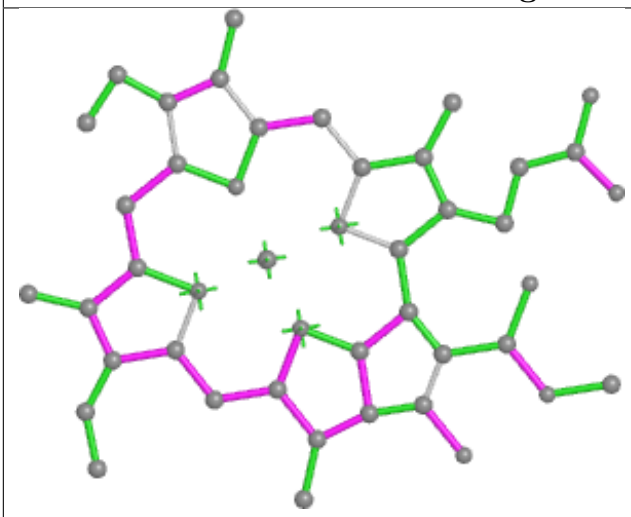
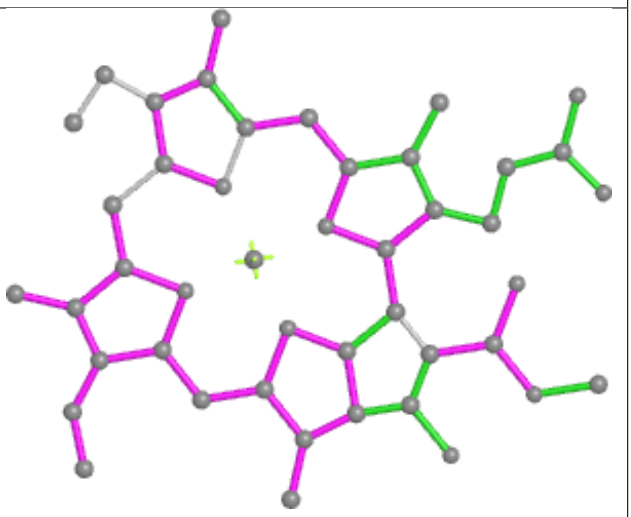
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 1 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

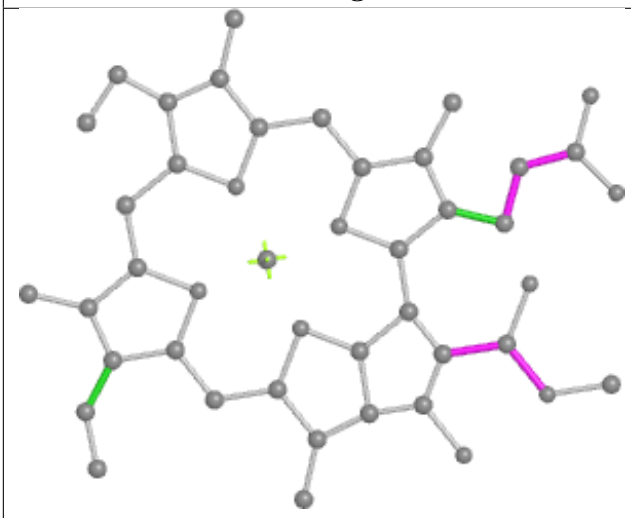
Ligand CLA 12 508



Bond lengths



Bond angles



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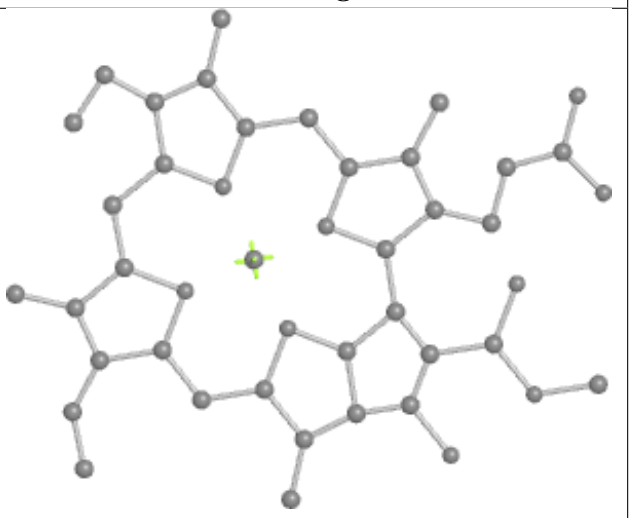
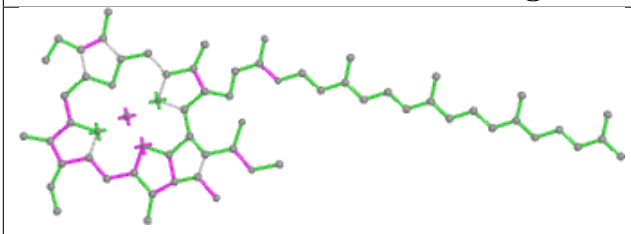


Rings

Ligand CLA B 806



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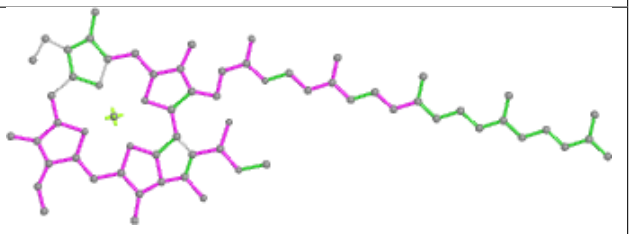
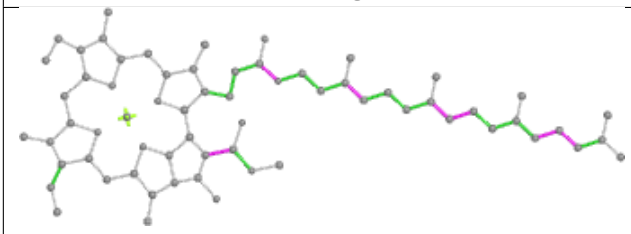


Bond angles



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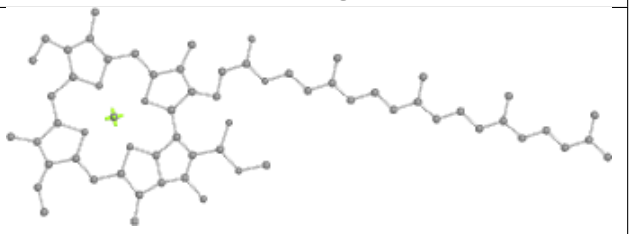
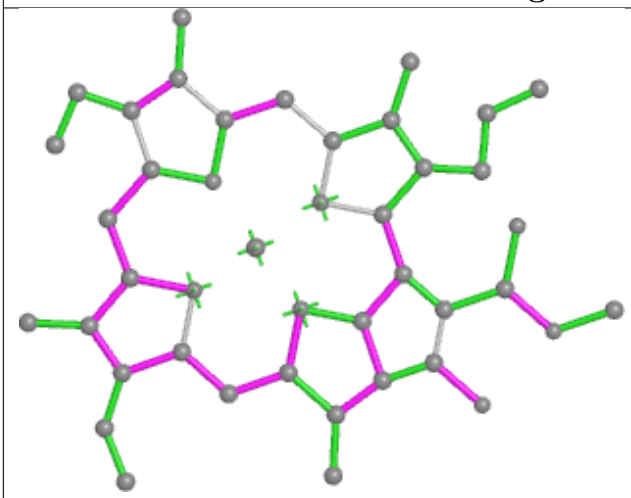


Rings

Ligand CLA 4 708



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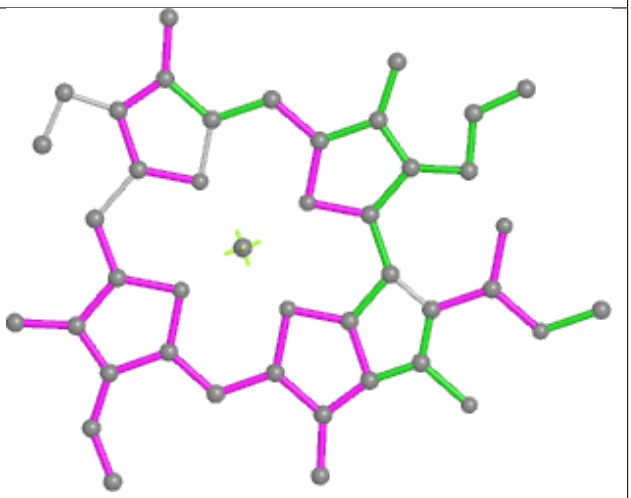

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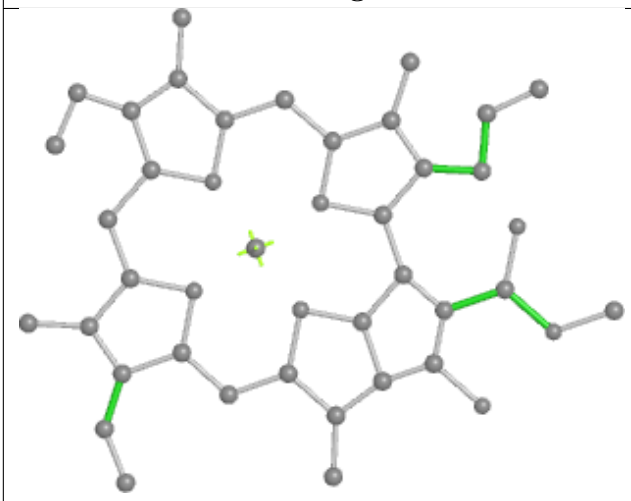

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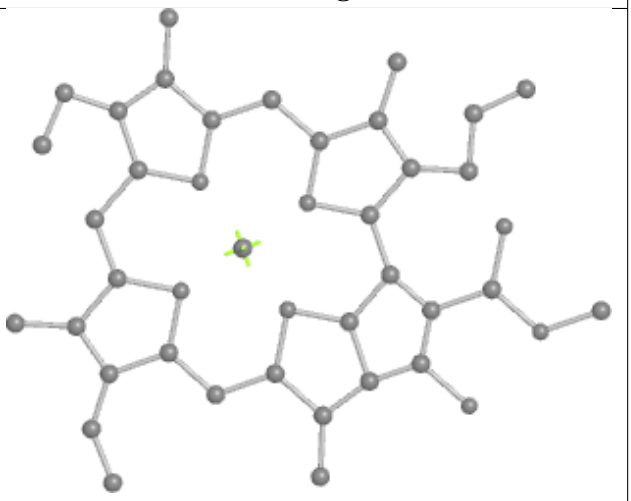
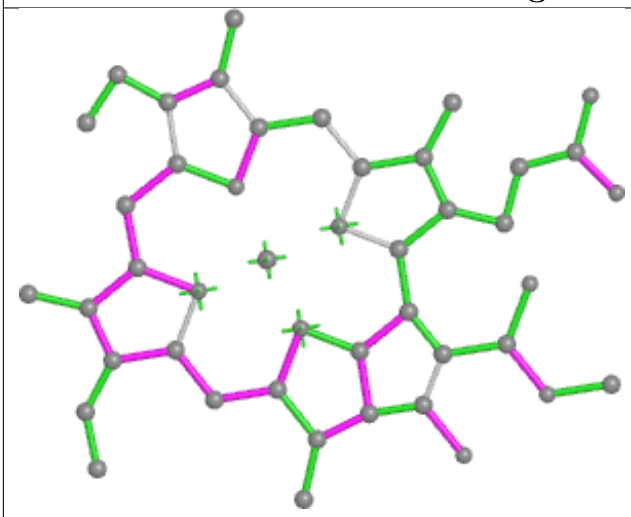


Rings

Ligand CLA 4 709



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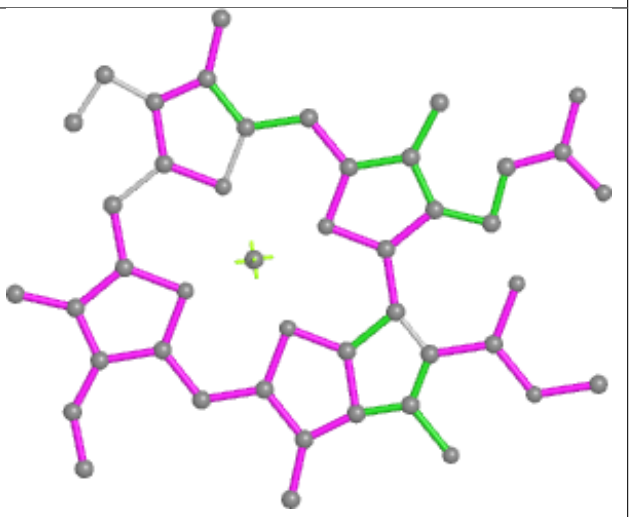
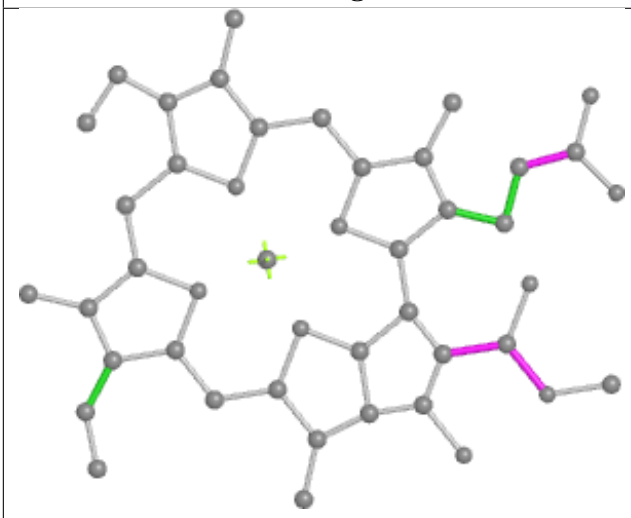


Bond angles



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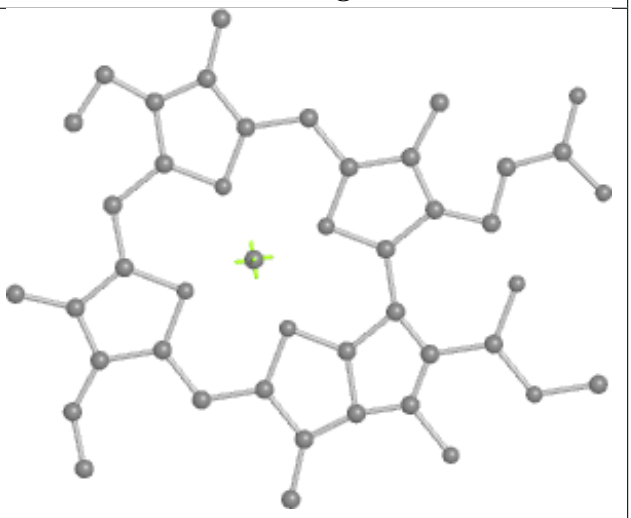
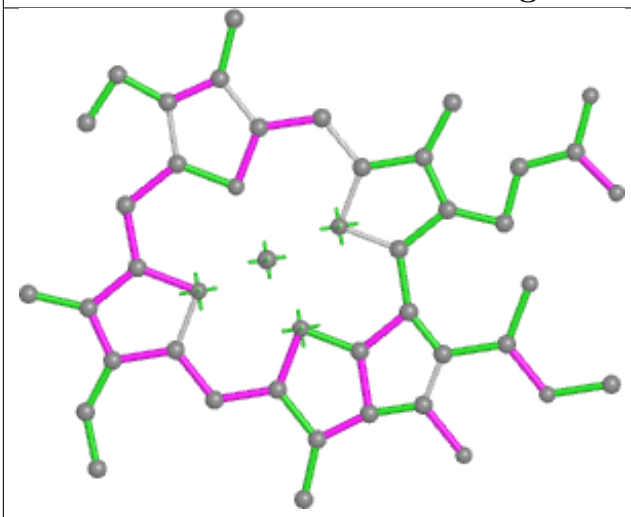


Rings

Ligand CLA 12 503



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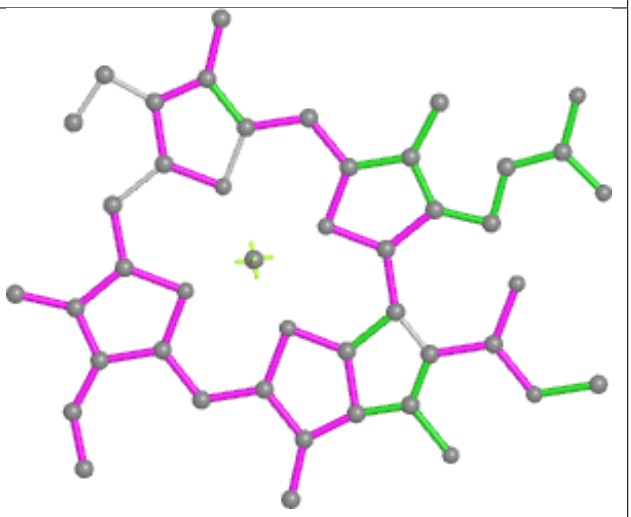
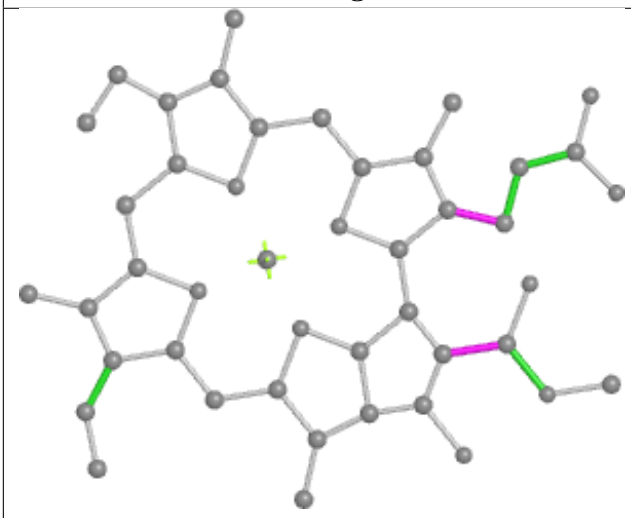


Bond angles



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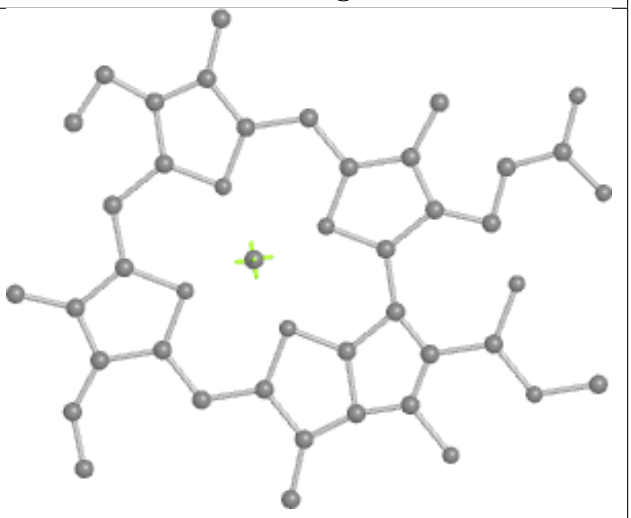
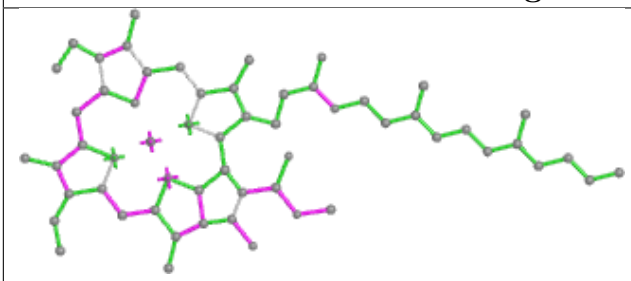
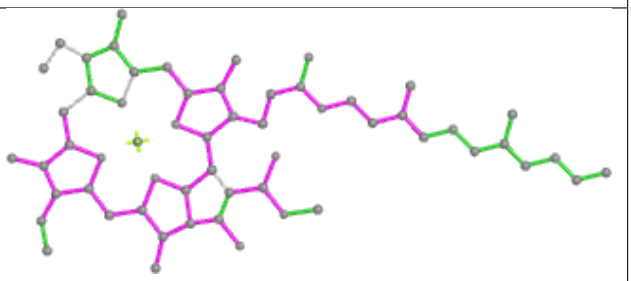
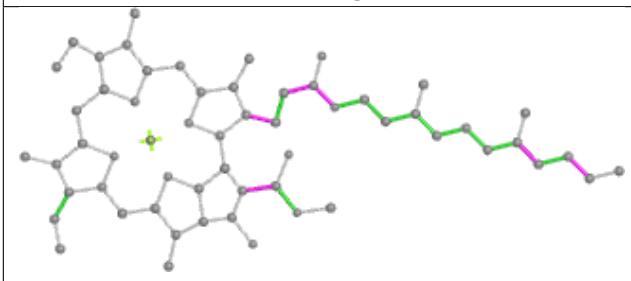
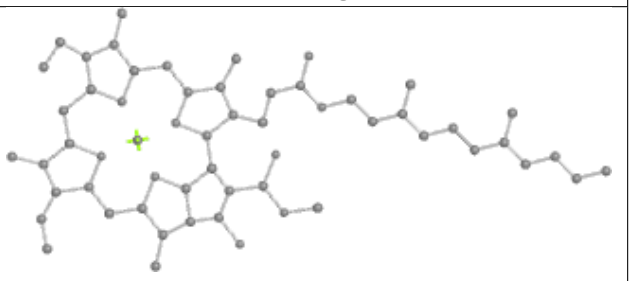
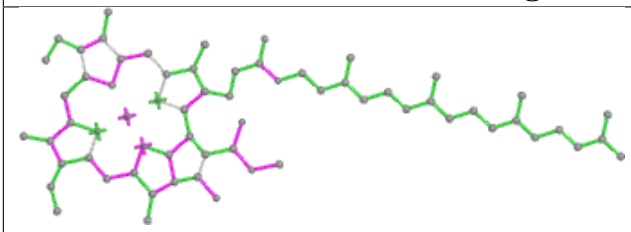
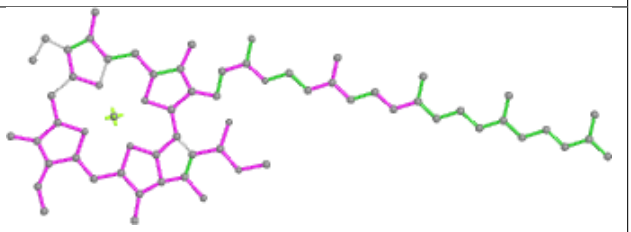
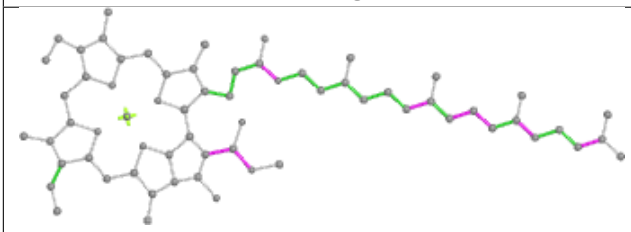
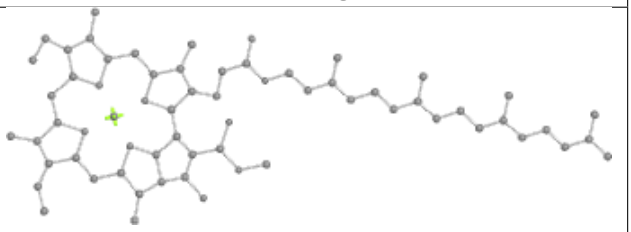
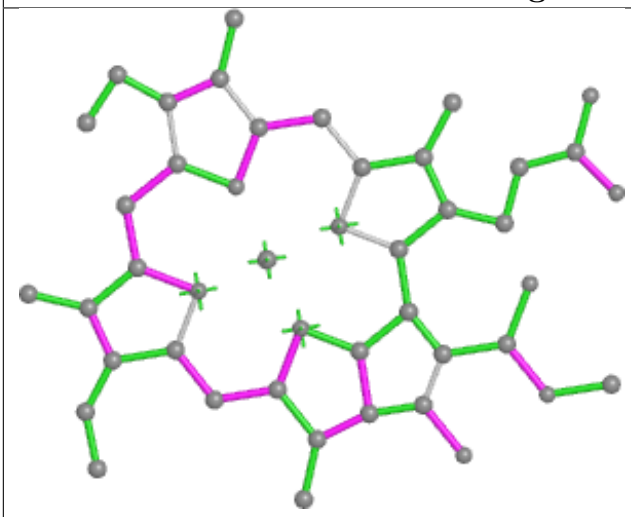


Rings

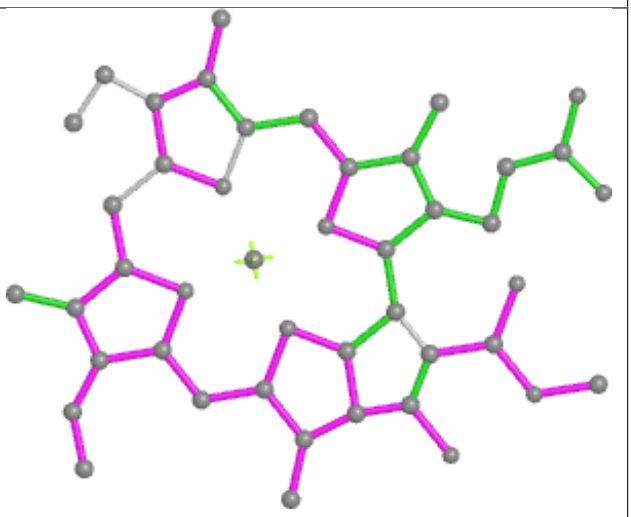
Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

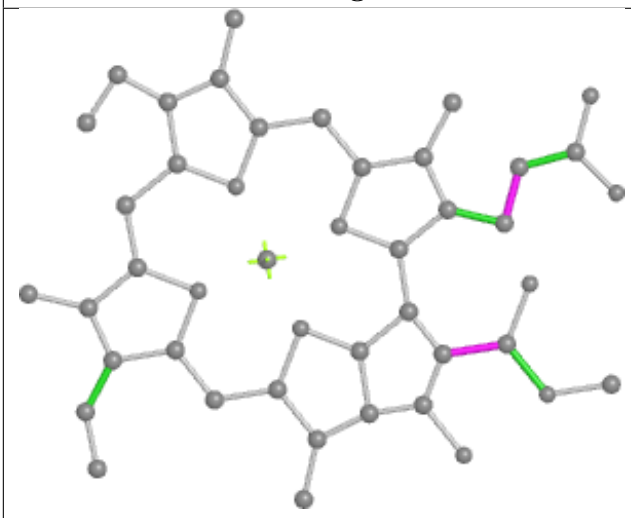
Ligand CLA 2 503



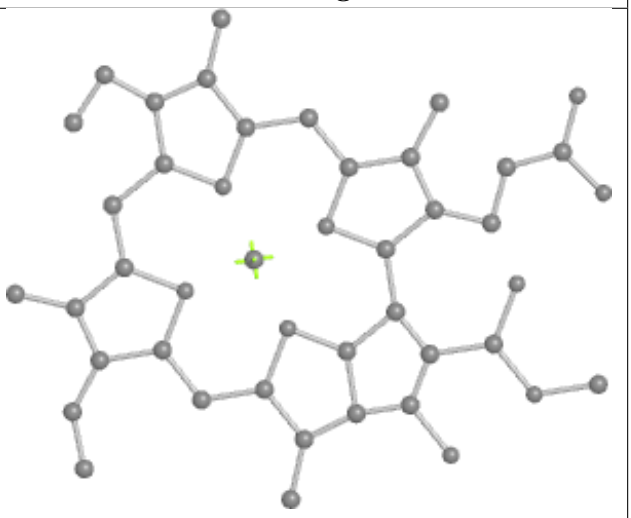
Bond lengths



Bond angles

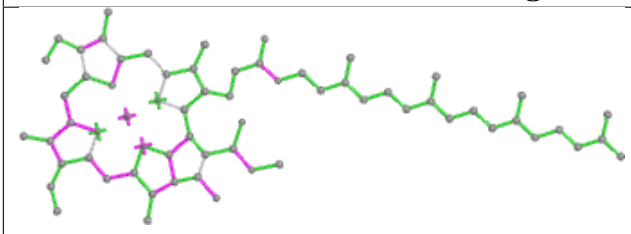


Torsions



Rings

Ligand CLA B 812



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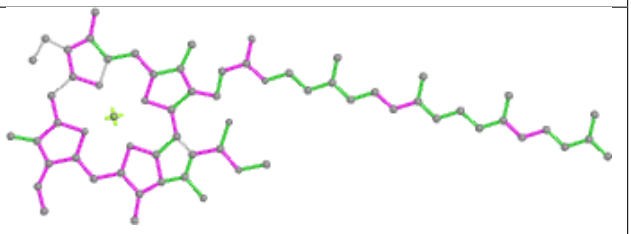
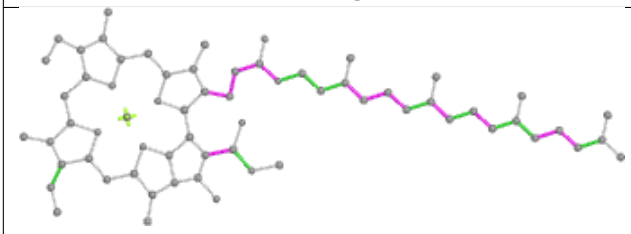


Bond angles



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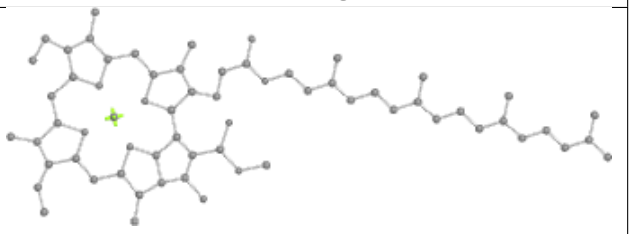
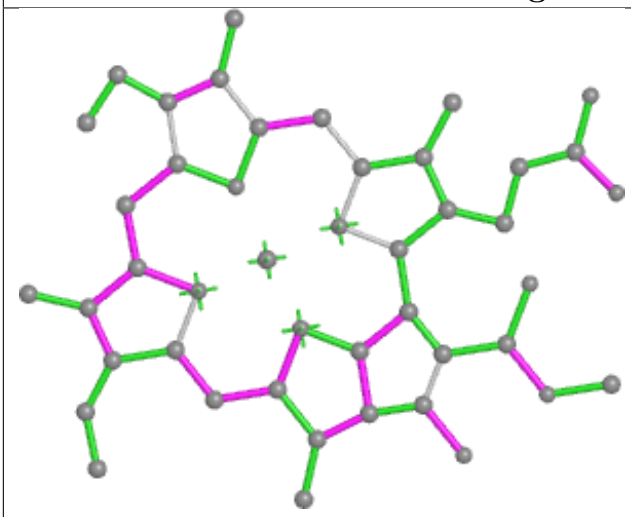


Rings

Ligand CLA 8 611



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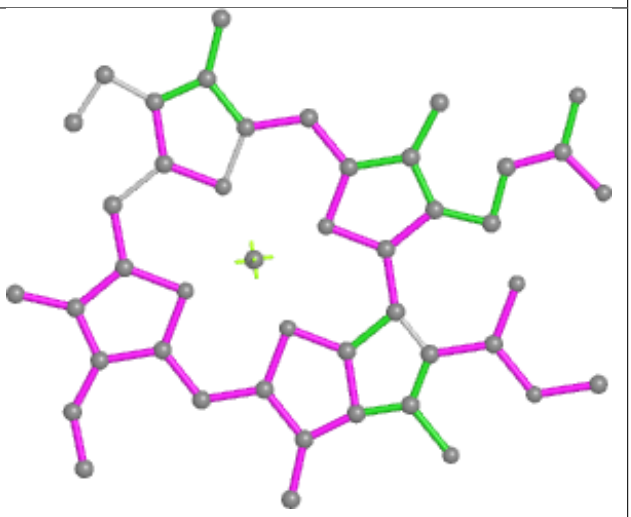
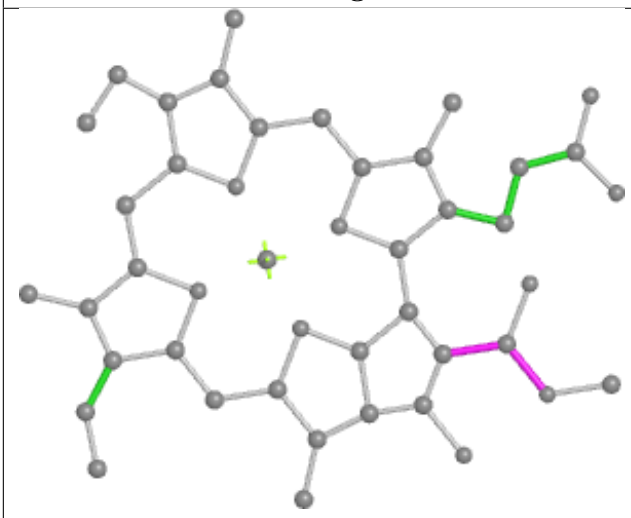


Bond angles



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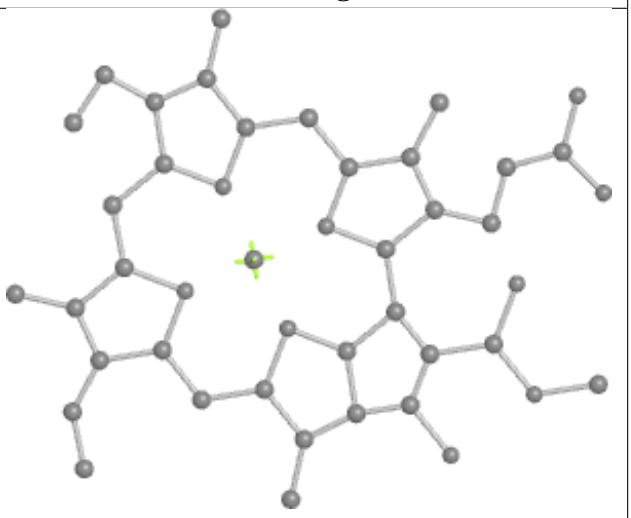
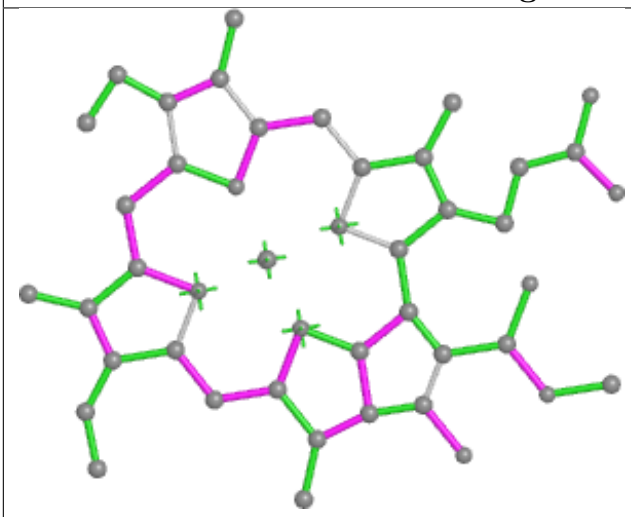


Rings

Ligand CLA 12 502



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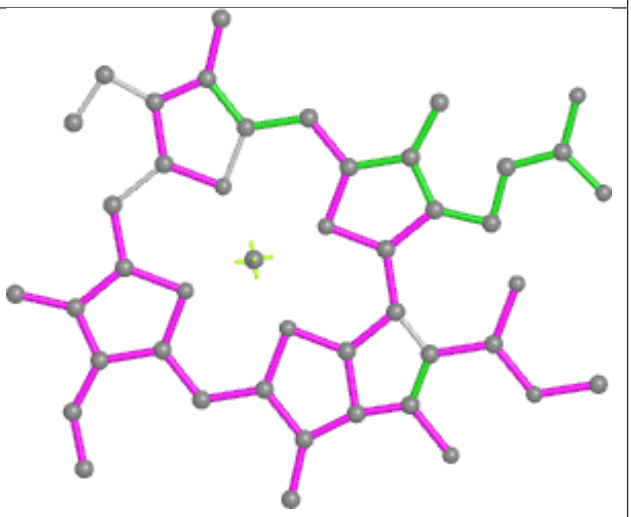
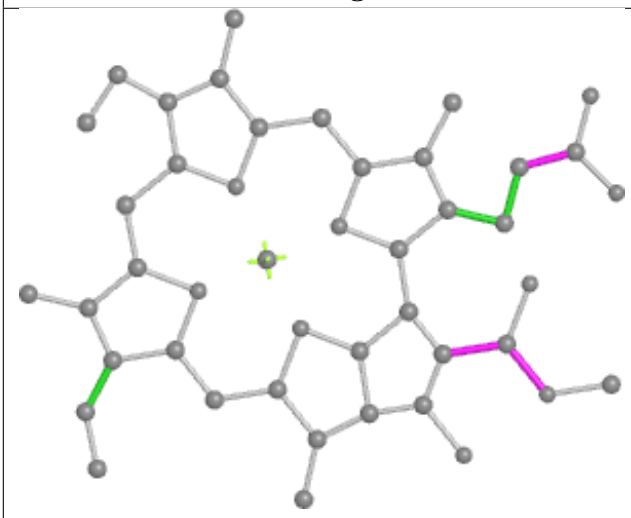
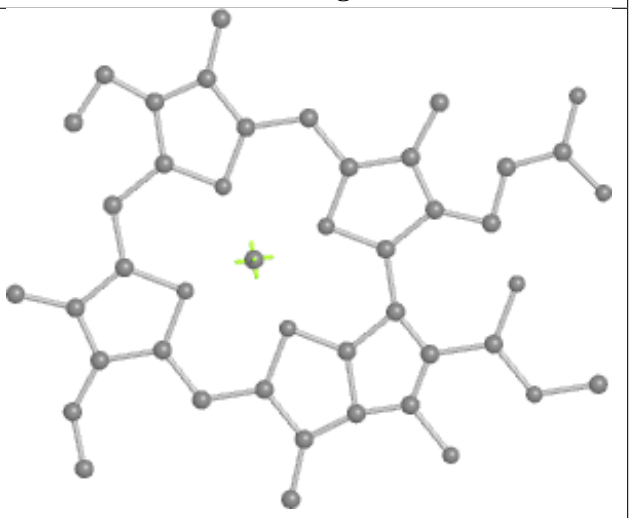


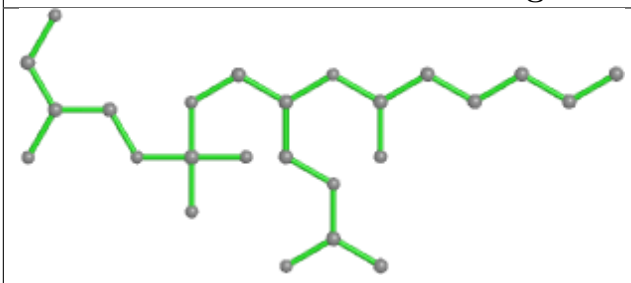
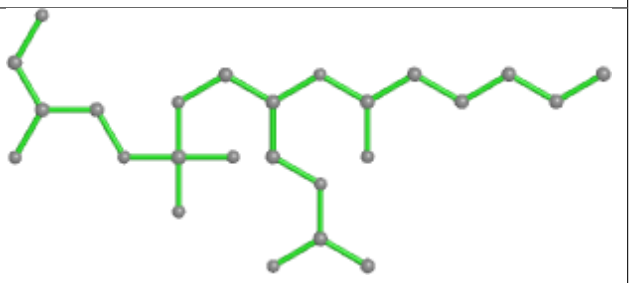
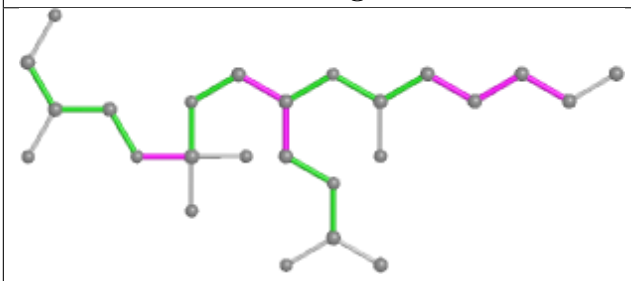
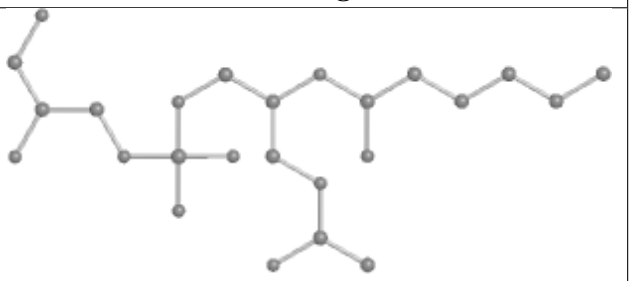
Bond angles



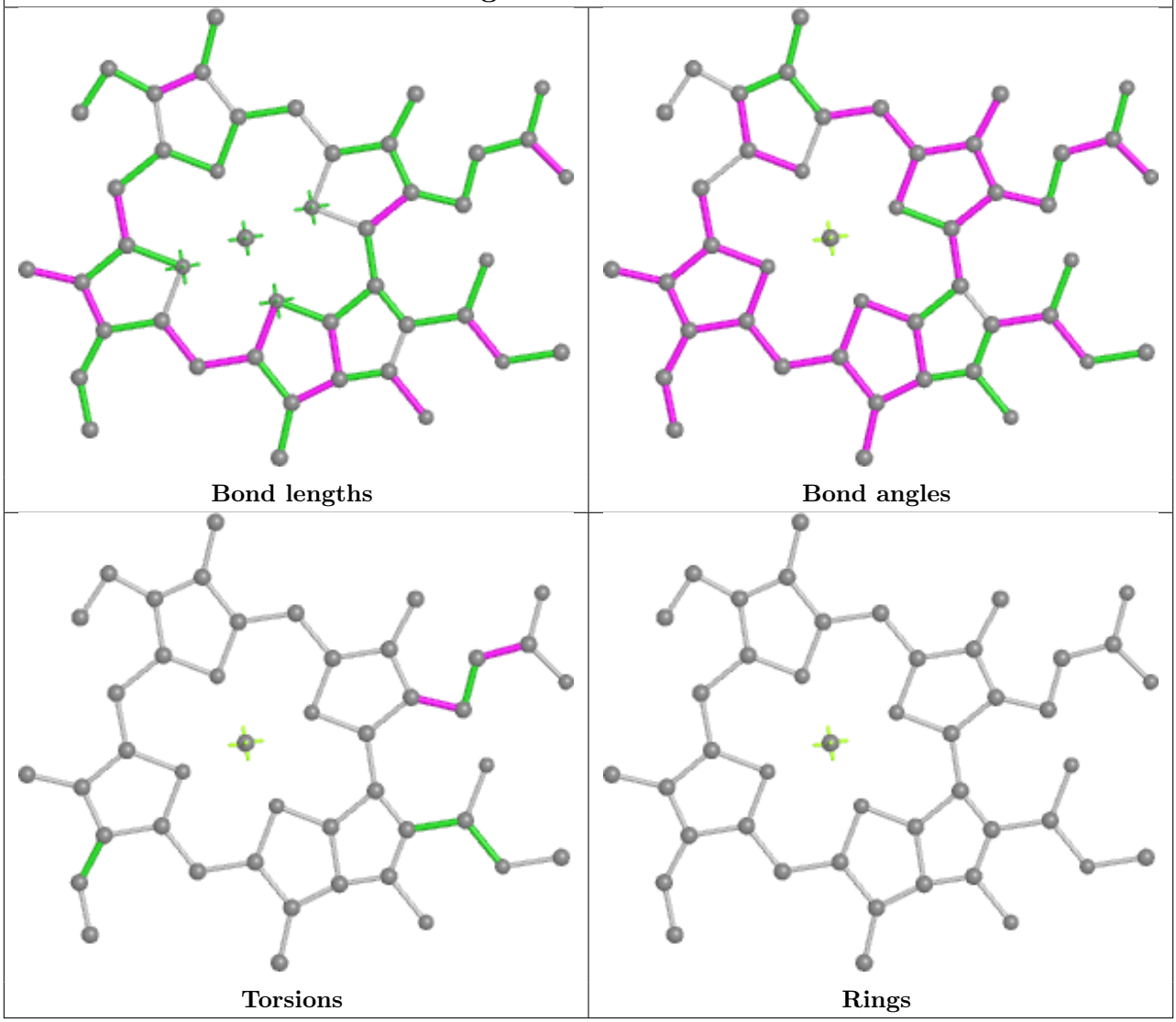
Torsions



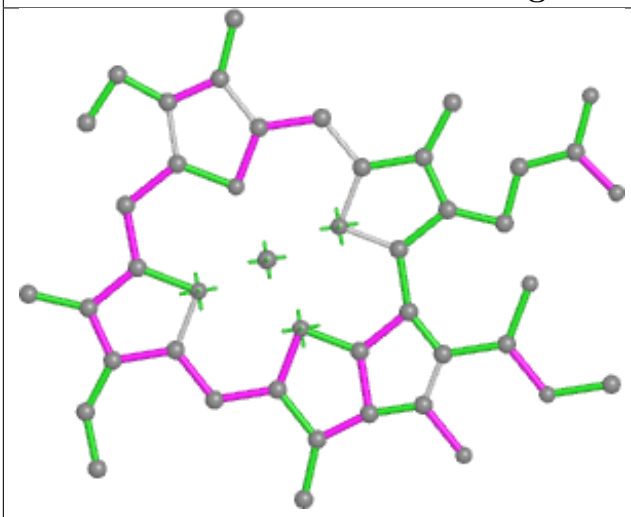
Rings

Ligand LHG 3 719	
 Bond lengths	 Bond angles
 Torsions	 Rings

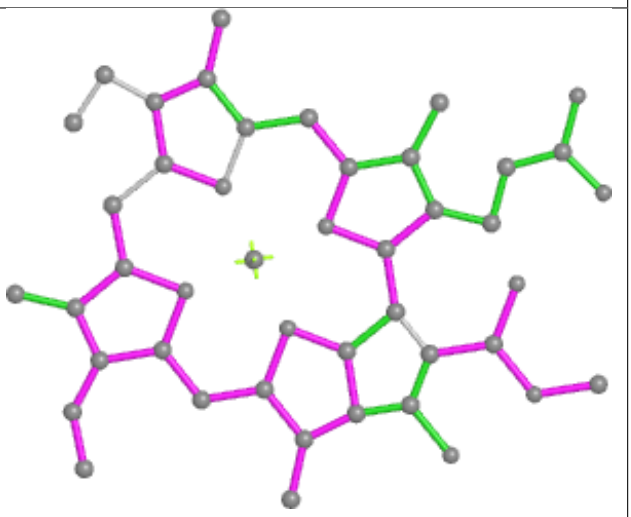
Ligand CLA A 823



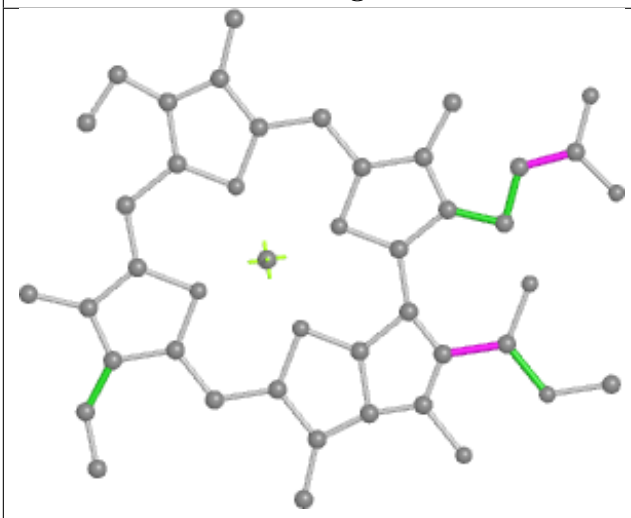
Ligand CLA 9 904



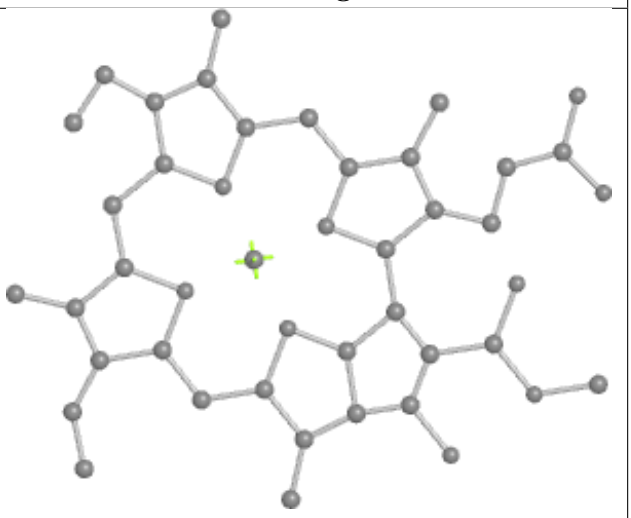
Bond lengths



Bond angles

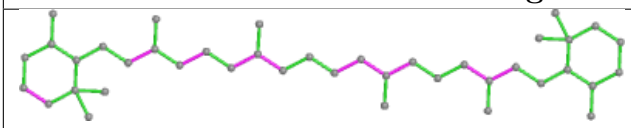


Torsions



Rings

Ligand BCR J 102



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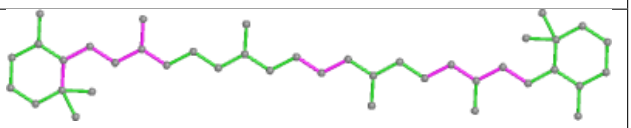

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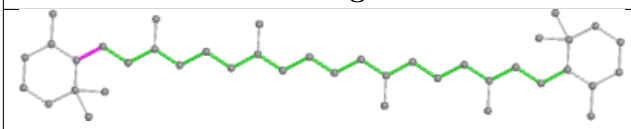
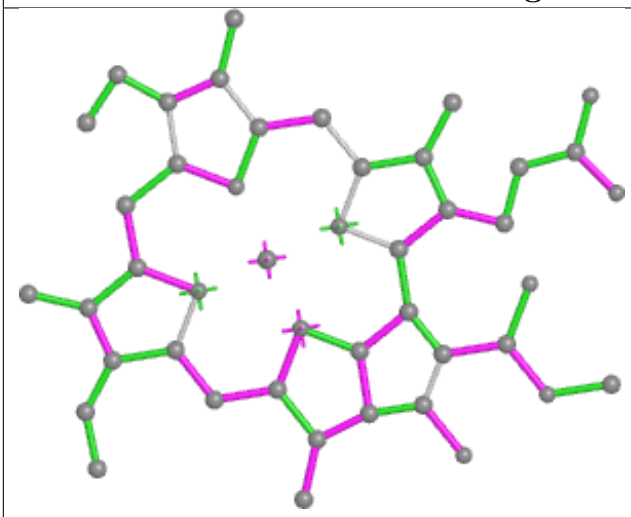


Torsions

Rings

Ligand CLA B 808



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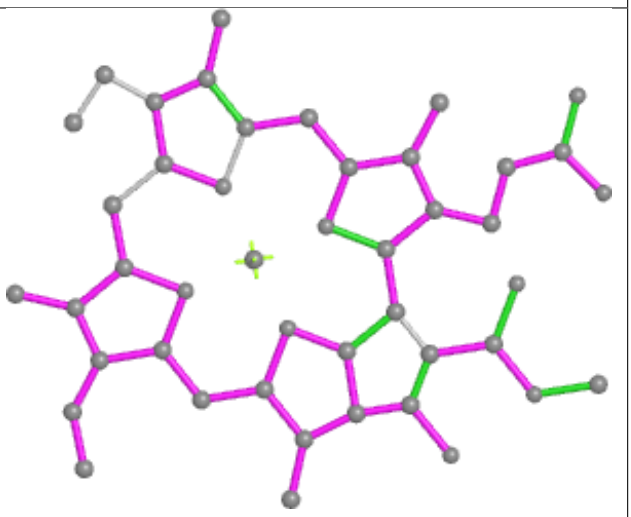
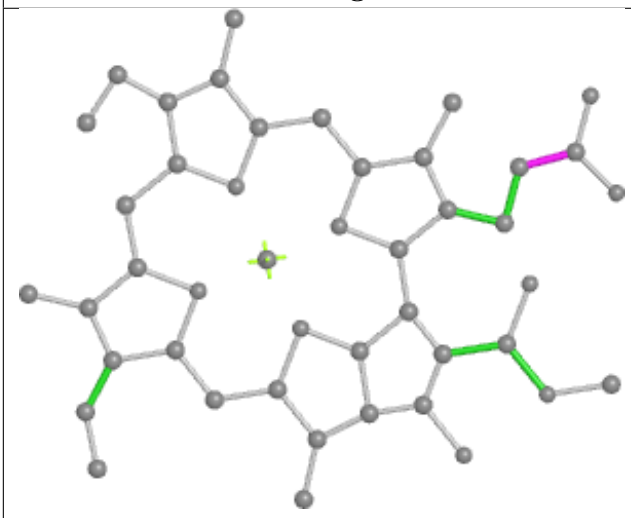


Bond angles



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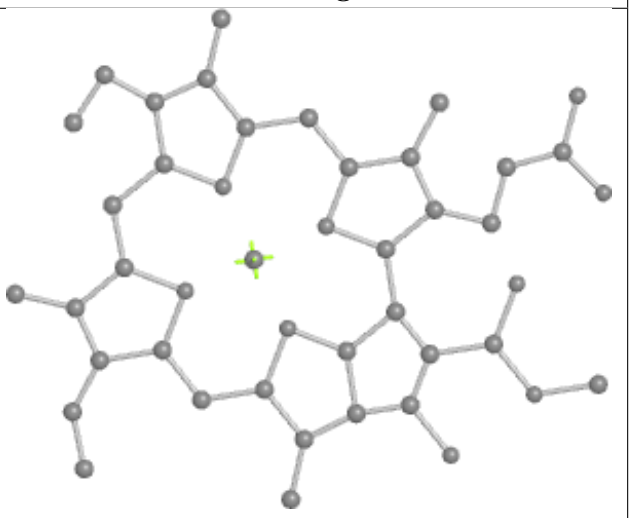
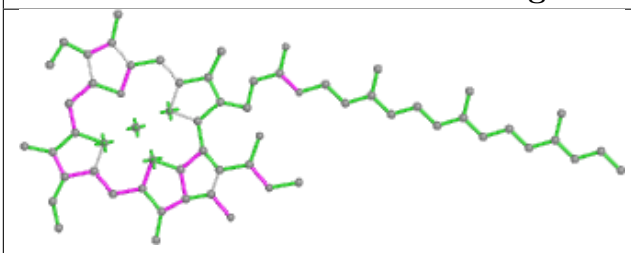
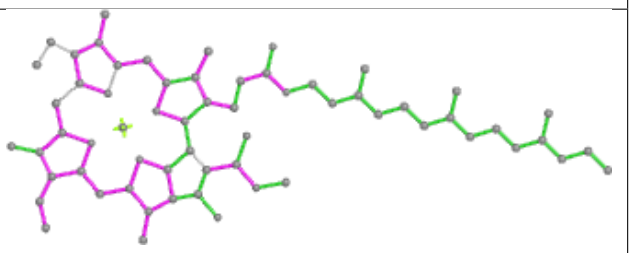


Rings

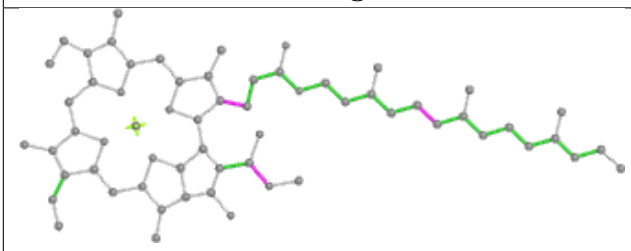
Ligand CLA 8 609



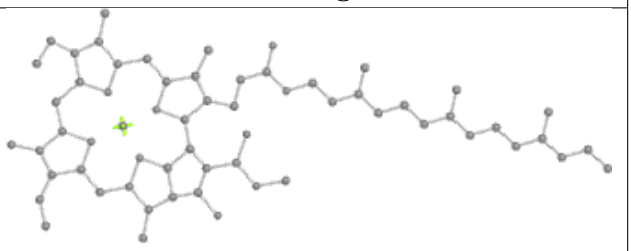
Bond lengths



Bond angles



Torsions



Rings

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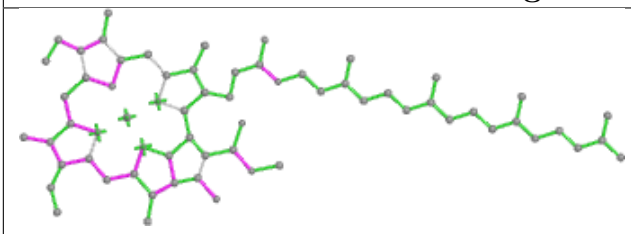
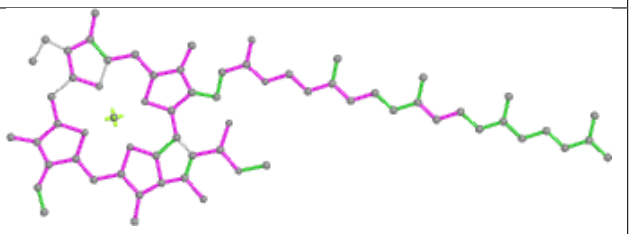
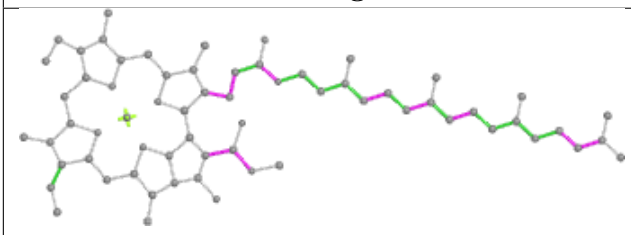
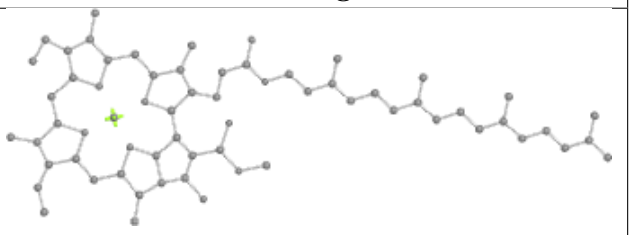
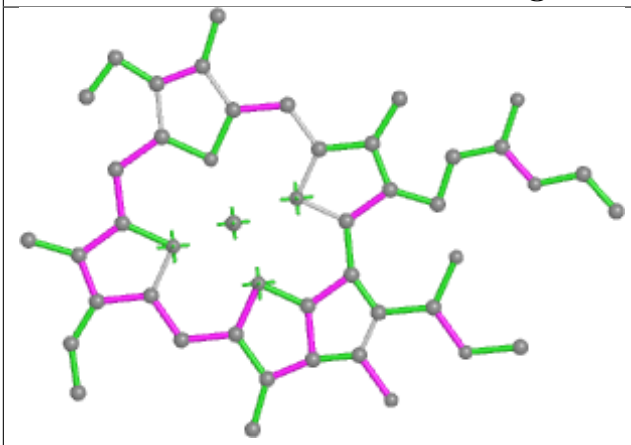
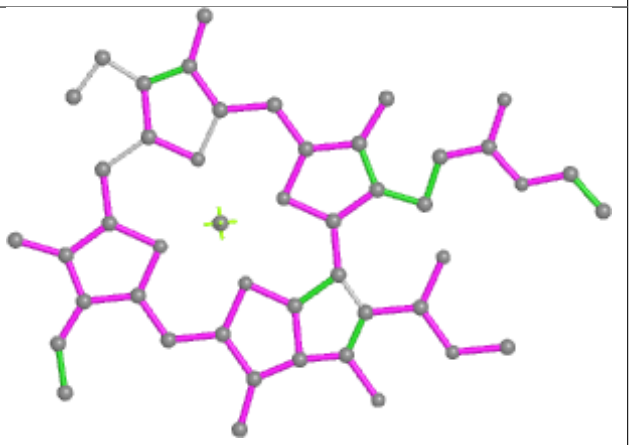
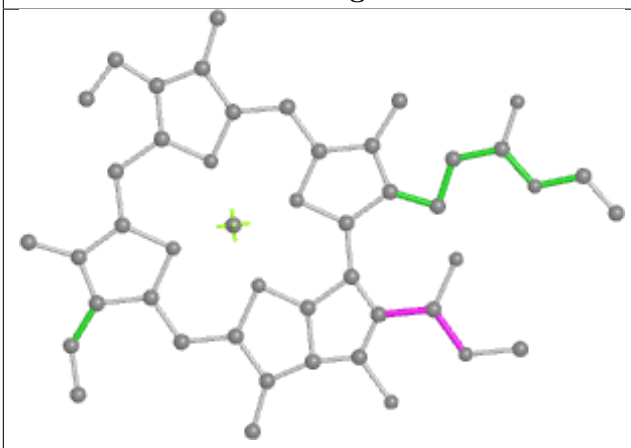
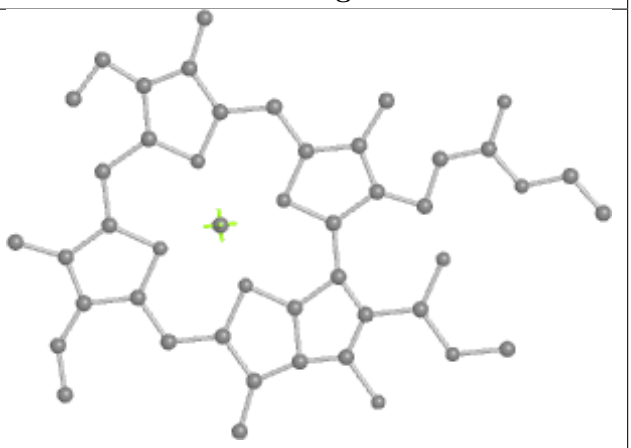
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

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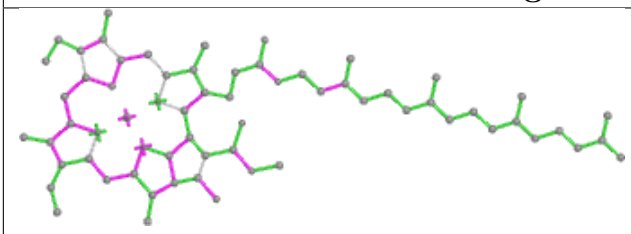
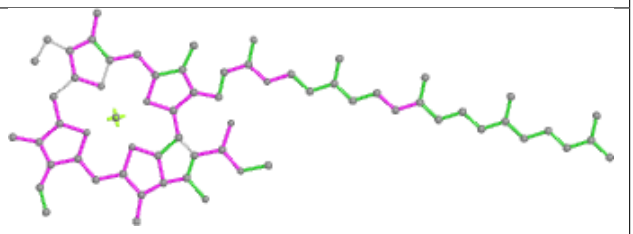
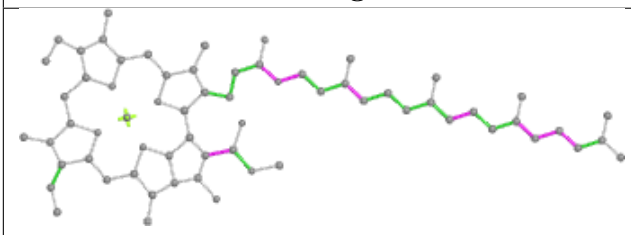
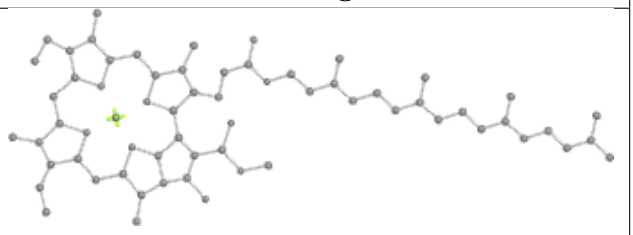
 Bond lengths	 Bond angles
 Torsions	 Rings

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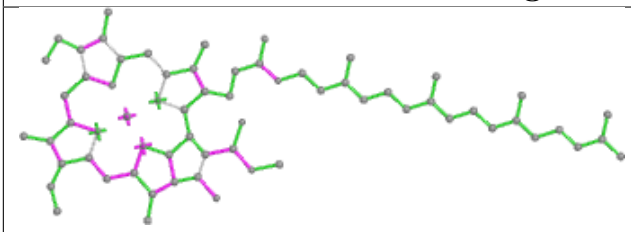
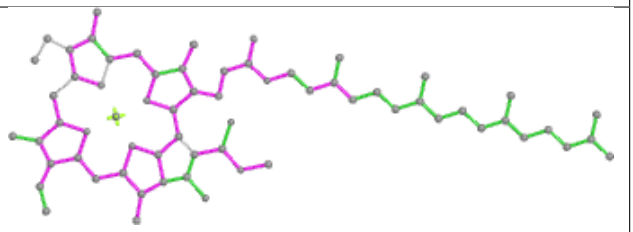
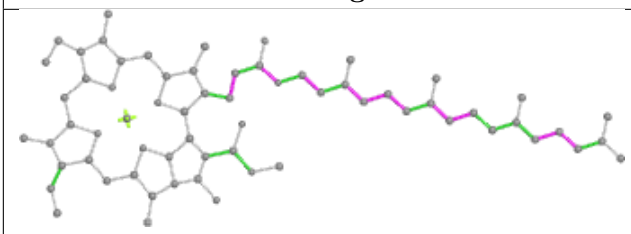
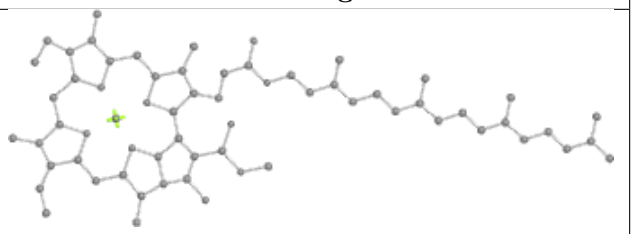
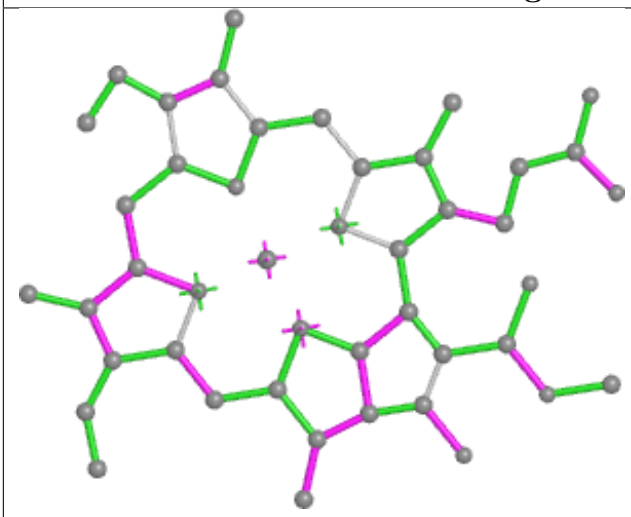
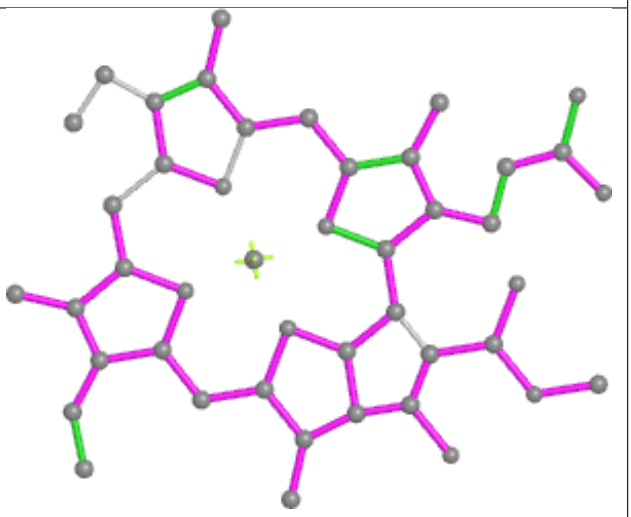
 Bond lengths	 Bond angles
 Torsions	 Rings

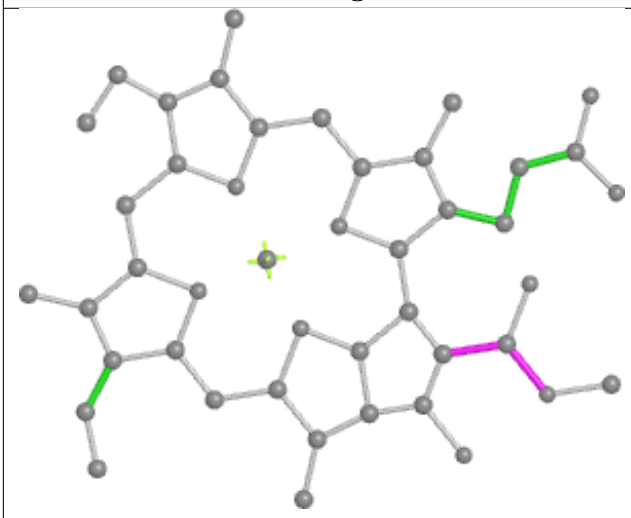
Ligand CLA B 838



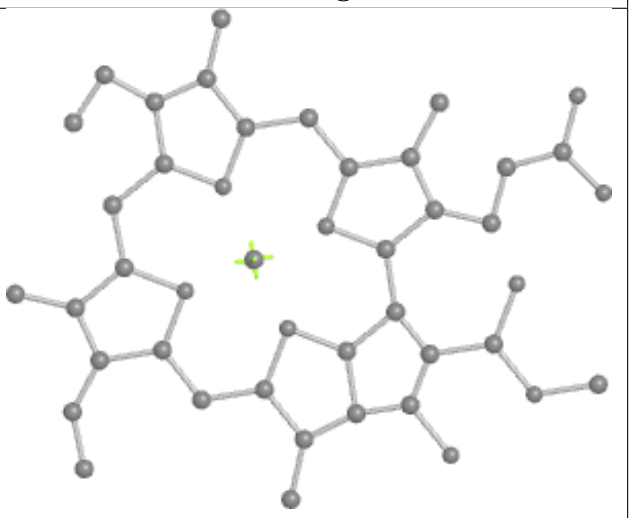
Bond lengths



Bond angles

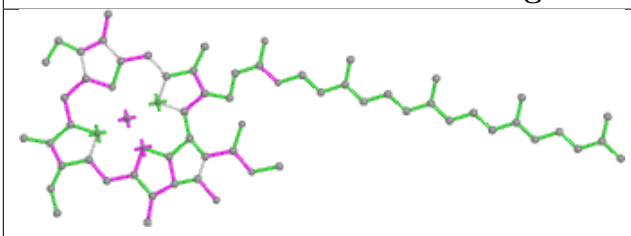


Torsions

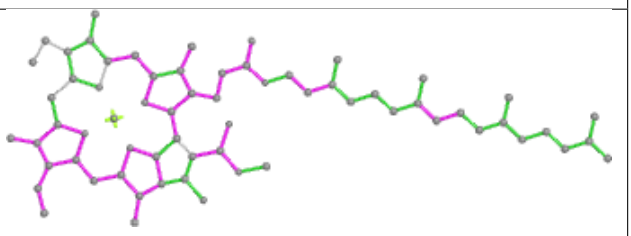


Rings

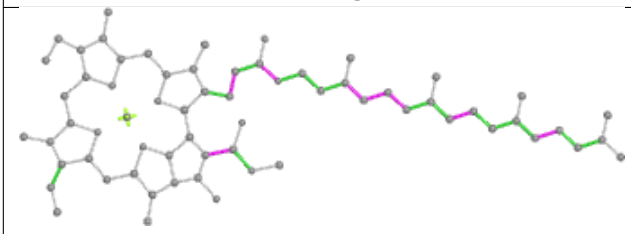
Ligand CLA B 807



Bond lengths



Bond angles



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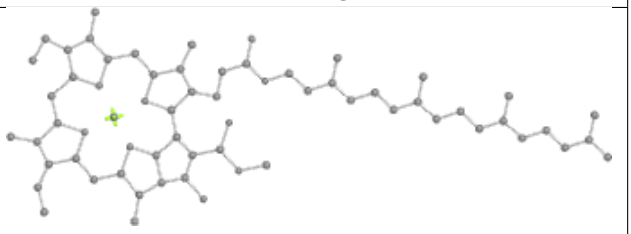
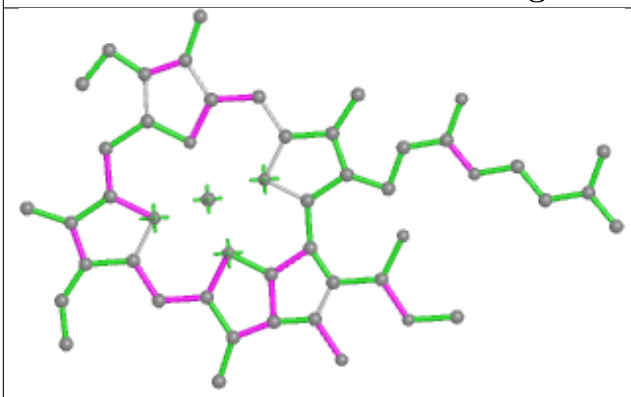
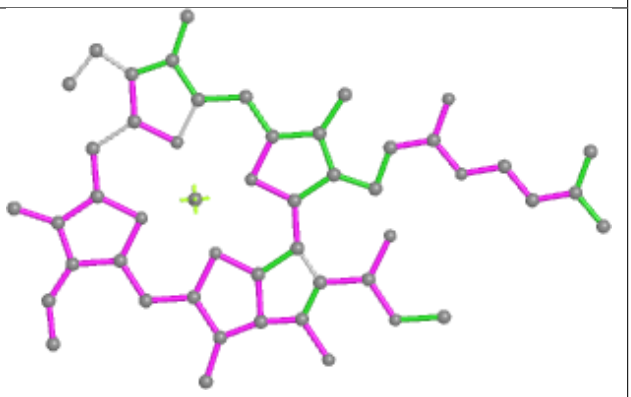
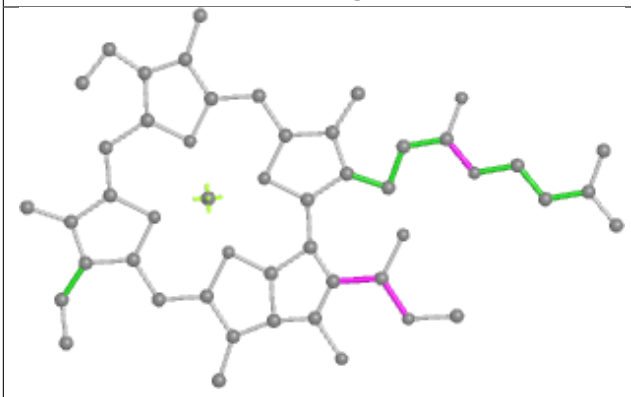
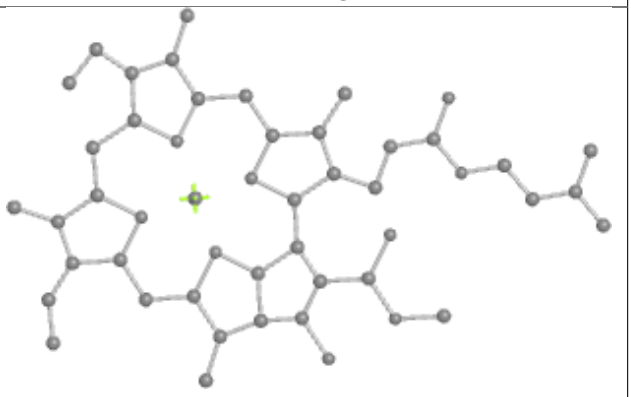
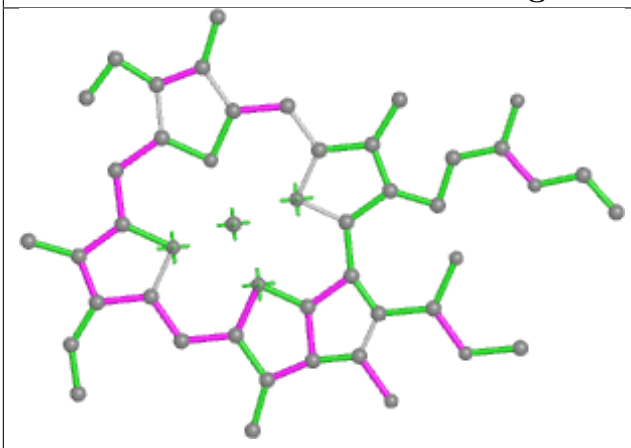
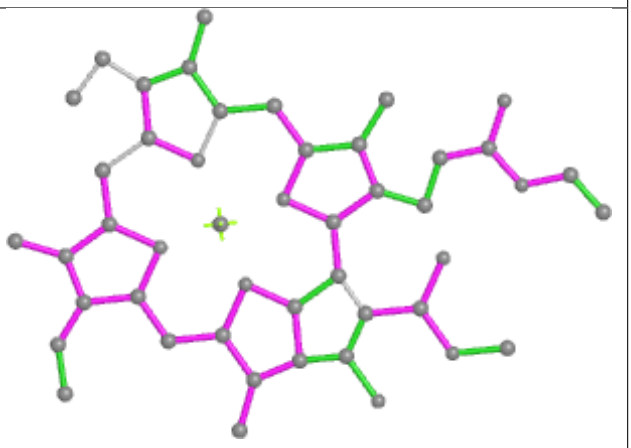
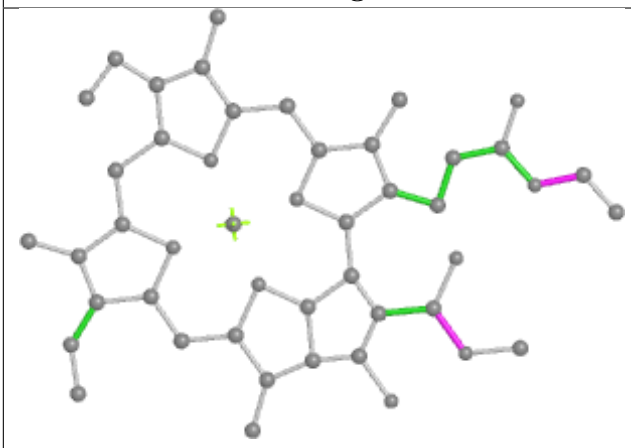
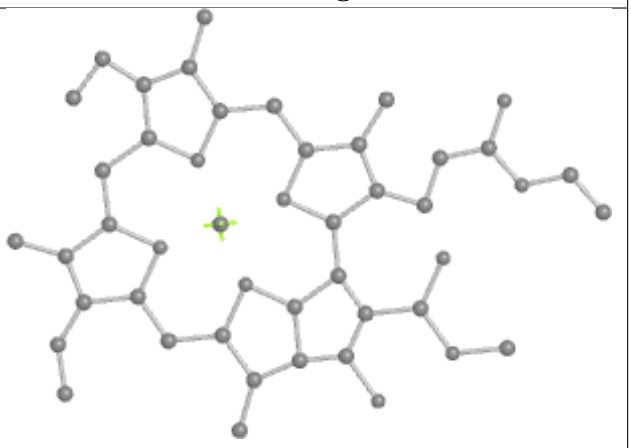
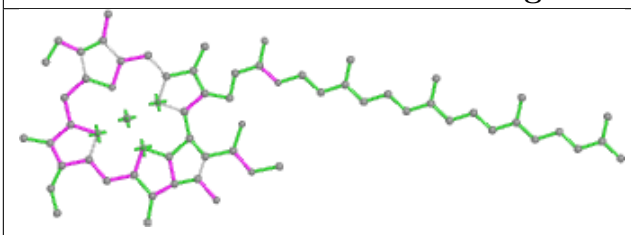
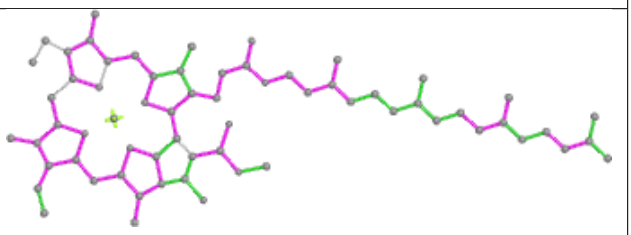
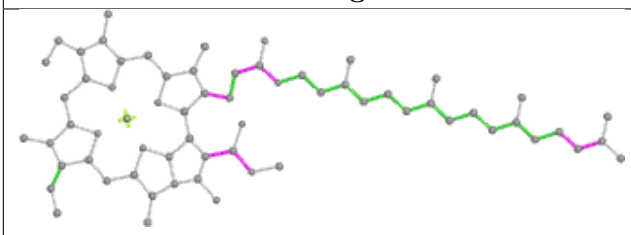
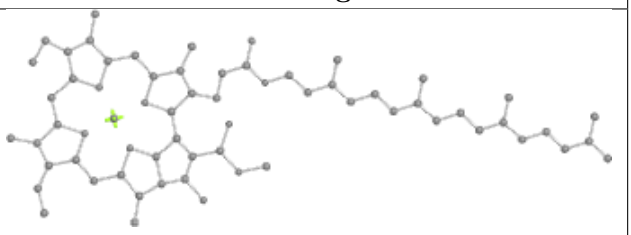


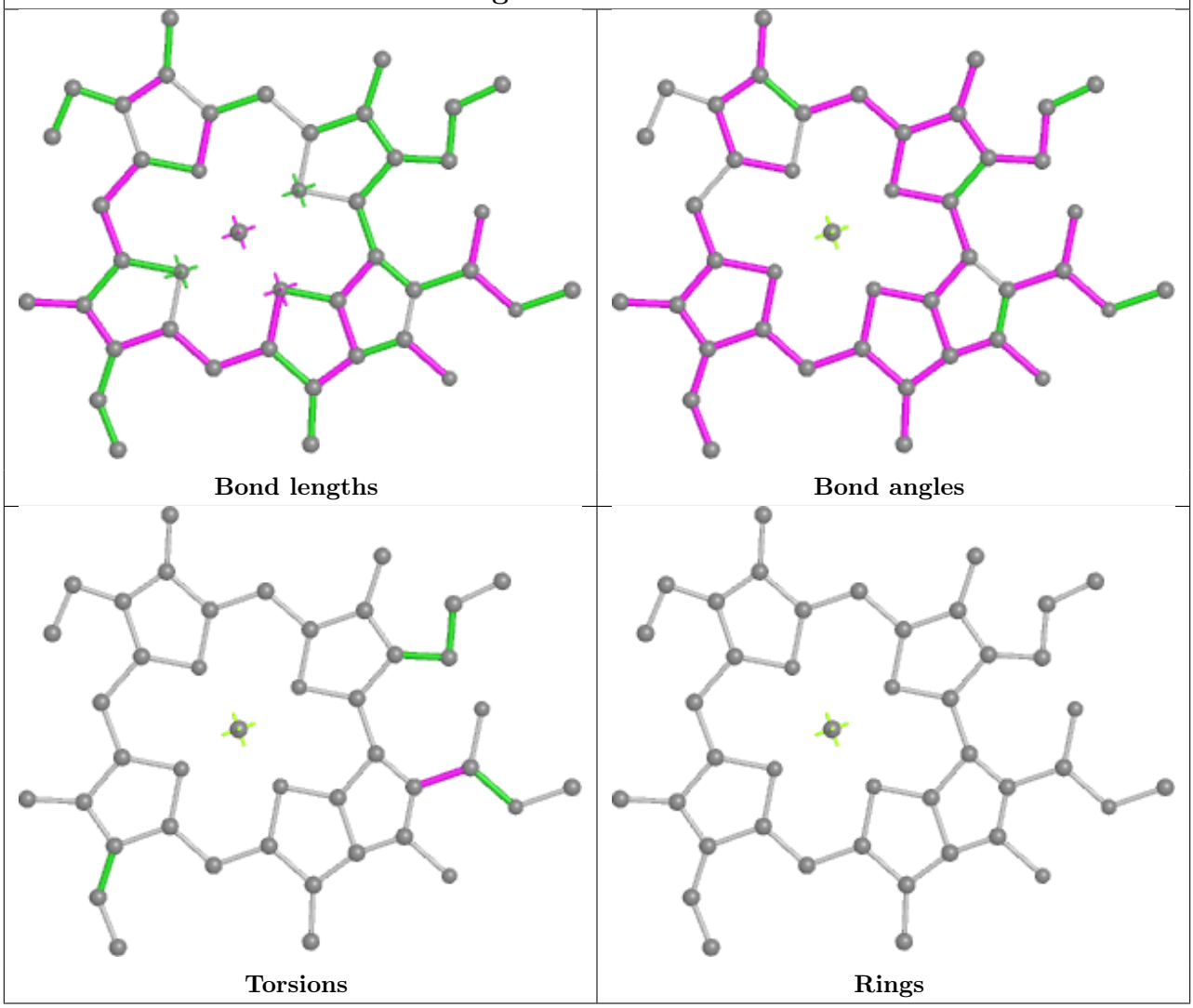
Rings

Ligand CLA 7 705	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 4 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 709



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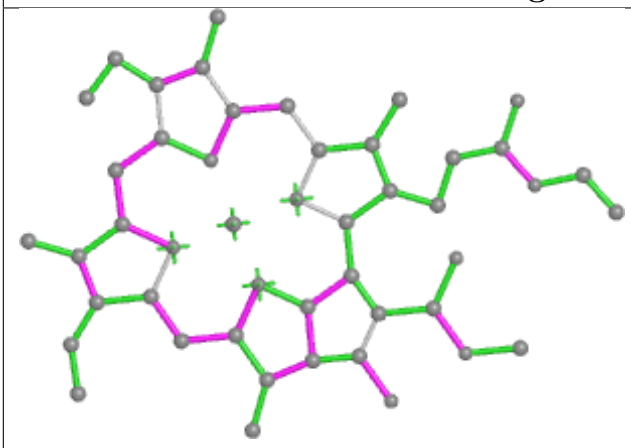
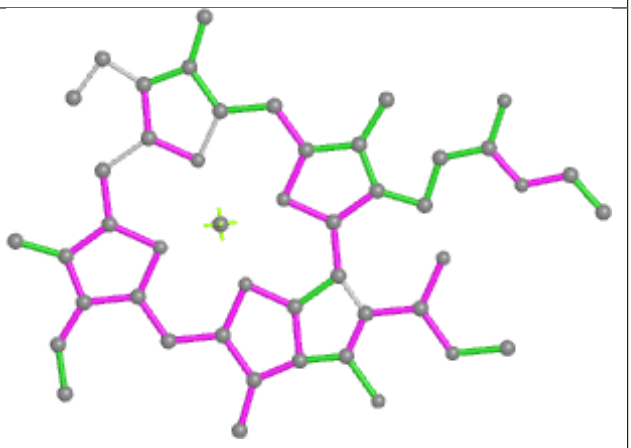
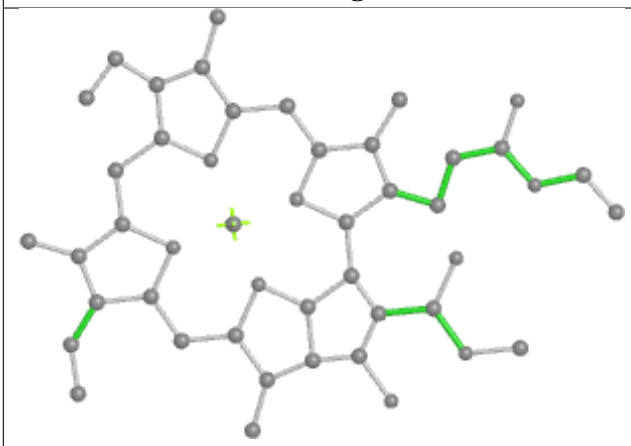
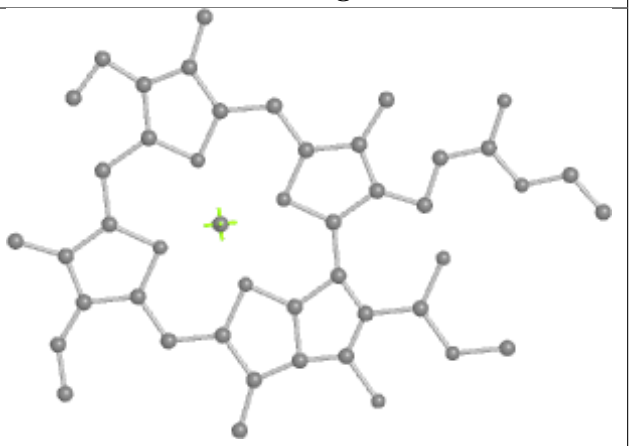
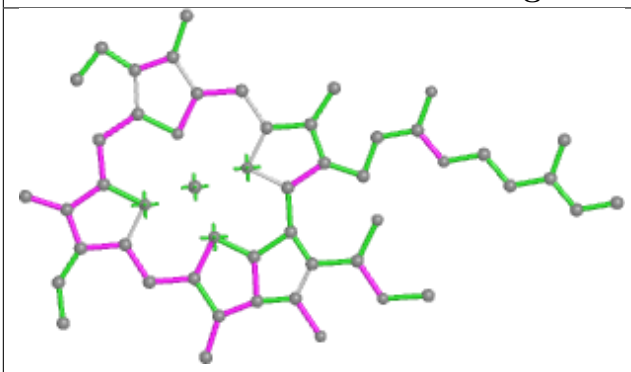
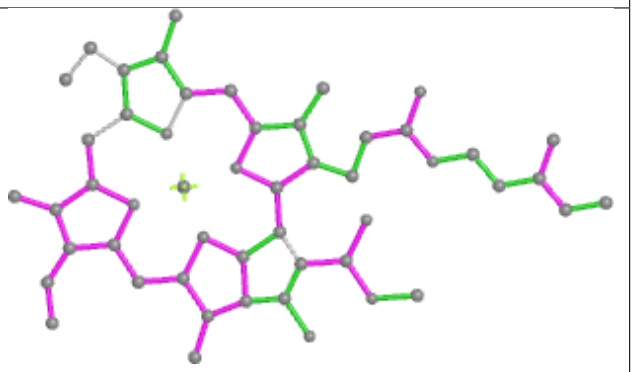
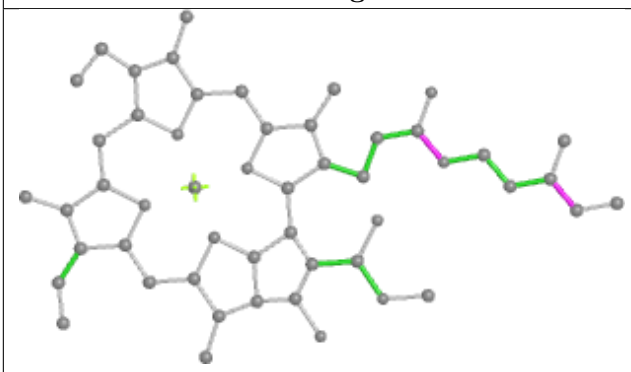
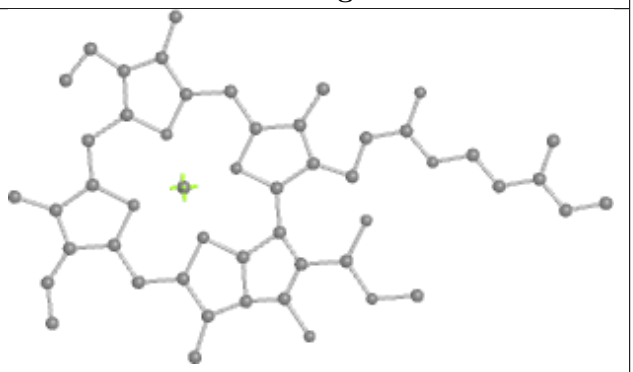
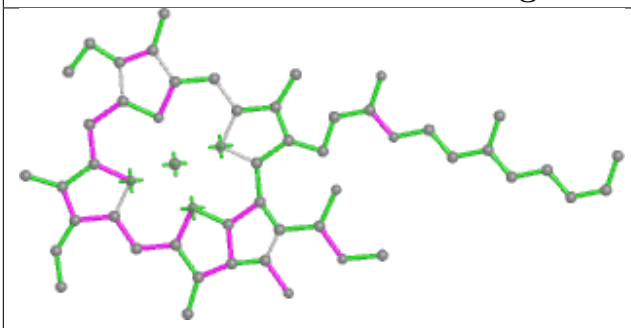
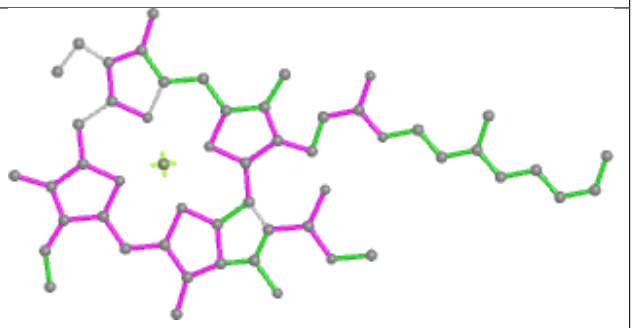
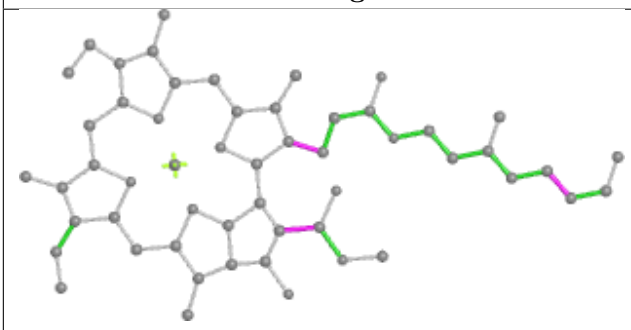
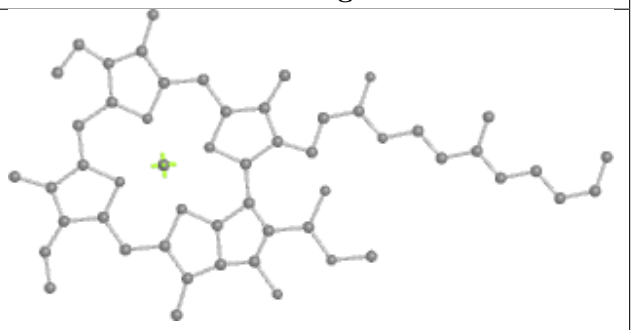
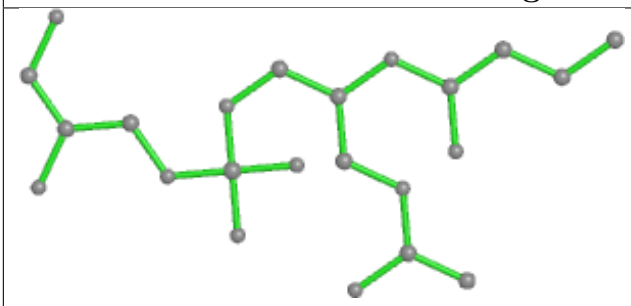
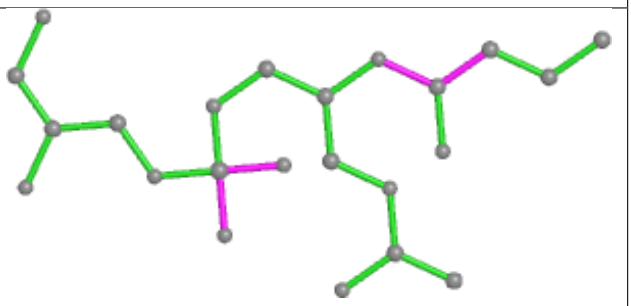
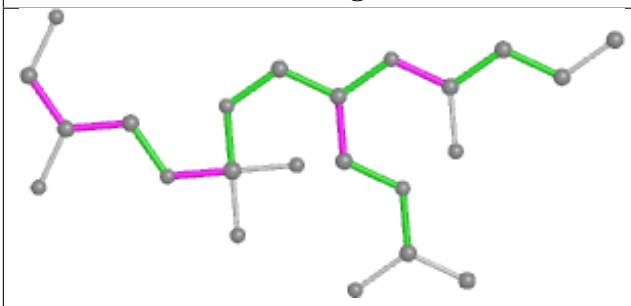
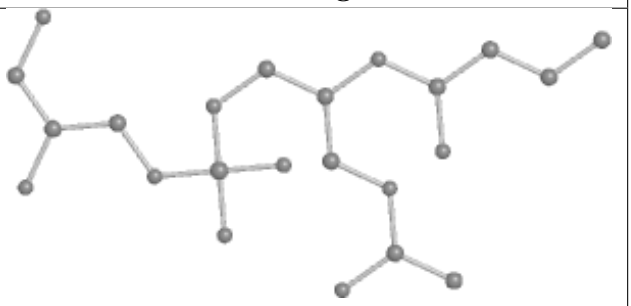
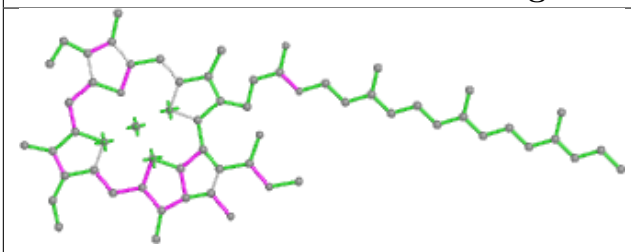
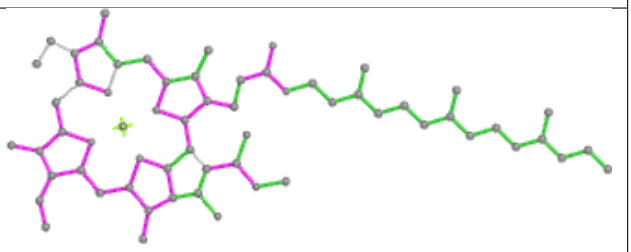
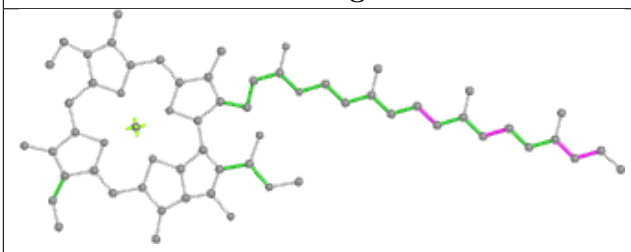
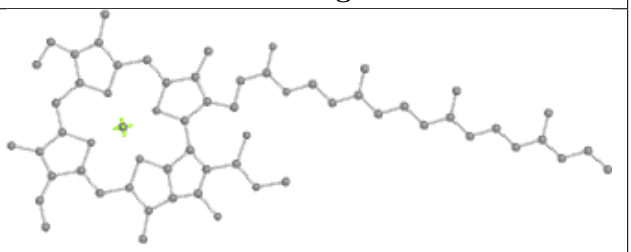
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

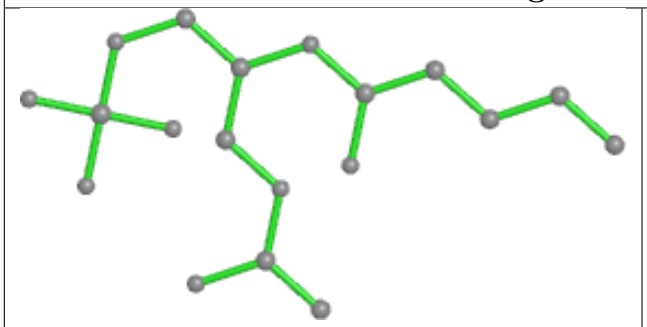
Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 11 707	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 4 714



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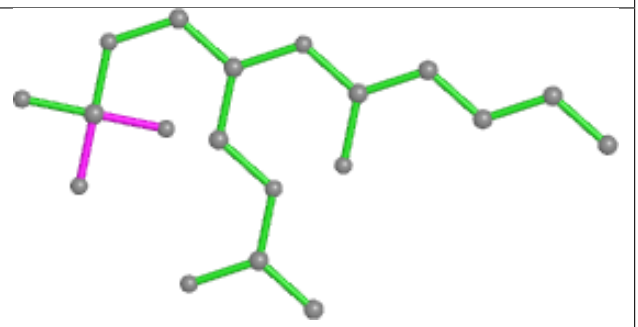
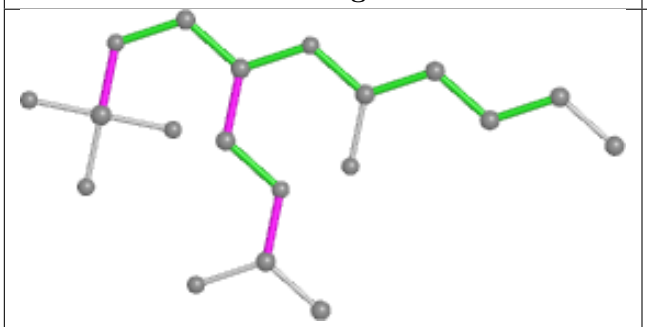
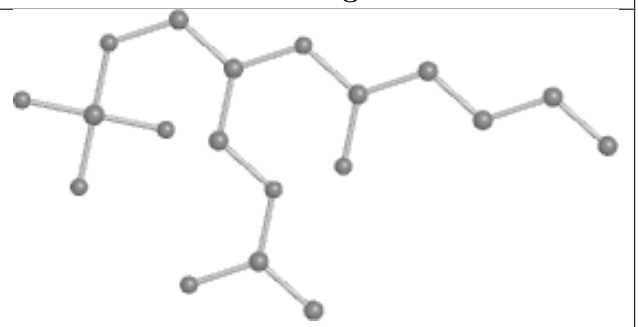


Bond angles

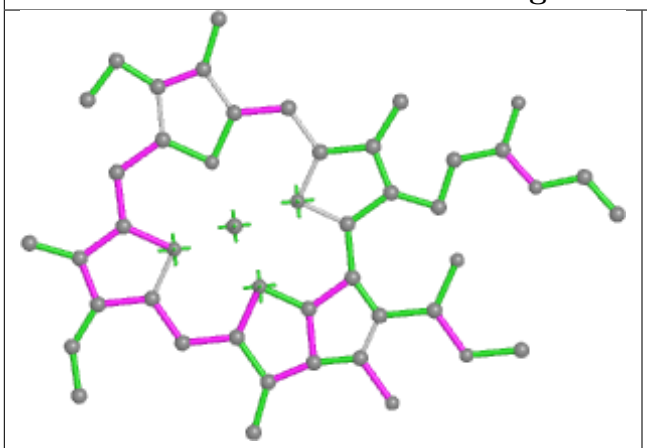


Torsions



Rings

Ligand CLA 8 607



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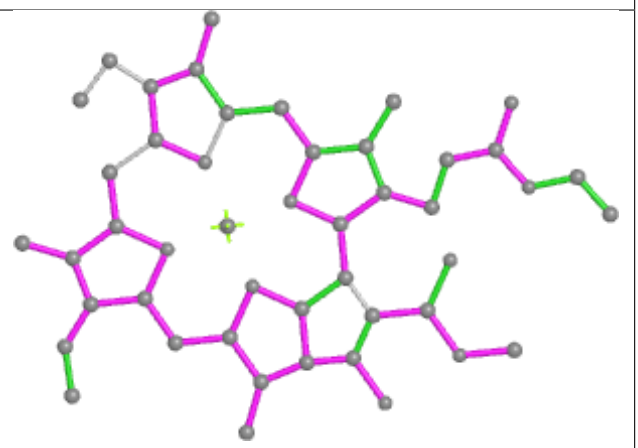
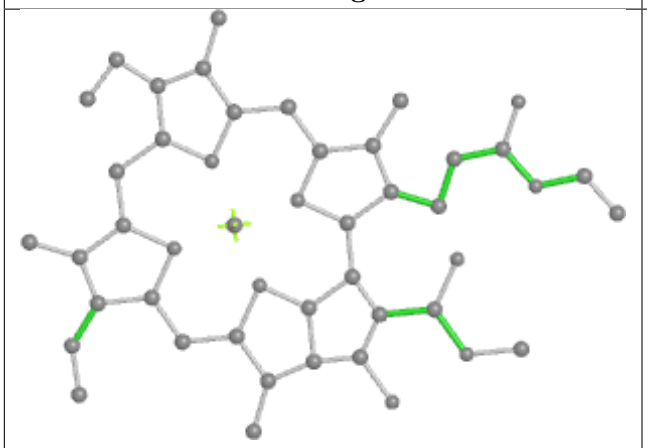


Bond angles



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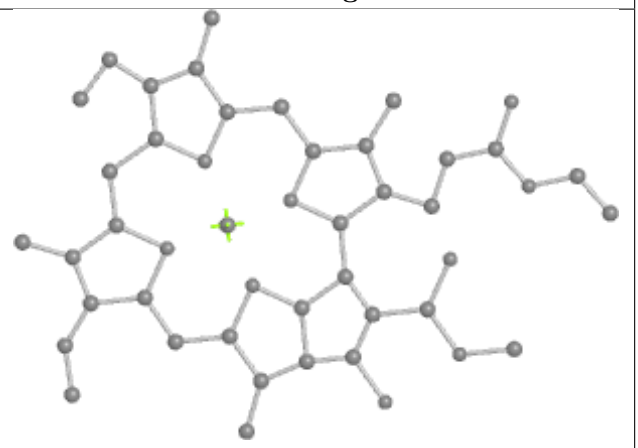
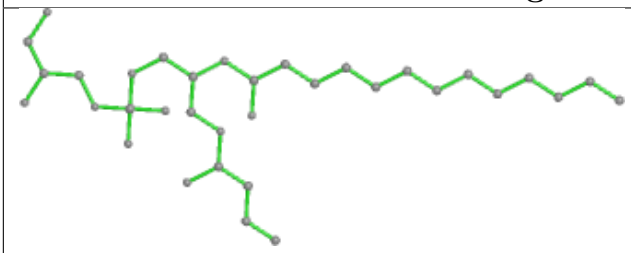
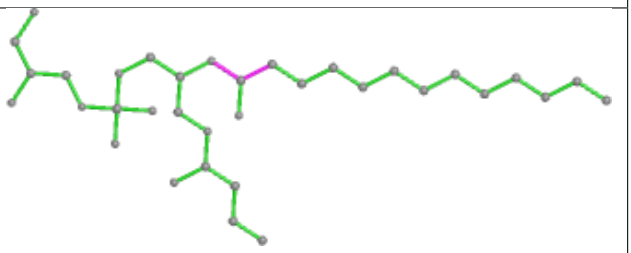
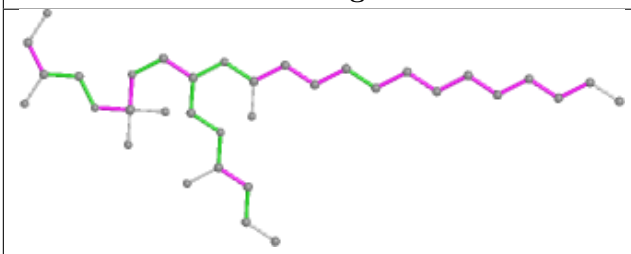
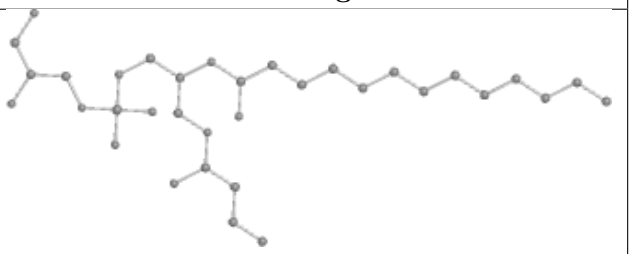
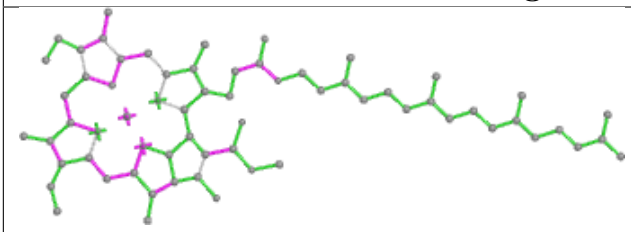
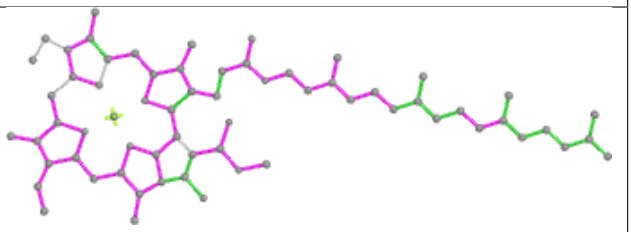
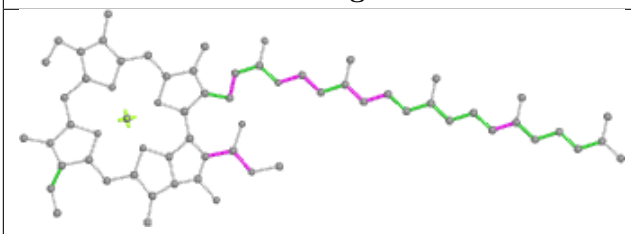
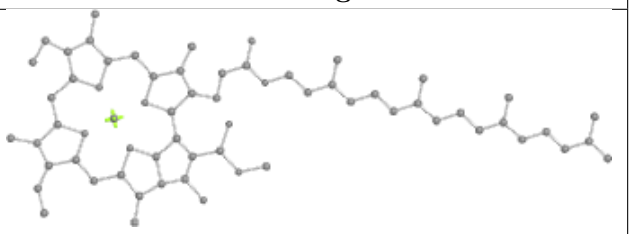
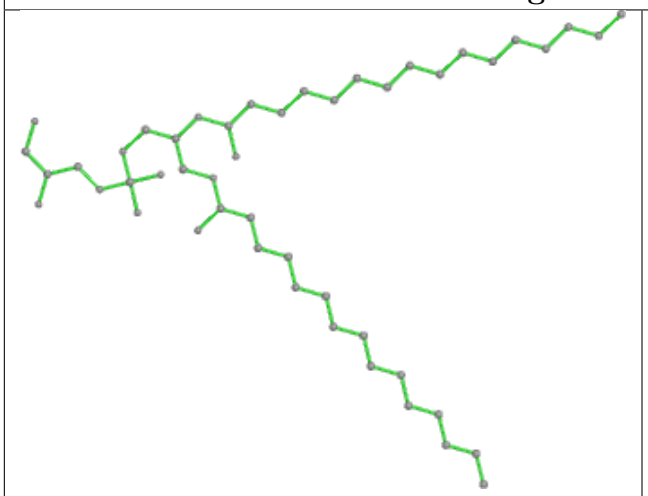


Rings

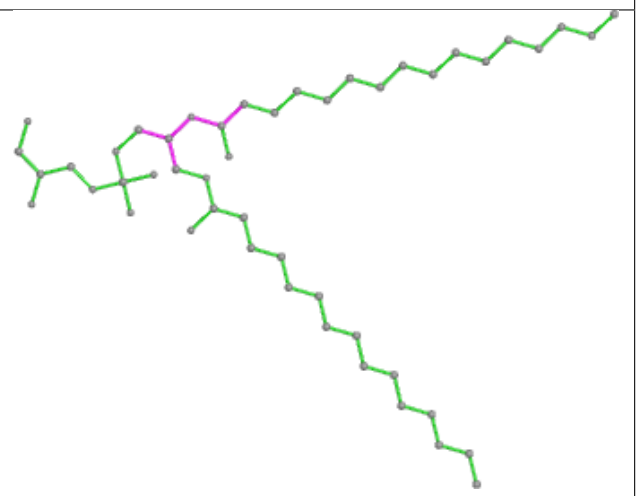
Ligand LHG 9 917	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 862	
 Bond lengths	 Bond angles
 Torsions	 Rings

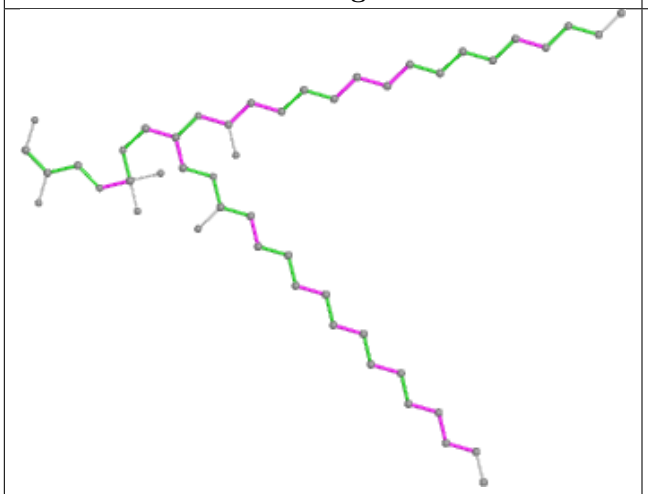
Ligand LHG 7 717



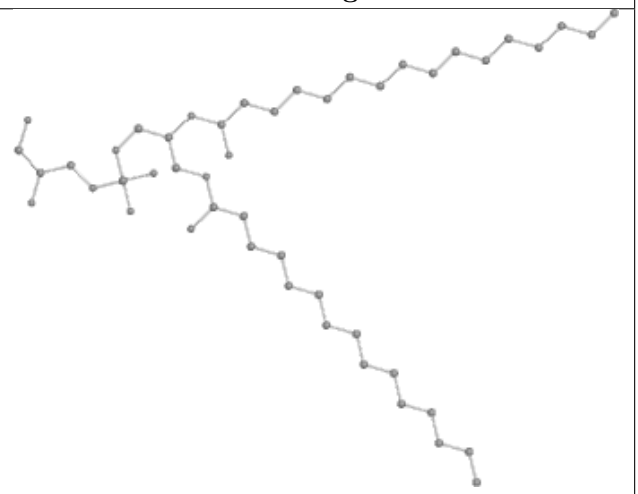
Bond lengths



Bond angles

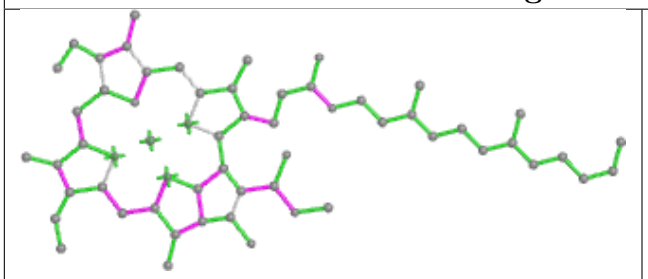


Torsions



Rings

Ligand CLA A 825



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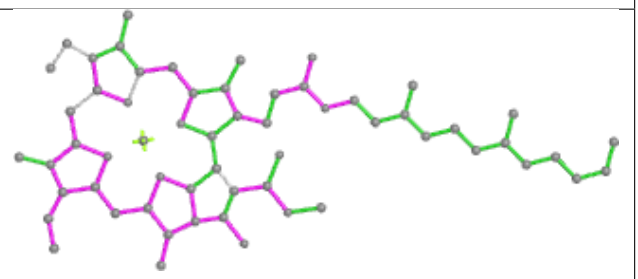
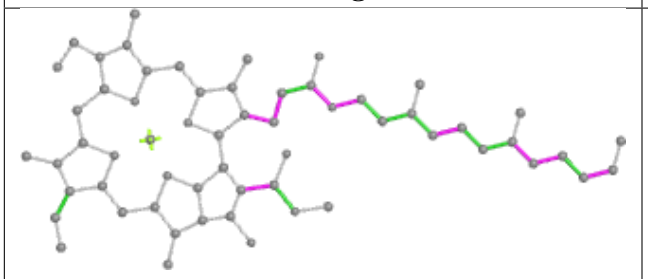


Bond angles



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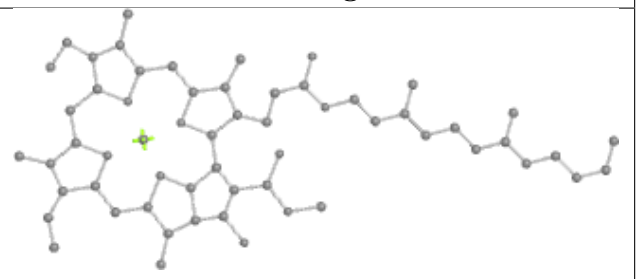
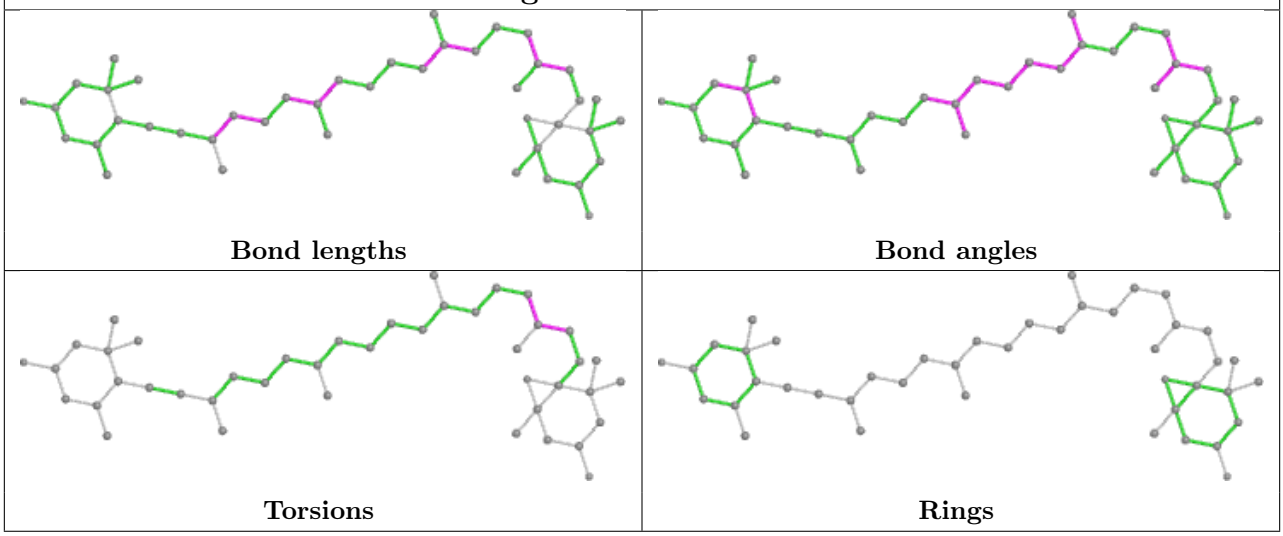
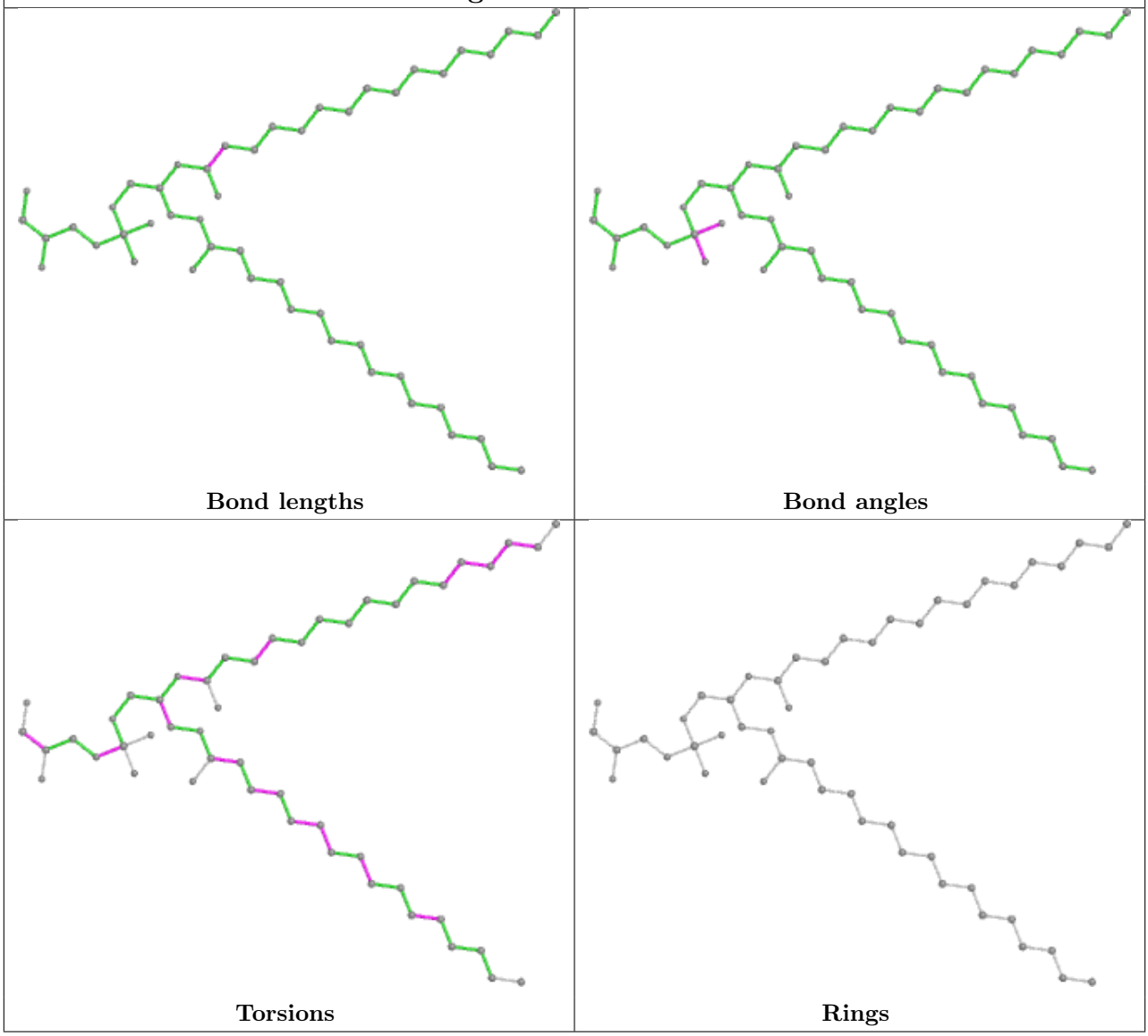


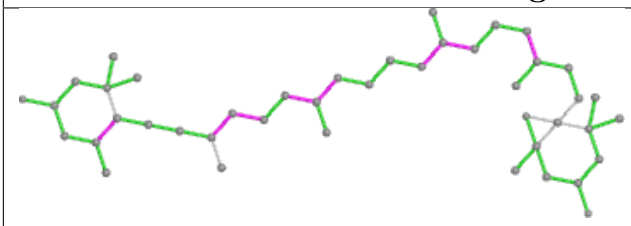
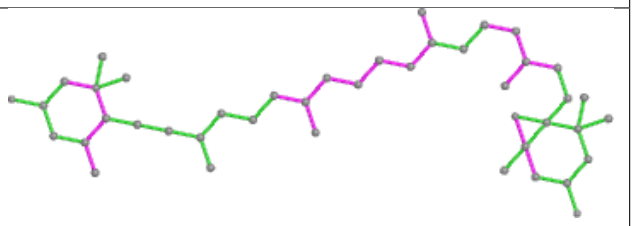
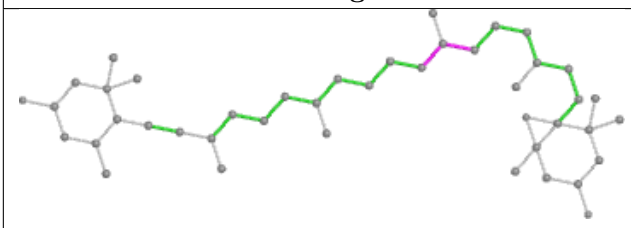
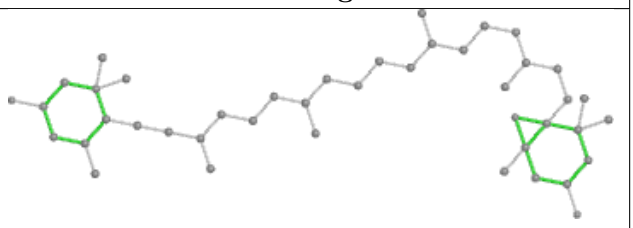
Rings

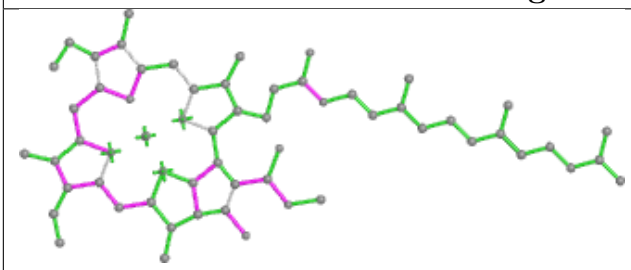
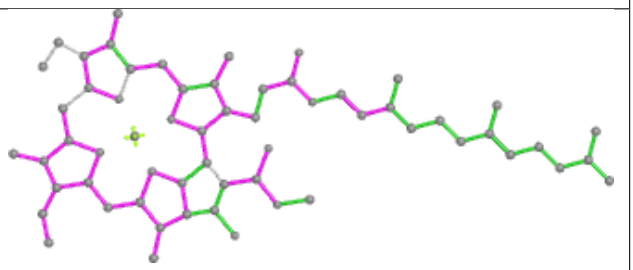
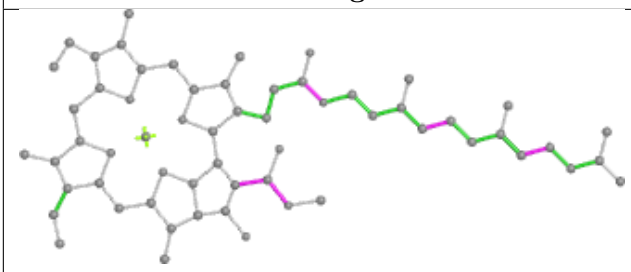
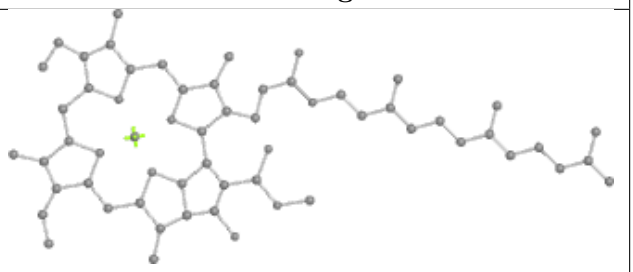
Ligand DD6 11 712



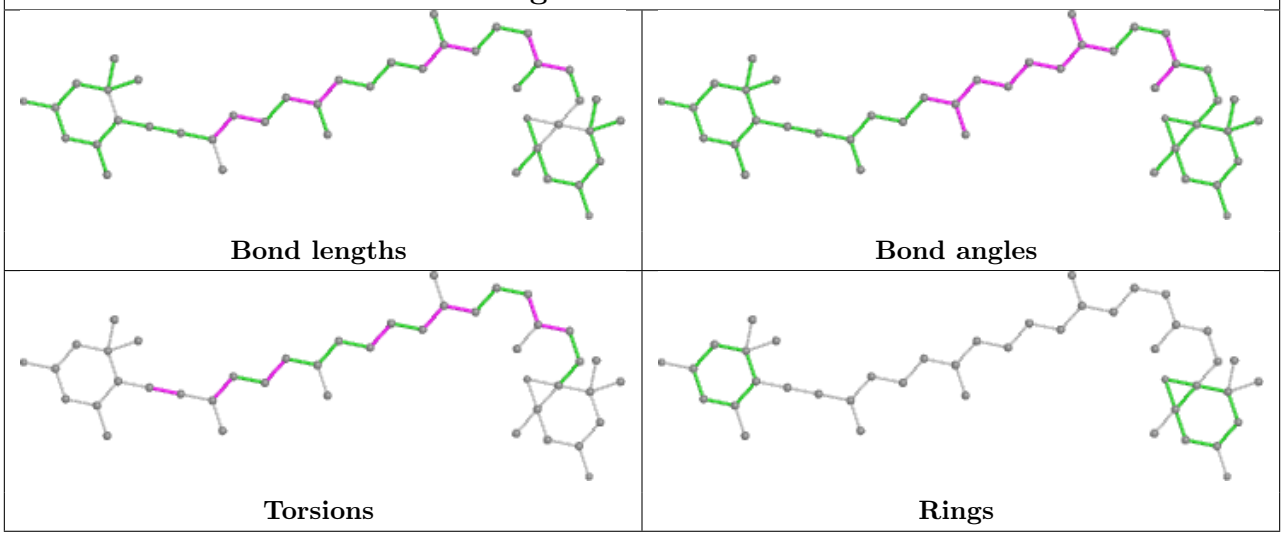
Ligand LHG A 853



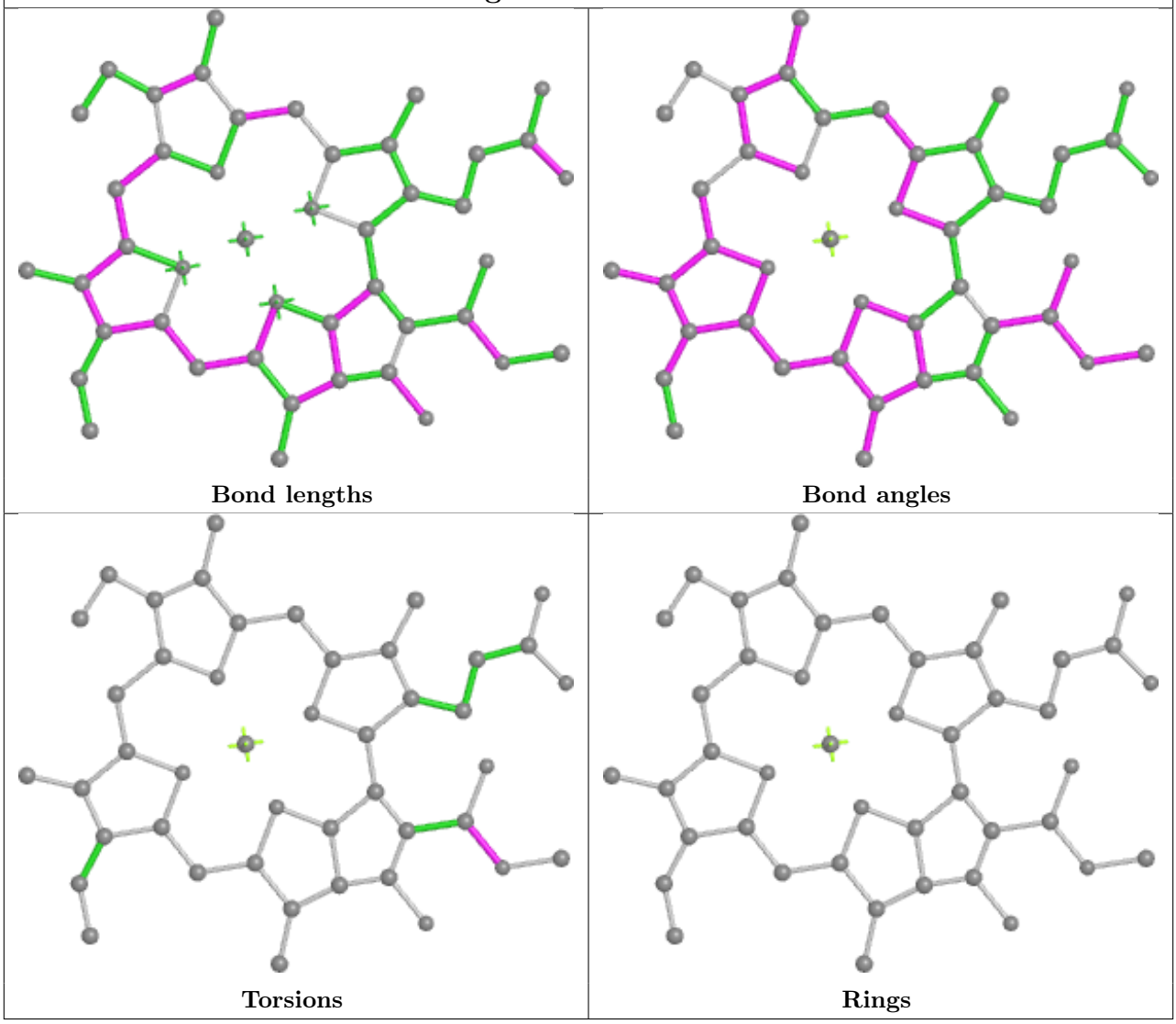
Ligand DD6 4 712	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 7 715



Ligand CLA 5 711



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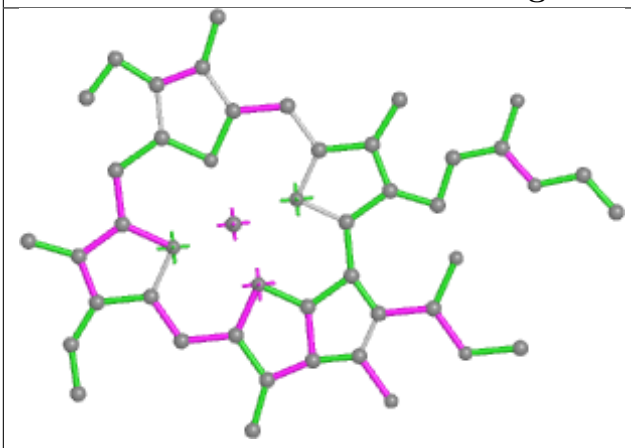
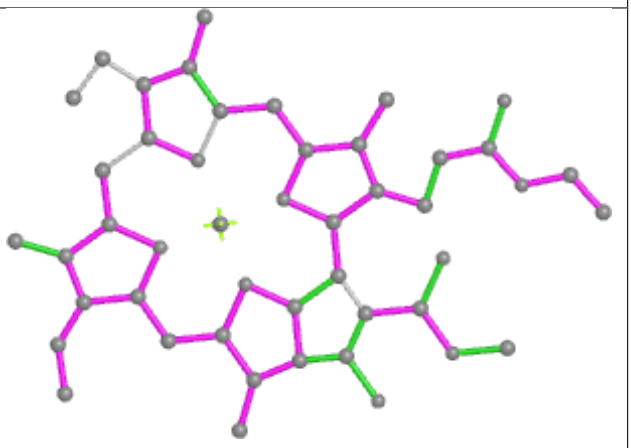
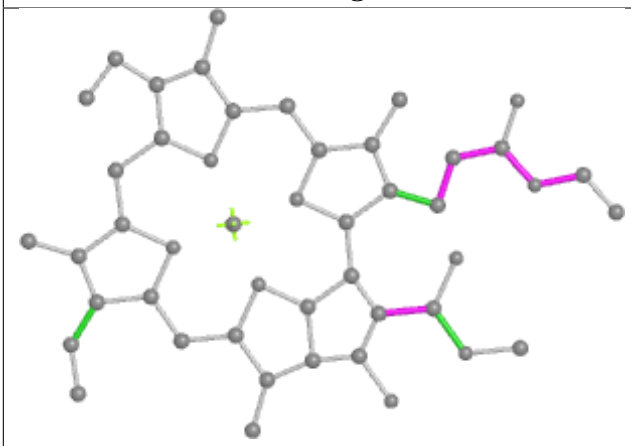
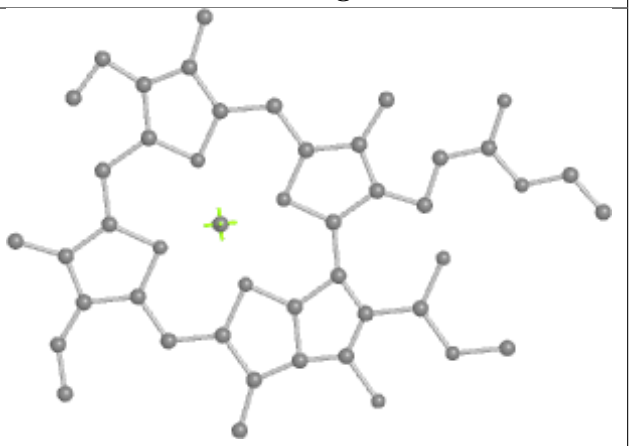
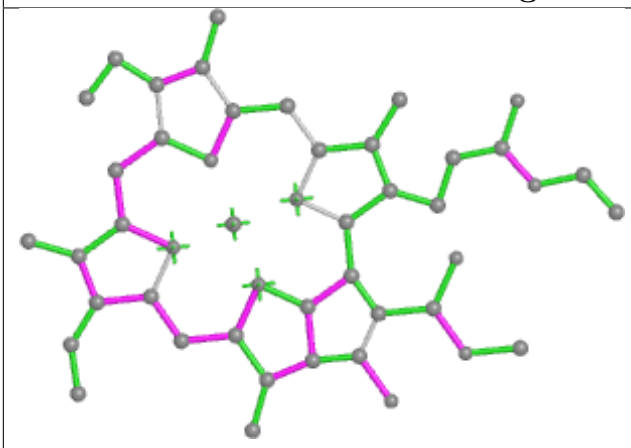
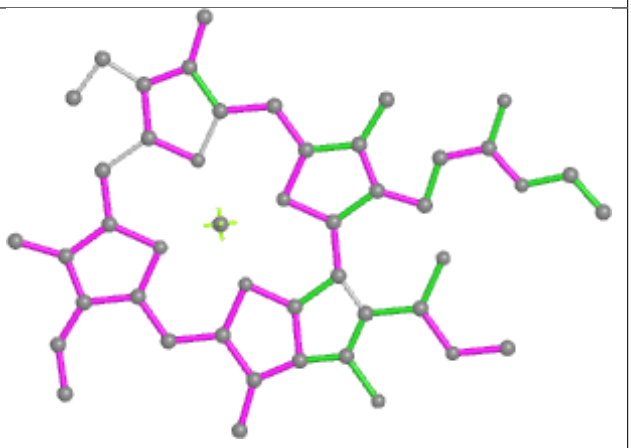
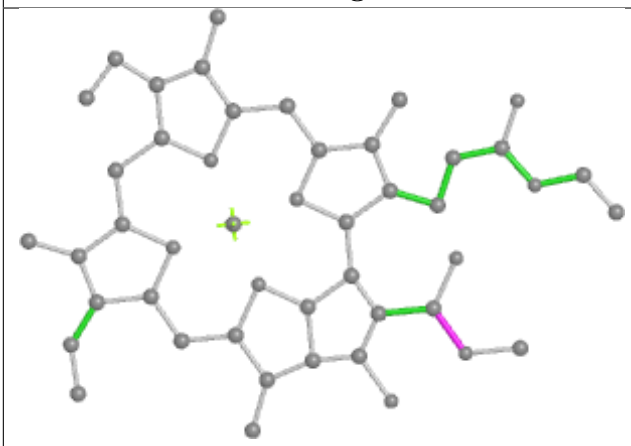
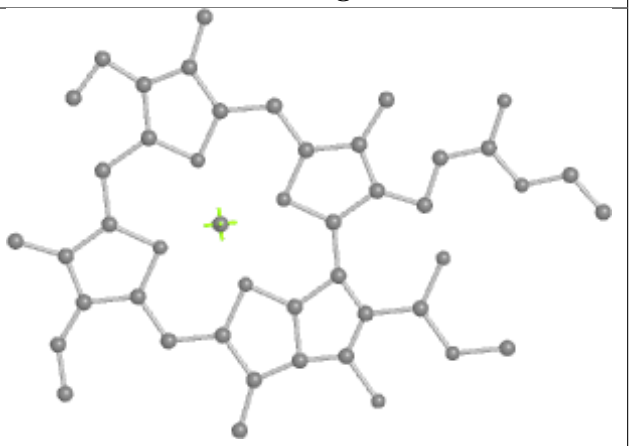
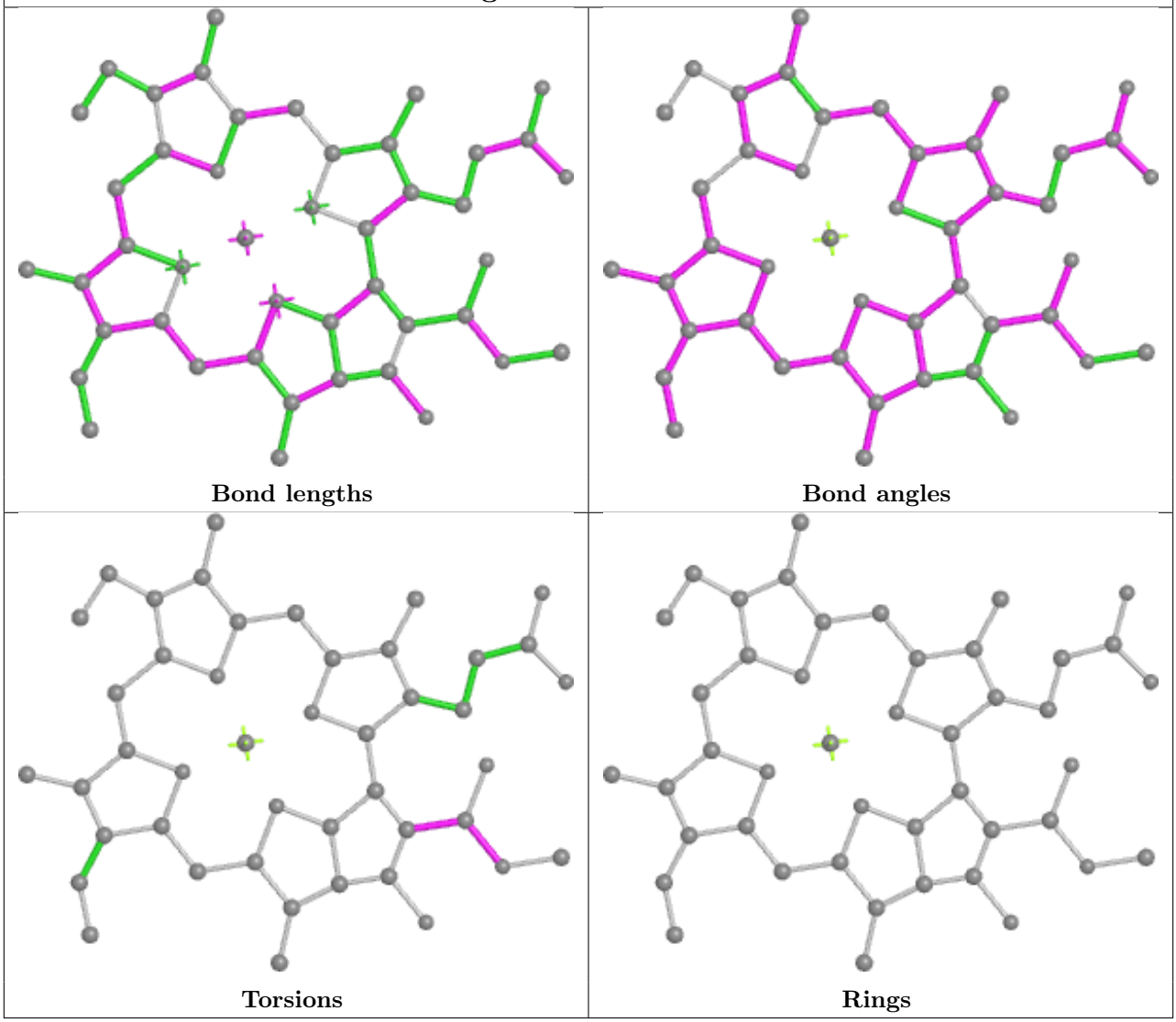
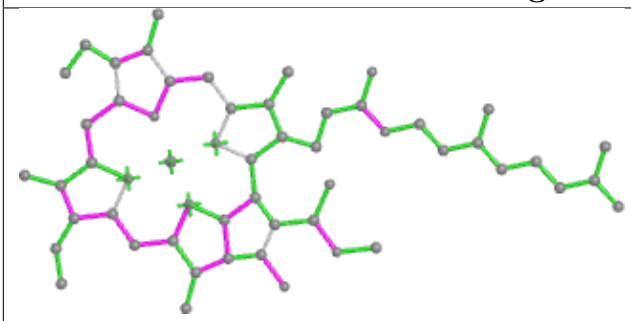
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 13 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

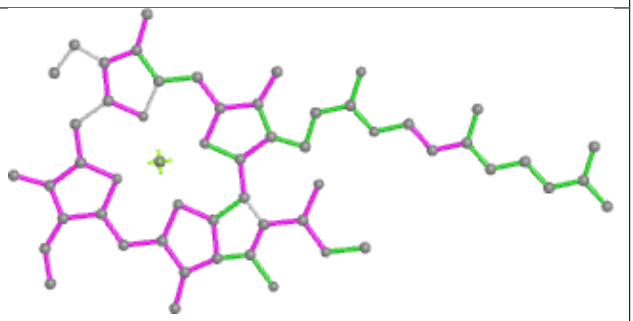
Ligand CLA B 822



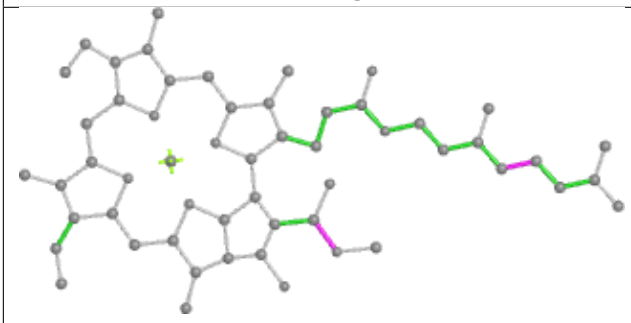
Ligand CLA 4 702



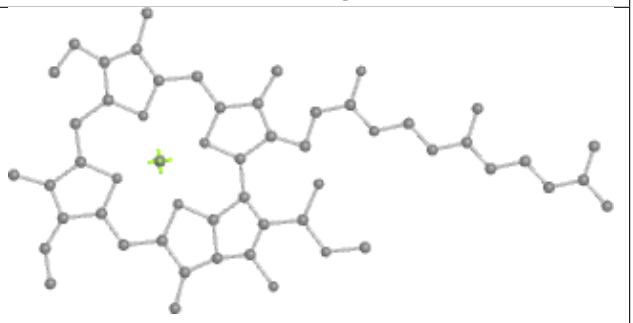
Bond lengths



Bond angles

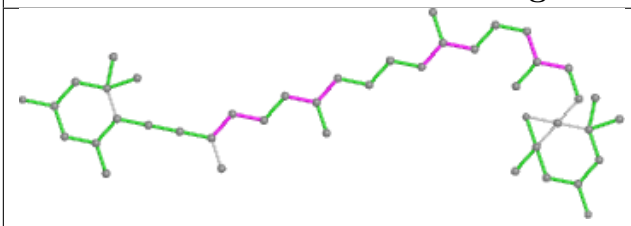


Torsions



Rings

Ligand DD6 2 520



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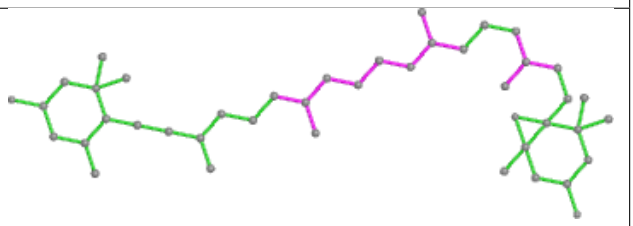
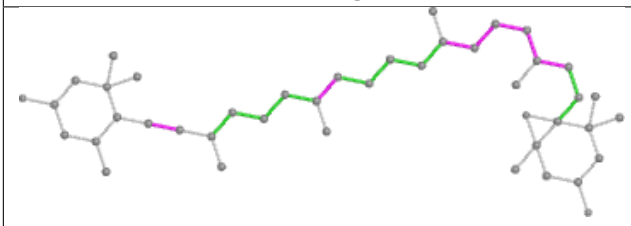


Bond angles



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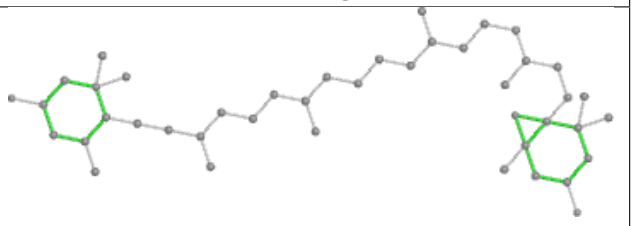
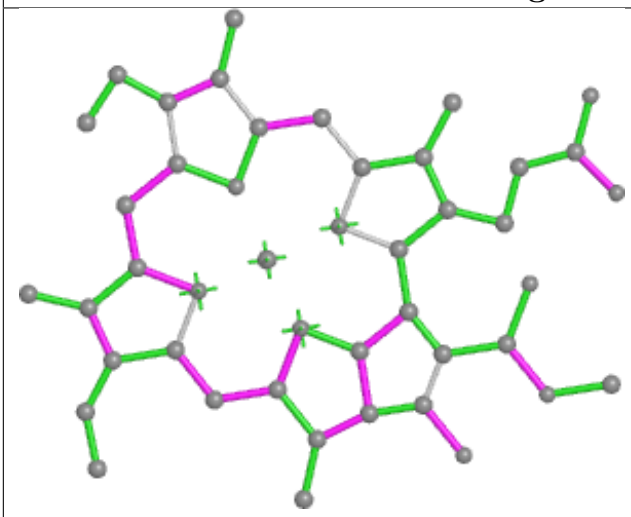


Rings

Ligand CLA 7 712



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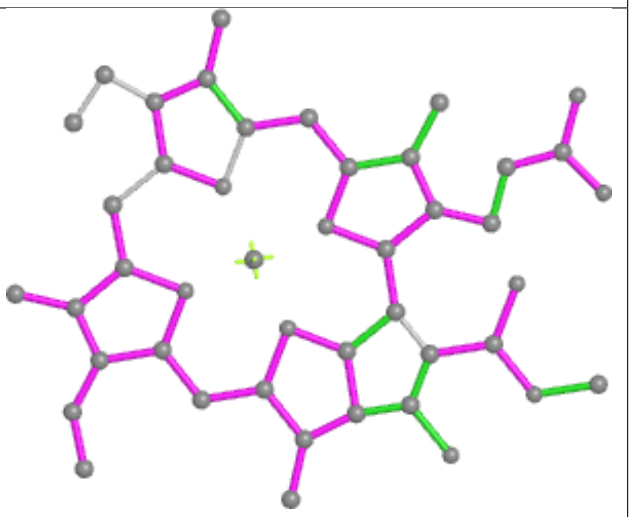

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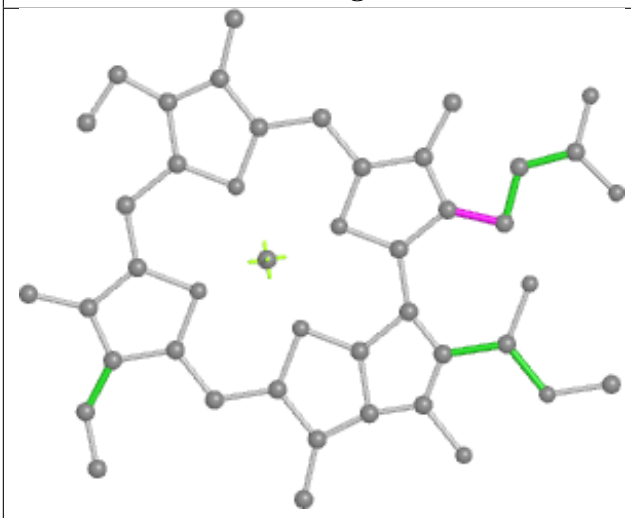

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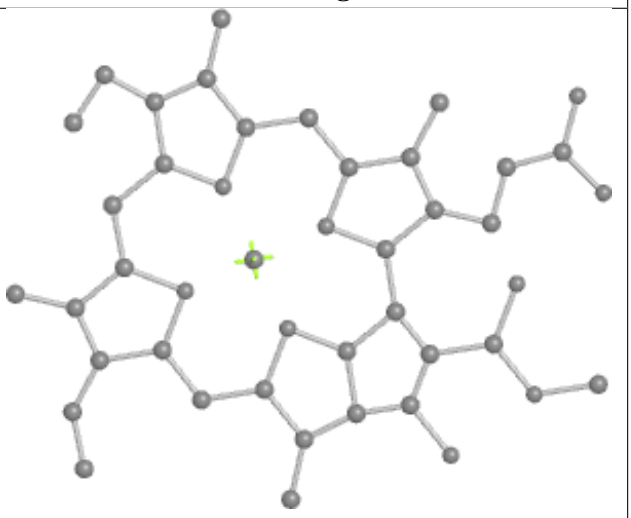
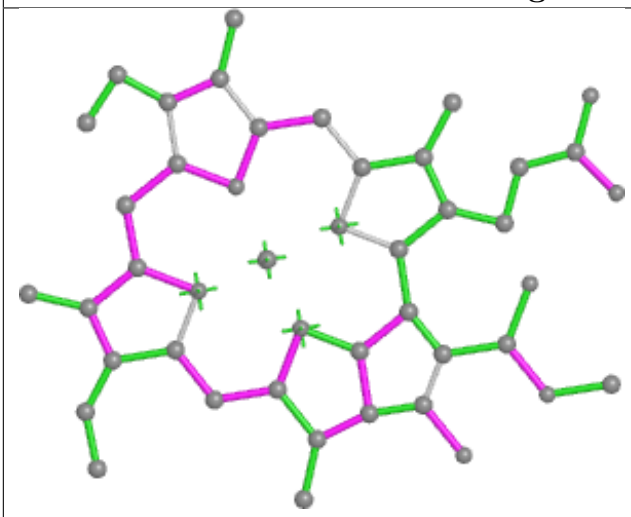


Rings

Ligand CLA 9 912



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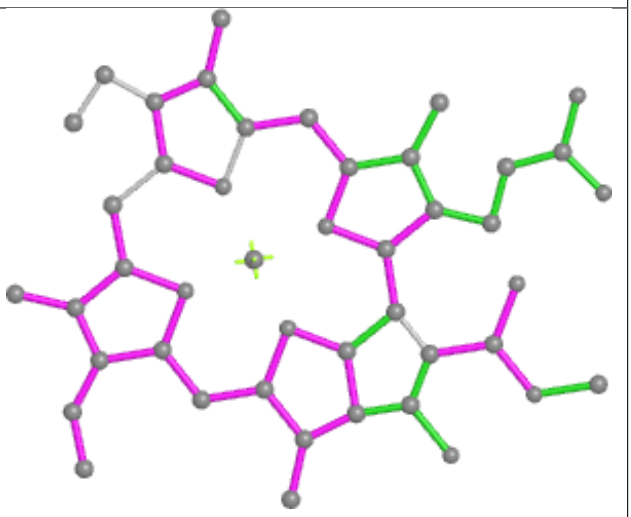

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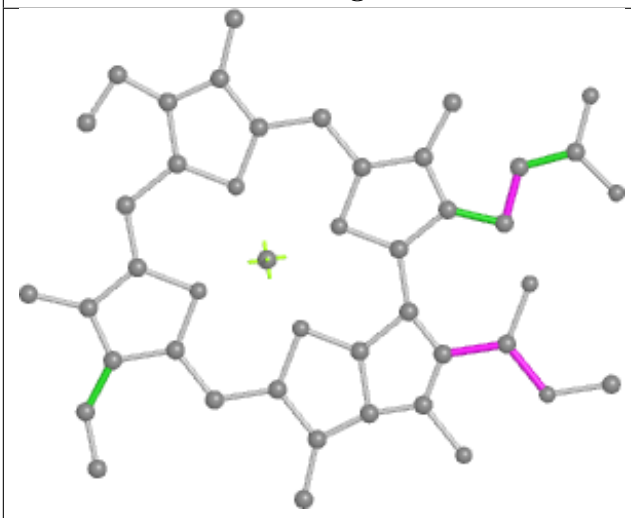

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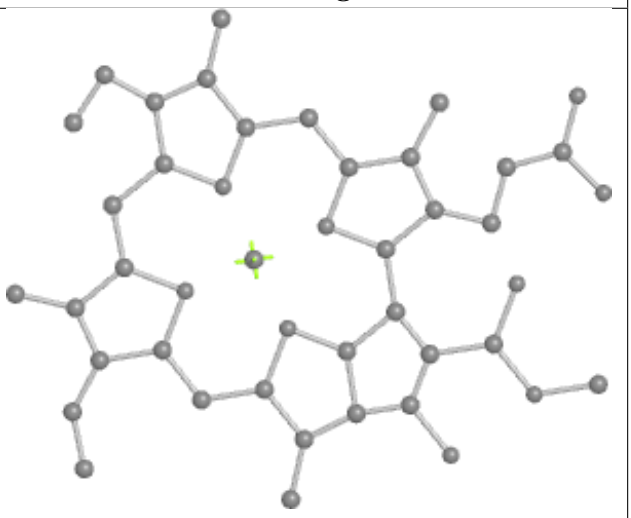
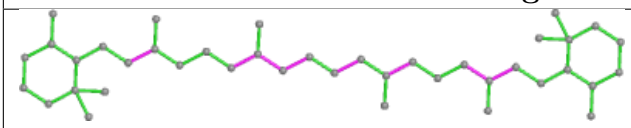


Rings

Ligand BCR A 848



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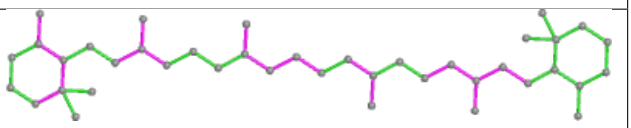

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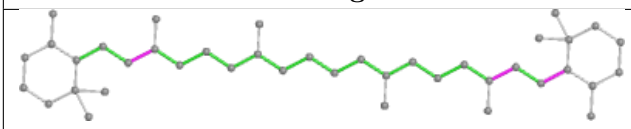
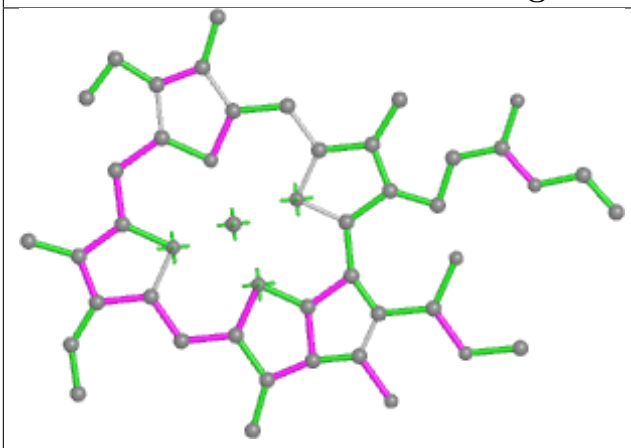
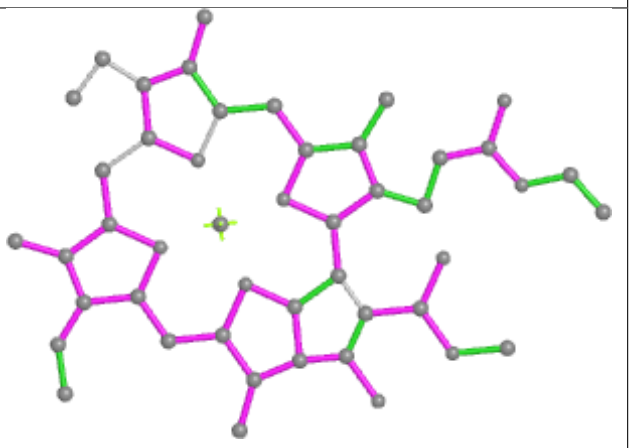
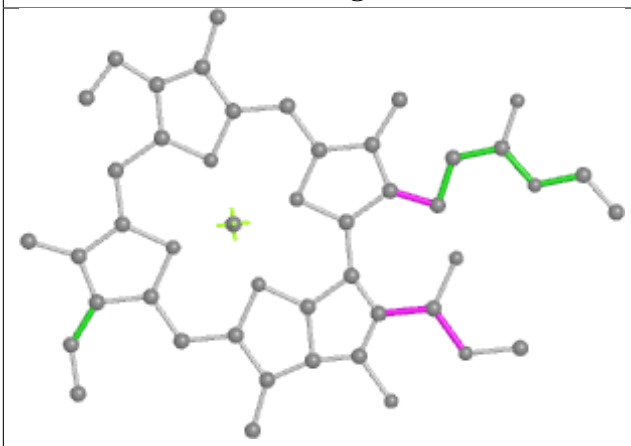
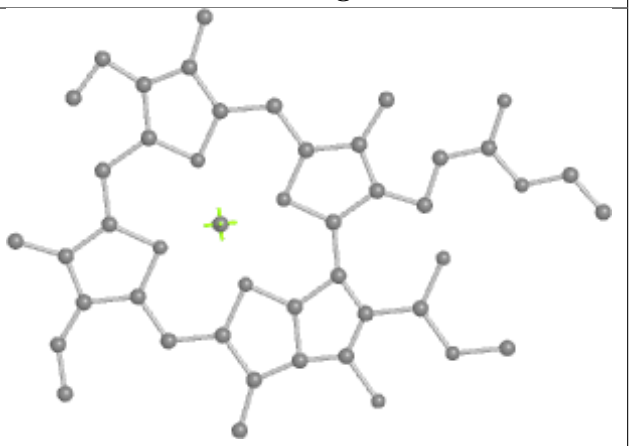
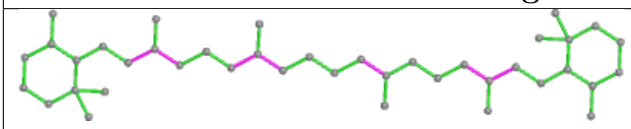
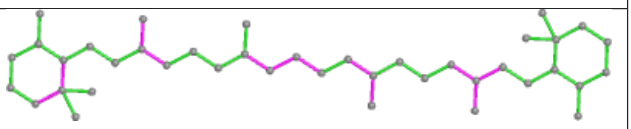
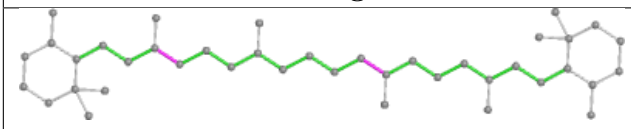
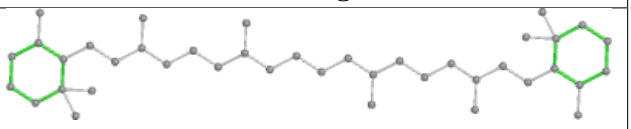


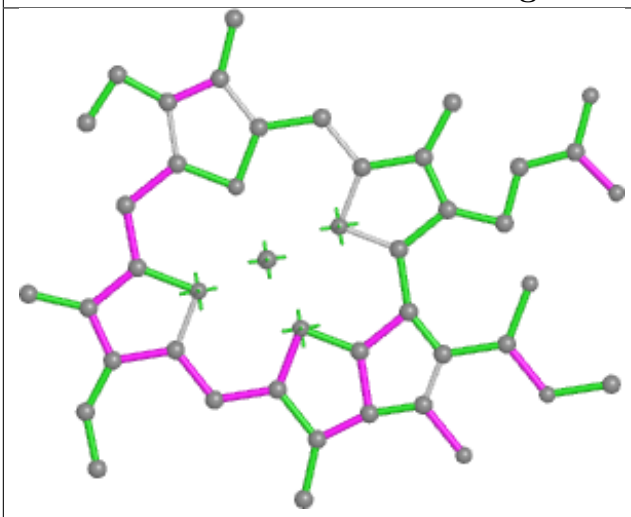
Torsions

Rings

Ligand CLA 5 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 12 507



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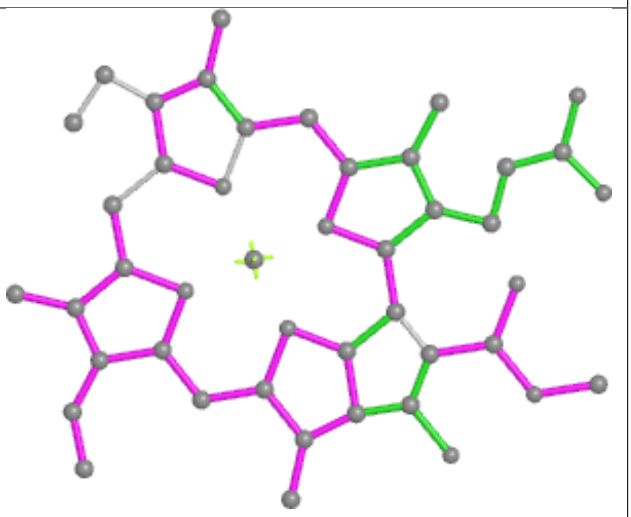
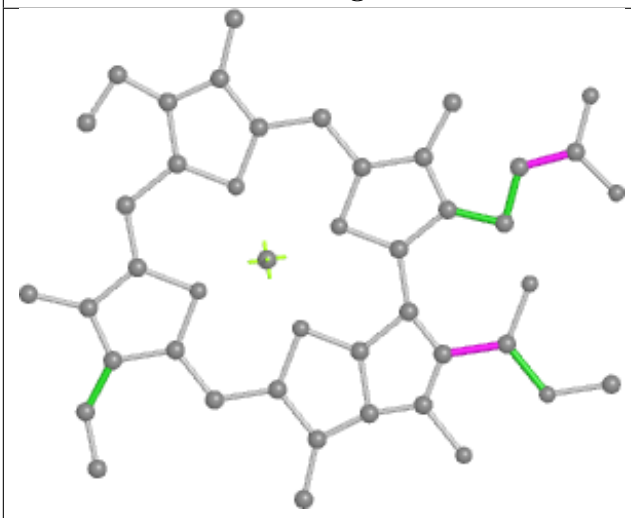


Bond angles



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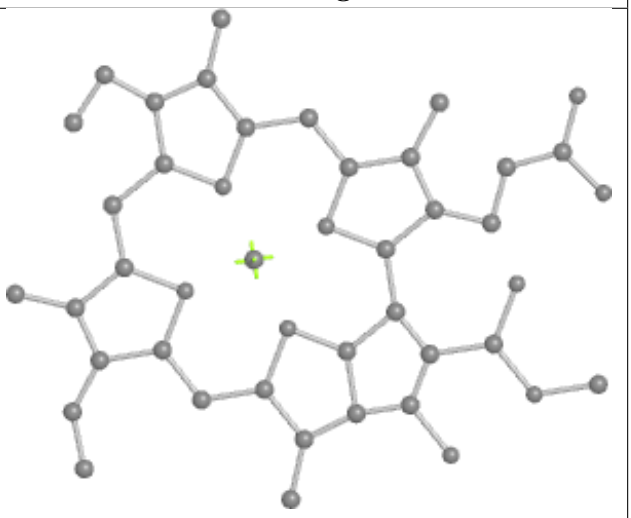
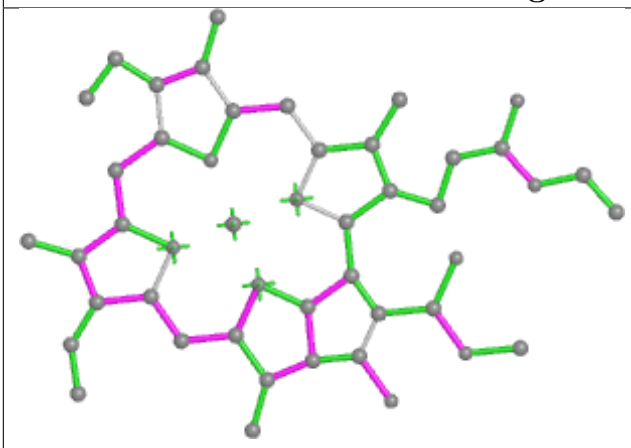


Rings

Ligand CLA 6 903



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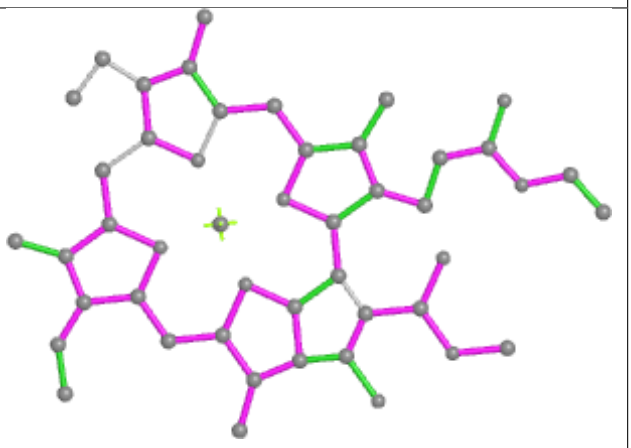
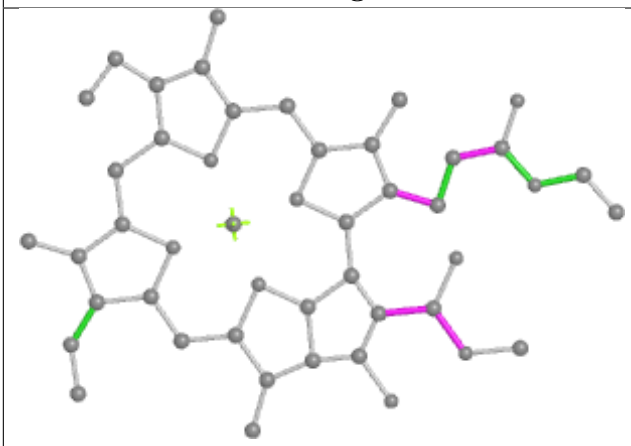


Bond angles



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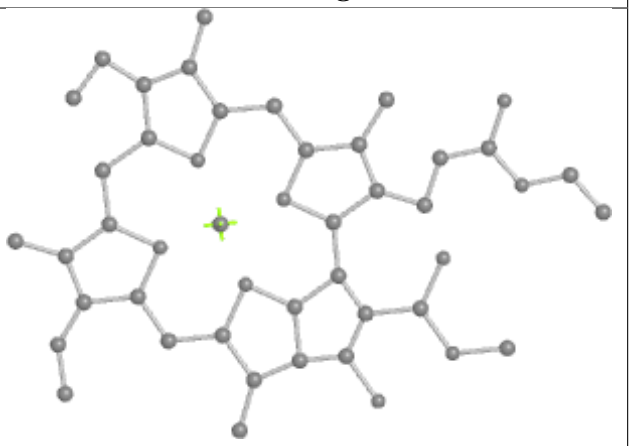
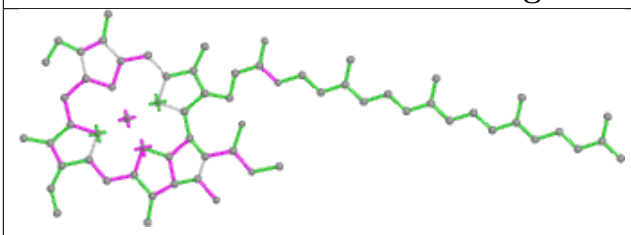


Rings

Ligand CLA A 822



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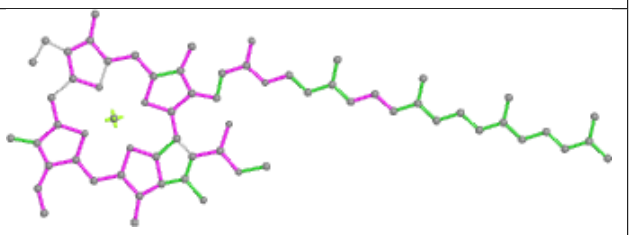
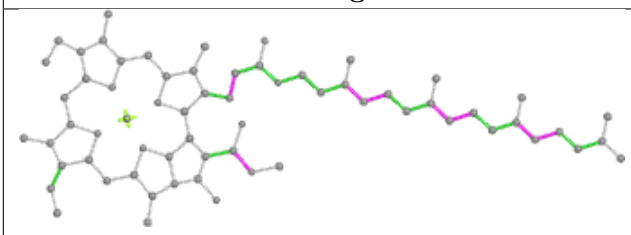


Bond angles



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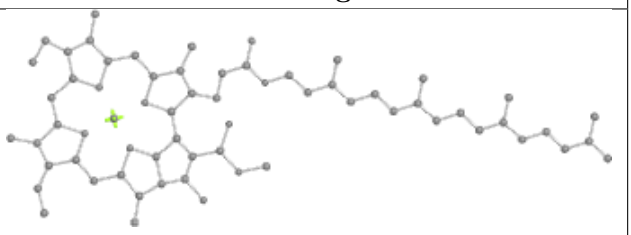
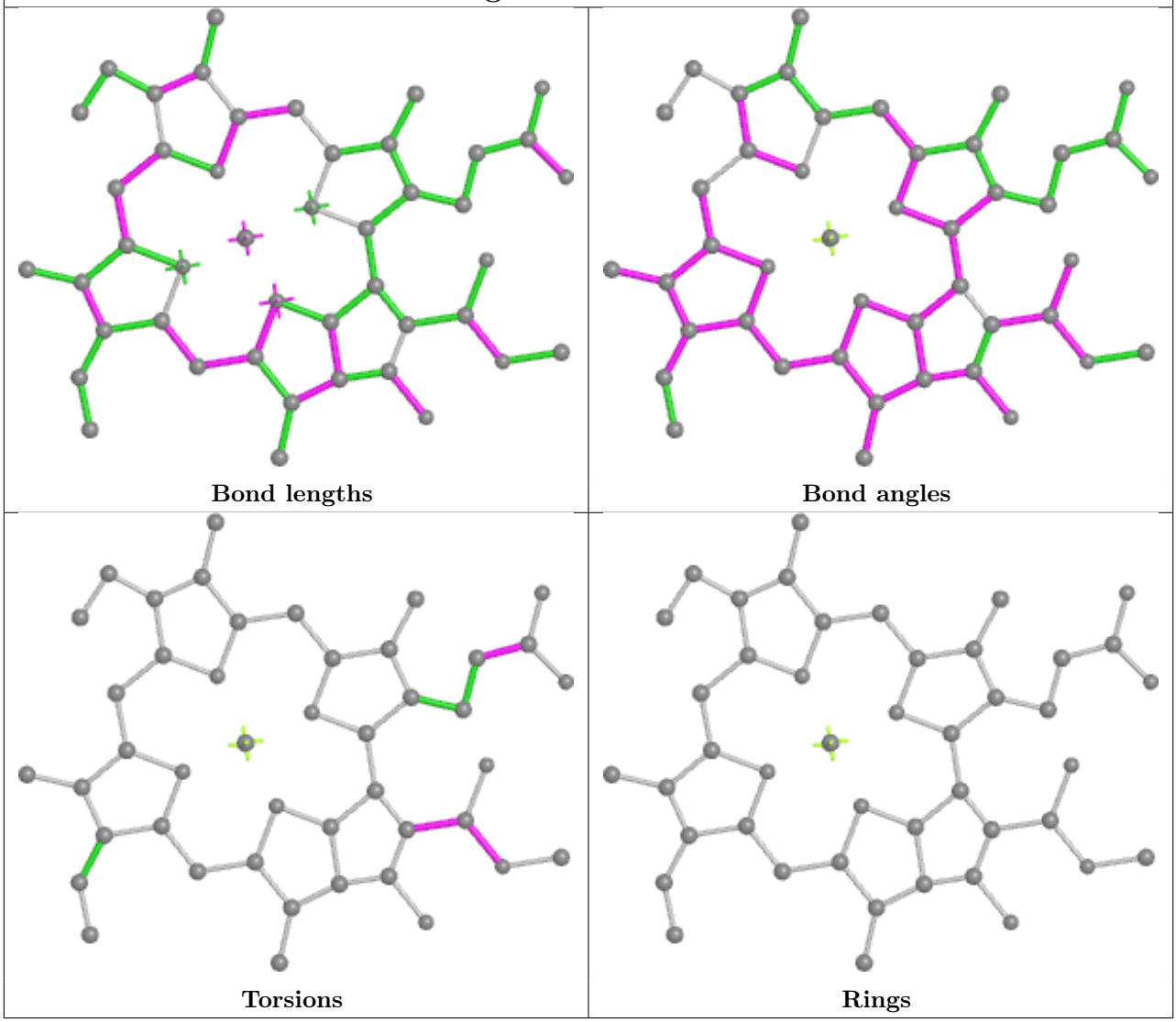


Rings

Ligand CLA 2 505



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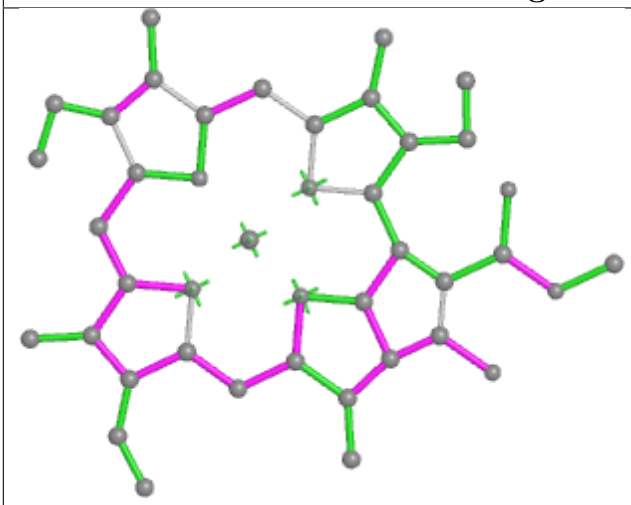
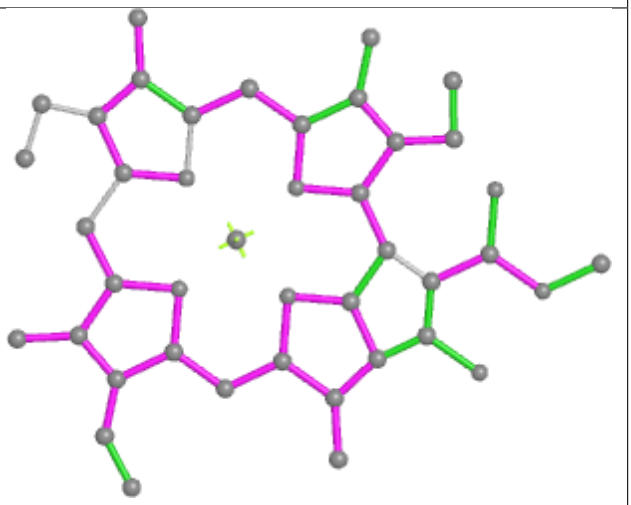
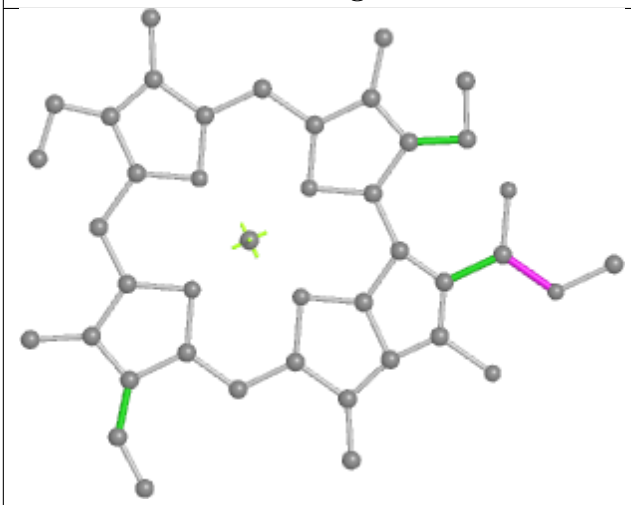


Bond lengths



Bond angles



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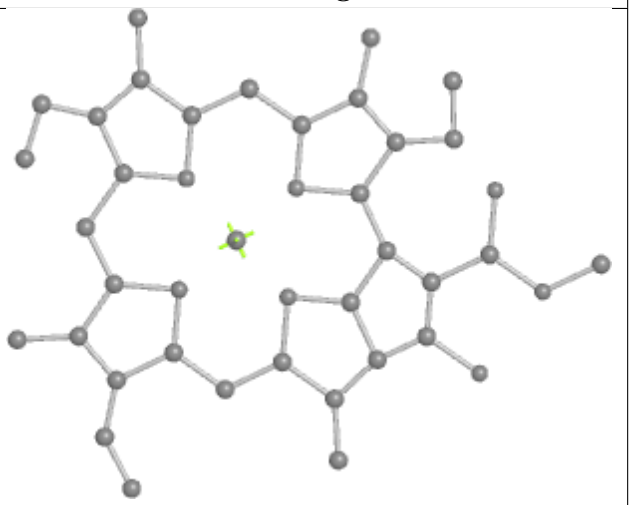
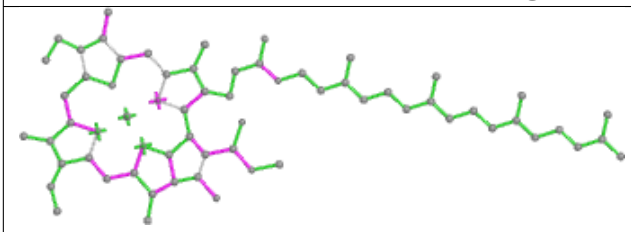


Rings

Ligand CLA A 806



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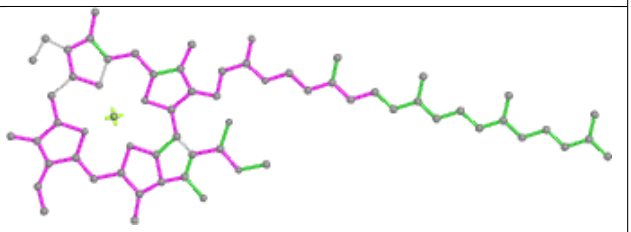
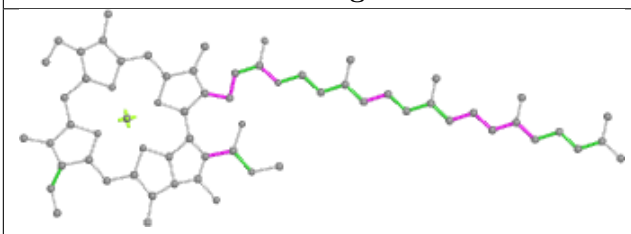


Bond angles



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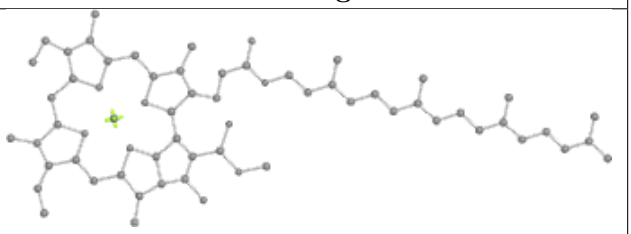
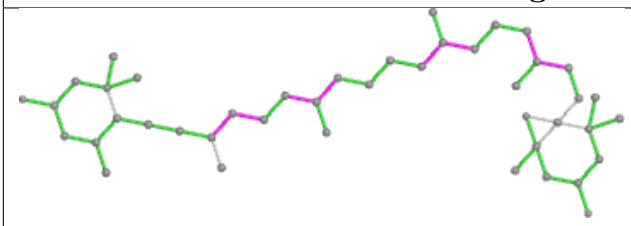
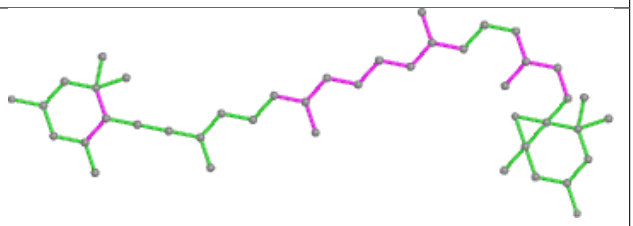
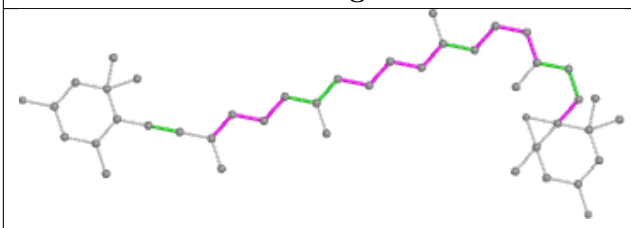
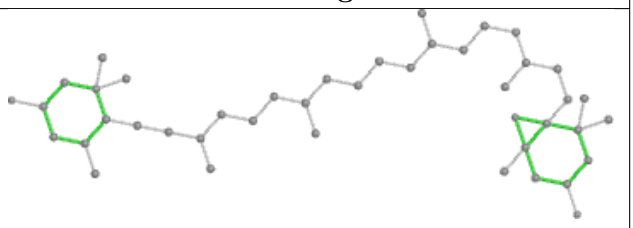
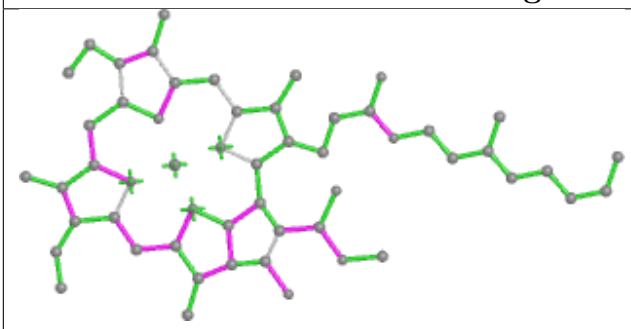
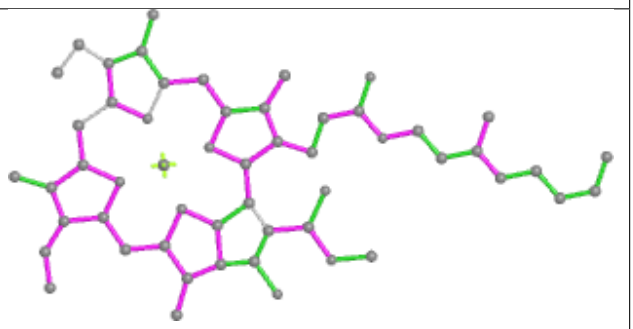
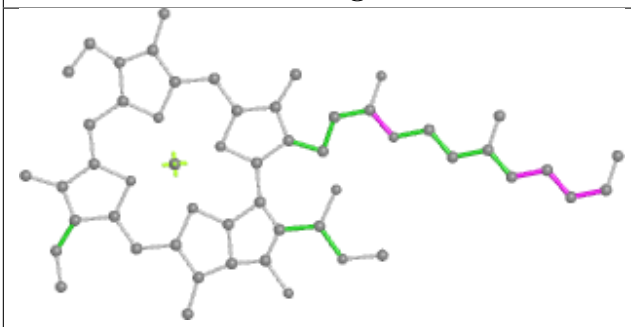
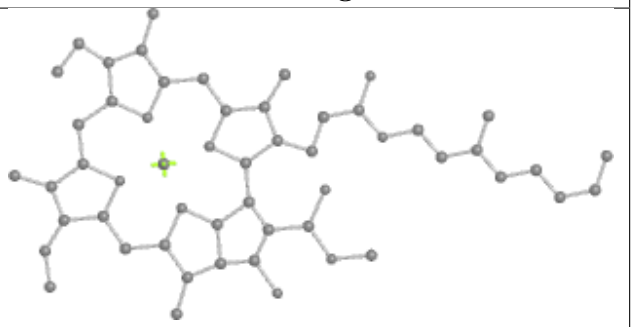


Rings

Ligand DD6 1 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

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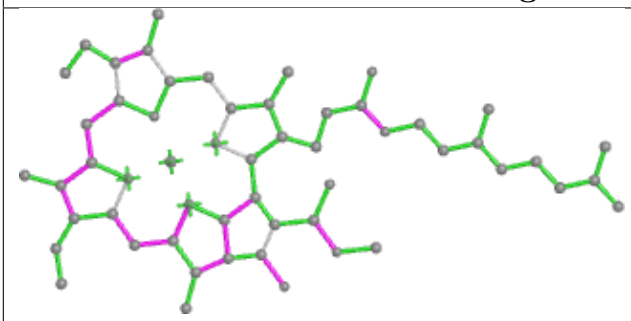
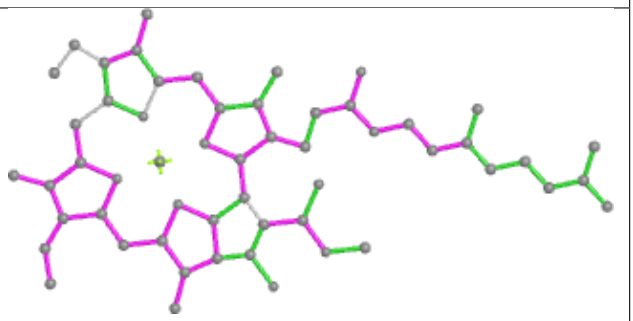
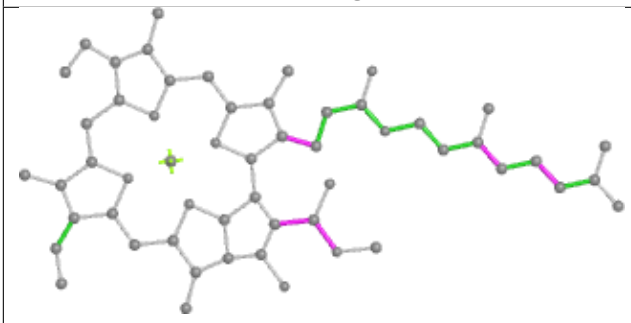
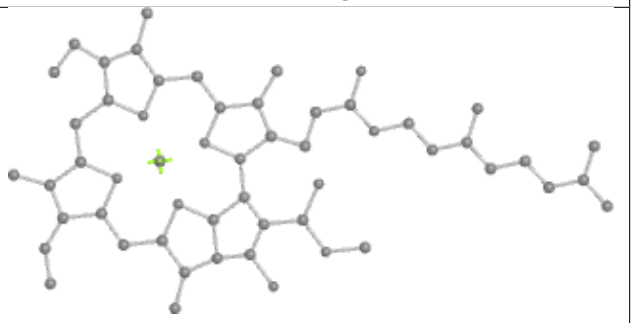
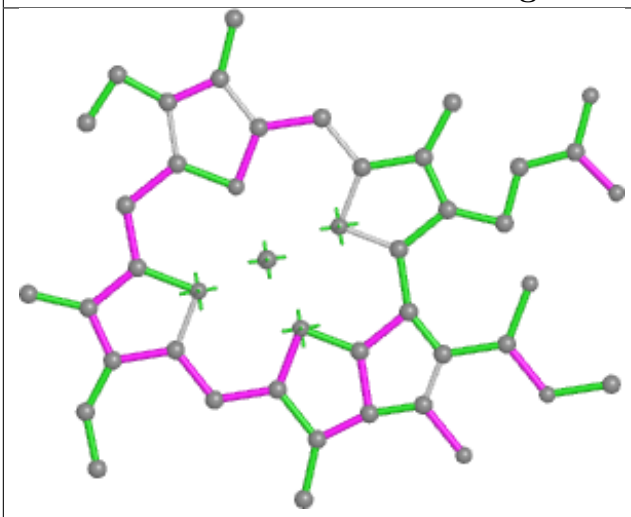
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 11 709



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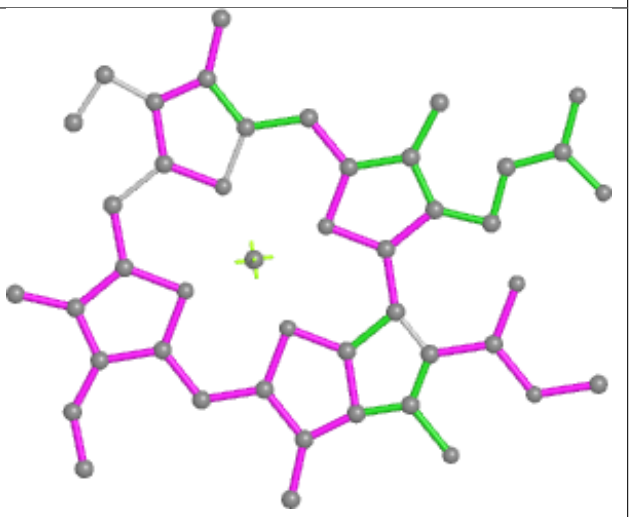

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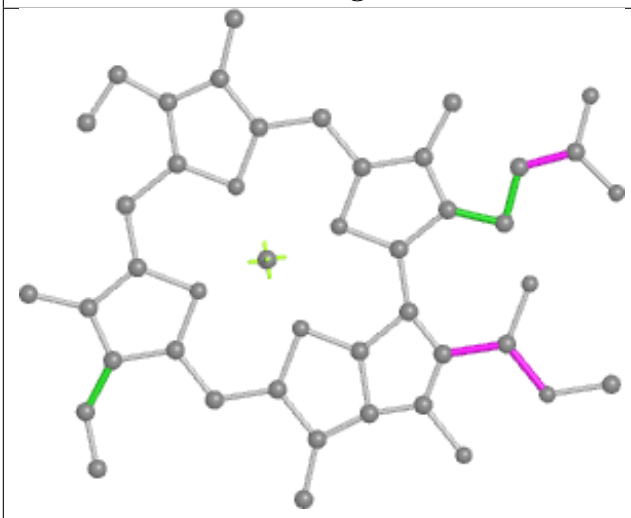

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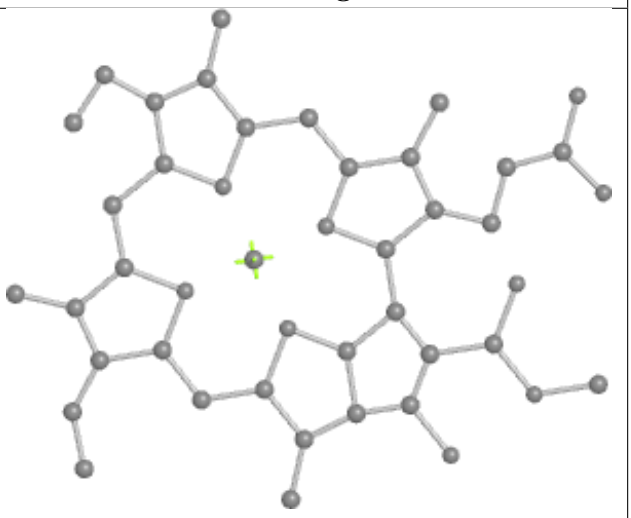
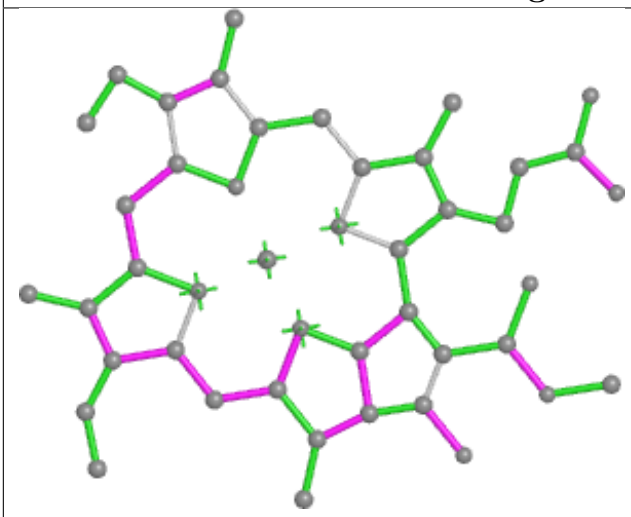


Rings

Ligand CLA 1 512



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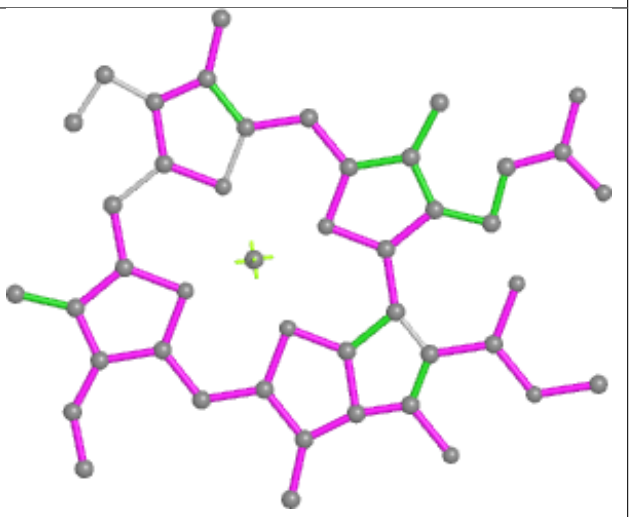

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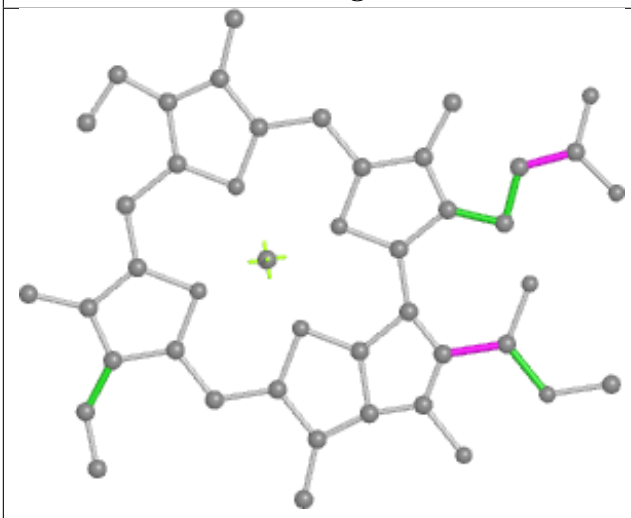

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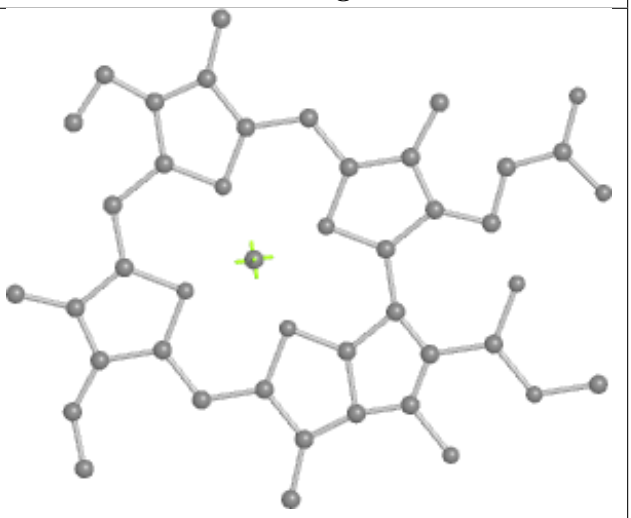
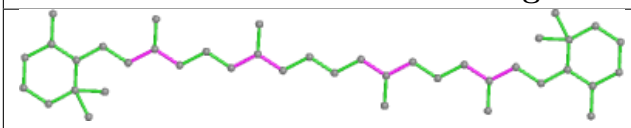


Rings

Ligand BCR B 842



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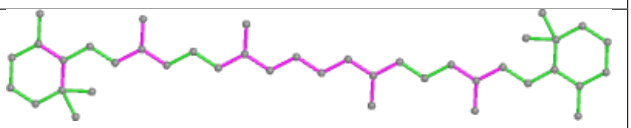

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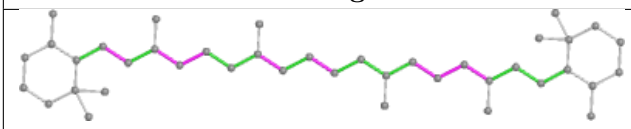
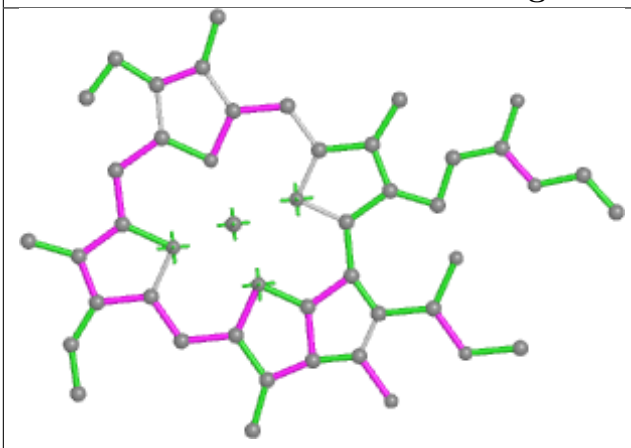
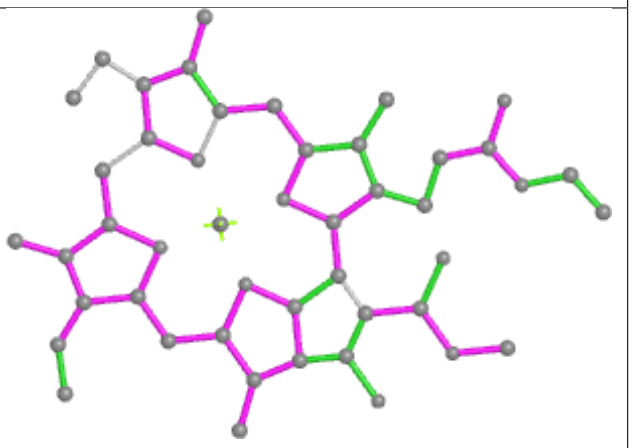


Torsions

Rings

Ligand CLA 9 906	
	
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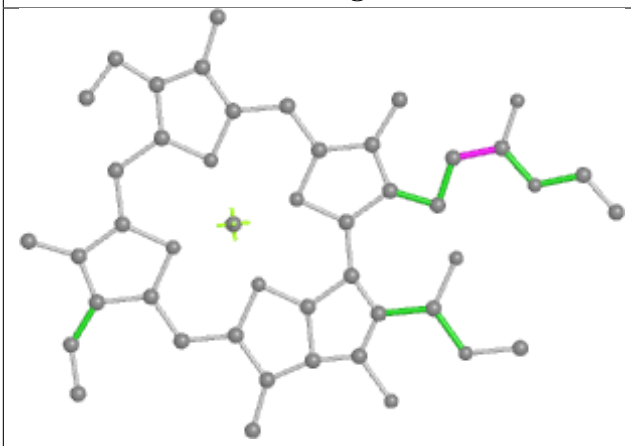
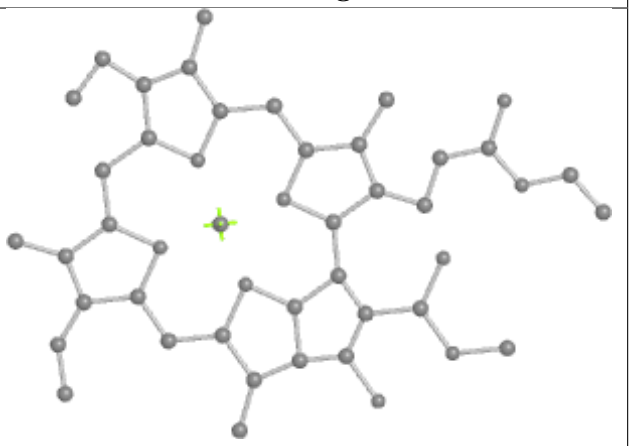
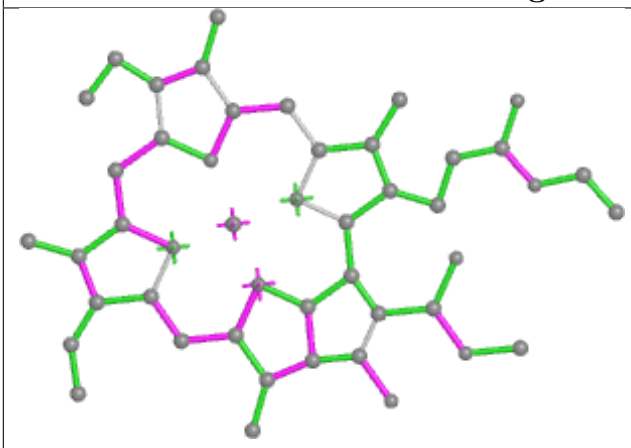
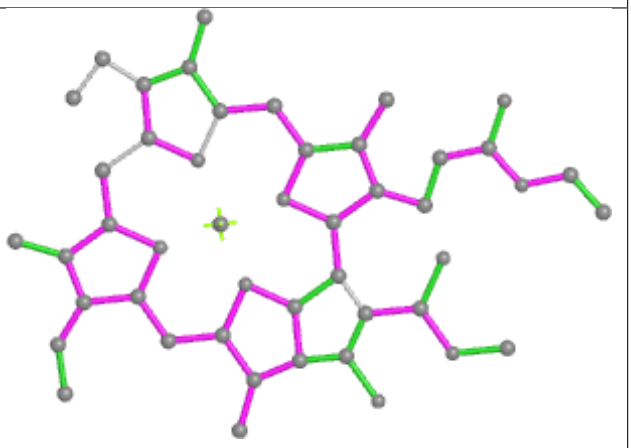
	
Torsions	**Rings**

Ligand CLA 7 707	
	
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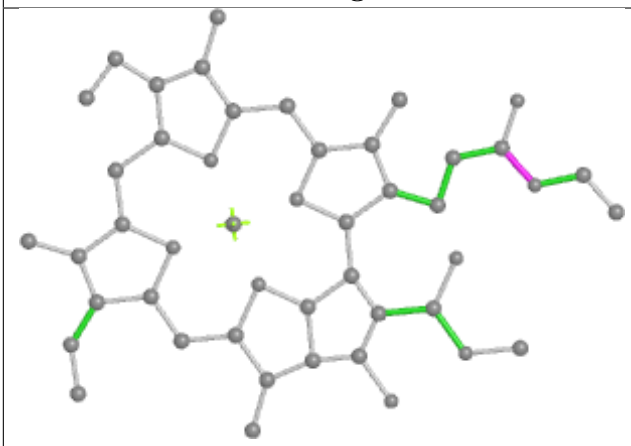
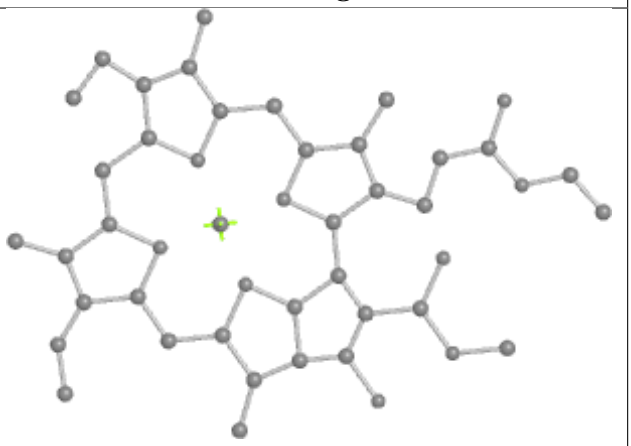
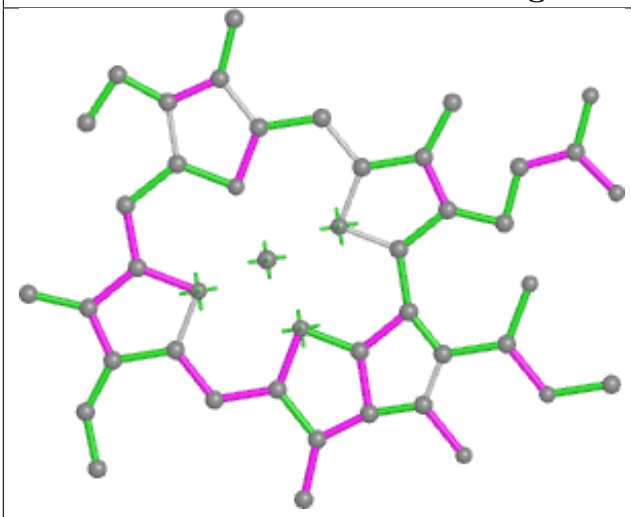
	
Torsions	**Rings**

Ligand CLA J 101



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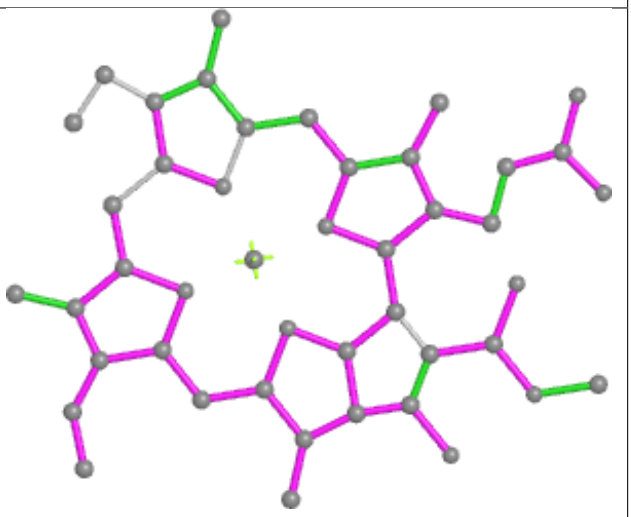
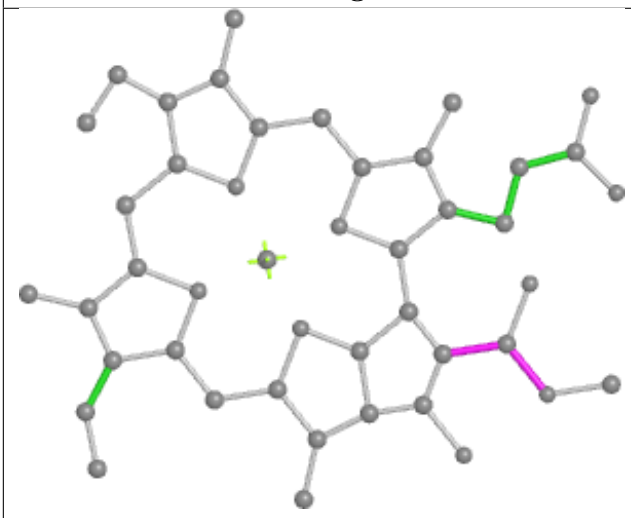
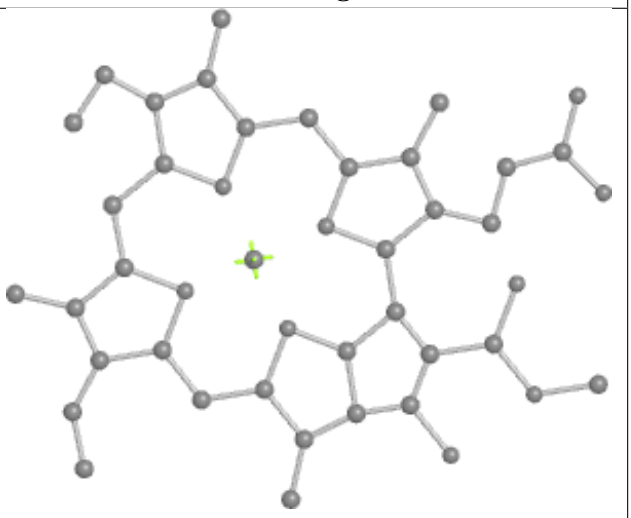


Bond angles



Torsions



Rings

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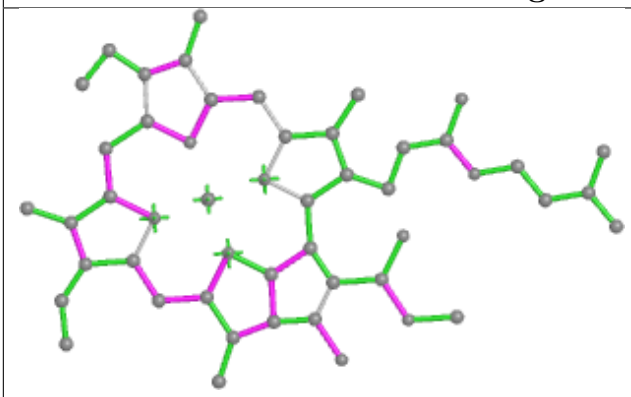
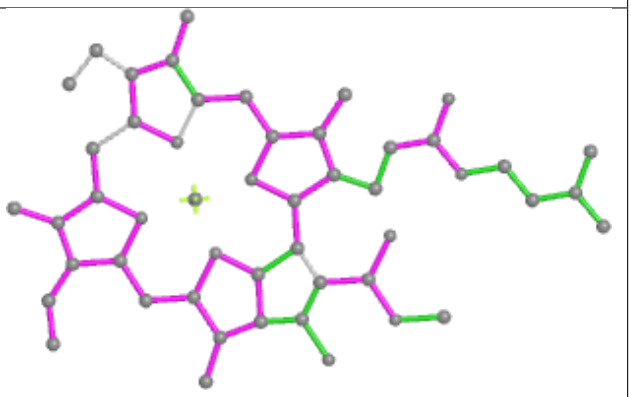
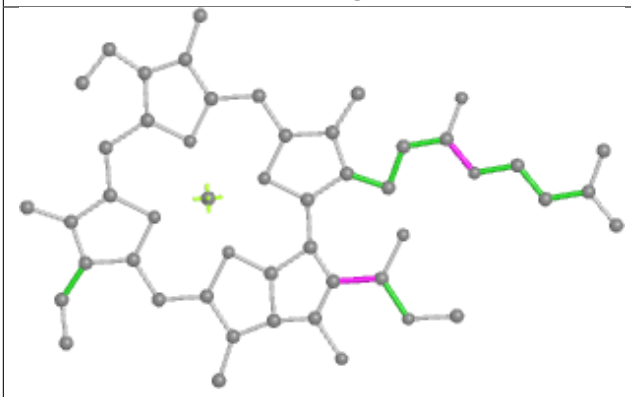
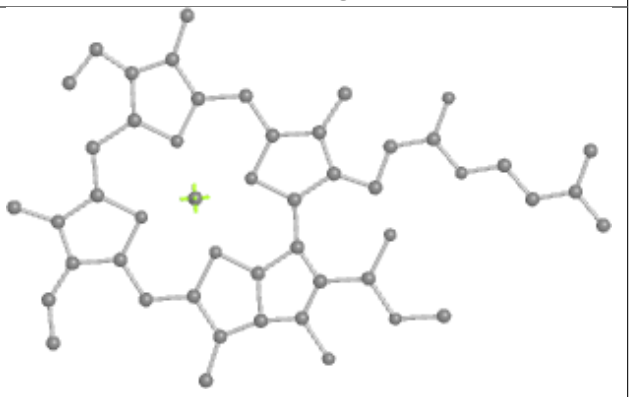
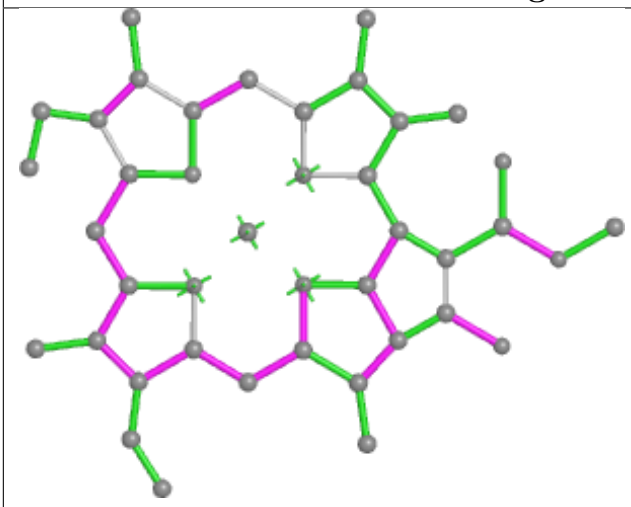
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 701



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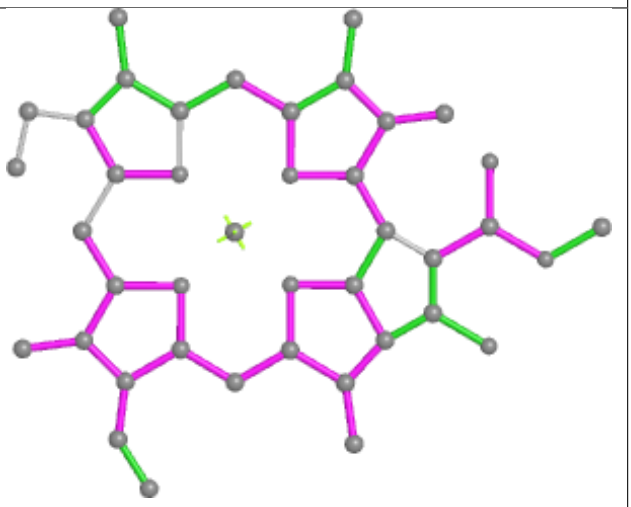

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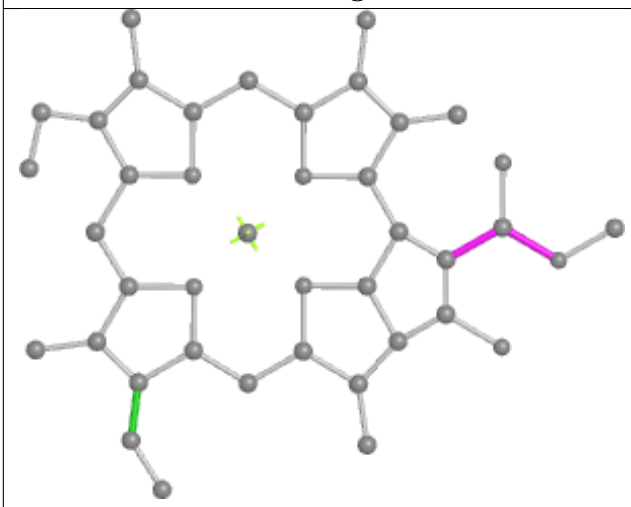
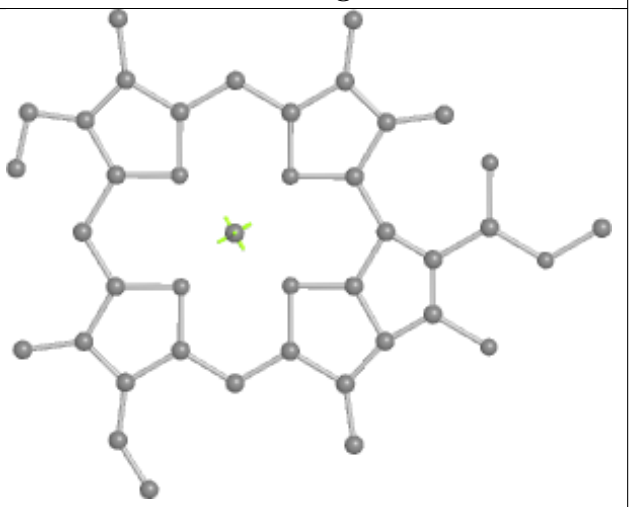
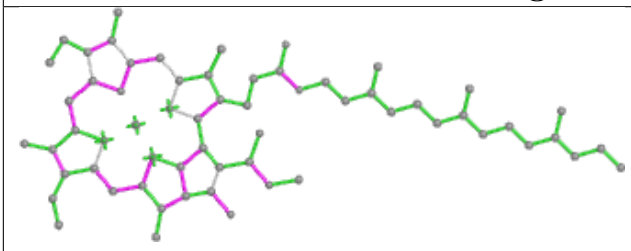


Torsions



Rings

Ligand CLA 7 708



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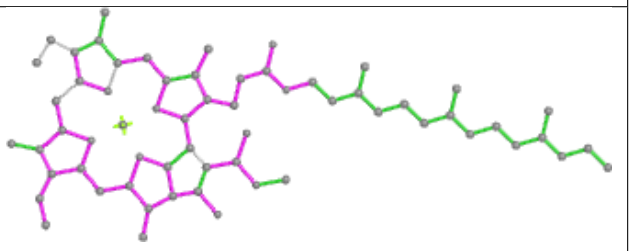

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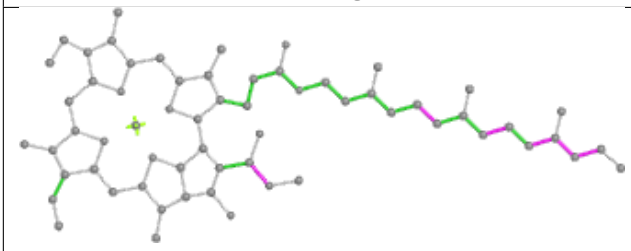

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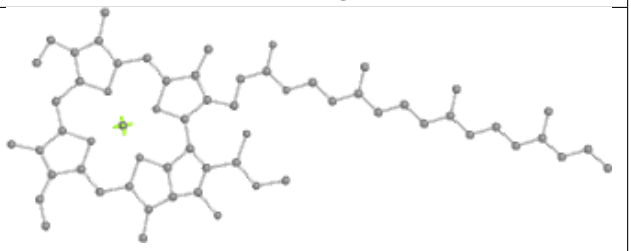
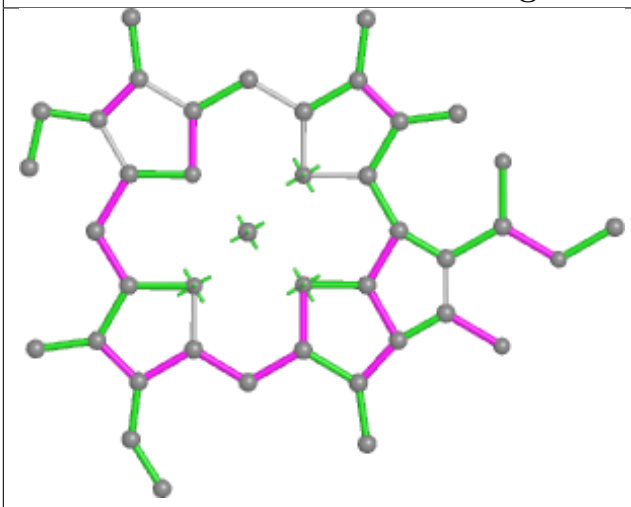


Rings

Ligand CLA 10 703



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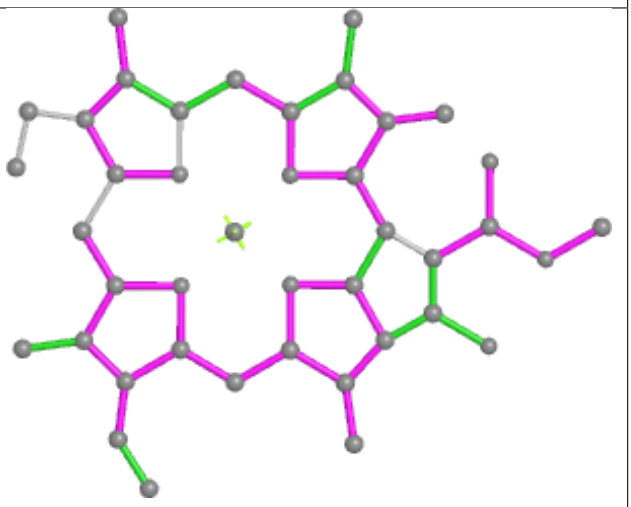
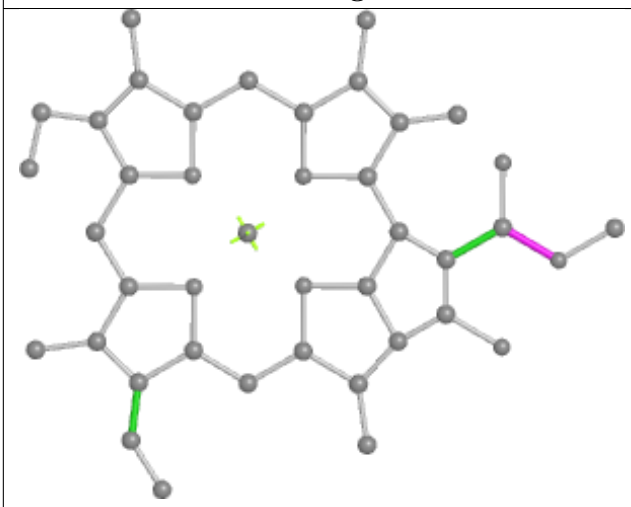


Bond angles



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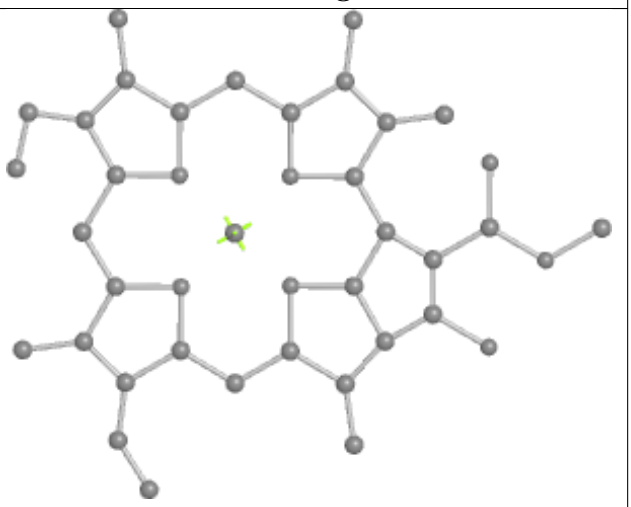
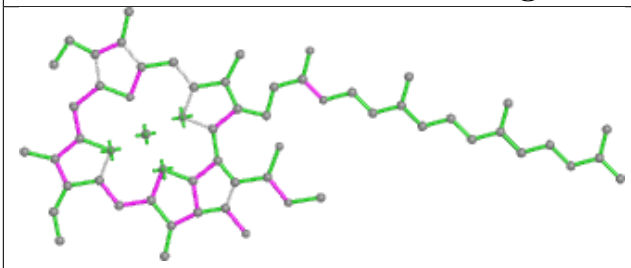


Rings

Ligand CLA 11 702



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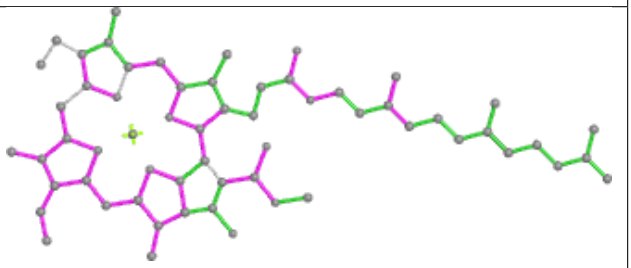
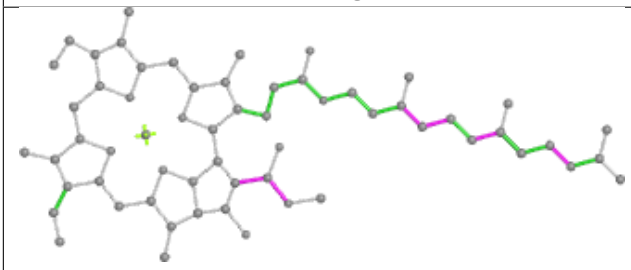


Bond angles



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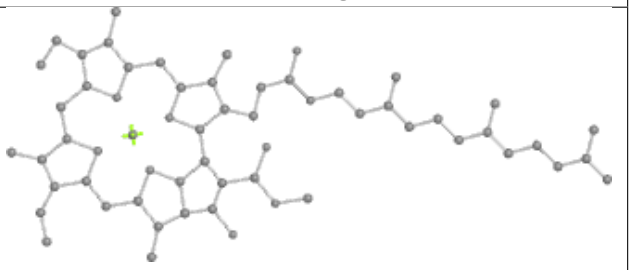
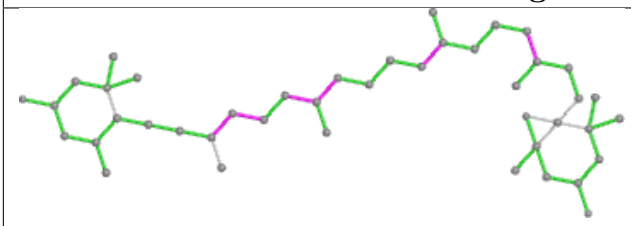
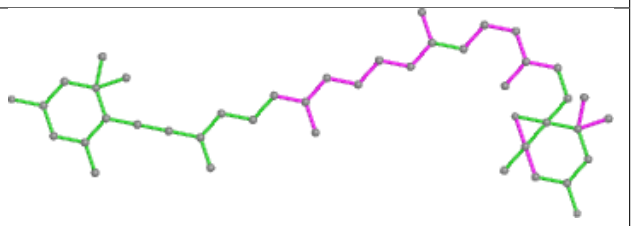
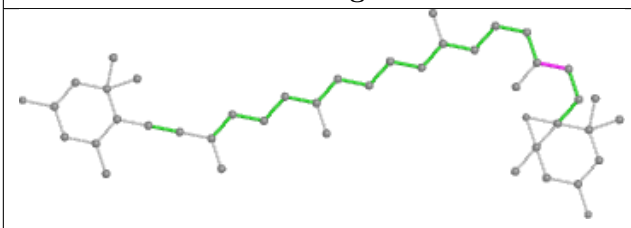
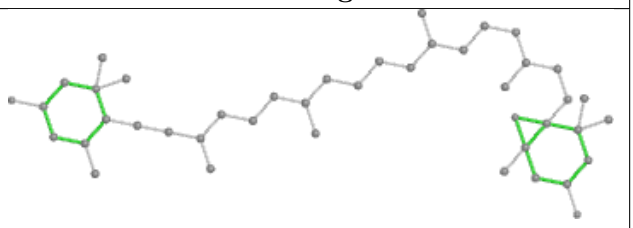
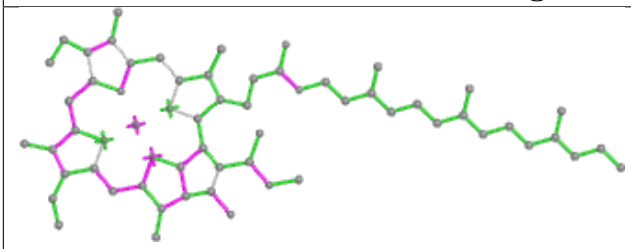
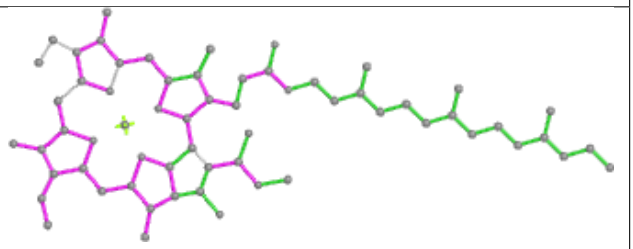
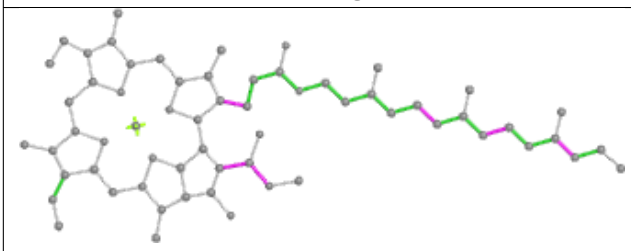
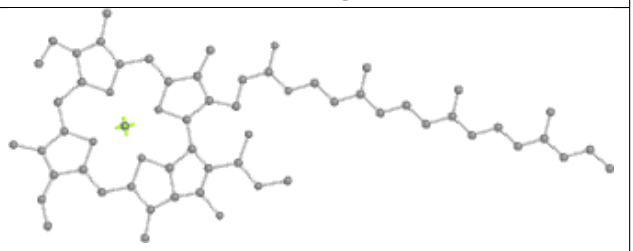
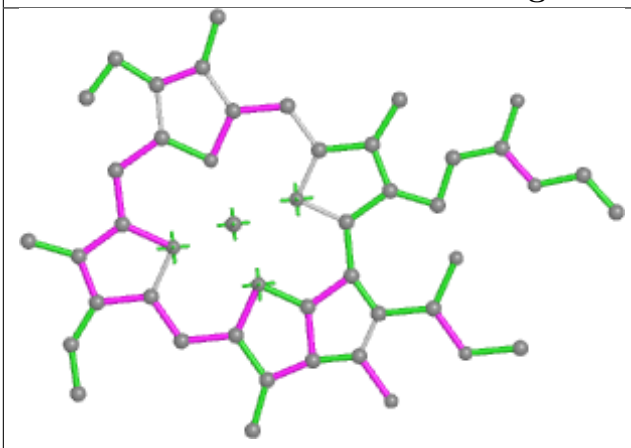


Rings

Ligand DD6 2 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 913



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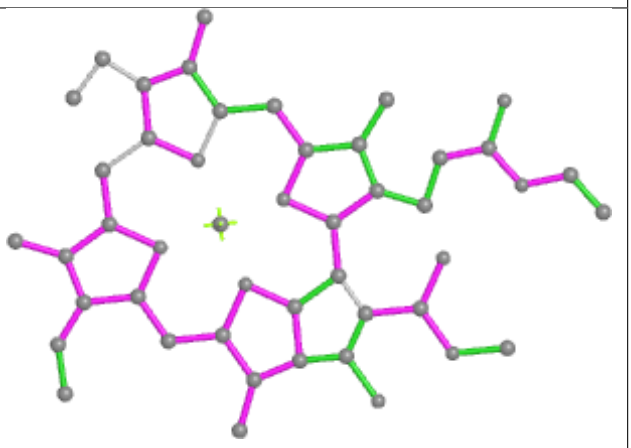
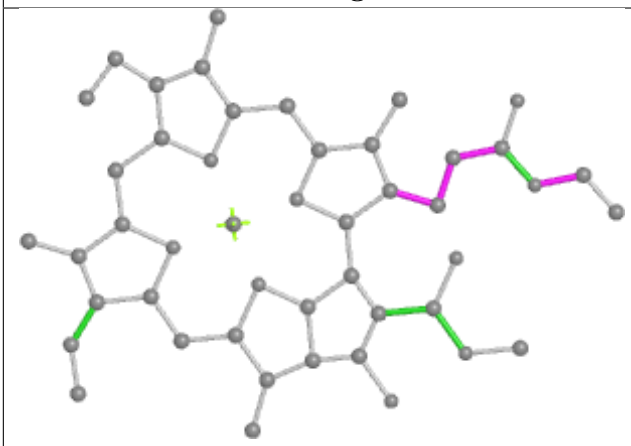
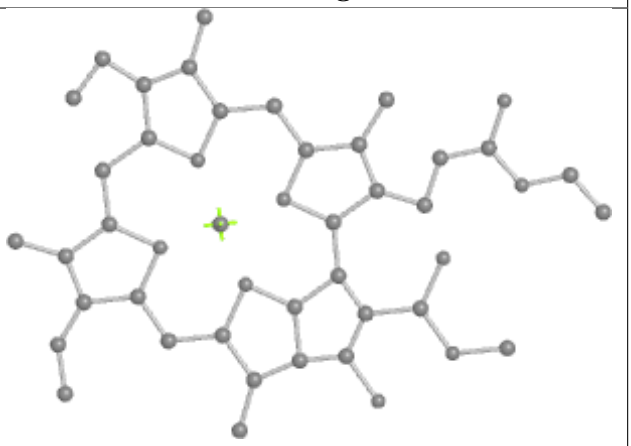


Bond angles

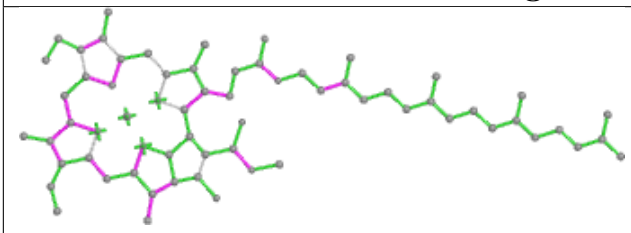


Torsions



Rings

Ligand CLA B 827



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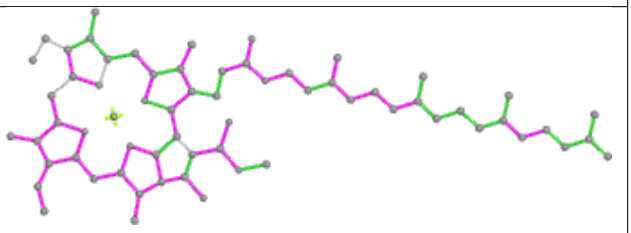

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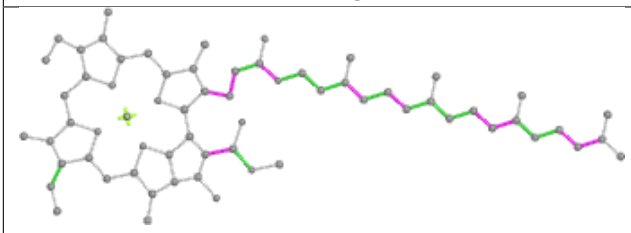

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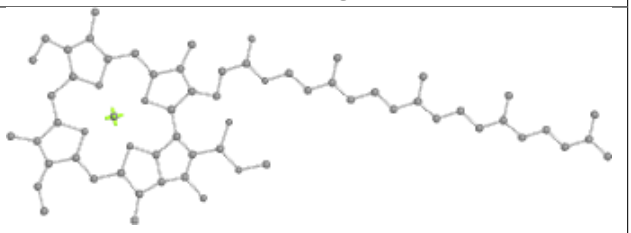
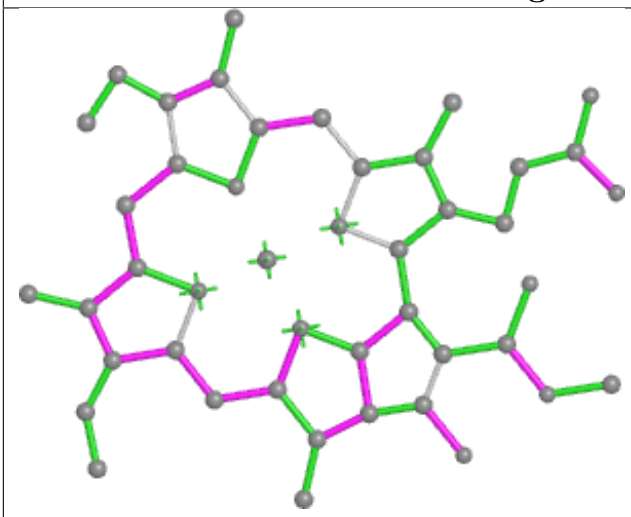


Rings

Ligand CLA 8 605



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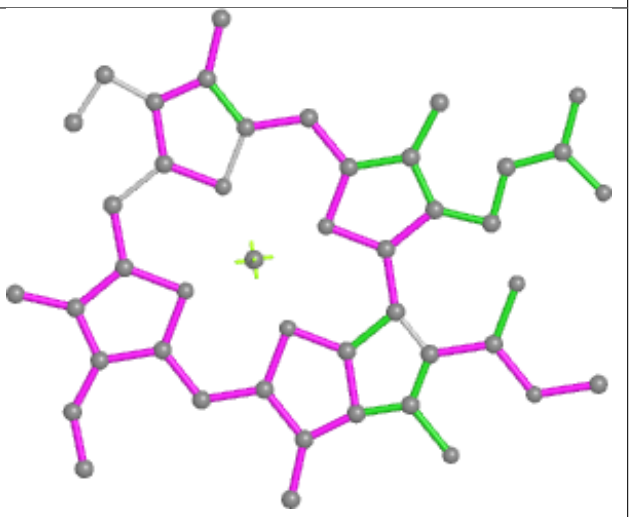
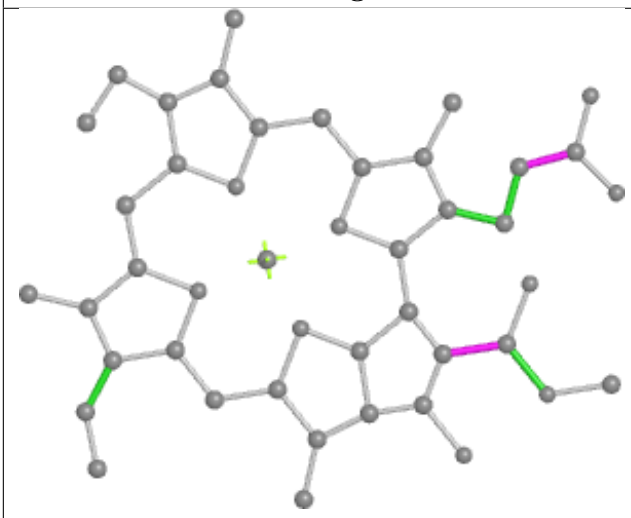


Bond angles



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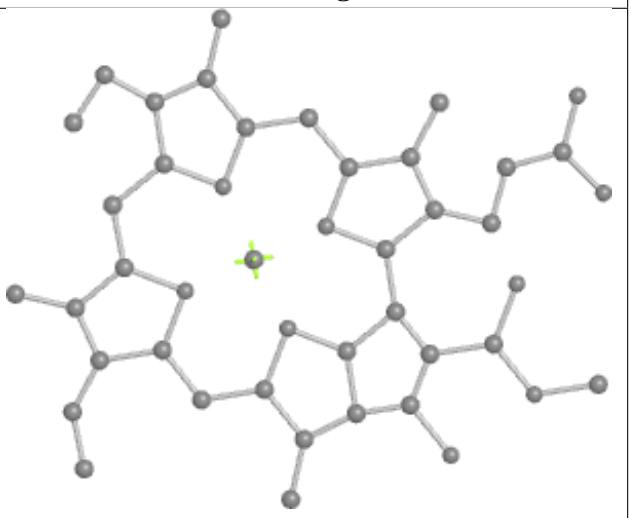
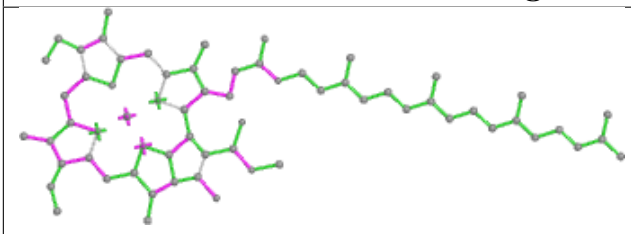


Rings

Ligand CLA B 828



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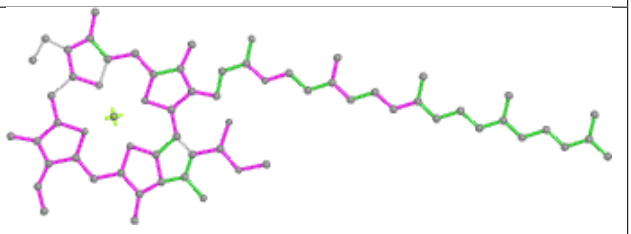

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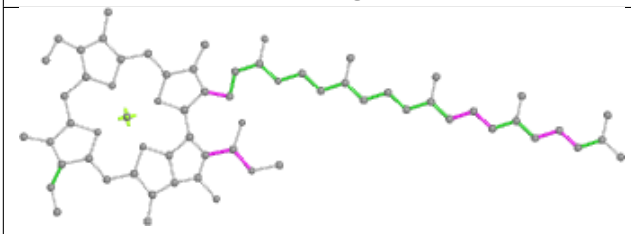

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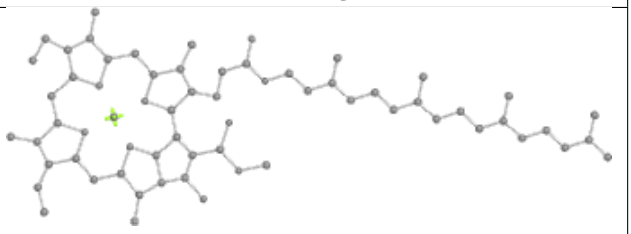
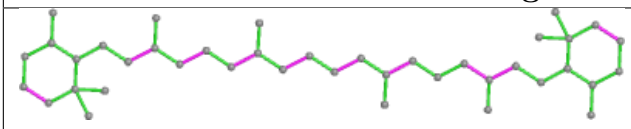
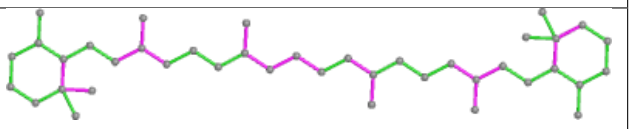
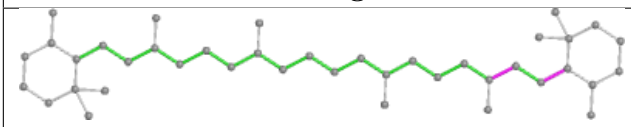


Rings

Ligand BCR A 847	
 Bond lengths	 Bond angles
 Torsions	Rings

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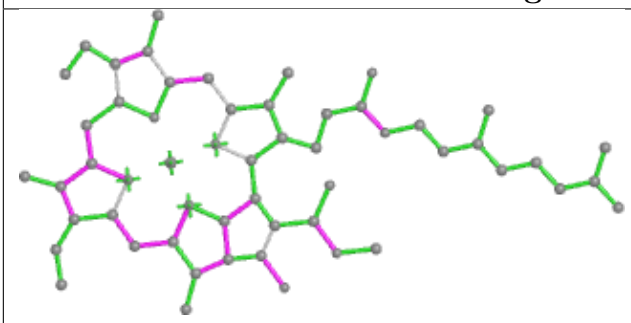
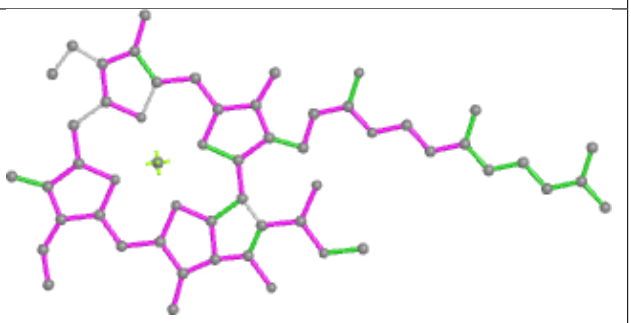
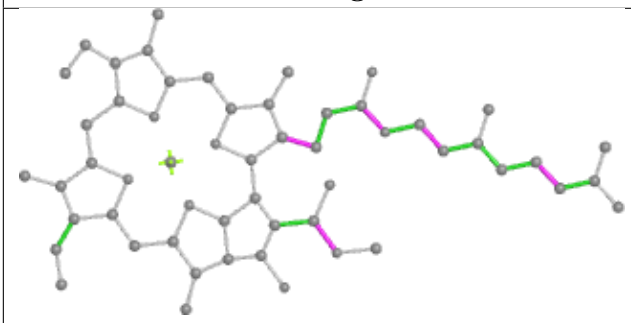
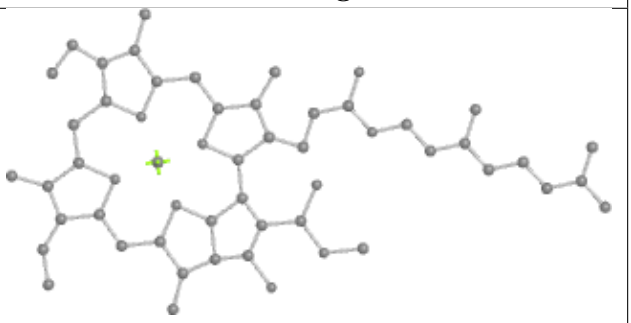
 Bond lengths	 Bond angles
 Torsions	 Rings

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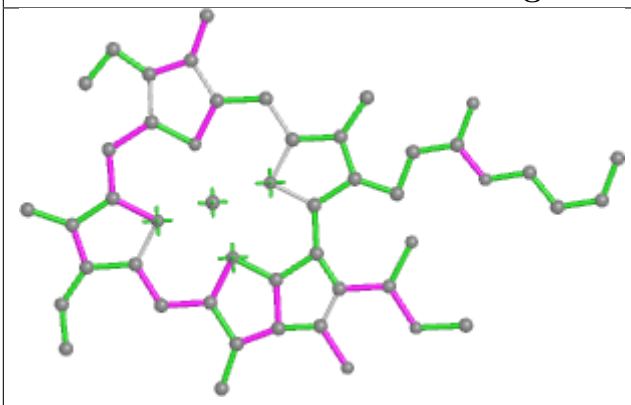
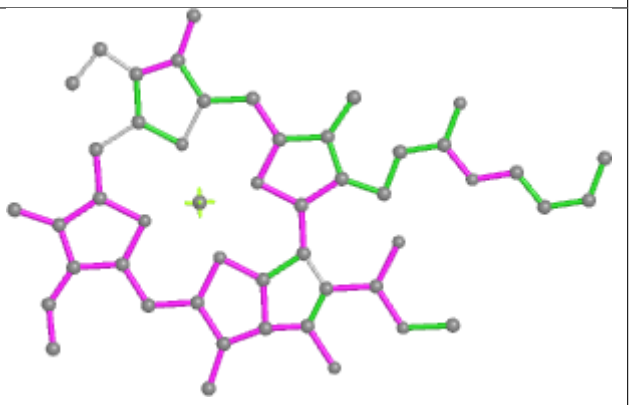
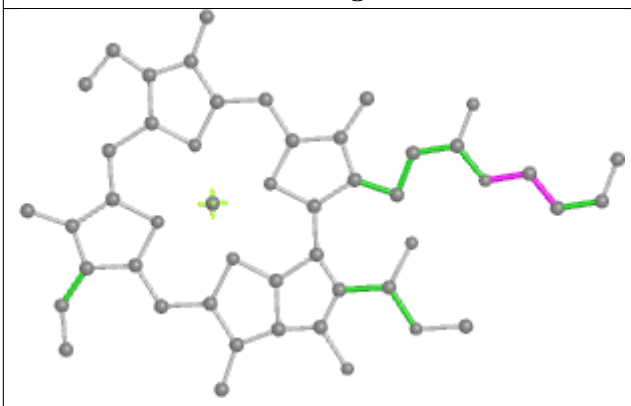
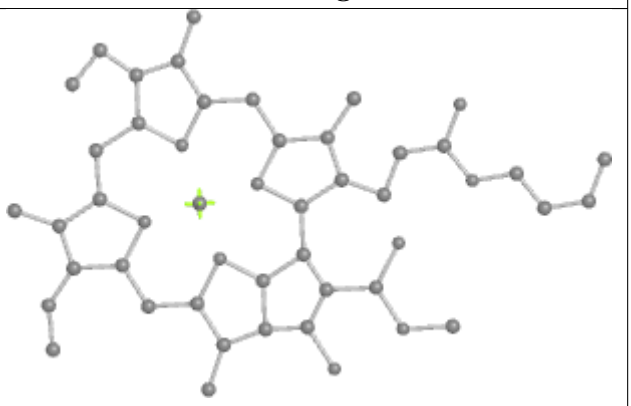
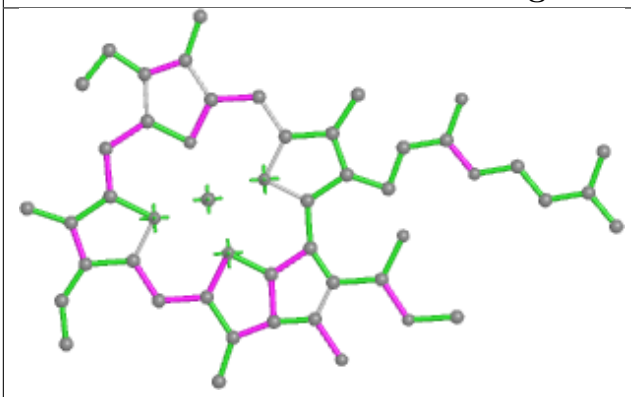
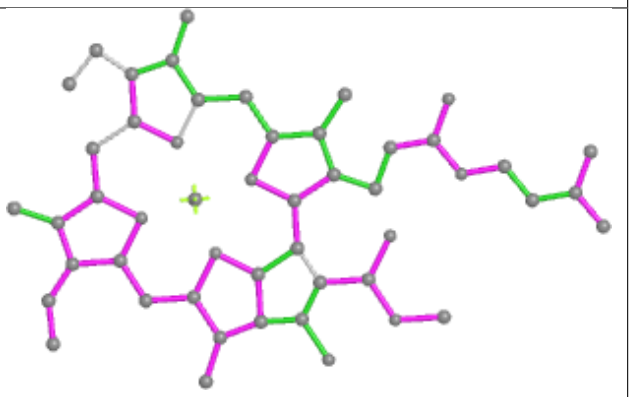
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 704



Bond lengths



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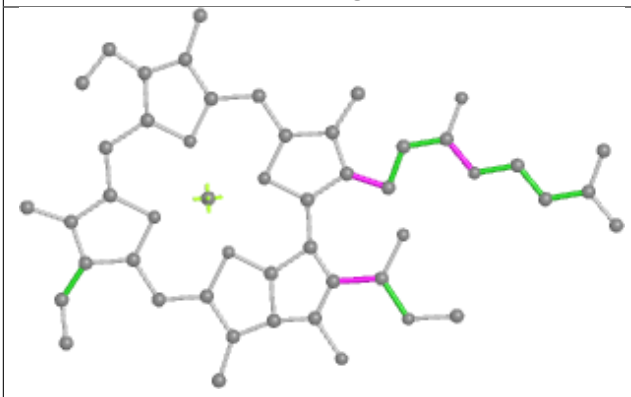
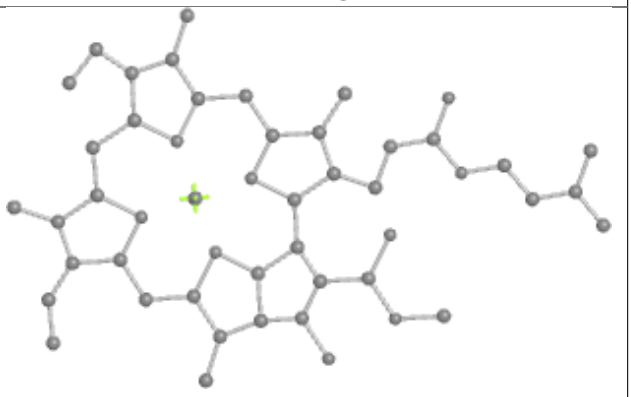
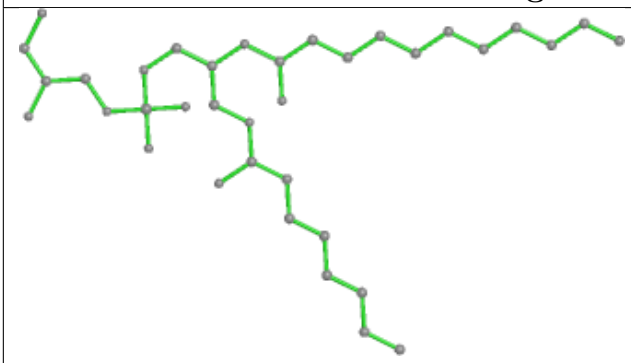


Torsions



Rings

Ligand LHG 1 521



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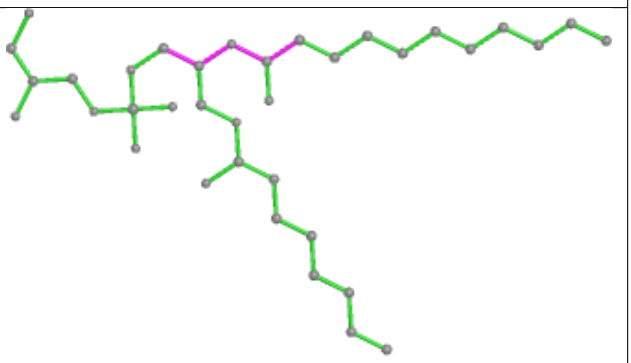
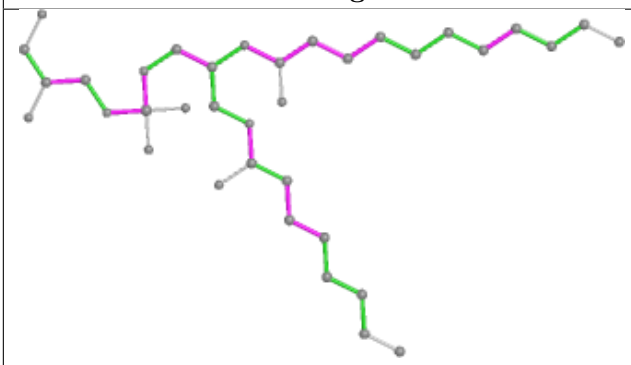
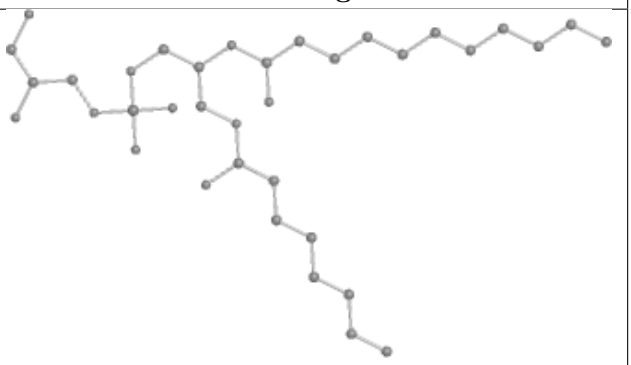


Bond angles

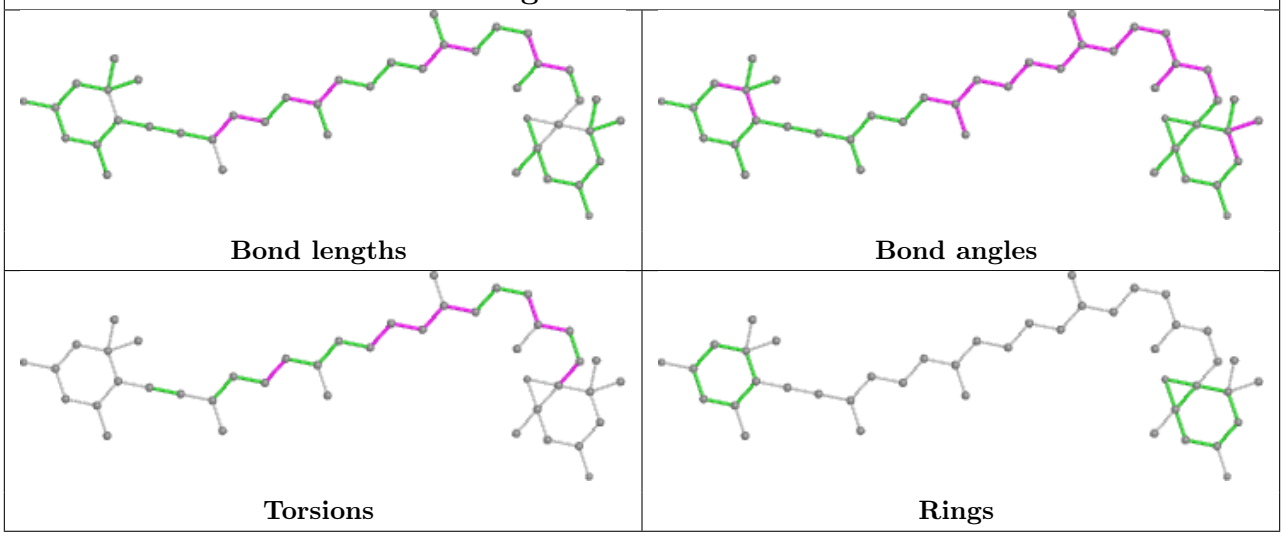


Torsions

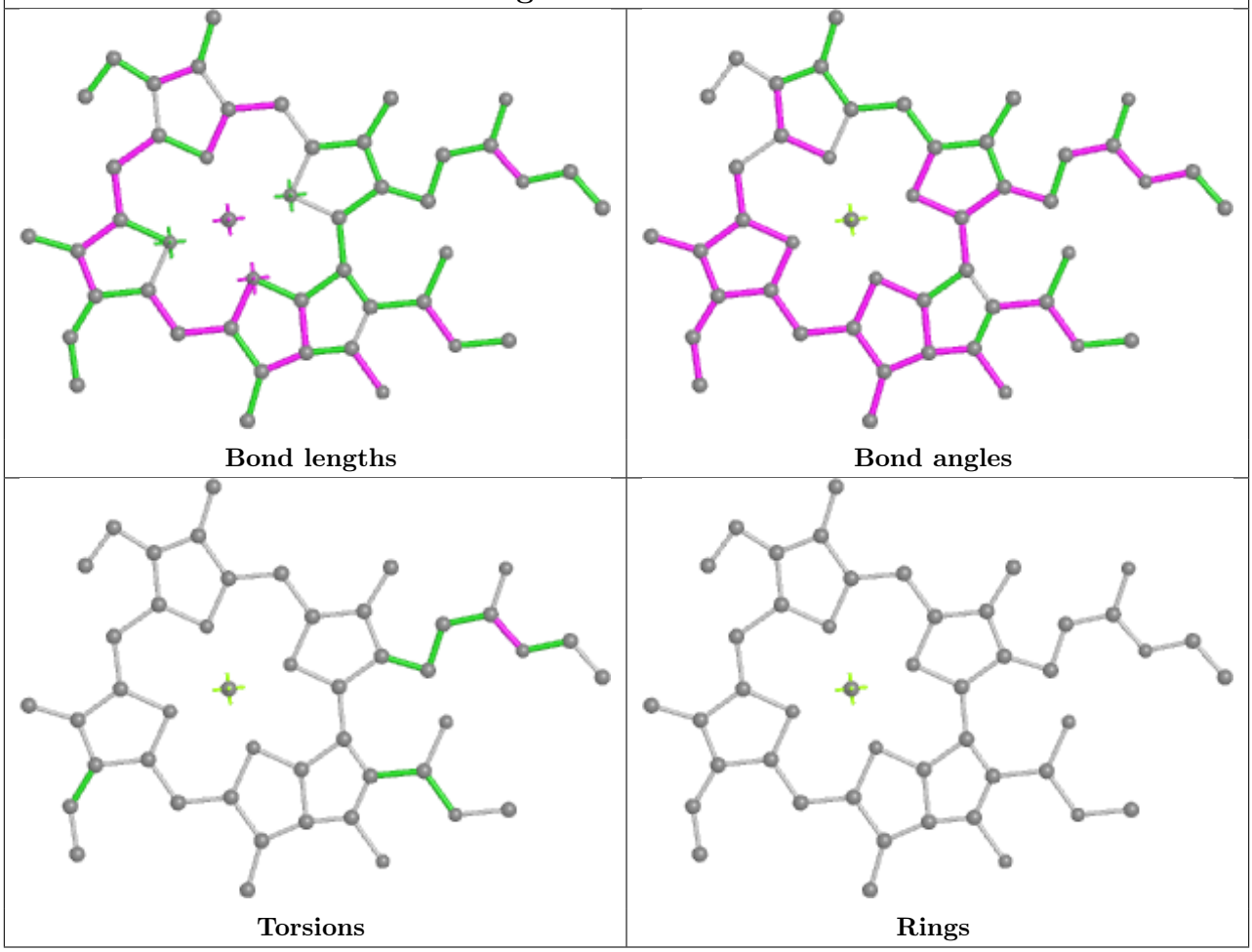


Rings

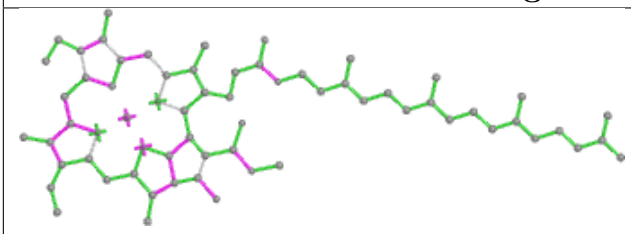
Ligand DD6 12 510



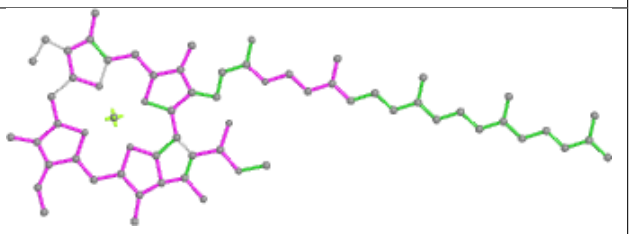
Ligand CLA 7 714



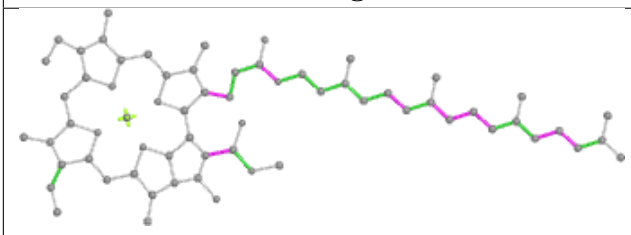
Ligand CLA A 804



Bond lengths



Bond angles



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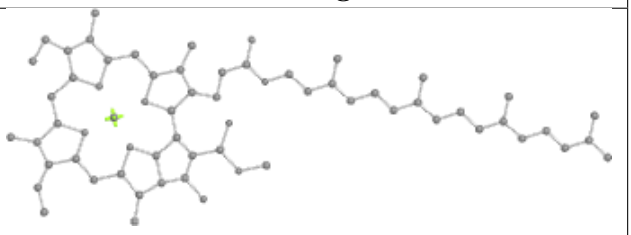
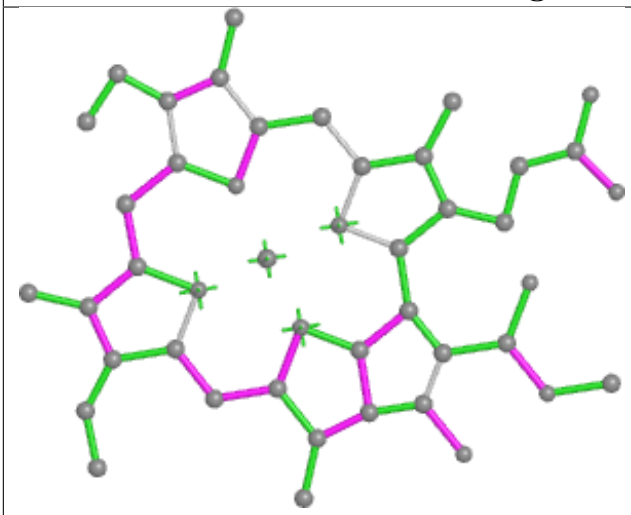


Rings

Ligand CLA 2 511



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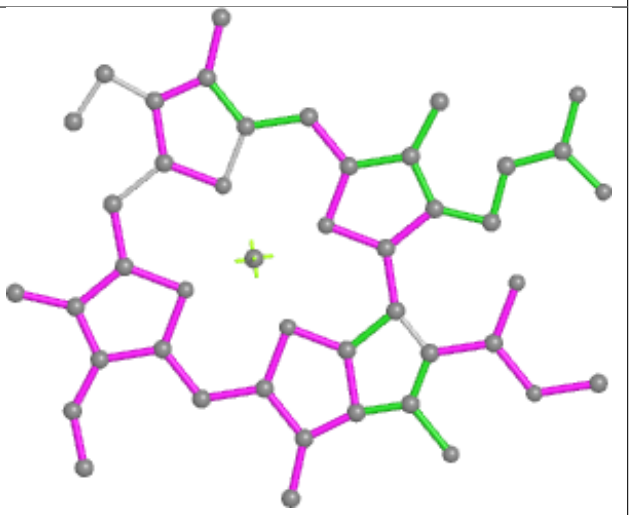
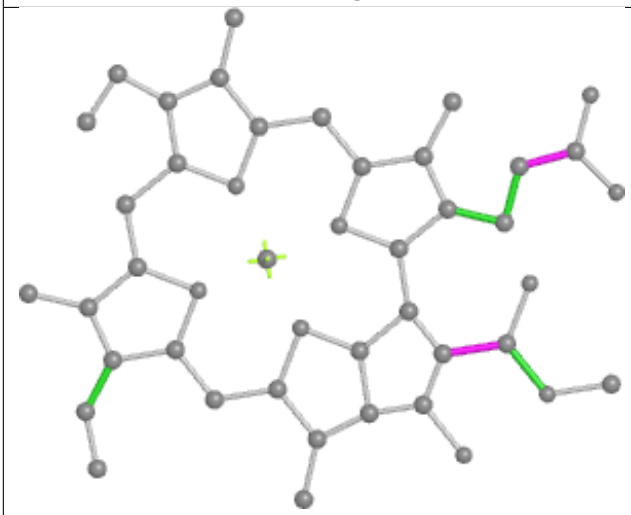


Bond angles



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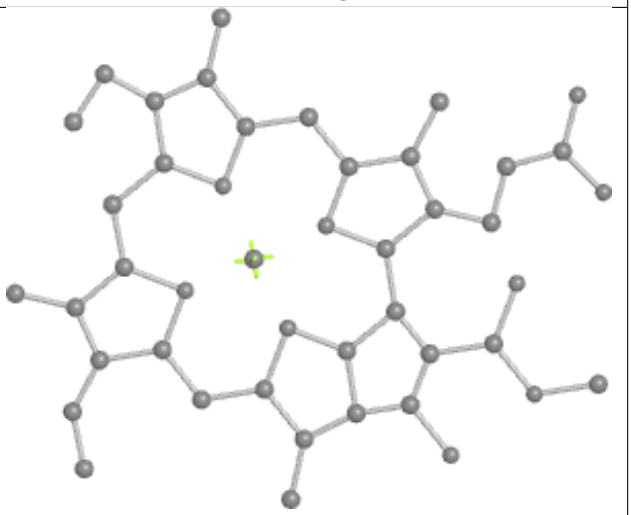
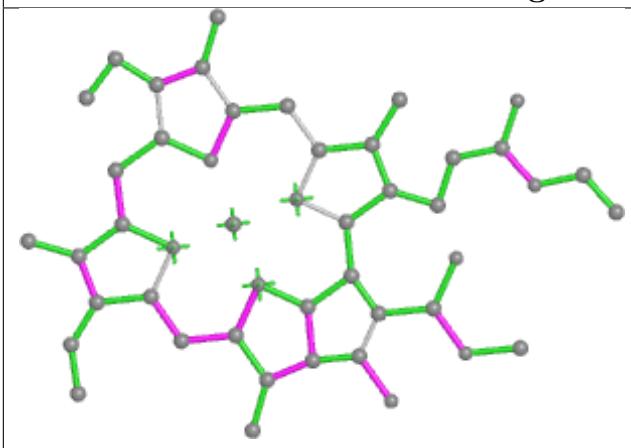
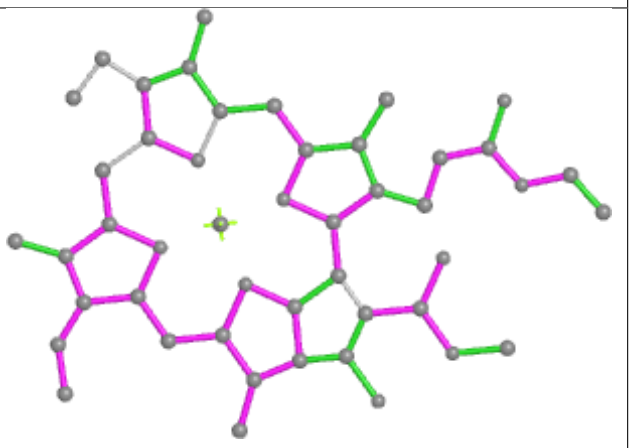


Rings

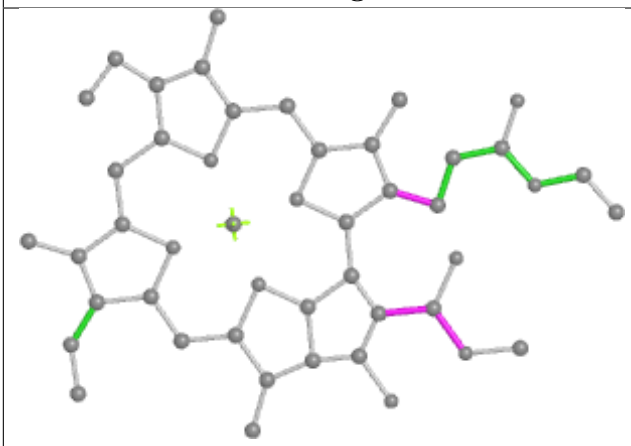
Ligand CLA 8 603



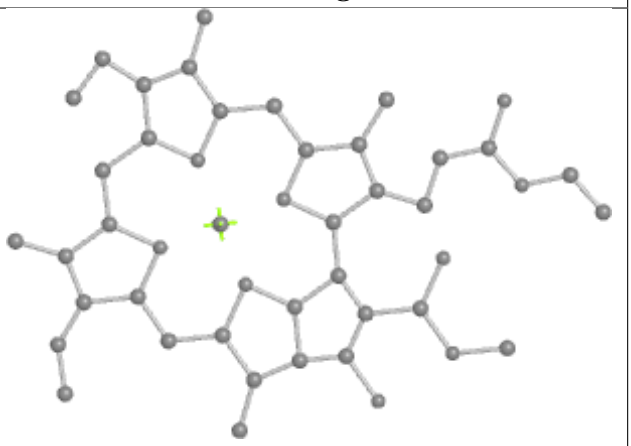
Bond lengths



Bond angles

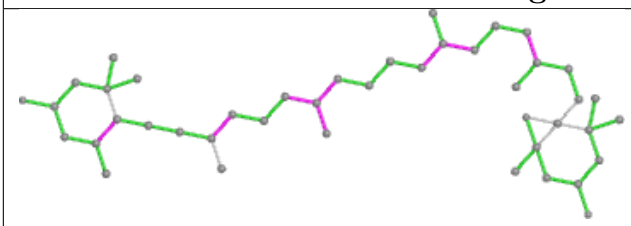


Torsions



Rings

Ligand DD6 7 716



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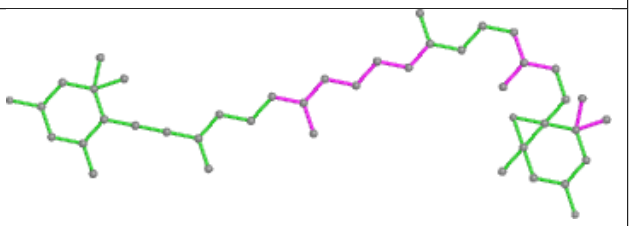

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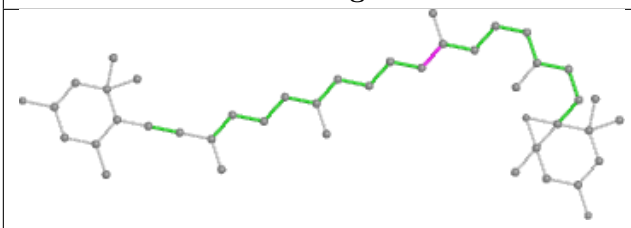

Torsions

Rings

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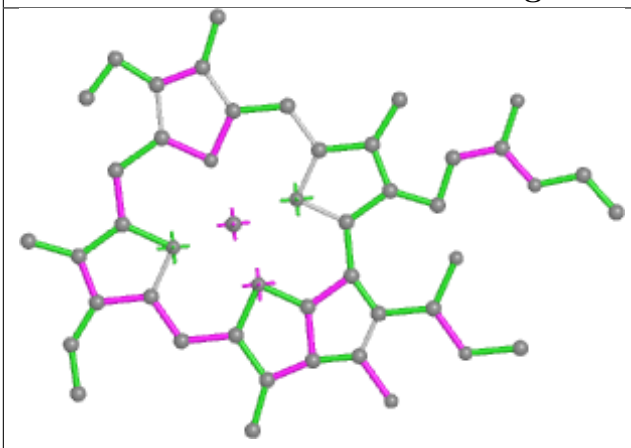
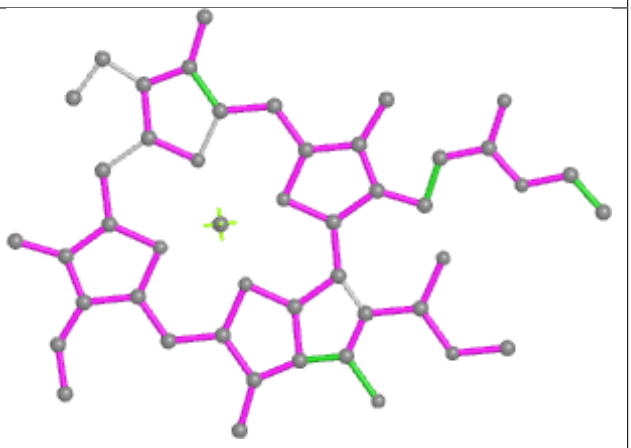
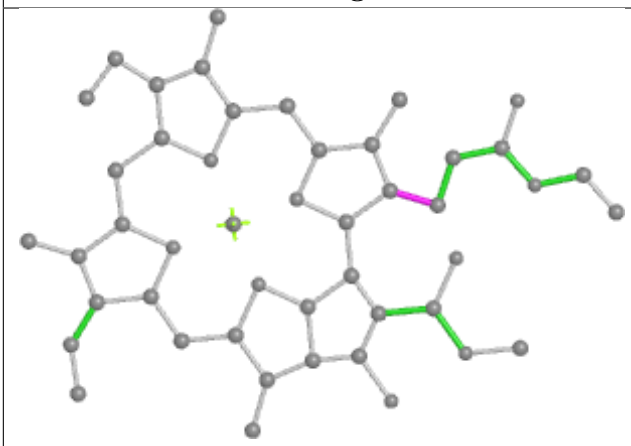
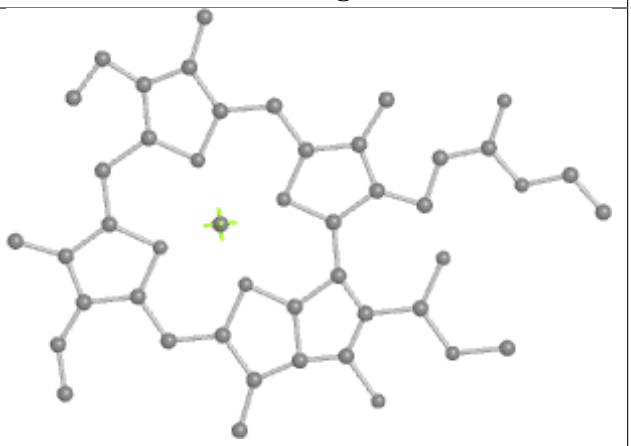
 Bond lengths	 Bond angles
 Torsions	 Rings

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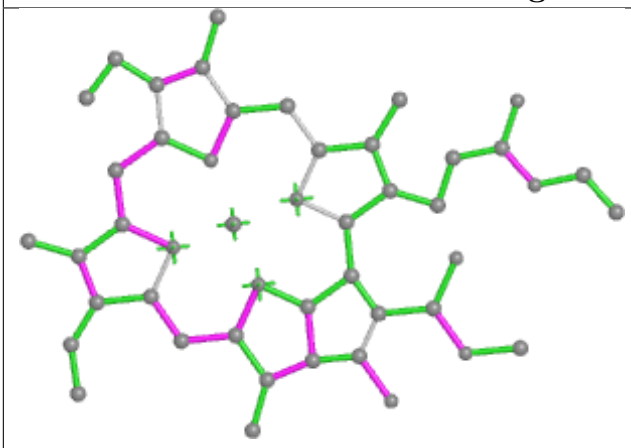
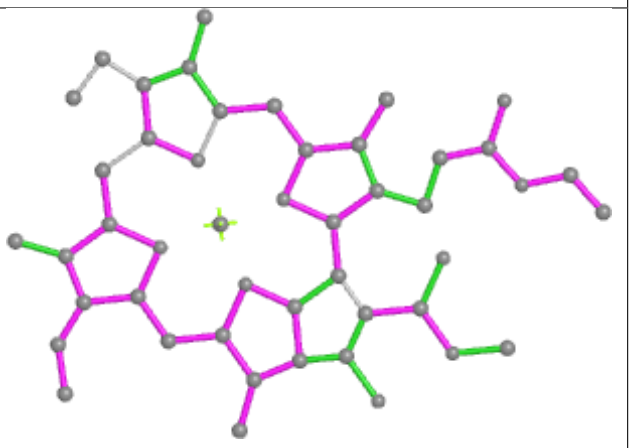
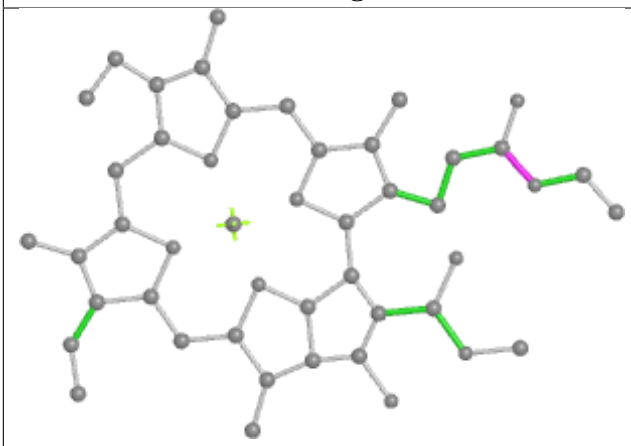
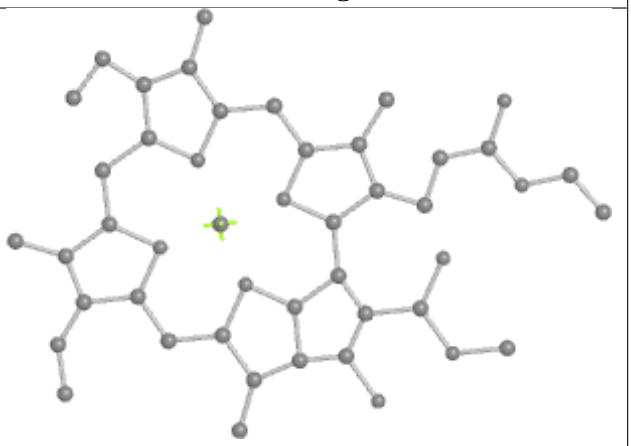
 Bond lengths	 Bond angles
 Torsions	 Rings

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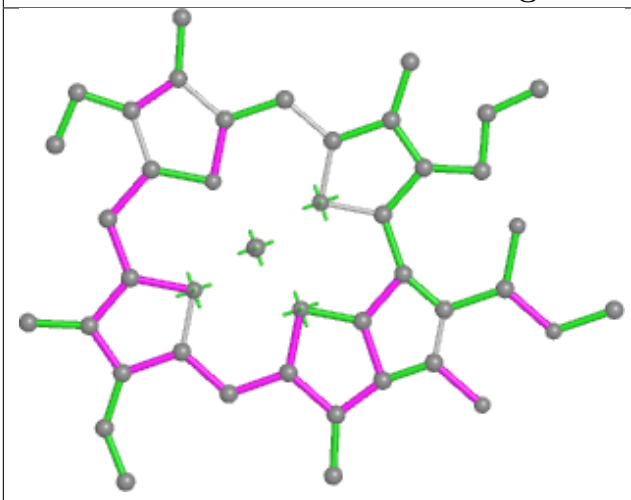
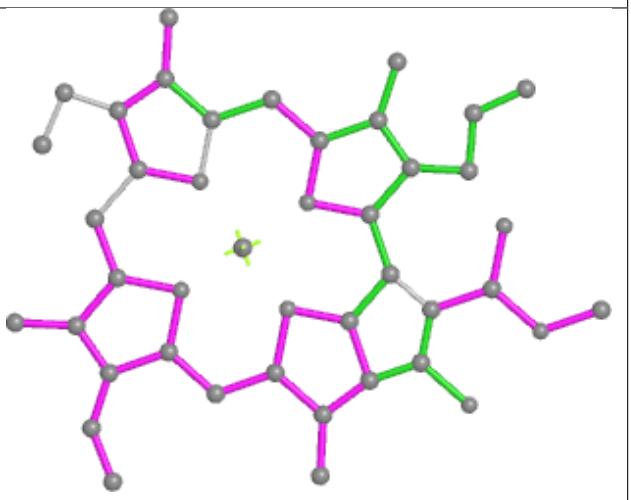
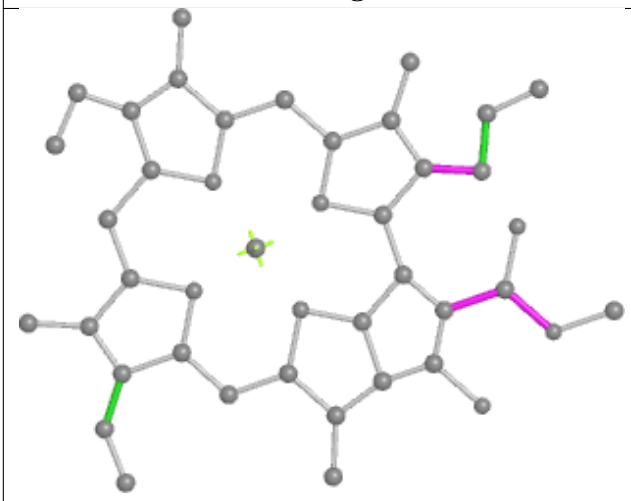


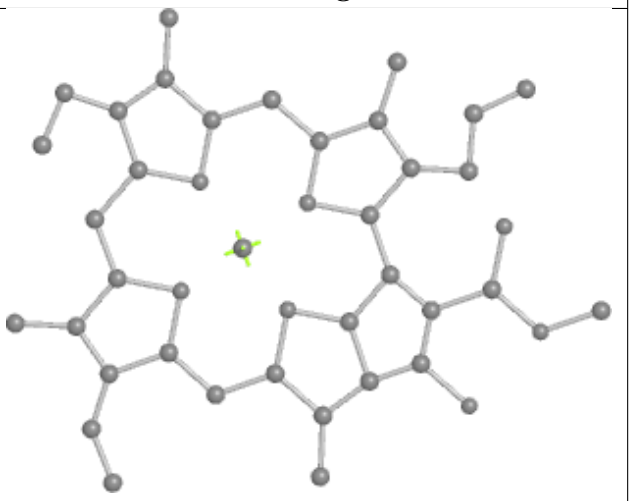
Bond lengths



Bond angles



Torsions



Rings

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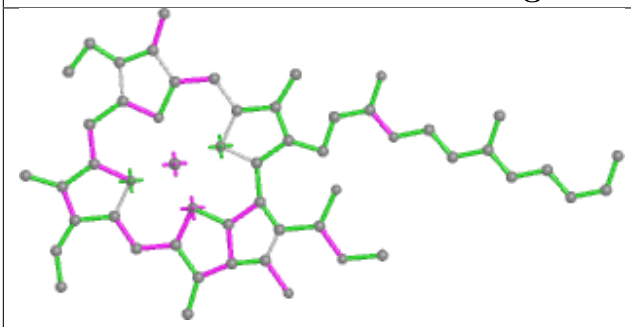
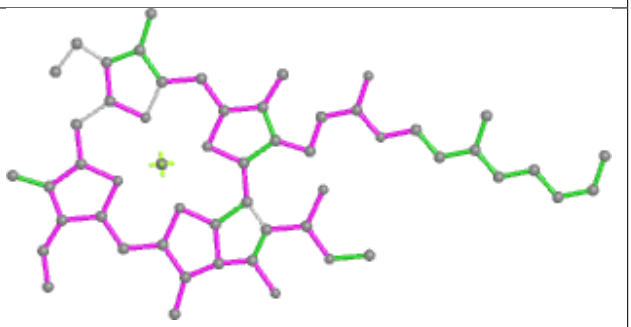
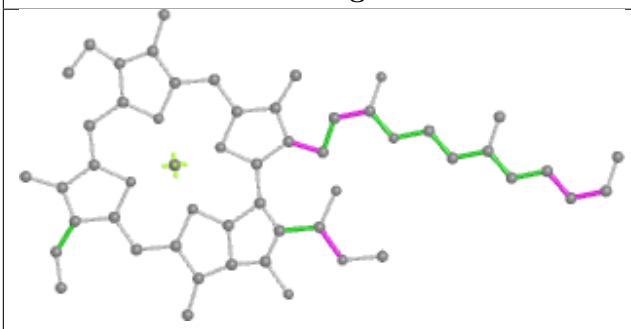
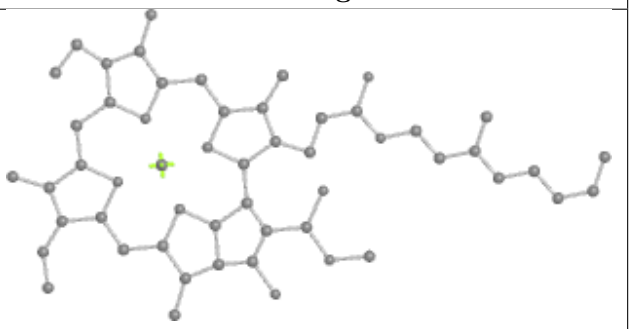
 Bond lengths	 Bond angles
 Torsions	 Rings

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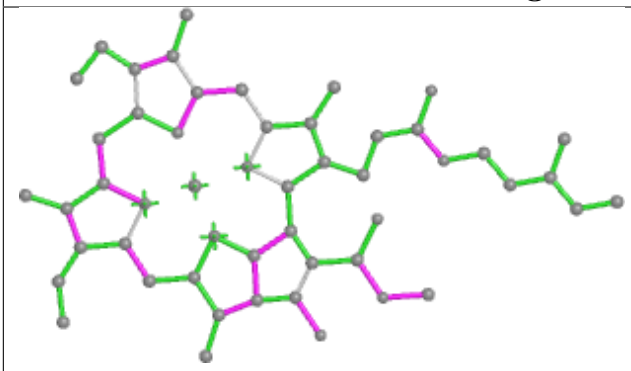
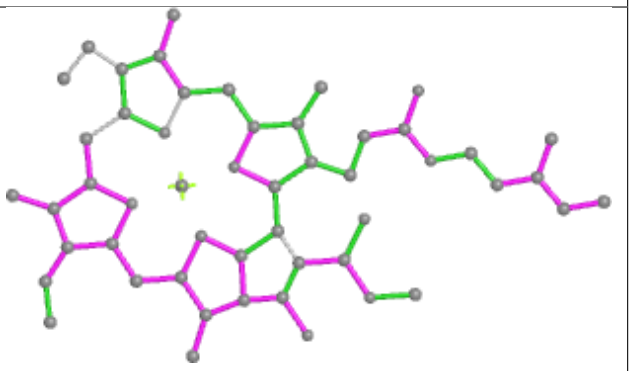
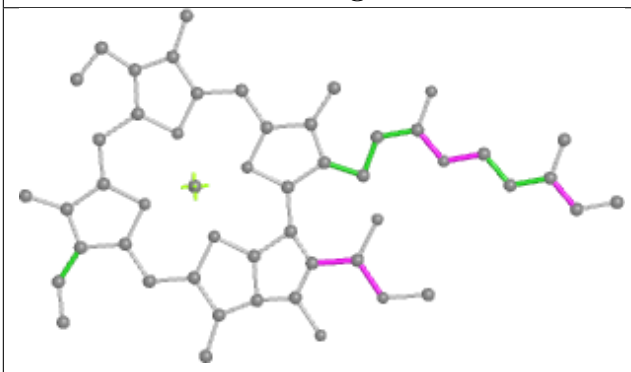
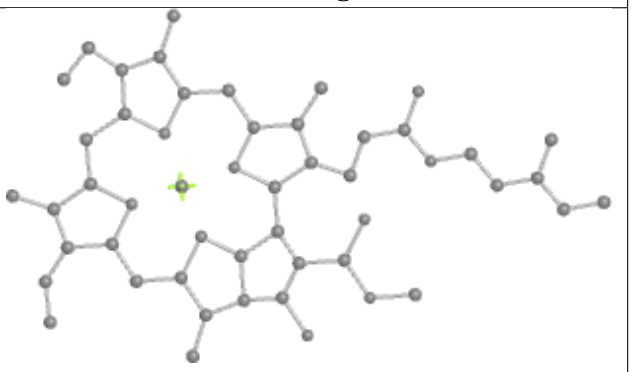
 Bond lengths	 Bond angles
 Torsions	 Rings

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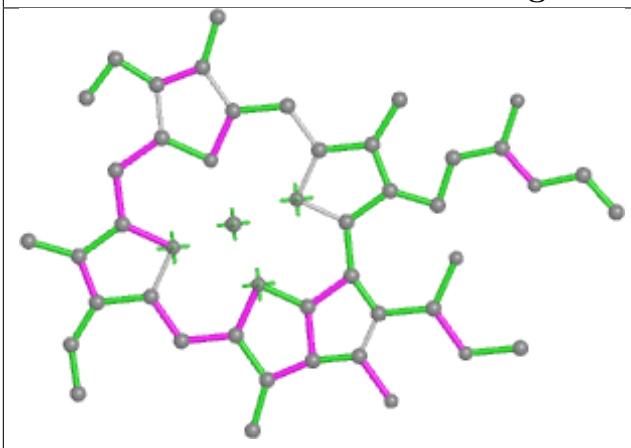
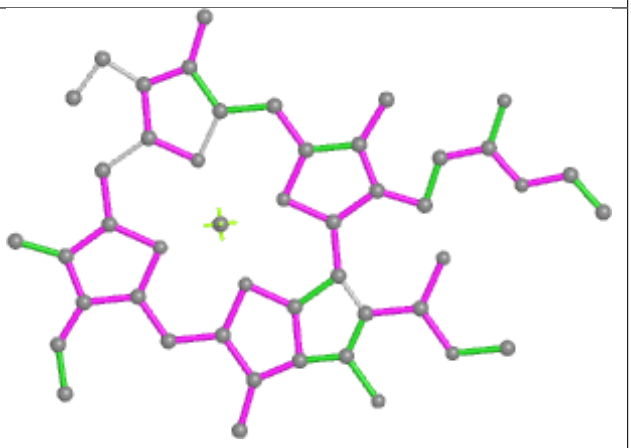
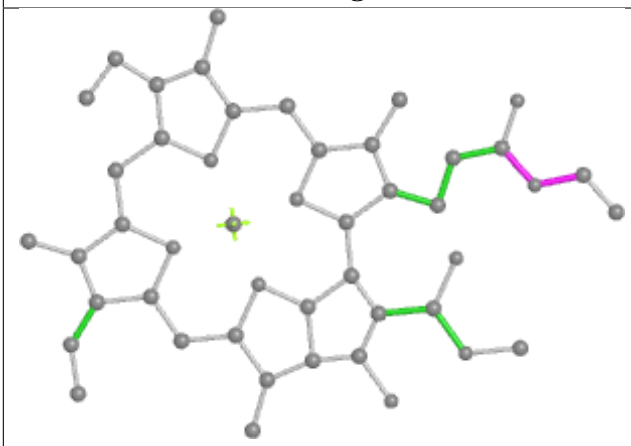
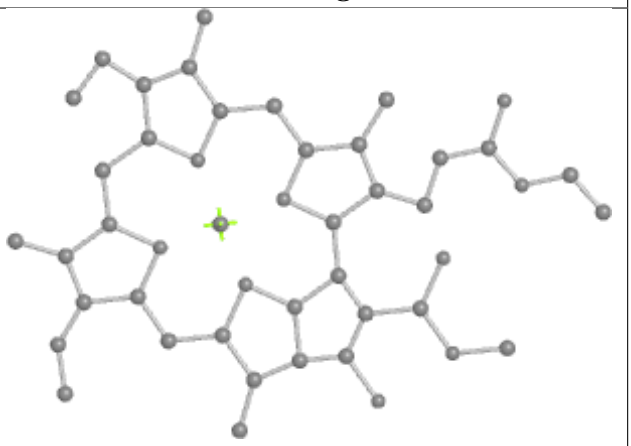
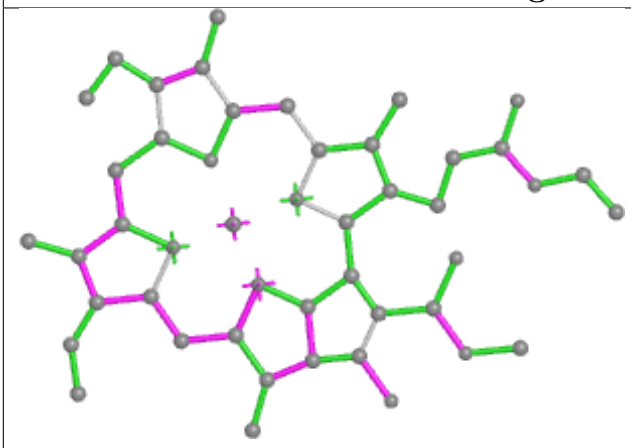
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 509



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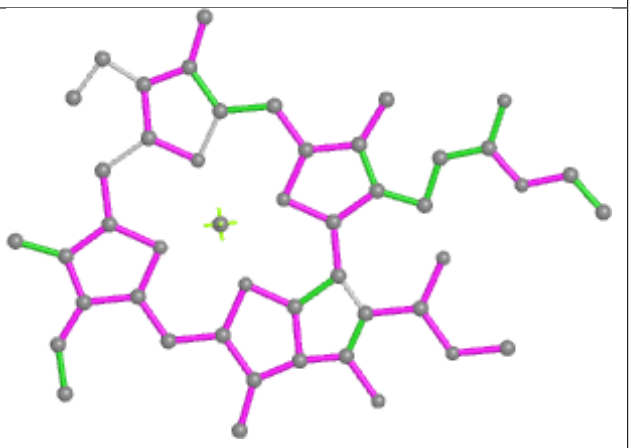
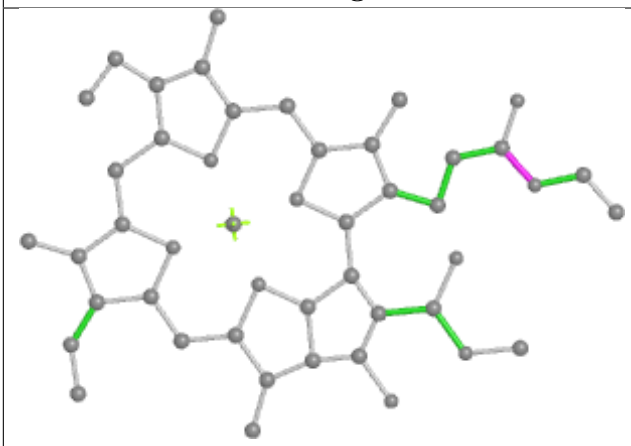


Bond angles



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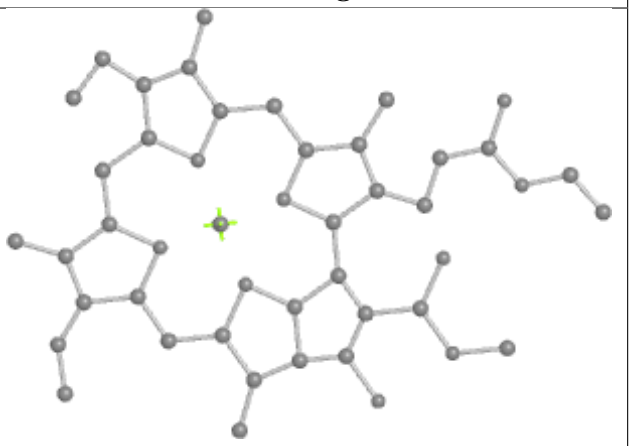
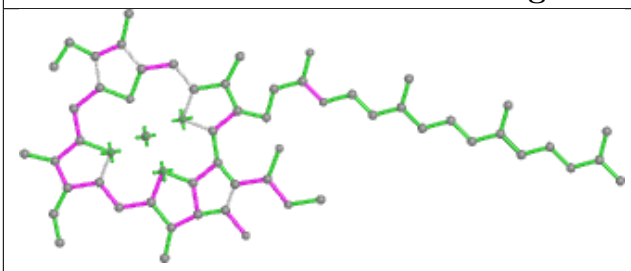


Rings

Ligand CLA 5 702



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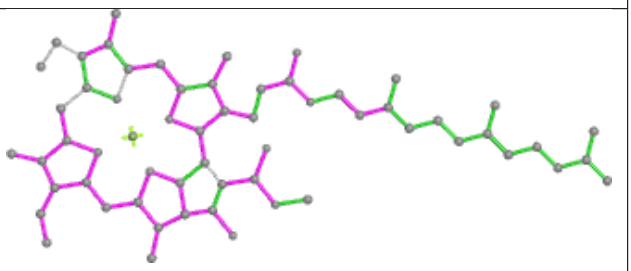

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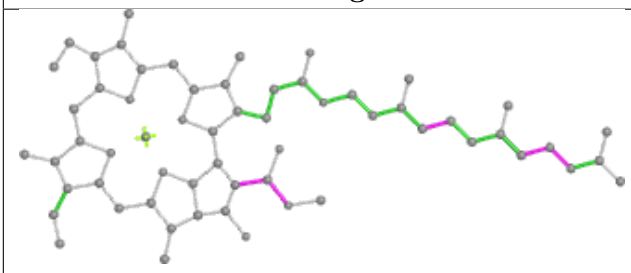

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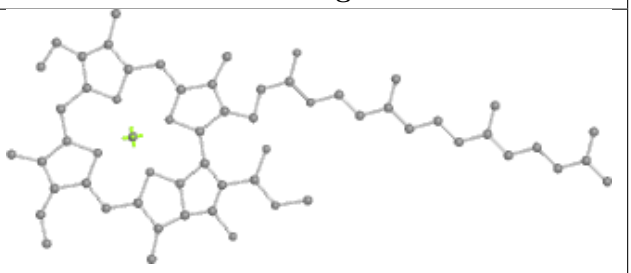

Rings

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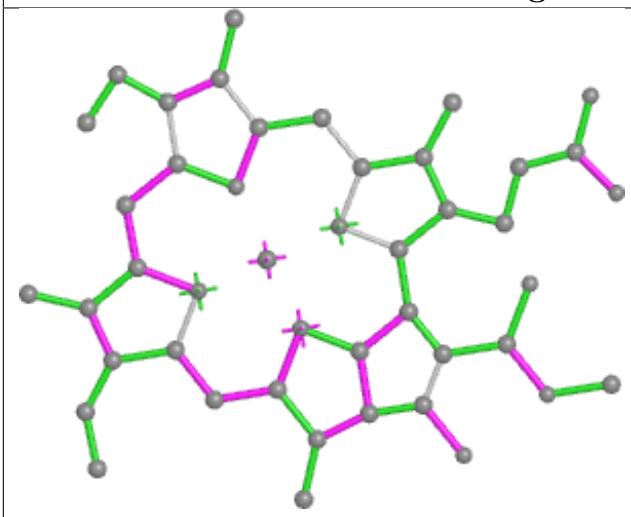

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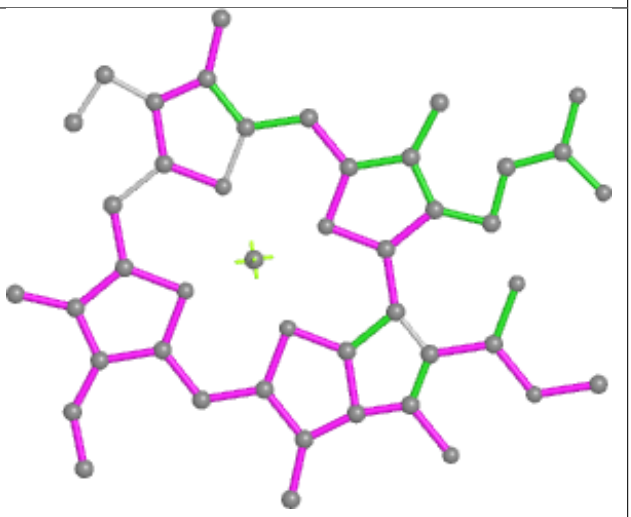

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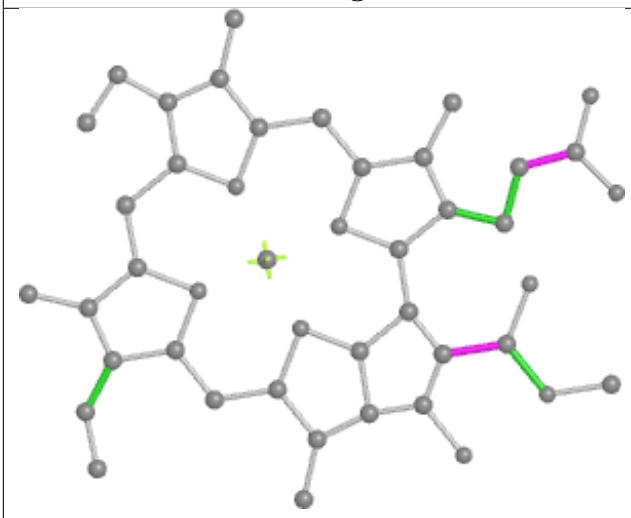

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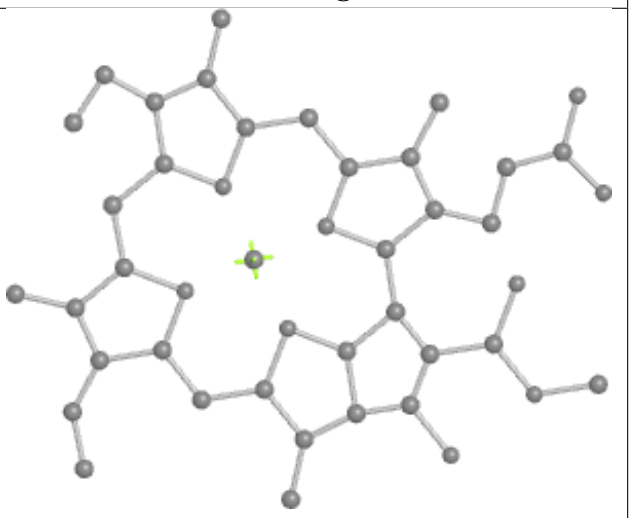
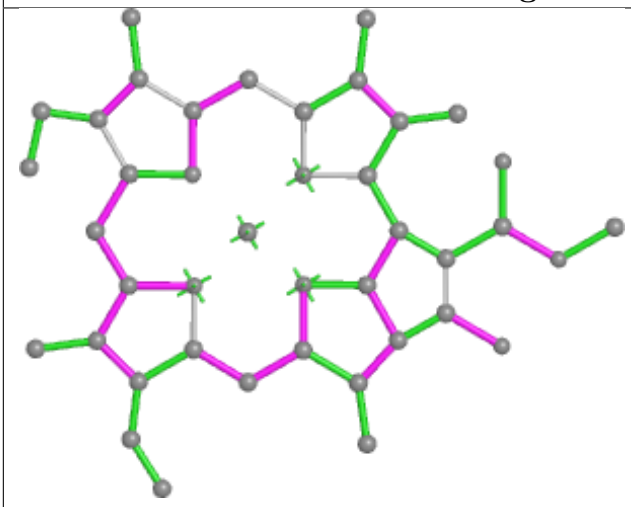
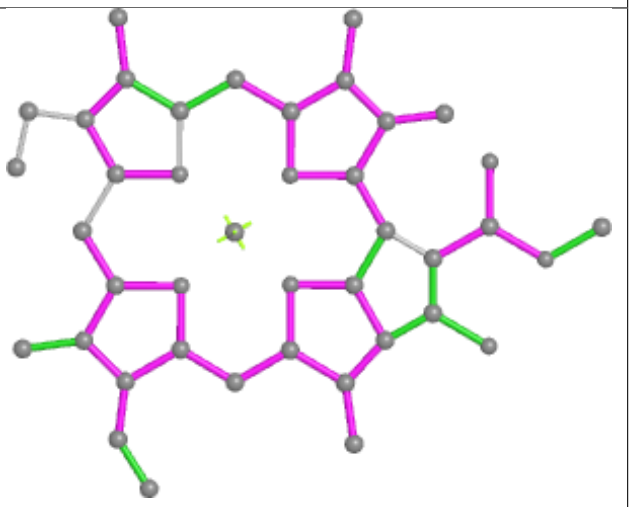
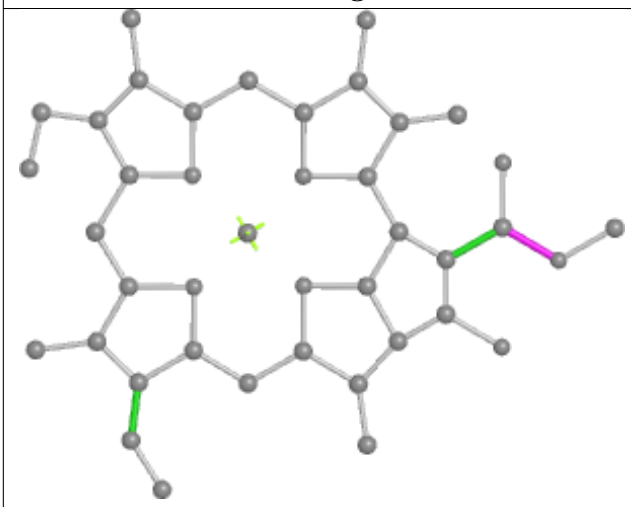
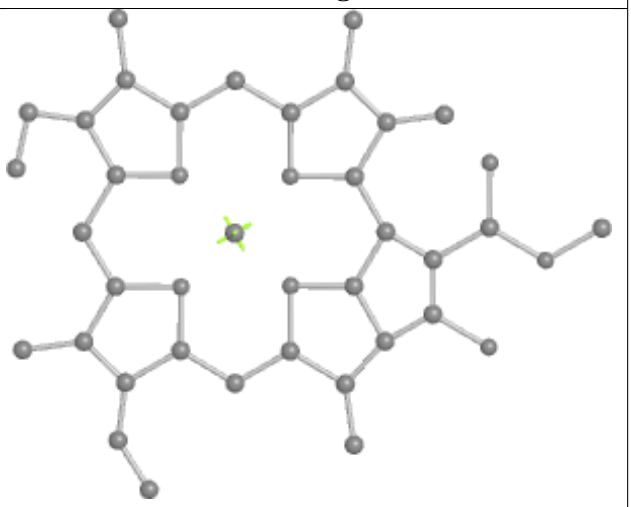


Rings

Ligand CLA 11 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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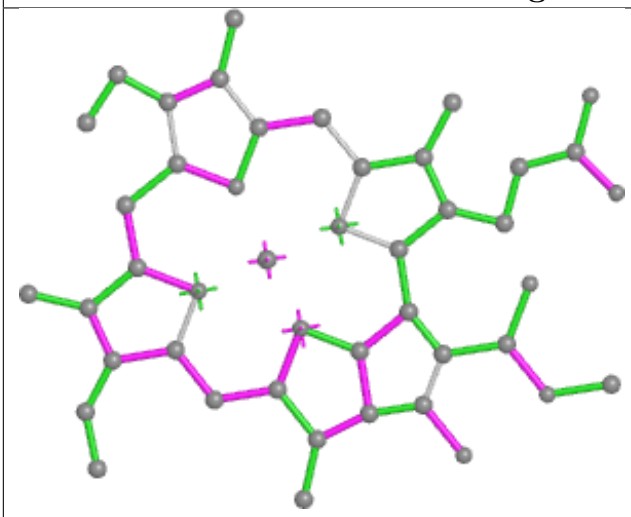

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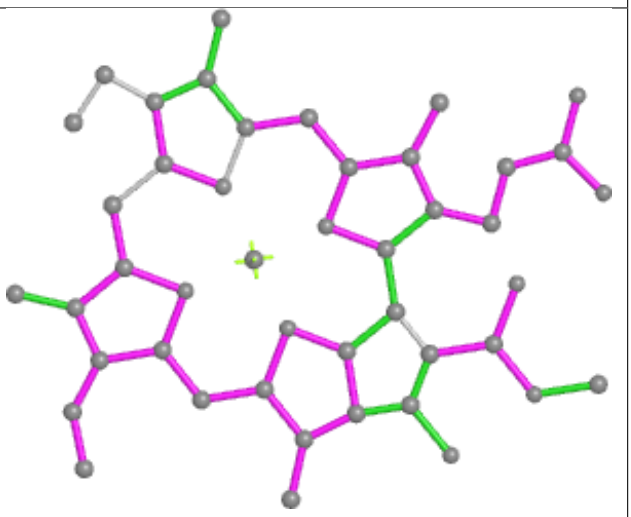
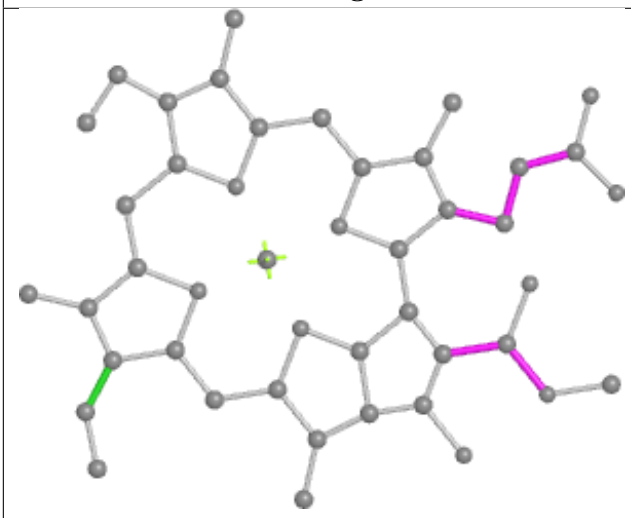


Bond angles



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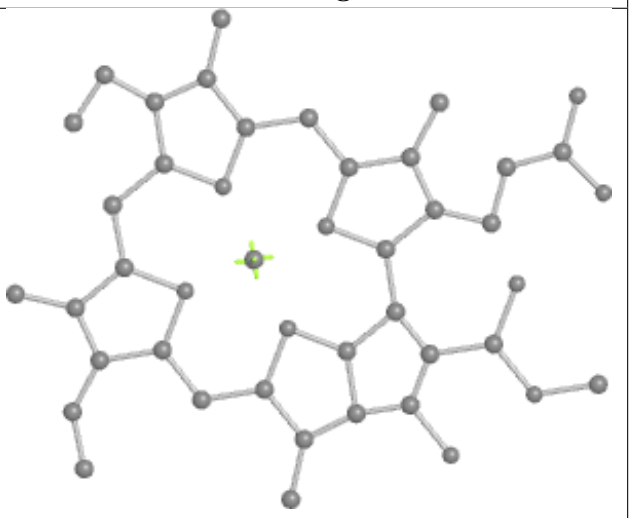
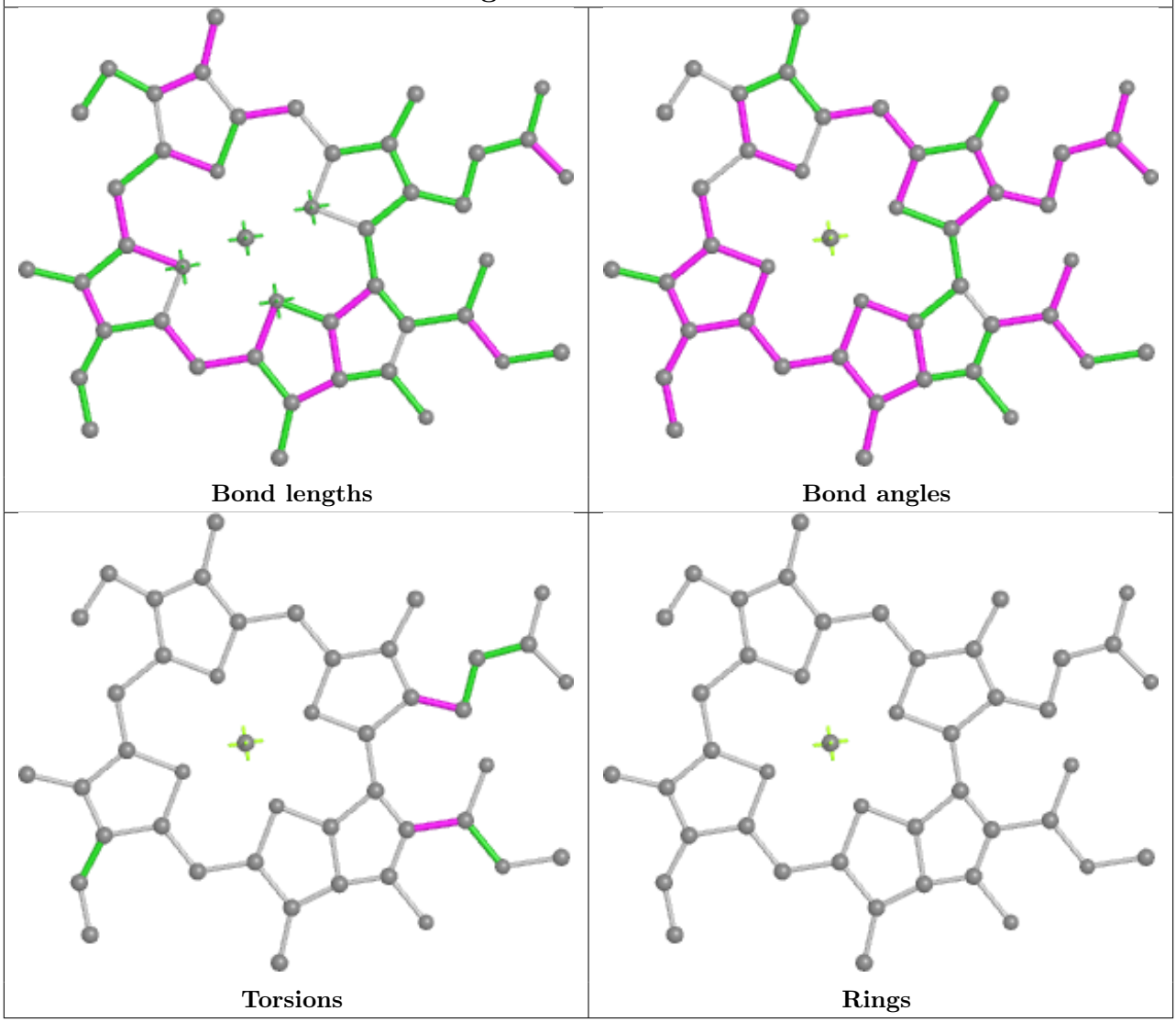
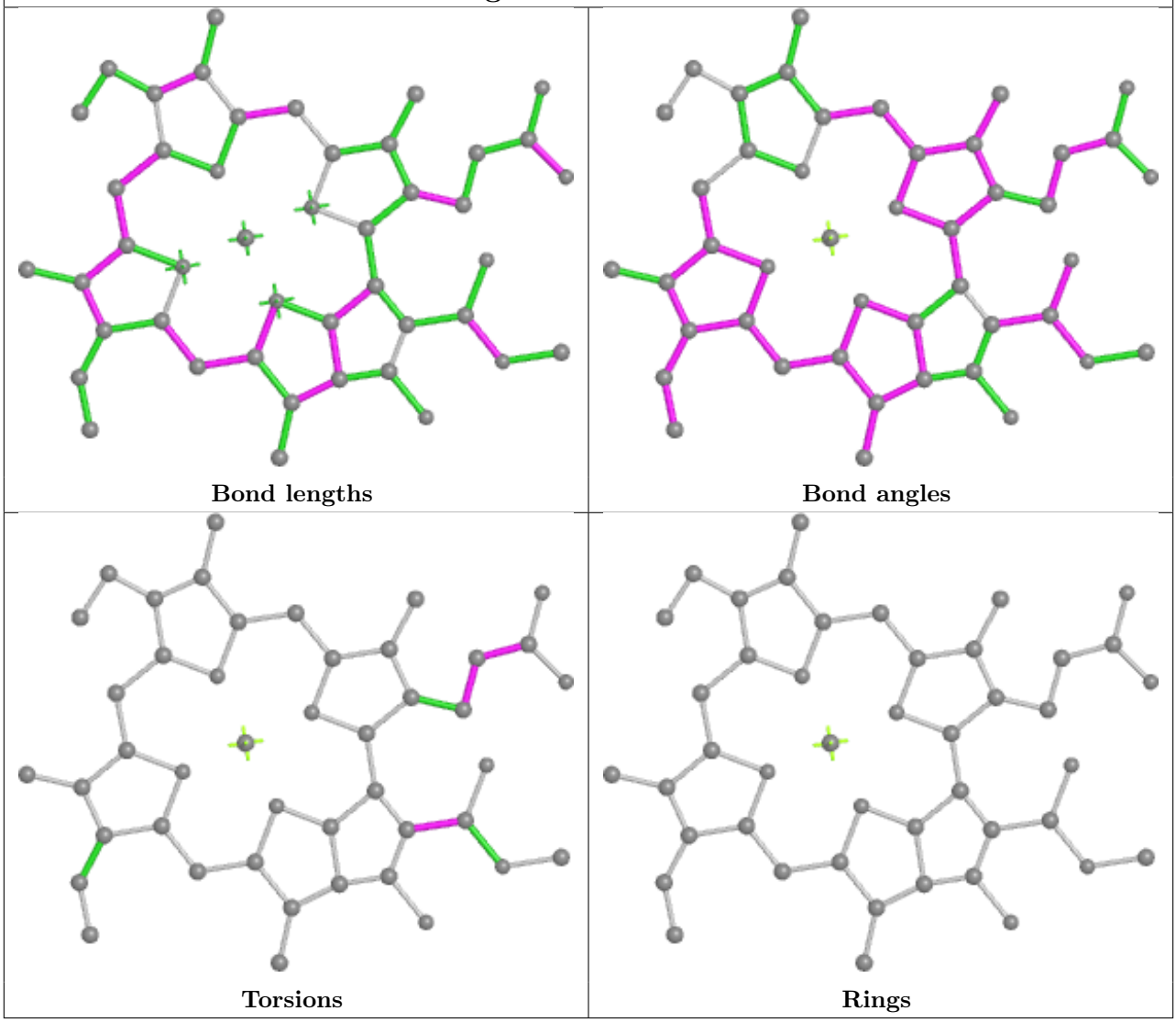


Rings

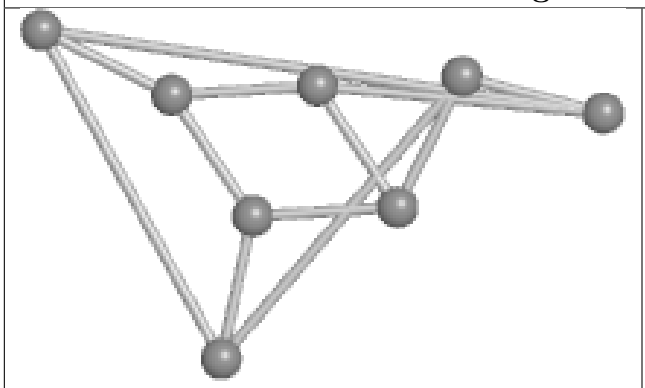
Ligand CLA A 816



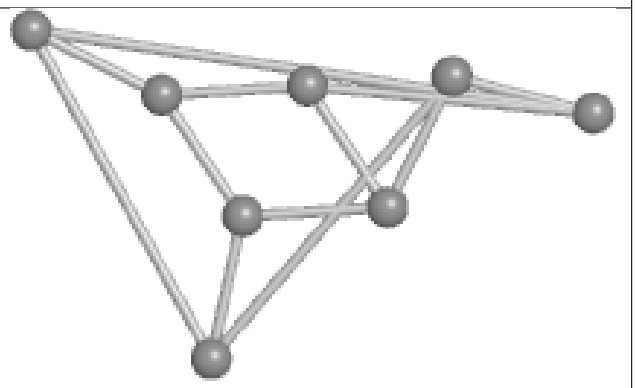
Ligand CLA 7 710



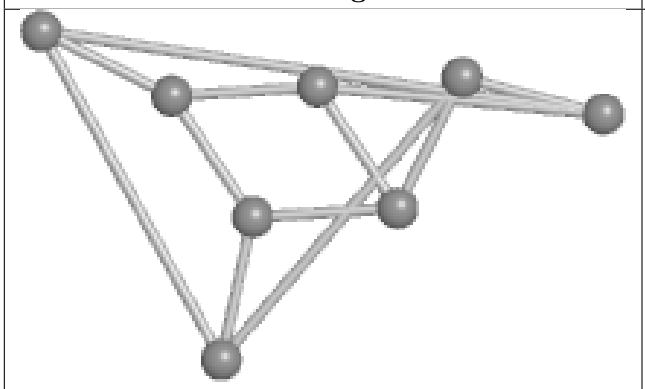
Ligand SF4 C 101



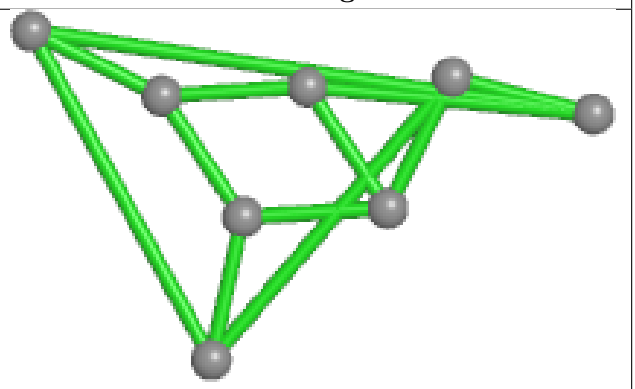
Bond lengths



Bond angles

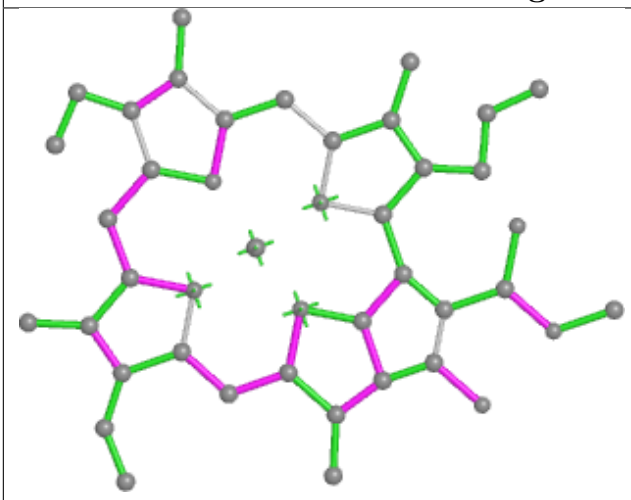


Torsions

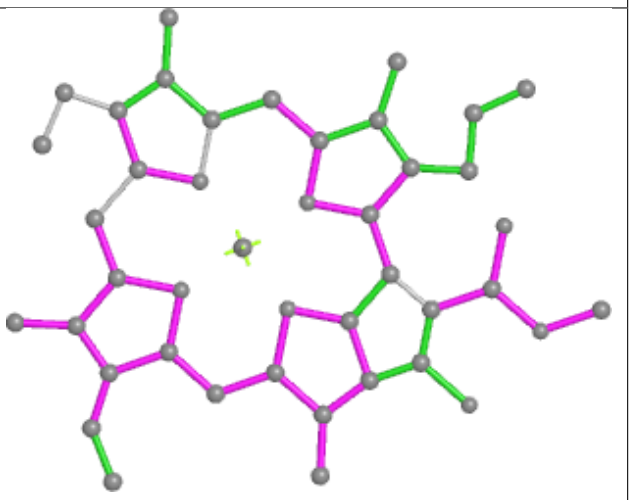


Rings

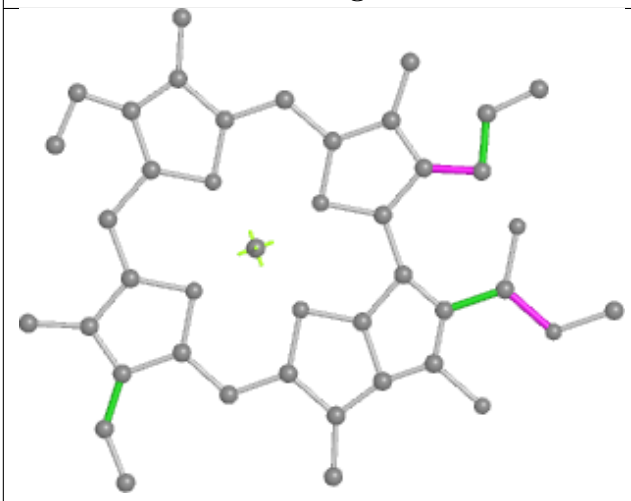
Ligand CLA 2 510



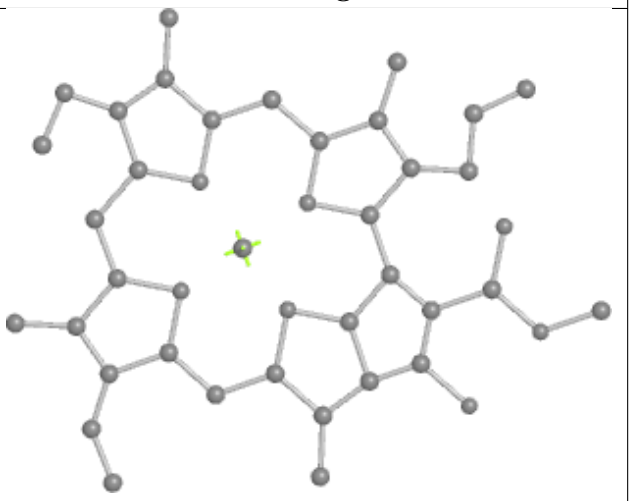
Bond lengths



Bond angles

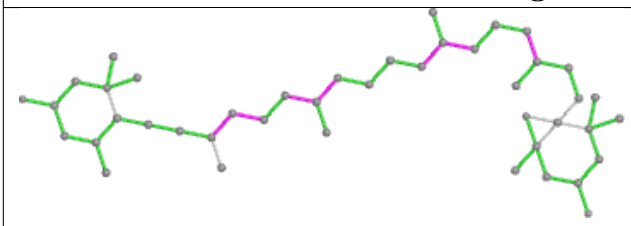


Torsions



Rings

Ligand DD6 1 519



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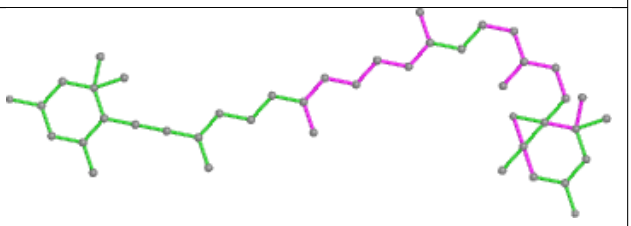
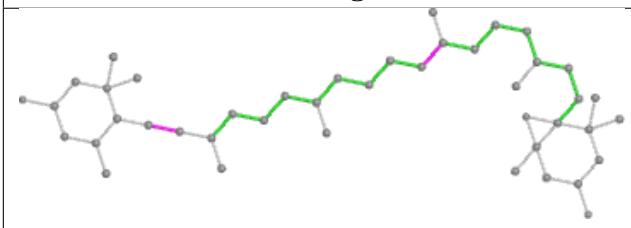


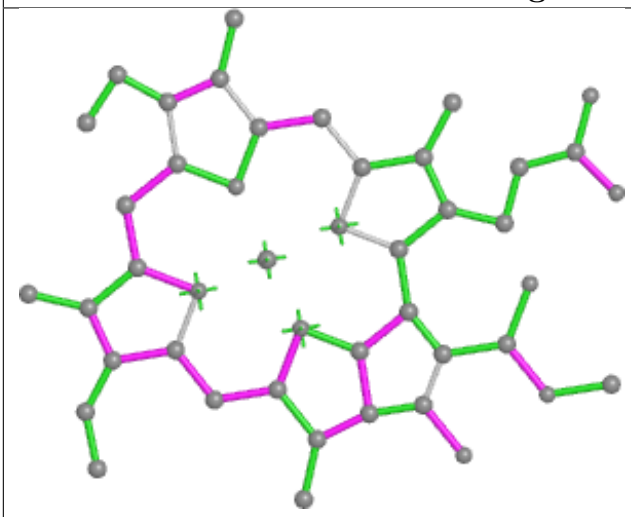
Bond angles



Torsions

Rings

Ligand CLA 4 710



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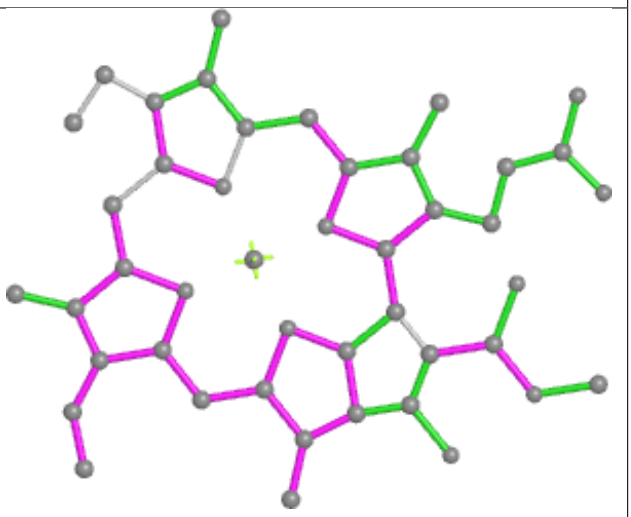
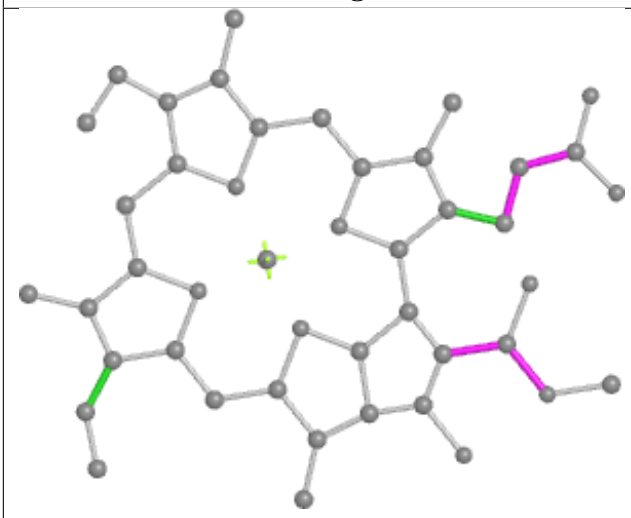
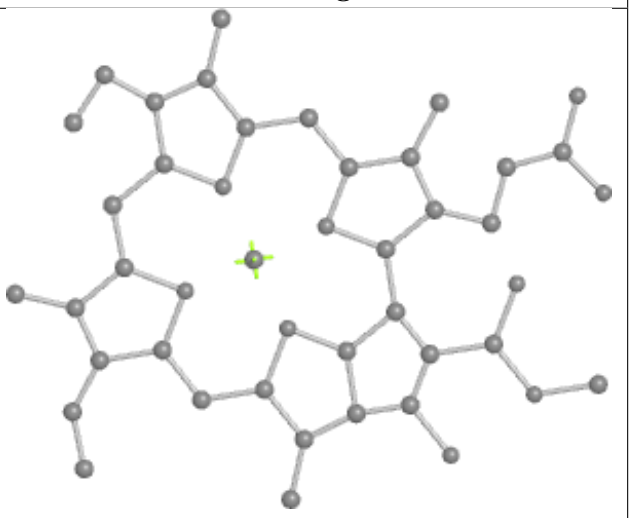


Bond angles

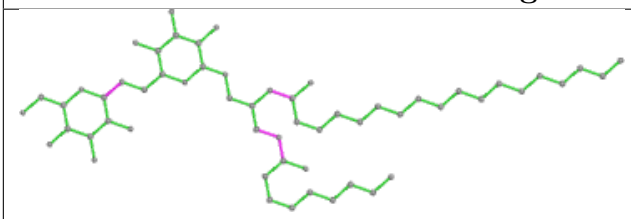


Torsions

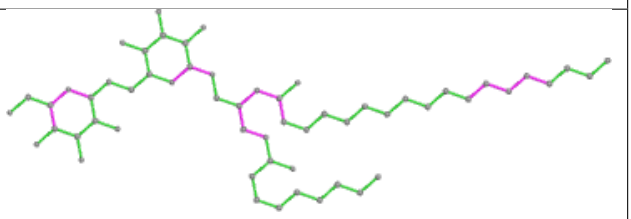


Rings

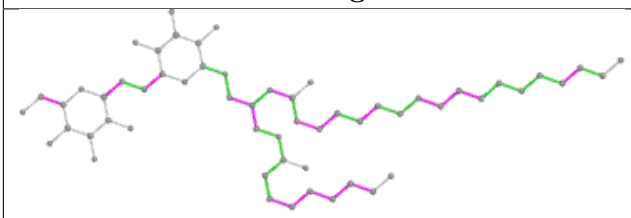
Ligand DGD B 847



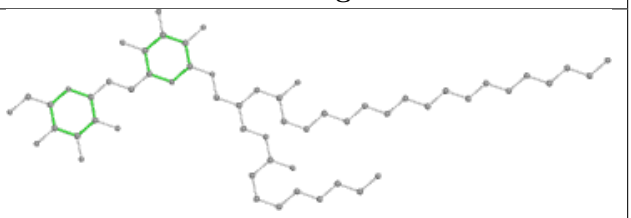
Bond lengths



Bond angles

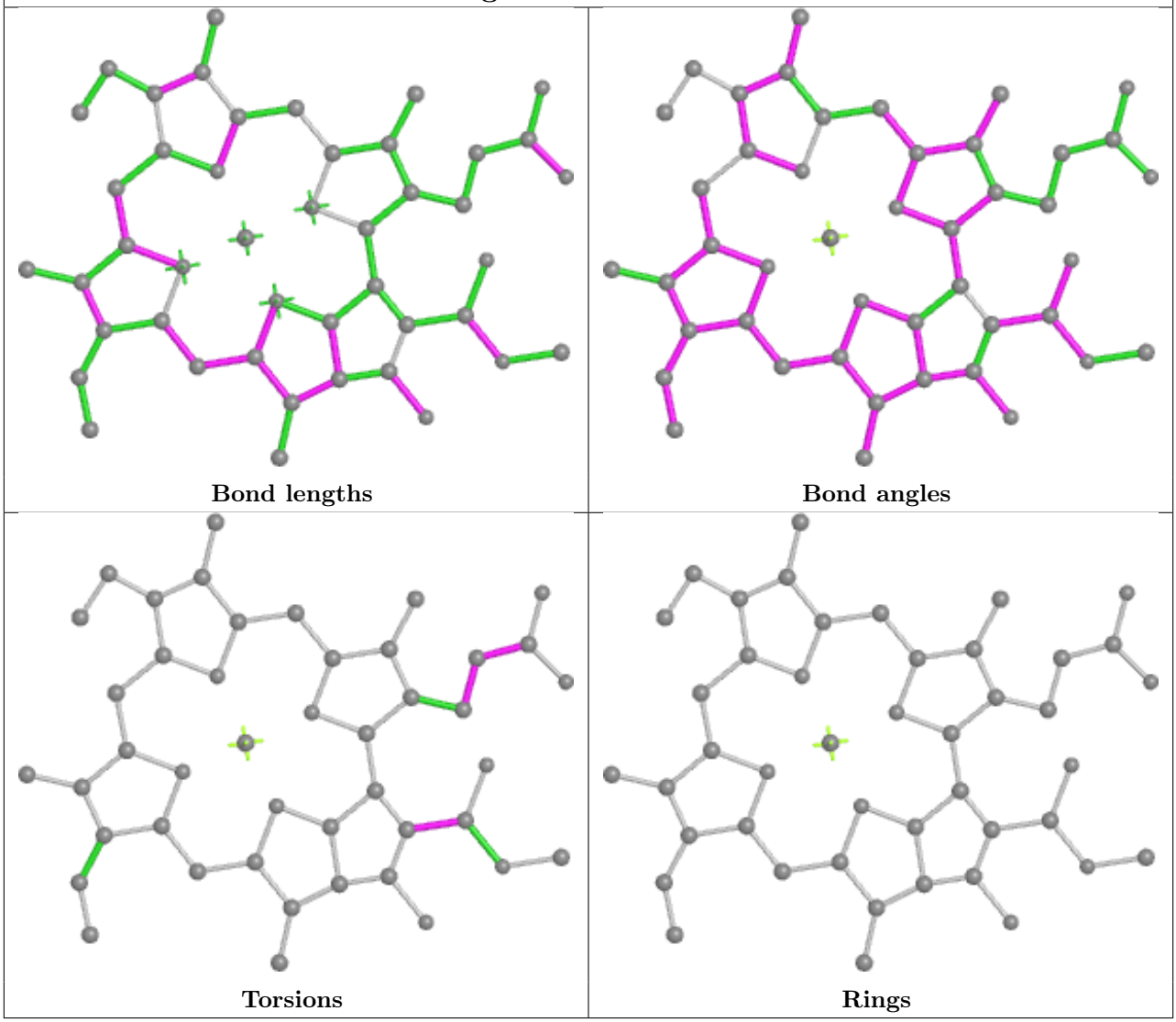


Torsions

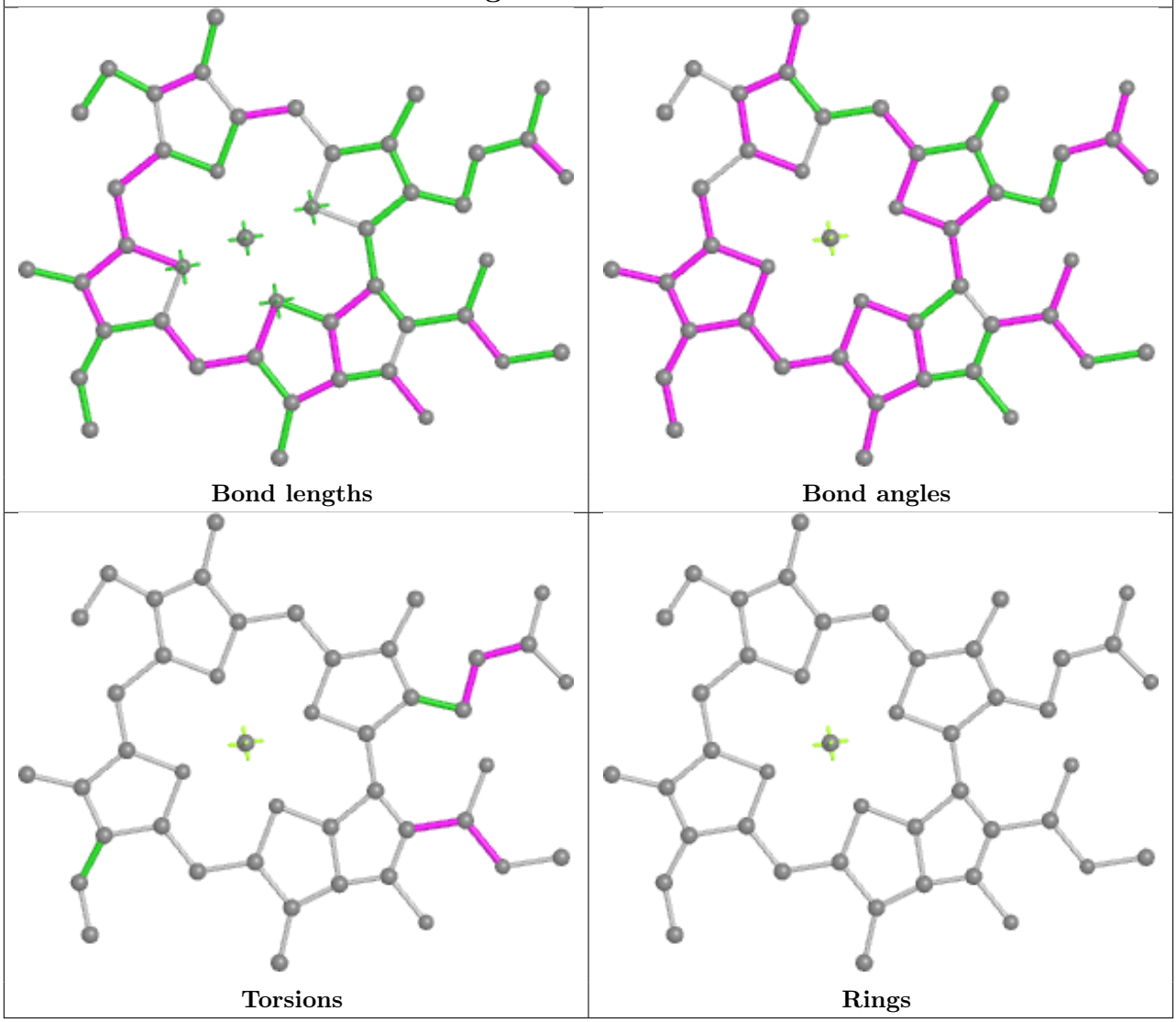


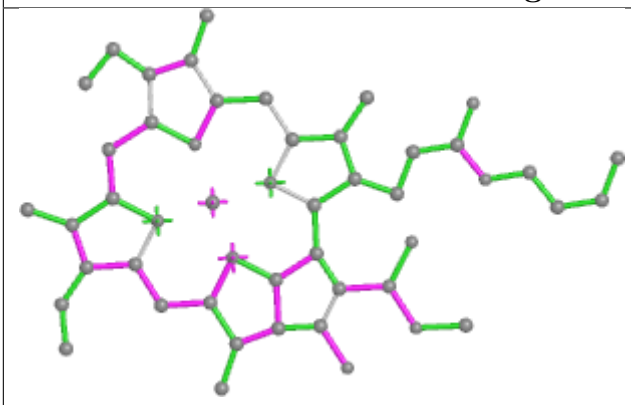
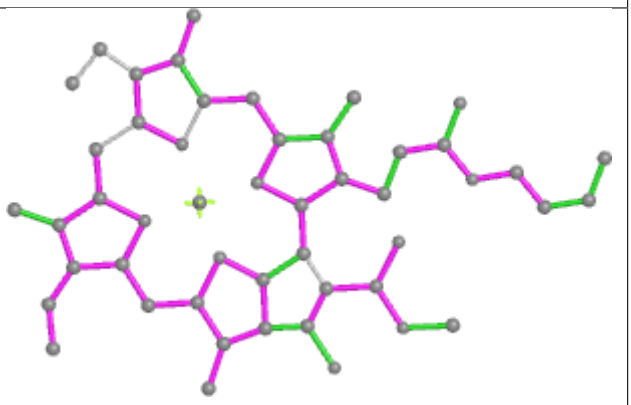
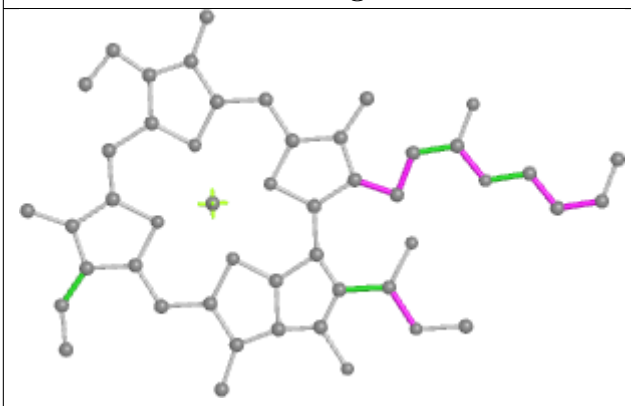
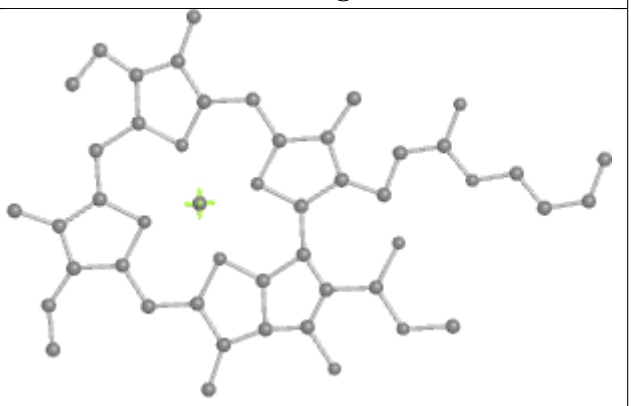
Rings

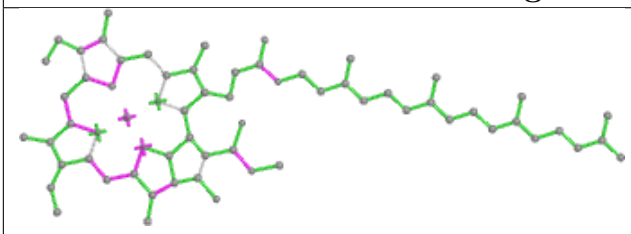
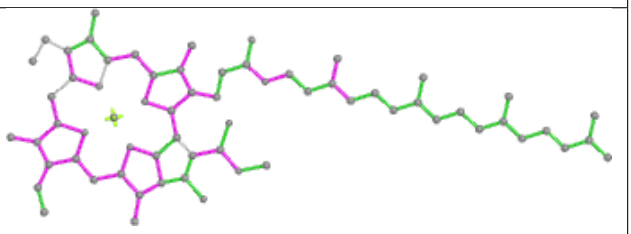
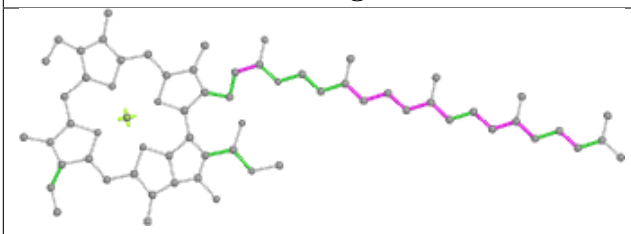
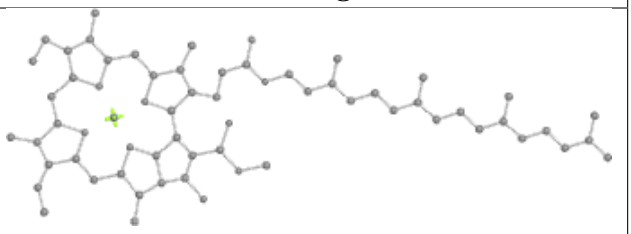
Ligand CLA B 811



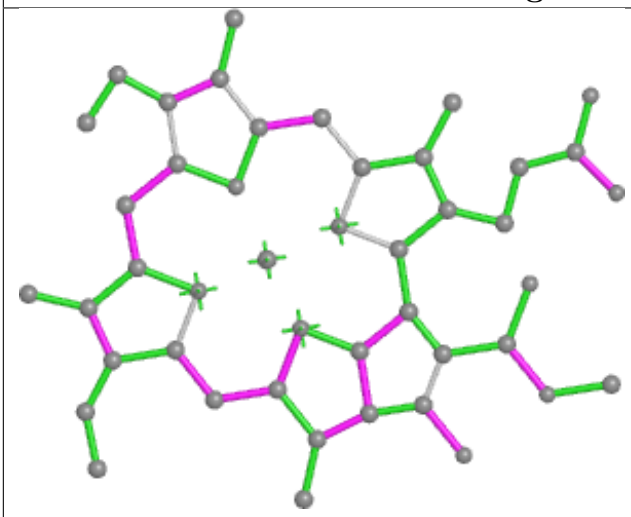
Ligand CLA 4 703



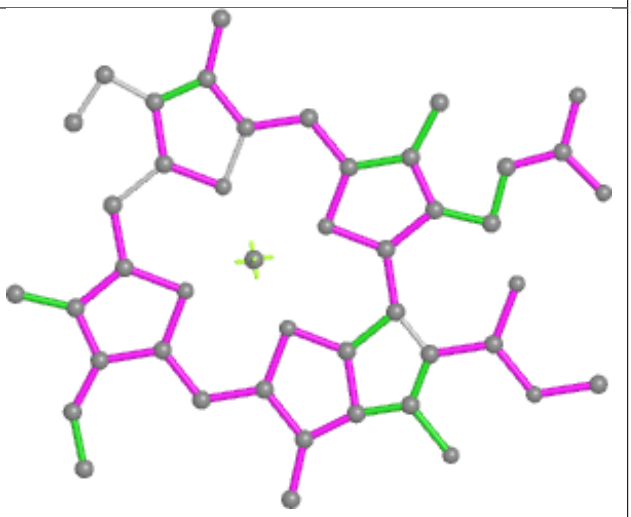
Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

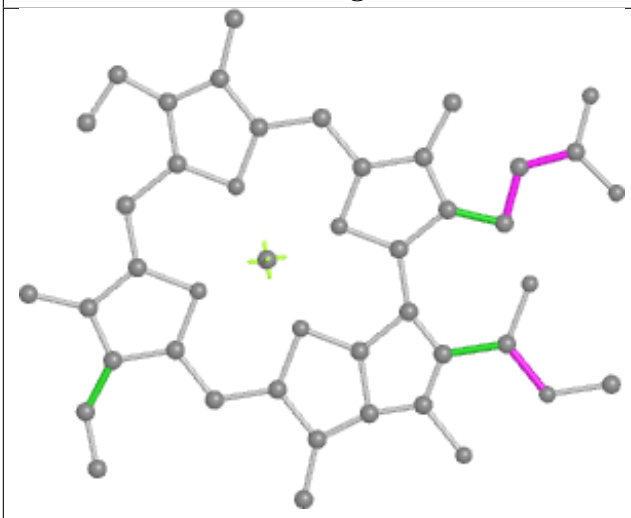
Ligand CLA F 403



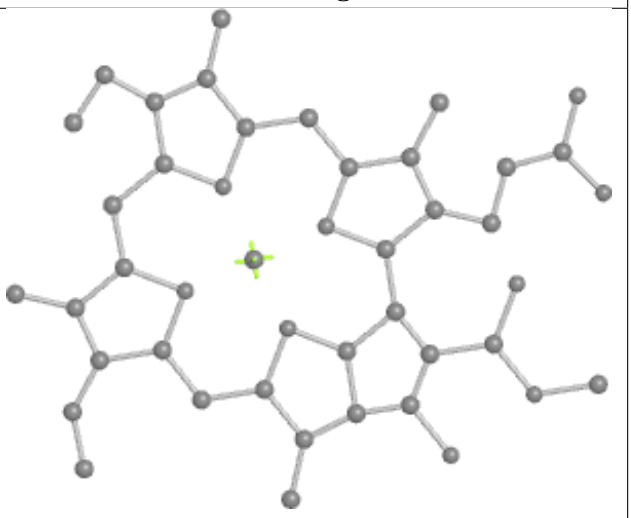
Bond lengths



Bond angles

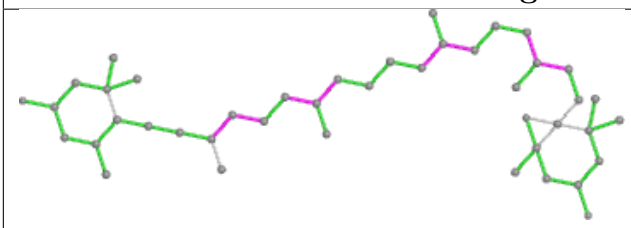


Torsions



Rings

Ligand DD6 12 509



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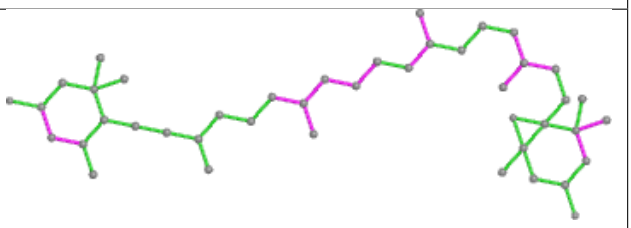
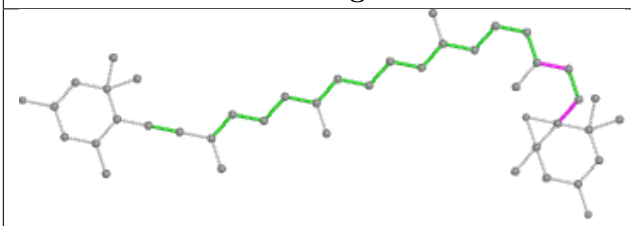


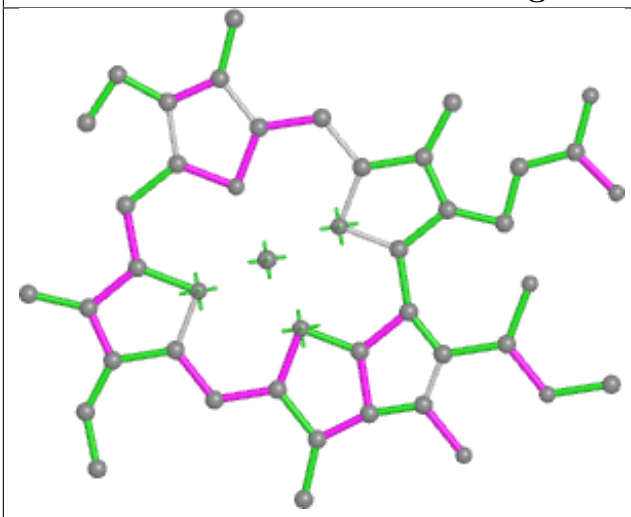
Bond angles



Torsions

Rings

Ligand CLA 3 703



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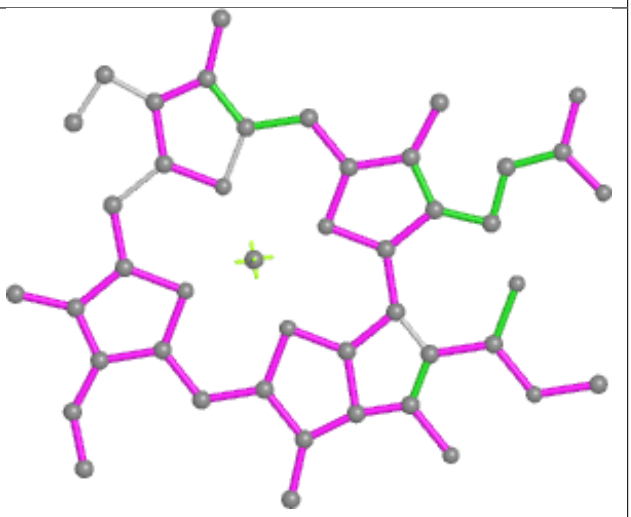
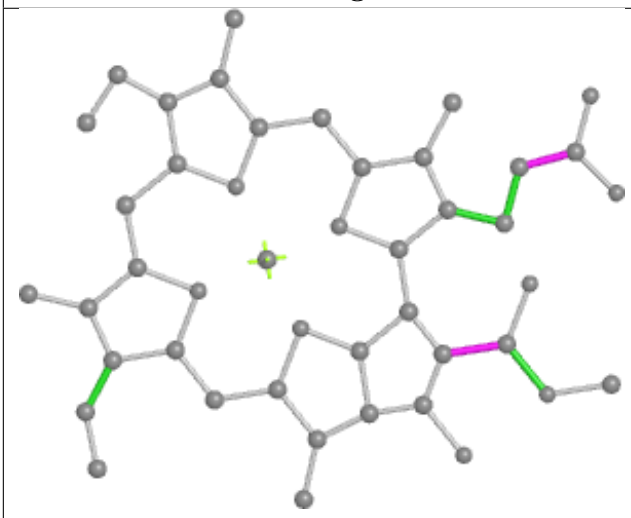
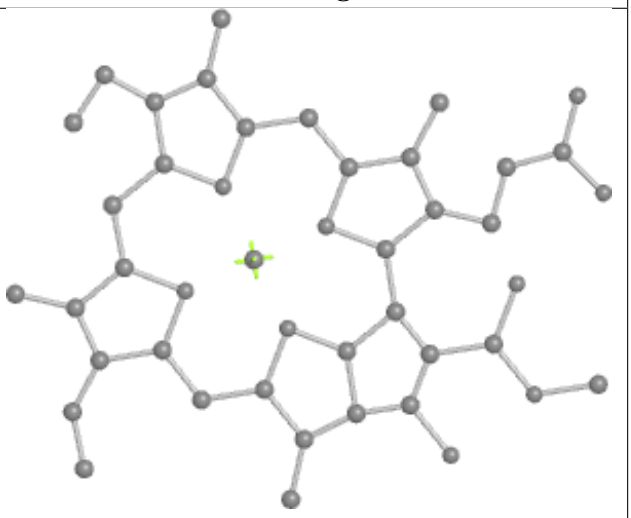


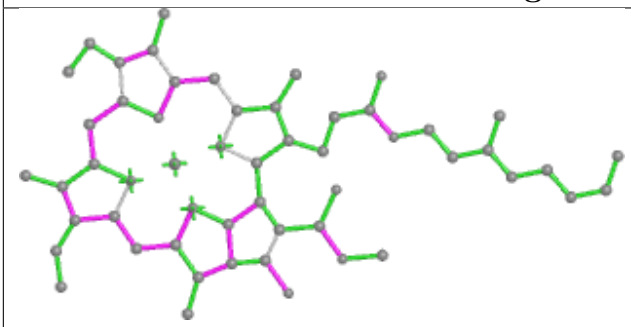
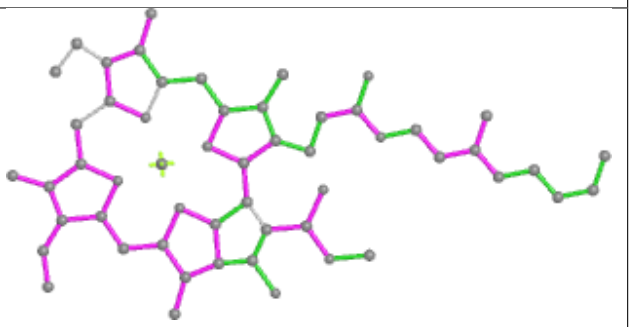
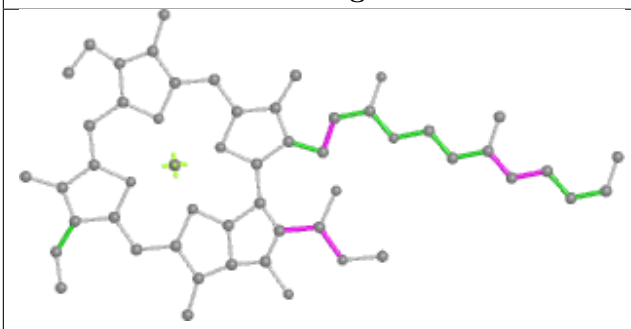
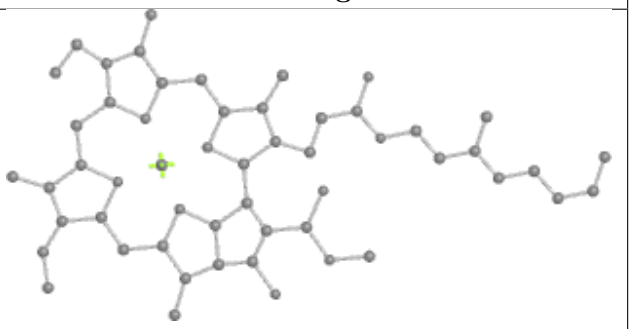
Bond angles



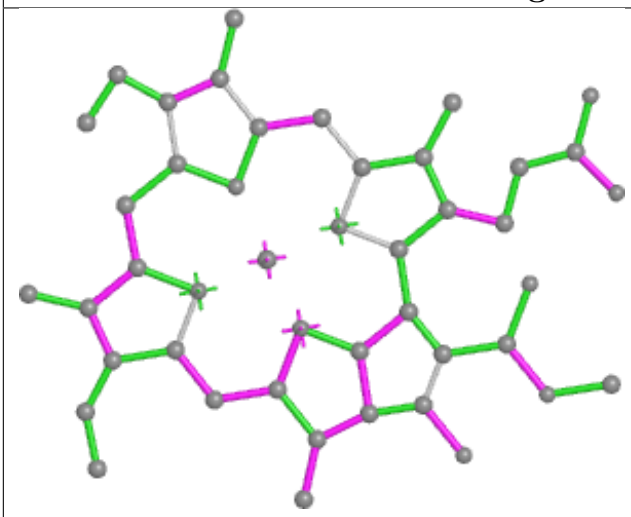
Torsions



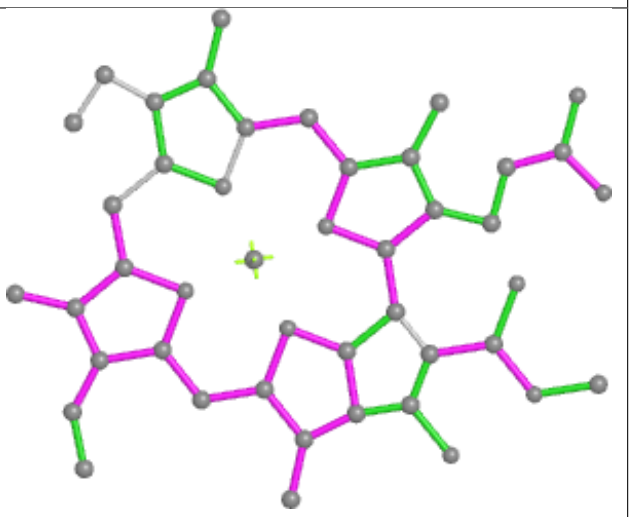
Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

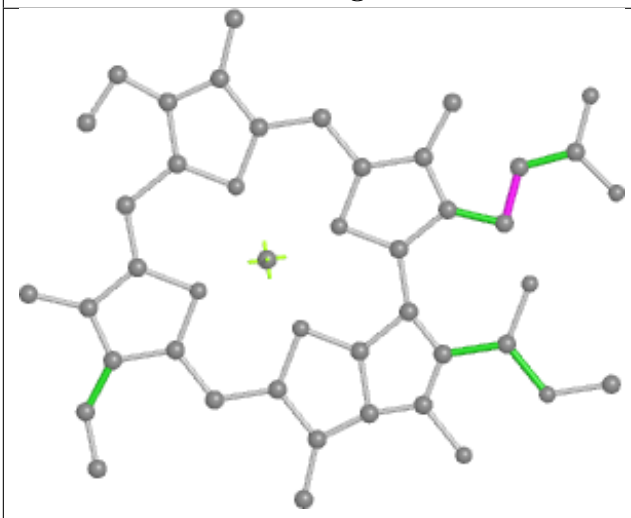
Ligand CLA 2 516



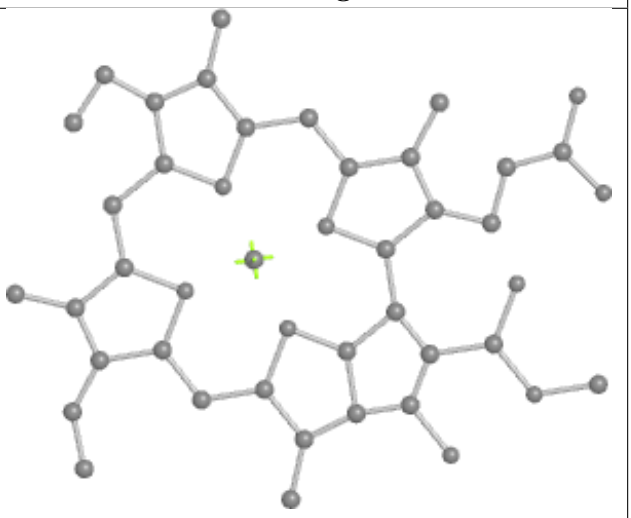
Bond lengths



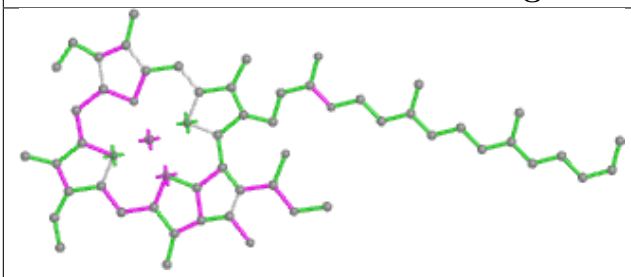
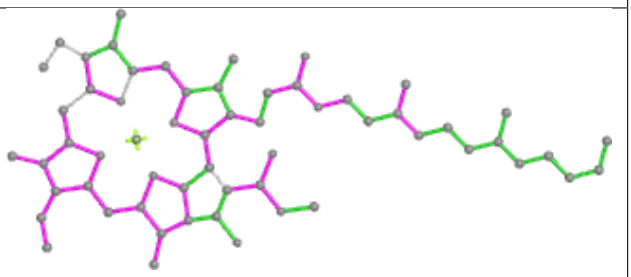
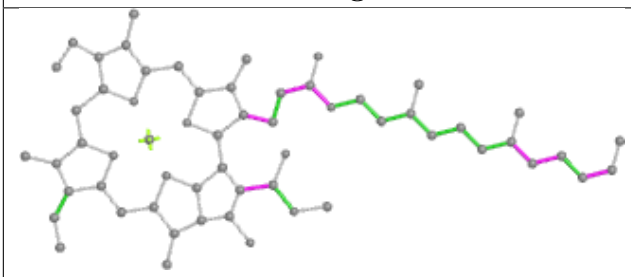
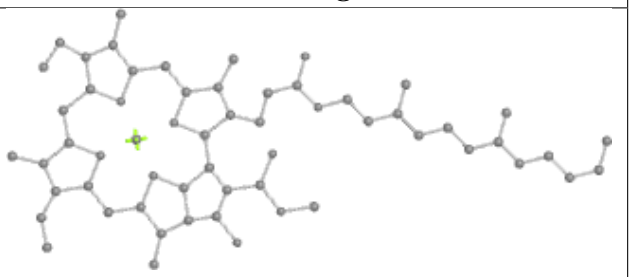
Bond angles

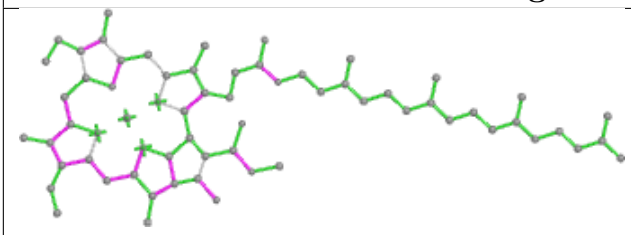
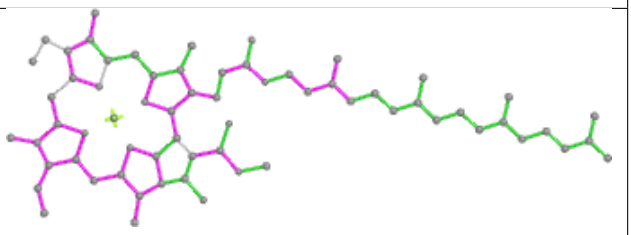
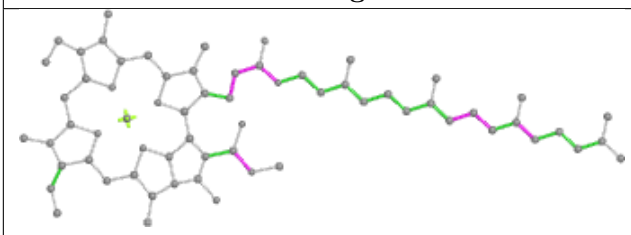
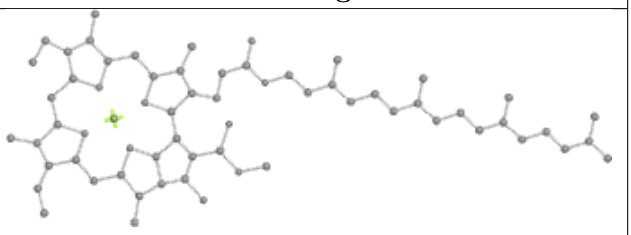


Torsions

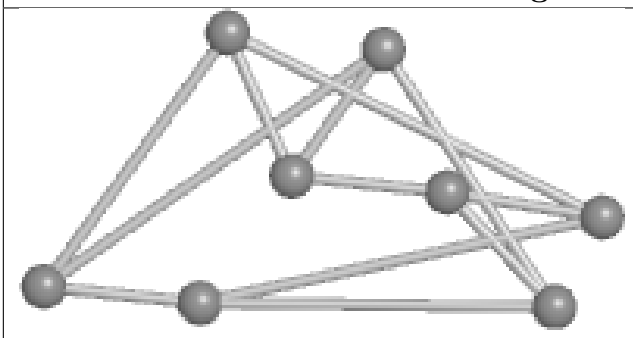


Rings

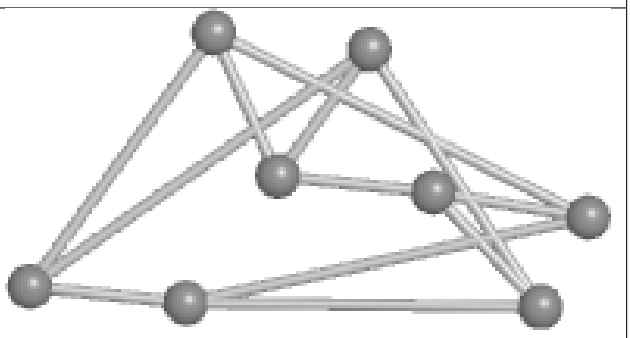
Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

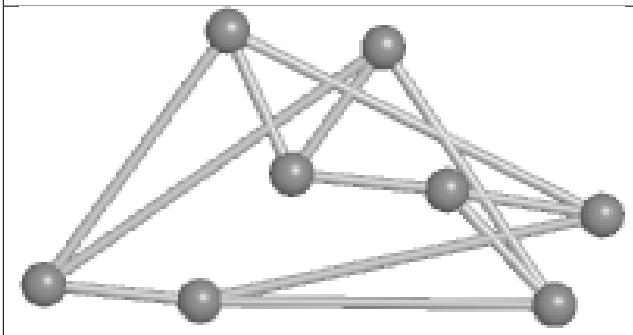
Ligand SF4 A 846



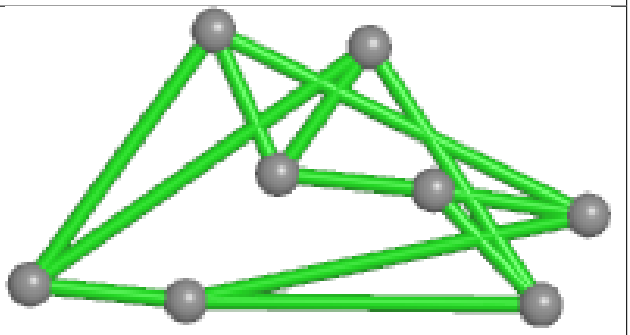
Bond lengths



Bond angles

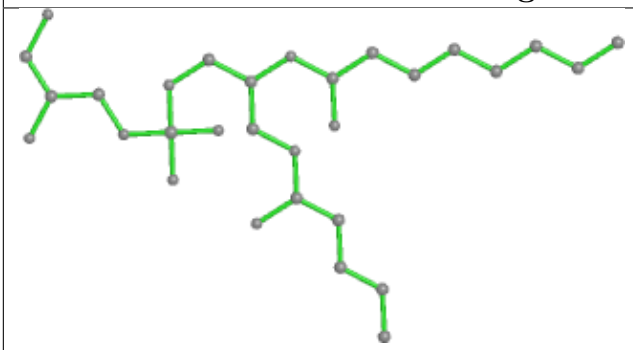


Torsions

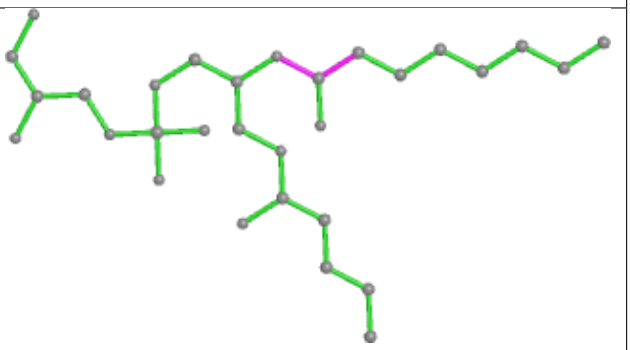


Rings

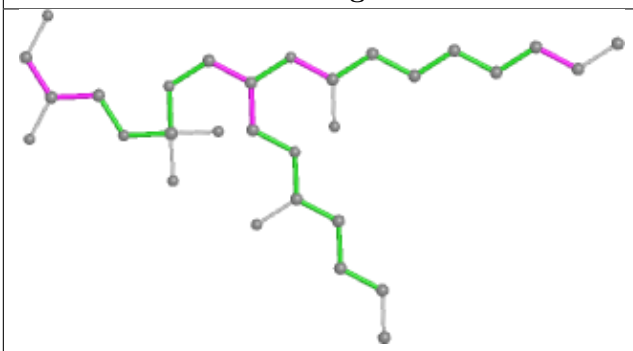
Ligand LHG 11 714



Bond lengths



Bond angles



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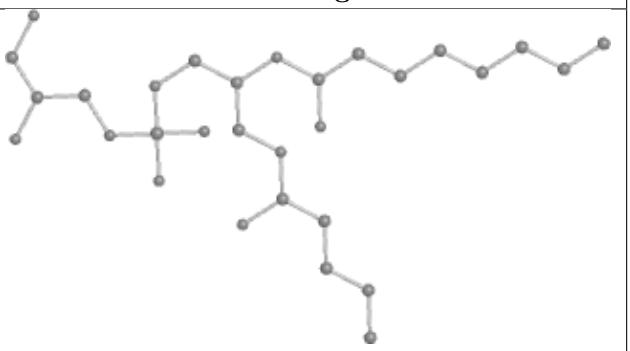
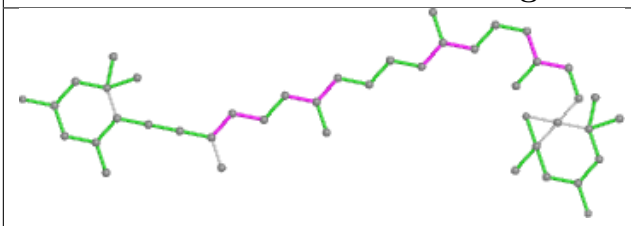
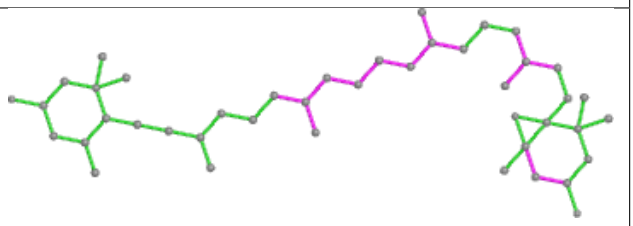
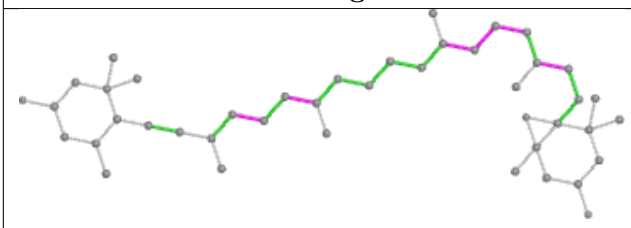
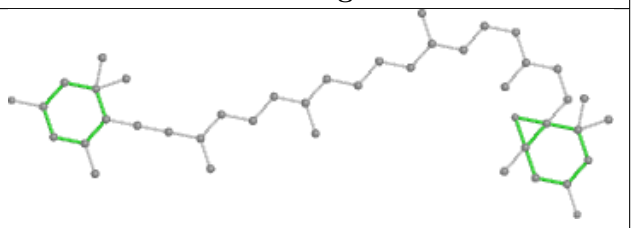
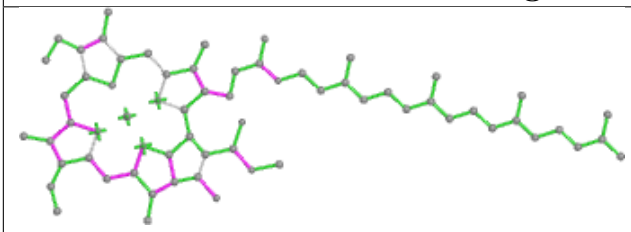
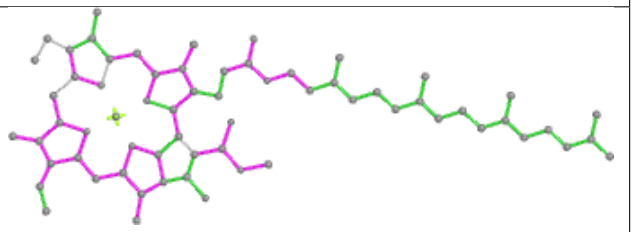
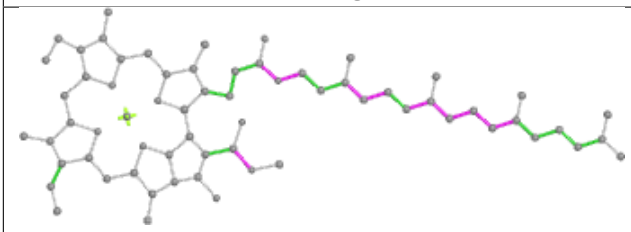
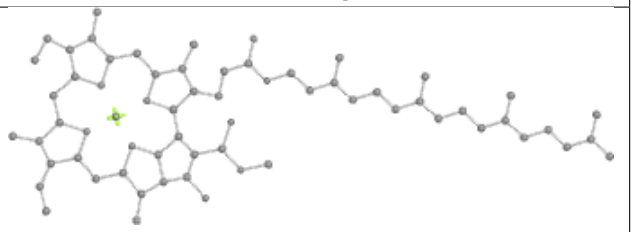
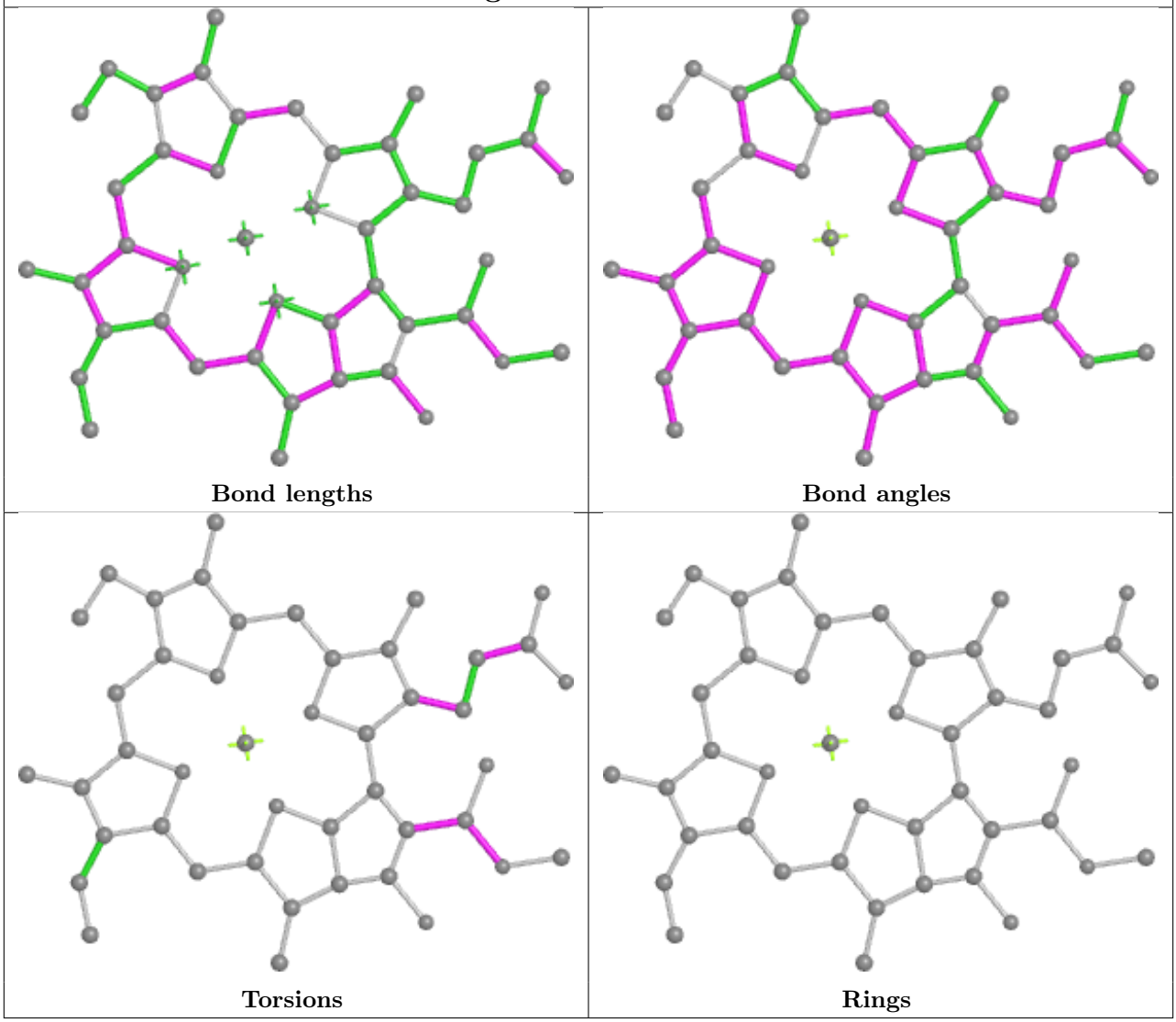


Rings

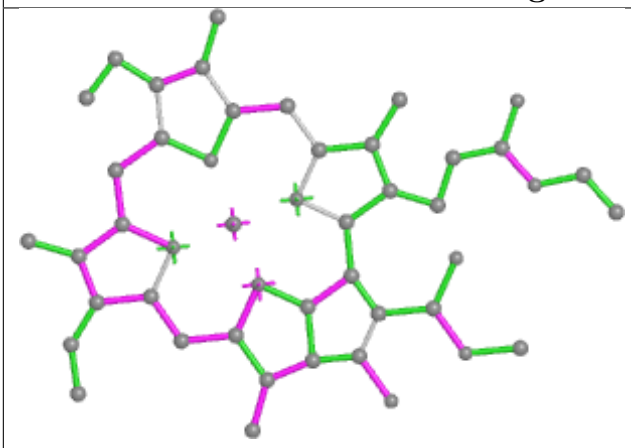
Ligand DD6 11 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

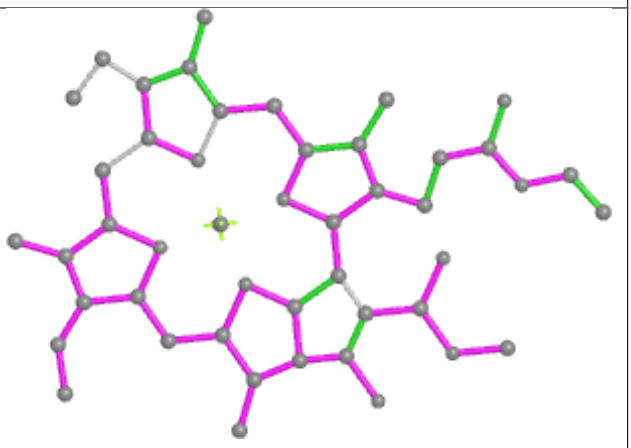
Ligand CLA 3 712



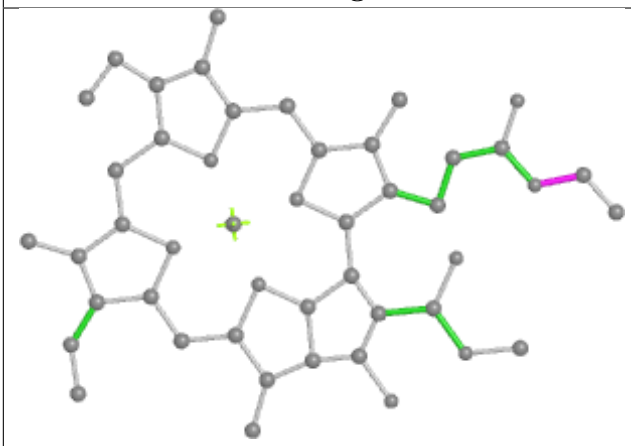
Ligand CLA 6 907



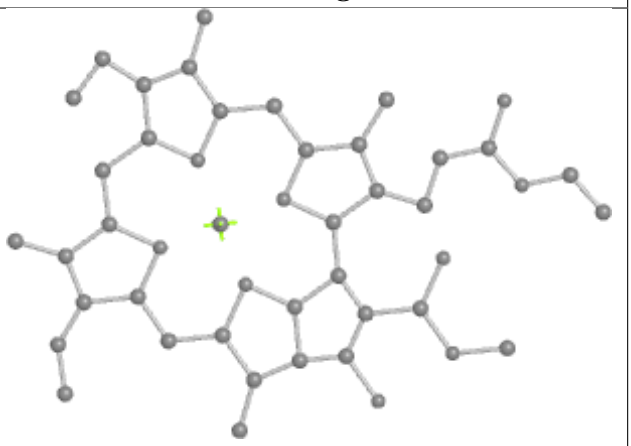
Bond lengths



Bond angles

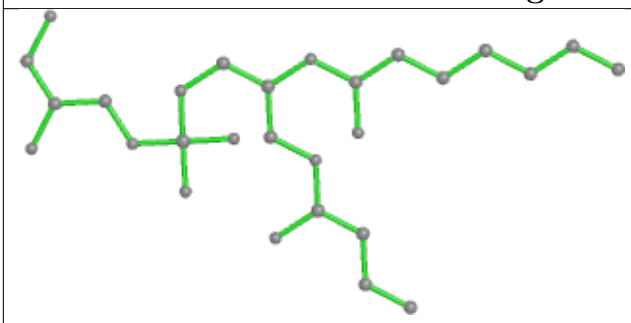


Torsions

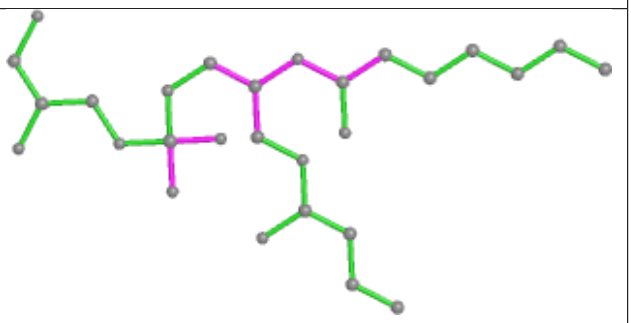


Rings

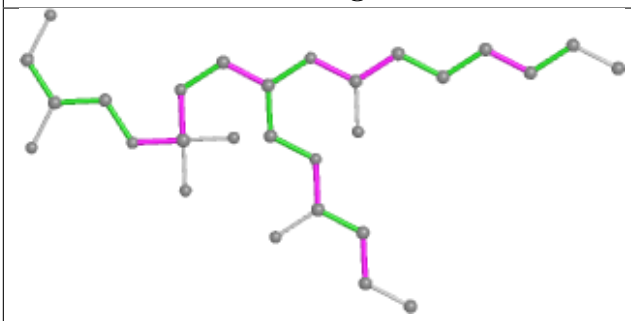
Ligand LHG 6 917



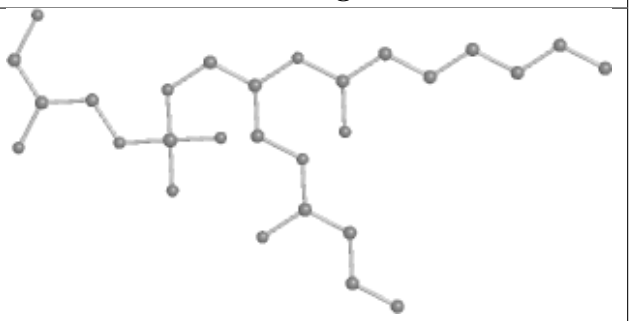
Bond lengths



Bond angles

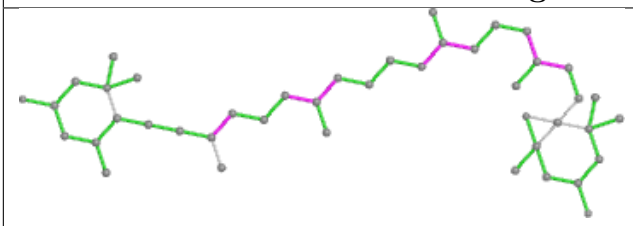


Torsions



Rings

Ligand DD6 2 519



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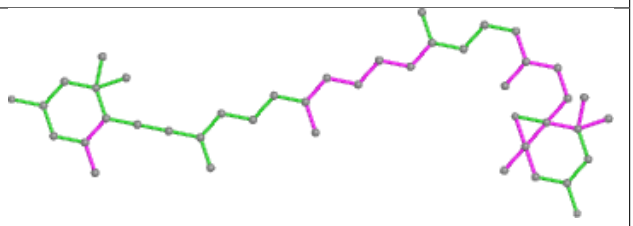
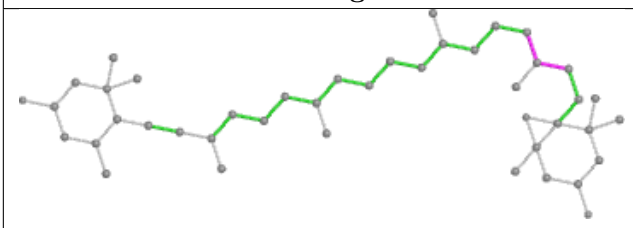


Bond angles



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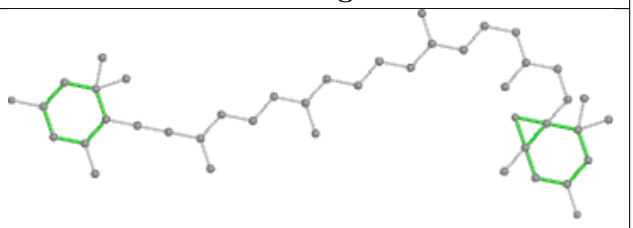
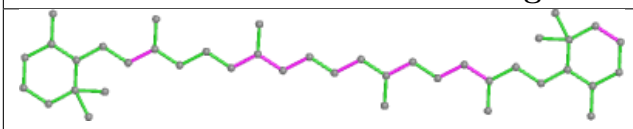


Rings

Ligand BCR F 405



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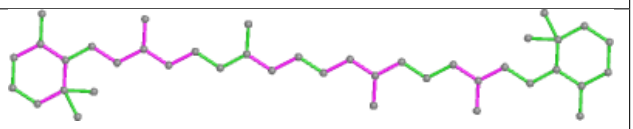
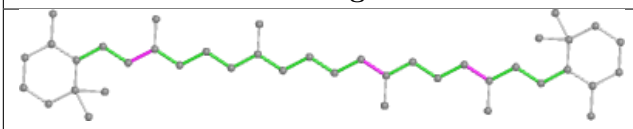


Bond angles



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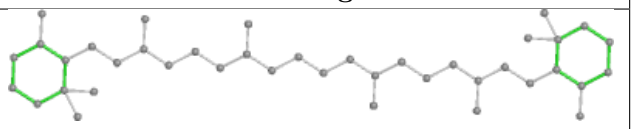
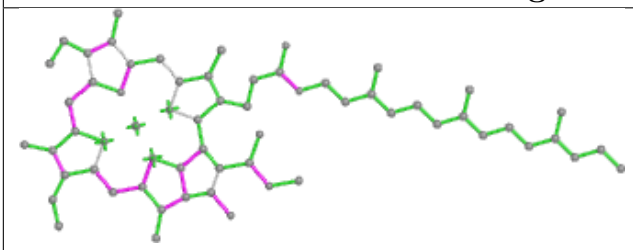
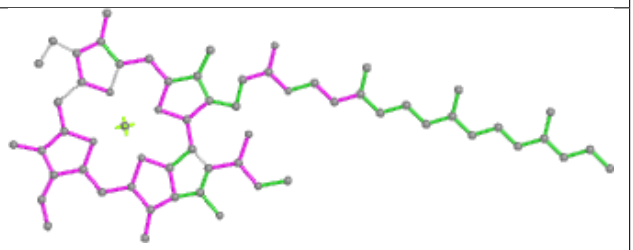


Rings

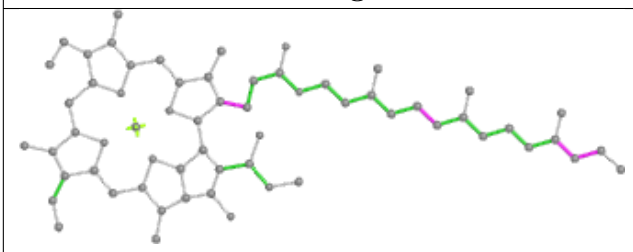
Ligand CLA 3 707



Bond lengths



Bond angles



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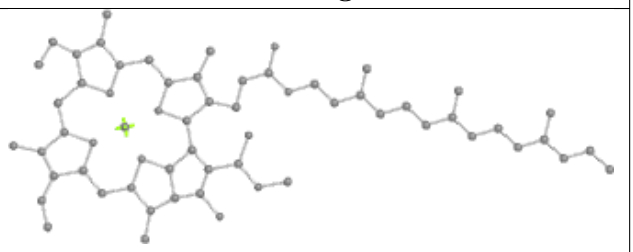
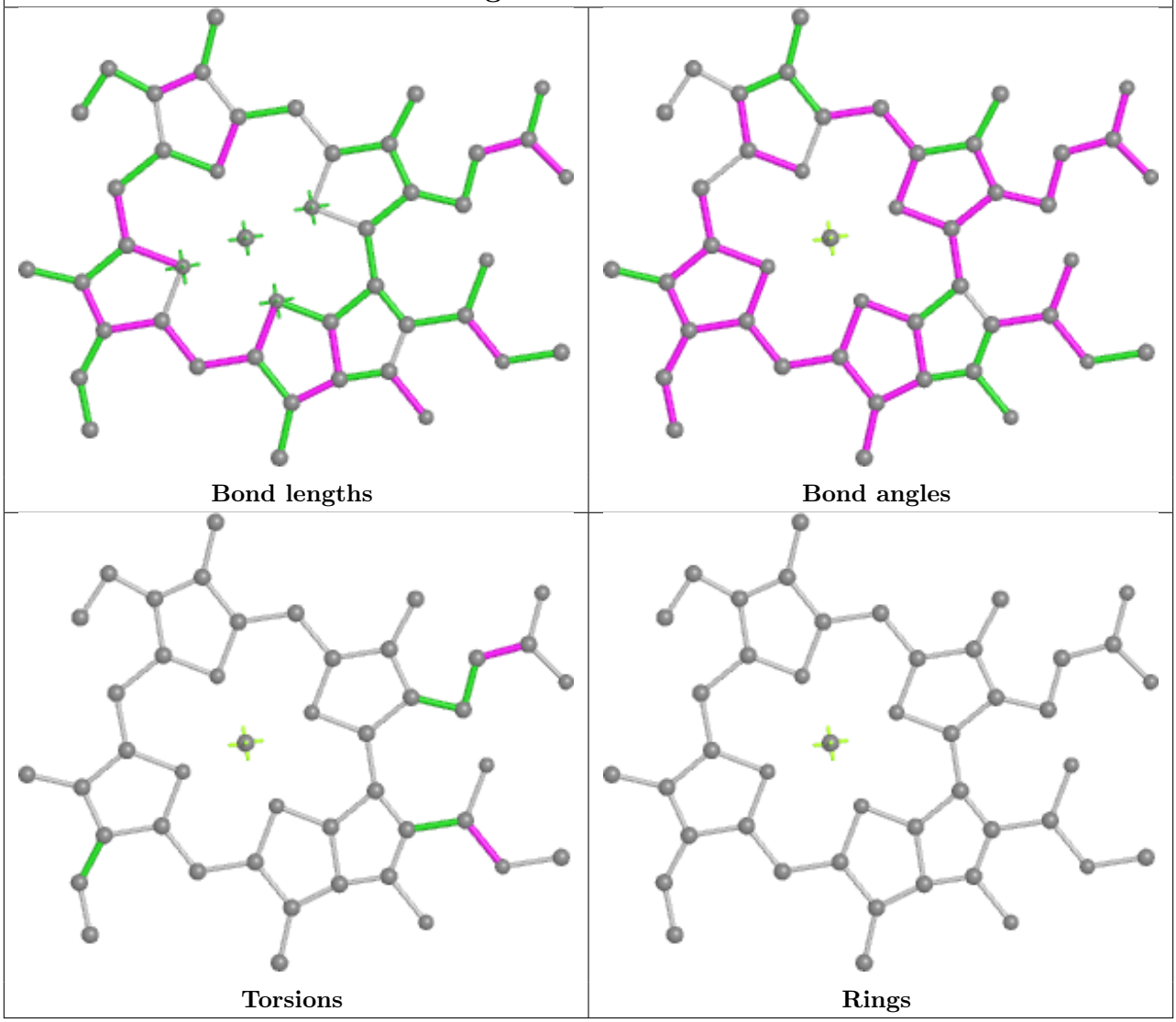
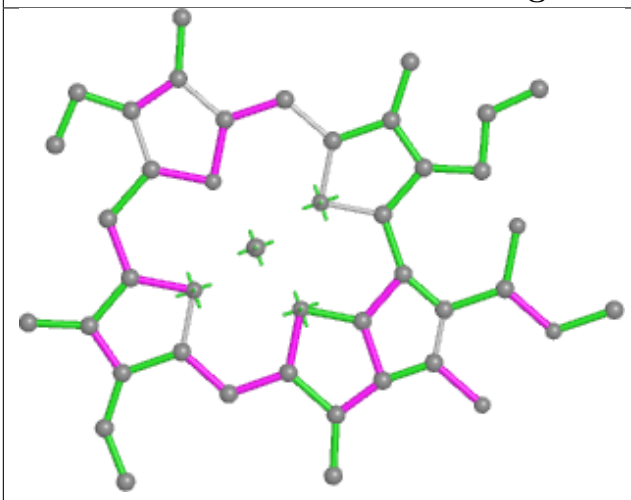


Rings

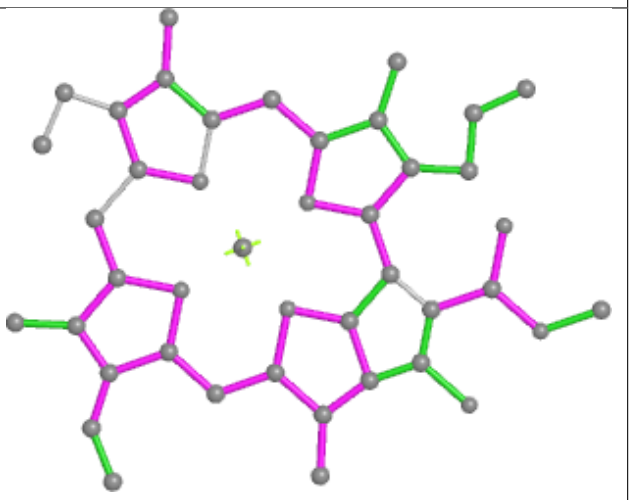
Ligand CLA 4 711



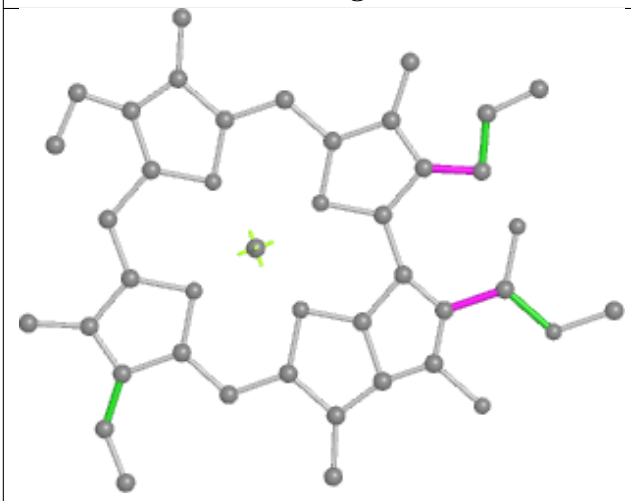
Ligand CLA 5 708



Bond lengths



Bond angles



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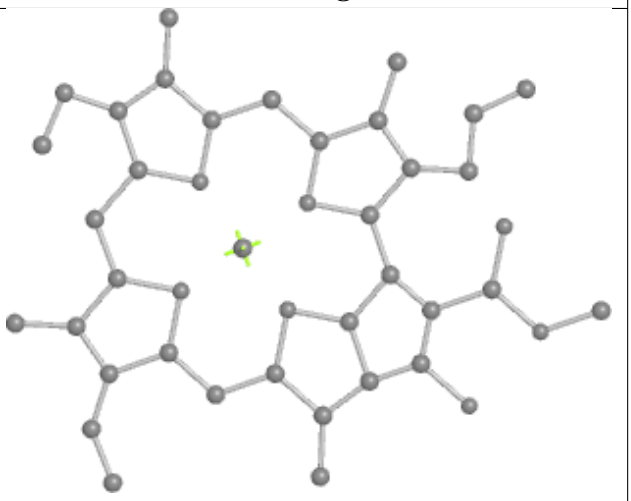
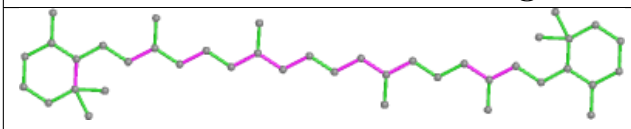


Rings

Ligand BCR M 102



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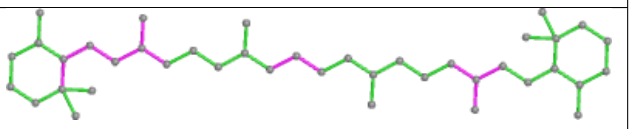
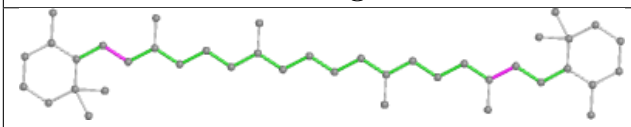


Bond angles



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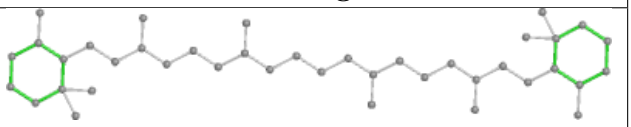
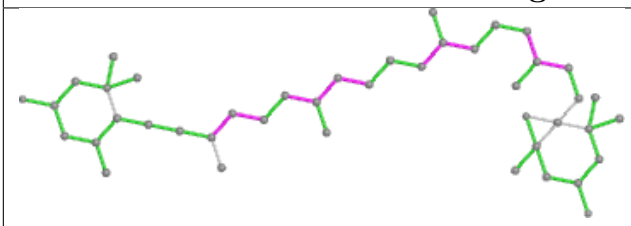
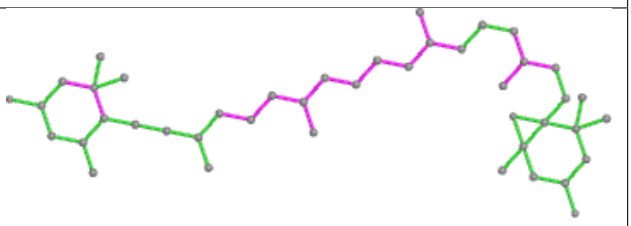
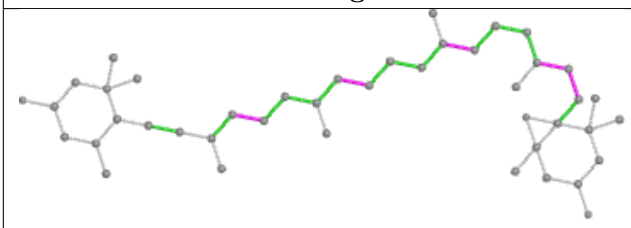
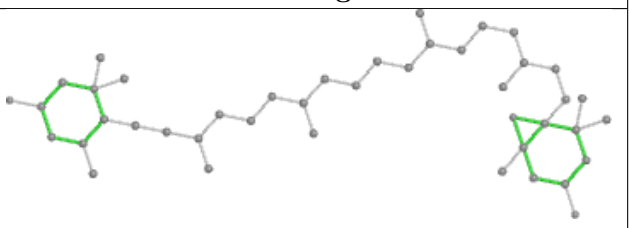
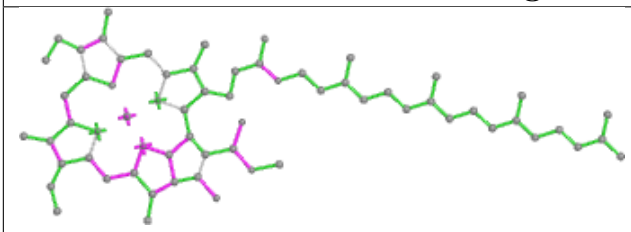
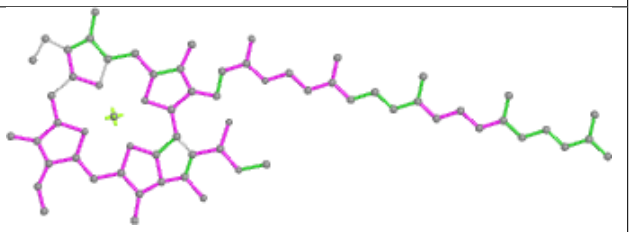
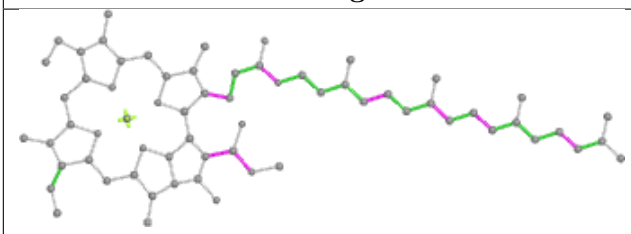
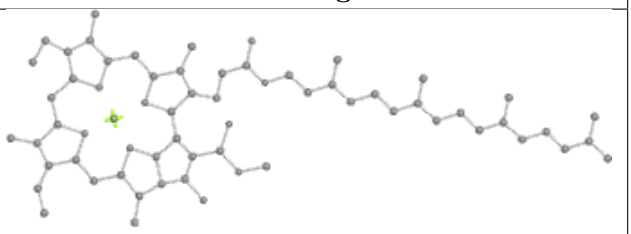
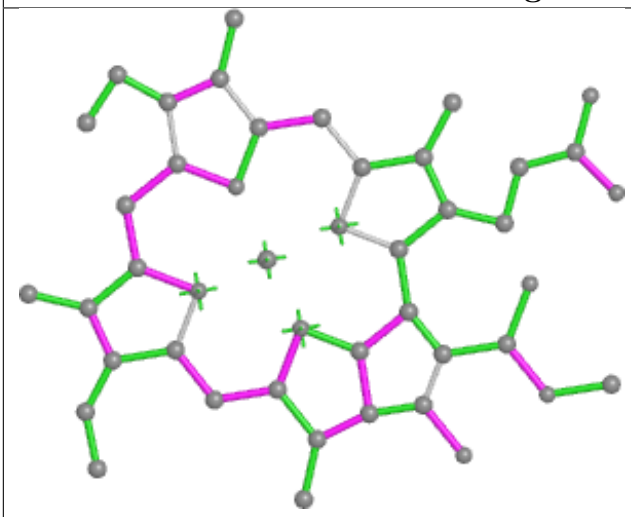


Rings

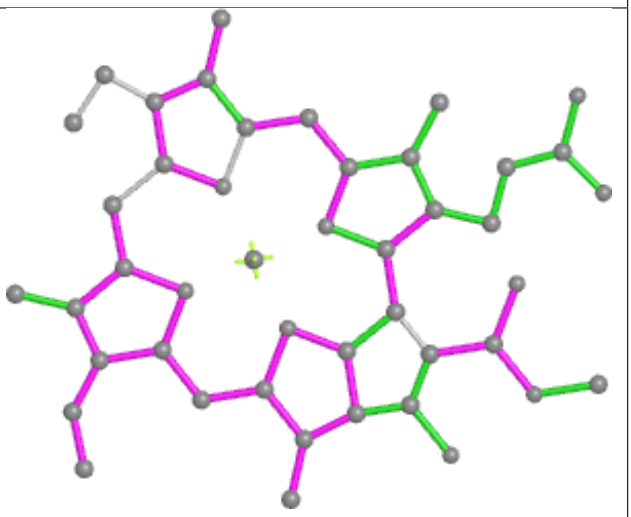
Ligand DD6 3 718	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

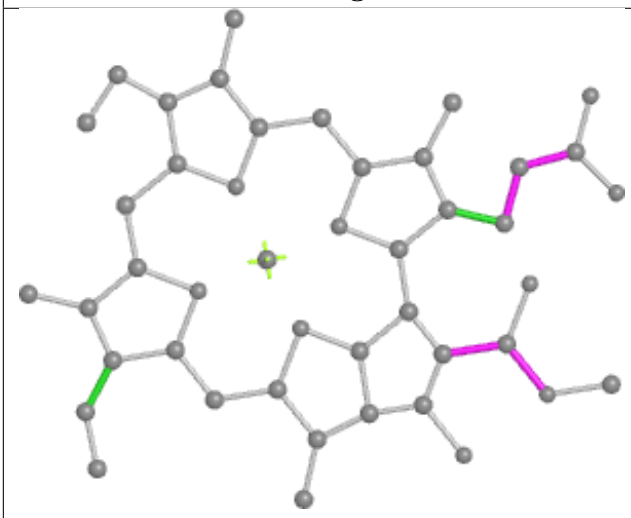
Ligand CLA B 820



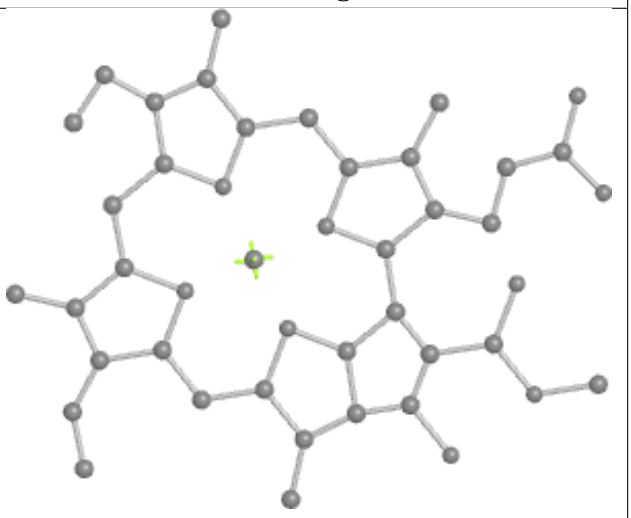
Bond lengths



Bond angles

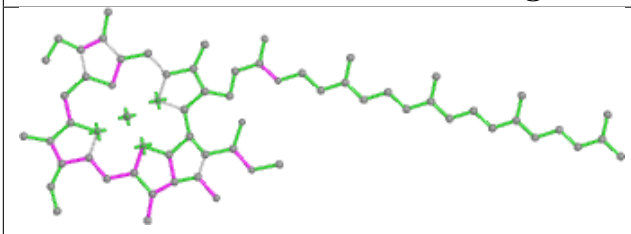


Torsions



Rings

Ligand CLA B 831



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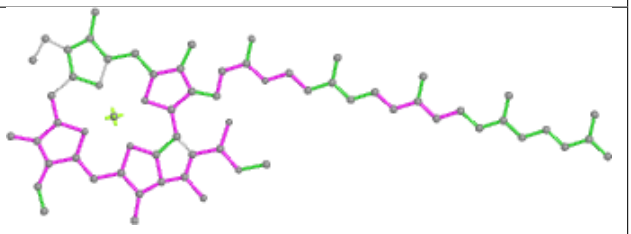

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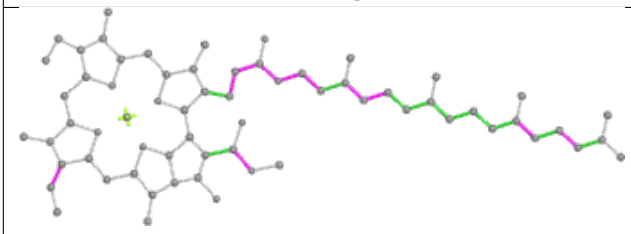

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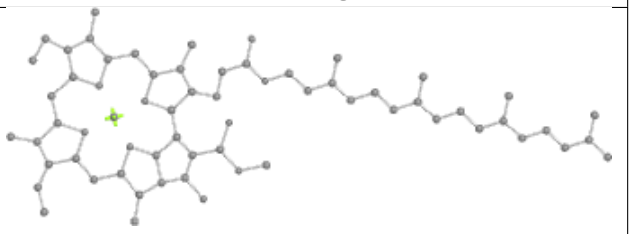
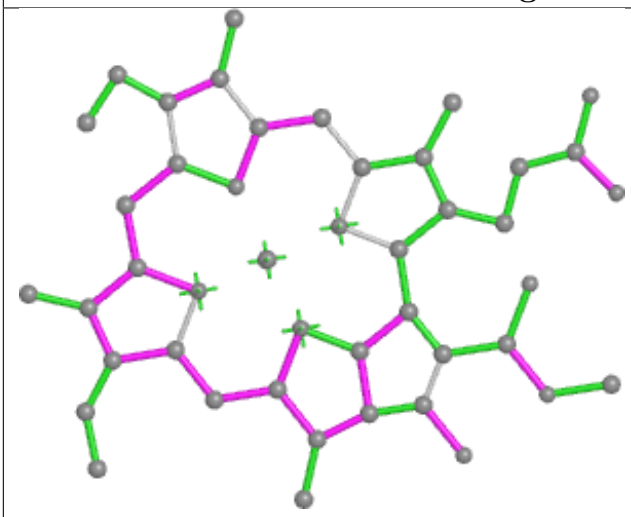


Rings

Ligand CLA 11 710



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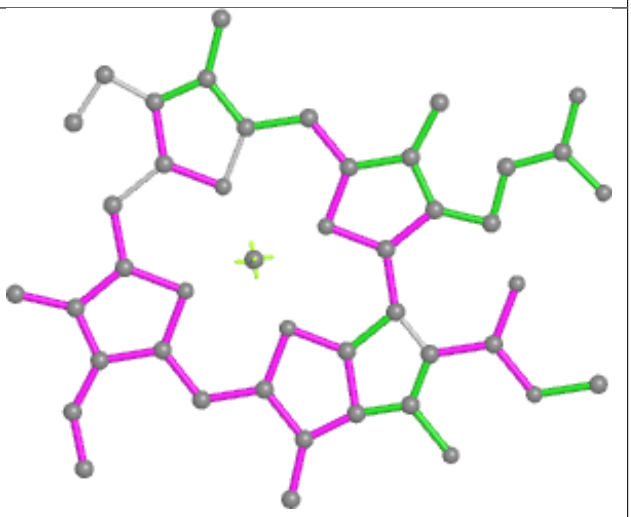
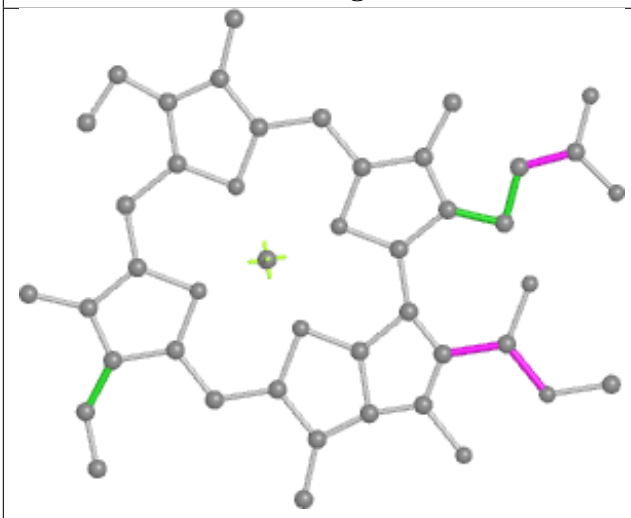


Bond angles



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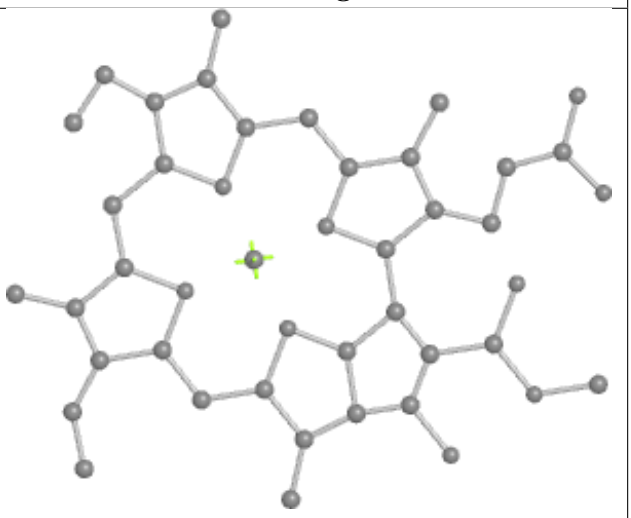
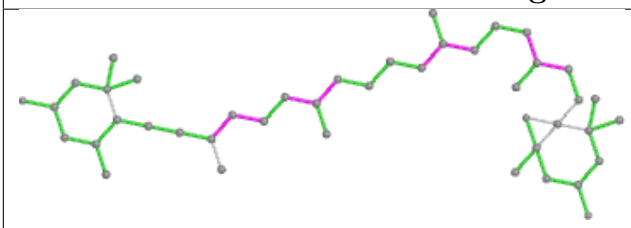


Rings

Ligand DD6 8 616



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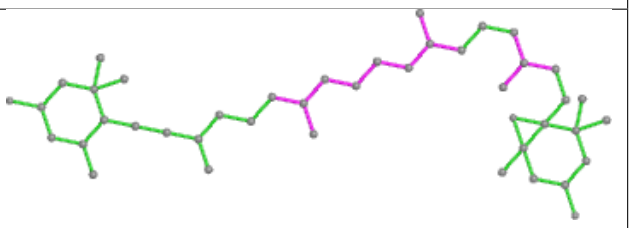
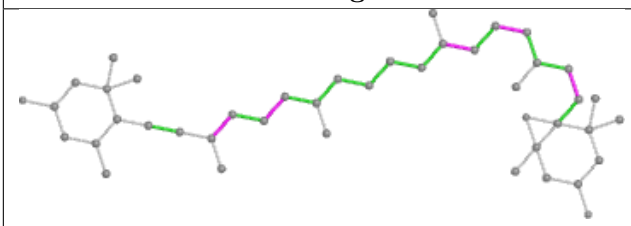
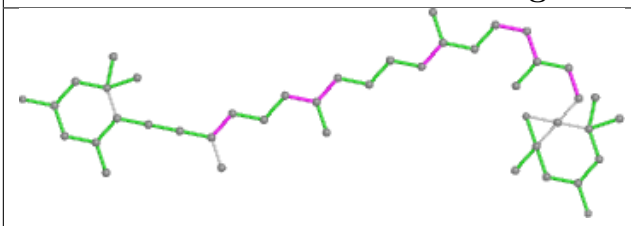
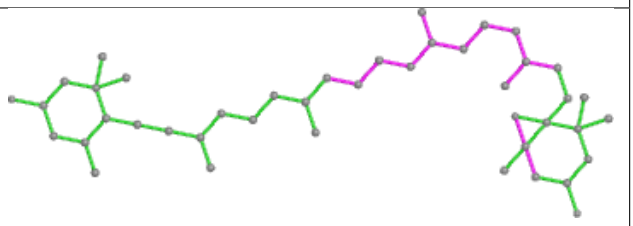
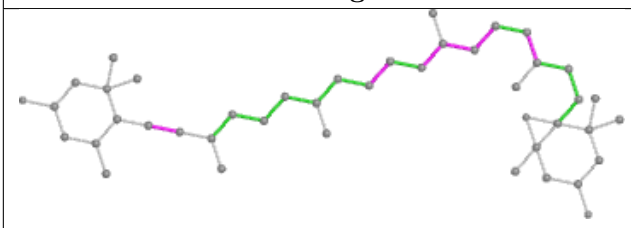
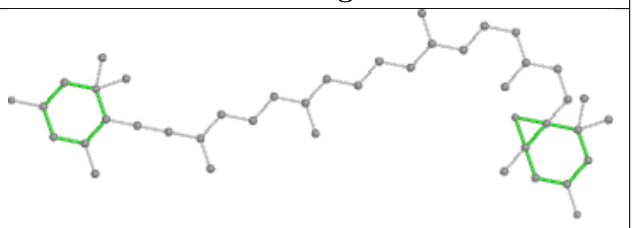


Bond angles



Torsions

Rings

Ligand DD6 3 717	
 Bond lengths	 Bond angles
 Torsions	 Rings

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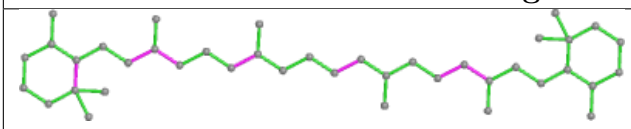
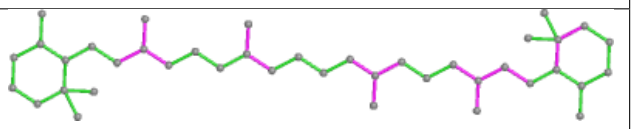
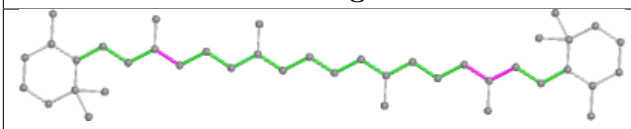
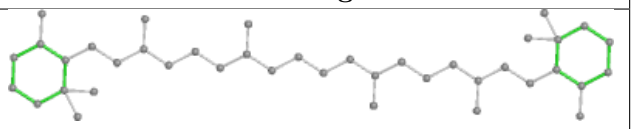
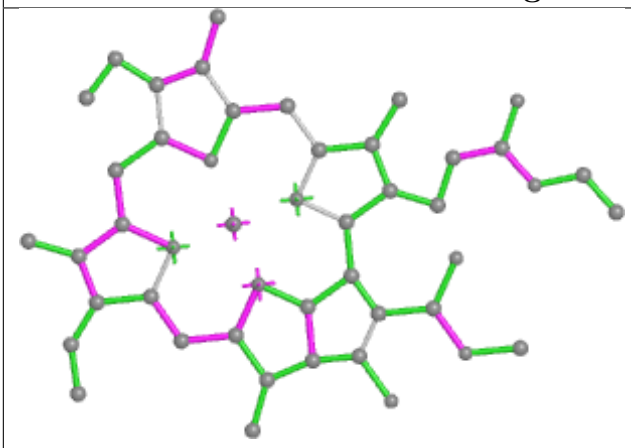
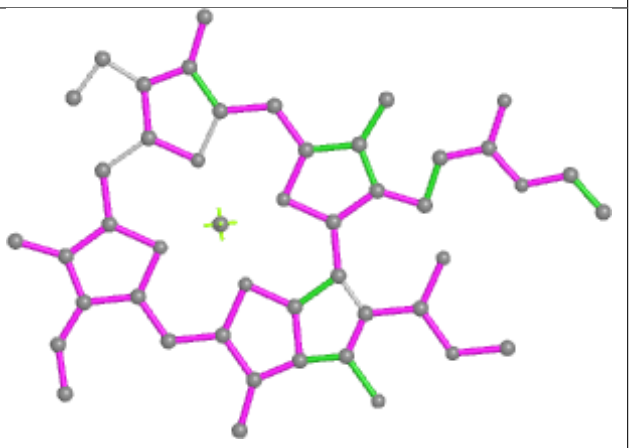
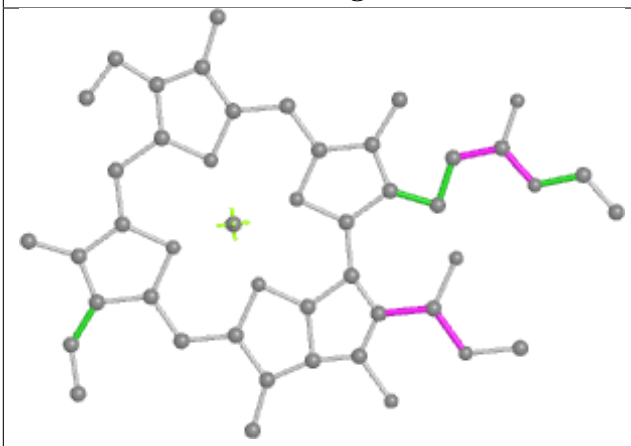
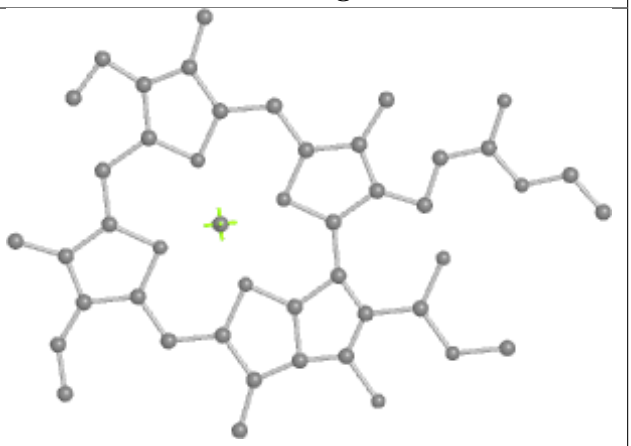
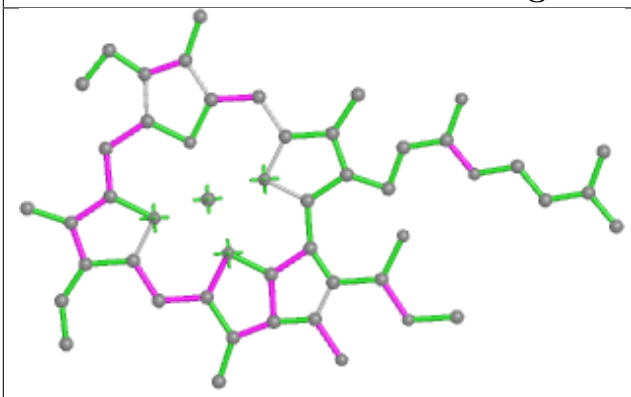
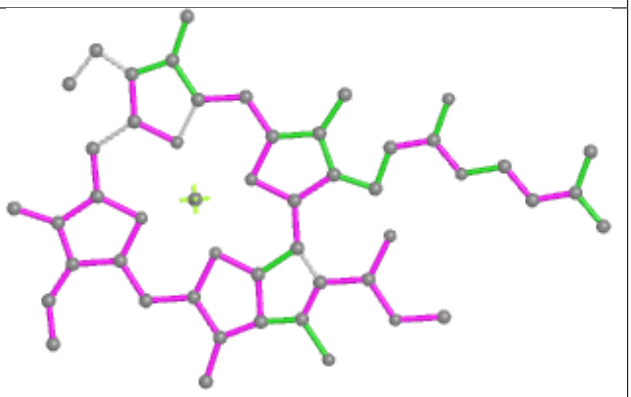
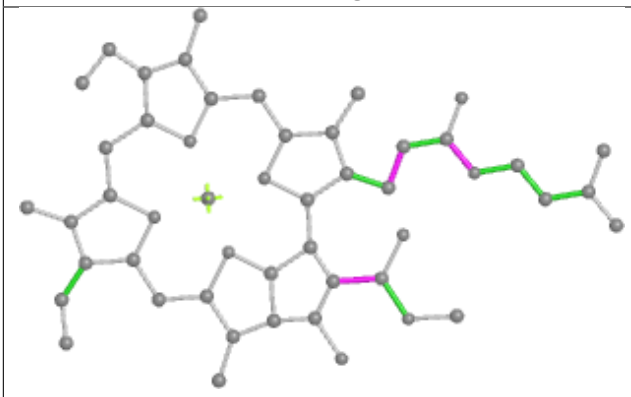
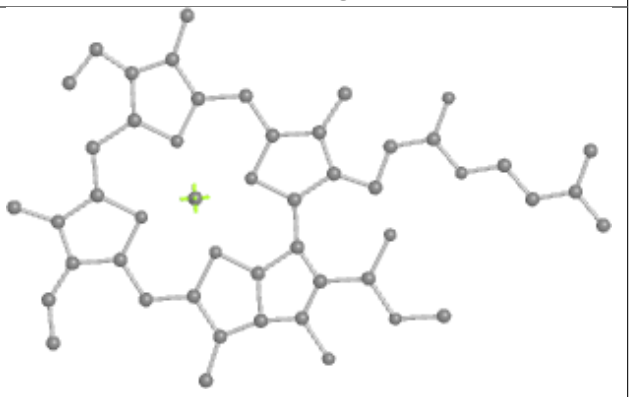
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 905	
 Bond lengths	 Bond angles
 Torsions	 Rings

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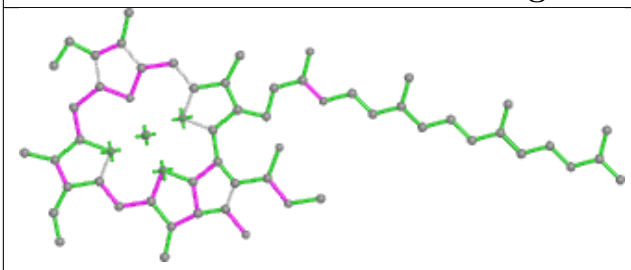
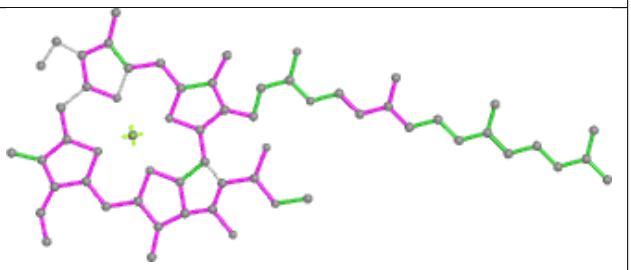
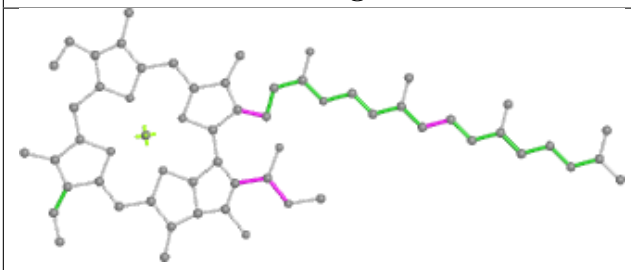
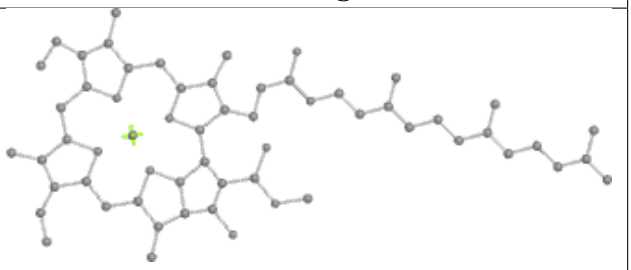
 Bond lengths	 Bond angles
 Torsions	 Rings

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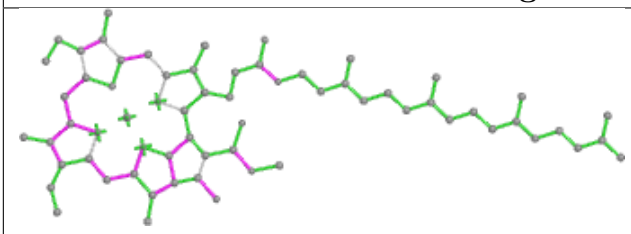
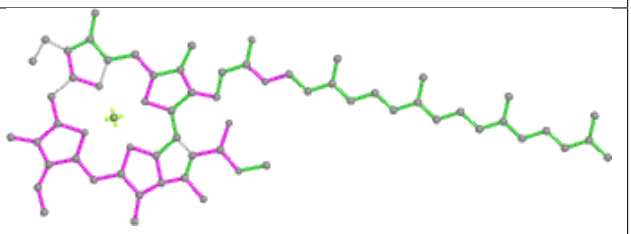
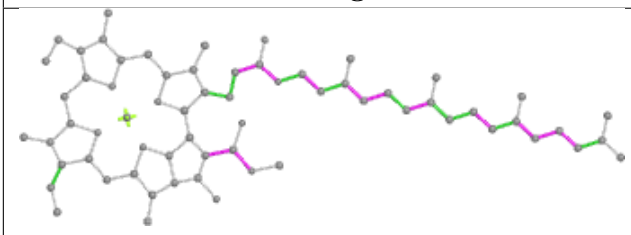
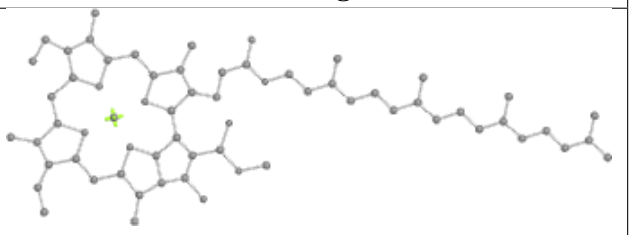
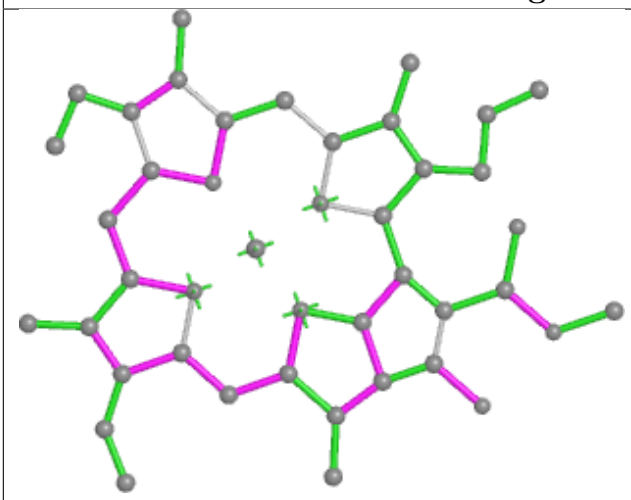
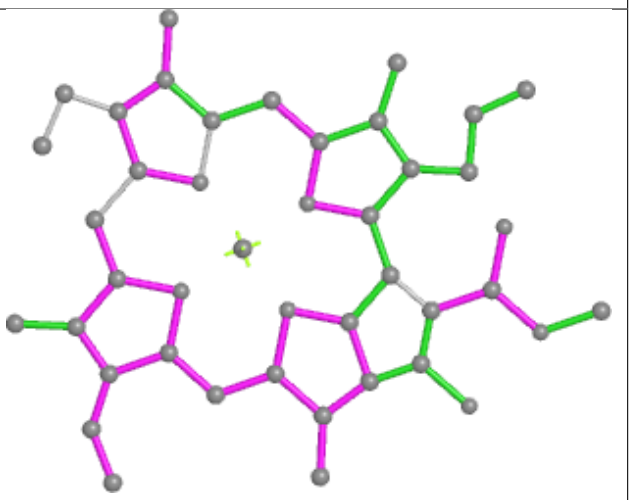
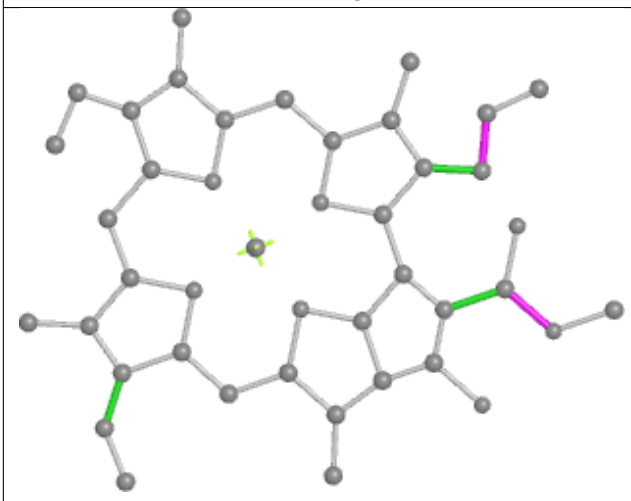
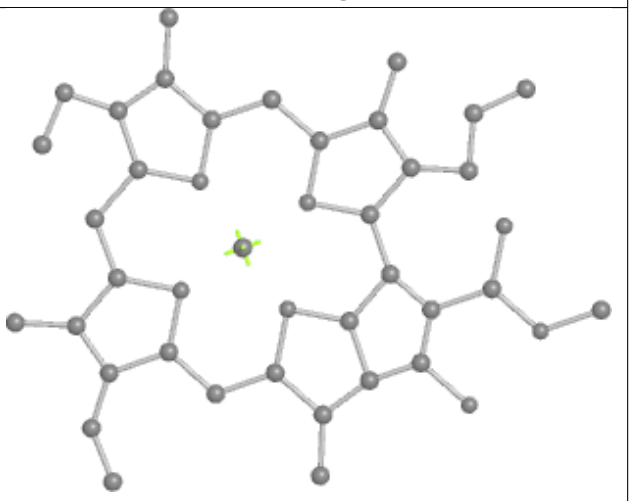
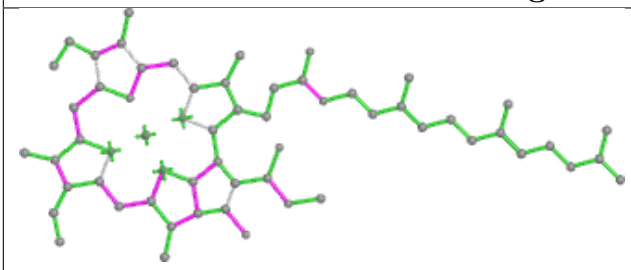
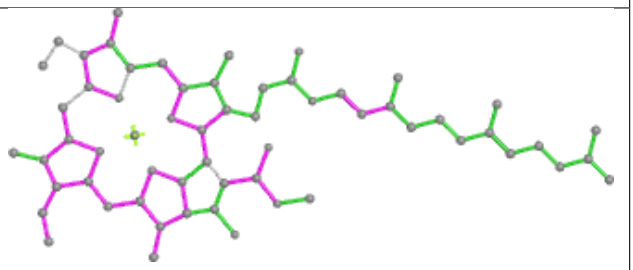
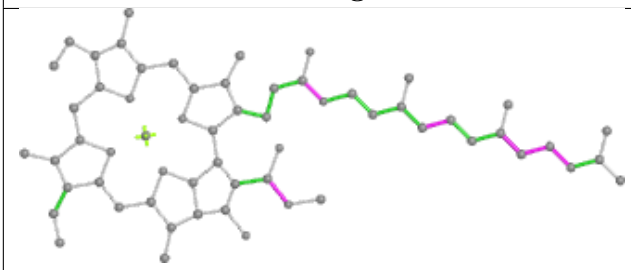
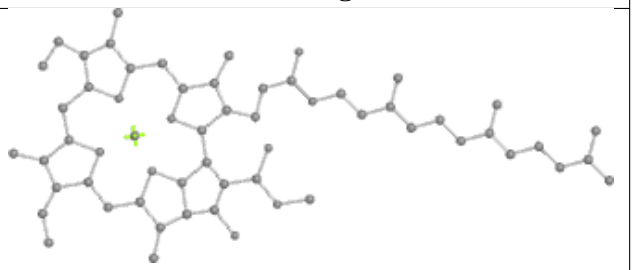
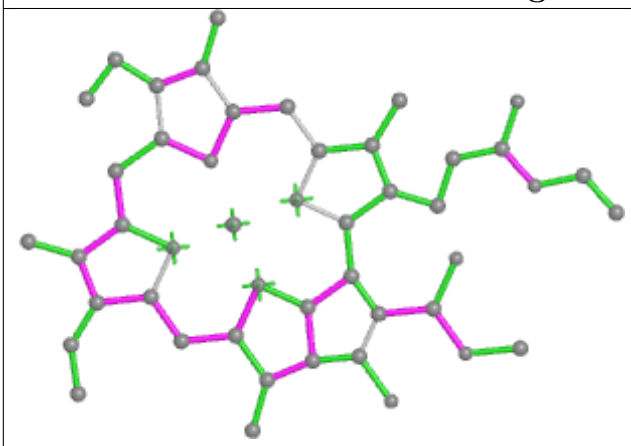
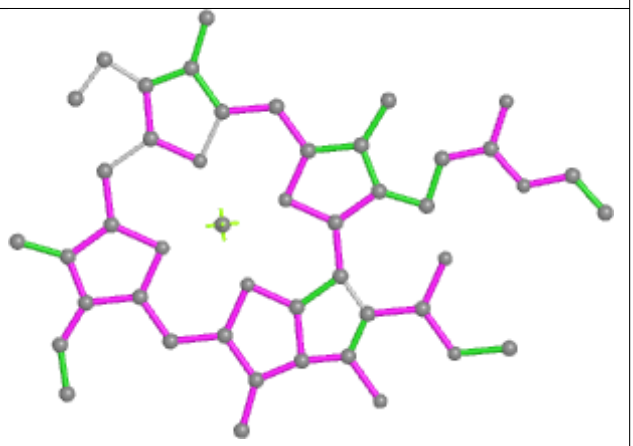
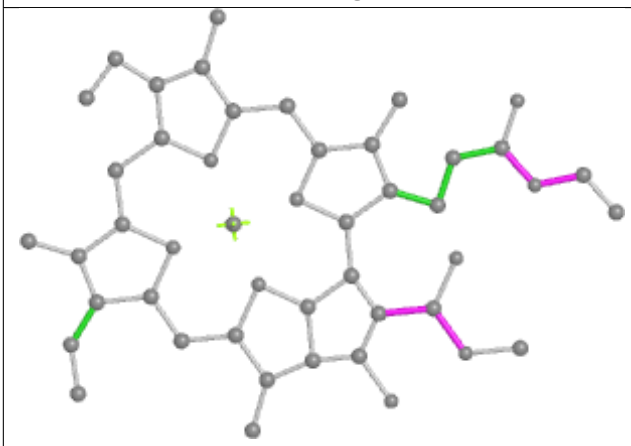
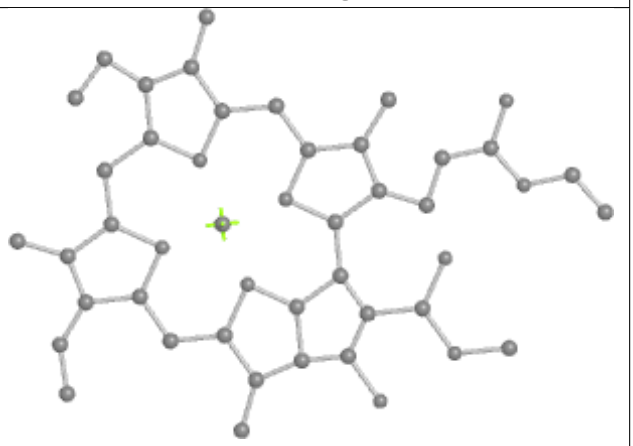
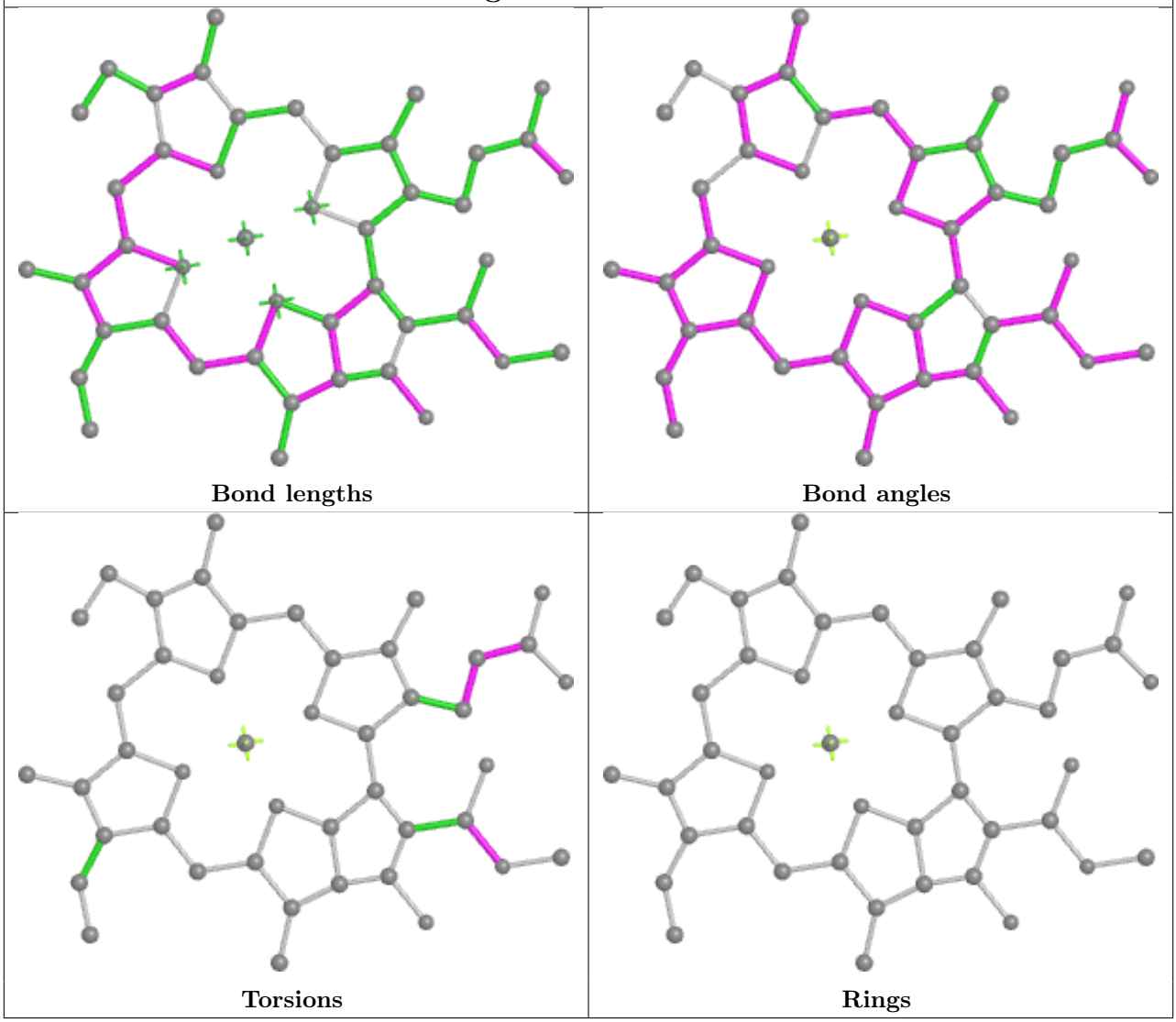
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 909	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 613



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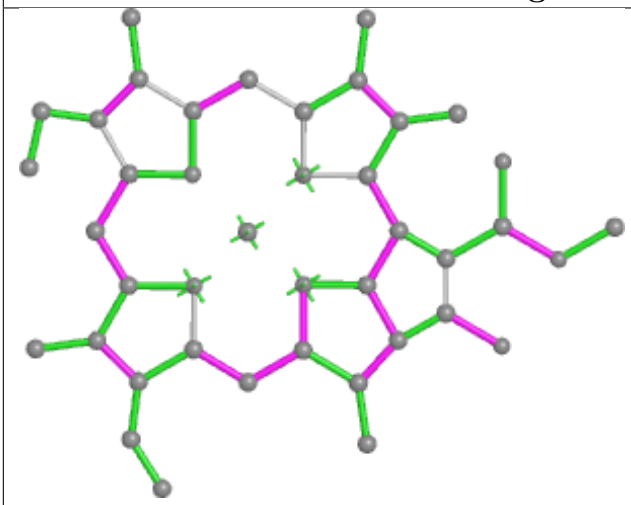
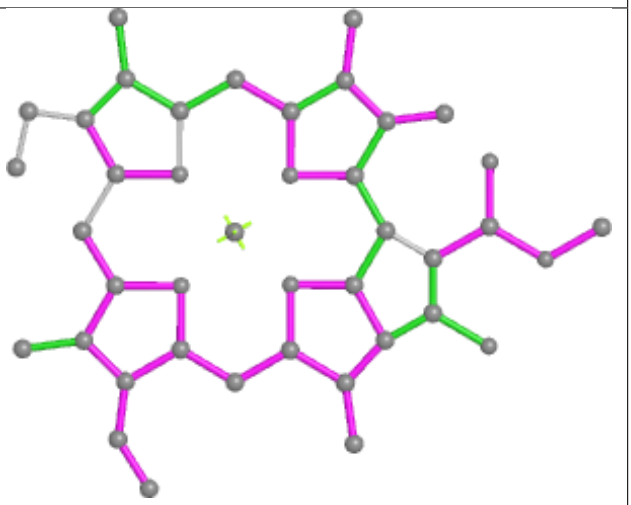
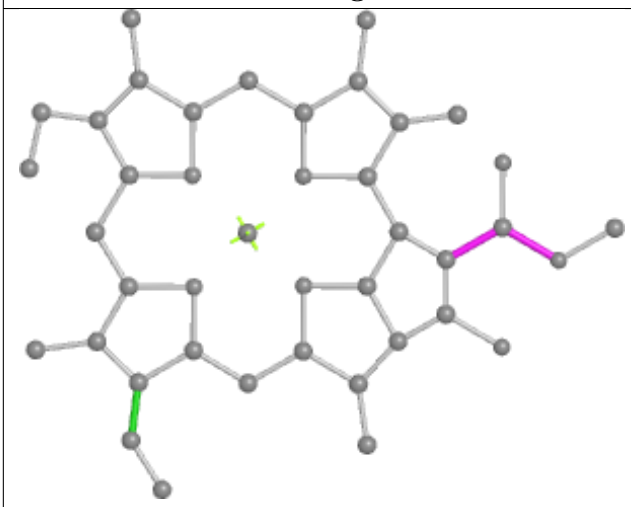
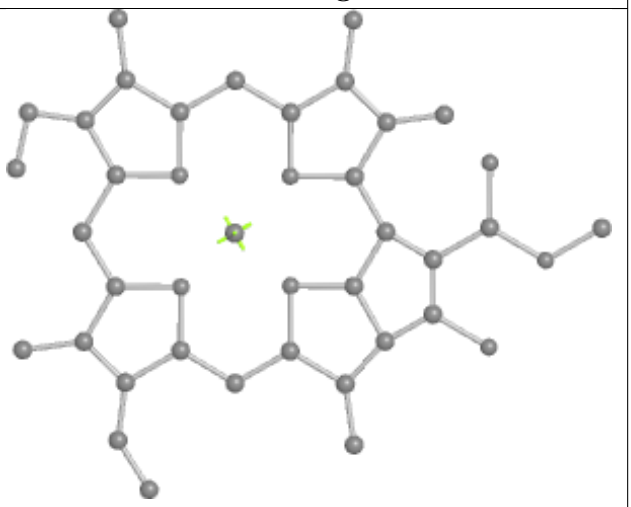
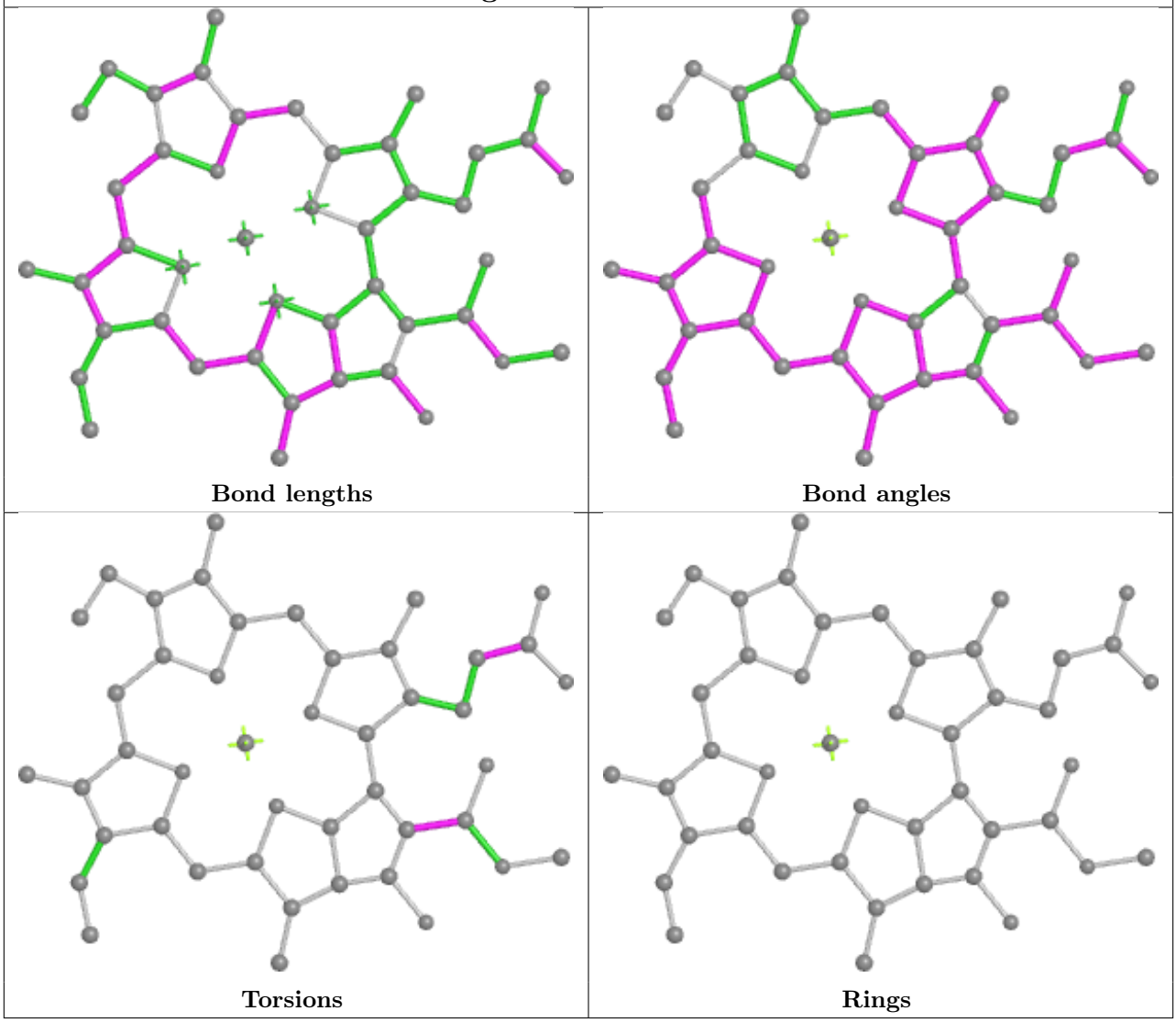
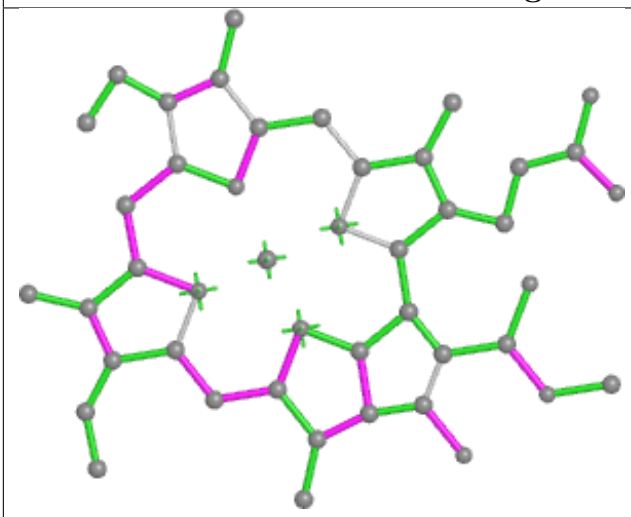
 Bond lengths	 Bond angles
 Torsions	 Rings

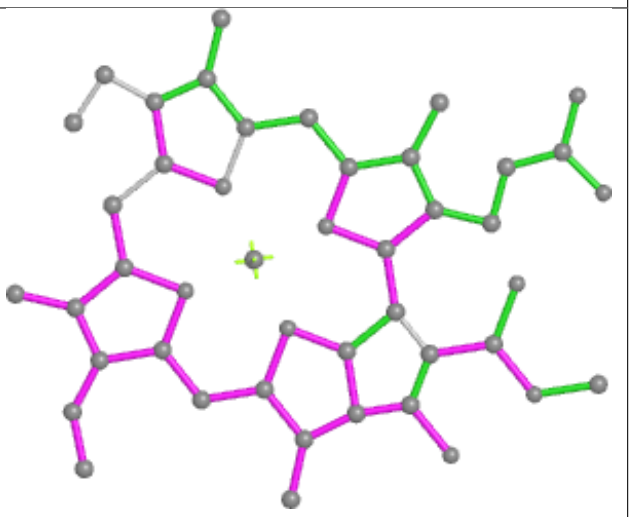
Ligand CLA B 809



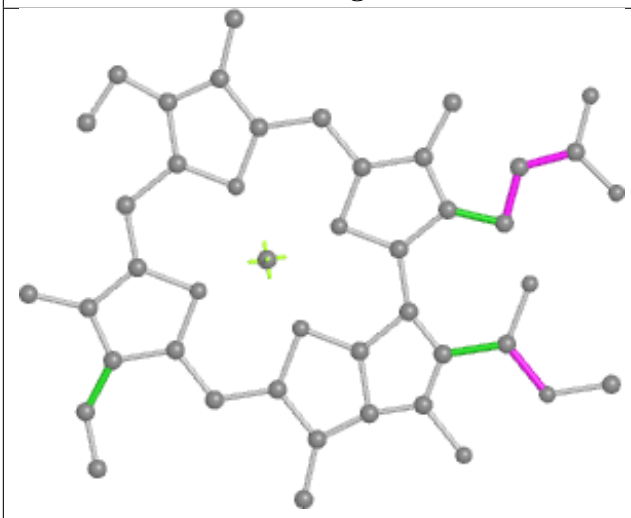
Ligand CLA B 837



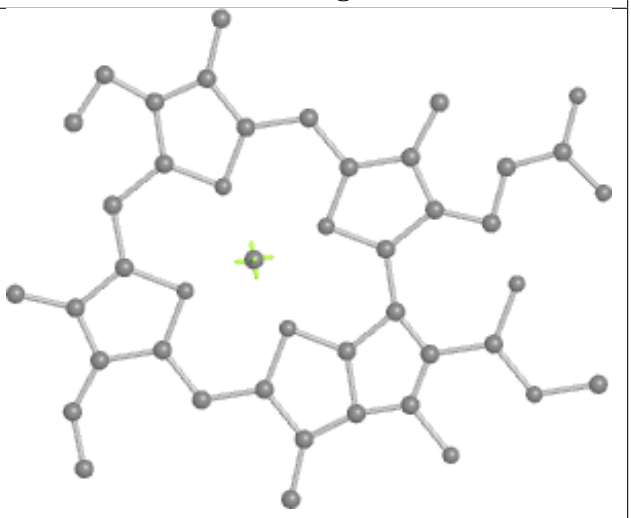
Bond lengths



Bond angles

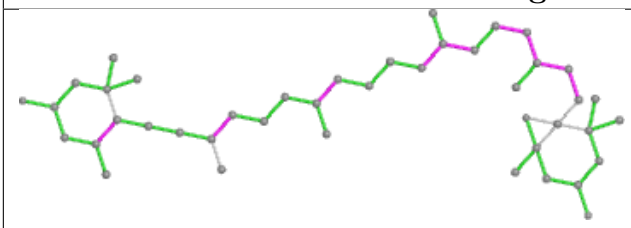


Torsions



Rings

Ligand DD6 5 713



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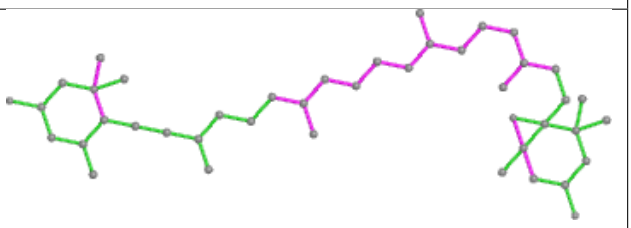
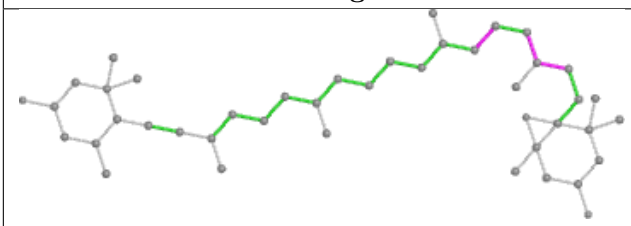
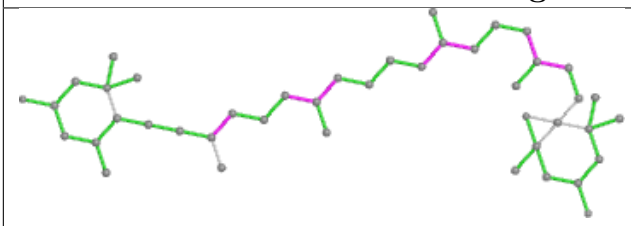
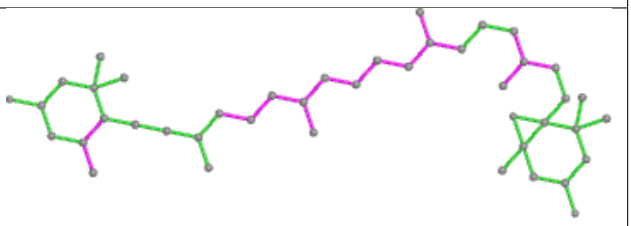
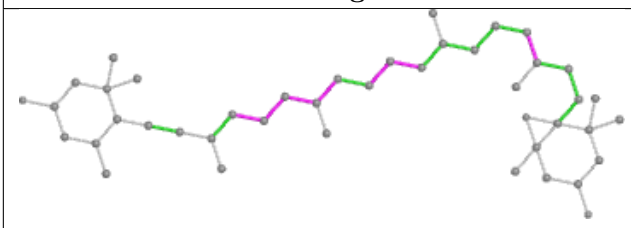
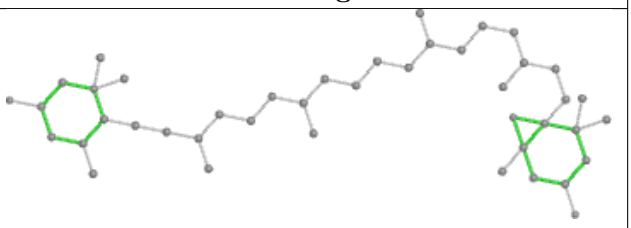


Bond angles



Torsions

Rings

Ligand DD6 9 916	
 Bond lengths	 Bond angles
 Torsions	 Rings

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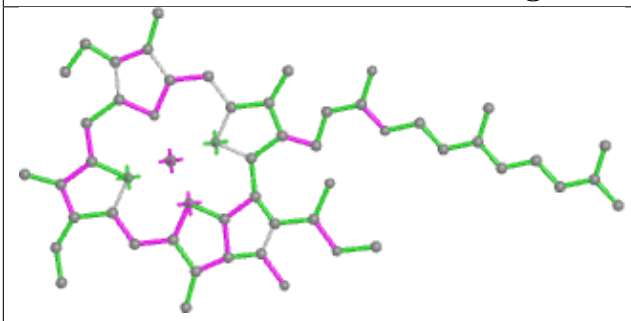
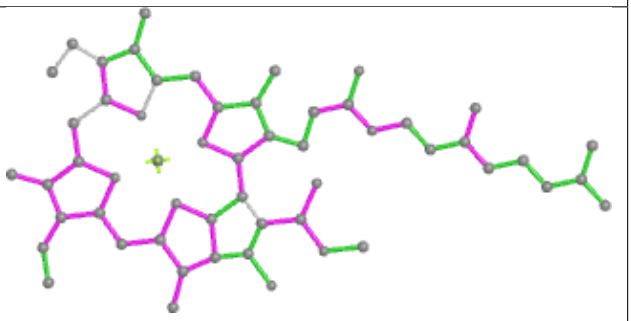
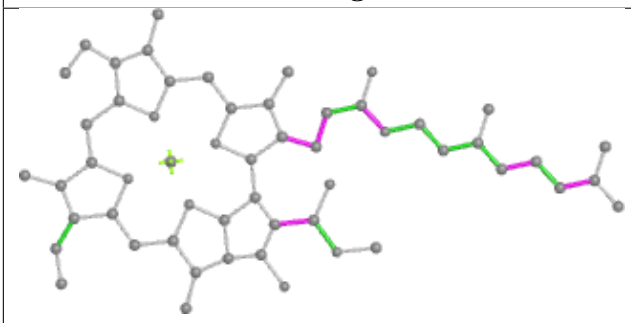
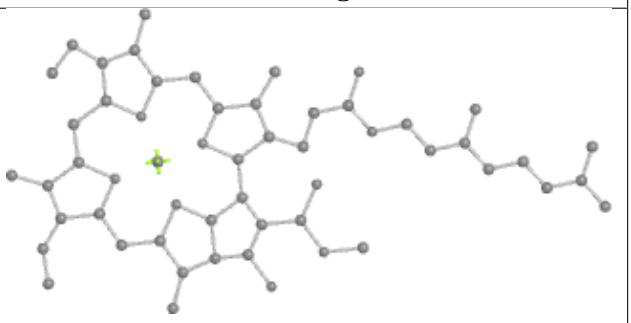
 Bond lengths	 Bond angles
 Torsions	 Rings

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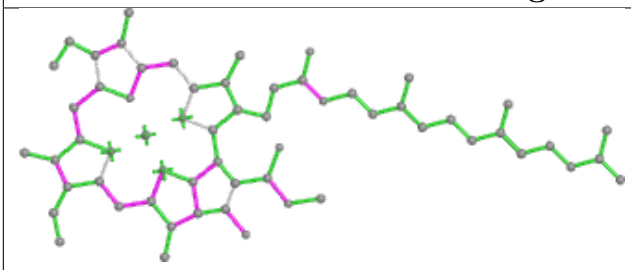
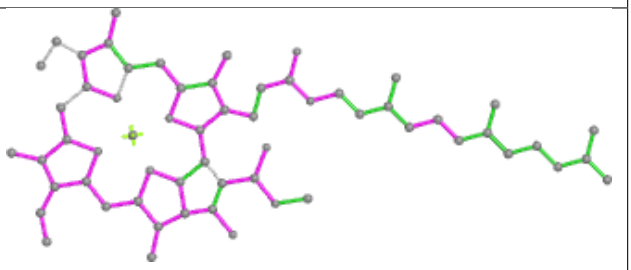
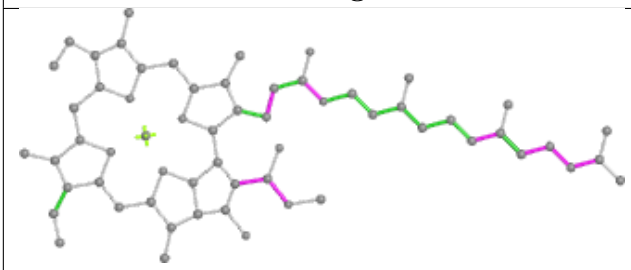
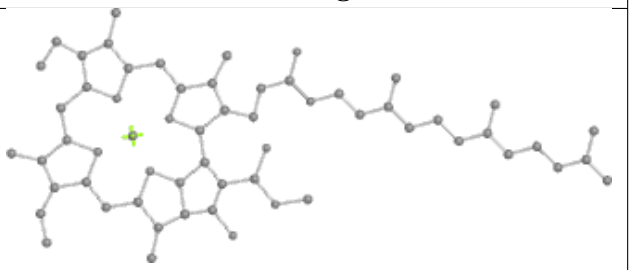
 Bond lengths	 Bond angles
 Torsions	 Rings

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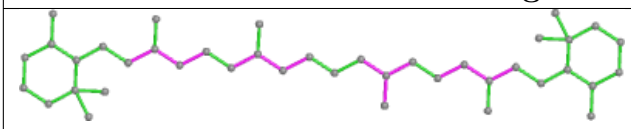
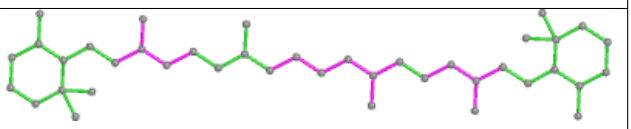
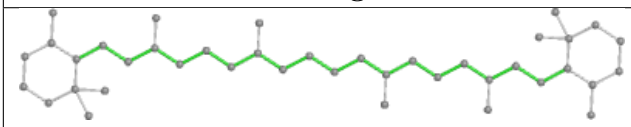
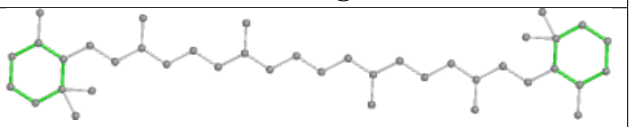
 Bond lengths	 Bond angles
 Torsions	 Rings

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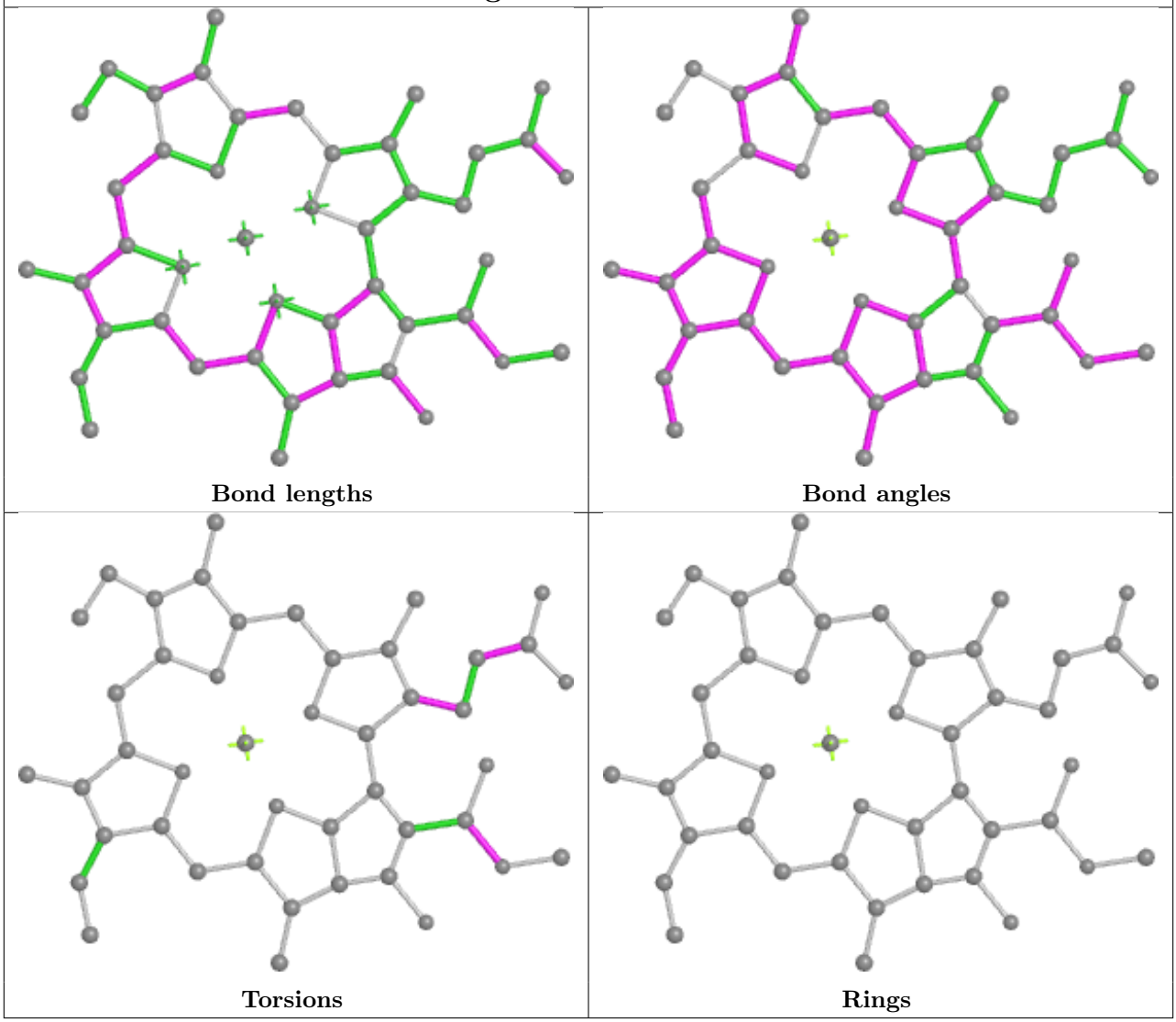

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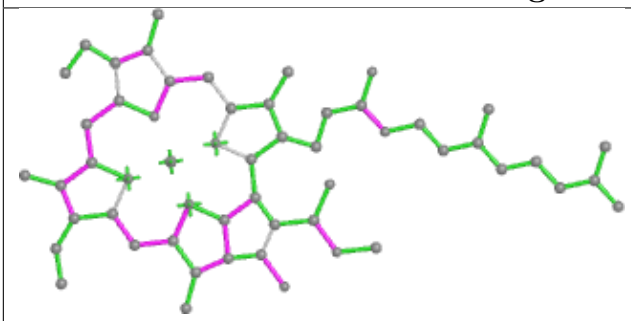
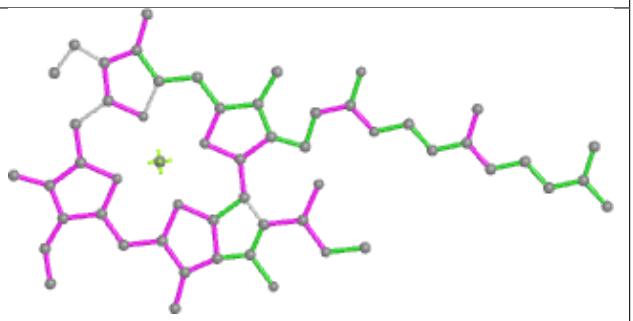
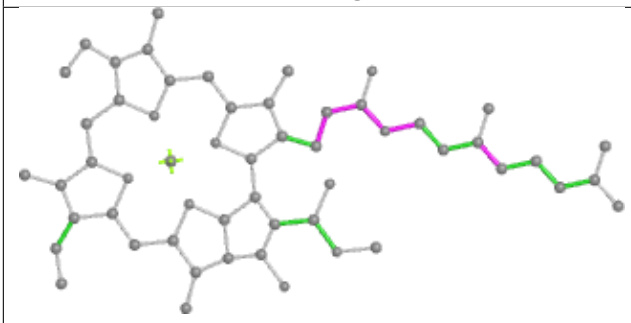
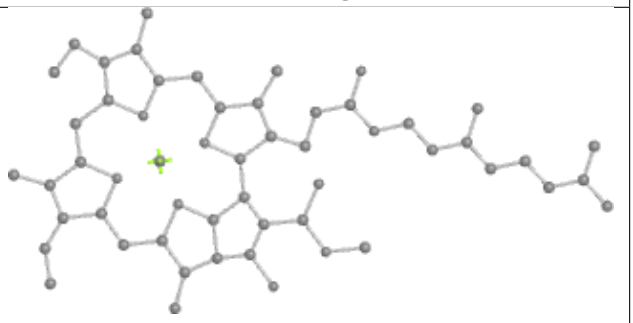
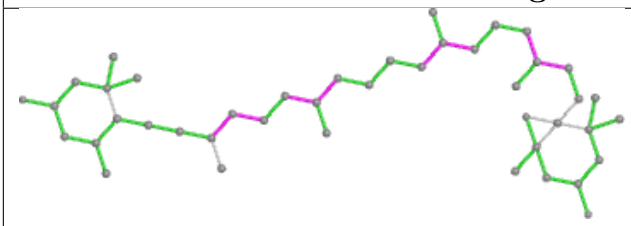
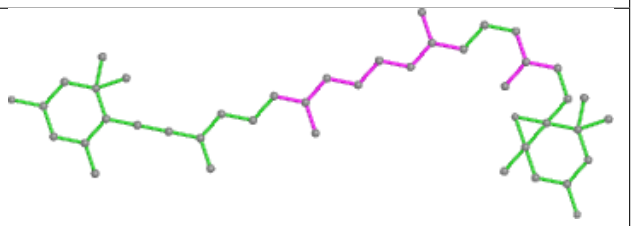
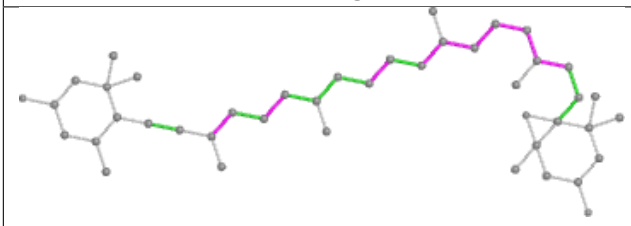
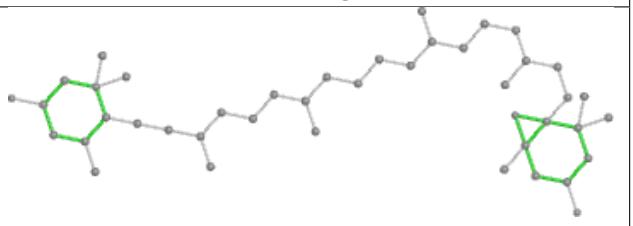
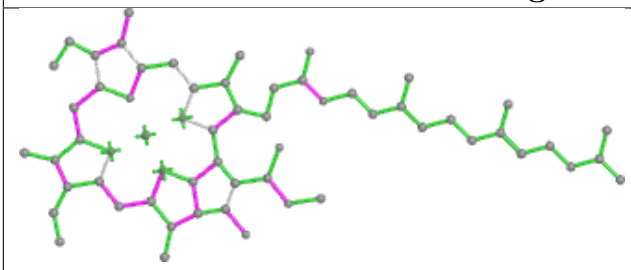
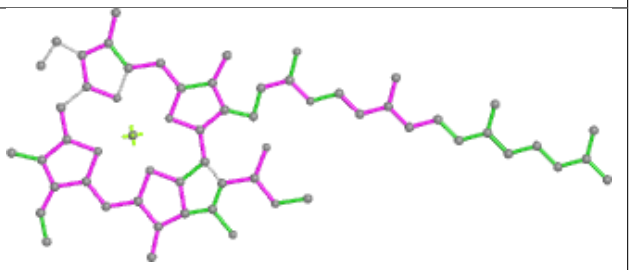
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 1 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 604



Bond lengths



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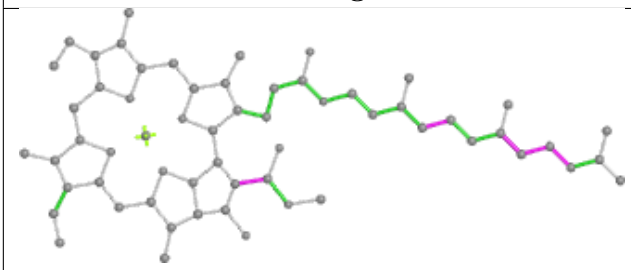

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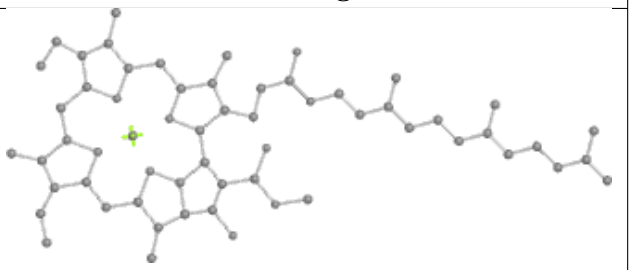
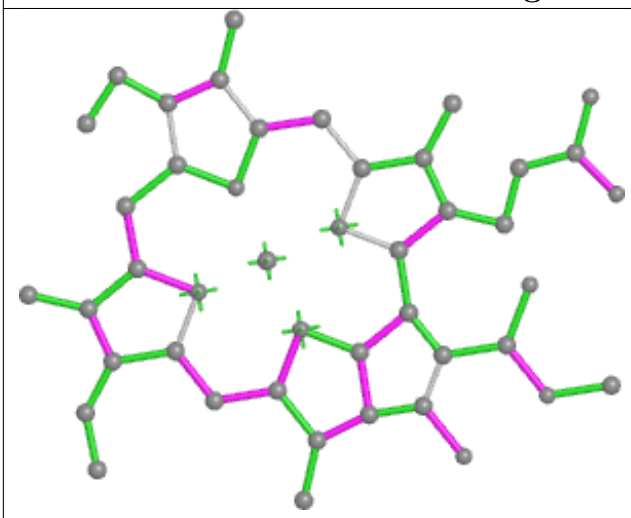


Rings

Ligand CLA A 837



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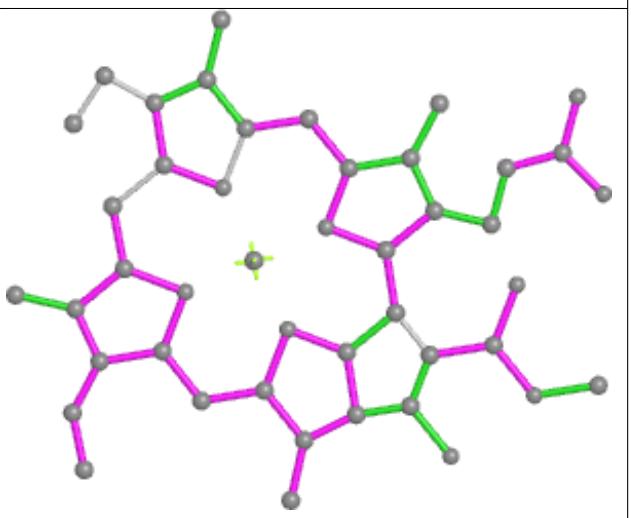

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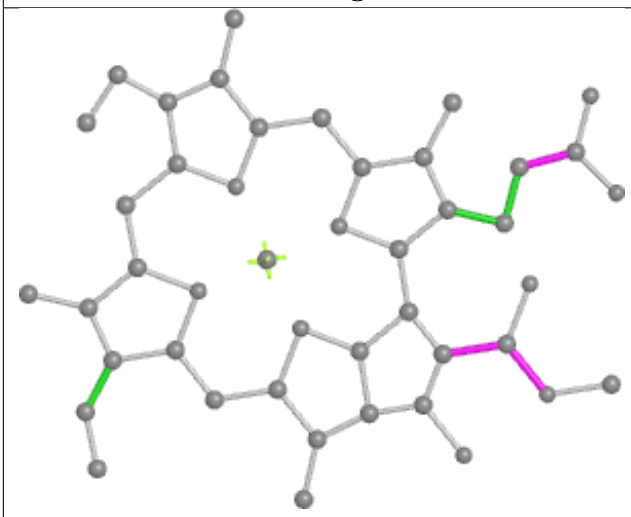

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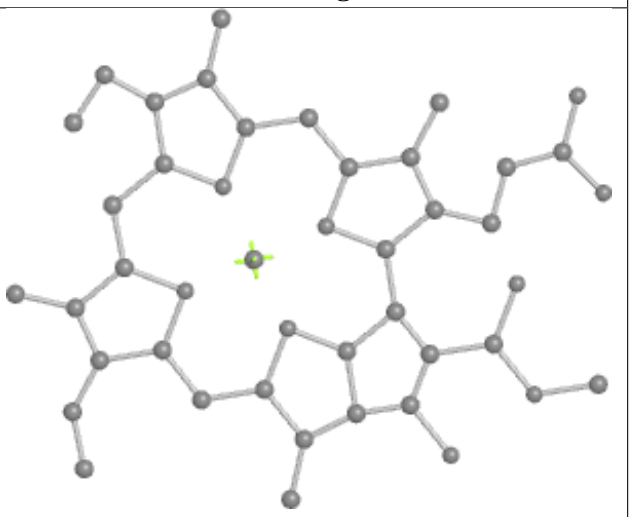
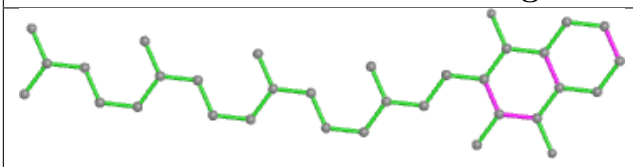


Rings

Ligand PQN A 845



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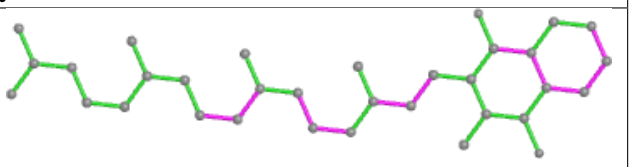

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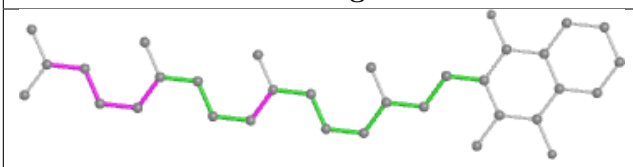

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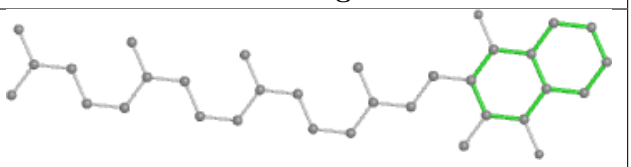

Rings

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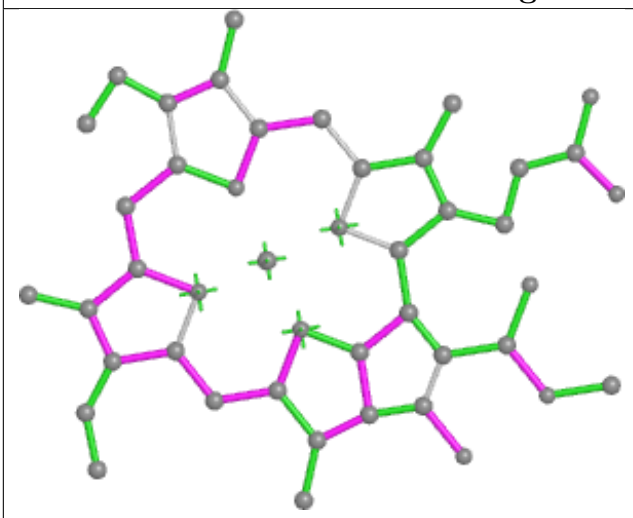

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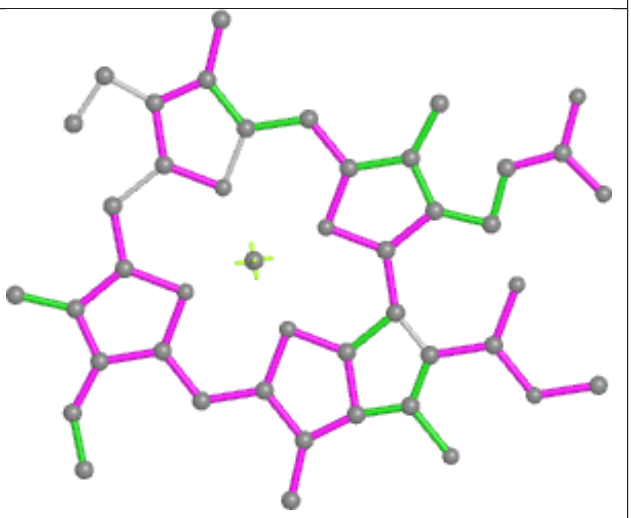
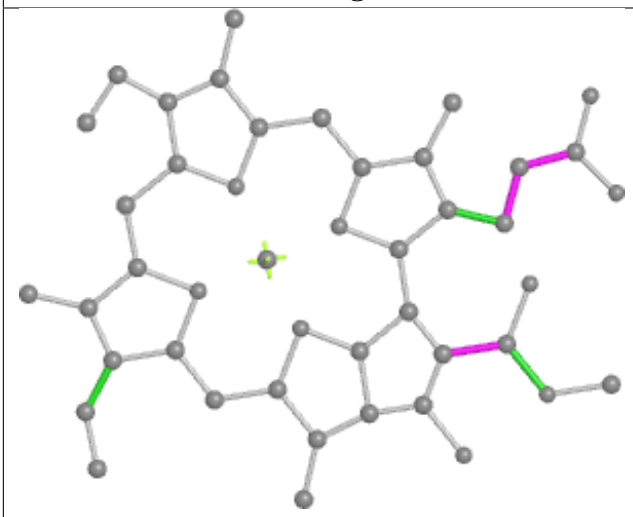


Bond angles



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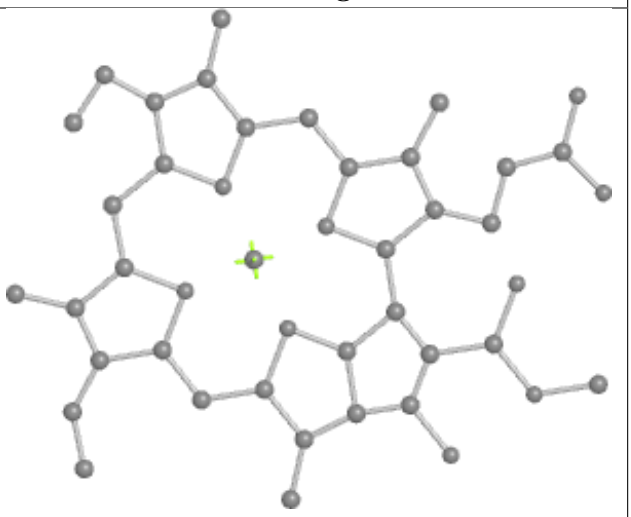

Rings

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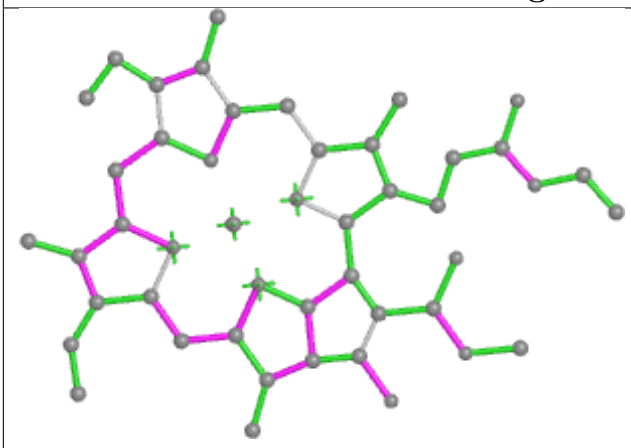	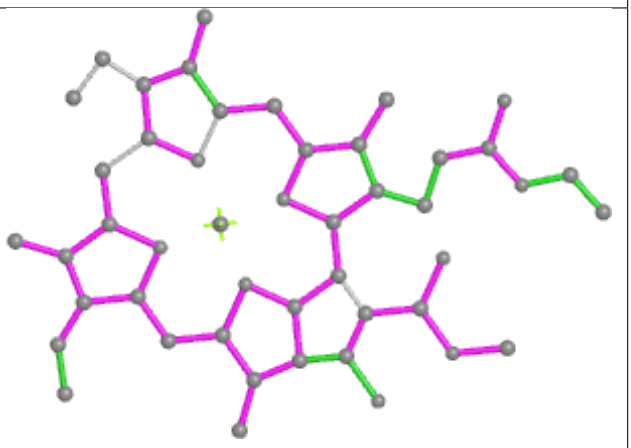
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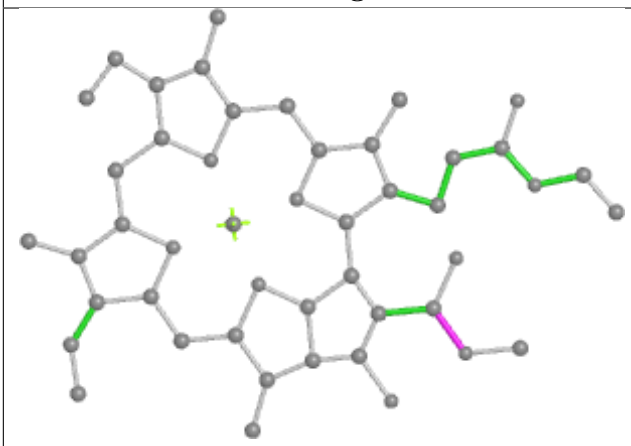
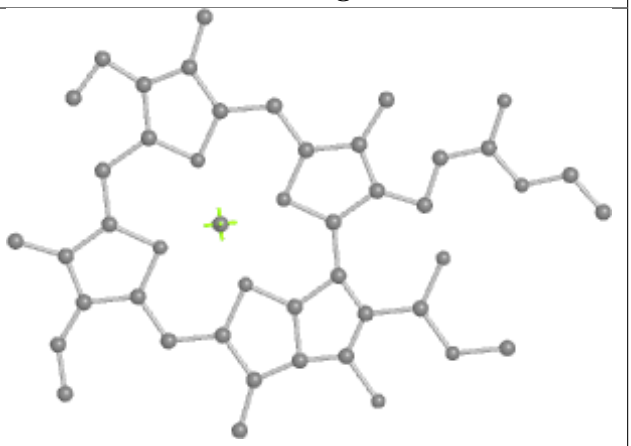
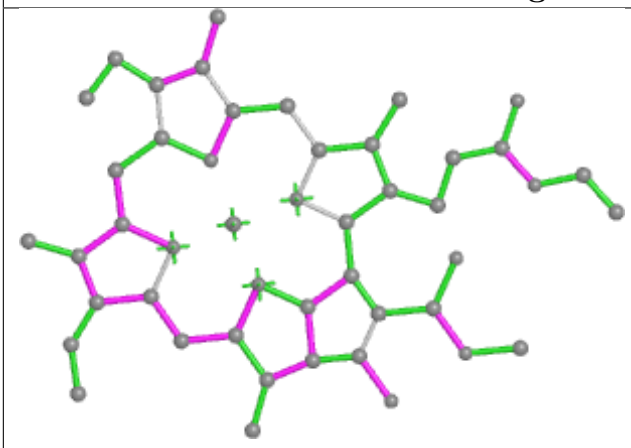
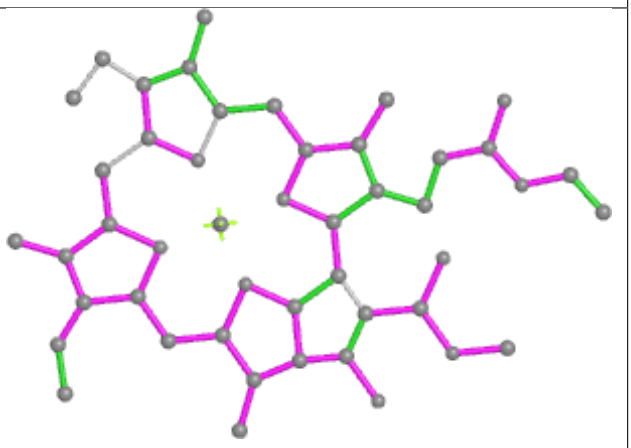
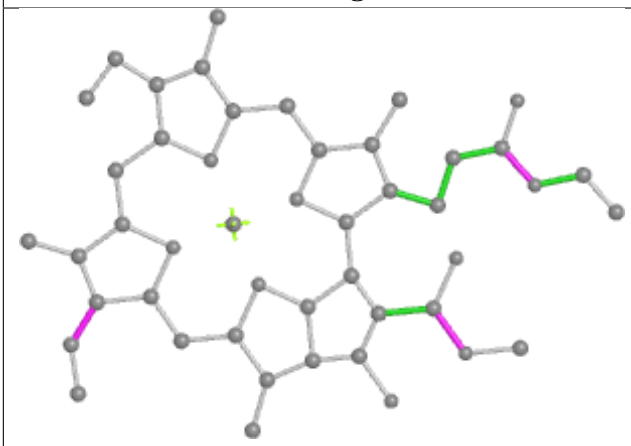
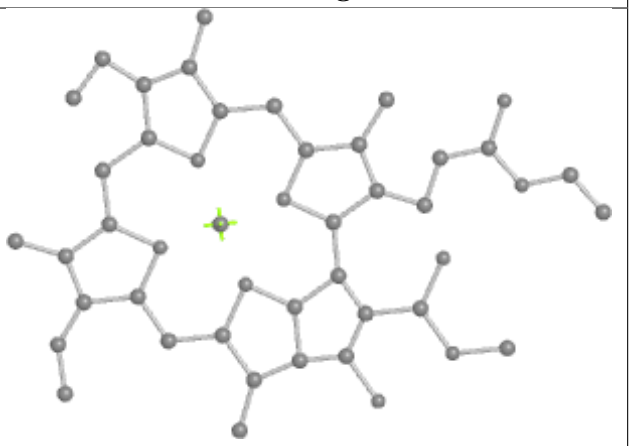
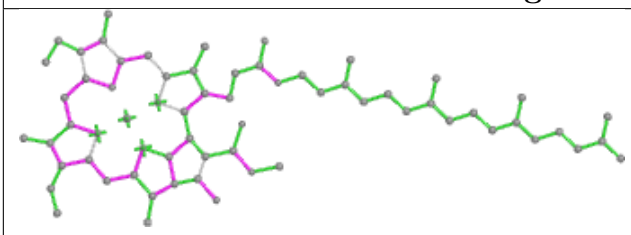
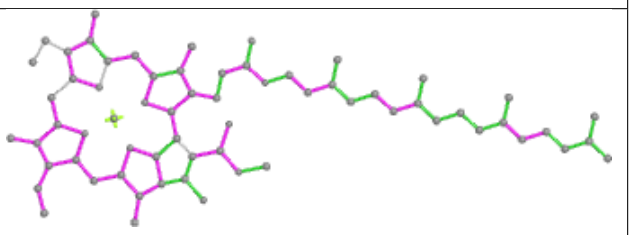
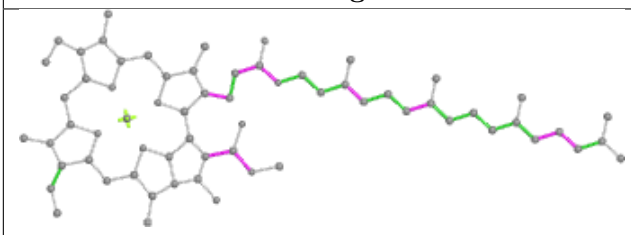
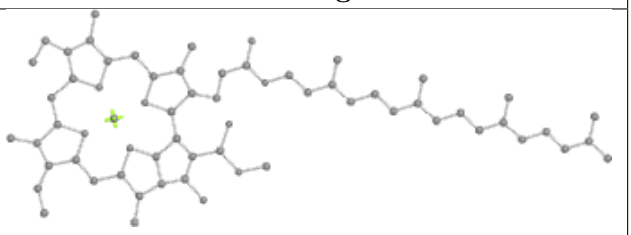
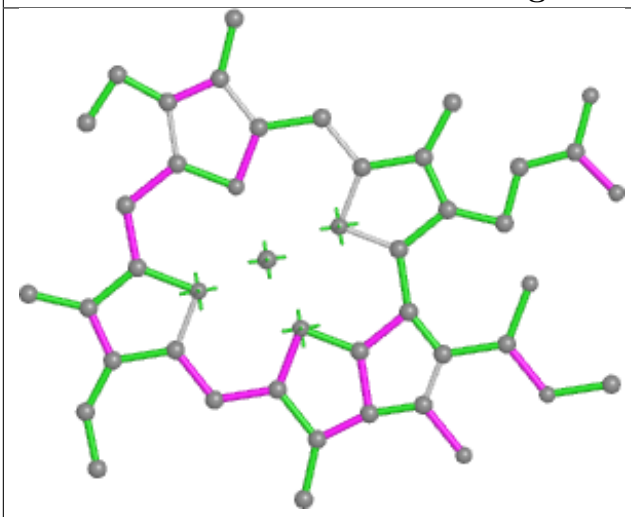
	
Torsions	**Rings**

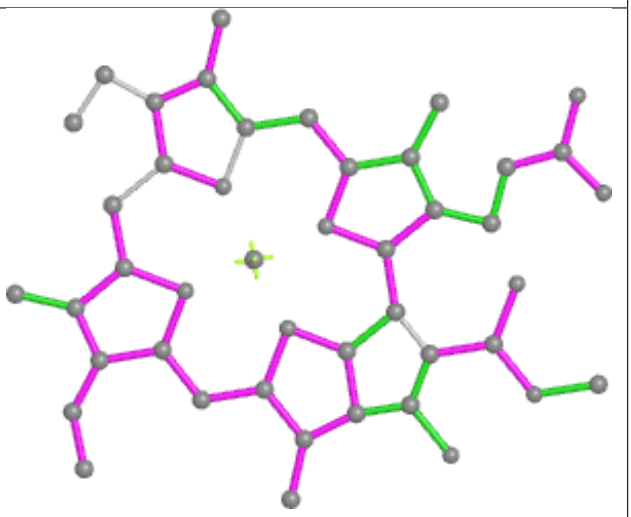
Ligand CLA 7 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

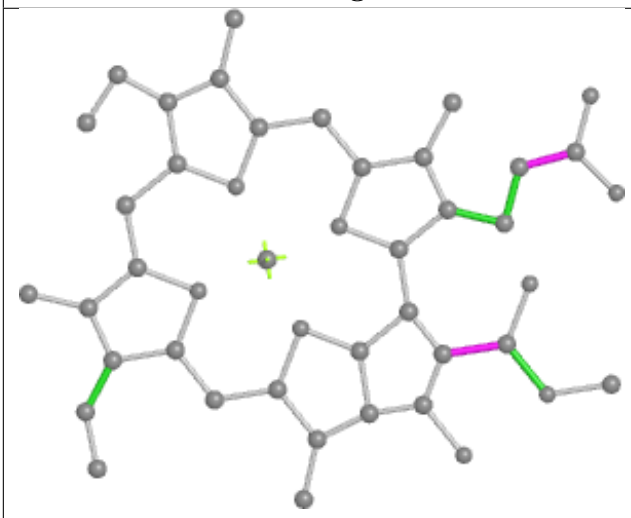
Ligand CLA 6 911



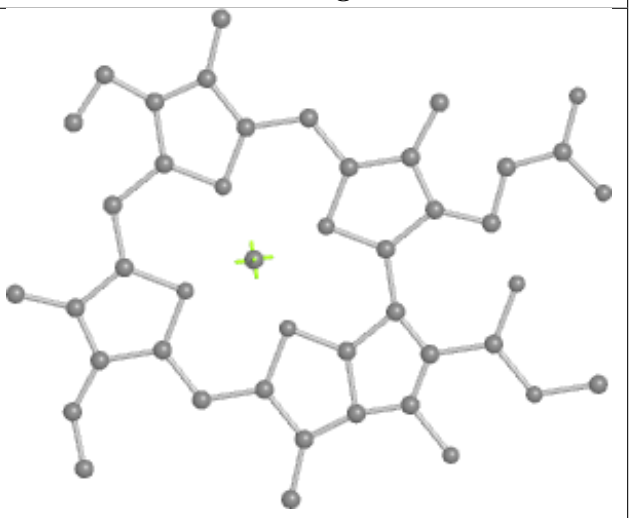
Bond lengths



Bond angles

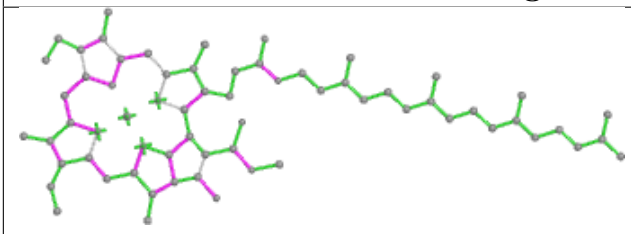


Torsions



Rings

Ligand CLA A 810



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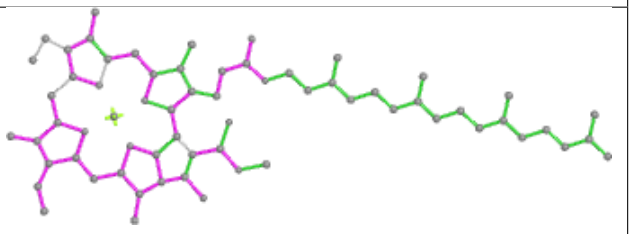
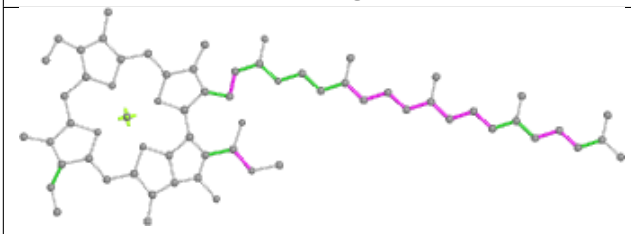
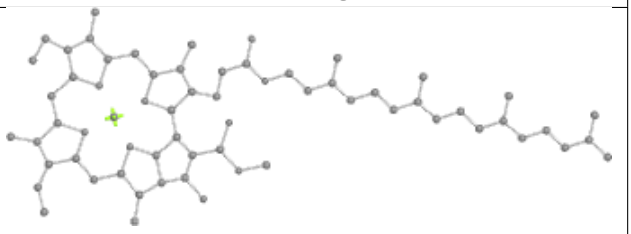


Bond angles

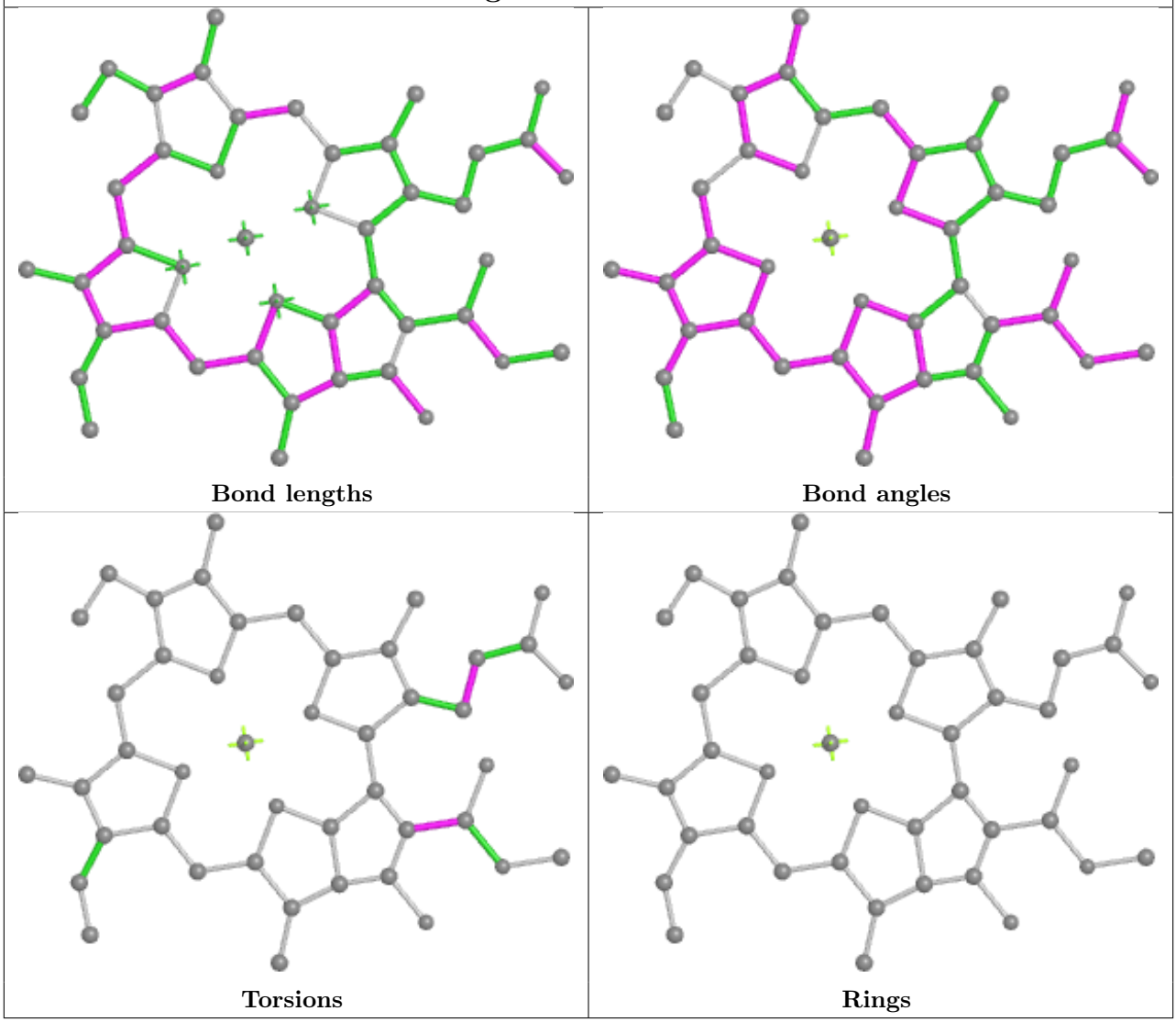


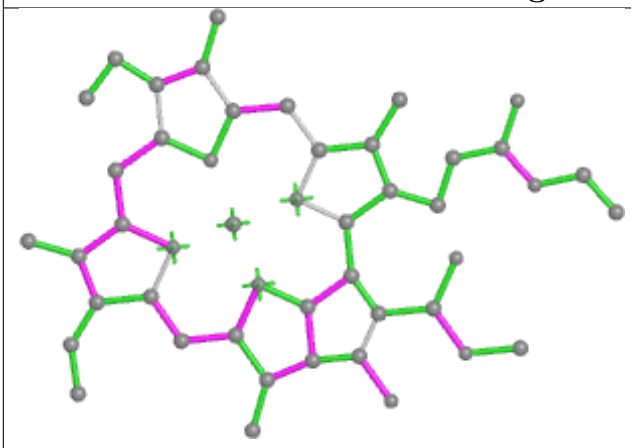
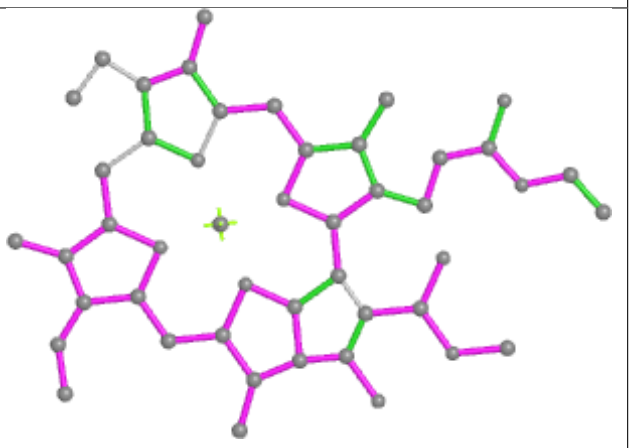
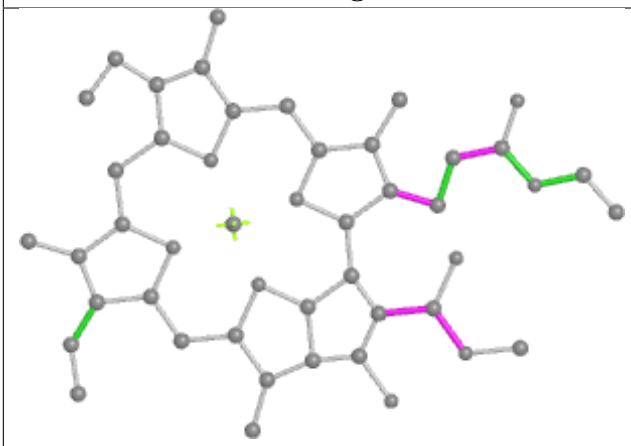
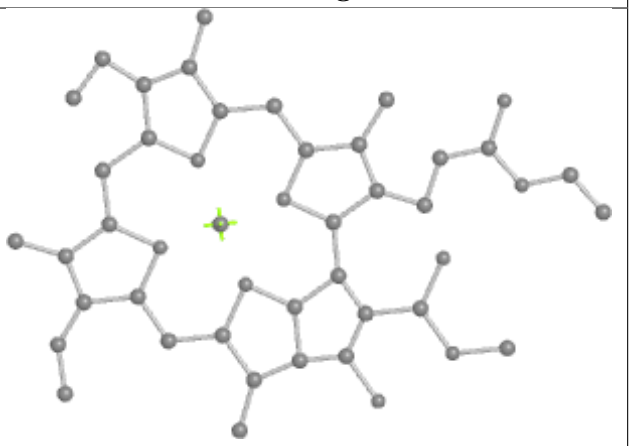
Torsions



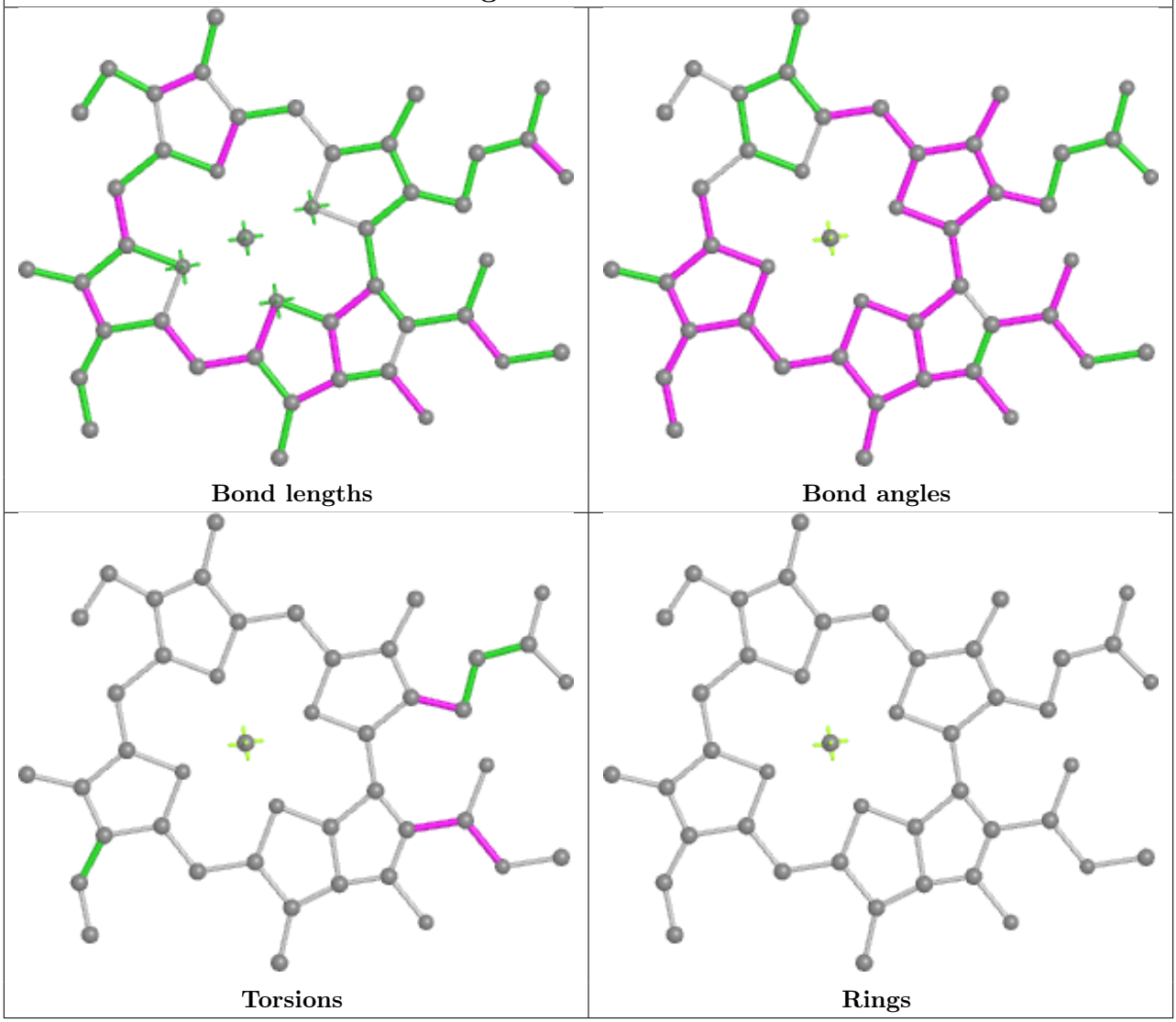
Rings

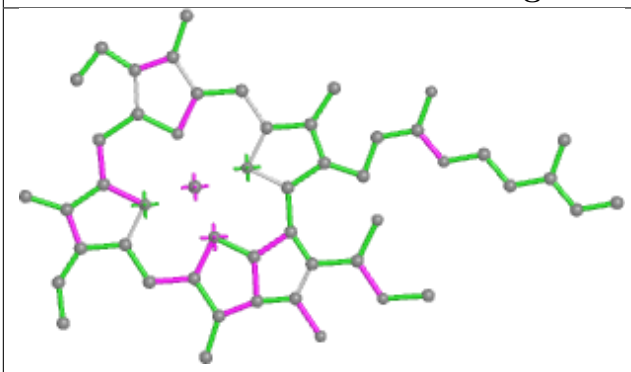
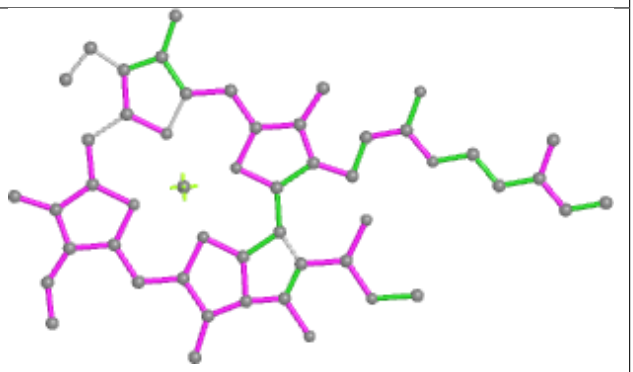
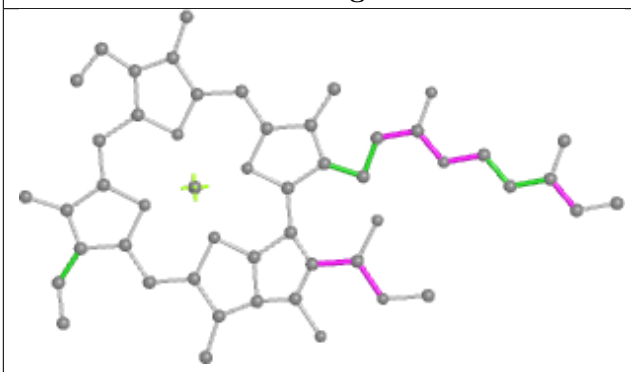
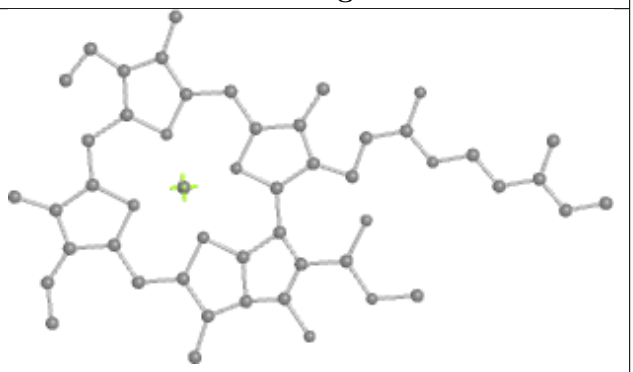
Ligand CLA 2 517

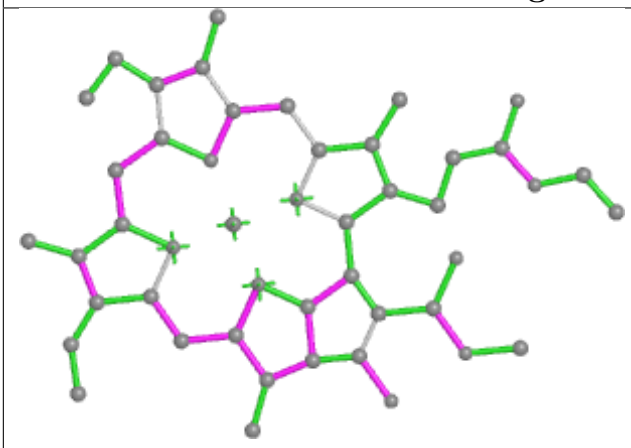
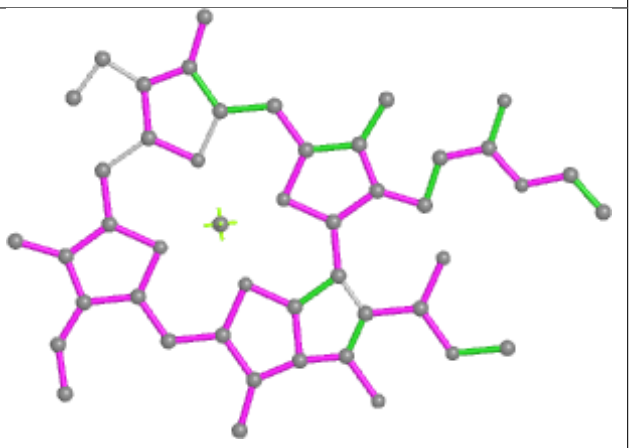
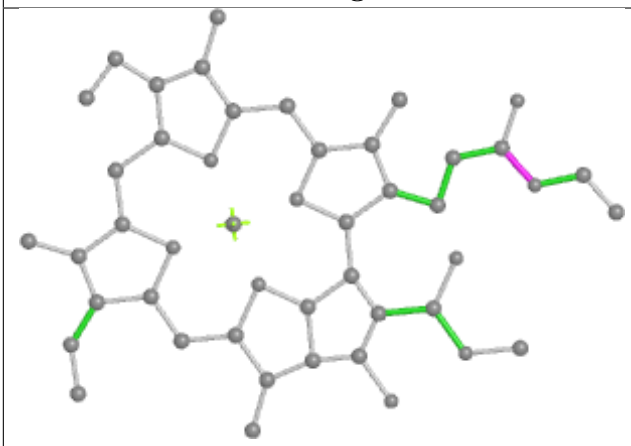
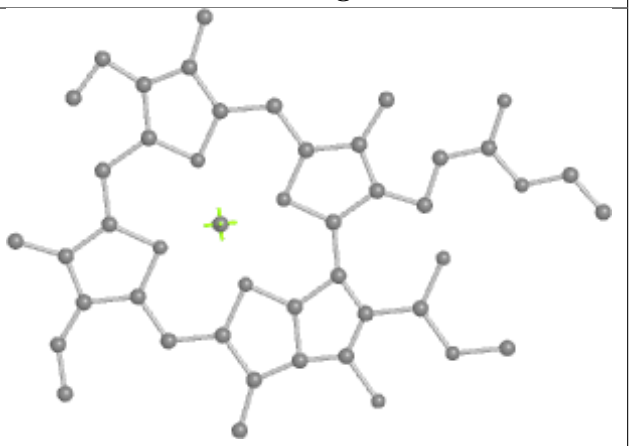


Ligand CLA 3 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

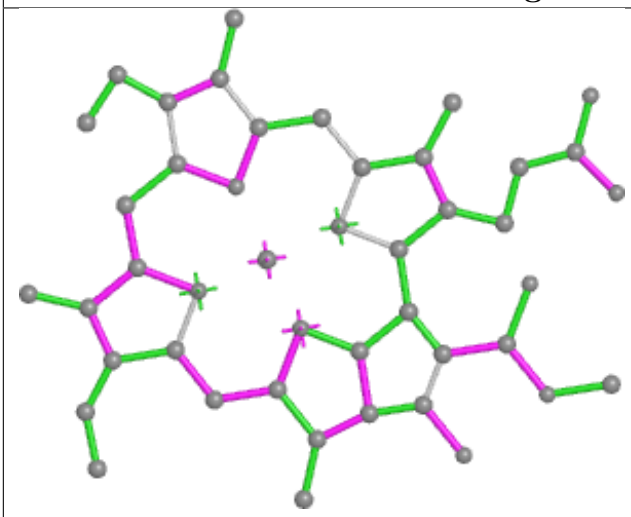
Ligand CLA A 811



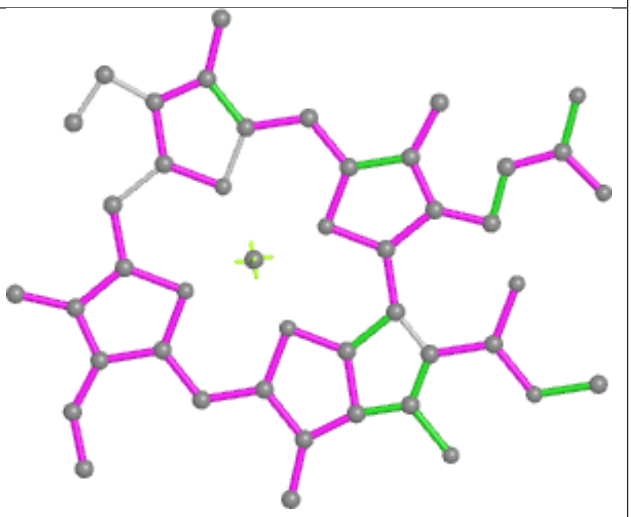
Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

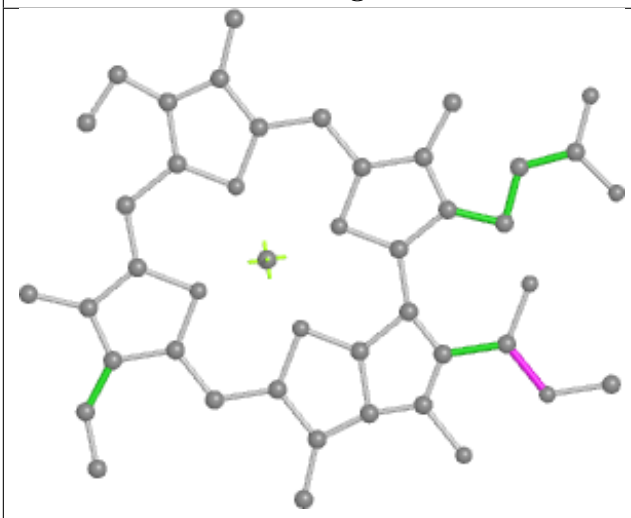
Ligand CLA B 814



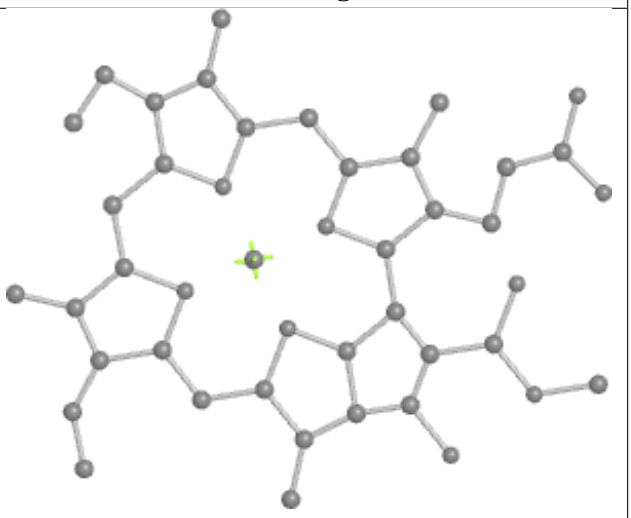
Bond lengths



Bond angles

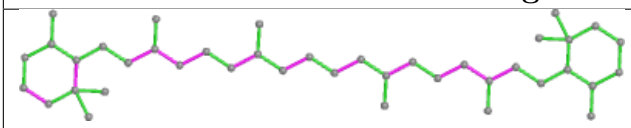


Torsions

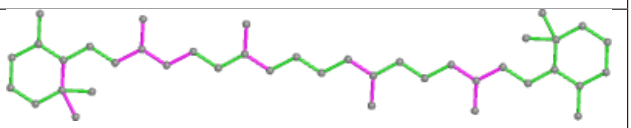


Rings

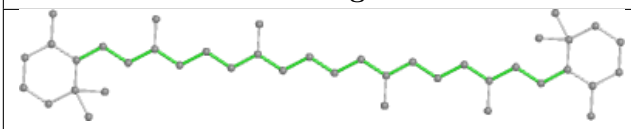
Ligand BCR A 851



Bond lengths

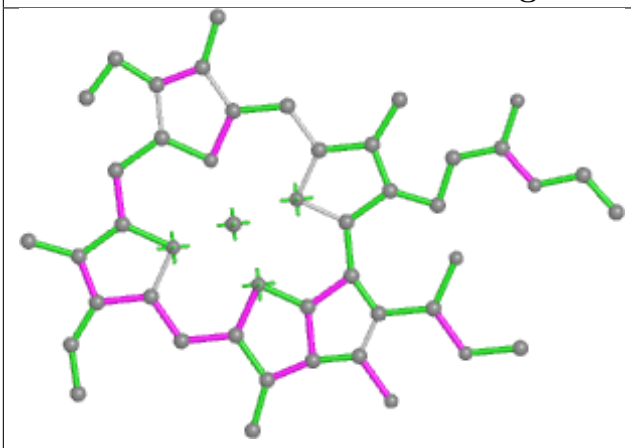
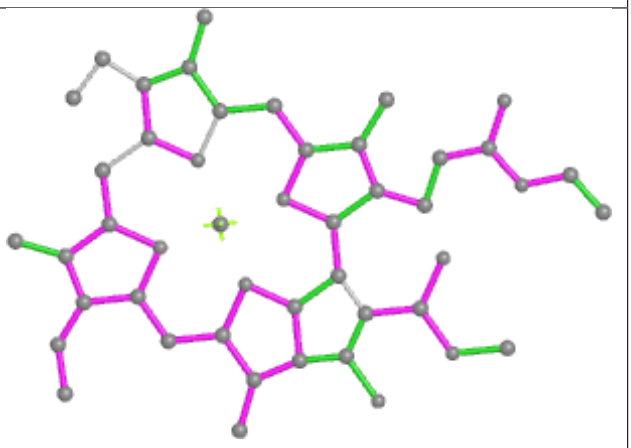
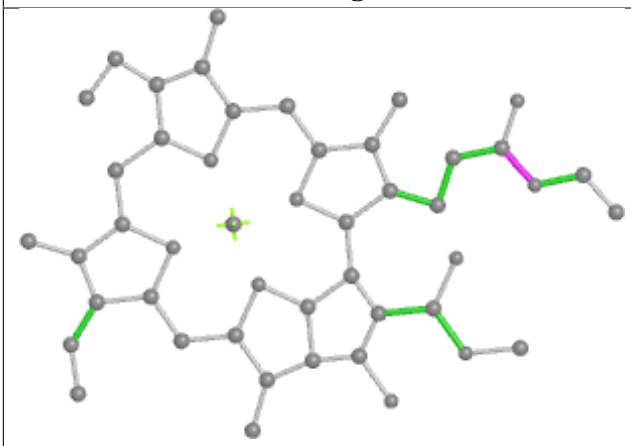
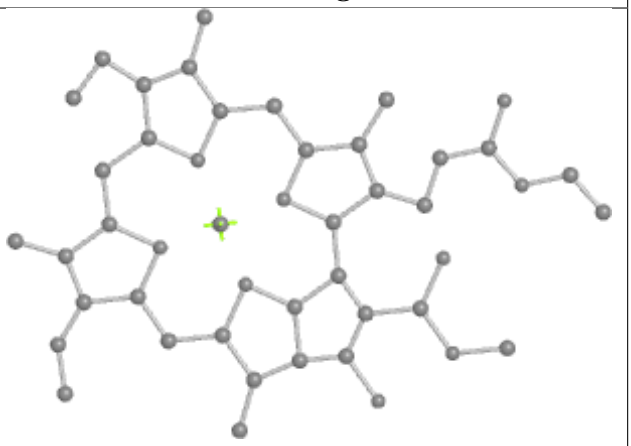


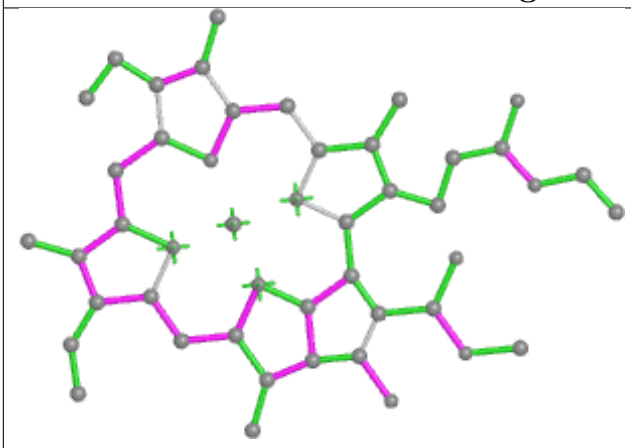
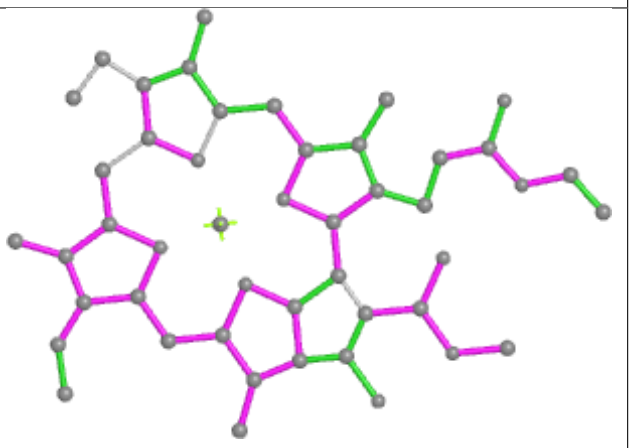
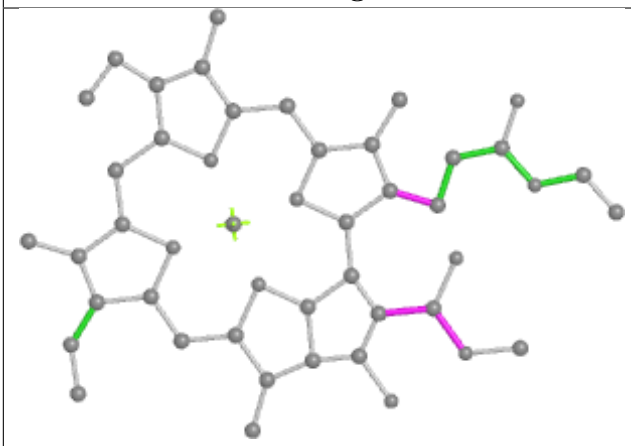
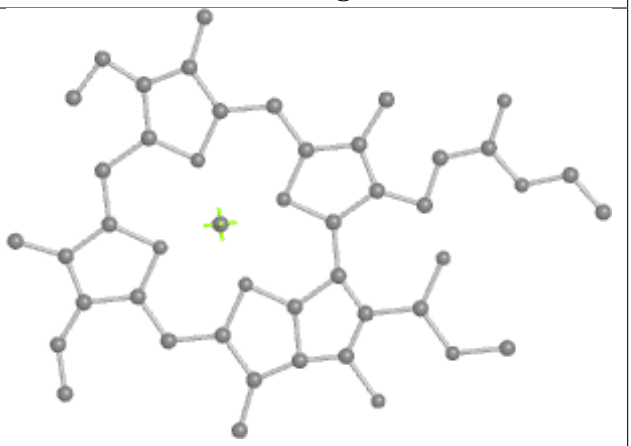
Bond angles

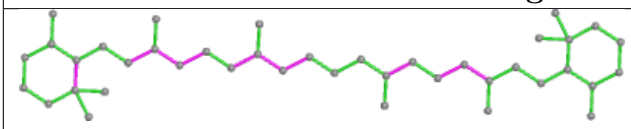
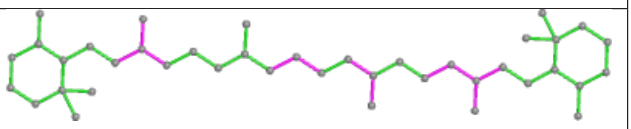
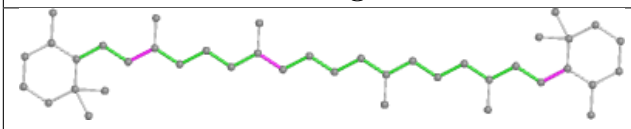
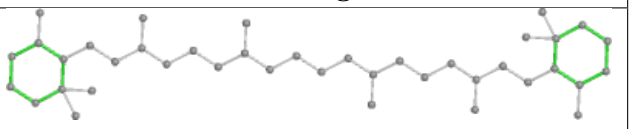


Torsions

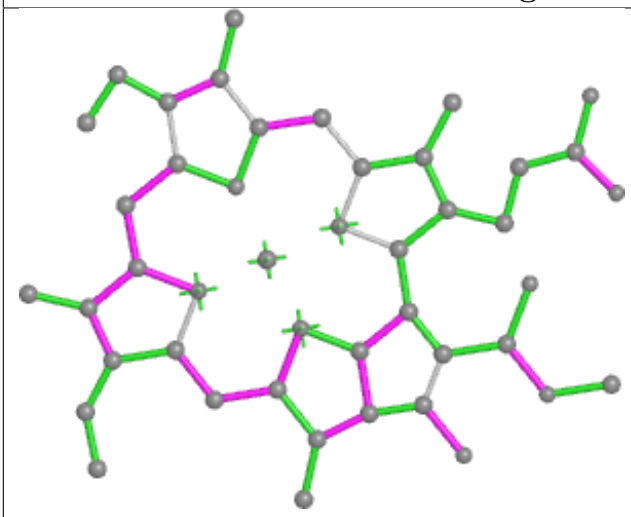
Rings

Ligand CLA 12 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

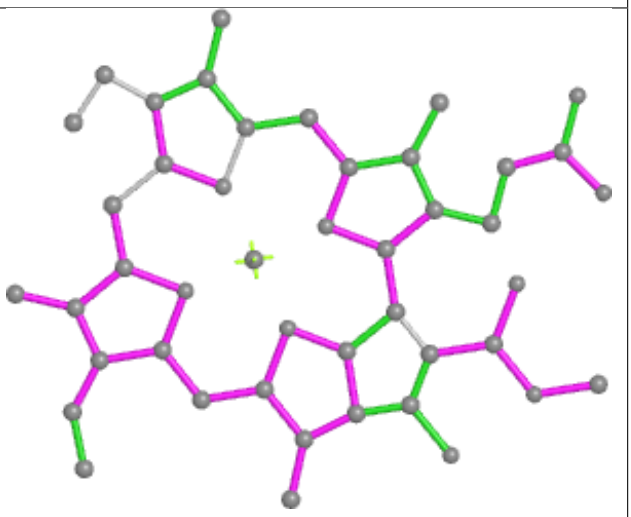
Ligand CLA 13 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

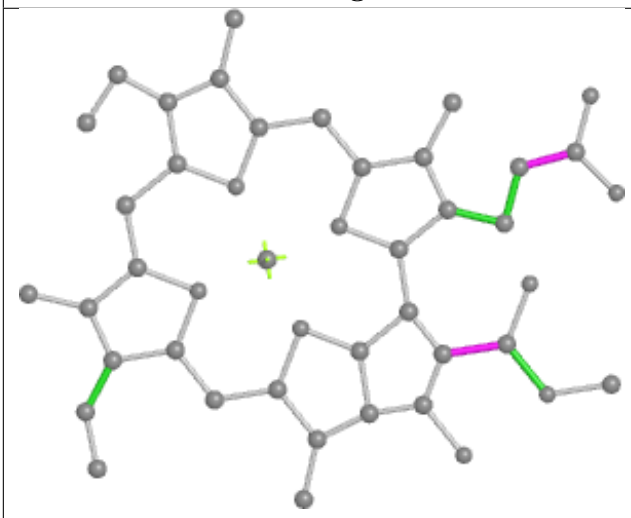
Ligand CLA 10 709



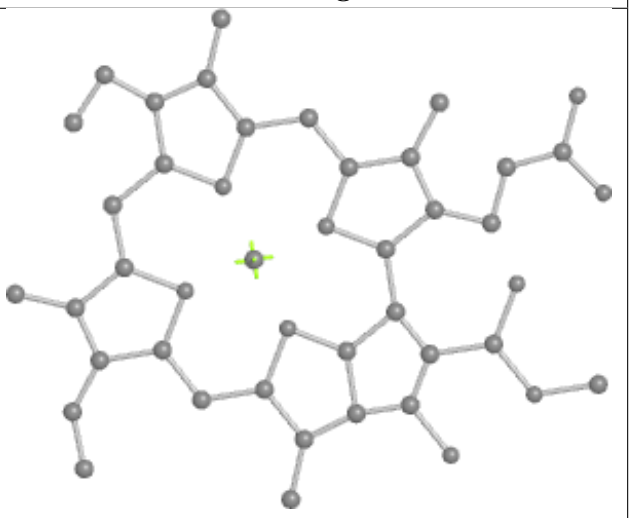
Bond lengths



Bond angles

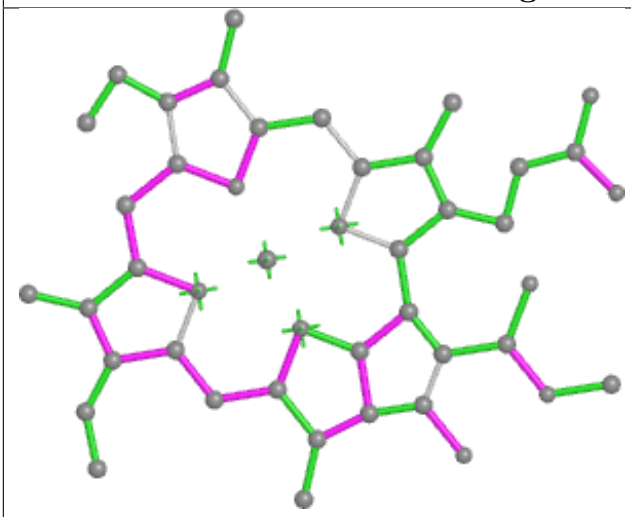


Torsions

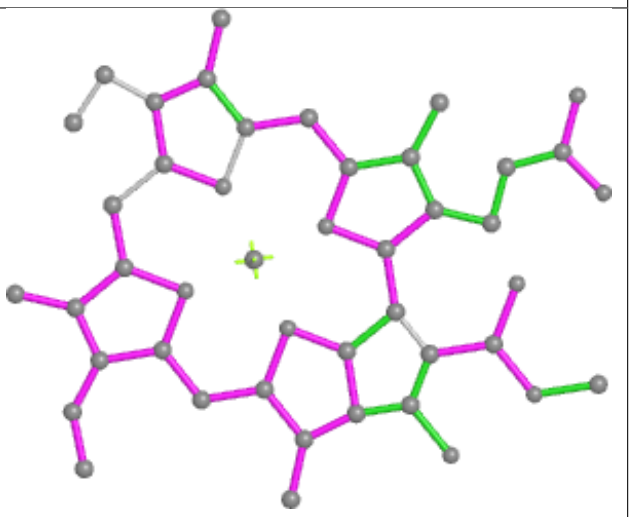


Rings

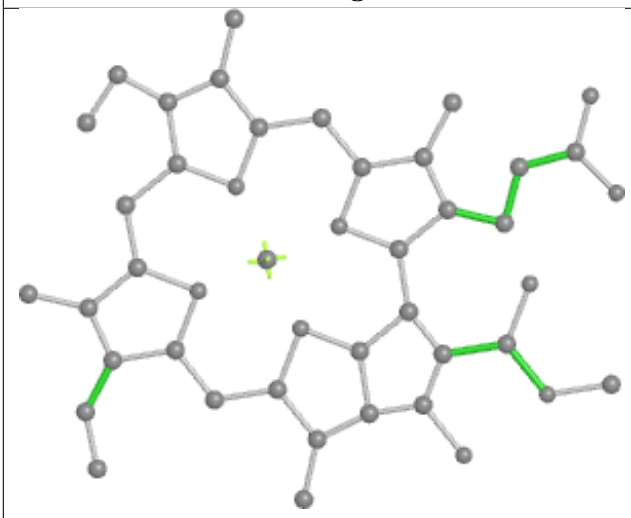
Ligand CLA 11 704



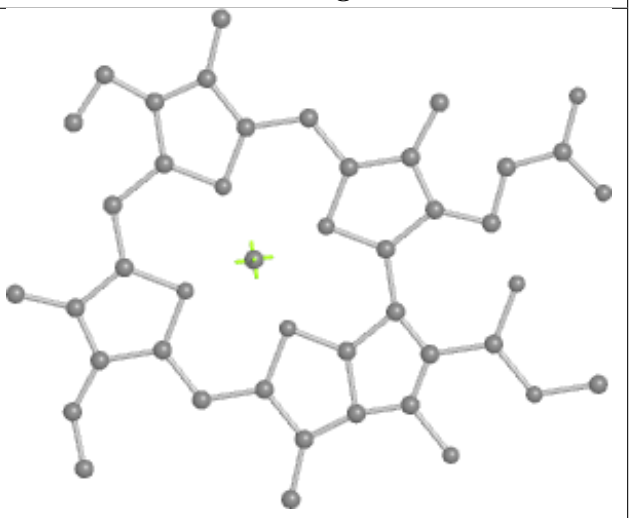
Bond lengths



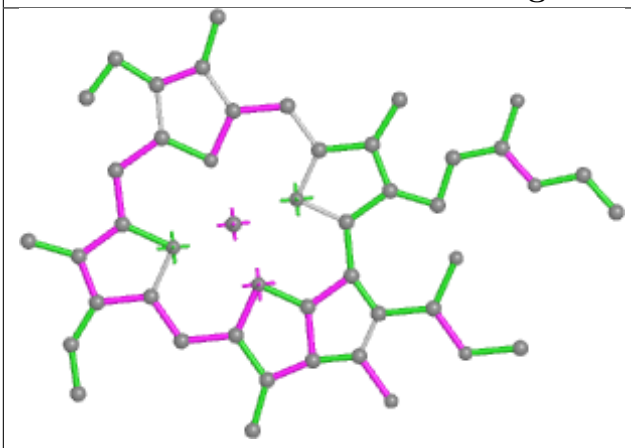
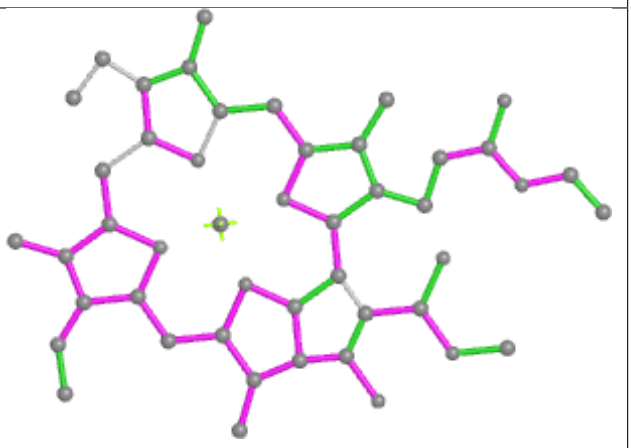
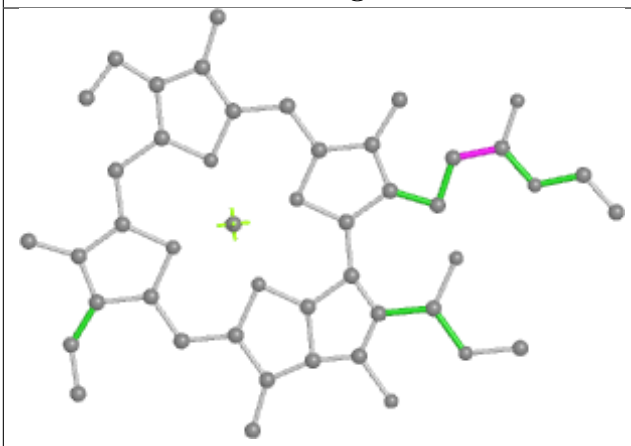
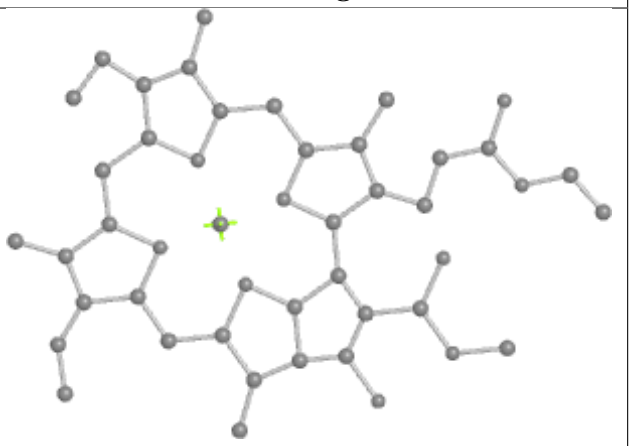
Bond angles



Torsions



Rings

Ligand CLA 8 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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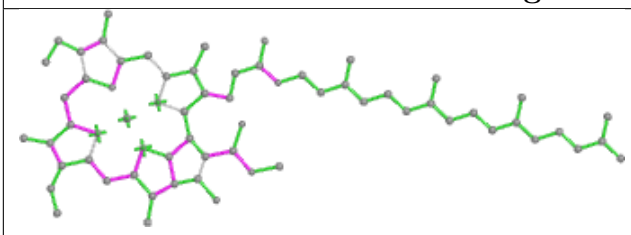
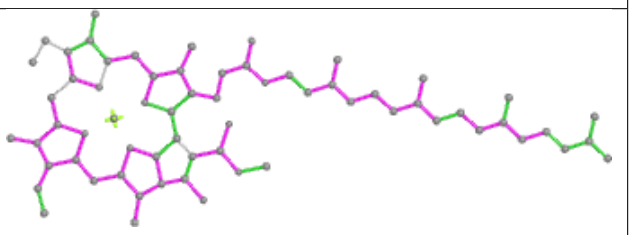
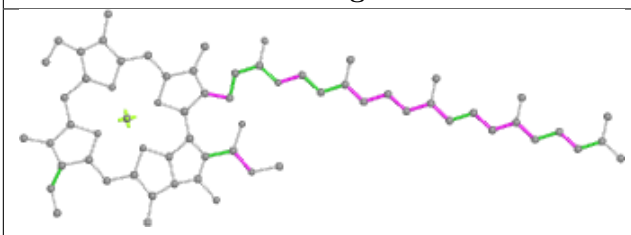
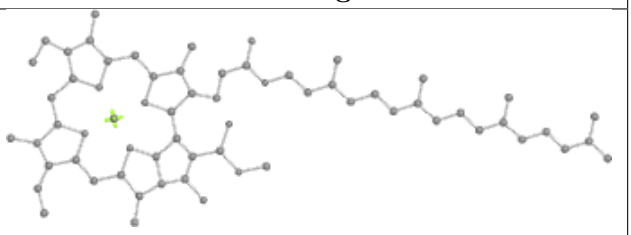
 Bond lengths	 Bond angles
 Torsions	 Rings

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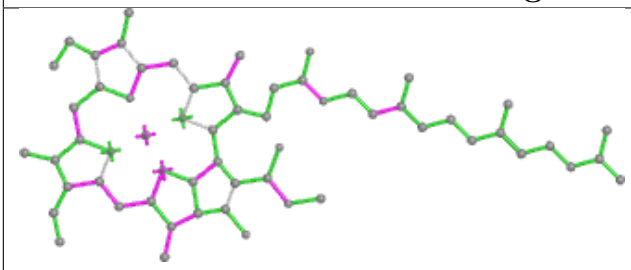
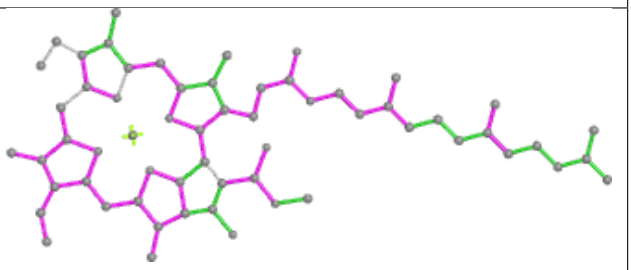
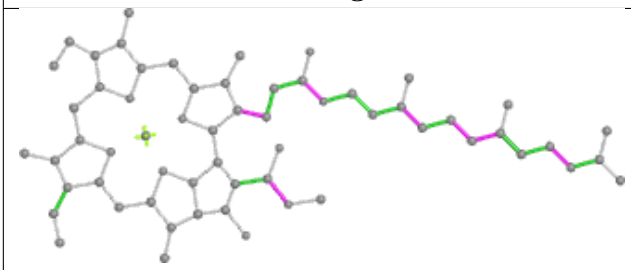
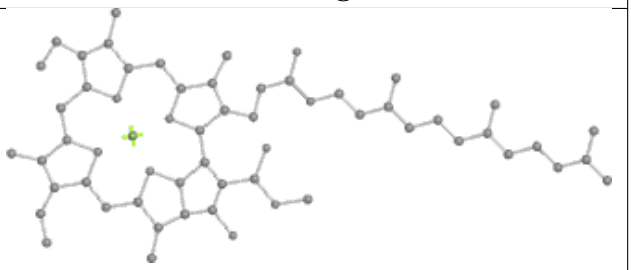
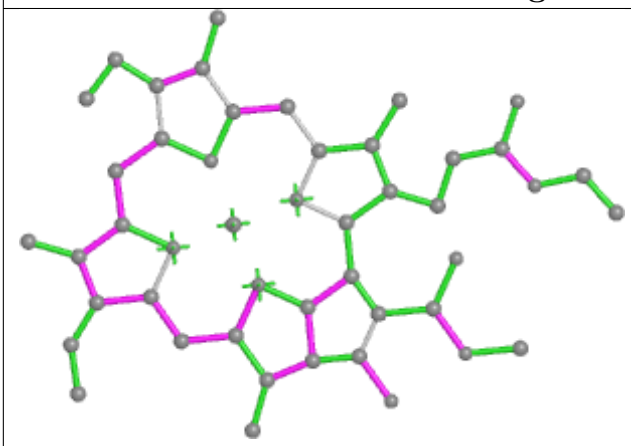
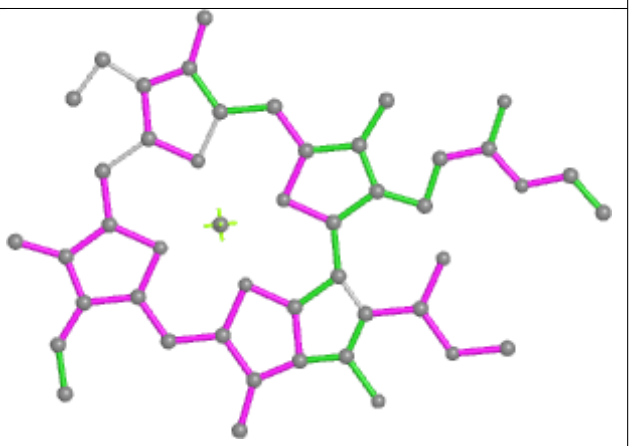
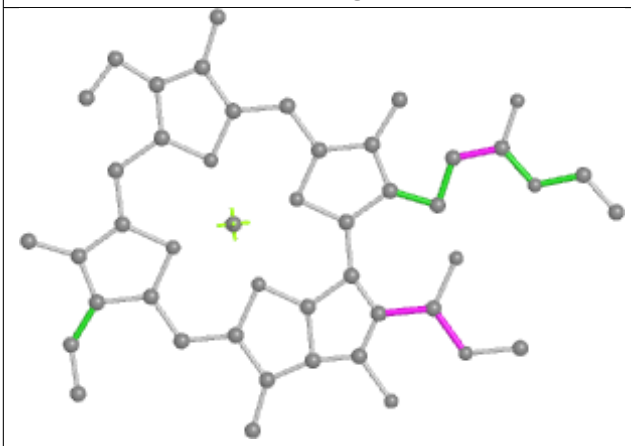
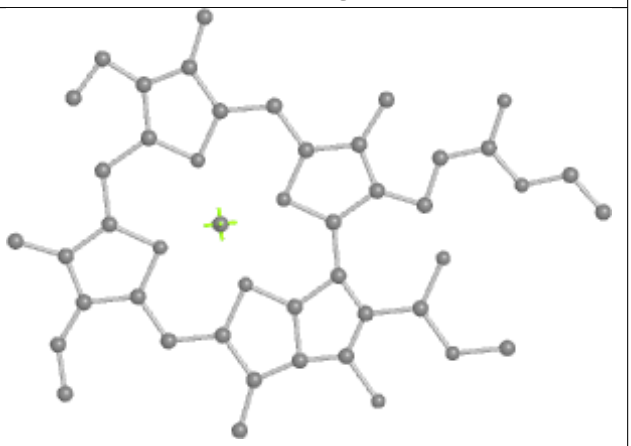
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 914	
 Bond lengths	 Bond angles
 Torsions	 Rings

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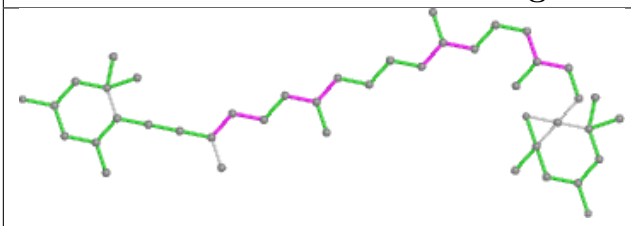
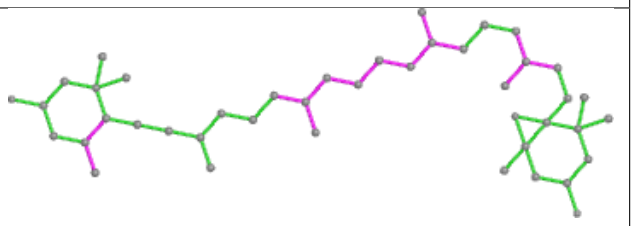
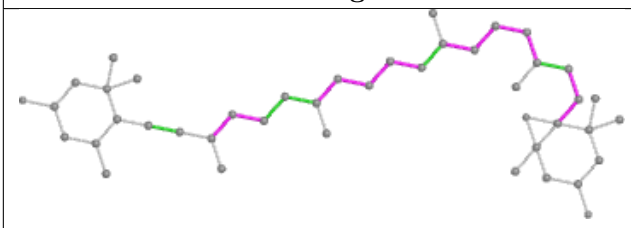
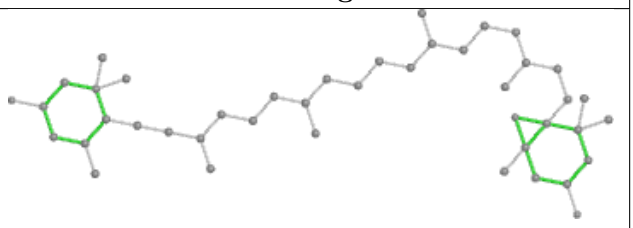
 Bond lengths	 Bond angles
 Torsions	 Rings

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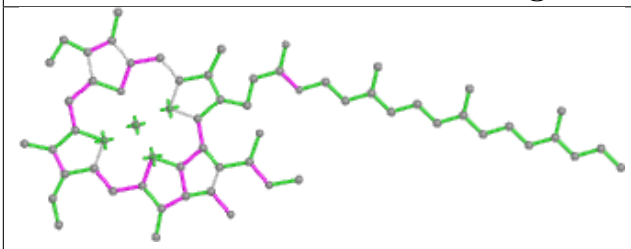
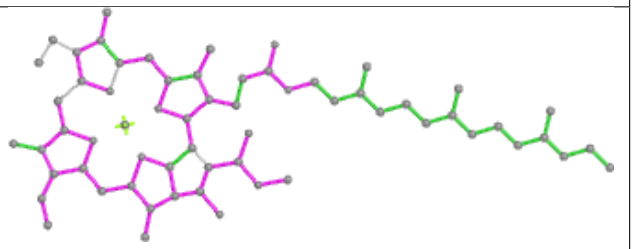
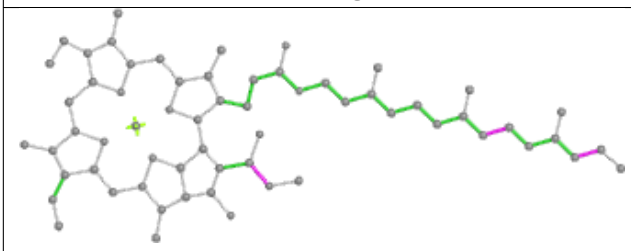
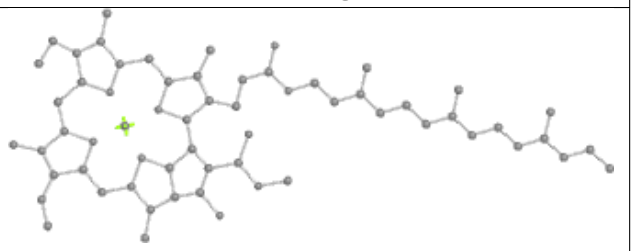
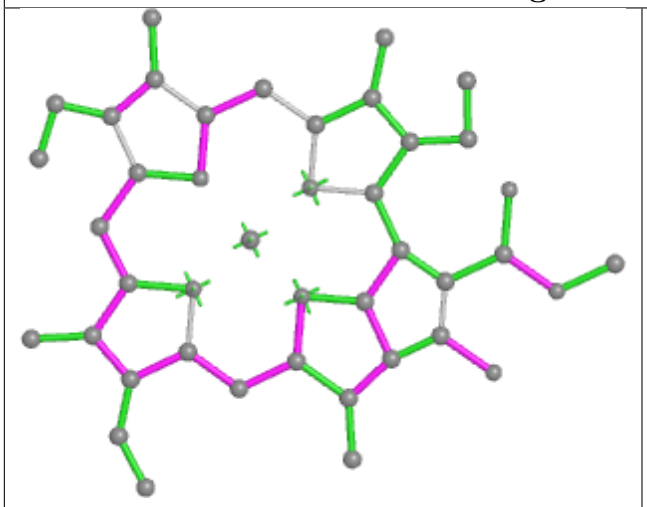
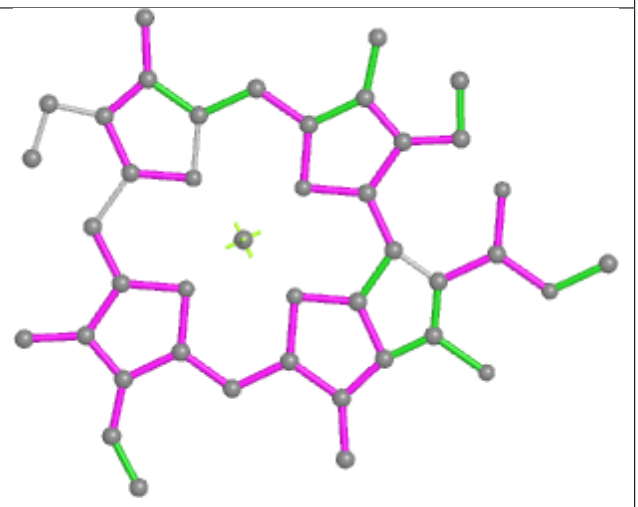
 Bond lengths	 Bond angles
 Torsions	 Rings

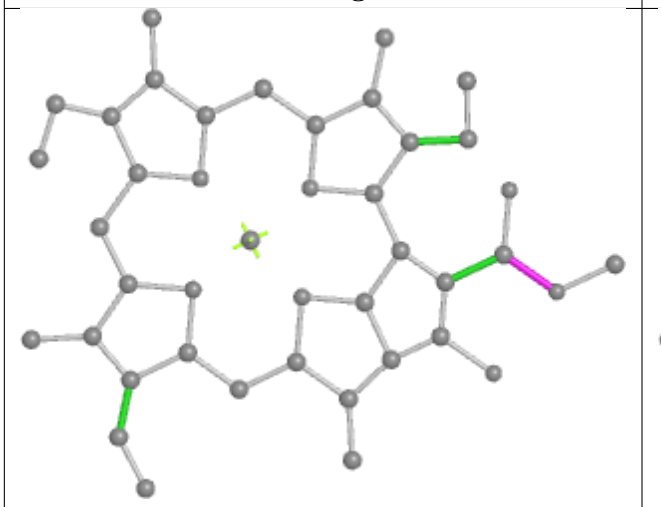
Ligand CLA 1 504



Bond lengths



Bond angles



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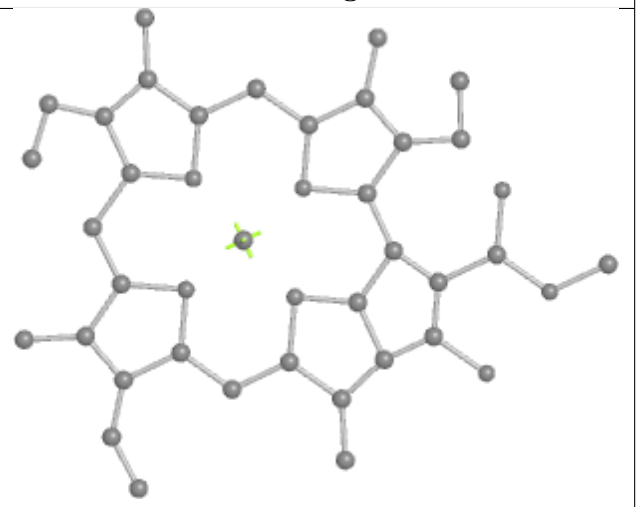
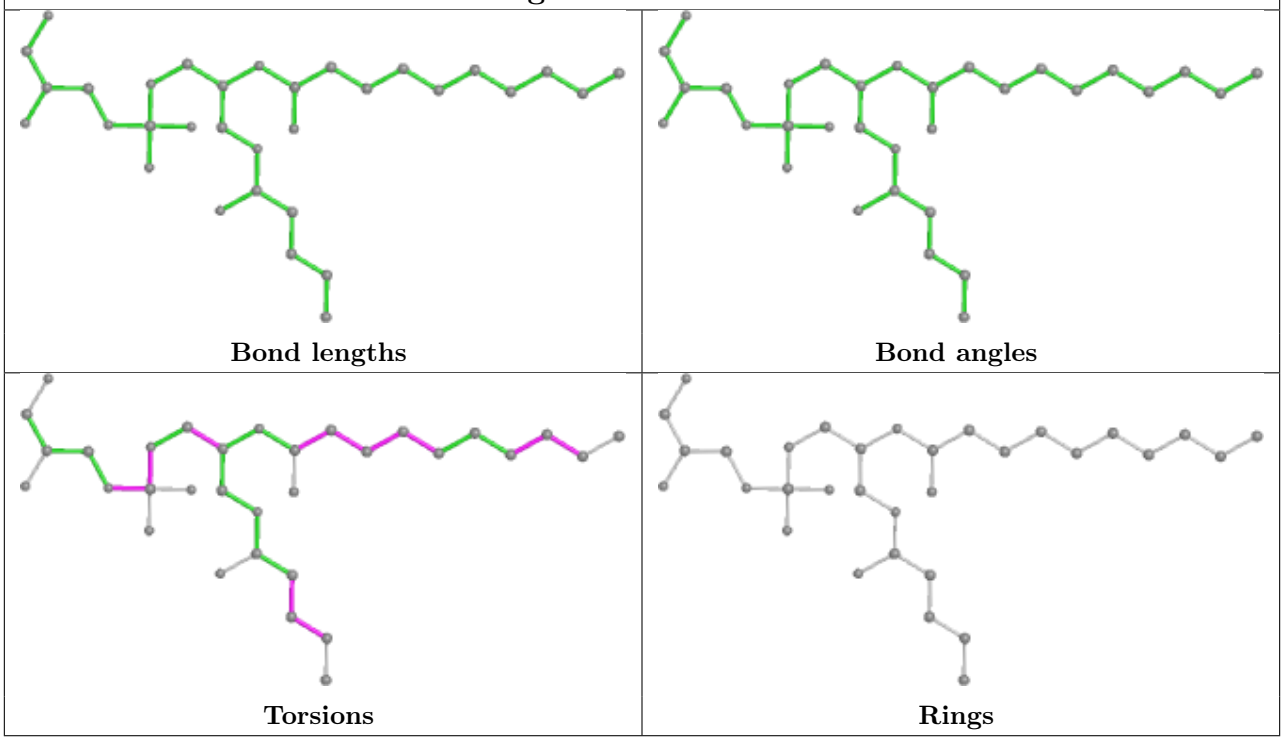
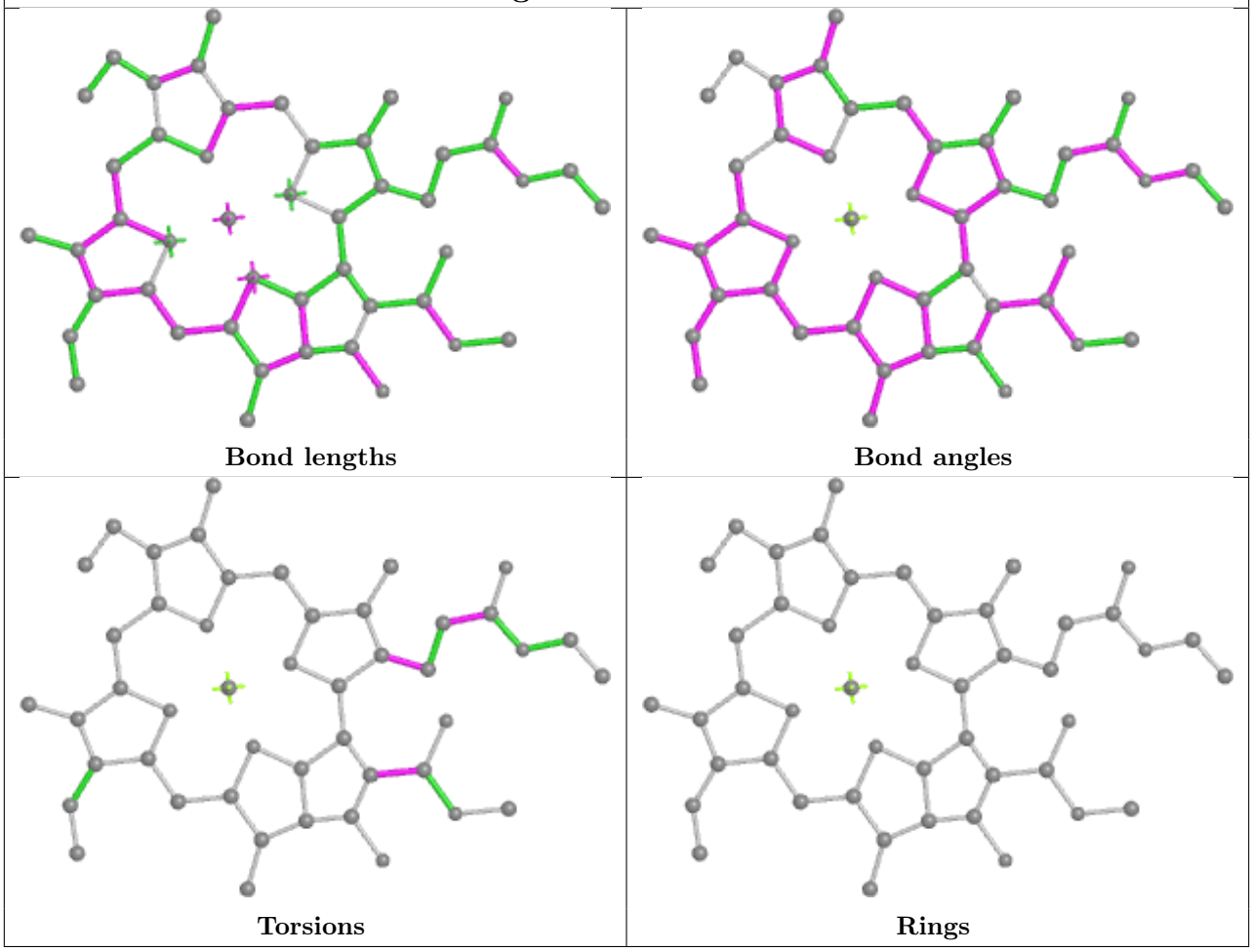


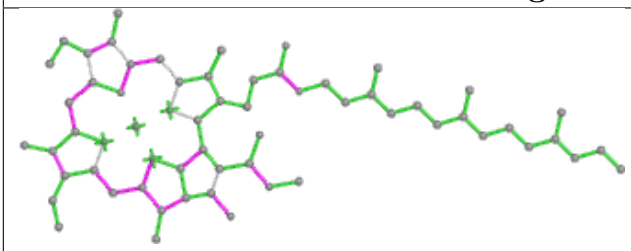
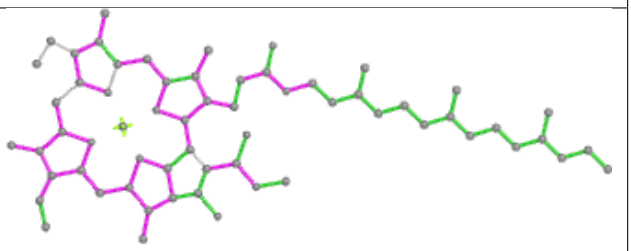
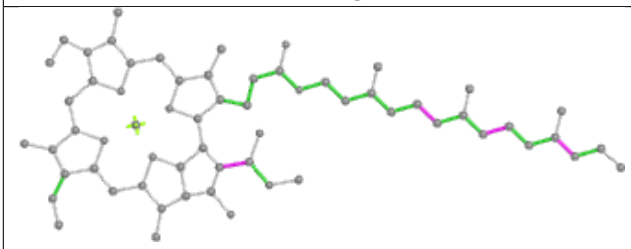
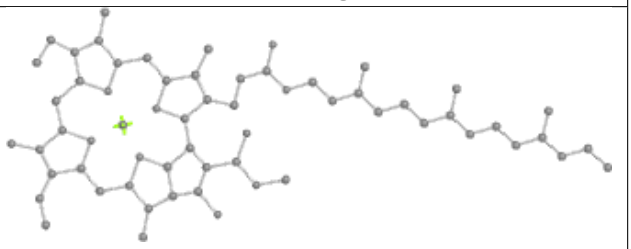
Rings

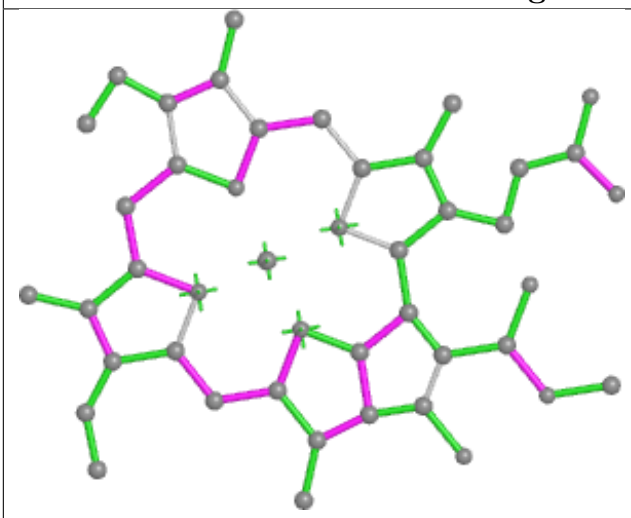
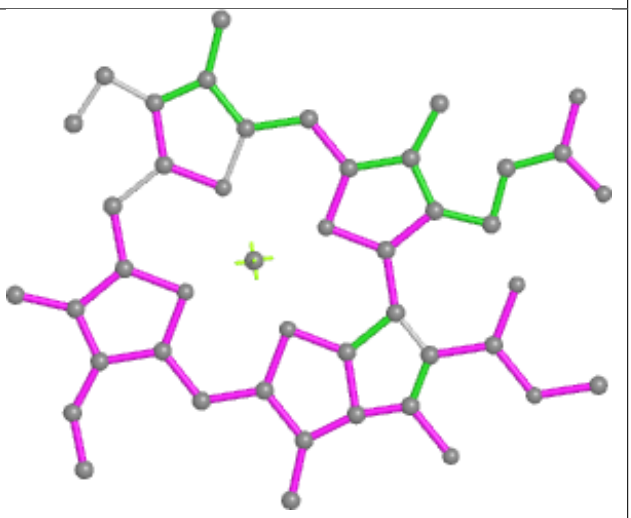
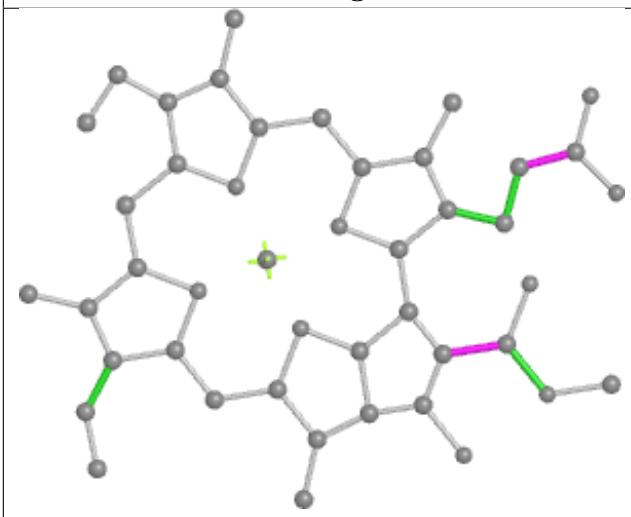
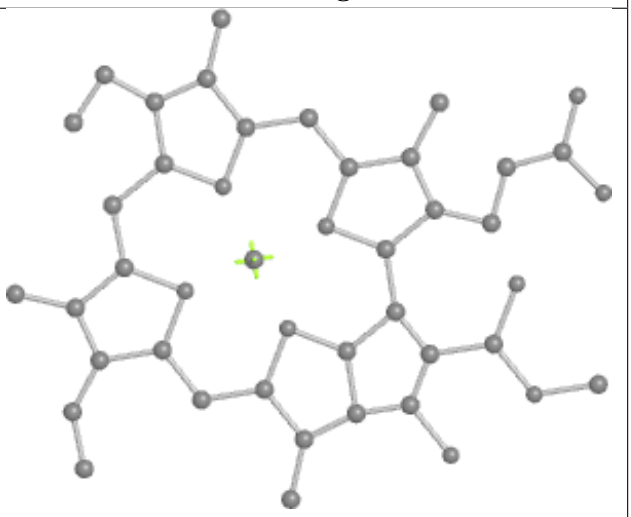
Ligand LHG 5 714

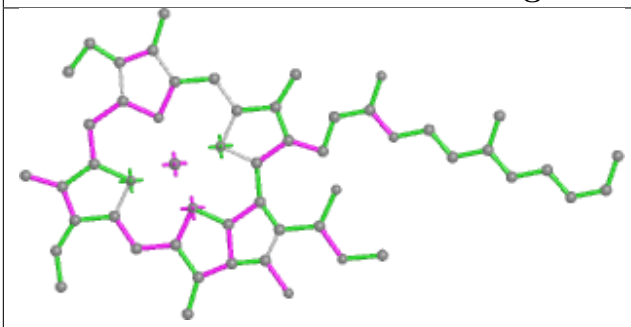
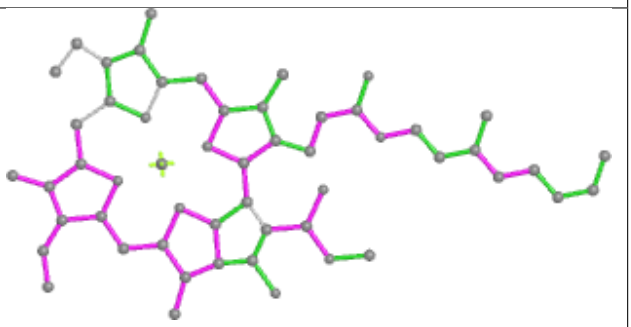
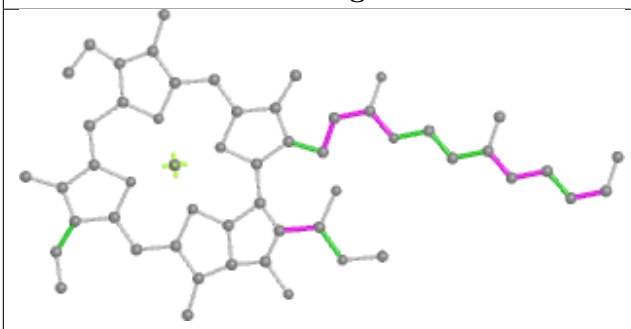
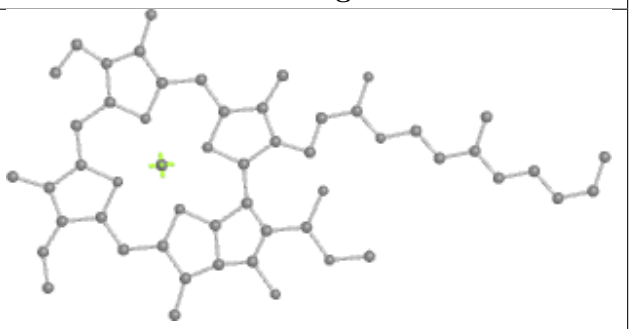


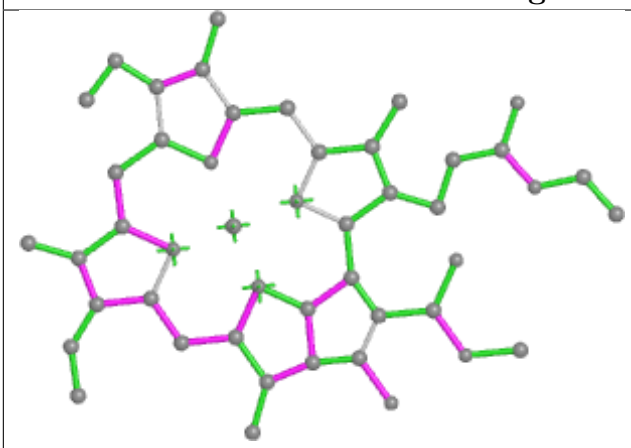
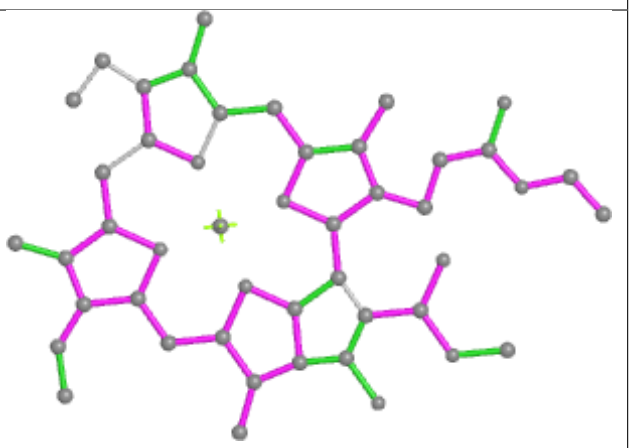
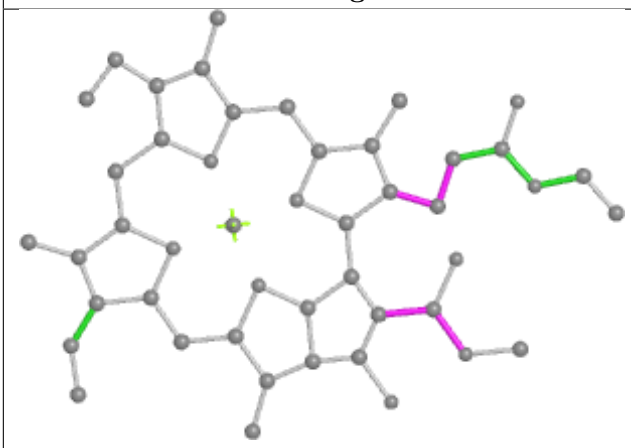
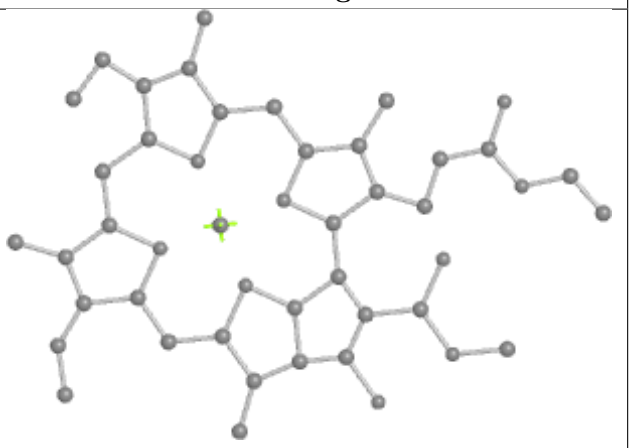
Ligand CLA B 819



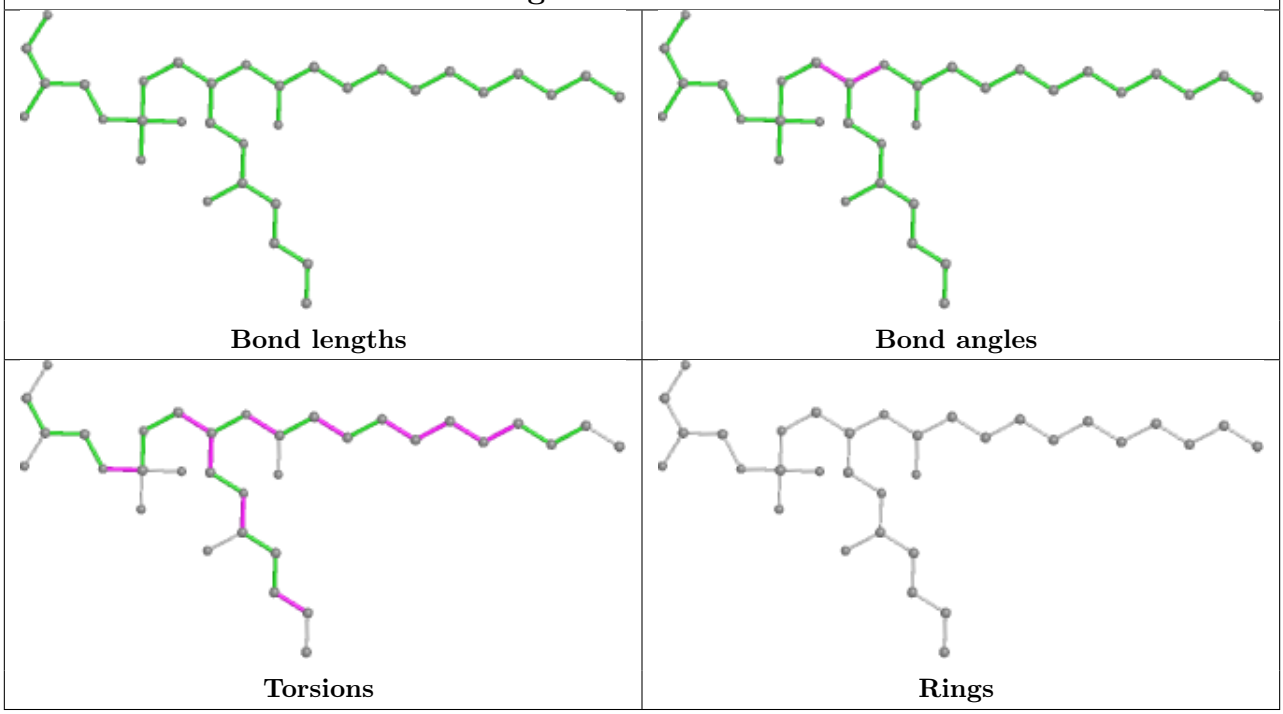
Ligand CLA 6 909	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

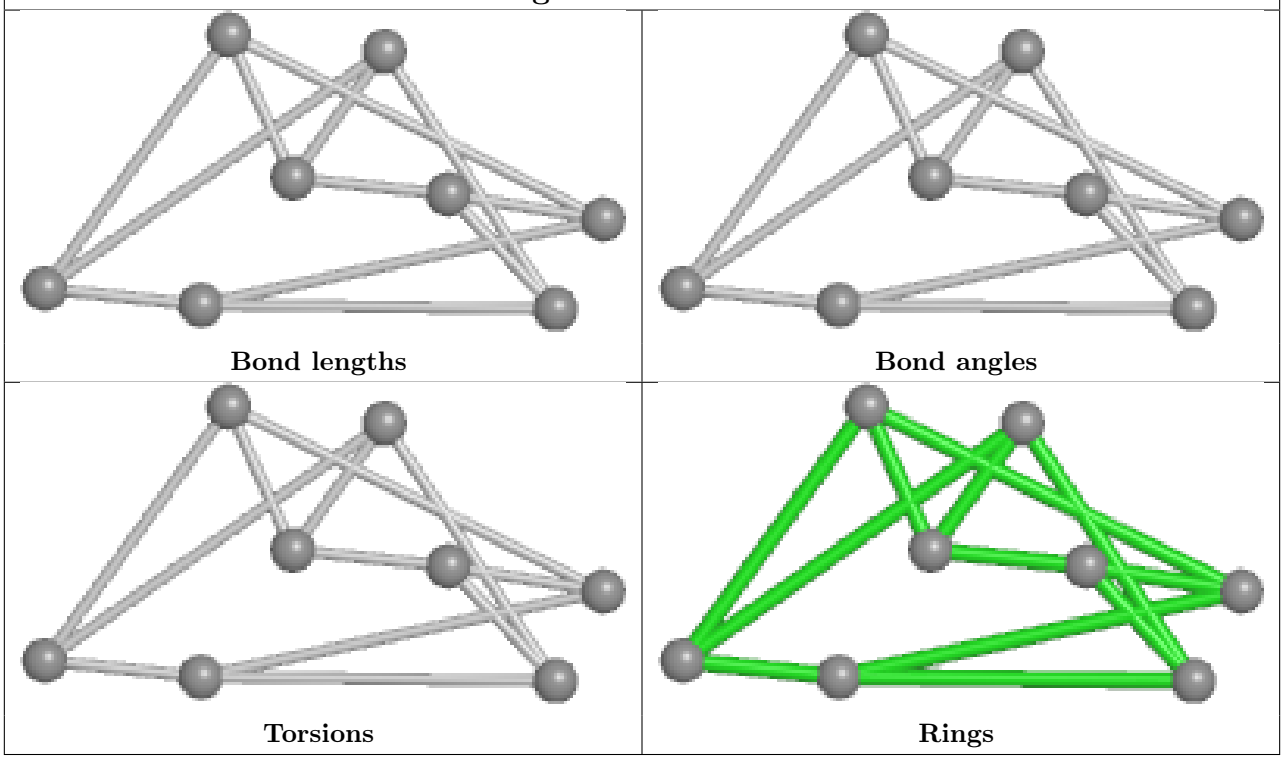
Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 914	
 Bond lengths	 Bond angles
 Torsions	 Rings

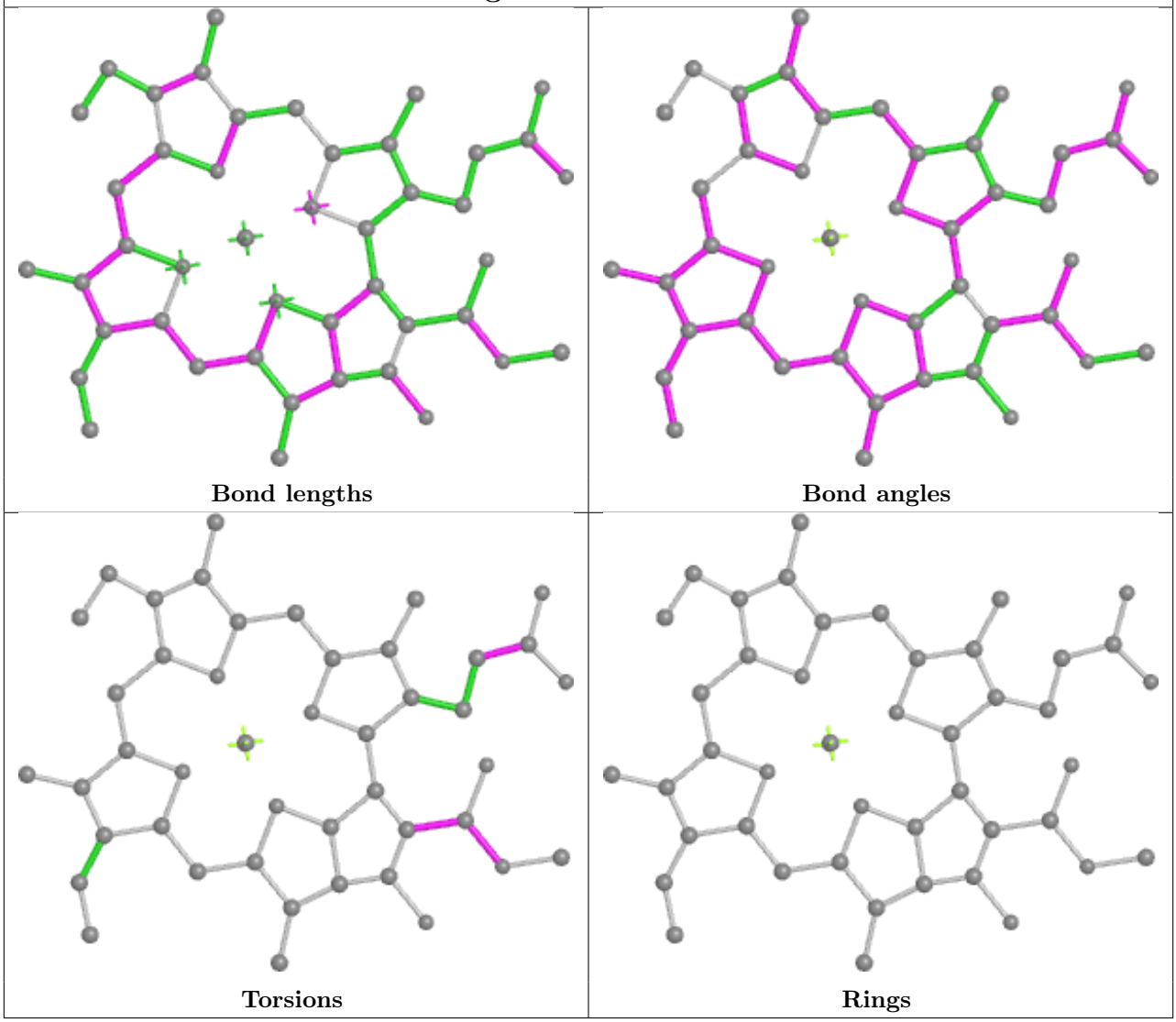
Ligand LHG 8 617

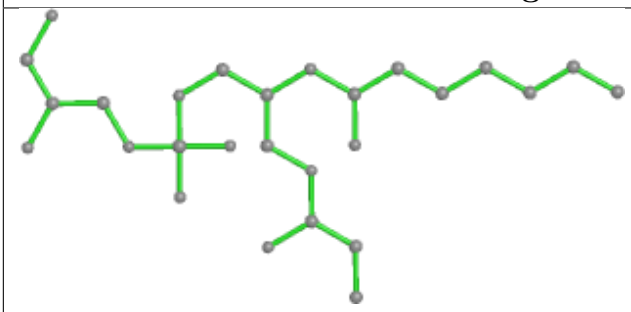
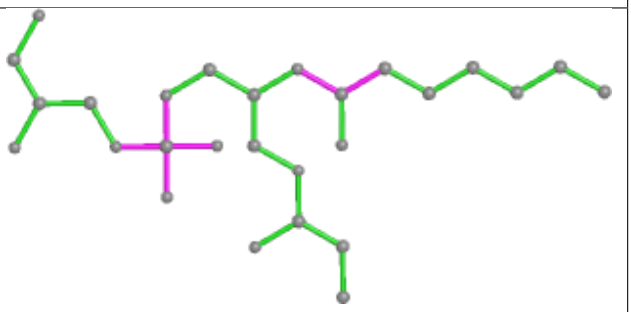
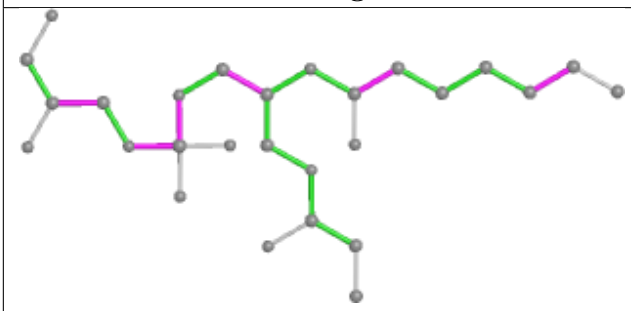
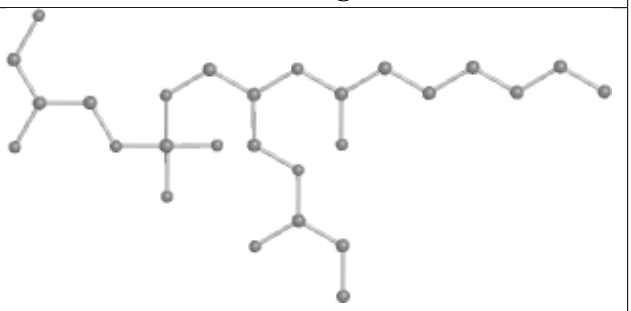


Ligand SF4 C 102

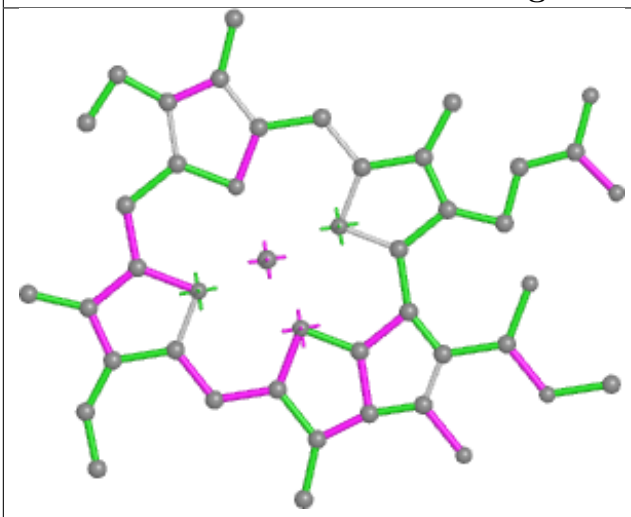


Ligand CLA 9 910

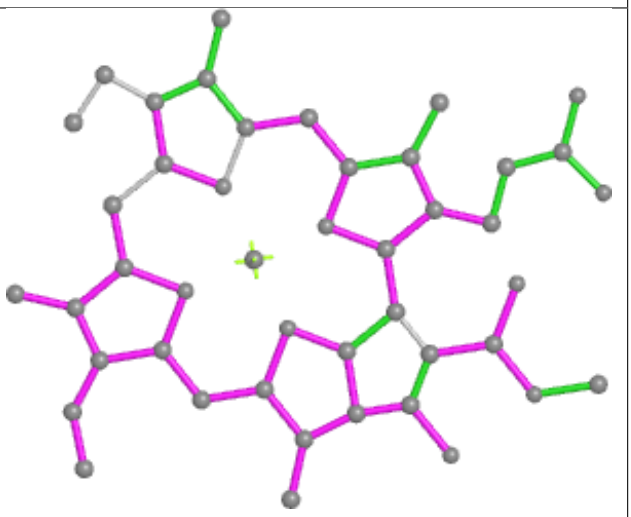


Ligand LHG A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

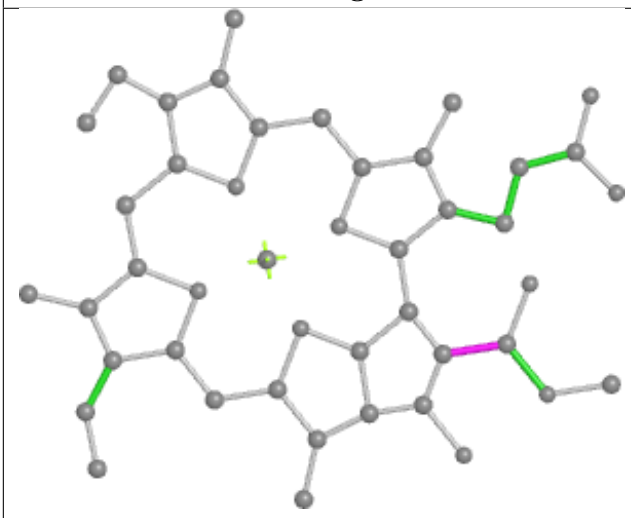
Ligand CLA 6 908



Bond lengths



Bond angles



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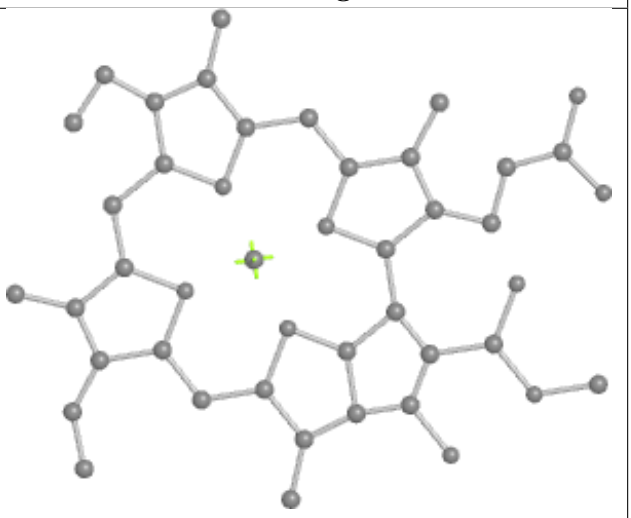
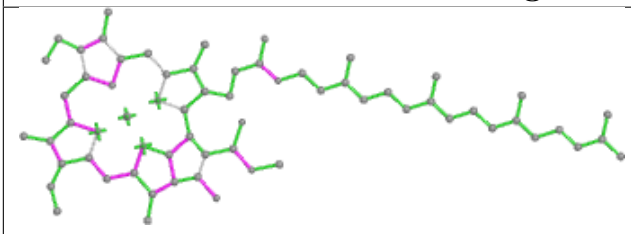


Rings

Ligand CLA A 812



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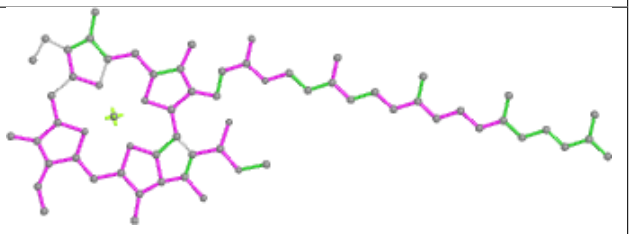

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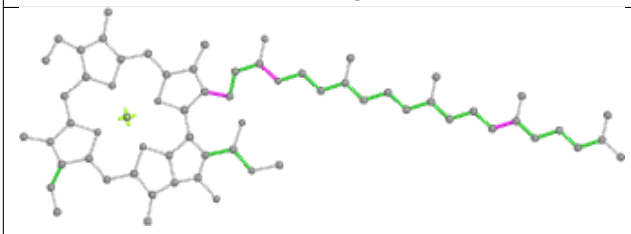

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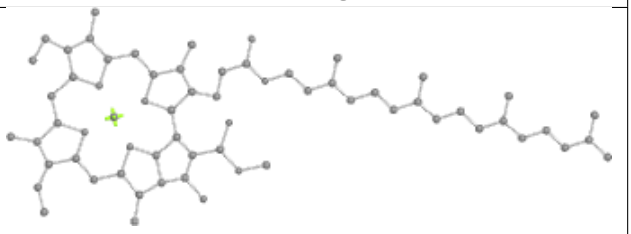
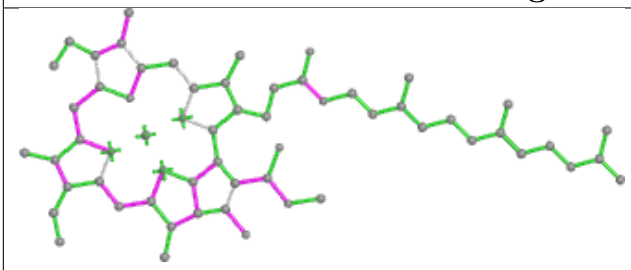
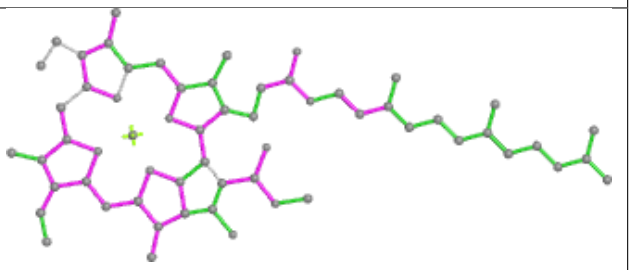
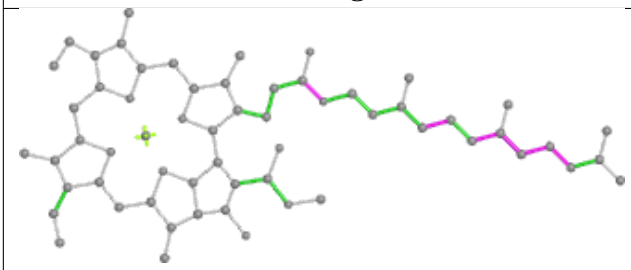
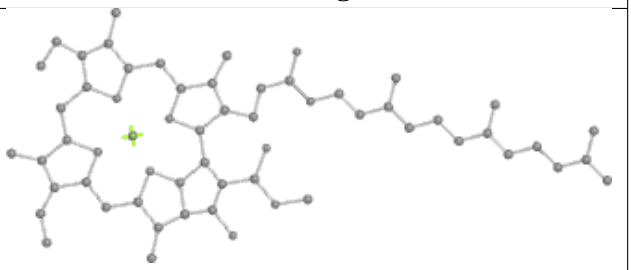


Rings

Ligand CLA 7 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

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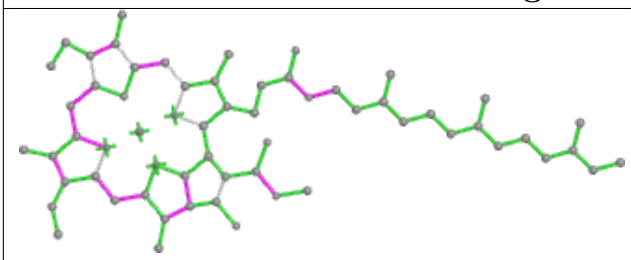
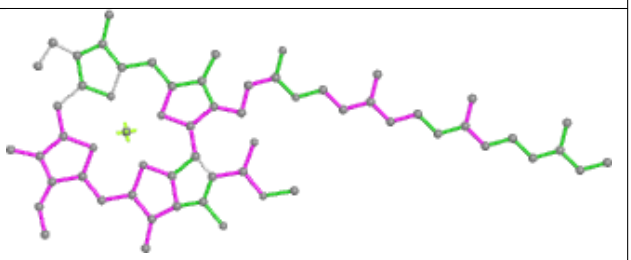
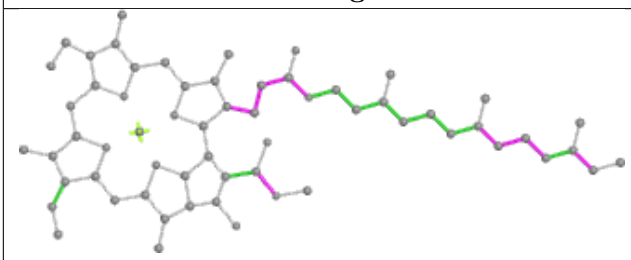
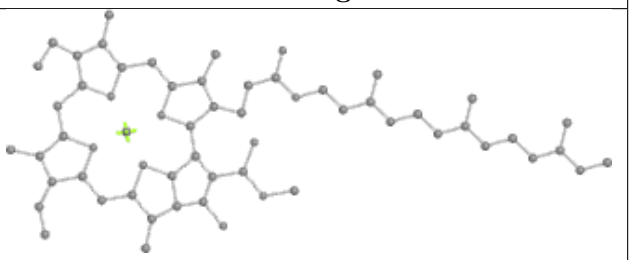
 Bond lengths	 Bond angles
 Torsions	 Rings

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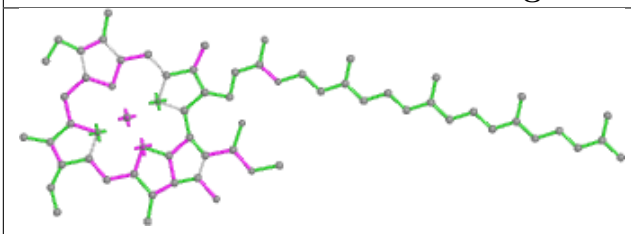
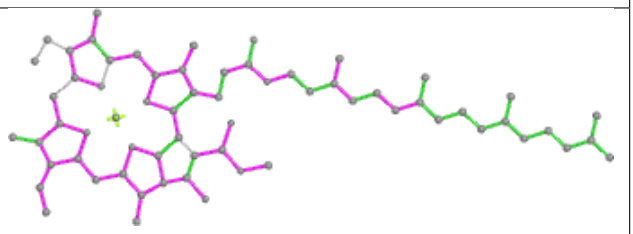
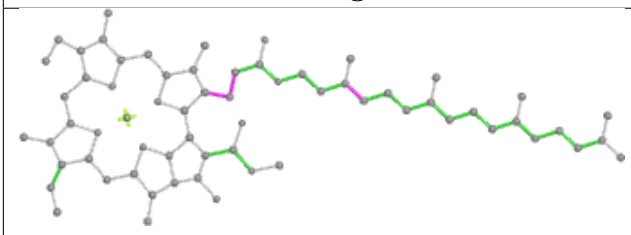
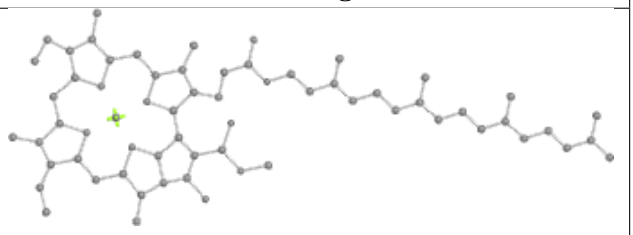
 Bond lengths	 Bond angles
 Torsions	 Rings

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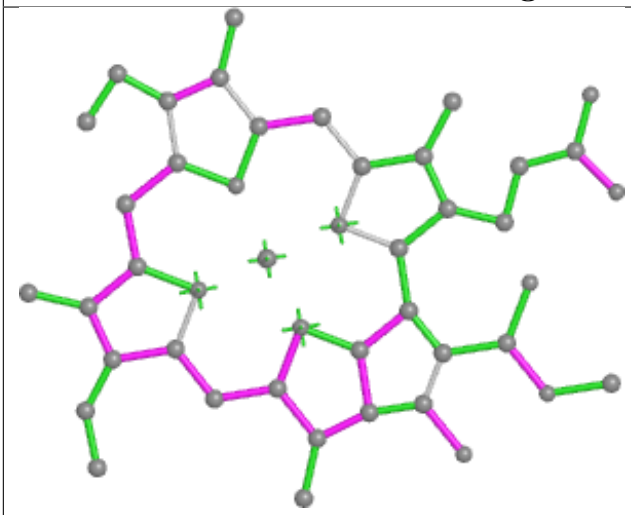
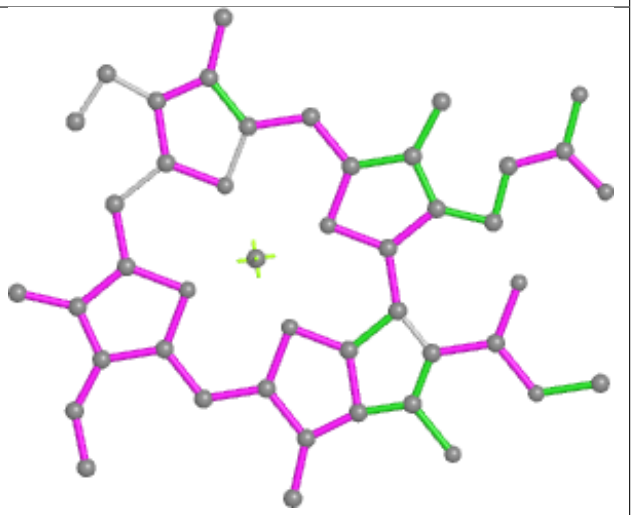
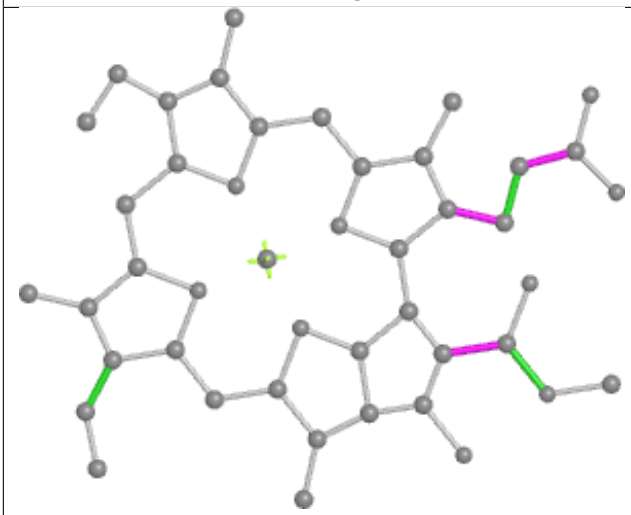
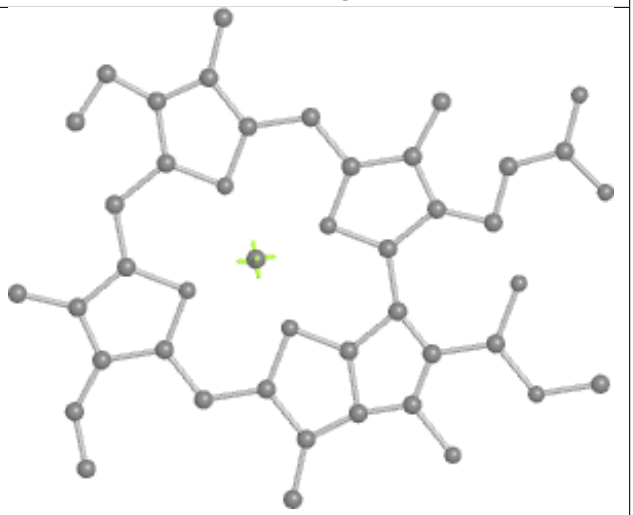
 Bond lengths	 Bond angles
 Torsions	 Rings

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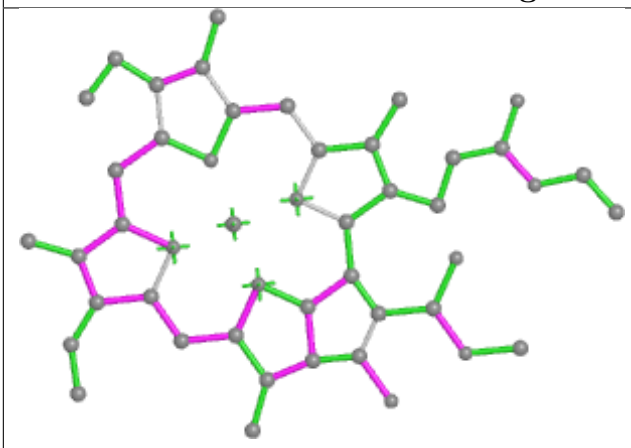
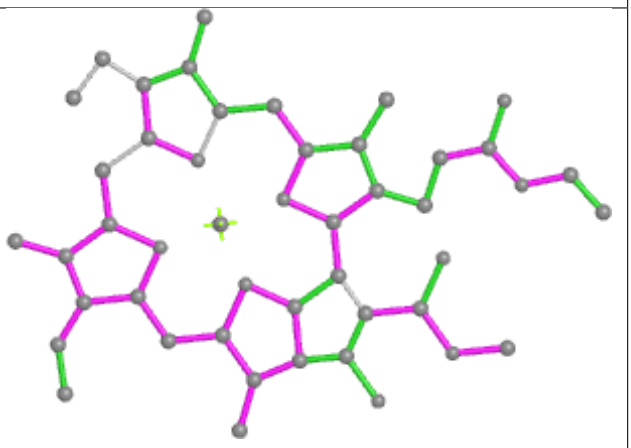
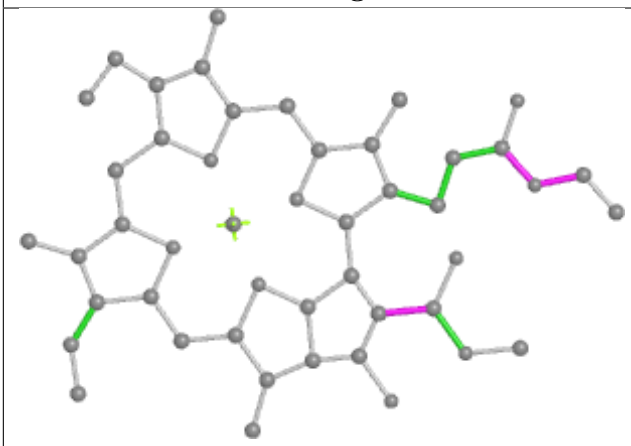
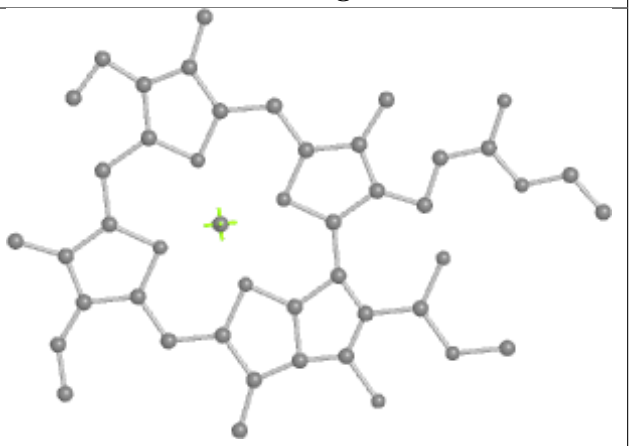
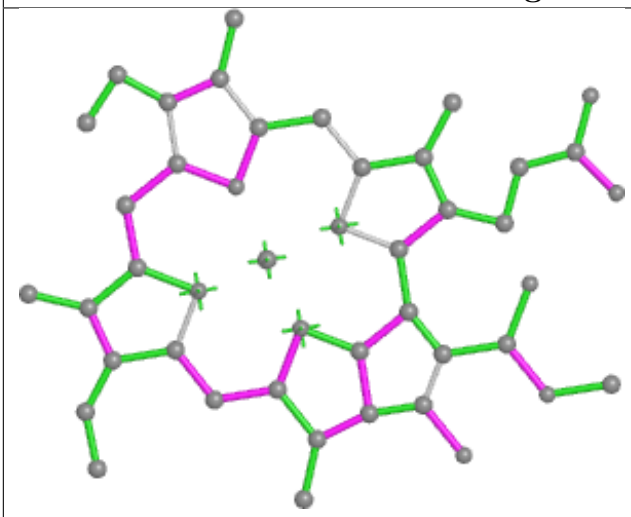
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 829



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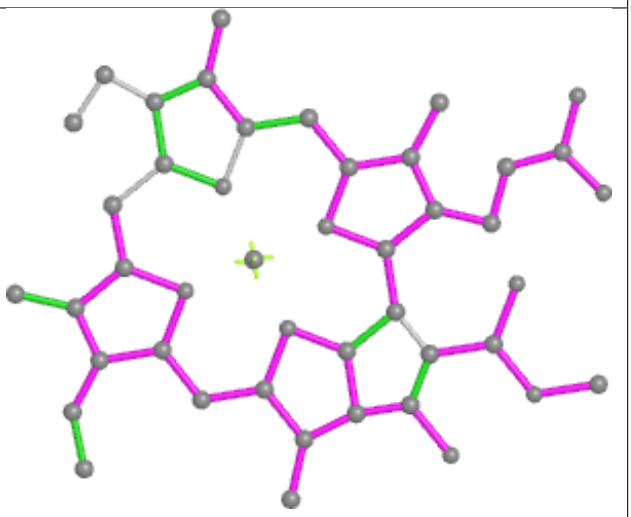
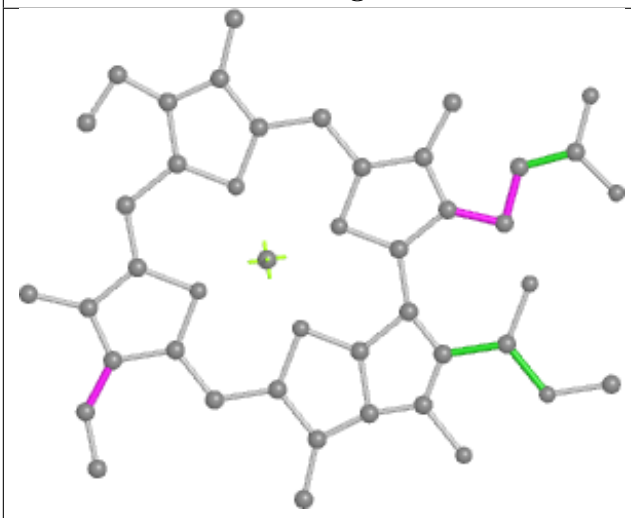


Bond angles



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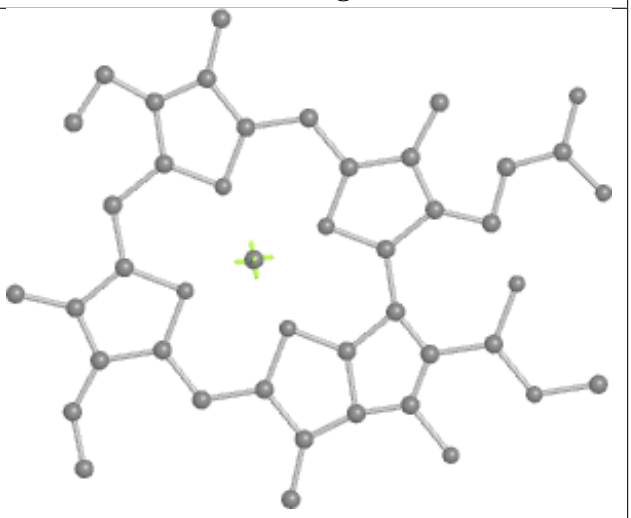
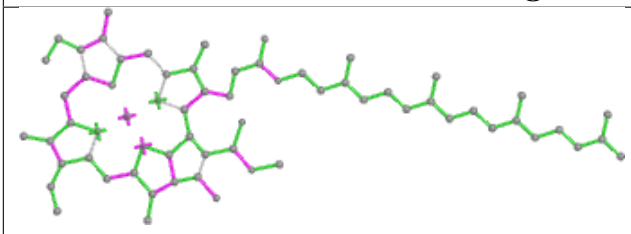


Rings

Ligand CLA B 825



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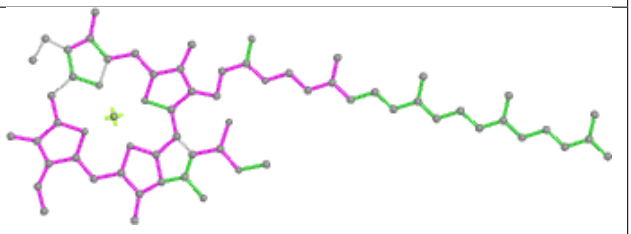

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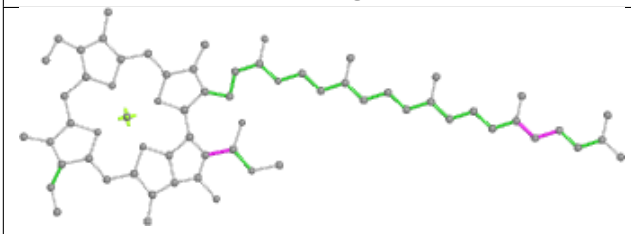

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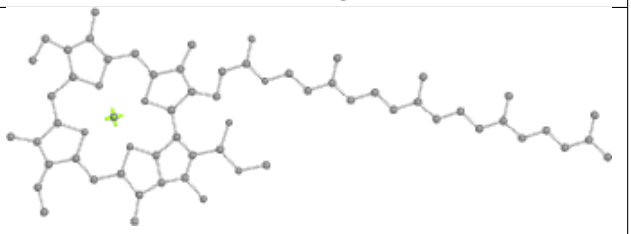
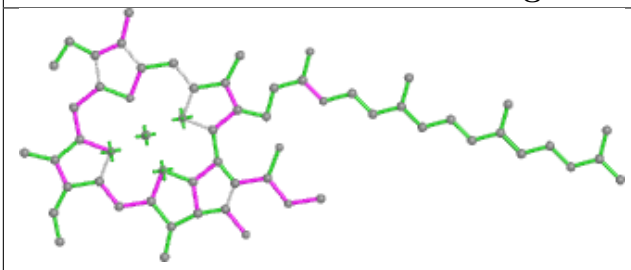


Rings

Ligand CLA A 827



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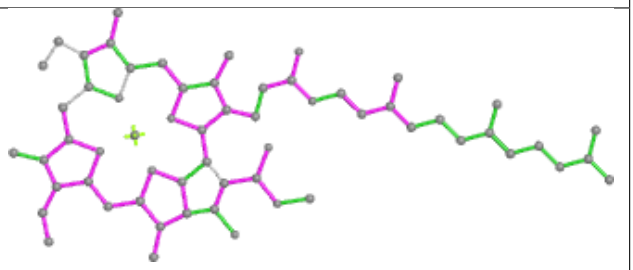

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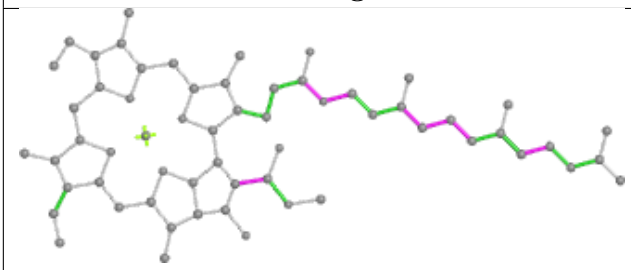

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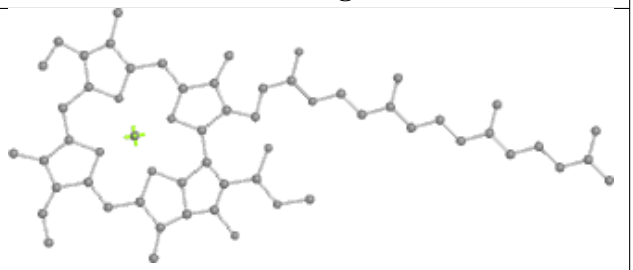
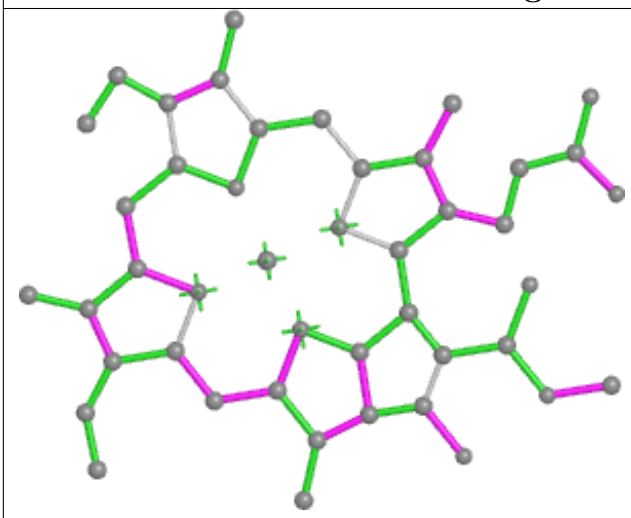


Rings

Ligand CLA B 833



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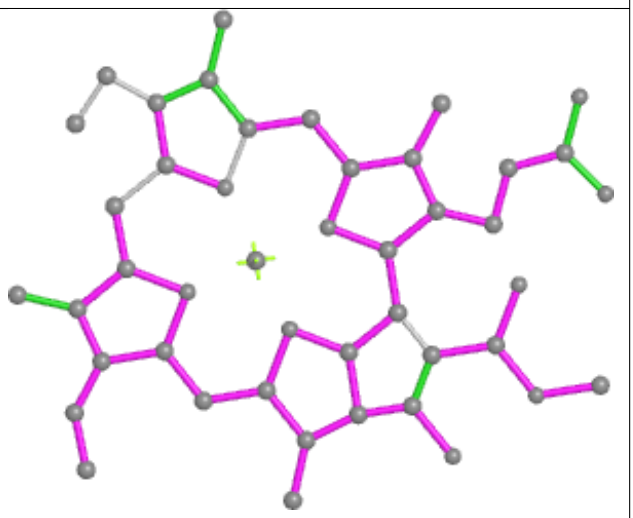
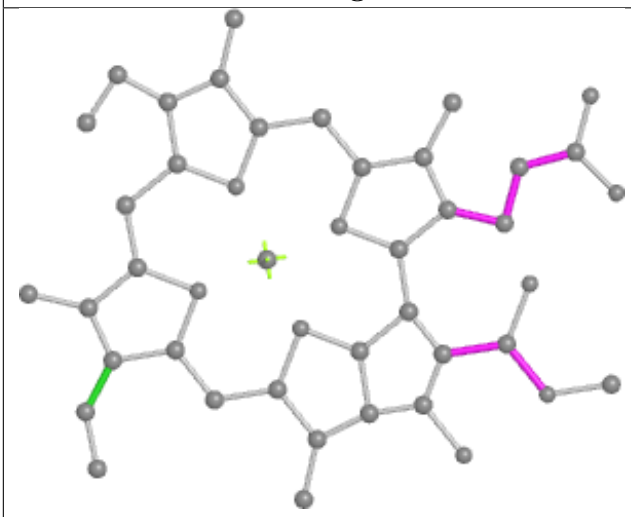


Bond angles



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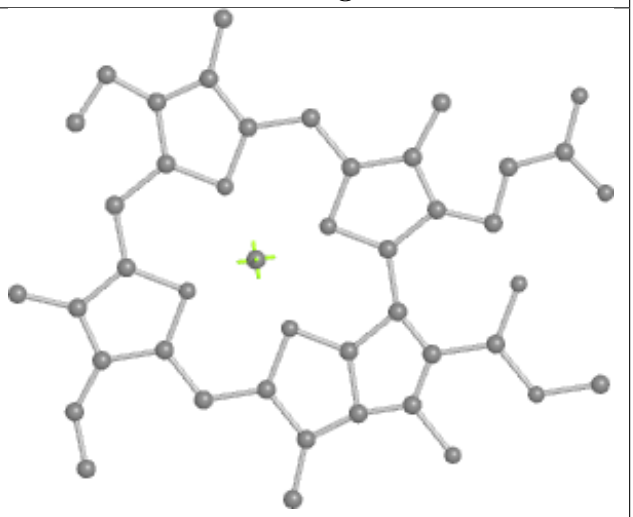
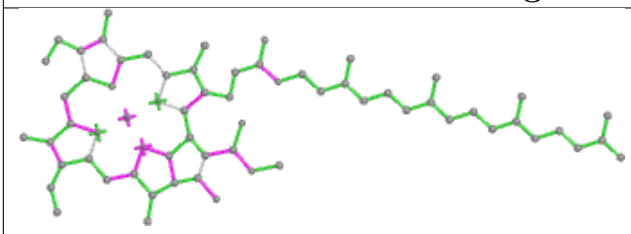
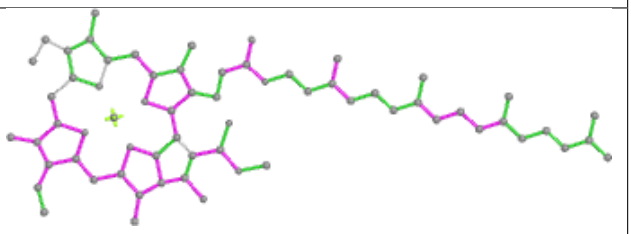
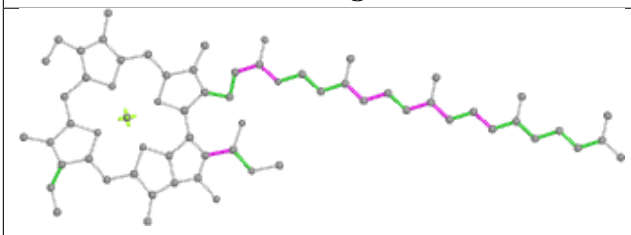
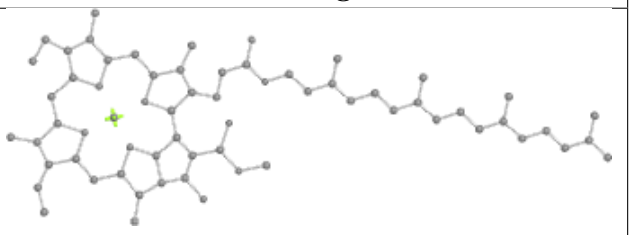


Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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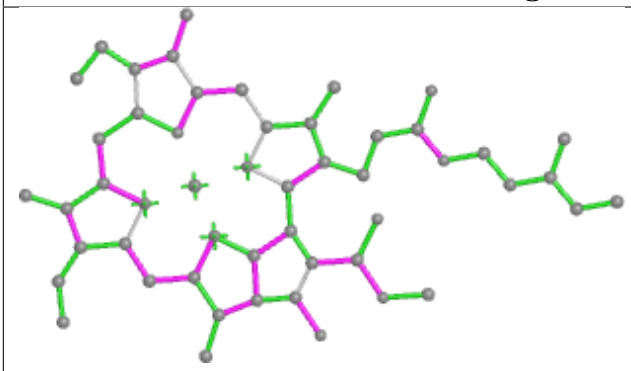
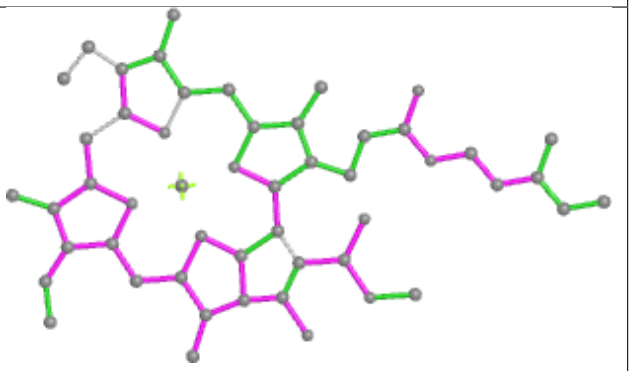
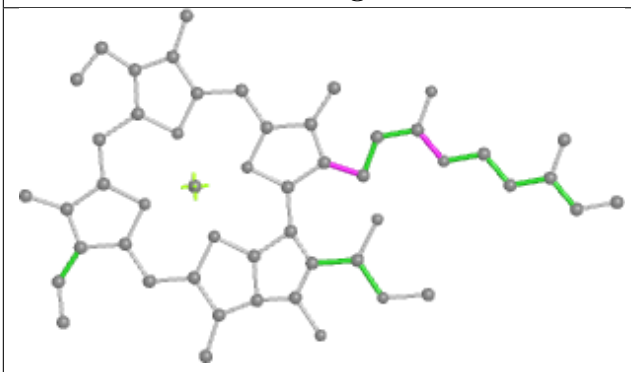
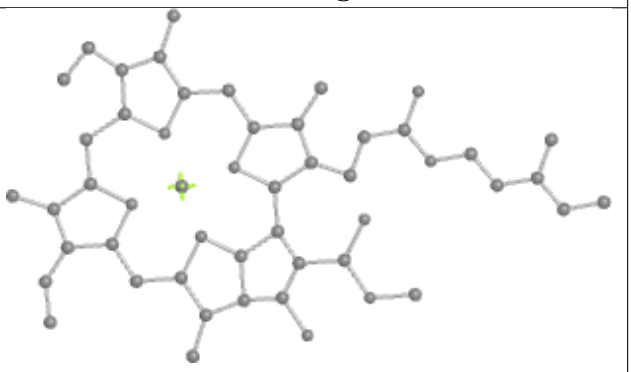
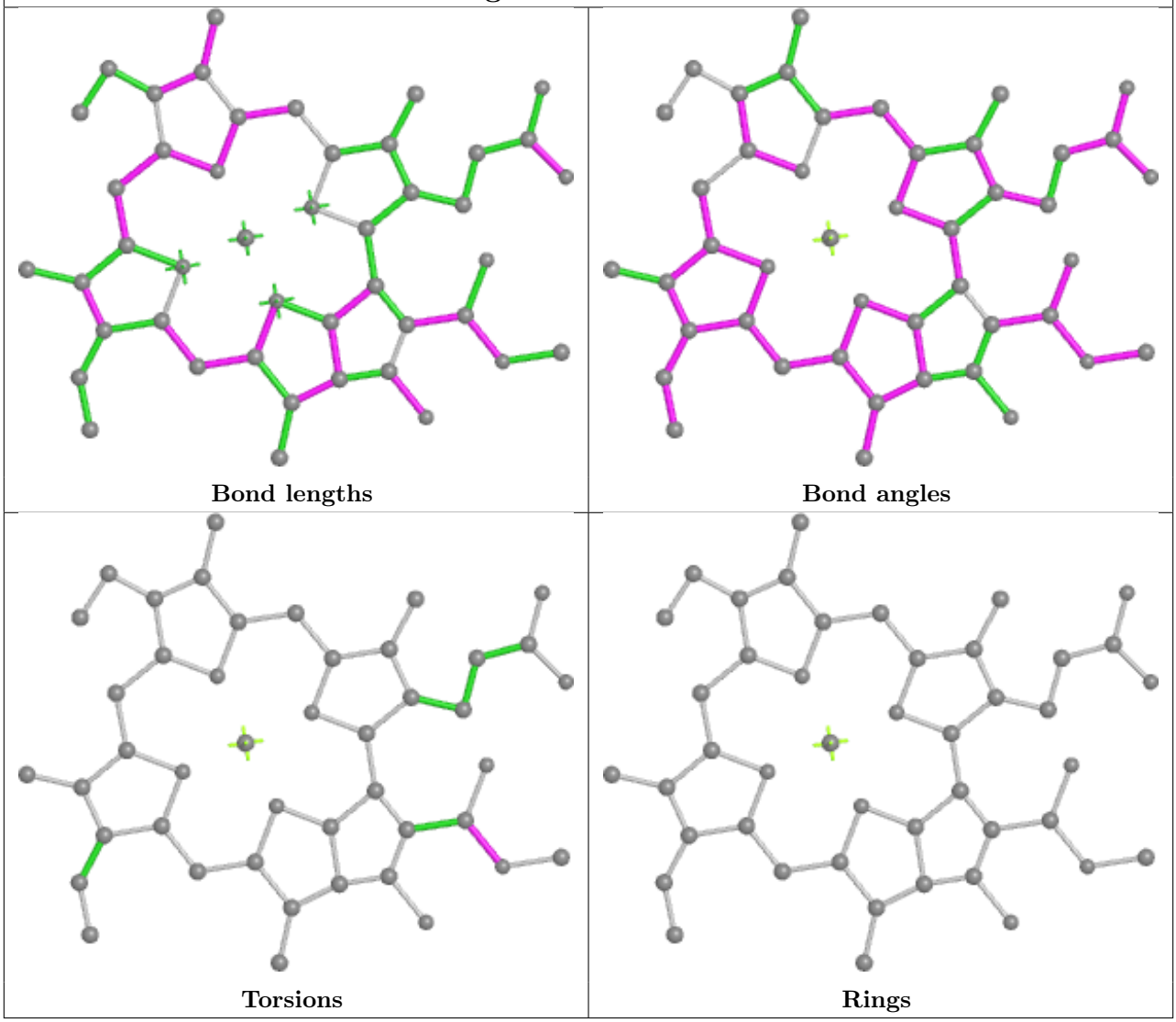
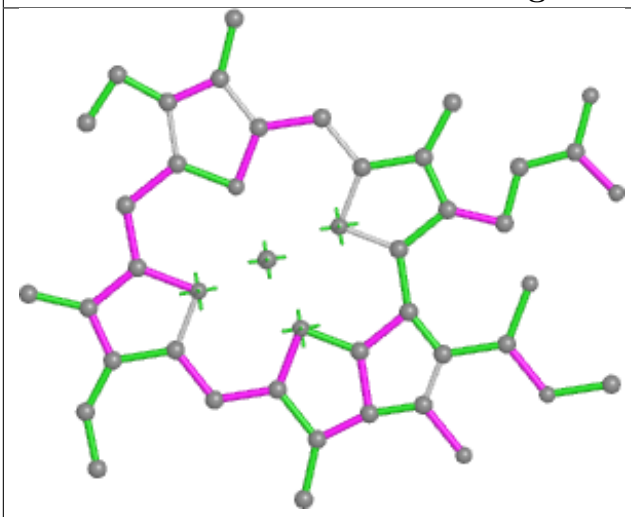
 Bond lengths	 Bond angles
 Torsions	 Rings

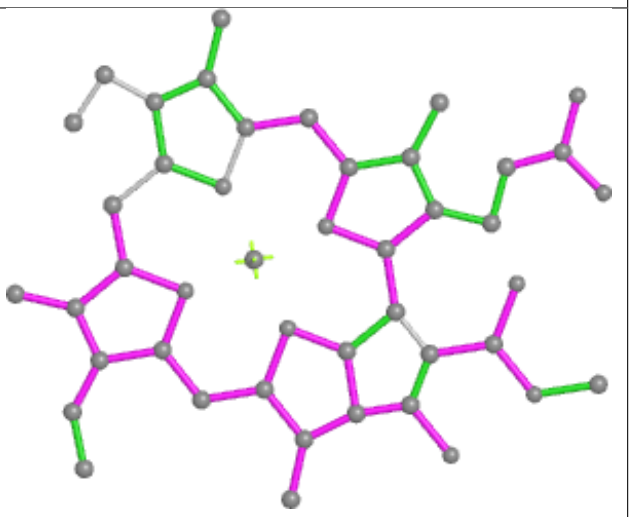
Ligand CLA 1 501



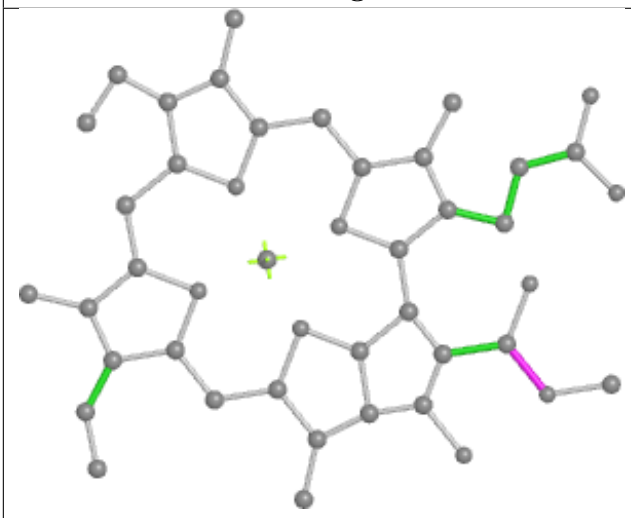
Ligand CLA 1 517



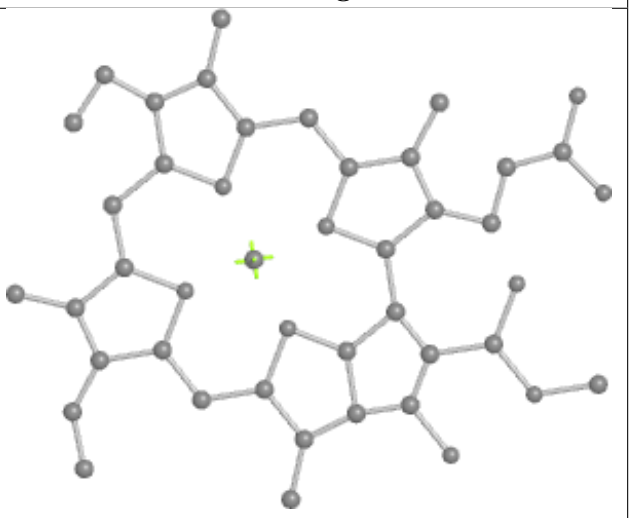
Bond lengths



Bond angles

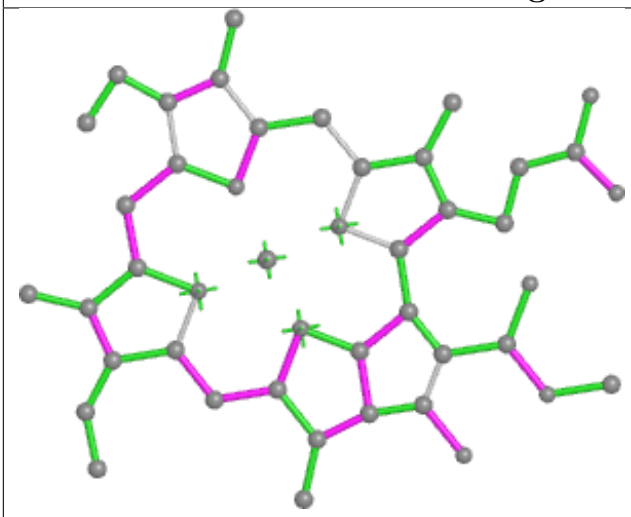


Torsions



Rings

Ligand CLA 3 715



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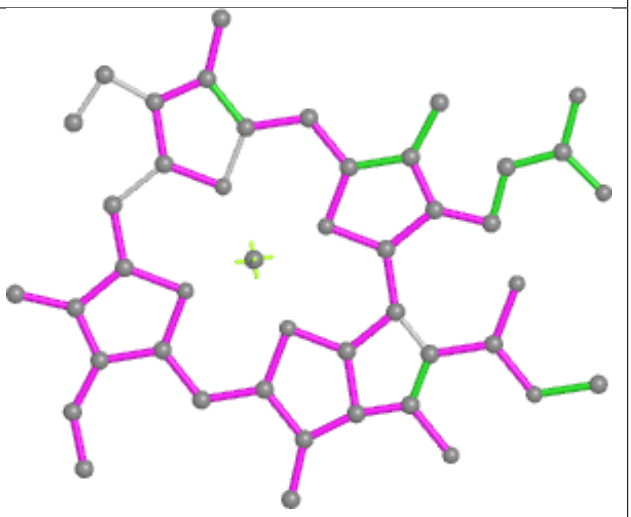
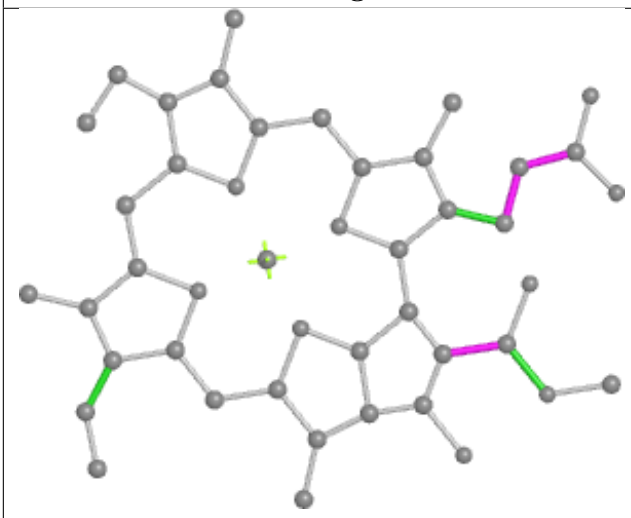


Bond angles



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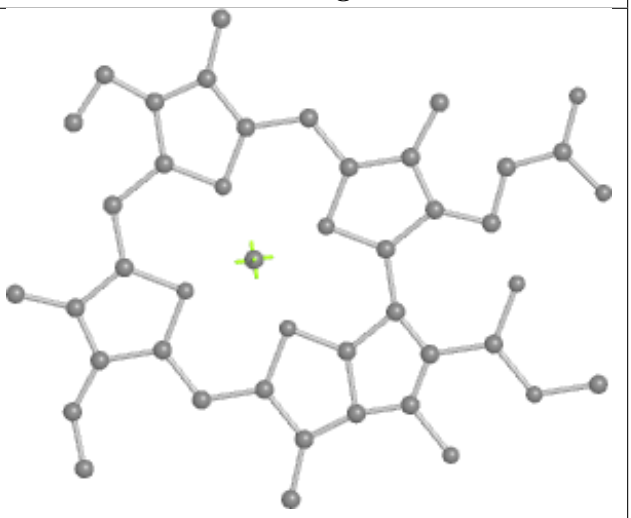
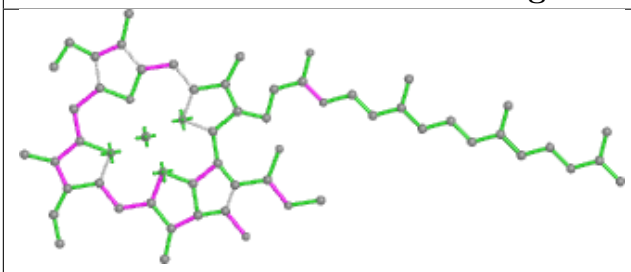


Rings

Ligand CLA 9 903



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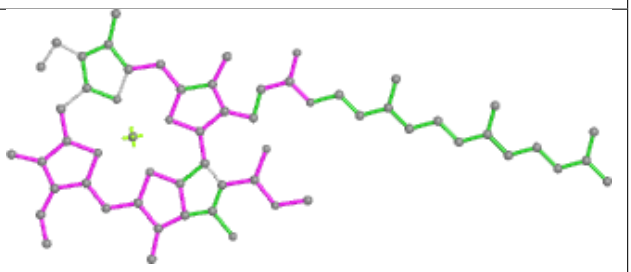

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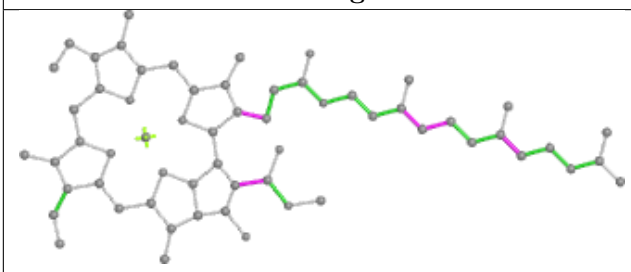

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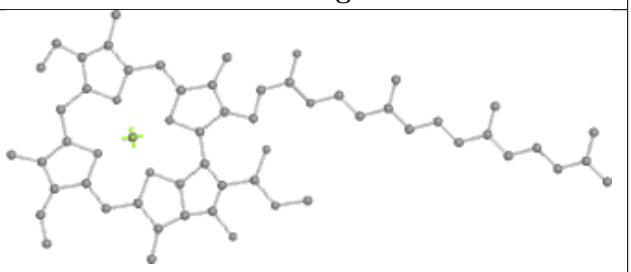
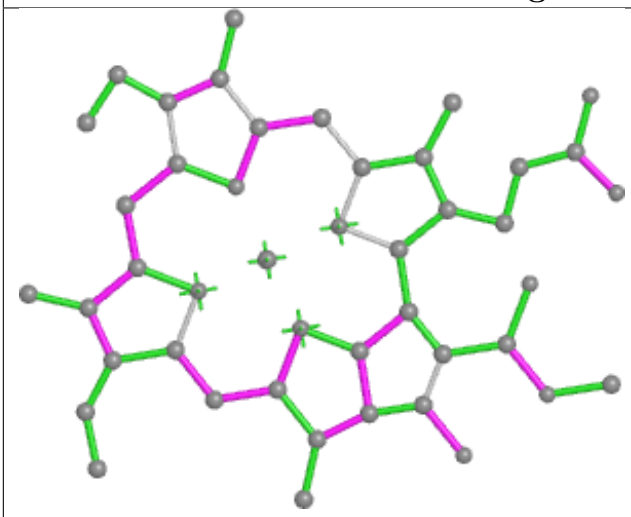


Rings

Ligand CLA 2 513



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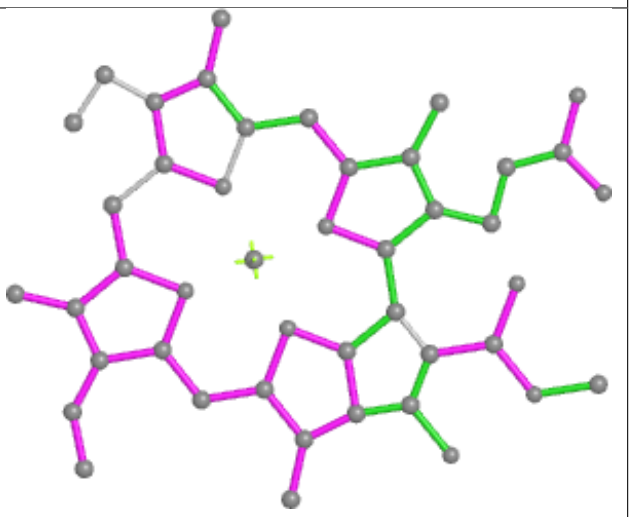
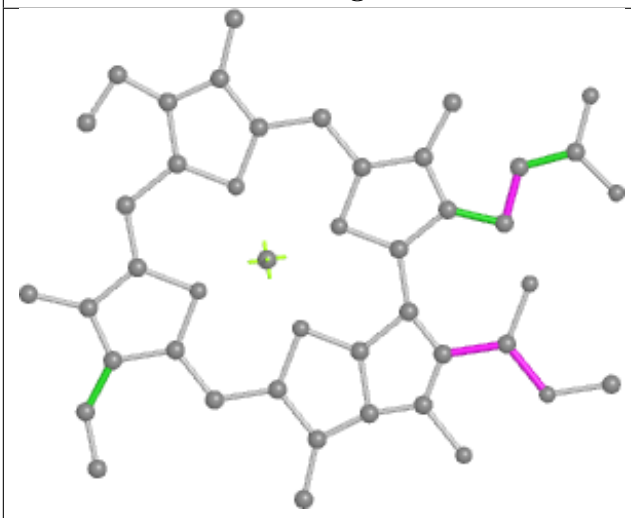


Bond angles



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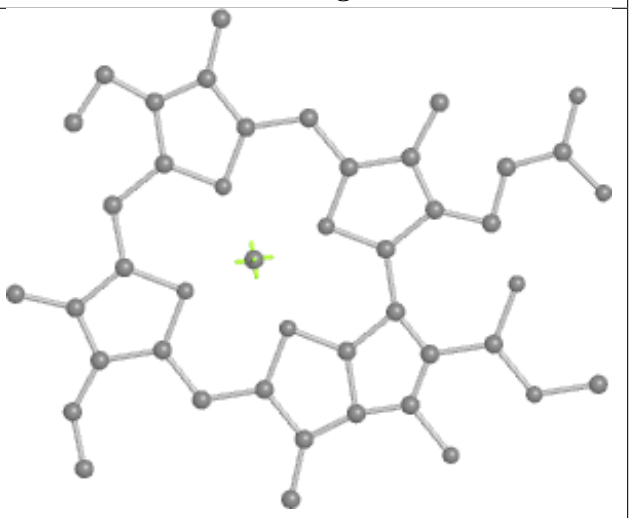
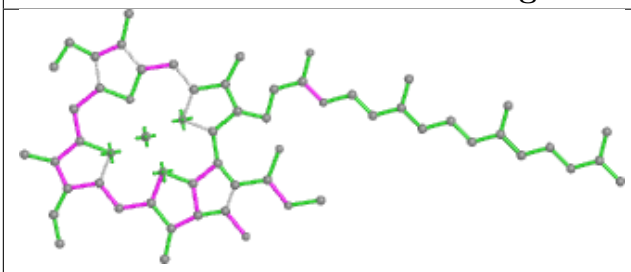


Rings

Ligand CLA 10 704



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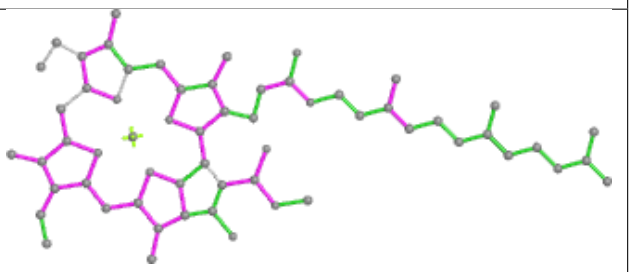
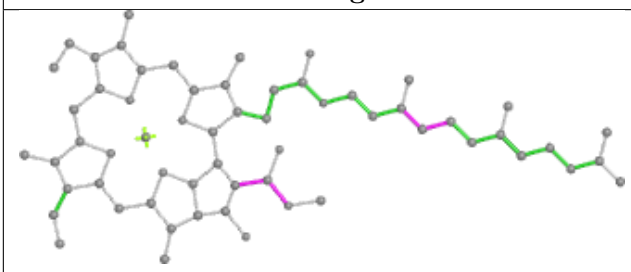


Bond angles



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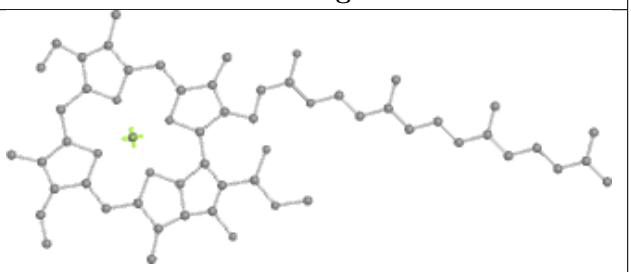
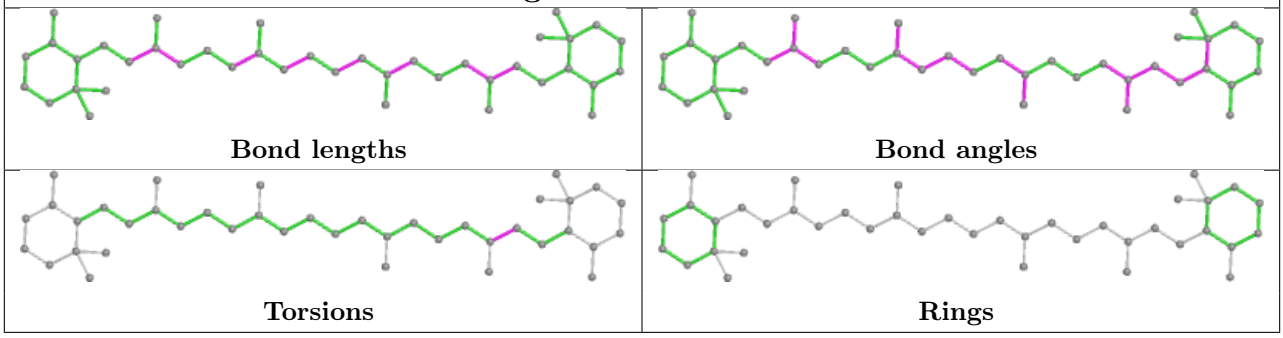


Rings

Ligand BCR B 841



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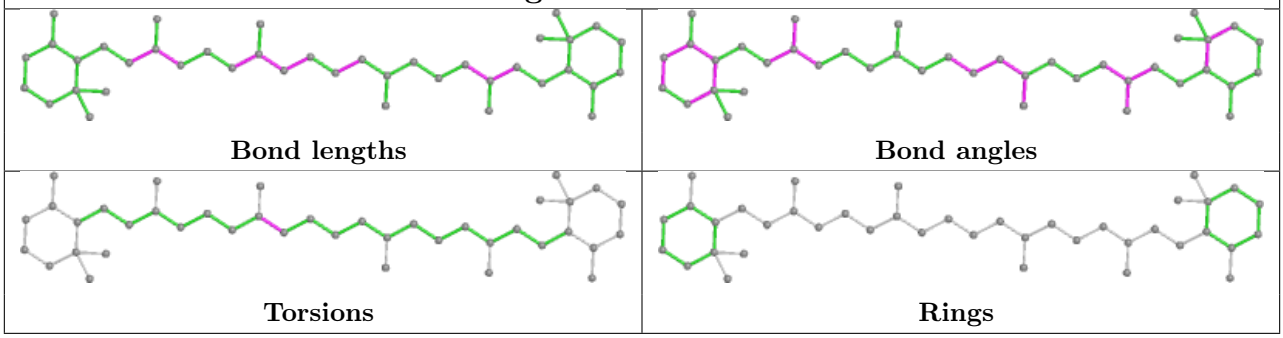
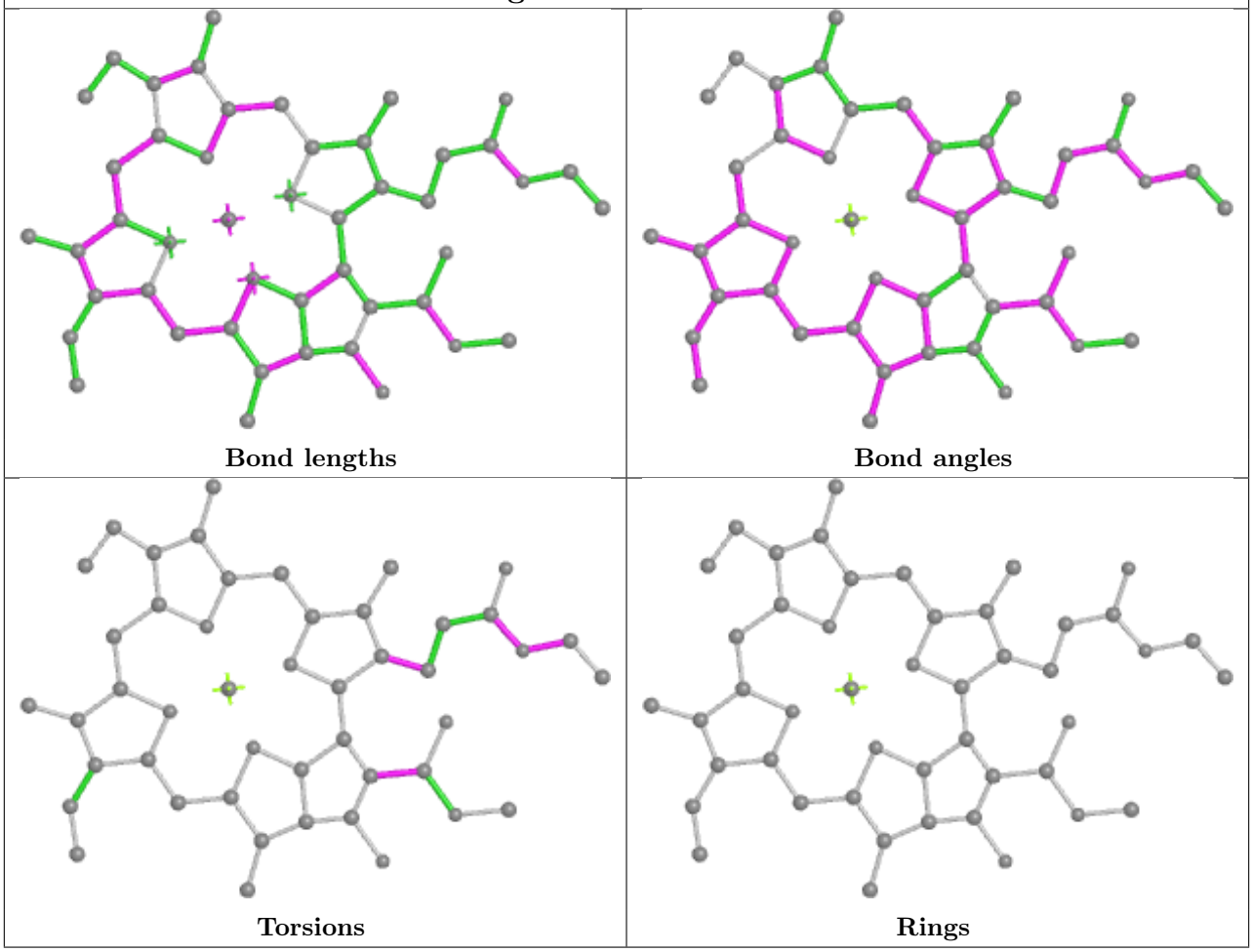
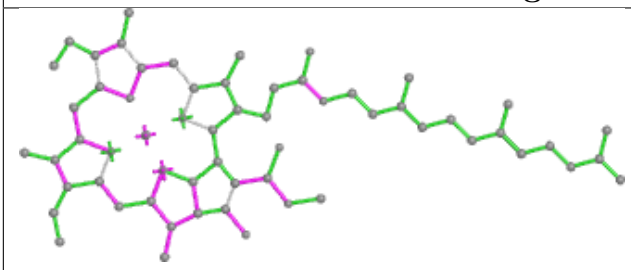


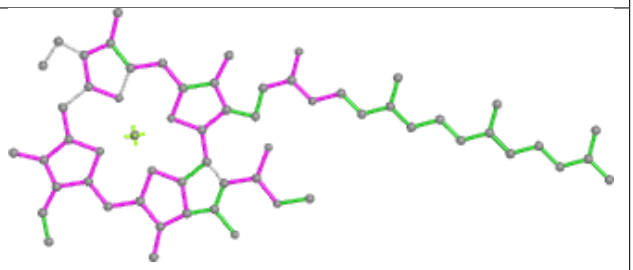
Ligand CLA 11 705



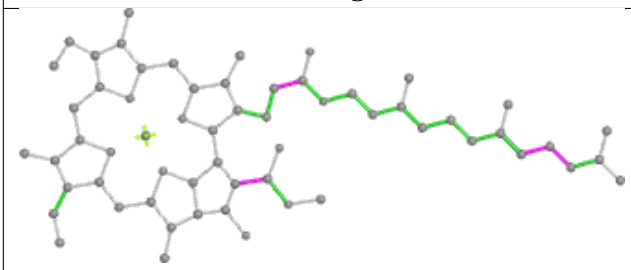
Ligand CLA A 814



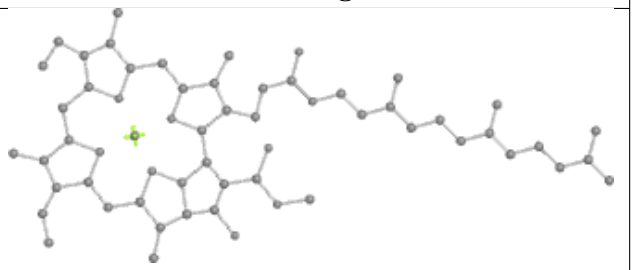
Bond lengths



Bond angles

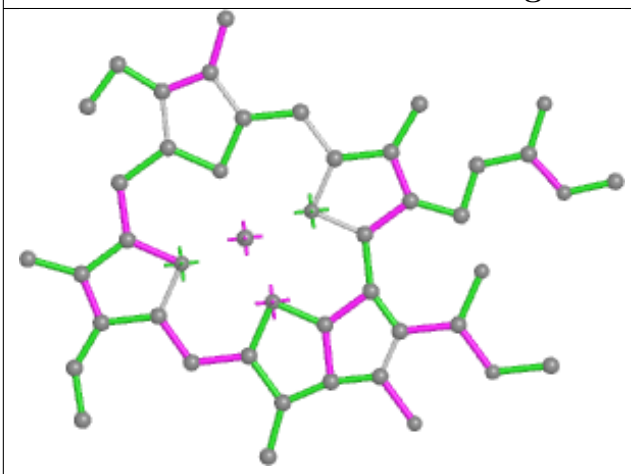


Torsions



Rings

Ligand CLA B 824



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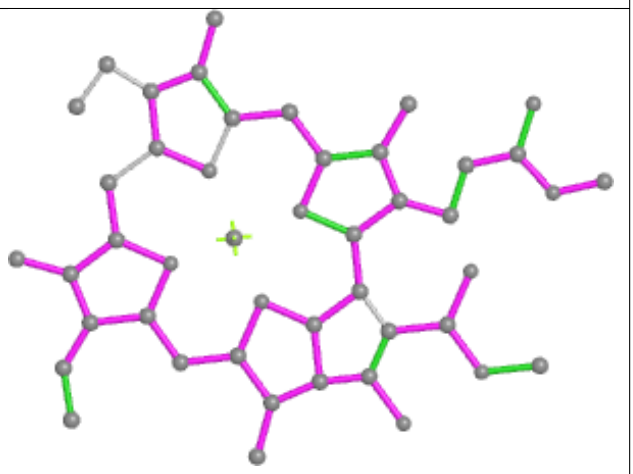
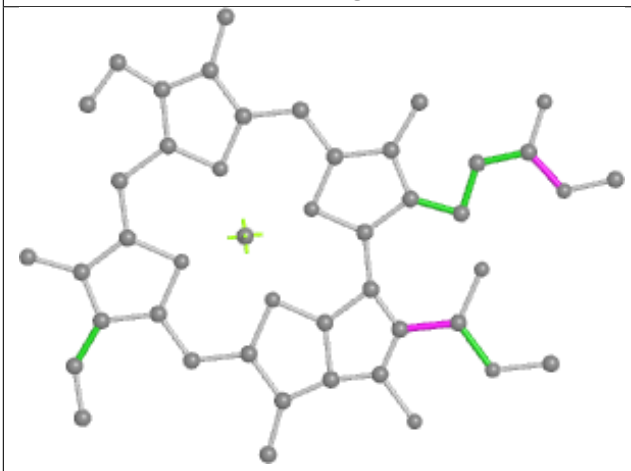


Bond angles



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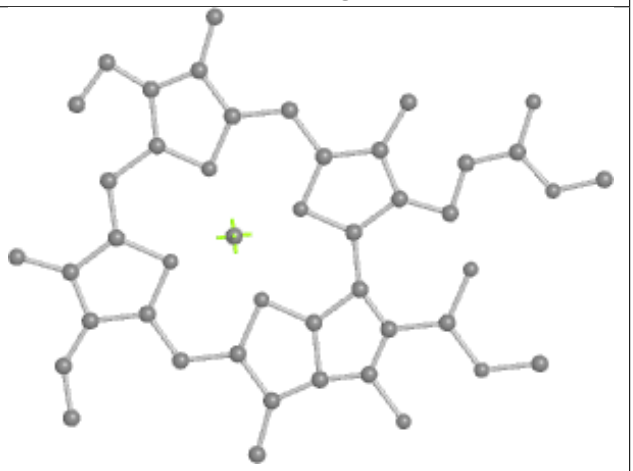
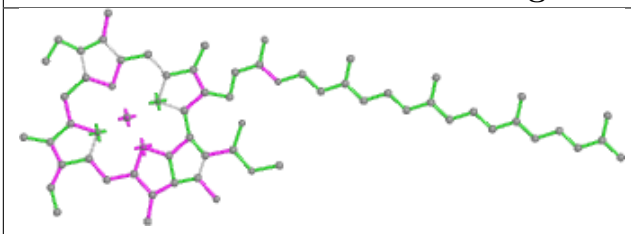
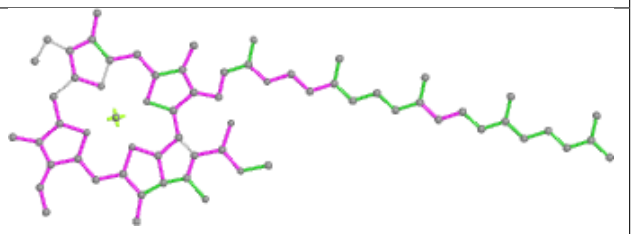
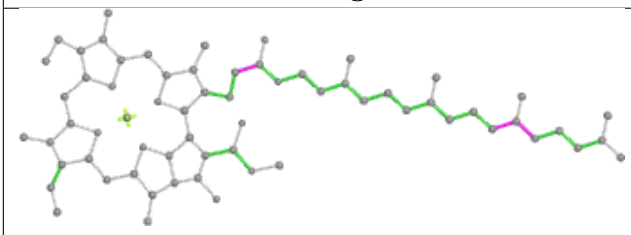
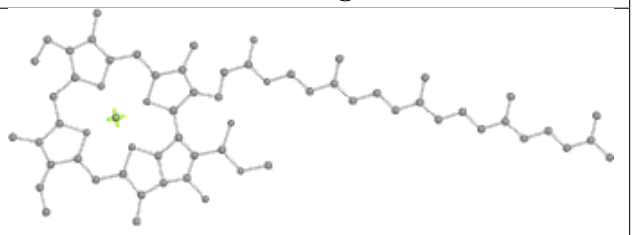
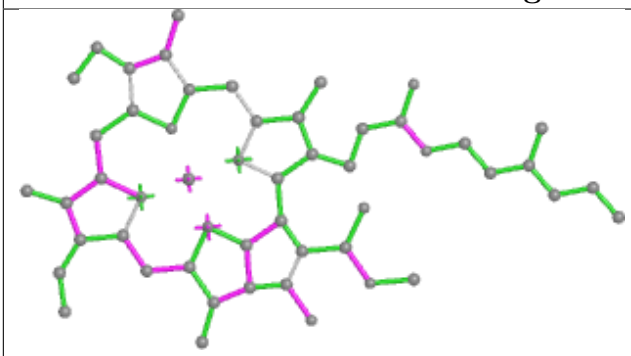
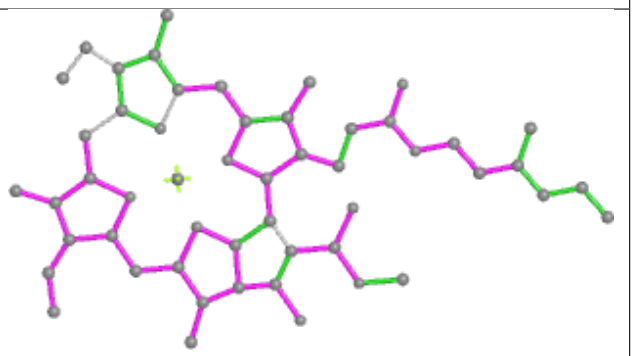
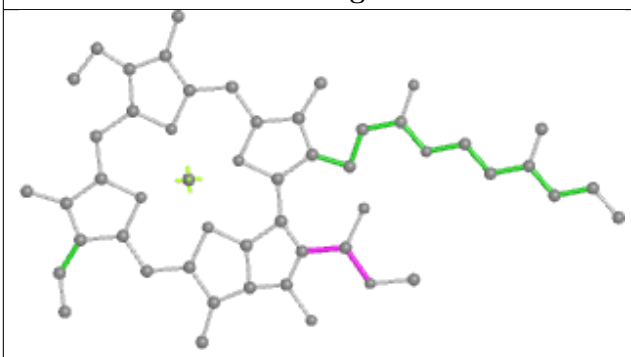
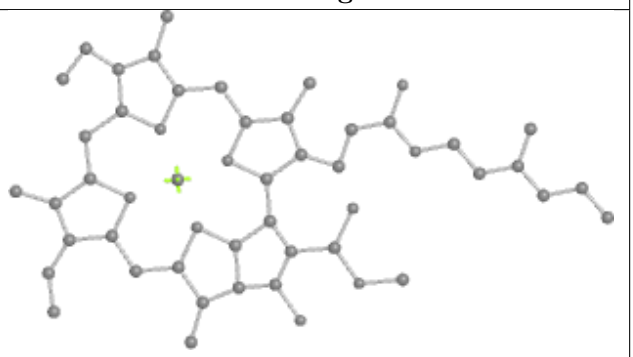
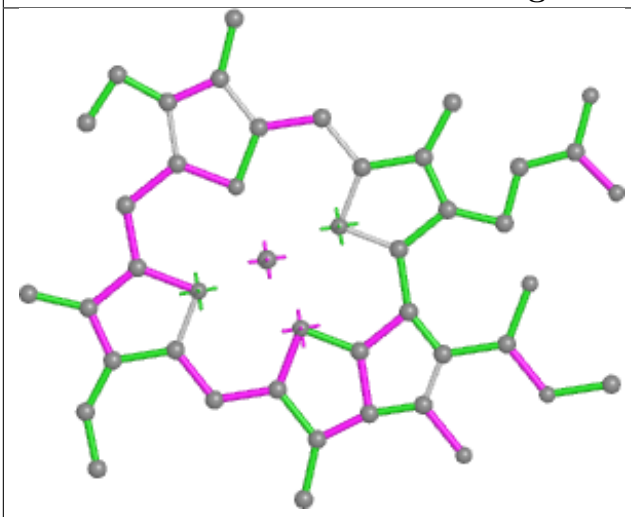


Rings

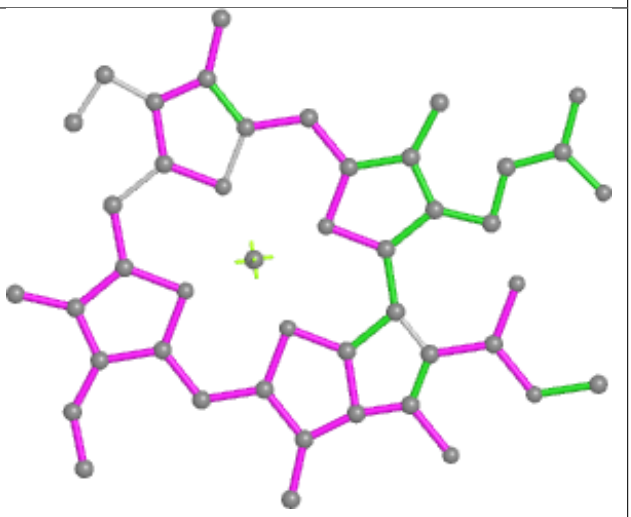
Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

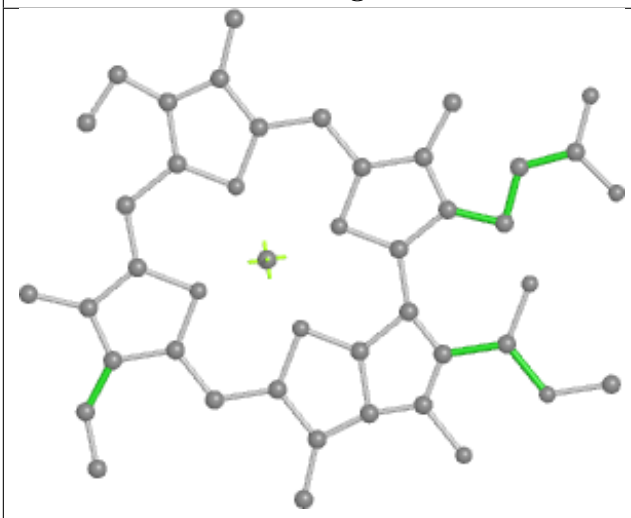
Ligand CLA 8 606



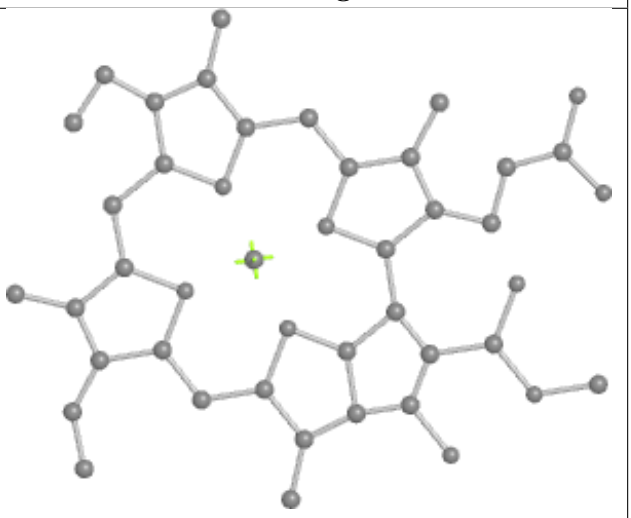
Bond lengths



Bond angles

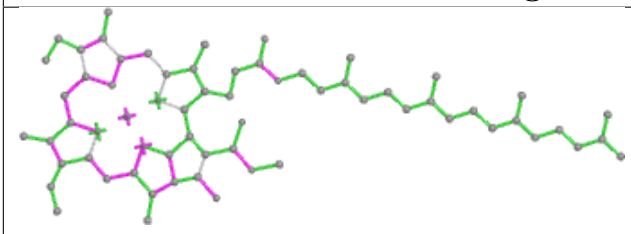


Torsions



Rings

Ligand CLA A 833



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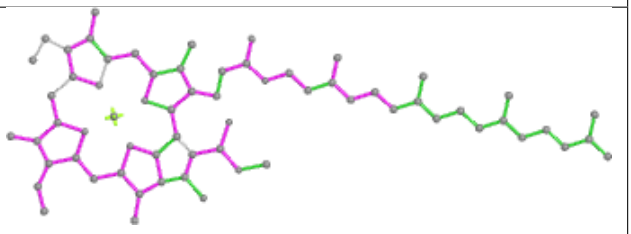
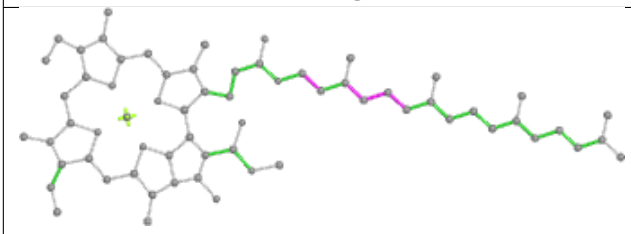
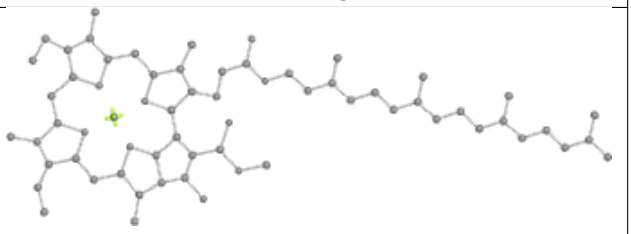


Bond angles

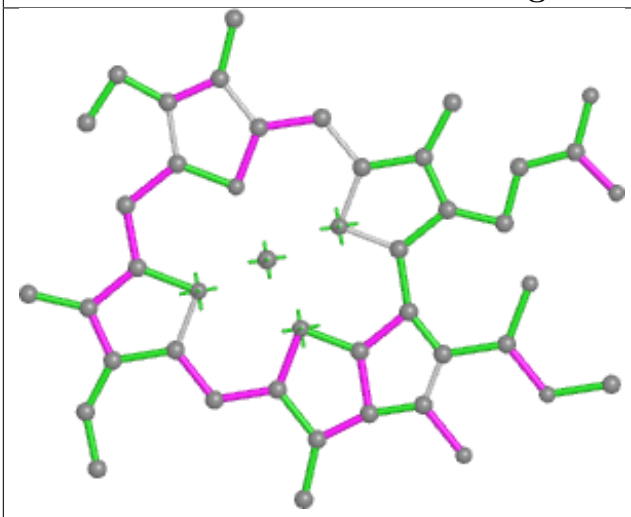


Torsions



Rings

Ligand CLA 3 709



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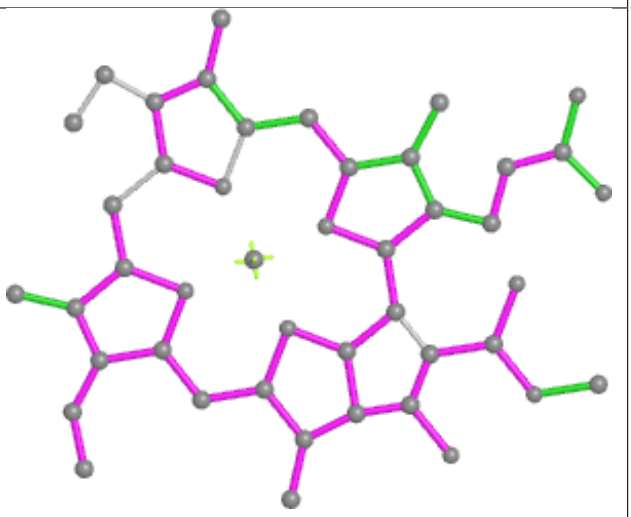
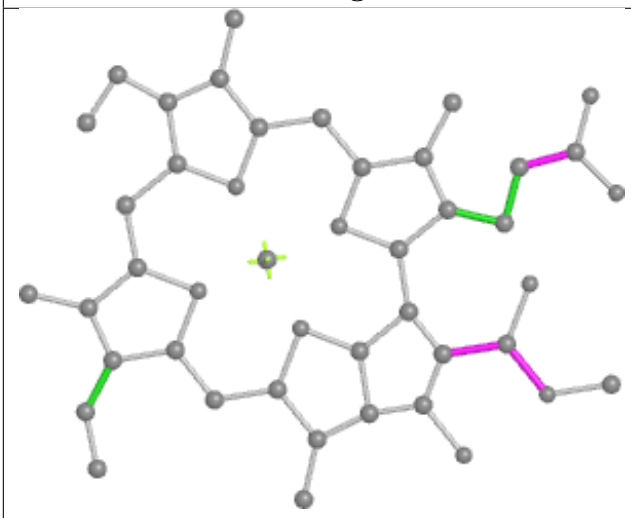
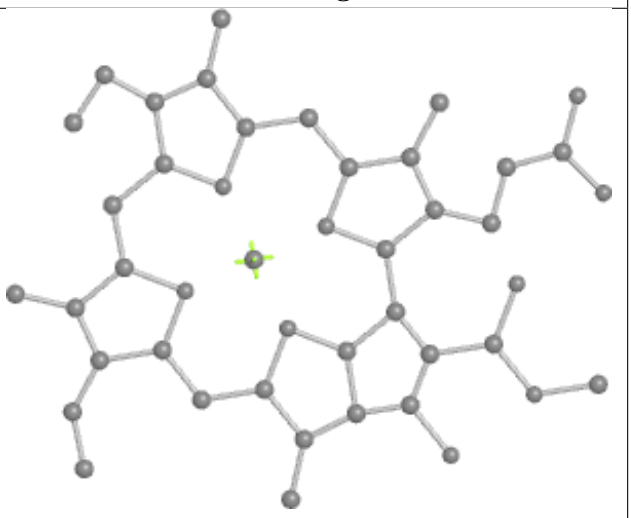


Bond angles

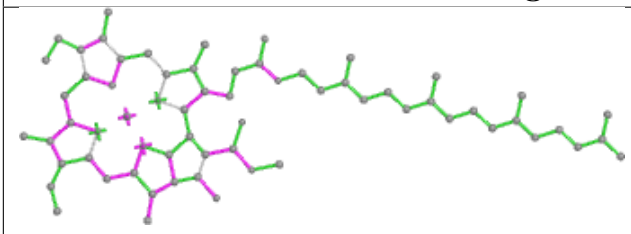


Torsions

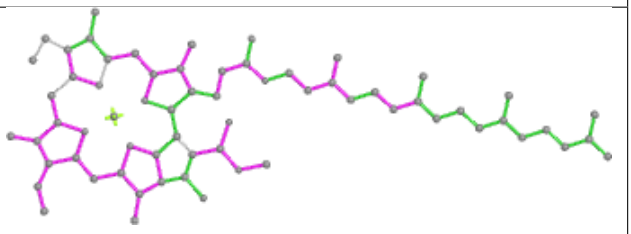


Rings

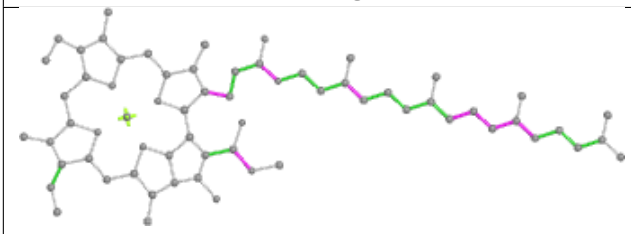
Ligand CLA B 826



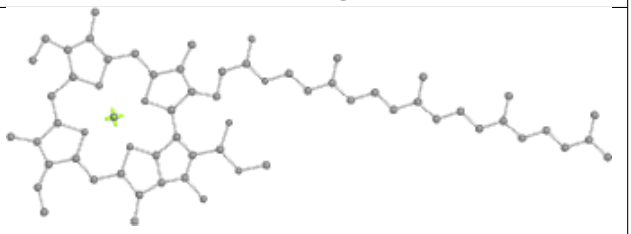
Bond lengths



Bond angles

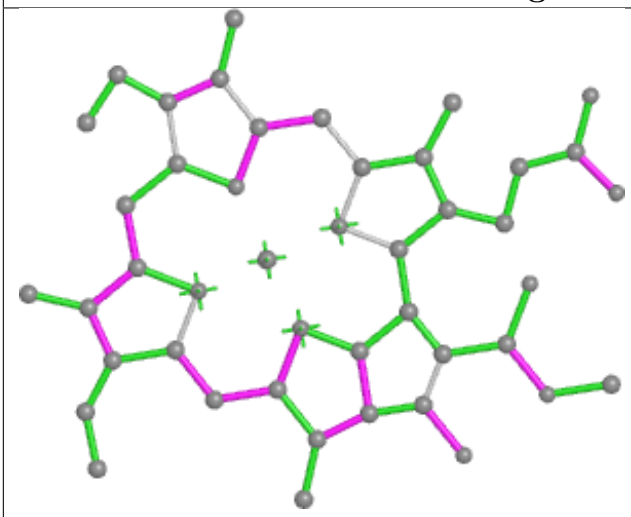


Torsions

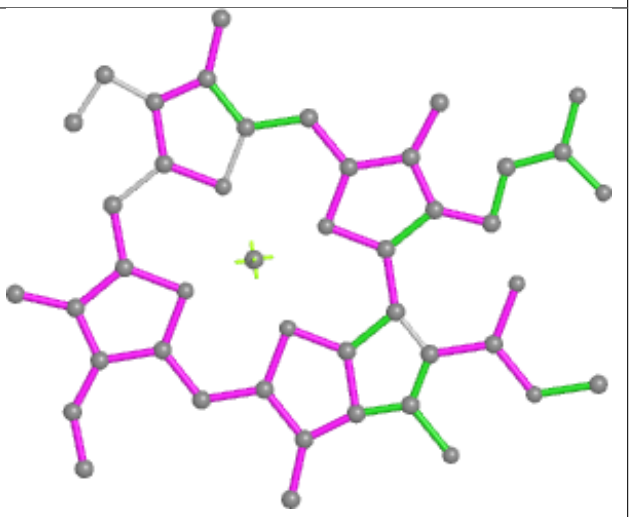


Rings

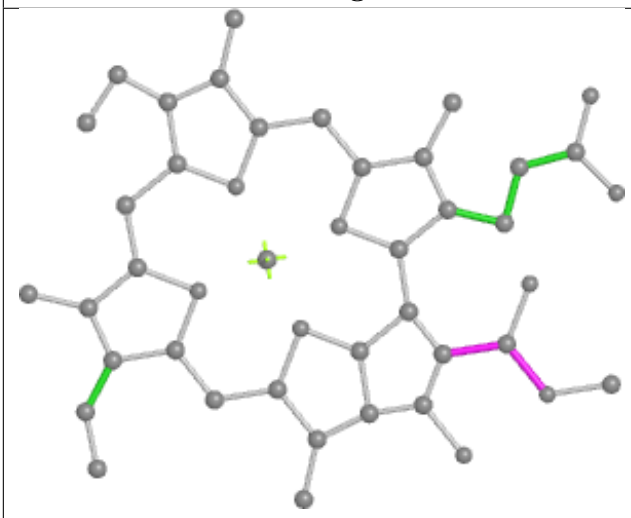
Ligand CLA 5 706



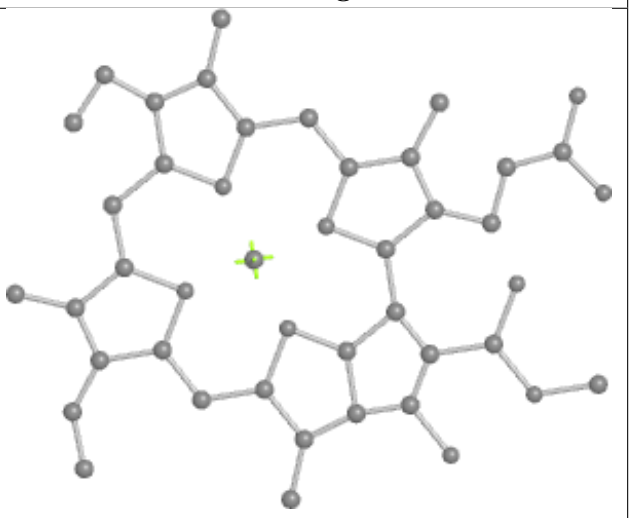
Bond lengths



Bond angles

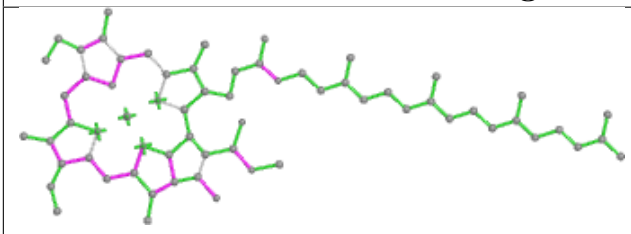


Torsions



Rings

Ligand CLA 11 706



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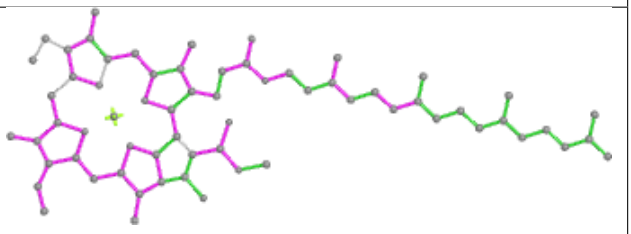
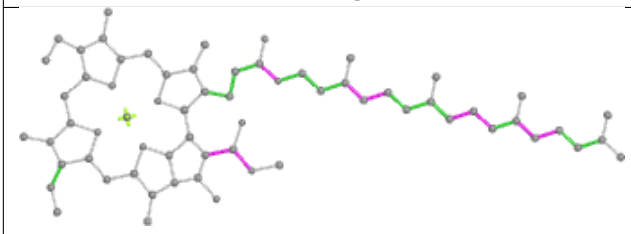


Bond angles



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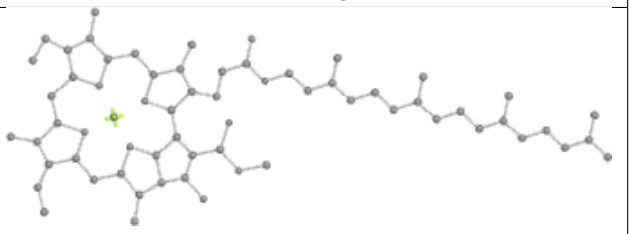
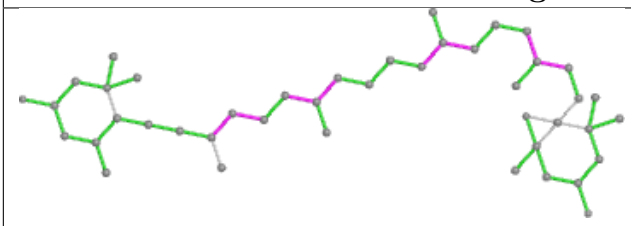


Rings

Ligand DD6 9 915



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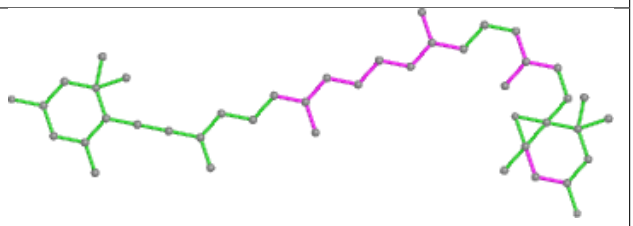
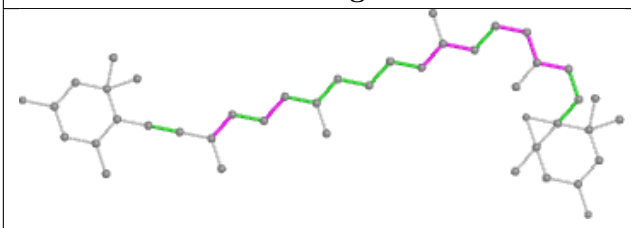


Bond angles



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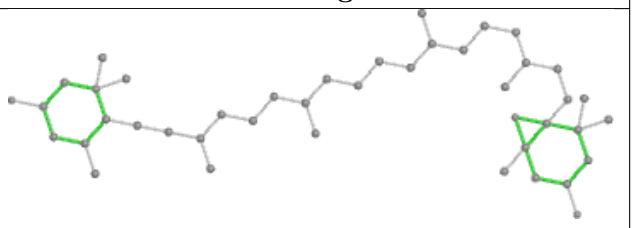
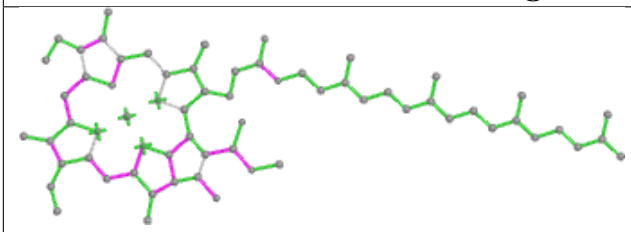


Rings

Ligand CLA B 818



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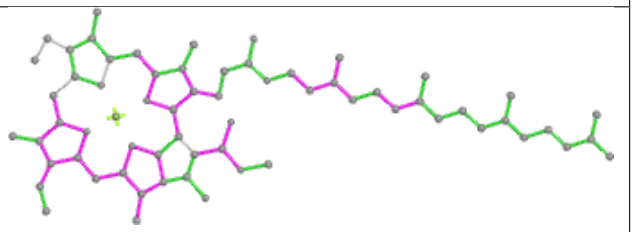

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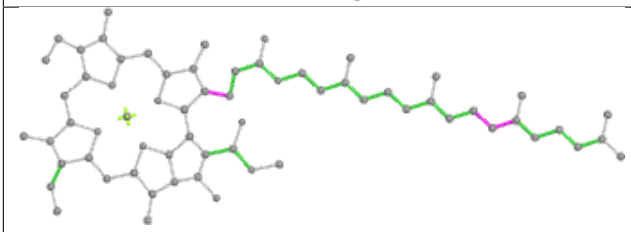

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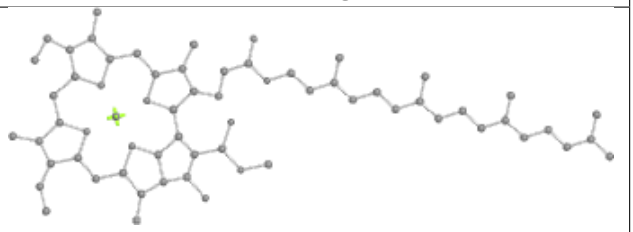
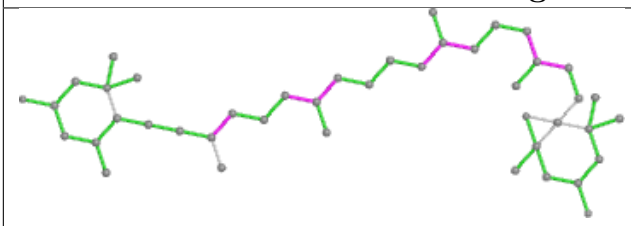


Rings

Ligand DD6 4 713



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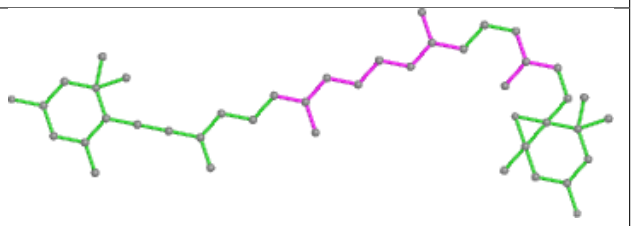
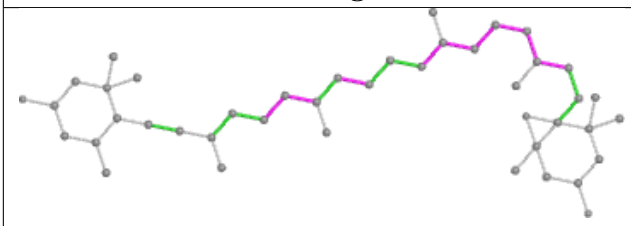


Bond angles



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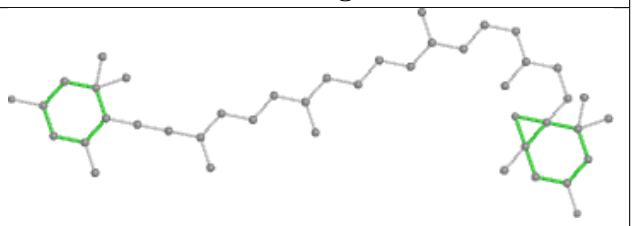
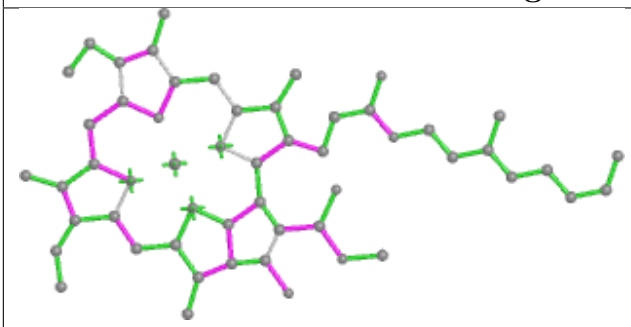
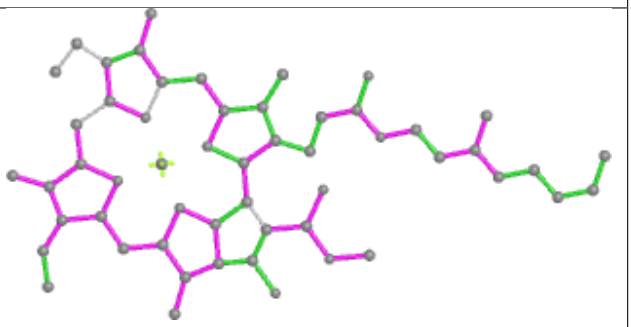
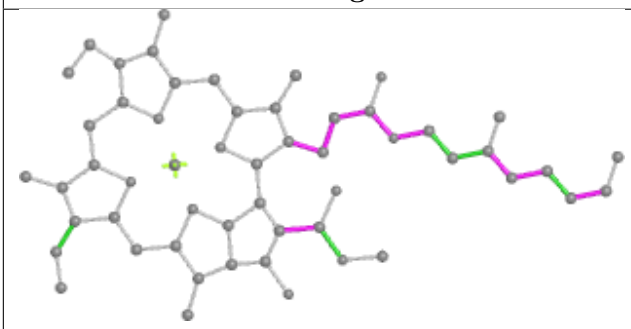
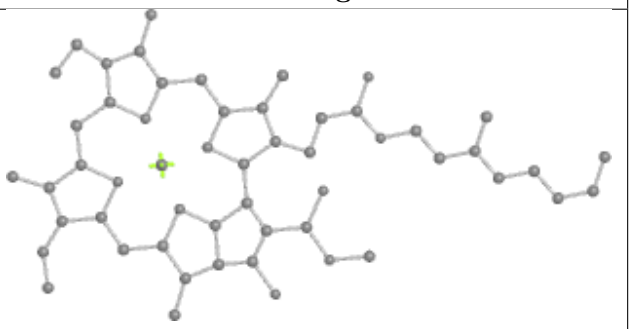


Rings

Ligand CLA B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

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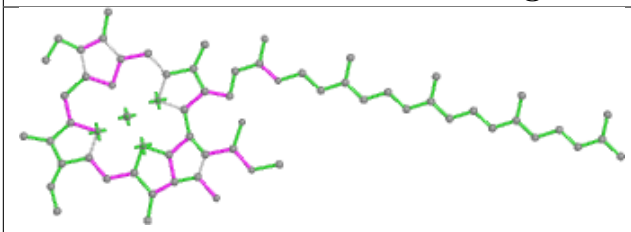
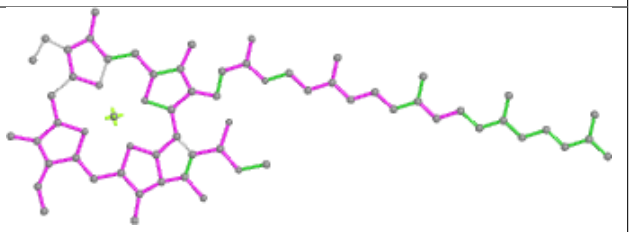
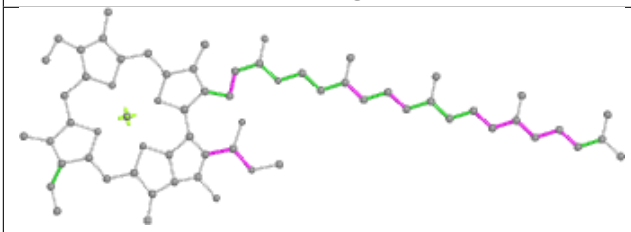
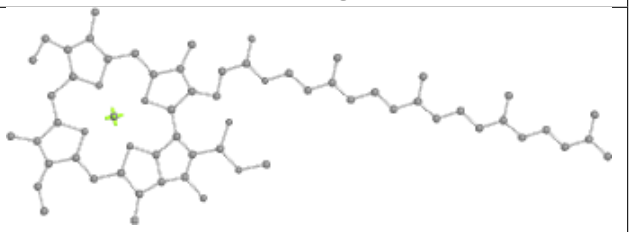
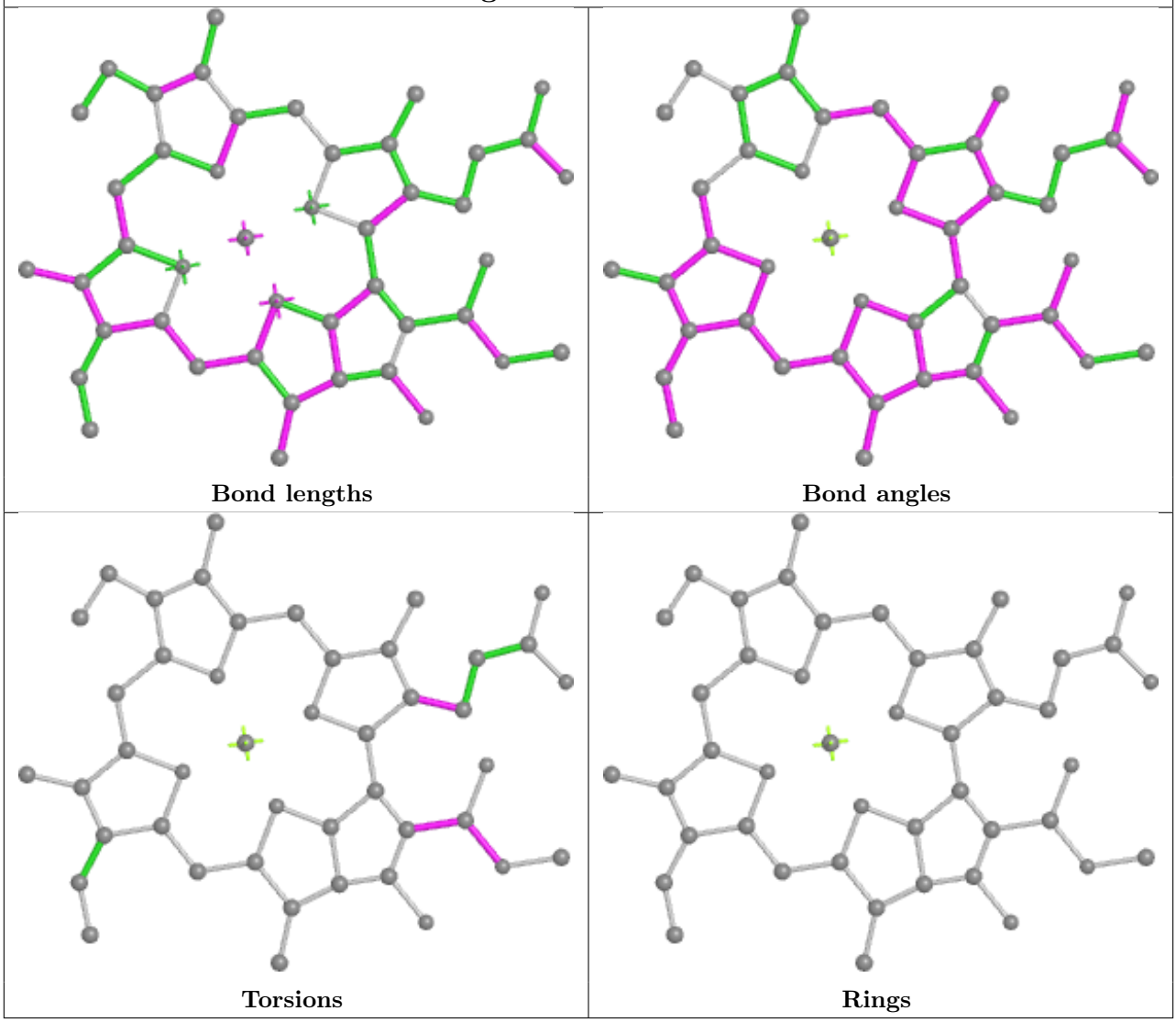
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 835



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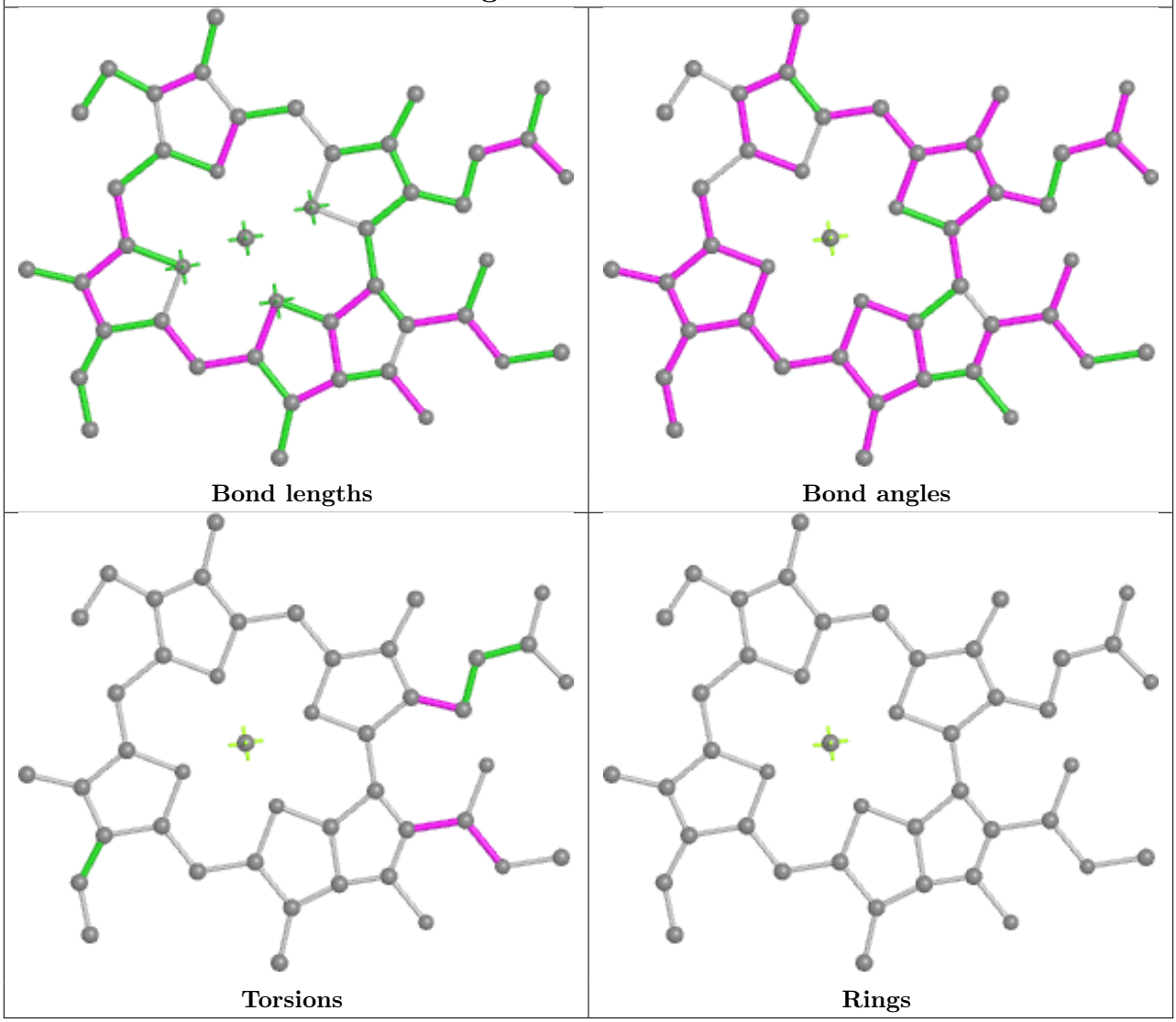
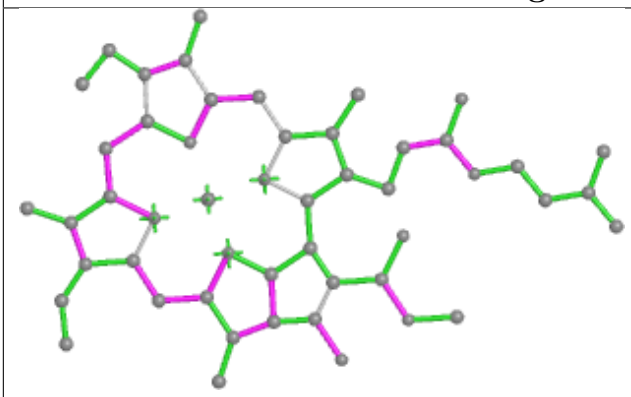
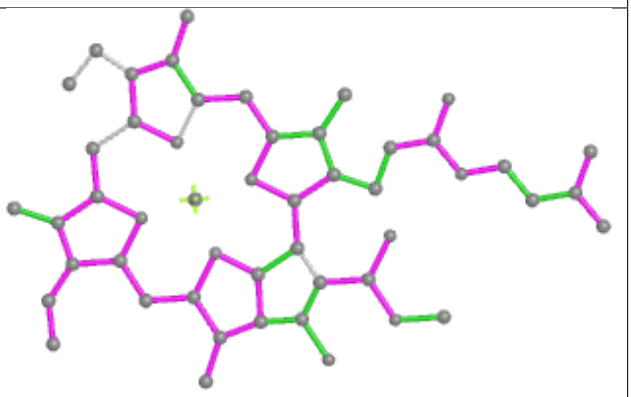


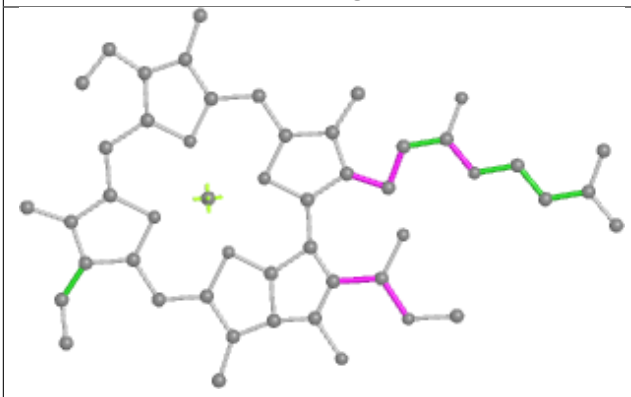
Ligand CLA 5 710



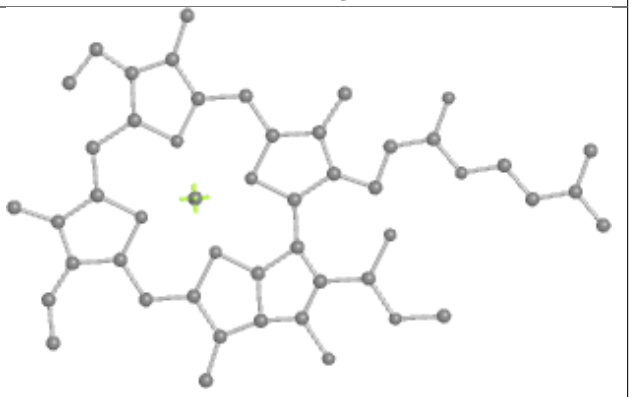
Bond lengths



Bond angles

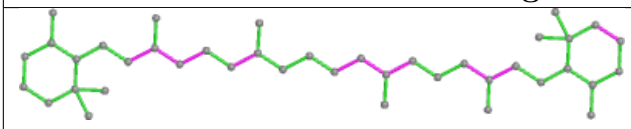


Torsions



Rings

Ligand BCR A 849



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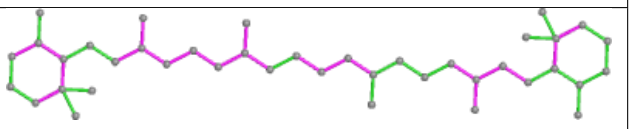
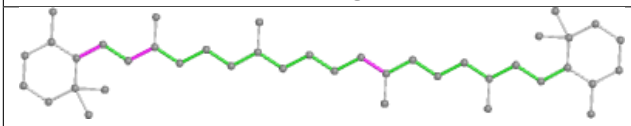


Bond angles



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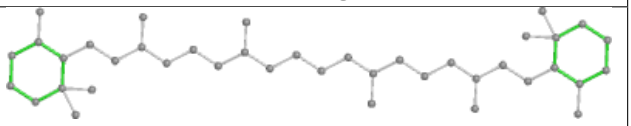
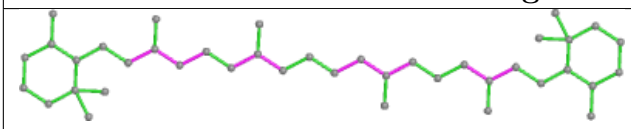


Rings

Ligand BCR A 850



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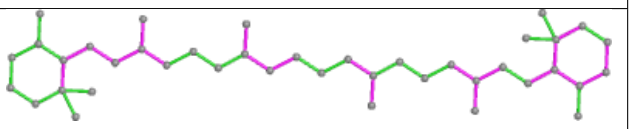
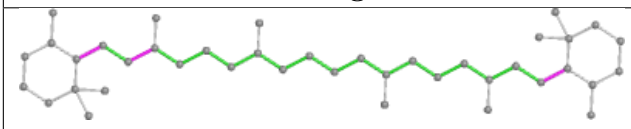


Bond angles



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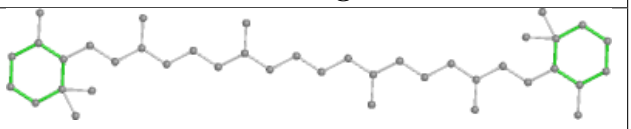
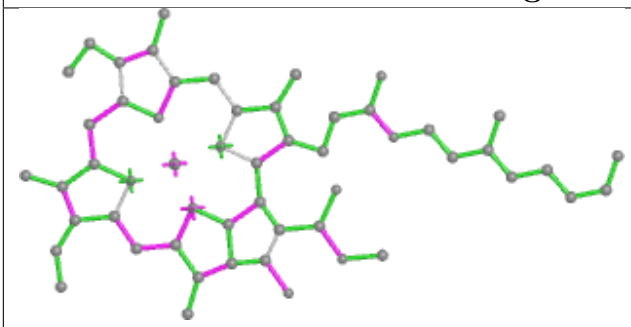
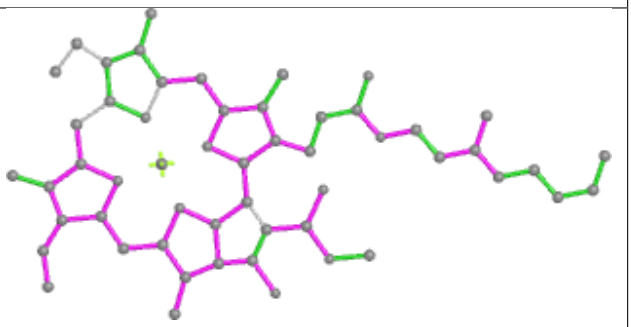
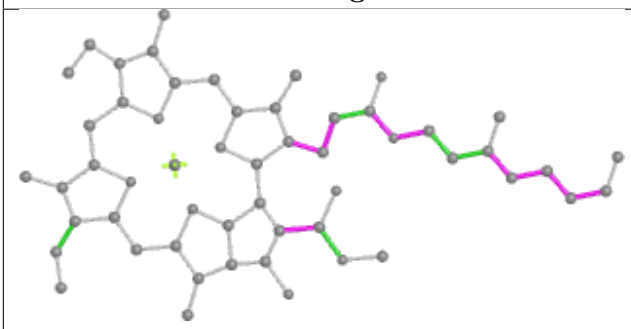
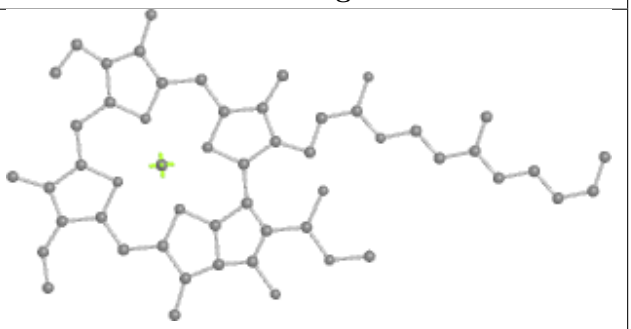
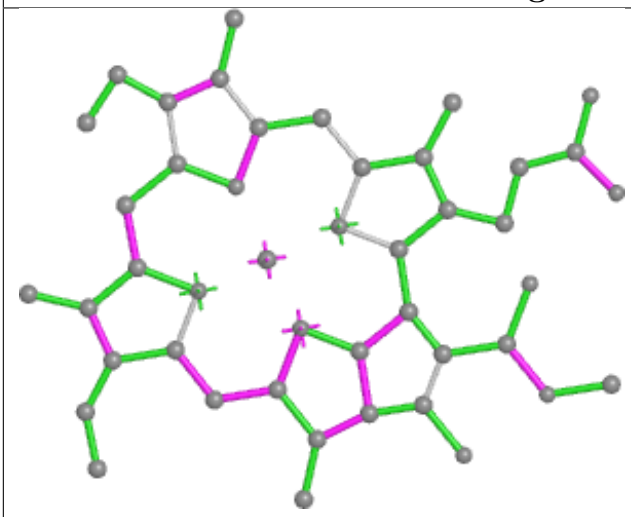


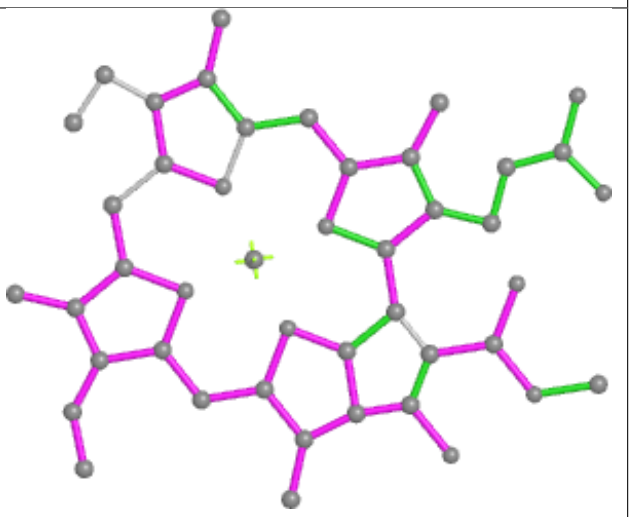
Rings

Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

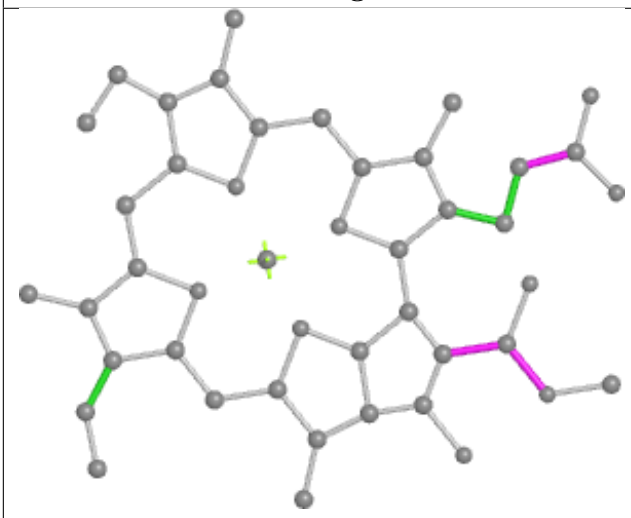
Ligand CLA 5 703



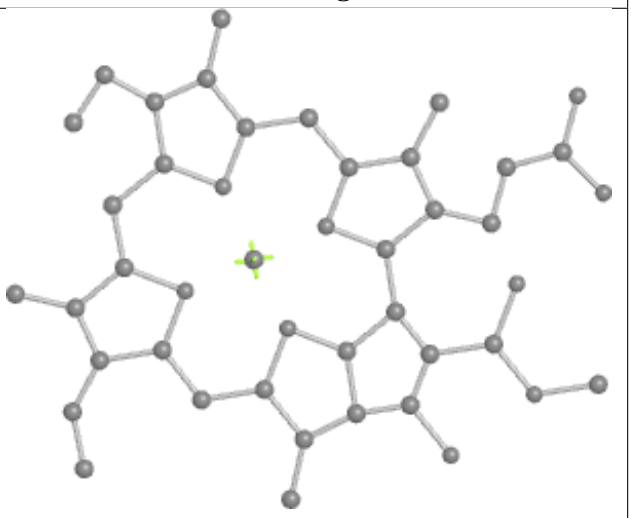
Bond lengths



Bond angles

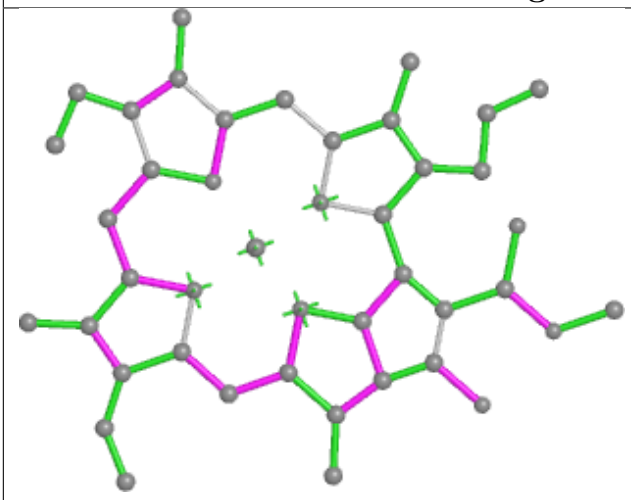


Torsions



Rings

Ligand CLA 8 610



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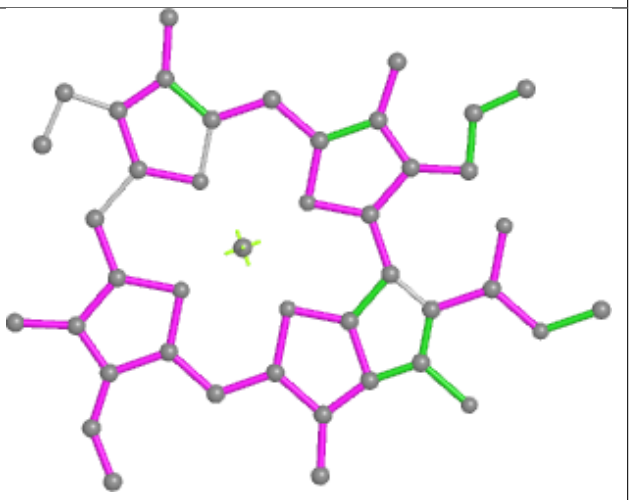
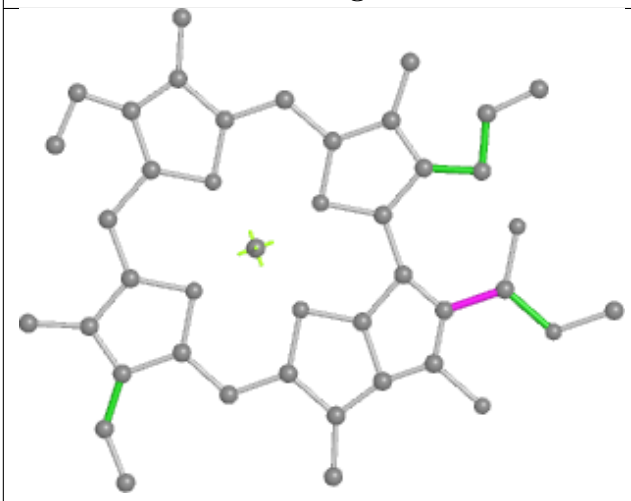


Bond angles



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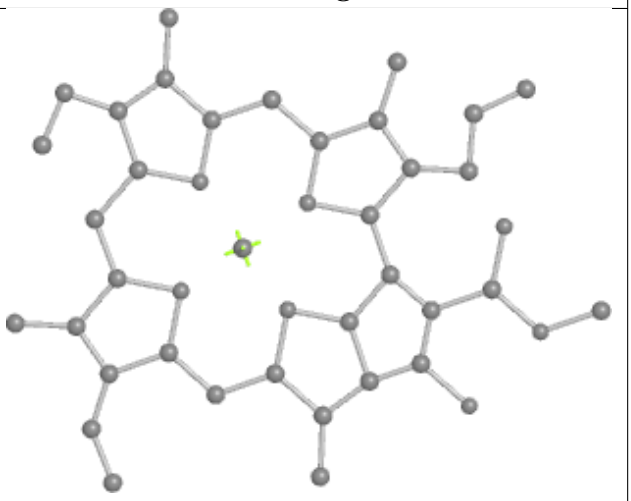
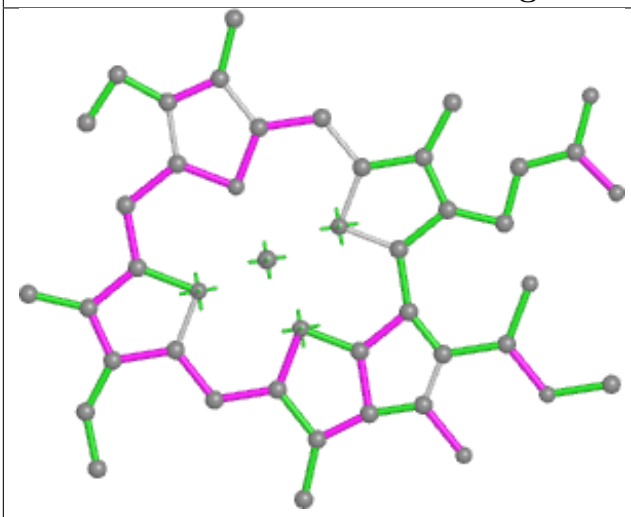
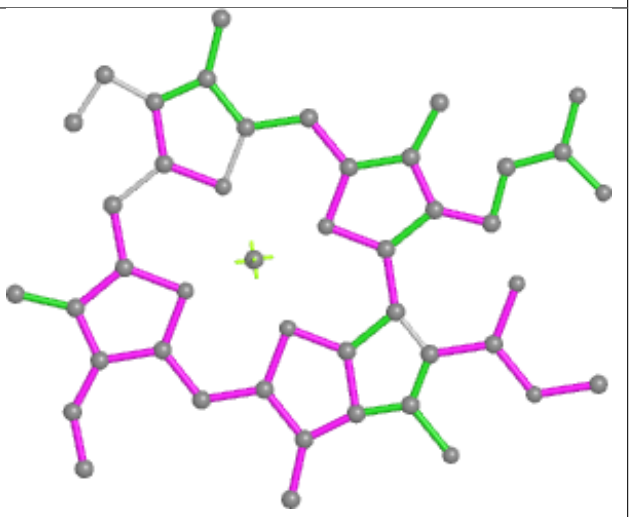


Rings

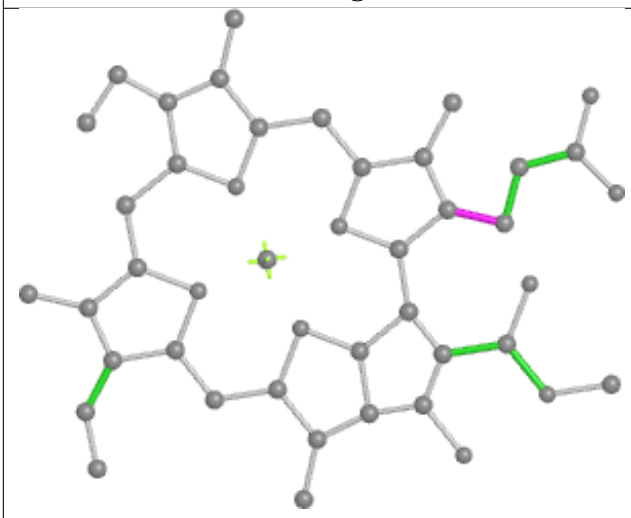
Ligand CLA 10 711



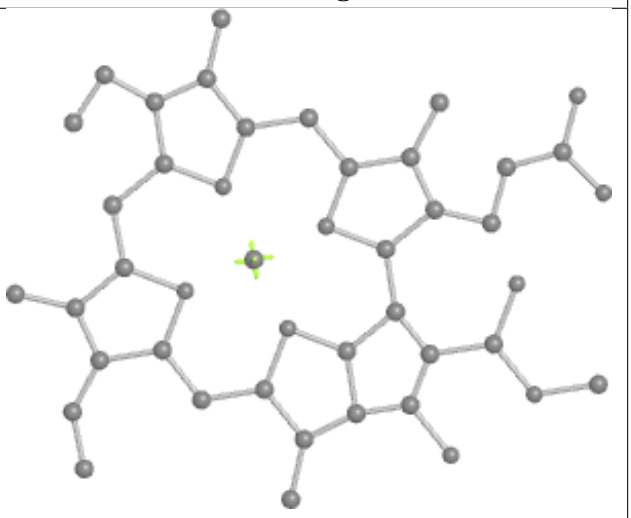
Bond lengths



Bond angles

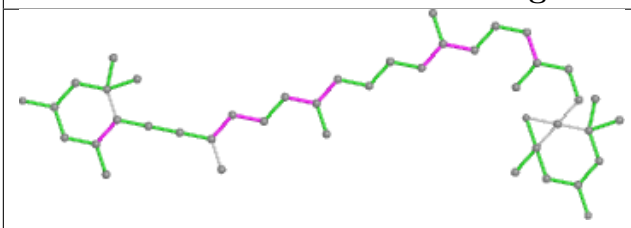


Torsions



Rings

Ligand DD6 6 915



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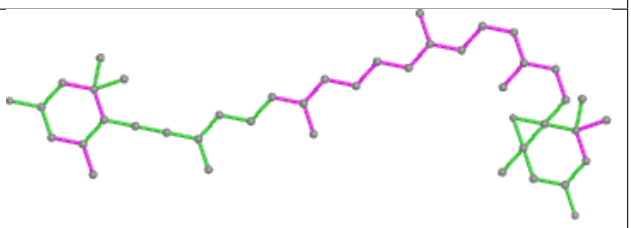

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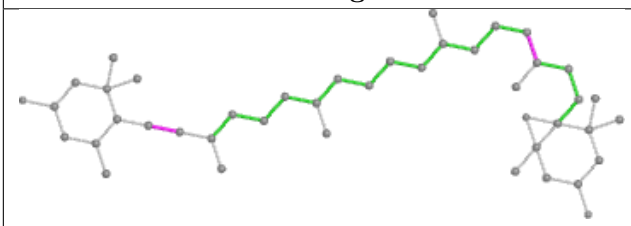
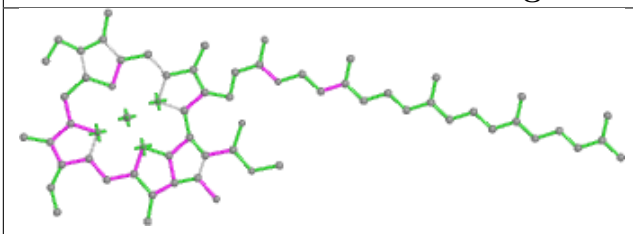


Torsions

Rings

Ligand CLA A 820



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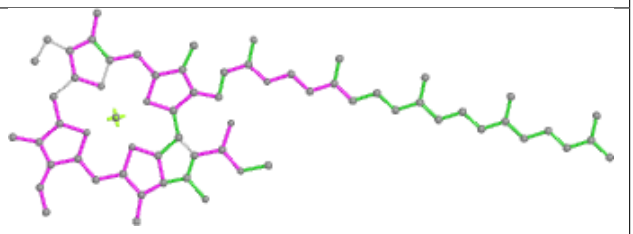
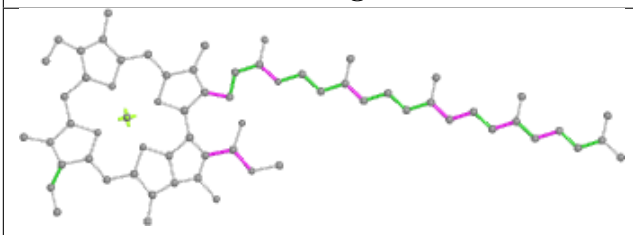


Bond angles



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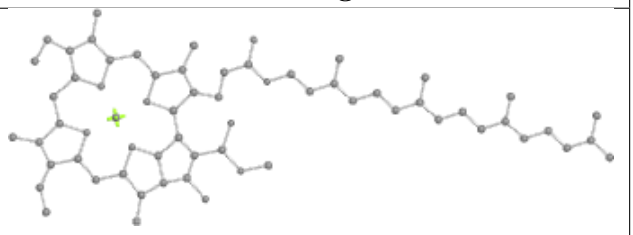
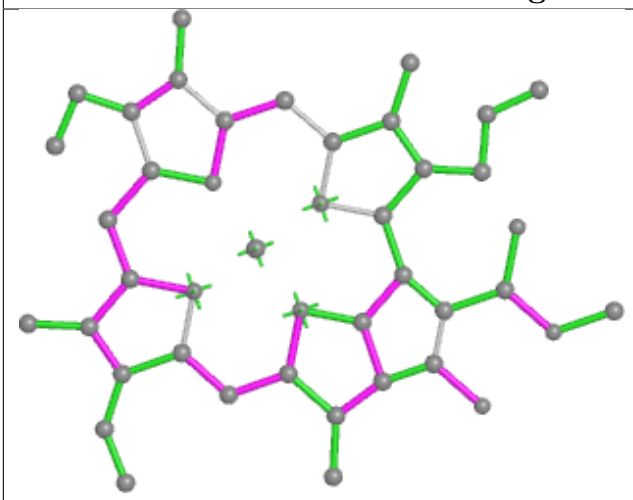


Rings

Ligand CLA 1 511



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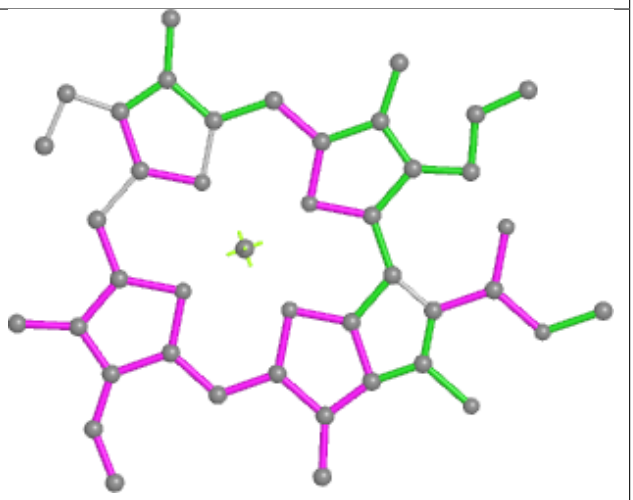

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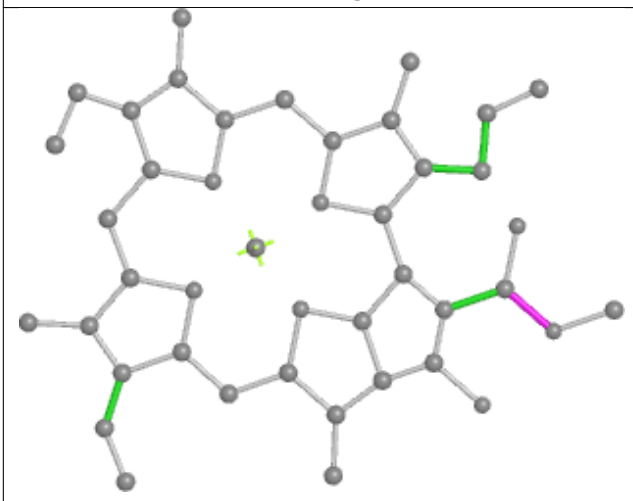

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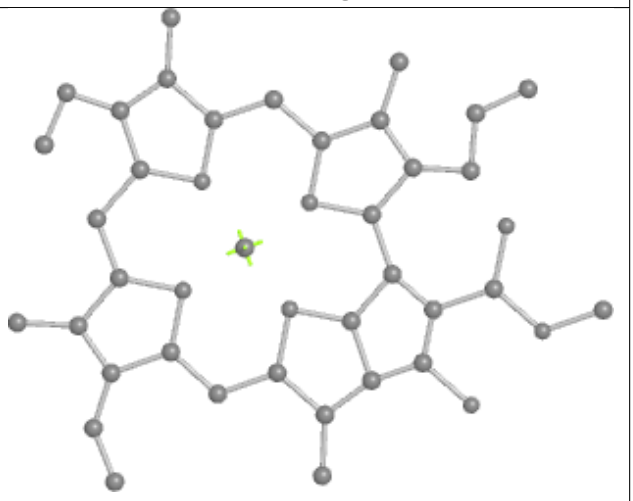
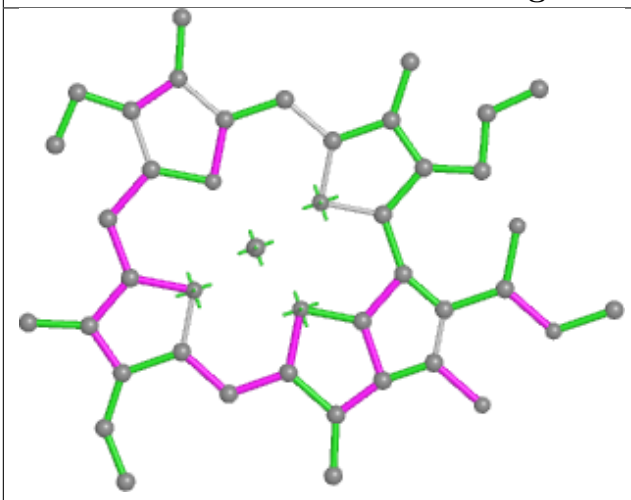


Rings

Ligand CLA 6 910



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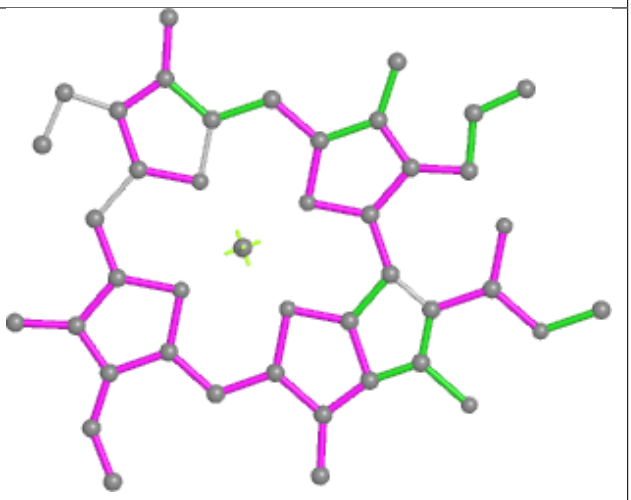

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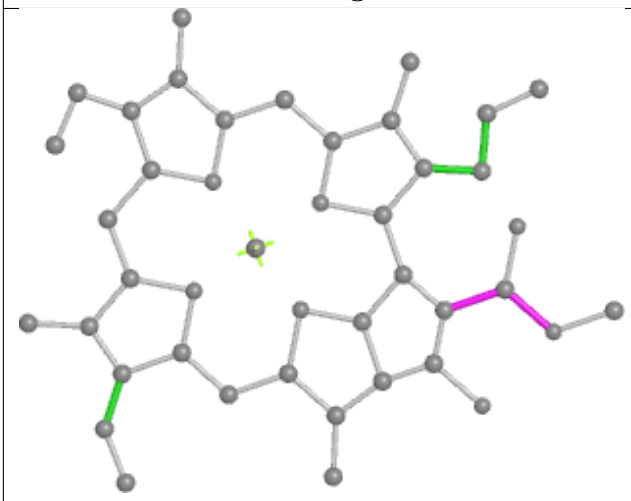

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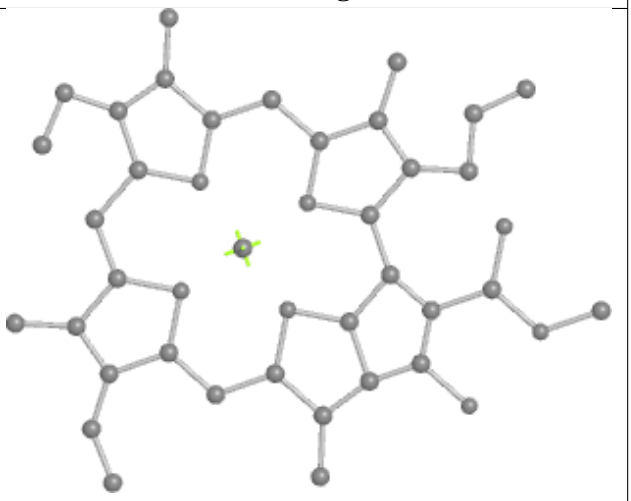
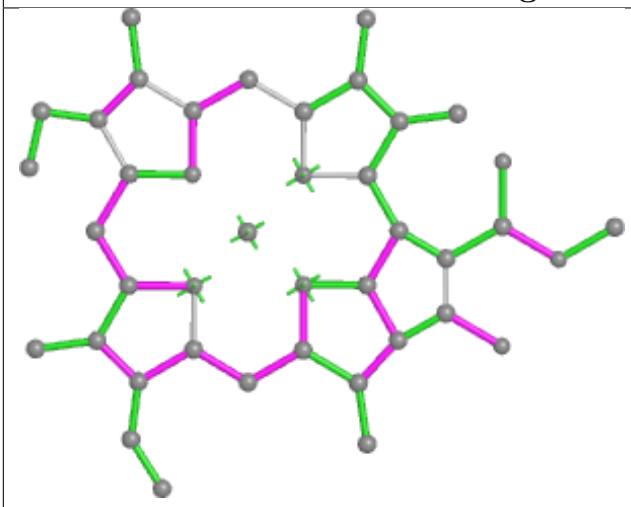


Rings

Ligand CLA 12 504



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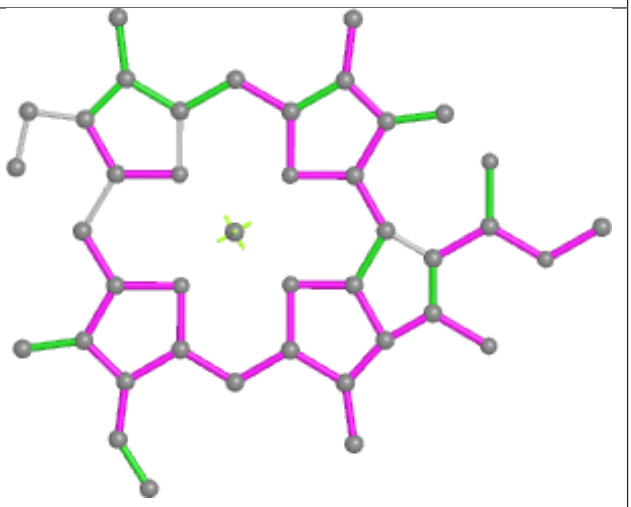
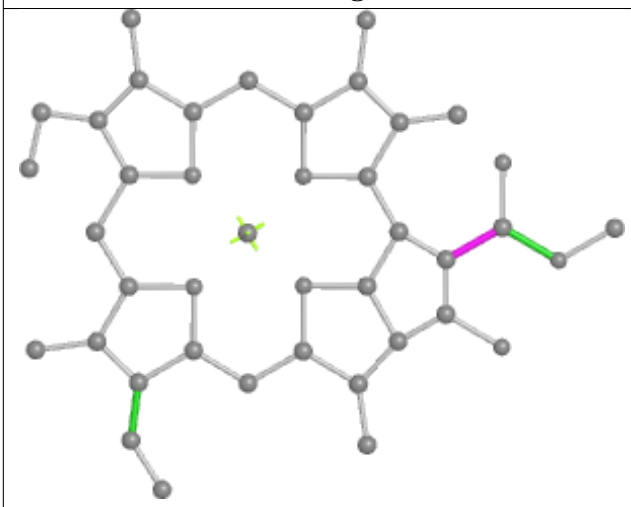


Bond angles



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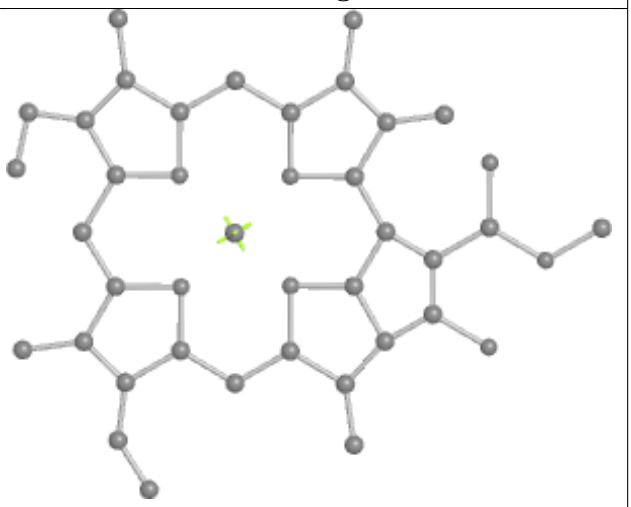
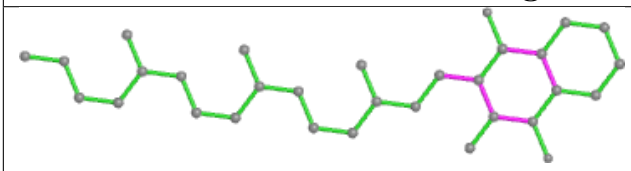


Rings

Ligand PQN B 840



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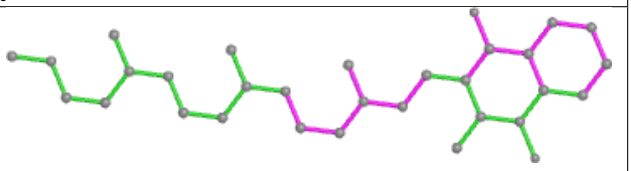
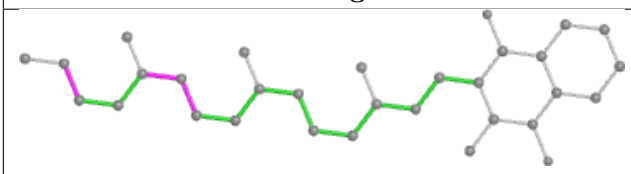


Bond angles



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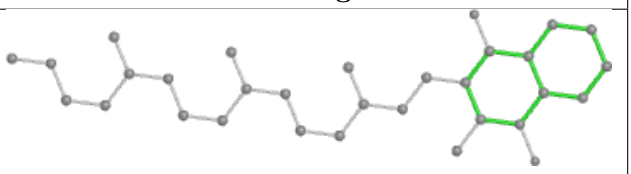
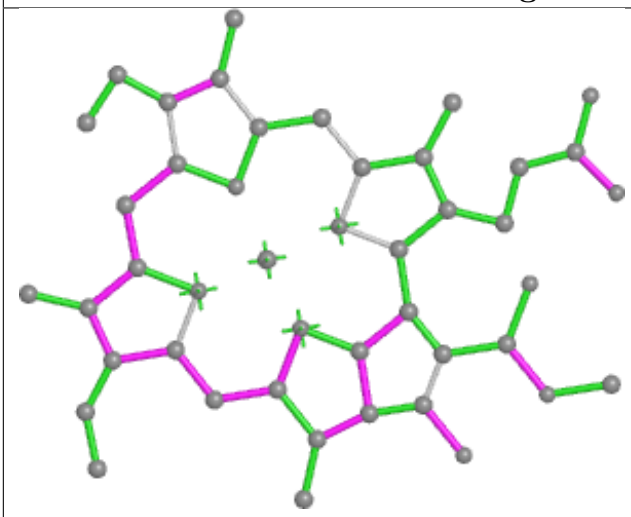


Rings

Ligand CLA 10 705



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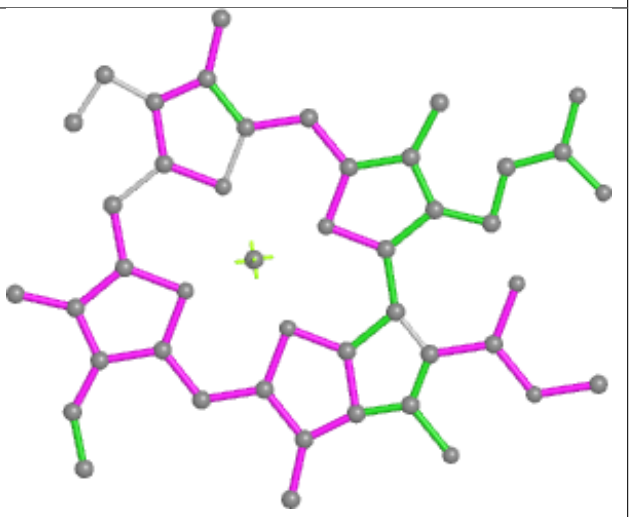

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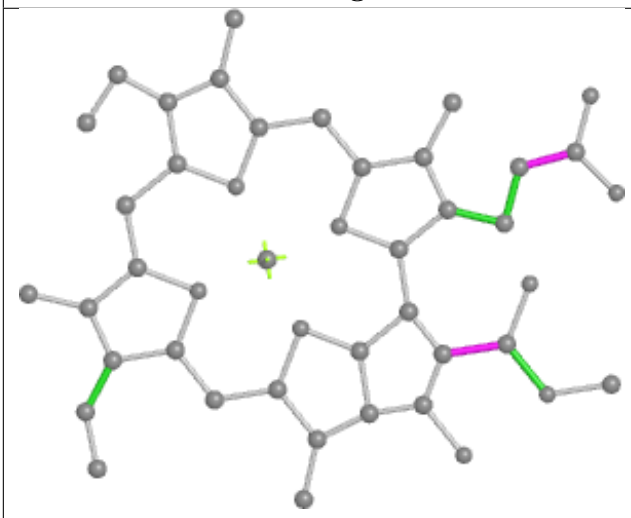

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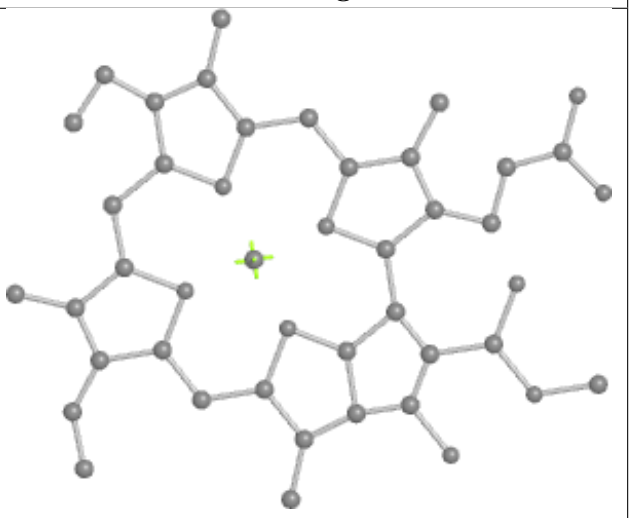
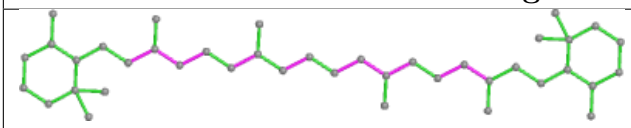


Rings

Ligand BCR B 845



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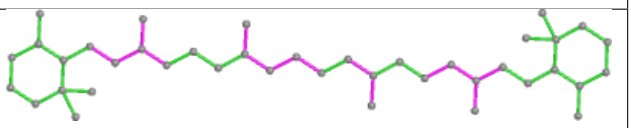
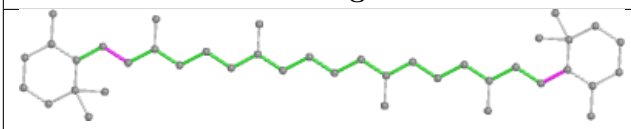


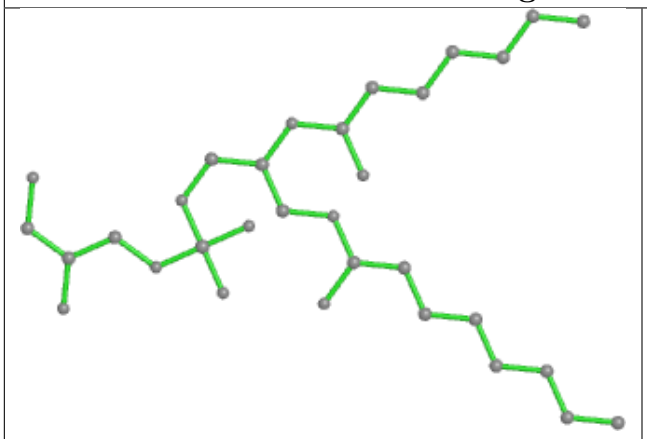
Bond angles



Torsions

Rings

Ligand LHG 10 713



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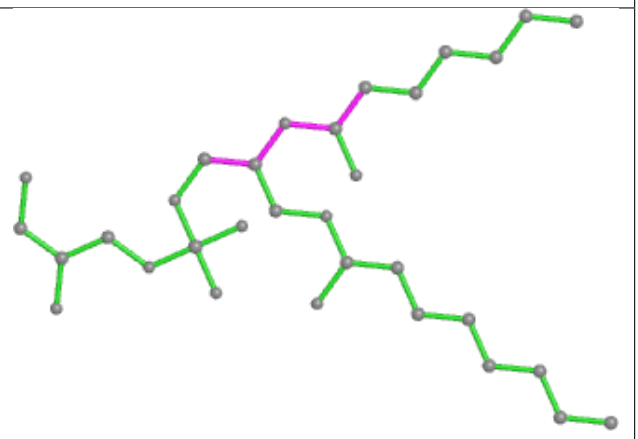
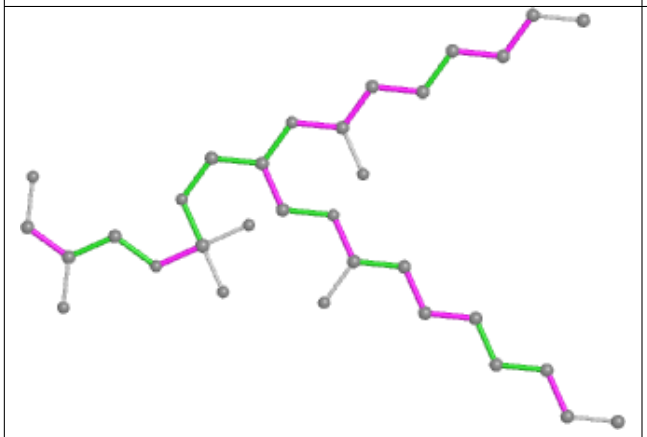


Bond angles



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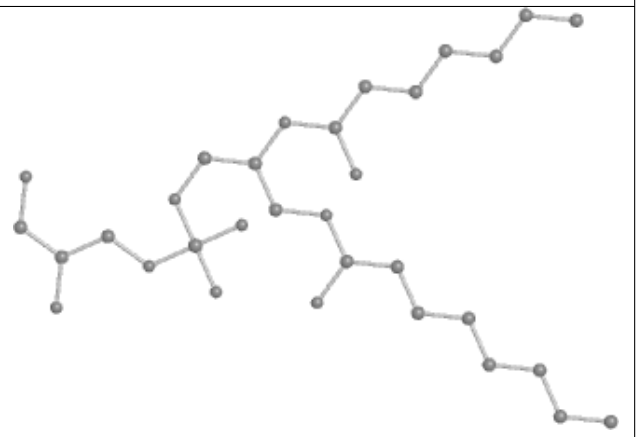
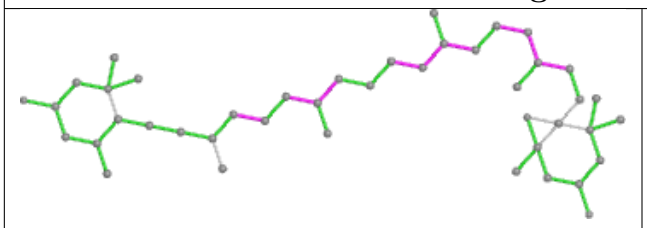


Rings

Ligand DD6 5 712



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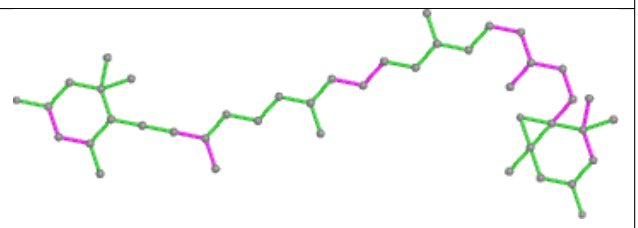

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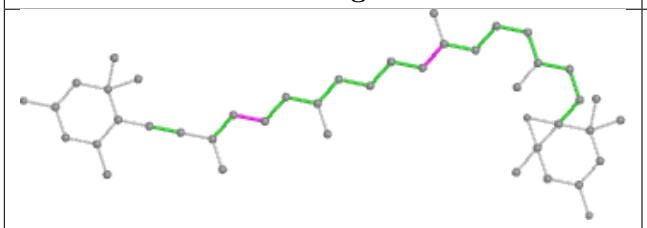

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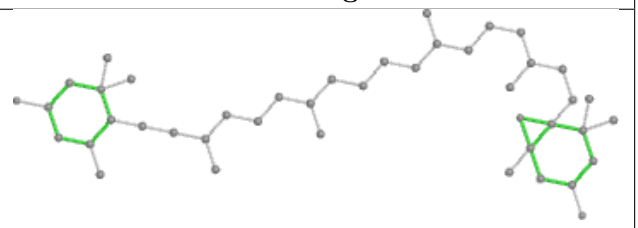
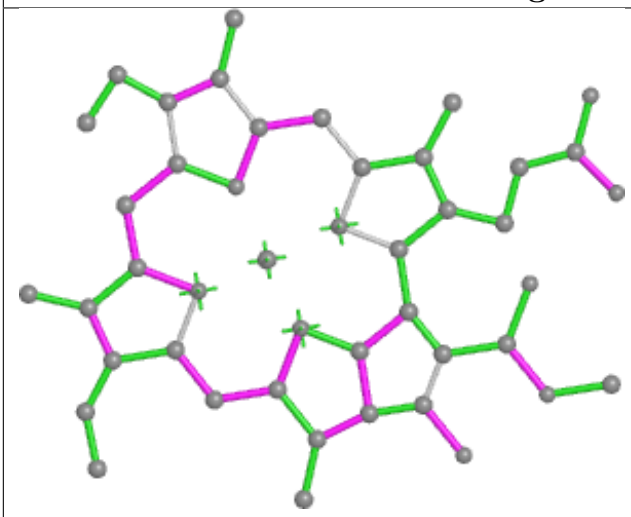


Rings

Ligand CLA 6 912



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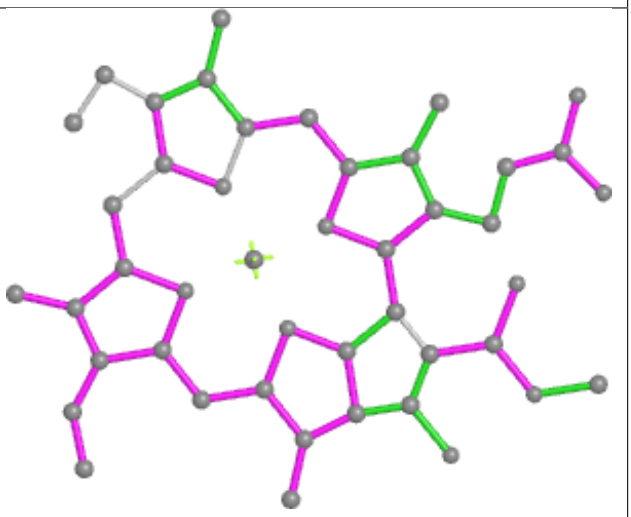
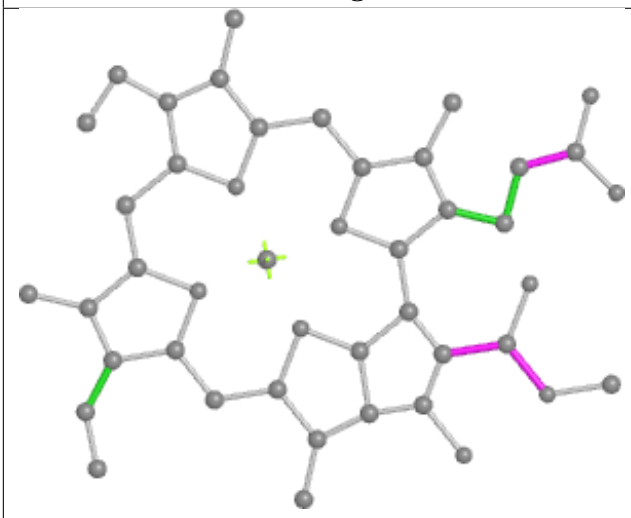


Bond angles



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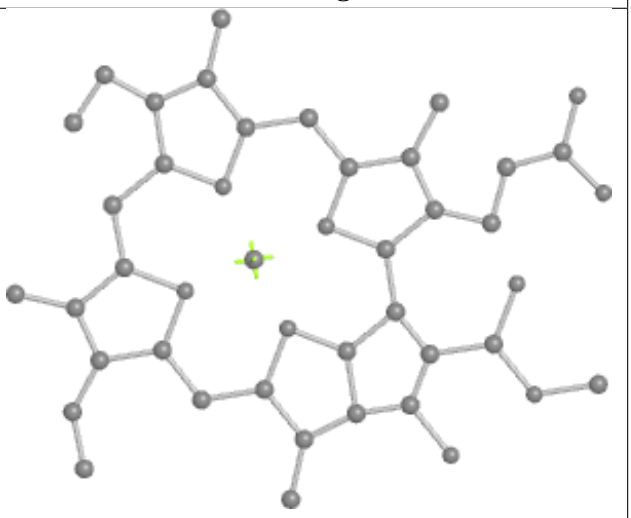
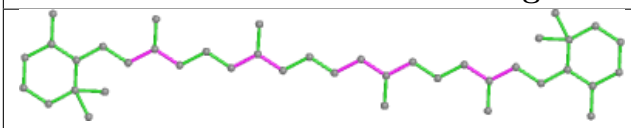


Rings

Ligand BCR B 844



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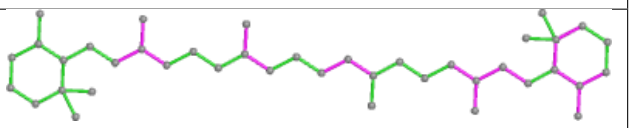
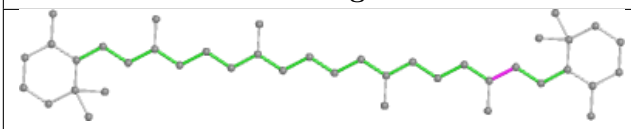
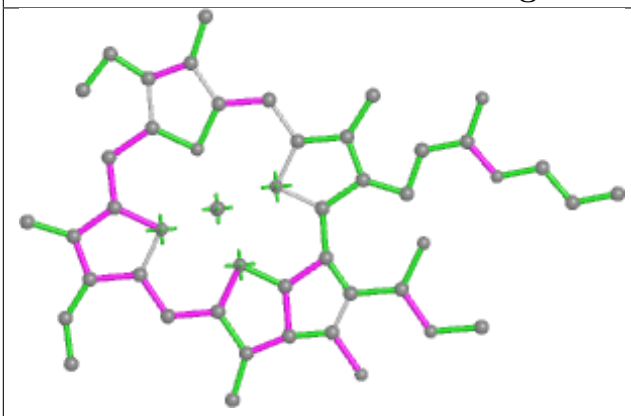
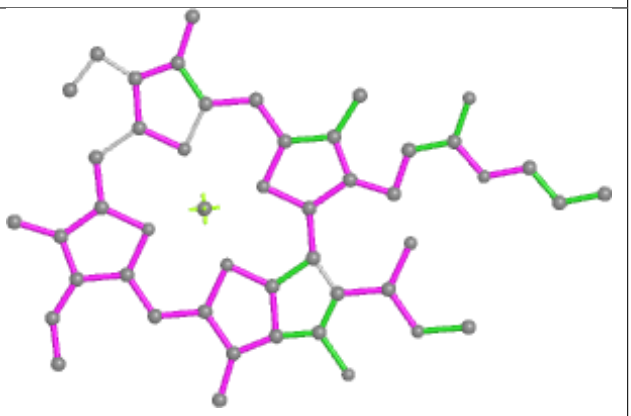
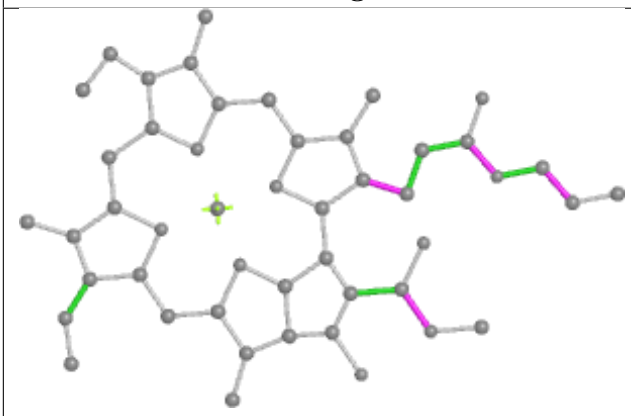
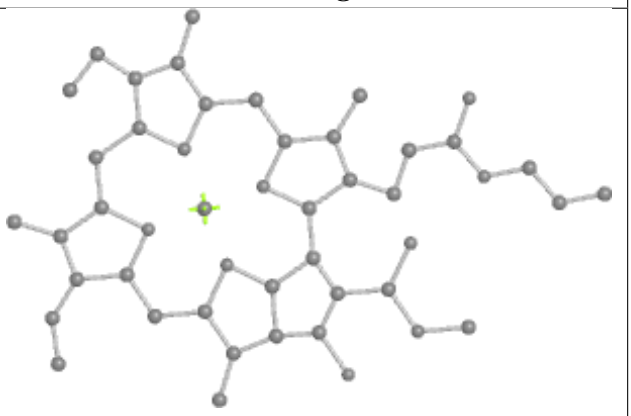


Bond angles

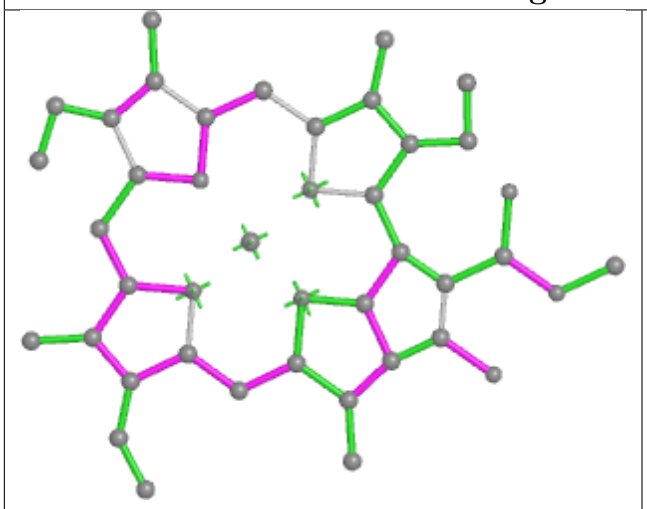


Torsions

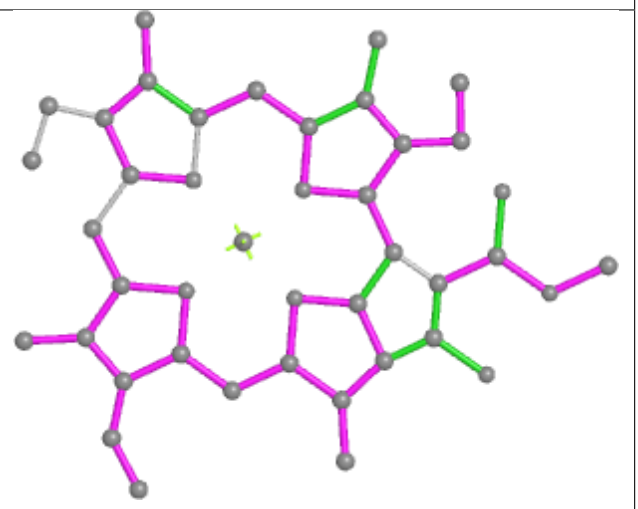
Rings

Ligand CLA 10 707	
 Bond lengths	 Bond angles
 Torsions	 Rings

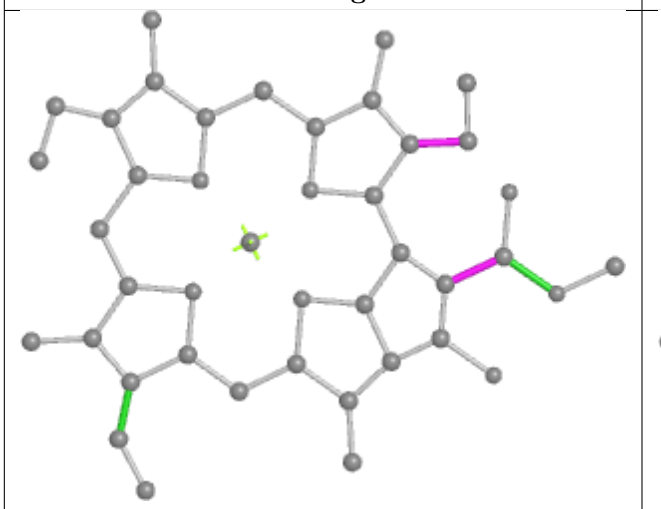
Ligand CLA 3 704



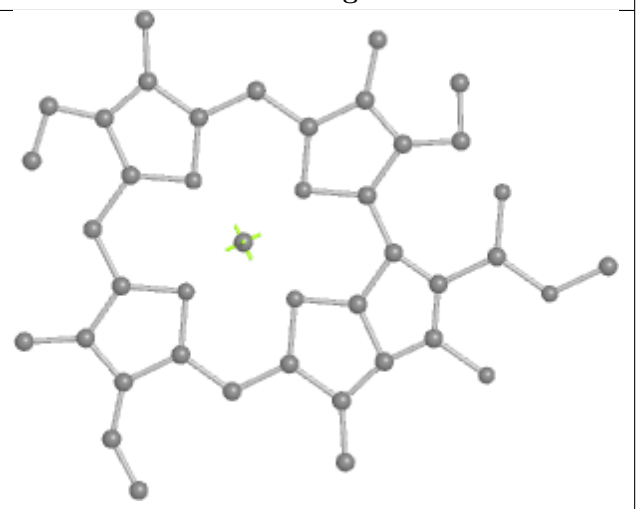
Bond lengths



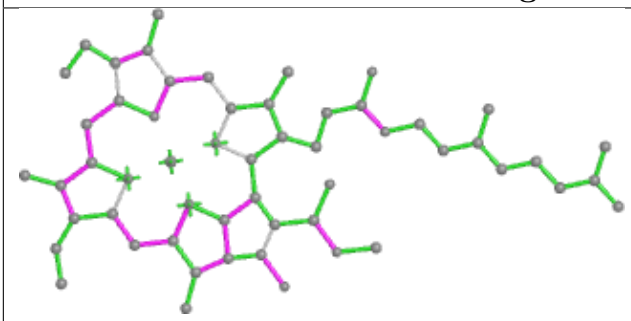
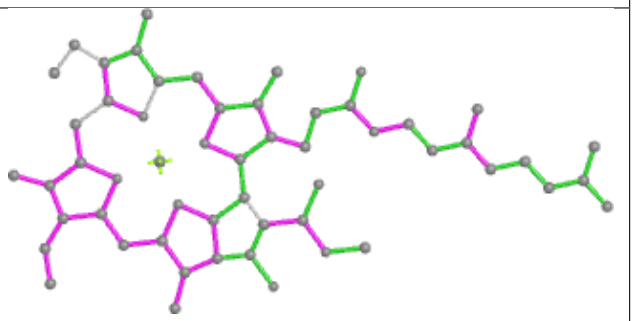
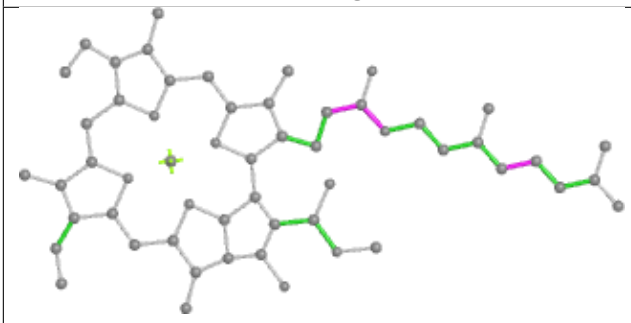
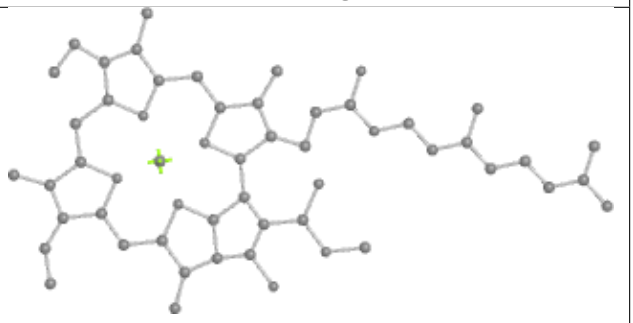
Bond angles

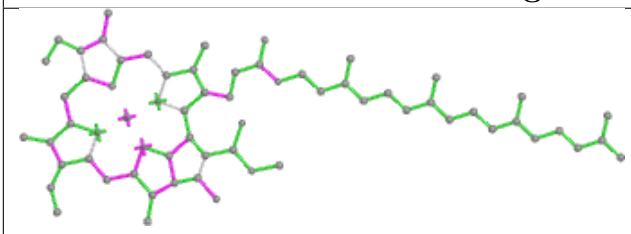
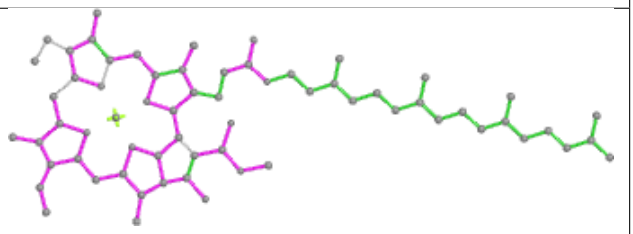
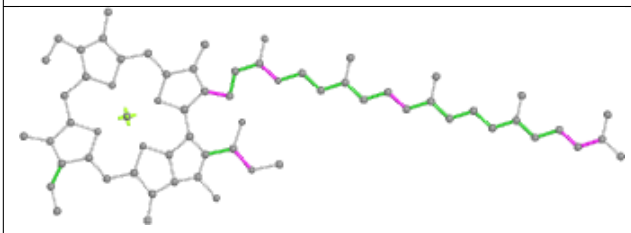
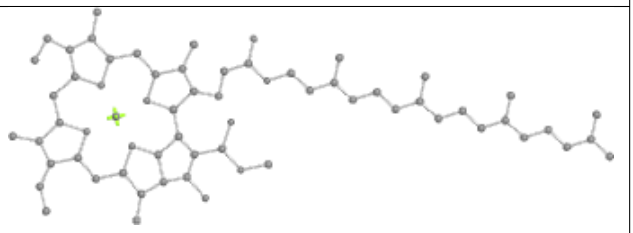


Torsions

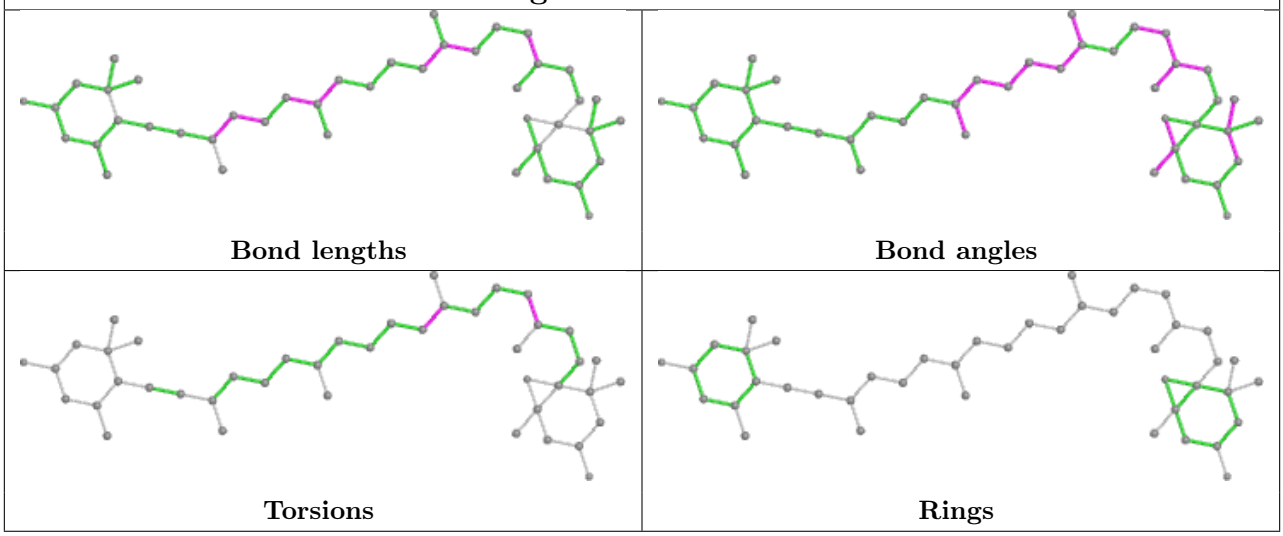


Rings

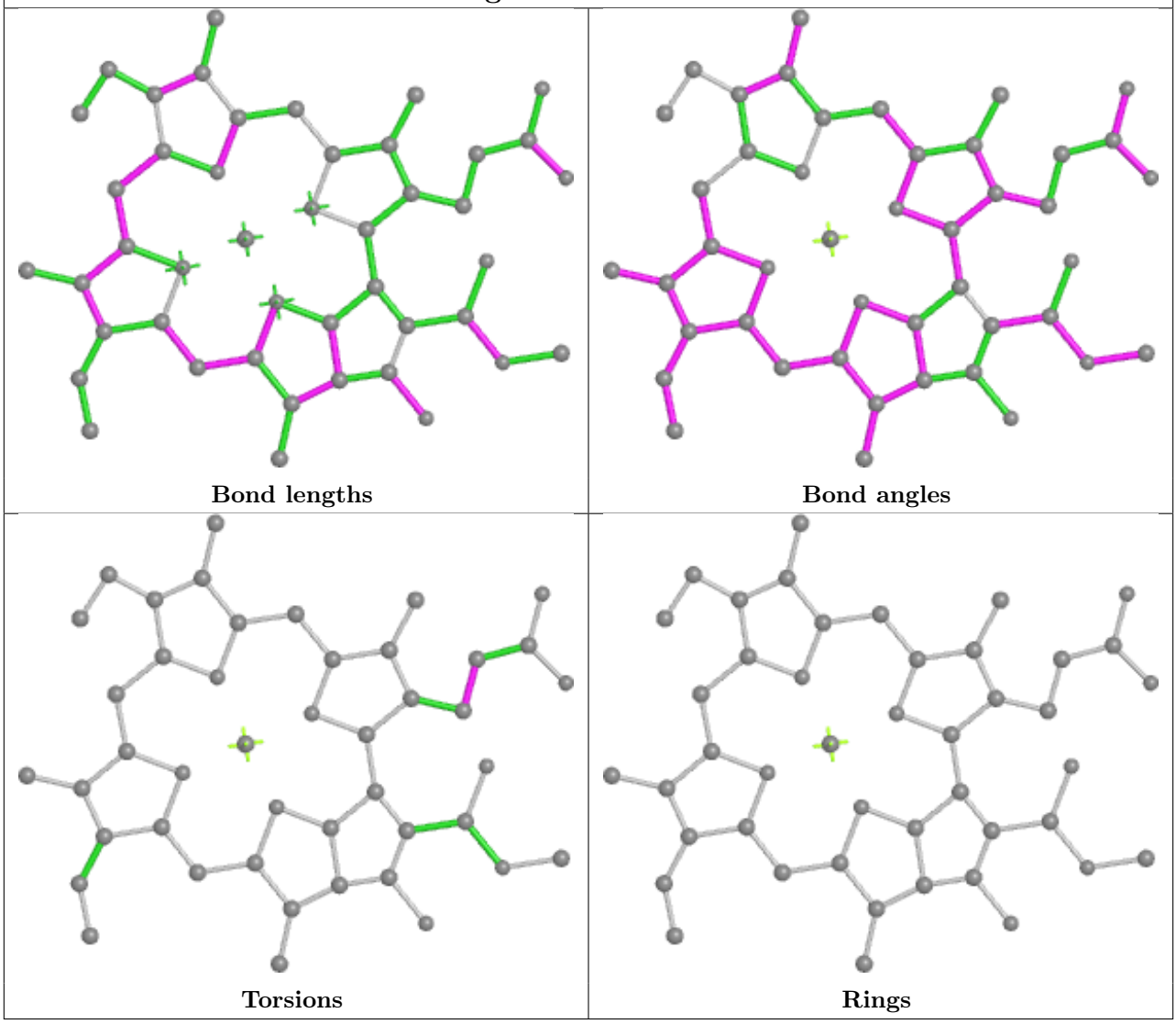
Ligand CLA 10 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

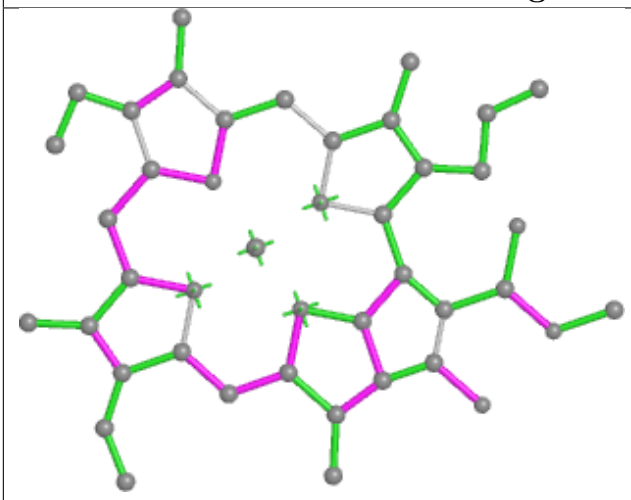
Ligand DD6 3 716



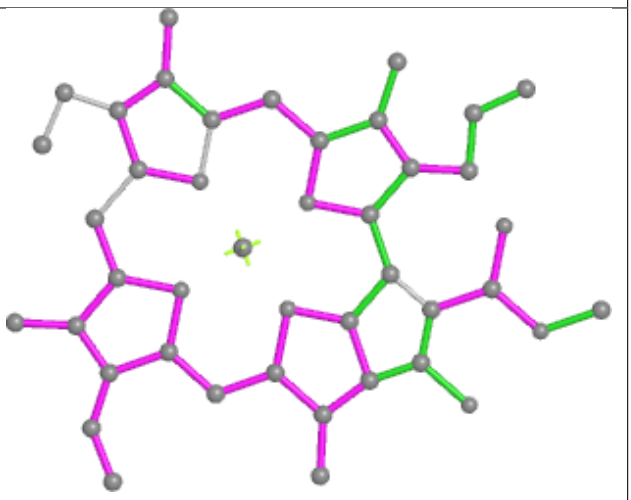
Ligand CLA 1 515



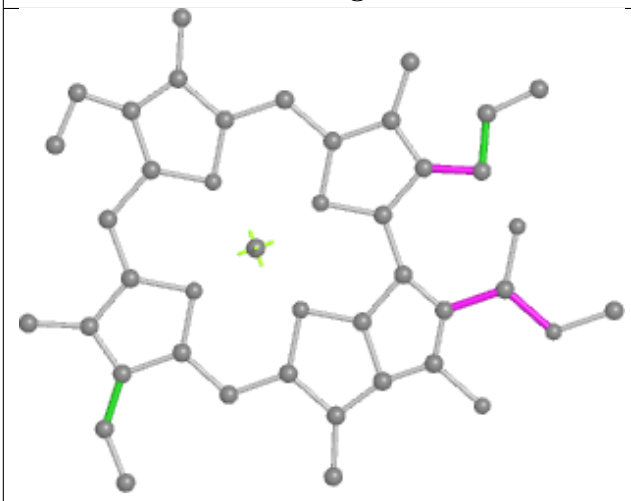
Ligand CLA 3 708



Bond lengths



Bond angles



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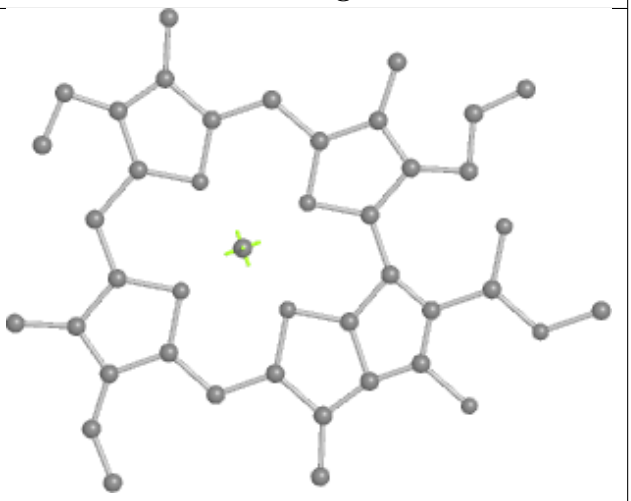
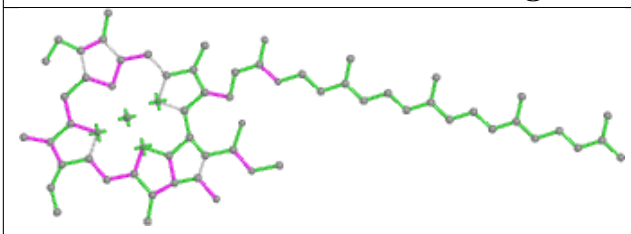
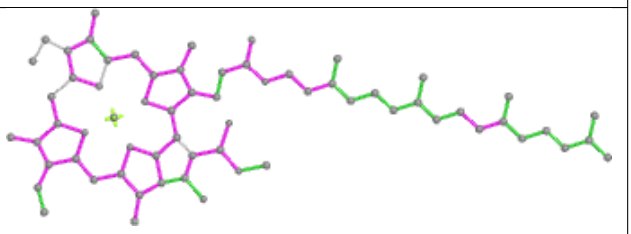


Rings

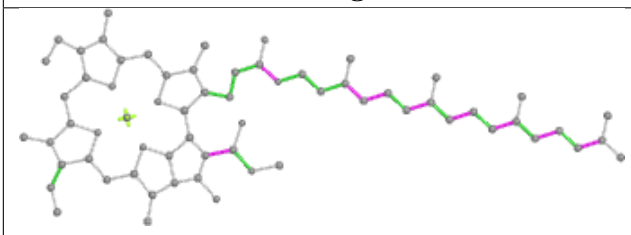
Ligand CLA B 835



Bond lengths



Bond angles



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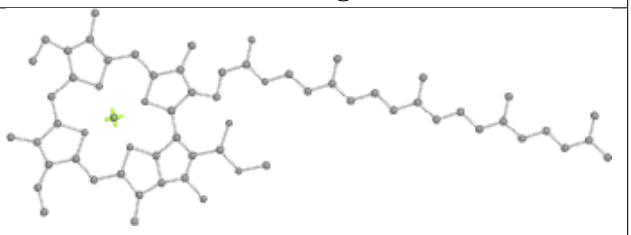
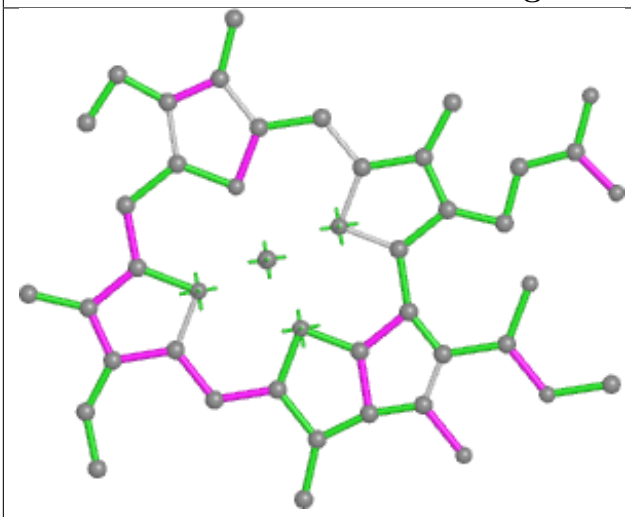


Rings

Ligand CLA A 834



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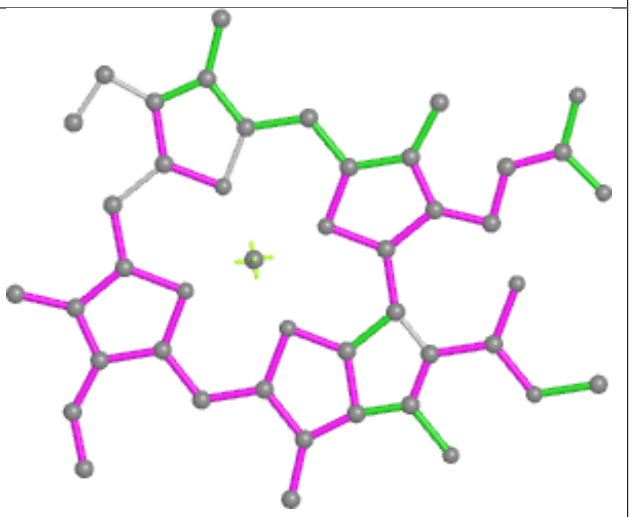
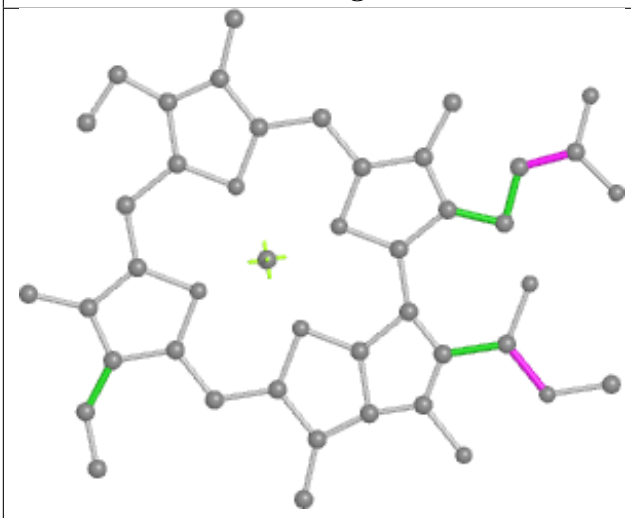


Bond angles



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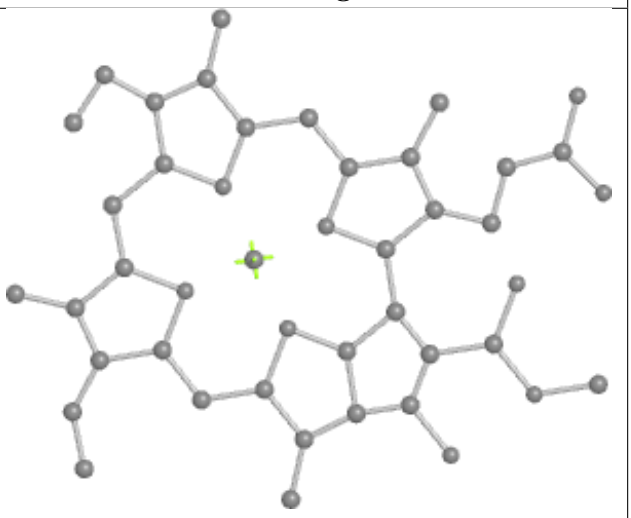
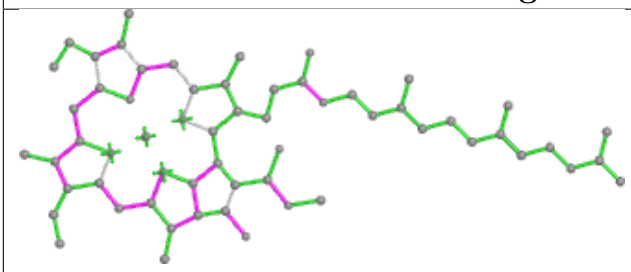


Rings

Ligand CLA 12 501



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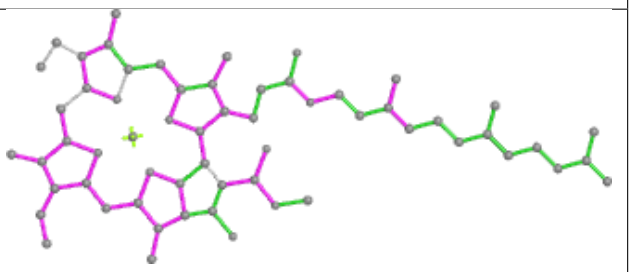
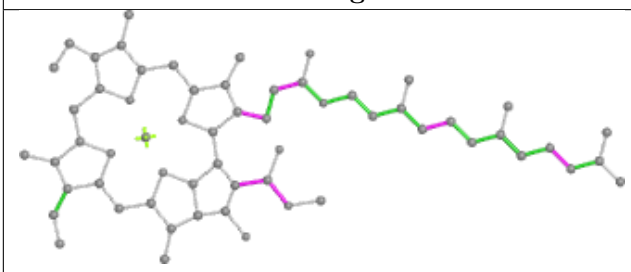


Bond angles



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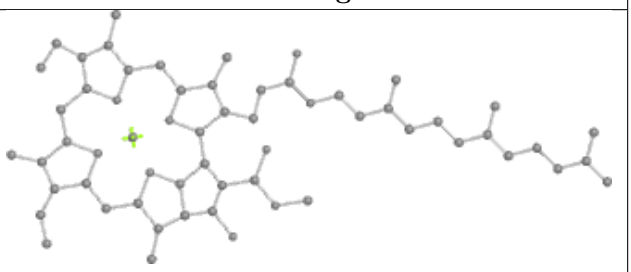
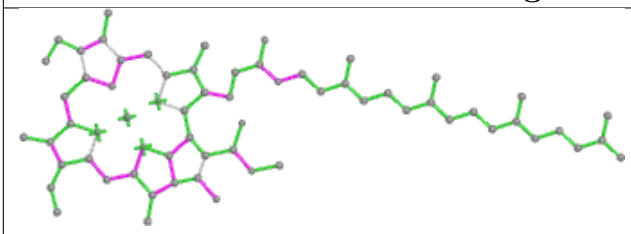


Rings

Ligand CLA A 826



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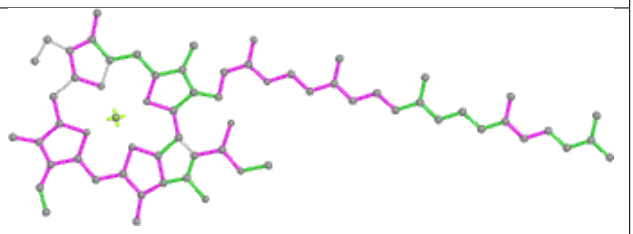
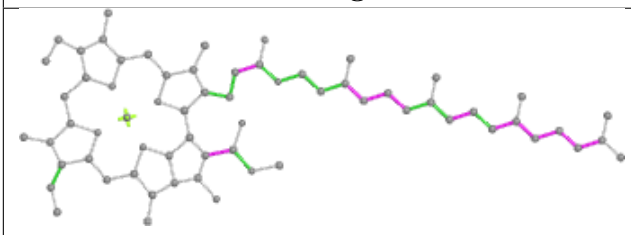


Bond angles



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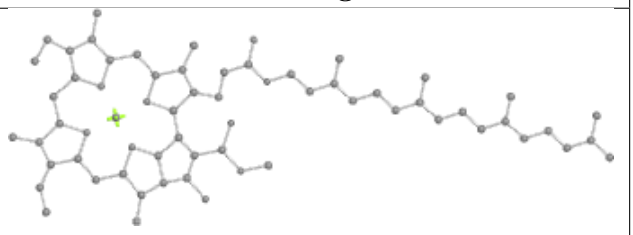
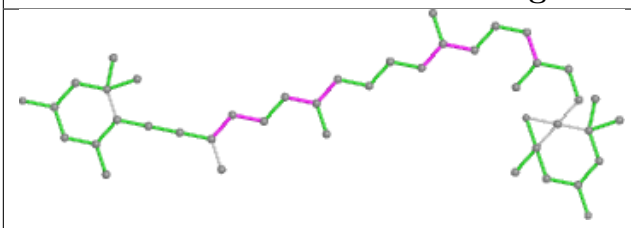


Rings

Ligand DD6 6 916



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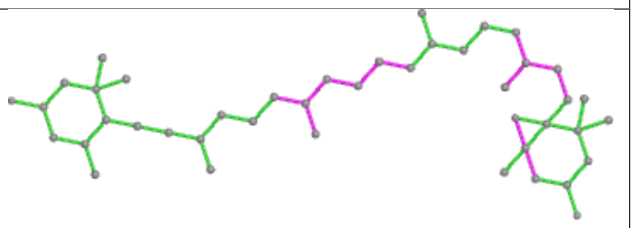
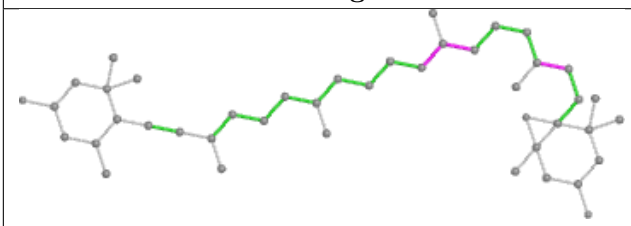


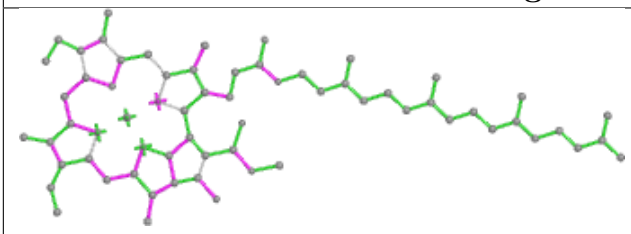
Bond angles



Torsions

Rings

Ligand CLA B 801



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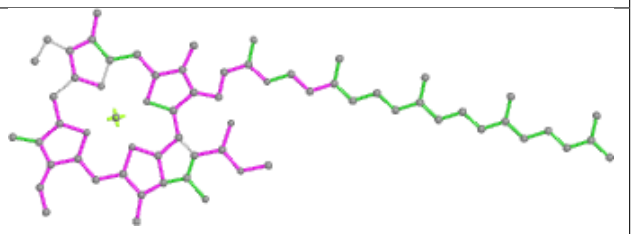

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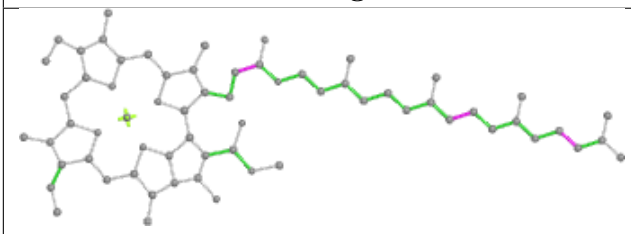

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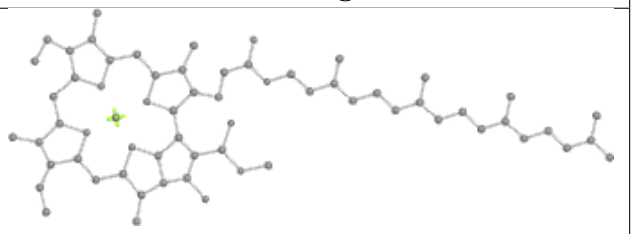
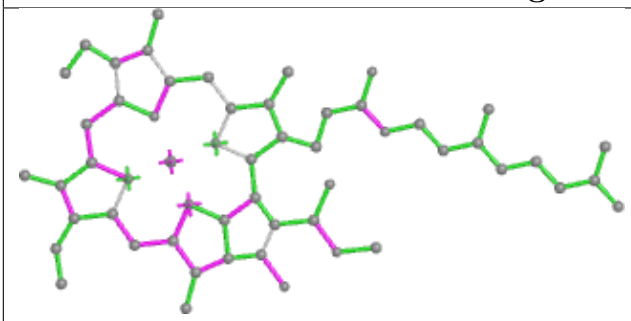
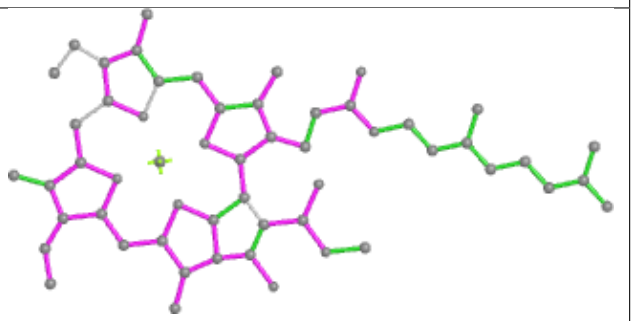
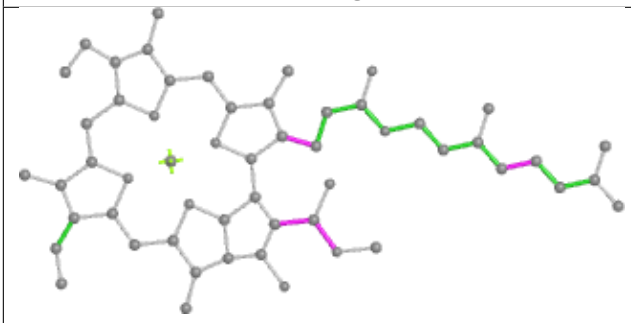
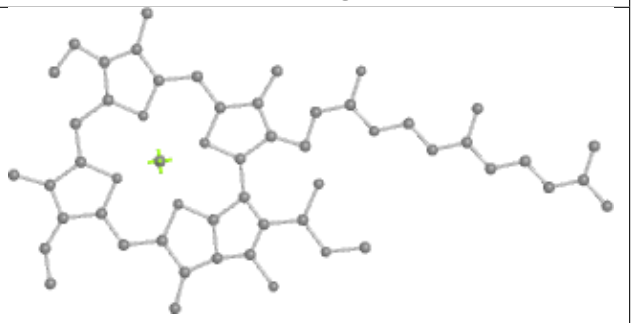
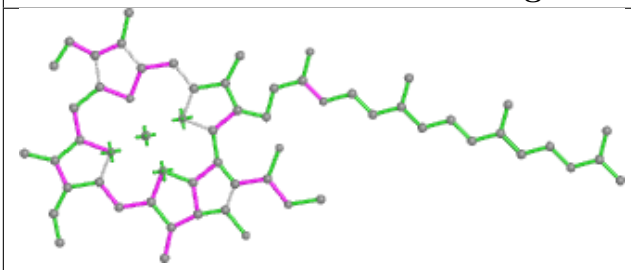
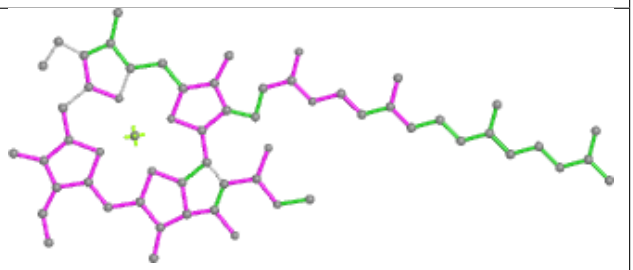
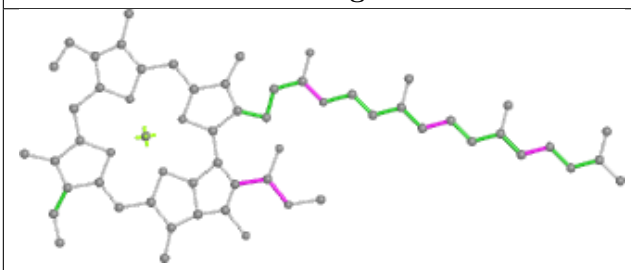
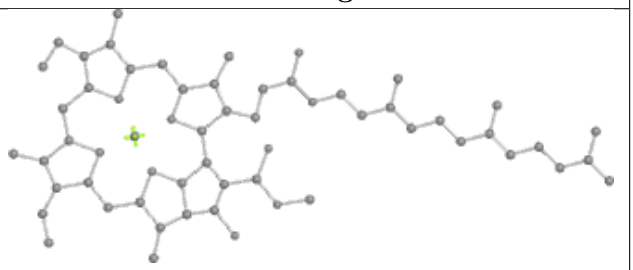
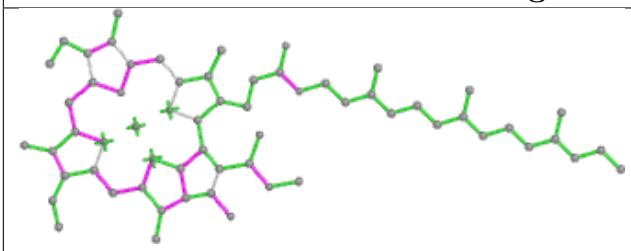
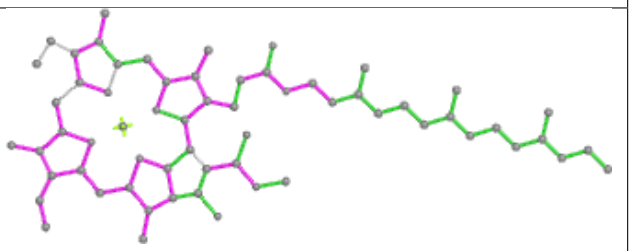
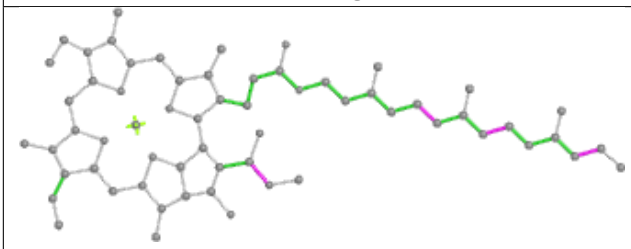
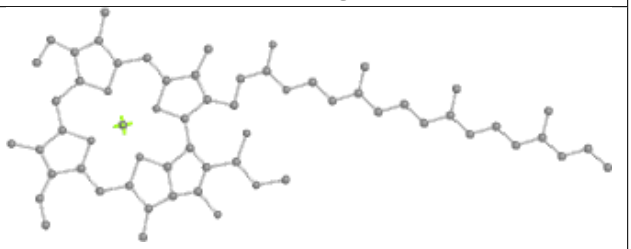
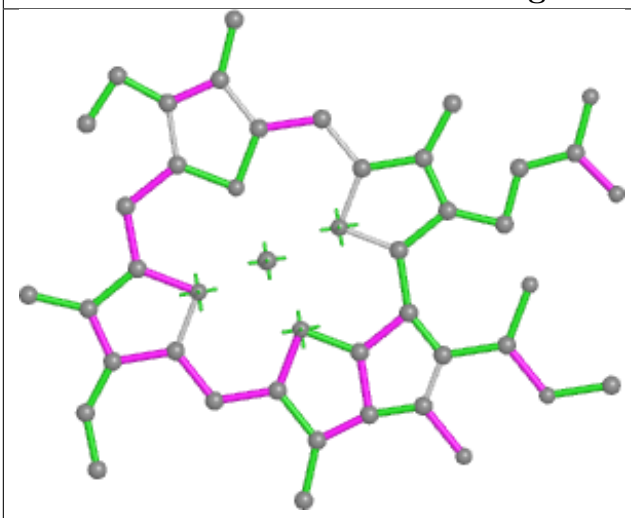
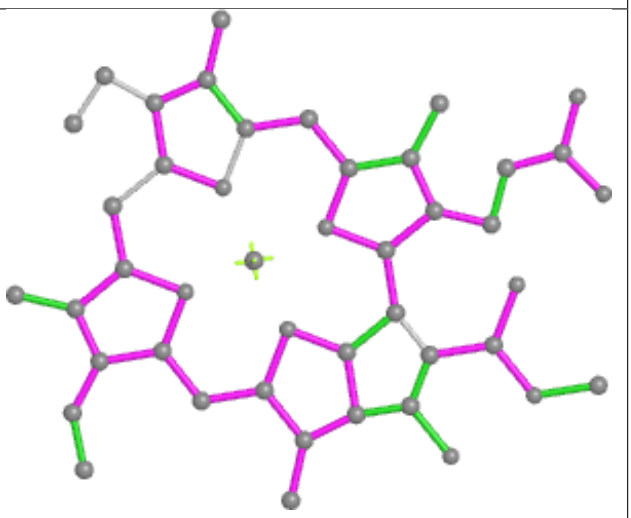
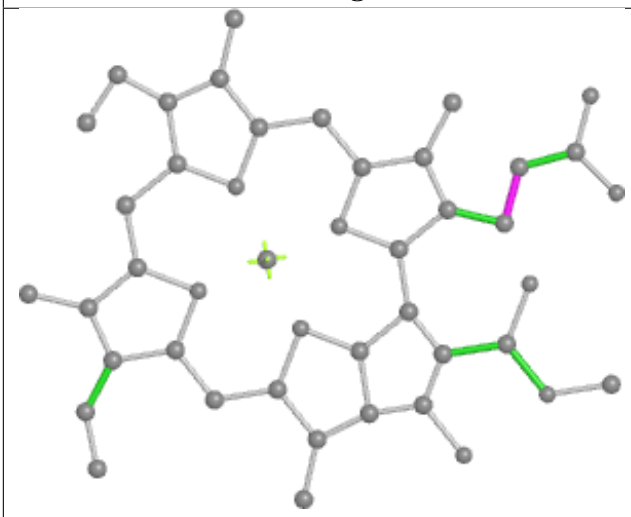
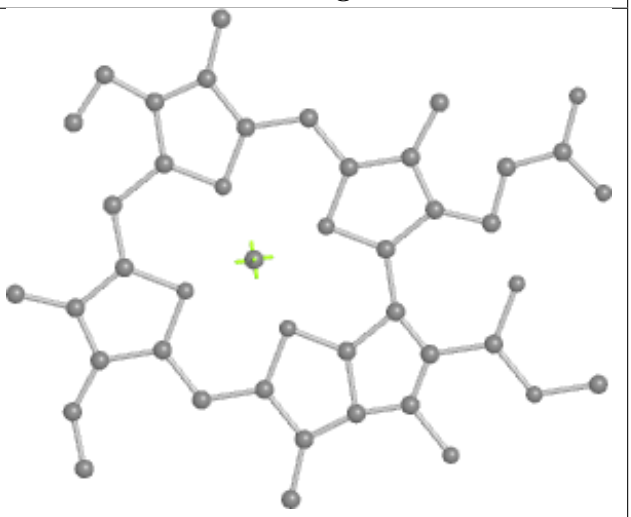


Rings

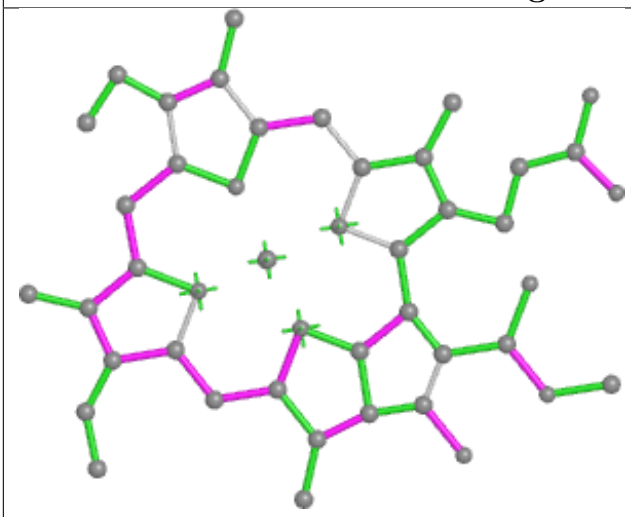
Ligand CLA 5 707	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 514



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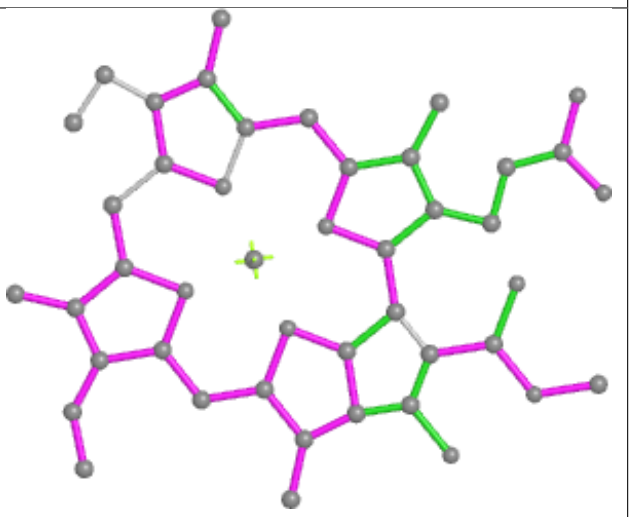

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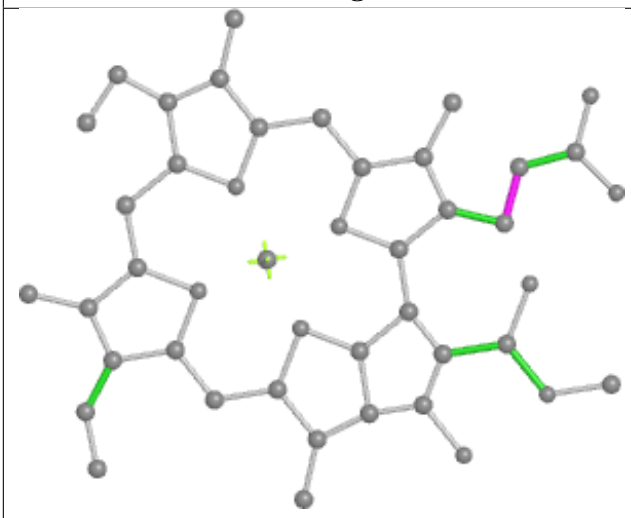

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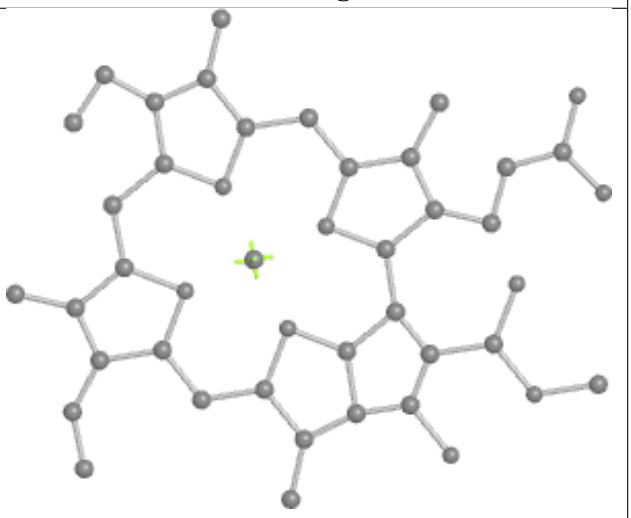
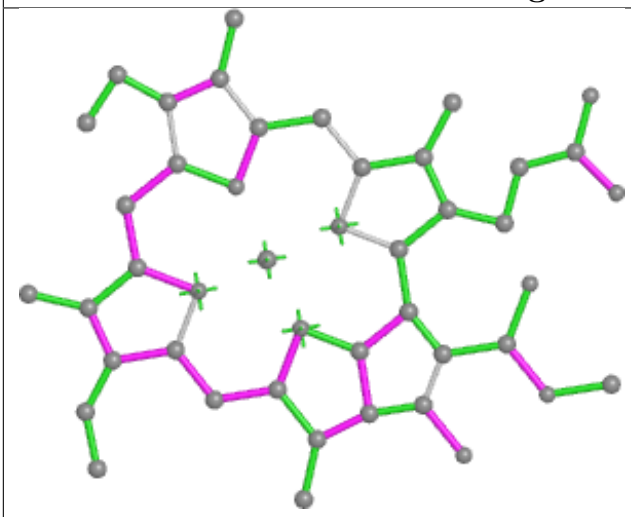


Rings

Ligand CLA 3 713



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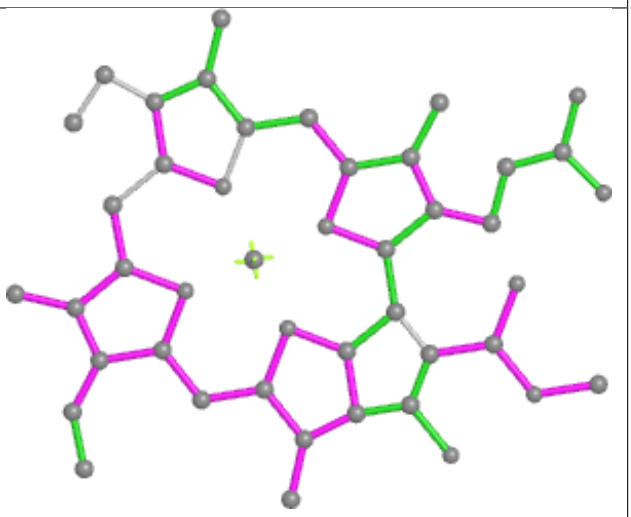

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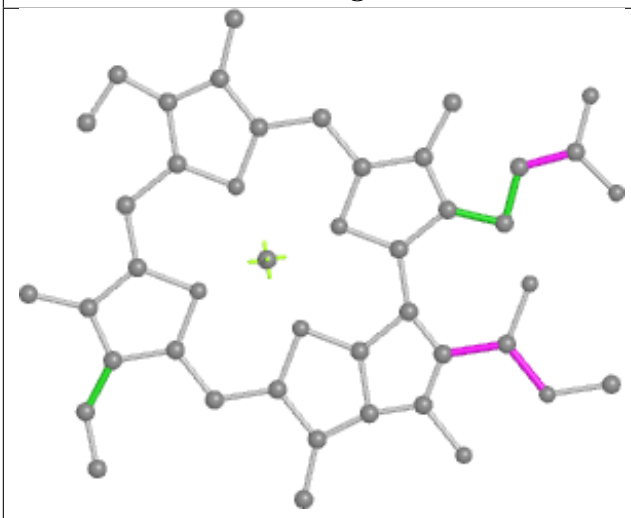

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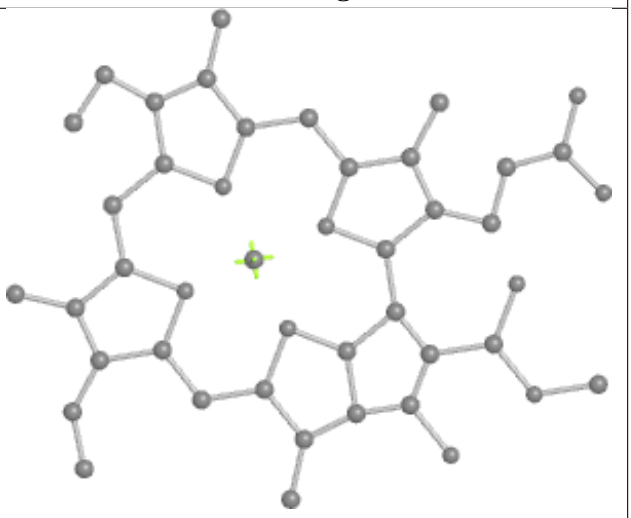
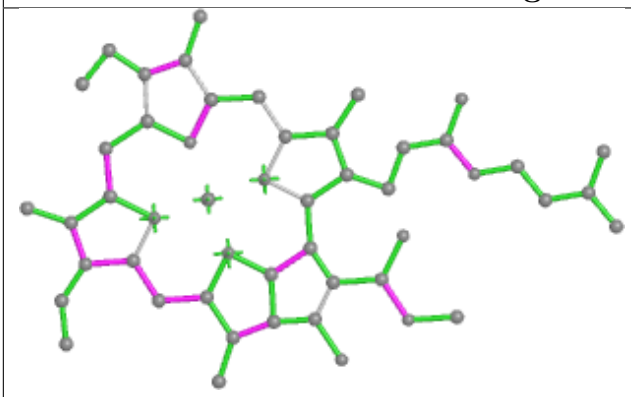
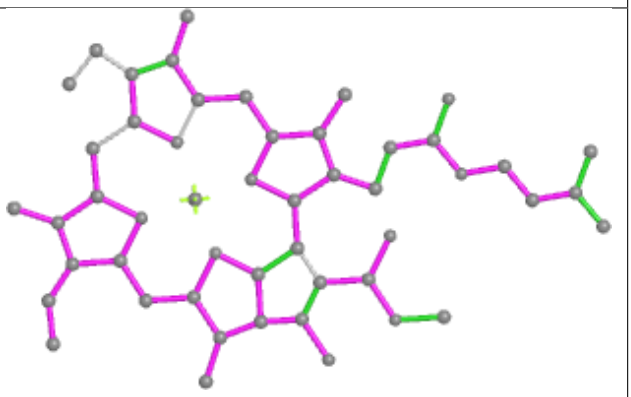


Rings

Ligand CLA A 832	
	
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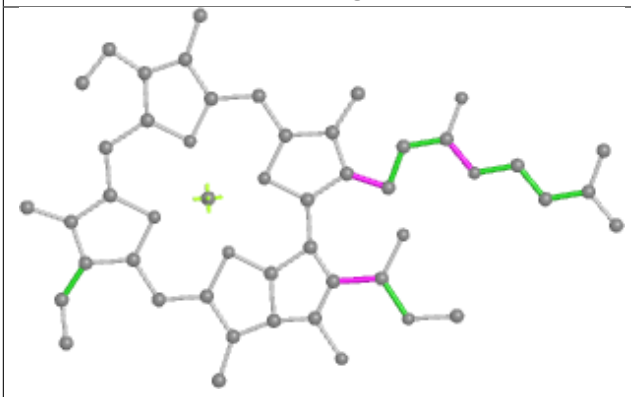
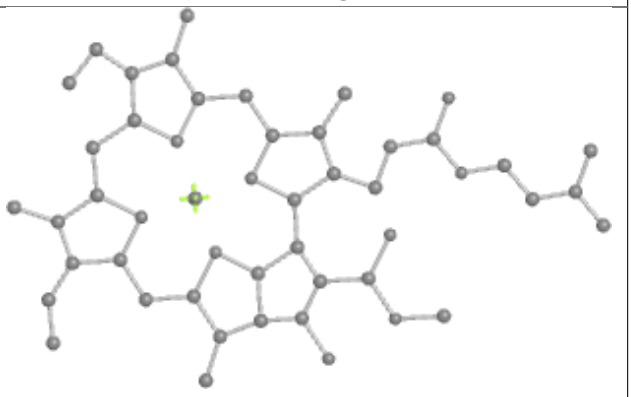
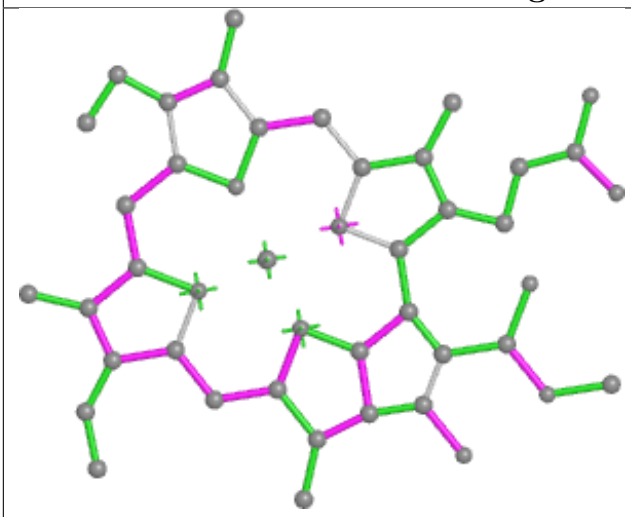
	
Torsions	**Rings**

Ligand CLA 5 709



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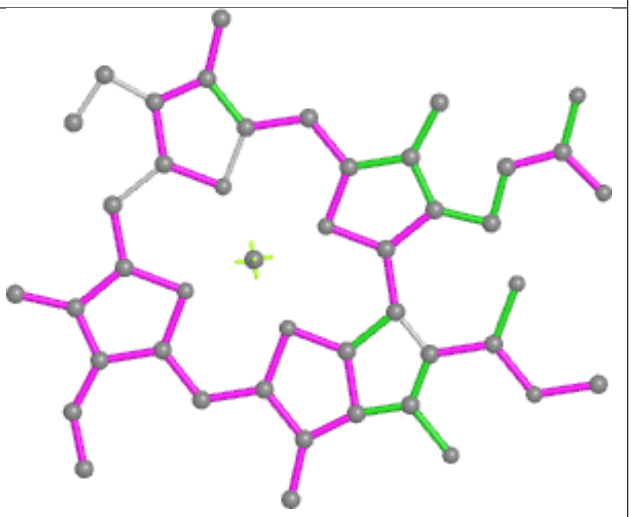

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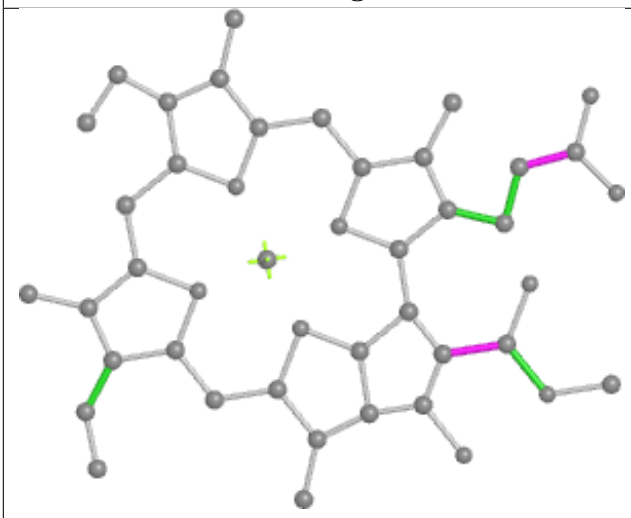

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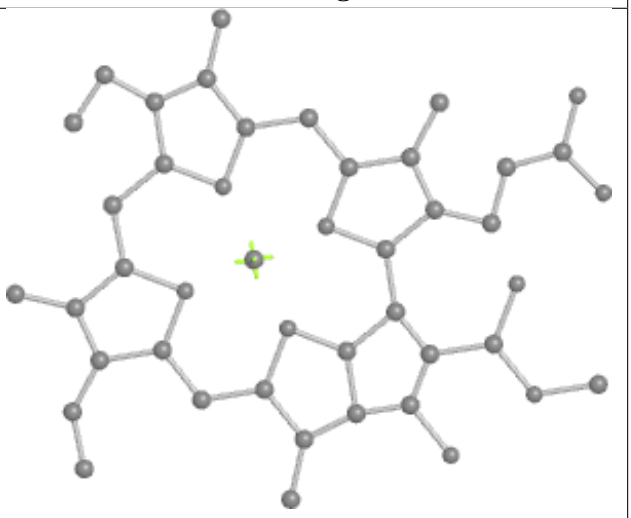
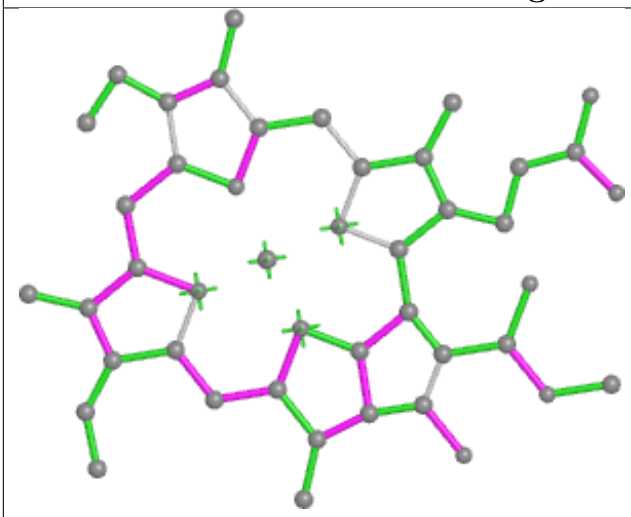


Rings

Ligand CLA 7 704



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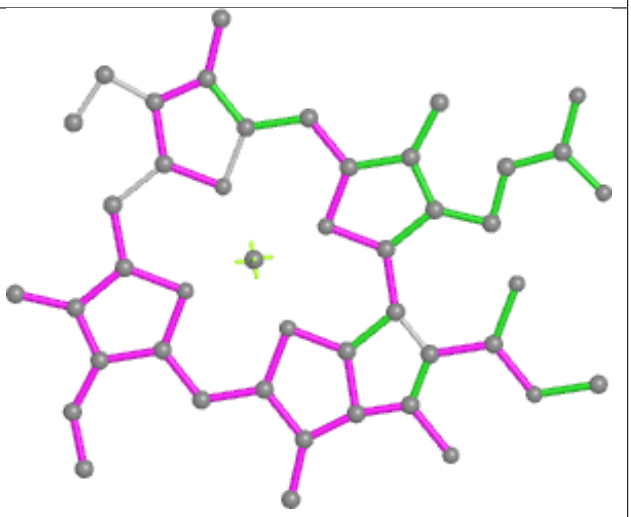

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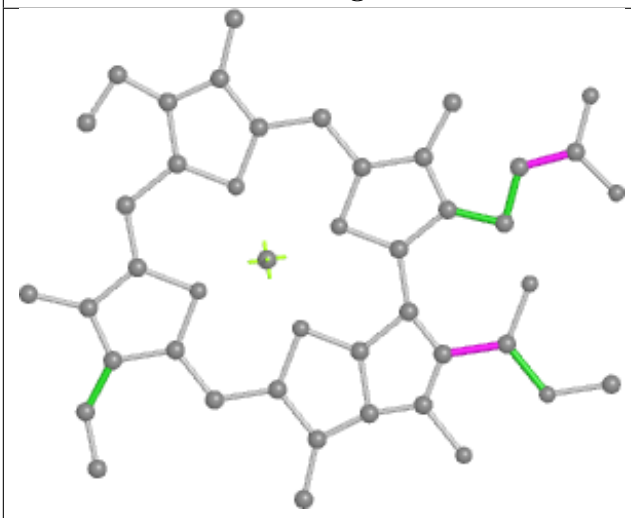

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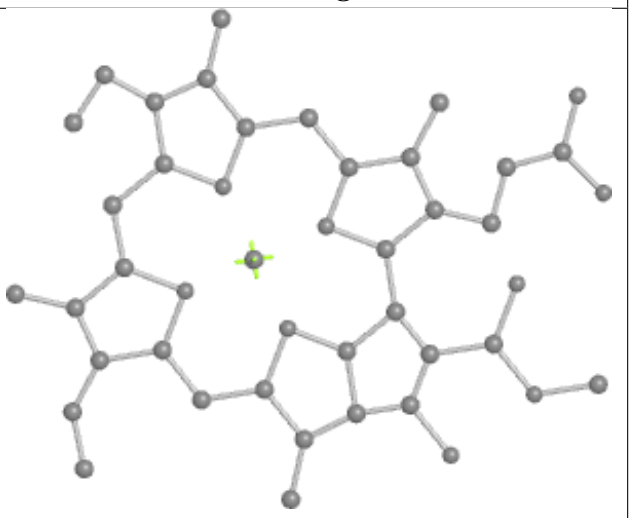
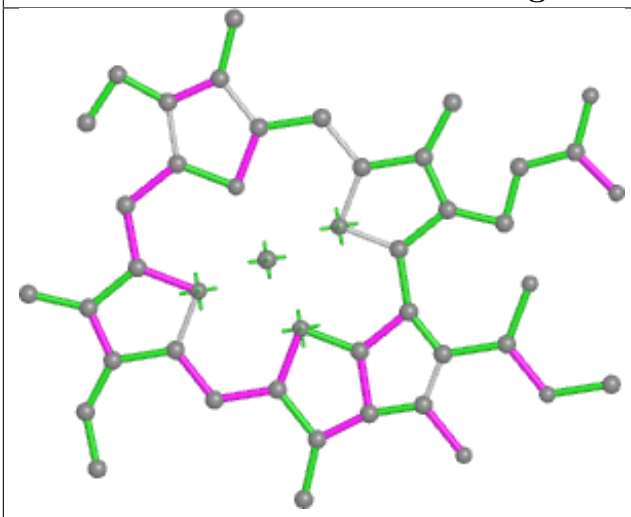


Rings

Ligand CLA 3 711



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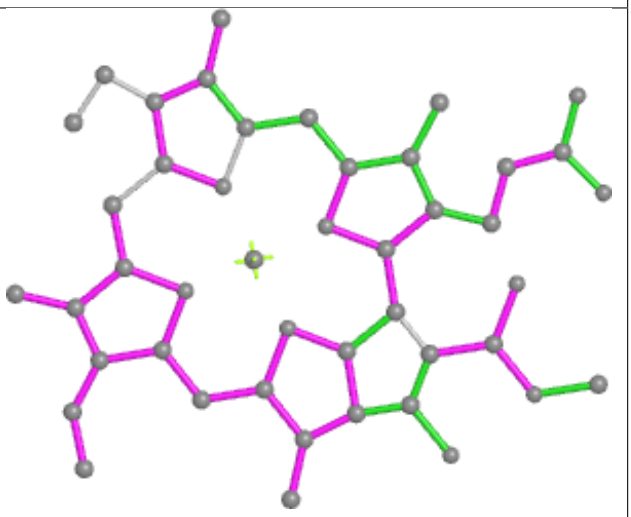

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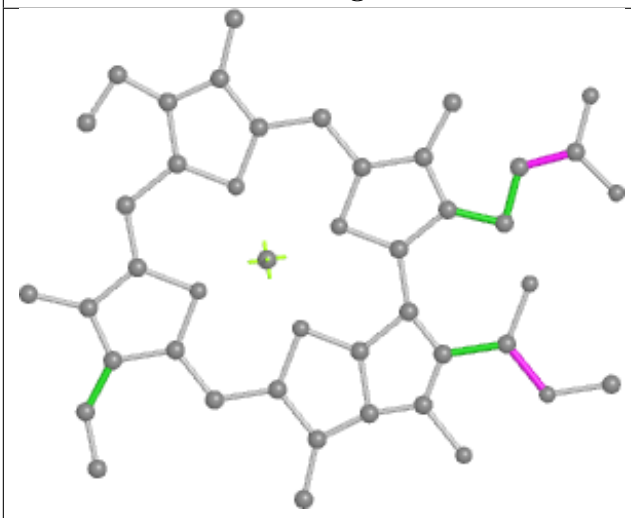

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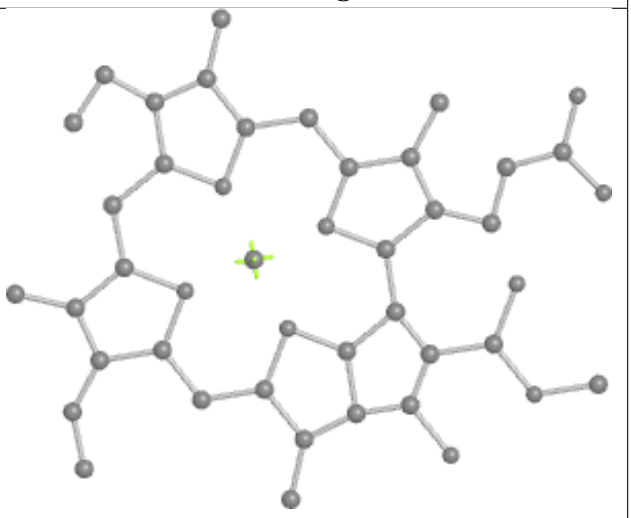
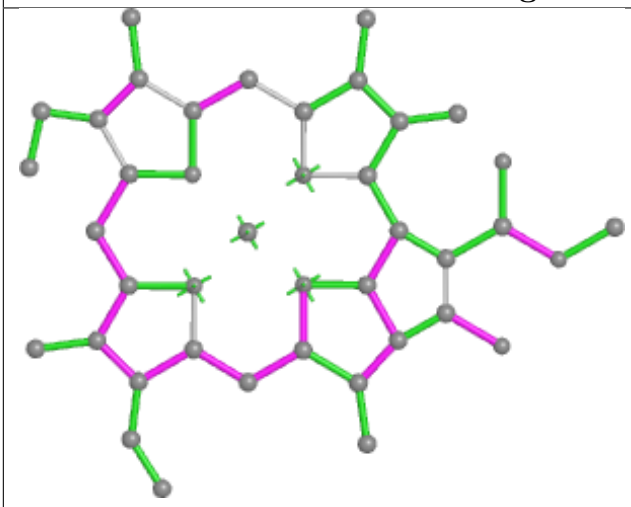


Rings

Ligand CLA 10 706



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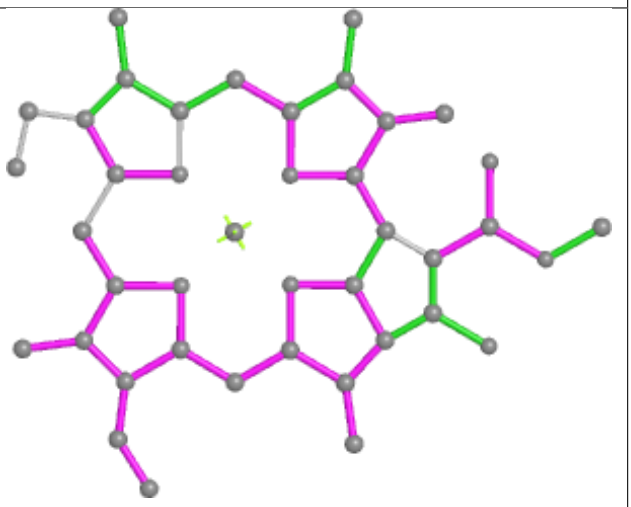

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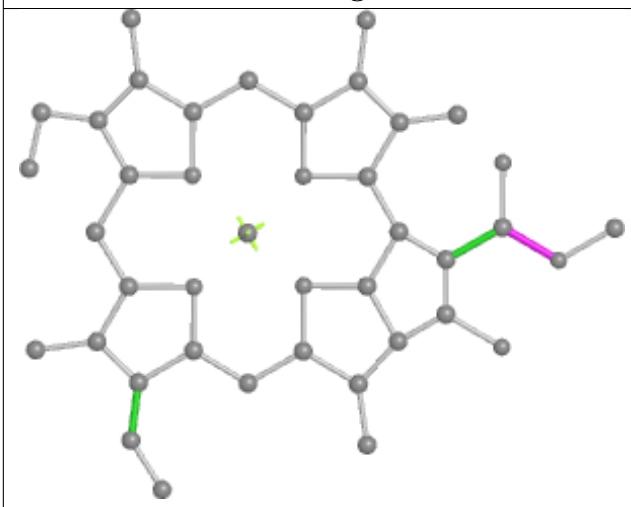

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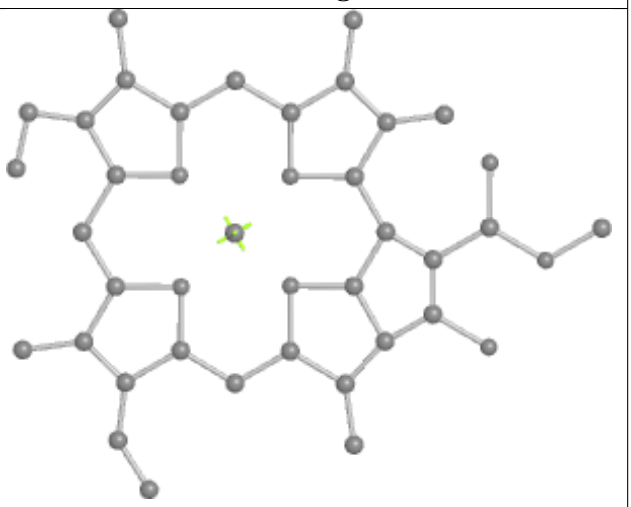
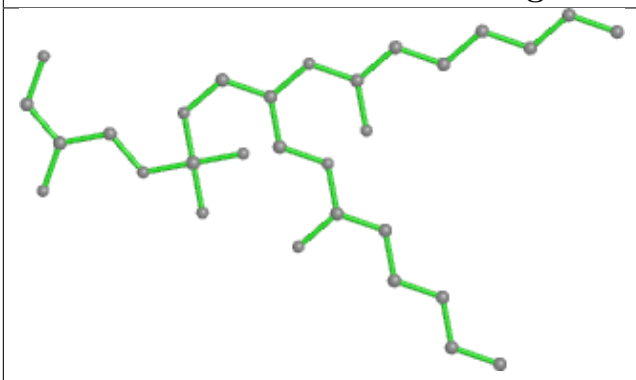
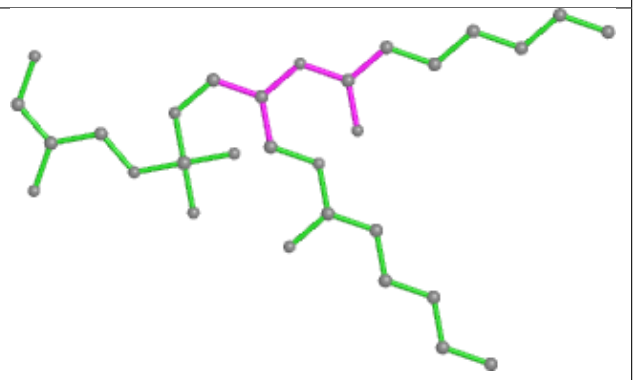
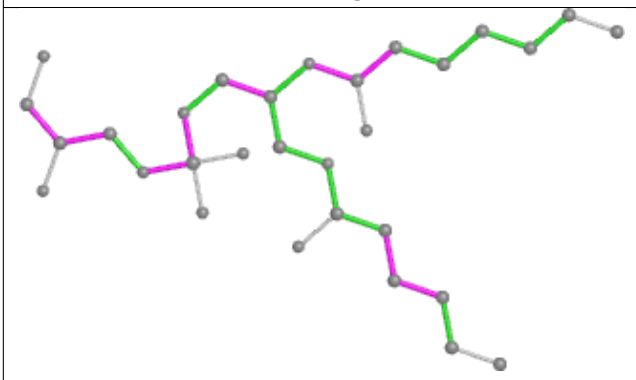
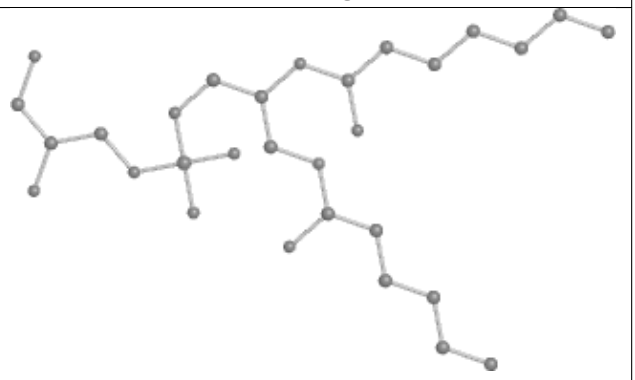
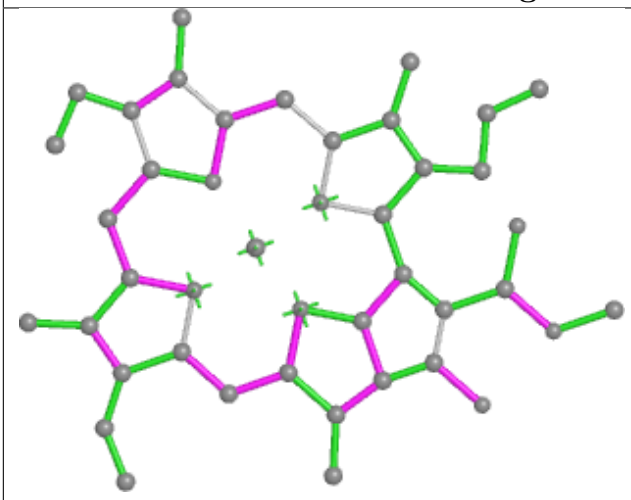


Rings

Ligand LHG 2 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 10 708



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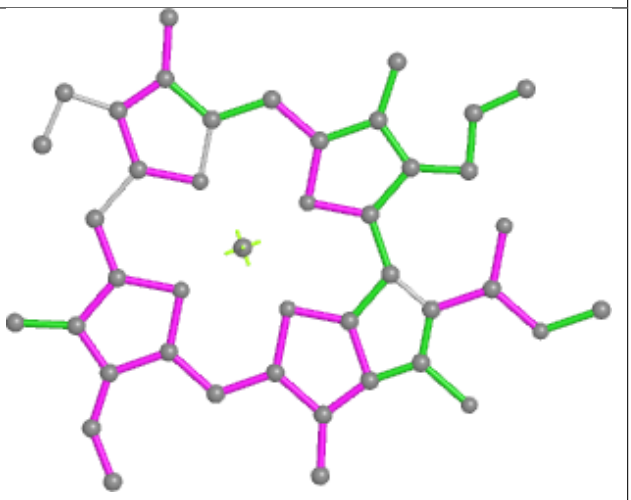

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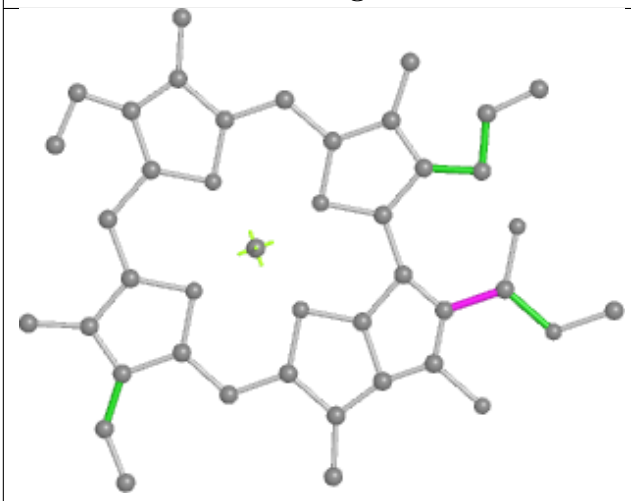

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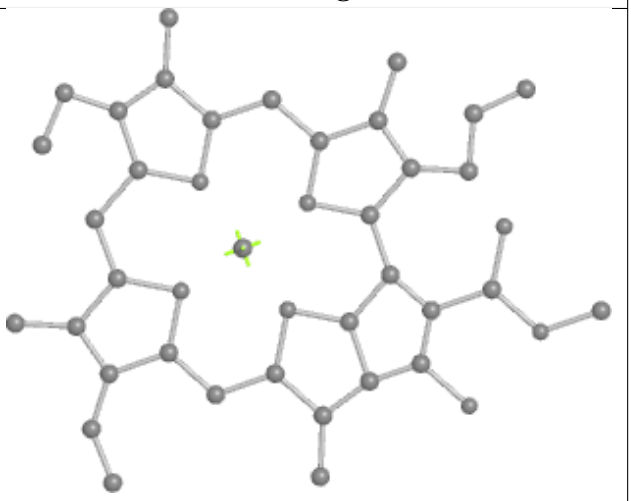
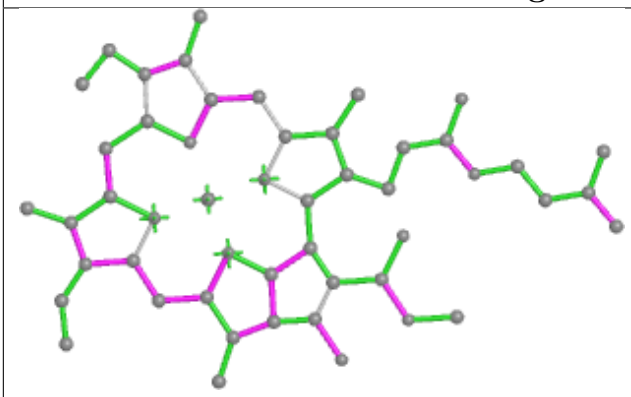
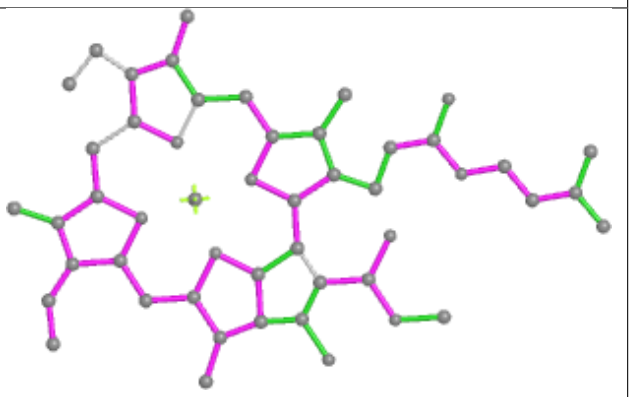
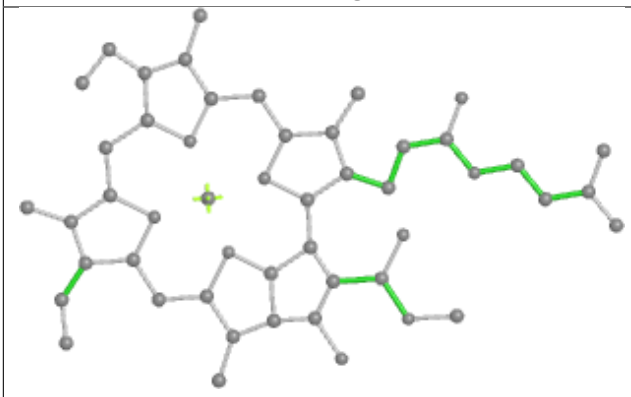
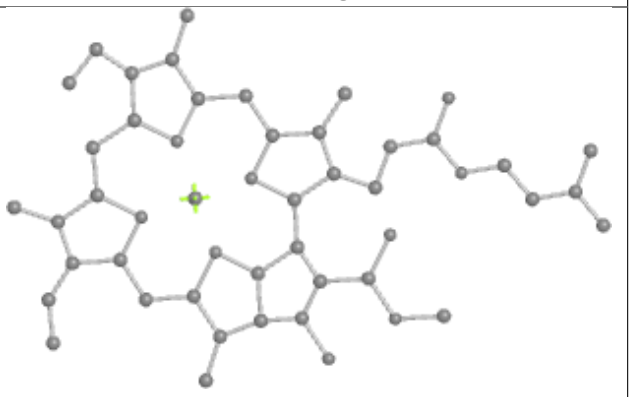
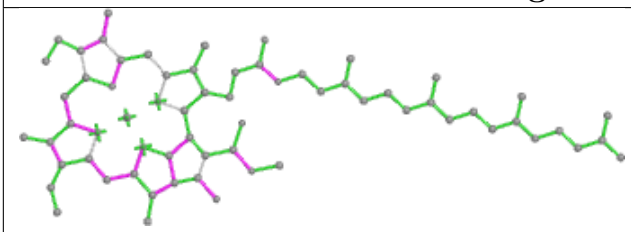
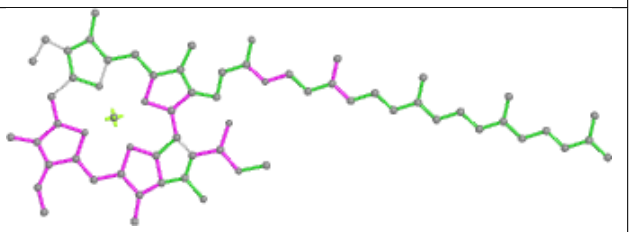
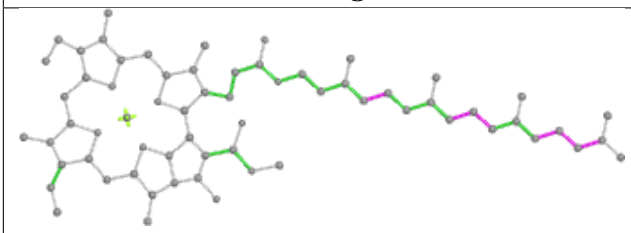
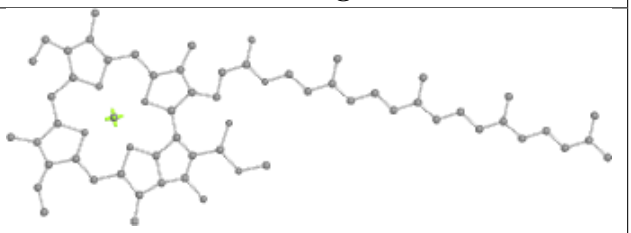


Rings

Ligand CLA 4 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 711	
 Bond lengths	 Bond angles
 Torsions	 Rings

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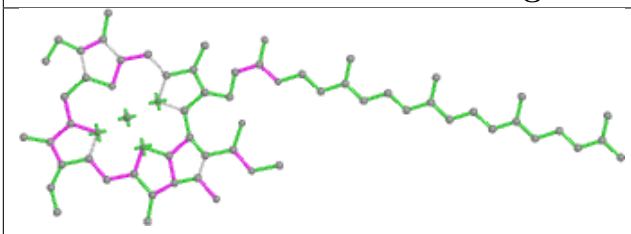
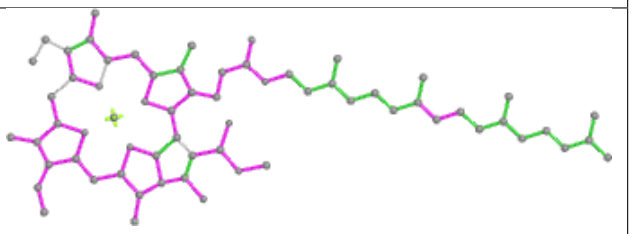
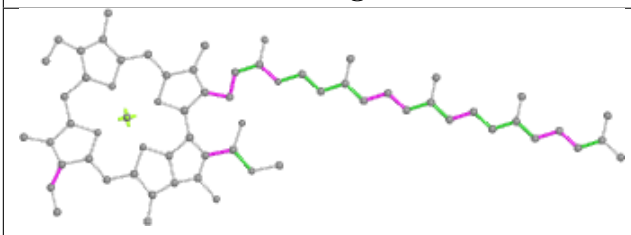
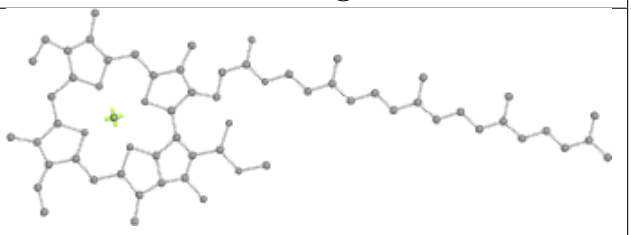
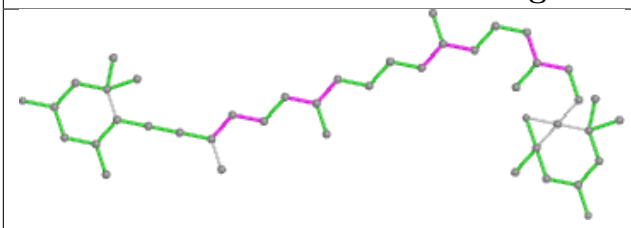
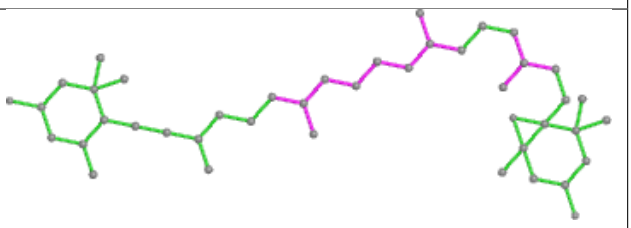
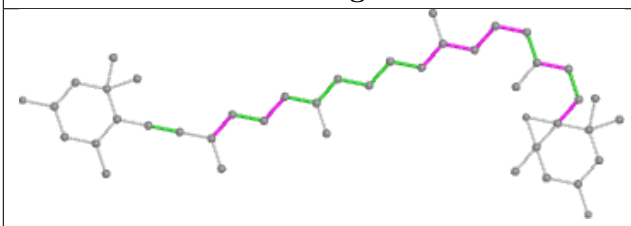
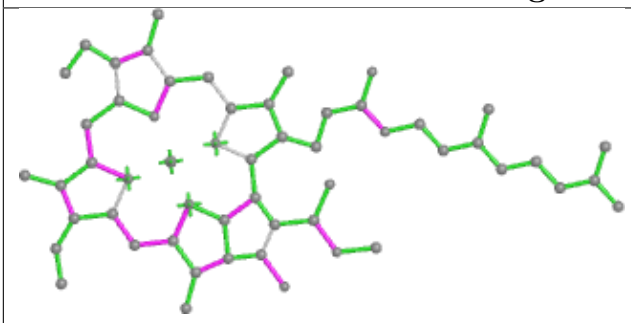
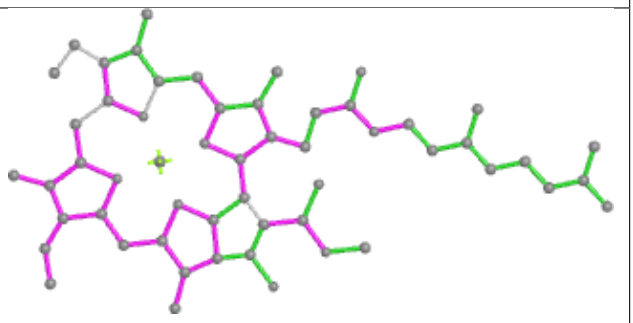
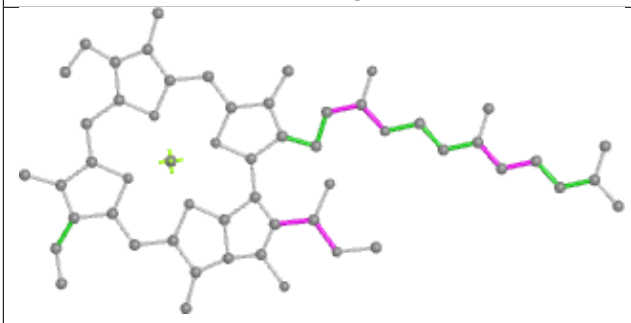
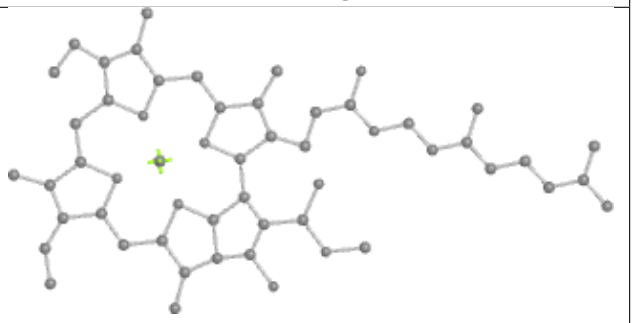
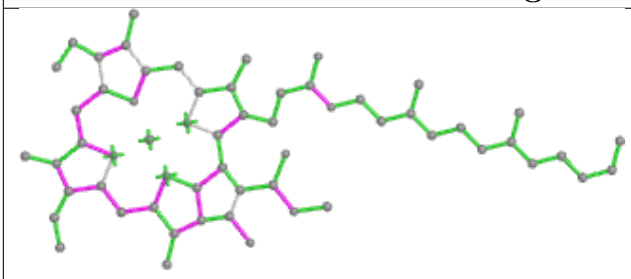
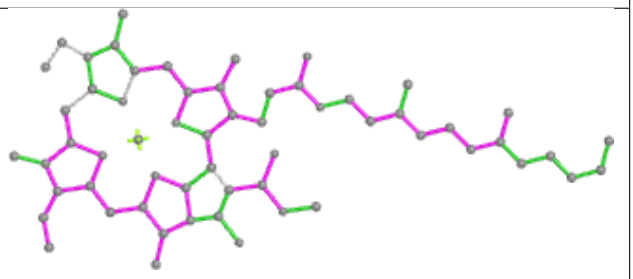
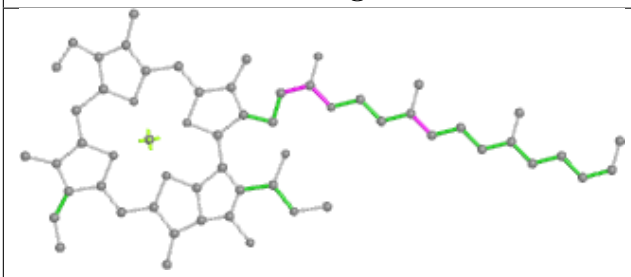
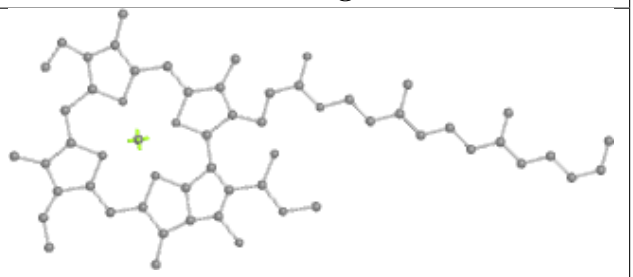
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 8 615	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 3 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 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.

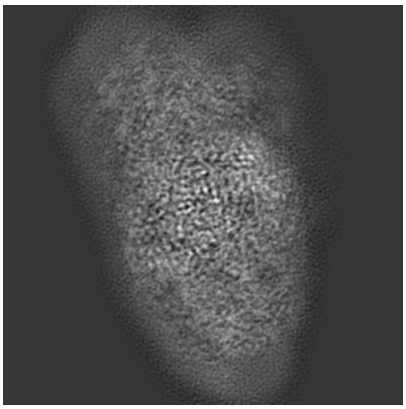
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-65026. These allow visual inspection of the internal detail of the map and identification of artifacts.

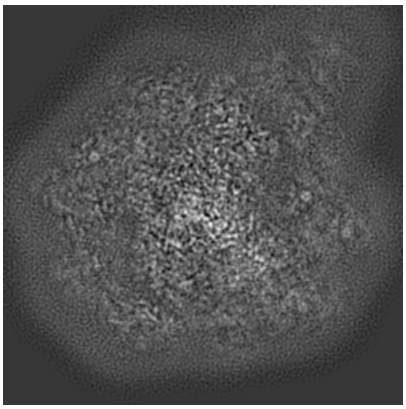
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

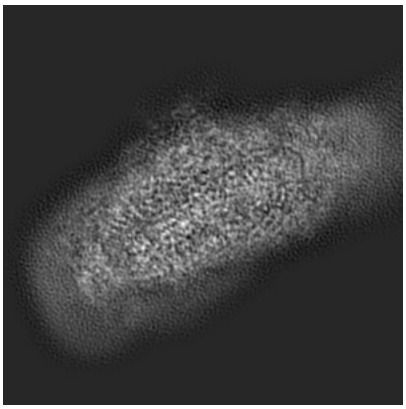
6.1.1 Primary map



X

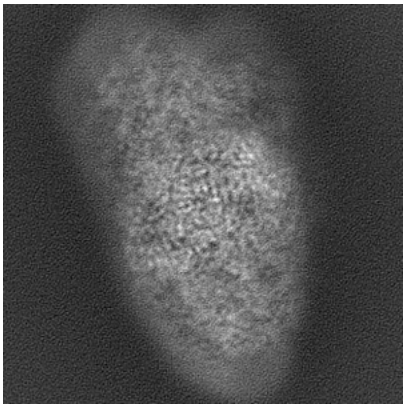


Y

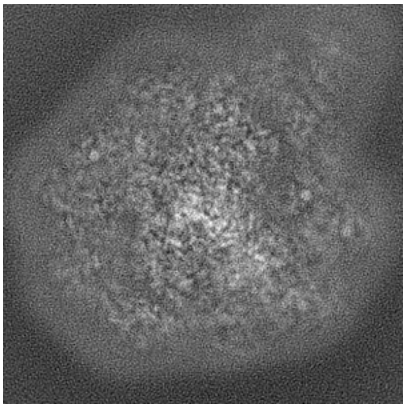


Z

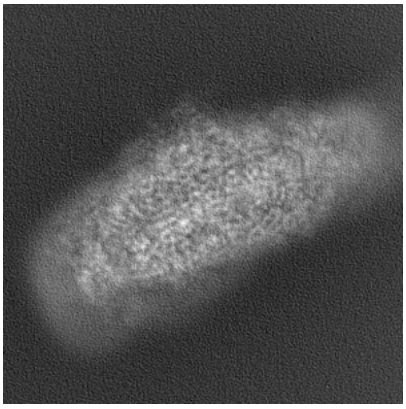
6.1.2 Raw map



X



Y

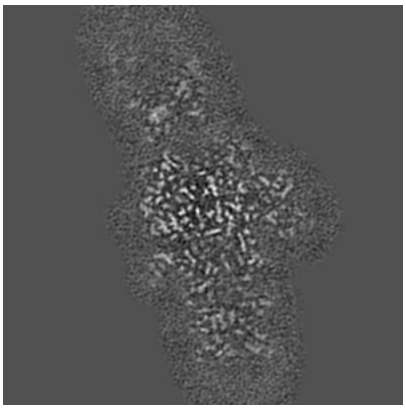


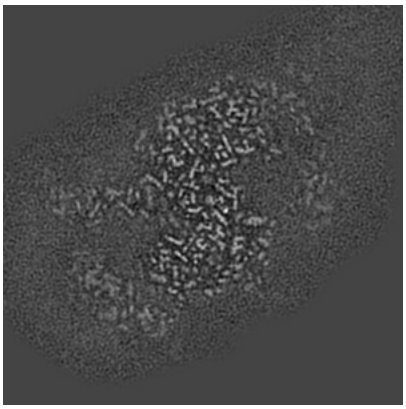
Z

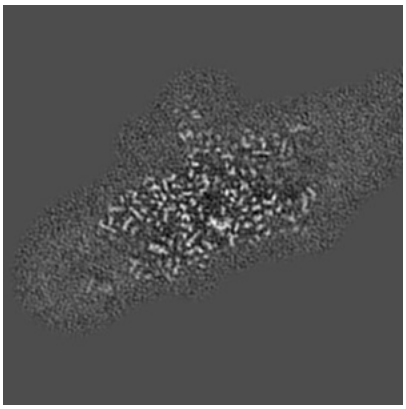
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

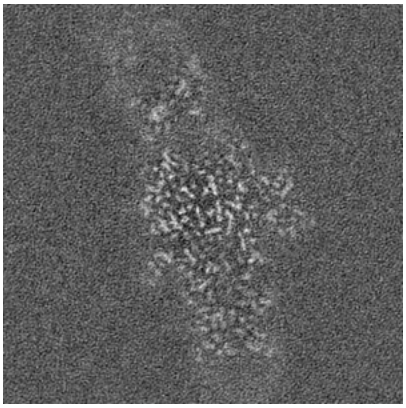
6.2.1 Primary map

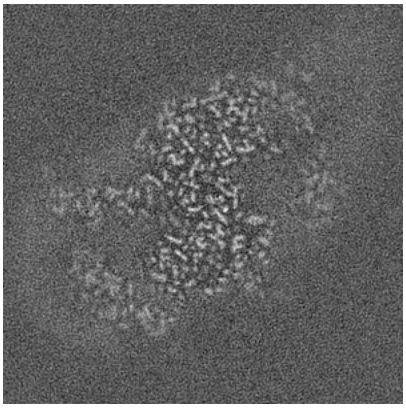

X Index: 144

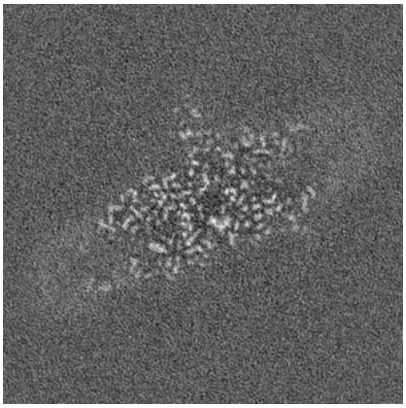

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

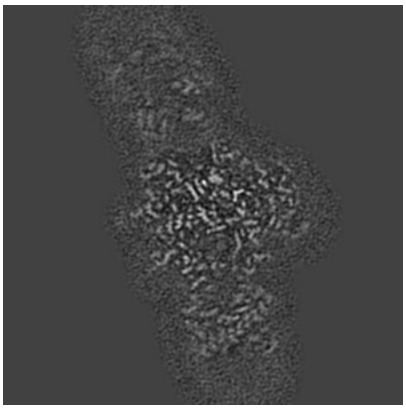

Y Index: 144

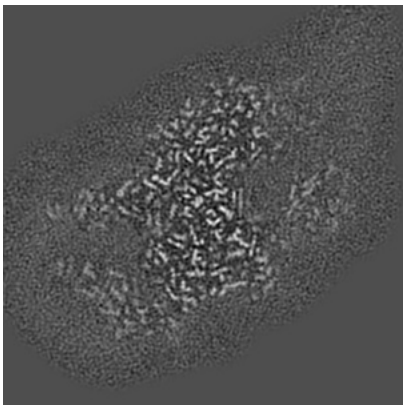

Z Index: 144

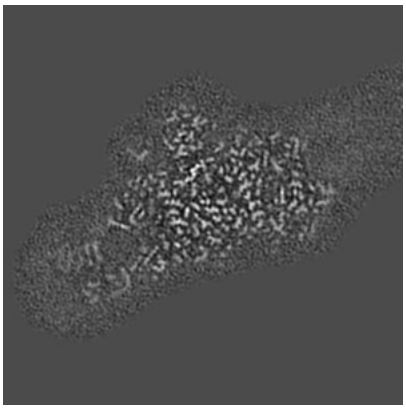
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

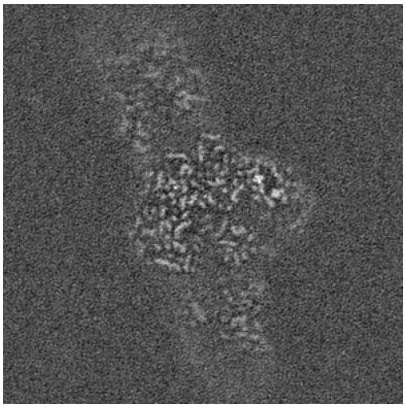
6.3.1 Primary map

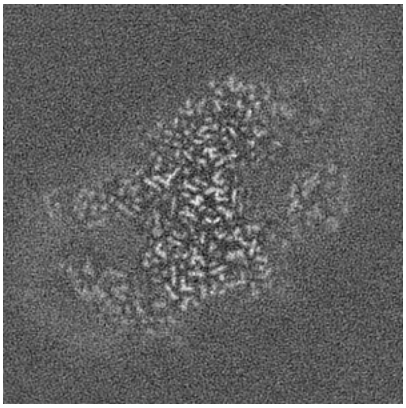

X Index: 139

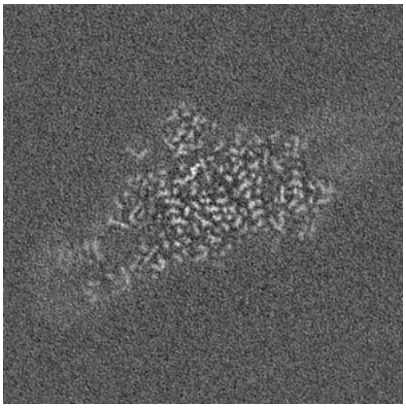

Y Index: 139


Z Index: 154

6.3.2 Raw map


X Index: 129

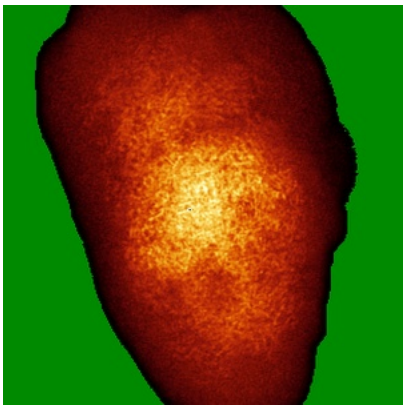

Y Index: 140

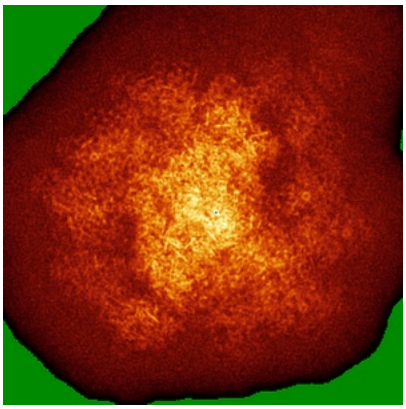

Z Index: 154

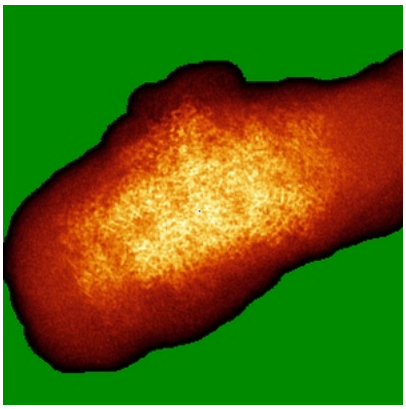
The images above show the largest variance slices of the map in three orthogonal directions.

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

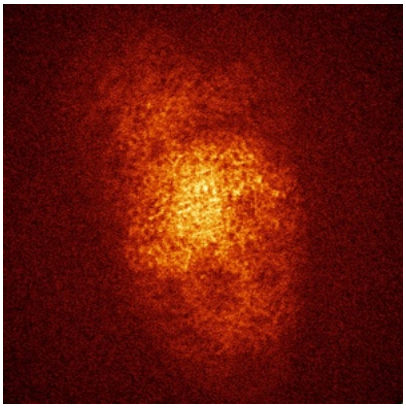
6.4.1 Primary map

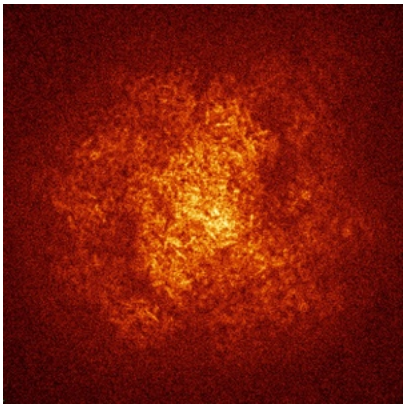

X

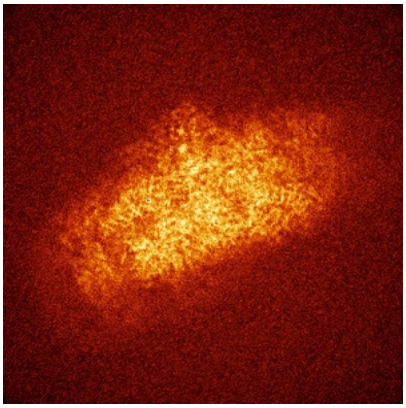

Y


Z

6.4.2 Raw map


X

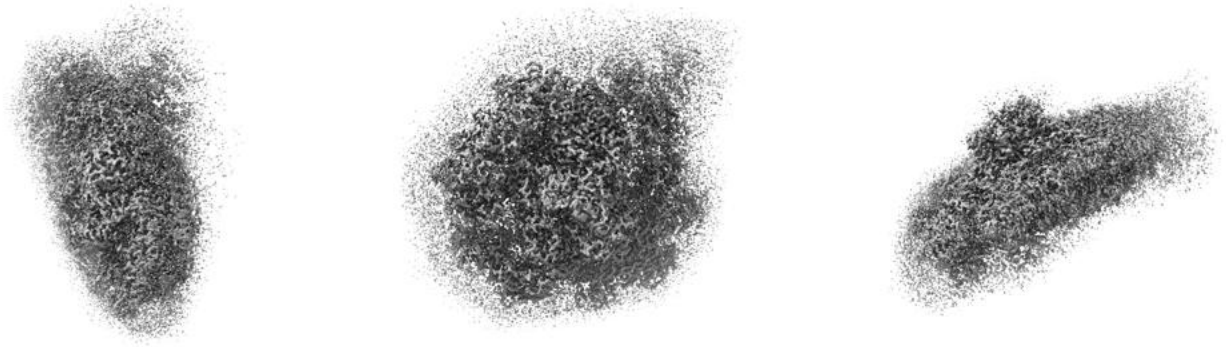

Y


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)

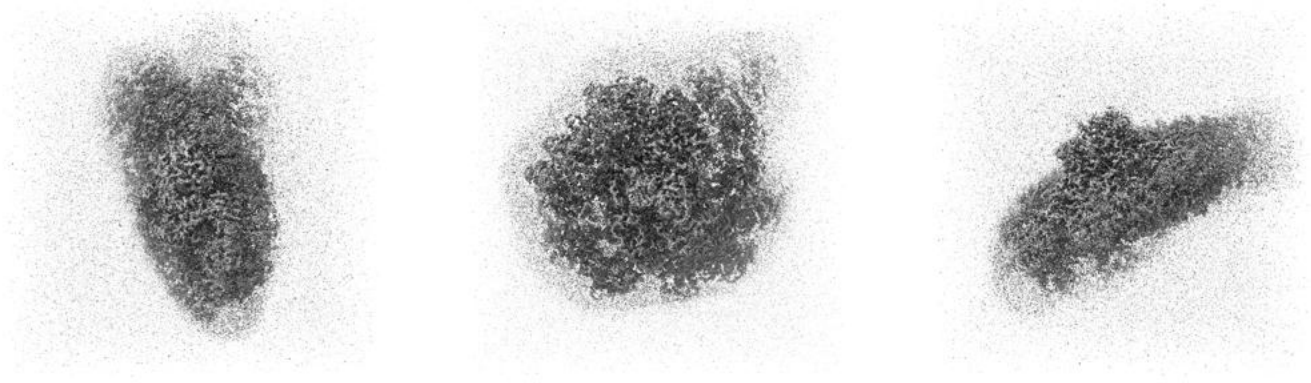
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

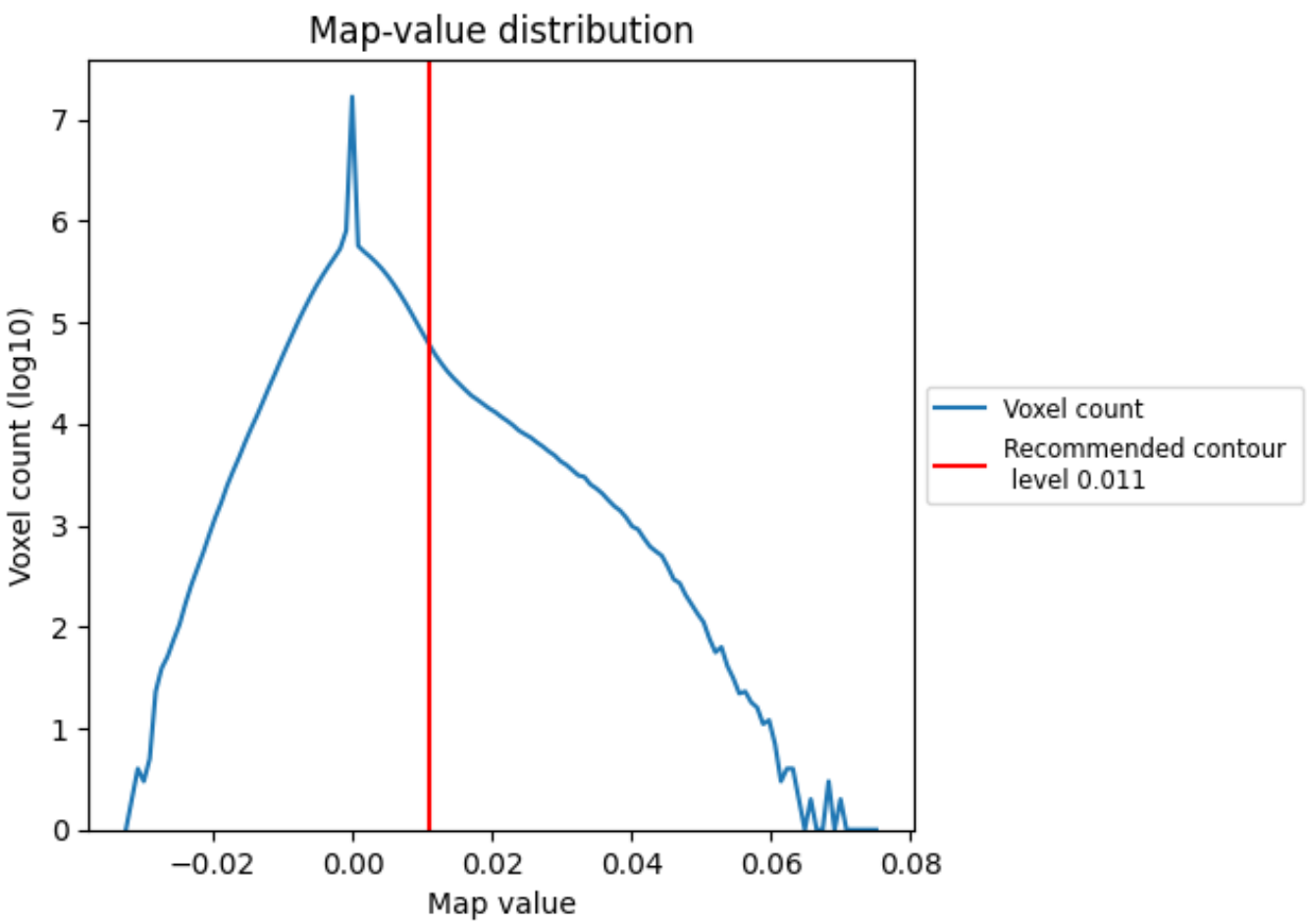
6.6 Mask visualisation (i)

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

7 Map analysis (i)

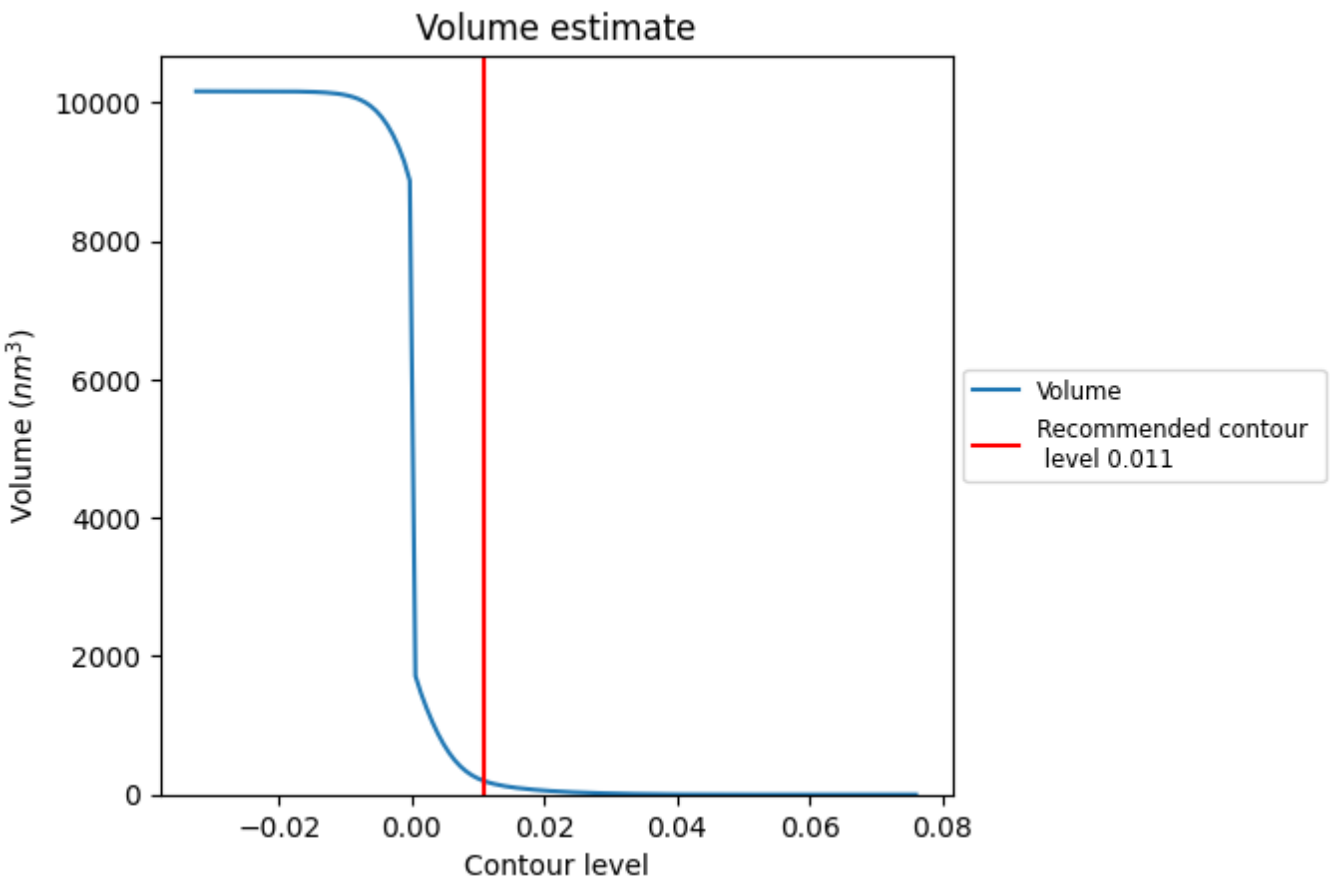
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

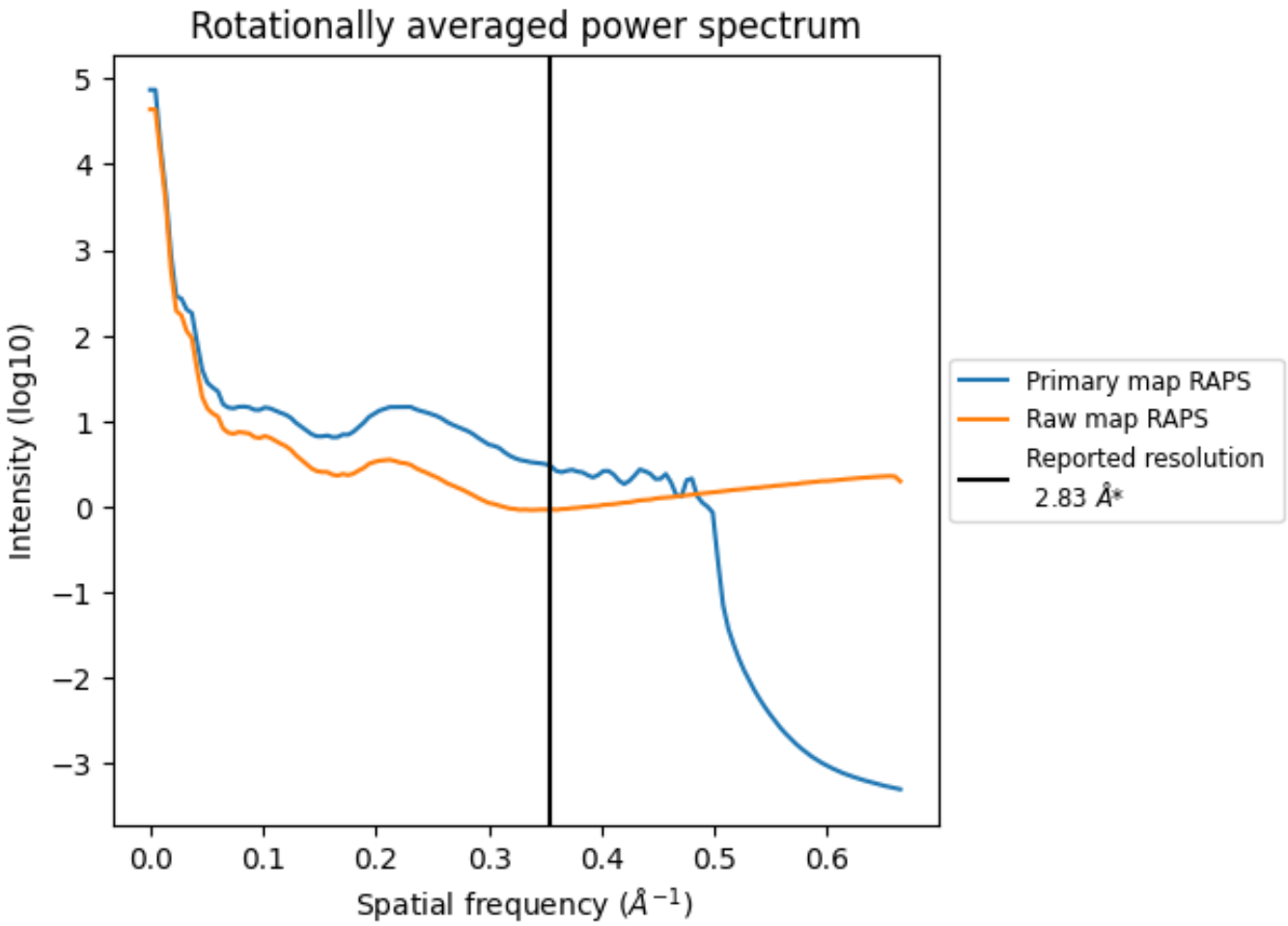
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 175 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)

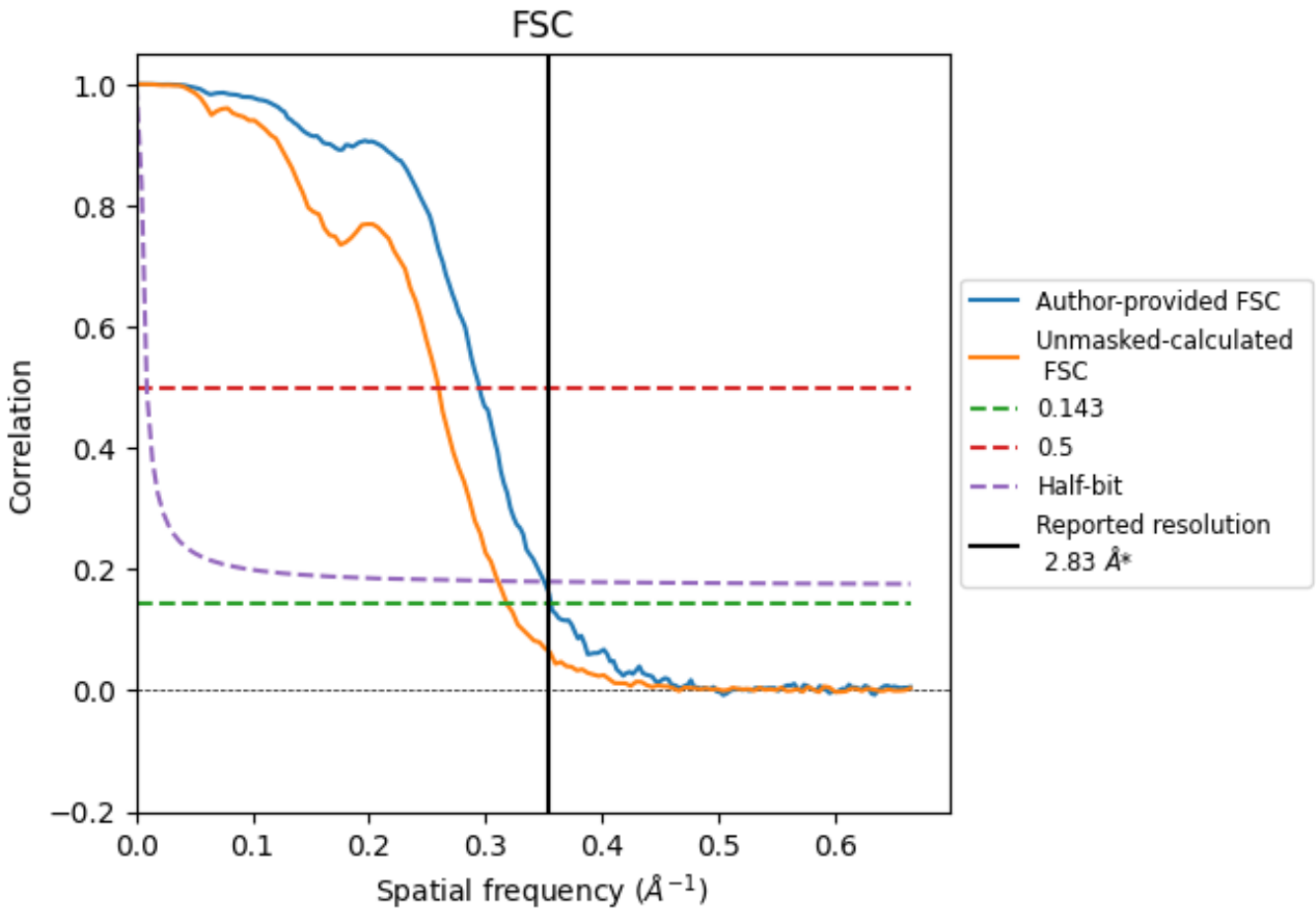


*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

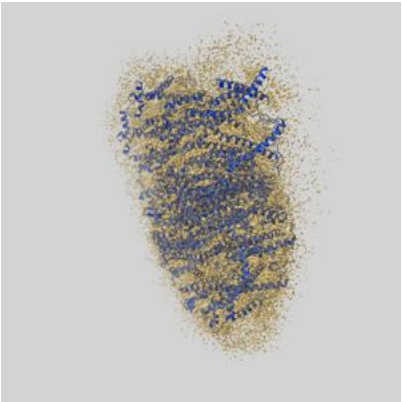
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.81	3.39	2.85
Unmasked-calculated*	3.14	3.85	3.22

*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 3.14 differs from the reported value 2.83 by more than 10 %

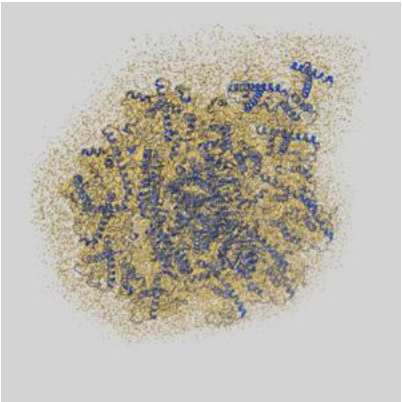
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-65026 and PDB model 9VFJ. Per-residue inclusion information can be found in section 3 on page 32.

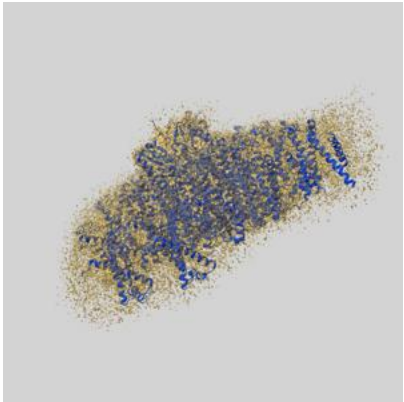
9.1 Map-model overlay (i)



X



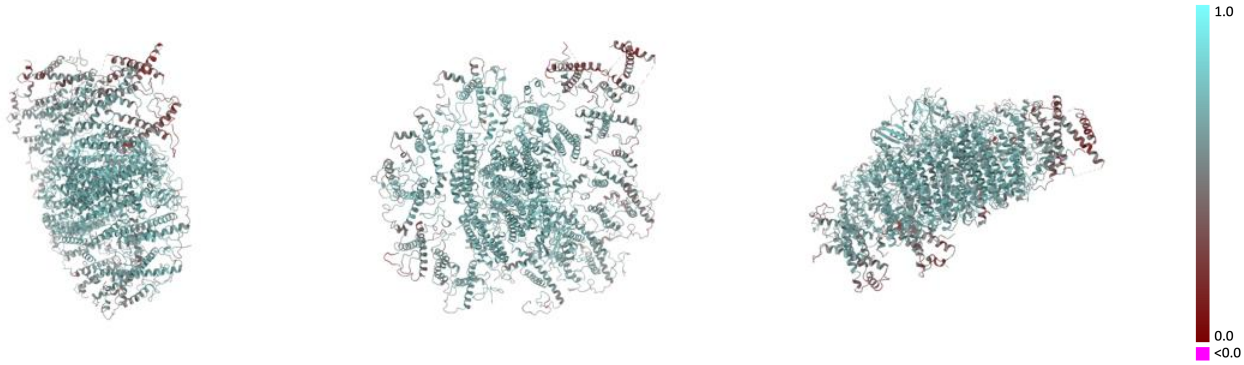
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

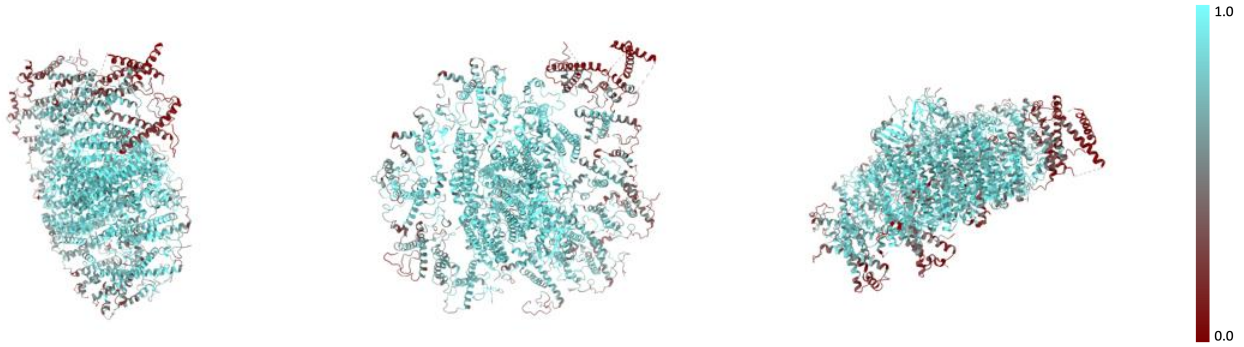
9.2 Q-score mapped to coordinate model (i)



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.

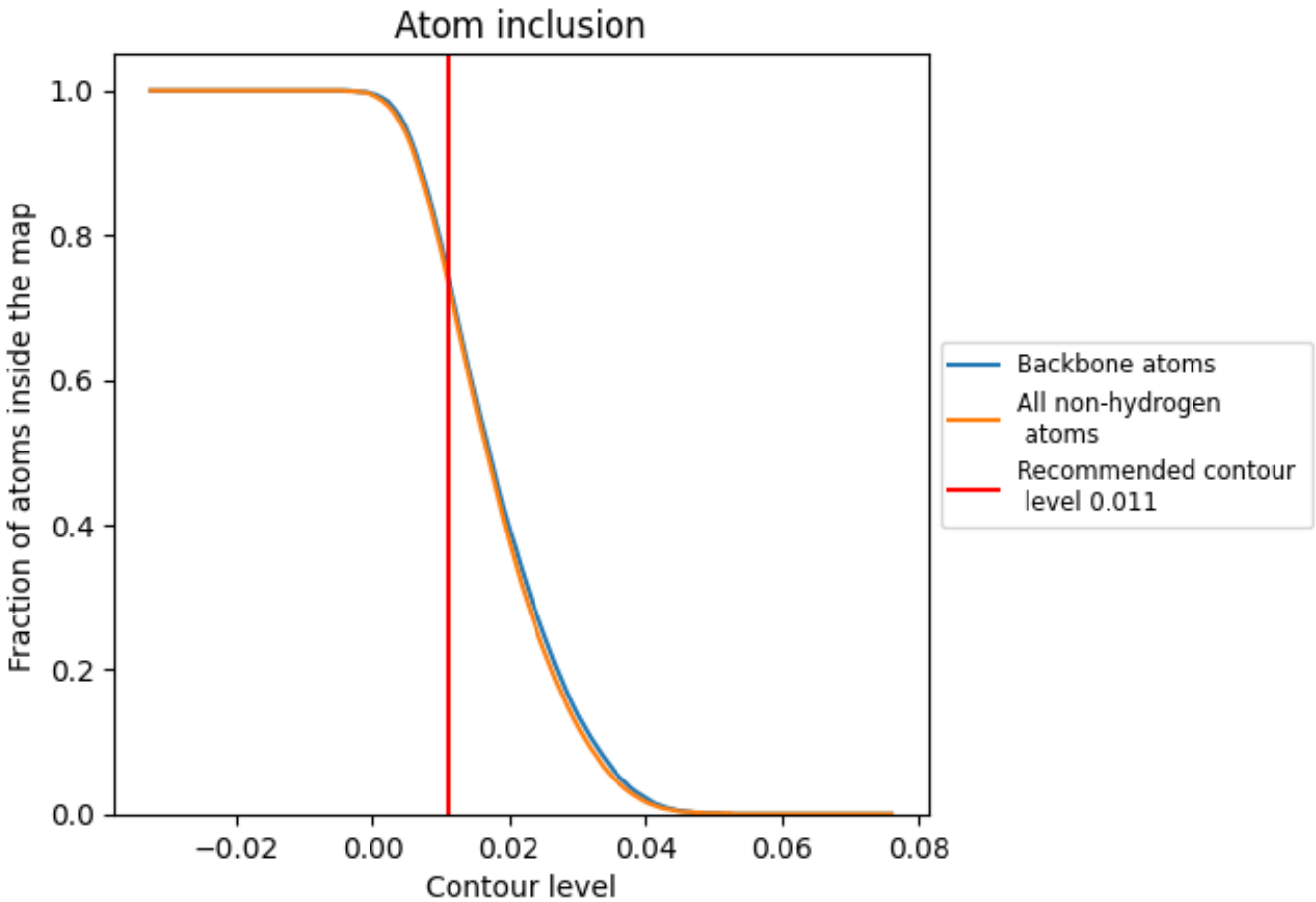
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.6050
1	0.6770	0.5760
10	0.3090	0.4220
11	0.5030	0.4990
12	0.3990	0.4450
13	0.1900	0.3910
2	0.7590	0.6050
3	0.6850	0.5760
4	0.5140	0.4940
5	0.7340	0.5930
6	0.6070	0.5390
7	0.8140	0.6320
8	0.6480	0.5640
9	0.5320	0.5300
A	0.9130	0.6890
B	0.9010	0.6820
C	0.9420	0.6960
D	0.7840	0.6280
E	0.7630	0.6290
F	0.8350	0.6510
J	0.8400	0.6600
M	0.7410	0.6100