Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 02:09 AM JST

PDB ID	:	8WEY / pdb_00008wey
EMDB ID	:	EMD-37480
Title	:	PSI-LHCI of the red alga Cyanidium caldarium RK-1 (NIES-2137)
Authors	:	Kato, K.; Hamaguchi, T.; Nakajima, Y.; Kawakami, K.; Yonekura, K.; Shen, J.R.; Nagao, R.
Deposited on	:	2023-09-19
Resolution	:	1.92 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:

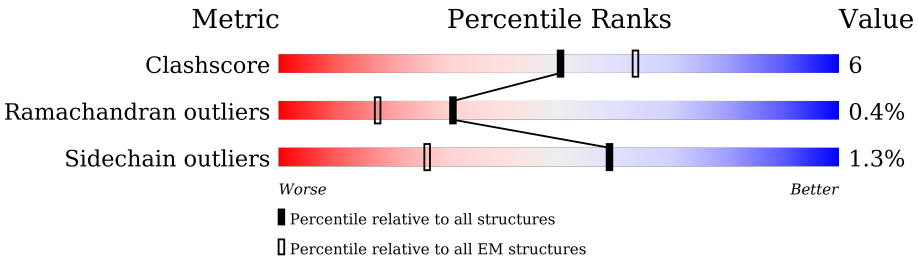
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

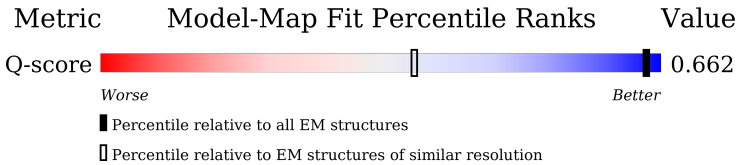
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1227 (1.42 - 2.42)

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	748	90% 9%
2	B	732	91% 9%
3	C	81	96%
4	D	139	81% 16%

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Mol	Chain	Length	Quality of chain
5	E	61	5% 100%
6	F	178	80% 9% 11%
7	I	32	84% 16%
8	J	38	92% 8%
9	K	68	19% 84% 9% 7%
10	L	141	13% 81% 5% 14%
11	M	28	82% 18%
12	O	155	50% 50% 46%
13	1	214	31% 73% 7% 20%
13	4	214	54% 69% 10% 20%
14	2	222	24% 74% 8% 18%
14	5	222	18% 76% 6% 18%
15	3	219	27% 65% 31%

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
25	5X6	1	312	-	X	-	-
25	5X6	1	313	-	X	-	-
25	5X6	1	314	-	X	-	-
25	5X6	1	315	-	X	-	-
25	5X6	1	316	-	X	-	-
25	5X6	2	317	-	X	-	-
25	5X6	2	318	-	X	-	-
25	5X6	2	319	-	X	-	-
25	5X6	2	320	-	X	-	-
25	5X6	2	321	-	X	-	-
25	5X6	3	316	-	X	-	-
25	5X6	3	317	-	X	-	-
25	5X6	3	318	-	X	-	-
25	5X6	4	312	-	X	-	-
25	5X6	4	313	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	5X6	4	314	-	X	-	-
25	5X6	5	301	-	X	-	-
25	5X6	5	315	-	X	-	-
25	5X6	5	316	-	X	-	-
25	5X6	5	317	-	X	-	-
25	5X6	5	318	-	X	-	-
25	5X6	F	205	-	X	-	-
25	5X6	J	105	-	X	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36163 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	5794	3784	996	987	27	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	730	5818	3829	981	990	18	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	598	367	104	115	12	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	117	938	594	165	176	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	61	491	321	77	92	1	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	158	1296	829	225	238	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	32	238	163	33	40	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	38	313	214	46	52	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	63	454	294	75	83	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	121	923	610	146	164	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	28	208	138	32	35	3	0	0

- Molecule 12 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	O	83	634	432	97	105	0	0

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	172	1365	892	228	235	10	0	0
13	4	172	1365	892	228	235	10	0	0

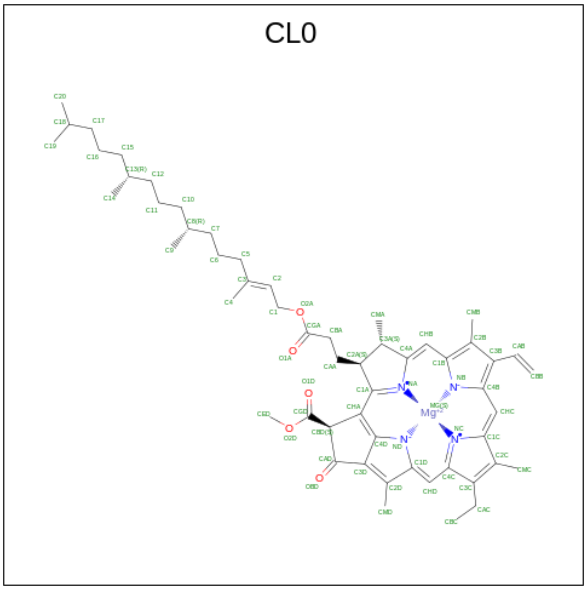
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2	183	1428	926	243	250	9	0	0
			Total	C	N	O	S		
14	5	183	1428	926	243	250	9	0	0

- Molecule 15 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	151	1169	759	198	206	6	0	0

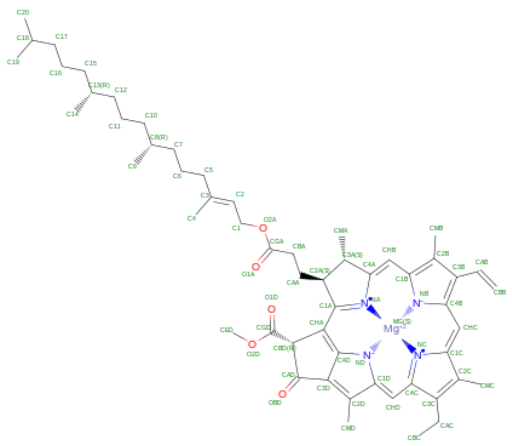
- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

CLA



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	62	52	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
17	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	F	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	K	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	L	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
17	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
17	O	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	O	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
17	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	59	49	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	2	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	3	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
17	3	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	4	1	45	35	1	4	5	0

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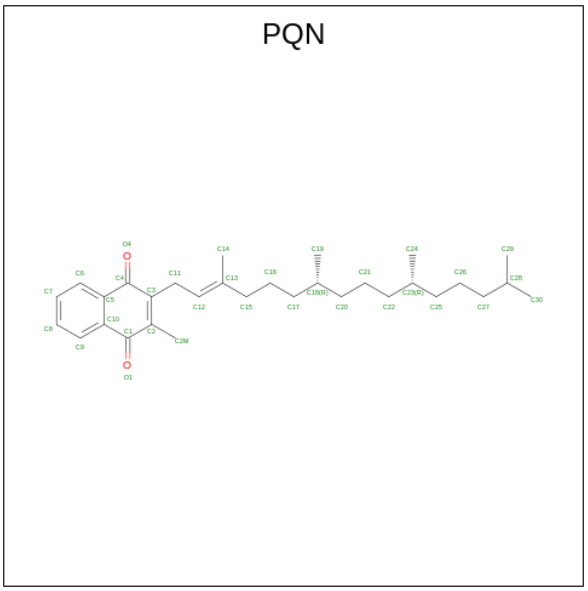
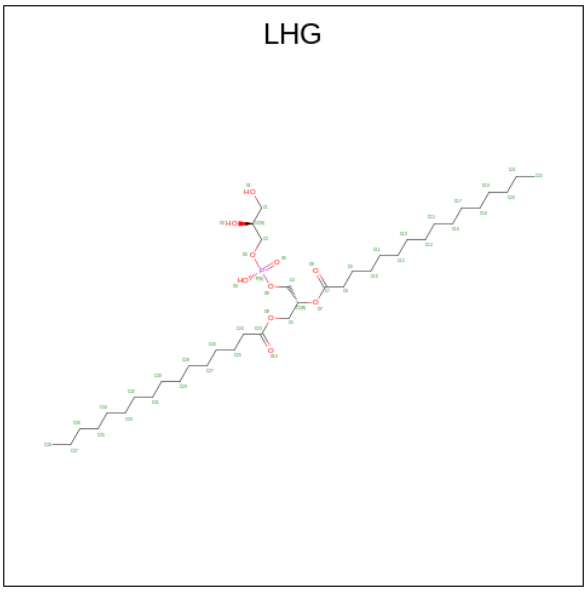
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	5	1	44	36	1	4	3	0

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	A	1	49	38	10	1	0

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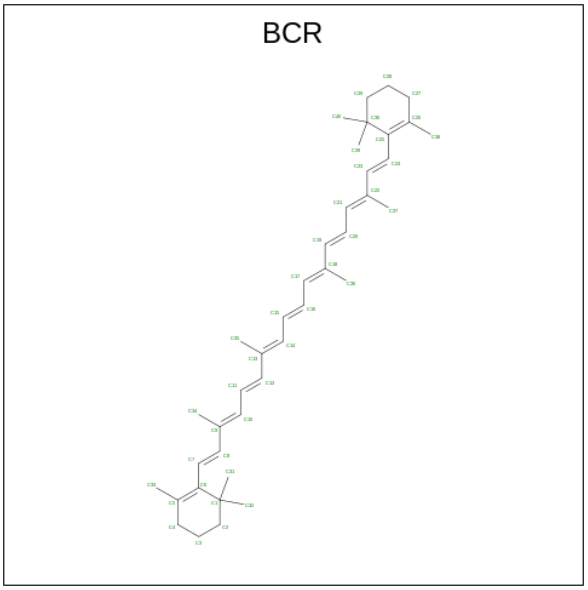
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	A	1	40	29	10	1	0
			Total	C	O	P	
19	J	1	49	38	10	1	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	A	1	40	40	0
			Total	C	
20	A	1	40	40	0
			Total	C	
20	A	1	40	40	0
			Total	C	
20	A	1	40	40	0
			Total	C	
20	A	1	40	40	0
			Total	C	
20	B	1	40	40	0
			Total	C	
20	B	1	40	40	0
			Total	C	
20	B	1	40	40	0
			Total	C	
20	B	1	40	40	0

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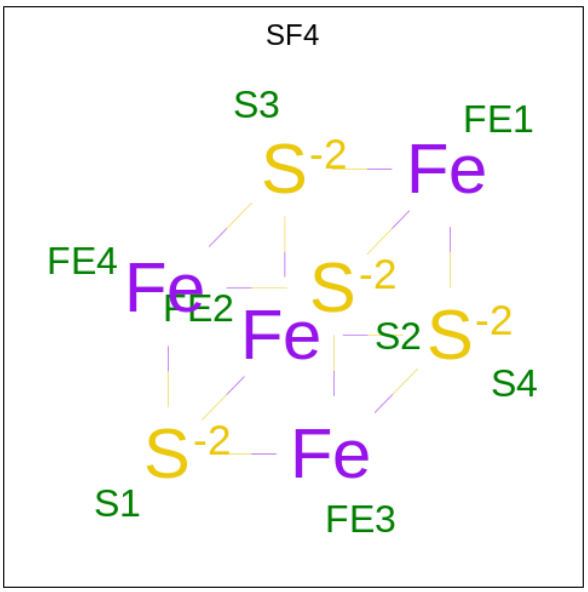
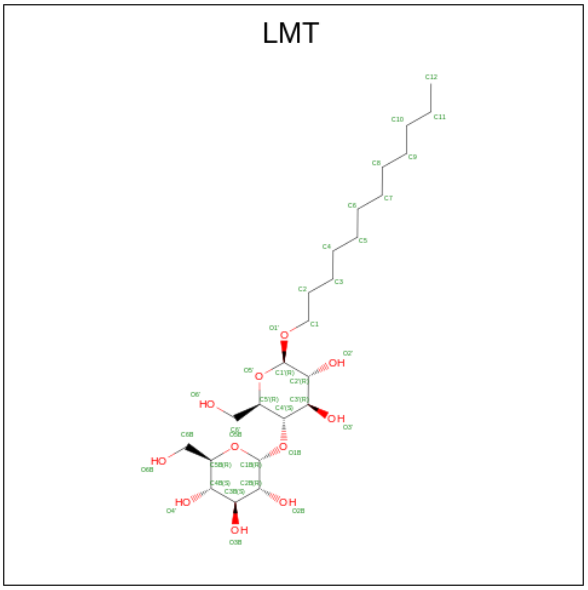
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	B	1	40	40	0
			Total	C	
20	B	1	40	40	0
			Total	C	
20	B	1	40	40	0
			Total	C	
20	I	1	40	40	0
			Total	C	
20	J	1	40	40	0
			Total	C	
20	K	1	40	40	0
			Total	C	
20	L	1	40	40	0
			Total	C	
20	L	1	40	40	0
			Total	C	
20	L	1	40	40	0
			Total	C	
20	M	1	40	40	0
			Total	C	
20	O	1	40	40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

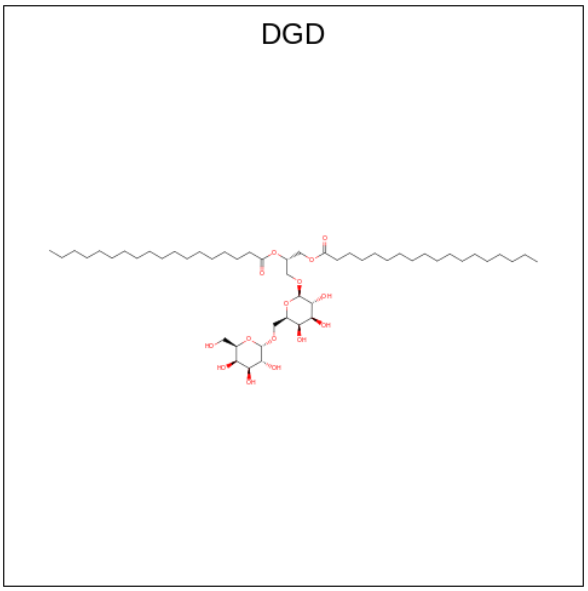


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	A	1	35	24	11	0
22	B	1	35	24	11	0
22	B	1	35	24	11	0
22	B	1	35	24	11	0
22	F	1	35	24	11	0
22	L	1	35	24	11	0
22	3	1	35	24	11	0

- Molecule 23 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

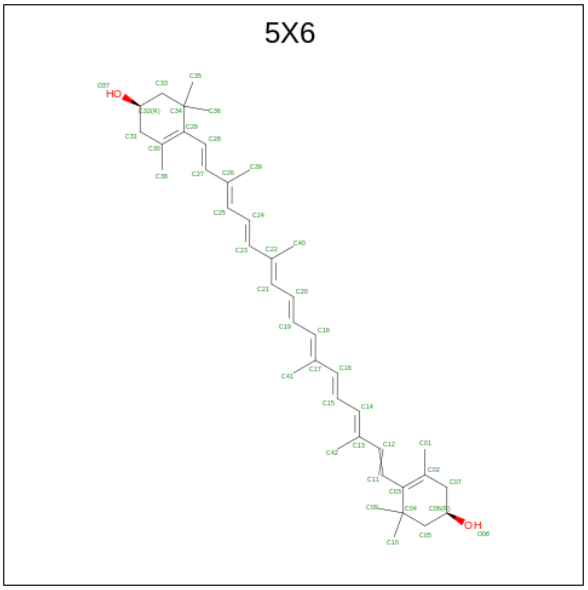
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
23	A	4	48	48	0
			Total	C	
23	B	5	54	54	0
			Total	C	
23	F	1	9	9	0
			Total	C	
23	I	1	12	12	0
			Total	C	
23	J	1	13	13	0
			Total	C	
23	K	1	13	13	0
			Total	C	
23	L	1	13	13	0
			Total	C	
23	O	1	6	6	0
			Total	C	
23	1	1	8	8	0
			Total	C	
23	2	3	32	32	0
			Total	C	
23	3	3	37	37	0
			Total	C	
23	4	2	24	24	0
			Total	C	
23	5	1	8	8	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	B	1	66	51	15	0

- Molecule 25 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	F	1	42	40	2	0
			Total	C	O	
25	J	1	42	40	2	0
			Total	C	O	
25	1	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	1	1	42	40	2	0
25	1	1	42	40	2	0
25	1	1	42	40	2	0
25	1	1	42	40	2	0
25	2	1	42	40	2	0
25	2	1	42	40	2	0
25	2	1	42	40	2	0
25	2	1	42	40	2	0
25	2	1	42	40	2	0
25	3	1	42	40	2	0
25	3	1	42	40	2	0
25	3	1	42	40	2	0
25	4	1	42	40	2	0
25	4	1	42	40	2	0
25	4	1	42	40	2	0
25	5	1	42	40	2	0
25	5	1	42	40	2	0
25	5	1	42	40	2	0
25	5	1	42	40	2	0
25	5	1	42	40	2	0

- Molecule 26 is water.

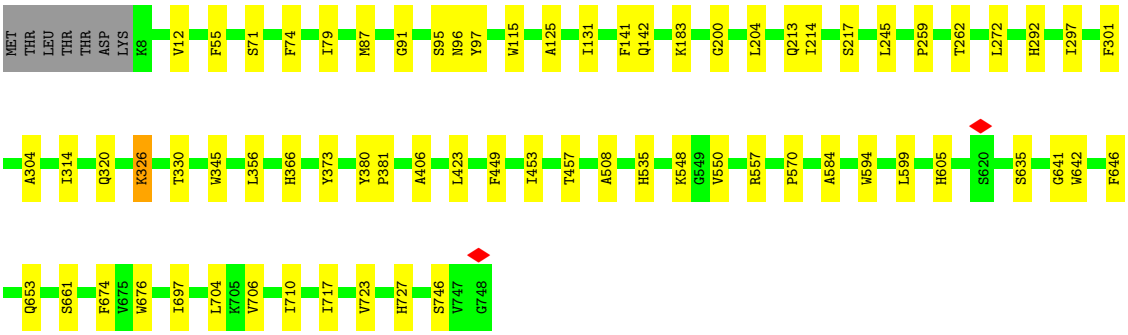
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
26	A	203	203	203	0
			Total	O	
26	B	220	220	220	0
			Total	O	
26	C	41	41	41	0
			Total	O	
26	D	18	18	18	0
			Total	O	
26	E	23	23	23	0
			Total	O	
26	F	22	22	22	0
			Total	O	
26	I	2	2	2	0
			Total	O	
26	J	7	7	7	0
			Total	O	
26	K	2	2	2	0
			Total	O	
26	L	7	7	7	0
			Total	O	
26	M	2	2	2	0
			Total	O	
26	1	3	3	3	0
			Total	O	
26	3	1	1	1	0
			Total	O	
26	4	3	3	3	0
			Total	O	
26	5	6	6	6	0

3 Residue-property plots (i)

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

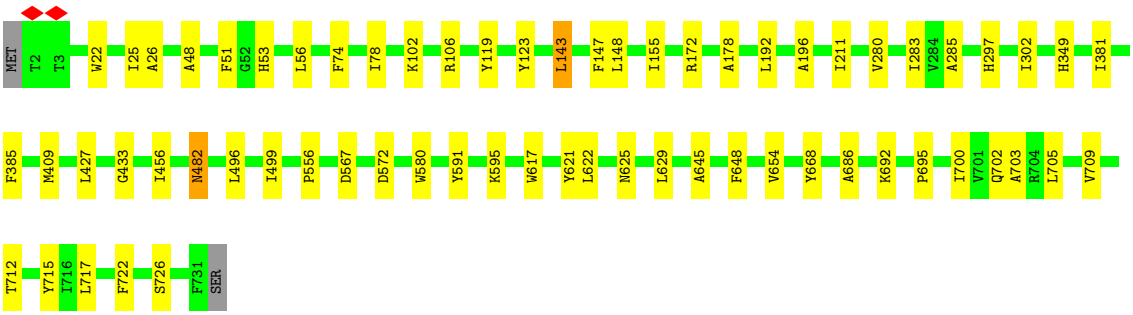
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



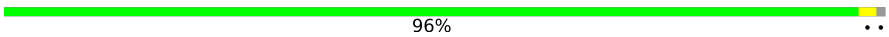
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

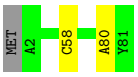
Chain B:



• Molecule 3: Photosystem I iron-sulfur center

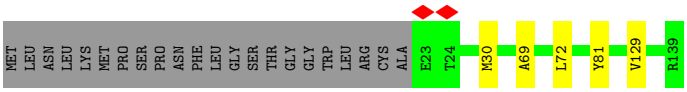
Chain C:





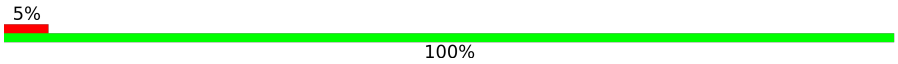
• Molecule 4: Photosystem I reaction center subunit II

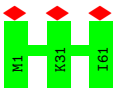
Chain D:



• Molecule 5: Photosystem I reaction center subunit IV

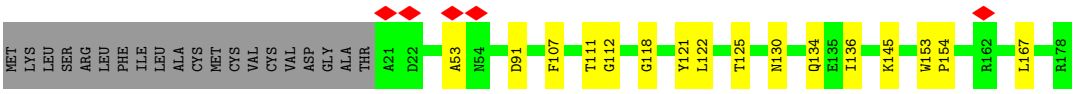
Chain E:





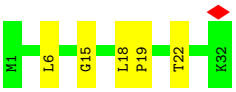
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



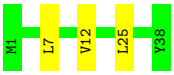
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



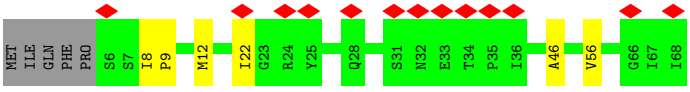
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



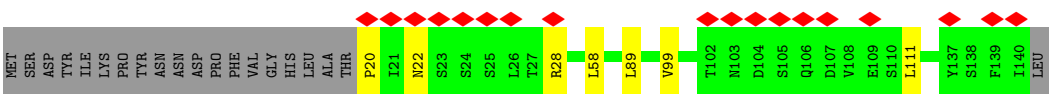
• Molecule 9: Photosystem I reaction center subunit X

Chain K:



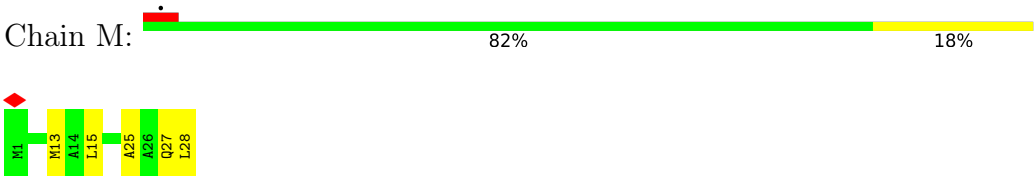
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



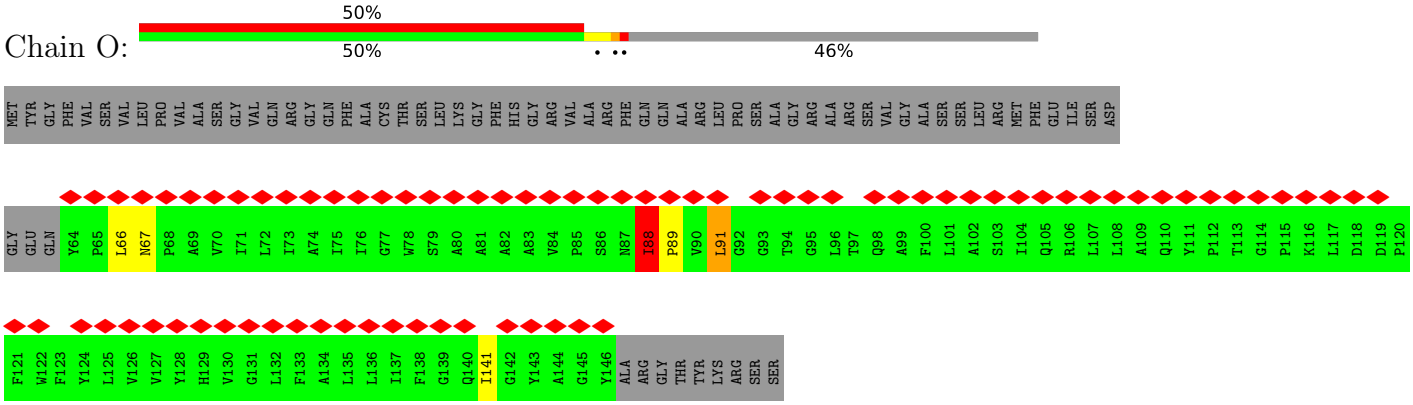
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:



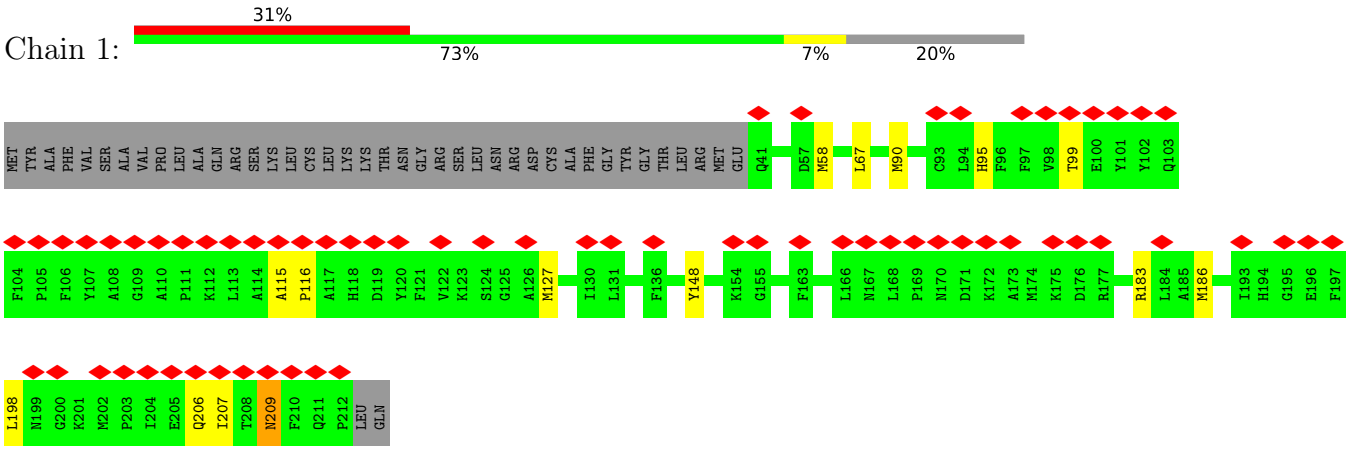
- Molecule 12: Photosystem I subunit O

Chain O:



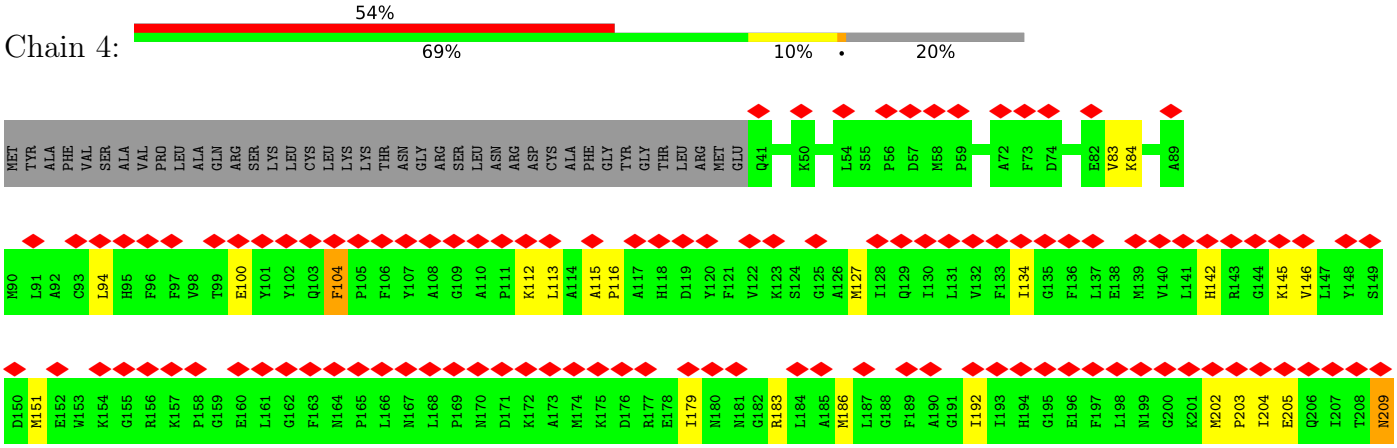
- Molecule 13: Lhcr1

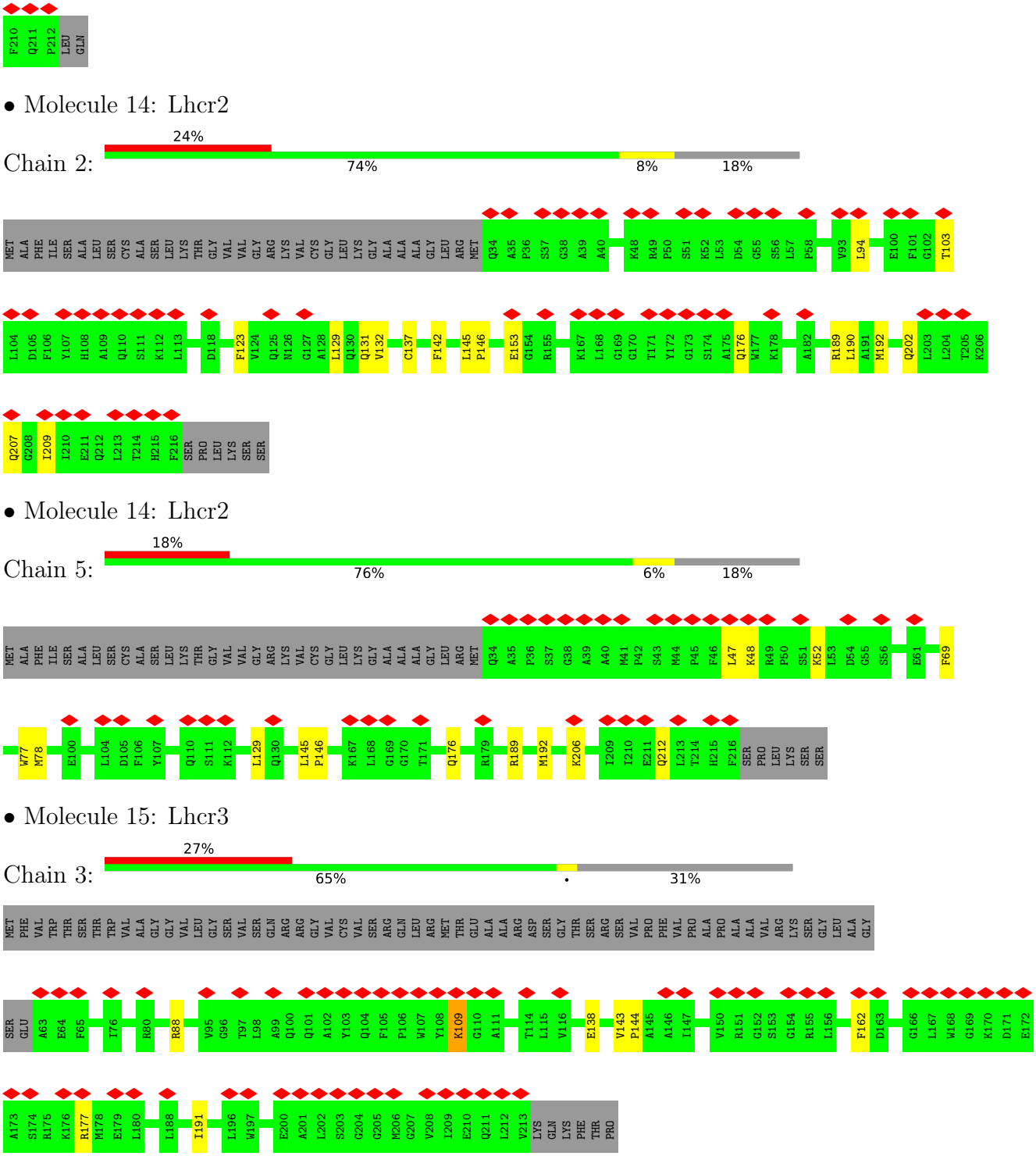
Chain 1:



- Molecule 13: Lhcr1

Chain 4:




F210 Q211 P212 LEU GLN
• Molecule 14: Lhcr2
Chain 2:
24%
74%
8%
18%
MET ALA PHE ILE SER ALA LEU SER CYS ALA SER LEU LYS THR GLY VAL VAL GLY ARG LYS VAL CYS GLY LEU LYS GLY ALA ALA ALA GLY LEU ARG MET Q34 A35 P36 S37 G38 A39 A40 K48 R49 P50 S51 K52 L53 D54 G55 S56 L57 P58 V93 L94 E100 F101 G102 T103
L104 D105 F106 Y107 H108 A109 Q110 S111 K112 L113 D118 F123 V124 Q125 N126 G127 A128 L129 Q130 Q131 V132 C137 F142 L145 P146 E153 G154 R155 K167 L168 G169 G170 T171 Y172 G173 S174 A175 Q176 W177 K178 A182 R189 L190 A191 M192 Q202 L203 L204 T205 K206
Q207 G208 I209 I210 E211 Q212 L213 T214 H215 F216 SER PRO LEU LYS SER SER
• Molecule 14: Lhcr2
Chain 5:
18%
76%
6%
18%
MET ALA PHE ILE SER ALA LEU SER CYS ALA SER LEU LYS THR GLY VAL VAL GLY ARG LYS VAL CYS GLY LEU LYS GLY ALA ALA ALA GLY LEU ARG MET Q34 A35 P36 S37 G38 A39 A40 M41 P42 S43 M44 P45 F46 L47 K48 R49 P50 S51 K52 L53 D54 G55 S56 E61 F69
W77 M78 E100 L104 D105 F106 Y107 Q110 S111 K112 L129 Q130 L145 P146 K167 L168 G169 G170 T171 Q176 R179 R189 M192 K206 I209 I210 E211 Q212 L213 T214 H215 F216 SER PRO LEU LYS SER SER
• Molecule 15: Lhcr3
Chain 3:
27%
65%
31%
MET PHE VAL TRP THR SER THR TRP VAL ALA GLY GLY VAL LEU GLY SER VAL SER GLN ARG ARG GLY VAL CYS VAL SER ARG GLN LEU ARG MET THR GLU ALA ALA ARG ASP SER GLY THR SER ARG SER VAL PRO PHE VAL PRO ALA PRO ALA ALA VAL ARG LYS SER GLY LEU ALA GLY
SER GLU A63 E64 F65 I76 R80 R88 V95 G96 T97 L98 A99 Q100 Q101 A102 Y103 Q104 F105 P106 W107 Y108 K109 G110 A111 T114 L115 V116 E138 V143 P144 A145 A146 I147 V150 R151 G152 S153 G154 R155 L156 F162 D163 G166 L167 W168 G169 K170 D171 E172
A173 S174 R175 K176 R177 M178 E179 L180 L188 I191 L196 W197 E200 A201 L202 S203 G204 G205 M206 G207 V208 I209 E210 Q211 L212 V213 LYS GLN LYS PHE THR PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228449	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 ($e^-/Å^2$)	39.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	202.752, 202.752, 202.752	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.792, 0.792, 0.792	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: SF4, PQN, CL0, LHG, UNL, LMT, 5X6, CLA, BCR, DGD

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	0.92	0/5979	1.43	0/8148
2	B	0.90	0/6027	1.45	0/8236
3	C	0.91	0/608	1.32	0/822
4	D	0.95	0/957	1.31	0/1292
5	E	0.99	0/500	1.26	0/676
6	F	0.95	0/1329	1.52	0/1799
7	I	1.02	0/243	1.52	0/332
8	J	0.88	0/322	1.39	0/439
9	K	1.05	0/459	1.76	2/627 (0.3%)
10	L	0.99	0/945	1.69	0/1281
11	M	1.00	0/209	1.71	0/283
12	O	1.06	0/656	1.65	0/903
13	1	1.01	0/1407	1.58	0/1903
13	4	1.02	0/1407	1.59	0/1903
14	2	1.00	0/1467	1.65	2/1980 (0.1%)
14	5	0.99	0/1467	1.64	0/1980
15	3	1.02	0/1199	1.67	0/1627
All	All	0.96	0/25181	1.51	4/34231 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	O	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	22	ILE	CA-C-N	5.29	125.85	119.98
9	K	22	ILE	C-N-CA	5.29	125.85	119.98
14	2	207	GLN	CA-C-N	5.05	124.90	120.10
14	2	207	GLN	C-N-CA	5.05	124.90	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	O	88	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5794	0	5722	55	0
2	B	5818	0	5649	60	0
3	C	598	0	576	2	0
4	D	938	0	933	4	0
5	E	491	0	509	0	0
6	F	1296	0	1263	14	0
7	I	238	0	265	6	0
8	J	313	0	327	2	0
9	K	454	0	490	3	0
10	L	923	0	939	2	0
11	M	208	0	230	5	0
12	O	634	0	644	2	0
13	1	1365	0	1351	12	0
13	4	1365	0	1351	13	0
14	2	1428	0	1406	17	0
14	5	1428	0	1406	5	0
15	3	1169	0	1172	6	0
16	A	65	0	72	1	0
17	1	540	0	442	17	0
17	2	618	0	494	23	0
17	3	530	0	423	13	0
17	4	418	0	321	14	0
17	5	680	0	619	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A	2664	0	2743	71	0
17	B	2513	0	2633	98	0
17	F	86	0	62	5	0
17	J	42	0	31	1	0
17	K	97	0	80	3	0
17	L	172	0	164	2	0
17	O	136	0	101	4	0
18	A	33	0	46	1	0
18	B	33	0	46	2	0
19	A	89	0	127	1	0
19	J	49	0	74	1	0
20	A	200	0	280	13	0
20	B	280	0	392	8	0
20	I	40	0	56	0	0
20	J	40	0	56	3	0
20	K	40	0	56	1	0
20	L	120	0	168	4	0
20	M	40	0	56	3	0
20	O	40	0	56	0	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	3	35	0	46	0	0
22	A	35	0	46	0	0
22	B	105	0	138	0	0
22	F	35	0	46	0	0
22	L	35	0	46	0	0
23	1	8	0	0	0	0
23	2	32	0	0	0	0
23	3	37	0	0	0	0
23	4	24	0	0	0	0
23	5	8	0	0	0	0
23	A	48	0	0	0	0
23	B	54	0	0	0	0
23	F	9	0	0	0	0
23	I	12	0	0	0	0
23	J	13	0	0	0	0
23	K	13	0	0	0	0
23	L	13	0	0	0	0
23	O	6	0	0	0	0
24	B	66	0	96	3	0
25	1	210	0	0	2	0
25	2	210	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	126	0	0	2	0
25	4	126	0	0	0	0
25	5	210	0	0	2	0
25	F	42	0	0	0	0
25	J	42	0	0	0	0
26	1	3	0	0	0	0
26	3	1	0	0	0	0
26	4	3	0	0	0	0
26	5	6	0	0	0	0
26	A	203	0	0	1	0
26	B	220	0	0	1	0
26	C	41	0	0	0	0
26	D	18	0	0	0	0
26	E	23	0	0	0	0
26	F	22	0	0	0	0
26	I	2	0	0	0	0
26	J	7	0	0	0	0
26	K	2	0	0	0	0
26	L	7	0	0	0	0
26	M	2	0	0	0	0
All	All	36163	0	34249	390	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 (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:190:LEU:HD21	17:2:313:CLA:HBC3	1.66	0.77
14:2:132:VAL:CG2	17:2:309:CLA:HBC1	2.17	0.74
14:2:129:LEU:HD22	17:2:309:CLA:HBC3	1.69	0.74
1:A:535:HIS:HE1	1:A:605:HIS:HD2	1.37	0.72
17:K:103:CLA:HMC3	20:K:104:BCR:H332	1.72	0.71
17:1:302:CLA:H41	17:1:303:CLA:HMA3	1.71	0.71
17:B:839:CLA:H192	10:L:58:LEU:HD21	1.77	0.65
2:B:78:ILE:HD12	2:B:123:TYR:CD1	2.31	0.65
1:A:535:HIS:HE1	1:A:605:HIS:CD2	2.15	0.65
2:B:705:LEU:HD22	24:B:849:DGD:HB22	1.80	0.63
20:M:101:BCR:H321	20:M:101:BCR:HC8	1.82	0.62
17:A:852:CLA:CGA	17:A:852:CLA:H3A	2.30	0.61
17:B:826:CLA:H102	17:B:837:CLA:H43	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:123:PHE:CE1	17:2:307:CLA:HED1	2.36	0.60
17:B:837:CLA:H41	17:B:837:CLA:C7	2.31	0.60
2:B:26:ALA:HA	17:B:830:CLA:H42	1.83	0.60
17:B:839:CLA:HBB2	18:B:842:PQN:H141	1.83	0.60
20:L:201:BCR:H383	20:L:201:BCR:H23C	1.83	0.59
14:2:132:VAL:HG21	17:2:309:CLA:HBC1	1.84	0.58
1:A:259:PRO:O	1:A:262:THR:O	2.22	0.58
17:5:313:CLA:HBC2	25:5:318:5X6:C14	2.33	0.58
1:A:115:TRP:CD2	17:A:807:CLA:HED3	2.38	0.58
17:J:103:CLA:HHC	17:J:103:CLA:HBB1	1.85	0.58
2:B:591:TYR:CZ	17:B:836:CLA:HBC3	2.38	0.58
17:B:840:CLA:HHC	17:B:840:CLA:HBB1	1.85	0.58
14:2:132:VAL:HG23	17:2:309:CLA:HBC1	1.85	0.58
17:B:826:CLA:HBB1	17:B:826:CLA:HMB1	1.86	0.57
13:1:206:GLN:HE22	17:1:310:CLA:HED1	1.69	0.57
17:A:802:CLA:HBB1	17:A:802:CLA:HMB1	1.84	0.57
6:F:107:PHE:CZ	6:F:111:THR:HG21	2.40	0.57
17:B:837:CLA:HBB1	17:B:837:CLA:HMB3	1.87	0.57
1:A:314:ILE:HD13	9:K:46:ALA:HB2	1.87	0.57
2:B:385:PHE:CE2	20:B:847:BCR:H373	2.38	0.57
17:B:807:CLA:H142	17:B:828:CLA:H143	1.85	0.57
9:K:12:MET:HE1	9:K:56:VAL:HG23	1.87	0.57
17:A:826:CLA:H43	17:A:826:CLA:O1A	2.05	0.56
2:B:56:LEU:HD21	17:B:807:CLA:HMD1	1.87	0.56
20:B:843:BCR:H331	20:B:843:BCR:C8	2.36	0.56
17:F:204:CLA:HBC3	17:F:204:CLA:HHD	1.88	0.56
17:L:202:CLA:HHC	17:L:202:CLA:HBB1	1.87	0.56
2:B:297:HIS:HB3	2:B:302:ILE:HD11	1.88	0.56
17:2:309:CLA:HHC	17:2:309:CLA:HBB1	1.88	0.56
17:A:809:CLA:HHC	17:A:809:CLA:HBB1	1.87	0.56
6:F:145:LYS:HA	13:1:148:TYR:CD2	2.41	0.56
1:A:674:PHE:CG	20:A:846:BCR:H363	2.41	0.55
2:B:22:TRP:CG	2:B:702:GLN:HE22	2.24	0.55
17:B:805:CLA:HBA1	17:B:805:CLA:HBD	1.88	0.55
17:A:834:CLA:HHC	17:A:834:CLA:HBB1	1.89	0.55
1:A:449:PHE:CZ	1:A:453:ILE:HD11	2.42	0.55
20:L:206:BCR:C8	20:L:206:BCR:H331	2.35	0.55
1:A:304:ALA:HB2	17:A:819:CLA:HBC2	1.87	0.55
17:B:826:CLA:H43	17:B:834:CLA:HBB2	1.87	0.55
13:4:134:ILE:HD13	17:4:307:CLA:HBC2	1.88	0.55
18:A:840:PQN:H141	17:A:855:CLA:HBB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:203:CLA:HMB2	8:J:25:LEU:HD21	1.89	0.55
1:A:345:TRP:HB3	17:A:803:CLA:HAC1	1.89	0.54
17:A:853:CLA:OBD	17:B:804:CLA:HMB2	2.08	0.54
17:B:823:CLA:CHC	17:B:841:CLA:HED1	2.37	0.54
17:B:829:CLA:HBB1	17:B:829:CLA:HMB3	1.89	0.54
9:K:8:ILE:HB	9:K:9:PRO:HD3	1.88	0.54
2:B:48:ALA:HB3	11:M:28:LEU:HD21	1.90	0.54
11:M:25:ALA:HB2	20:M:101:BCR:H312	1.89	0.54
17:A:823:CLA:HMB2	17:A:825:CLA:H93	1.89	0.54
1:A:550:VAL:HG21	20:A:845:BCR:HC31	1.89	0.54
14:2:94:LEU:HD23	17:2:307:CLA:HBC2	1.90	0.54
17:B:838:CLA:HMB3	17:B:838:CLA:HBB1	1.89	0.54
2:B:56:LEU:HD21	17:B:807:CLA:CMD	2.38	0.53
4:D:30:MET:HE2	4:D:72:LEU:HD12	1.89	0.53
2:B:717:LEU:HD22	17:B:828:CLA:H41	1.91	0.53
17:B:836:CLA:HBB1	17:B:836:CLA:HMB1	1.90	0.53
1:A:214:ILE:HD13	17:A:813:CLA:C3C	2.39	0.53
17:B:810:CLA:H201	7:I:22:THR:HG22	1.91	0.53
2:B:56:LEU:CD1	17:B:808:CLA:H141	2.38	0.53
1:A:74:PHE:CZ	17:A:811:CLA:HED1	2.44	0.53
1:A:406:ALA:HB1	1:A:584:ALA:HB1	1.89	0.53
2:B:78:ILE:HG23	2:B:123:TYR:CE1	2.43	0.53
17:A:833:CLA:HHC	17:A:833:CLA:HBB1	1.90	0.53
1:A:366:HIS:ND1	17:A:816:CLA:OBD	2.41	0.52
17:A:820:CLA:H142	17:A:820:CLA:H91	1.92	0.52
20:A:857:BCR:H331	20:A:857:BCR:C8	2.39	0.52
17:A:815:CLA:CHD	17:A:816:CLA:HBB2	2.40	0.52
17:A:814:CLA:HHC	17:A:814:CLA:HBB1	1.92	0.52
14:2:123:PHE:CZ	17:2:307:CLA:HED1	2.44	0.52
17:B:818:CLA:HBB1	17:B:818:CLA:HHC	1.91	0.52
1:A:674:PHE:CD2	20:A:846:BCR:H363	2.44	0.52
17:A:834:CLA:HMB1	20:A:845:BCR:H281	1.91	0.52
13:1:207:ILE:HG23	13:1:207:ILE:O	2.10	0.52
17:A:816:CLA:CMD	17:A:817:CLA:H202	2.40	0.52
1:A:297:ILE:CD1	17:A:816:CLA:HBC2	2.39	0.52
17:B:807:CLA:H142	17:B:828:CLA:C14	2.40	0.52
17:K:103:CLA:HHC	17:K:103:CLA:HBB1	1.92	0.51
17:A:839:CLA:HHC	17:A:839:CLA:HBB1	1.92	0.51
17:B:832:CLA:HBC2	17:B:838:CLA:HMC2	1.92	0.51
17:A:816:CLA:HHC	17:A:816:CLA:HBB1	1.92	0.51
17:B:811:CLA:CBB	7:I:15:GLY:HA3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:811:CLA:HBB2	7:I:15:GLY:HA3	1.90	0.51
17:5:304:CLA:HHC	17:5:304:CLA:HBB1	1.93	0.51
17:5:307:CLA:HHC	17:5:307:CLA:HBB1	1.91	0.51
17:A:855:CLA:HHC	17:A:855:CLA:HBB1	1.93	0.51
13:4:204:ILE:HD12	13:4:205:GLU:N	2.26	0.51
17:2:308:CLA:HHC	17:2:308:CLA:HBB1	1.93	0.51
17:B:831:CLA:HMB3	17:B:831:CLA:HBB1	1.91	0.51
1:A:213:GLN:HA	1:A:217:SER:HB2	1.93	0.50
17:B:813:CLA:HHC	17:B:813:CLA:HBB1	1.92	0.50
17:A:827:CLA:HBB1	17:A:827:CLA:HMB1	1.94	0.50
17:A:829:CLA:CBB	17:A:837:CLA:CBB	2.90	0.50
17:A:859:CLA:HBC2	17:A:859:CLA:HMC3	1.92	0.50
13:4:112:LYS:HB2	13:4:202:MET:HE1	1.94	0.50
2:B:695:PRO:HB3	17:B:839:CLA:C1C	2.42	0.50
2:B:155:ILE:HD13	11:M:27:GLN:HB3	1.94	0.50
1:A:55:PHE:CD2	17:A:803:CLA:HMC2	2.47	0.50
17:A:805:CLA:HMB1	17:A:805:CLA:HBB1	1.94	0.50
17:3:306:CLA:HHC	17:3:306:CLA:HBB1	1.94	0.50
17:B:823:CLA:HMB1	17:B:823:CLA:HBB1	1.94	0.50
17:5:311:CLA:HHC	17:5:311:CLA:HBB1	1.93	0.50
1:A:96:ASN:HB3	1:A:131:ILE:HG12	1.94	0.49
17:A:838:CLA:HHC	17:A:838:CLA:HBB1	1.94	0.49
17:B:802:CLA:HMB1	17:B:802:CLA:HBB1	1.94	0.49
2:B:280:VAL:HG21	17:B:817:CLA:CBB	2.42	0.49
17:B:815:CLA:H93	17:5:304:CLA:H191	1.93	0.49
17:1:311:CLA:HBB1	17:1:311:CLA:HHC	1.95	0.49
17:5:303:CLA:HBB1	17:5:303:CLA:HMB3	1.94	0.49
17:B:812:CLA:H11	17:B:813:CLA:C3D	2.42	0.49
25:1:314:5X6:C24	14:2:131:GLN:HE22	2.26	0.49
1:A:97:TYR:HA	1:A:141:PHE:CE2	2.48	0.49
17:1:301:CLA:HHC	17:1:301:CLA:HBB1	1.94	0.49
1:A:697:ILE:HD13	17:A:854:CLA:HMD1	1.95	0.49
17:1:306:CLA:HHC	17:1:306:CLA:HBB1	1.95	0.49
17:K:102:CLA:HHC	17:K:102:CLA:HBB1	1.95	0.49
17:4:303:CLA:HHC	17:4:303:CLA:HBB1	1.95	0.49
17:A:822:CLA:HHC	17:A:822:CLA:HBB1	1.94	0.49
17:B:841:CLA:HHC	17:B:841:CLA:HBB1	1.95	0.49
1:A:356:LEU:HD21	17:A:804:CLA:HBB1	1.94	0.48
17:B:817:CLA:CHD	17:B:818:CLA:HBB2	2.42	0.48
14:2:94:LEU:CD2	17:2:307:CLA:HBC2	2.44	0.48
1:A:548:LYS:HE3	2:B:668:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:808:CLA:HHC	17:A:808:CLA:HBB1	1.94	0.48
2:B:715:TYR:CE1	17:B:804:CLA:HED1	2.48	0.48
17:5:305:CLA:HBA1	17:5:305:CLA:HBD	1.95	0.48
17:5:308:CLA:HBB1	17:5:308:CLA:HMB1	1.94	0.48
1:A:71:SER:OG	17:A:809:CLA:HHD	2.12	0.48
13:4:183:ARG:HA	13:4:186:MET:HE3	1.95	0.48
17:A:831:CLA:H142	20:B:848:BCR:H15C	1.96	0.48
17:B:829:CLA:HBA1	17:B:829:CLA:C4A	2.44	0.48
4:D:30:MET:HE1	4:D:69:ALA:HA	1.95	0.48
17:2:313:CLA:HBC2	17:2:313:CLA:HHD	1.95	0.48
17:A:839:CLA:HMA3	2:B:686:ALA:CB	2.43	0.48
1:A:74:PHE:CE1	17:A:811:CLA:HED1	2.49	0.48
17:F:203:CLA:HBB1	17:F:203:CLA:HHC	1.95	0.48
13:1:58:MET:HE2	17:1:302:CLA:HED2	1.95	0.48
13:1:183:ARG:HA	13:1:186:MET:HE3	1.95	0.48
17:1:305:CLA:HBB1	17:1:305:CLA:HHC	1.95	0.48
15:3:143:VAL:HB	15:3:144:PRO:HD3	1.96	0.48
2:B:48:ALA:CB	11:M:28:LEU:HD21	2.44	0.48
2:B:456:ILE:HG21	6:F:91:ASP:HB3	1.95	0.48
13:4:192:ILE:HG23	13:4:203:PRO:HG3	1.94	0.48
17:4:310:CLA:HHC	17:4:310:CLA:HBB1	1.96	0.48
2:B:433:GLY:HA3	17:B:857:CLA:CBB	2.43	0.48
2:B:595:LYS:HG2	17:B:836:CLA:HBC1	1.95	0.48
2:B:51:PHE:CZ	17:B:814:CLA:HED1	2.49	0.47
2:B:703:ALA:CB	18:B:842:PQN:C8	2.92	0.47
1:A:326:LYS:O	17:A:859:CLA:HBC3	2.13	0.47
17:B:834:CLA:HHC	17:B:834:CLA:HBB1	1.96	0.47
17:4:311:CLA:HHC	17:4:311:CLA:HBB1	1.96	0.47
17:3:309:CLA:HHC	17:3:309:CLA:HBB1	1.96	0.47
17:5:306:CLA:HHC	17:5:306:CLA:HBB1	1.96	0.47
17:A:821:CLA:HHC	17:A:821:CLA:HBB1	1.97	0.47
6:F:145:LYS:HA	13:1:148:TYR:CE2	2.49	0.47
2:B:717:LEU:CD2	17:B:828:CLA:H41	2.45	0.47
17:O:203:CLA:HHC	17:O:203:CLA:HBB1	1.97	0.47
17:3:308:CLA:HHC	17:3:308:CLA:HBB1	1.95	0.47
14:5:129:LEU:HD21	17:5:305:CLA:HMA1	1.95	0.47
2:B:625:ASN:HB3	2:B:726:SER:HB2	1.97	0.47
17:B:837:CLA:H41	17:B:837:CLA:H72	1.97	0.47
15:3:177:ARG:HG2	17:3:312:CLA:HED1	1.96	0.47
13:4:151:MET:HE1	17:4:307:CLA:HED2	1.97	0.47
17:A:854:CLA:H193	6:F:121:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:204:CLA:HHC	17:F:204:CLA:HBB1	1.96	0.47
17:3:315:CLA:HHC	17:3:315:CLA:HBB1	1.96	0.47
16:A:801:CL0:H12	17:B:802:CLA:OBD	2.15	0.47
20:L:205:BCR:H403	20:L:205:BCR:H23C	1.97	0.47
14:2:103:THR:HG22	17:2:307:CLA:O1D	2.14	0.47
1:A:200:GLY:O	1:A:204:LEU:HB2	2.15	0.47
2:B:629:LEU:HD22	2:B:722:PHE:HA	1.97	0.47
20:A:857:BCR:H383	20:A:857:BCR:H23C	1.97	0.47
2:B:381:ILE:HG21	17:B:826:CLA:C3C	2.44	0.47
2:B:617:TRP:O	2:B:621:TYR:HB3	2.15	0.47
17:B:821:CLA:HHC	17:B:821:CLA:HBB1	1.97	0.47
17:O:204:CLA:HHC	17:O:204:CLA:HBB1	1.97	0.47
17:1:307:CLA:HMC1	25:1:312:5X6:C24	2.45	0.47
17:5:307:CLA:HMB2	25:5:318:5X6:C12	2.44	0.47
1:A:457:THR:HG21	17:A:832:CLA:HBC3	1.97	0.46
17:5:313:CLA:HHC	17:5:313:CLA:HBB1	1.97	0.46
17:A:815:CLA:HHC	17:A:815:CLA:HBB1	1.96	0.46
17:1:308:CLA:HHC	17:1:308:CLA:HBB1	1.97	0.46
17:2:304:CLA:HHC	17:2:304:CLA:HBB1	1.98	0.46
17:2:315:CLA:HHC	17:2:315:CLA:HBB1	1.97	0.46
17:A:835:CLA:HBB1	17:A:835:CLA:HMB1	1.97	0.46
17:B:820:CLA:HBC3	17:B:820:CLA:HHD	1.98	0.46
17:3:314:CLA:HHC	17:3:314:CLA:HBB1	1.97	0.46
2:B:143:LEU:HD22	2:B:147:PHE:CE2	2.50	0.46
17:3:313:CLA:HHC	17:3:313:CLA:HBB1	1.96	0.46
17:5:309:CLA:HMB3	17:5:309:CLA:HBB1	1.95	0.46
17:A:818:CLA:H202	20:A:844:BCR:C38	2.45	0.46
17:B:833:CLA:HBC2	17:B:833:CLA:HHD	1.97	0.46
4:D:30:MET:HE3	4:D:81:TYR:HB2	1.96	0.46
13:4:127:MET:SD	17:4:306:CLA:HBC3	2.55	0.46
17:5:302:CLA:HHC	17:5:302:CLA:HBB1	1.98	0.46
1:A:704:LEU:HD23	6:F:167:LEU:HD23	1.97	0.46
17:B:835:CLA:HBD	17:B:835:CLA:HAA1	1.98	0.46
20:B:844:BCR:H331	20:B:844:BCR:C8	2.46	0.46
13:1:67:LEU:HD11	14:2:142:PHE:HE1	1.81	0.46
17:3:305:CLA:HMC2	25:3:317:5X6:C23	2.46	0.46
17:5:310:CLA:HHC	17:5:310:CLA:HBB1	1.97	0.46
17:2:304:CLA:HBC1	15:3:162:PHE:HA	1.98	0.46
17:4:306:CLA:HHC	17:4:306:CLA:HBB1	1.98	0.46
17:A:854:CLA:H172	6:F:118:GLY:HA2	1.98	0.46
17:A:859:CLA:HHC	17:A:859:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:HIS:CE1	17:B:806:CLA:HMA2	2.51	0.46
17:1:309:CLA:HHC	17:1:309:CLA:HBB1	1.97	0.46
17:A:807:CLA:HMB3	17:A:807:CLA:HBB1	1.97	0.46
17:B:833:CLA:HBC2	17:B:833:CLA:CHD	2.44	0.46
8:J:7:LEU:HA	8:J:12:VAL:HG11	1.98	0.46
17:O:205:CLA:HHC	17:O:205:CLA:HBB1	1.98	0.46
13:1:90:MET:HE2	17:1:307:CLA:CBB	2.46	0.46
1:A:142:GLN:HB3	1:A:373:TYR:HB3	1.97	0.45
17:B:820:CLA:HMB2	17:B:825:CLA:HMA3	1.98	0.45
17:A:803:CLA:H42	17:A:803:CLA:O1A	2.15	0.45
2:B:349:HIS:ND1	17:B:818:CLA:OBD	2.47	0.45
17:F:203:CLA:HAA2	17:F:203:CLA:HBD	1.97	0.45
17:A:819:CLA:HBB1	17:A:819:CLA:HMB3	1.97	0.45
2:B:285:ALA:HB2	17:B:820:CLA:HBC2	1.97	0.45
17:B:808:CLA:HHC	17:B:808:CLA:HBB1	1.98	0.45
17:2:312:CLA:HHC	17:2:312:CLA:HBB1	1.97	0.45
17:3:312:CLA:HHC	17:3:312:CLA:HBB1	1.97	0.45
17:A:810:CLA:HBB1	17:A:810:CLA:HMB3	1.97	0.45
17:A:836:CLA:CHD	17:A:836:CLA:H42	2.46	0.45
17:A:819:CLA:CMB	17:A:823:CLA:HMA2	2.47	0.45
17:A:852:CLA:HMB1	17:A:852:CLA:HBB1	1.99	0.45
2:B:567:ASP:HA	2:B:572:ASP:CG	2.42	0.45
2:B:629:LEU:HD21	2:B:648:PHE:CD1	2.52	0.45
20:B:803:BCR:H331	20:B:803:BCR:C8	2.47	0.45
17:4:307:CLA:HHC	17:4:307:CLA:HBB1	1.98	0.45
17:B:835:CLA:HHC	17:B:835:CLA:HBB1	1.99	0.45
20:J:104:BCR:H331	20:J:104:BCR:C8	2.46	0.45
1:A:380:TYR:N	1:A:381:PRO:CD	2.80	0.45
1:A:653:GLN:HG2	1:A:746:SER:HB2	1.99	0.45
17:B:812:CLA:H11	17:B:813:CLA:C4D	2.47	0.45
2:B:192:LEU:HA	2:B:196:ALA:HB3	1.99	0.45
17:B:816:CLA:H43	20:B:845:BCR:HC21	1.99	0.45
4:D:30:MET:HE1	4:D:69:ALA:CA	2.47	0.45
6:F:125:THR:HG22	6:F:134:GLN:HB3	1.98	0.45
17:2:307:CLA:C1A	17:2:307:CLA:CGA	2.95	0.45
17:4:309:CLA:HHC	17:4:309:CLA:HBB1	1.98	0.45
17:B:807:CLA:HMC1	20:B:844:BCR:H401	1.99	0.44
17:1:302:CLA:HBB1	17:1:302:CLA:HMB3	1.98	0.44
17:2:313:CLA:HHC	17:2:313:CLA:HBB1	1.98	0.44
17:2:316:CLA:HHC	17:2:316:CLA:HBB1	1.99	0.44
1:A:635:SER:O	1:A:641:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:802:CLA:HAA2	17:B:802:CLA:HBD	1.98	0.44
17:B:830:CLA:H92	17:B:830:CLA:H52	1.99	0.44
14:2:189:ARG:HA	14:2:192:MET:HE3	1.98	0.44
14:5:189:ARG:HA	14:5:192:MET:HE3	1.98	0.44
1:A:557:ARG:HD2	3:C:80:ALA:HB3	1.99	0.44
20:A:846:BCR:H331	20:A:846:BCR:C8	2.46	0.44
17:A:853:CLA:HBB1	17:A:853:CLA:HMB1	2.00	0.44
2:B:280:VAL:HG21	17:B:817:CLA:HBB1	2.00	0.44
17:L:204:CLA:HHC	17:L:204:CLA:HBB1	2.00	0.44
1:A:642:TRP:O	1:A:646:PHE:HB3	2.18	0.44
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.52	0.44
13:4:146:VAL:HB	17:4:307:CLA:HMA2	1.99	0.44
17:5:312:CLA:HHC	17:5:312:CLA:HBB1	1.99	0.44
17:A:804:CLA:H152	17:A:804:CLA:H112	1.87	0.44
2:B:622:LEU:HD22	17:B:804:CLA:HMD2	1.99	0.44
17:1:304:CLA:HHC	17:1:304:CLA:HBB1	1.99	0.44
1:A:570:PRO:HB3	1:A:717:ILE:HB	2.00	0.44
17:A:859:CLA:HBC2	17:A:859:CLA:CMC	2.48	0.44
1:A:297:ILE:HD13	17:A:816:CLA:HBC2	2.00	0.44
17:B:817:CLA:C4C	17:B:818:CLA:HBB2	2.47	0.44
6:F:112:GLY:HA3	6:F:153:TRP:CZ2	2.52	0.44
12:O:88:ILE:HG13	12:O:89:PRO:HD3	2.00	0.44
13:1:95:HIS:HB2	17:1:304:CLA:C1C	2.48	0.44
13:4:202:MET:HG3	13:4:203:PRO:HD2	2.00	0.44
17:A:854:CLA:HBB2	6:F:118:GLY:HA3	2.00	0.43
14:2:202:GLN:HG3	14:2:209:ILE:HD11	2.00	0.43
2:B:580:TRP:CZ2	17:B:802:CLA:HAB	2.53	0.43
17:1:310:CLA:HHC	17:1:310:CLA:HBB1	2.00	0.43
1:A:79:ILE:HG23	20:J:104:BCR:HC21	2.00	0.43
1:A:204:LEU:HD13	20:A:844:BCR:H21C	2.00	0.43
1:A:330:THR:OG1	19:A:842:LHG:HC12	2.18	0.43
2:B:25:ILE:HA	17:B:805:CLA:HMD2	2.00	0.43
17:B:828:CLA:HAA1	17:B:828:CLA:HBD	1.99	0.43
2:B:211:ILE:HG23	17:5:313:CLA:HMD1	2.00	0.43
17:B:824:CLA:H52	17:B:825:CLA:H143	2.00	0.43
14:2:137:CYS:SG	17:2:310:CLA:CBB	3.06	0.43
15:3:88:ARG:NH2	17:3:311:CLA:O1D	2.51	0.43
17:4:308:CLA:HHC	17:4:308:CLA:HBB1	2.00	0.43
17:A:818:CLA:HMB3	17:A:818:CLA:HBB1	2.00	0.43
17:B:813:CLA:H62	17:B:813:CLA:H41	1.83	0.43
17:2:307:CLA:HHC	17:2:307:CLA:HBB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB2	1:A:661:SER:HB2	2.00	0.43
20:A:843:BCR:H11C	20:A:843:BCR:H341	1.91	0.43
17:A:832:CLA:HHC	17:A:832:CLA:HBB1	1.99	0.43
17:B:823:CLA:HBC2	17:B:824:CLA:HBA1	2.01	0.43
14:2:145:LEU:HB3	14:2:146:PRO:HD3	2.01	0.43
17:3:307:CLA:HHC	17:3:307:CLA:HBB1	2.00	0.43
13:4:83:VAL:HG22	13:4:179:ILE:HD11	2.00	0.43
17:A:859:CLA:ND	12:O:141:ILE:HG22	2.34	0.43
13:4:115:ALA:HB3	13:4:116:PRO:HD3	2.00	0.43
13:4:142:HIS:NE2	17:4:307:CLA:HED1	2.34	0.43
6:F:153:TRP:N	6:F:154:PRO:CD	2.82	0.43
17:4:305:CLA:HHC	17:4:305:CLA:HBB1	2.00	0.43
1:A:272:LEU:HD22	1:A:292:HIS:HA	2.01	0.42
1:A:301:PHE:HE1	17:A:819:CLA:HAB	1.84	0.42
2:B:178:ALA:HA	2:B:283:ILE:HA	2.01	0.42
2:B:712:THR:HG21	24:B:849:DGD:HBH2	2.01	0.42
17:B:824:CLA:HMA2	17:B:841:CLA:HED3	2.01	0.42
17:A:826:CLA:H202	20:J:104:BCR:C17	2.49	0.42
17:B:807:CLA:H91	24:B:849:DGD:HBN1	2.00	0.42
17:5:313:CLA:HBC3	17:5:313:CLA:HHD	2.01	0.42
1:A:676:TRP:HZ3	17:B:802:CLA:HMD3	1.84	0.42
17:B:839:CLA:H171	10:L:89:LEU:HD11	2.02	0.42
13:1:115:ALA:HB3	13:1:116:PRO:HD3	2.00	0.42
2:B:629:LEU:O	2:B:645:ALA:HB2	2.20	0.42
6:F:122:LEU:HD12	6:F:122:LEU:HA	1.94	0.42
17:5:308:CLA:HBA2	17:5:308:CLA:H3A	1.90	0.42
2:B:74:PHE:HA	2:B:119:TYR:CE2	2.54	0.42
20:A:843:BCR:H362	20:A:844:BCR:H21C	2.02	0.42
2:B:427:LEU:HD11	17:B:837:CLA:HMB2	2.02	0.42
17:B:823:CLA:HHC	17:B:841:CLA:HED1	2.01	0.42
1:A:12:VAL:HG22	1:A:183:LYS:HG3	2.01	0.42
2:B:148:LEU:HD21	20:M:101:BCR:H342	2.02	0.42
2:B:297:HIS:CB	2:B:302:ILE:HD11	2.50	0.42
2:B:709:VAL:HG21	17:B:830:CLA:H91	2.01	0.42
17:2:314:CLA:HHC	17:2:314:CLA:HBB1	2.02	0.42
1:A:320:GLN:NE2	26:A:912:HOH:O	2.50	0.42
17:B:812:CLA:H61	17:B:812:CLA:H41	1.85	0.42
15:3:191:ILE:HD11	17:3:305:CLA:HAC1	2.01	0.42
20:A:846:BCR:H362	17:B:802:CLA:H11	2.01	0.41
17:B:801:CLA:H3A	17:B:801:CLA:CGA	2.49	0.41
13:1:127:MET:SD	17:1:305:CLA:HBC3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:LEU:HA	2:B:499:ILE:HG22	2.02	0.41
17:B:816:CLA:HBB1	17:B:816:CLA:HMB1	2.01	0.41
17:B:834:CLA:CMB	17:B:836:CLA:HED2	2.50	0.41
17:B:857:CLA:H42	19:J:102:LHG:HC62	2.02	0.41
17:3:306:CLA:CAB	25:3:317:5X6:C21	2.97	0.41
14:5:145:LEU:HB3	14:5:146:PRO:HD3	2.01	0.41
1:A:594:TRP:CH2	17:A:853:CLA:HAB	2.55	0.41
1:A:204:LEU:HD22	20:A:843:BCR:H361	2.02	0.41
2:B:409:MET:SD	17:B:831:CLA:CHD	3.08	0.41
2:B:556:PRO:HB3	2:B:700:ILE:HB	2.02	0.41
1:A:91:GLY:O	1:A:95:SER:OG	2.29	0.41
2:B:172:ARG:NH2	26:B:922:HOH:O	2.54	0.41
2:B:385:PHE:CZ	20:B:847:BCR:H373	2.54	0.41
17:B:810:CLA:CMB	17:B:811:CLA:C1C	2.98	0.41
17:B:822:CLA:HBB1	17:B:822:CLA:HHC	2.03	0.41
17:5:314:CLA:HHC	17:5:314:CLA:HBB1	2.02	0.41
1:A:423:LEU:HD13	17:A:819:CLA:H202	2.02	0.41
1:A:723:VAL:HG13	1:A:727:HIS:CE1	2.55	0.41
3:C:58:CYS:HA	21:C:102:SF4:S4	2.61	0.41
6:F:153:TRP:CG	6:F:154:PRO:HD3	2.56	0.41
1:A:87:MET:HE2	1:A:87:MET:N	2.36	0.41
17:A:810:CLA:HBC1	17:A:811:CLA:H142	2.02	0.41
13:4:151:MET:HE1	17:4:307:CLA:CED	2.50	0.41
2:B:654:VAL:HG22	17:B:840:CLA:HMB3	2.02	0.41
17:B:805:CLA:H92	11:M:25:ALA:HB2	2.03	0.41
17:B:812:CLA:CMD	14:5:77:TRP:CD2	3.03	0.41
1:A:706:VAL:O	1:A:706:VAL:HG22	2.21	0.41
17:B:836:CLA:HBC2	17:B:836:CLA:HHD	2.03	0.41
17:A:815:CLA:C4C	17:A:816:CLA:HBB2	2.51	0.40
2:B:482:ASN:N	2:B:482:ASN:HD22	2.19	0.40
2:B:591:TYR:CE1	17:B:836:CLA:HBC3	2.56	0.40
7:I:18:LEU:HB3	7:I:19:PRO:HD3	2.02	0.40
13:1:198:LEU:HD23	17:1:310:CLA:HED3	2.03	0.40
17:5:305:CLA:HHC	17:5:305:CLA:HBB1	2.04	0.40
17:B:810:CLA:H172	17:B:840:CLA:H43	2.02	0.40
17:B:827:CLA:H201	17:B:841:CLA:H172	2.02	0.40
17:B:839:CLA:HHC	17:B:839:CLA:HBB1	2.02	0.40
17:O:203:CLA:HBC2	17:O:204:CLA:H11	2.03	0.40
14:2:129:LEU:HA	14:2:132:VAL:HG22	2.04	0.40
14:5:69:PHE:HB3	14:5:78:MET:HE3	2.03	0.40
1:A:214:ILE:HD13	17:A:813:CLA:CAC	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ILE:CD1	6:F:136:ILE:HG23	2.51	0.40
17:A:831:CLA:HMB2	20:L:201:BCR:C36	2.51	0.40
17:A:853:CLA:HAA2	17:A:853:CLA:HBD	2.04	0.40
17:B:810:CLA:H201	7:I:22:THR:CG2	2.50	0.40
7:I:6:LEU:HD23	7:I:6:LEU:HA	1.98	0.40
2:B:48:ALA:HB2	2:B:155:ILE:HG23	2.03	0.40
17:B:831:CLA:HAA1	17:B:841:CLA:H41	2.04	0.40
15:3:138:GLU:O	15:3:143:VAL:N	2.53	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	739/748 (99%)	716 (97%)	22 (3%)	1 (0%)	48 40
2	B	728/732 (100%)	712 (98%)	16 (2%)	0	100 100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100 100
4	D	115/139 (83%)	112 (97%)	3 (3%)	0	100 100
5	E	59/61 (97%)	55 (93%)	4 (7%)	0	100 100
6	F	156/178 (88%)	153 (98%)	2 (1%)	1 (1%)	21 10
7	I	30/32 (94%)	29 (97%)	1 (3%)	0	100 100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
9	K	61/68 (90%)	58 (95%)	3 (5%)	0	100 100
10	L	119/141 (84%)	113 (95%)	5 (4%)	1 (1%)	16 6
11	M	26/28 (93%)	26 (100%)	0	0	100 100
12	O	81/155 (52%)	70 (86%)	7 (9%)	4 (5%)	1 0
13	1	170/214 (79%)	149 (88%)	19 (11%)	2 (1%)	10 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	4	170/214 (79%)	150 (88%)	17 (10%)	3 (2%)	6	1
14	2	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
14	5	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
15	3	149/219 (68%)	137 (92%)	11 (7%)	1 (1%)	18	9
All	All	3079/3492 (88%)	2933 (95%)	133 (4%)	13 (0%)	31	19

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	99	THR
12	O	88	ILE
1	A	508	ALA
6	F	53	ALA
10	L	22	ASN
12	O	91	LEU
13	4	209	ASN
12	O	66	LEU
13	1	209	ASN
13	4	104	PHE
13	4	100	GLU
15	3	109	LYS
12	O	67	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/608 (99%)	598 (100%)	3 (0%)	81	80
2	B	596/598 (100%)	591 (99%)	5 (1%)	73	71
3	C	66/67 (98%)	66 (100%)	0	100	100
4	D	98/116 (84%)	97 (99%)	1 (1%)	68	64
5	E	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	136/153 (89%)	135 (99%)	1 (1%)	76	73
7	I	27/27 (100%)	27 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
9	K	51/56 (91%)	51 (100%)	0	100	100
10	L	96/114 (84%)	92 (96%)	4 (4%)	26	11
11	M	22/22 (100%)	20 (91%)	2 (9%)	9	1
12	O	63/118 (53%)	61 (97%)	2 (3%)	34	18
13	1	143/178 (80%)	142 (99%)	1 (1%)	76	73
13	4	143/178 (80%)	137 (96%)	6 (4%)	26	11
14	2	146/174 (84%)	144 (99%)	2 (1%)	59	50
14	5	146/174 (84%)	140 (96%)	6 (4%)	27	12
15	3	117/171 (68%)	116 (99%)	1 (1%)	70	67
All	All	2542/2845 (89%)	2508 (99%)	34 (1%)	59	53

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
1	A	326	LYS
1	A	599	LEU
2	B	102	LYS
2	B	106	ARG
2	B	143	LEU
2	B	482	ASN
2	B	692	LYS
4	D	129	VAL
6	F	130	ASN
10	L	20	PRO
10	L	28	ARG
10	L	99	VAL
10	L	111	LEU
11	M	13	MET
11	M	15	LEU
12	O	88	ILE
12	O	91	LEU
13	1	209	ASN
14	2	153	GLU
14	2	176	GLN

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Mol	Chain	Res	Type
15	3	109	LYS
13	4	84	LYS
13	4	94	LEU
13	4	104	PHE
13	4	113	LEU
13	4	145	LYS
13	4	209	ASN
14	5	47	LEU
14	5	48	LYS
14	5	52	LYS
14	5	176	GLN
14	5	206	LYS
14	5	212	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	244	ASN
1	A	320	GLN
1	A	493	ASN
1	A	535	HIS
1	A	564	ASN
1	A	605	HIS
2	B	169	ASN
2	B	227	ASN
2	B	264	GLN
2	B	446	ASN
2	B	482	ASN
2	B	489	GLN
2	B	601	GLN
2	B	603	ASN
4	D	93	GLN
4	D	112	GLN
6	F	67	GLN
9	K	16	ASN
10	L	116	GLN
11	M	5	ASN
11	M	27	GLN
12	O	98	GLN
13	1	85	ASN
13	1	206	GLN

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Mol	Chain	Res	Type
14	2	131	GLN
14	2	176	GLN
14	2	187	ASN
14	2	201	GLN
14	2	212	GLN
15	3	199	GLN
13	4	85	ASN
13	4	180	ASN
13	4	194	HIS
14	5	126	ASN
14	5	201	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 238 ligands modelled in this entry, 25 are unknown - leaving 213 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	$\#\|Z\| > 2$
17	CLA	B	801	-	69,73,73	1.83	18 (26%)	83,113,113	2.47	25 (30%)
16	CL0	A	801	1	69,73,73	1.85	18 (26%)	83,113,113	2.71	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	L	203	10	69,73,73	1.99	20 (28%)	83,113,113	2.66	26 (31%)
17	CLA	B	837	2	69,73,73	1.92	20 (28%)	83,113,113	2.82	32 (38%)
17	CLA	B	829	2	69,73,73	1.88	20 (28%)	83,113,113	2.80	28 (33%)
17	CLA	B	826	26	69,73,73	1.87	20 (28%)	83,113,113	2.77	29 (34%)
17	CLA	5	310	-	45,49,73	2.55	20 (44%)	54,84,113	3.37	26 (48%)
17	CLA	B	838	2	51,55,73	2.24	19 (37%)	61,91,113	3.32	27 (44%)
25	5X6	1	314	-	43,43,43	5.91	23 (53%)	58,60,60	4.67	34 (58%)
20	BCR	B	844	-	41,41,41	1.60	8 (19%)	56,56,56	1.32	5 (8%)
25	5X6	1	316	-	43,43,43	6.01	23 (53%)	58,60,60	4.31	29 (50%)
17	CLA	A	830	1	60,64,73	2.06	20 (33%)	72,102,113	2.92	29 (40%)
22	LMT	B	850	-	36,36,36	0.41	0	47,47,47	0.67	0
25	5X6	4	314	-	43,43,43	6.09	24 (55%)	58,60,60	4.61	33 (56%)
17	CLA	5	311	14	49,53,73	2.50	21 (42%)	59,89,113	3.17	26 (44%)
21	SF4	C	102	3	0,12,12	-	-	-		
17	CLA	A	855	26	65,69,73	1.96	19 (29%)	78,108,113	2.91	27 (34%)
17	CLA	B	833	2	69,73,73	1.82	18 (26%)	83,113,113	2.89	31 (37%)
17	CLA	K	103	9	46,50,73	2.34	20 (43%)	55,85,113	3.23	28 (50%)
17	CLA	A	812	1	69,73,73	1.92	18 (26%)	83,113,113	2.84	24 (28%)
17	CLA	A	856	1	69,73,73	1.83	20 (28%)	83,113,113	2.78	28 (33%)
17	CLA	3	313	15	46,50,73	2.49	20 (43%)	55,85,113	3.28	26 (47%)
17	CLA	3	308	-	49,53,73	2.46	20 (40%)	59,89,113	3.11	25 (42%)
25	5X6	3	318	-	43,43,43	6.05	25 (58%)	58,60,60	4.43	30 (51%)
17	CLA	1	309	13	49,53,73	2.47	20 (40%)	59,89,113	3.21	26 (44%)
17	CLA	3	309	15	49,53,73	2.46	20 (40%)	59,89,113	3.25	26 (44%)
20	BCR	L	201	-	41,41,41	1.56	10 (24%)	56,56,56	1.52	8 (14%)
17	CLA	5	304	14	69,73,73	2.01	19 (27%)	83,113,113	2.77	29 (34%)
17	CLA	4	309	-	45,49,73	2.54	20 (44%)	54,84,113	3.34	27 (50%)
17	CLA	B	822	2	50,54,73	2.34	19 (38%)	60,90,113	3.32	27 (45%)
17	CLA	2	313	14	46,50,73	2.52	19 (41%)	55,85,113	3.31	27 (49%)
17	CLA	A	824	26	59,63,73	1.93	19 (32%)	71,101,113	3.18	31 (43%)
20	BCR	A	845	-	41,41,41	1.55	11 (26%)	56,56,56	1.44	9 (16%)
17	CLA	1	301	13	49,53,73	2.44	20 (40%)	59,89,113	3.02	25 (42%)
20	BCR	B	847	-	41,41,41	1.55	9 (21%)	56,56,56	1.42	9 (16%)
21	SF4	A	847	2,1	0,12,12	-	-	-		
17	CLA	B	857	2	62,66,73	2.00	18 (29%)	74,104,113	3.08	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	LMT	3	301	-	36,36,36	0.48	0	47,47,47	0.52	0
18	PQN	B	842	-	34,34,34	1.45	2 (5%)	42,45,45	1.12	3 (7%)
20	BCR	J	104	-	41,41,41	1.58	9 (21%)	56,56,56	1.36	8 (14%)
22	LMT	B	851	-	36,36,36	0.45	0	47,47,47	0.54	0
17	CLA	A	803	1	69,73,73	1.91	21 (30%)	83,113,113	2.81	27 (32%)
17	CLA	5	313	14	49,53,73	2.43	20 (40%)	59,89,113	3.12	30 (50%)
17	CLA	A	823	26	69,73,73	1.90	21 (30%)	83,113,113	2.80	28 (33%)
17	CLA	2	314	14	49,53,73	2.50	20 (40%)	59,89,113	3.22	27 (45%)
20	BCR	I	101	-	41,41,41	1.55	10 (24%)	56,56,56	1.37	9 (16%)
20	BCR	B	845	-	41,41,41	1.62	9 (21%)	56,56,56	1.41	8 (14%)
20	BCR	B	803	-	41,41,41	1.61	7 (17%)	56,56,56	1.67	10 (17%)
17	CLA	O	204	12	54,58,73	2.39	20 (37%)	65,95,113	3.21	30 (46%)
25	5X6	J	105	-	43,43,43	5.34	23 (53%)	58,60,60	4.97	28 (48%)
17	CLA	B	806	2	69,73,73	1.91	20 (28%)	83,113,113	2.85	29 (34%)
17	CLA	2	310	14	49,53,73	2.50	19 (38%)	59,89,113	3.16	26 (44%)
17	CLA	4	307	13	49,53,73	2.44	20 (40%)	59,89,113	3.16	31 (52%)
17	CLA	1	305	13	49,53,73	2.54	21 (42%)	59,89,113	3.12	25 (42%)
17	CLA	A	826	1	69,73,73	1.93	21 (30%)	83,113,113	2.78	28 (33%)
25	5X6	1	312	-	43,43,43	6.04	24 (55%)	58,60,60	4.32	30 (51%)
17	CLA	B	817	2	59,63,73	2.13	18 (30%)	71,101,113	3.09	28 (39%)
17	CLA	A	828	1	69,73,73	1.83	17 (24%)	83,113,113	2.83	27 (32%)
17	CLA	B	823	2	47,51,73	2.37	20 (42%)	56,86,113	3.25	25 (44%)
17	CLA	5	305	14	69,73,73	2.14	20 (28%)	83,113,113	3.07	37 (44%)
20	BCR	A	844	-	41,41,41	1.59	9 (21%)	56,56,56	1.42	8 (14%)
20	BCR	B	846	-	41,41,41	1.82	7 (17%)	56,56,56	1.70	10 (17%)
17	CLA	5	314	-	47,52,73	2.44	20 (42%)	58,87,113	3.17	27 (46%)
25	5X6	F	205	-	43,43,43	5.20	25 (58%)	58,60,60	5.49	33 (56%)
22	LMT	F	201	-	36,36,36	0.49	0	47,47,47	0.55	0
19	LHG	A	842	17	39,39,48	0.28	0	42,45,54	0.37	0
17	CLA	B	828	2	69,73,73	1.82	20 (28%)	83,113,113	2.82	31 (37%)
17	CLA	B	818	2	63,67,73	1.98	20 (31%)	75,105,113	2.99	30 (40%)
17	CLA	B	809	2	69,73,73	1.83	19 (27%)	83,113,113	2.87	32 (38%)
25	5X6	1	315	-	43,43,43	6.05	23 (53%)	58,60,60	4.73	31 (53%)
17	CLA	5	303	14	69,73,73	2.09	20 (28%)	83,113,113	2.84	32 (38%)
17	CLA	B	819	2	64,68,73	1.94	19 (29%)	77,107,113	3.05	31 (40%)
22	LMT	L	207	-	36,36,36	0.44	0	47,47,47	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	5X6	2	321	-	43,43,43	5.96	23 (53%)	58,60,60	4.85	30 (51%)
17	CLA	A	825	1	69,73,73	1.89	20 (28%)	83,113,113	2.84	30 (36%)
17	CLA	A	835	1	55,59,73	2.17	21 (38%)	66,96,113	2.96	27 (40%)
17	CLA	1	306	13	59,63,73	2.22	21 (35%)	71,101,113	2.80	32 (45%)
17	CLA	3	311	15	56,60,73	2.33	19 (33%)	67,97,113	3.17	27 (40%)
17	CLA	B	834	26	69,73,73	1.95	17 (24%)	83,113,113	2.78	31 (37%)
22	LMT	A	848	-	36,36,36	0.50	0	47,47,47	1.09	4 (8%)
17	CLA	A	805	1	54,58,73	2.18	19 (35%)	65,95,113	3.15	28 (43%)
17	CLA	A	822	1	59,63,73	2.07	18 (30%)	71,101,113	3.11	23 (32%)
17	CLA	B	832	2	69,73,73	1.96	20 (28%)	83,113,113	2.70	27 (32%)
17	CLA	B	835	26	49,53,73	2.35	18 (36%)	59,89,113	3.13	29 (49%)
25	5X6	5	317	-	43,43,43	6.12	24 (55%)	58,60,60	4.60	32 (55%)
25	5X6	4	312	-	43,43,43	6.03	23 (53%)	58,60,60	4.49	28 (48%)
17	CLA	B	810	2	69,73,73	1.92	17 (24%)	83,113,113	2.63	28 (33%)
20	BCR	L	205	-	41,41,41	1.68	8 (19%)	56,56,56	1.31	6 (10%)
17	CLA	F	203	26	49,53,73	2.28	20 (40%)	59,89,113	3.03	25 (42%)
25	5X6	5	316	-	43,43,43	5.70	24 (55%)	58,60,60	4.64	27 (46%)
17	CLA	4	304	13	63,67,73	2.21	19 (30%)	75,105,113	2.98	32 (42%)
17	CLA	A	814	26	49,53,73	2.39	20 (40%)	59,89,113	3.16	25 (42%)
17	CLA	B	821	2	49,53,73	2.34	20 (40%)	59,89,113	3.21	28 (47%)
17	CLA	4	311	-	49,53,73	2.49	21 (42%)	59,89,113	3.26	26 (44%)
25	5X6	5	315	-	43,43,43	5.93	24 (55%)	58,60,60	4.76	31 (53%)
25	5X6	2	318	-	43,43,43	5.90	24 (55%)	58,60,60	4.38	29 (50%)
20	BCR	B	848	-	41,41,41	1.61	8 (19%)	56,56,56	1.52	9 (16%)
17	CLA	B	820	26	69,73,73	2.03	19 (27%)	83,113,113	2.64	28 (33%)
20	BCR	M	101	-	41,41,41	1.87	6 (14%)	56,56,56	1.63	11 (19%)
25	5X6	2	320	-	43,43,43	6.03	25 (58%)	58,60,60	4.30	32 (55%)
20	BCR	A	857	-	41,41,41	1.58	10 (24%)	56,56,56	1.43	7 (12%)
17	CLA	A	831	1	69,73,73	1.92	19 (27%)	83,113,113	2.75	29 (34%)
20	BCR	A	846	-	41,41,41	1.57	10 (24%)	56,56,56	1.32	8 (14%)
17	CLA	O	205	-	49,53,73	2.51	21 (42%)	59,89,113	3.20	28 (47%)
17	CLA	O	203	-	45,49,73	2.53	20 (44%)	54,84,113	3.35	28 (51%)
25	5X6	1	313	-	43,43,43	6.02	24 (55%)	58,60,60	4.63	33 (56%)
24	DGD	B	849	-	67,67,67	0.88	2 (2%)	81,81,81	0.88	4 (4%)
17	CLA	1	303	13	59,63,73	2.26	18 (30%)	71,101,113	2.99	28 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	A	836	1	60,64,73	2.09	21 (35%)	72,102,113	2.92	28 (38%)
17	CLA	3	305	15	67,71,73	2.13	19 (28%)	80,110,113	2.87	30 (37%)
17	CLA	A	818	1	69,73,73	1.98	20 (28%)	83,113,113	2.79	33 (39%)
17	CLA	2	312	-	45,49,73	2.52	20 (44%)	54,84,113	3.40	28 (51%)
25	5X6	4	313	-	43,43,43	6.17	24 (55%)	58,60,60	4.05	31 (53%)
17	CLA	A	827	1	69,73,73	1.87	18 (26%)	83,113,113	2.74	26 (31%)
17	CLA	1	302	13	63,67,73	2.11	19 (30%)	75,105,113	2.76	28 (37%)
17	CLA	1	304	13	49,53,73	2.48	20 (40%)	59,89,113	3.30	27 (45%)
17	CLA	2	304	14	49,53,73	2.45	21 (42%)	59,89,113	3.25	28 (47%)
17	CLA	A	815	1	66,70,73	1.98	19 (28%)	79,109,113	2.79	27 (34%)
17	CLA	3	314	-	50,54,73	2.46	20 (40%)	60,90,113	3.19	29 (48%)
20	BCR	K	104	-	41,41,41	1.78	8 (19%)	56,56,56	1.66	12 (21%)
17	CLA	L	204	26	54,58,73	2.36	19 (35%)	65,95,113	3.00	29 (44%)
17	CLA	A	853	26	69,73,73	1.82	20 (28%)	83,113,113	2.86	30 (36%)
17	CLA	3	310	15	49,53,73	2.42	19 (38%)	59,89,113	3.24	28 (47%)
17	CLA	2	305	14	69,73,73	2.09	19 (27%)	83,113,113	2.83	30 (36%)
17	CLA	B	836	2	64,68,73	1.95	19 (29%)	77,107,113	2.82	29 (37%)
17	CLA	B	816	2	69,73,73	1.97	19 (27%)	83,113,113	2.75	28 (33%)
19	LHG	J	102	-	48,48,48	0.27	0	51,54,54	0.36	0
17	CLA	A	832	1	69,73,73	1.89	19 (27%)	83,113,113	2.78	30 (36%)
17	CLA	A	834	1	69,73,73	2.00	21 (30%)	83,113,113	2.73	31 (37%)
25	5X6	3	317	-	43,43,43	6.00	23 (53%)	58,60,60	4.32	28 (48%)
21	SF4	C	101	3	0,12,12	-	-	-		
17	CLA	B	815	2	69,73,73	1.94	20 (28%)	83,113,113	2.74	26 (31%)
17	CLA	5	307	14	49,53,73	2.32	21 (42%)	59,89,113	3.31	27 (45%)
17	CLA	B	840	2	69,73,73	1.82	19 (27%)	83,113,113	2.87	29 (34%)
25	5X6	5	318	-	43,43,43	5.97	24 (55%)	58,60,60	4.77	34 (58%)
17	CLA	A	811	1	69,73,73	1.88	20 (28%)	83,113,113	2.72	29 (34%)
17	CLA	A	839	26	69,73,73	1.93	20 (28%)	83,113,113	2.80	27 (32%)
17	CLA	5	308	14	69,73,73	2.09	21 (30%)	83,113,113	2.79	31 (37%)
17	CLA	5	302	14	49,53,73	2.51	21 (42%)	59,89,113	3.19	25 (42%)
25	5X6	2	317	-	43,43,43	6.11	24 (55%)	58,60,60	4.29	30 (51%)
17	CLA	B	807	2	69,73,73	1.85	20 (28%)	83,113,113	2.74	30 (36%)
17	CLA	A	802	17,1	59,63,73	2.06	16 (27%)	71,101,113	2.97	29 (40%)
17	CLA	B	805	2	69,73,73	1.91	20 (28%)	83,113,113	4.12	38 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	A	813	1	46,50,73	2.33	19 (41%)	55,85,113	3.31	27 (49%)
17	CLA	B	825	26	69,73,73	1.88	21 (30%)	83,113,113	2.70	28 (33%)
19	LHG	A	841	-	48,48,48	0.31	0	51,54,54	0.36	0
17	CLA	3	307	-	59,63,73	2.30	20 (33%)	71,101,113	3.09	30 (42%)
17	CLA	B	841	-	69,73,73	2.01	19 (27%)	83,113,113	2.80	28 (33%)
20	BCR	B	843	-	41,41,41	1.78	6 (14%)	56,56,56	1.41	9 (16%)
17	CLA	A	821	1	55,59,73	2.18	19 (34%)	66,96,113	3.14	29 (43%)
17	CLA	B	811	2	69,73,73	1.91	19 (27%)	83,113,113	2.69	28 (33%)
17	CLA	B	839	26	69,73,73	1.90	19 (27%)	83,113,113	2.78	23 (27%)
17	CLA	1	311	13	49,53,73	2.50	21 (42%)	59,89,113	3.26	28 (47%)
17	CLA	B	824	2	59,63,73	2.17	18 (30%)	71,101,113	3.17	31 (43%)
17	CLA	1	310	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
17	CLA	2	311	14	59,63,73	2.27	19 (32%)	71,101,113	3.14	29 (40%)
17	CLA	B	802	26	69,73,73	1.78	17 (24%)	83,113,113	2.96	34 (40%)
17	CLA	B	813	2	59,63,73	2.15	21 (35%)	71,101,113	3.00	31 (43%)
17	CLA	2	307	14	59,63,73	2.23	20 (33%)	71,101,113	3.18	32 (45%)
17	CLA	L	202	10	61,65,73	2.16	21 (34%)	73,103,113	2.90	29 (39%)
17	CLA	2	306	14	49,53,73	2.41	20 (40%)	59,89,113	3.16	27 (45%)
25	5X6	3	316	-	43,43,43	6.07	24 (55%)	58,60,60	4.52	30 (51%)
17	CLA	A	837	1	69,73,73	1.86	17 (24%)	83,113,113	2.96	26 (31%)
17	CLA	1	308	-	45,49,73	2.51	19 (42%)	54,84,113	3.32	27 (50%)
17	CLA	F	204	6	45,49,73	2.45	19 (42%)	54,84,113	3.40	28 (51%)
17	CLA	4	303	13	52,56,73	2.39	20 (38%)	62,92,113	3.13	28 (45%)
22	LMT	B	852	-	36,36,36	0.48	0	47,47,47	0.54	0
17	CLA	A	852	-	69,73,73	1.79	20 (28%)	83,113,113	2.57	31 (37%)
17	CLA	A	804	1	69,73,73	1.91	17 (24%)	83,113,113	2.75	29 (34%)
17	CLA	A	859	19	50,54,73	2.32	20 (40%)	60,90,113	3.25	26 (43%)
17	CLA	4	310	-	49,53,73	2.51	21 (42%)	59,89,113	3.18	28 (47%)
18	PQN	A	840	-	34,34,34	1.51	2 (5%)	42,45,45	1.03	2 (4%)
17	CLA	A	820	1	69,73,73	1.97	19 (27%)	83,113,113	2.84	31 (37%)
17	CLA	2	308	14	49,53,73	2.50	21 (42%)	59,89,113	3.16	27 (45%)
17	CLA	3	306	15	49,53,73	2.43	20 (40%)	59,89,113	3.19	30 (50%)
25	5X6	5	301	-	43,43,43	6.07	24 (55%)	58,60,60	4.27	28 (48%)
17	CLA	B	827	2	69,73,73	1.85	21 (30%)	83,113,113	2.78	30 (36%)
17	CLA	5	312	14	49,53,73	2.46	20 (40%)	59,89,113	3.18	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	B	814	2	69,73,73	1.90	19 (27%)	83,113,113	2.72	27 (32%)
17	CLA	B	808	2	69,73,73	1.92	17 (24%)	83,113,113	2.91	26 (31%)
17	CLA	1	307	13	64,68,73	2.16	19 (29%)	77,107,113	2.94	29 (37%)
17	CLA	A	808	1	59,63,73	2.11	18 (30%)	71,101,113	3.00	32 (45%)
17	CLA	A	806	1	69,73,73	1.82	17 (24%)	83,113,113	2.85	29 (34%)
17	CLA	A	816	1	69,73,73	1.88	19 (27%)	83,113,113	2.68	27 (32%)
17	CLA	B	831	2	69,73,73	1.93	20 (28%)	83,113,113	2.75	33 (39%)
17	CLA	B	830	2	69,73,73	1.82	18 (26%)	83,113,113	2.94	29 (34%)
17	CLA	2	309	14	49,53,73	2.41	20 (40%)	59,89,113	3.23	28 (47%)
17	CLA	3	312	-	45,49,73	2.54	20 (44%)	54,84,113	3.37	25 (46%)
17	CLA	5	306	14	49,53,73	2.46	21 (42%)	59,89,113	3.22	27 (45%)
17	CLA	4	308	13	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
17	CLA	A	807	1	69,73,73	1.90	20 (28%)	83,113,113	2.94	30 (36%)
17	CLA	A	838	1	69,73,73	1.79	19 (27%)	83,113,113	2.73	32 (38%)
17	CLA	A	854	1	69,73,73	1.86	19 (27%)	83,113,113	2.83	25 (30%)
17	CLA	A	817	1	69,73,73	1.90	17 (24%)	83,113,113	2.81	28 (33%)
17	CLA	4	306	13	49,53,73	2.52	21 (42%)	59,89,113	3.18	26 (44%)
20	BCR	A	843	-	41,41,41	1.65	9 (21%)	56,56,56	1.43	12 (21%)
17	CLA	5	309	14	69,73,73	2.05	19 (27%)	83,113,113	2.88	32 (38%)
17	CLA	B	812	2	69,73,73	2.00	19 (27%)	83,113,113	2.65	29 (34%)
17	CLA	3	315	-	55,59,73	2.36	21 (38%)	66,96,113	3.11	28 (42%)
17	CLA	A	833	1	69,73,73	1.91	17 (24%)	83,113,113	2.67	33 (39%)
17	CLA	A	809	17,1	69,73,73	1.86	21 (30%)	83,113,113	2.76	28 (33%)
25	5X6	2	319	-	43,43,43	6.21	24 (55%)	58,60,60	4.13	29 (50%)
17	CLA	K	102	26	59,63,73	2.21	21 (35%)	71,101,113	2.94	30 (42%)
17	CLA	A	819	26	69,73,73	1.94	17 (24%)	83,113,113	2.68	27 (32%)
17	CLA	2	315	14	49,53,73	2.47	20 (40%)	59,89,113	3.19	26 (44%)
17	CLA	A	829	1	54,58,73	2.17	19 (35%)	65,95,113	3.03	31 (47%)
17	CLA	2	316	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	27 (45%)
17	CLA	A	810	1	58,62,73	2.12	22 (37%)	69,99,113	3.05	28 (40%)
17	CLA	B	804	2	69,73,73	1.86	19 (27%)	83,113,113	2.73	27 (32%)
20	BCR	L	206	-	41,41,41	1.74	7 (17%)	56,56,56	1.48	11 (19%)
17	CLA	4	305	13	49,53,73	2.47	21 (42%)	59,89,113	3.17	27 (45%)
20	BCR	O	202	-	41,41,41	1.72	7 (17%)	56,56,56	1.44	10 (17%)
17	CLA	J	103	8	46,50,73	2.30	19 (41%)	55,85,113	3.22	27 (49%)

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
17	CLA	B	801	-	-	7/39/115/115	-
16	CL0	A	801	1	-	2/39/115/115	-
17	CLA	L	203	10	-	8/39/115/115	-
17	CLA	B	837	2	-	10/39/115/115	-
17	CLA	B	829	2	-	2/39/115/115	-
17	CLA	B	826	26	-	13/39/115/115	-
17	CLA	5	310	-	-	4/10/86/115	-
17	CLA	B	838	2	-	3/18/94/115	-
25	5X6	1	314	-	-	22/29/67/67	0/2/2/2
20	BCR	B	844	-	-	8/29/63/63	0/2/2/2
25	5X6	1	316	-	-	23/29/67/67	0/2/2/2
17	CLA	A	830	1	-	4/29/105/115	-
22	LMT	B	850	-	-	7/21/61/61	0/2/2/2
25	5X6	4	314	-	-	22/29/67/67	0/2/2/2
17	CLA	5	311	14	-	8/15/91/115	-
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	A	855	26	-	11/35/111/115	-
17	CLA	B	833	2	-	10/39/115/115	-
17	CLA	K	103	9	-	2/12/88/115	-
17	CLA	A	812	1	-	17/39/115/115	-
17	CLA	A	856	1	-	6/39/115/115	-
17	CLA	3	313	15	-	4/12/88/115	-
17	CLA	3	308	-	-	7/15/91/115	-
25	5X6	3	318	-	-	16/29/67/67	0/2/2/2
17	CLA	1	309	13	-	4/15/91/115	-
17	CLA	3	309	15	-	3/15/91/115	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2
17	CLA	5	304	14	-	7/39/115/115	-
17	CLA	4	309	-	-	3/10/86/115	-
17	CLA	B	822	2	-	3/17/93/115	-
17	CLA	2	313	14	-	5/12/88/115	-
17	CLA	A	824	26	-	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	A	845	-	-	6/29/63/63	0/2/2/2
17	CLA	1	301	13	-	7/15/91/115	-
20	BCR	B	847	-	-	7/29/63/63	0/2/2/2
22	LMT	3	301	-	-	10/21/61/61	0/2/2/2
17	CLA	B	857	2	-	4/31/107/115	-
21	SF4	A	847	2,1	-	-	0/6/5/5
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
20	BCR	J	104	-	-	6/29/63/63	0/2/2/2
22	LMT	B	851	-	-	8/21/61/61	0/2/2/2
17	CLA	A	803	1	-	9/39/115/115	-
17	CLA	5	313	14	-	6/15/91/115	-
17	CLA	A	823	26	-	8/39/115/115	-
17	CLA	2	314	14	-	5/15/91/115	-
20	BCR	I	101	-	-	6/29/63/63	0/2/2/2
20	BCR	B	845	-	-	11/29/63/63	0/2/2/2
20	BCR	B	803	-	-	6/29/63/63	0/2/2/2
17	CLA	O	204	12	-	7/21/97/115	-
25	5X6	J	105	-	-	19/29/67/67	0/2/2/2
17	CLA	B	806	2	-	11/39/115/115	-
17	CLA	2	310	14	-	1/15/91/115	-
17	CLA	4	307	13	-	9/15/91/115	-
17	CLA	1	305	13	-	7/15/91/115	-
17	CLA	A	826	1	-	8/39/115/115	-
25	5X6	1	312	-	-	15/29/67/67	0/2/2/2
17	CLA	B	817	2	-	8/27/103/115	-
17	CLA	A	828	1	-	8/39/115/115	-
17	CLA	B	823	2	-	3/13/89/115	-
17	CLA	5	305	14	-	12/39/115/115	-
20	BCR	A	844	-	-	8/29/63/63	0/2/2/2
20	BCR	B	846	-	-	6/29/63/63	0/2/2/2
17	CLA	5	314	-	-	3/12/88/115	-
25	5X6	F	205	-	-	16/29/67/67	0/2/2/2
22	LMT	F	201	-	-	13/21/61/61	0/2/2/2
19	LHG	A	842	17	-	19/44/44/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	828	2	-	11/39/115/115	-
17	CLA	B	818	2	-	11/32/108/115	-
17	CLA	B	809	2	-	8/39/115/115	-
25	5X6	1	315	-	-	25/29/67/67	0/2/2/2
17	CLA	5	303	14	-	12/39/115/115	-
17	CLA	B	819	2	-	4/33/109/115	-
22	LMT	L	207	-	-	8/21/61/61	0/2/2/2
25	5X6	2	321	-	-	25/29/67/67	0/2/2/2
17	CLA	A	825	1	-	8/39/115/115	-
17	CLA	A	835	1	-	3/23/99/115	-
17	CLA	1	306	13	-	5/27/103/115	-
17	CLA	3	311	15	-	3/24/100/115	-
17	CLA	B	834	26	-	9/39/115/115	-
22	LMT	A	848	-	-	7/21/61/61	0/2/2/2
17	CLA	A	805	1	-	2/21/97/115	-
17	CLA	A	822	1	-	7/27/103/115	-
17	CLA	B	832	2	-	11/39/115/115	-
17	CLA	B	835	26	-	6/15/91/115	-
25	5X6	5	317	-	-	22/29/67/67	0/2/2/2
25	5X6	4	312	-	-	22/29/67/67	0/2/2/2
17	CLA	B	810	2	-	12/39/115/115	-
20	BCR	L	205	-	-	4/29/63/63	0/2/2/2
17	CLA	F	203	26	-	0/15/91/115	-
25	5X6	5	316	-	-	18/29/67/67	0/2/2/2
17	CLA	4	304	13	-	8/32/108/115	-
17	CLA	A	814	26	-	3/15/91/115	-
17	CLA	B	821	2	-	4/15/91/115	-
17	CLA	4	311	-	-	6/15/91/115	-
25	5X6	5	315	-	-	20/29/67/67	0/2/2/2
25	5X6	2	318	-	-	18/29/67/67	0/2/2/2
20	BCR	B	848	-	-	4/29/63/63	0/2/2/2
17	CLA	B	820	26	-	10/39/115/115	-
20	BCR	M	101	-	-	11/29/63/63	0/2/2/2
25	5X6	2	320	-	-	22/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	A	857	-	-	4/29/63/63	0/2/2/2
17	CLA	A	831	1	-	10/39/115/115	-
20	BCR	A	846	-	-	4/29/63/63	0/2/2/2
17	CLA	O	205	-	-	7/15/91/115	-
17	CLA	O	203	-	-	4/10/86/115	-
25	5X6	1	313	-	-	17/29/67/67	0/2/2/2
24	DGD	B	849	-	-	23/55/95/95	0/2/2/2
17	CLA	1	303	13	-	9/27/103/115	-
17	CLA	A	836	1	-	5/29/105/115	-
17	CLA	3	305	15	-	10/37/113/115	-
17	CLA	A	818	1	-	9/39/115/115	-
17	CLA	2	312	-	-	5/10/86/115	-
25	5X6	4	313	-	-	22/29/67/67	0/2/2/2
17	CLA	A	827	1	-	6/39/115/115	-
17	CLA	1	302	13	-	6/32/108/115	-
17	CLA	1	304	13	-	7/15/91/115	-
17	CLA	2	304	14	-	6/15/91/115	-
17	CLA	A	815	1	-	10/36/112/115	-
17	CLA	3	314	-	-	8/17/93/115	-
20	BCR	K	104	-	-	7/29/63/63	0/2/2/2
17	CLA	L	204	26	-	7/21/97/115	-
17	CLA	A	853	26	-	3/39/115/115	-
17	CLA	3	310	15	-	6/15/91/115	-
17	CLA	2	305	14	-	7/39/115/115	-
17	CLA	B	836	2	-	7/33/109/115	-
17	CLA	B	816	2	-	14/39/115/115	-
19	LHG	J	102	-	-	24/53/53/53	-
17	CLA	A	832	1	-	7/39/115/115	-
17	CLA	A	834	1	-	14/39/115/115	-
25	5X6	3	317	-	-	23/29/67/67	0/2/2/2
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	B	815	2	-	14/39/115/115	-
17	CLA	5	307	14	-	4/15/91/115	-
17	CLA	B	840	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5X6	5	318	-	-	19/29/67/67	0/2/2/2
17	CLA	A	811	1	-	7/39/115/115	-
17	CLA	A	839	26	-	9/39/115/115	-
17	CLA	5	308	14	-	12/39/115/115	-
17	CLA	5	302	14	-	8/15/91/115	-
25	5X6	2	317	-	-	22/29/67/67	0/2/2/2
17	CLA	B	807	2	-	11/39/115/115	-
17	CLA	A	802	17,1	-	9/27/103/115	-
17	CLA	B	805	2	-	14/39/115/115	-
17	CLA	A	813	1	-	5/12/88/115	-
17	CLA	B	825	26	-	7/39/115/115	-
19	LHG	A	841	-	-	18/53/53/53	-
17	CLA	3	307	-	-	4/27/103/115	-
17	CLA	B	841	-	-	5/39/115/115	-
20	BCR	B	843	-	-	1/29/63/63	0/2/2/2
17	CLA	A	821	1	-	5/23/99/115	-
17	CLA	B	811	2	-	11/39/115/115	-
17	CLA	B	839	26	-	10/39/115/115	-
17	CLA	1	311	13	-	8/15/91/115	-
17	CLA	B	824	2	-	6/27/103/115	-
17	CLA	1	310	-	-	5/15/91/115	-
17	CLA	2	311	14	-	10/27/103/115	-
17	CLA	B	802	26	-	15/39/115/115	-
17	CLA	B	813	2	-	5/27/103/115	-
17	CLA	2	307	14	-	12/27/103/115	-
17	CLA	L	202	10	-	13/30/106/115	-
17	CLA	2	306	14	-	4/15/91/115	-
25	5X6	3	316	-	-	21/29/67/67	0/2/2/2
17	CLA	A	837	1	-	9/39/115/115	-
17	CLA	1	308	-	-	6/10/86/115	-
17	CLA	F	204	6	-	5/10/86/115	-
17	CLA	4	303	13	-	9/19/95/115	-
22	LMT	B	852	-	-	12/21/61/61	0/2/2/2
17	CLA	A	852	-	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	804	1	-	17/39/115/115	-
17	CLA	A	859	19	-	10/17/93/115	-
17	CLA	4	310	-	-	4/15/91/115	-
18	PQN	A	840	-	-	4/23/43/43	0/2/2/2
17	CLA	A	820	1	-	10/39/115/115	-
17	CLA	2	308	14	-	4/15/91/115	-
17	CLA	3	306	15	-	5/15/91/115	-
25	5X6	5	301	-	-	20/29/67/67	0/2/2/2
17	CLA	B	827	2	-	7/39/115/115	-
17	CLA	5	312	14	-	5/15/91/115	-
17	CLA	B	814	2	-	8/39/115/115	-
17	CLA	B	808	2	-	7/39/115/115	-
17	CLA	1	307	13	-	7/33/109/115	-
17	CLA	A	808	1	-	7/27/103/115	-
17	CLA	A	806	1	-	10/39/115/115	-
17	CLA	A	816	1	-	7/39/115/115	-
17	CLA	B	831	2	-	13/39/115/115	-
17	CLA	B	830	2	-	9/39/115/115	-
17	CLA	2	309	14	-	7/15/91/115	-
17	CLA	3	312	-	-	2/10/86/115	-
17	CLA	5	306	14	-	7/15/91/115	-
17	CLA	4	308	13	-	4/15/91/115	-
17	CLA	A	807	1	-	12/39/115/115	-
17	CLA	A	838	1	-	5/39/115/115	-
17	CLA	A	854	1	-	6/39/115/115	-
17	CLA	A	817	1	-	6/39/115/115	-
17	CLA	4	306	13	-	6/15/91/115	-
20	BCR	A	843	-	-	10/29/63/63	0/2/2/2
17	CLA	5	309	14	-	11/39/115/115	-
17	CLA	B	812	2	-	14/39/115/115	-
17	CLA	3	315	-	-	11/23/99/115	-
17	CLA	A	833	1	-	7/39/115/115	-
17	CLA	A	809	17,1	-	6/39/115/115	-
25	5X6	2	319	-	-	20/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	K	102	26	-	7/27/103/115	-
17	CLA	A	819	26	-	7/39/115/115	-
17	CLA	2	315	14	-	0/15/91/115	-
17	CLA	A	829	1	-	7/21/97/115	-
17	CLA	2	316	-	-	6/15/91/115	-
17	CLA	A	810	1	-	10/26/102/115	-
17	CLA	B	804	2	-	7/39/115/115	-
20	BCR	L	206	-	-	5/29/63/63	0/2/2/2
17	CLA	4	305	13	-	8/15/91/115	-
20	BCR	O	202	-	-	2/29/63/63	0/2/2/2
17	CLA	J	103	8	-	5/12/88/115	-

All (3727) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	319	5X6	C18-C17	16.24	1.57	1.35
25	4	313	5X6	C18-C17	15.98	1.57	1.35
25	1	313	5X6	C18-C17	15.87	1.56	1.35
25	5	318	5X6	C18-C17	15.73	1.56	1.35
25	2	320	5X6	C18-C17	15.71	1.56	1.35
25	2	319	5X6	C14-C13	15.71	1.56	1.35
25	5	317	5X6	C14-C13	15.62	1.56	1.35
25	2	317	5X6	C18-C17	15.62	1.56	1.35
25	5	301	5X6	C18-C17	15.60	1.56	1.35
25	1	312	5X6	C18-C17	15.59	1.56	1.35
25	2	319	5X6	C21-C22	15.59	1.56	1.35
25	3	316	5X6	C18-C17	15.57	1.56	1.35
25	4	313	5X6	C25-C26	15.53	1.56	1.35
25	5	317	5X6	C18-C17	15.53	1.56	1.35
25	4	313	5X6	C21-C22	15.53	1.56	1.35
25	2	318	5X6	C21-C22	15.49	1.56	1.35
25	4	314	5X6	C18-C17	15.48	1.56	1.35
25	1	316	5X6	C18-C17	15.46	1.56	1.35
25	4	314	5X6	C21-C22	15.46	1.56	1.35
25	3	318	5X6	C18-C17	15.43	1.56	1.35
25	2	317	5X6	C21-C22	15.40	1.56	1.35
25	5	301	5X6	C14-C13	15.40	1.56	1.35
25	1	313	5X6	C21-C22	15.39	1.56	1.35
25	4	312	5X6	C14-C13	15.38	1.56	1.35
25	3	318	5X6	C21-C22	15.37	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	317	5X6	C21-C22	15.37	1.56	1.35
25	1	316	5X6	C14-C13	15.36	1.56	1.35
25	5	317	5X6	C21-C22	15.36	1.56	1.35
25	1	315	5X6	C18-C17	15.36	1.56	1.35
25	4	314	5X6	C14-C13	15.34	1.56	1.35
25	1	314	5X6	C18-C17	15.34	1.56	1.35
25	4	313	5X6	C14-C13	15.34	1.56	1.35
25	5	301	5X6	C21-C22	15.34	1.56	1.35
25	1	312	5X6	C14-C13	15.31	1.56	1.35
25	1	315	5X6	C21-C22	15.27	1.56	1.35
25	3	316	5X6	C21-C22	15.27	1.56	1.35
25	3	318	5X6	C14-C13	15.26	1.56	1.35
25	4	312	5X6	C21-C22	15.26	1.56	1.35
25	2	317	5X6	C14-C13	15.25	1.56	1.35
25	3	317	5X6	C18-C17	15.24	1.56	1.35
25	2	318	5X6	C18-C17	15.23	1.56	1.35
25	1	315	5X6	C14-C13	15.23	1.56	1.35
25	1	313	5X6	C14-C13	15.22	1.56	1.35
25	4	312	5X6	C18-C17	15.22	1.56	1.35
25	5	317	5X6	C25-C26	15.20	1.55	1.35
25	3	316	5X6	C14-C13	15.19	1.55	1.35
25	2	317	5X6	C25-C26	15.15	1.55	1.35
25	3	317	5X6	C14-C13	15.15	1.55	1.35
25	1	312	5X6	C21-C22	15.12	1.55	1.35
25	2	321	5X6	C21-C22	15.08	1.55	1.35
25	2	320	5X6	C21-C22	15.07	1.55	1.35
25	5	315	5X6	C18-C17	15.06	1.55	1.35
25	2	320	5X6	C25-C26	15.02	1.55	1.35
25	5	315	5X6	C25-C26	15.01	1.55	1.35
25	5	318	5X6	C14-C13	14.98	1.55	1.35
25	4	314	5X6	C25-C26	14.97	1.55	1.35
25	2	321	5X6	C14-C13	14.97	1.55	1.35
25	2	319	5X6	C25-C26	14.94	1.55	1.35
25	3	316	5X6	C25-C26	14.94	1.55	1.35
25	2	321	5X6	C18-C17	14.93	1.55	1.35
25	5	301	5X6	C25-C26	14.90	1.55	1.35
25	1	314	5X6	C25-C26	14.90	1.55	1.35
25	1	316	5X6	C21-C22	14.89	1.55	1.35
25	1	315	5X6	C25-C26	14.86	1.55	1.35
25	5	315	5X6	C14-C13	14.84	1.55	1.35
25	1	312	5X6	C25-C26	14.82	1.55	1.35
25	5	315	5X6	C21-C22	14.82	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	321	5X6	C25-C26	14.82	1.55	1.35
25	1	316	5X6	C25-C26	14.81	1.55	1.35
25	5	318	5X6	C21-C22	14.78	1.55	1.35
25	3	317	5X6	C25-C26	14.75	1.55	1.35
25	1	314	5X6	C21-C22	14.70	1.55	1.35
25	4	312	5X6	C25-C26	14.68	1.55	1.35
25	3	318	5X6	C25-C26	14.64	1.55	1.35
25	5	318	5X6	C25-C26	14.62	1.55	1.35
25	2	318	5X6	C14-C13	14.61	1.55	1.35
25	2	320	5X6	C14-C13	14.59	1.55	1.35
25	1	313	5X6	C25-C26	14.53	1.55	1.35
25	5	316	5X6	C18-C17	14.50	1.55	1.35
25	5	316	5X6	C21-C22	14.43	1.54	1.35
25	2	318	5X6	C25-C26	14.27	1.54	1.35
25	1	314	5X6	C14-C13	14.25	1.54	1.35
25	5	316	5X6	C14-C13	14.10	1.54	1.35
25	J	105	5X6	C14-C13	14.09	1.54	1.35
25	5	316	5X6	C25-C26	13.83	1.54	1.35
25	F	205	5X6	C21-C22	13.71	1.54	1.35
25	J	105	5X6	C21-C22	13.48	1.53	1.35
25	J	105	5X6	C18-C17	13.32	1.53	1.35
25	F	205	5X6	C18-C17	13.24	1.53	1.35
25	F	205	5X6	C14-C13	13.02	1.53	1.35
25	J	105	5X6	C25-C26	12.99	1.53	1.35
25	F	205	5X6	C25-C26	12.86	1.52	1.35
25	2	317	5X6	C24-C23	8.49	1.56	1.34
25	2	319	5X6	C15-C16	8.47	1.56	1.34
25	4	313	5X6	C24-C23	8.44	1.56	1.34
25	3	316	5X6	C24-C23	8.42	1.56	1.34
25	4	313	5X6	C30-C29	8.41	1.49	1.34
25	5	317	5X6	C24-C23	8.41	1.56	1.34
25	4	314	5X6	C24-C23	8.37	1.56	1.34
25	2	321	5X6	C24-C23	8.34	1.56	1.34
25	2	320	5X6	C24-C23	8.33	1.56	1.34
25	1	315	5X6	C24-C23	8.33	1.56	1.34
25	3	316	5X6	C15-C16	8.32	1.56	1.34
25	4	313	5X6	C15-C16	8.30	1.56	1.34
25	3	318	5X6	C24-C23	8.28	1.55	1.34
25	4	312	5X6	C24-C23	8.27	1.55	1.34
25	5	315	5X6	C24-C23	8.25	1.55	1.34
25	3	317	5X6	C24-C23	8.25	1.55	1.34
25	2	317	5X6	C15-C16	8.24	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	312	5X6	C15-C16	8.24	1.55	1.34
25	1	315	5X6	C15-C16	8.23	1.55	1.34
25	2	319	5X6	C24-C23	8.22	1.55	1.34
25	1	312	5X6	C24-C23	8.21	1.55	1.34
25	3	318	5X6	C30-C29	8.19	1.48	1.34
25	1	314	5X6	C24-C23	8.19	1.55	1.34
25	5	317	5X6	C15-C16	8.18	1.55	1.34
25	1	316	5X6	C15-C16	8.17	1.55	1.34
25	3	317	5X6	C15-C16	8.16	1.55	1.34
25	4	312	5X6	C30-C29	8.15	1.48	1.34
25	1	313	5X6	C24-C23	8.14	1.55	1.34
25	3	317	5X6	C30-C29	8.14	1.48	1.34
25	5	318	5X6	C24-C23	8.14	1.55	1.34
25	4	312	5X6	C15-C16	8.13	1.55	1.34
25	3	318	5X6	C15-C16	8.12	1.55	1.34
25	5	301	5X6	C24-C23	8.10	1.55	1.34
25	5	301	5X6	C15-C16	8.09	1.55	1.34
25	4	314	5X6	C15-C16	8.09	1.55	1.34
25	2	319	5X6	C20-C19	8.08	1.57	1.36
25	1	313	5X6	C15-C16	8.07	1.55	1.34
25	2	320	5X6	C02-C03	8.06	1.48	1.34
25	5	316	5X6	C30-C29	8.03	1.48	1.34
25	2	321	5X6	C15-C16	8.01	1.55	1.34
25	1	316	5X6	C30-C29	8.00	1.48	1.34
25	5	315	5X6	C15-C16	7.99	1.55	1.34
25	2	317	5X6	C20-C19	7.97	1.56	1.36
25	3	316	5X6	C30-C29	7.97	1.48	1.34
25	2	320	5X6	C15-C16	7.97	1.55	1.34
25	1	316	5X6	C24-C23	7.96	1.55	1.34
25	5	318	5X6	C15-C16	7.96	1.55	1.34
25	2	318	5X6	C15-C16	7.92	1.55	1.34
25	2	317	5X6	C30-C29	7.91	1.48	1.34
25	1	312	5X6	C30-C29	7.91	1.48	1.34
25	1	315	5X6	C30-C29	7.90	1.48	1.34
25	2	318	5X6	C24-C23	7.90	1.54	1.34
25	5	316	5X6	C24-C23	7.90	1.54	1.34
25	3	316	5X6	C20-C19	7.87	1.56	1.36
25	2	319	5X6	C02-C03	7.87	1.48	1.34
25	2	320	5X6	C30-C29	7.85	1.48	1.34
25	4	314	5X6	C30-C29	7.85	1.48	1.34
25	5	315	5X6	C30-C29	7.84	1.48	1.34
25	4	314	5X6	C20-C19	7.84	1.56	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	317	5X6	C30-C29	7.83	1.48	1.34
25	4	312	5X6	C20-C19	7.81	1.56	1.36
25	1	314	5X6	C15-C16	7.79	1.54	1.34
25	2	318	5X6	C30-C29	7.78	1.47	1.34
25	1	313	5X6	C30-C29	7.78	1.47	1.34
25	2	319	5X6	C30-C29	7.77	1.47	1.34
25	1	316	5X6	C20-C19	7.75	1.56	1.36
25	5	301	5X6	C20-C19	7.75	1.56	1.36
25	5	317	5X6	C20-C19	7.75	1.56	1.36
25	1	313	5X6	C20-C19	7.74	1.56	1.36
25	3	318	5X6	C20-C19	7.73	1.56	1.36
25	4	313	5X6	C20-C19	7.73	1.56	1.36
25	5	318	5X6	C30-C29	7.72	1.47	1.34
25	1	315	5X6	C20-C19	7.70	1.56	1.36
25	1	314	5X6	C30-C29	7.69	1.47	1.34
25	2	319	5X6	C27-C28	7.68	1.56	1.33
25	1	312	5X6	C20-C19	7.66	1.55	1.36
25	5	315	5X6	C20-C19	7.65	1.55	1.36
25	1	314	5X6	C27-C28	7.63	1.56	1.33
25	2	320	5X6	C20-C19	7.63	1.55	1.36
25	3	318	5X6	C27-C28	7.63	1.56	1.33
25	1	315	5X6	C27-C28	7.62	1.56	1.33
25	4	314	5X6	C27-C28	7.62	1.56	1.33
25	5	301	5X6	C30-C29	7.61	1.47	1.34
25	1	312	5X6	C27-C28	7.61	1.56	1.33
25	2	317	5X6	C27-C28	7.60	1.56	1.33
25	2	321	5X6	C30-C29	7.59	1.47	1.34
25	5	318	5X6	C20-C19	7.59	1.55	1.36
25	4	312	5X6	C12-C11	7.59	1.56	1.33
25	5	301	5X6	C02-C03	7.58	1.47	1.34
25	4	313	5X6	C27-C28	7.58	1.56	1.33
25	2	318	5X6	C02-C03	7.58	1.47	1.34
25	3	317	5X6	C20-C19	7.57	1.55	1.36
25	5	317	5X6	C27-C28	7.57	1.56	1.33
25	5	316	5X6	C15-C16	7.57	1.54	1.34
25	2	319	5X6	C12-C11	7.57	1.56	1.33
25	1	313	5X6	C12-C11	7.57	1.56	1.33
25	2	321	5X6	C27-C28	7.57	1.56	1.33
25	2	321	5X6	C20-C19	7.57	1.55	1.36
25	J	105	5X6	C24-C23	7.57	1.54	1.34
25	1	316	5X6	C27-C28	7.56	1.55	1.33
25	5	316	5X6	C02-C03	7.56	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	317	5X6	C02-C03	7.54	1.47	1.34
25	3	316	5X6	C02-C03	7.51	1.47	1.34
25	2	320	5X6	C27-C28	7.49	1.55	1.33
25	1	314	5X6	C20-C19	7.49	1.55	1.36
25	3	316	5X6	C27-C28	7.49	1.55	1.33
25	4	312	5X6	C27-C28	7.49	1.55	1.33
25	J	105	5X6	C30-C29	7.48	1.47	1.34
25	5	318	5X6	C02-C03	7.48	1.47	1.34
25	5	301	5X6	C12-C11	7.48	1.55	1.33
25	3	318	5X6	C02-C03	7.47	1.47	1.34
25	4	313	5X6	C02-C03	7.47	1.47	1.34
25	3	317	5X6	C02-C03	7.45	1.47	1.34
25	5	301	5X6	C27-C28	7.44	1.55	1.33
25	3	317	5X6	C27-C28	7.44	1.55	1.33
25	5	317	5X6	C12-C11	7.43	1.55	1.33
25	2	321	5X6	C12-C11	7.41	1.55	1.33
25	2	317	5X6	C02-C03	7.40	1.47	1.34
25	1	315	5X6	C02-C03	7.39	1.47	1.34
25	1	312	5X6	C02-C03	7.39	1.47	1.34
25	5	318	5X6	C27-C28	7.38	1.55	1.33
25	5	315	5X6	C27-C28	7.38	1.55	1.33
25	4	314	5X6	C02-C03	7.37	1.47	1.34
25	1	312	5X6	C12-C11	7.36	1.55	1.33
25	1	315	5X6	C12-C11	7.35	1.55	1.33
25	2	320	5X6	C12-C11	7.34	1.55	1.33
25	4	314	5X6	C12-C11	7.34	1.55	1.33
25	3	316	5X6	C12-C11	7.34	1.55	1.33
25	5	316	5X6	C20-C19	7.32	1.55	1.36
25	3	318	5X6	C12-C11	7.31	1.55	1.33
25	1	314	5X6	C02-C03	7.31	1.47	1.34
18	A	840	PQN	C3-C2	7.30	1.48	1.35
25	2	318	5X6	C20-C19	7.30	1.55	1.36
25	F	205	5X6	C02-C03	7.29	1.47	1.34
25	1	314	5X6	C12-C11	7.29	1.55	1.33
25	2	317	5X6	C12-C11	7.28	1.55	1.33
25	5	316	5X6	C27-C28	7.26	1.55	1.33
25	1	316	5X6	C02-C03	7.26	1.47	1.34
25	1	316	5X6	C12-C11	7.25	1.55	1.33
25	2	318	5X6	C27-C28	7.24	1.55	1.33
25	5	315	5X6	C02-C03	7.22	1.46	1.34
25	3	317	5X6	C12-C11	7.18	1.54	1.33
25	2	318	5X6	C12-C11	7.17	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	313	5X6	C12-C11	7.15	1.54	1.33
25	2	321	5X6	C02-C03	7.11	1.46	1.34
25	J	105	5X6	C27-C28	7.10	1.54	1.33
25	1	313	5X6	C02-C03	7.07	1.46	1.34
25	F	205	5X6	C15-C16	7.05	1.52	1.34
25	4	312	5X6	C02-C03	7.05	1.46	1.34
25	1	313	5X6	C27-C28	7.04	1.54	1.33
25	5	315	5X6	C12-C11	7.00	1.54	1.33
25	5	318	5X6	C12-C11	6.98	1.54	1.33
25	5	316	5X6	C12-C11	6.97	1.54	1.33
25	F	205	5X6	C24-C23	6.93	1.52	1.34
25	F	205	5X6	C27-C28	6.89	1.53	1.33
25	J	105	5X6	C15-C16	6.87	1.52	1.34
25	F	205	5X6	C20-C19	6.83	1.53	1.36
18	B	842	PQN	C3-C2	6.80	1.47	1.35
25	J	105	5X6	C20-C19	6.66	1.53	1.36
25	J	105	5X6	C12-C11	6.50	1.52	1.33
25	F	205	5X6	C30-C29	6.42	1.45	1.34
25	F	205	5X6	C12-C11	6.42	1.52	1.33
25	J	105	5X6	C02-C03	5.91	1.44	1.34
17	A	859	CLA	C3C-C2C	5.71	1.48	1.36
17	1	305	CLA	C3C-C2C	5.64	1.48	1.36
17	2	313	CLA	C3C-C2C	5.55	1.48	1.36
17	1	308	CLA	C3C-C2C	5.52	1.48	1.36
25	2	319	5X6	C27-C26	5.52	1.57	1.45
17	1	303	CLA	C3C-C2C	5.48	1.48	1.36
17	B	810	CLA	C1B-NB	-5.47	1.31	1.37
20	M	101	BCR	C10-C9	5.44	1.43	1.35
17	O	205	CLA	C3C-C2C	5.44	1.48	1.36
17	5	311	CLA	C3C-C2C	5.44	1.48	1.36
17	5	310	CLA	C1D-ND	5.44	1.44	1.37
17	A	833	CLA	C3C-C2C	5.43	1.48	1.36
17	1	310	CLA	C3C-C2C	5.43	1.48	1.36
17	O	204	CLA	C1D-ND	5.42	1.44	1.37
17	4	310	CLA	O2D-CGD	5.42	1.46	1.33
17	1	304	CLA	O2D-CGD	5.42	1.46	1.33
17	2	310	CLA	C3C-C2C	5.42	1.48	1.36
17	2	311	CLA	O2D-CGD	5.41	1.46	1.33
17	4	305	CLA	O2D-CGD	5.41	1.46	1.33
17	4	310	CLA	C3C-C2C	5.41	1.48	1.36
17	3	315	CLA	O2D-CGD	5.41	1.46	1.33
17	3	312	CLA	C1D-ND	5.41	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	302	CLA	C3C-C2C	5.40	1.48	1.36
17	O	205	CLA	C1D-ND	5.40	1.44	1.37
17	4	304	CLA	C3C-C2C	5.39	1.48	1.36
17	B	834	CLA	C3C-C2C	5.38	1.48	1.36
17	5	314	CLA	C1D-ND	5.38	1.44	1.37
17	2	304	CLA	O2D-CGD	5.38	1.46	1.33
17	2	308	CLA	C3C-C2C	5.37	1.48	1.36
17	3	311	CLA	CHC-C1C	5.37	1.49	1.38
17	3	313	CLA	C3C-C2C	5.37	1.48	1.36
17	5	303	CLA	O2D-CGD	5.37	1.46	1.33
17	3	307	CLA	O2D-CGD	5.37	1.46	1.33
17	3	309	CLA	O2D-CGD	5.37	1.46	1.33
17	B	823	CLA	C3C-C2C	5.36	1.48	1.36
17	2	305	CLA	CHC-C1C	5.36	1.49	1.38
17	O	203	CLA	C3C-C2C	5.36	1.48	1.36
17	O	203	CLA	C1D-ND	5.35	1.44	1.37
17	B	820	CLA	C3C-C2C	5.35	1.48	1.36
17	5	309	CLA	O2D-CGD	5.35	1.46	1.33
17	4	306	CLA	C3C-C2C	5.35	1.48	1.36
17	4	303	CLA	C3C-C2C	5.34	1.48	1.36
17	3	307	CLA	C1D-ND	5.34	1.44	1.37
17	4	305	CLA	C1D-ND	5.34	1.44	1.37
17	1	311	CLA	O2D-CGD	5.34	1.46	1.33
17	A	813	CLA	C3C-C2C	5.33	1.48	1.36
17	1	305	CLA	O2D-CGD	5.33	1.46	1.33
17	5	314	CLA	C3C-C2C	5.33	1.48	1.36
17	3	313	CLA	O2D-CGD	5.33	1.46	1.33
17	5	305	CLA	O2D-CGD	5.33	1.46	1.33
17	3	311	CLA	C3C-C2C	5.32	1.48	1.36
17	4	304	CLA	O2D-CGD	5.32	1.46	1.33
17	1	309	CLA	O2D-CGD	5.32	1.46	1.33
17	1	311	CLA	C3C-C2C	5.32	1.48	1.36
17	1	301	CLA	C3C-C2C	5.32	1.48	1.36
17	5	311	CLA	C1D-ND	5.32	1.44	1.37
17	3	313	CLA	C1D-ND	5.32	1.44	1.37
17	2	316	CLA	C1D-ND	5.31	1.44	1.37
17	A	827	CLA	C4B-NB	-5.31	1.31	1.37
17	K	103	CLA	O2D-CGD	5.31	1.46	1.33
17	1	310	CLA	C1D-ND	5.30	1.44	1.37
17	L	204	CLA	C3C-C2C	5.30	1.48	1.36
17	1	307	CLA	O2D-CGD	5.30	1.46	1.33
17	2	305	CLA	O2D-CGD	5.30	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	315	CLA	C3C-C2C	5.30	1.48	1.36
17	A	821	CLA	C3C-C2C	5.30	1.48	1.36
17	5	311	CLA	O2D-CGD	5.30	1.46	1.33
17	O	204	CLA	C3C-C2C	5.29	1.48	1.36
17	4	310	CLA	C1D-ND	5.29	1.44	1.37
17	2	306	CLA	O2D-CGD	5.29	1.46	1.33
17	4	308	CLA	O2D-CGD	5.29	1.46	1.33
17	4	309	CLA	C1D-ND	5.28	1.44	1.37
17	1	308	CLA	O2D-CGD	5.28	1.46	1.33
17	3	314	CLA	O2D-CGD	5.28	1.46	1.33
17	5	302	CLA	C1D-ND	5.28	1.44	1.37
17	3	306	CLA	O2D-CGD	5.28	1.46	1.33
17	B	812	CLA	O2D-CGD	5.28	1.46	1.33
17	5	306	CLA	O2D-CGD	5.28	1.46	1.33
17	1	311	CLA	C1D-ND	5.28	1.44	1.37
17	2	313	CLA	O2D-CGD	5.28	1.46	1.33
17	3	314	CLA	C1D-ND	5.27	1.44	1.37
17	4	311	CLA	O2D-CGD	5.27	1.46	1.33
17	4	306	CLA	O2D-CGD	5.27	1.46	1.33
17	5	302	CLA	O2D-CGD	5.27	1.46	1.33
17	3	307	CLA	C3C-C2C	5.27	1.47	1.36
17	3	312	CLA	O2D-CGD	5.26	1.46	1.33
17	1	304	CLA	CHC-C1C	5.26	1.49	1.38
17	4	309	CLA	O2D-CGD	5.26	1.46	1.33
17	O	203	CLA	O2D-CGD	5.26	1.46	1.33
17	5	305	CLA	CHC-C1C	5.26	1.49	1.38
17	L	202	CLA	C3C-C2C	5.26	1.47	1.36
17	2	312	CLA	C3C-C2C	5.26	1.47	1.36
17	3	306	CLA	C3C-C2C	5.26	1.47	1.36
17	3	310	CLA	C3C-C2C	5.25	1.47	1.36
17	3	312	CLA	C3C-C2C	5.25	1.47	1.36
25	2	317	5X6	C27-C26	5.25	1.57	1.45
17	A	823	CLA	C1B-NB	-5.25	1.31	1.37
17	2	315	CLA	O2D-CGD	5.25	1.46	1.33
17	4	304	CLA	CHC-C1C	5.25	1.49	1.38
17	2	311	CLA	C3C-C2C	5.25	1.47	1.36
17	1	309	CLA	C1D-ND	5.25	1.44	1.37
17	4	303	CLA	O2D-CGD	5.24	1.46	1.33
17	2	312	CLA	O2D-CGD	5.24	1.46	1.33
17	L	202	CLA	O2D-CGD	5.24	1.46	1.33
17	5	310	CLA	O2D-CGD	5.24	1.46	1.33
17	4	306	CLA	C1D-ND	5.24	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	314	CLA	C3C-C2C	5.24	1.47	1.36
17	2	309	CLA	O2D-CGD	5.24	1.46	1.33
17	4	309	CLA	C3C-C2C	5.23	1.47	1.36
17	5	312	CLA	O2D-CGD	5.23	1.46	1.33
17	2	314	CLA	O2D-CGD	5.23	1.46	1.33
17	5	310	CLA	C3C-C2C	5.23	1.47	1.36
17	3	309	CLA	C3C-C2C	5.23	1.47	1.36
17	4	311	CLA	C1D-ND	5.23	1.44	1.37
17	2	308	CLA	O2D-CGD	5.22	1.45	1.33
17	A	836	CLA	C3C-C2C	5.22	1.47	1.36
17	B	841	CLA	C3C-C2C	5.22	1.47	1.36
17	5	304	CLA	C3C-C2C	5.22	1.47	1.36
17	3	308	CLA	C1D-ND	5.22	1.44	1.37
17	2	316	CLA	O2D-CGD	5.22	1.45	1.33
17	5	307	CLA	O2D-CGD	5.21	1.45	1.33
17	2	309	CLA	C1D-ND	5.21	1.44	1.37
17	3	315	CLA	C1D-ND	5.21	1.44	1.37
17	4	308	CLA	C3C-C2C	5.21	1.47	1.36
17	A	829	CLA	O2D-CGD	5.21	1.45	1.33
17	4	305	CLA	C3C-C2C	5.21	1.47	1.36
17	A	819	CLA	C3C-C2C	5.21	1.47	1.36
17	B	835	CLA	O2D-CGD	5.21	1.45	1.33
17	O	205	CLA	O2D-CGD	5.20	1.45	1.33
17	2	310	CLA	CHC-C1C	5.20	1.49	1.38
17	2	314	CLA	C1D-ND	5.20	1.44	1.37
17	5	308	CLA	C3C-C2C	5.19	1.47	1.36
17	2	315	CLA	C3C-C2C	5.19	1.47	1.36
17	2	304	CLA	C3C-C2C	5.19	1.47	1.36
17	1	301	CLA	O2D-CGD	5.19	1.45	1.33
17	B	824	CLA	O2D-CGD	5.19	1.45	1.33
17	1	302	CLA	O2D-CGD	5.19	1.45	1.33
17	2	311	CLA	CHC-C1C	5.19	1.49	1.38
17	B	821	CLA	C3C-C2C	5.18	1.47	1.36
17	4	307	CLA	C3C-C2C	5.18	1.47	1.36
17	3	305	CLA	O2D-CGD	5.18	1.45	1.33
17	3	314	CLA	C3C-C2C	5.18	1.47	1.36
17	4	311	CLA	C3C-C2C	5.18	1.47	1.36
25	5	301	5X6	C27-C26	5.17	1.57	1.45
17	3	305	CLA	C3C-C2C	5.17	1.47	1.36
17	1	307	CLA	CHC-C1C	5.17	1.49	1.38
17	1	309	CLA	C3C-C2C	5.17	1.47	1.36
17	2	308	CLA	C1D-ND	5.16	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	813	CLA	O2D-CGD	5.16	1.45	1.33
17	5	306	CLA	C3C-C2C	5.16	1.47	1.36
17	A	802	CLA	C3C-C2C	5.16	1.47	1.36
25	5	317	5X6	C27-C26	5.16	1.57	1.45
17	3	309	CLA	C1D-ND	5.16	1.44	1.37
25	4	314	5X6	C27-C26	5.16	1.57	1.45
17	2	312	CLA	C1D-ND	5.15	1.44	1.37
17	1	303	CLA	C1D-ND	5.15	1.44	1.37
17	3	308	CLA	O2D-CGD	5.15	1.45	1.33
17	5	313	CLA	O2D-CGD	5.15	1.45	1.33
17	B	813	CLA	C3C-C2C	5.14	1.47	1.36
17	1	306	CLA	C3C-C2C	5.14	1.47	1.36
17	5	303	CLA	C3C-C2C	5.14	1.47	1.36
17	3	311	CLA	O2D-CGD	5.14	1.45	1.33
17	2	304	CLA	C1D-ND	5.14	1.44	1.37
17	5	305	CLA	C3C-C2C	5.14	1.47	1.36
25	3	317	5X6	C27-C26	5.14	1.57	1.45
17	J	103	CLA	O2D-CGD	5.14	1.45	1.33
17	1	310	CLA	O2D-CGD	5.13	1.45	1.33
25	1	316	5X6	C27-C26	5.13	1.57	1.45
17	A	855	CLA	C3C-C2C	5.13	1.47	1.36
17	5	312	CLA	C3C-C2C	5.13	1.47	1.36
25	1	314	5X6	C27-C26	5.13	1.57	1.45
25	2	320	5X6	C27-C26	5.13	1.57	1.45
17	2	316	CLA	C3C-C2C	5.12	1.47	1.36
17	1	302	CLA	C3C-C2C	5.12	1.47	1.36
17	A	810	CLA	O2D-CGD	5.12	1.45	1.33
17	2	313	CLA	C1D-ND	5.12	1.44	1.37
17	2	306	CLA	C3C-C2C	5.12	1.47	1.36
17	1	303	CLA	O2D-CGD	5.12	1.45	1.33
17	B	824	CLA	CHC-C1C	5.12	1.48	1.38
17	3	310	CLA	O2D-CGD	5.11	1.45	1.33
17	2	307	CLA	C3C-C2C	5.11	1.47	1.36
17	B	823	CLA	O2D-CGD	5.11	1.45	1.33
17	A	826	CLA	C4B-NB	-5.11	1.31	1.37
17	3	308	CLA	C3C-C2C	5.11	1.47	1.36
17	5	313	CLA	C3C-C2C	5.11	1.47	1.36
25	4	313	5X6	C27-C26	5.10	1.56	1.45
17	B	826	CLA	C3C-C2C	5.10	1.47	1.36
17	B	822	CLA	O2D-CGD	5.10	1.45	1.33
17	L	204	CLA	O2D-CGD	5.10	1.45	1.33
17	B	817	CLA	C3C-C2C	5.10	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	307	CLA	CHC-C1C	5.10	1.48	1.38
17	2	314	CLA	CHC-C1C	5.09	1.48	1.38
17	2	307	CLA	O2D-CGD	5.09	1.45	1.33
17	A	805	CLA	C3C-C2C	5.09	1.47	1.36
17	B	841	CLA	O2D-CGD	5.09	1.45	1.33
17	A	821	CLA	O2D-CGD	5.09	1.45	1.33
17	1	305	CLA	C1D-ND	5.09	1.44	1.37
17	A	814	CLA	O2D-CGD	5.09	1.45	1.33
17	A	815	CLA	O2D-CGD	5.09	1.45	1.33
17	3	305	CLA	CHC-C1C	5.09	1.48	1.38
17	5	309	CLA	C3C-C2C	5.08	1.47	1.36
16	A	801	CL0	C1B-NB	-5.08	1.31	1.37
17	F	204	CLA	O2D-CGD	5.07	1.45	1.33
17	4	308	CLA	C1D-ND	5.07	1.44	1.37
17	B	822	CLA	C3C-C2C	5.07	1.47	1.36
17	A	820	CLA	O2D-CGD	5.07	1.45	1.33
17	5	308	CLA	O2D-CGD	5.07	1.45	1.33
17	L	204	CLA	C1D-ND	5.07	1.44	1.37
17	B	831	CLA	C3C-C2C	5.07	1.47	1.36
17	4	308	CLA	CHC-C1C	5.06	1.48	1.38
17	1	303	CLA	CHC-C1C	5.06	1.48	1.38
17	B	812	CLA	C3C-C2C	5.06	1.47	1.36
20	K	104	BCR	C10-C9	5.06	1.42	1.35
17	B	811	CLA	C3C-C2C	5.06	1.47	1.36
25	3	318	5X6	C27-C26	5.06	1.56	1.45
17	2	305	CLA	C3C-C2C	5.05	1.47	1.36
17	2	315	CLA	C1D-ND	5.05	1.44	1.37
17	O	204	CLA	O2D-CGD	5.05	1.45	1.33
17	A	832	CLA	C3C-C2C	5.05	1.47	1.36
17	1	308	CLA	C1D-ND	5.05	1.44	1.37
17	B	808	CLA	C3C-C2C	5.05	1.47	1.36
17	5	306	CLA	C1D-ND	5.05	1.44	1.37
17	B	832	CLA	O2D-CGD	5.04	1.45	1.33
17	1	304	CLA	C3C-C2C	5.04	1.47	1.36
20	M	101	BCR	C14-C13	5.04	1.42	1.35
17	K	102	CLA	O2D-CGD	5.04	1.45	1.33
17	A	814	CLA	C3C-C2C	5.03	1.47	1.36
17	4	303	CLA	C1D-ND	5.03	1.44	1.37
17	3	305	CLA	C1D-ND	5.03	1.44	1.37
17	1	310	CLA	CHC-C1C	5.02	1.48	1.38
17	L	203	CLA	O2D-CGD	5.02	1.45	1.33
25	3	316	5X6	C27-C26	5.02	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	304	CLA	C1D-ND	5.01	1.43	1.37
17	B	835	CLA	C3C-C2C	5.01	1.47	1.36
17	2	310	CLA	C1D-ND	5.01	1.43	1.37
17	F	204	CLA	C3C-C2C	5.01	1.47	1.36
17	2	307	CLA	CHC-C1C	5.01	1.48	1.38
25	1	315	5X6	C27-C26	5.00	1.56	1.45
17	5	312	CLA	C1D-ND	5.00	1.43	1.37
17	K	102	CLA	C3C-C2C	4.99	1.47	1.36
17	A	854	CLA	O2D-CGD	4.99	1.45	1.33
17	K	102	CLA	C1D-ND	4.99	1.43	1.37
17	4	306	CLA	CHC-C1C	4.99	1.48	1.38
25	2	319	5X6	C12-C13	4.98	1.56	1.45
17	1	307	CLA	C3C-C2C	4.98	1.47	1.36
25	5	318	5X6	C27-C26	4.98	1.56	1.45
17	5	305	CLA	C1D-ND	4.98	1.43	1.37
17	B	816	CLA	C3C-C2C	4.97	1.47	1.36
17	2	313	CLA	CHC-C1C	4.97	1.48	1.38
17	A	803	CLA	C1B-NB	-4.97	1.31	1.37
17	B	821	CLA	O2D-CGD	4.97	1.45	1.33
17	B	827	CLA	C3C-C2C	4.97	1.47	1.36
17	B	813	CLA	O2D-CGD	4.96	1.45	1.33
17	A	808	CLA	O2D-CGD	4.96	1.45	1.33
17	A	859	CLA	O2D-CGD	4.96	1.45	1.33
17	A	808	CLA	C3C-C2C	4.96	1.47	1.36
17	B	824	CLA	C3C-C2C	4.96	1.47	1.36
17	5	305	CLA	O2A-CGA	4.96	1.47	1.33
17	A	829	CLA	C3C-C2C	4.96	1.47	1.36
17	4	304	CLA	C1D-ND	4.96	1.43	1.37
17	A	831	CLA	O2D-CGD	4.95	1.45	1.33
17	A	820	CLA	C3C-C2C	4.95	1.47	1.36
17	B	820	CLA	O2D-CGD	4.95	1.45	1.33
17	A	819	CLA	O2D-CGD	4.95	1.45	1.33
17	2	305	CLA	C1D-ND	4.95	1.43	1.37
17	A	817	CLA	C3C-C2C	4.94	1.47	1.36
17	3	311	CLA	C1D-ND	4.94	1.43	1.37
25	5	317	5X6	C12-C13	4.94	1.56	1.45
17	5	304	CLA	O2D-CGD	4.94	1.45	1.33
17	B	831	CLA	O2D-CGD	4.94	1.45	1.33
17	B	857	CLA	C3C-C2C	4.93	1.47	1.36
17	2	306	CLA	C1D-ND	4.93	1.43	1.37
25	1	312	5X6	C27-C26	4.92	1.56	1.45
25	4	312	5X6	C12-C13	4.92	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	310	CLA	O2D-CGD	4.92	1.45	1.33
17	A	804	CLA	C3C-C2C	4.92	1.47	1.36
17	B	807	CLA	C3C-C2C	4.91	1.47	1.36
17	3	309	CLA	CHC-C1C	4.91	1.48	1.38
17	5	308	CLA	CHC-C1C	4.91	1.48	1.38
17	B	817	CLA	O2D-CGD	4.91	1.45	1.33
17	1	306	CLA	O2D-CGD	4.91	1.45	1.33
17	O	204	CLA	CHC-C1C	4.90	1.48	1.38
17	5	312	CLA	CHC-C1C	4.90	1.48	1.38
17	5	314	CLA	CHC-C1C	4.90	1.48	1.38
17	B	813	CLA	C1D-ND	4.90	1.43	1.37
17	B	838	CLA	C3C-C2C	4.90	1.47	1.36
20	B	846	BCR	C21-C22	4.90	1.42	1.35
17	A	809	CLA	C3C-C2C	4.89	1.47	1.36
20	L	206	BCR	C10-C9	4.89	1.42	1.35
17	A	833	CLA	O2D-CGD	4.89	1.45	1.33
25	2	321	5X6	C12-C13	4.89	1.56	1.45
17	4	309	CLA	CHC-C1C	4.88	1.48	1.38
17	B	839	CLA	C1B-NB	-4.88	1.31	1.37
17	B	807	CLA	O2D-CGD	4.88	1.45	1.33
17	B	837	CLA	C3C-C2C	4.87	1.47	1.36
17	B	822	CLA	CHC-C1C	4.87	1.48	1.38
17	4	307	CLA	CHC-C1C	4.87	1.48	1.38
17	4	307	CLA	O2D-CGD	4.87	1.45	1.33
17	1	305	CLA	CHC-C1C	4.87	1.48	1.38
17	A	855	CLA	O2D-CGD	4.87	1.45	1.33
17	3	310	CLA	CHC-C1C	4.87	1.48	1.38
25	2	318	5X6	C27-C26	4.87	1.56	1.45
17	3	306	CLA	C1D-ND	4.86	1.43	1.37
17	A	815	CLA	C3C-C2C	4.86	1.47	1.36
17	5	310	CLA	CHC-C1C	4.86	1.48	1.38
17	A	834	CLA	C3C-C2C	4.86	1.47	1.36
17	A	812	CLA	C3C-C2C	4.86	1.47	1.36
17	A	839	CLA	O2D-CGD	4.86	1.45	1.33
17	B	832	CLA	C3C-C2C	4.86	1.47	1.36
17	2	311	CLA	C1D-ND	4.86	1.43	1.37
17	O	205	CLA	CHC-C1C	4.86	1.48	1.38
17	3	314	CLA	CHC-C1C	4.86	1.48	1.38
17	J	103	CLA	C3C-C2C	4.85	1.47	1.36
17	B	838	CLA	C4B-NB	-4.85	1.31	1.37
17	3	312	CLA	CHC-C1C	4.85	1.48	1.38
17	5	302	CLA	CHC-C1C	4.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	308	CLA	CHC-C1C	4.84	1.48	1.38
17	4	310	CLA	CHC-C1C	4.84	1.48	1.38
17	B	838	CLA	O2D-CGD	4.83	1.45	1.33
17	3	315	CLA	CHC-C1C	4.83	1.48	1.38
17	L	202	CLA	C1D-ND	4.83	1.43	1.37
17	A	828	CLA	C1B-NB	-4.83	1.31	1.37
17	2	316	CLA	CHC-C1C	4.83	1.48	1.38
17	2	309	CLA	C3C-C2C	4.83	1.47	1.36
17	A	838	CLA	C3C-C2C	4.83	1.47	1.36
17	B	811	CLA	O2D-CGD	4.83	1.45	1.33
25	5	315	5X6	C27-C26	4.82	1.56	1.45
17	1	307	CLA	C1D-ND	4.82	1.43	1.37
17	A	818	CLA	C3C-C2C	4.81	1.47	1.36
17	2	315	CLA	CHC-C1C	4.80	1.48	1.38
25	4	312	5X6	C27-C26	4.80	1.56	1.45
17	4	311	CLA	CHC-C1C	4.80	1.48	1.38
17	A	810	CLA	C3C-C2C	4.80	1.46	1.36
17	B	829	CLA	C3C-C2C	4.79	1.46	1.36
17	B	834	CLA	O2D-CGD	4.79	1.44	1.33
17	K	103	CLA	C3C-C2C	4.79	1.46	1.36
17	1	306	CLA	C1D-ND	4.79	1.43	1.37
17	A	807	CLA	C3C-C2C	4.79	1.46	1.36
25	4	313	5X6	C12-C13	4.79	1.56	1.45
17	3	307	CLA	O2A-CGA	4.79	1.47	1.33
17	B	818	CLA	O2D-CGD	4.78	1.44	1.33
17	B	808	CLA	O2D-CGD	4.78	1.44	1.33
17	4	305	CLA	CHC-C1C	4.78	1.48	1.38
17	A	822	CLA	O2D-CGD	4.78	1.44	1.33
17	A	803	CLA	O2D-CGD	4.78	1.44	1.33
17	B	828	CLA	C4B-NB	-4.78	1.31	1.37
17	3	310	CLA	C1D-ND	4.78	1.43	1.37
17	A	856	CLA	O2D-CGD	4.78	1.44	1.33
25	1	312	5X6	C12-C13	4.77	1.56	1.45
25	1	313	5X6	C12-C13	4.77	1.56	1.45
17	3	313	CLA	CHC-C1C	4.77	1.48	1.38
17	A	856	CLA	C3C-C2C	4.77	1.46	1.36
25	5	301	5X6	C12-C13	4.77	1.56	1.45
17	B	825	CLA	O2D-CGD	4.77	1.44	1.33
17	B	814	CLA	O2D-CGD	4.77	1.44	1.33
25	5	316	5X6	C27-C26	4.77	1.56	1.45
17	O	203	CLA	CHC-C1C	4.77	1.48	1.38
25	3	316	5X6	C12-C13	4.77	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	833	CLA	C3C-C2C	4.76	1.46	1.36
20	B	843	BCR	C10-C9	4.75	1.42	1.35
17	2	312	CLA	CHC-C1C	4.75	1.48	1.38
17	A	837	CLA	C3C-C2C	4.75	1.46	1.36
25	2	321	5X6	C27-C26	4.75	1.56	1.45
17	A	832	CLA	O2D-CGD	4.75	1.44	1.33
17	B	837	CLA	O2D-CGD	4.74	1.44	1.33
25	1	313	5X6	C27-C26	4.74	1.56	1.45
25	4	314	5X6	C12-C13	4.74	1.56	1.45
17	1	309	CLA	CHC-C1C	4.74	1.48	1.38
17	L	204	CLA	CHC-C1C	4.74	1.48	1.38
17	A	853	CLA	C3C-C2C	4.74	1.46	1.36
17	B	802	CLA	C3C-C2C	4.74	1.46	1.36
25	1	315	5X6	C12-C13	4.74	1.56	1.45
17	A	834	CLA	O2D-CGD	4.74	1.44	1.33
17	B	801	CLA	O2D-CGD	4.74	1.44	1.33
17	B	805	CLA	C3C-C2C	4.73	1.46	1.36
17	A	805	CLA	O2D-CGD	4.73	1.44	1.33
25	2	320	5X6	C12-C13	4.72	1.56	1.45
17	A	829	CLA	C1B-NB	-4.72	1.32	1.37
17	A	806	CLA	O2D-CGD	4.72	1.44	1.33
17	A	830	CLA	O2D-CGD	4.71	1.44	1.33
17	A	836	CLA	O2D-CGD	4.71	1.44	1.33
17	5	303	CLA	C1D-ND	4.71	1.43	1.37
17	A	830	CLA	C3C-C2C	4.71	1.46	1.36
17	B	805	CLA	O2D-CGD	4.71	1.44	1.33
17	A	818	CLA	O2D-CGD	4.71	1.44	1.33
17	A	812	CLA	C1B-NB	-4.71	1.32	1.37
17	B	804	CLA	C1B-NB	-4.71	1.32	1.37
17	A	810	CLA	O2A-CGA	4.71	1.47	1.33
17	A	804	CLA	O2A-CGA	4.70	1.47	1.33
17	A	852	CLA	O2D-CGD	4.70	1.44	1.33
17	A	824	CLA	C3C-C2C	4.70	1.46	1.36
25	2	318	5X6	C12-C13	4.70	1.56	1.45
17	4	307	CLA	C1D-ND	4.70	1.43	1.37
17	A	826	CLA	O2D-CGD	4.70	1.44	1.33
17	B	822	CLA	C1D-ND	4.69	1.43	1.37
17	B	827	CLA	O2D-CGD	4.69	1.44	1.33
17	B	815	CLA	C1B-NB	-4.69	1.32	1.37
25	5	316	5X6	C12-C13	4.69	1.56	1.45
25	1	314	5X6	C12-C13	4.69	1.56	1.45
25	3	318	5X6	C12-C13	4.69	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	304	CLA	C1D-ND	4.69	1.43	1.37
17	5	313	CLA	CHC-C1C	4.69	1.48	1.38
17	2	307	CLA	C1D-ND	4.69	1.43	1.37
17	B	840	CLA	O2D-CGD	4.68	1.44	1.33
17	5	303	CLA	CHC-C1C	4.68	1.48	1.38
17	B	801	CLA	C3C-C2C	4.68	1.46	1.36
17	L	203	CLA	C3C-C2C	4.68	1.46	1.36
17	B	814	CLA	C3C-C2C	4.68	1.46	1.36
17	A	814	CLA	O2A-CGA	4.68	1.46	1.30
17	F	204	CLA	C1D-ND	4.68	1.43	1.37
17	1	311	CLA	CHC-C1C	4.68	1.48	1.38
17	5	306	CLA	CHC-C1C	4.67	1.48	1.38
17	B	804	CLA	C3C-C2C	4.67	1.46	1.36
17	A	816	CLA	C3C-C2C	4.67	1.46	1.36
17	A	817	CLA	O2D-CGD	4.67	1.44	1.33
17	F	203	CLA	C3C-C2C	4.67	1.46	1.36
17	5	311	CLA	CHC-C1C	4.67	1.48	1.38
25	2	317	5X6	C12-C13	4.67	1.56	1.45
25	1	316	5X6	C12-C13	4.66	1.56	1.45
17	B	828	CLA	C3C-C2C	4.66	1.46	1.36
17	B	829	CLA	C4B-NB	-4.66	1.32	1.37
17	F	203	CLA	O2D-CGD	4.66	1.44	1.33
17	A	804	CLA	C4B-NB	-4.66	1.32	1.37
17	A	831	CLA	C3C-C2C	4.66	1.46	1.36
25	2	317	5X6	C23-C22	4.65	1.55	1.45
25	4	313	5X6	C23-C22	4.65	1.55	1.45
17	A	854	CLA	C3C-C2C	4.64	1.46	1.36
17	1	301	CLA	C1D-ND	4.64	1.43	1.37
25	2	319	5X6	C23-C22	4.64	1.55	1.45
17	B	829	CLA	C1B-NB	-4.64	1.32	1.37
17	5	309	CLA	C1D-ND	4.64	1.43	1.37
17	B	823	CLA	CHC-C1C	4.64	1.47	1.38
25	5	318	5X6	C33-C32	4.63	1.59	1.52
17	A	827	CLA	C3C-C2C	4.63	1.46	1.36
17	B	841	CLA	CHC-C1C	4.63	1.47	1.38
20	M	101	BCR	C21-C22	4.63	1.41	1.35
16	A	801	CL0	C3C-C2C	4.63	1.46	1.36
17	5	304	CLA	O2A-CGA	4.62	1.46	1.33
17	2	308	CLA	CHD-C1D	4.62	1.47	1.38
17	5	309	CLA	CHC-C1C	4.62	1.47	1.38
17	5	309	CLA	O2A-CGA	4.62	1.46	1.33
16	A	801	CL0	C4B-NB	-4.62	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	311	CLA	O2A-CGA	4.62	1.46	1.33
17	A	852	CLA	C1B-NB	-4.62	1.32	1.37
17	A	835	CLA	O2D-CGD	4.62	1.44	1.33
20	B	843	BCR	C21-C22	4.61	1.41	1.35
17	A	816	CLA	O2D-CGD	4.61	1.44	1.33
17	B	835	CLA	O2A-CGA	4.61	1.46	1.30
17	B	836	CLA	O2D-CGD	4.61	1.44	1.33
17	A	852	CLA	C3C-C2C	4.61	1.46	1.36
17	5	308	CLA	C1D-ND	4.61	1.43	1.37
20	M	101	BCR	C17-C18	4.60	1.41	1.35
17	B	820	CLA	C1D-ND	4.60	1.43	1.37
17	A	835	CLA	C3C-C2C	4.60	1.46	1.36
18	B	842	PQN	C10-C5	4.60	1.48	1.40
17	K	102	CLA	CHC-C1C	4.60	1.47	1.38
17	A	826	CLA	C3C-C2C	4.59	1.46	1.36
17	A	855	CLA	C1B-NB	-4.59	1.32	1.37
17	A	834	CLA	O2A-CGA	4.59	1.46	1.33
25	3	317	5X6	C12-C13	4.59	1.55	1.45
17	A	828	CLA	C3C-C2C	4.59	1.46	1.36
17	B	809	CLA	O2D-CGD	4.59	1.44	1.33
17	A	835	CLA	O2A-CGA	4.59	1.46	1.33
17	A	804	CLA	O2D-CGD	4.59	1.44	1.33
17	B	806	CLA	O2D-CGD	4.58	1.44	1.33
17	2	315	CLA	O2A-CGA	4.58	1.46	1.30
17	3	310	CLA	O2A-CGA	4.58	1.46	1.30
17	2	304	CLA	CHC-C1C	4.58	1.47	1.38
17	B	823	CLA	C1D-ND	4.58	1.43	1.37
20	B	846	BCR	C10-C9	4.57	1.41	1.35
25	2	321	5X6	C33-C32	4.57	1.58	1.52
17	2	306	CLA	O2A-CGA	4.57	1.46	1.30
17	5	303	CLA	O2A-CGA	4.57	1.46	1.33
17	1	306	CLA	CHC-C1C	4.57	1.47	1.38
17	3	311	CLA	O2A-CGA	4.57	1.46	1.33
17	B	817	CLA	O2A-CGA	4.56	1.46	1.33
17	B	817	CLA	C1D-ND	4.56	1.43	1.37
17	4	303	CLA	CHC-C1C	4.56	1.47	1.38
17	B	820	CLA	CHC-C1C	4.56	1.47	1.38
17	2	310	CLA	O2A-CGA	4.56	1.46	1.30
17	5	313	CLA	C1D-ND	4.56	1.43	1.37
17	A	811	CLA	C3C-C2C	4.56	1.46	1.36
17	4	307	CLA	O2A-CGA	4.55	1.46	1.30
17	5	313	CLA	O2A-CGA	4.55	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	307	CLA	O2A-CGA	4.55	1.46	1.30
17	3	306	CLA	CHC-C1C	4.55	1.47	1.38
17	3	306	CLA	O2A-CGA	4.55	1.46	1.30
17	3	308	CLA	CHC-C1C	4.55	1.47	1.38
17	1	305	CLA	O2A-CGA	4.55	1.46	1.30
17	3	309	CLA	O2A-CGA	4.55	1.46	1.30
20	B	848	BCR	C10-C9	4.55	1.41	1.35
17	A	812	CLA	O2A-CGA	4.54	1.46	1.33
17	A	802	CLA	O2D-CGD	4.54	1.44	1.33
20	B	846	BCR	C17-C18	4.54	1.41	1.35
17	B	841	CLA	C1D-ND	4.54	1.43	1.37
17	A	828	CLA	O2A-CGA	4.54	1.46	1.33
17	B	813	CLA	O2A-CGA	4.54	1.46	1.33
17	1	310	CLA	O2A-CGA	4.54	1.46	1.30
17	B	836	CLA	C3C-C2C	4.54	1.46	1.36
17	B	818	CLA	O2A-CGA	4.54	1.46	1.33
17	2	309	CLA	O2A-CGA	4.54	1.46	1.30
17	A	825	CLA	C3C-C2C	4.54	1.46	1.36
17	4	306	CLA	O2A-CGA	4.54	1.46	1.30
17	2	314	CLA	O2A-CGA	4.53	1.46	1.30
17	5	312	CLA	O2A-CGA	4.53	1.46	1.30
17	3	308	CLA	O2A-CGA	4.53	1.46	1.30
17	1	309	CLA	O2A-CGA	4.53	1.46	1.30
17	1	301	CLA	CHC-C1C	4.53	1.47	1.38
17	A	839	CLA	C1B-NB	-4.53	1.32	1.37
20	K	104	BCR	C14-C13	4.53	1.41	1.35
17	1	311	CLA	O2A-CGA	4.53	1.46	1.30
17	B	830	CLA	C3C-C2C	4.53	1.46	1.36
17	1	301	CLA	O2A-CGA	4.52	1.45	1.30
17	B	819	CLA	O2D-CGD	4.52	1.44	1.33
25	1	315	5X6	C16-C17	4.52	1.55	1.45
17	A	833	CLA	O2A-CGA	4.52	1.46	1.33
17	B	821	CLA	O2A-CGA	4.51	1.45	1.30
25	2	319	5X6	C16-C17	4.51	1.55	1.45
17	2	316	CLA	O2A-CGA	4.51	1.45	1.30
17	B	816	CLA	O2D-CGD	4.51	1.44	1.33
17	2	304	CLA	O2A-CGA	4.51	1.45	1.30
17	A	817	CLA	C4B-NB	-4.51	1.32	1.37
17	A	809	CLA	O2D-CGD	4.51	1.44	1.33
17	B	812	CLA	C1B-NB	-4.51	1.32	1.37
17	1	304	CLA	O2A-CGA	4.51	1.45	1.30
20	B	803	BCR	C10-C9	4.51	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	836	CLA	C4B-NB	-4.50	1.32	1.37
17	4	311	CLA	O2A-CGA	4.50	1.45	1.30
17	B	815	CLA	C3C-C2C	4.50	1.46	1.36
17	5	311	CLA	O2A-CGA	4.50	1.45	1.30
17	A	823	CLA	O2D-CGD	4.50	1.44	1.33
25	1	312	5X6	C16-C17	4.50	1.55	1.45
17	5	310	CLA	CHD-C1D	4.50	1.47	1.38
17	O	205	CLA	O2A-CGA	4.50	1.45	1.30
17	2	308	CLA	O2A-CGA	4.50	1.45	1.30
17	1	305	CLA	CHD-C1D	4.49	1.47	1.38
17	A	814	CLA	CHC-C1C	4.49	1.47	1.38
17	3	312	CLA	CHD-C1D	4.49	1.47	1.38
17	5	306	CLA	O2A-CGA	4.49	1.45	1.30
17	5	302	CLA	O2A-CGA	4.49	1.45	1.30
17	B	824	CLA	O2A-CGA	4.49	1.46	1.33
17	B	830	CLA	C1B-NB	-4.49	1.32	1.37
17	B	816	CLA	O2A-CGA	4.49	1.46	1.33
25	1	314	5X6	C33-C32	4.49	1.58	1.52
17	4	310	CLA	O2A-CGA	4.48	1.45	1.30
17	A	815	CLA	O2A-CGA	4.48	1.46	1.33
17	4	308	CLA	O2A-CGA	4.48	1.45	1.30
20	O	202	BCR	C10-C9	4.48	1.41	1.35
17	A	859	CLA	CHC-C1C	4.48	1.47	1.38
17	B	809	CLA	C3C-C2C	4.48	1.46	1.36
17	B	815	CLA	O2D-CGD	4.48	1.44	1.33
17	5	308	CLA	CHD-C1D	4.47	1.47	1.38
17	4	309	CLA	CHD-C1D	4.47	1.47	1.38
17	5	307	CLA	C3C-C2C	4.46	1.46	1.36
17	B	833	CLA	O2D-CGD	4.46	1.44	1.33
17	3	305	CLA	O2A-CGA	4.46	1.46	1.33
17	5	314	CLA	CHD-C1D	4.46	1.47	1.38
18	A	840	PQN	C10-C5	4.46	1.48	1.40
17	A	823	CLA	C3C-C2C	4.45	1.46	1.36
20	B	843	BCR	C17-C18	4.45	1.41	1.35
17	2	307	CLA	O2A-CGA	4.45	1.46	1.33
17	B	829	CLA	O2D-CGD	4.45	1.44	1.33
17	A	818	CLA	O2A-CGA	4.45	1.46	1.33
17	4	303	CLA	O2A-CGA	4.45	1.46	1.33
25	4	314	5X6	C33-C32	4.45	1.58	1.52
17	B	837	CLA	O2A-CGA	4.45	1.46	1.33
17	2	308	CLA	CHC-C1C	4.44	1.47	1.38
17	A	812	CLA	CHC-C1C	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	315	5X6	C12-C13	4.44	1.55	1.45
17	F	203	CLA	O2A-CGA	4.44	1.45	1.30
25	5	317	5X6	C23-C22	4.44	1.55	1.45
17	2	306	CLA	CHC-C1C	4.44	1.47	1.38
17	B	805	CLA	O2A-CGA	4.44	1.46	1.33
25	5	301	5X6	C23-C22	4.44	1.55	1.45
17	B	810	CLA	O2D-CGD	4.43	1.44	1.33
17	A	814	CLA	C1D-ND	4.43	1.43	1.37
17	A	822	CLA	C3C-C2C	4.43	1.46	1.36
17	2	310	CLA	CHD-C1D	4.43	1.47	1.38
17	O	205	CLA	CHD-C1D	4.43	1.47	1.38
25	2	321	5X6	C23-C22	4.43	1.55	1.45
17	B	839	CLA	C3C-C2C	4.42	1.46	1.36
25	2	320	5X6	C23-C22	4.42	1.55	1.45
17	A	821	CLA	CHC-C1C	4.42	1.47	1.38
25	3	316	5X6	C23-C22	4.42	1.55	1.45
17	A	821	CLA	O2A-CGA	4.42	1.46	1.33
17	B	819	CLA	C3C-C2C	4.42	1.46	1.36
17	O	203	CLA	CHD-C1D	4.42	1.47	1.38
25	3	316	5X6	C16-C17	4.42	1.55	1.45
17	4	310	CLA	CHD-C1D	4.41	1.47	1.38
17	2	316	CLA	CHD-C1D	4.41	1.47	1.38
25	5	301	5X6	C16-C17	4.41	1.55	1.45
17	A	803	CLA	C3C-C2C	4.41	1.46	1.36
17	L	203	CLA	O2A-CGA	4.41	1.46	1.33
17	4	311	CLA	CHD-C1D	4.41	1.46	1.38
17	A	824	CLA	O2D-CGD	4.41	1.44	1.33
17	1	310	CLA	CHD-C1D	4.41	1.46	1.38
17	3	314	CLA	CHD-C1D	4.40	1.46	1.38
17	5	306	CLA	CHD-C1D	4.40	1.46	1.38
25	4	314	5X6	C23-C22	4.40	1.55	1.45
17	B	857	CLA	O2D-CGD	4.40	1.43	1.33
17	L	202	CLA	O2A-CGA	4.40	1.46	1.33
25	1	313	5X6	C16-C17	4.40	1.55	1.45
17	B	806	CLA	C1B-NB	-4.40	1.32	1.37
17	B	818	CLA	C3C-C2C	4.40	1.46	1.36
17	K	103	CLA	C1D-ND	4.39	1.43	1.37
17	A	829	CLA	O2A-CGA	4.39	1.46	1.33
17	B	835	CLA	CHC-C1C	4.39	1.47	1.38
17	B	810	CLA	C3C-C2C	4.39	1.46	1.36
17	O	204	CLA	CHD-C1D	4.39	1.46	1.38
17	A	825	CLA	O2D-CGD	4.39	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	311	CLA	CHD-C1D	4.39	1.46	1.38
17	B	805	CLA	CHC-C1C	4.39	1.47	1.38
25	5	318	5X6	C12-C13	4.38	1.55	1.45
17	4	306	CLA	CHD-C1D	4.38	1.46	1.38
17	B	812	CLA	C4B-NB	-4.38	1.32	1.37
17	B	830	CLA	C4B-NB	-4.38	1.32	1.37
25	2	317	5X6	C16-C17	4.38	1.55	1.45
25	5	317	5X6	C16-C17	4.38	1.55	1.45
17	L	203	CLA	C1D-ND	4.38	1.43	1.37
17	3	315	CLA	O2A-CGA	4.38	1.46	1.33
17	B	821	CLA	CHC-C1C	4.38	1.47	1.38
17	1	304	CLA	CHC-C4B	4.37	1.49	1.39
17	B	836	CLA	C4B-NB	-4.37	1.32	1.37
20	L	206	BCR	C21-C22	4.37	1.41	1.35
17	3	313	CLA	CHD-C1D	4.37	1.46	1.38
17	A	805	CLA	O2A-CGA	4.37	1.46	1.33
17	A	807	CLA	O2D-CGD	4.37	1.43	1.33
17	A	805	CLA	C1B-NB	-4.37	1.32	1.37
17	B	834	CLA	O2A-CGA	4.37	1.46	1.33
17	5	307	CLA	C1D-ND	4.37	1.43	1.37
17	B	839	CLA	CHC-C1C	4.37	1.47	1.38
25	5	315	5X6	C23-C22	4.37	1.55	1.45
17	4	305	CLA	CHD-C1D	4.36	1.46	1.38
17	A	830	CLA	O2A-CGA	4.36	1.46	1.33
17	A	807	CLA	CHC-C1C	4.36	1.47	1.38
17	1	302	CLA	C1D-ND	4.36	1.43	1.37
17	5	302	CLA	CHD-C1D	4.36	1.46	1.38
20	B	843	BCR	C14-C13	4.36	1.41	1.35
17	B	837	CLA	C4B-NB	-4.35	1.32	1.37
17	2	315	CLA	CHD-C1D	4.35	1.46	1.38
17	3	315	CLA	CHD-C1D	4.35	1.46	1.38
17	5	310	CLA	CHD-C4C	4.35	1.49	1.39
17	A	820	CLA	O2A-CGA	4.35	1.46	1.33
17	A	822	CLA	O2A-CGA	4.35	1.46	1.33
17	A	832	CLA	C3D-C2D	4.35	1.51	1.39
25	3	318	5X6	C23-C22	4.35	1.55	1.45
17	5	314	CLA	O2A-CGA	4.34	1.46	1.33
17	A	819	CLA	O2A-CGA	4.34	1.46	1.33
17	B	839	CLA	O2D-CGD	4.34	1.43	1.33
17	4	306	CLA	CHD-C4C	4.34	1.49	1.39
17	1	305	CLA	CHD-C4C	4.34	1.49	1.39
17	B	825	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	204	CLA	O2A-CGA	4.33	1.46	1.33
17	B	817	CLA	CHC-C1C	4.33	1.47	1.38
17	A	819	CLA	C4B-NB	-4.33	1.32	1.37
17	4	305	CLA	O2A-CGA	4.33	1.45	1.30
25	J	105	5X6	C27-C26	4.33	1.55	1.45
17	2	312	CLA	CHD-C1D	4.33	1.46	1.38
25	5	318	5X6	C16-C17	4.33	1.55	1.45
17	1	306	CLA	CHD-C1D	4.33	1.46	1.38
17	A	837	CLA	CHC-C1C	4.33	1.47	1.38
17	3	307	CLA	CHD-C1D	4.33	1.46	1.38
17	B	804	CLA	O2D-CGD	4.33	1.43	1.33
17	5	308	CLA	O2A-CGA	4.33	1.46	1.33
17	A	820	CLA	CHC-C1C	4.32	1.47	1.38
17	B	840	CLA	C3C-C2C	4.32	1.45	1.36
25	5	318	5X6	C23-C22	4.32	1.55	1.45
17	A	815	CLA	C1D-ND	4.32	1.43	1.37
17	5	311	CLA	CHD-C1D	4.32	1.46	1.38
17	A	831	CLA	O2A-CGA	4.32	1.46	1.33
25	4	313	5X6	C16-C17	4.32	1.55	1.45
20	K	104	BCR	C21-C22	4.32	1.41	1.35
17	K	103	CLA	CHC-C1C	4.32	1.47	1.38
17	B	810	CLA	O2A-CGA	4.32	1.46	1.33
25	1	314	5X6	C23-C22	4.32	1.55	1.45
17	1	307	CLA	O2A-CGA	4.31	1.45	1.33
17	A	834	CLA	C1D-ND	4.31	1.43	1.37
17	A	813	CLA	CHC-C1C	4.31	1.47	1.38
25	4	312	5X6	C23-C22	4.31	1.55	1.45
17	A	826	CLA	O2A-CGA	4.31	1.45	1.33
17	B	828	CLA	O2A-CGA	4.31	1.45	1.33
25	4	312	5X6	C16-C17	4.30	1.55	1.45
17	5	313	CLA	CHD-C1D	4.30	1.46	1.38
17	2	309	CLA	CHD-C1D	4.30	1.46	1.38
17	B	815	CLA	O2A-CGA	4.30	1.45	1.33
17	1	307	CLA	CHC-C4B	4.30	1.49	1.39
17	B	830	CLA	O2A-CGA	4.30	1.45	1.33
17	5	302	CLA	CHD-C4C	4.30	1.49	1.39
17	A	808	CLA	O2A-CGA	4.30	1.45	1.33
17	3	308	CLA	CHD-C1D	4.30	1.46	1.38
17	L	202	CLA	CHC-C1C	4.30	1.47	1.38
17	5	304	CLA	CHC-C1C	4.30	1.47	1.38
25	2	317	5X6	C33-C32	4.29	1.58	1.52
17	L	204	CLA	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	315	5X6	C33-C32	4.29	1.58	1.52
25	2	319	5X6	C19-C18	4.29	1.56	1.43
25	1	315	5X6	C23-C22	4.29	1.55	1.45
17	2	314	CLA	CHD-C1D	4.29	1.46	1.38
17	B	806	CLA	C3C-C2C	4.29	1.45	1.36
17	A	834	CLA	CHD-C1D	4.29	1.46	1.38
17	2	308	CLA	CHD-C4C	4.29	1.49	1.39
17	1	303	CLA	O2A-CGA	4.28	1.45	1.33
17	5	312	CLA	CHD-C1D	4.28	1.46	1.38
17	B	816	CLA	CHC-C1C	4.28	1.47	1.38
17	1	302	CLA	CHC-C1C	4.28	1.47	1.38
17	4	309	CLA	CHD-C4C	4.28	1.49	1.39
17	B	826	CLA	O2D-CGD	4.27	1.43	1.33
17	1	301	CLA	CHD-C1D	4.27	1.46	1.38
17	B	837	CLA	CHC-C1C	4.27	1.47	1.38
17	2	305	CLA	O2A-CGA	4.27	1.45	1.33
17	A	833	CLA	CHC-C1C	4.27	1.47	1.38
17	B	809	CLA	C1B-NB	-4.26	1.32	1.37
17	K	102	CLA	O2A-CGA	4.26	1.45	1.33
17	L	204	CLA	CHD-C1D	4.26	1.46	1.38
17	F	204	CLA	CHC-C1C	4.26	1.47	1.38
17	5	305	CLA	CHD-C4C	4.26	1.49	1.39
25	4	314	5X6	C16-C17	4.26	1.55	1.45
17	A	838	CLA	O2D-CGD	4.26	1.43	1.33
17	2	310	CLA	CHC-C4B	4.26	1.49	1.39
20	B	846	BCR	C14-C13	4.26	1.41	1.35
17	B	828	CLA	C1B-NB	-4.25	1.32	1.37
17	B	838	CLA	O2A-CGA	4.25	1.45	1.33
17	4	311	CLA	CHD-C4C	4.25	1.48	1.39
17	2	304	CLA	CHD-C1D	4.25	1.46	1.38
17	4	303	CLA	CHD-C1D	4.25	1.46	1.38
17	1	306	CLA	O2A-CGA	4.25	1.45	1.33
17	A	807	CLA	C1B-NB	-4.25	1.32	1.37
17	A	822	CLA	C1B-NB	-4.25	1.32	1.37
17	B	834	CLA	CHC-C1C	4.25	1.47	1.38
17	1	309	CLA	CHD-C1D	4.25	1.46	1.38
17	O	205	CLA	CHD-C4C	4.25	1.48	1.39
17	3	312	CLA	CHD-C4C	4.24	1.48	1.39
17	B	808	CLA	C1B-NB	-4.24	1.32	1.37
17	A	828	CLA	O2D-CGD	4.24	1.43	1.33
17	B	820	CLA	CHD-C1D	4.24	1.46	1.38
17	B	831	CLA	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	854	CLA	C1B-NB	-4.24	1.32	1.37
17	B	811	CLA	C4B-NB	-4.24	1.32	1.37
17	2	309	CLA	CHC-C1C	4.24	1.47	1.38
17	B	802	CLA	O2A-CGA	4.24	1.45	1.33
17	B	827	CLA	C1B-NB	-4.24	1.32	1.37
25	3	317	5X6	C16-C17	4.24	1.55	1.45
17	2	316	CLA	CHD-C4C	4.23	1.48	1.39
17	B	831	CLA	C1B-NB	-4.23	1.32	1.37
17	A	822	CLA	CHC-C1C	4.23	1.47	1.38
17	O	203	CLA	CHD-C4C	4.23	1.48	1.39
17	B	832	CLA	O2A-CGA	4.23	1.45	1.33
17	A	818	CLA	C1D-ND	4.23	1.43	1.37
17	5	305	CLA	CHC-C4B	4.23	1.48	1.39
17	B	825	CLA	C1B-NB	-4.23	1.32	1.37
17	5	305	CLA	CHD-C1D	4.23	1.46	1.38
17	1	311	CLA	CHD-C4C	4.23	1.48	1.39
17	4	310	CLA	CHD-C4C	4.22	1.48	1.39
17	3	307	CLA	CHD-C4C	4.22	1.48	1.39
17	A	802	CLA	C1B-NB	-4.22	1.32	1.37
17	B	828	CLA	O2D-CGD	4.22	1.43	1.33
17	5	307	CLA	CHC-C1C	4.22	1.47	1.38
17	2	312	CLA	CHD-C4C	4.22	1.48	1.39
17	4	304	CLA	CHC-C4B	4.21	1.48	1.39
17	B	808	CLA	O2A-CGA	4.21	1.45	1.33
17	B	833	CLA	O2A-CGA	4.21	1.45	1.33
17	5	303	CLA	CHD-C4C	4.21	1.48	1.39
17	2	313	CLA	CHD-C1D	4.21	1.46	1.38
25	1	316	5X6	C23-C22	4.21	1.55	1.45
17	5	304	CLA	CHD-C1D	4.21	1.46	1.38
17	A	825	CLA	C1D-ND	4.21	1.43	1.37
17	A	824	CLA	C4B-NB	-4.21	1.32	1.37
17	B	811	CLA	O2A-CGA	4.21	1.45	1.33
25	2	321	5X6	C16-C17	4.21	1.55	1.45
17	4	307	CLA	CHD-C1D	4.21	1.46	1.38
17	A	802	CLA	CHC-C1C	4.20	1.47	1.38
17	A	834	CLA	CHC-C1C	4.20	1.47	1.38
17	A	856	CLA	O2A-CGA	4.20	1.45	1.33
17	1	310	CLA	CHD-C4C	4.20	1.48	1.39
25	2	320	5X6	C16-C17	4.20	1.55	1.45
17	2	304	CLA	CHD-C4C	4.20	1.48	1.39
17	A	839	CLA	C3C-C2C	4.20	1.45	1.36
17	L	203	CLA	CHC-C1C	4.20	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	305	CLA	CHD-C4C	4.20	1.48	1.39
24	B	849	DGD	O1G-C1A	4.19	1.45	1.33
17	A	829	CLA	CHC-C1C	4.19	1.47	1.38
17	A	859	CLA	C1B-NB	-4.19	1.32	1.37
17	2	305	CLA	CHC-C4B	4.19	1.48	1.39
17	3	310	CLA	CHD-C1D	4.19	1.46	1.38
17	A	837	CLA	O2A-CGA	4.19	1.45	1.33
17	2	307	CLA	CHD-C4C	4.19	1.48	1.39
17	A	839	CLA	O2A-CGA	4.19	1.45	1.33
17	A	827	CLA	O2D-CGD	4.19	1.43	1.33
17	3	309	CLA	CHD-C1D	4.19	1.46	1.38
25	3	318	5X6	C16-C17	4.19	1.54	1.45
17	5	314	CLA	CHD-C4C	4.19	1.48	1.39
17	2	313	CLA	CHD-C4C	4.19	1.48	1.39
25	1	316	5X6	C33-C32	4.19	1.58	1.52
17	B	826	CLA	CHC-C1C	4.18	1.47	1.38
17	B	839	CLA	C1D-ND	4.18	1.42	1.37
17	3	313	CLA	CHD-C4C	4.18	1.48	1.39
17	1	303	CLA	CHD-C1D	4.18	1.46	1.38
17	3	305	CLA	CHD-C4C	4.18	1.48	1.39
17	B	834	CLA	C1B-NB	-4.18	1.32	1.37
17	A	811	CLA	C1B-NB	-4.18	1.32	1.37
17	5	311	CLA	CHD-C4C	4.18	1.48	1.39
25	2	320	5X6	C33-C32	4.18	1.58	1.52
17	4	308	CLA	CHD-C1D	4.17	1.46	1.38
17	B	819	CLA	C1B-NB	-4.17	1.32	1.37
17	1	308	CLA	CHD-C4C	4.17	1.48	1.39
25	1	313	5X6	C23-C22	4.17	1.54	1.45
17	O	204	CLA	CHD-C4C	4.17	1.48	1.39
25	1	316	5X6	C16-C17	4.17	1.54	1.45
17	4	305	CLA	CHD-C4C	4.17	1.48	1.39
17	3	314	CLA	CHD-C4C	4.17	1.48	1.39
17	4	304	CLA	CHD-C4C	4.17	1.48	1.39
17	B	857	CLA	O2A-CGA	4.17	1.45	1.33
17	3	311	CLA	CHD-C4C	4.17	1.48	1.39
17	B	826	CLA	C4B-NB	-4.16	1.32	1.37
17	4	304	CLA	CHD-C1D	4.16	1.46	1.38
17	3	311	CLA	CHC-C4B	4.16	1.48	1.39
17	B	857	CLA	CHC-C1C	4.16	1.47	1.38
17	A	823	CLA	O2A-CGA	4.16	1.45	1.33
17	A	808	CLA	CHC-C1C	4.16	1.47	1.38
17	2	311	CLA	CHD-C4C	4.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	315	CLA	CHD-C4C	4.16	1.48	1.39
17	B	838	CLA	CHC-C1C	4.16	1.47	1.38
20	L	205	BCR	C14-C13	4.16	1.41	1.35
17	A	828	CLA	C4B-NB	-4.15	1.32	1.37
17	2	314	CLA	CHD-C4C	4.15	1.48	1.39
17	5	308	CLA	CHD-C4C	4.15	1.48	1.39
17	1	304	CLA	CHD-C1D	4.15	1.46	1.38
17	A	816	CLA	C1B-NB	-4.15	1.32	1.37
17	A	809	CLA	C1B-NB	-4.15	1.32	1.37
17	B	831	CLA	C1D-ND	4.15	1.42	1.37
17	3	305	CLA	CHC-C4B	4.14	1.48	1.39
17	B	819	CLA	C4B-NB	-4.14	1.32	1.37
17	F	204	CLA	CHD-C1D	4.14	1.46	1.38
17	B	820	CLA	O2A-CGA	4.14	1.45	1.33
17	B	839	CLA	OBD-CAD	4.14	1.29	1.22
17	F	204	CLA	CHD-C4C	4.14	1.48	1.39
17	B	824	CLA	CHC-C4B	4.14	1.48	1.39
17	B	832	CLA	C1B-NB	-4.14	1.32	1.37
17	1	303	CLA	CHC-C4B	4.13	1.48	1.39
17	A	859	CLA	C1D-ND	4.13	1.42	1.37
17	B	813	CLA	CHC-C1C	4.13	1.46	1.38
17	A	802	CLA	O2A-CGA	4.13	1.45	1.33
17	A	822	CLA	C1D-ND	4.13	1.42	1.37
17	A	812	CLA	O2D-CGD	4.13	1.43	1.33
17	1	302	CLA	O2A-CGA	4.13	1.45	1.33
17	A	837	CLA	O2D-CGD	4.13	1.43	1.33
20	L	206	BCR	C14-C13	4.13	1.41	1.35
17	A	854	CLA	C4B-NB	-4.13	1.32	1.37
17	A	855	CLA	O2A-CGA	4.13	1.45	1.33
17	3	305	CLA	CHD-C1D	4.13	1.46	1.38
17	B	804	CLA	C4B-NB	-4.13	1.32	1.37
17	5	303	CLA	CHD-C1D	4.13	1.46	1.38
17	2	310	CLA	CHD-C4C	4.13	1.48	1.39
17	B	823	CLA	CHD-C1D	4.12	1.46	1.38
17	A	819	CLA	CHC-C1C	4.12	1.46	1.38
17	F	203	CLA	C1D-ND	4.12	1.42	1.37
17	4	304	CLA	O2A-CGA	4.12	1.45	1.33
20	B	844	BCR	C10-C9	4.12	1.41	1.35
17	A	831	CLA	CHC-C1C	4.12	1.46	1.38
17	A	804	CLA	C1B-NB	-4.12	1.32	1.37
17	4	307	CLA	CHD-C4C	4.12	1.48	1.39
25	5	317	5X6	C24-C25	4.12	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	306	CLA	CHD-C4C	4.12	1.48	1.39
17	B	822	CLA	O2A-CGA	4.12	1.46	1.33
17	A	817	CLA	C1B-NB	-4.11	1.32	1.37
17	A	818	CLA	CHC-C1C	4.11	1.46	1.38
17	1	310	CLA	CHC-C4B	4.11	1.48	1.39
17	B	806	CLA	CHC-C1C	4.11	1.46	1.38
17	A	839	CLA	CHC-C1C	4.11	1.46	1.38
17	2	311	CLA	CHC-C4B	4.11	1.48	1.39
17	4	303	CLA	CHD-C4C	4.11	1.48	1.39
17	B	808	CLA	C1D-ND	4.11	1.42	1.37
17	B	857	CLA	C1B-NB	-4.11	1.32	1.37
17	2	315	CLA	CHD-C4C	4.11	1.48	1.39
17	B	825	CLA	C3C-C2C	4.11	1.45	1.36
25	2	319	5X6	C15-C14	4.10	1.56	1.43
17	A	817	CLA	CHC-C1C	4.10	1.46	1.38
17	A	811	CLA	CHC-C1C	4.10	1.46	1.38
17	B	819	CLA	CHC-C1C	4.10	1.46	1.38
17	2	314	CLA	CHC-C4B	4.10	1.48	1.39
17	1	309	CLA	CHD-C4C	4.10	1.48	1.39
17	B	821	CLA	C1D-ND	4.10	1.42	1.37
17	B	833	CLA	C1B-NB	-4.10	1.32	1.37
17	B	832	CLA	CHD-C1D	4.10	1.46	1.38
17	2	309	CLA	CHD-C4C	4.09	1.48	1.39
17	A	809	CLA	O2A-CGA	4.09	1.45	1.33
17	3	307	CLA	CHC-C4B	4.09	1.48	1.39
17	2	307	CLA	CHD-C1D	4.09	1.46	1.38
25	4	313	5X6	C19-C18	4.09	1.56	1.43
17	A	825	CLA	CHC-C1C	4.09	1.46	1.38
17	K	102	CLA	CHD-C1D	4.09	1.46	1.38
17	A	827	CLA	C1B-NB	-4.09	1.32	1.37
24	B	849	DGD	O2G-C1B	4.09	1.45	1.34
17	B	857	CLA	C4B-NB	-4.09	1.32	1.37
25	5	301	5X6	C19-C18	4.09	1.56	1.43
25	5	317	5X6	C33-C32	4.09	1.58	1.52
25	2	318	5X6	C16-C17	4.09	1.54	1.45
17	B	801	CLA	C4B-NB	-4.09	1.32	1.37
17	B	839	CLA	O2A-CGA	4.09	1.45	1.33
17	J	103	CLA	C1D-ND	4.09	1.42	1.37
17	3	306	CLA	CHD-C1D	4.09	1.46	1.38
17	4	308	CLA	CHC-C4B	4.08	1.48	1.39
17	A	819	CLA	C1D-ND	4.08	1.42	1.37
17	B	816	CLA	C4B-NB	-4.08	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	306	CLA	CHD-C4C	4.08	1.48	1.39
25	3	317	5X6	C23-C22	4.08	1.54	1.45
25	2	319	5X6	C20-C21	4.08	1.56	1.43
25	5	315	5X6	C16-C17	4.08	1.54	1.45
25	1	314	5X6	C16-C17	4.08	1.54	1.45
17	4	308	CLA	CHD-C4C	4.07	1.48	1.39
17	1	301	CLA	CHD-C4C	4.07	1.48	1.39
17	3	309	CLA	CHD-C4C	4.07	1.48	1.39
17	A	814	CLA	C1B-NB	-4.07	1.32	1.37
25	2	317	5X6	C24-C25	4.07	1.56	1.43
17	5	313	CLA	CHD-C4C	4.07	1.48	1.39
16	A	801	CL0	O2D-CGD	4.06	1.43	1.33
17	L	204	CLA	C1B-NB	-4.06	1.32	1.37
17	A	836	CLA	CHD-C1D	4.06	1.46	1.38
17	A	859	CLA	O2A-CGA	4.06	1.45	1.33
17	A	811	CLA	O2D-CGD	4.06	1.43	1.33
17	1	307	CLA	CHD-C4C	4.06	1.48	1.39
17	A	815	CLA	CHC-C1C	4.05	1.46	1.38
17	3	308	CLA	CHD-C4C	4.05	1.48	1.39
17	A	825	CLA	C1B-NB	-4.05	1.32	1.37
17	1	302	CLA	CHD-C1D	4.05	1.46	1.38
17	B	836	CLA	O2A-CGA	4.05	1.45	1.33
17	B	830	CLA	O2D-CGD	4.05	1.43	1.33
17	B	812	CLA	CHC-C1C	4.05	1.46	1.38
17	B	814	CLA	C1D-ND	4.05	1.42	1.37
17	B	832	CLA	C1D-ND	4.05	1.42	1.37
17	A	813	CLA	CHD-C1D	4.04	1.46	1.38
17	A	855	CLA	CHC-C1C	4.04	1.46	1.38
17	A	820	CLA	C4B-NB	-4.04	1.32	1.37
17	A	806	CLA	C1B-NB	-4.04	1.32	1.37
17	1	303	CLA	CHD-C4C	4.04	1.48	1.39
17	A	837	CLA	C1B-NB	-4.04	1.32	1.37
25	1	312	5X6	C23-C22	4.04	1.54	1.45
17	A	806	CLA	C4B-NB	-4.04	1.32	1.37
25	4	314	5X6	C19-C18	4.04	1.56	1.43
17	1	308	CLA	CHD-C1D	4.04	1.46	1.38
17	3	309	CLA	CHC-C4B	4.04	1.48	1.39
25	2	318	5X6	C33-C32	4.04	1.58	1.52
25	3	316	5X6	C19-C18	4.04	1.55	1.43
17	B	815	CLA	CHC-C1C	4.03	1.46	1.38
17	B	822	CLA	C3D-C2D	4.03	1.50	1.39
17	A	853	CLA	CHD-C1D	4.03	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	314	CLA	O2A-CGA	4.02	1.45	1.33
20	O	202	BCR	C14-C13	4.02	1.41	1.35
20	L	205	BCR	C10-C9	4.02	1.41	1.35
17	5	312	CLA	CHD-C4C	4.02	1.48	1.39
17	A	819	CLA	C1B-NB	-4.02	1.32	1.37
17	K	103	CLA	C1B-NB	-4.02	1.32	1.37
17	3	311	CLA	CHD-C1D	4.02	1.46	1.38
17	4	311	CLA	CHC-C4B	4.01	1.48	1.39
17	B	841	CLA	CHD-C4C	4.01	1.48	1.39
25	F	205	5X6	C27-C26	4.01	1.54	1.45
17	5	305	CLA	C3B-C4B	4.01	1.52	1.42
17	B	835	CLA	C1D-ND	4.01	1.42	1.37
17	B	812	CLA	CHD-C1D	4.00	1.46	1.38
25	2	320	5X6	C24-C25	4.00	1.55	1.43
17	5	304	CLA	CHD-C4C	4.00	1.48	1.39
17	B	819	CLA	O2A-CGA	4.00	1.45	1.33
17	B	810	CLA	C4B-NB	-4.00	1.32	1.37
17	B	838	CLA	C1B-NB	-4.00	1.32	1.37
17	B	808	CLA	C4B-NB	-3.99	1.32	1.37
17	3	306	CLA	CHD-C4C	3.99	1.48	1.39
17	2	305	CLA	CHD-C1D	3.99	1.46	1.38
17	A	808	CLA	C1B-NB	-3.99	1.32	1.37
17	B	840	CLA	C4B-NB	-3.99	1.32	1.37
17	B	822	CLA	CHC-C4B	3.99	1.48	1.39
17	2	306	CLA	CHD-C4C	3.99	1.48	1.39
17	1	304	CLA	CHD-C4C	3.98	1.48	1.39
17	B	820	CLA	CHD-C4C	3.98	1.48	1.39
17	5	302	CLA	CHC-C4B	3.98	1.48	1.39
17	A	820	CLA	C3D-C2D	3.98	1.50	1.39
17	F	203	CLA	CHC-C1C	3.98	1.46	1.38
17	A	812	CLA	OBD-CAD	3.98	1.29	1.22
17	A	838	CLA	O2A-CGA	3.98	1.45	1.33
17	2	306	CLA	CHD-C1D	3.98	1.46	1.38
17	A	836	CLA	C3D-C2D	3.98	1.50	1.39
17	L	202	CLA	CHD-C1D	3.98	1.46	1.38
20	L	201	BCR	C10-C9	3.98	1.41	1.35
17	5	312	CLA	CHC-C4B	3.97	1.48	1.39
17	A	805	CLA	C4B-NB	-3.97	1.32	1.37
17	B	836	CLA	CHC-C1C	3.97	1.46	1.38
17	A	838	CLA	C1B-NB	-3.97	1.32	1.37
25	4	314	5X6	C24-C25	3.97	1.55	1.43
17	B	840	CLA	O2A-CGA	3.97	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	845	BCR	C21-C22	3.97	1.41	1.35
17	1	307	CLA	C3B-C4B	3.97	1.52	1.42
25	1	312	5X6	C19-C18	3.97	1.55	1.43
25	5	317	5X6	C15-C14	3.97	1.55	1.43
17	B	818	CLA	CHC-C1C	3.97	1.46	1.38
25	1	315	5X6	C24-C25	3.97	1.55	1.43
25	1	313	5X6	C19-C18	3.96	1.55	1.43
17	4	310	CLA	CHC-C4B	3.96	1.48	1.39
17	A	836	CLA	O2A-CGA	3.96	1.44	1.33
17	A	816	CLA	O2A-CGA	3.96	1.44	1.33
17	B	807	CLA	O2A-CGA	3.96	1.44	1.33
17	A	806	CLA	C3C-C2C	3.96	1.45	1.36
17	A	856	CLA	CHC-C1C	3.96	1.46	1.38
17	4	306	CLA	CHC-C4B	3.96	1.48	1.39
17	2	316	CLA	CHC-C4B	3.96	1.48	1.39
17	2	313	CLA	CHC-C4B	3.96	1.48	1.39
17	1	302	CLA	CHD-C4C	3.96	1.48	1.39
17	B	816	CLA	CHD-C1D	3.96	1.46	1.38
17	J	103	CLA	CHD-C1D	3.96	1.46	1.38
20	K	104	BCR	C17-C18	3.95	1.41	1.35
17	B	802	CLA	O2D-CGD	3.95	1.42	1.33
25	3	316	5X6	C15-C14	3.95	1.55	1.43
17	B	815	CLA	C1D-ND	3.95	1.42	1.37
17	A	835	CLA	C4B-NB	-3.95	1.32	1.37
17	B	825	CLA	C1D-ND	3.95	1.42	1.37
17	B	841	CLA	O2A-CGA	3.95	1.44	1.33
17	5	311	CLA	CHC-C4B	3.95	1.48	1.39
17	B	806	CLA	O2A-CGA	3.95	1.44	1.33
17	3	310	CLA	CHC-C4B	3.94	1.48	1.39
17	F	203	CLA	CHD-C1D	3.94	1.46	1.38
17	A	818	CLA	C4B-NB	-3.94	1.32	1.37
17	O	204	CLA	CHC-C4B	3.94	1.48	1.39
17	5	314	CLA	CHC-C4B	3.94	1.48	1.39
17	A	835	CLA	C1B-NB	-3.94	1.32	1.37
17	2	311	CLA	CHD-C1D	3.94	1.46	1.38
17	O	205	CLA	CHC-C4B	3.94	1.48	1.39
25	5	318	5X6	C24-C25	3.94	1.55	1.43
25	2	317	5X6	C19-C18	3.94	1.55	1.43
17	5	309	CLA	CHD-C4C	3.94	1.48	1.39
17	A	827	CLA	CHC-C1C	3.94	1.46	1.38
17	A	814	CLA	CHD-C1D	3.94	1.46	1.38
25	3	318	5X6	C24-C25	3.94	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	835	CLA	CHC-C1C	3.94	1.46	1.38
17	O	203	CLA	CHC-C4B	3.93	1.48	1.39
25	3	318	5X6	C33-C32	3.93	1.58	1.52
17	2	307	CLA	CHC-C4B	3.93	1.48	1.39
25	3	316	5X6	C24-C25	3.93	1.55	1.43
17	A	826	CLA	C1B-NB	-3.93	1.32	1.37
17	3	310	CLA	CHD-C4C	3.93	1.48	1.39
17	L	204	CLA	CHC-C4B	3.93	1.48	1.39
17	A	823	CLA	C1D-ND	3.93	1.42	1.37
17	K	102	CLA	CHD-C4C	3.92	1.48	1.39
17	B	816	CLA	C1D-ND	3.92	1.42	1.37
25	5	317	5X6	C20-C21	3.92	1.55	1.43
25	1	313	5X6	C15-C14	3.92	1.55	1.43
25	2	321	5X6	C24-C25	3.92	1.55	1.43
17	A	825	CLA	O2A-CGA	3.92	1.44	1.33
17	B	801	CLA	C1B-NB	-3.92	1.33	1.37
17	B	816	CLA	CHD-C4C	3.92	1.48	1.39
17	B	827	CLA	O2A-CGA	3.91	1.44	1.33
25	4	313	5X6	C15-C14	3.91	1.55	1.43
17	L	203	CLA	CHD-C1D	3.91	1.46	1.38
25	5	301	5X6	C20-C21	3.91	1.55	1.43
17	B	841	CLA	CHD-C1D	3.91	1.46	1.38
17	A	811	CLA	C4B-NB	-3.91	1.33	1.37
25	1	315	5X6	C19-C18	3.91	1.55	1.43
17	1	302	CLA	C1B-NB	-3.91	1.33	1.37
25	3	318	5X6	C19-C18	3.91	1.55	1.43
17	3	312	CLA	CHC-C4B	3.91	1.48	1.39
17	A	824	CLA	O2A-CGA	3.91	1.44	1.33
17	3	315	CLA	CHC-C4B	3.91	1.48	1.39
25	5	317	5X6	C19-C18	3.91	1.55	1.43
17	A	806	CLA	CHC-C1C	3.91	1.46	1.38
17	5	309	CLA	CHD-C1D	3.90	1.46	1.38
17	4	309	CLA	CHC-C4B	3.90	1.48	1.39
17	A	816	CLA	C1D-ND	3.90	1.42	1.37
25	2	319	5X6	C33-C32	3.90	1.57	1.52
25	5	315	5X6	C24-C25	3.90	1.55	1.43
25	4	313	5X6	C24-C25	3.90	1.55	1.43
17	A	832	CLA	C4B-NB	-3.90	1.33	1.37
25	5	301	5X6	C24-C25	3.90	1.55	1.43
25	5	315	5X6	C19-C18	3.90	1.55	1.43
17	2	308	CLA	C3D-C2D	3.90	1.49	1.39
17	A	834	CLA	C3D-C2D	3.89	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	316	5X6	C33-C32	3.89	1.57	1.52
25	1	312	5X6	C15-C14	3.89	1.55	1.43
25	2	319	5X6	C24-C25	3.89	1.55	1.43
20	L	206	BCR	C17-C18	3.89	1.40	1.35
25	3	317	5X6	C19-C18	3.89	1.55	1.43
17	A	833	CLA	C1B-NB	-3.89	1.33	1.37
17	3	313	CLA	CHC-C4B	3.89	1.48	1.39
17	1	308	CLA	CHC-C4B	3.89	1.48	1.39
25	5	316	5X6	C23-C22	3.89	1.54	1.45
17	A	803	CLA	O2A-CGA	3.89	1.44	1.33
17	2	311	CLA	C3B-C4B	3.89	1.51	1.42
17	A	832	CLA	O2A-CGA	3.89	1.44	1.33
17	2	312	CLA	CHC-C4B	3.89	1.48	1.39
25	4	312	5X6	C20-C21	3.89	1.55	1.43
17	3	314	CLA	CHC-C4B	3.89	1.48	1.39
17	B	836	CLA	C1B-NB	-3.88	1.33	1.37
17	B	817	CLA	CHC-C4B	3.88	1.48	1.39
25	3	317	5X6	C24-C25	3.88	1.55	1.43
17	A	808	CLA	C1D-ND	3.88	1.42	1.37
17	5	310	CLA	CHC-C4B	3.88	1.48	1.39
25	4	314	5X6	C15-C14	3.88	1.55	1.43
17	1	304	CLA	C3B-C4B	3.88	1.51	1.42
17	A	813	CLA	C1D-ND	3.88	1.42	1.37
17	B	817	CLA	CHD-C4C	3.88	1.48	1.39
17	B	802	CLA	C4B-NB	-3.88	1.33	1.37
17	3	315	CLA	OBD-CAD	3.88	1.29	1.22
17	B	831	CLA	CHD-C1D	3.88	1.45	1.38
17	1	305	CLA	CHC-C4B	3.88	1.48	1.39
17	A	830	CLA	C1D-ND	3.88	1.42	1.37
25	3	318	5X6	C15-C14	3.88	1.55	1.43
17	L	204	CLA	CHD-C4C	3.88	1.48	1.39
17	3	311	CLA	C3B-C4B	3.87	1.51	1.42
17	O	204	CLA	OBD-CAD	3.87	1.29	1.22
25	1	315	5X6	C15-C14	3.87	1.55	1.43
25	5	301	5X6	C15-C14	3.87	1.55	1.43
17	A	852	CLA	O2A-CGA	3.87	1.44	1.33
25	3	316	5X6	C33-C32	3.87	1.57	1.52
17	3	308	CLA	OBD-CAD	3.87	1.29	1.22
17	4	307	CLA	CHC-C4B	3.87	1.48	1.39
17	5	312	CLA	C3D-C2D	3.87	1.49	1.39
17	A	853	CLA	C1B-NB	-3.87	1.33	1.37
17	B	818	CLA	C1D-ND	3.87	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	315	CLA	CHC-C4B	3.87	1.48	1.39
17	5	306	CLA	C3D-C2D	3.87	1.49	1.39
25	4	314	5X6	C20-C21	3.86	1.55	1.43
17	A	803	CLA	C4B-NB	-3.86	1.33	1.37
17	5	307	CLA	C1B-NB	-3.86	1.33	1.37
17	5	311	CLA	CHB-C1B	3.86	1.48	1.39
25	4	312	5X6	C15-C14	3.86	1.55	1.43
17	B	809	CLA	O2A-CGA	3.86	1.44	1.33
20	A	843	BCR	C21-C22	3.86	1.40	1.35
17	1	305	CLA	C3D-C2D	3.86	1.49	1.39
25	4	312	5X6	C24-C25	3.86	1.55	1.43
17	A	811	CLA	O2A-CGA	3.86	1.44	1.33
17	B	801	CLA	O2A-CGA	3.86	1.44	1.33
25	1	316	5X6	C19-C18	3.86	1.55	1.43
25	2	317	5X6	C15-C14	3.86	1.55	1.43
17	A	814	CLA	CHB-C1B	3.86	1.48	1.39
25	2	318	5X6	C23-C22	3.86	1.54	1.45
17	2	312	CLA	C3D-C2D	3.85	1.49	1.39
17	B	814	CLA	O2A-CGA	3.85	1.44	1.33
17	B	822	CLA	CHD-C4C	3.85	1.48	1.39
17	3	305	CLA	C3B-C4B	3.85	1.51	1.42
17	A	813	CLA	C1B-NB	-3.85	1.33	1.37
17	A	825	CLA	C4B-NB	-3.85	1.33	1.37
17	A	808	CLA	C3D-C2D	3.85	1.49	1.39
17	B	811	CLA	CHC-C1C	3.85	1.46	1.38
25	1	315	5X6	C20-C21	3.85	1.55	1.43
17	B	822	CLA	CHD-C1D	3.85	1.45	1.38
25	1	316	5X6	C15-C14	3.85	1.55	1.43
17	B	814	CLA	CHC-C4B	3.85	1.48	1.39
17	A	805	CLA	C1D-ND	3.85	1.42	1.37
17	A	807	CLA	O2A-CGA	3.85	1.44	1.33
17	2	314	CLA	C3B-C4B	3.85	1.51	1.42
25	1	316	5X6	C24-C25	3.84	1.55	1.43
17	A	821	CLA	CHD-C1D	3.84	1.45	1.38
25	1	314	5X6	C24-C25	3.84	1.55	1.43
17	2	306	CLA	CHB-C1B	3.84	1.48	1.39
17	1	310	CLA	C3B-C4B	3.84	1.51	1.42
25	1	312	5X6	C24-C25	3.84	1.55	1.43
17	4	309	CLA	C3D-C2D	3.84	1.49	1.39
25	1	313	5X6	C24-C25	3.84	1.55	1.43
17	1	311	CLA	CHC-C4B	3.84	1.48	1.39
17	2	313	CLA	OBD-CAD	3.84	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	306	CLA	C3D-C2D	3.84	1.49	1.39
17	B	821	CLA	CHD-C4C	3.84	1.48	1.39
17	1	308	CLA	CHB-C1B	3.84	1.48	1.39
25	1	313	5X6	C33-C32	3.84	1.57	1.52
25	5	318	5X6	C19-C18	3.84	1.55	1.43
17	1	307	CLA	CHD-C1D	3.84	1.45	1.38
17	A	854	CLA	CHC-C1C	3.84	1.46	1.38
25	2	318	5X6	C19-C18	3.84	1.55	1.43
17	B	824	CLA	C1B-NB	-3.84	1.33	1.37
17	B	835	CLA	C3D-C2D	3.83	1.49	1.39
25	1	312	5X6	C33-C32	3.83	1.57	1.52
25	1	316	5X6	C20-C21	3.83	1.55	1.43
17	B	807	CLA	C4B-NB	-3.83	1.33	1.37
17	O	203	CLA	CHB-C1B	3.83	1.48	1.39
17	1	306	CLA	CHC-C4B	3.83	1.48	1.39
17	1	309	CLA	CHC-C4B	3.83	1.48	1.39
17	A	834	CLA	CHD-C4C	3.83	1.48	1.39
17	L	202	CLA	CHD-C4C	3.83	1.48	1.39
17	A	806	CLA	O2A-CGA	3.83	1.44	1.33
17	3	312	CLA	C3D-C2D	3.83	1.49	1.39
17	A	815	CLA	CHD-C4C	3.83	1.48	1.39
25	2	320	5X6	C15-C14	3.83	1.55	1.43
17	A	853	CLA	O2D-CGD	3.83	1.42	1.33
17	2	315	CLA	OBD-CAD	3.83	1.29	1.22
17	5	309	CLA	CHC-C4B	3.82	1.48	1.39
17	5	303	CLA	OBD-CAD	3.82	1.29	1.22
17	5	311	CLA	C3D-C2D	3.82	1.49	1.39
17	A	802	CLA	CHD-C1D	3.82	1.45	1.38
17	A	830	CLA	CHB-C1B	3.82	1.48	1.39
20	A	843	BCR	C10-C9	3.82	1.40	1.35
25	1	315	5X6	C33-C32	3.82	1.57	1.52
17	B	825	CLA	CHC-C1C	3.82	1.46	1.38
17	1	311	CLA	C3D-C2D	3.82	1.49	1.39
16	A	801	CL0	O2A-CGA	3.82	1.44	1.33
17	3	312	CLA	CHB-C1B	3.82	1.48	1.39
17	5	302	CLA	C3D-C2D	3.82	1.49	1.39
17	1	311	CLA	OBD-CAD	3.82	1.29	1.22
17	A	830	CLA	C1B-NB	-3.82	1.33	1.37
17	1	308	CLA	C3D-C2D	3.82	1.49	1.39
25	3	317	5X6	C33-C32	3.82	1.57	1.52
17	2	305	CLA	C3B-C4B	3.81	1.51	1.42
17	4	310	CLA	C3D-C2D	3.81	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	307	CLA	CHD-C4C	3.81	1.47	1.39
17	2	309	CLA	OBD-CAD	3.81	1.29	1.22
25	4	313	5X6	C20-C21	3.81	1.55	1.43
17	B	837	CLA	CHD-C1D	3.81	1.45	1.38
25	1	313	5X6	C20-C21	3.81	1.55	1.43
17	A	820	CLA	C1D-ND	3.81	1.42	1.37
17	4	303	CLA	CHC-C4B	3.81	1.48	1.39
17	B	835	CLA	CHD-C1D	3.81	1.45	1.38
17	B	814	CLA	C1B-NB	-3.81	1.33	1.37
17	4	304	CLA	C3D-C2D	3.81	1.49	1.39
17	B	834	CLA	C1D-ND	3.81	1.42	1.37
25	5	301	5X6	C33-C32	3.81	1.57	1.52
17	5	314	CLA	OBD-CAD	3.81	1.29	1.22
17	A	831	CLA	C3D-C2D	3.81	1.49	1.39
17	A	818	CLA	CHD-C4C	3.81	1.47	1.39
17	A	836	CLA	CHC-C1C	3.81	1.46	1.38
17	1	301	CLA	C3D-C2D	3.81	1.49	1.39
17	A	810	CLA	CHC-C1C	3.81	1.46	1.38
17	B	802	CLA	C1B-NB	-3.81	1.33	1.37
25	2	321	5X6	C15-C14	3.80	1.55	1.43
17	2	304	CLA	OBD-CAD	3.80	1.29	1.22
17	3	315	CLA	C3D-C2D	3.80	1.49	1.39
17	1	310	CLA	C3D-C2D	3.80	1.49	1.39
17	O	203	CLA	OBD-CAD	3.80	1.29	1.22
17	1	303	CLA	C1B-NB	-3.80	1.33	1.37
17	A	811	CLA	C1D-ND	3.80	1.42	1.37
25	2	320	5X6	C19-C18	3.80	1.55	1.43
17	O	203	CLA	C3D-C2D	3.80	1.49	1.39
17	3	315	CLA	CHB-C1B	3.80	1.47	1.39
25	2	318	5X6	C20-C21	3.80	1.55	1.43
17	5	307	CLA	C3D-C2D	3.80	1.49	1.39
17	A	813	CLA	CHD-C4C	3.80	1.47	1.39
25	1	314	5X6	C19-C18	3.80	1.55	1.43
17	4	309	CLA	OBD-CAD	3.80	1.29	1.22
17	B	837	CLA	C1B-NB	-3.80	1.33	1.37
25	4	312	5X6	C19-C18	3.80	1.55	1.43
17	B	826	CLA	O2A-CGA	3.80	1.44	1.33
17	5	305	CLA	OBD-CAD	3.80	1.29	1.22
17	2	304	CLA	CHB-C1B	3.80	1.47	1.39
17	5	311	CLA	OBD-CAD	3.79	1.29	1.22
17	4	304	CLA	C3B-C4B	3.79	1.51	1.42
17	A	818	CLA	CHD-C1D	3.79	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	841	CLA	CHC-C4B	3.79	1.47	1.39
25	3	317	5X6	C15-C14	3.79	1.55	1.43
17	2	312	CLA	CHB-C1B	3.79	1.47	1.39
17	5	314	CLA	C3B-C4B	3.79	1.51	1.42
17	1	305	CLA	OBD-CAD	3.79	1.29	1.22
17	4	310	CLA	OBD-CAD	3.79	1.29	1.22
17	4	309	CLA	CHB-C1B	3.79	1.47	1.39
17	O	205	CLA	C3D-C2D	3.79	1.49	1.39
17	3	313	CLA	C3D-C2D	3.79	1.49	1.39
17	5	310	CLA	C3D-C2D	3.78	1.49	1.39
17	4	311	CLA	OBD-CAD	3.78	1.29	1.22
17	A	830	CLA	C3D-C2D	3.78	1.49	1.39
17	5	306	CLA	CHC-C4B	3.78	1.47	1.39
17	5	310	CLA	CHB-C1B	3.78	1.47	1.39
17	B	812	CLA	O2A-CGA	3.78	1.44	1.33
17	L	202	CLA	OBD-CAD	3.78	1.29	1.22
17	5	302	CLA	CHB-C1B	3.78	1.47	1.39
17	5	308	CLA	CHC-C4B	3.78	1.47	1.39
17	1	302	CLA	C3D-C2D	3.78	1.49	1.39
17	A	831	CLA	CHD-C1D	3.78	1.45	1.38
17	A	837	CLA	C4B-NB	-3.78	1.33	1.37
17	2	315	CLA	C3D-C2D	3.78	1.49	1.39
17	A	810	CLA	C1B-NB	-3.77	1.33	1.37
17	2	309	CLA	C3D-C2D	3.77	1.49	1.39
17	F	204	CLA	C3D-C2D	3.77	1.49	1.39
17	2	313	CLA	C3D-C2D	3.77	1.49	1.39
17	4	305	CLA	CHC-C4B	3.77	1.47	1.39
17	3	309	CLA	C3D-C2D	3.77	1.49	1.39
17	4	307	CLA	C3D-C2D	3.77	1.49	1.39
17	4	308	CLA	C3B-C4B	3.77	1.51	1.42
17	B	823	CLA	CHD-C4C	3.77	1.47	1.39
17	5	314	CLA	C3D-C2D	3.77	1.49	1.39
17	2	314	CLA	OBD-CAD	3.77	1.29	1.22
17	B	835	CLA	C1B-NB	-3.77	1.33	1.37
17	A	805	CLA	CHB-C1B	3.77	1.47	1.39
17	A	815	CLA	C3D-C2D	3.77	1.49	1.39
17	3	314	CLA	C3D-C2D	3.77	1.49	1.39
17	3	305	CLA	C3D-C2D	3.77	1.49	1.39
25	3	318	5X6	C20-C21	3.76	1.55	1.43
17	2	310	CLA	C3D-C2D	3.76	1.49	1.39
17	3	307	CLA	C3D-C2D	3.76	1.49	1.39
20	A	844	BCR	C10-C9	3.76	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	307	CLA	C3D-C2D	3.76	1.49	1.39
17	A	818	CLA	CHB-C1B	3.76	1.47	1.39
17	4	308	CLA	OBD-CAD	3.76	1.29	1.22
17	2	309	CLA	CHB-C1B	3.76	1.47	1.39
17	A	833	CLA	C3D-C2D	3.76	1.49	1.39
17	2	314	CLA	C3D-C2D	3.76	1.49	1.39
17	2	304	CLA	C3D-C2D	3.76	1.49	1.39
17	3	314	CLA	OBD-CAD	3.76	1.29	1.22
17	A	817	CLA	CHD-C1D	3.76	1.45	1.38
25	5	318	5X6	C15-C14	3.76	1.55	1.43
17	O	205	CLA	OBD-CAD	3.76	1.29	1.22
17	A	833	CLA	C4B-NB	-3.76	1.33	1.37
17	A	814	CLA	CHD-C4C	3.76	1.47	1.39
17	2	305	CLA	OBD-CAD	3.75	1.28	1.22
17	3	307	CLA	OBD-CAD	3.75	1.28	1.22
17	5	302	CLA	OBD-CAD	3.75	1.28	1.22
17	5	303	CLA	C3D-C2D	3.75	1.49	1.39
17	L	204	CLA	OBD-CAD	3.75	1.28	1.22
17	B	833	CLA	C4B-NB	-3.75	1.33	1.37
17	1	309	CLA	OBD-CAD	3.75	1.28	1.22
17	B	817	CLA	CHD-C1D	3.75	1.45	1.38
17	5	303	CLA	CHC-C4B	3.75	1.47	1.39
17	A	802	CLA	OBD-CAD	3.75	1.28	1.22
17	1	311	CLA	CHB-C1B	3.75	1.47	1.39
17	A	817	CLA	C3D-C2D	3.75	1.49	1.39
17	B	827	CLA	CHC-C1C	3.75	1.46	1.38
17	4	304	CLA	OBD-CAD	3.75	1.28	1.22
17	5	309	CLA	C3D-C2D	3.75	1.49	1.39
17	A	831	CLA	C1B-NB	-3.75	1.33	1.37
20	O	202	BCR	C21-C22	3.75	1.40	1.35
17	5	312	CLA	CHB-C1B	3.75	1.47	1.39
17	3	311	CLA	OBD-CAD	3.75	1.28	1.22
17	3	313	CLA	OBD-CAD	3.75	1.28	1.22
25	5	318	5X6	C20-C21	3.75	1.55	1.43
17	B	840	CLA	C1B-NB	-3.75	1.33	1.37
17	B	815	CLA	OBD-CAD	3.75	1.28	1.22
17	4	306	CLA	OBD-CAD	3.74	1.28	1.22
17	J	103	CLA	C4B-NB	-3.74	1.33	1.37
17	4	311	CLA	C3D-C2D	3.74	1.49	1.39
17	2	316	CLA	OBD-CAD	3.74	1.28	1.22
25	2	320	5X6	C20-C21	3.74	1.55	1.43
17	B	821	CLA	CHC-C4B	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	832	CLA	CHC-C1C	3.74	1.46	1.38
17	4	303	CLA	OBD-CAD	3.74	1.28	1.22
17	K	103	CLA	CHD-C1D	3.74	1.45	1.38
17	2	316	CLA	C3D-C2D	3.74	1.49	1.39
17	3	306	CLA	CHC-C4B	3.74	1.47	1.39
17	A	855	CLA	C4B-NB	-3.74	1.33	1.37
17	B	815	CLA	CHB-C1B	3.74	1.47	1.39
25	2	317	5X6	C20-C21	3.74	1.55	1.43
17	A	810	CLA	CHD-C1D	3.74	1.45	1.38
17	3	305	CLA	OBD-CAD	3.74	1.28	1.22
17	A	827	CLA	CHD-C1D	3.74	1.45	1.38
17	2	313	CLA	C3B-C4B	3.74	1.51	1.42
17	4	308	CLA	C3D-C2D	3.73	1.49	1.39
17	4	303	CLA	CHB-C1B	3.73	1.47	1.39
17	1	304	CLA	OBD-CAD	3.73	1.28	1.22
17	B	813	CLA	CHC-C4B	3.73	1.47	1.39
17	5	308	CLA	C3D-C2D	3.73	1.49	1.39
17	A	818	CLA	OBD-CAD	3.73	1.28	1.22
17	A	816	CLA	CHC-C1C	3.73	1.46	1.38
17	2	313	CLA	CHB-C1B	3.73	1.47	1.39
17	3	311	CLA	C3D-C2D	3.73	1.49	1.39
17	3	310	CLA	C3D-C2D	3.73	1.49	1.39
17	5	310	CLA	OBD-CAD	3.73	1.28	1.22
17	1	301	CLA	CHC-C4B	3.73	1.47	1.39
17	B	831	CLA	CHC-C1C	3.72	1.46	1.38
17	O	204	CLA	C3D-C2D	3.72	1.49	1.39
17	1	309	CLA	C3D-C2D	3.72	1.49	1.39
17	A	808	CLA	C4B-NB	-3.72	1.33	1.37
25	2	321	5X6	C19-C18	3.72	1.55	1.43
17	B	814	CLA	CHC-C1C	3.72	1.46	1.38
17	B	807	CLA	C1B-NB	-3.72	1.33	1.37
17	2	316	CLA	CHB-C1B	3.72	1.47	1.39
17	3	308	CLA	CHC-C4B	3.72	1.47	1.39
17	A	815	CLA	C1B-NB	-3.72	1.33	1.37
17	4	306	CLA	CHB-C1B	3.72	1.47	1.39
25	3	317	5X6	C20-C21	3.72	1.55	1.43
17	L	202	CLA	CHB-C1B	3.72	1.47	1.39
17	5	313	CLA	OBD-CAD	3.72	1.28	1.22
25	4	312	5X6	C33-C32	3.72	1.57	1.52
17	2	304	CLA	CHC-C4B	3.72	1.47	1.39
17	B	823	CLA	CHC-C4B	3.72	1.47	1.39
17	A	839	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	813	CLA	CHD-C4C	3.71	1.47	1.39
17	B	820	CLA	C3D-C2D	3.71	1.49	1.39
17	B	806	CLA	CHD-C1D	3.71	1.45	1.38
17	3	313	CLA	C3B-C4B	3.71	1.51	1.42
17	4	303	CLA	C3D-C2D	3.71	1.49	1.39
17	A	837	CLA	CHC-C4B	3.71	1.47	1.39
17	B	818	CLA	C4B-NB	-3.71	1.33	1.37
20	B	845	BCR	C14-C13	3.71	1.40	1.35
17	J	103	CLA	CHB-C1B	3.71	1.47	1.39
17	A	859	CLA	CHB-C1B	3.71	1.47	1.39
17	A	816	CLA	CHD-C1D	3.71	1.45	1.38
17	A	834	CLA	C1B-NB	-3.71	1.33	1.37
17	2	310	CLA	C3B-C4B	3.71	1.51	1.42
17	4	307	CLA	C3B-C4B	3.71	1.51	1.42
17	A	853	CLA	C3D-C2D	3.71	1.49	1.39
17	1	304	CLA	C3D-C2D	3.71	1.49	1.39
17	B	812	CLA	C1D-ND	3.70	1.42	1.37
17	B	801	CLA	CHD-C1D	3.70	1.45	1.38
17	1	302	CLA	OBD-CAD	3.70	1.28	1.22
17	L	203	CLA	CHB-C1B	3.70	1.47	1.39
17	B	813	CLA	CHD-C1D	3.70	1.45	1.38
17	2	316	CLA	C3B-C4B	3.70	1.51	1.42
17	5	312	CLA	C3B-C4B	3.70	1.51	1.42
17	A	821	CLA	CHC-C4B	3.70	1.47	1.39
17	K	103	CLA	CHB-C1B	3.70	1.47	1.39
17	A	810	CLA	CHB-C1B	3.70	1.47	1.39
17	A	839	CLA	C1D-ND	3.70	1.42	1.37
17	3	313	CLA	CHB-C1B	3.70	1.47	1.39
17	B	831	CLA	C4B-NB	-3.70	1.33	1.37
20	B	803	BCR	C17-C18	3.69	1.40	1.35
17	A	826	CLA	C1C-NC	-3.69	1.32	1.37
17	B	811	CLA	C3D-C2D	3.69	1.49	1.39
17	1	309	CLA	C3B-C4B	3.69	1.51	1.42
17	A	859	CLA	OBD-CAD	3.69	1.28	1.22
17	A	823	CLA	C4B-NB	-3.69	1.33	1.37
25	J	105	5X6	C23-C22	3.69	1.53	1.45
17	A	811	CLA	CHB-C1B	3.69	1.47	1.39
17	A	830	CLA	CHC-C1C	3.69	1.46	1.38
17	O	205	CLA	CHB-C1B	3.69	1.47	1.39
17	3	314	CLA	C3B-C4B	3.69	1.51	1.42
20	L	205	BCR	C21-C22	3.69	1.40	1.35
17	2	308	CLA	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	CHC-C4B	3.69	1.47	1.39
25	5	316	5X6	C16-C17	3.69	1.53	1.45
17	2	305	CLA	C3D-C2D	3.69	1.49	1.39
17	K	102	CLA	C3D-C2D	3.68	1.49	1.39
17	A	815	CLA	CHD-C1D	3.68	1.45	1.38
17	4	305	CLA	CHB-C1B	3.68	1.47	1.39
17	5	308	CLA	C1B-NB	-3.68	1.33	1.37
17	2	312	CLA	OBD-CAD	3.68	1.28	1.22
17	4	311	CLA	C3B-C4B	3.68	1.51	1.42
17	B	835	CLA	CHC-C4B	3.68	1.47	1.39
20	O	202	BCR	C17-C18	3.68	1.40	1.35
17	4	305	CLA	C3D-C2D	3.68	1.49	1.39
17	2	311	CLA	C3D-C2D	3.68	1.49	1.39
17	B	832	CLA	CHD-C4C	3.68	1.47	1.39
17	B	809	CLA	CHC-C1C	3.68	1.46	1.38
17	1	307	CLA	OBD-CAD	3.67	1.28	1.22
17	3	308	CLA	C3D-C2D	3.67	1.49	1.39
17	3	314	CLA	CHB-C1B	3.67	1.47	1.39
17	O	205	CLA	C3B-C4B	3.67	1.51	1.42
17	A	816	CLA	C4B-NB	-3.67	1.33	1.37
17	J	103	CLA	CHD-C4C	3.67	1.47	1.39
17	B	810	CLA	C1D-ND	3.67	1.42	1.37
17	B	813	CLA	CHB-C1B	3.67	1.47	1.39
17	B	824	CLA	CHD-C4C	3.67	1.47	1.39
25	4	313	5X6	C33-C32	3.67	1.57	1.52
17	B	835	CLA	C4B-NB	-3.67	1.33	1.37
17	5	312	CLA	OBD-CAD	3.67	1.28	1.22
17	O	203	CLA	C3B-C4B	3.67	1.51	1.42
17	A	827	CLA	O2A-CGA	3.67	1.44	1.33
17	B	817	CLA	C3D-C2D	3.67	1.49	1.39
25	3	316	5X6	C20-C21	3.66	1.54	1.43
17	O	204	CLA	C3B-C4B	3.66	1.51	1.42
17	5	306	CLA	C3B-C4B	3.66	1.51	1.42
17	F	203	CLA	C3D-C2D	3.66	1.49	1.39
17	4	310	CLA	C3B-C4B	3.66	1.51	1.42
17	3	308	CLA	CHB-C1B	3.66	1.47	1.39
17	A	835	CLA	CHC-C4B	3.66	1.47	1.39
17	B	816	CLA	C1B-NB	-3.66	1.33	1.37
17	3	312	CLA	OBD-CAD	3.66	1.28	1.22
17	3	309	CLA	OBD-CAD	3.66	1.28	1.22
17	A	824	CLA	CHC-C1C	3.66	1.46	1.38
17	A	804	CLA	CHB-C1B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	CHD-C1D	3.66	1.45	1.38
17	K	102	CLA	CHB-C1B	3.65	1.47	1.39
17	A	814	CLA	OBD-CAD	3.65	1.28	1.22
17	B	810	CLA	CHB-C1B	3.65	1.47	1.39
17	4	308	CLA	CHB-C1B	3.65	1.47	1.39
17	A	832	CLA	CHD-C1D	3.65	1.45	1.38
17	4	310	CLA	CHB-C1B	3.65	1.47	1.39
17	B	822	CLA	C3B-C4B	3.65	1.51	1.42
17	5	302	CLA	C3B-C4B	3.65	1.51	1.42
25	5	316	5X6	C19-C18	3.65	1.54	1.43
17	5	306	CLA	OBD-CAD	3.65	1.28	1.22
17	A	836	CLA	C1B-NB	-3.65	1.33	1.37
17	4	305	CLA	C3B-C4B	3.65	1.51	1.42
17	4	306	CLA	C3B-C4B	3.65	1.51	1.42
17	A	820	CLA	CHD-C4C	3.65	1.47	1.39
17	3	306	CLA	C3D-C2D	3.65	1.49	1.39
17	B	821	CLA	CHD-C1D	3.64	1.45	1.38
17	L	203	CLA	C1B-NB	-3.64	1.33	1.37
17	4	311	CLA	CHB-C1B	3.64	1.47	1.39
17	A	803	CLA	CHD-C1D	3.64	1.45	1.38
17	K	102	CLA	C1B-NB	-3.64	1.33	1.37
17	1	305	CLA	CHB-C1B	3.64	1.47	1.39
17	A	820	CLA	CHB-C1B	3.64	1.47	1.39
17	B	816	CLA	OBD-CAD	3.64	1.28	1.22
17	L	202	CLA	C3D-C2D	3.64	1.49	1.39
17	2	315	CLA	C3B-C4B	3.64	1.51	1.42
17	2	314	CLA	CHB-C1B	3.64	1.47	1.39
17	B	804	CLA	CHB-C1B	3.64	1.47	1.39
17	K	102	CLA	CHC-C4B	3.64	1.47	1.39
17	1	307	CLA	CHB-C1B	3.64	1.47	1.39
17	1	306	CLA	C3D-C2D	3.64	1.49	1.39
17	4	309	CLA	C3B-C4B	3.64	1.51	1.42
25	1	313	5X6	C05-C06	3.64	1.57	1.52
25	4	312	5X6	C05-C06	3.64	1.57	1.52
17	L	204	CLA	CHB-C1B	3.64	1.47	1.39
25	1	312	5X6	C20-C21	3.63	1.54	1.43
25	1	316	5X6	C28-C29	3.63	1.58	1.45
17	F	203	CLA	C1B-NB	-3.63	1.33	1.37
17	A	819	CLA	CHD-C1D	3.63	1.45	1.38
17	A	811	CLA	CHC-C4B	3.63	1.47	1.39
25	5	315	5X6	C15-C14	3.63	1.54	1.43
17	3	307	CLA	C3B-C4B	3.63	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	C1B-NB	-3.63	1.33	1.37
17	2	312	CLA	C3B-C4B	3.63	1.51	1.42
17	5	307	CLA	CHD-C1D	3.63	1.45	1.38
17	4	307	CLA	OBD-CAD	3.63	1.28	1.22
17	A	813	CLA	C4B-NB	-3.63	1.33	1.37
17	1	302	CLA	CHB-C1B	3.63	1.47	1.39
17	1	310	CLA	OBD-CAD	3.63	1.28	1.22
17	2	307	CLA	C3B-C4B	3.63	1.51	1.42
17	2	306	CLA	CHC-C4B	3.63	1.47	1.39
17	3	312	CLA	C3B-C4B	3.63	1.51	1.42
17	A	839	CLA	CHB-C1B	3.63	1.47	1.39
17	5	313	CLA	CHC-C4B	3.63	1.47	1.39
17	B	841	CLA	C3D-C2D	3.63	1.49	1.39
17	B	832	CLA	C3D-C2D	3.63	1.49	1.39
17	1	311	CLA	C3B-C4B	3.63	1.51	1.42
17	B	819	CLA	CHD-C1D	3.62	1.45	1.38
17	B	824	CLA	CHD-C1D	3.62	1.45	1.38
17	A	829	CLA	C4B-NB	-3.62	1.33	1.37
17	3	311	CLA	CHB-C1B	3.62	1.47	1.39
17	5	310	CLA	C3B-C4B	3.62	1.51	1.42
17	5	304	CLA	C3D-C2D	3.62	1.49	1.39
17	A	825	CLA	CHB-C1B	3.62	1.47	1.39
20	J	104	BCR	C17-C18	3.62	1.40	1.35
25	1	315	5X6	C28-C29	3.62	1.57	1.45
17	2	315	CLA	CHB-C1B	3.62	1.47	1.39
17	J	103	CLA	CHC-C1C	3.62	1.45	1.38
17	B	824	CLA	C3B-C4B	3.62	1.51	1.42
17	1	309	CLA	CHB-C1B	3.62	1.47	1.39
17	A	856	CLA	C1B-NB	-3.62	1.33	1.37
17	A	831	CLA	C1D-ND	3.62	1.42	1.37
17	B	829	CLA	O2A-CGA	3.62	1.43	1.33
25	3	318	5X6	C28-C29	3.62	1.57	1.45
17	1	302	CLA	CHC-C4B	3.61	1.47	1.39
17	B	821	CLA	C3D-C2D	3.61	1.49	1.39
17	A	817	CLA	C1D-ND	3.61	1.42	1.37
17	A	809	CLA	C3D-C2D	3.61	1.49	1.39
17	B	835	CLA	CHD-C4C	3.61	1.47	1.39
17	B	814	CLA	C3D-C2D	3.61	1.49	1.39
17	B	821	CLA	CHB-C1B	3.61	1.47	1.39
25	1	312	5X6	C05-C06	3.61	1.57	1.52
17	K	103	CLA	CHD-C4C	3.61	1.47	1.39
25	1	316	5X6	C05-C06	3.61	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	839	CLA	C3D-C2D	3.61	1.49	1.39
17	B	806	CLA	C3D-C2D	3.61	1.49	1.39
17	A	807	CLA	C4B-NB	-3.61	1.33	1.37
17	3	309	CLA	C3B-C4B	3.61	1.51	1.42
25	2	318	5X6	C15-C14	3.61	1.54	1.43
17	B	808	CLA	CHC-C1C	3.61	1.45	1.38
17	A	820	CLA	CHD-C1D	3.61	1.45	1.38
17	A	854	CLA	CHC-C4B	3.61	1.47	1.39
17	1	301	CLA	CHB-C1B	3.61	1.47	1.39
17	A	821	CLA	C1D-ND	3.61	1.42	1.37
17	4	305	CLA	C1B-NB	-3.61	1.33	1.37
17	A	826	CLA	C3D-C2D	3.61	1.49	1.39
17	5	307	CLA	CHC-C4B	3.61	1.47	1.39
25	1	314	5X6	C15-C14	3.60	1.54	1.43
17	1	308	CLA	C3B-C4B	3.60	1.51	1.42
17	B	841	CLA	CHB-C1B	3.60	1.47	1.39
20	A	845	BCR	C23-C22	-3.60	1.38	1.45
17	5	311	CLA	C3B-C4B	3.60	1.51	1.42
17	A	831	CLA	CHD-C4C	3.60	1.47	1.39
17	1	308	CLA	OBD-CAD	3.60	1.28	1.22
17	5	309	CLA	OBD-CAD	3.60	1.28	1.22
17	5	313	CLA	C1B-NB	-3.60	1.33	1.37
17	B	835	CLA	OBD-CAD	3.60	1.28	1.22
17	2	307	CLA	OBD-CAD	3.60	1.28	1.22
25	2	318	5X6	C24-C25	3.59	1.54	1.43
25	1	315	5X6	C05-C06	3.59	1.57	1.52
17	A	852	CLA	C3D-C2D	3.59	1.48	1.39
17	K	103	CLA	CHC-C4B	3.59	1.47	1.39
17	A	810	CLA	CHD-C4C	3.59	1.47	1.39
17	5	314	CLA	CHB-C1B	3.58	1.47	1.39
17	B	838	CLA	C1D-ND	3.58	1.42	1.37
17	B	823	CLA	CHB-C1B	3.58	1.47	1.39
17	A	831	CLA	C4B-NB	-3.58	1.33	1.37
17	2	305	CLA	CHB-C1B	3.58	1.47	1.39
25	F	205	5X6	C16-C17	3.58	1.53	1.45
25	4	312	5X6	C28-C29	3.58	1.57	1.45
17	1	301	CLA	OBD-CAD	3.58	1.28	1.22
17	4	304	CLA	CHB-C1B	3.58	1.47	1.39
17	5	313	CLA	C3B-C4B	3.57	1.51	1.42
16	A	801	CL0	CHB-C1B	3.57	1.47	1.39
17	1	310	CLA	CHB-C1B	3.57	1.47	1.39
25	4	313	5X6	C28-C29	3.57	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	204	CLA	OBD-CAD	3.57	1.28	1.22
25	5	317	5X6	C28-C29	3.57	1.57	1.45
25	2	320	5X6	C28-C29	3.57	1.57	1.45
17	B	814	CLA	CHB-C1B	3.57	1.47	1.39
17	1	305	CLA	C1B-NB	-3.57	1.33	1.37
17	A	838	CLA	CHC-C1C	3.57	1.45	1.38
17	3	306	CLA	CHB-C1B	3.57	1.47	1.39
17	B	811	CLA	C1B-NB	-3.57	1.33	1.37
25	2	317	5X6	C28-C29	3.57	1.57	1.45
17	2	306	CLA	C3D-C2D	3.57	1.48	1.39
17	L	202	CLA	CHC-C4B	3.57	1.47	1.39
17	B	829	CLA	CHD-C4C	3.56	1.47	1.39
17	A	855	CLA	OBD-CAD	3.56	1.28	1.22
17	2	308	CLA	CHC-C4B	3.56	1.47	1.39
17	B	834	CLA	C3D-C2D	3.56	1.48	1.39
17	5	309	CLA	CHB-C1B	3.56	1.47	1.39
17	5	307	CLA	OBD-CAD	3.56	1.28	1.22
17	B	831	CLA	C3D-C2D	3.56	1.48	1.39
17	A	818	CLA	C3D-C2D	3.56	1.48	1.39
17	B	802	CLA	CHB-C1B	3.56	1.47	1.39
17	B	829	CLA	CHD-C1D	3.56	1.45	1.38
20	B	847	BCR	C10-C9	3.55	1.40	1.35
17	A	806	CLA	CHB-C1B	3.55	1.47	1.39
17	1	303	CLA	C3B-C4B	3.55	1.51	1.42
17	B	820	CLA	C1B-NB	-3.55	1.33	1.37
17	B	820	CLA	C4B-NB	-3.55	1.33	1.37
17	L	203	CLA	OBD-CAD	3.55	1.28	1.22
17	A	835	CLA	CHD-C1D	3.55	1.45	1.38
17	B	818	CLA	CHC-C4B	3.55	1.47	1.39
17	A	804	CLA	C3D-C2D	3.55	1.48	1.39
17	2	311	CLA	OBD-CAD	3.55	1.28	1.22
17	2	307	CLA	CHB-C1B	3.55	1.47	1.39
17	F	204	CLA	CHB-C1B	3.55	1.47	1.39
17	L	204	CLA	C3D-C2D	3.55	1.48	1.39
17	A	855	CLA	C1D-ND	3.55	1.42	1.37
17	L	203	CLA	C3D-C2D	3.54	1.48	1.39
17	3	315	CLA	C3B-C4B	3.54	1.51	1.42
17	A	856	CLA	CHD-C4C	3.54	1.47	1.39
17	B	857	CLA	C3D-C2D	3.54	1.48	1.39
17	A	852	CLA	CHC-C1C	3.54	1.45	1.38
25	2	321	5X6	C28-C29	3.54	1.57	1.45
17	1	305	CLA	C3B-C4B	3.54	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	818	CLA	C3D-C2D	3.54	1.48	1.39
17	1	304	CLA	CHB-C1B	3.54	1.47	1.39
25	J	105	5X6	C12-C13	3.54	1.53	1.45
17	B	828	CLA	C3D-C2D	3.54	1.48	1.39
20	B	844	BCR	C14-C13	3.54	1.40	1.35
17	A	837	CLA	C3D-C2D	3.53	1.48	1.39
17	3	309	CLA	CHB-C1B	3.53	1.47	1.39
17	L	203	CLA	CHC-C4B	3.53	1.47	1.39
25	2	319	5X6	C28-C29	3.53	1.57	1.45
20	B	845	BCR	C17-C18	3.53	1.40	1.35
17	A	829	CLA	C3D-C2D	3.53	1.48	1.39
17	B	841	CLA	C3B-C4B	3.53	1.51	1.42
17	A	837	CLA	C1D-ND	3.53	1.42	1.37
17	1	303	CLA	C3D-C2D	3.53	1.48	1.39
17	B	809	CLA	CHB-C1B	3.53	1.47	1.39
17	5	306	CLA	CHB-C1B	3.53	1.47	1.39
17	B	839	CLA	C4B-NB	-3.53	1.33	1.37
17	B	838	CLA	CHC-C4B	3.53	1.47	1.39
17	A	807	CLA	CHC-C4B	3.52	1.47	1.39
17	3	305	CLA	CHB-C1B	3.52	1.47	1.39
20	A	857	BCR	C10-C9	3.52	1.40	1.35
17	A	853	CLA	CHB-C1B	3.52	1.47	1.39
17	A	802	CLA	CHD-C4C	3.52	1.47	1.39
25	4	314	5X6	C05-C06	3.52	1.57	1.52
17	B	806	CLA	CHB-C1B	3.52	1.47	1.39
17	A	813	CLA	CHC-C4B	3.52	1.47	1.39
17	B	836	CLA	C3D-C2D	3.52	1.48	1.39
17	B	807	CLA	C3D-C2D	3.51	1.48	1.39
17	3	306	CLA	C1B-NB	-3.51	1.33	1.37
20	A	843	BCR	C14-C13	3.51	1.40	1.35
17	B	814	CLA	CHD-C1D	3.51	1.45	1.38
17	5	304	CLA	CHC-C4B	3.51	1.47	1.39
17	5	313	CLA	CHB-C1B	3.51	1.47	1.39
17	F	203	CLA	CHD-C4C	3.51	1.47	1.39
17	B	819	CLA	C1D-ND	3.51	1.42	1.37
17	B	824	CLA	OBD-CAD	3.51	1.28	1.22
17	A	811	CLA	C3D-C2D	3.51	1.48	1.39
25	2	321	5X6	C20-C21	3.51	1.54	1.43
17	B	826	CLA	C3D-C2D	3.51	1.48	1.39
17	B	801	CLA	C3D-C2D	3.51	1.48	1.39
17	A	854	CLA	CHB-C1B	3.51	1.47	1.39
17	B	824	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	203	CLA	C3B-C4B	3.51	1.51	1.42
17	A	812	CLA	CHB-C1B	3.51	1.47	1.39
17	3	310	CLA	C3B-C4B	3.51	1.51	1.42
17	A	805	CLA	C3D-C2D	3.51	1.48	1.39
17	B	808	CLA	CHC-C4B	3.51	1.47	1.39
17	A	822	CLA	CHC-C4B	3.51	1.47	1.39
17	5	303	CLA	CHB-C1B	3.50	1.47	1.39
17	B	834	CLA	C4B-NB	-3.50	1.33	1.37
25	4	314	5X6	C28-C29	3.50	1.57	1.45
17	A	809	CLA	CHC-C1C	3.50	1.45	1.38
17	K	103	CLA	C3D-C2D	3.50	1.48	1.39
17	3	306	CLA	C3B-C4B	3.50	1.50	1.42
17	O	204	CLA	CHB-C1B	3.50	1.47	1.39
17	2	307	CLA	C1B-NB	-3.50	1.33	1.37
17	B	837	CLA	C3D-C2D	3.50	1.48	1.39
17	A	803	CLA	CHC-C1C	3.50	1.45	1.38
17	B	811	CLA	CHC-C4B	3.50	1.47	1.39
17	B	804	CLA	O2A-CGA	3.50	1.43	1.33
25	3	316	5X6	C28-C29	3.50	1.57	1.45
17	A	836	CLA	CHB-C1B	3.50	1.47	1.39
25	1	314	5X6	C05-C06	3.49	1.57	1.52
17	A	829	CLA	CHC-C4B	3.49	1.47	1.39
25	5	315	5X6	C20-C21	3.49	1.54	1.43
17	A	814	CLA	C3D-C2D	3.49	1.48	1.39
17	2	308	CLA	CHB-C1B	3.49	1.47	1.39
17	A	825	CLA	C3D-C2D	3.49	1.48	1.39
17	B	833	CLA	CHB-C1B	3.49	1.47	1.39
17	F	204	CLA	C1B-NB	-3.49	1.33	1.37
17	A	808	CLA	C3B-C4B	3.49	1.50	1.42
17	B	829	CLA	C3D-C2D	3.48	1.48	1.39
17	B	804	CLA	C1D-ND	3.48	1.42	1.37
25	5	316	5X6	C15-C14	3.48	1.54	1.43
17	A	853	CLA	C4B-NB	-3.48	1.33	1.37
25	1	312	5X6	C28-C29	3.48	1.57	1.45
17	B	818	CLA	CHD-C1D	3.48	1.45	1.38
16	A	801	CL0	C3D-C2D	3.48	1.48	1.39
17	2	308	CLA	C3B-C4B	3.48	1.50	1.42
20	I	101	BCR	C10-C9	3.48	1.40	1.35
17	B	816	CLA	C3D-C2D	3.48	1.48	1.39
17	A	803	CLA	CHB-C1B	3.48	1.47	1.39
17	4	307	CLA	C1B-NB	-3.48	1.33	1.37
17	B	815	CLA	CHD-C4C	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	832	CLA	CHB-C1B	3.48	1.47	1.39
25	5	315	5X6	C28-C29	3.48	1.57	1.45
17	B	810	CLA	CHC-C1C	3.47	1.45	1.38
17	B	815	CLA	CHD-C1D	3.47	1.45	1.38
17	1	306	CLA	CHB-C1B	3.47	1.47	1.39
17	A	809	CLA	CHD-C4C	3.47	1.47	1.39
17	F	203	CLA	CHC-C4B	3.47	1.47	1.39
17	A	836	CLA	CHC-C4B	3.47	1.47	1.39
17	B	822	CLA	CHB-C1B	3.47	1.47	1.39
17	A	812	CLA	CHD-C4C	3.47	1.47	1.39
17	L	203	CLA	CHD-C4C	3.47	1.47	1.39
17	B	824	CLA	C3D-C2D	3.47	1.48	1.39
17	4	303	CLA	C3B-C4B	3.47	1.50	1.42
17	B	825	CLA	CHB-C1B	3.47	1.47	1.39
17	A	853	CLA	O2A-CGA	3.46	1.43	1.33
17	A	819	CLA	C3D-C2D	3.46	1.48	1.39
17	B	820	CLA	CHC-C4B	3.46	1.47	1.39
17	1	307	CLA	C1B-NB	-3.46	1.33	1.37
20	A	846	BCR	C21-C22	3.46	1.40	1.35
17	B	823	CLA	C3D-C2D	3.46	1.48	1.39
20	A	843	BCR	C17-C18	3.46	1.40	1.35
20	L	205	BCR	C17-C18	3.46	1.40	1.35
17	A	833	CLA	CHD-C1D	3.46	1.45	1.38
17	A	829	CLA	CHD-C1D	3.46	1.45	1.38
25	1	314	5X6	C20-C21	3.46	1.54	1.43
20	L	201	BCR	C14-C13	3.46	1.40	1.35
17	A	820	CLA	CHC-C4B	3.46	1.47	1.39
17	5	313	CLA	C3D-C2D	3.46	1.48	1.39
17	B	817	CLA	C3B-C4B	3.45	1.50	1.42
25	5	318	5X6	C05-C06	3.45	1.57	1.52
17	3	307	CLA	CHB-C1B	3.45	1.47	1.39
17	B	811	CLA	CHD-C1D	3.45	1.45	1.38
17	B	825	CLA	CHD-C1D	3.45	1.45	1.38
17	5	307	CLA	C3B-C4B	3.45	1.50	1.42
17	2	304	CLA	C3B-C4B	3.45	1.50	1.42
17	A	808	CLA	CHD-C1D	3.45	1.45	1.38
20	A	846	BCR	C23-C22	-3.45	1.38	1.45
17	B	804	CLA	C3D-C2D	3.45	1.48	1.39
17	K	102	CLA	OBD-CAD	3.45	1.28	1.22
17	A	810	CLA	CHC-C4B	3.45	1.47	1.39
25	J	105	5X6	C16-C17	3.45	1.53	1.45
17	A	854	CLA	O2A-CGA	3.45	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	821	CLA	OBD-CAD	3.45	1.28	1.22
17	A	829	CLA	CHD-C4C	3.44	1.47	1.39
17	A	817	CLA	O2A-CGA	3.44	1.43	1.33
20	B	847	BCR	C21-C22	3.44	1.40	1.35
17	J	103	CLA	C3D-C2D	3.44	1.48	1.39
25	5	316	5X6	C05-C06	3.44	1.57	1.52
17	B	822	CLA	OBD-CAD	3.44	1.28	1.22
17	B	806	CLA	C1D-ND	3.44	1.42	1.37
17	B	838	CLA	CHD-C1D	3.44	1.45	1.38
25	3	316	5X6	C05-C06	3.44	1.57	1.52
17	A	859	CLA	C3D-C2D	3.44	1.48	1.39
17	A	859	CLA	CHD-C4C	3.44	1.47	1.39
17	B	836	CLA	CHD-C1D	3.44	1.45	1.38
17	2	310	CLA	OBD-CAD	3.44	1.28	1.22
17	4	307	CLA	CHB-C1B	3.44	1.47	1.39
17	2	309	CLA	C1B-NB	-3.44	1.33	1.37
17	A	808	CLA	CHD-C4C	3.44	1.47	1.39
20	A	846	BCR	C14-C13	3.44	1.40	1.35
17	K	102	CLA	C3B-C4B	3.43	1.50	1.42
17	1	306	CLA	C3B-C4B	3.43	1.50	1.42
17	A	830	CLA	CHD-C1D	3.43	1.45	1.38
25	2	318	5X6	C28-C29	3.43	1.57	1.45
17	A	802	CLA	C4B-NB	-3.43	1.33	1.37
17	5	305	CLA	C3D-C2D	3.43	1.48	1.39
17	B	827	CLA	C4B-NB	-3.43	1.33	1.37
17	1	306	CLA	C1B-NB	-3.43	1.33	1.37
17	A	853	CLA	CHC-C1C	3.43	1.45	1.38
17	A	822	CLA	C4B-NB	-3.42	1.33	1.37
17	5	304	CLA	C1B-NB	-3.42	1.33	1.37
17	B	805	CLA	CHD-C4C	3.42	1.47	1.39
25	2	321	5X6	C05-C06	3.42	1.57	1.52
17	1	306	CLA	OBD-CAD	3.42	1.28	1.22
17	2	307	CLA	C3D-C2D	3.42	1.48	1.39
17	B	821	CLA	C1B-NB	-3.42	1.33	1.37
25	1	314	5X6	C28-C29	3.42	1.57	1.45
17	A	802	CLA	CHB-C1B	3.42	1.47	1.39
17	3	308	CLA	C3B-C4B	3.42	1.50	1.42
17	B	805	CLA	C1D-ND	3.42	1.42	1.37
17	A	832	CLA	C1B-NB	-3.42	1.33	1.37
17	B	823	CLA	C1B-NB	-3.42	1.33	1.37
17	A	805	CLA	CHC-C1C	3.41	1.45	1.38
17	B	820	CLA	OBD-CAD	3.41	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	812	CLA	CHB-C1B	3.41	1.47	1.39
25	5	301	5X6	C28-C29	3.41	1.57	1.45
17	5	303	CLA	C1B-NB	-3.41	1.33	1.37
17	A	821	CLA	C3D-C2D	3.41	1.48	1.39
17	A	805	CLA	CHD-C4C	3.41	1.47	1.39
17	A	830	CLA	OBD-CAD	3.41	1.28	1.22
17	A	807	CLA	CHD-C1D	3.41	1.45	1.38
17	A	809	CLA	CHB-C1B	3.41	1.47	1.39
17	B	827	CLA	CHB-C1B	3.40	1.47	1.39
17	B	820	CLA	C3B-C4B	3.40	1.50	1.42
17	A	853	CLA	CHC-C4B	3.40	1.47	1.39
20	O	202	BCR	C23-C22	-3.40	1.38	1.45
17	B	825	CLA	C4B-NB	-3.40	1.33	1.37
17	L	204	CLA	C3B-C4B	3.40	1.50	1.42
17	2	311	CLA	CHB-C1B	3.40	1.47	1.39
17	A	807	CLA	OBD-CAD	3.40	1.28	1.22
17	B	808	CLA	CHD-C1D	3.40	1.45	1.38
20	B	848	BCR	C23-C22	-3.40	1.38	1.45
17	B	812	CLA	CHD-C4C	3.40	1.47	1.39
17	B	831	CLA	CHD-C4C	3.40	1.47	1.39
20	B	848	BCR	C17-C18	3.40	1.40	1.35
17	2	309	CLA	CHC-C4B	3.40	1.47	1.39
17	A	822	CLA	OBD-CAD	3.40	1.28	1.22
17	B	833	CLA	CHC-C1C	3.40	1.45	1.38
17	B	810	CLA	C3D-C2D	3.40	1.48	1.39
17	B	838	CLA	C3D-C2D	3.40	1.48	1.39
17	A	826	CLA	CHC-C1C	3.40	1.45	1.38
25	5	318	5X6	C28-C29	3.39	1.57	1.45
17	B	813	CLA	C3B-C4B	3.39	1.50	1.42
17	L	202	CLA	C1B-NB	-3.39	1.33	1.37
17	A	828	CLA	OBD-CAD	3.39	1.28	1.22
25	4	313	5X6	C05-C06	3.39	1.57	1.52
17	A	818	CLA	CHC-C4B	3.39	1.47	1.39
17	B	839	CLA	CHB-C1B	3.39	1.47	1.39
17	B	840	CLA	C3D-C2D	3.39	1.48	1.39
17	B	838	CLA	CHD-C4C	3.39	1.47	1.39
17	B	840	CLA	CHB-C1B	3.39	1.47	1.39
25	3	317	5X6	C28-C29	3.39	1.57	1.45
17	A	830	CLA	C4B-NB	-3.39	1.33	1.37
17	F	203	CLA	CHB-C1B	3.39	1.47	1.39
17	A	836	CLA	CHD-C4C	3.38	1.47	1.39
17	F	204	CLA	CHC-C4B	3.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	821	CLA	C3B-C4B	3.38	1.50	1.42
25	5	315	5X6	C05-C06	3.38	1.57	1.52
17	J	103	CLA	CHC-C4B	3.38	1.47	1.39
17	B	801	CLA	CHC-C1C	3.38	1.45	1.38
17	A	855	CLA	CHB-C1B	3.38	1.47	1.39
17	2	306	CLA	C1B-NB	-3.38	1.33	1.37
17	B	809	CLA	CHD-C1D	3.38	1.44	1.38
17	3	306	CLA	OBD-CAD	3.38	1.28	1.22
17	B	834	CLA	CHC-C4B	3.38	1.47	1.39
17	B	813	CLA	C3D-C2D	3.38	1.48	1.39
17	B	826	CLA	CHD-C1D	3.37	1.44	1.38
17	B	826	CLA	CHD-C4C	3.37	1.46	1.39
17	B	802	CLA	CHC-C1C	3.37	1.45	1.38
17	A	852	CLA	OBD-CAD	3.37	1.28	1.22
17	A	816	CLA	CHC-C4B	3.37	1.47	1.39
17	5	308	CLA	OBD-CAD	3.37	1.28	1.22
17	B	813	CLA	C1B-NB	-3.37	1.33	1.37
20	B	803	BCR	C14-C13	3.37	1.40	1.35
25	J	105	5X6	C05-C06	3.37	1.57	1.52
17	A	813	CLA	C3D-C2D	3.37	1.48	1.39
17	A	807	CLA	CHB-C1B	3.37	1.47	1.39
17	1	301	CLA	C3B-C4B	3.37	1.50	1.42
25	5	317	5X6	C05-C06	3.36	1.57	1.52
17	4	305	CLA	OBD-CAD	3.36	1.28	1.22
17	3	310	CLA	OBD-CAD	3.36	1.28	1.22
25	J	105	5X6	C20-C21	3.36	1.53	1.43
17	B	807	CLA	CHD-C4C	3.36	1.46	1.39
17	1	309	CLA	C1B-NB	-3.36	1.33	1.37
17	2	310	CLA	C1B-NB	-3.36	1.33	1.37
17	1	301	CLA	C1B-NB	-3.36	1.33	1.37
17	2	308	CLA	C1B-NB	-3.36	1.33	1.37
25	J	105	5X6	C24-C25	3.36	1.53	1.43
17	A	856	CLA	CHC-C4B	3.36	1.46	1.39
17	B	841	CLA	OBD-CAD	3.35	1.28	1.22
17	B	807	CLA	CHC-C1C	3.35	1.45	1.38
17	B	837	CLA	CHB-C1B	3.35	1.46	1.39
20	B	848	BCR	C14-C13	3.35	1.40	1.35
17	A	804	CLA	CHD-C1D	3.35	1.44	1.38
17	A	831	CLA	CHC-C4B	3.35	1.46	1.39
17	J	103	CLA	OBD-CAD	3.35	1.28	1.22
17	4	304	CLA	C1B-NB	-3.35	1.33	1.37
17	A	833	CLA	CHD-C4C	3.35	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	823	CLA	C4B-NB	-3.35	1.33	1.37
17	B	831	CLA	CHB-C1B	3.34	1.46	1.39
17	A	834	CLA	CHC-C4B	3.34	1.46	1.39
20	A	844	BCR	C8-C9	-3.34	1.38	1.45
20	I	101	BCR	C21-C22	3.34	1.40	1.35
17	A	820	CLA	OBD-CAD	3.34	1.28	1.22
17	B	806	CLA	C4B-NB	-3.34	1.33	1.37
17	A	825	CLA	C1C-NC	-3.34	1.32	1.37
17	B	830	CLA	CHB-C1B	3.34	1.46	1.39
17	B	828	CLA	CHC-C1C	3.34	1.45	1.38
17	B	841	CLA	C1B-NB	-3.33	1.33	1.37
17	5	305	CLA	C1B-NB	-3.33	1.33	1.37
17	B	815	CLA	C3D-C2D	3.33	1.48	1.39
17	B	857	CLA	CHD-C1D	3.33	1.44	1.38
25	5	316	5X6	C24-C25	3.33	1.53	1.43
17	A	838	CLA	CHB-C1B	3.33	1.46	1.39
17	A	838	CLA	CHC-C4B	3.33	1.46	1.39
17	B	802	CLA	C1D-ND	3.33	1.41	1.37
17	A	835	CLA	CHB-C1B	3.32	1.46	1.39
17	A	808	CLA	OBD-CAD	3.32	1.28	1.22
17	B	825	CLA	C3D-C2D	3.32	1.48	1.39
17	5	307	CLA	CHB-C1B	3.32	1.46	1.39
17	A	821	CLA	C1B-NB	-3.32	1.33	1.37
17	A	854	CLA	C1D-ND	3.32	1.41	1.37
17	A	827	CLA	CHB-C1B	3.32	1.46	1.39
17	B	857	CLA	CHC-C4B	3.32	1.46	1.39
17	B	807	CLA	CHC-C4B	3.32	1.46	1.39
17	A	802	CLA	C3D-C2D	3.32	1.48	1.39
20	O	202	BCR	C8-C9	-3.31	1.38	1.45
17	A	823	CLA	CHB-C1B	3.31	1.46	1.39
17	B	802	CLA	C3D-C2D	3.31	1.48	1.39
17	5	306	CLA	C1B-NB	-3.31	1.33	1.37
17	B	805	CLA	OBD-CAD	3.31	1.28	1.22
17	B	819	CLA	CHB-C1B	3.31	1.46	1.39
17	A	856	CLA	CHB-C1B	3.31	1.46	1.39
17	B	801	CLA	CHD-C4C	3.31	1.46	1.39
17	B	832	CLA	CHC-C4B	3.31	1.46	1.39
17	A	834	CLA	CHB-C1B	3.31	1.46	1.39
17	5	304	CLA	C3B-C4B	3.31	1.50	1.42
17	A	853	CLA	CHD-C4C	3.30	1.46	1.39
17	A	859	CLA	CHD-C1D	3.30	1.44	1.38
17	A	859	CLA	CHC-C4B	3.30	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	810	CLA	C1D-ND	3.30	1.41	1.37
17	A	828	CLA	C1C-NC	-3.30	1.32	1.37
17	B	816	CLA	CHC-C4B	3.30	1.46	1.39
17	A	856	CLA	CHD-C1D	3.30	1.44	1.38
17	B	835	CLA	C3B-C4B	3.30	1.50	1.42
17	B	832	CLA	C4B-NB	-3.30	1.33	1.37
17	B	834	CLA	CHB-C1B	3.29	1.46	1.39
17	A	815	CLA	CHC-C4B	3.29	1.46	1.39
25	2	318	5X6	C05-C06	3.29	1.57	1.52
17	A	812	CLA	C3D-C2D	3.29	1.48	1.39
17	A	821	CLA	CHD-C4C	3.29	1.46	1.39
17	A	816	CLA	C3D-C2D	3.29	1.48	1.39
17	A	830	CLA	CHD-C4C	3.29	1.46	1.39
17	A	827	CLA	C1D-ND	3.29	1.41	1.37
17	A	809	CLA	OBD-CAD	3.29	1.28	1.22
17	F	204	CLA	C3B-C4B	3.29	1.50	1.42
17	A	822	CLA	C3D-C2D	3.28	1.48	1.39
17	A	803	CLA	OBD-CAD	3.28	1.28	1.22
17	A	837	CLA	C3B-C4B	3.28	1.50	1.42
17	A	805	CLA	CHD-C1D	3.28	1.44	1.38
17	B	812	CLA	OBD-CAD	3.28	1.28	1.22
17	B	805	CLA	CHD-C1D	3.28	1.44	1.38
17	A	812	CLA	C1D-ND	3.27	1.41	1.37
25	F	205	5X6	C23-C22	3.27	1.53	1.45
17	B	827	CLA	C1D-ND	3.27	1.41	1.37
17	B	807	CLA	C1D-ND	3.27	1.41	1.37
17	B	808	CLA	CHB-C1B	3.27	1.46	1.39
20	A	844	BCR	C14-C13	3.27	1.40	1.35
17	A	828	CLA	CHB-C1B	3.27	1.46	1.39
17	B	809	CLA	CHC-C4B	3.27	1.46	1.39
17	B	812	CLA	C3D-C2D	3.27	1.48	1.39
17	B	818	CLA	CHD-C4C	3.26	1.46	1.39
17	A	823	CLA	CHC-C1C	3.26	1.45	1.38
25	5	316	5X6	C20-C21	3.26	1.53	1.43
20	A	857	BCR	C21-C22	3.26	1.40	1.35
20	A	857	BCR	C14-C13	3.26	1.40	1.35
17	2	313	CLA	C1B-NB	-3.26	1.33	1.37
17	A	839	CLA	C1C-NC	-3.26	1.32	1.37
17	5	308	CLA	C4B-NB	-3.26	1.33	1.37
17	5	304	CLA	C4B-NB	-3.26	1.33	1.37
17	J	103	CLA	C1B-NB	-3.26	1.33	1.37
17	3	314	CLA	C1B-NB	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	837	CLA	CHD-C4C	3.25	1.46	1.39
17	2	305	CLA	C1B-NB	-3.25	1.33	1.37
25	5	301	5X6	C05-C06	3.25	1.57	1.52
17	2	310	CLA	CHB-C1B	3.25	1.46	1.39
17	A	826	CLA	CHC-C4B	3.25	1.46	1.39
17	B	834	CLA	CHD-C4C	3.25	1.46	1.39
17	B	805	CLA	C3D-C2D	3.25	1.48	1.39
17	3	310	CLA	CHB-C1B	3.24	1.46	1.39
17	A	821	CLA	CHB-C1B	3.24	1.46	1.39
20	A	844	BCR	C21-C22	3.24	1.40	1.35
25	1	313	5X6	C28-C29	3.24	1.56	1.45
17	A	809	CLA	CHC-C4B	3.24	1.46	1.39
17	B	804	CLA	CHC-C1C	3.24	1.45	1.38
17	B	830	CLA	CHD-C1D	3.24	1.44	1.38
17	A	804	CLA	CHC-C4B	3.24	1.46	1.39
17	B	840	CLA	OBD-CAD	3.23	1.28	1.22
17	B	857	CLA	CHD-C4C	3.23	1.46	1.39
17	B	807	CLA	CHD-C1D	3.23	1.44	1.38
17	3	305	CLA	C1B-NB	-3.23	1.33	1.37
17	A	824	CLA	CHD-C4C	3.23	1.46	1.39
17	3	308	CLA	C1B-NB	-3.23	1.33	1.37
17	B	811	CLA	CHD-C4C	3.22	1.46	1.39
17	A	810	CLA	C3D-C2D	3.22	1.47	1.39
17	5	309	CLA	C3B-C4B	3.22	1.50	1.42
25	2	319	5X6	C11-C03	3.22	1.56	1.45
17	A	822	CLA	C1C-NC	-3.22	1.33	1.37
17	A	834	CLA	C4B-NB	-3.22	1.33	1.37
17	B	819	CLA	C1C-NC	-3.22	1.33	1.37
17	A	819	CLA	CHD-C4C	3.22	1.46	1.39
17	A	811	CLA	OBD-CAD	3.22	1.28	1.22
17	A	802	CLA	CHC-C4B	3.22	1.46	1.39
17	B	837	CLA	CHD-C4C	3.22	1.46	1.39
17	B	840	CLA	CHC-C4B	3.22	1.46	1.39
17	B	838	CLA	CHB-C1B	3.22	1.46	1.39
17	A	803	CLA	C3D-C2D	3.22	1.47	1.39
17	B	833	CLA	CHD-C4C	3.22	1.46	1.39
17	B	801	CLA	CHC-C4B	3.22	1.46	1.39
17	5	309	CLA	C4B-NB	-3.22	1.33	1.37
17	A	835	CLA	C3D-C2D	3.22	1.47	1.39
25	F	205	5X6	C19-C18	3.22	1.53	1.43
20	J	104	BCR	C23-C22	-3.21	1.39	1.45
17	4	310	CLA	C1B-NB	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	105	5X6	C33-C32	3.21	1.56	1.52
17	B	812	CLA	CHC-C4B	3.21	1.46	1.39
17	A	818	CLA	C1B-NB	-3.21	1.33	1.37
17	2	315	CLA	C1B-NB	-3.21	1.33	1.37
17	A	835	CLA	CHD-C4C	3.21	1.46	1.39
17	B	837	CLA	CHC-C4B	3.21	1.46	1.39
17	2	309	CLA	C3B-C4B	3.20	1.50	1.42
17	B	839	CLA	CHD-C4C	3.20	1.46	1.39
17	A	838	CLA	CHD-C1D	3.20	1.44	1.38
17	A	831	CLA	CHB-C1B	3.20	1.46	1.39
17	L	203	CLA	C4B-NB	-3.20	1.33	1.37
17	A	804	CLA	C1D-ND	3.20	1.41	1.37
17	A	828	CLA	C3D-C2D	3.20	1.47	1.39
17	B	839	CLA	CHD-C1D	3.20	1.44	1.38
25	2	317	5X6	C05-C06	3.20	1.56	1.52
17	A	830	CLA	CHC-C4B	3.20	1.46	1.39
17	A	804	CLA	CHD-C4C	3.20	1.46	1.39
20	B	847	BCR	C14-C13	3.20	1.40	1.35
17	B	808	CLA	CHD-C4C	3.20	1.46	1.39
17	A	805	CLA	CHC-C4B	3.20	1.46	1.39
25	J	105	5X6	C15-C14	3.20	1.53	1.43
25	3	317	5X6	C05-C06	3.19	1.56	1.52
17	A	813	CLA	CHB-C1B	3.19	1.46	1.39
17	B	806	CLA	C1C-NC	-3.19	1.33	1.37
17	A	837	CLA	CHB-C1B	3.19	1.46	1.39
16	A	801	CL0	CHC-C1C	3.19	1.45	1.38
17	B	833	CLA	CHC-C4B	3.19	1.46	1.39
17	A	807	CLA	C1D-ND	3.19	1.41	1.37
17	3	311	CLA	C1B-NB	-3.19	1.33	1.37
17	B	817	CLA	OBD-CAD	3.19	1.28	1.22
17	A	815	CLA	CHB-C1B	3.19	1.46	1.39
17	B	811	CLA	CHB-C1B	3.19	1.46	1.39
17	B	827	CLA	CHD-C4C	3.18	1.46	1.39
17	B	830	CLA	CHC-C1C	3.18	1.45	1.38
17	A	854	CLA	C3D-C2D	3.18	1.47	1.39
17	B	808	CLA	C3D-C2D	3.18	1.47	1.39
25	J	105	5X6	C19-C18	3.18	1.53	1.43
17	B	824	CLA	C4B-NB	-3.18	1.33	1.37
17	A	833	CLA	C1D-ND	3.18	1.41	1.37
20	A	857	BCR	C12-C13	-3.18	1.39	1.45
25	3	318	5X6	C05-C06	3.17	1.56	1.52
17	K	103	CLA	OBD-CAD	3.17	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	838	CLA	C3D-C2D	3.17	1.47	1.39
17	B	827	CLA	C3D-C2D	3.17	1.47	1.39
17	A	829	CLA	C1D-ND	3.17	1.41	1.37
17	A	824	CLA	C1B-NB	-3.17	1.33	1.37
17	A	803	CLA	C1D-ND	3.17	1.41	1.37
17	3	313	CLA	C1B-NB	-3.17	1.33	1.37
17	B	829	CLA	CHB-C1B	3.17	1.46	1.39
17	K	103	CLA	C3B-C4B	3.17	1.50	1.42
17	B	808	CLA	C1C-NC	-3.16	1.33	1.37
20	I	101	BCR	C8-C9	-3.16	1.39	1.45
17	B	819	CLA	CHD-C4C	3.16	1.46	1.39
20	B	803	BCR	C21-C22	3.16	1.40	1.35
17	1	303	CLA	CHB-C1B	3.16	1.46	1.39
17	B	826	CLA	C1B-NB	-3.16	1.33	1.37
17	A	821	CLA	C3B-C4B	3.16	1.50	1.42
17	B	826	CLA	CHB-C1B	3.16	1.46	1.39
20	L	201	BCR	C23-C22	-3.16	1.39	1.45
17	A	854	CLA	OBD-CAD	3.16	1.27	1.22
25	5	316	5X6	C28-C29	3.16	1.56	1.45
17	J	103	CLA	C3B-C4B	3.16	1.50	1.42
17	B	818	CLA	CHB-C1B	3.16	1.46	1.39
17	B	807	CLA	CHB-C1B	3.15	1.46	1.39
17	3	310	CLA	C1B-NB	-3.15	1.33	1.37
17	4	303	CLA	C1B-NB	-3.15	1.33	1.37
17	A	834	CLA	C3B-C4B	3.15	1.50	1.42
17	B	805	CLA	C4B-NB	-3.15	1.33	1.37
17	2	304	CLA	C1B-NB	-3.15	1.33	1.37
17	2	312	CLA	C1B-NB	-3.15	1.33	1.37
17	B	802	CLA	CHC-C4B	3.15	1.46	1.39
20	B	845	BCR	C10-C9	3.15	1.40	1.35
17	A	855	CLA	CHD-C4C	3.15	1.46	1.39
17	O	204	CLA	C1B-NB	-3.15	1.33	1.37
17	B	810	CLA	CHD-C4C	3.15	1.46	1.39
17	B	804	CLA	CHD-C1D	3.15	1.44	1.38
17	A	817	CLA	CHD-C4C	3.14	1.46	1.39
17	A	819	CLA	OBD-CAD	3.14	1.27	1.22
17	B	806	CLA	OBD-CAD	3.14	1.27	1.22
17	5	304	CLA	CHB-C1B	3.14	1.46	1.39
17	A	839	CLA	C4B-NB	-3.14	1.33	1.37
17	5	314	CLA	C1B-NB	-3.14	1.33	1.37
17	B	818	CLA	OBD-CAD	3.14	1.27	1.22
16	A	801	CL0	CHD-C4C	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	834	CLA	OBD-CAD	3.14	1.27	1.22
17	B	836	CLA	CHD-C4C	3.14	1.46	1.39
17	A	817	CLA	CHB-C1B	3.14	1.46	1.39
17	B	832	CLA	OBD-CAD	3.13	1.27	1.22
17	A	812	CLA	CHC-C4B	3.13	1.46	1.39
20	A	843	BCR	C23-C22	-3.13	1.39	1.45
17	B	840	CLA	CHC-C1C	3.13	1.44	1.38
17	A	856	CLA	C4B-NB	-3.13	1.33	1.37
17	1	311	CLA	C1B-NB	-3.13	1.33	1.37
17	4	308	CLA	C1B-NB	-3.13	1.33	1.37
17	A	832	CLA	C3D-C4D	-3.13	1.37	1.44
17	5	312	CLA	C1B-NB	-3.13	1.33	1.37
17	A	806	CLA	CHC-C4B	3.13	1.46	1.39
20	A	845	BCR	C8-C9	-3.12	1.39	1.45
17	A	812	CLA	CHD-C1D	3.12	1.44	1.38
17	A	827	CLA	C3D-C2D	3.12	1.47	1.39
17	A	810	CLA	C4B-NB	-3.12	1.33	1.37
17	B	814	CLA	CHD-C4C	3.12	1.46	1.39
17	2	314	CLA	C1B-NB	-3.12	1.33	1.37
17	A	825	CLA	CHC-C4B	3.12	1.46	1.39
17	5	308	CLA	C3B-C4B	3.12	1.50	1.42
17	A	805	CLA	OBD-CAD	3.12	1.27	1.22
17	B	802	CLA	CHD-C1D	3.12	1.44	1.38
17	B	825	CLA	CHC-C4B	3.12	1.46	1.39
17	B	817	CLA	CHB-C1B	3.11	1.46	1.39
25	2	320	5X6	C11-C03	3.11	1.56	1.45
17	3	315	CLA	C1B-NB	-3.11	1.34	1.37
17	B	835	CLA	CHB-C1B	3.11	1.46	1.39
17	A	820	CLA	C1B-NB	-3.11	1.34	1.37
17	5	303	CLA	C4B-NB	-3.11	1.34	1.37
17	B	857	CLA	CHB-C1B	3.11	1.46	1.39
20	A	857	BCR	C8-C9	-3.11	1.39	1.45
17	A	806	CLA	C3D-C2D	3.11	1.47	1.39
17	A	815	CLA	OBD-CAD	3.11	1.27	1.22
17	L	202	CLA	C3B-C4B	3.11	1.50	1.42
17	A	832	CLA	OBD-CAD	3.11	1.27	1.22
17	A	808	CLA	CHC-C4B	3.11	1.46	1.39
17	B	818	CLA	C1B-NB	-3.11	1.34	1.37
17	B	839	CLA	C3D-C2D	3.10	1.47	1.39
17	A	813	CLA	OBD-CAD	3.10	1.27	1.22
17	B	810	CLA	OBD-CAD	3.10	1.27	1.22
17	5	304	CLA	OBD-CAD	3.10	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	814	CLA	CHC-C4B	3.10	1.46	1.39
17	A	839	CLA	CHC-C4B	3.10	1.46	1.39
17	A	824	CLA	C3D-C2D	3.10	1.47	1.39
17	B	830	CLA	C3D-C2D	3.10	1.47	1.39
17	B	802	CLA	OBD-CAD	3.10	1.27	1.22
17	A	822	CLA	CHD-C1D	3.10	1.44	1.38
17	A	824	CLA	CHC-C4B	3.10	1.46	1.39
17	A	812	CLA	C4B-NB	-3.10	1.34	1.37
16	A	801	CL0	OBD-CAD	3.09	1.27	1.22
17	O	203	CLA	C1B-NB	-3.09	1.34	1.37
17	2	306	CLA	OBD-CAD	3.09	1.27	1.22
17	B	809	CLA	C3D-C2D	3.09	1.47	1.39
17	B	826	CLA	CHC-C4B	3.09	1.46	1.39
17	F	204	CLA	C4C-C3C	3.09	1.50	1.45
17	B	806	CLA	CHD-C4C	3.09	1.46	1.39
17	A	832	CLA	CHC-C4B	3.08	1.46	1.39
17	B	814	CLA	C4B-NB	-3.08	1.34	1.37
17	A	832	CLA	CHD-C4C	3.08	1.46	1.39
20	A	846	BCR	C12-C13	-3.08	1.39	1.45
17	O	205	CLA	C1B-NB	-3.08	1.34	1.37
17	2	316	CLA	C1B-NB	-3.08	1.34	1.37
17	B	805	CLA	CHB-C1B	3.08	1.46	1.39
17	B	831	CLA	CHC-C4B	3.08	1.46	1.39
17	A	814	CLA	C3B-C4B	3.08	1.50	1.42
17	4	311	CLA	C1B-NB	-3.07	1.34	1.37
17	A	821	CLA	C4B-NB	-3.07	1.34	1.37
17	B	806	CLA	CHC-C4B	3.07	1.46	1.39
17	1	305	CLA	C4C-C3C	3.07	1.50	1.45
17	A	824	CLA	C1C-NC	-3.07	1.33	1.37
17	A	819	CLA	CHC-C4B	3.07	1.46	1.39
17	B	810	CLA	CHC-C4B	3.07	1.46	1.39
17	1	302	CLA	C4B-NB	-3.06	1.34	1.37
17	B	827	CLA	CHD-C1D	3.06	1.44	1.38
17	A	811	CLA	CHD-C1D	3.06	1.44	1.38
17	2	311	CLA	C1B-NB	-3.06	1.34	1.37
17	A	856	CLA	OBD-CAD	3.06	1.27	1.22
17	B	814	CLA	OBD-CAD	3.06	1.27	1.22
17	B	823	CLA	OBD-CAD	3.06	1.27	1.22
20	B	844	BCR	C17-C18	3.06	1.39	1.35
17	5	305	CLA	CHB-C1B	3.06	1.46	1.39
17	A	824	CLA	CHB-C1B	3.06	1.46	1.39
17	A	806	CLA	CHD-C1D	3.06	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	828	CLA	CHD-C1D	3.06	1.44	1.38
17	A	822	CLA	CHB-C1B	3.06	1.46	1.39
17	2	306	CLA	C4B-NB	-3.05	1.34	1.37
17	B	840	CLA	C3B-C4B	3.05	1.49	1.42
17	3	309	CLA	C1B-NB	-3.05	1.34	1.37
17	1	304	CLA	C1C-C2C	3.05	1.50	1.44
17	A	825	CLA	CHD-C1D	3.05	1.44	1.38
17	A	856	CLA	C3D-C2D	3.05	1.47	1.39
17	A	853	CLA	C1D-ND	3.04	1.41	1.37
17	B	829	CLA	CHC-C1C	3.04	1.44	1.38
17	4	306	CLA	C1B-NB	-3.04	1.34	1.37
17	A	827	CLA	CHC-C4B	3.04	1.46	1.39
17	A	822	CLA	CHD-C4C	3.04	1.46	1.39
17	1	304	CLA	C1B-NB	-3.04	1.34	1.37
17	A	855	CLA	C3D-C2D	3.04	1.47	1.39
17	A	809	CLA	C1D-ND	3.04	1.41	1.37
17	A	803	CLA	CHD-C4C	3.04	1.46	1.39
25	J	105	5X6	C28-C29	3.03	1.55	1.45
20	B	846	BCR	C8-C9	-3.03	1.39	1.45
17	2	308	CLA	C4C-C3C	3.03	1.50	1.45
17	A	825	CLA	OBD-CAD	3.03	1.27	1.22
17	A	833	CLA	CHC-C4B	3.03	1.46	1.39
17	B	829	CLA	CHC-C4B	3.03	1.46	1.39
17	A	826	CLA	C1D-ND	3.03	1.41	1.37
17	B	840	CLA	C1D-ND	3.02	1.41	1.37
17	4	309	CLA	C1B-NB	-3.02	1.34	1.37
17	1	310	CLA	C1B-NB	-3.02	1.34	1.37
17	A	832	CLA	CHB-C1B	3.02	1.46	1.39
25	2	318	5X6	C11-C03	3.02	1.55	1.45
17	5	310	CLA	C1B-NB	-3.02	1.34	1.37
17	B	834	CLA	OBD-CAD	3.02	1.27	1.22
17	B	833	CLA	CHD-C1D	3.02	1.44	1.38
17	B	804	CLA	CHC-C4B	3.01	1.46	1.39
20	L	205	BCR	C23-C22	-3.01	1.39	1.45
17	B	827	CLA	C1C-NC	-3.01	1.33	1.37
17	5	305	CLA	C1C-C2C	3.01	1.50	1.44
17	B	836	CLA	CHB-C1B	3.01	1.46	1.39
17	A	804	CLA	CHC-C1C	3.01	1.44	1.38
17	B	857	CLA	C3B-C4B	3.01	1.49	1.42
17	A	839	CLA	CHD-C1D	3.01	1.44	1.38
16	A	801	CL0	CHC-C4B	3.01	1.46	1.39
20	B	845	BCR	C8-C9	-3.00	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	845	BCR	C12-C13	-3.00	1.39	1.45
20	J	104	BCR	C14-C13	3.00	1.39	1.35
17	B	810	CLA	C1C-NC	-3.00	1.33	1.37
25	F	205	5X6	C24-C25	3.00	1.52	1.43
17	A	823	CLA	C3D-C2D	3.00	1.47	1.39
20	J	104	BCR	C8-C9	-3.00	1.39	1.45
17	B	840	CLA	CHD-C1D	2.99	1.44	1.38
17	B	807	CLA	OBD-CAD	2.99	1.27	1.22
17	A	832	CLA	CHC-C1C	2.99	1.44	1.38
17	A	807	CLA	C1C-NC	-2.99	1.33	1.37
17	B	816	CLA	CHB-C1B	2.99	1.46	1.39
17	B	809	CLA	CHD-C4C	2.99	1.46	1.39
17	B	839	CLA	C1C-NC	-2.99	1.33	1.37
25	4	314	5X6	C11-C03	2.99	1.55	1.45
17	A	838	CLA	C3B-C4B	2.99	1.49	1.42
17	B	828	CLA	CHB-C1B	2.99	1.46	1.39
17	A	821	CLA	C1C-NC	-2.98	1.33	1.37
17	B	829	CLA	OBD-CAD	2.98	1.27	1.22
20	J	104	BCR	C10-C9	2.98	1.39	1.35
17	3	307	CLA	C1B-NB	-2.98	1.34	1.37
17	A	811	CLA	CHD-C4C	2.98	1.46	1.39
25	F	205	5X6	C12-C13	2.97	1.52	1.45
17	A	859	CLA	C3B-C4B	2.97	1.49	1.42
17	4	308	CLA	C1C-C2C	2.97	1.50	1.44
17	A	856	CLA	C1D-ND	2.97	1.41	1.37
17	5	311	CLA	C1B-NB	-2.97	1.34	1.37
25	5	301	5X6	C11-C03	2.97	1.55	1.45
17	B	808	CLA	OBD-CAD	2.97	1.27	1.22
20	B	844	BCR	C19-C18	-2.97	1.39	1.45
17	5	302	CLA	C1B-NB	-2.97	1.34	1.37
17	F	203	CLA	OBD-CAD	2.97	1.27	1.22
17	5	303	CLA	C3B-C4B	2.96	1.49	1.42
25	F	205	5X6	C33-C32	2.96	1.56	1.52
17	B	811	CLA	C3D-C4D	-2.96	1.37	1.44
17	B	836	CLA	C3B-C4B	2.96	1.49	1.42
17	B	836	CLA	CHC-C4B	2.96	1.46	1.39
25	1	315	5X6	C11-C03	2.96	1.55	1.45
20	A	843	BCR	C8-C9	-2.96	1.39	1.45
17	3	312	CLA	C1B-NB	-2.96	1.34	1.37
20	B	847	BCR	C23-C22	-2.96	1.39	1.45
17	A	809	CLA	C3D-C4D	-2.95	1.37	1.44
17	A	833	CLA	OBD-CAD	2.95	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	829	CLA	C3B-C4B	2.95	1.49	1.42
17	B	838	CLA	C1C-NC	-2.95	1.33	1.37
17	B	834	CLA	C3B-C4B	2.95	1.49	1.42
20	A	845	BCR	C14-C13	2.95	1.39	1.35
17	1	307	CLA	C1C-C2C	2.95	1.50	1.44
17	2	306	CLA	C3B-C4B	2.95	1.49	1.42
17	B	833	CLA	C1D-ND	2.95	1.41	1.37
25	2	320	5X6	C05-C06	2.94	1.56	1.52
17	A	817	CLA	OBD-CAD	2.94	1.27	1.22
17	A	835	CLA	OBD-CAD	2.94	1.27	1.22
17	B	819	CLA	C3D-C2D	2.94	1.47	1.39
17	B	825	CLA	OBD-CAD	2.94	1.27	1.22
17	B	812	CLA	C3D-C4D	-2.93	1.37	1.44
17	5	302	CLA	C4C-C3C	2.93	1.50	1.45
17	A	838	CLA	CHD-C4C	2.93	1.45	1.39
17	A	855	CLA	CHD-C1D	2.93	1.44	1.38
17	2	313	CLA	C4C-C3C	2.93	1.50	1.45
17	A	839	CLA	C1C-C2C	2.92	1.50	1.44
25	2	317	5X6	C11-C03	2.92	1.55	1.45
17	B	819	CLA	CHC-C4B	2.92	1.46	1.39
25	3	316	5X6	C11-C03	2.92	1.55	1.45
17	B	815	CLA	C4B-NB	-2.92	1.34	1.37
17	1	308	CLA	C1B-NB	-2.92	1.34	1.37
17	B	804	CLA	C1C-NC	-2.92	1.33	1.37
17	A	835	CLA	C3B-C4B	2.92	1.49	1.42
17	B	809	CLA	C3B-C4B	2.92	1.49	1.42
17	O	204	CLA	C1C-C2C	2.92	1.50	1.44
17	B	830	CLA	CHD-C4C	2.92	1.45	1.39
17	A	802	CLA	C1B-C2B	2.91	1.50	1.43
17	A	852	CLA	CHB-C1B	2.91	1.45	1.39
25	4	312	5X6	C11-C03	2.91	1.55	1.45
17	A	833	CLA	C3B-C4B	2.91	1.49	1.42
17	B	833	CLA	C3D-C2D	2.91	1.47	1.39
25	3	317	5X6	C11-C03	2.91	1.55	1.45
17	A	837	CLA	CHD-C1D	2.91	1.44	1.38
17	2	310	CLA	C1C-C2C	2.91	1.50	1.44
17	B	827	CLA	OBD-CAD	2.91	1.27	1.22
25	1	312	5X6	C11-C03	2.90	1.55	1.45
17	A	810	CLA	C3D-C4D	-2.90	1.37	1.44
17	B	823	CLA	C3B-C4B	2.90	1.49	1.42
25	5	317	5X6	C11-C03	2.90	1.55	1.45
17	A	804	CLA	OBD-CAD	2.90	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	823	CLA	CHD-C4C	2.90	1.45	1.39
17	A	806	CLA	C1D-ND	2.90	1.41	1.37
20	I	101	BCR	C23-C22	-2.90	1.39	1.45
17	B	825	CLA	CHD-C4C	2.90	1.45	1.39
20	J	104	BCR	C21-C22	2.90	1.39	1.35
20	L	201	BCR	C17-C18	2.90	1.39	1.35
20	B	803	BCR	C8-C9	-2.90	1.39	1.45
17	2	306	CLA	C1B-C2B	2.90	1.50	1.43
17	A	817	CLA	CHC-C4B	2.89	1.45	1.39
17	B	817	CLA	C1B-NB	-2.89	1.34	1.37
17	B	824	CLA	C1C-C2C	2.89	1.50	1.44
25	F	205	5X6	C15-C14	2.89	1.52	1.43
25	4	313	5X6	C11-C03	2.89	1.55	1.45
17	B	826	CLA	C1C-NC	-2.89	1.33	1.37
17	A	826	CLA	C1C-C2C	2.89	1.50	1.44
25	3	318	5X6	C11-C03	2.89	1.55	1.45
17	F	204	CLA	C4B-NB	-2.89	1.34	1.37
17	B	811	CLA	C1D-ND	2.88	1.41	1.37
17	1	303	CLA	C1C-C2C	2.88	1.50	1.44
17	B	801	CLA	CHB-C1B	2.88	1.45	1.39
25	1	316	5X6	C11-C03	2.88	1.55	1.45
17	2	311	CLA	C1C-C2C	2.88	1.50	1.44
20	A	845	BCR	C19-C18	-2.88	1.39	1.45
17	A	809	CLA	C3B-C4B	2.88	1.49	1.42
17	A	826	CLA	CHB-C1B	2.88	1.45	1.39
20	B	844	BCR	C23-C22	-2.88	1.39	1.45
17	A	833	CLA	CHB-C1B	2.87	1.45	1.39
17	B	841	CLA	C1C-C2C	2.87	1.50	1.44
17	A	825	CLA	CHD-C4C	2.87	1.45	1.39
25	5	318	5X6	C11-C03	2.87	1.55	1.45
17	A	828	CLA	CHD-C4C	2.86	1.45	1.39
17	B	825	CLA	C1C-C2C	2.86	1.50	1.44
17	A	829	CLA	CHB-C1B	2.86	1.45	1.39
20	A	845	BCR	C17-C18	2.86	1.39	1.35
17	2	305	CLA	C1C-C2C	2.86	1.50	1.44
17	A	832	CLA	C1D-ND	2.85	1.41	1.37
25	1	313	5X6	C11-C03	2.85	1.55	1.45
20	B	803	BCR	C23-C22	-2.85	1.39	1.45
17	A	815	CLA	C4B-NB	-2.85	1.34	1.37
17	A	826	CLA	CHD-C1D	2.85	1.43	1.38
20	I	101	BCR	C12-C13	-2.85	1.39	1.45
20	A	846	BCR	C10-C9	2.85	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	817	CLA	C1C-NC	-2.85	1.33	1.37
17	B	833	CLA	C3D-C4D	-2.85	1.37	1.44
17	B	837	CLA	C1C-NC	-2.84	1.33	1.37
17	A	803	CLA	CHC-C4B	2.84	1.45	1.39
17	B	809	CLA	C3D-C4D	-2.84	1.37	1.44
17	B	837	CLA	OBD-CAD	2.84	1.27	1.22
17	2	314	CLA	C1C-C2C	2.84	1.50	1.44
17	A	823	CLA	CHD-C1D	2.84	1.43	1.38
17	B	809	CLA	C1B-C2B	2.84	1.49	1.43
17	1	301	CLA	C4C-C3C	2.83	1.49	1.45
17	4	306	CLA	C4C-C3C	2.83	1.49	1.45
17	B	857	CLA	C1D-ND	2.83	1.41	1.37
17	B	820	CLA	CHB-C1B	2.83	1.45	1.39
17	3	311	CLA	C1C-C2C	2.83	1.50	1.44
17	A	832	CLA	C1C-NC	-2.83	1.33	1.37
20	L	205	BCR	C12-C13	-2.83	1.39	1.45
17	A	804	CLA	C1C-NC	-2.83	1.33	1.37
17	B	811	CLA	OBD-CAD	2.83	1.27	1.22
17	A	806	CLA	OBD-CAD	2.83	1.27	1.22
17	A	808	CLA	C1C-NC	-2.83	1.33	1.37
17	B	805	CLA	C3B-C4B	2.83	1.49	1.42
17	B	828	CLA	CHC-C4B	2.82	1.45	1.39
20	A	843	BCR	C12-C13	-2.82	1.39	1.45
17	B	829	CLA	C1C-NC	-2.82	1.33	1.37
17	A	816	CLA	C1C-NC	-2.82	1.33	1.37
17	A	839	CLA	CHD-C4C	2.82	1.45	1.39
17	A	810	CLA	C1B-C2B	2.82	1.49	1.43
17	A	823	CLA	C1B-C2B	2.82	1.49	1.43
17	1	310	CLA	C1C-C2C	2.82	1.50	1.44
17	2	307	CLA	C1C-C2C	2.82	1.50	1.44
25	2	319	5X6	C05-C06	2.81	1.56	1.52
17	A	836	CLA	OBD-CAD	2.81	1.27	1.22
17	B	830	CLA	C1C-NC	-2.81	1.33	1.37
17	B	809	CLA	C1D-ND	2.81	1.41	1.37
17	B	806	CLA	C4D-CHA	2.81	1.48	1.38
17	B	816	CLA	C3B-C4B	2.81	1.49	1.42
17	A	803	CLA	C1C-NC	-2.81	1.33	1.37
17	B	810	CLA	CHD-C1D	2.81	1.43	1.38
17	A	806	CLA	C1C-NC	-2.81	1.33	1.37
17	B	815	CLA	C1B-C2B	2.81	1.49	1.43
17	A	836	CLA	C1D-ND	2.81	1.41	1.37
17	A	855	CLA	C1C-NC	-2.81	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	314	CLA	C1C-C2C	2.80	1.50	1.44
17	B	815	CLA	CHC-C4B	2.80	1.45	1.39
17	2	316	CLA	C1C-C2C	2.80	1.50	1.44
17	A	835	CLA	C3D-C4D	-2.80	1.37	1.44
17	A	806	CLA	CHD-C4C	2.80	1.45	1.39
17	A	816	CLA	CHB-C1B	2.80	1.45	1.39
17	B	829	CLA	C3D-C4D	-2.80	1.37	1.44
17	A	816	CLA	CHD-C4C	2.80	1.45	1.39
17	B	802	CLA	CHD-C4C	2.80	1.45	1.39
17	4	304	CLA	C1C-C2C	2.80	1.50	1.44
17	A	823	CLA	CHC-C4B	2.80	1.45	1.39
17	A	815	CLA	C3B-C4B	2.80	1.49	1.42
17	A	856	CLA	C1B-C2B	2.80	1.49	1.43
17	5	308	CLA	CHB-C1B	2.80	1.45	1.39
25	1	314	5X6	C11-C03	2.79	1.55	1.45
17	4	311	CLA	C1C-C2C	2.79	1.50	1.44
20	B	848	BCR	C19-C18	-2.79	1.39	1.45
25	F	205	5X6	C20-C21	2.79	1.52	1.43
17	1	311	CLA	C4C-C3C	2.79	1.49	1.45
17	A	838	CLA	OBD-CAD	2.79	1.27	1.22
17	3	314	CLA	C1C-C2C	2.79	1.50	1.44
17	B	829	CLA	C1D-ND	2.78	1.41	1.37
17	4	309	CLA	C1C-C2C	2.78	1.49	1.44
17	A	823	CLA	C1C-NC	-2.78	1.33	1.37
17	B	824	CLA	CHB-C1B	2.78	1.45	1.39
17	A	819	CLA	C1C-NC	-2.78	1.33	1.37
17	4	306	CLA	C1C-C2C	2.77	1.49	1.44
17	5	312	CLA	C1C-C2C	2.77	1.49	1.44
17	5	310	CLA	C1C-C2C	2.77	1.49	1.44
17	2	313	CLA	C1C-C2C	2.77	1.49	1.44
20	L	205	BCR	C8-C9	-2.77	1.40	1.45
16	A	801	CL0	CHD-C1D	2.77	1.43	1.38
17	3	305	CLA	C1C-C2C	2.77	1.49	1.44
20	B	844	BCR	C21-C22	2.77	1.39	1.35
20	A	845	BCR	C21-C22	2.77	1.39	1.35
17	3	307	CLA	C1C-C2C	2.76	1.49	1.44
20	I	101	BCR	C14-C13	2.76	1.39	1.35
20	B	847	BCR	C8-C9	-2.76	1.40	1.45
17	A	820	CLA	C1C-NC	-2.76	1.33	1.37
17	B	827	CLA	CHC-C4B	2.76	1.45	1.39
17	A	807	CLA	CHD-C4C	2.76	1.45	1.39
20	B	847	BCR	C12-C13	-2.76	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	822	CLA	C3B-C4B	2.76	1.49	1.42
17	3	309	CLA	C1C-C2C	2.75	1.49	1.44
17	4	303	CLA	C4C-C3C	2.75	1.49	1.45
17	A	807	CLA	C3D-C2D	2.75	1.46	1.39
17	A	855	CLA	CHC-C4B	2.75	1.45	1.39
17	A	806	CLA	C1B-C2B	2.75	1.49	1.43
17	K	103	CLA	C3D-C4D	-2.75	1.38	1.44
17	B	830	CLA	CHC-C4B	2.75	1.45	1.39
17	A	830	CLA	C3D-C4D	-2.74	1.38	1.44
25	2	321	5X6	C11-C03	2.74	1.54	1.45
17	A	859	CLA	C1C-NC	-2.74	1.33	1.37
17	B	857	CLA	C1C-NC	-2.74	1.33	1.37
20	A	844	BCR	C12-C13	-2.74	1.40	1.45
17	A	819	CLA	CHB-C1B	2.74	1.45	1.39
17	B	802	CLA	C1C-NC	-2.73	1.33	1.37
20	B	846	BCR	C23-C22	-2.73	1.40	1.45
17	1	303	CLA	C4B-NB	-2.73	1.34	1.37
17	L	204	CLA	C1C-C2C	2.73	1.49	1.44
20	B	844	BCR	C8-C9	-2.73	1.40	1.45
17	B	830	CLA	OBD-CAD	2.73	1.27	1.22
17	B	808	CLA	C1C-C2C	2.73	1.49	1.44
17	5	303	CLA	C1B-C2B	2.73	1.49	1.43
17	5	308	CLA	C1C-C2C	2.73	1.49	1.44
17	B	818	CLA	C3B-C4B	2.72	1.49	1.42
17	B	840	CLA	C1C-NC	-2.72	1.33	1.37
17	B	822	CLA	C1B-NB	-2.72	1.34	1.37
17	3	308	CLA	C1C-C2C	2.72	1.49	1.44
17	1	303	CLA	C3D-C4D	-2.72	1.38	1.44
17	3	312	CLA	C1C-C2C	2.72	1.49	1.44
17	5	310	CLA	C4C-C3C	2.72	1.49	1.45
17	K	103	CLA	C4B-NB	-2.72	1.34	1.37
17	L	203	CLA	C3B-C4B	2.72	1.49	1.42
17	A	823	CLA	C1C-C2C	2.72	1.49	1.44
17	K	102	CLA	C1C-C2C	2.72	1.49	1.44
17	O	205	CLA	C1C-C2C	2.71	1.49	1.44
17	B	857	CLA	OBD-CAD	2.71	1.27	1.22
17	3	310	CLA	C1C-C2C	2.71	1.49	1.44
17	A	816	CLA	OBD-CAD	2.71	1.27	1.22
17	3	306	CLA	C4B-NB	-2.71	1.34	1.37
17	L	203	CLA	C1B-C2B	2.71	1.49	1.43
17	A	831	CLA	C1C-C2C	2.71	1.49	1.44
17	2	315	CLA	C1C-C2C	2.71	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	812	CLA	C1C-NC	-2.71	1.33	1.37
17	A	814	CLA	C4B-NB	-2.70	1.34	1.37
17	5	313	CLA	C4B-NB	-2.70	1.34	1.37
17	A	808	CLA	CHB-C1B	2.70	1.45	1.39
17	4	310	CLA	C1C-C2C	2.70	1.49	1.44
17	A	828	CLA	CHC-C4B	2.70	1.45	1.39
17	L	202	CLA	C4B-NB	-2.70	1.34	1.37
25	5	315	5X6	C11-C03	2.70	1.54	1.45
17	A	859	CLA	C1C-C2C	2.70	1.49	1.44
17	A	823	CLA	OBD-CAD	2.70	1.27	1.22
17	5	309	CLA	C1C-C2C	2.70	1.49	1.44
17	A	821	CLA	OBD-CAD	2.70	1.27	1.22
17	A	827	CLA	CHD-C4C	2.70	1.45	1.39
17	A	853	CLA	C1B-C2B	2.69	1.49	1.43
17	A	820	CLA	C3B-C4B	2.69	1.49	1.42
17	5	304	CLA	C3D-C4D	-2.69	1.38	1.44
17	3	315	CLA	C1C-C2C	2.69	1.49	1.44
17	B	828	CLA	C3D-C4D	-2.69	1.38	1.44
20	A	844	BCR	C23-C22	-2.69	1.40	1.45
17	A	852	CLA	CHD-C4C	2.69	1.45	1.39
17	B	818	CLA	C1C-NC	-2.68	1.33	1.37
20	L	206	BCR	C8-C9	-2.68	1.40	1.45
17	A	838	CLA	C4B-NB	-2.68	1.34	1.37
16	A	801	CL0	C1C-NC	-2.68	1.33	1.37
17	A	829	CLA	C3D-C4D	-2.68	1.38	1.44
20	L	201	BCR	C21-C22	2.68	1.39	1.35
17	A	807	CLA	C3D-C4D	-2.68	1.38	1.44
17	A	828	CLA	CHC-C1C	2.68	1.44	1.38
17	B	823	CLA	C1B-C2B	2.68	1.49	1.43
17	A	813	CLA	C1C-NC	-2.68	1.33	1.37
17	B	822	CLA	C1C-C2C	2.68	1.49	1.44
17	3	313	CLA	C1C-C2C	2.68	1.49	1.44
17	2	308	CLA	C4B-NB	-2.68	1.34	1.37
17	B	826	CLA	C3B-C4B	2.67	1.49	1.42
17	A	804	CLA	C3D-C4D	-2.67	1.38	1.44
17	B	828	CLA	C1D-ND	2.67	1.41	1.37
17	A	835	CLA	C1C-C2C	2.67	1.49	1.44
17	B	826	CLA	OBD-CAD	2.67	1.27	1.22
17	A	802	CLA	C3B-C4B	2.67	1.49	1.42
17	5	309	CLA	C1B-C2B	2.67	1.49	1.43
20	J	104	BCR	C19-C18	-2.67	1.40	1.45
17	2	312	CLA	C4C-C3C	2.67	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	822	CLA	C1C-C2C	2.66	1.49	1.44
17	B	801	CLA	C1C-NC	-2.66	1.33	1.37
17	B	817	CLA	C1C-C2C	2.66	1.49	1.44
17	B	832	CLA	C3D-C4D	-2.66	1.38	1.44
17	5	313	CLA	C4C-C3C	2.66	1.49	1.45
17	1	309	CLA	C1C-C2C	2.66	1.49	1.44
17	A	831	CLA	OBD-CAD	2.65	1.27	1.22
17	A	826	CLA	C3D-C4D	-2.65	1.38	1.44
17	A	814	CLA	C4C-C3C	2.65	1.49	1.45
17	B	836	CLA	C1C-NC	-2.65	1.33	1.37
17	B	823	CLA	C1C-C2C	2.65	1.49	1.44
17	A	830	CLA	C1B-C2B	2.65	1.49	1.43
17	B	838	CLA	C3D-C4D	-2.65	1.38	1.44
17	A	859	CLA	C4B-NB	-2.65	1.34	1.37
17	5	311	CLA	C1C-C2C	2.64	1.49	1.44
17	1	301	CLA	C4B-NB	-2.64	1.34	1.37
17	B	814	CLA	C3D-C4D	-2.64	1.38	1.44
17	A	827	CLA	C1C-NC	-2.64	1.33	1.37
17	1	303	CLA	OBD-CAD	2.64	1.27	1.22
17	3	312	CLA	C4C-C3C	2.64	1.49	1.45
17	1	305	CLA	C1C-C2C	2.63	1.49	1.44
17	A	809	CLA	C4B-NB	-2.63	1.34	1.37
17	O	203	CLA	C1C-C2C	2.63	1.49	1.44
17	B	828	CLA	CHD-C1D	2.63	1.43	1.38
17	A	810	CLA	OBD-CAD	2.63	1.27	1.22
20	A	857	BCR	C23-C22	-2.63	1.40	1.45
17	2	304	CLA	C1B-C2B	2.63	1.49	1.43
17	2	312	CLA	C1B-C2B	2.63	1.49	1.43
17	O	205	CLA	C4D-CHA	2.63	1.47	1.38
17	A	809	CLA	CHD-C1D	2.62	1.43	1.38
17	5	302	CLA	C1C-C2C	2.62	1.49	1.44
17	A	813	CLA	C3B-C4B	2.62	1.48	1.42
20	L	206	BCR	C23-C22	-2.62	1.40	1.45
20	B	848	BCR	C8-C9	-2.62	1.40	1.45
17	1	306	CLA	C4B-NB	-2.62	1.34	1.37
20	K	104	BCR	C23-C22	-2.62	1.40	1.45
17	B	813	CLA	OBD-CAD	2.62	1.27	1.22
17	5	309	CLA	C1B-NB	-2.62	1.34	1.37
20	B	843	BCR	C8-C9	-2.61	1.40	1.45
17	B	812	CLA	C3B-C4B	2.61	1.48	1.42
17	O	204	CLA	C4D-CHA	2.61	1.47	1.38
17	A	832	CLA	C3B-C4B	2.61	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	C1C-C2C	2.61	1.49	1.44
20	B	844	BCR	C12-C13	-2.61	1.40	1.45
17	4	309	CLA	C1B-C2B	2.60	1.49	1.43
17	B	801	CLA	C3D-C4D	-2.60	1.38	1.44
17	A	854	CLA	CHD-C1D	2.60	1.43	1.38
17	2	308	CLA	C4D-CHA	2.60	1.47	1.38
17	B	834	CLA	C3D-C4D	-2.60	1.38	1.44
17	A	836	CLA	C3B-C4B	2.60	1.48	1.42
17	B	827	CLA	C3D-C4D	-2.60	1.38	1.44
17	A	826	CLA	OBD-CAD	2.60	1.27	1.22
17	A	852	CLA	CHD-C1D	2.60	1.43	1.38
17	3	310	CLA	C4B-NB	-2.59	1.34	1.37
20	B	848	BCR	C21-C22	2.59	1.39	1.35
17	B	825	CLA	C4D-CHA	2.59	1.47	1.38
16	A	801	CL0	C3D-C4D	-2.59	1.38	1.44
20	M	101	BCR	C8-C9	-2.59	1.40	1.45
17	B	817	CLA	C3D-C4D	-2.59	1.38	1.44
17	B	840	CLA	C3D-C4D	-2.58	1.38	1.44
17	A	824	CLA	C3D-C4D	-2.58	1.38	1.44
17	A	827	CLA	C3B-C4B	2.58	1.48	1.42
17	4	305	CLA	C1C-C2C	2.58	1.49	1.44
20	A	844	BCR	C17-C18	2.58	1.39	1.35
20	I	101	BCR	C19-C18	-2.58	1.40	1.45
17	4	307	CLA	C1C-C2C	2.58	1.49	1.44
17	2	304	CLA	C1C-C2C	2.58	1.49	1.44
17	A	827	CLA	C3D-C4D	-2.58	1.38	1.44
17	1	301	CLA	C1C-C2C	2.58	1.49	1.44
17	2	312	CLA	C4D-CHA	2.58	1.47	1.38
17	5	302	CLA	C1B-C2B	2.57	1.49	1.43
17	A	838	CLA	C3D-C4D	-2.57	1.38	1.44
17	A	818	CLA	C1C-C2C	2.57	1.49	1.44
17	K	103	CLA	C1B-C2B	2.57	1.49	1.43
17	5	310	CLA	C1B-C2B	2.57	1.49	1.43
17	B	807	CLA	C3D-C4D	-2.57	1.38	1.44
17	B	821	CLA	C4B-NB	-2.57	1.34	1.37
17	1	303	CLA	C4D-CHA	2.57	1.47	1.38
17	B	833	CLA	C1B-C2B	2.57	1.49	1.43
17	3	308	CLA	C1B-C2B	2.57	1.49	1.43
17	1	310	CLA	C4C-C3C	2.57	1.49	1.45
25	F	205	5X6	C28-C29	2.57	1.54	1.45
17	A	854	CLA	CHD-C4C	2.57	1.45	1.39
17	5	303	CLA	C1C-C2C	2.56	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	852	CLA	CHC-C4B	2.56	1.45	1.39
20	A	846	BCR	C17-C18	2.56	1.39	1.35
17	B	832	CLA	C3B-C4B	2.56	1.48	1.42
17	1	308	CLA	C1B-C2B	2.56	1.49	1.43
17	2	316	CLA	C4D-CHA	2.56	1.47	1.38
17	A	852	CLA	C4B-NB	-2.56	1.34	1.37
17	1	308	CLA	C4C-C3C	2.56	1.49	1.45
20	J	104	BCR	C12-C13	-2.56	1.40	1.45
17	A	831	CLA	C1C-NC	-2.56	1.34	1.37
17	3	312	CLA	C1B-C2B	2.56	1.49	1.43
20	B	847	BCR	C19-C18	-2.56	1.40	1.45
17	A	838	CLA	C1D-ND	2.56	1.40	1.37
17	B	804	CLA	C1B-C2B	2.56	1.49	1.43
17	B	821	CLA	C4D-CHA	2.55	1.47	1.38
17	B	819	CLA	OBD-CAD	2.55	1.26	1.22
17	B	810	CLA	C3D-C4D	-2.55	1.38	1.44
17	5	314	CLA	C4D-CHA	2.55	1.47	1.38
17	B	836	CLA	C1B-C2B	2.55	1.49	1.43
17	3	308	CLA	C4D-CHA	2.55	1.47	1.38
17	B	817	CLA	C4B-NB	-2.55	1.34	1.37
17	5	306	CLA	C4C-C3C	2.55	1.49	1.45
17	B	823	CLA	C3D-C4D	-2.55	1.38	1.44
17	B	833	CLA	C1C-C2C	2.55	1.49	1.44
17	A	805	CLA	C1B-C2B	2.55	1.49	1.43
17	O	203	CLA	C1B-C2B	2.55	1.49	1.43
20	B	803	BCR	C19-C18	-2.55	1.40	1.45
17	3	314	CLA	C4D-CHA	2.55	1.47	1.38
17	A	835	CLA	C1C-NC	-2.54	1.34	1.37
17	B	811	CLA	C3B-C4B	2.54	1.48	1.42
17	5	310	CLA	C4D-CHA	2.54	1.47	1.38
17	A	836	CLA	C1B-C2B	2.54	1.49	1.43
17	B	836	CLA	C1D-ND	2.54	1.40	1.37
17	2	316	CLA	C1B-C2B	2.54	1.49	1.43
17	B	830	CLA	C1D-ND	2.54	1.40	1.37
17	B	828	CLA	CHD-C4C	2.54	1.45	1.39
17	A	810	CLA	C3B-C4B	2.54	1.48	1.42
17	5	302	CLA	C4D-CHA	2.54	1.47	1.38
17	4	303	CLA	C4D-CHA	2.54	1.47	1.38
17	A	816	CLA	C3D-C4D	-2.54	1.38	1.44
17	1	302	CLA	C3B-C4B	2.53	1.48	1.42
17	B	831	CLA	OBD-CAD	2.53	1.26	1.22
20	A	846	BCR	C8-C9	-2.53	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	831	CLA	C3D-C4D	-2.53	1.38	1.44
17	A	852	CLA	C3D-C4D	-2.53	1.38	1.44
17	4	307	CLA	C4D-CHA	2.53	1.47	1.38
17	3	315	CLA	C1B-C2B	2.53	1.49	1.43
17	1	308	CLA	C1C-C2C	2.53	1.49	1.44
17	K	102	CLA	C4D-CHA	2.53	1.47	1.38
17	A	823	CLA	C3D-C4D	-2.53	1.38	1.44
17	B	831	CLA	C3D-C4D	-2.53	1.38	1.44
17	4	310	CLA	C4C-C3C	2.53	1.49	1.45
17	2	309	CLA	C1B-C2B	2.53	1.49	1.43
17	B	828	CLA	OBD-CAD	2.53	1.26	1.22
17	B	805	CLA	C1C-C2C	2.53	1.49	1.44
17	A	818	CLA	C3D-C4D	-2.53	1.38	1.44
17	B	813	CLA	C3D-C4D	-2.53	1.38	1.44
17	5	306	CLA	C1C-C2C	2.53	1.49	1.44
17	4	310	CLA	C4D-CHA	2.52	1.47	1.38
17	B	836	CLA	C3D-C4D	-2.52	1.38	1.44
17	B	837	CLA	C1B-C2B	2.52	1.49	1.43
17	1	309	CLA	C4D-CHA	2.52	1.47	1.38
17	2	316	CLA	C4C-C3C	2.52	1.49	1.45
17	A	831	CLA	C3B-C4B	2.52	1.48	1.42
17	4	309	CLA	C4C-C3C	2.52	1.49	1.45
20	A	857	BCR	C19-C18	-2.52	1.40	1.45
17	B	820	CLA	C1C-C2C	2.52	1.49	1.44
17	1	306	CLA	C1C-C2C	2.52	1.49	1.44
17	A	818	CLA	C3B-C4B	2.52	1.48	1.42
17	5	306	CLA	C4D-CHA	2.51	1.47	1.38
17	A	814	CLA	C1C-NC	-2.51	1.34	1.37
17	1	305	CLA	C4D-CHA	2.51	1.47	1.38
17	A	802	CLA	C1D-ND	2.51	1.40	1.37
17	5	313	CLA	C4D-CHA	2.51	1.47	1.38
17	1	310	CLA	C4D-CHA	2.51	1.47	1.38
17	3	312	CLA	C4D-CHA	2.51	1.47	1.38
17	2	312	CLA	C1C-C2C	2.51	1.49	1.44
17	F	204	CLA	C3D-C4D	-2.51	1.38	1.44
25	5	316	5X6	C11-C03	2.51	1.54	1.45
17	A	818	CLA	C4D-CHA	2.51	1.47	1.38
17	A	823	CLA	C4D-CHA	2.50	1.47	1.38
17	A	829	CLA	OBD-CAD	2.50	1.26	1.22
17	A	823	CLA	C3B-C2B	2.50	1.49	1.41
17	2	309	CLA	C4B-NB	-2.50	1.34	1.37
17	4	303	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	204	CLA	C1C-C2C	2.50	1.49	1.44
17	A	802	CLA	C3D-C4D	-2.50	1.38	1.44
17	B	809	CLA	C4B-NB	-2.50	1.34	1.37
17	A	835	CLA	C4D-CHA	2.50	1.47	1.38
17	A	836	CLA	C4D-CHA	2.50	1.47	1.38
17	B	832	CLA	C1B-C2B	2.50	1.49	1.43
17	3	314	CLA	C1B-C2B	2.50	1.49	1.43
17	B	836	CLA	OBD-CAD	2.49	1.26	1.22
17	B	813	CLA	C4D-CHA	2.49	1.47	1.38
17	5	311	CLA	C1B-C2B	2.49	1.49	1.43
17	2	310	CLA	C4B-NB	-2.49	1.34	1.37
17	A	824	CLA	CHD-C1D	2.49	1.43	1.38
17	2	310	CLA	C4D-CHA	2.49	1.47	1.38
17	L	202	CLA	C4D-CHA	2.49	1.47	1.38
17	A	810	CLA	C4D-CHA	2.49	1.47	1.38
20	B	845	BCR	C23-C22	-2.49	1.40	1.45
17	5	307	CLA	C4B-NB	-2.49	1.34	1.37
17	4	303	CLA	C4B-NB	-2.49	1.34	1.37
17	3	315	CLA	C4D-CHA	2.49	1.47	1.38
17	A	813	CLA	C3D-C4D	-2.49	1.38	1.44
17	4	311	CLA	C4C-C3C	2.49	1.49	1.45
17	L	202	CLA	C1B-C2B	2.49	1.49	1.43
17	K	102	CLA	C4C-C3C	2.48	1.49	1.45
20	A	845	BCR	C15-C14	-2.48	1.35	1.43
17	5	312	CLA	C4D-CHA	2.48	1.47	1.38
17	2	306	CLA	C4D-CHA	2.48	1.47	1.38
17	B	816	CLA	C1C-NC	-2.48	1.34	1.37
17	L	204	CLA	C4B-NB	-2.48	1.34	1.37
17	B	857	CLA	C3D-C4D	-2.48	1.38	1.44
17	O	204	CLA	C1B-C2B	2.48	1.49	1.43
17	A	839	CLA	C3B-C4B	2.48	1.48	1.42
17	B	823	CLA	C3B-C2B	2.48	1.49	1.41
17	L	204	CLA	C4D-CHA	2.48	1.47	1.38
17	2	310	CLA	C4C-C3C	2.48	1.49	1.45
17	4	309	CLA	C4D-CHA	2.48	1.47	1.38
17	A	837	CLA	C1C-C2C	2.47	1.49	1.44
17	O	205	CLA	C4C-C3C	2.47	1.49	1.45
17	A	835	CLA	C1D-ND	2.47	1.40	1.37
17	O	205	CLA	C1B-C2B	2.47	1.49	1.43
17	1	311	CLA	C1C-C2C	2.47	1.49	1.44
17	2	315	CLA	C1B-C2B	2.47	1.49	1.43
17	A	853	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	306	CLA	C4D-CHA	2.47	1.47	1.38
17	B	827	CLA	C3B-C4B	2.47	1.48	1.42
17	J	103	CLA	C3D-C4D	-2.47	1.38	1.44
17	A	833	CLA	C1C-NC	-2.47	1.34	1.37
17	K	102	CLA	C3D-C4D	-2.47	1.38	1.44
17	B	801	CLA	OBD-CAD	2.47	1.26	1.22
17	B	826	CLA	C1D-ND	2.47	1.40	1.37
17	B	815	CLA	C1C-C2C	2.47	1.49	1.44
17	A	812	CLA	C1B-C2B	2.47	1.49	1.43
17	B	825	CLA	C1B-C2B	2.47	1.49	1.43
17	2	307	CLA	C3D-C4D	-2.47	1.38	1.44
17	4	305	CLA	C4D-CHA	2.47	1.47	1.38
17	5	305	CLA	C4B-NB	-2.47	1.34	1.37
17	A	826	CLA	C3B-C4B	2.47	1.48	1.42
17	B	830	CLA	C3D-C4D	-2.47	1.38	1.44
17	A	836	CLA	C3D-C4D	-2.47	1.38	1.44
17	B	841	CLA	C1B-C2B	2.46	1.49	1.43
17	B	815	CLA	C3B-C4B	2.46	1.48	1.42
17	1	302	CLA	C3D-C4D	-2.46	1.38	1.44
17	B	821	CLA	C1C-C2C	2.46	1.49	1.44
17	J	103	CLA	C1C-NC	-2.46	1.34	1.37
17	A	811	CLA	C4D-CHA	2.46	1.47	1.38
17	B	837	CLA	C1D-ND	2.46	1.40	1.37
17	2	311	CLA	C4B-NB	-2.46	1.34	1.37
20	A	843	BCR	C19-C18	-2.46	1.40	1.45
17	2	314	CLA	C4D-CHA	2.46	1.47	1.38
17	1	308	CLA	C4D-CHA	2.46	1.47	1.38
17	A	825	CLA	C3D-C4D	-2.46	1.38	1.44
17	F	203	CLA	C4D-CHA	2.46	1.47	1.38
17	O	203	CLA	C4D-CHA	2.46	1.47	1.38
17	1	306	CLA	C4C-C3C	2.46	1.49	1.45
17	B	840	CLA	C1B-C2B	2.46	1.49	1.43
17	L	203	CLA	C4D-CHA	2.46	1.47	1.38
17	2	313	CLA	C4D-CHA	2.46	1.47	1.38
17	L	203	CLA	C1C-C2C	2.46	1.49	1.44
17	B	804	CLA	OBD-CAD	2.45	1.26	1.22
17	3	308	CLA	C4C-C3C	2.45	1.49	1.45
17	2	313	CLA	C1B-C2B	2.45	1.49	1.43
17	A	803	CLA	C3D-C4D	-2.45	1.38	1.44
17	1	311	CLA	C1B-C2B	2.45	1.49	1.43
17	1	311	CLA	C4B-NB	-2.45	1.34	1.37
17	B	837	CLA	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	102	CLA	C4B-NB	-2.45	1.34	1.37
17	2	311	CLA	C3D-C4D	-2.45	1.38	1.44
25	F	205	5X6	O37-C32	-2.45	1.36	1.43
17	A	815	CLA	C3D-C4D	-2.45	1.38	1.44
17	1	301	CLA	C4D-CHA	2.45	1.47	1.38
17	3	313	CLA	C4D-CHA	2.45	1.47	1.38
20	L	201	BCR	C8-C9	-2.44	1.40	1.45
17	L	204	CLA	C4C-C3C	2.44	1.49	1.45
17	B	838	CLA	OBD-CAD	2.44	1.26	1.22
17	5	308	CLA	C4D-CHA	2.44	1.47	1.38
17	B	814	CLA	C1B-C2B	2.44	1.49	1.43
20	K	104	BCR	C8-C9	-2.44	1.40	1.45
17	4	306	CLA	C4B-NB	-2.44	1.34	1.37
17	3	313	CLA	C4C-C3C	2.44	1.49	1.45
17	B	812	CLA	C1B-C2B	2.44	1.49	1.43
17	3	309	CLA	C4D-CHA	2.44	1.47	1.38
17	4	308	CLA	C1B-C2B	2.44	1.49	1.43
17	A	834	CLA	C3D-C4D	-2.43	1.38	1.44
17	B	806	CLA	C1C-C2C	2.43	1.49	1.44
17	1	302	CLA	C1B-C2B	2.43	1.49	1.43
17	A	830	CLA	C3B-C2B	2.43	1.49	1.41
17	B	819	CLA	C3B-C2B	2.43	1.49	1.41
17	2	308	CLA	C1B-C2B	2.43	1.49	1.43
17	4	305	CLA	C3D-C4D	-2.43	1.38	1.44
25	F	205	5X6	C05-C06	2.43	1.55	1.52
17	B	841	CLA	C4B-NB	-2.43	1.34	1.37
17	K	103	CLA	C1C-NC	-2.43	1.34	1.37
17	A	836	CLA	C1C-NC	-2.43	1.34	1.37
17	B	823	CLA	C4D-CHA	2.43	1.47	1.38
17	A	855	CLA	C3B-C4B	2.43	1.48	1.42
17	3	314	CLA	C4C-C3C	2.43	1.49	1.45
17	5	308	CLA	C1B-C2B	2.43	1.49	1.43
17	B	820	CLA	C3D-C4D	-2.43	1.38	1.44
17	A	805	CLA	C1C-NC	-2.43	1.34	1.37
17	3	306	CLA	C1C-C2C	2.42	1.49	1.44
17	2	305	CLA	C3D-C4D	-2.42	1.38	1.44
17	B	815	CLA	C4C-C3C	2.42	1.49	1.45
17	A	825	CLA	C3B-C4B	2.42	1.48	1.42
17	B	819	CLA	C3D-C4D	-2.42	1.38	1.44
17	A	838	CLA	C4D-CHA	2.42	1.47	1.38
17	2	307	CLA	C4C-C3C	2.42	1.49	1.45
17	B	816	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	C3D-C4D	-2.42	1.38	1.44
20	M	101	BCR	C23-C22	-2.42	1.40	1.45
20	B	845	BCR	C12-C13	-2.42	1.40	1.45
17	A	854	CLA	C1B-C2B	2.42	1.49	1.43
17	5	305	CLA	C3D-C4D	-2.42	1.38	1.44
17	B	813	CLA	C1C-C2C	2.42	1.49	1.44
17	3	306	CLA	C4C-C3C	2.42	1.49	1.45
17	3	313	CLA	C1B-C2B	2.42	1.48	1.43
17	1	311	CLA	C4D-CHA	2.42	1.47	1.38
17	B	829	CLA	C4D-CHA	2.42	1.47	1.38
17	2	304	CLA	C4D-CHA	2.41	1.47	1.38
17	3	306	CLA	C4D-CHA	2.41	1.47	1.38
17	4	306	CLA	C1B-C2B	2.41	1.48	1.43
17	A	856	CLA	C3D-C4D	-2.41	1.38	1.44
17	2	309	CLA	C4D-CHA	2.41	1.47	1.38
17	F	204	CLA	C4D-CHA	2.41	1.47	1.38
17	4	311	CLA	C1B-C2B	2.41	1.48	1.43
17	2	306	CLA	C1C-C2C	2.41	1.49	1.44
17	A	837	CLA	OBD-CAD	2.41	1.26	1.22
17	5	309	CLA	C3B-C2B	2.41	1.49	1.41
17	B	805	CLA	C3D-C4D	-2.41	1.38	1.44
17	A	819	CLA	C3B-C4B	2.41	1.48	1.42
17	A	811	CLA	C1B-C2B	2.41	1.48	1.43
17	5	312	CLA	C1B-C2B	2.41	1.48	1.43
17	5	311	CLA	C4D-CHA	2.41	1.47	1.38
17	F	204	CLA	C1B-C2B	2.41	1.48	1.43
17	A	822	CLA	C4D-CHA	2.41	1.47	1.38
17	F	203	CLA	C4C-C3C	2.41	1.49	1.45
17	B	825	CLA	C3D-C4D	-2.41	1.38	1.44
20	B	847	BCR	C16-C17	-2.41	1.36	1.43
20	A	844	BCR	C19-C18	-2.41	1.40	1.45
17	A	814	CLA	C1C-C2C	2.40	1.49	1.44
17	5	314	CLA	C1B-C2B	2.40	1.48	1.43
20	L	201	BCR	C19-C18	-2.40	1.40	1.45
17	B	818	CLA	C3D-C4D	-2.40	1.38	1.44
25	J	105	5X6	C11-C03	2.40	1.53	1.45
17	O	204	CLA	C4C-C3C	2.40	1.49	1.45
17	L	202	CLA	C3D-C4D	-2.40	1.38	1.44
17	B	839	CLA	CHC-C4B	2.40	1.44	1.39
17	3	305	CLA	C4D-CHA	2.40	1.46	1.38
17	A	820	CLA	C1B-C2B	2.40	1.48	1.43
17	B	804	CLA	C4D-CHA	2.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	308	CLA	C4D-CHA	2.40	1.46	1.38
17	2	314	CLA	C4C-C3C	2.40	1.49	1.45
17	J	103	CLA	C1C-C2C	2.39	1.49	1.44
17	2	315	CLA	C4D-CHA	2.39	1.46	1.38
17	B	806	CLA	C3B-C4B	2.39	1.48	1.42
17	3	308	CLA	C4B-NB	-2.39	1.34	1.37
17	L	203	CLA	C3D-C4D	-2.39	1.38	1.44
17	K	103	CLA	C4D-CHA	2.39	1.46	1.38
17	A	853	CLA	C4C-C3C	2.39	1.49	1.45
17	5	311	CLA	C4C-C3C	2.39	1.49	1.45
17	B	831	CLA	C4C-C3C	2.39	1.49	1.45
17	5	307	CLA	C4D-CHA	2.39	1.46	1.38
17	4	311	CLA	C4D-CHA	2.39	1.46	1.38
17	5	308	CLA	C3D-C4D	-2.39	1.38	1.44
17	A	815	CLA	C1B-C2B	2.39	1.48	1.43
17	A	832	CLA	C1B-C2B	2.39	1.48	1.43
17	B	807	CLA	C3B-C4B	2.39	1.48	1.42
17	4	307	CLA	C4C-C3C	2.39	1.49	1.45
20	A	857	BCR	C17-C18	2.38	1.38	1.35
17	A	806	CLA	C3B-C4B	2.38	1.48	1.42
17	A	834	CLA	C4C-C3C	2.38	1.49	1.45
17	3	310	CLA	C4D-CHA	2.38	1.46	1.38
17	B	828	CLA	C4D-CHA	2.38	1.46	1.38
17	A	830	CLA	C1C-NC	-2.38	1.34	1.37
17	B	832	CLA	C1C-NC	-2.38	1.34	1.37
17	3	307	CLA	C4B-NB	-2.38	1.34	1.37
17	5	306	CLA	C1B-C2B	2.38	1.48	1.43
17	3	315	CLA	C4C-C3C	2.38	1.49	1.45
17	2	306	CLA	C3B-C2B	2.38	1.49	1.41
17	A	824	CLA	C1B-C2B	2.38	1.48	1.43
17	A	805	CLA	C3D-C4D	-2.38	1.38	1.44
17	4	307	CLA	C4B-NB	-2.38	1.34	1.37
17	J	103	CLA	C4D-CHA	2.38	1.46	1.38
17	B	828	CLA	C1C-NC	-2.38	1.34	1.37
17	1	310	CLA	C1B-C2B	2.38	1.48	1.43
17	1	302	CLA	C1C-C2C	2.38	1.49	1.44
17	B	841	CLA	C4D-CHA	2.38	1.46	1.38
17	J	103	CLA	C4C-C3C	2.37	1.49	1.45
17	A	804	CLA	C1B-C2B	2.37	1.48	1.43
17	B	822	CLA	C4D-CHA	2.37	1.46	1.38
17	B	826	CLA	C3D-C4D	-2.37	1.38	1.44
17	5	313	CLA	C3D-C4D	-2.37	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	204	CLA	C3A-C2A	-2.37	1.52	1.54
17	A	826	CLA	CHD-C4C	2.37	1.44	1.39
17	A	809	CLA	C1B-C2B	2.37	1.48	1.43
17	F	203	CLA	C1C-C2C	2.37	1.49	1.44
17	B	805	CLA	C1B-C2B	2.37	1.48	1.43
17	B	826	CLA	C1B-C2B	2.37	1.48	1.43
17	A	810	CLA	C1C-C2C	2.37	1.49	1.44
17	2	306	CLA	C3D-C4D	-2.37	1.38	1.44
17	4	307	CLA	C1B-C2B	2.37	1.48	1.43
17	5	313	CLA	C1B-C2B	2.37	1.48	1.43
17	5	303	CLA	C4D-CHA	2.37	1.46	1.38
17	2	315	CLA	C4B-NB	-2.36	1.34	1.37
17	A	826	CLA	CHB-C4A	-2.36	1.32	1.37
17	B	824	CLA	C1C-NC	-2.36	1.34	1.37
17	4	305	CLA	C4C-C3C	2.36	1.49	1.45
17	2	313	CLA	C4B-NB	-2.36	1.34	1.37
17	A	809	CLA	C4D-CHA	2.36	1.46	1.38
17	B	824	CLA	C4D-CHA	2.36	1.46	1.38
17	J	103	CLA	C1B-C2B	2.36	1.48	1.43
17	1	309	CLA	C1B-C2B	2.36	1.48	1.43
17	A	824	CLA	OBD-CAD	2.36	1.26	1.22
17	3	313	CLA	C4B-NB	-2.36	1.34	1.37
17	3	307	CLA	C4D-CHA	2.36	1.46	1.38
17	1	304	CLA	C4B-NB	-2.36	1.34	1.37
17	2	308	CLA	C1C-C2C	2.36	1.49	1.44
17	F	203	CLA	C3D-C4D	-2.36	1.38	1.44
17	A	859	CLA	C3D-C4D	-2.36	1.38	1.44
17	B	833	CLA	OBD-CAD	2.36	1.26	1.22
17	A	830	CLA	C4D-CHA	2.36	1.46	1.38
17	A	817	CLA	C3D-C4D	-2.35	1.38	1.44
17	A	807	CLA	C4D-CHA	2.35	1.46	1.38
17	1	302	CLA	C4D-CHA	2.35	1.46	1.38
17	O	203	CLA	C4C-C3C	2.35	1.49	1.45
17	B	805	CLA	C4D-CHA	2.35	1.46	1.38
17	3	309	CLA	C1B-C2B	2.35	1.48	1.43
17	B	804	CLA	CHD-C4C	2.35	1.44	1.39
17	1	306	CLA	C4D-CHA	2.35	1.46	1.38
17	1	307	CLA	C4D-CHA	2.35	1.46	1.38
17	5	314	CLA	C4C-C3C	2.35	1.49	1.45
17	1	308	CLA	C4B-NB	-2.35	1.34	1.37
17	2	307	CLA	C4B-NB	-2.35	1.34	1.37
17	B	815	CLA	C3B-C2B	2.35	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	811	CLA	C3D-C4D	-2.35	1.38	1.44
17	4	303	CLA	C1C-C2C	2.35	1.49	1.44
17	A	852	CLA	C3B-C2B	2.34	1.49	1.41
17	B	822	CLA	C4B-NB	-2.34	1.34	1.37
17	4	310	CLA	C1B-C2B	2.34	1.48	1.43
17	A	824	CLA	C3B-C2B	2.34	1.49	1.41
17	3	309	CLA	C3D-C4D	-2.34	1.38	1.44
20	I	101	BCR	C17-C18	2.34	1.38	1.35
17	1	304	CLA	C4D-CHA	2.34	1.46	1.38
17	A	807	CLA	C1C-C2C	2.34	1.49	1.44
17	5	304	CLA	C4D-CHA	2.34	1.46	1.38
17	1	303	CLA	C4C-C3C	2.34	1.49	1.45
17	A	812	CLA	C1C-NC	-2.34	1.34	1.37
17	5	309	CLA	C3D-C4D	-2.34	1.38	1.44
20	L	201	BCR	C20-C21	-2.34	1.36	1.43
17	B	802	CLA	C1B-C2B	2.34	1.48	1.43
17	5	308	CLA	C3B-C2B	2.34	1.49	1.41
17	A	829	CLA	C4D-CHA	2.33	1.46	1.38
17	L	202	CLA	C1C-C2C	2.33	1.49	1.44
17	1	306	CLA	C3D-C4D	-2.33	1.38	1.44
17	1	305	CLA	C4B-NB	-2.33	1.34	1.37
17	5	311	CLA	C4B-NB	-2.33	1.34	1.37
17	5	306	CLA	C4B-NB	-2.33	1.34	1.37
17	A	831	CLA	C4D-CHA	2.33	1.46	1.38
17	A	832	CLA	C4D-CHA	2.33	1.46	1.38
17	3	309	CLA	C4C-C3C	2.33	1.49	1.45
17	5	304	CLA	C1C-C2C	2.33	1.49	1.44
17	2	314	CLA	C1B-C2B	2.33	1.48	1.43
17	2	305	CLA	C4D-CHA	2.33	1.46	1.38
17	A	814	CLA	C1B-C2B	2.33	1.48	1.43
17	1	309	CLA	C3B-C2B	2.33	1.49	1.41
17	B	814	CLA	C4D-CHA	2.33	1.46	1.38
17	3	306	CLA	C1B-C2B	2.33	1.48	1.43
17	B	821	CLA	C3D-C4D	-2.33	1.38	1.44
17	A	820	CLA	C4D-CHA	2.33	1.46	1.38
17	4	304	CLA	C4D-CHA	2.33	1.46	1.38
17	A	839	CLA	C1B-C2B	2.33	1.48	1.43
17	3	311	CLA	C3D-C4D	-2.32	1.38	1.44
17	B	827	CLA	MG-ND	-2.32	2.01	2.05
17	A	820	CLA	C3D-C4D	-2.32	1.38	1.44
17	A	816	CLA	C1C-C2C	2.32	1.49	1.44
17	F	203	CLA	C4B-NB	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	825	CLA	C3B-C4B	2.32	1.48	1.42
17	5	305	CLA	C4D-CHA	2.32	1.46	1.38
20	L	205	BCR	C19-C18	-2.32	1.41	1.45
17	B	835	CLA	C1C-C2C	2.32	1.49	1.44
17	A	854	CLA	C1C-NC	-2.32	1.34	1.37
17	2	309	CLA	C3D-C4D	-2.32	1.38	1.44
17	A	835	CLA	C1B-C2B	2.32	1.48	1.43
17	B	838	CLA	C1B-C2B	2.32	1.48	1.43
17	A	803	CLA	C4D-CHA	2.32	1.46	1.38
17	5	308	CLA	C4C-C3C	2.31	1.49	1.45
17	5	303	CLA	C3D-C4D	-2.31	1.39	1.44
17	A	827	CLA	C1B-C2B	2.31	1.48	1.43
17	B	832	CLA	C1C-C2C	2.31	1.49	1.44
17	B	837	CLA	C3B-C4B	2.31	1.48	1.42
17	A	816	CLA	C4D-CHA	2.31	1.46	1.38
17	B	817	CLA	C4D-CHA	2.31	1.46	1.38
17	3	310	CLA	C4C-C3C	2.31	1.49	1.45
17	B	811	CLA	C1C-NC	-2.31	1.34	1.37
17	B	829	CLA	C1B-C2B	2.31	1.48	1.43
17	2	312	CLA	C4B-NB	-2.31	1.34	1.37
17	A	815	CLA	C4D-CHA	2.31	1.46	1.38
17	B	832	CLA	C4D-CHA	2.31	1.46	1.38
17	A	833	CLA	C3D-C4D	-2.31	1.39	1.44
17	A	807	CLA	C3B-C2B	2.31	1.49	1.41
17	K	103	CLA	C4C-C3C	2.31	1.49	1.45
17	2	306	CLA	C4C-C3C	2.31	1.49	1.45
17	B	817	CLA	C1B-C2B	2.31	1.48	1.43
17	5	313	CLA	C1C-C2C	2.31	1.49	1.44
17	O	204	CLA	C4B-NB	-2.30	1.35	1.37
17	B	805	CLA	C1C-NC	-2.30	1.34	1.37
20	B	843	BCR	C23-C22	-2.30	1.41	1.45
17	3	305	CLA	C4B-NB	-2.30	1.35	1.37
17	4	311	CLA	C4B-NB	-2.30	1.35	1.37
17	3	305	CLA	C3D-C4D	-2.30	1.39	1.44
17	B	808	CLA	C3B-C4B	2.30	1.48	1.42
17	2	311	CLA	C4D-CHA	2.30	1.46	1.38
17	3	310	CLA	C3D-C4D	-2.30	1.39	1.44
17	3	307	CLA	C4C-C3C	2.30	1.49	1.45
17	B	824	CLA	CHB-C4A	-2.30	1.32	1.37
17	A	818	CLA	C1C-NC	-2.30	1.34	1.37
17	B	811	CLA	C4D-CHA	2.30	1.46	1.38
17	A	854	CLA	C3B-C4B	2.29	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	311	CLA	C3D-C4D	-2.29	1.39	1.44
17	B	830	CLA	C1B-C2B	2.29	1.48	1.43
17	B	819	CLA	C3B-C4B	2.29	1.48	1.42
17	B	807	CLA	C4D-CHA	2.29	1.46	1.38
17	L	203	CLA	C3B-C2B	2.29	1.49	1.41
17	A	803	CLA	C1C-C2C	2.29	1.49	1.44
17	A	828	CLA	C3B-C2B	2.29	1.49	1.41
17	B	840	CLA	C4D-CHA	2.29	1.46	1.38
17	3	305	CLA	C1B-C2B	2.29	1.48	1.43
17	B	816	CLA	C4D-CHA	2.29	1.46	1.38
17	B	807	CLA	C1B-C2B	2.29	1.48	1.43
17	5	303	CLA	C3B-C2B	2.29	1.48	1.41
17	3	312	CLA	C4B-NB	-2.29	1.35	1.37
17	B	818	CLA	C4D-CHA	2.29	1.46	1.38
17	A	811	CLA	C1C-NC	-2.29	1.34	1.37
17	B	819	CLA	C1B-C2B	2.29	1.48	1.43
17	A	838	CLA	C1C-NC	-2.29	1.34	1.37
17	1	305	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	812	CLA	C3B-C2B	2.29	1.48	1.41
17	1	309	CLA	C4B-NB	-2.29	1.35	1.37
17	A	808	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	824	CLA	C3B-C4B	2.29	1.48	1.42
17	A	821	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	813	CLA	C4C-C3C	2.28	1.49	1.45
17	4	304	CLA	C3D-C4D	-2.28	1.39	1.44
17	3	307	CLA	C1B-C2B	2.28	1.48	1.43
17	A	853	CLA	OBD-CAD	2.28	1.26	1.22
17	B	839	CLA	C1B-C2B	2.28	1.48	1.43
17	3	309	CLA	C4B-NB	-2.28	1.35	1.37
17	B	831	CLA	C4D-CHA	2.28	1.46	1.38
17	1	304	CLA	C3D-C4D	-2.28	1.39	1.44
17	3	314	CLA	C4B-NB	-2.28	1.35	1.37
17	B	812	CLA	C4D-CHA	2.28	1.46	1.38
17	A	816	CLA	C3B-C4B	2.28	1.48	1.42
17	4	309	CLA	C4B-NB	-2.28	1.35	1.37
17	1	306	CLA	C1B-C2B	2.28	1.48	1.43
17	1	301	CLA	C3D-C4D	-2.28	1.39	1.44
17	1	308	CLA	C3D-C4D	-2.28	1.39	1.44
17	1	307	CLA	C1B-C2B	2.28	1.48	1.43
17	A	809	CLA	C1C-C2C	2.28	1.49	1.44
17	A	837	CLA	C3D-C4D	-2.28	1.39	1.44
17	A	859	CLA	C4D-CHA	2.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	811	CLA	C1B-C2B	2.27	1.48	1.43
17	A	852	CLA	MG-ND	-2.27	2.01	2.05
17	B	829	CLA	C3B-C4B	2.27	1.48	1.42
17	B	809	CLA	OBD-CAD	2.27	1.26	1.22
17	1	305	CLA	C3B-C2B	2.27	1.48	1.41
17	A	814	CLA	C4D-CHA	2.27	1.46	1.38
17	A	839	CLA	C3D-C4D	-2.27	1.39	1.44
17	4	310	CLA	C3B-C2B	2.27	1.48	1.41
17	B	826	CLA	C3B-C2B	2.27	1.48	1.41
17	4	310	CLA	C3D-C4D	-2.27	1.39	1.44
17	B	839	CLA	C3B-C4B	2.27	1.48	1.42
17	B	835	CLA	C3D-C4D	-2.27	1.39	1.44
17	4	305	CLA	C4B-NB	-2.27	1.35	1.37
17	1	310	CLA	C3D-C4D	-2.27	1.39	1.44
17	3	311	CLA	C1B-C2B	2.27	1.48	1.43
17	A	859	CLA	C1B-C2B	2.27	1.48	1.43
17	4	306	CLA	C3D-C4D	-2.27	1.39	1.44
17	5	310	CLA	C4B-NB	-2.27	1.35	1.37
17	A	830	CLA	C3B-C4B	2.27	1.48	1.42
16	A	801	CL0	C4D-CHA	2.27	1.46	1.38
17	B	806	CLA	C3D-C4D	-2.26	1.39	1.44
17	A	826	CLA	C4D-CHA	2.26	1.46	1.38
17	4	307	CLA	C3D-C4D	-2.26	1.39	1.44
17	4	310	CLA	C4B-NB	-2.26	1.35	1.37
17	5	307	CLA	C1C-C2C	2.26	1.48	1.44
17	B	822	CLA	C3D-C4D	-2.26	1.39	1.44
17	3	315	CLA	C3D-C4D	-2.26	1.39	1.44
17	A	813	CLA	C3B-C2B	2.26	1.48	1.41
17	B	840	CLA	CHD-C4C	2.26	1.44	1.39
16	A	801	CL0	C1B-C2B	2.26	1.48	1.43
17	3	308	CLA	C3D-C4D	-2.26	1.39	1.44
17	B	840	CLA	C4C-C3C	2.26	1.48	1.45
17	2	308	CLA	C3B-C2B	2.26	1.48	1.41
17	A	834	CLA	C4D-CHA	2.26	1.46	1.38
17	A	852	CLA	C1C-NC	-2.26	1.34	1.37
17	1	311	CLA	C3D-C4D	-2.26	1.39	1.44
20	L	201	BCR	C12-C13	-2.25	1.41	1.45
17	B	826	CLA	C4D-CHA	2.25	1.46	1.38
17	A	811	CLA	C3B-C2B	2.25	1.48	1.41
17	5	312	CLA	C4B-NB	-2.25	1.35	1.37
17	A	825	CLA	C4D-CHA	2.25	1.46	1.38
17	3	312	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	C4D-CHA	2.25	1.46	1.38
17	2	304	CLA	C3D-C4D	-2.25	1.39	1.44
17	O	203	CLA	C3B-C2B	2.25	1.48	1.41
17	B	826	CLA	C1C-C2C	2.25	1.48	1.44
17	A	838	CLA	C1B-C2B	2.25	1.48	1.43
17	A	808	CLA	C4D-CHA	2.25	1.46	1.38
17	B	838	CLA	C4D-CHA	2.25	1.46	1.38
17	3	307	CLA	C3D-C4D	-2.25	1.39	1.44
17	A	839	CLA	C4C-C3C	2.25	1.48	1.45
17	3	313	CLA	C3B-C2B	2.25	1.48	1.41
17	1	301	CLA	C1B-C2B	2.25	1.48	1.43
17	B	813	CLA	C4B-NB	-2.25	1.35	1.37
20	B	847	BCR	C15-C14	-2.25	1.36	1.43
17	1	310	CLA	C4B-NB	-2.24	1.35	1.37
17	5	307	CLA	C3D-C4D	-2.24	1.39	1.44
17	B	836	CLA	C4D-CHA	2.24	1.46	1.38
17	1	304	CLA	C1B-C2B	2.24	1.48	1.43
17	5	311	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	803	CLA	C4C-C3C	2.24	1.48	1.45
17	1	309	CLA	C4C-C3C	2.24	1.48	1.45
17	1	302	CLA	C3B-C2B	2.24	1.48	1.41
20	B	845	BCR	C19-C18	-2.24	1.41	1.45
17	1	305	CLA	C1B-C2B	2.24	1.48	1.43
17	2	313	CLA	C3D-C4D	-2.24	1.39	1.44
17	B	834	CLA	C1C-NC	-2.24	1.34	1.37
17	1	307	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	856	CLA	C3B-C4B	2.24	1.48	1.42
17	5	305	CLA	C4C-C3C	2.24	1.48	1.45
17	B	828	CLA	MG-ND	-2.24	2.01	2.05
17	B	831	CLA	C1C-NC	-2.24	1.34	1.37
17	2	305	CLA	C1B-C2B	2.23	1.48	1.43
17	B	832	CLA	C4C-C3C	2.23	1.48	1.45
17	3	311	CLA	C4D-CHA	2.23	1.46	1.38
20	A	845	BCR	C11-C10	-2.23	1.36	1.43
17	B	820	CLA	C1C-NC	-2.23	1.34	1.37
17	5	310	CLA	C3D-C4D	-2.23	1.39	1.44
17	A	836	CLA	C3B-C2B	2.23	1.48	1.41
17	1	308	CLA	C3B-C2B	2.23	1.48	1.41
17	O	203	CLA	C3D-C4D	-2.23	1.39	1.44
17	4	303	CLA	C3D-C4D	-2.23	1.39	1.44
17	4	309	CLA	C3D-C4D	-2.23	1.39	1.44
17	A	825	CLA	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	306	CLA	C3B-C2B	2.22	1.48	1.41
17	3	314	CLA	C3B-C2B	2.22	1.48	1.41
17	5	302	CLA	C4B-NB	-2.22	1.35	1.37
17	5	311	CLA	C3B-C2B	2.22	1.48	1.41
17	L	202	CLA	C3B-C2B	2.22	1.48	1.41
17	3	308	CLA	C3B-C2B	2.22	1.48	1.41
17	B	831	CLA	C1B-C2B	2.22	1.48	1.43
17	4	308	CLA	C3D-C4D	-2.22	1.39	1.44
17	5	309	CLA	C4D-CHA	2.22	1.46	1.38
17	5	312	CLA	C4C-C3C	2.22	1.48	1.45
17	B	837	CLA	C4D-CHA	2.22	1.46	1.38
17	A	817	CLA	C3B-C2B	2.22	1.48	1.41
17	2	309	CLA	C4C-C3C	2.22	1.48	1.45
17	O	204	CLA	C3D-C4D	-2.22	1.39	1.44
17	3	313	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	808	CLA	C1C-C2C	2.22	1.48	1.44
17	2	307	CLA	C1B-C2B	2.22	1.48	1.43
17	A	821	CLA	C4D-CHA	2.22	1.46	1.38
17	A	807	CLA	C3B-C4B	2.22	1.48	1.42
17	A	817	CLA	C3B-C4B	2.22	1.48	1.42
17	2	314	CLA	C4B-NB	-2.21	1.35	1.37
17	4	305	CLA	C1B-C2B	2.21	1.48	1.43
17	B	814	CLA	C3B-C2B	2.21	1.48	1.41
17	A	815	CLA	C4C-C3C	2.21	1.48	1.45
17	A	828	CLA	C1D-ND	2.21	1.40	1.37
17	B	809	CLA	C4C-C3C	2.21	1.48	1.45
25	5	318	5X6	C41-C17	2.21	1.55	1.50
17	B	829	CLA	C3B-C2B	2.21	1.48	1.41
17	A	835	CLA	C3B-C2B	2.21	1.48	1.41
17	A	803	CLA	C3B-C2B	2.21	1.48	1.41
17	B	835	CLA	C1C-NC	-2.21	1.34	1.37
17	2	316	CLA	C4B-NB	-2.21	1.35	1.37
17	3	311	CLA	C4B-NB	-2.21	1.35	1.37
17	A	818	CLA	C3B-C2B	2.21	1.48	1.41
17	4	305	CLA	C3B-C2B	2.21	1.48	1.41
17	2	310	CLA	C3D-C4D	-2.21	1.39	1.44
17	5	313	CLA	C3B-C2B	2.21	1.48	1.41
17	A	803	CLA	C1B-C2B	2.21	1.48	1.43
17	A	812	CLA	C1C-C2C	2.21	1.48	1.44
20	A	846	BCR	C19-C18	-2.21	1.41	1.45
17	B	814	CLA	C1C-C2C	2.21	1.48	1.44
17	A	855	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	308	CLA	C3D-C4D	-2.21	1.39	1.44
17	B	812	CLA	C3B-C2B	2.21	1.48	1.41
17	4	311	CLA	C3B-C2B	2.21	1.48	1.41
17	2	304	CLA	C4C-C3C	2.21	1.48	1.45
17	4	306	CLA	C3B-C2B	2.20	1.48	1.41
20	B	848	BCR	C20-C21	-2.20	1.36	1.43
17	1	311	CLA	C3B-C2B	2.20	1.48	1.41
17	B	838	CLA	C3B-C4B	2.20	1.47	1.42
17	A	820	CLA	C3B-C2B	2.20	1.48	1.41
17	2	314	CLA	C3D-C4D	-2.20	1.39	1.44
17	A	805	CLA	C3B-C2B	2.20	1.48	1.41
17	4	311	CLA	C1D-C2D	2.20	1.49	1.45
17	2	307	CLA	C4D-CHA	2.20	1.46	1.38
17	5	302	CLA	C3B-C2B	2.20	1.48	1.41
17	3	312	CLA	C3B-C2B	2.20	1.48	1.41
17	A	818	CLA	C1B-C2B	2.20	1.48	1.43
17	5	310	CLA	C3B-C2B	2.20	1.48	1.41
17	O	205	CLA	C4B-NB	-2.20	1.35	1.37
17	A	856	CLA	C3B-C2B	2.20	1.48	1.41
17	3	306	CLA	C3B-C2B	2.20	1.48	1.41
17	B	830	CLA	C3B-C4B	2.20	1.47	1.42
17	2	313	CLA	C3B-C2B	2.19	1.48	1.41
17	2	315	CLA	C3D-C4D	-2.19	1.39	1.44
17	5	312	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	809	CLA	C1C-NC	-2.19	1.34	1.37
17	5	302	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	832	CLA	C4C-C3C	2.19	1.48	1.45
17	2	312	CLA	C3B-C2B	2.19	1.48	1.41
17	3	315	CLA	C3B-C2B	2.19	1.48	1.41
25	1	313	5X6	C41-C17	2.19	1.55	1.50
17	4	309	CLA	C3B-C2B	2.19	1.48	1.41
17	A	828	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	825	CLA	C3B-C2B	2.19	1.48	1.41
17	A	816	CLA	C4C-C3C	2.19	1.48	1.45
17	4	307	CLA	C3B-C2B	2.19	1.48	1.41
17	5	306	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	834	CLA	C1C-C2C	2.19	1.48	1.44
17	B	836	CLA	C1C-C2C	2.19	1.48	1.44
17	2	312	CLA	C3D-C4D	-2.19	1.39	1.44
20	K	104	BCR	C12-C13	-2.19	1.41	1.45
17	2	304	CLA	C4B-NB	-2.19	1.35	1.37
17	A	811	CLA	C3B-C4B	2.19	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	854	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	810	CLA	C3B-C2B	2.18	1.48	1.41
17	B	814	CLA	C4C-C3C	2.18	1.48	1.45
17	A	821	CLA	C1C-C2C	2.18	1.48	1.44
17	B	806	CLA	C1B-C2B	2.18	1.48	1.43
17	A	804	CLA	C4D-CHA	2.18	1.46	1.38
17	O	205	CLA	C3B-C2B	2.18	1.48	1.41
17	A	813	CLA	C4D-CHA	2.18	1.46	1.38
17	O	203	CLA	C4B-NB	-2.18	1.35	1.37
17	1	306	CLA	C3B-C2B	2.18	1.48	1.41
17	K	103	CLA	C1C-C2C	2.18	1.48	1.44
17	K	102	CLA	C3B-C2B	2.18	1.48	1.41
17	3	310	CLA	C1B-C2B	2.18	1.48	1.43
25	2	319	5X6	C01-C02	2.17	1.54	1.50
17	2	310	CLA	C1B-C2B	2.17	1.48	1.43
17	5	314	CLA	C3D-C4D	-2.17	1.39	1.44
17	4	308	CLA	C4C-C3C	2.17	1.48	1.45
17	B	830	CLA	C3B-C2B	2.17	1.48	1.41
17	B	841	CLA	C3B-C2B	2.17	1.48	1.41
17	B	813	CLA	C1B-C2B	2.17	1.48	1.43
17	A	834	CLA	C3B-C2B	2.17	1.48	1.41
17	L	204	CLA	C1B-C2B	2.17	1.48	1.43
17	5	310	CLA	C1D-C2D	2.17	1.49	1.45
17	B	827	CLA	C4D-CHA	2.17	1.46	1.38
17	B	839	CLA	C3D-C4D	-2.17	1.39	1.44
17	L	204	CLA	C3D-C4D	-2.17	1.39	1.44
17	F	203	CLA	C1B-C2B	2.17	1.48	1.43
17	1	309	CLA	C3D-C4D	-2.17	1.39	1.44
17	A	805	CLA	C3B-C4B	2.17	1.47	1.42
17	B	821	CLA	C3B-C2B	2.17	1.48	1.41
17	2	316	CLA	C3D-C4D	-2.17	1.39	1.44
17	A	853	CLA	C1C-C2C	2.16	1.48	1.44
17	B	816	CLA	C3D-C4D	-2.16	1.39	1.44
17	A	838	CLA	C3B-C2B	2.16	1.48	1.41
17	4	308	CLA	C3B-C2B	2.16	1.48	1.41
17	L	202	CLA	C1C-NC	-2.16	1.34	1.37
17	2	305	CLA	C4B-NB	-2.16	1.35	1.37
20	A	844	BCR	C15-C14	-2.16	1.36	1.43
20	A	857	BCR	C15-C14	-2.16	1.36	1.43
17	A	812	CLA	C4D-CHA	2.16	1.46	1.38
17	B	815	CLA	C4D-CHA	2.16	1.46	1.38
17	A	811	CLA	C1C-C2C	2.16	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	C1C-NC	-2.16	1.34	1.37
17	2	311	CLA	C1B-C2B	2.16	1.48	1.43
20	I	101	BCR	C15-C14	-2.16	1.36	1.43
17	B	821	CLA	C1C-NC	-2.16	1.34	1.37
17	5	314	CLA	C4B-NB	-2.16	1.35	1.37
17	L	202	CLA	C4C-C3C	2.16	1.48	1.45
17	2	316	CLA	C3B-C2B	2.16	1.48	1.41
17	A	819	CLA	C3D-C4D	-2.16	1.39	1.44
25	F	205	5X6	O08-C06	-2.15	1.37	1.43
17	2	315	CLA	C4C-C3C	2.15	1.48	1.45
17	B	804	CLA	C3D-C4D	-2.15	1.39	1.44
17	B	815	CLA	C3D-C4D	-2.15	1.39	1.44
17	A	805	CLA	C4D-CHA	2.15	1.46	1.38
17	A	810	CLA	C4C-C3C	2.15	1.48	1.45
17	3	315	CLA	C4B-NB	-2.15	1.35	1.37
17	B	801	CLA	C1B-C2B	2.15	1.48	1.43
17	A	829	CLA	C1C-NC	-2.15	1.34	1.37
17	4	303	CLA	C3B-C2B	2.15	1.48	1.41
17	2	315	CLA	C3B-C2B	2.15	1.48	1.41
17	A	826	CLA	C3B-C2B	2.15	1.48	1.41
17	A	827	CLA	C4D-CHA	2.15	1.46	1.38
17	B	810	CLA	C1C-C2C	2.14	1.48	1.44
16	A	801	CL0	C1D-ND	2.14	1.40	1.37
17	2	309	CLA	C1C-C2C	2.14	1.48	1.44
17	A	855	CLA	C4D-CHA	2.14	1.46	1.38
17	A	855	CLA	C1C-C2C	2.14	1.48	1.44
17	K	103	CLA	C3B-C2B	2.14	1.48	1.41
17	B	809	CLA	C1C-C2C	2.14	1.48	1.44
20	A	845	BCR	C16-C17	-2.14	1.36	1.43
17	B	810	CLA	C4D-CHA	2.14	1.46	1.38
17	4	308	CLA	C4B-NB	-2.14	1.35	1.37
17	1	307	CLA	C3B-C2B	2.14	1.48	1.41
17	B	818	CLA	C1C-C2C	2.14	1.48	1.44
17	B	801	CLA	C3B-C4B	2.14	1.47	1.42
20	I	101	BCR	C16-C17	-2.14	1.36	1.43
17	5	312	CLA	C3B-C2B	2.14	1.48	1.41
20	O	202	BCR	C19-C18	-2.14	1.41	1.45
17	B	827	CLA	C1B-C2B	2.14	1.48	1.43
17	A	853	CLA	C3B-C4B	2.13	1.47	1.42
17	L	203	CLA	C4C-C3C	2.13	1.48	1.45
17	A	814	CLA	C3D-C4D	-2.13	1.39	1.44
17	2	309	CLA	C3B-C2B	2.13	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	813	CLA	C1C-C2C	2.13	1.48	1.44
17	1	301	CLA	C3B-C2B	2.13	1.48	1.41
17	B	839	CLA	C4D-CHA	2.13	1.46	1.38
17	B	805	CLA	C3B-C2B	2.13	1.48	1.41
17	B	811	CLA	C3B-C2B	2.13	1.48	1.41
17	A	853	CLA	C1C-NC	-2.13	1.34	1.37
17	A	854	CLA	C4D-CHA	2.13	1.46	1.38
25	4	313	5X6	C38-C30	2.13	1.54	1.50
17	B	835	CLA	C4D-CHA	2.13	1.46	1.38
17	A	833	CLA	C4D-CHA	2.13	1.46	1.38
17	A	803	CLA	C3B-C4B	2.13	1.47	1.42
17	5	308	CLA	C1C-NC	-2.13	1.34	1.37
25	5	315	5X6	C41-C17	2.13	1.55	1.50
17	B	828	CLA	C3B-C4B	2.13	1.47	1.42
17	B	841	CLA	C3D-C4D	-2.13	1.39	1.44
17	4	304	CLA	C1B-C2B	2.13	1.48	1.43
17	A	856	CLA	C4D-CHA	2.13	1.46	1.38
17	A	826	CLA	MG-NB	-2.13	2.01	2.05
17	4	309	CLA	C1D-C2D	2.13	1.49	1.45
17	A	837	CLA	C4D-CHA	2.12	1.46	1.38
17	2	311	CLA	C3B-C2B	2.12	1.48	1.41
20	A	857	BCR	C11-C10	-2.12	1.36	1.43
20	J	104	BCR	C15-C14	-2.12	1.36	1.43
17	A	806	CLA	C3D-C4D	-2.12	1.39	1.44
17	A	827	CLA	OBD-CAD	2.12	1.26	1.22
17	O	205	CLA	C3D-C4D	-2.12	1.39	1.44
20	L	206	BCR	C12-C13	-2.12	1.41	1.45
17	B	820	CLA	C4C-C3C	2.12	1.48	1.45
17	A	839	CLA	C4D-CHA	2.12	1.45	1.38
17	B	818	CLA	C4C-C3C	2.12	1.48	1.45
17	1	307	CLA	C4B-NB	-2.12	1.35	1.37
17	B	833	CLA	C3B-C2B	2.12	1.48	1.41
17	3	314	CLA	C3D-C4D	-2.11	1.39	1.44
17	B	813	CLA	MG-ND	-2.11	2.01	2.05
25	2	320	5X6	C01-C02	2.11	1.54	1.50
17	3	311	CLA	C3B-C2B	2.11	1.48	1.41
20	K	104	BCR	C19-C18	-2.11	1.41	1.45
17	2	314	CLA	C3B-C2B	2.11	1.48	1.41
17	5	303	CLA	C4C-C3C	2.11	1.48	1.45
17	B	833	CLA	C1C-NC	-2.10	1.34	1.37
17	A	824	CLA	C4D-CHA	2.10	1.45	1.38
17	1	305	CLA	C1D-C2D	2.10	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	828	CLA	C3B-C2B	2.10	1.48	1.41
17	5	304	CLA	C1B-C2B	2.10	1.48	1.43
17	3	312	CLA	C1D-C2D	2.10	1.49	1.45
17	B	827	CLA	C3B-C2B	2.10	1.48	1.41
17	A	813	CLA	C1B-C2B	2.10	1.48	1.43
17	B	816	CLA	C3B-C2B	2.10	1.48	1.41
17	1	310	CLA	C3B-C2B	2.10	1.48	1.41
17	O	204	CLA	C3B-C2B	2.09	1.48	1.41
17	5	311	CLA	C1D-C2D	2.09	1.49	1.45
17	A	809	CLA	C1C-NC	-2.09	1.34	1.37
17	B	822	CLA	C3B-C2B	2.09	1.48	1.41
17	3	307	CLA	C1D-C2D	2.09	1.49	1.45
17	3	313	CLA	C1D-C2D	2.09	1.49	1.45
17	B	823	CLA	C1C-NC	-2.09	1.34	1.37
17	A	809	CLA	MG-ND	-2.09	2.01	2.05
17	A	835	CLA	MG-ND	-2.09	2.01	2.05
17	B	802	CLA	C3D-C4D	-2.09	1.39	1.44
17	B	821	CLA	C1B-C2B	2.09	1.48	1.43
17	B	802	CLA	C3B-C4B	2.09	1.47	1.42
17	5	314	CLA	C3B-C2B	2.08	1.48	1.41
25	2	320	5X6	C41-C17	2.08	1.55	1.50
17	1	311	CLA	C1D-C2D	2.08	1.49	1.45
17	A	852	CLA	C1B-C2B	2.08	1.48	1.43
17	A	834	CLA	CHB-C4A	-2.08	1.32	1.37
17	B	806	CLA	C3B-C2B	2.08	1.48	1.41
17	A	856	CLA	C1C-C2C	2.08	1.48	1.44
17	A	822	CLA	C3B-C2B	2.08	1.48	1.41
17	2	312	CLA	C3A-C2A	-2.08	1.52	1.54
17	A	824	CLA	C1C-C2C	2.08	1.48	1.44
17	B	839	CLA	C1C-C2C	2.08	1.48	1.44
20	L	201	BCR	C15-C14	-2.08	1.37	1.43
17	5	307	CLA	C3B-C2B	2.08	1.48	1.41
17	3	309	CLA	C3B-C2B	2.08	1.48	1.41
17	A	825	CLA	C1C-C2C	2.08	1.48	1.44
17	B	818	CLA	CHB-C4A	-2.07	1.32	1.37
17	5	305	CLA	C1B-C2B	2.07	1.48	1.43
17	A	852	CLA	C4D-CHA	2.07	1.45	1.38
20	A	846	BCR	C16-C17	-2.07	1.37	1.43
17	B	820	CLA	C4D-CHA	2.07	1.45	1.38
17	B	813	CLA	C3B-C2B	2.07	1.48	1.41
17	B	838	CLA	C3B-C2B	2.07	1.48	1.41
20	A	846	BCR	C20-C21	-2.07	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	825	CLA	C3B-C2B	2.07	1.48	1.41
17	5	307	CLA	C4C-C3C	2.06	1.48	1.45
17	A	823	CLA	C3B-C4B	2.06	1.47	1.42
17	A	828	CLA	C4D-CHA	2.06	1.45	1.38
25	4	314	5X6	C38-C30	2.06	1.54	1.50
17	B	837	CLA	C3B-C2B	2.06	1.48	1.41
17	B	825	CLA	C1C-NC	-2.06	1.34	1.37
17	B	804	CLA	MG-ND	-2.06	2.01	2.05
17	A	810	CLA	C1C-NC	-2.06	1.34	1.37
17	A	810	CLA	MG-ND	-2.06	2.01	2.05
17	A	856	CLA	C4C-C3C	2.06	1.48	1.45
17	O	203	CLA	C1D-C2D	2.06	1.49	1.45
17	2	308	CLA	C1D-C2D	2.06	1.49	1.45
17	A	852	CLA	C1D-ND	2.06	1.40	1.37
25	F	205	5X6	C01-C02	2.06	1.54	1.50
17	A	831	CLA	C4C-C3C	2.06	1.48	1.45
17	A	836	CLA	C1C-C2C	2.05	1.48	1.44
17	B	808	CLA	C4D-CHA	2.05	1.45	1.38
25	5	317	5X6	C38-C30	2.05	1.54	1.50
17	A	855	CLA	C1B-C2B	2.05	1.48	1.43
17	A	836	CLA	C4C-C3C	2.05	1.48	1.45
25	2	317	5X6	C41-C17	2.05	1.55	1.50
17	B	857	CLA	C1C-C2C	2.05	1.48	1.44
17	A	823	CLA	C4C-C3C	2.05	1.48	1.45
17	4	304	CLA	C3B-C2B	2.05	1.48	1.41
17	B	825	CLA	C4C-C3C	2.05	1.48	1.45
17	5	302	CLA	C1D-C2D	2.04	1.49	1.45
17	5	304	CLA	C4C-C3C	2.04	1.48	1.45
17	A	815	CLA	C1C-C2C	2.04	1.48	1.44
17	4	305	CLA	C1D-C2D	2.04	1.49	1.45
17	1	304	CLA	C4C-C3C	2.04	1.48	1.45
25	3	318	5X6	C01-C02	2.04	1.54	1.50
16	A	801	CL0	C3B-C2B	2.04	1.48	1.41
17	A	809	CLA	C4C-C3C	2.04	1.48	1.45
17	3	315	CLA	C1D-C2D	2.04	1.49	1.45
17	5	306	CLA	C1D-C2D	2.04	1.49	1.45
17	B	801	CLA	MG-ND	-2.04	2.01	2.05
17	B	807	CLA	C4C-C3C	2.04	1.48	1.45
17	K	102	CLA	C1B-C2B	2.04	1.48	1.43
17	B	819	CLA	C4D-CHA	2.04	1.45	1.38
17	A	830	CLA	MG-ND	-2.04	2.01	2.05
17	B	857	CLA	C4D-CHA	2.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	304	CLA	C3B-C2B	2.04	1.48	1.41
17	O	205	CLA	C1D-C2D	2.04	1.49	1.45
17	B	829	CLA	CHB-C4A	-2.04	1.32	1.37
17	2	305	CLA	C3B-C2B	2.04	1.48	1.41
25	5	316	5X6	C01-C02	2.03	1.54	1.50
17	3	305	CLA	C3B-C2B	2.03	1.48	1.41
17	A	852	CLA	C1C-C2C	2.03	1.48	1.44
17	B	807	CLA	C3B-C2B	2.03	1.48	1.41
17	A	854	CLA	C1C-C2C	2.03	1.48	1.44
17	B	831	CLA	C3B-C4B	2.03	1.47	1.42
25	2	318	5X6	C41-C17	2.03	1.55	1.50
17	4	310	CLA	C1D-C2D	2.03	1.49	1.45
17	1	306	CLA	C1C-NC	-2.03	1.34	1.37
17	B	822	CLA	C1B-C2B	2.03	1.48	1.43
25	5	301	5X6	C01-C02	2.02	1.54	1.50
17	2	307	CLA	C1D-C2D	2.02	1.49	1.45
17	A	821	CLA	C4C-C3C	2.02	1.48	1.45
17	F	203	CLA	C1C-NC	-2.02	1.34	1.37
17	A	859	CLA	C3B-C2B	2.02	1.48	1.41
17	A	834	CLA	C1B-C2B	2.02	1.48	1.43
20	A	845	BCR	C20-C21	-2.02	1.37	1.43
25	3	318	5X6	C38-C30	2.02	1.54	1.50
17	2	316	CLA	C1D-C2D	2.02	1.49	1.45
17	A	819	CLA	C4D-CHA	2.01	1.45	1.38
17	B	827	CLA	C1C-C2C	2.01	1.48	1.44
17	2	304	CLA	C3B-C2B	2.01	1.48	1.41
17	B	804	CLA	C1C-C2C	2.01	1.48	1.44
20	A	843	BCR	C15-C14	-2.01	1.37	1.43
17	5	305	CLA	CHB-C4A	-2.01	1.32	1.37
17	5	314	CLA	C1D-C2D	2.01	1.49	1.45
20	B	845	BCR	C16-C17	-2.01	1.37	1.43
17	A	853	CLA	C4D-CHA	2.01	1.45	1.38
25	1	312	5X6	C41-C17	2.01	1.55	1.50
17	B	801	CLA	C4D-CHA	2.01	1.45	1.38
17	A	807	CLA	C4C-C3C	2.01	1.48	1.45
17	5	307	CLA	C1B-C2B	2.01	1.48	1.43
17	4	306	CLA	C1D-C2D	2.01	1.49	1.45
17	B	823	CLA	C4C-C3C	2.01	1.48	1.45
17	A	829	CLA	C1C-C2C	2.01	1.48	1.44
17	5	307	CLA	C1C-NC	-2.01	1.34	1.37
17	B	831	CLA	C3B-C2B	2.01	1.48	1.41
17	4	304	CLA	C4B-NB	-2.00	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	316	5X6	C41-C17	2.00	1.55	1.50
17	A	829	CLA	CHB-C4A	-2.00	1.32	1.37
17	B	828	CLA	CHB-C4A	-2.00	1.32	1.37
20	B	846	BCR	C15-C14	-2.00	1.37	1.43
17	K	102	CLA	C1C-NC	-2.00	1.34	1.37
17	2	304	CLA	C1D-C2D	2.00	1.49	1.45

All (5264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	805	CLA	O2A-CGA-O1A	-17.93	78.34	123.59
17	B	805	CLA	O2A-CGA-CBA	16.54	163.81	111.91
25	2	321	5X6	C01-C02-C03	-14.63	108.10	124.53
25	F	205	5X6	C28-C27-C26	-14.17	104.83	126.23
25	1	316	5X6	C01-C02-C03	-13.59	109.26	124.53
25	1	314	5X6	C38-C30-C29	-13.57	109.30	124.53
25	2	321	5X6	C38-C30-C29	-13.31	109.58	124.53
25	F	205	5X6	C24-C25-C26	-13.29	108.34	127.31
25	F	205	5X6	C19-C18-C17	-13.18	108.50	127.31
25	5	318	5X6	C38-C30-C29	-13.17	109.74	124.53
25	1	313	5X6	C01-C02-C03	-13.12	109.79	124.53
25	J	105	5X6	C24-C25-C26	-13.00	108.76	127.31
25	5	317	5X6	C38-C30-C29	-12.76	110.20	124.53
25	1	315	5X6	C38-C30-C29	-12.76	110.20	124.53
25	3	316	5X6	C38-C30-C29	-12.68	110.29	124.53
25	4	314	5X6	C38-C30-C29	-12.41	110.59	124.53
25	5	317	5X6	C01-C02-C03	-12.41	110.59	124.53
25	1	315	5X6	C01-C02-C03	-12.20	110.83	124.53
25	F	205	5X6	C20-C21-C22	-12.06	110.10	127.31
25	5	315	5X6	C01-C02-C03	-12.05	110.99	124.53
25	1	312	5X6	C01-C02-C03	-11.85	111.22	124.53
25	4	312	5X6	C01-C02-C03	-11.83	111.25	124.53
17	B	808	CLA	C1D-ND-C4D	-11.66	98.05	106.33
25	5	318	5X6	C01-C02-C03	-11.57	111.54	124.53
25	5	318	5X6	C15-C14-C13	-11.50	110.89	127.31
25	5	316	5X6	C38-C30-C29	-11.46	111.66	124.53
25	F	205	5X6	C15-C14-C13	-11.41	111.02	127.31
25	5	315	5X6	C20-C21-C22	-11.40	111.04	127.31
25	5	316	5X6	C20-C21-C22	-11.32	111.16	127.31
25	2	319	5X6	C01-C02-C03	-11.19	111.96	124.53
25	2	321	5X6	C15-C14-C13	-11.08	111.49	127.31
25	2	318	5X6	C24-C25-C26	-11.05	111.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	822	CLA	C1D-ND-C4D	-11.02	98.51	106.33
25	5	301	5X6	C01-C02-C03	-10.98	112.20	124.53
25	2	317	5X6	C01-C02-C03	-10.93	112.25	124.53
25	3	316	5X6	C01-C02-C03	-10.82	112.38	124.53
25	J	105	5X6	C20-C21-C22	-10.80	111.90	127.31
17	2	307	CLA	C1D-ND-C4D	-10.78	98.68	106.33
17	B	857	CLA	C1D-ND-C4D	-10.76	98.69	106.33
17	B	839	CLA	C1D-ND-C4D	-10.74	98.71	106.33
25	4	314	5X6	C01-C02-C03	-10.73	112.48	124.53
17	B	833	CLA	C2D-C1D-ND	10.71	118.00	110.10
17	B	824	CLA	C1D-ND-C4D	-10.71	98.73	106.33
17	B	819	CLA	C1D-ND-C4D	-10.68	98.75	106.33
17	A	807	CLA	C1D-ND-C4D	-10.66	98.77	106.33
25	2	320	5X6	C15-C14-C13	-10.65	112.11	127.31
17	A	812	CLA	C1D-ND-C4D	-10.65	98.77	106.33
25	J	105	5X6	C15-C14-C13	-10.65	112.11	127.31
25	3	318	5X6	C38-C30-C29	-10.64	112.58	124.53
25	2	319	5X6	C38-C30-C29	-10.61	112.61	124.53
17	A	854	CLA	C1D-ND-C4D	-10.60	98.80	106.33
17	A	859	CLA	C1D-ND-C4D	-10.59	98.81	106.33
25	5	315	5X6	C15-C14-C13	-10.56	112.23	127.31
25	2	321	5X6	C20-C21-C22	-10.55	112.25	127.31
25	3	317	5X6	C01-C02-C03	-10.53	112.71	124.53
25	F	205	5X6	C38-C30-C29	-10.51	112.73	124.53
25	1	312	5X6	C38-C30-C29	-10.51	112.73	124.53
17	3	311	CLA	C1D-ND-C4D	-10.44	98.92	106.33
17	A	812	CLA	C2D-C1D-ND	10.43	117.79	110.10
17	B	808	CLA	C2D-C1D-ND	10.40	117.77	110.10
25	4	312	5X6	C38-C30-C29	-10.40	112.85	124.53
25	1	314	5X6	C15-C14-C13	-10.40	112.47	127.31
17	A	824	CLA	C2D-C1D-ND	10.40	117.77	110.10
17	2	311	CLA	C1D-ND-C4D	-10.38	98.96	106.33
17	A	824	CLA	C1D-ND-C4D	-10.38	98.96	106.33
17	A	855	CLA	C1D-ND-C4D	-10.37	98.97	106.33
17	B	822	CLA	C1D-ND-C4D	-10.34	98.99	106.33
17	1	307	CLA	C1D-ND-C4D	-10.32	99.00	106.33
25	1	313	5X6	C38-C30-C29	-10.30	112.97	124.53
17	A	806	CLA	C1D-ND-C4D	-10.27	99.04	106.33
17	2	305	CLA	C1D-ND-C4D	-10.26	99.05	106.33
17	A	814	CLA	C1D-ND-C4D	-10.25	99.05	106.33
17	A	820	CLA	C1D-ND-C4D	-10.24	99.06	106.33
25	1	314	5X6	C20-C21-C22	-10.23	112.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	839	CLA	C1D-ND-C4D	-10.23	99.07	106.33
17	A	837	CLA	C2D-C1D-ND	10.22	117.64	110.10
25	3	318	5X6	C20-C21-C22	-10.22	112.72	127.31
25	4	312	5X6	C15-C14-C13	-10.19	112.76	127.31
17	B	833	CLA	C1D-ND-C4D	-10.18	99.10	106.33
17	5	305	CLA	C1D-ND-C4D	-10.18	99.10	106.33
25	3	317	5X6	C38-C30-C29	-10.16	113.12	124.53
17	A	855	CLA	C2D-C1D-ND	10.14	117.58	110.10
17	A	817	CLA	C1D-ND-C4D	-10.13	99.14	106.33
17	5	309	CLA	C1D-ND-C4D	-10.12	99.15	106.33
17	4	308	CLA	C1D-ND-C4D	-10.11	99.15	106.33
17	A	837	CLA	C1D-ND-C4D	-10.11	99.15	106.33
17	B	857	CLA	C2D-C1D-ND	10.11	117.55	110.10
17	A	805	CLA	C1D-ND-C4D	-10.10	99.16	106.33
17	A	806	CLA	C2D-C1D-ND	10.10	117.55	110.10
17	3	307	CLA	C1D-ND-C4D	-10.09	99.17	106.33
17	A	821	CLA	C1D-ND-C4D	-10.08	99.17	106.33
17	2	304	CLA	C1D-ND-C4D	-10.07	99.18	106.33
17	4	304	CLA	C1D-ND-C4D	-10.05	99.19	106.33
25	2	321	5X6	C19-C18-C17	-10.05	112.96	127.31
17	A	822	CLA	C2D-C1D-ND	10.05	117.51	110.10
17	3	305	CLA	C1D-ND-C4D	-10.03	99.21	106.33
25	3	317	5X6	C19-C18-C17	-10.01	113.02	127.31
25	2	320	5X6	C38-C30-C29	-9.99	113.31	124.53
17	1	308	CLA	C1D-ND-C4D	-9.98	99.25	106.33
17	1	304	CLA	C1D-ND-C4D	-9.97	99.25	106.33
17	B	841	CLA	C1D-ND-C4D	-9.94	99.28	106.33
17	A	856	CLA	C1D-ND-C4D	-9.94	99.28	106.33
17	A	819	CLA	C1D-ND-C4D	-9.93	99.28	106.33
25	3	318	5X6	C24-C25-C26	-9.93	113.14	127.31
17	A	818	CLA	C1D-ND-C4D	-9.91	99.29	106.33
17	A	807	CLA	C2D-C1D-ND	9.91	117.41	110.10
17	B	805	CLA	C2D-C1D-ND	9.89	117.39	110.10
25	1	313	5X6	C28-C27-C26	-9.89	111.29	126.23
17	O	203	CLA	C1D-ND-C4D	-9.88	99.32	106.33
25	4	313	5X6	C38-C30-C29	-9.88	113.43	124.53
17	B	830	CLA	C1D-ND-C4D	-9.87	99.32	106.33
17	5	312	CLA	C1D-ND-C4D	-9.87	99.33	106.33
17	B	824	CLA	C2D-C1D-ND	9.86	117.37	110.10
25	5	315	5X6	C28-C27-C26	-9.84	111.37	126.23
25	2	320	5X6	C01-C02-C03	-9.82	113.50	124.53
17	B	805	CLA	O1A-CGA-CBA	-9.81	85.47	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	311	CLA	C1D-ND-C4D	-9.80	99.38	106.33
17	5	303	CLA	C1D-ND-C4D	-9.80	99.38	106.33
17	2	315	CLA	C1D-ND-C4D	-9.79	99.38	106.33
17	3	309	CLA	C1D-ND-C4D	-9.79	99.38	106.33
25	1	316	5X6	C24-C25-C26	-9.79	113.34	127.31
17	B	838	CLA	C1D-ND-C4D	-9.78	99.39	106.33
17	4	311	CLA	C1D-ND-C4D	-9.77	99.39	106.33
17	2	310	CLA	C1D-ND-C4D	-9.77	99.40	106.33
17	A	859	CLA	C2D-C1D-ND	9.77	117.30	110.10
17	B	815	CLA	C1D-ND-C4D	-9.77	99.40	106.33
25	5	301	5X6	C38-C30-C29	-9.76	113.57	124.53
17	2	314	CLA	C1D-ND-C4D	-9.76	99.40	106.33
25	2	317	5X6	C15-C14-C13	-9.76	113.38	127.31
25	3	317	5X6	C15-C14-C13	-9.75	113.39	127.31
17	A	813	CLA	C1D-ND-C4D	-9.74	99.42	106.33
17	B	828	CLA	C2D-C1D-ND	9.74	117.28	110.10
17	2	309	CLA	C1D-ND-C4D	-9.70	99.45	106.33
17	B	840	CLA	C1D-ND-C4D	-9.69	99.45	106.33
17	5	302	CLA	C1D-ND-C4D	-9.69	99.45	106.33
17	B	816	CLA	C1D-ND-C4D	-9.68	99.46	106.33
25	5	301	5X6	C15-C14-C13	-9.68	113.50	127.31
25	3	316	5X6	C20-C21-C22	-9.68	113.50	127.31
17	3	315	CLA	C1D-ND-C4D	-9.68	99.46	106.33
25	J	105	5X6	C38-C30-C29	-9.67	113.67	124.53
17	A	854	CLA	C2D-C1D-ND	9.67	117.23	110.10
25	3	318	5X6	C15-C14-C13	-9.65	113.53	127.31
17	4	306	CLA	C1D-ND-C4D	-9.65	99.48	106.33
17	B	817	CLA	C1D-ND-C4D	-9.64	99.48	106.33
17	B	823	CLA	C1D-ND-C4D	-9.64	99.49	106.33
17	3	312	CLA	C1D-ND-C4D	-9.64	99.49	106.33
25	4	314	5X6	C15-C14-C13	-9.64	113.56	127.31
25	2	320	5X6	C28-C27-C26	-9.63	111.68	126.23
17	2	313	CLA	C1D-ND-C4D	-9.63	99.49	106.33
17	2	316	CLA	C1D-ND-C4D	-9.63	99.50	106.33
17	B	818	CLA	C1D-ND-C4D	-9.63	99.50	106.33
17	A	820	CLA	C2D-C1D-ND	9.62	117.20	110.10
17	5	310	CLA	C1D-ND-C4D	-9.62	99.50	106.33
17	B	840	CLA	C2D-C1D-ND	9.61	117.19	110.10
17	A	817	CLA	C2D-C1D-ND	9.61	117.19	110.10
25	5	316	5X6	C15-C14-C13	-9.60	113.61	127.31
17	3	310	CLA	C1D-ND-C4D	-9.59	99.52	106.33
17	4	309	CLA	C1D-ND-C4D	-9.59	99.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	310	CLA	C1D-ND-C4D	-9.59	99.52	106.33
25	1	315	5X6	C20-C21-C22	-9.58	113.63	127.31
17	4	310	CLA	C1D-ND-C4D	-9.58	99.53	106.33
25	1	312	5X6	C24-C25-C26	-9.57	113.64	127.31
25	1	315	5X6	C15-C14-C13	-9.57	113.65	127.31
25	1	313	5X6	C15-C14-C13	-9.56	113.66	127.31
17	L	202	CLA	C1D-ND-C4D	-9.56	99.55	106.33
25	5	315	5X6	C11-C12-C13	-9.55	111.80	126.23
17	B	809	CLA	C1D-ND-C4D	-9.55	99.55	106.33
17	A	828	CLA	C1D-ND-C4D	-9.54	99.55	106.33
17	5	311	CLA	C1D-ND-C4D	-9.54	99.56	106.33
17	2	312	CLA	C1D-ND-C4D	-9.52	99.58	106.33
17	A	838	CLA	C1D-ND-C4D	-9.51	99.58	106.33
17	B	829	CLA	C1D-ND-C4D	-9.51	99.58	106.33
17	A	802	CLA	C1D-ND-C4D	-9.51	99.58	106.33
17	1	309	CLA	C1D-ND-C4D	-9.50	99.58	106.33
17	A	803	CLA	C1D-ND-C4D	-9.50	99.59	106.33
17	B	839	CLA	C2D-C1D-ND	9.49	117.10	110.10
17	3	314	CLA	C1D-ND-C4D	-9.49	99.59	106.33
17	3	313	CLA	C1D-ND-C4D	-9.48	99.60	106.33
25	5	315	5X6	C38-C30-C29	-9.47	113.89	124.53
17	B	838	CLA	C2D-C1D-ND	9.47	117.08	110.10
17	B	822	CLA	C2D-C1D-ND	9.47	117.08	110.10
17	O	204	CLA	C1D-ND-C4D	-9.46	99.61	106.33
17	L	204	CLA	C1D-ND-C4D	-9.46	99.62	106.33
17	5	314	CLA	C1D-ND-C4D	-9.44	99.63	106.33
17	A	818	CLA	C2D-C1D-ND	9.42	117.05	110.10
17	B	821	CLA	C1D-ND-C4D	-9.41	99.65	106.33
17	5	306	CLA	C1D-ND-C4D	-9.41	99.65	106.33
17	B	837	CLA	C1D-ND-C4D	-9.41	99.65	106.33
17	5	307	CLA	C1D-ND-C4D	-9.40	99.66	106.33
25	3	316	5X6	C15-C14-C13	-9.40	113.89	127.31
17	3	306	CLA	C1D-ND-C4D	-9.39	99.66	106.33
17	B	834	CLA	C1D-ND-C4D	-9.39	99.66	106.33
17	B	826	CLA	C2D-C1D-ND	9.39	117.02	110.10
17	B	802	CLA	C2D-C1D-ND	9.39	117.02	110.10
17	A	805	CLA	C2D-C1D-ND	9.38	117.01	110.10
17	1	305	CLA	C1D-ND-C4D	-9.37	99.68	106.33
17	B	802	CLA	C1D-ND-C4D	-9.37	99.68	106.33
17	O	205	CLA	C1D-ND-C4D	-9.36	99.68	106.33
25	4	314	5X6	C20-C21-C22	-9.36	113.95	127.31
17	B	830	CLA	C2D-C1D-ND	9.35	117.00	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	853	CLA	C2D-C1D-ND	9.35	116.99	110.10
25	2	321	5X6	C28-C27-C26	-9.33	112.14	126.23
17	A	810	CLA	C2D-C1D-ND	9.33	116.98	110.10
17	B	821	CLA	C2D-C1D-ND	9.32	116.97	110.10
17	A	810	CLA	C1D-ND-C4D	-9.31	99.72	106.33
25	1	315	5X6	C19-C18-C17	-9.31	114.02	127.31
17	1	303	CLA	C1D-ND-C4D	-9.30	99.73	106.33
17	B	805	CLA	C1D-ND-C4D	-9.29	99.74	106.33
17	4	305	CLA	C1D-ND-C4D	-9.28	99.74	106.33
25	1	316	5X6	C15-C14-C13	-9.28	114.07	127.31
17	A	839	CLA	C2D-C1D-ND	9.27	116.93	110.10
17	B	818	CLA	C2D-C1D-ND	9.26	116.93	110.10
17	B	809	CLA	C2D-C1D-ND	9.25	116.92	110.10
25	2	319	5X6	C24-C25-C26	-9.24	114.12	127.31
17	B	819	CLA	C2D-C1D-ND	9.24	116.91	110.10
17	4	303	CLA	C1D-ND-C4D	-9.22	99.78	106.33
25	1	316	5X6	C19-C18-C17	-9.22	114.15	127.31
17	K	103	CLA	C1D-ND-C4D	-9.22	99.79	106.33
25	5	317	5X6	C19-C18-C17	-9.21	114.17	127.31
25	J	105	5X6	C20-C19-C18	-9.21	104.61	123.47
17	A	833	CLA	C1D-ND-C4D	-9.19	99.80	106.33
25	3	318	5X6	C01-C02-C03	-9.19	114.20	124.53
17	A	856	CLA	C2D-C1D-ND	9.19	116.88	110.10
25	5	318	5X6	C20-C21-C22	-9.19	114.19	127.31
17	F	204	CLA	C1D-ND-C4D	-9.19	99.81	106.33
25	J	105	5X6	C01-C02-C03	-9.18	114.21	124.53
25	1	315	5X6	C24-C25-C26	-9.18	114.21	127.31
25	4	314	5X6	C24-C25-C26	-9.18	114.22	127.31
17	A	808	CLA	C1D-ND-C4D	-9.17	99.82	106.33
17	2	306	CLA	C1D-ND-C4D	-9.17	99.82	106.33
17	4	307	CLA	C1D-ND-C4D	-9.17	99.82	106.33
25	2	318	5X6	C15-C14-C13	-9.17	114.22	127.31
25	4	312	5X6	C19-C18-C17	-9.17	114.22	127.31
25	2	319	5X6	C15-C14-C13	-9.16	114.24	127.31
25	1	314	5X6	C01-C02-C03	-9.16	114.24	124.53
25	2	317	5X6	C11-C12-C13	-9.16	112.40	126.23
17	1	306	CLA	C1D-ND-C4D	-9.15	99.83	106.33
25	1	314	5X6	C24-C25-C26	-9.14	114.26	127.31
17	B	837	CLA	C2D-C1D-ND	9.14	116.84	110.10
25	4	313	5X6	C01-C02-C03	-9.14	114.27	124.53
25	2	318	5X6	C19-C18-C17	-9.13	114.28	127.31
17	B	832	CLA	C1D-ND-C4D	-9.13	99.85	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	102	CLA	C1D-ND-C4D	-9.12	99.85	106.33
17	A	815	CLA	C1D-ND-C4D	-9.12	99.86	106.33
17	B	829	CLA	C2D-C1D-ND	9.11	116.81	110.10
17	B	827	CLA	C1D-ND-C4D	-9.10	99.87	106.33
25	4	313	5X6	C11-C12-C13	-9.10	112.48	126.23
25	4	312	5X6	C24-C25-C26	-9.10	114.33	127.31
25	2	318	5X6	C38-C30-C29	-9.10	114.31	124.53
25	2	320	5X6	C20-C21-C22	-9.09	114.33	127.31
25	5	318	5X6	C24-C25-C26	-9.09	114.33	127.31
17	B	826	CLA	C1D-ND-C4D	-9.09	99.88	106.33
17	5	307	CLA	C2D-C1D-ND	9.08	116.80	110.10
17	B	835	CLA	C1D-ND-C4D	-9.08	99.89	106.33
17	B	813	CLA	C1D-ND-C4D	-9.08	99.89	106.33
17	A	828	CLA	C2D-C1D-ND	9.07	116.78	110.10
25	5	316	5X6	C01-C02-C03	-9.04	114.38	124.53
17	5	308	CLA	C1D-ND-C4D	-9.04	99.92	106.33
17	5	308	CLA	C2B-C1B-NB	9.03	116.28	110.23
17	A	811	CLA	C2D-C1D-ND	9.02	116.75	110.10
17	A	809	CLA	C1D-ND-C4D	-9.02	99.93	106.33
17	5	313	CLA	C1D-ND-C4D	-9.00	99.94	106.33
17	B	820	CLA	C1D-ND-C4D	-9.00	99.94	106.33
17	2	308	CLA	C1D-ND-C4D	-8.99	99.95	106.33
25	5	318	5X6	C28-C27-C26	-8.99	112.64	126.23
17	A	836	CLA	C1D-ND-C4D	-8.99	99.95	106.33
17	B	827	CLA	C2D-C1D-ND	8.97	116.72	110.10
17	B	806	CLA	C1D-ND-C4D	-8.97	99.96	106.33
17	B	813	CLA	C2D-C1D-ND	8.97	116.71	110.10
17	1	302	CLA	C1D-ND-C4D	-8.97	99.97	106.33
25	3	317	5X6	C24-C25-C26	-8.96	114.52	127.31
17	1	301	CLA	C1D-ND-C4D	-8.96	99.97	106.33
16	A	801	CL0	C2D-C1D-ND	8.95	116.70	110.10
25	3	318	5X6	C19-C18-C17	-8.94	114.55	127.31
17	A	811	CLA	C1D-ND-C4D	-8.93	99.99	106.33
25	5	317	5X6	C20-C21-C22	-8.93	114.57	127.31
17	5	305	CLA	C2B-C1B-NB	8.92	116.21	110.23
17	A	825	CLA	C2D-C1D-ND	8.92	116.67	110.10
17	B	814	CLA	C1D-ND-C4D	-8.91	100.01	106.33
17	A	809	CLA	C2D-C1D-ND	8.91	116.67	110.10
17	A	815	CLA	C2D-C1D-ND	8.89	116.66	110.10
25	5	315	5X6	C19-C18-C17	-8.87	114.65	127.31
17	B	807	CLA	C2D-C1D-ND	8.87	116.64	110.10
25	2	318	5X6	C01-C02-C03	-8.86	114.57	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	203	CLA	C1D-ND-C4D	-8.86	100.04	106.33
17	A	825	CLA	C1D-ND-C4D	-8.85	100.05	106.33
17	A	821	CLA	C2D-C1D-ND	8.85	116.63	110.10
25	3	316	5X6	C41-C17-C18	-8.85	110.53	122.92
17	B	824	CLA	C2B-C1B-NB	8.84	116.16	110.23
17	A	804	CLA	C2D-C1D-ND	8.81	116.60	110.10
17	5	309	CLA	C2D-C1D-ND	8.81	116.60	110.10
25	5	316	5X6	C16-C17-C18	-8.80	105.44	118.94
17	5	304	CLA	C2B-C1B-NB	8.79	116.12	110.23
17	A	836	CLA	C2D-C1D-ND	8.79	116.58	110.10
17	B	804	CLA	C2D-C1D-ND	8.78	116.58	110.10
17	A	838	CLA	C2D-C1D-ND	8.77	116.57	110.10
25	3	316	5X6	C11-C12-C13	-8.77	112.98	126.23
17	B	817	CLA	C2D-C1D-ND	8.76	116.56	110.10
25	2	317	5X6	C20-C21-C22	-8.76	114.81	127.31
17	B	810	CLA	C1D-ND-C4D	-8.76	100.11	106.33
25	5	301	5X6	C24-C25-C26	-8.76	114.81	127.31
17	1	307	CLA	C2D-C1D-ND	8.75	116.55	110.10
17	3	308	CLA	C1D-ND-C4D	-8.74	100.13	106.33
25	4	314	5X6	C11-C12-C13	-8.72	113.06	126.23
17	A	808	CLA	C2B-C1B-NB	8.70	116.06	110.23
17	B	831	CLA	C1D-ND-C4D	-8.69	100.16	106.33
17	A	823	CLA	C1D-ND-C4D	-8.69	100.16	106.33
17	A	827	CLA	C1D-ND-C4D	-8.69	100.16	106.33
25	5	317	5X6	C28-C27-C26	-8.68	113.11	126.23
17	2	311	CLA	C2D-C1D-ND	8.68	116.50	110.10
25	5	315	5X6	C24-C25-C26	-8.67	114.93	127.31
25	5	317	5X6	C15-C14-C13	-8.67	114.94	127.31
17	A	823	CLA	C2D-C1D-ND	8.66	116.49	110.10
17	J	103	CLA	C1D-ND-C4D	-8.66	100.18	106.33
25	1	314	5X6	C28-C27-C26	-8.62	113.21	126.23
17	5	304	CLA	C1D-ND-C4D	-8.62	100.21	106.33
25	2	320	5X6	C24-C25-C26	-8.61	115.03	127.31
17	A	819	CLA	C2D-C1D-ND	8.60	116.44	110.10
17	A	852	CLA	C2D-C1D-ND	8.60	116.44	110.10
17	A	853	CLA	C1D-ND-C4D	-8.59	100.23	106.33
25	J	105	5X6	C16-C17-C18	-8.59	105.76	118.94
17	A	834	CLA	C1D-ND-C4D	-8.59	100.23	106.33
25	1	315	5X6	C11-C12-C13	-8.58	113.26	126.23
17	A	831	CLA	C2D-C1D-ND	8.58	116.43	110.10
17	A	803	CLA	C2D-C1D-ND	8.58	116.43	110.10
17	B	810	CLA	C2D-C1D-ND	8.58	116.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	814	CLA	C2D-C1D-ND	8.58	116.42	110.10
17	A	802	CLA	C2D-C1D-ND	8.57	116.42	110.10
25	J	105	5X6	C12-C13-C14	-8.57	105.79	118.94
17	A	830	CLA	C1D-ND-C4D	-8.56	100.26	106.33
17	F	203	CLA	C1D-ND-C4D	-8.55	100.26	106.33
17	A	829	CLA	C1D-ND-C4D	-8.54	100.27	106.33
25	5	318	5X6	C42-C13-C14	-8.54	110.96	122.92
17	A	830	CLA	C2D-C1D-ND	8.53	116.39	110.10
17	B	815	CLA	C2D-C1D-ND	8.50	116.37	110.10
17	3	311	CLA	C2D-C1D-ND	8.49	116.36	110.10
17	B	804	CLA	C1D-ND-C4D	-8.49	100.30	106.33
25	5	301	5X6	C20-C21-C22	-8.47	115.22	127.31
17	B	836	CLA	C2D-C1D-ND	8.47	116.35	110.10
17	A	831	CLA	C1D-ND-C4D	-8.47	100.32	106.33
25	4	312	5X6	C20-C21-C22	-8.47	115.22	127.31
17	A	813	CLA	C2D-C1D-ND	8.47	116.34	110.10
17	B	841	CLA	C2D-C1D-ND	8.46	116.34	110.10
17	5	312	CLA	C2D-C1D-ND	8.46	116.34	110.10
17	A	827	CLA	C2D-C1D-ND	8.44	116.33	110.10
17	2	305	CLA	C2D-C1D-ND	8.44	116.33	110.10
17	1	308	CLA	C2D-C1D-ND	8.44	116.33	110.10
17	A	808	CLA	C2D-C1D-ND	8.44	116.32	110.10
17	4	308	CLA	C2D-C1D-ND	8.44	116.32	110.10
16	A	801	CL0	C1D-ND-C4D	-8.42	100.36	106.33
17	5	307	CLA	C2B-C1B-NB	8.41	115.87	110.23
17	3	309	CLA	C2D-C1D-ND	8.40	116.29	110.10
17	A	835	CLA	C1D-ND-C4D	-8.38	100.38	106.33
17	B	825	CLA	C1D-ND-C4D	-8.37	100.39	106.33
17	B	806	CLA	C2D-C1D-ND	8.36	116.27	110.10
17	B	812	CLA	C1D-ND-C4D	-8.36	100.39	106.33
25	F	205	5X6	C11-C12-C13	-8.34	113.64	126.23
25	2	319	5X6	C11-C12-C13	-8.34	113.64	126.23
25	2	318	5X6	C11-C12-C13	-8.33	113.64	126.23
17	B	836	CLA	C1D-ND-C4D	-8.33	100.42	106.33
25	5	301	5X6	C28-C27-C26	-8.33	113.66	126.23
17	B	801	CLA	C2D-C1D-ND	8.31	116.23	110.10
17	L	202	CLA	C2D-C1D-ND	8.31	116.23	110.10
17	B	828	CLA	C1D-ND-C4D	-8.30	100.44	106.33
25	4	312	5X6	C41-C17-C18	-8.30	111.30	122.92
17	A	833	CLA	C2D-C1D-ND	8.30	116.22	110.10
25	F	205	5X6	C20-C19-C18	-8.29	106.49	123.47
17	B	816	CLA	C2D-C1D-ND	8.29	116.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	313	5X6	C20-C21-C22	-8.28	115.49	127.31
17	B	807	CLA	C1D-ND-C4D	-8.27	100.46	106.33
17	B	835	CLA	C2D-C1D-ND	8.27	116.20	110.10
17	4	304	CLA	C2D-C1D-ND	8.26	116.19	110.10
17	B	834	CLA	C2D-C1D-ND	8.26	116.19	110.10
25	1	312	5X6	C15-C14-C13	-8.25	115.53	127.31
17	K	103	CLA	C2D-C1D-ND	8.25	116.18	110.10
25	1	312	5X6	C20-C21-C22	-8.24	115.55	127.31
17	2	304	CLA	C2D-C1D-ND	8.24	116.17	110.10
17	A	816	CLA	C1D-ND-C4D	-8.22	100.50	106.33
17	B	814	CLA	C2D-C1D-ND	8.22	116.16	110.10
25	4	313	5X6	C40-C22-C21	-8.21	111.42	122.92
25	3	317	5X6	C11-C12-C13	-8.19	113.85	126.23
17	2	312	CLA	C2D-C1D-ND	8.19	116.14	110.10
25	2	321	5X6	C24-C25-C26	-8.17	115.65	127.31
25	1	314	5X6	C42-C13-C14	-8.16	111.49	122.92
17	1	303	CLA	C2B-C1B-NB	8.16	115.70	110.23
17	5	303	CLA	C2D-C1D-ND	8.16	116.12	110.10
17	2	307	CLA	C2D-C1D-ND	8.15	116.11	110.10
25	2	317	5X6	C40-C22-C21	-8.15	111.51	122.92
17	2	306	CLA	C2D-C1D-ND	8.14	116.11	110.10
17	K	102	CLA	C2D-C1D-ND	8.14	116.10	110.10
17	2	314	CLA	C2D-C1D-ND	8.14	116.10	110.10
17	3	306	CLA	C2D-C1D-ND	8.13	116.10	110.10
17	3	305	CLA	C2D-C1D-ND	8.13	116.10	110.10
17	A	835	CLA	C2D-C1D-ND	8.13	116.09	110.10
17	B	811	CLA	C1D-ND-C4D	-8.13	100.56	106.33
25	5	316	5X6	C11-C12-C13	-8.12	113.96	126.23
17	2	309	CLA	C2D-C1D-ND	8.12	116.09	110.10
17	B	831	CLA	C2D-C1D-ND	8.11	116.08	110.10
17	B	820	CLA	C2B-C1B-NB	8.11	115.67	110.23
17	2	315	CLA	C2D-C1D-ND	8.10	116.07	110.10
17	2	310	CLA	C2B-C1B-NB	8.09	115.66	110.23
25	J	105	5X6	C19-C18-C17	-8.08	115.77	127.31
25	4	313	5X6	C15-C14-C13	-8.08	115.78	127.31
25	1	316	5X6	C38-C30-C29	-8.08	115.45	124.53
17	5	306	CLA	C2B-C1B-NB	8.06	115.64	110.23
17	2	313	CLA	C2D-C1D-ND	8.06	116.04	110.10
17	1	304	CLA	C2D-C1D-ND	8.04	116.03	110.10
25	2	321	5X6	C41-C17-C18	-8.04	111.66	122.92
25	1	315	5X6	C39-C26-C25	-8.04	111.66	122.92
17	B	825	CLA	C2D-C1D-ND	8.03	116.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	315	CLA	C2D-C1D-ND	8.02	116.02	110.10
17	A	829	CLA	C2D-C1D-ND	8.02	116.02	110.10
17	4	307	CLA	C2B-C1B-NB	8.02	115.61	110.23
17	3	307	CLA	C2D-C1D-ND	8.02	116.01	110.10
25	2	317	5X6	C38-C30-C29	-8.01	115.53	124.53
17	5	309	CLA	C2B-C1B-NB	8.01	115.60	110.23
17	1	303	CLA	C2D-C1D-ND	8.00	116.00	110.10
17	4	303	CLA	C2D-C1D-ND	7.99	115.99	110.10
25	1	313	5X6	C20-C21-C22	-7.99	115.91	127.31
17	O	203	CLA	C2D-C1D-ND	7.99	115.99	110.10
17	3	314	CLA	C2D-C1D-ND	7.97	115.98	110.10
17	2	316	CLA	C2D-C1D-ND	7.96	115.97	110.10
17	5	302	CLA	C2D-C1D-ND	7.95	115.96	110.10
25	5	318	5X6	C40-C22-C21	-7.95	111.79	122.92
25	4	314	5X6	C19-C18-C17	-7.95	115.97	127.31
17	1	310	CLA	C2B-C1B-NB	7.95	115.56	110.23
17	F	203	CLA	C2D-C1D-ND	7.95	115.96	110.10
17	3	310	CLA	C2D-C1D-ND	7.94	115.96	110.10
17	1	304	CLA	C2B-C1B-NB	7.94	115.56	110.23
17	1	309	CLA	C2D-C1D-ND	7.94	115.95	110.10
17	O	204	CLA	C2D-C1D-ND	7.93	115.95	110.10
17	1	310	CLA	C2D-C1D-ND	7.93	115.95	110.10
17	A	816	CLA	C2D-C1D-ND	7.92	115.94	110.10
17	2	311	CLA	C2B-C1B-NB	7.92	115.54	110.23
25	1	315	5X6	C28-C27-C26	-7.92	114.28	126.23
17	B	817	CLA	C2B-C1B-NB	7.91	115.53	110.23
17	2	310	CLA	C2D-C1D-ND	7.91	115.93	110.10
17	1	311	CLA	C2D-C1D-ND	7.90	115.93	110.10
17	A	804	CLA	C1D-ND-C4D	-7.90	100.72	106.33
25	1	313	5X6	C42-C13-C14	-7.90	111.86	122.92
25	1	315	5X6	C41-C17-C18	-7.90	111.86	122.92
25	2	317	5X6	C41-C17-C18	-7.90	111.86	122.92
17	5	313	CLA	C2B-C1B-NB	7.89	115.52	110.23
25	1	313	5X6	C24-C25-C26	-7.89	116.05	127.31
25	J	105	5X6	C28-C27-C26	-7.89	114.32	126.23
17	B	832	CLA	C2D-C1D-ND	7.88	115.91	110.10
17	3	311	CLA	C2B-C1B-NB	7.88	115.52	110.23
17	5	314	CLA	C2D-C1D-ND	7.87	115.90	110.10
25	1	314	5X6	C40-C22-C21	-7.86	111.91	122.92
17	5	305	CLA	C2D-C1D-ND	7.86	115.90	110.10
17	5	311	CLA	C2D-C1D-ND	7.85	115.89	110.10
17	A	834	CLA	C2D-C1D-ND	7.84	115.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	825	CLA	C2B-C1B-NB	7.84	115.49	110.23
17	A	813	CLA	C2B-C1B-NB	7.84	115.49	110.23
17	B	812	CLA	C2B-C1B-NB	7.84	115.49	110.23
25	5	315	5X6	C40-C22-C21	-7.84	111.95	122.92
17	5	314	CLA	C2B-C1B-NB	7.83	115.48	110.23
17	3	305	CLA	C2B-C1B-NB	7.83	115.48	110.23
17	A	826	CLA	C2D-C1D-ND	7.83	115.87	110.10
17	B	811	CLA	C2B-C1B-NB	7.83	115.48	110.23
17	5	306	CLA	C2D-C1D-ND	7.82	115.86	110.10
17	4	311	CLA	C2D-C1D-ND	7.81	115.86	110.10
25	3	317	5X6	C28-C27-C26	-7.81	114.44	126.23
17	L	203	CLA	C2D-C1D-ND	7.80	115.85	110.10
17	3	310	CLA	C2B-C1B-NB	7.79	115.46	110.23
25	2	318	5X6	C42-C13-C14	-7.79	112.01	122.92
25	4	314	5X6	C39-C26-C25	-7.79	112.01	122.92
17	B	801	CLA	C1D-ND-C4D	-7.78	100.81	106.33
17	O	205	CLA	C2D-C1D-ND	7.78	115.84	110.10
17	3	312	CLA	C2D-C1D-ND	7.78	115.83	110.10
17	3	307	CLA	C2B-C1B-NB	7.77	115.44	110.23
17	1	307	CLA	C2B-C1B-NB	7.77	115.44	110.23
17	B	832	CLA	C2B-C1B-NB	7.76	115.44	110.23
17	B	822	CLA	C2B-C1B-NB	7.76	115.44	110.23
17	A	852	CLA	C1D-ND-C4D	-7.76	100.82	106.33
17	4	309	CLA	C2D-C1D-ND	7.76	115.82	110.10
17	O	204	CLA	C2B-C1B-NB	7.76	115.43	110.23
25	5	301	5X6	C19-C18-C17	-7.75	116.25	127.31
17	4	306	CLA	C2D-C1D-ND	7.75	115.82	110.10
17	A	832	CLA	C4A-NA-C1A	-7.75	103.22	106.71
17	5	310	CLA	C2D-C1D-ND	7.75	115.81	110.10
17	2	314	CLA	C2B-C1B-NB	7.73	115.42	110.23
17	5	303	CLA	C2B-C1B-NB	7.73	115.42	110.23
17	4	310	CLA	C2D-C1D-ND	7.73	115.80	110.10
17	A	827	CLA	C2B-C1B-NB	7.71	115.40	110.23
25	2	317	5X6	C24-C25-C26	-7.71	116.30	127.31
25	3	316	5X6	C40-C22-C21	-7.70	112.13	122.92
17	3	313	CLA	C2D-C1D-ND	7.70	115.78	110.10
25	4	312	5X6	C28-C27-C26	-7.68	114.63	126.23
25	1	316	5X6	C11-C12-C13	-7.67	114.64	126.23
25	2	320	5X6	C19-C18-C17	-7.66	116.37	127.31
25	F	205	5X6	C39-C26-C25	-7.65	112.21	122.92
17	2	308	CLA	C2B-C1B-NB	7.65	115.36	110.23
25	5	301	5X6	C42-C13-C14	-7.64	112.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	204	CLA	C2D-C1D-ND	7.64	115.73	110.10
25	1	312	5X6	C28-C27-C26	-7.63	114.71	126.23
17	B	802	CLA	O2D-CGD-CBD	7.63	124.83	111.27
17	B	811	CLA	C2D-C1D-ND	7.62	115.72	110.10
25	3	318	5X6	C11-C12-C13	-7.62	114.72	126.23
17	1	309	CLA	C2B-C1B-NB	7.62	115.34	110.23
17	J	103	CLA	C2D-C1D-ND	7.62	115.72	110.10
17	3	309	CLA	C2B-C1B-NB	7.61	115.34	110.23
17	2	305	CLA	C2B-C1B-NB	7.60	115.33	110.23
17	1	301	CLA	C2D-C1D-ND	7.59	115.70	110.10
17	1	302	CLA	C2D-C1D-ND	7.59	115.70	110.10
17	4	307	CLA	C2D-C1D-ND	7.59	115.69	110.10
17	4	310	CLA	C2B-C1B-NB	7.58	115.31	110.23
17	B	823	CLA	C2D-C1D-ND	7.58	115.69	110.10
17	B	806	CLA	C2B-C1B-NB	7.57	115.31	110.23
17	O	205	CLA	C2B-C1B-NB	7.56	115.30	110.23
25	F	205	5X6	C41-C17-C18	-7.53	112.37	122.92
17	B	830	CLA	O2D-CGD-CBD	7.53	124.64	111.27
17	5	304	CLA	C2D-C1D-ND	7.52	115.64	110.10
17	1	305	CLA	C2D-C1D-ND	7.50	115.63	110.10
17	B	834	CLA	C2B-C1B-NB	7.50	115.26	110.23
17	1	305	CLA	C2B-C1B-NB	7.50	115.26	110.23
17	5	305	CLA	CMD-C2D-C1D	7.49	137.92	124.71
25	5	317	5X6	C24-C25-C26	-7.49	116.63	127.31
17	3	306	CLA	C2B-C1B-NB	7.49	115.25	110.23
17	3	313	CLA	C2B-C1B-NB	7.48	115.24	110.23
17	4	311	CLA	C2B-C1B-NB	7.48	115.24	110.23
17	B	818	CLA	C2B-C1B-NB	7.47	115.24	110.23
17	L	204	CLA	C2D-C1D-ND	7.47	115.61	110.10
17	2	316	CLA	C2B-C1B-NB	7.47	115.24	110.23
17	B	805	CLA	C2B-C1B-NB	7.47	115.24	110.23
25	5	317	5X6	C11-C12-C13	-7.45	114.98	126.23
17	4	306	CLA	C2B-C1B-NB	7.45	115.23	110.23
17	3	314	CLA	C2B-C1B-NB	7.45	115.22	110.23
25	3	318	5X6	C42-C13-C14	-7.44	112.51	122.92
17	1	311	CLA	C2B-C1B-NB	7.43	115.22	110.23
25	4	313	5X6	C19-C18-C17	-7.42	116.72	127.31
17	B	816	CLA	C2B-C1B-NB	7.42	115.20	110.23
17	4	305	CLA	C2D-C1D-ND	7.41	115.57	110.10
17	2	308	CLA	C2D-C1D-ND	7.41	115.56	110.10
17	A	832	CLA	O2D-CGD-CBD	7.40	124.41	111.27
17	A	802	CLA	C2B-C1B-NB	7.38	115.18	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	807	CLA	C2B-C1B-NB	7.38	115.18	110.23
17	A	820	CLA	C2B-C1B-NB	7.36	115.16	110.23
25	J	105	5X6	C11-C12-C13	-7.36	115.12	126.23
17	3	308	CLA	C2D-C1D-ND	7.34	115.51	110.10
17	2	315	CLA	C2B-C1B-NB	7.34	115.15	110.23
25	5	318	5X6	C11-C12-C13	-7.32	115.17	126.23
25	5	316	5X6	C24-C25-C26	-7.32	116.87	127.31
25	5	316	5X6	C28-C27-C26	-7.30	115.20	126.23
17	1	306	CLA	C2B-C1B-NB	7.30	115.12	110.23
17	4	308	CLA	C2B-C1B-NB	7.30	115.12	110.23
25	3	318	5X6	C28-C27-C26	-7.29	115.22	126.23
25	J	105	5X6	C12-C11-C03	-7.29	106.72	127.20
17	B	827	CLA	C2B-C1B-NB	7.29	115.12	110.23
17	B	841	CLA	C2B-C1B-NB	7.29	115.12	110.23
17	5	310	CLA	C2B-C1B-NB	7.28	115.11	110.23
25	2	319	5X6	C39-C26-C25	-7.27	112.73	122.92
17	F	204	CLA	C2B-C1B-NB	7.26	115.10	110.23
25	5	316	5X6	C19-C18-C17	-7.26	116.95	127.31
25	5	318	5X6	C19-C18-C17	-7.25	116.96	127.31
17	2	313	CLA	C2B-C1B-NB	7.25	115.09	110.23
17	2	307	CLA	CMD-C2D-C1D	7.25	137.49	124.71
17	A	829	CLA	C2B-C1B-NB	7.24	115.08	110.23
17	5	312	CLA	C2B-C1B-NB	7.23	115.08	110.23
25	5	301	5X6	C41-C17-C18	-7.23	112.80	122.92
25	1	313	5X6	C11-C12-C13	-7.23	115.31	126.23
17	A	828	CLA	O2D-CGD-CBD	7.23	124.11	111.27
17	4	304	CLA	C2B-C1B-NB	7.23	115.08	110.23
25	5	317	5X6	C41-C17-C18	-7.21	112.82	122.92
25	2	318	5X6	C39-C26-C25	-7.21	112.83	122.92
17	B	836	CLA	C2B-C1B-NB	7.20	115.06	110.23
17	5	302	CLA	C2B-C1B-NB	7.20	115.06	110.23
17	2	306	CLA	C2B-C1B-NB	7.20	115.06	110.23
17	5	308	CLA	C2D-C1D-ND	7.20	115.41	110.10
17	5	313	CLA	C2D-C1D-ND	7.19	115.40	110.10
25	2	317	5X6	C28-C27-C26	-7.19	115.37	126.23
17	B	840	CLA	C2C-C1C-NC	7.18	116.70	109.97
17	A	826	CLA	C1D-ND-C4D	-7.18	101.23	106.33
17	1	308	CLA	C2B-C1B-NB	7.18	115.05	110.23
25	2	317	5X6	C19-C18-C17	-7.17	117.07	127.31
25	2	318	5X6	C28-C27-C26	-7.17	115.41	126.23
17	A	824	CLA	C2B-C1B-NB	7.17	115.04	110.23
17	2	307	CLA	O2D-CGD-CBD	7.15	123.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	312	CLA	C2B-C1B-NB	7.15	115.03	110.23
17	A	837	CLA	C2B-C1B-NB	7.15	115.03	110.23
17	A	833	CLA	C2B-C1B-NB	7.15	115.02	110.23
17	B	829	CLA	C2B-C1B-NB	7.14	115.02	110.23
17	B	823	CLA	C2B-C1B-NB	7.14	115.02	110.23
25	1	316	5X6	C20-C21-C22	-7.14	117.12	127.31
17	B	820	CLA	C2D-C1D-ND	7.14	115.37	110.10
25	2	319	5X6	C42-C13-C14	-7.14	112.92	122.92
17	O	203	CLA	C2B-C1B-NB	7.14	115.02	110.23
17	1	306	CLA	C2D-C1D-ND	7.12	115.35	110.10
17	3	308	CLA	C2B-C1B-NB	7.12	115.00	110.23
25	5	317	5X6	C42-C13-C14	-7.11	112.96	122.92
17	B	821	CLA	C2B-C1B-NB	7.11	115.00	110.23
17	4	305	CLA	C2B-C1B-NB	7.11	115.00	110.23
25	2	319	5X6	C20-C21-C22	-7.11	117.17	127.31
17	A	822	CLA	C2B-C1B-NB	7.11	115.00	110.23
17	A	817	CLA	C2B-C1B-NB	7.09	114.99	110.23
17	K	102	CLA	C2B-C1B-NB	7.09	114.99	110.23
17	2	312	CLA	C2B-C1B-NB	7.09	114.98	110.23
17	4	309	CLA	C2B-C1B-NB	7.08	114.98	110.23
25	1	316	5X6	C41-C17-C18	-7.08	113.00	122.92
25	1	312	5X6	C11-C12-C13	-7.08	115.54	126.23
17	4	303	CLA	C2B-C1B-NB	7.06	114.96	110.23
17	A	810	CLA	C2B-C1B-NB	7.05	114.96	110.23
25	5	317	5X6	C40-C22-C21	-7.05	113.04	122.92
25	5	315	5X6	C42-C13-C14	-7.05	113.05	122.92
25	F	205	5X6	C01-C02-C03	-7.05	116.61	124.53
17	B	830	CLA	C2B-C1B-NB	7.05	114.95	110.23
17	2	307	CLA	C2B-C1B-NB	7.04	114.95	110.23
17	B	819	CLA	C2B-C1B-NB	7.03	114.94	110.23
25	4	314	5X6	C42-C13-C14	-7.01	113.11	122.92
25	3	316	5X6	C42-C13-C14	-6.99	113.13	122.92
17	3	307	CLA	CMD-C2D-C1D	6.97	137.00	124.71
25	1	315	5X6	C42-C13-C14	-6.97	113.16	122.92
17	B	857	CLA	O2D-CGD-CBD	6.96	123.64	111.27
17	4	305	CLA	CMD-C2D-C1D	6.96	136.98	124.71
17	B	804	CLA	C2C-C1C-NC	6.96	116.49	109.97
17	4	311	CLA	CMD-C2D-C1D	6.95	136.97	124.71
25	3	317	5X6	C39-C26-C25	-6.95	113.19	122.92
25	2	318	5X6	C20-C19-C18	-6.95	109.24	123.47
25	1	316	5X6	C42-C13-C14	-6.93	113.22	122.92
17	5	310	CLA	CMD-C2D-C1D	6.93	136.92	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	314	5X6	C28-C27-C26	-6.93	115.77	126.23
17	1	309	CLA	CMD-C2D-C1D	6.92	136.91	124.71
17	B	809	CLA	O2D-CGD-CBD	6.91	123.55	111.27
17	5	311	CLA	C2B-C1B-NB	6.90	114.86	110.23
17	1	301	CLA	C2B-C1B-NB	6.90	114.86	110.23
17	3	315	CLA	C2B-C1B-NB	6.89	114.85	110.23
25	1	313	5X6	C40-C22-C21	-6.87	113.30	122.92
25	5	316	5X6	C40-C22-C21	-6.87	113.31	122.92
25	1	312	5X6	C19-C18-C17	-6.86	117.52	127.31
25	F	205	5X6	C12-C11-C03	-6.86	107.95	127.20
25	1	313	5X6	C19-C18-C17	-6.85	117.54	127.31
17	L	204	CLA	C2B-C1B-NB	6.85	114.82	110.23
17	A	835	CLA	C2B-C1B-NB	6.85	114.82	110.23
17	O	204	CLA	CMD-C2D-C1D	6.84	136.76	124.71
17	3	315	CLA	CMD-C2D-C1D	6.84	136.76	124.71
25	4	312	5X6	C39-C26-C25	-6.81	113.38	122.92
25	2	320	5X6	C40-C22-C21	-6.81	113.38	122.92
17	A	834	CLA	C2B-C1B-NB	6.81	114.80	110.23
25	5	318	5X6	C39-C26-C25	-6.80	113.40	122.92
17	B	857	CLA	C2B-C1B-NB	6.79	114.79	110.23
17	A	828	CLA	C2C-C1C-NC	6.79	116.34	109.97
25	5	316	5X6	C20-C19-C18	-6.79	109.57	123.47
17	A	807	CLA	C2B-C1B-NB	6.79	114.78	110.23
17	B	813	CLA	C2B-C1B-NB	6.79	114.78	110.23
25	3	316	5X6	C24-C25-C26	-6.78	117.63	127.31
17	B	838	CLA	C2B-C1B-NB	6.78	114.77	110.23
17	3	312	CLA	CMD-C2D-C1D	6.77	136.65	124.71
17	B	813	CLA	CMD-C2D-C1D	6.77	136.65	124.71
25	3	317	5X6	C41-C17-C18	-6.77	113.44	122.92
17	3	308	CLA	CMD-C2D-C1D	6.77	136.64	124.71
25	5	316	5X6	C42-C13-C14	-6.76	113.46	122.92
17	3	305	CLA	CMD-C2D-C1D	6.75	136.62	124.71
25	3	317	5X6	C42-C13-C14	-6.74	113.48	122.92
17	F	203	CLA	C2B-C1B-NB	6.74	114.75	110.23
17	2	304	CLA	CMD-C2D-C1D	6.74	136.59	124.71
17	O	205	CLA	CMD-C2D-C1D	6.73	136.58	124.71
25	3	316	5X6	C19-C18-C17	-6.73	117.70	127.31
17	1	311	CLA	CMD-C2D-C1D	6.73	136.57	124.71
17	2	312	CLA	O2D-CGD-CBD	6.72	123.22	111.27
17	5	311	CLA	CMD-C2D-C1D	6.72	136.56	124.71
17	B	819	CLA	CHD-C1D-ND	-6.72	118.28	124.45
17	A	823	CLA	C2C-C1C-NC	6.72	116.26	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	316	CLA	CMD-C2D-C1D	6.71	136.54	124.71
17	A	853	CLA	O2D-CGD-CBD	6.71	123.19	111.27
17	A	821	CLA	CHD-C1D-ND	-6.70	118.29	124.45
17	O	203	CLA	CMD-C2D-C1D	6.70	136.52	124.71
25	4	313	5X6	C24-C25-C26	-6.70	117.75	127.31
20	B	803	BCR	C8-C9-C10	6.69	129.21	118.94
17	3	313	CLA	CMD-C2D-C1D	6.69	136.51	124.71
17	A	826	CLA	C2B-C1B-NB	6.69	114.72	110.23
25	2	317	5X6	C42-C13-C14	-6.69	113.55	122.92
25	1	314	5X6	C39-C26-C25	-6.69	113.56	122.92
17	A	815	CLA	C2B-C1B-NB	6.68	114.71	110.23
17	2	313	CLA	CMD-C2D-C1D	6.68	136.49	124.71
17	1	310	CLA	CMD-C2D-C1D	6.68	136.49	124.71
17	5	314	CLA	CMD-C2D-C1D	6.68	136.49	124.71
17	K	102	CLA	CMD-C2D-C1D	6.68	136.49	124.71
17	3	311	CLA	CHD-C1D-ND	-6.68	118.32	124.45
17	B	819	CLA	CMD-C2D-C1D	6.68	136.48	124.71
17	2	311	CLA	CMD-C2D-C1D	6.68	136.48	124.71
25	J	105	5X6	C40-C22-C21	-6.67	113.58	122.92
25	3	318	5X6	C41-C17-C18	-6.67	113.58	122.92
25	2	319	5X6	C40-C22-C21	-6.67	113.58	122.92
17	4	309	CLA	CMD-C2D-C1D	6.67	136.47	124.71
25	1	312	5X6	C39-C26-C25	-6.67	113.58	122.92
17	2	305	CLA	CMD-C2D-C1D	6.67	136.46	124.71
17	2	307	CLA	CHD-C1D-ND	-6.67	118.33	124.45
17	2	314	CLA	CMD-C2D-C1D	6.67	136.46	124.71
17	1	303	CLA	CMD-C2D-C1D	6.66	136.45	124.71
17	4	310	CLA	CMD-C2D-C1D	6.64	136.42	124.71
17	2	311	CLA	CHD-C1D-ND	-6.64	118.35	124.45
17	F	204	CLA	CMD-C2D-C1D	6.64	136.41	124.71
17	3	314	CLA	CMD-C2D-C1D	6.64	136.41	124.71
17	3	305	CLA	CHD-C1D-ND	-6.63	118.36	124.45
17	A	804	CLA	C2B-C1B-NB	6.63	114.68	110.23
17	A	853	CLA	CHD-C1D-ND	-6.62	118.37	124.45
25	5	301	5X6	C11-C12-C13	-6.62	116.23	126.23
17	A	832	CLA	C2C-C1C-NC	6.62	116.17	109.97
25	4	314	5X6	C41-C17-C18	-6.61	113.66	122.92
17	5	304	CLA	CMD-C2D-C1D	6.61	136.36	124.71
17	3	307	CLA	CHD-C1D-ND	-6.60	118.39	124.45
17	3	311	CLA	CMD-C2D-C1D	6.60	136.34	124.71
17	4	308	CLA	CMD-C2D-C1D	6.60	136.34	124.71
25	3	318	5X6	C39-C26-C25	-6.59	113.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	807	CLA	CMD-C2D-C1D	6.58	136.32	124.71
17	2	315	CLA	CMD-C2D-C1D	6.58	136.31	124.71
17	A	826	CLA	C4A-NA-C1A	-6.58	103.75	106.71
17	1	305	CLA	CMD-C2D-C1D	6.57	136.30	124.71
17	5	302	CLA	CMD-C2D-C1D	6.57	136.30	124.71
17	A	830	CLA	C2B-C1B-NB	6.57	114.64	110.23
17	3	309	CLA	CMD-C2D-C1D	6.57	136.29	124.71
17	A	853	CLA	C2C-C1C-NC	6.56	116.12	109.97
17	A	803	CLA	C2C-C1C-NC	6.56	116.12	109.97
17	A	821	CLA	CMD-C2D-C1D	6.56	136.27	124.71
17	4	306	CLA	CMD-C2D-C1D	6.56	136.27	124.71
25	2	320	5X6	C39-C26-C25	-6.55	113.74	122.92
17	2	309	CLA	C2B-C1B-NB	6.55	114.62	110.23
17	3	306	CLA	CMD-C2D-C1D	6.55	136.26	124.71
17	5	306	CLA	CMD-C2D-C1D	6.54	136.25	124.71
25	3	316	5X6	C27-C26-C25	-6.54	108.91	118.94
17	5	305	CLA	CHD-C1D-ND	-6.54	118.45	124.45
25	4	313	5X6	C28-C27-C26	-6.52	116.38	126.23
25	5	316	5X6	C27-C26-C25	-6.52	108.93	118.94
25	4	313	5X6	C42-C13-C14	-6.52	113.79	122.92
17	A	816	CLA	C4A-NA-C1A	-6.52	103.78	106.71
25	2	319	5X6	C28-C27-C26	-6.52	116.39	126.23
17	J	103	CLA	C2B-C1B-NB	6.51	114.60	110.23
17	A	826	CLA	C2C-C1C-NC	6.51	116.07	109.97
17	B	822	CLA	CHD-C1D-ND	-6.51	118.47	124.45
17	5	303	CLA	CHD-C1D-ND	-6.51	118.48	124.45
17	L	202	CLA	CMD-C2D-C1D	6.50	136.17	124.71
17	2	309	CLA	CMD-C2D-C1D	6.49	136.15	124.71
17	4	311	CLA	CHD-C1D-ND	-6.49	118.49	124.45
17	A	832	CLA	C2D-C1D-ND	6.48	114.88	110.10
17	5	303	CLA	CMD-C2D-C1D	6.48	136.13	124.71
17	B	835	CLA	C2B-C1B-NB	6.48	114.57	110.23
17	5	309	CLA	CMD-C2D-C1D	6.47	136.12	124.71
17	L	203	CLA	C2B-C1B-NB	6.47	114.57	110.23
25	4	312	5X6	C40-C22-C21	-6.46	113.87	122.92
17	A	832	CLA	C1D-ND-C4D	-6.46	101.75	106.33
25	J	105	5X6	C19-C20-C21	-6.45	110.26	123.47
17	4	303	CLA	CMD-C2D-C1D	6.45	136.08	124.71
17	B	810	CLA	C2C-C1C-NC	6.45	116.02	109.97
17	2	304	CLA	CHD-C1D-ND	-6.44	118.54	124.45
17	A	859	CLA	C2B-C1B-NB	6.44	114.55	110.23
17	A	836	CLA	C2B-C1B-NB	6.43	114.55	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	302	CLA	C2B-C1B-NB	6.42	114.54	110.23
25	2	318	5X6	C41-C17-C18	-6.42	113.92	122.92
17	A	806	CLA	C2B-C1B-NB	6.41	114.53	110.23
25	5	316	5X6	C23-C22-C21	-6.41	109.10	118.94
17	O	203	CLA	CHD-C1D-ND	-6.40	118.57	124.45
17	5	313	CLA	CMD-C2D-C1D	6.39	135.97	124.71
17	5	306	CLA	CHD-C1D-ND	-6.39	118.59	124.45
17	2	305	CLA	CHD-C1D-ND	-6.38	118.59	124.45
17	A	804	CLA	CMD-C2D-C1D	6.38	135.96	124.71
17	4	304	CLA	CMD-C2D-C1D	6.38	135.95	124.71
17	L	202	CLA	C2B-C1B-NB	6.37	114.50	110.23
17	5	310	CLA	CHD-C1D-ND	-6.36	118.61	124.45
17	A	854	CLA	C2B-C1B-NB	6.36	114.49	110.23
17	3	312	CLA	CHD-C1D-ND	-6.35	118.61	124.45
25	F	205	5X6	C16-C17-C18	-6.35	109.19	118.94
17	1	311	CLA	CHD-C1D-ND	-6.35	118.62	124.45
25	1	314	5X6	C11-C12-C13	-6.35	116.64	126.23
17	2	306	CLA	CMD-C2D-C1D	6.35	135.90	124.71
17	B	823	CLA	CMD-C2D-C1D	6.34	135.89	124.71
17	A	832	CLA	C2B-C1B-NB	6.34	114.48	110.23
17	5	309	CLA	CHD-C1D-ND	-6.34	118.63	124.45
17	B	812	CLA	C2D-C1D-ND	6.34	114.77	110.10
17	A	855	CLA	CMD-C2D-C1D	6.34	135.88	124.71
17	2	312	CLA	CMD-C2D-C1D	6.33	135.87	124.71
25	J	105	5X6	C23-C22-C21	-6.33	109.23	118.94
17	A	825	CLA	CMD-C2D-C1D	6.32	135.85	124.71
17	L	203	CLA	C2C-C1C-NC	6.32	115.89	109.97
17	A	818	CLA	C2B-C1B-NB	6.32	114.47	110.23
17	2	315	CLA	CHD-C1D-ND	-6.32	118.65	124.45
25	2	318	5X6	C20-C21-C22	-6.31	118.30	127.31
25	5	315	5X6	C41-C17-C18	-6.31	114.08	122.92
17	B	825	CLA	O2D-CGD-CBD	6.31	122.48	111.27
25	1	312	5X6	C16-C17-C18	-6.30	109.27	118.94
17	2	304	CLA	C2B-C1B-NB	6.30	114.46	110.23
25	1	316	5X6	C28-C27-C26	-6.30	116.72	126.23
17	2	310	CLA	CMD-C2D-C1D	6.29	135.81	124.71
17	B	817	CLA	CMD-C2D-C1D	6.29	135.80	124.71
17	4	304	CLA	CHD-C1D-ND	-6.28	118.68	124.45
17	2	308	CLA	CMD-C2D-C1D	6.28	135.78	124.71
17	A	811	CLA	C2B-C1B-NB	6.28	114.44	110.23
17	1	304	CLA	CMD-C2D-C1D	6.27	135.77	124.71
25	1	314	5X6	C20-C19-C18	-6.27	110.62	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	315	5X6	C16-C17-C18	-6.26	109.33	118.94
17	A	856	CLA	O2D-CGD-CBD	6.26	122.39	111.27
17	O	204	CLA	O2D-CGD-CBD	6.25	122.38	111.27
17	A	812	CLA	C2B-C1B-NB	6.25	114.42	110.23
17	B	828	CLA	C2C-C1C-NC	6.25	115.82	109.97
17	B	828	CLA	C2B-C1B-NB	6.25	114.42	110.23
17	A	804	CLA	C2C-C1C-NC	6.24	115.82	109.97
25	J	105	5X6	C42-C13-C14	-6.24	114.18	122.92
17	3	315	CLA	CHD-C1D-ND	-6.23	118.73	124.45
25	5	317	5X6	C39-C26-C25	-6.23	114.20	122.92
17	5	314	CLA	CHD-C1D-ND	-6.23	118.73	124.45
17	B	806	CLA	O2D-CGD-CBD	6.23	122.33	111.27
17	4	305	CLA	CHD-C1D-ND	-6.23	118.73	124.45
16	A	801	CL0	C2C-C1C-NC	6.23	115.80	109.97
17	A	823	CLA	CMD-C2D-C1D	6.22	135.68	124.71
17	A	837	CLA	C4A-NA-C1A	-6.21	103.91	106.71
17	B	807	CLA	C2C-C1C-NC	6.21	115.79	109.97
17	B	838	CLA	C2C-C1C-NC	6.21	115.79	109.97
17	4	308	CLA	CHD-C1D-ND	-6.21	118.75	124.45
17	B	831	CLA	C2C-C1C-NC	6.20	115.78	109.97
17	1	310	CLA	CHD-C1D-ND	-6.19	118.76	124.45
17	3	313	CLA	CHD-C1D-ND	-6.19	118.76	124.45
17	4	303	CLA	O2D-CGD-CBD	6.19	122.27	111.27
17	B	834	CLA	CHD-C1D-ND	-6.19	118.76	124.45
17	B	832	CLA	CMD-C2D-C1D	6.19	135.62	124.71
17	4	309	CLA	CHD-C1D-ND	-6.19	118.77	124.45
17	B	824	CLA	CHD-C1D-ND	-6.19	118.77	124.45
17	1	309	CLA	CHD-C1D-ND	-6.19	118.77	124.45
17	A	839	CLA	C2C-C1C-NC	6.18	115.77	109.97
17	A	809	CLA	C2C-C1C-NC	6.18	115.77	109.97
17	B	834	CLA	CMD-C2D-C1D	6.18	135.61	124.71
17	A	856	CLA	C2B-C1B-NB	6.18	114.38	110.23
17	A	859	CLA	CMD-C2D-C1D	6.18	135.61	124.71
17	L	204	CLA	CMD-C2D-C1D	6.18	135.61	124.71
17	2	316	CLA	CHD-C1D-ND	-6.18	118.78	124.45
17	B	804	CLA	C2B-C1B-NB	6.17	114.37	110.23
17	B	833	CLA	CMD-C2D-C1D	6.17	135.59	124.71
17	A	821	CLA	C2B-C1B-NB	6.17	114.37	110.23
17	A	806	CLA	C2C-C1C-NC	6.17	115.75	109.97
17	2	314	CLA	CHD-C1D-ND	-6.16	118.79	124.45
17	5	311	CLA	CHD-C1D-ND	-6.16	118.79	124.45
25	4	314	5X6	C40-C22-C21	-6.16	114.30	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	830	CLA	C2C-C1C-NC	6.16	115.74	109.97
17	1	305	CLA	CHD-C1D-ND	-6.15	118.80	124.45
25	F	205	5X6	C42-C13-C14	-6.15	114.31	122.92
17	A	822	CLA	CMD-C2D-C1D	6.15	135.55	124.71
17	A	825	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
17	B	826	CLA	C2B-C1B-NB	6.14	114.35	110.23
17	3	311	CLA	O2D-CGD-CBD	6.14	122.18	111.27
17	A	810	CLA	CMD-C2D-C1D	6.14	135.53	124.71
17	B	801	CLA	CHD-C1D-ND	-6.14	118.81	124.45
17	A	826	CLA	C3C-C4C-NC	6.14	117.45	110.57
17	K	103	CLA	C2B-C1B-NB	6.14	114.34	110.23
25	2	321	5X6	C11-C12-C13	-6.13	116.97	126.23
17	B	833	CLA	C3D-C2D-C1D	-6.13	97.46	105.83
17	3	309	CLA	CHD-C1D-ND	-6.13	118.82	124.45
17	4	310	CLA	CHD-C1D-ND	-6.13	118.82	124.45
17	A	853	CLA	C2B-C1B-NB	6.11	114.33	110.23
17	B	831	CLA	C2B-C1B-NB	6.11	114.33	110.23
17	A	819	CLA	C2B-C1B-NB	6.10	114.32	110.23
17	B	802	CLA	C2B-C1B-NB	6.10	114.32	110.23
17	F	204	CLA	CHD-C1D-ND	-6.09	118.85	124.45
17	B	805	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
17	F	204	CLA	CAC-C3C-C4C	6.09	132.71	124.81
17	B	810	CLA	CMD-C2D-C1D	6.09	135.45	124.71
17	3	314	CLA	CHD-C1D-ND	-6.09	118.86	124.45
17	A	814	CLA	CMD-C2D-C1D	6.08	135.43	124.71
17	K	103	CLA	CMD-C2D-C1D	6.08	135.43	124.71
17	A	809	CLA	CMD-C2D-C1D	6.08	135.43	124.71
17	4	306	CLA	CHD-C1D-ND	-6.07	118.87	124.45
25	3	316	5X6	C28-C27-C26	-6.07	117.06	126.23
17	1	307	CLA	CMD-C2D-C1D	6.06	135.40	124.71
17	2	310	CLA	CHD-C1D-ND	-6.06	118.88	124.45
17	A	855	CLA	C2B-C1B-NB	6.06	114.29	110.23
25	2	321	5X6	C42-C13-C14	-6.06	114.44	122.92
17	A	831	CLA	C2C-C1C-NC	6.05	115.64	109.97
25	F	205	5X6	C19-C20-C21	-6.05	111.08	123.47
17	A	820	CLA	CHD-C1D-ND	-6.05	118.89	124.45
17	A	831	CLA	C2B-C1B-NB	6.05	114.29	110.23
17	2	308	CLA	CHD-C1D-ND	-6.05	118.89	124.45
17	1	308	CLA	CMD-C2D-C1D	6.05	135.38	124.71
17	B	841	CLA	CHD-C1D-ND	-6.04	118.90	124.45
17	1	307	CLA	CHD-C1D-ND	-6.03	118.91	124.45
25	F	205	5X6	C12-C13-C14	-6.03	109.68	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	805	CLA	C2C-C1C-NC	6.03	115.62	109.97
25	5	316	5X6	C19-C20-C21	-6.03	111.13	123.47
17	A	809	CLA	C2B-C1B-NB	6.02	114.27	110.23
17	O	205	CLA	CHD-C1D-ND	-6.02	118.92	124.45
17	B	832	CLA	CHD-C1D-ND	-6.02	118.92	124.45
17	5	302	CLA	CHD-C1D-ND	-6.02	118.92	124.45
17	B	809	CLA	CMD-C2D-C1D	6.01	135.31	124.71
17	3	310	CLA	CMD-C2D-C1D	6.01	135.31	124.71
17	3	310	CLA	CHD-C1D-ND	-6.01	118.93	124.45
17	B	841	CLA	CMD-C2D-C1D	6.01	135.30	124.71
17	O	204	CLA	CHD-C1D-ND	-6.01	118.93	124.45
17	A	833	CLA	CHD-C1D-ND	-6.01	118.93	124.45
17	2	309	CLA	CHD-C1D-ND	-6.00	118.94	124.45
17	B	840	CLA	C2B-C1B-NB	5.99	114.25	110.23
17	B	831	CLA	CMD-C2D-C1D	5.98	135.25	124.71
17	B	839	CLA	C2B-C1B-NB	5.98	114.24	110.23
17	B	806	CLA	C2C-C1C-NC	5.98	115.57	109.97
17	B	829	CLA	C2C-C1C-NC	5.97	115.56	109.97
17	1	306	CLA	CMD-C2D-C1D	5.96	135.22	124.71
17	B	820	CLA	CMD-C2D-C1D	5.96	135.22	124.71
17	B	840	CLA	CMD-C2D-C1D	5.96	135.22	124.71
17	B	815	CLA	C2B-C1B-NB	5.95	114.22	110.23
17	B	809	CLA	C2C-C1C-NC	5.95	115.55	109.97
17	B	802	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
17	A	823	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
17	2	313	CLA	CHD-C1D-ND	-5.94	118.99	124.45
17	A	803	CLA	C2B-C1B-NB	5.93	114.21	110.23
17	A	855	CLA	C2C-C1C-NC	5.93	115.53	109.97
17	A	825	CLA	O2D-CGD-CBD	5.93	121.81	111.27
25	2	321	5X6	C20-C19-C18	-5.93	111.32	123.47
17	B	833	CLA	C2C-C1C-NC	5.93	115.53	109.97
17	A	824	CLA	CHD-C1D-ND	-5.93	119.01	124.45
17	A	854	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
17	A	819	CLA	CHD-C1D-ND	-5.92	119.01	124.45
17	F	204	CLA	O2D-CGD-CBD	5.91	121.77	111.27
17	B	808	CLA	CHD-C1D-ND	-5.91	119.03	124.45
17	B	824	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
17	A	824	CLA	C2C-C1C-NC	5.90	115.50	109.97
17	J	103	CLA	C2C-C1C-NC	5.90	115.50	109.97
17	A	803	CLA	CMD-C2D-C1D	5.90	135.11	124.71
17	B	830	CLA	C2C-C1C-NC	5.90	115.50	109.97
17	A	812	CLA	CHD-C4C-C3C	-5.90	116.17	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	814	CLA	O2D-CGD-CBD	5.89	121.74	111.27
25	5	316	5X6	C12-C13-C14	-5.89	109.90	118.94
17	A	834	CLA	CHD-C1D-ND	-5.89	119.04	124.45
17	5	308	CLA	CHD-C1D-ND	-5.89	119.04	124.45
17	B	825	CLA	C2C-C1C-NC	5.89	115.49	109.97
17	B	820	CLA	CHD-C1D-ND	-5.89	119.04	124.45
25	F	205	5X6	C23-C22-C21	-5.89	109.91	118.94
17	3	306	CLA	CHD-C1D-ND	-5.89	119.05	124.45
17	B	825	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
17	2	308	CLA	C2C-C1C-NC	5.88	115.48	109.97
17	B	815	CLA	C2C-C1C-NC	5.88	115.48	109.97
25	J	105	5X6	C14-C15-C16	-5.87	104.89	123.22
17	5	307	CLA	CMD-C2D-C1D	5.87	135.06	124.71
17	B	816	CLA	CMD-C2D-C1D	5.87	135.06	124.71
17	A	834	CLA	C2C-C1C-NC	5.87	115.47	109.97
17	B	814	CLA	CAC-C3C-C4C	5.87	132.42	124.81
17	5	312	CLA	CHD-C1D-ND	-5.87	119.06	124.45
17	2	312	CLA	CHD-C1D-ND	-5.87	119.06	124.45
25	2	321	5X6	C40-C22-C21	-5.86	114.71	122.92
17	B	837	CLA	C2B-C1B-NB	5.86	114.16	110.23
17	5	308	CLA	CMD-C2D-C1D	5.86	135.04	124.71
17	1	304	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
17	B	814	CLA	C2B-C1B-NB	5.85	114.16	110.23
17	B	827	CLA	CMD-C2D-C1D	5.85	135.03	124.71
17	A	854	CLA	C2C-C1C-NC	5.85	115.45	109.97
17	A	823	CLA	O2D-CGD-CBD	5.85	121.66	111.27
17	B	835	CLA	CMD-C2D-C1D	5.84	135.01	124.71
17	A	808	CLA	CHD-C1D-ND	-5.84	119.08	124.45
17	A	832	CLA	CHD-C1D-ND	-5.84	119.09	124.45
17	A	813	CLA	CMD-C2D-C1D	5.84	135.00	124.71
17	1	307	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
17	A	837	CLA	O2D-CGD-CBD	5.83	121.62	111.27
17	A	835	CLA	C2C-C1C-NC	5.83	115.43	109.97
17	A	810	CLA	CHD-C1D-ND	-5.83	119.10	124.45
17	B	817	CLA	O2D-CGD-CBD	5.83	121.62	111.27
17	B	817	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
17	A	818	CLA	CHD-C1D-ND	-5.82	119.10	124.45
17	5	312	CLA	CMD-C2D-C1D	5.82	134.98	124.71
17	B	814	CLA	CMD-C2D-C1D	5.82	134.97	124.71
17	A	809	CLA	O2D-CGD-CBD	5.82	121.61	111.27
17	A	816	CLA	C2C-C1C-NC	5.81	115.42	109.97
17	A	827	CLA	CMD-C2D-C1D	5.81	134.96	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	311	CLA	O2D-CGD-CBD	5.81	121.59	111.27
17	A	824	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
17	A	839	CLA	CMD-C2D-C1D	5.81	134.94	124.71
17	B	821	CLA	CMD-C2D-C1D	5.80	134.94	124.71
25	1	312	5X6	C20-C19-C18	-5.80	111.59	123.47
17	L	202	CLA	C2C-C1C-NC	5.80	115.40	109.97
17	B	805	CLA	CAA-C2A-C3A	-5.79	96.93	112.78
17	A	802	CLA	C2C-C1C-NC	5.79	115.39	109.97
17	A	811	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
17	F	203	CLA	CMD-C2D-C1D	5.78	134.91	124.71
17	A	814	CLA	CHD-C1D-ND	-5.78	119.14	124.45
17	A	822	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
17	1	304	CLA	CHD-C1D-ND	-5.78	119.14	124.45
17	B	839	CLA	C2C-C1C-NC	5.78	115.39	109.97
17	B	835	CLA	CHD-C1D-ND	-5.78	119.14	124.45
17	B	808	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
17	2	311	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
17	B	821	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
17	B	838	CLA	O2D-CGD-CBD	5.77	121.52	111.27
17	A	803	CLA	CHD-C1D-ND	-5.77	119.16	124.45
17	A	838	CLA	C2C-C1C-NC	5.76	115.37	109.97
17	B	839	CLA	CMD-C2D-C1D	5.76	134.87	124.71
25	2	320	5X6	C16-C17-C18	-5.76	110.10	118.94
17	1	303	CLA	CHD-C1D-ND	-5.76	119.16	124.45
17	A	808	CLA	CMD-C2D-C1D	5.76	134.86	124.71
17	B	802	CLA	C2C-C1C-NC	5.76	115.37	109.97
25	F	205	5X6	C27-C26-C25	-5.75	110.11	118.94
25	1	313	5X6	C39-C26-C25	-5.75	114.86	122.92
17	B	807	CLA	CMD-C2D-C1D	5.75	134.85	124.71
17	J	103	CLA	CMD-C2D-C1D	5.75	134.85	124.71
17	B	823	CLA	CHD-C1D-ND	-5.75	119.17	124.45
17	A	854	CLA	CMD-C2D-C1D	5.75	134.84	124.71
17	A	837	CLA	CHD-C1D-ND	-5.74	119.18	124.45
17	A	834	CLA	CMD-C2D-C1D	5.74	134.83	124.71
17	B	811	CLA	CMD-C2D-C1D	5.74	134.83	124.71
17	A	828	CLA	C2B-C1B-NB	5.74	114.08	110.23
17	B	828	CLA	C3D-C2D-C1D	-5.73	98.01	105.83
17	B	805	CLA	CMD-C2D-C1D	5.73	134.81	124.71
17	B	836	CLA	C2C-C1C-NC	5.73	115.34	109.97
25	1	313	5X6	C23-C22-C21	-5.73	110.16	118.94
17	A	824	CLA	C3D-C2D-C1D	-5.73	98.02	105.83
17	A	818	CLA	CMD-C2D-C1D	5.72	134.80	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	859	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
17	B	839	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
17	A	837	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
17	3	315	CLA	O2D-CGD-CBD	5.71	121.42	111.27
17	A	815	CLA	C2C-C1C-NC	5.71	115.32	109.97
17	A	838	CLA	CMD-C2D-C1D	5.71	134.78	124.71
17	B	822	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
17	A	826	CLA	CMD-C2D-C1D	5.70	134.77	124.71
17	A	816	CLA	CMD-C2D-C1D	5.70	134.76	124.71
17	A	855	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
25	3	316	5X6	C39-C26-C25	-5.70	114.94	122.92
17	O	205	CLA	O2D-CGD-CBD	5.70	121.39	111.27
25	1	314	5X6	C19-C18-C17	-5.70	119.18	127.31
17	K	102	CLA	CHD-C1D-ND	-5.70	119.22	124.45
17	A	839	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
17	1	308	CLA	CHD-C1D-ND	-5.69	119.22	124.45
17	A	821	CLA	C4A-NA-C1A	-5.69	104.15	106.71
17	B	828	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
25	3	317	5X6	C20-C19-C18	-5.69	111.83	123.47
17	B	822	CLA	CMD-C2D-C1D	5.68	134.73	124.71
17	B	837	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
17	B	833	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
17	4	307	CLA	CMD-C2D-C1D	5.68	134.72	124.71
17	1	302	CLA	C2C-C1C-NC	5.68	115.29	109.97
17	3	311	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
17	B	831	CLA	CHD-C1D-ND	-5.67	119.24	124.45
17	B	805	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
17	B	814	CLA	C2C-C1C-NC	5.67	115.28	109.97
17	5	305	CLA	O2D-CGD-CBD	5.66	121.32	111.27
17	A	806	CLA	CHD-C1D-ND	-5.66	119.25	124.45
17	B	813	CLA	CHD-C1D-ND	-5.66	119.25	124.45
17	A	827	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
17	B	827	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
25	5	316	5X6	C27-C28-C29	-5.65	111.33	127.20
25	5	318	5X6	C20-C19-C18	-5.65	111.91	123.47
17	A	814	CLA	C2B-C1B-NB	5.64	114.02	110.23
17	4	307	CLA	O2D-CGD-CBD	5.64	121.29	111.27
25	5	318	5X6	C23-C22-C21	-5.64	110.28	118.94
25	1	315	5X6	C40-C22-C21	-5.64	115.03	122.92
17	A	824	CLA	CMD-C2D-C1D	5.63	134.64	124.71
17	A	805	CLA	CMD-C2D-C1D	5.63	134.63	124.71
25	1	312	5X6	C41-C17-C18	-5.63	115.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	832	CLA	C2C-C1C-NC	5.63	115.24	109.97
17	4	304	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
17	B	817	CLA	CHD-C1D-ND	-5.62	119.28	124.45
17	2	309	CLA	C2C-C1C-NC	5.62	115.24	109.97
17	A	816	CLA	C2B-C1B-NB	5.62	114.00	110.23
17	A	822	CLA	CHD-C1D-ND	-5.61	119.29	124.45
17	A	811	CLA	CMD-C2D-C1D	5.61	134.60	124.71
17	B	841	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
17	B	827	CLA	O2D-CGD-CBD	5.61	121.23	111.27
17	5	304	CLA	CHD-C1D-ND	-5.61	119.30	124.45
17	B	826	CLA	C2C-C1C-NC	5.61	115.23	109.97
17	L	204	CLA	CHD-C1D-ND	-5.61	119.30	124.45
17	4	308	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
17	2	306	CLA	CHD-C1D-ND	-5.60	119.31	124.45
25	1	314	5X6	C16-C17-C18	-5.59	110.36	118.94
17	A	831	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	B	808	CLA	CMD-C2D-C1D	5.59	134.57	124.71
17	B	816	CLA	O2D-CGD-CBD	5.59	121.20	111.27
25	2	319	5X6	C19-C18-C17	-5.59	119.33	127.31
17	A	838	CLA	O2D-CGD-CBD	5.59	121.19	111.27
17	5	309	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
17	B	837	CLA	C2C-C1C-NC	5.58	115.20	109.97
17	3	305	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
17	B	812	CLA	C4A-NA-C1A	-5.58	104.20	106.71
17	2	305	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
17	B	805	CLA	O2D-CGD-CBD	5.58	121.18	111.27
17	B	813	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
17	A	831	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
17	A	829	CLA	CHD-C1D-ND	-5.57	119.34	124.45
17	L	202	CLA	CHD-C1D-ND	-5.57	119.34	124.45
17	B	809	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
25	2	317	5X6	C39-C26-C25	-5.57	115.12	122.92
17	5	305	CLA	CAA-C2A-C3A	-5.57	97.54	112.78
17	A	856	CLA	C2C-C1C-NC	5.56	115.19	109.97
17	A	810	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
17	A	838	CLA	C2B-C1B-NB	5.56	113.96	110.23
17	5	307	CLA	CHD-C1D-ND	-5.55	119.35	124.45
25	4	312	5X6	C20-C19-C18	-5.55	112.11	123.47
17	5	308	CLA	C3B-C2B-C1B	-5.55	100.47	107.16
17	A	827	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	2	311	CLA	C4A-NA-C1A	-5.55	104.21	106.71
17	F	203	CLA	C2C-C1C-NC	5.54	115.16	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	801	CL0	C2B-C1B-NB	5.54	113.94	110.23
17	A	810	CLA	C2C-C1C-NC	5.54	115.16	109.97
17	B	811	CLA	C2C-C1C-NC	5.53	115.16	109.97
17	J	103	CLA	O2D-CGD-CBD	5.53	121.09	111.27
17	A	819	CLA	CMD-C2D-C1D	5.53	134.46	124.71
17	A	805	CLA	C2B-C1B-NB	5.53	113.94	110.23
17	B	826	CLA	CMD-C2D-C1D	5.53	134.46	124.71
17	B	824	CLA	CMD-C2D-C1D	5.53	134.45	124.71
17	1	306	CLA	CHD-C1D-ND	-5.53	119.38	124.45
25	2	320	5X6	C19-C20-C21	-5.53	112.15	123.47
17	A	807	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
17	A	852	CLA	C2B-C1B-NB	5.52	113.93	110.23
17	B	808	CLA	O2D-CGD-CBD	5.52	121.08	111.27
17	A	855	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
17	B	835	CLA	C2C-C1C-NC	5.52	115.14	109.97
17	A	804	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
17	B	818	CLA	CMD-C2D-C1D	5.51	134.43	124.71
25	5	301	5X6	C39-C26-C25	-5.51	115.20	122.92
17	A	818	CLA	O2D-CGD-CBD	5.51	121.06	111.27
17	A	826	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	B	838	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
17	A	816	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
17	5	313	CLA	CHD-C1D-ND	-5.51	119.39	124.45
17	A	817	CLA	CHD-C1D-ND	-5.50	119.39	124.45
17	1	303	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
17	B	813	CLA	C3D-C2D-C1D	-5.49	98.33	105.83
17	A	852	CLA	C2C-C1C-NC	5.49	115.12	109.97
17	4	303	CLA	CHD-C1D-ND	-5.49	119.41	124.45
17	L	203	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
17	B	827	CLA	C2C-C1C-NC	5.48	115.11	109.97
17	B	806	CLA	CMD-C2D-C1D	5.48	134.37	124.71
17	K	102	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
17	B	804	CLA	CMD-C2D-C1D	5.48	134.37	124.71
25	3	316	5X6	C27-C28-C29	-5.47	111.83	127.20
25	1	312	5X6	C24-C23-C22	-5.47	111.04	126.42
17	5	311	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
17	A	853	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
17	A	837	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
17	A	810	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
17	B	810	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
25	J	105	5X6	C39-C26-C25	-5.46	115.28	122.92
17	B	828	CLA	O2D-CGD-CBD	5.46	120.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	308	CLA	CHD-C1D-ND	-5.45	119.44	124.45
17	1	309	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
17	B	829	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
17	5	312	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
25	1	314	5X6	C12-C11-C03	-5.44	111.91	127.20
17	B	823	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
17	L	203	CLA	CMD-C2D-C1D	5.44	134.30	124.71
17	5	307	CLA	O2D-CGD-CBD	5.44	120.93	111.27
17	A	811	CLA	CAC-C3C-C4C	5.44	131.86	124.81
17	A	802	CLA	O2D-CGD-CBD	5.43	120.92	111.27
17	A	827	CLA	C3B-C2B-C1B	-5.43	100.61	107.16
17	A	854	CLA	CHD-C1D-ND	-5.43	119.46	124.45
25	4	312	5X6	C23-C22-C21	-5.43	110.61	118.94
17	B	838	CLA	CMD-C2D-C1D	5.43	134.28	124.71
17	A	839	CLA	CHD-C1D-ND	-5.42	119.47	124.45
25	1	312	5X6	C42-C13-C14	-5.42	115.33	122.92
17	A	825	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
17	A	823	CLA	C2B-C1B-NB	5.42	113.86	110.23
17	A	812	CLA	C2C-C1C-NC	5.42	115.05	109.97
25	1	312	5X6	C27-C26-C25	-5.42	110.63	118.94
17	A	830	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
17	B	818	CLA	CHD-C1D-ND	-5.41	119.48	124.45
17	1	301	CLA	CMD-C2D-C1D	5.41	134.25	124.71
17	L	202	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
17	A	830	CLA	CMD-C2D-C1D	5.41	134.24	124.71
17	B	838	CLA	C3B-C2B-C1B	-5.41	100.64	107.16
17	B	826	CLA	CHD-C1D-ND	-5.40	119.49	124.45
17	A	836	CLA	C2C-C1C-NC	5.40	115.03	109.97
17	B	812	CLA	CMD-C2D-C1D	5.40	134.22	124.71
17	A	813	CLA	CHD-C1D-ND	-5.40	119.50	124.45
17	A	838	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
17	B	826	CLA	O2D-CGD-CBD	5.39	120.85	111.27
17	3	315	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
17	5	314	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
17	A	826	CLA	CHD-C1D-ND	-5.39	119.50	124.45
17	B	815	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
17	1	301	CLA	C2C-C1C-NC	5.39	115.02	109.97
17	A	817	CLA	C2C-C1C-NC	5.39	115.02	109.97
17	A	806	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
17	A	818	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
17	A	853	CLA	CMD-C2D-C1D	5.38	134.19	124.71
17	B	818	CLA	C2C-C1C-NC	5.38	115.01	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	304	CLA	O2D-CGD-CBD	5.38	120.82	111.27
17	B	833	CLA	C2B-C1B-NB	5.37	113.83	110.23
17	B	804	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
17	5	309	CLA	O2D-CGD-CBD	5.37	120.81	111.27
17	B	833	CLA	CHD-C1D-ND	-5.37	119.52	124.45
17	3	308	CLA	C2C-C1C-NC	5.37	115.00	109.97
17	3	310	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
17	F	204	CLA	C2C-C1C-NC	5.36	115.00	109.97
17	B	808	CLA	C2C-C1C-NC	5.36	114.99	109.97
17	A	834	CLA	O2D-CGD-CBD	5.36	120.79	111.27
17	B	838	CLA	C3D-C2D-C1D	-5.35	98.52	105.83
17	B	821	CLA	CHD-C1D-ND	-5.35	119.53	124.45
17	B	825	CLA	C2B-C1B-NB	5.35	113.82	110.23
17	B	819	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
17	2	304	CLA	O2D-CGD-CBD	5.35	120.78	111.27
17	B	825	CLA	C3C-C4C-NC	5.35	116.57	110.57
17	2	315	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
17	B	840	CLA	CAC-C3C-C4C	5.35	131.75	124.81
25	5	315	5X6	C20-C19-C18	-5.34	112.53	123.47
17	A	859	CLA	CHD-C1D-ND	-5.34	119.54	124.45
17	2	314	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
17	A	832	CLA	CMD-C2D-C1D	5.34	134.13	124.71
17	A	822	CLA	CAC-C3C-C4C	5.34	131.74	124.81
17	A	802	CLA	CHD-C1D-ND	-5.34	119.55	124.45
17	B	837	CLA	O2D-CGD-CBD	5.34	120.75	111.27
17	A	824	CLA	C3B-C2B-C1B	-5.34	100.72	107.16
17	1	302	CLA	CHD-C1D-ND	-5.34	119.55	124.45
17	1	302	CLA	CMD-C2D-C1D	5.33	134.11	124.71
17	A	856	CLA	CHD-C1D-ND	-5.33	119.56	124.45
17	K	103	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
17	5	307	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
17	2	304	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
17	B	801	CLA	C2B-C1B-NB	5.33	113.80	110.23
17	A	803	CLA	O2D-CGD-CBD	5.32	120.73	111.27
17	1	302	CLA	O2D-CGD-CBD	5.32	120.72	111.27
17	2	306	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
17	B	857	CLA	CHD-C1D-ND	-5.32	119.57	124.45
17	3	313	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
17	B	835	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
17	K	103	CLA	C2C-C1C-NC	5.31	114.95	109.97
17	A	814	CLA	C2C-C1C-NC	5.31	114.94	109.97
17	A	815	CLA	CHD-C4C-C3C	-5.30	117.05	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	841	CLA	O2D-CGD-CBD	5.30	120.68	111.27
17	3	307	CLA	O2D-CGD-CBD	5.30	120.68	111.27
17	B	832	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
17	B	813	CLA	C2C-C1C-NC	5.30	114.94	109.97
17	A	839	CLA	C2B-C1B-NB	5.30	113.78	110.23
17	B	830	CLA	CHD-C1D-ND	-5.29	119.59	124.45
25	F	205	5X6	C25-C24-C23	-5.29	106.70	123.22
17	F	203	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
17	A	829	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
17	3	306	CLA	O2D-CGD-CBD	5.28	120.66	111.27
25	3	317	5X6	C20-C21-C22	-5.28	119.77	127.31
17	4	305	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
17	L	202	CLA	O2D-CGD-CBD	5.28	120.65	111.27
17	O	204	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
17	B	810	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
17	B	834	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
17	4	305	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	A	856	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
17	B	807	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
17	A	827	CLA	C2C-C1C-NC	5.27	114.91	109.97
17	A	833	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	2	311	CLA	O2D-CGD-CBD	5.27	120.63	111.27
17	B	812	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
17	B	840	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
17	A	805	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
17	A	820	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
17	2	313	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	B	829	CLA	CMD-C2D-C1D	5.26	133.99	124.71
17	B	812	CLA	C2C-C1C-NC	5.26	114.90	109.97
17	A	859	CLA	O2D-CGD-CBD	5.26	120.62	111.27
25	1	314	5X6	C19-C20-C21	-5.26	112.70	123.47
17	B	825	CLA	CMD-C2D-C1D	5.26	133.98	124.71
17	A	818	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
17	A	805	CLA	CHD-C1D-ND	-5.25	119.62	124.45
25	1	312	5X6	C40-C22-C21	-5.25	115.56	122.92
25	1	313	5X6	C20-C19-C18	-5.25	112.71	123.47
17	B	840	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
17	B	804	CLA	C3C-C4C-NC	5.25	116.46	110.57
17	4	303	CLA	C2C-C1C-NC	5.25	114.89	109.97
17	3	309	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
17	A	836	CLA	CHD-C1D-ND	-5.25	119.63	124.45
17	A	823	CLA	C3C-C4C-NC	5.24	116.45	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	801	CLA	C2C-C1C-NC	5.24	114.89	109.97
17	B	821	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
17	A	837	CLA	CMD-C2D-C1D	5.24	133.95	124.71
17	B	829	CLA	C3B-C2B-C1B	-5.24	100.84	107.16
17	B	806	CLA	CHD-C1D-ND	-5.24	119.64	124.45
17	A	812	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
17	F	203	CLA	C4A-NA-C1A	-5.24	104.35	106.71
17	4	304	CLA	O2D-CGD-CBD	5.24	120.57	111.27
17	2	307	CLA	C3D-C4D-ND	5.23	118.70	110.24
17	F	203	CLA	CHD-C1D-ND	-5.23	119.65	124.45
17	4	310	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
25	1	315	5X6	C20-C19-C18	-5.23	112.77	123.47
17	4	304	CLA	C4A-NA-C1A	-5.22	104.36	106.71
17	A	817	CLA	O2D-CGD-CBD	5.22	120.55	111.27
17	O	205	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
17	2	312	CLA	C2C-C1C-NC	5.22	114.87	109.97
25	2	318	5X6	C40-C22-C23	-5.22	109.85	118.08
17	A	809	CLA	CHD-C1D-ND	-5.22	119.65	124.45
17	B	821	CLA	O2D-CGD-CBD	5.22	120.55	111.27
17	B	816	CLA	CHD-C1D-ND	-5.22	119.66	124.45
17	B	824	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
17	4	306	CLA	C4A-NA-C1A	-5.22	104.36	106.71
17	4	305	CLA	O2D-CGD-CBD	5.22	120.54	111.27
17	1	305	CLA	C2C-C1C-NC	5.22	114.86	109.97
17	B	857	CLA	C4A-NA-C1A	-5.22	104.36	106.71
25	3	318	5X6	C40-C22-C21	-5.22	115.61	122.92
17	2	310	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
17	2	307	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	A	856	CLA	CMD-C2D-C1D	5.21	133.90	124.71
17	5	304	CLA	C2C-C1C-NC	5.21	114.86	109.97
25	F	205	5X6	C15-C16-C17	-5.21	111.78	126.42
17	3	306	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
17	B	811	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	B	811	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
17	3	307	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
25	F	205	5X6	C24-C23-C22	-5.20	111.80	126.42
17	B	829	CLA	CHD-C1D-ND	-5.20	119.67	124.45
17	1	310	CLA	C4A-NA-C1A	-5.20	104.37	106.71
16	A	801	CL0	CHD-C4C-C3C	-5.19	117.20	124.84
17	A	821	CLA	CAC-C3C-C4C	5.19	131.55	124.81
17	B	816	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
17	A	823	CLA	C3D-C2D-C1D	-5.19	98.75	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	830	CLA	O2D-CGD-CBD	5.19	120.49	111.27
25	1	313	5X6	C27-C26-C25	-5.19	110.98	118.94
17	A	835	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
25	1	313	5X6	C19-C20-C21	-5.19	112.85	123.47
17	1	310	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
17	B	834	CLA	C4A-NA-C1A	-5.18	104.38	106.71
17	3	314	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
17	A	859	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
17	5	303	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
17	B	811	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
17	5	304	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
25	3	318	5X6	C20-C19-C18	-5.17	112.89	123.47
17	A	831	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
25	4	312	5X6	C42-C13-C14	-5.16	115.69	122.92
17	4	307	CLA	CHD-C1D-ND	-5.16	119.71	124.45
17	5	304	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
17	B	836	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
17	O	203	CLA	CHD-C4C-C3C	-5.15	117.26	124.84
17	A	807	CLA	CAC-C3C-C4C	5.15	131.49	124.81
17	A	806	CLA	O2D-CGD-CBD	5.15	120.42	111.27
17	B	814	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
20	B	846	BCR	C15-C16-C17	5.15	134.02	123.47
17	1	310	CLA	O2D-CGD-CBD	5.14	120.40	111.27
17	A	829	CLA	CMD-C2D-C1D	5.14	133.77	124.71
17	2	304	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	3	308	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
17	A	802	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
25	5	301	5X6	C40-C22-C21	-5.13	115.73	122.92
17	A	818	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	2	306	CLA	C2C-C1C-NC	5.13	114.78	109.97
25	5	315	5X6	C12-C11-C03	-5.13	112.79	127.20
17	A	831	CLA	O2D-CGD-CBD	5.13	120.38	111.27
17	B	823	CLA	C2C-C1C-NC	5.13	114.78	109.97
17	5	309	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
25	2	321	5X6	C16-C17-C18	-5.12	111.08	118.94
17	B	809	CLA	C2B-C1B-NB	5.12	113.67	110.23
17	O	203	CLA	O2D-CGD-CBD	5.12	120.37	111.27
17	O	205	CLA	C2C-C1C-NC	5.12	114.77	109.97
17	5	313	CLA	C2C-C1C-NC	5.12	114.77	109.97
17	B	837	CLA	C4A-NA-C1A	-5.12	104.40	106.71
17	A	827	CLA	CHD-C1D-ND	-5.12	119.75	124.45
17	2	316	CLA	CHD-C4C-C3C	-5.12	117.31	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	833	CLA	O2D-CGD-CBD	5.11	120.36	111.27
17	1	307	CLA	O2D-CGD-CBD	5.11	120.36	111.27
17	L	204	CLA	C4A-NA-C1A	-5.11	104.41	106.71
20	K	104	BCR	C16-C15-C14	5.11	133.94	123.47
25	2	321	5X6	C39-C26-C25	-5.11	115.76	122.92
17	2	308	CLA	CAC-C3C-C4C	5.11	131.44	124.81
17	L	204	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
17	1	304	CLA	C4A-NA-C1A	-5.10	104.41	106.71
17	B	819	CLA	O2D-CGD-CBD	5.10	120.34	111.27
17	B	824	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
17	1	311	CLA	C2C-C1C-NC	5.10	114.75	109.97
16	A	801	CL0	O2D-CGD-CBD	5.10	120.33	111.27
17	A	826	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
17	B	805	CLA	C3C-C4C-NC	5.10	116.29	110.57
17	B	819	CLA	C2C-C1C-NC	5.10	114.75	109.97
25	1	312	5X6	C11-C03-C02	-5.10	109.11	121.46
17	A	807	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
25	1	313	5X6	C11-C03-C02	-5.09	109.13	121.46
17	A	814	CLA	CAC-C3C-C4C	5.09	131.41	124.81
17	B	826	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
25	1	316	5X6	C40-C22-C21	-5.09	115.79	122.92
17	4	310	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	A	822	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
17	B	821	CLA	C2C-C1C-NC	5.09	114.74	109.97
17	A	853	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
17	A	811	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
17	5	307	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
17	A	809	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
17	A	828	CLA	C1C-C2C-C3C	-5.08	101.62	106.96
17	3	306	CLA	C2C-C1C-NC	5.08	114.73	109.97
25	2	318	5X6	C27-C26-C25	-5.08	111.15	118.94
17	A	855	CLA	CHD-C1D-ND	-5.08	119.79	124.45
17	A	820	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
17	A	817	CLA	CMD-C2D-C1D	5.07	133.66	124.71
17	A	821	CLA	CHD-C4C-C3C	-5.07	117.38	124.84
17	B	807	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
17	B	822	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
17	A	815	CLA	CMD-C2D-C1D	5.07	133.65	124.71
17	4	311	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
17	3	305	CLA	C4A-NA-C1A	-5.07	104.43	106.71
17	B	807	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
17	A	819	CLA	CHD-C4C-C3C	-5.06	117.40	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	305	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
17	B	812	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
17	3	310	CLA	O2D-CGD-CBD	5.06	120.26	111.27
17	5	306	CLA	C2C-C1C-NC	5.06	114.71	109.97
17	A	854	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
25	5	316	5X6	C14-C15-C16	-5.06	107.44	123.22
17	B	830	CLA	CMD-C2D-C1D	5.06	133.62	124.71
25	5	317	5X6	C20-C19-C18	-5.05	113.12	123.47
25	1	316	5X6	C39-C26-C25	-5.05	115.85	122.92
17	B	808	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
17	4	309	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
25	2	321	5X6	C19-C20-C21	-5.05	113.13	123.47
17	A	802	CLA	CMD-C2D-C1D	5.05	133.61	124.71
17	B	826	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
17	A	805	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
17	B	837	CLA	CMD-C2D-C1D	5.04	133.60	124.71
17	B	809	CLA	CHD-C1D-ND	-5.04	119.82	124.45
17	B	818	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
17	2	305	CLA	O2D-CGD-CBD	5.04	120.23	111.27
17	A	813	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
17	B	828	CLA	C3C-C4C-NC	5.04	116.22	110.57
17	J	103	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
17	O	203	CLA	C2C-C1C-NC	5.04	114.69	109.97
17	5	311	CLA	C2C-C1C-NC	5.04	114.69	109.97
25	1	315	5X6	C19-C20-C21	-5.03	113.16	123.47
17	B	808	CLA	C2B-C1B-NB	5.03	113.61	110.23
17	B	816	CLA	C2C-C1C-NC	5.03	114.69	109.97
17	B	802	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
17	B	830	CLA	CAA-C2A-C3A	-5.03	99.01	112.78
17	B	808	CLA	C3C-C4C-NC	5.03	116.21	110.57
17	A	829	CLA	C2C-C1C-NC	5.03	114.68	109.97
17	B	814	CLA	CMC-C2C-C1C	5.03	132.69	125.04
17	4	311	CLA	C4A-NA-C1A	-5.02	104.45	106.71
25	2	317	5X6	C16-C17-C18	-5.02	111.23	118.94
17	1	305	CLA	C4A-NA-C1A	-5.02	104.45	106.71
17	L	203	CLA	O2D-CGD-CBD	5.02	120.19	111.27
25	3	318	5X6	C19-C20-C21	-5.02	113.19	123.47
25	2	320	5X6	C42-C13-C14	-5.02	115.89	122.92
17	B	827	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
17	A	820	CLA	CMD-C2D-C1D	5.02	133.56	124.71
17	5	303	CLA	O2D-CGD-CBD	5.02	120.19	111.27
17	B	840	CLA	C3C-C4C-NC	5.02	116.20	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	811	CLA	C2C-C1C-NC	5.01	114.67	109.97
17	A	815	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
25	3	317	5X6	C19-C20-C21	-5.01	113.20	123.47
17	5	308	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
17	B	831	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
17	3	311	CLA	C3D-C4D-ND	5.01	118.34	110.24
17	B	806	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
17	A	807	CLA	C3C-C4C-NC	5.00	116.18	110.57
17	A	808	CLA	C2C-C1C-NC	5.00	114.66	109.97
17	5	310	CLA	CAC-C3C-C4C	5.00	131.30	124.81
17	B	810	CLA	O2D-CGD-CBD	5.00	120.16	111.27
25	5	301	5X6	C27-C26-C25	-5.00	111.27	118.94
17	K	103	CLA	O2D-CGD-CBD	5.00	120.15	111.27
17	5	302	CLA	C2C-C1C-NC	4.99	114.65	109.97
17	B	805	CLA	C2C-C1C-NC	4.99	114.64	109.97
17	3	312	CLA	C2C-C1C-NC	4.99	114.64	109.97
17	A	859	CLA	C2C-C1C-NC	4.98	114.64	109.97
17	B	802	CLA	CHD-C1D-ND	-4.98	119.88	124.45
17	A	824	CLA	C3C-C4C-NC	4.98	116.16	110.57
17	5	305	CLA	O2A-CGA-CBA	4.98	127.54	111.91
17	A	808	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
17	1	303	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
17	B	811	CLA	O2D-CGD-CBD	4.98	120.12	111.27
17	A	854	CLA	C3C-C4C-NC	4.98	116.15	110.57
25	3	318	5X6	C12-C11-C03	-4.98	113.23	127.20
17	3	309	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	A	804	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
17	B	817	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
17	A	809	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
17	1	302	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
17	A	831	CLA	CHD-C1D-ND	-4.97	119.89	124.45
25	4	314	5X6	C19-C20-C21	-4.97	113.30	123.47
25	J	105	5X6	C24-C23-C22	-4.97	112.46	126.42
25	3	316	5X6	C12-C11-C03	-4.97	113.26	127.20
17	A	831	CLA	CMD-C2D-C1D	4.97	133.46	124.71
17	1	301	CLA	CHD-C1D-ND	-4.97	119.89	124.45
17	A	808	CLA	C4A-NA-C1A	-4.96	104.47	106.71
17	A	803	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
17	B	836	CLA	C4A-NA-C1A	-4.96	104.48	106.71
17	B	818	CLA	C3B-C2B-C1B	-4.96	101.18	107.16
20	A	844	BCR	C37-C22-C21	-4.96	115.98	122.92
17	1	308	CLA	C2C-C1C-NC	4.96	114.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	829	CLA	C4A-NA-C1A	-4.96	104.48	106.71
17	B	820	CLA	CHD-C4C-C3C	-4.96	117.56	124.84
25	4	312	5X6	C27-C26-C25	-4.95	111.34	118.94
17	B	808	CLA	C3D-C4D-ND	4.95	118.25	110.24
25	2	318	5X6	C12-C11-C03	-4.95	113.29	127.20
17	1	307	CLA	CMC-C2C-C1C	4.95	132.58	125.04
17	K	102	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
17	5	313	CLA	CAC-C3C-C4C	4.95	131.23	124.81
17	A	854	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
17	B	807	CLA	CHD-C1D-ND	-4.95	119.91	124.45
25	2	318	5X6	C15-C16-C17	-4.95	112.52	126.42
25	5	315	5X6	C39-C26-C25	-4.95	116.00	122.92
17	A	835	CLA	C3C-C4C-NC	4.94	116.11	110.57
17	A	806	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
17	B	836	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
17	B	818	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
17	B	831	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
17	B	836	CLA	CHD-C1D-ND	-4.94	119.92	124.45
17	A	807	CLA	C2C-C1C-NC	4.94	114.60	109.97
17	3	313	CLA	C2C-C1C-NC	4.94	114.60	109.97
17	B	823	CLA	O2D-CGD-CBD	4.94	120.04	111.27
17	B	829	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
17	B	838	CLA	CHD-C1D-ND	-4.93	119.93	124.45
25	2	317	5X6	C12-C11-C03	-4.93	113.36	127.20
17	A	804	CLA	CHD-C1D-ND	-4.93	119.93	124.45
17	A	852	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
17	A	812	CLA	CHD-C1D-ND	-4.92	119.93	124.45
25	1	315	5X6	C24-C23-C22	-4.92	112.60	126.42
17	A	811	CLA	C3C-C4C-NC	4.92	116.08	110.57
25	5	318	5X6	C19-C20-C21	-4.92	113.40	123.47
17	B	815	CLA	CMD-C2D-C1D	4.91	133.37	124.71
17	A	830	CLA	CHD-C1D-ND	-4.91	119.94	124.45
17	A	826	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
25	1	314	5X6	C15-C16-C17	-4.91	112.62	126.42
17	B	818	CLA	O2D-CGD-CBD	4.91	120.00	111.27
25	2	321	5X6	C23-C22-C21	-4.91	111.41	118.94
17	A	835	CLA	CMD-C2D-C1D	4.91	133.36	124.71
17	A	830	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
17	2	305	CLA	C4A-NA-C1A	-4.91	104.50	106.71
17	A	838	CLA	CHD-C1D-ND	-4.91	119.94	124.45
17	A	820	CLA	C2C-C1C-NC	4.91	114.57	109.97
17	B	805	CLA	C3B-C2B-C1B	-4.91	101.24	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	313	5X6	C41-C17-C18	-4.90	116.06	122.92
17	5	309	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
17	1	303	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	2	309	CLA	CAC-C3C-C4C	4.89	131.16	124.81
17	1	309	CLA	C2C-C1C-NC	4.89	114.56	109.97
17	A	831	CLA	C3C-C4C-NC	4.89	116.06	110.57
17	B	819	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
17	A	853	CLA	C1C-C2C-C3C	-4.89	101.82	106.96
17	A	815	CLA	CHD-C1D-ND	-4.89	119.96	124.45
17	3	310	CLA	C4A-NA-C1A	-4.89	104.51	106.71
17	B	839	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
17	A	821	CLA	C2C-C1C-NC	4.88	114.55	109.97
17	A	822	CLA	C3D-C4D-ND	4.88	118.14	110.24
17	3	314	CLA	C2C-C1C-NC	4.88	114.55	109.97
17	5	303	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
17	B	824	CLA	C3D-C4D-ND	4.88	118.13	110.24
17	4	309	CLA	C2C-C1C-NC	4.88	114.54	109.97
17	A	839	CLA	O2D-CGD-CBD	4.88	119.93	111.27
17	2	311	CLA	C3D-C4D-ND	4.88	118.13	110.24
17	4	307	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
17	B	804	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
17	A	825	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
17	A	814	CLA	C3D-C4D-ND	4.87	118.12	110.24
17	A	834	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
17	A	804	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
17	A	828	CLA	CMD-C2D-C1D	4.87	133.30	124.71
17	2	311	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
17	3	315	CLA	C2C-C1C-NC	4.87	114.53	109.97
17	A	816	CLA	C3C-C4C-NC	4.87	116.03	110.57
17	B	827	CLA	C3C-C4C-NC	4.87	116.03	110.57
16	A	801	CL0	CMD-C2D-C1D	4.87	133.29	124.71
17	5	302	CLA	O2D-CGD-CBD	4.87	119.92	111.27
17	A	835	CLA	O2D-CGD-CBD	4.87	119.92	111.27
17	A	806	CLA	CMD-C2D-C1D	4.87	133.29	124.71
17	K	102	CLA	C2C-C1C-NC	4.87	114.53	109.97
17	2	313	CLA	C2C-C1C-NC	4.87	114.53	109.97
17	B	828	CLA	C4A-NA-C1A	-4.86	104.52	106.71
17	5	307	CLA	C2C-C1C-NC	4.86	114.53	109.97
17	5	306	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
17	5	305	CLA	CMC-C2C-C1C	4.86	132.44	125.04
17	5	310	CLA	C2C-C1C-NC	4.86	114.53	109.97
17	3	309	CLA	C3D-C2D-C1D	-4.86	99.20	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	802	CLA	C3C-C4C-NC	4.86	116.02	110.57
17	2	313	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
17	2	306	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
17	L	204	CLA	C2C-C1C-NC	4.86	114.52	109.97
17	A	817	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
25	4	313	5X6	C27-C26-C25	-4.86	111.49	118.94
17	O	204	CLA	C2C-C1C-NC	4.86	114.52	109.97
17	A	817	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
25	1	313	5X6	C16-C17-C18	-4.85	111.49	118.94
17	B	810	CLA	C3C-C4C-NC	4.85	116.02	110.57
17	A	833	CLA	C2C-C1C-NC	4.85	114.52	109.97
17	3	307	CLA	C3D-C4D-ND	4.85	118.09	110.24
25	5	318	5X6	C42-C13-C12	-4.85	110.43	118.08
17	A	825	CLA	C3C-C4C-NC	4.85	116.01	110.57
25	2	320	5X6	C23-C22-C21	-4.85	111.50	118.94
17	A	820	CLA	O2D-CGD-CBD	4.85	119.89	111.27
25	2	318	5X6	C12-C13-C14	-4.85	111.50	118.94
17	B	857	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
17	4	304	CLA	C3D-C4D-ND	4.84	118.07	110.24
17	5	305	CLA	C3D-C4D-ND	4.84	118.07	110.24
20	A	857	BCR	C37-C22-C21	-4.84	116.14	122.92
17	B	815	CLA	CMC-C2C-C1C	4.84	132.41	125.04
17	2	305	CLA	C3D-C4D-ND	4.84	118.07	110.24
25	3	316	5X6	C20-C19-C18	-4.84	113.56	123.47
17	A	837	CLA	C2C-C1C-NC	4.84	114.50	109.97
17	B	816	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
17	1	307	CLA	C3D-C4D-ND	4.84	118.06	110.24
17	2	307	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
25	5	317	5X6	C19-C20-C21	-4.84	113.57	123.47
17	A	819	CLA	C2C-C1C-NC	4.84	114.50	109.97
25	5	301	5X6	C12-C11-C03	-4.83	113.63	127.20
17	3	305	CLA	C3D-C4D-ND	4.83	118.06	110.24
17	3	312	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
17	1	308	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
25	2	320	5X6	C41-C17-C18	-4.83	116.16	122.92
17	1	306	CLA	C2C-C1C-NC	4.82	114.49	109.97
17	A	816	CLA	CAC-C3C-C4C	4.82	131.07	124.81
17	K	103	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
17	B	840	CLA	CHD-C1D-ND	-4.82	120.02	124.45
25	1	316	5X6	C24-C23-C22	-4.82	112.87	126.42
17	B	825	CLA	CAC-C3C-C4C	4.82	131.06	124.81
17	5	314	CLA	C4A-NA-C1A	-4.82	104.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	313	CLA	O2D-CGD-CBD	4.82	119.83	111.27
17	1	306	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
17	B	823	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	B	857	CLA	C3D-C4D-ND	4.82	118.03	110.24
17	B	809	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
17	A	854	CLA	C3D-C4D-ND	4.81	118.03	110.24
17	A	813	CLA	C3B-C2B-C1B	-4.81	101.35	107.16
25	1	313	5X6	C28-C29-C30	-4.81	109.80	121.46
17	J	103	CLA	CAC-C3C-C4C	4.81	131.05	124.81
17	2	304	CLA	C3D-C4D-ND	4.81	118.02	110.24
17	B	834	CLA	O2D-CGD-CBD	4.81	119.82	111.27
17	4	308	CLA	O2D-CGD-CBD	4.81	119.81	111.27
17	A	839	CLA	C3D-C4D-ND	4.81	118.02	110.24
17	A	836	CLA	CHD-C4C-C3C	-4.81	117.78	124.84
17	1	304	CLA	C3D-C4D-ND	4.81	118.01	110.24
17	B	822	CLA	O2D-CGD-CBD	4.80	119.81	111.27
17	A	811	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
17	A	802	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
17	A	828	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
17	2	314	CLA	C4A-NA-C1A	-4.80	104.55	106.71
17	A	833	CLA	CMD-C2D-C1D	4.80	133.18	124.71
17	3	306	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
17	2	314	CLA	O2D-CGD-CBD	4.80	119.80	111.27
17	A	820	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
17	5	307	CLA	CAC-C3C-C4C	4.79	131.03	124.81
17	A	853	CLA	O2D-CGD-O1D	-4.79	114.47	123.84
17	B	815	CLA	O2D-CGD-CBD	4.79	119.78	111.27
17	A	855	CLA	C3C-C4C-NC	4.79	115.94	110.57
17	5	314	CLA	C2C-C1C-NC	4.79	114.46	109.97
17	A	827	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
17	B	805	CLA	CHD-C1D-ND	-4.78	120.06	124.45
17	3	314	CLA	O2D-CGD-CBD	4.78	119.77	111.27
25	J	105	5X6	C11-C03-C02	-4.78	109.88	121.46
25	3	318	5X6	C12-C13-C14	-4.78	111.61	118.94
17	B	806	CLA	C3B-C4B-NB	4.77	114.94	110.52
17	B	837	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
17	1	311	CLA	C3D-C4D-ND	4.77	117.96	110.24
17	A	836	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	4	303	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
17	B	823	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
17	2	313	CLA	O2D-CGD-CBD	4.77	119.74	111.27
17	3	312	CLA	C4A-NA-C1A	-4.77	104.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	316	5X6	C12-C11-C03	-4.77	113.81	127.20
17	4	311	CLA	C3D-C4D-ND	4.77	117.95	110.24
17	A	856	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
17	5	309	CLA	C3D-C4D-ND	4.76	117.94	110.24
17	B	815	CLA	CAC-C3C-C4C	4.76	130.99	124.81
25	4	314	5X6	C20-C19-C18	-4.76	113.72	123.47
17	5	311	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	3	313	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	B	817	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
17	2	316	CLA	O2D-CGD-CBD	4.76	119.72	111.27
17	A	834	CLA	CMC-C2C-C1C	4.75	132.28	125.04
17	A	820	CLA	C3D-C4D-ND	4.75	117.93	110.24
25	5	318	5X6	C27-C28-C29	-4.75	113.85	127.20
17	2	316	CLA	C2C-C1C-NC	4.75	114.42	109.97
25	4	312	5X6	C27-C28-C29	-4.75	113.85	127.20
17	B	839	CLA	C3D-C4D-ND	4.75	117.92	110.24
25	1	313	5X6	C27-C28-C29	-4.75	113.86	127.20
17	B	806	CLA	CAC-C3C-C4C	4.75	130.97	124.81
17	A	836	CLA	CAC-C3C-C4C	4.75	130.97	124.81
17	A	808	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
25	2	320	5X6	C11-C12-C13	-4.75	119.06	126.23
17	A	829	CLA	O2D-CGD-CBD	4.75	119.70	111.27
17	A	821	CLA	C3D-C4D-ND	4.75	117.92	110.24
17	J	103	CLA	CMC-C2C-C1C	4.75	132.27	125.04
17	5	313	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
17	5	303	CLA	C3D-C4D-ND	4.75	117.91	110.24
17	B	841	CLA	C3D-C4D-ND	4.74	117.91	110.24
25	3	317	5X6	C40-C22-C21	-4.74	116.28	122.92
17	2	306	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
17	4	308	CLA	C3D-C4D-ND	4.74	117.91	110.24
25	J	105	5X6	C25-C24-C23	-4.74	108.42	123.22
17	4	311	CLA	O2D-CGD-CBD	4.74	119.69	111.27
17	A	839	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
17	2	310	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
17	B	815	CLA	CHD-C1D-ND	-4.74	120.10	124.45
17	4	309	CLA	C4A-NA-C1A	-4.74	104.58	106.71
25	1	316	5X6	C27-C28-C29	-4.74	113.90	127.20
17	A	816	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
17	B	826	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
17	A	839	CLA	C3C-C4C-NC	4.73	115.88	110.57
17	B	837	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
17	5	306	CLA	O2D-CGD-CBD	4.73	119.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	812	CLA	CMD-C2D-C1D	4.73	133.05	124.71
17	O	203	CLA	C3D-C4D-ND	4.73	117.89	110.24
17	4	306	CLA	C3D-C4D-ND	4.73	117.89	110.24
17	1	303	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
17	B	826	CLA	C1C-C2C-C3C	-4.73	101.99	106.96
17	A	819	CLA	C3D-C4D-ND	4.73	117.88	110.24
17	A	813	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
17	2	312	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
17	B	802	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
17	A	803	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
17	B	841	CLA	C2C-C1C-NC	4.72	114.40	109.97
17	B	804	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
17	4	305	CLA	C2C-C1C-NC	4.72	114.39	109.97
17	3	308	CLA	O2D-CGD-CBD	4.72	119.66	111.27
17	5	305	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
17	A	823	CLA	CAC-C3C-C4C	4.72	130.93	124.81
17	2	310	CLA	C3D-C4D-ND	4.72	117.87	110.24
17	B	814	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
17	4	309	CLA	O2D-CGD-CBD	4.72	119.65	111.27
17	B	819	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
17	B	819	CLA	C3D-C4D-ND	4.71	117.86	110.24
17	A	824	CLA	C3D-C4D-ND	4.71	117.86	110.24
17	A	832	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
17	2	315	CLA	C2C-C1C-NC	4.71	114.38	109.97
17	5	303	CLA	C2C-C1C-NC	4.71	114.38	109.97
17	B	836	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
17	A	813	CLA	O2D-CGD-CBD	4.71	119.63	111.27
17	3	310	CLA	C3D-C4D-ND	4.71	117.85	110.24
17	A	811	CLA	O2D-CGD-CBD	4.71	119.63	111.27
25	4	313	5X6	C41-C17-C18	-4.71	116.33	122.92
17	2	305	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
17	A	814	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
17	1	309	CLA	C4A-NA-C1A	-4.70	104.59	106.71
17	B	837	CLA	C3C-C4C-NC	4.70	115.85	110.57
17	2	315	CLA	C3D-C4D-ND	4.70	117.85	110.24
17	A	812	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
17	A	836	CLA	CMD-C2D-C1D	4.70	133.00	124.71
17	4	308	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
17	2	313	CLA	CAC-C3C-C4C	4.70	130.91	124.81
17	L	202	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
17	B	822	CLA	C3D-C4D-ND	4.70	117.83	110.24
17	A	830	CLA	C3C-C4C-NC	4.70	115.84	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	801	CL0	C1C-C2C-C3C	-4.69	102.02	106.96
17	B	804	CLA	CHD-C1D-ND	-4.69	120.14	124.45
17	1	304	CLA	CMC-C2C-C1C	4.69	132.18	125.04
17	A	807	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
17	A	811	CLA	CMC-C2C-C1C	4.69	132.18	125.04
17	B	823	CLA	C3D-C4D-ND	4.69	117.82	110.24
17	1	307	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
17	B	857	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
17	A	809	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
17	A	802	CLA	C3D-C4D-ND	4.69	117.82	110.24
17	5	310	CLA	C4A-NA-C1A	-4.68	104.60	106.71
17	A	807	CLA	CHD-C1D-ND	-4.68	120.15	124.45
17	A	837	CLA	C3C-C4C-NC	4.68	115.82	110.57
17	B	838	CLA	C3C-C4C-NC	4.68	115.82	110.57
25	1	315	5X6	C16-C17-C18	-4.68	111.76	118.94
17	A	803	CLA	C3D-C4D-ND	4.68	117.81	110.24
17	A	833	CLA	C3D-C4D-ND	4.68	117.81	110.24
25	F	205	5X6	C27-C28-C29	-4.68	114.07	127.20
17	A	827	CLA	C3C-C4C-NC	4.68	115.81	110.57
17	1	307	CLA	C4A-NA-C1A	-4.68	104.60	106.71
17	A	822	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
25	5	315	5X6	C23-C22-C21	-4.67	111.77	118.94
25	3	318	5X6	C15-C16-C17	-4.67	113.29	126.42
17	4	309	CLA	C3D-C4D-ND	4.67	117.80	110.24
17	5	310	CLA	CHD-C4C-C3C	-4.67	117.97	124.84
17	B	836	CLA	C3C-C4C-NC	4.67	115.81	110.57
17	5	304	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
17	4	310	CLA	C3D-C4D-ND	4.67	117.79	110.24
16	A	801	CL0	C3D-C2D-C1D	-4.67	99.46	105.83
17	3	315	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
17	B	820	CLA	C2C-C1C-NC	4.67	114.34	109.97
17	3	310	CLA	C2C-C1C-NC	4.67	114.34	109.97
17	A	826	CLA	CAC-C3C-C4C	4.67	130.87	124.81
17	A	817	CLA	C3D-C4D-ND	4.67	117.79	110.24
25	5	316	5X6	C24-C23-C22	-4.67	113.31	126.42
17	1	305	CLA	C3D-C4D-ND	4.66	117.78	110.24
17	A	817	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
17	B	815	CLA	C3C-C4C-NC	4.66	115.80	110.57
20	B	848	BCR	C8-C9-C10	4.66	126.09	118.94
17	2	312	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
17	3	311	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
17	O	204	CLA	C3D-C2D-C1D	-4.66	99.47	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	839	CLA	CHD-C1D-ND	-4.66	120.17	124.45
17	A	808	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
17	5	311	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
17	A	816	CLA	C3B-C2B-C1B	-4.65	101.54	107.16
17	5	302	CLA	CHD-C4C-C3C	-4.65	118.00	124.84
17	A	821	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
17	A	852	CLA	C3C-C4C-NC	4.65	115.79	110.57
17	A	835	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
17	B	801	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
17	L	203	CLA	C3C-C4C-NC	4.65	115.79	110.57
17	B	827	CLA	CHD-C1D-ND	-4.65	120.18	124.45
25	4	314	5X6	C28-C29-C30	-4.65	110.21	121.46
17	A	852	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
17	B	832	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
17	5	312	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
25	5	301	5X6	C12-C13-C14	-4.64	111.82	118.94
17	4	306	CLA	O2D-CGD-CBD	4.64	119.52	111.27
17	B	826	CLA	C3C-C4C-NC	4.64	115.78	110.57
25	4	314	5X6	C16-C17-C18	-4.64	111.82	118.94
17	F	204	CLA	C4A-NA-C1A	-4.64	104.62	106.71
17	A	833	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
17	1	308	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
25	3	317	5X6	C15-C16-C17	-4.64	113.38	126.42
17	2	309	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
17	A	853	CLA	C3C-C4C-NC	4.64	115.77	110.57
17	1	308	CLA	C3D-C4D-ND	4.64	117.74	110.24
17	B	817	CLA	C4A-NA-C1A	-4.64	104.62	106.71
25	5	317	5X6	C24-C23-C22	-4.64	113.39	126.42
17	3	312	CLA	C3D-C4D-ND	4.64	117.74	110.24
17	A	822	CLA	C2C-C1C-NC	4.64	114.32	109.97
17	3	315	CLA	C3D-C4D-ND	4.64	117.74	110.24
17	A	803	CLA	C3B-C4B-NB	4.64	114.82	110.52
17	5	302	CLA	C3D-C4D-ND	4.64	117.74	110.24
17	5	312	CLA	O2D-CGD-CBD	4.63	119.50	111.27
17	2	314	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
17	1	310	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
17	4	306	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
17	5	312	CLA	C3D-C4D-ND	4.63	117.73	110.24
17	4	303	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
17	2	304	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
17	1	301	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
17	5	311	CLA	C3D-C4D-ND	4.63	117.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	307	CLA	C4A-NA-C1A	-4.63	104.62	106.71
25	5	318	5X6	C15-C16-C17	-4.63	113.42	126.42
17	2	316	CLA	C4A-NA-C1A	-4.63	104.63	106.71
17	5	308	CLA	C3D-C4D-ND	4.62	117.72	110.24
17	4	307	CLA	C2C-C1C-NC	4.62	114.30	109.97
17	4	306	CLA	CAC-C3C-C4C	4.62	130.81	124.81
17	A	829	CLA	C4A-NA-C1A	-4.62	104.63	106.71
17	B	824	CLA	C4A-NA-C1A	-4.62	104.63	106.71
17	2	308	CLA	O2D-CGD-CBD	4.62	119.48	111.27
17	5	310	CLA	C3D-C4D-ND	4.62	117.71	110.24
17	2	313	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
17	A	812	CLA	C3D-C4D-ND	4.62	117.71	110.24
17	K	102	CLA	C4A-NA-C1A	-4.62	104.63	106.71
17	3	313	CLA	C3D-C4D-ND	4.61	117.70	110.24
17	A	835	CLA	C4A-NA-C1A	-4.61	104.63	106.71
17	B	830	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
17	1	309	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
17	B	834	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
17	2	314	CLA	C3D-C4D-ND	4.61	117.70	110.24
25	4	313	5X6	C27-C28-C29	-4.61	114.26	127.20
17	1	311	CLA	CHD-C4C-C3C	-4.61	118.07	124.84
17	B	816	CLA	C3D-C4D-ND	4.61	117.69	110.24
17	A	813	CLA	C2C-C1C-NC	4.61	114.29	109.97
17	5	314	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
17	B	857	CLA	C2C-C1C-NC	4.60	114.29	109.97
17	4	311	CLA	C2C-C1C-NC	4.60	114.29	109.97
17	A	804	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
17	A	812	CLA	C3C-C4C-NC	4.60	115.73	110.57
17	L	203	CLA	CHD-C1D-ND	-4.60	120.23	124.45
17	4	306	CLA	C2C-C1C-NC	4.60	114.28	109.97
17	5	303	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
17	A	852	CLA	CHD-C1D-ND	-4.60	120.23	124.45
25	2	319	5X6	C15-C16-C17	-4.60	113.50	126.42
17	A	859	CLA	C3C-C4C-NC	4.60	115.73	110.57
17	3	309	CLA	C2C-C1C-NC	4.60	114.28	109.97
17	3	305	CLA	CMC-C2C-C1C	4.59	132.04	125.04
17	A	814	CLA	O2D-CGD-CBD	4.59	119.43	111.27
17	1	304	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
25	3	317	5X6	C11-C03-C02	-4.59	110.34	121.46
17	B	836	CLA	CAC-C3C-C4C	4.59	130.77	124.81
17	3	311	CLA	C4A-NA-C1A	-4.59	104.64	106.71
17	A	813	CLA	C3D-C4D-ND	4.59	117.66	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	820	CLA	C3D-C4D-ND	4.59	117.66	110.24
25	2	317	5X6	C20-C19-C18	-4.59	114.08	123.47
17	B	820	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
17	B	801	CLA	CHD-C4C-C3C	-4.59	118.10	124.84
17	A	805	CLA	C3D-C4D-ND	4.59	117.66	110.24
17	2	309	CLA	C3D-C4D-ND	4.58	117.66	110.24
17	A	836	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
17	B	805	CLA	CAC-C3C-C4C	4.58	130.75	124.81
17	1	311	CLA	C4A-NA-C1A	-4.58	104.65	106.71
17	5	306	CLA	C3D-C4D-ND	4.58	117.65	110.24
17	B	835	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
25	2	321	5X6	C12-C11-C03	-4.58	114.34	127.20
17	B	806	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
17	2	316	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
25	4	314	5X6	C27-C28-C29	-4.58	114.35	127.20
17	4	303	CLA	CAC-C3C-C4C	4.57	130.75	124.81
17	B	830	CLA	C3B-C4B-NB	4.57	114.76	110.52
17	K	103	CLA	CHD-C1D-ND	-4.57	120.25	124.45
17	2	312	CLA	CAC-C3C-C4C	4.57	130.74	124.81
17	B	815	CLA	C3D-C4D-ND	4.57	117.63	110.24
17	5	313	CLA	O2D-CGD-CBD	4.57	119.39	111.27
25	5	301	5X6	C15-C16-C17	-4.57	113.58	126.42
17	2	313	CLA	C3D-C4D-ND	4.57	117.63	110.24
17	2	309	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
17	4	311	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
17	1	310	CLA	C3D-C4D-ND	4.57	117.63	110.24
17	B	814	CLA	CHD-C1D-ND	-4.57	120.26	124.45
17	A	834	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
17	3	314	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
17	3	312	CLA	O2D-CGD-CBD	4.57	119.38	111.27
17	A	859	CLA	C3D-C4D-ND	4.56	117.62	110.24
17	A	834	CLA	C4A-NA-C1A	-4.56	104.66	106.71
17	B	839	CLA	CAC-C3C-C4C	4.56	130.73	124.81
17	4	305	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
17	B	839	CLA	C3C-C4C-NC	4.56	115.68	110.57
17	5	302	CLA	CAC-C3C-C4C	4.56	130.72	124.81
17	B	841	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
17	B	830	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
17	1	301	CLA	C4A-NA-C1A	-4.55	104.66	106.71
17	4	304	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	K	104	BCR	C15-C16-C17	4.55	132.80	123.47
17	5	310	CLA	C3D-C2D-C1D	-4.55	99.62	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	837	CLA	CMC-C2C-C1C	4.55	131.97	125.04
25	5	317	5X6	C15-C16-C17	-4.55	113.64	126.42
17	O	203	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
17	A	818	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
25	1	316	5X6	C15-C16-C17	-4.55	113.64	126.42
25	5	316	5X6	C25-C24-C23	-4.55	109.03	123.22
17	1	301	CLA	O2D-CGD-CBD	4.55	119.35	111.27
17	5	302	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
17	1	311	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
17	B	833	CLA	C3C-C4C-NC	4.54	115.67	110.57
17	3	309	CLA	C3D-C4D-ND	4.54	117.58	110.24
17	A	814	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
25	4	312	5X6	C28-C29-C30	-4.54	110.46	121.46
17	A	836	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
17	F	204	CLA	C3D-C4D-ND	4.54	117.58	110.24
17	A	835	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
17	5	312	CLA	C4A-NA-C1A	-4.54	104.67	106.71
17	B	832	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
17	3	305	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
17	A	810	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
25	3	317	5X6	C12-C11-C03	-4.53	114.47	127.20
17	B	836	CLA	CMD-C2D-C1D	4.53	132.70	124.71
17	J	103	CLA	CHD-C1D-ND	-4.53	120.29	124.45
17	1	302	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
17	1	306	CLA	C3D-C4D-ND	4.53	117.57	110.24
17	3	313	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
17	A	804	CLA	O2D-CGD-CBD	4.53	119.32	111.27
17	L	204	CLA	C3D-C4D-ND	4.53	117.57	110.24
17	F	204	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
17	B	809	CLA	C3C-C4C-NC	4.53	115.65	110.57
17	1	303	CLA	C2C-C1C-NC	4.53	114.21	109.97
17	5	307	CLA	C3B-C2B-C1B	-4.53	101.70	107.16
17	O	205	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
17	A	856	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
25	1	312	5X6	C19-C20-C21	-4.52	114.21	123.47
17	2	316	CLA	C3D-C4D-ND	4.52	117.55	110.24
17	2	310	CLA	C4A-NA-C1A	-4.52	104.67	106.71
17	2	315	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
17	A	819	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	4	313	5X6	C24-C23-C22	-4.52	113.73	126.42
25	3	318	5X6	C24-C23-C22	-4.52	113.73	126.42
17	A	853	CLA	C3B-C2B-C1B	-4.52	101.71	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	828	CLA	CHD-C1D-ND	-4.52	120.30	124.45
17	3	312	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
17	3	310	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
17	3	307	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
25	2	317	5X6	C27-C26-C25	-4.51	112.02	118.94
17	F	203	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
17	B	814	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
17	A	803	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
25	1	316	5X6	C16-C17-C18	-4.51	112.02	118.94
17	4	305	CLA	C3D-C4D-ND	4.51	117.53	110.24
17	B	802	CLA	CMD-C2D-C1D	4.51	132.66	124.71
17	A	836	CLA	O2D-CGD-CBD	4.51	119.28	111.27
17	4	308	CLA	C2C-C1C-NC	4.51	114.19	109.97
17	A	830	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
17	A	828	CLA	C3D-C4D-ND	4.50	117.52	110.24
17	A	832	CLA	CHD-C4C-C3C	-4.50	118.22	124.84
17	A	822	CLA	C3C-C4C-NC	4.50	115.62	110.57
25	4	314	5X6	C15-C16-C17	-4.50	113.78	126.42
17	B	832	CLA	C3D-C4D-ND	4.50	117.52	110.24
17	B	837	CLA	CHD-C1D-ND	-4.50	120.32	124.45
25	4	312	5X6	C11-C12-C13	-4.50	119.44	126.23
17	4	309	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
17	B	822	CLA	C4A-NA-C1A	-4.50	104.69	106.71
17	A	856	CLA	C3D-C4D-ND	4.49	117.50	110.24
17	1	309	CLA	C3D-C4D-ND	4.49	117.50	110.24
17	A	836	CLA	C3D-C4D-ND	4.49	117.50	110.24
17	3	312	CLA	CAC-C3C-C4C	4.49	130.63	124.81
17	B	836	CLA	O2D-CGD-CBD	4.49	119.25	111.27
17	3	309	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
17	3	305	CLA	O2D-CGD-CBD	4.49	119.24	111.27
17	A	810	CLA	C3C-C4C-NC	4.49	115.60	110.57
17	B	830	CLA	C1C-C2C-C3C	-4.48	102.24	106.96
17	A	828	CLA	CHD-C1D-ND	-4.48	120.33	124.45
17	4	310	CLA	C4A-NA-C1A	-4.48	104.69	106.71
17	1	302	CLA	C3D-C4D-ND	4.48	117.49	110.24
25	4	313	5X6	C11-C03-C02	-4.48	110.61	121.46
25	1	314	5X6	C27-C28-C29	-4.48	114.62	127.20
25	1	316	5X6	C19-C20-C21	-4.48	114.30	123.47
17	5	306	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
17	4	310	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
17	1	310	CLA	C2C-C1C-NC	4.48	114.17	109.97
25	1	312	5X6	C12-C11-C03	-4.48	114.63	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	311	CLA	CAC-C3C-C4C	4.48	130.62	124.81
25	5	315	5X6	C11-C03-C02	-4.48	110.62	121.46
17	B	835	CLA	C4A-NA-C1A	-4.48	104.69	106.71
17	5	311	CLA	O2D-CGD-CBD	4.48	119.22	111.27
17	A	838	CLA	C3C-C4C-NC	4.47	115.59	110.57
17	B	825	CLA	CMC-C2C-C1C	4.47	131.85	125.04
17	B	837	CLA	C3D-C4D-ND	4.47	117.47	110.24
25	2	320	5X6	C20-C19-C18	-4.47	114.31	123.47
17	B	830	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
16	A	801	CL0	C3C-C4C-NC	4.46	115.58	110.57
17	5	305	CLA	C4A-NA-C1A	-4.46	104.70	106.71
17	B	827	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
17	L	203	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
17	B	831	CLA	O2D-CGD-CBD	4.45	119.18	111.27
17	B	812	CLA	CHD-C1D-ND	-4.45	120.36	124.45
25	4	312	5X6	C19-C20-C21	-4.45	114.35	123.47
17	1	308	CLA	C4A-NA-C1A	-4.45	104.70	106.71
25	1	314	5X6	C24-C23-C22	-4.45	113.91	126.42
17	B	820	CLA	C4A-NA-C1A	-4.45	104.71	106.71
17	3	315	CLA	C4A-NA-C1A	-4.45	104.71	106.71
17	A	802	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
17	A	825	CLA	C2C-C1C-NC	4.45	114.14	109.97
17	A	819	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
17	L	203	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
17	2	308	CLA	C3D-C4D-ND	4.44	117.43	110.24
17	3	314	CLA	C3D-C4D-ND	4.44	117.43	110.24
17	4	307	CLA	CAC-C3C-C4C	4.44	130.57	124.81
17	5	305	CLA	CAC-C3C-C4C	4.44	130.57	124.81
17	A	815	CLA	C3C-C4C-NC	4.44	115.55	110.57
25	2	319	5X6	C23-C22-C21	-4.44	112.13	118.94
25	1	313	5X6	C25-C24-C23	-4.44	109.37	123.22
25	4	312	5X6	C39-C26-C27	-4.44	111.09	118.08
17	5	310	CLA	O2D-CGD-CBD	4.44	119.15	111.27
17	B	834	CLA	C3D-C4D-ND	4.43	117.41	110.24
17	3	310	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
17	A	819	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
17	5	308	CLA	O2D-CGD-CBD	4.43	119.14	111.27
17	B	814	CLA	C3C-C4C-NC	4.43	115.54	110.57
17	B	834	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
17	B	827	CLA	C4A-NA-C1A	-4.43	104.72	106.71
17	2	308	CLA	C4A-NA-C1A	-4.43	104.72	106.71
17	A	811	CLA	CHD-C1D-ND	-4.43	120.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	312	CLA	C3D-C4D-ND	4.42	117.39	110.24
25	3	318	5X6	C27-C28-C29	-4.42	114.78	127.20
25	2	320	5X6	C01-C02-C07	-4.42	106.16	114.36
17	4	306	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
17	5	314	CLA	C3D-C4D-ND	4.42	117.39	110.24
17	B	815	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
17	B	816	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
17	A	837	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
17	4	307	CLA	C3D-C4D-ND	4.42	117.39	110.24
17	A	834	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
25	5	301	5X6	C24-C23-C22	-4.42	114.00	126.42
17	B	813	CLA	C3C-C4C-NC	4.42	115.53	110.57
17	B	835	CLA	O2D-CGD-CBD	4.42	119.12	111.27
17	A	808	CLA	C3D-C4D-ND	4.42	117.38	110.24
17	2	311	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
17	O	205	CLA	C3D-C4D-ND	4.41	117.38	110.24
17	A	812	CLA	CAC-C3C-C4C	4.41	130.53	124.81
17	1	301	CLA	C3D-C4D-ND	4.41	117.37	110.24
17	B	833	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
17	A	838	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
17	1	304	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
17	1	305	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
17	B	835	CLA	C3D-C4D-ND	4.40	117.35	110.24
17	B	806	CLA	C3C-C4C-NC	4.40	115.50	110.57
17	5	305	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
17	2	308	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
17	A	829	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
20	B	848	BCR	C37-C22-C23	4.40	125.00	118.08
20	L	201	BCR	C34-C9-C10	-4.40	116.76	122.92
25	5	301	5X6	C20-C19-C18	-4.40	114.47	123.47
17	3	307	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
25	2	318	5X6	C27-C28-C29	-4.39	114.86	127.20
17	B	836	CLA	CMC-C2C-C1C	4.39	131.73	125.04
17	2	309	CLA	O2D-CGD-CBD	4.39	119.07	111.27
25	5	316	5X6	C12-C11-C03	-4.39	114.87	127.20
17	A	833	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
17	A	823	CLA	C3B-C4B-NB	4.39	114.58	110.52
17	B	825	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
25	2	318	5X6	C40-C22-C21	-4.38	116.78	122.92
17	B	841	CLA	C4A-NA-C1A	-4.38	104.73	106.71
17	A	837	CLA	CAC-C3C-C4C	4.38	130.50	124.81
17	3	306	CLA	C3D-C4D-ND	4.38	117.33	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	831	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
17	A	806	CLA	C3D-C4D-ND	4.38	117.33	110.24
17	A	806	CLA	C3C-C4C-NC	4.38	115.48	110.57
25	4	313	5X6	C12-C11-C03	-4.38	114.91	127.20
17	A	805	CLA	O2D-CGD-CBD	4.38	119.05	111.27
17	1	308	CLA	O2D-CGD-CBD	4.38	119.05	111.27
17	B	828	CLA	CMD-C2D-C1D	4.38	132.43	124.71
25	4	314	5X6	C27-C26-C25	-4.37	112.23	118.94
17	A	802	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
17	5	302	CLA	C4A-NA-C1A	-4.37	104.74	106.71
17	A	806	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
17	B	811	CLA	CHD-C1D-ND	-4.37	120.44	124.45
17	5	313	CLA	C3D-C4D-ND	4.37	117.31	110.24
17	4	307	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
20	B	846	BCR	C12-C13-C14	4.37	125.65	118.94
17	2	310	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
17	A	831	CLA	CMC-C2C-C1C	4.37	131.69	125.04
17	B	807	CLA	C1C-C2C-C3C	-4.37	102.37	106.96
17	B	807	CLA	C3C-C4C-NC	4.37	115.47	110.57
17	1	310	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
17	B	815	CLA	C4-C3-C5	4.37	122.61	115.27
17	A	805	CLA	C3C-C4C-NC	4.36	115.47	110.57
17	B	809	CLA	CMB-C2B-C1B	4.36	132.01	125.37
25	4	314	5X6	C12-C11-C03	-4.36	114.95	127.20
17	A	828	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
17	B	857	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
17	B	834	CLA	C2C-C1C-NC	4.36	114.06	109.97
17	A	807	CLA	CAA-C2A-C3A	-4.36	100.84	112.78
17	A	829	CLA	CMB-C2B-C1B	4.36	132.00	125.37
17	A	812	CLA	CMC-C2C-C1C	4.36	131.67	125.04
17	3	308	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
17	2	307	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
17	K	103	CLA	C3C-C4C-NC	4.35	115.44	110.57
17	B	840	CLA	CMB-C2B-C1B	4.35	131.99	125.37
20	B	845	BCR	C37-C22-C21	-4.35	116.84	122.92
25	5	317	5X6	C11-C03-C02	-4.35	110.94	121.46
17	K	102	CLA	C3C-C4C-NC	4.35	115.44	110.57
17	B	818	CLA	CAC-C3C-C4C	4.34	130.45	124.81
17	B	811	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
17	1	305	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
17	O	204	CLA	C4A-NA-C1A	-4.34	104.75	106.71
17	O	203	CLA	C4A-NA-C1A	-4.34	104.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	201	BCR	C37-C22-C23	4.34	124.92	118.08
17	O	204	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
17	B	816	CLA	C4A-NA-C1A	-4.34	104.75	106.71
17	A	825	CLA	CHD-C1D-ND	-4.34	120.47	124.45
17	B	817	CLA	C2C-C1C-NC	4.34	114.03	109.97
17	A	816	CLA	CHD-C1D-ND	-4.33	120.47	124.45
17	B	804	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
17	A	832	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
17	2	307	CLA	C2C-C1C-NC	4.33	114.03	109.97
17	B	806	CLA	C3D-C4D-ND	4.33	117.24	110.24
17	L	202	CLA	C3D-C4D-ND	4.33	117.23	110.24
17	O	204	CLA	C3D-C4D-ND	4.33	117.23	110.24
17	A	839	CLA	CMC-C2C-C1C	4.32	131.62	125.04
17	3	305	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
17	A	815	CLA	CMB-C2B-C1B	4.32	131.95	125.37
17	B	817	CLA	C3C-C4C-NC	4.32	115.42	110.57
25	4	312	5X6	C24-C23-C22	-4.32	114.28	126.42
17	J	103	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
25	2	319	5X6	C19-C20-C21	-4.32	114.62	123.47
17	B	817	CLA	C3D-C4D-ND	4.32	117.23	110.24
17	A	837	CLA	C3D-C4D-ND	4.32	117.22	110.24
17	1	309	CLA	O2D-CGD-CBD	4.32	118.94	111.27
17	2	309	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
17	A	838	CLA	C3D-C4D-ND	4.32	117.22	110.24
17	B	812	CLA	C3C-C4C-NC	4.32	115.41	110.57
17	B	818	CLA	C3C-C4C-NC	4.32	115.41	110.57
17	A	825	CLA	C4A-NA-C1A	-4.32	104.77	106.71
25	4	314	5X6	C24-C23-C22	-4.31	114.30	126.42
17	B	830	CLA	C3D-C4D-ND	4.31	117.22	110.24
17	A	855	CLA	C3D-C4D-ND	4.31	117.21	110.24
17	A	834	CLA	C3D-C4D-ND	4.31	117.20	110.24
17	3	309	CLA	O2D-CGD-CBD	4.31	118.92	111.27
17	A	806	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
17	B	817	CLA	CMC-C2C-C1C	4.30	131.59	125.04
17	B	829	CLA	C3D-C4D-ND	4.30	117.20	110.24
25	3	317	5X6	C27-C28-C29	-4.30	115.13	127.20
17	3	314	CLA	CMC-C2C-C1C	4.30	131.59	125.04
25	1	314	5X6	C23-C22-C21	-4.30	112.35	118.94
17	5	304	CLA	O2D-CGD-CBD	4.29	118.90	111.27
17	A	826	CLA	O2D-CGD-CBD	4.29	118.90	111.27
17	2	305	CLA	CMC-C2C-C1C	4.29	131.58	125.04
17	A	807	CLA	C3D-C4D-ND	4.29	117.18	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	311	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
17	5	306	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
17	A	831	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
17	2	310	CLA	C2C-C1C-NC	4.28	113.98	109.97
17	A	828	CLA	C3C-C4C-NC	4.28	115.37	110.57
25	4	313	5X6	C19-C20-C21	-4.28	114.71	123.47
17	1	301	CLA	CAC-C3C-C4C	4.28	130.36	124.81
25	2	319	5X6	C24-C23-C22	-4.28	114.41	126.42
25	2	318	5X6	C16-C17-C18	-4.27	112.38	118.94
25	5	315	5X6	C19-C20-C21	-4.27	114.73	123.47
17	B	822	CLA	CMC-C2C-C1C	4.27	131.54	125.04
25	1	315	5X6	C11-C03-C02	-4.27	111.12	121.46
17	B	822	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
17	5	312	CLA	C2C-C1C-NC	4.27	113.97	109.97
17	B	818	CLA	C3D-C4D-ND	4.26	117.14	110.24
17	2	307	CLA	CMC-C2C-C1C	4.26	131.53	125.04
20	K	104	BCR	C37-C22-C21	-4.26	116.95	122.92
17	5	308	CLA	C4A-NA-C1A	-4.26	104.79	106.71
17	O	204	CLA	CMC-C2C-C1C	4.26	131.53	125.04
17	A	823	CLA	CMC-C2C-C1C	4.26	131.53	125.04
17	A	806	CLA	C3B-C4B-NB	4.26	114.47	110.52
17	4	303	CLA	C3D-C4D-ND	4.26	117.12	110.24
25	5	317	5X6	C12-C11-C03	-4.26	115.25	127.20
17	B	835	CLA	C1C-C2C-C3C	-4.25	102.48	106.96
17	B	829	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
17	A	805	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
17	B	812	CLA	C3D-C4D-ND	4.25	117.11	110.24
25	3	318	5X6	C16-C17-C18	-4.25	112.42	118.94
17	A	837	CLA	O2D-CGD-O1D	-4.25	115.54	123.84
17	B	821	CLA	C3C-C4C-NC	4.25	115.33	110.57
17	B	840	CLA	C3D-C4D-ND	4.25	117.11	110.24
25	J	105	5X6	C27-C26-C25	-4.25	112.43	118.94
17	4	306	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
17	5	307	CLA	C3D-C4D-ND	4.24	117.10	110.24
17	A	809	CLA	C3C-C4C-NC	4.24	115.33	110.57
17	B	802	CLA	C4A-NA-C1A	-4.24	104.80	106.71
17	O	205	CLA	C4A-NA-C1A	-4.24	104.80	106.71
17	B	808	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
17	B	841	CLA	CMC-C2C-C1C	4.24	131.49	125.04
17	2	311	CLA	CMC-C2C-C1C	4.24	131.49	125.04
25	5	316	5X6	C41-C17-C18	-4.24	116.99	122.92
17	A	839	CLA	CAC-C3C-C4C	4.24	130.31	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	314	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
17	3	308	CLA	C4A-NA-C1A	-4.24	104.80	106.71
17	A	810	CLA	CMC-C2C-C1C	4.23	131.49	125.04
17	5	308	CLA	C2C-C1C-NC	4.23	113.94	109.97
25	5	317	5X6	C27-C26-C25	-4.23	112.44	118.94
17	B	806	CLA	CMC-C2C-C1C	4.23	131.49	125.04
17	B	838	CLA	C3D-C4D-ND	4.23	117.09	110.24
25	1	313	5X6	C12-C11-C03	-4.23	115.31	127.20
17	3	307	CLA	C2C-C1C-NC	4.23	113.94	109.97
17	1	306	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
17	L	203	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
17	5	310	CLA	CMC-C2C-C1C	4.23	131.47	125.04
17	5	313	CLA	C3B-C2B-C1B	-4.23	102.06	107.16
17	B	831	CLA	C3D-C4D-ND	4.23	117.07	110.24
17	B	804	CLA	C3B-C4B-NB	4.22	114.43	110.52
17	4	311	CLA	CMC-C2C-C1C	4.22	131.47	125.04
17	3	306	CLA	C3B-C2B-C1B	-4.22	102.06	107.16
17	B	838	CLA	C4A-NA-C1A	-4.22	104.81	106.71
17	A	854	CLA	CMC-C2C-C1C	4.22	131.47	125.04
20	B	803	BCR	C37-C22-C21	-4.22	117.01	122.92
25	1	314	5X6	C14-C15-C16	-4.22	110.05	123.22
25	4	312	5X6	C16-C17-C18	-4.22	112.47	118.94
17	A	818	CLA	C3D-C4D-ND	4.22	117.06	110.24
17	B	810	CLA	C2B-C1B-NB	4.22	113.06	110.23
17	5	309	CLA	C2C-C1C-NC	4.22	113.92	109.97
17	B	831	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
17	4	308	CLA	C4A-NA-C1A	-4.22	104.81	106.71
25	5	315	5X6	C27-C26-C25	-4.22	112.47	118.94
17	B	808	CLA	CMB-C2B-C1B	4.21	131.79	125.37
17	A	824	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
25	1	316	5X6	C41-C17-C16	-4.21	111.44	118.08
17	3	314	CLA	C4A-NA-C1A	-4.21	104.81	106.71
25	2	321	5X6	C15-C16-C17	-4.21	114.58	126.42
17	1	302	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
17	A	832	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
17	B	829	CLA	C3C-C4C-NC	4.21	115.29	110.57
25	5	301	5X6	C16-C17-C18	-4.21	112.48	118.94
17	A	805	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
25	5	318	5X6	C24-C23-C22	-4.20	114.61	126.42
17	A	828	CLA	C4A-NA-C1A	-4.20	104.82	106.71
16	A	801	CL0	C3B-C2B-C1B	-4.20	102.09	107.16
17	B	811	CLA	C1C-C2C-C3C	-4.20	102.54	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	314	5X6	C28-C29-C30	-4.20	111.29	121.46
17	A	805	CLA	CAC-C3C-C4C	4.20	130.26	124.81
17	2	316	CLA	CMC-C2C-C1C	4.20	131.43	125.04
17	L	204	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
17	1	301	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
25	5	315	5X6	C12-C13-C14	-4.20	112.50	118.94
17	B	814	CLA	C3D-C4D-ND	4.19	117.02	110.24
17	K	103	CLA	CAC-C3C-C4C	4.19	130.25	124.81
25	1	313	5X6	C15-C16-C17	-4.19	114.65	126.42
17	J	103	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
17	A	829	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
25	F	205	5X6	C40-C22-C21	-4.19	117.06	122.92
17	A	809	CLA	CMC-C2C-C1C	4.19	131.41	125.04
17	A	832	CLA	CAC-C3C-C4C	4.19	130.24	124.81
17	B	817	CLA	CMB-C2B-C1B	4.18	131.74	125.37
17	B	833	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
17	B	828	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
17	A	809	CLA	C3D-C4D-ND	4.18	117.00	110.24
17	A	815	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
17	L	204	CLA	CAC-C3C-C4C	4.18	130.23	124.81
17	L	203	CLA	C3D-C4D-ND	4.18	116.99	110.24
17	A	830	CLA	C1C-C2C-C3C	-4.18	102.57	106.96
17	2	305	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
17	5	309	CLA	C4A-NA-C1A	-4.17	104.83	106.71
17	A	828	CLA	C3B-C4B-NB	4.17	114.38	110.52
17	B	823	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
17	2	308	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
17	O	204	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
17	F	204	CLA	CMC-C2C-C1C	4.16	131.38	125.04
17	B	828	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
17	A	823	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
17	2	314	CLA	CAC-C3C-C4C	4.16	130.21	124.81
17	1	307	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
17	A	803	CLA	C3C-C4C-NC	4.16	115.24	110.57
17	2	316	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
17	2	306	CLA	C3D-C4D-ND	4.16	116.97	110.24
17	2	315	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
17	B	839	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
17	A	813	CLA	C4A-NA-C1A	-4.15	104.84	106.71
17	B	813	CLA	CMC-C2C-C1C	4.15	131.37	125.04
17	O	205	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
25	3	316	5X6	C23-C22-C21	-4.15	112.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	308	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
17	A	855	CLA	CMB-C2B-C1B	4.15	131.68	125.37
17	5	308	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
25	5	316	5X6	C15-C16-C17	-4.14	114.77	126.42
17	B	815	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
17	1	303	CLA	C3D-C4D-ND	4.14	116.94	110.24
17	2	312	CLA	C4A-NA-C1A	-4.14	104.84	106.71
25	1	315	5X6	C12-C11-C03	-4.14	115.58	127.20
25	J	105	5X6	C27-C28-C29	-4.14	115.58	127.20
17	A	833	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
17	A	852	CLA	CMC-C2C-C1C	4.14	131.34	125.04
17	B	818	CLA	C4A-NA-C1A	-4.14	104.85	106.71
17	4	309	CLA	CAC-C3C-C4C	4.14	130.18	124.81
17	B	802	CLA	C3D-C4D-ND	4.14	116.93	110.24
17	K	102	CLA	C3D-C4D-ND	4.14	116.93	110.24
20	M	101	BCR	C8-C9-C10	4.14	125.29	118.94
17	1	308	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
17	2	314	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
17	5	304	CLA	C3D-C4D-ND	4.13	116.92	110.24
17	4	311	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
17	B	812	CLA	O2D-CGD-CBD	4.13	118.61	111.27
17	A	835	CLA	CHD-C1D-ND	-4.13	120.66	124.45
17	B	841	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
17	4	303	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
17	F	203	CLA	C3C-C4C-NC	4.12	115.19	110.57
17	1	309	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
17	4	310	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
17	B	840	CLA	O2D-CGD-CBD	4.12	118.59	111.27
17	2	316	CLA	CAC-C3C-C4C	4.12	130.16	124.81
17	B	822	CLA	C2C-C1C-NC	4.12	113.83	109.97
17	A	833	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
17	A	835	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
17	B	811	CLA	C3C-C4C-NC	4.12	115.19	110.57
20	B	845	BCR	C34-C9-C10	-4.12	117.15	122.92
17	B	810	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
25	5	301	5X6	C11-C03-C02	-4.12	111.49	121.46
25	3	316	5X6	C11-C03-C02	-4.12	111.49	121.46
17	A	853	CLA	C3D-C4D-ND	4.12	116.89	110.24
17	L	203	CLA	CMC-C2C-C1C	4.12	131.31	125.04
17	B	810	CLA	CHD-C1D-ND	-4.11	120.67	124.45
17	5	306	CLA	CAC-C3C-C4C	4.11	130.15	124.81
20	J	104	BCR	C37-C22-C21	-4.11	117.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	801	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
17	5	303	CLA	C1-O2A-CGA	4.11	127.23	116.44
17	A	856	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
17	B	809	CLA	C3D-C4D-ND	4.11	116.89	110.24
25	1	313	5X6	C40-C22-C23	-4.11	111.60	118.08
25	5	318	5X6	C16-C17-C18	-4.11	112.64	118.94
17	4	311	CLA	CAC-C3C-C4C	4.11	130.14	124.81
17	A	806	CLA	CMC-C2C-C1C	4.11	131.29	125.04
17	3	308	CLA	C3B-C2B-C1B	-4.11	102.21	107.16
17	1	311	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
17	3	313	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
17	F	204	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
17	A	802	CLA	C3C-C4C-NC	4.10	115.17	110.57
17	A	822	CLA	CMC-C2C-C1C	4.10	131.28	125.04
25	5	315	5X6	C24-C23-C22	-4.10	114.91	126.42
17	A	854	CLA	CAC-C3C-C4C	4.10	130.13	124.81
17	2	307	CLA	CAC-C3C-C4C	4.10	130.13	124.81
25	1	312	5X6	C27-C28-C29	-4.10	115.70	127.20
20	B	843	BCR	C37-C22-C21	-4.10	117.19	122.92
17	A	821	CLA	C3C-C4C-NC	4.10	115.16	110.57
17	B	826	CLA	C3D-C4D-ND	4.09	116.86	110.24
17	B	809	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
17	5	310	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
17	A	815	CLA	C3D-C4D-ND	4.09	116.85	110.24
17	A	827	CLA	CMC-C2C-C1C	4.09	131.26	125.04
17	A	814	CLA	C3C-C4C-NC	4.09	115.15	110.57
17	1	305	CLA	O2D-CGD-CBD	4.09	118.53	111.27
17	3	308	CLA	C3D-C4D-ND	4.09	116.85	110.24
17	B	802	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
17	5	302	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
20	B	846	BCR	C35-C13-C14	-4.08	117.21	122.92
17	K	103	CLA	C3D-C4D-ND	4.08	116.84	110.24
17	A	815	CLA	CMC-C2C-C1C	4.08	131.25	125.04
17	B	840	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
17	A	804	CLA	C3C-C4C-NC	4.08	115.14	110.57
17	1	304	CLA	C3C-C4C-NC	4.08	115.14	110.57
17	B	811	CLA	C3D-C4D-ND	4.08	116.83	110.24
17	4	310	CLA	O2D-CGD-CBD	4.08	118.51	111.27
25	2	318	5X6	C11-C03-C02	-4.08	111.59	121.46
17	4	309	CLA	C3B-C2B-C1B	-4.07	102.24	107.16
17	J	103	CLA	C3D-C4D-ND	4.07	116.83	110.24
17	A	803	CLA	CMC-C2C-C1C	4.07	131.24	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	312	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
17	B	831	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
25	F	205	5X6	C14-C15-C16	-4.06	110.54	123.22
17	1	301	CLA	C3C-C4C-NC	4.06	115.13	110.57
17	B	832	CLA	C3C-C4C-NC	4.06	115.12	110.57
17	J	103	CLA	C3C-C4C-NC	4.06	115.12	110.57
17	A	804	CLA	CMC-C2C-C1C	4.06	131.22	125.04
17	B	838	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
17	3	308	CLA	CAC-C3C-C4C	4.06	130.07	124.81
17	B	821	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
17	B	820	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
17	B	836	CLA	C3D-C4D-ND	4.06	116.80	110.24
25	4	312	5X6	C15-C16-C17	-4.05	115.03	126.42
17	B	802	CLA	O2A-CGA-CBA	4.05	124.62	111.91
17	2	315	CLA	C4A-NA-C1A	-4.05	104.89	106.71
17	A	852	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
25	1	316	5X6	C20-C19-C18	-4.05	115.18	123.47
17	4	308	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
17	A	839	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
17	A	830	CLA	C3B-C4B-NB	4.05	114.27	110.52
17	B	806	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
17	A	817	CLA	C4A-NA-C1A	-4.05	104.89	106.71
17	1	303	CLA	C4-C3-C5	4.05	122.08	115.27
17	3	308	CLA	CMC-C2C-C1C	4.05	131.20	125.04
17	A	828	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
17	A	818	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
17	1	301	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
17	5	313	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
17	A	815	CLA	C4A-NA-C1A	-4.04	104.89	106.71
17	2	315	CLA	O2D-CGD-CBD	4.04	118.44	111.27
17	B	806	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
17	3	314	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
17	3	312	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
25	4	313	5X6	C12-C13-C14	-4.04	112.75	118.94
17	B	801	CLA	CMD-C2D-C1D	4.04	131.82	124.71
17	A	834	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
25	2	317	5X6	C12-C13-C14	-4.03	112.75	118.94
17	B	837	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
17	L	202	CLA	C3C-C4C-NC	4.03	115.09	110.57
17	A	829	CLA	C3D-C4D-ND	4.03	116.76	110.24
17	5	307	CLA	C4A-NA-C1A	-4.03	104.89	106.71
17	B	823	CLA	C3C-C4C-NC	4.03	115.09	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	857	CLA	CMD-C2D-C1D	4.03	131.82	124.71
25	4	313	5X6	C16-C17-C18	-4.03	112.76	118.94
17	3	312	CLA	CMC-C2C-C1C	4.03	131.18	125.04
17	4	307	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
17	A	807	CLA	CED-O2D-CGD	4.02	125.03	115.94
17	1	302	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
17	A	855	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
17	2	314	CLA	C2C-C1C-NC	4.02	113.74	109.97
17	B	833	CLA	C3D-C4D-ND	4.02	116.74	110.24
17	A	812	CLA	O2D-CGD-CBD	4.02	118.41	111.27
17	2	313	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
25	1	314	5X6	C41-C17-C16	-4.01	111.75	118.08
17	B	801	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
20	A	846	BCR	C34-C9-C10	-4.01	117.30	122.92
17	2	304	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
17	1	303	CLA	C3C-C4C-NC	4.01	115.07	110.57
17	2	306	CLA	C4A-NA-C1A	-4.01	104.90	106.71
17	A	823	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
17	A	832	CLA	C3C-C4C-NC	4.01	115.06	110.57
17	4	303	CLA	C4A-NA-C1A	-4.01	104.91	106.71
17	B	818	CLA	O2A-CGA-CBA	4.01	124.48	111.91
20	I	101	BCR	C37-C22-C21	-4.01	117.31	122.92
17	A	818	CLA	C3C-C4C-NC	4.00	115.06	110.57
17	A	810	CLA	C3B-C4B-NB	4.00	114.23	110.52
25	1	314	5X6	C41-C17-C18	-4.00	117.31	122.92
17	B	829	CLA	O2D-CGD-CBD	4.00	118.38	111.27
17	2	306	CLA	O2D-CGD-CBD	4.00	118.38	111.27
17	5	311	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
17	B	816	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
17	3	307	CLA	CMB-C2B-C1B	4.00	131.46	125.37
17	5	312	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
25	2	317	5X6	C23-C22-C21	-4.00	112.81	118.94
17	B	831	CLA	C3C-C4C-NC	4.00	115.05	110.57
17	B	824	CLA	CMC-C2C-C1C	4.00	131.12	125.04
25	3	316	5X6	C24-C23-C22	-3.99	115.20	126.42
25	5	316	5X6	C39-C26-C25	-3.99	117.33	122.92
17	1	305	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
17	A	810	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
17	L	202	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
17	B	840	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
25	2	318	5X6	C14-C15-C16	-3.98	110.79	123.22
17	B	827	CLA	C3D-C4D-ND	3.98	116.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	313	5X6	C20-C19-C18	-3.98	115.33	123.47
25	3	317	5X6	C42-C13-C12	-3.98	111.81	118.08
25	1	314	5X6	C12-C13-C14	-3.98	112.84	118.94
17	O	203	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
17	K	103	CLA	C4A-NA-C1A	-3.97	104.92	106.71
17	A	836	CLA	C3C-C4C-NC	3.97	115.02	110.57
25	1	316	5X6	C42-C13-C12	-3.97	111.82	118.08
17	B	828	CLA	C3B-C4B-NB	3.97	114.20	110.52
17	B	821	CLA	C3D-C4D-ND	3.97	116.65	110.24
20	A	846	BCR	C37-C22-C21	-3.97	117.37	122.92
17	A	859	CLA	C4A-NA-C1A	-3.96	104.92	106.71
16	A	801	CL0	C3B-C4B-NB	3.96	114.19	110.52
17	A	855	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
25	3	317	5X6	C27-C26-C25	-3.96	112.86	118.94
25	2	320	5X6	C24-C23-C22	-3.96	115.29	126.42
16	A	801	CL0	CMC-C2C-C1C	3.96	131.07	125.04
17	F	203	CLA	C3D-C4D-ND	3.96	116.64	110.24
17	5	304	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
25	2	320	5X6	C12-C11-C03	-3.96	116.09	127.20
17	A	820	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
17	B	802	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
17	B	857	CLA	C3C-C4C-NC	3.96	115.01	110.57
17	1	304	CLA	CAC-C3C-C4C	3.96	129.94	124.81
17	A	852	CLA	CMD-C2D-C1D	3.96	131.69	124.71
17	A	824	CLA	O2D-CGD-CBD	3.96	118.30	111.27
17	5	312	CLA	C3C-C4C-NC	3.95	115.01	110.57
25	1	313	5X6	C39-C26-C27	-3.95	111.85	118.08
20	I	101	BCR	C37-C22-C23	3.95	124.30	118.08
25	1	315	5X6	C28-C29-C30	-3.95	111.89	121.46
25	1	316	5X6	C11-C03-C02	-3.95	111.90	121.46
17	A	852	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
17	3	314	CLA	CAC-C3C-C4C	3.95	129.93	124.81
17	4	308	CLA	CMC-C2C-C1C	3.95	131.05	125.04
17	3	315	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
25	2	317	5X6	C19-C20-C21	-3.94	115.40	123.47
17	A	805	CLA	CMC-C2C-C1C	3.94	131.04	125.04
17	L	202	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
17	3	305	CLA	C2C-C1C-NC	3.94	113.66	109.97
17	B	838	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
17	B	837	CLA	CMC-C2C-C1C	3.94	131.03	125.04
17	B	807	CLA	C4-C3-C5	3.94	121.89	115.27
25	4	314	5X6	C23-C22-C21	-3.93	112.90	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	835	CLA	C3D-C4D-ND	3.93	116.59	110.24
17	B	819	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
17	J	103	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
20	L	205	BCR	C37-C22-C21	-3.93	117.42	122.92
17	B	841	CLA	C3C-C4C-NC	3.93	114.97	110.57
17	A	826	CLA	C4C-C3C-C2C	-3.93	101.18	106.90
25	5	301	5X6	C19-C20-C21	-3.93	115.43	123.47
17	A	826	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
17	2	309	CLA	C4A-NA-C1A	-3.92	104.94	106.71
17	5	303	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
17	A	817	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
20	M	101	BCR	C16-C15-C14	3.92	131.51	123.47
17	4	304	CLA	C2C-C1C-NC	3.92	113.64	109.97
17	A	832	CLA	C3D-C4D-ND	3.92	116.58	110.24
17	B	833	CLA	CMC-C2C-C1C	3.92	131.00	125.04
17	B	832	CLA	O2D-CGD-CBD	3.91	118.22	111.27
17	A	803	CLA	CAC-C3C-C4C	3.91	129.88	124.81
17	4	307	CLA	C4A-NA-C1A	-3.91	104.95	106.71
17	A	807	CLA	C4C-C3C-C2C	-3.91	101.20	106.90
17	A	810	CLA	C3D-C4D-ND	3.91	116.56	110.24
25	3	316	5X6	C19-C20-C21	-3.91	115.47	123.47
17	1	306	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
17	A	831	CLA	C3D-C4D-ND	3.91	116.56	110.24
17	4	309	CLA	CMC-C2C-C1C	3.91	130.99	125.04
17	A	831	CLA	CMB-C2B-C1B	3.90	131.31	125.37
17	L	204	CLA	C3C-C4C-NC	3.90	114.95	110.57
20	M	101	BCR	C37-C22-C21	-3.90	117.45	122.92
17	A	813	CLA	C3C-C4C-NC	3.90	114.95	110.57
17	2	304	CLA	CMB-C2B-C1B	3.90	131.31	125.37
17	A	830	CLA	C3D-C4D-ND	3.90	116.55	110.24
17	F	204	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
17	K	102	CLA	O2D-CGD-CBD	3.90	118.19	111.27
17	4	303	CLA	C3C-C4C-NC	3.90	114.94	110.57
17	5	311	CLA	C3C-C4C-NC	3.89	114.94	110.57
17	B	806	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
17	A	815	CLA	O2D-CGD-CBD	3.88	118.16	111.27
17	B	813	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
17	B	825	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
17	2	313	CLA	C3C-C4C-NC	3.87	114.91	110.57
17	3	307	CLA	CMC-C2C-C1C	3.87	130.93	125.04
17	5	304	CLA	C4A-NA-C1A	-3.87	104.97	106.71
17	A	829	CLA	C3C-C4C-NC	3.87	114.91	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	801	CLA	C3C-C4C-NC	3.87	114.91	110.57
17	F	203	CLA	CMC-C2C-C1C	3.87	130.93	125.04
25	2	319	5X6	C27-C26-C25	-3.87	113.01	118.94
17	B	836	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
17	B	819	CLA	C3B-C4B-NB	3.86	114.10	110.52
17	A	821	CLA	O2D-CGD-CBD	3.86	118.13	111.27
17	B	810	CLA	C3D-C4D-ND	3.86	116.48	110.24
17	B	830	CLA	CAC-C3C-C4C	3.86	129.82	124.81
20	B	803	BCR	C15-C16-C17	3.86	131.38	123.47
20	A	843	BCR	C37-C22-C21	-3.86	117.52	122.92
17	B	832	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
25	5	318	5X6	C27-C26-C25	-3.85	113.03	118.94
20	L	206	BCR	C37-C22-C21	-3.85	117.53	122.92
17	A	829	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
25	2	317	5X6	C11-C03-C02	-3.85	112.14	121.46
20	B	848	BCR	C37-C22-C21	-3.85	117.53	122.92
25	2	319	5X6	C41-C17-C18	-3.85	117.53	122.92
16	A	801	CL0	C3D-C4D-ND	3.85	116.46	110.24
17	K	102	CLA	CAC-C3C-C4C	3.84	129.80	124.81
17	2	314	CLA	C3C-C4C-NC	3.84	114.88	110.57
17	5	306	CLA	C4A-NA-C1A	-3.84	104.98	106.71
17	A	826	CLA	CMC-C2C-C1C	3.84	130.89	125.04
17	5	312	CLA	CMC-C2C-C1C	3.84	130.89	125.04
17	A	804	CLA	CAC-C3C-C4C	3.84	129.79	124.81
17	B	840	CLA	C4-C3-C5	3.84	121.73	115.27
17	A	804	CLA	C3B-C4B-NB	3.84	114.08	110.52
17	A	828	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
20	B	844	BCR	C34-C9-C10	-3.84	117.55	122.92
17	1	303	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
17	K	103	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
17	B	826	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
17	O	205	CLA	C3C-C4C-NC	3.83	114.87	110.57
17	A	811	CLA	C3D-C4D-ND	3.83	116.44	110.24
25	2	319	5X6	C27-C28-C29	-3.83	116.44	127.20
17	3	306	CLA	C4A-NA-C1A	-3.83	104.98	106.71
17	A	815	CLA	CAC-C3C-C4C	3.83	129.78	124.81
17	1	310	CLA	C3C-C4C-NC	3.83	114.86	110.57
17	A	859	CLA	C3B-C2B-C1B	-3.82	102.55	107.16
17	A	825	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
17	A	855	CLA	CMC-C2C-C1C	3.82	130.85	125.04
17	2	314	CLA	CMC-C2C-C1C	3.82	130.85	125.04
17	A	835	CLA	CMC-C2C-C1C	3.81	130.85	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	303	CLA	CMC-C2C-C1C	3.81	130.85	125.04
17	B	805	CLA	C3D-C4D-ND	3.81	116.41	110.24
17	B	813	CLA	C4-C3-C5	3.81	121.69	115.27
17	2	304	CLA	C4A-NA-C1A	-3.81	104.99	106.71
17	A	822	CLA	O2D-CGD-CBD	3.81	118.04	111.27
17	A	856	CLA	CMC-C2C-C1C	3.81	130.84	125.04
20	A	843	BCR	C34-C9-C10	-3.81	117.59	122.92
17	B	816	CLA	C3C-C4C-NC	3.81	114.84	110.57
20	L	201	BCR	C37-C22-C21	-3.81	117.59	122.92
20	L	206	BCR	C34-C9-C10	-3.81	117.59	122.92
17	B	813	CLA	C4A-NA-C1A	-3.81	105.00	106.71
17	2	307	CLA	C3B-C2B-C1B	-3.80	102.57	107.16
17	B	809	CLA	CAC-C3C-C4C	3.80	129.74	124.81
17	A	825	CLA	CAC-C3C-C4C	3.80	129.74	124.81
25	5	317	5X6	C42-C13-C12	-3.79	112.10	118.08
25	2	320	5X6	C14-C15-C16	-3.79	111.38	123.22
25	3	316	5X6	C12-C13-C14	-3.79	113.12	118.94
17	5	312	CLA	CAC-C3C-C4C	3.79	129.73	124.81
25	5	318	5X6	C41-C17-C18	-3.79	117.61	122.92
17	1	308	CLA	CAC-C3C-C4C	3.79	129.73	124.81
17	B	802	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
17	B	819	CLA	CAC-C3C-C4C	3.79	129.72	124.81
17	B	829	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
25	1	313	5X6	C12-C13-C14	-3.79	113.13	118.94
17	B	832	CLA	C3B-C4B-NB	3.79	114.03	110.52
20	O	202	BCR	C37-C22-C21	-3.79	117.62	122.92
17	F	203	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
17	3	306	CLA	C3C-C4C-NC	3.79	114.82	110.57
17	A	854	CLA	O2D-CGD-CBD	3.79	118.00	111.27
17	3	308	CLA	C3C-C4C-NC	3.78	114.81	110.57
17	A	808	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	3	308	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	A	815	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
17	A	816	CLA	C3D-C4D-ND	3.78	116.35	110.24
17	A	817	CLA	CAC-C3C-C4C	3.78	129.71	124.81
17	4	304	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
17	5	309	CLA	CMC-C2C-C1C	3.78	130.79	125.04
20	B	844	BCR	C37-C22-C23	3.78	124.03	118.08
17	5	314	CLA	C3C-C4C-NC	3.77	114.80	110.57
17	4	308	CLA	C3C-C4C-NC	3.77	114.80	110.57
20	A	857	BCR	C37-C22-C23	3.77	124.02	118.08
17	2	315	CLA	CMC-C2C-C1C	3.77	130.78	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	838	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
25	2	320	5X6	C39-C26-C27	-3.77	112.14	118.08
17	A	825	CLA	C3D-C4D-ND	3.76	116.33	110.24
25	2	320	5X6	C27-C28-C29	-3.76	116.64	127.20
16	A	801	CL0	CHD-C1D-ND	-3.76	121.00	124.45
17	2	306	CLA	C3C-C4C-NC	3.76	114.79	110.57
17	K	103	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
17	O	203	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
17	A	808	CLA	O2D-CGD-CBD	3.76	117.95	111.27
17	A	836	CLA	C3B-C4B-NB	3.76	114.00	110.52
25	F	205	5X6	C39-C26-C27	-3.76	112.16	118.08
17	4	310	CLA	C3C-C4C-NC	3.76	114.78	110.57
20	J	104	BCR	C34-C9-C8	3.76	124.00	118.08
20	L	206	BCR	C8-C9-C10	3.75	124.70	118.94
17	A	852	CLA	CAC-C3C-C4C	3.75	129.68	124.81
17	A	827	CLA	C3D-C4D-ND	3.75	116.31	110.24
17	1	302	CLA	C4A-NA-C1A	-3.75	105.02	106.71
17	1	305	CLA	CAC-C3C-C4C	3.75	129.68	124.81
17	3	310	CLA	C3C-C4C-NC	3.75	114.78	110.57
17	O	204	CLA	C3C-C4C-NC	3.75	114.78	110.57
17	A	830	CLA	CAC-C3C-C4C	3.75	129.67	124.81
17	3	309	CLA	C3C-C4C-NC	3.75	114.77	110.57
17	2	309	CLA	C3B-C2B-C1B	-3.74	102.65	107.16
17	A	856	CLA	C3C-C4C-NC	3.74	114.76	110.57
17	J	103	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
17	2	309	CLA	CMC-C2C-C1C	3.74	130.73	125.04
17	3	315	CLA	C3C-C4C-NC	3.74	114.76	110.57
25	5	315	5X6	C15-C16-C17	-3.73	115.93	126.42
17	A	821	CLA	C3B-C2B-C1B	-3.73	102.66	107.16
17	A	836	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
17	1	302	CLA	C3B-C4B-NB	3.73	113.97	110.52
17	B	821	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
25	F	205	5X6	C11-C03-C02	-3.73	112.43	121.46
25	5	301	5X6	C27-C28-C29	-3.73	116.73	127.20
17	B	835	CLA	CMC-C2C-C1C	3.73	130.71	125.04
17	F	203	CLA	CAC-C3C-C4C	3.73	129.65	124.81
17	5	307	CLA	C3C-C4C-NC	3.72	114.75	110.57
17	L	204	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
17	5	302	CLA	C3C-C4C-NC	3.72	114.74	110.57
17	1	304	CLA	C2C-C1C-NC	3.72	113.46	109.97
17	A	825	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
17	5	308	CLA	O2A-CGA-CBA	3.72	123.57	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	313	5X6	C39-C26-C25	-3.72	117.72	122.92
17	B	857	CLA	O1D-CGD-CBD	-3.72	116.88	124.48
17	B	839	CLA	C1D-CHD-C4C	-3.71	118.04	126.06
17	5	313	CLA	C4A-NA-C1A	-3.71	105.04	106.71
25	3	317	5X6	C16-C17-C18	-3.71	113.24	118.94
17	2	308	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
25	5	318	5X6	C28-C29-C30	-3.71	112.47	121.46
17	B	801	CLA	C3D-C4D-ND	3.71	116.24	110.24
17	1	308	CLA	C3C-C4C-NC	3.71	114.73	110.57
17	L	203	CLA	CAC-C3C-C4C	3.71	129.62	124.81
17	B	805	CLA	CMC-C2C-C1C	3.71	130.68	125.04
17	3	310	CLA	CMB-C2B-C1B	3.71	131.01	125.37
25	5	315	5X6	C42-C13-C12	-3.70	112.24	118.08
17	A	839	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
17	A	825	CLA	C3B-C4B-NB	3.70	113.95	110.52
17	2	312	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	3	311	CLA	C2C-C1C-NC	3.70	113.44	109.97
17	1	307	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	1	309	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	B	834	CLA	C3C-C4C-NC	3.70	114.72	110.57
17	B	839	CLA	CMB-C2B-C1B	3.70	131.00	125.37
17	K	102	CLA	C3B-C2B-C1B	-3.69	102.71	107.16
17	A	819	CLA	C3C-C4C-NC	3.69	114.71	110.57
25	F	205	5X6	C42-C13-C12	-3.69	112.27	118.08
17	3	313	CLA	C3C-C4C-NC	3.69	114.71	110.57
17	B	824	CLA	C3C-C4C-NC	3.69	114.70	110.57
17	B	828	CLA	CMC-C2C-C1C	3.68	130.65	125.04
17	5	304	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
17	B	821	CLA	C4A-NA-C1A	-3.68	105.05	106.71
17	B	841	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
17	1	304	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
17	B	835	CLA	C3C-C4C-NC	3.68	114.70	110.57
17	B	825	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
17	O	204	CLA	CMB-C2B-C1B	3.68	130.97	125.37
25	4	313	5X6	C14-C15-C16	-3.68	111.75	123.22
25	3	316	5X6	C16-C17-C18	-3.68	113.30	118.94
17	4	306	CLA	CMC-C2C-C1C	3.67	130.63	125.04
17	A	809	CLA	C1-O2A-CGA	3.67	126.07	116.44
17	B	835	CLA	C3B-C2B-C1B	-3.67	102.73	107.16
17	B	813	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
17	1	310	CLA	CAC-C3C-C4C	3.67	129.57	124.81
25	1	315	5X6	C27-C26-C25	-3.67	113.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	846	BCR	C16-C15-C14	3.67	130.99	123.47
20	B	848	BCR	C34-C9-C10	-3.67	117.79	122.92
17	B	825	CLA	C3D-C4D-ND	3.67	116.17	110.24
17	A	820	CLA	C3B-C4B-NB	3.66	113.91	110.52
17	A	852	CLA	C3D-C4D-ND	3.66	116.16	110.24
17	A	816	CLA	CMB-C2B-C1B	3.66	130.95	125.37
20	B	846	BCR	C34-C9-C10	-3.66	117.79	122.92
17	B	825	CLA	CHD-C1D-ND	-3.66	121.09	124.45
17	A	835	CLA	CAC-C3C-C4C	3.66	129.56	124.81
17	B	823	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
17	2	316	CLA	C3C-C4C-NC	3.66	114.67	110.57
17	B	833	CLA	C3B-C4B-NB	3.66	113.91	110.52
17	B	857	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
17	B	857	CLA	CMB-C2B-C1B	3.65	130.93	125.37
17	3	314	CLA	C3C-C4C-NC	3.65	114.67	110.57
17	A	808	CLA	C3C-C4C-NC	3.65	114.67	110.57
25	5	317	5X6	C27-C28-C29	-3.65	116.96	127.20
17	2	315	CLA	C3C-C4C-NC	3.65	114.66	110.57
17	A	803	CLA	C3B-C2B-C1B	-3.65	102.76	107.16
17	1	305	CLA	C3C-C4C-NC	3.64	114.66	110.57
17	O	204	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
17	5	311	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
17	A	830	CLA	C1-O2A-CGA	3.64	125.99	116.44
25	5	317	5X6	C23-C22-C21	-3.64	113.36	118.94
17	O	205	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
25	2	318	5X6	C24-C23-C22	-3.64	116.20	126.42
17	B	825	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
17	2	306	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
17	A	813	CLA	CAC-C3C-C4C	3.63	129.52	124.81
17	B	834	CLA	CMB-C2B-C1B	3.63	130.90	125.37
17	A	809	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
17	B	812	CLA	C3B-C4B-NB	3.63	113.88	110.52
17	1	306	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
17	B	809	CLA	CMC-C2C-C1C	3.63	130.56	125.04
17	3	313	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
17	4	305	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
17	A	817	CLA	C3C-C4C-NC	3.62	114.64	110.57
17	B	830	CLA	C4A-NA-C1A	-3.62	105.08	106.71
17	L	203	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
20	B	847	BCR	C34-C9-C10	-3.62	117.85	122.92
17	5	313	CLA	C3C-C4C-NC	3.62	114.63	110.57
17	B	805	CLA	C4C-C3C-C2C	-3.62	101.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	309	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
17	A	820	CLA	C4A-NA-C1A	-3.62	105.08	106.71
17	5	308	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
17	4	307	CLA	CMC-C2C-C1C	3.61	130.54	125.04
17	A	805	CLA	C3B-C4B-NB	3.61	113.87	110.52
17	B	819	CLA	C3C-C4C-NC	3.61	114.62	110.57
17	B	827	CLA	C4C-C3C-C2C	-3.61	101.63	106.90
17	2	309	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
25	3	316	5X6	C25-C24-C23	-3.61	111.95	123.22
17	4	310	CLA	CED-O2D-CGD	3.61	124.10	115.94
17	B	830	CLA	O1D-CGD-CBD	-3.61	117.10	124.48
17	A	819	CLA	O2D-CGD-CBD	3.61	117.68	111.27
25	4	313	5X6	C42-C13-C12	-3.61	112.39	118.08
25	4	312	5X6	C25-C24-C23	-3.61	111.96	123.22
17	2	304	CLA	C3B-C2B-C1B	-3.61	102.81	107.16
17	A	859	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
17	A	824	CLA	CMC-C2C-C1C	3.60	130.53	125.04
17	A	816	CLA	C4C-C3C-C2C	-3.60	101.65	106.90
17	4	309	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	1	311	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	B	828	CLA	CAC-C3C-C4C	3.60	129.48	124.81
17	3	310	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
17	5	309	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
17	A	832	CLA	CMB-C2B-C1B	3.60	130.85	125.37
25	1	313	5X6	C42-C13-C12	-3.59	112.41	118.08
17	A	834	CLA	CAC-C3C-C4C	3.59	129.47	124.81
25	2	321	5X6	C24-C23-C22	-3.59	116.32	126.42
17	2	306	CLA	CAC-C3C-C4C	3.59	129.47	124.81
17	B	818	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
25	4	314	5X6	C41-C17-C16	-3.59	112.42	118.08
25	5	317	5X6	C39-C26-C27	-3.59	112.42	118.08
17	B	826	CLA	C4A-NA-C1A	-3.59	105.09	106.71
17	F	204	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	4	310	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
17	3	307	CLA	CAC-C3C-C4C	3.59	129.46	124.81
17	4	305	CLA	C3B-C2B-C1B	-3.59	102.83	107.16
17	2	310	CLA	C3C-C4C-NC	3.59	114.59	110.57
17	B	831	CLA	CAC-C3C-C4C	3.59	129.46	124.81
25	2	318	5X6	C41-C17-C16	-3.59	112.43	118.08
17	A	832	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
17	B	825	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
17	4	307	CLA	C3C-C4C-NC	3.58	114.59	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	833	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
17	4	304	CLA	C3C-C4C-NC	3.58	114.59	110.57
17	4	304	CLA	O2A-CGA-CBA	3.58	123.14	111.91
17	2	309	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
17	5	305	CLA	C2C-C1C-NC	3.58	113.33	109.97
17	A	838	CLA	C4-C3-C2	-3.58	114.50	123.68
17	5	306	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
17	4	305	CLA	C3C-C4C-NC	3.58	114.58	110.57
17	L	202	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
17	5	306	CLA	CMC-C2C-C1C	3.58	130.49	125.04
17	3	308	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
17	3	313	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
17	B	837	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
17	B	822	CLA	C3C-C4C-NC	3.57	114.58	110.57
17	A	839	CLA	CMB-C2B-C1B	3.57	130.81	125.37
17	3	305	CLA	CMB-C2B-C1B	3.57	130.81	125.37
17	B	805	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
25	2	321	5X6	C27-C26-C25	-3.57	113.47	118.94
17	B	820	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
17	2	315	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
17	1	306	CLA	C4A-NA-C1A	-3.57	105.10	106.71
17	B	810	CLA	CAC-C3C-C4C	3.56	129.44	124.81
17	B	811	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
20	A	857	BCR	C16-C15-C14	3.56	130.77	123.47
17	A	813	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
17	1	309	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
20	A	845	BCR	C34-C9-C8	3.56	123.69	118.08
17	1	306	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
25	J	105	5X6	C41-C17-C18	-3.56	117.94	122.92
17	A	833	CLA	CMB-C2B-C1B	3.56	130.79	125.37
17	4	306	CLA	C3C-C4C-NC	3.56	114.56	110.57
25	3	317	5X6	C24-C23-C22	-3.56	116.42	126.42
20	L	201	BCR	C16-C15-C14	3.56	130.76	123.47
17	2	311	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
17	B	808	CLA	C4C-C3C-C2C	-3.56	101.72	106.90
17	B	820	CLA	C3C-C4C-NC	3.56	114.56	110.57
17	A	807	CLA	O2A-CGA-CBA	3.55	123.06	111.91
17	B	835	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
25	2	320	5X6	C15-C16-C17	-3.55	116.43	126.42
17	1	309	CLA	CMC-C2C-C1C	3.55	130.45	125.04
17	5	303	CLA	C4A-NA-C1A	-3.55	105.11	106.71
17	A	827	CLA	C1C-C2C-C3C	-3.55	103.22	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	822	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
17	2	305	CLA	C2C-C1C-NC	3.55	113.30	109.97
17	B	831	CLA	C3B-C4B-NB	3.55	113.81	110.52
17	A	819	CLA	CAC-C3C-C4C	3.55	129.41	124.81
17	A	822	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
17	A	855	CLA	C1-C2-C3	-3.55	119.91	126.04
17	3	314	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	L	203	CLA	C4A-NA-C1A	-3.54	105.11	106.71
17	B	827	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
17	4	308	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
20	M	101	BCR	C34-C9-C10	-3.54	117.96	122.92
25	2	317	5X6	C24-C23-C22	-3.54	116.47	126.42
17	B	812	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
17	B	829	CLA	CMC-C2C-C1C	3.54	130.43	125.04
17	A	821	CLA	CMB-C2B-C1B	3.54	130.76	125.37
17	5	309	CLA	C3C-C4C-NC	3.54	114.54	110.57
17	B	813	CLA	O2D-CGD-CBD	3.54	117.56	111.27
17	5	310	CLA	CMB-C2B-C1B	3.54	130.76	125.37
16	A	801	CL0	CAA-C2A-C3A	-3.54	103.09	112.78
17	2	305	CLA	CMB-C2B-C1B	3.54	130.76	125.37
17	5	307	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
17	2	311	CLA	C2C-C1C-NC	3.54	113.28	109.97
17	1	302	CLA	C3C-C4C-NC	3.54	114.54	110.57
17	O	204	CLA	CAC-C3C-C4C	3.53	129.40	124.81
17	F	203	CLA	C3B-C2B-C1B	-3.53	102.89	107.16
17	2	310	CLA	CMB-C2B-C1B	3.53	130.75	125.37
17	2	311	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	A	838	CLA	C5-C3-C2	3.53	128.26	121.12
17	A	838	CLA	C3B-C2B-C1B	-3.53	102.90	107.16
17	A	823	CLA	CHD-C1D-ND	-3.53	121.21	124.45
20	K	104	BCR	C36-C18-C17	-3.53	117.98	122.92
17	B	812	CLA	CAC-C3C-C4C	3.53	129.39	124.81
17	3	311	CLA	C3C-C4C-NC	3.53	114.53	110.57
17	5	304	CLA	C3C-C4C-NC	3.53	114.53	110.57
25	1	315	5X6	C23-C22-C21	-3.53	113.53	118.94
17	B	830	CLA	C3C-C4C-NC	3.53	114.53	110.57
18	B	842	PQN	C2M-C2-C3	-3.53	118.65	124.40
17	2	307	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
17	3	312	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
17	B	812	CLA	C4C-C3C-C2C	-3.53	101.76	106.90
17	B	804	CLA	C4A-NA-C1A	-3.53	105.12	106.71
17	B	813	CLA	C1D-CHD-C4C	-3.52	118.46	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	306	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
17	5	314	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
17	K	102	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
17	B	818	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
17	3	307	CLA	CED-O2D-CGD	3.52	123.90	115.94
17	A	830	CLA	CMC-C2C-C1C	3.52	130.40	125.04
17	B	828	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
25	5	315	5X6	C39-C26-C27	-3.52	112.53	118.08
17	A	809	CLA	CAC-C3C-C4C	3.52	129.38	124.81
17	B	808	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
17	B	834	CLA	CMC-C2C-C1C	3.52	130.40	125.04
17	A	836	CLA	C2A-C1A-CHA	-3.52	117.71	123.86
17	A	823	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
17	2	308	CLA	C3C-C4C-NC	3.52	114.52	110.57
17	A	811	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
17	3	312	CLA	CMB-C2B-C1B	3.51	130.72	125.37
17	B	822	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
25	2	321	5X6	C25-C24-C23	-3.51	112.25	123.22
25	1	313	5X6	C24-C23-C22	-3.51	116.55	126.42
25	1	315	5X6	C27-C28-C29	-3.51	117.34	127.20
25	5	318	5X6	C25-C24-C23	-3.51	112.26	123.22
17	5	313	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
17	A	856	CLA	C3B-C4B-NB	3.51	113.77	110.52
17	3	311	CLA	CMC-C2C-C1C	3.51	130.38	125.04
17	A	821	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
17	A	824	CLA	C4A-NA-C1A	-3.51	105.13	106.71
17	B	817	CLA	CAC-C3C-C4C	3.51	129.36	124.81
17	A	815	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
17	B	824	CLA	C2C-C1C-NC	3.50	113.25	109.97
17	4	308	CLA	CMB-C2B-C1B	3.50	130.71	125.37
25	4	312	5X6	C12-C11-C03	-3.50	117.36	127.20
17	B	813	CLA	C3D-C4D-ND	3.50	115.90	110.24
17	B	823	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
17	1	307	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
25	4	312	5X6	C14-C15-C16	-3.50	112.29	123.22
17	2	316	CLA	CMB-C2B-C1B	3.50	130.70	125.37
17	A	814	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
17	3	315	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
17	B	804	CLA	C3D-C4D-ND	3.50	115.89	110.24
17	O	203	CLA	C3C-C4C-NC	3.50	114.49	110.57
17	5	302	CLA	CMB-C2B-C1B	3.50	130.69	125.37
17	5	306	CLA	C3C-C4C-NC	3.50	114.49	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	309	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
17	A	826	CLA	CAA-C2A-C3A	-3.49	103.21	112.78
17	A	823	CLA	C3D-C4D-ND	3.49	115.89	110.24
17	4	309	CLA	CMB-C2B-C1B	3.49	130.69	125.37
17	3	309	CLA	CMB-C2B-C1B	3.49	130.69	125.37
20	A	843	BCR	C15-C16-C17	3.49	130.62	123.47
17	B	817	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
20	B	803	BCR	C34-C9-C8	-3.49	112.58	118.08
25	2	321	5X6	C11-C03-C02	-3.49	113.01	121.46
17	4	305	CLA	CAC-C3C-C4C	3.49	129.34	124.81
20	O	202	BCR	C8-C9-C10	3.49	124.29	118.94
17	F	204	CLA	CMB-C2B-C1B	3.49	130.68	125.37
17	2	310	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
25	1	314	5X6	C11-C03-C02	-3.48	113.03	121.46
17	B	838	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
17	A	833	CLA	CMC-C2C-C1C	3.48	130.34	125.04
25	2	319	5X6	C11-C03-C02	-3.48	113.03	121.46
17	A	816	CLA	CMC-C2C-C1C	3.48	130.34	125.04
17	B	820	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
17	A	818	CLA	CMC-C2C-C1C	3.48	130.33	125.04
17	4	307	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
17	B	808	CLA	C2A-C1A-CHA	-3.47	117.78	123.86
17	2	306	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
22	A	848	LMT	O1B-C4'-C3'	3.47	116.52	107.28
17	4	304	CLA	CMC-C2C-C1C	3.47	130.33	125.04
25	1	315	5X6	C39-C26-C27	-3.47	112.60	118.08
17	5	311	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
17	3	312	CLA	C3C-C4C-NC	3.47	114.47	110.57
17	A	832	CLA	CMC-C2C-C1C	3.47	130.32	125.04
17	4	311	CLA	C3C-C4C-NC	3.47	114.46	110.57
17	2	305	CLA	C3C-C4C-NC	3.47	114.46	110.57
17	A	854	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
17	3	315	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
17	2	304	CLA	CMC-C2C-C1C	3.46	130.31	125.04
17	5	309	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
17	5	312	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
17	A	807	CLA	CMC-C2C-C1C	3.46	130.31	125.04
17	A	816	CLA	O2A-CGA-CBA	3.46	122.77	111.91
20	L	205	BCR	C16-C15-C14	3.46	130.56	123.47
17	A	819	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
17	K	103	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
17	3	311	CLA	C1D-CHD-C4C	-3.46	118.60	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	816	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
17	A	822	CLA	CMB-C2B-C1B	3.45	130.63	125.37
17	2	312	CLA	CMB-C2B-C1B	3.45	130.63	125.37
17	B	840	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
25	5	315	5X6	C27-C28-C29	-3.45	117.51	127.20
17	5	304	CLA	CMC-C2C-C1C	3.45	130.29	125.04
17	A	810	CLA	O2D-CGD-CBD	3.45	117.40	111.27
17	A	812	CLA	C1-O2A-CGA	3.45	125.49	116.44
17	B	839	CLA	CMC-C2C-C1C	3.45	130.29	125.04
17	B	815	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
17	5	310	CLA	C3C-C4C-NC	3.45	114.44	110.57
20	L	205	BCR	C34-C9-C10	-3.45	118.09	122.92
17	3	306	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
17	B	834	CLA	CAC-C3C-C4C	3.45	129.28	124.81
17	B	837	CLA	CAC-C3C-C4C	3.45	129.28	124.81
17	B	814	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
17	B	840	CLA	CMC-C2C-C1C	3.45	130.29	125.04
17	3	315	CLA	CMC-C2C-C1C	3.45	130.29	125.04
20	B	847	BCR	C29-C30-C25	3.45	115.78	110.48
25	2	319	5X6	C41-C17-C16	-3.44	112.65	118.08
17	4	304	CLA	C1-O2A-CGA	3.44	125.48	116.44
17	B	815	CLA	C3B-C4B-NB	3.44	113.71	110.52
17	3	307	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	5	314	CLA	CMC-C2C-C1C	3.44	130.28	125.04
17	4	308	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
17	B	808	CLA	CAC-C3C-C4C	3.44	129.28	124.81
17	B	805	CLA	C4A-NA-C1A	-3.44	105.16	106.71
17	3	305	CLA	C3C-C4C-NC	3.44	114.43	110.57
17	B	828	CLA	C3D-C4D-ND	3.44	115.80	110.24
17	B	813	CLA	CAC-C3C-C4C	3.43	129.27	124.81
17	3	310	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
17	B	808	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
25	4	314	5X6	C14-C15-C16	-3.43	112.51	123.22
17	2	310	CLA	CAC-C3C-C4C	3.43	129.26	124.81
25	5	317	5X6	C40-C22-C23	-3.43	112.67	118.08
17	B	807	CLA	C3D-C4D-ND	3.43	115.79	110.24
17	2	309	CLA	CHC-C1C-C2C	-3.43	117.20	126.73
17	5	307	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
17	2	304	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
17	4	310	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
17	A	854	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
17	1	307	CLA	C2C-C1C-NC	3.43	113.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	314	5X6	C01-C02-C07	-3.43	108.01	114.36
20	J	104	BCR	C37-C22-C23	3.43	123.47	118.08
17	A	814	CLA	CMB-C2B-C1B	3.42	130.59	125.37
17	A	811	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
17	2	304	CLA	C3C-C4C-NC	3.42	114.41	110.57
17	B	821	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
17	2	307	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
25	2	317	5X6	C27-C28-C29	-3.42	117.59	127.20
17	A	855	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
17	1	308	CLA	CMB-C2B-C1B	3.42	130.58	125.37
17	2	305	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
17	2	306	CLA	CMC-C2C-C1C	3.42	130.24	125.04
17	A	834	CLA	C3C-C4C-NC	3.42	114.40	110.57
17	B	825	CLA	CBC-CAC-C3C	-3.42	103.01	112.43
17	B	824	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
17	4	304	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
17	A	812	CLA	C1C-C2C-C3C	-3.42	103.37	106.96
17	1	310	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
20	M	101	BCR	C15-C16-C17	3.41	130.47	123.47
17	A	820	CLA	C3C-C4C-NC	3.41	114.40	110.57
20	A	846	BCR	C37-C22-C23	3.41	123.46	118.08
17	5	308	CLA	CAA-C2A-C1A	-3.41	100.79	111.97
17	5	308	CLA	CAC-C3C-C4C	3.41	129.24	124.81
17	B	809	CLA	C4A-NA-C1A	-3.41	105.17	106.71
17	B	802	CLA	O2A-C1-C2	3.41	117.60	108.64
17	2	311	CLA	C1-O2A-CGA	3.41	125.39	116.44
17	2	306	CLA	C3B-C4B-NB	3.41	113.68	110.52
25	5	318	5X6	C01-C02-C07	-3.40	108.05	114.36
25	5	315	5X6	C25-C24-C23	-3.40	112.60	123.22
17	4	311	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
17	3	309	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
20	B	844	BCR	C37-C22-C21	-3.40	118.16	122.92
20	B	846	BCR	C36-C18-C17	-3.40	118.16	122.92
17	B	841	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
17	2	315	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
17	K	102	CLA	CMC-C2C-C1C	3.40	130.21	125.04
17	B	816	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
17	B	830	CLA	CHC-C1C-C2C	-3.40	117.29	126.73
17	1	305	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
17	1	303	CLA	O2D-CGD-CBD	3.40	117.30	111.27
17	L	204	CLA	O2D-CGD-CBD	3.40	117.30	111.27
17	B	839	CLA	O2D-CGD-CBD	3.39	117.30	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	845	BCR	C37-C22-C21	-3.39	118.17	122.92
17	A	814	CLA	C4A-NA-C1A	-3.39	105.18	106.71
17	B	807	CLA	CAC-C3C-C4C	3.39	129.21	124.81
17	O	203	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
25	3	318	5X6	C14-C15-C16	-3.39	112.64	123.22
17	5	314	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
20	B	843	BCR	C15-C16-C17	3.39	130.42	123.47
17	3	307	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
17	B	841	CLA	CMB-C2B-C1B	3.39	130.53	125.37
20	B	803	BCR	C34-C9-C10	-3.38	118.18	122.92
17	2	308	CLA	CHC-C1C-C2C	-3.38	117.33	126.73
17	B	806	CLA	CHB-C4A-NA	3.38	129.19	124.51
17	4	305	CLA	CMC-C2C-C1C	3.38	130.19	125.04
17	2	311	CLA	CMB-C2B-C1B	3.38	130.51	125.37
17	A	827	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
17	3	305	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
25	3	318	5X6	C25-C24-C23	-3.38	112.68	123.22
17	A	802	CLA	C3B-C4B-NB	3.38	113.65	110.52
17	B	812	CLA	C3D-C2D-C1D	-3.38	101.22	105.83
17	3	309	CLA	CAC-C3C-C4C	3.38	129.19	124.81
17	L	204	CLA	CMC-C2C-C1C	3.38	130.18	125.04
17	4	309	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
17	B	827	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
17	1	307	CLA	CAC-C3C-C4C	3.37	129.19	124.81
17	5	310	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
17	A	829	CLA	CED-O2D-CGD	3.37	123.56	115.94
17	A	827	CLA	CAC-C3C-C4C	3.37	129.19	124.81
17	A	826	CLA	C3D-C4D-ND	3.37	115.69	110.24
17	5	303	CLA	O2A-CGA-CBA	3.37	122.48	111.91
17	A	828	CLA	C2A-C1A-CHA	-3.37	117.97	123.86
17	1	303	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
17	O	205	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
17	3	314	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
17	A	824	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
17	A	808	CLA	CMB-C2B-C1B	3.37	130.50	125.37
17	2	314	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
17	2	316	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
17	A	829	CLA	CMC-C2C-C1C	3.37	130.16	125.04
17	1	301	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
17	A	809	CLA	CMB-C2B-C1B	3.36	130.49	125.37
17	B	801	CLA	C3B-C4B-NB	3.36	113.64	110.52
17	5	307	CLA	CMC-C2C-C1C	3.36	130.16	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	847	BCR	C34-C9-C8	3.36	123.37	118.08
17	1	302	CLA	CMC-C2C-C1C	3.36	130.16	125.04
17	4	304	CLA	CMB-C2B-C1B	3.36	130.49	125.37
25	4	314	5X6	C12-C13-C14	-3.36	113.79	118.94
25	3	316	5X6	C15-C16-C17	-3.36	116.98	126.42
17	3	310	CLA	CMC-C2C-C1C	3.36	130.15	125.04
17	A	834	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
17	B	816	CLA	C3B-C4B-NB	3.35	113.63	110.52
17	5	304	CLA	O2A-CGA-CBA	3.35	122.43	111.91
17	B	805	CLA	CBA-CAA-C2A	3.35	123.76	113.86
17	O	204	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
25	3	318	5X6	C23-C22-C21	-3.35	113.80	118.94
17	1	302	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
17	A	804	CLA	C3D-C4D-ND	3.35	115.66	110.24
17	3	309	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
17	1	308	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
17	B	840	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
17	B	830	CLA	CBA-CAA-C2A	3.34	123.74	113.86
17	2	312	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
25	2	321	5X6	C27-C28-C29	-3.34	117.81	127.20
25	F	205	5X6	C01-C02-C07	-3.34	108.16	114.36
25	2	321	5X6	C14-C15-C16	-3.34	112.79	123.22
17	4	305	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
25	1	315	5X6	C12-C13-C14	-3.34	113.82	118.94
17	A	837	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	1	308	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	B	834	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
17	5	303	CLA	C3B-C4B-NB	3.34	113.61	110.52
17	A	813	CLA	C4C-C3C-C2C	-3.34	102.04	106.90
17	A	838	CLA	CMC-C2C-C1C	3.34	130.12	125.04
17	L	204	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
17	3	309	CLA	CMC-C2C-C1C	3.33	130.12	125.04
17	K	102	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
17	2	307	CLA	CMB-C2B-C1B	3.33	130.44	125.37
25	2	319	5X6	C20-C19-C18	-3.33	116.65	123.47
17	B	831	CLA	CHC-C1C-C2C	-3.33	117.48	126.73
17	2	307	CLA	C2A-C1A-CHA	-3.33	118.04	123.86
17	5	303	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
17	A	831	CLA	CAC-C3C-C4C	3.33	129.13	124.81
17	B	827	CLA	C3B-C4B-NB	3.33	113.60	110.52
17	4	303	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
17	A	831	CLA	C1D-CHD-C4C	-3.33	118.88	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	816	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
17	A	859	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
25	2	319	5X6	C25-C24-C23	-3.32	112.85	123.22
17	1	306	CLA	CAC-C3C-C4C	3.32	129.12	124.81
17	A	812	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
17	B	828	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
17	2	316	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
17	B	838	CLA	O2A-CGA-CBA	3.32	122.33	111.91
17	B	836	CLA	CED-O2D-CGD	3.32	123.45	115.94
17	A	813	CLA	C3B-C4B-NB	3.32	113.59	110.52
17	3	305	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
17	B	809	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
20	A	844	BCR	C16-C15-C14	3.32	130.27	123.47
17	A	838	CLA	CAC-C3C-C4C	3.32	129.12	124.81
17	5	304	CLA	C4-C3-C2	-3.32	115.17	123.68
17	B	811	CLA	C3B-C4B-NB	3.32	113.59	110.52
25	3	316	5X6	C40-C22-C23	-3.31	112.85	118.08
17	A	859	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
17	5	313	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
17	A	820	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
17	B	839	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
17	4	311	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
20	B	847	BCR	C16-C15-C14	3.31	130.25	123.47
17	B	819	CLA	C4A-NA-C1A	-3.31	105.22	106.71
17	A	829	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
25	5	316	5X6	C41-C17-C16	-3.31	112.87	118.08
17	L	204	CLA	CMB-C2B-C1B	3.31	130.41	125.37
17	A	855	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
17	5	308	CLA	C3C-C4C-NC	3.30	114.27	110.57
17	J	103	CLA	CMB-C2B-C1B	3.30	130.40	125.37
17	B	811	CLA	CMC-C2C-C1C	3.30	130.06	125.04
20	B	846	BCR	C37-C22-C21	-3.30	118.30	122.92
17	F	203	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
17	1	301	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
20	J	104	BCR	C34-C9-C10	-3.30	118.30	122.92
17	B	814	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
25	3	318	5X6	C41-C17-C16	-3.30	112.88	118.08
17	5	313	CLA	CMC-C2C-C1C	3.30	130.06	125.04
17	B	824	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
17	A	825	CLA	CMC-C2C-C1C	3.29	130.05	125.04
17	B	823	CLA	CAC-C3C-C4C	3.29	129.08	124.81
17	B	839	CLA	C4C-C3C-C2C	-3.29	102.10	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	204	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
25	2	318	5X6	C25-C24-C23	-3.29	112.95	123.22
17	1	306	CLA	C3C-C4C-NC	3.28	114.25	110.57
25	2	317	5X6	C25-C24-C23	-3.28	112.97	123.22
17	B	804	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
17	3	310	CLA	CAC-C3C-C4C	3.28	129.07	124.81
17	2	312	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
17	3	305	CLA	CAC-C3C-C4C	3.28	129.06	124.81
20	A	845	BCR	C34-C9-C10	-3.28	118.33	122.92
25	2	319	5X6	C40-C22-C23	-3.27	112.92	118.08
17	B	857	CLA	CMC-C2C-C1C	3.27	130.02	125.04
17	B	813	CLA	OBD-CAD-C3D	-3.27	120.65	128.52
17	5	305	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
17	4	303	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
17	2	313	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
17	A	807	CLA	C1-C2-C3	-3.27	120.39	126.04
17	2	307	CLA	C3C-C4C-NC	3.27	114.23	110.57
17	A	853	CLA	C3B-C4B-NB	3.27	113.54	110.52
17	A	808	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
17	B	838	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
17	B	809	CLA	C3B-C4B-NB	3.26	113.54	110.52
17	B	810	CLA	C3B-C4B-NB	3.26	113.54	110.52
17	A	807	CLA	O2D-CGD-CBD	3.26	117.06	111.27
25	2	317	5X6	C15-C16-C17	-3.26	117.26	126.42
17	2	309	CLA	C3B-C4B-NB	3.26	113.54	110.52
17	A	809	CLA	O1D-CGD-CBD	-3.26	117.82	124.48
17	L	202	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
20	M	101	BCR	C36-C18-C17	-3.26	118.36	122.92
17	1	301	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
17	B	825	CLA	C3B-C4B-NB	3.26	113.54	110.52
17	A	812	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
17	3	309	CLA	CED-O2D-CGD	3.25	123.30	115.94
17	A	836	CLA	C1-O2A-CGA	3.25	124.98	116.44
17	4	304	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
17	2	310	CLA	CMC-C2C-C1C	3.25	129.99	125.04
17	1	311	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
17	2	313	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
17	A	807	CLA	O2A-CGA-O1A	-3.25	115.39	123.59
25	1	314	5X6	C25-C24-C23	-3.25	113.09	123.22
25	J	105	5X6	C15-C16-C17	-3.24	117.30	126.42
25	4	312	5X6	C11-C03-C02	-3.24	113.60	121.46
17	A	823	CLA	C4C-C3C-C2C	-3.24	102.17	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	206	BCR	C15-C16-C17	3.24	130.12	123.47
17	B	829	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
25	5	315	5X6	C14-C15-C16	-3.24	113.10	123.22
17	A	819	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
17	1	309	CLA	CAC-C3C-C4C	3.24	129.01	124.81
17	A	809	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
17	3	307	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
17	A	837	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
17	3	315	CLA	CAC-C3C-C4C	3.23	129.01	124.81
17	B	823	CLA	C3B-C4B-NB	3.23	113.51	110.52
17	A	806	CLA	CAC-C3C-C4C	3.23	129.00	124.81
17	B	802	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
17	B	810	CLA	C3B-C2B-C1B	-3.23	103.26	107.16
17	B	810	CLA	CMC-C2C-C1C	3.23	129.96	125.04
17	A	827	CLA	O2D-CGD-CBD	3.23	117.01	111.27
17	A	833	CLA	C3C-C4C-NC	3.23	114.19	110.57
17	4	307	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
17	K	103	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
17	2	310	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
17	A	830	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
17	B	822	CLA	CAC-C3C-C4C	3.22	128.99	124.81
17	B	825	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
17	A	856	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
17	3	312	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
17	A	821	CLA	C1C-C2C-C3C	-3.22	103.58	106.96
17	A	835	CLA	C1-O2A-CGA	3.22	124.88	116.44
17	B	836	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
17	4	306	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
25	2	319	5X6	C42-C13-C12	-3.21	113.02	118.08
17	5	305	CLA	C3C-C4C-NC	3.21	114.17	110.57
17	5	307	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
17	5	308	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
17	A	803	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
17	B	826	CLA	O1D-CGD-CBD	-3.21	117.92	124.48
17	3	311	CLA	CMB-C2B-C1B	3.21	130.26	125.37
17	B	815	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
25	5	317	5X6	C14-C15-C16	-3.21	113.20	123.22
17	B	804	CLA	CHC-C1C-C2C	-3.21	117.82	126.73
25	1	312	5X6	C28-C29-C30	-3.21	113.69	121.46
17	A	836	CLA	CMC-C2C-C1C	3.21	129.92	125.04
17	A	827	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
20	O	202	BCR	C37-C22-C23	3.21	123.13	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	203	CLA	C3B-C4B-NB	3.21	113.49	110.52
25	2	317	5X6	C14-C15-C16	-3.21	113.21	123.22
17	B	818	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
22	A	848	LMT	C1B-O5B-C5B	3.20	119.97	113.69
25	4	314	5X6	C25-C24-C23	-3.20	113.23	123.22
17	B	817	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
17	5	313	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
17	B	824	CLA	O2D-CGD-CBD	3.20	116.95	111.27
17	A	856	CLA	CAC-C3C-C4C	3.20	128.96	124.81
17	A	828	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
17	F	204	CLA	C3C-C4C-NC	3.19	114.15	110.57
17	B	815	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
25	2	320	5X6	C27-C26-C25	-3.19	114.04	118.94
17	A	814	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
17	2	312	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
17	2	308	CLA	C3B-C4B-NB	3.19	113.47	110.52
17	A	805	CLA	C2A-C1A-CHA	-3.19	118.28	123.86
17	1	310	CLA	CMB-C2B-C1B	3.19	130.23	125.37
20	A	845	BCR	C2-C3-C4	3.19	118.50	111.38
17	B	824	CLA	O2A-CGA-CBA	3.19	121.92	111.91
25	2	318	5X6	C23-C22-C21	-3.19	114.05	118.94
17	B	802	CLA	CAC-C3C-C4C	3.19	128.95	124.81
17	B	831	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
17	B	805	CLA	C4-C3-C5	3.19	120.63	115.27
25	2	317	5X6	C41-C17-C16	-3.19	113.05	118.08
25	3	318	5X6	C27-C26-C25	-3.19	114.05	118.94
25	3	316	5X6	C14-C15-C16	-3.19	113.27	123.22
25	2	319	5X6	C12-C11-C03	-3.19	118.25	127.20
25	2	320	5X6	C11-C03-C02	-3.19	113.75	121.46
17	5	303	CLA	C3C-C4C-NC	3.18	114.14	110.57
17	A	814	CLA	C3B-C2B-C1B	-3.18	103.32	107.16
17	A	837	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
17	1	310	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
17	B	830	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
17	3	315	CLA	CMB-C2B-C1B	3.18	130.21	125.37
17	B	802	CLA	C7-C6-C5	-3.18	104.74	113.36
17	5	310	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
25	3	317	5X6	C25-C24-C23	-3.17	113.31	123.22
17	B	809	CLA	C3B-C2B-C1B	-3.17	103.33	107.16
17	1	311	CLA	C1D-CHD-C4C	-3.17	119.21	126.06
25	1	315	5X6	C25-C24-C23	-3.17	113.33	123.22
17	J	103	CLA	C4A-NA-C1A	-3.17	105.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	302	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
17	B	824	CLA	CED-O2D-CGD	3.17	123.11	115.94
17	B	804	CLA	CAC-C3C-C4C	3.17	128.92	124.81
17	B	801	CLA	CAC-C3C-C4C	3.17	128.92	124.81
17	B	857	CLA	C1D-CHD-C4C	-3.16	119.23	126.06
17	B	857	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
17	A	832	CLA	CHC-C1C-C2C	-3.16	117.94	126.73
25	1	316	5X6	C14-C15-C16	-3.16	113.35	123.22
17	B	828	CLA	OBD-CAD-C3D	-3.16	120.91	128.52
25	2	320	5X6	C41-C17-C16	-3.16	113.10	118.08
17	3	306	CLA	CAC-C3C-C4C	3.16	128.91	124.81
17	A	859	CLA	CMB-C2B-C1B	3.16	130.18	125.37
17	5	302	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
17	5	308	CLA	CMC-C2C-C1C	3.15	129.84	125.04
20	B	843	BCR	C16-C15-C14	3.15	129.93	123.47
17	B	837	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
25	4	312	5X6	C40-C22-C23	-3.15	113.11	118.08
17	B	817	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
17	A	852	CLA	CHB-C4A-NA	3.15	128.87	124.51
17	2	314	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
17	B	807	CLA	CHB-C4A-NA	3.15	128.86	124.51
17	4	303	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
17	A	819	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
17	2	307	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
17	B	828	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
17	5	314	CLA	CMB-C2B-C1B	3.15	130.16	125.37
25	5	318	5X6	C40-C22-C23	-3.14	113.12	118.08
17	4	310	CLA	CMC-C2C-C1C	3.14	129.83	125.04
25	1	312	5X6	C15-C16-C17	-3.14	117.58	126.42
17	5	302	CLA	CMC-C2C-C1C	3.14	129.82	125.04
17	A	836	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
17	5	305	CLA	CBA-CAA-C2A	3.14	123.13	113.86
16	A	801	CL0	C1D-CHD-C4C	-3.14	119.29	126.06
17	A	854	CLA	CED-O2D-CGD	3.14	123.03	115.94
25	1	315	5X6	C42-C13-C12	-3.14	113.13	118.08
20	L	206	BCR	C36-C18-C17	-3.14	118.53	122.92
17	A	839	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
25	4	313	5X6	C15-C16-C17	-3.14	117.61	126.42
25	2	318	5X6	C42-C13-C12	-3.14	113.14	118.08
17	B	804	CLA	CAA-C2A-C3A	-3.14	104.19	112.78
17	B	820	CLA	CAC-C3C-C4C	3.13	128.88	124.81
17	A	838	CLA	C4C-C3C-C2C	-3.13	102.33	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	304	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
17	B	806	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
17	A	829	CLA	CAC-C3C-C4C	3.13	128.87	124.81
17	A	824	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
17	B	816	CLA	CAC-C3C-C4C	3.13	128.87	124.81
17	A	839	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
17	A	820	CLA	O2A-CGA-CBA	3.13	121.72	111.91
20	B	845	BCR	C15-C16-C17	3.13	129.88	123.47
17	1	302	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
17	A	814	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
17	1	304	CLA	CMB-C2B-C1B	3.13	130.13	125.37
17	1	311	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
17	2	312	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
17	2	311	CLA	CED-O2D-CGD	3.13	123.01	115.94
17	B	820	CLA	CMC-C2C-C1C	3.12	129.80	125.04
25	5	301	5X6	C14-C15-C16	-3.12	113.48	123.22
17	A	823	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
17	5	306	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
17	2	311	CLA	CHD-C4C-NC	3.12	129.12	124.20
17	A	809	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
17	B	814	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
17	B	838	CLA	CMC-C2C-C1C	3.12	129.79	125.04
17	B	819	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
25	1	315	5X6	C14-C15-C16	-3.12	113.49	123.22
17	B	809	CLA	CHC-C1C-C2C	-3.12	118.08	126.73
17	B	812	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
17	B	824	CLA	CHD-C4C-NC	3.11	129.11	124.20
17	A	824	CLA	C3B-C4B-NB	3.11	113.40	110.52
20	B	847	BCR	C37-C22-C21	-3.11	118.56	122.92
17	B	813	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
17	4	303	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
17	B	819	CLA	CMC-C2C-C1C	3.11	129.78	125.04
25	5	317	5X6	C41-C17-C16	-3.11	113.18	118.08
17	B	822	CLA	CMB-C2B-C1B	3.11	130.10	125.37
17	A	818	CLA	C4A-NA-C1A	-3.11	105.31	106.71
17	B	857	CLA	CAC-C3C-C4C	3.11	128.84	124.81
17	1	310	CLA	CMC-C2C-C1C	3.11	129.77	125.04
17	B	832	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
17	4	308	CLA	CAC-C3C-C4C	3.11	128.84	124.81
25	1	312	5X6	C39-C26-C27	-3.11	113.18	118.08
17	A	835	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
20	A	857	BCR	C36-C18-C17	-3.10	118.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	301	5X6	C23-C22-C21	-3.10	114.18	118.94
17	B	807	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	3	308	CLA	CMB-C2B-C1B	3.10	130.09	125.37
17	B	810	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
17	A	828	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	B	821	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	2	308	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
25	4	314	5X6	C42-C13-C12	-3.10	113.19	118.08
17	A	830	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
17	O	203	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	B	837	CLA	C1-O2A-CGA	3.10	124.58	116.44
17	2	315	CLA	CAC-C3C-C4C	3.10	128.83	124.81
17	5	302	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
17	A	810	CLA	C1D-CHD-C4C	-3.10	119.37	126.06
25	3	317	5X6	C40-C22-C23	-3.10	113.19	118.08
17	B	807	CLA	CED-O2D-CGD	3.10	122.94	115.94
20	A	857	BCR	C34-C9-C10	-3.10	118.58	122.92
17	3	306	CLA	CHC-C1C-C2C	-3.10	118.13	126.73
17	A	828	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
17	A	836	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
17	1	311	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
17	K	102	CLA	C1C-C2C-C3C	-3.09	103.70	106.96
17	B	818	CLA	CHB-C4A-NA	3.09	128.79	124.51
17	2	313	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
25	1	316	5X6	C12-C13-C14	-3.09	114.20	118.94
17	A	831	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
17	B	804	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
25	4	314	5X6	C33-C32-C31	3.09	114.53	110.30
17	F	204	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
16	A	801	CL0	CMA-C3A-C2A	-3.09	101.37	113.83
17	A	827	CLA	C3B-C4B-NB	3.09	113.38	110.52
17	A	834	CLA	CED-O2D-CGD	3.09	122.92	115.94
17	A	833	CLA	O2D-CGD-CBD	3.09	116.75	111.27
17	5	305	CLA	C1C-C2C-C3C	-3.08	103.71	106.96
17	A	810	CLA	OBD-CAD-C3D	-3.08	121.10	128.52
17	A	803	CLA	CAA-C2A-C1A	-3.08	101.87	111.97
17	A	852	CLA	C11-C10-C8	-3.08	105.95	115.92
17	B	808	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
17	B	831	CLA	C4-C3-C5	3.08	120.45	115.27
17	1	305	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
17	A	852	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
17	1	308	CLA	C4C-C3C-C2C	-3.08	102.41	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	312	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
20	B	803	BCR	C37-C22-C23	3.08	122.93	118.08
17	A	817	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
17	A	813	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
17	3	311	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
17	2	305	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
17	A	836	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
17	B	835	CLA	CMB-C2B-C1B	3.08	130.06	125.37
17	1	305	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
17	1	306	CLA	O2D-CGD-CBD	3.08	116.74	111.27
25	1	315	5X6	C15-C16-C17	-3.08	117.77	126.42
17	B	820	CLA	O2D-CGD-CBD	3.08	116.74	111.27
17	K	103	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
17	B	812	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
17	F	203	CLA	O2D-CGD-CBD	3.07	116.73	111.27
17	A	834	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
20	B	843	BCR	C36-C18-C17	-3.07	118.62	122.92
20	K	104	BCR	C34-C9-C10	-3.07	118.62	122.92
17	A	831	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
17	B	839	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
17	A	837	CLA	CMB-C2B-C1B	3.07	130.05	125.37
20	L	205	BCR	C34-C9-C8	3.07	122.91	118.08
17	A	818	CLA	CED-O2D-CGD	3.07	122.88	115.94
17	B	837	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
25	2	317	5X6	C42-C13-C12	-3.07	113.24	118.08
25	5	315	5X6	C28-C29-C30	-3.07	114.03	121.46
17	A	802	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
17	A	832	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
17	2	311	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
17	5	308	CLA	CBA-CAA-C2A	3.06	122.90	113.86
25	3	318	5X6	C42-C13-C12	-3.06	113.25	118.08
17	1	301	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
17	B	839	CLA	CED-O2D-CGD	3.06	122.86	115.94
17	1	308	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
17	B	808	CLA	CMC-C2C-C1C	3.06	129.70	125.04
17	B	831	CLA	C1-O2A-CGA	3.06	124.47	116.44
17	A	815	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
17	B	832	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
17	2	304	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
17	3	315	CLA	C4-C3-C5	3.06	119.48	115.98
17	B	802	CLA	C1-O2A-CGA	3.06	124.46	116.44
17	B	819	CLA	CHC-C1C-C2C	-3.06	118.24	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	304	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
17	5	314	CLA	CAC-C3C-C4C	3.05	128.77	124.81
17	5	306	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
17	A	806	CLA	C1-C2-C3	-3.05	120.76	126.04
25	3	316	5X6	C28-C29-C30	-3.05	114.07	121.46
17	A	839	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
17	A	810	CLA	CAC-C3C-C4C	3.05	128.77	124.81
17	1	307	CLA	CHD-C4C-NC	3.05	129.01	124.20
17	B	815	CLA	CED-O2D-CGD	3.05	122.84	115.94
17	A	824	CLA	CAC-C3C-C4C	3.05	128.77	124.81
17	O	203	CLA	CAC-C3C-C4C	3.05	128.77	124.81
17	B	857	CLA	O2A-CGA-CBA	3.05	121.48	111.91
17	A	825	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
17	5	311	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
17	A	822	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
17	B	857	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
17	5	309	CLA	O1D-CGD-CBD	-3.05	118.25	124.48
17	A	822	CLA	CED-O2D-CGD	3.05	122.83	115.94
17	5	302	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
17	4	306	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
17	A	838	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
17	A	856	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
17	B	838	CLA	CAC-C3C-C4C	3.04	128.76	124.81
17	5	304	CLA	C5-C3-C2	3.04	127.28	121.12
17	A	808	CLA	CAC-C3C-C4C	3.04	128.76	124.81
17	O	203	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
17	B	831	CLA	C4A-NA-C1A	-3.04	105.34	106.71
17	5	304	CLA	CMB-C2B-C1B	3.04	130.00	125.37
17	A	808	CLA	C4-C3-C5	3.04	120.38	115.27
17	5	308	CLA	CHB-C4A-NA	3.04	128.72	124.51
17	2	315	CLA	CMB-C2B-C1B	3.04	130.00	125.37
17	B	816	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
17	B	837	CLA	C4-C3-C2	-3.04	115.89	123.68
17	L	204	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
17	3	308	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
17	B	801	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
17	B	830	CLA	CMC-C2C-C1C	3.03	129.66	125.04
17	B	833	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	A	855	CLA	C4A-NA-C1A	-3.03	105.34	106.71
17	B	831	CLA	CBA-CAA-C2A	3.03	122.80	113.86
17	B	829	CLA	CAC-C3C-C4C	3.03	128.74	124.81
17	B	812	CLA	C4-C3-C2	-3.03	115.92	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	311	CLA	CHD-C4C-NC	3.03	128.97	124.20
17	B	807	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
17	B	822	CLA	CHD-C4C-NC	3.02	128.97	124.20
17	A	815	CLA	C4-C3-C5	3.02	120.36	115.27
25	3	317	5X6	C41-C17-C16	-3.02	113.31	118.08
17	A	824	CLA	CHB-C4A-NA	3.02	128.69	124.51
17	A	830	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
17	B	825	CLA	C4A-NA-C1A	-3.02	105.35	106.71
25	5	317	5X6	C28-C29-C30	-3.02	114.14	121.46
25	1	312	5X6	C14-C15-C16	-3.02	113.79	123.22
17	B	826	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
17	B	805	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
25	5	301	5X6	C41-C17-C16	-3.02	113.32	118.08
17	B	819	CLA	CED-O2D-CGD	3.02	122.77	115.94
17	A	834	CLA	C1-O2A-CGA	3.02	124.36	116.44
17	4	306	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
20	A	846	BCR	C36-C18-C17	-3.02	118.69	122.92
17	3	313	CLA	CAC-C3C-C4C	3.02	128.73	124.81
17	5	311	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
17	A	838	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
17	O	205	CLA	CAC-C3C-C4C	3.02	128.72	124.81
17	A	812	CLA	C4A-NA-C1A	-3.02	105.35	106.71
17	3	311	CLA	C2A-C1A-CHA	-3.02	118.59	123.86
17	B	810	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
17	A	817	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
17	5	305	CLA	O2A-C1-C2	3.01	116.55	108.64
17	1	303	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
17	F	204	CLA	C3B-C4B-NB	3.01	113.31	110.52
17	A	818	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
17	A	810	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
17	A	815	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
17	4	310	CLA	CAC-C3C-C4C	3.01	128.71	124.81
17	3	313	CLA	CMC-C2C-C1C	3.01	129.62	125.04
17	O	205	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
17	B	816	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
17	B	831	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
17	B	834	CLA	C1D-CHD-C4C	-3.01	119.58	126.06
17	B	836	CLA	C1D-CHD-C4C	-3.01	119.58	126.06
17	K	103	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
17	2	313	CLA	CMC-C2C-C1C	3.00	129.62	125.04
17	B	811	CLA	CHB-C4A-NA	3.00	128.67	124.51
17	4	303	CLA	CMB-C2B-C1B	3.00	129.94	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	832	CLA	C1-O2A-CGA	3.00	124.32	116.44
17	B	834	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
17	A	806	CLA	O1D-CGD-CBD	-3.00	118.34	124.48
25	4	312	5X6	C41-C17-C16	-3.00	113.35	118.08
17	5	309	CLA	C3B-C4B-NB	3.00	113.30	110.52
17	1	309	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
17	3	305	CLA	CHD-C4C-NC	3.00	128.93	124.20
17	A	853	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
16	A	801	CL0	O2D-CGD-O1D	-3.00	117.98	123.84
17	3	306	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
17	2	305	CLA	C1C-C2C-C3C	-3.00	103.81	106.96
17	2	305	CLA	CAC-C3C-C4C	3.00	128.70	124.81
17	B	821	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
17	A	819	CLA	C2A-C1A-CHA	-2.99	118.62	123.86
17	O	205	CLA	CMB-C2B-C1B	2.99	129.93	125.37
17	B	809	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
17	1	306	CLA	CMC-C2C-C1C	2.99	129.59	125.04
25	5	301	5X6	C25-C24-C23	-2.99	113.88	123.22
17	B	819	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
17	B	802	CLA	CMB-C2B-C1B	2.99	129.92	125.37
17	1	305	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
17	A	802	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
17	B	802	CLA	CMC-C2C-C1C	2.99	129.59	125.04
17	2	312	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
20	B	846	BCR	C10-C11-C12	2.99	132.53	123.22
17	A	814	CLA	C3B-C4B-NB	2.99	113.28	110.52
17	2	306	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
17	A	839	CLA	C1D-CHD-C4C	-2.99	119.62	126.06
17	K	102	CLA	O2A-CGA-CBA	2.98	121.27	111.91
17	A	805	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	F	203	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
17	5	313	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	A	804	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
17	A	821	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
17	4	305	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
17	B	809	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
17	5	305	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
17	B	826	CLA	CAC-C3C-C4C	2.98	128.67	124.81
17	A	805	CLA	C1-C2-C3	-2.98	121.94	126.75
17	1	310	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
17	2	305	CLA	CHD-C4C-NC	2.98	128.89	124.20
17	A	835	CLA	C1D-CHD-C4C	-2.97	119.64	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	313	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
17	A	833	CLA	C1-O2A-CGA	2.97	124.25	116.44
17	5	313	CLA	C3B-C4B-NB	2.97	113.27	110.52
17	B	806	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
17	B	840	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
17	B	819	CLA	O2A-CGA-CBA	2.97	121.23	111.91
17	B	832	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
18	A	840	PQN	C2M-C2-C1	2.97	121.19	116.27
17	B	814	CLA	C4A-NA-C1A	-2.96	105.37	106.71
17	B	829	CLA	C3B-C4B-NB	2.96	113.27	110.52
17	A	808	CLA	CMC-C2C-C1C	2.96	129.55	125.04
17	A	836	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
25	1	316	5X6	C01-C02-C07	-2.96	108.87	114.36
17	A	805	CLA	CED-O2D-CGD	2.96	122.63	115.94
17	A	805	CLA	O2A-CGA-CBA	2.96	121.20	111.91
17	B	835	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
17	B	801	CLA	O2A-CGA-CBA	2.96	121.19	111.91
17	5	312	CLA	CMB-C2B-C1B	2.96	129.88	125.37
17	2	307	CLA	CBA-CAA-C2A	2.96	122.60	113.86
18	B	842	PQN	C16-C15-C13	-2.96	105.70	113.45
17	J	103	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
17	B	823	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
17	B	821	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
25	1	313	5X6	C04-C03-C02	-2.96	118.45	122.61
17	B	837	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
17	B	809	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
25	1	312	5X6	C23-C22-C21	-2.95	114.41	118.94
17	B	831	CLA	CMC-C2C-C1C	2.95	129.54	125.04
17	B	801	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
17	A	802	CLA	CMB-C2B-C1B	2.95	129.87	125.37
20	J	104	BCR	C15-C16-C17	2.95	129.52	123.47
17	B	841	CLA	CAC-C3C-C4C	2.95	128.64	124.81
17	5	309	CLA	O2A-CGA-CBA	2.95	121.17	111.91
17	1	306	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
25	1	312	5X6	C41-C17-C16	-2.95	113.43	118.08
17	B	826	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	3	315	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
17	A	806	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
17	B	801	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
17	4	310	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
17	4	304	CLA	CHD-C4C-NC	2.94	128.84	124.20
17	A	802	CLA	CMC-C2C-C1C	2.94	129.52	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	307	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
20	M	101	BCR	C12-C13-C14	2.94	123.46	118.94
17	A	817	CLA	C3B-C4B-NB	2.94	113.24	110.52
18	A	840	PQN	C2M-C2-C3	-2.94	119.60	124.40
17	B	813	CLA	O2A-CGA-CBA	2.94	121.14	111.91
17	A	810	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
17	A	838	CLA	C1-O2A-CGA	2.94	124.15	116.44
17	A	820	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
17	A	810	CLA	O2A-CGA-CBA	2.94	121.12	111.91
25	5	317	5X6	C12-C13-C14	-2.94	114.44	118.94
17	A	820	CLA	CED-O2D-CGD	2.93	122.58	115.94
17	3	311	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
17	B	816	CLA	CMB-C2B-C1B	2.93	129.84	125.37
17	A	856	CLA	O1D-CGD-CBD	-2.93	118.48	124.48
17	2	311	CLA	O1D-CGD-CBD	-2.93	118.48	124.48
17	A	802	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	A	813	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
17	B	835	CLA	CAC-C3C-C4C	2.93	128.61	124.81
17	2	312	CLA	CMC-C2C-C1C	2.93	129.50	125.04
17	5	309	CLA	CHD-C4C-NC	2.93	128.82	124.20
17	B	814	CLA	C3B-C4B-NB	2.93	113.23	110.52
17	J	103	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
17	O	205	CLA	CMC-C2C-C1C	2.93	129.50	125.04
17	A	852	CLA	C3B-C4B-NB	2.92	113.23	110.52
17	5	308	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
17	1	306	CLA	CMB-C2B-C1B	2.92	129.82	125.37
17	1	306	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
20	O	202	BCR	C34-C9-C10	-2.92	118.83	122.92
17	L	204	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
20	K	104	BCR	C12-C13-C14	2.92	123.42	118.94
17	2	308	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
20	B	843	BCR	C34-C9-C10	-2.92	118.84	122.92
17	F	203	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
17	B	814	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
17	A	804	CLA	C1D-CHD-C4C	-2.92	119.77	126.06
17	B	820	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
17	B	817	CLA	C4-C3-C5	2.91	120.17	115.27
20	O	202	BCR	C16-C15-C14	2.91	129.44	123.47
17	B	818	CLA	CMB-C2B-C1B	2.91	129.81	125.37
17	A	834	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
17	2	309	CLA	CMB-C2B-C1B	2.91	129.81	125.37
17	2	313	CLA	CHC-C1C-C2C	-2.91	118.64	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	F	205	5X6	C34-C33-C32	-2.91	107.07	113.64
17	B	841	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
17	B	823	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
17	B	838	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
17	A	826	CLA	O2A-CGA-CBA	2.91	121.03	111.91
17	5	312	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
17	3	312	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
17	L	202	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
17	A	833	CLA	C1D-CHD-C4C	-2.90	119.79	126.06
17	A	808	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
17	A	802	CLA	C4A-NA-C1A	-2.90	105.40	106.71
17	A	808	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
17	B	818	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
17	B	807	CLA	C1D-CHD-C4C	-2.90	119.80	126.06
17	B	834	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
25	2	320	5X6	C25-C24-C23	-2.90	114.17	123.22
17	B	840	CLA	C3B-C4B-NB	2.90	113.20	110.52
17	A	805	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
17	1	307	CLA	CED-O2D-CGD	2.90	122.49	115.94
17	A	806	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
17	L	202	CLA	C3B-C4B-NB	2.89	113.20	110.52
17	L	202	CLA	C4A-NA-C1A	-2.89	105.41	106.71
25	3	316	5X6	C42-C13-C12	-2.89	113.52	118.08
17	4	307	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
17	B	811	CLA	CAC-C3C-C4C	2.89	128.56	124.81
17	3	310	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	K	103	CLA	CMB-C2B-C1B	2.89	129.77	125.37
17	4	303	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
17	A	813	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
17	1	307	CLA	CMB-C2B-C1B	2.89	129.77	125.37
17	A	817	CLA	CBC-CAC-C3C	-2.89	104.46	112.43
17	A	803	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
17	B	810	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
17	L	203	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
17	A	833	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
17	A	832	CLA	C1D-CHD-C4C	-2.89	119.82	126.06
17	4	309	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
17	5	304	CLA	CAC-C3C-C4C	2.89	128.55	124.81
17	B	809	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
17	3	309	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
17	F	204	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
17	A	835	CLA	C2A-C1A-CHA	-2.88	118.82	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	828	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
17	A	809	CLA	C3B-C4B-NB	2.88	113.19	110.52
17	B	807	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	5	306	CLA	CMB-C2B-C1B	2.88	129.76	125.37
17	B	829	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
25	2	321	5X6	C33-C32-C31	2.88	114.25	110.30
17	B	818	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
17	5	310	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
17	A	853	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
17	1	304	CLA	C2A-C1A-CHA	-2.88	118.83	123.86
17	B	806	CLA	C1-O2A-CGA	2.88	124.00	116.44
17	5	311	CLA	CAC-C3C-C4C	2.88	128.54	124.81
25	5	318	5X6	C14-C15-C16	-2.88	114.24	123.22
17	B	830	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
20	K	104	BCR	C19-C18-C17	2.88	123.36	118.94
17	A	817	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
17	A	807	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
17	A	814	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
17	3	306	CLA	CMC-C2C-C1C	2.88	129.42	125.04
17	B	833	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
17	A	837	CLA	O2A-CGA-CBA	2.88	120.93	111.91
17	J	103	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
16	A	801	CL0	CAC-C3C-C4C	2.87	128.54	124.81
17	A	803	CLA	CHB-C4A-NA	2.87	128.49	124.51
17	A	855	CLA	CAC-C3C-C4C	2.87	128.54	124.81
17	4	310	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
17	B	836	CLA	C3B-C4B-NB	2.87	113.18	110.52
17	5	314	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
17	B	834	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	B	830	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	O	205	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
17	3	308	CLA	C3B-C4B-NB	2.87	113.18	110.52
17	L	203	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
20	B	847	BCR	C37-C22-C23	2.87	122.59	118.08
17	A	833	CLA	CHB-C4A-NA	2.87	128.47	124.51
17	K	103	CLA	C3B-C4B-NB	2.87	113.17	110.52
17	5	309	CLA	CAC-C3C-C4C	2.86	128.53	124.81
17	A	829	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
17	B	807	CLA	OBD-CAD-C3D	-2.86	121.63	128.52
20	L	206	BCR	C16-C15-C14	2.86	129.34	123.47
17	A	834	CLA	C4-C3-C5	2.86	120.09	115.27
17	2	315	CLA	CED-O2D-CGD	2.86	122.41	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	307	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
20	L	205	BCR	C37-C22-C23	2.86	122.58	118.08
17	A	825	CLA	OBD-CAD-C3D	-2.86	121.64	128.52
17	A	817	CLA	C1-C2-C3	-2.86	121.10	126.04
17	B	824	CLA	CHB-C1B-C2B	-2.86	119.17	127.24
17	5	310	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	2	310	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	3	310	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
17	B	831	CLA	O2A-CGA-CBA	2.85	120.87	111.91
17	B	807	CLA	C3B-C4B-NB	2.85	113.16	110.52
17	3	310	CLA	CBA-CAA-C2A	2.85	122.29	113.86
17	A	853	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
17	A	803	CLA	CED-O2D-CGD	2.85	122.39	115.94
17	A	807	CLA	C1D-CHD-C4C	-2.85	119.90	126.06
17	B	811	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
17	A	829	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
17	B	826	CLA	CMC-C2C-C1C	2.85	129.38	125.04
17	A	818	CLA	C3B-C4B-NB	2.85	113.16	110.52
17	5	308	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
17	B	824	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
17	A	859	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
17	1	303	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
17	A	810	CLA	C4A-NA-C1A	-2.85	105.43	106.71
17	2	315	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
17	B	801	CLA	CMC-C2C-C1C	2.85	129.37	125.04
17	B	824	CLA	CAC-C3C-C4C	2.85	128.50	124.81
17	B	809	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
17	2	304	CLA	C3B-C4B-NB	2.84	113.15	110.52
17	4	306	CLA	CMB-C2B-C1B	2.84	129.70	125.37
17	A	822	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
20	I	101	BCR	C34-C9-C8	2.84	122.56	118.08
20	A	844	BCR	C34-C9-C10	-2.84	118.94	122.92
17	B	813	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
17	A	809	CLA	C4A-NA-C1A	-2.84	105.43	106.71
17	B	826	CLA	CMA-C3A-C2A	-2.84	102.37	113.83
17	3	310	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
17	B	829	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	B	809	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
17	K	102	CLA	CHC-C1C-C2C	-2.84	118.86	126.73
17	A	852	CLA	C1-O2A-CGA	2.83	123.88	116.44
17	3	307	CLA	O2A-CGA-CBA	2.83	120.80	111.91
17	B	835	CLA	CBA-CAA-C2A	2.83	122.22	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	304	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
17	4	311	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
17	A	819	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
17	3	314	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
17	2	306	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
17	5	303	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
17	B	813	CLA	CMB-C2B-C1B	2.83	129.68	125.37
17	3	315	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
17	A	855	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
17	B	801	CLA	O2D-CGD-CBD	2.83	116.29	111.27
25	3	317	5X6	C14-C15-C16	-2.82	114.40	123.22
17	A	816	CLA	O2D-CGD-CBD	2.82	116.29	111.27
17	A	821	CLA	C1D-CHD-C4C	-2.82	119.97	126.06
17	A	824	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	4	305	CLA	C3B-C4B-NB	2.82	113.13	110.52
24	B	849	DGD	O2G-C1B-C2B	2.82	117.58	111.50
17	B	815	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
17	2	316	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
17	4	305	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
25	1	314	5X6	C27-C26-C25	-2.82	114.61	118.94
17	3	313	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	B	811	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	5	314	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	5	303	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
17	1	307	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	B	807	CLA	CMB-C2B-C1B	2.82	129.66	125.37
17	4	306	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	J	103	CLA	C3B-C4B-NB	2.82	113.13	110.52
17	4	311	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
17	A	811	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
25	4	314	5X6	C11-C03-C02	-2.81	114.65	121.46
17	B	804	CLA	CMA-C3A-C2A	-2.81	102.48	113.83
25	2	320	5X6	C40-C22-C23	-2.81	113.65	118.08
17	A	838	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
16	A	801	CL0	CHC-C1C-C2C	-2.81	118.92	126.73
17	B	820	CLA	CED-O2D-CGD	2.81	122.29	115.94
17	B	826	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
25	4	314	5X6	C40-C22-C23	-2.81	113.65	118.08
25	5	317	5X6	C16-C17-C18	-2.81	114.63	118.94
17	B	832	CLA	CED-O2D-CGD	2.81	122.28	115.94
17	A	811	CLA	C3B-C4B-NB	2.81	113.12	110.52
17	5	303	CLA	CHD-C4C-NC	2.80	128.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	836	CLA	CED-O2D-CGD	2.80	122.28	115.94
17	B	825	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
17	B	839	CLA	C3B-C4B-NB	2.80	113.12	110.52
20	I	101	BCR	C11-C10-C9	2.80	131.31	127.31
17	1	307	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
17	A	832	CLA	O1D-CGD-CBD	-2.80	118.75	124.48
20	O	202	BCR	C35-C13-C14	-2.80	119.00	122.92
17	A	828	CLA	CAC-C3C-C4C	2.80	128.45	124.81
17	3	305	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
25	F	205	5X6	O08-C06-C05	-2.80	104.24	109.80
17	4	311	CLA	CMB-C2B-C1B	2.80	129.63	125.37
17	B	801	CLA	CHB-C4A-NA	2.80	128.38	124.51
17	B	820	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
17	A	816	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
17	1	304	CLA	CHD-C4C-NC	2.80	128.62	124.20
17	3	309	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
17	3	312	CLA	C2A-C1A-CHA	-2.80	118.97	123.85
17	A	831	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
17	A	854	CLA	C1D-CHD-C4C	-2.80	120.03	126.06
17	2	316	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
17	B	815	CLA	C5-C3-C2	-2.80	115.46	121.12
17	B	823	CLA	CMC-C2C-C1C	2.80	129.30	125.04
17	3	307	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
17	B	831	CLA	CED-O2D-CGD	2.79	122.25	115.94
17	2	311	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
17	F	204	CLA	C2A-C1A-CHA	-2.79	118.99	123.85
17	B	807	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
17	A	805	CLA	C1D-CHD-C4C	-2.79	120.05	126.06
17	A	823	CLA	CMA-C3A-C4A	2.78	119.26	111.77
17	3	307	CLA	O1D-CGD-CBD	-2.78	118.79	124.48
17	4	308	CLA	CHD-C4C-NC	2.78	128.59	124.20
25	3	316	5X6	C39-C26-C27	-2.78	113.69	118.08
17	L	202	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
17	3	311	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
17	B	838	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
17	A	833	CLA	C4-C3-C2	-2.78	116.54	123.68
20	I	101	BCR	C36-C18-C17	-2.78	119.03	122.92
17	L	202	CLA	C4-C3-C5	2.78	119.95	115.27
17	4	306	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
17	K	103	CLA	OBD-CAD-C3D	-2.78	121.83	128.52
17	1	306	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	1	301	CLA	CMC-C2C-C1C	2.78	129.27	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	812	CLA	C4-C3-C5	2.78	119.95	115.27
17	B	823	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
17	5	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	B	817	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
17	1	305	CLA	CMC-C2C-C1C	2.78	129.27	125.04
17	5	305	CLA	CHB-C1B-C2B	-2.78	119.39	127.24
17	B	816	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	A	807	CLA	O2A-C1-C2	2.78	115.93	108.64
17	2	313	CLA	CMB-C2B-C1B	2.78	129.60	125.37
17	2	311	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
17	5	309	CLA	CED-O2D-CGD	2.77	122.21	115.94
17	4	309	CLA	C2A-C1A-CHA	-2.77	119.01	123.85
17	2	314	CLA	CMB-C2B-C1B	2.77	129.59	125.37
17	2	310	CLA	O2D-CGD-CBD	2.77	116.20	111.27
17	B	841	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	A	825	CLA	O2A-CGA-CBA	2.77	120.61	111.91
25	3	316	5X6	C41-C17-C16	-2.77	113.71	118.08
17	B	819	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	2	308	CLA	CMC-C2C-C1C	2.77	129.26	125.04
17	A	828	CLA	CMA-C3A-C2A	-2.77	102.66	113.83
17	1	306	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
17	A	816	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
17	1	310	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
20	A	844	BCR	C36-C18-C17	-2.77	119.05	122.92
17	O	204	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
25	1	312	5X6	C25-C24-C23	-2.76	114.59	123.22
17	B	809	CLA	O2A-CGA-CBA	2.76	120.58	111.91
17	O	203	CLA	CMB-C2B-C1B	2.76	129.58	125.37
17	A	833	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
17	1	311	CLA	C3B-C4B-NB	2.76	113.08	110.52
17	3	311	CLA	O2A-CGA-CBA	2.76	120.57	111.91
17	3	307	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
17	B	808	CLA	C4A-NA-C1A	-2.76	105.47	106.71
17	L	204	CLA	CED-O2D-CGD	2.76	122.17	115.94
17	B	809	CLA	C1-C2-C3	-2.76	121.28	126.04
17	4	309	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	5	310	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
17	5	311	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
17	1	305	CLA	CED-O2D-CGD	2.75	122.17	115.94
17	A	802	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
17	A	806	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	A	802	CLA	C4-C3-C5	2.75	119.90	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	804	CLA	O2D-CGD-CBD	2.75	116.16	111.27
17	2	309	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
17	5	307	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
17	1	303	CLA	O2A-CGA-CBA	2.75	120.53	111.91
17	5	305	CLA	CED-O2D-CGD	2.75	122.15	115.94
17	2	314	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
17	A	804	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	4	307	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	2	304	CLA	CHD-C4C-NC	2.75	128.53	124.20
20	B	846	BCR	C19-C18-C17	2.75	123.16	118.94
17	3	314	CLA	C3B-C4B-NB	2.75	113.06	110.52
17	A	805	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	2	309	CLA	C3C-C4C-NC	2.74	113.65	110.57
20	O	202	BCR	C36-C18-C17	-2.74	119.08	122.92
17	4	307	CLA	CMB-C2B-C1B	2.74	129.55	125.37
17	3	311	CLA	CAC-C3C-C4C	2.74	128.37	124.81
20	B	843	BCR	C35-C13-C14	-2.74	119.08	122.92
17	A	803	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	5	306	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	B	837	CLA	C3B-C4B-NB	2.74	113.06	110.52
17	B	834	CLA	CED-O2D-CGD	2.74	122.14	115.94
17	F	204	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	B	836	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
17	1	311	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
17	5	314	CLA	O2A-CGA-CBA	2.74	120.50	111.91
17	A	853	CLA	CMC-C2C-C1C	2.74	129.21	125.04
17	A	821	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
17	A	813	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	1	314	5X6	C01-C02-C07	-2.74	109.28	114.36
17	B	818	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
17	A	812	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
17	1	302	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
17	4	305	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
17	B	857	CLA	CAA-C2A-C1A	-2.74	103.01	111.97
25	1	313	5X6	C14-C15-C16	-2.74	114.68	123.22
17	B	802	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
20	A	843	BCR	C36-C18-C17	-2.74	119.09	122.92
17	A	820	CLA	CAC-C3C-C4C	2.74	128.36	124.81
17	4	304	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
17	A	818	CLA	CHC-C1C-C2C	-2.73	119.13	126.73
17	4	304	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
20	O	202	BCR	C15-C16-C17	2.73	129.07	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	316	5X6	C25-C24-C23	-2.73	114.69	123.22
17	A	853	CLA	C1D-CHD-C4C	-2.73	120.16	126.06
17	K	102	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
17	2	307	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
17	B	804	CLA	CMA-C3A-C4A	-2.73	104.43	111.77
17	1	302	CLA	CED-O2D-CGD	2.73	122.11	115.94
16	A	801	CL0	C4C-C3C-C2C	-2.73	102.92	106.90
17	1	303	CLA	C5-C3-C2	-2.73	115.59	121.12
17	B	857	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
17	A	833	CLA	C3B-C4B-NB	2.73	113.05	110.52
17	A	852	CLA	C6-C7-C8	-2.73	107.10	115.92
17	3	314	CLA	CMB-C2B-C1B	2.73	129.53	125.37
17	2	311	CLA	CAC-C3C-C4C	2.73	128.35	124.81
17	1	309	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	1	306	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	4	311	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
17	B	824	CLA	CMB-C2B-C1B	2.73	129.52	125.37
17	2	316	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
17	1	308	CLA	C2A-C1A-CHA	-2.72	119.10	123.85
17	B	812	CLA	CED-O2D-CGD	2.72	122.10	115.94
17	O	205	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	3	317	5X6	C38-C30-C31	-2.72	109.31	114.36
17	B	824	CLA	CHC-C4B-NB	-2.72	121.38	124.26
17	B	827	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
17	B	804	CLA	CMC-C2C-C1C	2.72	129.18	125.04
17	B	821	CLA	O1D-CGD-CBD	-2.72	118.92	124.48
17	1	303	CLA	CMB-C2B-C1B	2.72	129.51	125.37
17	A	838	CLA	O2A-CGA-CBA	2.72	120.44	111.91
17	A	806	CLA	CMB-C2B-C1B	2.72	129.51	125.37
20	M	101	BCR	C35-C13-C14	-2.72	119.12	122.92
17	B	841	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
25	2	320	5X6	C38-C30-C31	-2.72	109.32	114.36
17	B	816	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
17	B	833	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	3	314	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
17	5	306	CLA	C3B-C4B-NB	2.72	113.03	110.52
17	5	310	CLA	C3B-C4B-NB	2.72	113.03	110.52
17	1	303	CLA	CHB-C1B-C2B	-2.72	119.57	127.24
17	3	308	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
17	5	308	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
17	A	815	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
25	1	314	5X6	C04-C03-C02	-2.71	118.79	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	820	CLA	CHD-C4C-NC	2.71	128.48	124.20
17	A	811	CLA	C4-C3-C5	2.71	119.83	115.27
17	B	834	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
17	1	310	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	A	845	BCR	C2-C1-C6	2.71	114.65	110.48
17	A	815	CLA	C1-O2A-CGA	2.71	123.56	116.44
17	3	312	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	B	820	CLA	CHB-C1B-C2B	-2.71	119.58	127.24
17	2	315	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	4	308	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
17	A	839	CLA	C3B-C4B-NB	2.71	113.03	110.52
17	A	852	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
17	4	303	CLA	O2A-CGA-CBA	2.71	120.40	111.91
17	O	203	CLA	C2A-C1A-CHA	-2.71	119.13	123.85
17	A	836	CLA	O2A-CGA-CBA	2.71	120.40	111.91
17	5	310	CLA	C2A-C1A-CHA	-2.70	119.13	123.85
17	5	302	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
17	A	818	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
17	1	301	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
17	3	312	CLA	C3B-C4B-NB	2.70	113.02	110.52
17	B	817	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	J	105	5X6	C40-C22-C23	-2.70	113.83	118.08
17	4	303	CLA	CMC-C2C-C1C	2.70	129.15	125.04
17	O	204	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
17	4	311	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
17	B	806	CLA	CAA-C2A-C1A	-2.70	103.14	111.97
17	A	811	CLA	C4A-NA-C1A	-2.70	105.49	106.71
20	A	843	BCR	C37-C22-C23	2.69	122.32	118.08
17	A	807	CLA	CBA-CAA-C2A	2.69	121.82	113.86
25	1	315	5X6	C40-C22-C23	-2.69	113.83	118.08
20	A	846	BCR	C15-C16-C17	2.69	128.99	123.47
17	A	820	CLA	CMC-C2C-C1C	2.69	129.14	125.04
17	2	305	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
17	B	828	CLA	C4-C3-C5	2.69	119.79	115.27
17	3	307	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
17	A	825	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
17	A	803	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
17	1	309	CLA	CHD-C4C-NC	2.69	128.44	124.20
17	1	301	CLA	CMB-C2B-C1B	2.69	129.46	125.37
17	A	814	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
17	B	819	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
17	B	802	CLA	CAA-C2A-C3A	-2.69	105.42	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	311	CLA	CMC-C2C-C1C	2.69	129.13	125.04
17	5	306	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	B	811	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	4	308	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
17	B	841	CLA	CHD-C4C-NC	2.68	128.43	124.20
17	5	311	CLA	CMC-C2C-C1C	2.68	129.12	125.04
25	5	318	5X6	C06-C07-C02	2.68	117.19	111.85
17	4	308	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
17	5	311	CLA	CMB-C2B-C1B	2.68	129.45	125.37
17	A	804	CLA	O2A-CGA-CBA	2.68	120.32	111.91
25	2	317	5X6	C40-C22-C23	-2.68	113.86	118.08
18	B	842	PQN	C2M-C2-C1	2.68	120.71	116.27
17	B	827	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
17	A	835	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
17	1	307	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
17	A	828	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
17	5	305	CLA	CHD-C4C-NC	2.68	128.42	124.20
17	A	852	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
17	A	856	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
17	K	102	CLA	C3B-C4B-NB	2.68	113.00	110.52
17	A	802	CLA	O1D-CGD-CBD	-2.68	119.01	124.48
17	5	312	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
17	A	839	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
20	L	206	BCR	C35-C13-C14	-2.67	119.18	122.92
17	O	204	CLA	O2A-CGA-CBA	2.67	120.29	111.91
17	A	824	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
17	A	853	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
17	F	204	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
20	B	845	BCR	C36-C18-C17	-2.67	119.19	122.92
17	A	810	CLA	CED-O2D-CGD	2.67	121.97	115.94
17	2	310	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
17	5	309	CLA	C1-O2A-CGA	2.66	123.43	116.44
17	1	309	CLA	CED-O2D-CGD	2.66	121.96	115.94
17	B	832	CLA	C4A-NA-C1A	-2.66	105.51	106.71
17	B	806	CLA	C1D-CHD-C4C	-2.66	120.31	126.06
25	4	313	5X6	C28-C29-C30	-2.66	115.01	121.46
17	1	302	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
17	1	305	CLA	C3B-C4B-NB	2.66	112.98	110.52
17	A	826	CLA	C1D-CHD-C4C	-2.66	120.32	126.06
17	B	835	CLA	CED-O2D-CGD	2.66	121.95	115.94
17	B	818	CLA	CMC-C2C-C1C	2.66	129.09	125.04
17	A	839	CLA	C4-C3-C5	2.66	119.74	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	808	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
17	O	203	CLA	C3B-C4B-NB	2.66	112.98	110.52
17	B	802	CLA	O1D-CGD-CBD	-2.66	119.05	124.48
17	1	304	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
17	A	812	CLA	C3B-C4B-NB	2.65	112.98	110.52
17	A	823	CLA	O2A-CGA-CBA	2.65	120.24	111.91
17	2	312	CLA	O1D-CGD-CBD	-2.65	119.05	124.48
17	A	852	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
17	A	803	CLA	O2A-CGA-CBA	2.65	120.23	111.91
17	2	309	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
20	K	104	BCR	C35-C13-C14	-2.65	119.21	122.92
17	A	832	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
25	4	314	5X6	C39-C26-C27	-2.65	113.90	118.08
25	5	317	5X6	C25-C24-C23	-2.65	114.95	123.22
25	J	105	5X6	C42-C13-C12	-2.65	113.90	118.08
17	5	304	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
17	2	307	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
17	5	305	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
17	B	830	CLA	CHB-C1B-NB	-2.65	121.45	124.26
17	A	804	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
17	3	307	CLA	CHD-C4C-NC	2.65	128.37	124.20
17	B	819	CLA	CHD-C4C-NC	2.64	128.37	124.20
17	A	859	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	A	855	CLA	C3B-C4B-NB	2.64	112.97	110.52
17	A	821	CLA	CMC-C2C-C1C	2.64	129.06	125.04
17	O	203	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
17	B	808	CLA	O2A-CGA-CBA	2.64	120.20	111.91
17	B	814	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
17	4	306	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
20	A	857	BCR	C34-C9-C8	2.64	122.24	118.08
17	5	306	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
17	A	819	CLA	CED-O2D-CGD	2.64	121.90	115.94
17	2	314	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
17	2	315	CLA	CHD-C4C-NC	2.64	128.36	124.20
17	B	805	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
17	B	834	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	A	807	CLA	C3B-C4B-NB	2.64	112.96	110.52
17	A	822	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
17	B	826	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
17	A	820	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
17	3	315	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
17	1	308	CLA	C3B-C4B-NB	2.63	112.96	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	809	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
17	A	804	CLA	C4A-NA-C1A	-2.63	105.52	106.71
17	A	835	CLA	C3B-C4B-NB	2.63	112.95	110.52
25	4	313	5X6	C41-C17-C16	-2.63	113.94	118.08
17	2	312	CLA	C3B-C4B-NB	2.63	112.95	110.52
17	K	103	CLA	CMC-C2C-C1C	2.63	129.04	125.04
17	B	831	CLA	CMB-C2B-C1B	2.62	129.37	125.37
17	A	827	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
17	O	204	CLA	C1-C2-C3	-2.62	122.51	126.75
17	5	308	CLA	CMB-C2B-C1B	2.62	129.36	125.37
17	2	307	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
17	B	822	CLA	CHC-C1C-C2C	-2.62	119.47	126.73
17	A	819	CLA	CMB-C2B-C1B	2.62	129.35	125.37
17	B	826	CLA	C1D-CHD-C4C	-2.62	120.42	126.06
17	A	808	CLA	CAA-C2A-C3A	-2.62	105.62	112.78
20	L	201	BCR	C35-C13-C14	-2.61	119.26	122.92
17	B	841	CLA	CED-O2D-CGD	2.61	121.85	115.94
17	3	315	CLA	CHD-C4C-NC	2.61	128.32	124.20
20	B	843	BCR	C37-C22-C23	2.61	122.19	118.08
17	B	820	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	5	309	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
17	5	304	CLA	C1-O2A-CGA	2.61	123.29	116.44
17	B	810	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
17	4	305	CLA	CHD-C4C-NC	2.61	128.31	124.20
17	5	304	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
17	B	817	CLA	CHC-C1C-C2C	-2.61	119.49	126.73
17	5	305	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
17	5	305	CLA	CMB-C2B-C1B	2.61	129.34	125.37
17	B	821	CLA	CHD-C4C-NC	2.60	128.31	124.20
17	1	304	CLA	CED-O2D-CGD	2.60	121.83	115.94
17	4	304	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
16	A	801	CL0	C4A-NA-C1A	-2.60	105.54	106.71
17	5	311	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	B	848	BCR	C15-C16-C17	2.60	128.80	123.47
17	5	304	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	B	810	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
17	1	303	CLA	CMC-C2C-C1C	2.60	129.00	125.04
17	J	103	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	B	836	CLA	CHC-C1C-C2C	-2.60	119.51	126.73
17	3	315	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
17	A	852	CLA	CED-O2D-CGD	2.60	121.82	115.94
17	B	814	CLA	CMB-C2B-C1B	2.60	129.32	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	821	CLA	CED-O2D-CGD	2.60	121.81	115.94
17	B	817	CLA	CHD-C4C-NC	2.60	128.29	124.20
17	B	833	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
17	B	841	CLA	C3B-C4B-NB	2.60	112.92	110.52
17	3	305	CLA	C1-O2A-CGA	2.59	123.25	116.44
17	A	825	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
25	5	318	5X6	C05-C06-C07	2.59	113.86	110.30
17	3	312	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
17	A	803	CLA	CAA-CBA-CGA	-2.59	105.67	113.25
17	1	302	CLA	CAC-C3C-C4C	2.59	128.17	124.81
25	5	318	5X6	C38-C30-C31	-2.59	109.55	114.36
17	1	306	CLA	C1-O2A-CGA	2.59	123.24	116.44
17	5	308	CLA	C3B-C4B-NB	2.59	112.92	110.52
25	4	313	5X6	C25-C24-C23	-2.59	115.13	123.22
17	O	204	CLA	CED-O2D-CGD	2.59	121.80	115.94
17	5	303	CLA	C5-C3-C2	2.59	126.36	121.12
17	A	834	CLA	C4-C3-C2	-2.59	117.03	123.68
17	L	202	CLA	CMB-C2B-C1B	2.59	129.31	125.37
17	A	859	CLA	C3B-C4B-NB	2.59	112.92	110.52
17	A	831	CLA	C4-C3-C2	-2.59	117.04	123.68
17	B	822	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
17	B	833	CLA	OBD-CAD-C3D	-2.59	122.29	128.52
17	3	305	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
25	2	321	5X6	C38-C30-C31	-2.59	109.56	114.36
17	5	309	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
17	5	302	CLA	C3B-C4B-NB	2.59	112.91	110.52
20	A	845	BCR	C37-C22-C23	2.59	122.15	118.08
16	A	801	CL0	CHB-C4A-NA	2.58	128.09	124.51
17	B	837	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
17	5	307	CLA	CHB-C1B-C2B	-2.58	119.94	127.24
17	5	314	CLA	CHD-C4C-NC	2.58	128.28	124.20
17	2	304	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
17	A	808	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
17	5	309	CLA	CMB-C2B-C1B	2.58	129.30	125.37
17	2	310	CLA	CHB-C1B-C2B	-2.58	119.95	127.24
17	3	310	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	A	844	BCR	C37-C22-C23	2.58	122.14	118.08
17	B	833	CLA	O2A-CGA-CBA	2.58	120.00	111.91
17	A	810	CLA	CMB-C2B-C1B	2.58	129.30	125.37
17	1	311	CLA	CMB-C2B-C1B	2.58	129.30	125.37
17	1	303	CLA	CAC-C3C-C4C	2.58	128.16	124.81
17	3	315	CLA	O2A-CGA-CBA	2.58	120.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	307	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
17	5	313	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	4	303	CLA	C3B-C4B-NB	2.58	112.91	110.52
17	5	305	CLA	CHC-C4B-NB	-2.58	121.53	124.26
17	A	830	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
17	3	306	CLA	C3B-C4B-NB	2.58	112.91	110.52
17	1	310	CLA	C2A-C1A-CHA	-2.58	119.36	123.86
17	2	312	CLA	C2A-C1A-CHA	-2.57	119.36	123.85
17	3	305	CLA	C4C-C3C-C2C	-2.57	103.14	106.90
17	A	818	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
17	B	812	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
17	B	824	CLA	CHB-C4A-NA	2.57	128.07	124.51
17	4	304	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
17	B	807	CLA	O2D-CGD-CBD	2.57	115.83	111.27
17	B	835	CLA	CHD-C4C-NC	2.57	128.25	124.20
17	3	310	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	5	318	5X6	C12-C11-C03	-2.57	119.99	127.20
17	A	833	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
17	5	311	CLA	CHD-C4C-NC	2.57	128.25	124.20
17	5	312	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	O	203	CLA	CHD-C4C-NC	2.56	128.24	124.20
17	B	834	CLA	C4-C3-C5	2.56	119.58	115.27
17	3	311	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
17	A	804	CLA	OBD-CAD-C3D	-2.56	122.35	128.52
17	5	309	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
17	3	313	CLA	C3B-C4B-NB	2.56	112.89	110.52
17	4	309	CLA	C3B-C4B-NB	2.56	112.89	110.52
20	A	843	BCR	C30-C25-C26	-2.56	119.01	122.61
17	3	313	CLA	CHD-C4C-NC	2.56	128.24	124.20
17	5	302	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
17	A	812	CLA	O2A-CGA-CBA	2.56	119.94	111.91
17	A	823	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
17	B	826	CLA	C3B-C4B-NB	2.56	112.89	110.52
17	B	838	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
17	A	820	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
17	A	854	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
17	B	837	CLA	O2A-CGA-CBA	2.55	119.92	111.91
17	B	857	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
17	2	313	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
17	1	309	CLA	C3B-C4B-NB	2.55	112.88	110.52
17	B	830	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
17	A	807	CLA	CHC-C1C-C2C	-2.55	119.64	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	817	CLA	CHB-C1B-C2B	-2.55	120.03	127.24
17	4	309	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	2	313	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
17	5	307	CLA	CHD-C4C-NC	2.55	128.22	124.20
17	A	834	CLA	C3B-C4B-NB	2.54	112.88	110.52
17	5	304	CLA	CHD-C4C-NC	2.54	128.21	124.20
17	A	859	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
17	4	308	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
25	3	318	5X6	C40-C22-C23	-2.54	114.07	118.08
17	5	303	CLA	CAC-C3C-C4C	2.54	128.11	124.81
17	3	314	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	O	205	CLA	C3B-C4B-NB	2.54	112.87	110.52
17	2	314	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
25	1	312	5X6	C40-C22-C23	-2.54	114.08	118.08
25	5	318	5X6	C33-C32-C31	2.54	113.78	110.30
17	2	310	CLA	CHD-C4C-NC	2.54	128.20	124.20
17	5	303	CLA	CMB-C2B-C1B	2.54	129.23	125.37
17	B	810	CLA	C4A-NA-C1A	-2.54	105.57	106.71
17	4	305	CLA	CED-O2D-CGD	2.53	121.67	115.94
17	B	832	CLA	CMC-C2C-C1C	2.53	128.90	125.04
17	L	204	CLA	O2A-CGA-CBA	2.53	119.86	111.91
17	5	308	CLA	CHD-C4C-NC	2.53	128.19	124.20
17	A	815	CLA	O2A-CGA-CBA	2.53	119.85	111.91
17	A	819	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	B	848	BCR	C35-C13-C14	-2.53	119.38	122.92
17	3	313	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
17	2	306	CLA	CHD-C4C-NC	2.53	128.19	124.20
25	4	313	5X6	C05-C06-C07	-2.53	106.84	110.30
17	3	315	CLA	C3B-C4B-NB	2.53	112.86	110.52
17	A	803	CLA	C1D-CHD-C4C	-2.53	120.60	126.06
17	A	829	CLA	CHB-C1B-C2B	-2.53	120.10	127.24
17	A	802	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
17	A	837	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
25	2	319	5X6	C38-C30-C31	-2.53	109.68	114.36
17	5	305	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	2	309	CLA	CHD-C4C-NC	2.52	128.18	124.20
25	1	313	5X6	C41-C17-C16	-2.52	114.10	118.08
17	5	307	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
17	A	818	CLA	C4-C3-C5	2.52	119.52	115.27
17	A	825	CLA	CHD-C4C-NC	2.52	128.18	124.20
17	A	808	CLA	O2A-CGA-CBA	2.52	119.82	111.91
25	1	314	5X6	C39-C26-C27	-2.52	114.11	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	204	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
25	2	320	5X6	C05-C06-C07	-2.52	106.86	110.30
17	A	837	CLA	CHB-C1B-C2B	-2.52	120.12	127.24
17	B	807	CLA	O2A-CGA-CBA	2.52	119.81	111.91
17	A	833	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
17	A	830	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
17	B	835	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
17	B	832	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
17	A	811	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	A	824	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
17	A	819	CLA	C3B-C4B-NB	2.51	112.85	110.52
17	A	824	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
17	A	856	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
17	B	830	CLA	C1-O2A-CGA	2.51	123.03	116.44
17	4	304	CLA	CED-O2D-CGD	2.51	121.62	115.94
17	A	804	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
17	5	312	CLA	CHD-C4C-NC	2.51	128.16	124.20
17	3	313	CLA	CMB-C2B-C1B	2.51	129.19	125.37
17	A	827	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
17	A	828	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
17	1	311	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
17	B	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B	834	CLA	CHD-C4C-NC	2.51	128.15	124.20
20	B	803	BCR	C36-C18-C17	-2.51	119.41	122.92
17	A	826	CLA	CMA-C3A-C2A	-2.51	103.72	113.83
17	B	841	CLA	C1-C2-C3	-2.51	121.71	126.04
17	3	311	CLA	CHC-C4B-NB	-2.50	121.61	124.26
17	A	824	CLA	C4-C3-C5	2.50	119.48	115.27
17	A	852	CLA	C1D-CHD-C4C	-2.50	120.66	126.06
17	4	310	CLA	C3B-C4B-NB	2.50	112.84	110.52
17	4	311	CLA	CHD-C4C-NC	2.50	128.15	124.20
17	4	304	CLA	O2A-C1-C2	2.50	115.21	108.64
17	L	203	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
17	A	818	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
17	A	827	CLA	CMB-C2B-C1B	2.50	129.18	125.37
17	F	203	CLA	C3B-C4B-NB	2.50	112.83	110.52
25	1	314	5X6	C33-C32-C31	2.50	113.72	110.30
17	O	204	CLA	CHD-C4C-NC	2.50	128.14	124.20
17	2	304	CLA	CAC-C3C-C4C	2.50	128.05	124.81
17	A	818	CLA	O2A-CGA-CBA	2.50	119.74	111.91
17	A	826	CLA	CHC-C1C-C2C	-2.50	119.80	126.73
17	K	103	CLA	C2A-C1A-CHA	-2.49	119.50	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	835	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	2	316	CLA	C3B-C4B-NB	2.49	112.83	110.52
17	K	102	CLA	C1-O2A-CGA	2.49	122.98	116.44
17	2	314	CLA	CHD-C4C-NC	2.49	128.13	124.20
20	B	847	BCR	C35-C13-C14	-2.49	119.43	122.92
17	1	303	CLA	CHD-C4C-NC	2.49	128.13	124.20
17	A	811	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
17	A	805	CLA	CMB-C2B-C1B	2.49	129.16	125.37
17	A	823	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
17	B	834	CLA	C1-O2A-CGA	2.49	122.97	116.44
17	B	840	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
17	A	832	CLA	C3B-C4B-NB	2.49	112.82	110.52
17	A	814	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
17	A	830	CLA	C4-C3-C5	2.49	119.45	115.27
17	A	856	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	B	809	CLA	C4-C3-C5	2.49	119.45	115.27
17	B	820	CLA	C2A-C1A-CHA	-2.48	119.51	123.86
17	B	826	CLA	C1-O2A-CGA	2.48	122.96	116.44
17	4	311	CLA	C3B-C4B-NB	2.48	112.82	110.52
17	A	856	CLA	CHD-C4C-NC	2.48	128.12	124.20
17	4	304	CLA	CAC-C3C-C4C	2.48	128.03	124.81
17	B	824	CLA	C1-O2A-CGA	2.48	122.95	116.44
17	1	308	CLA	CMC-C2C-C1C	2.48	128.82	125.04
17	A	830	CLA	CMB-C2B-C1B	2.48	129.15	125.37
17	B	840	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	1	314	5X6	C34-C29-C30	-2.48	119.12	122.61
17	A	818	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
17	3	312	CLA	CED-O2D-CGD	2.48	121.54	115.94
17	3	314	CLA	CHD-C4C-NC	2.48	128.11	124.20
17	A	829	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
17	A	817	CLA	CMC-C2C-C1C	2.48	128.81	125.04
20	K	104	BCR	C37-C22-C23	2.48	121.98	118.08
17	5	311	CLA	C3B-C4B-NB	2.47	112.81	110.52
17	2	314	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
17	3	309	CLA	CHD-C4C-NC	2.47	128.10	124.20
17	B	817	CLA	C5-C3-C2	-2.47	116.11	121.12
17	A	820	CLA	CMB-C2B-C1B	2.47	129.14	125.37
17	B	805	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
17	B	825	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
17	2	308	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	A	812	CLA	CHD-C4C-NC	2.47	128.10	124.20
16	A	801	CL0	CMA-C3A-C4A	-2.47	105.13	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	812	CLA	CMC-C2C-C1C	2.47	128.80	125.04
17	A	825	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
17	B	833	CLA	CMB-C2B-C1B	2.47	129.13	125.37
17	2	311	CLA	CHB-C1B-C2B	-2.47	120.27	127.24
17	5	305	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
20	B	844	BCR	C15-C14-C13	2.47	130.83	127.31
17	1	308	CLA	CED-O2D-CGD	2.47	121.51	115.94
25	2	321	5X6	C32-C31-C30	2.46	116.76	111.85
25	3	318	5X6	C11-C03-C02	-2.46	115.50	121.46
17	2	313	CLA	C3B-C4B-NB	2.46	112.80	110.52
20	B	803	BCR	C35-C13-C14	-2.46	119.47	122.92
20	B	845	BCR	C8-C9-C10	2.46	122.72	118.94
17	5	306	CLA	CED-O2D-CGD	2.46	121.50	115.94
17	1	304	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	5	303	CLA	C4-C3-C2	-2.46	117.37	123.68
17	3	310	CLA	CHB-C1B-C2B	-2.46	120.29	127.24
17	3	306	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	A	814	CLA	CMC-C2C-C1C	2.46	128.78	125.04
17	B	827	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
17	4	308	CLA	CED-O2D-CGD	2.46	121.50	115.94
17	B	841	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
17	3	309	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	4	314	5X6	C34-C29-C30	-2.46	119.15	122.61
17	A	856	CLA	C4A-NA-C1A	-2.46	105.60	106.71
17	B	802	CLA	C3B-C4B-NB	2.46	112.80	110.52
17	B	832	CLA	CAC-C3C-C4C	2.46	128.00	124.81
16	A	801	CL0	C2A-C1A-CHA	-2.46	119.56	123.86
17	O	203	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
25	F	205	5X6	C07-C02-C03	-2.45	115.38	120.85
20	I	101	BCR	C29-C30-C25	2.45	114.26	110.48
17	B	807	CLA	C4-C3-C2	-2.45	117.39	123.68
17	A	855	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
17	2	305	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
17	B	836	CLA	C4-C3-C5	2.45	119.39	115.27
17	5	304	CLA	CHB-C1B-C2B	-2.45	120.31	127.24
22	A	848	LMT	C1B-O1B-C4'	2.45	124.03	117.96
17	A	831	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
17	1	311	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
20	L	201	BCR	C36-C18-C17	-2.45	119.49	122.92
20	L	206	BCR	C37-C22-C23	2.45	121.93	118.08
17	4	310	CLA	CHD-C4C-NC	2.45	128.06	124.20
17	B	837	CLA	CED-O2D-CGD	2.45	121.47	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	I	101	BCR	C34-C9-C10	-2.45	119.50	122.92
17	A	815	CLA	C3B-C4B-NB	2.44	112.78	110.52
17	A	838	CLA	C3B-C4B-NB	2.44	112.78	110.52
25	5	318	5X6	C35-C34-C29	2.44	114.26	110.30
17	5	305	CLA	CHC-C1C-C2C	-2.44	119.94	126.73
24	B	849	DGD	O3G-C1D-C2D	2.44	112.12	108.30
17	B	829	CLA	C1-O2A-CGA	2.44	122.85	116.44
17	4	304	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
17	1	306	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	3	313	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	A	853	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	A	832	CLA	CHB-C1B-C2B	-2.44	120.35	127.24
17	B	823	CLA	CHD-C4C-NC	2.44	128.05	124.20
17	4	310	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
17	B	839	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
17	A	832	CLA	CED-O2D-CGD	2.44	121.45	115.94
17	2	314	CLA	CHC-C4B-NB	-2.44	121.68	124.26
17	2	306	CLA	CMB-C2B-C1B	2.43	129.08	125.37
17	2	311	CLA	O2A-CGA-CBA	2.43	119.54	111.91
25	5	315	5X6	C41-C17-C16	-2.43	114.24	118.08
17	2	304	CLA	CAA-C2A-C1A	2.43	119.95	111.97
17	2	305	CLA	C4-C3-C5	2.43	119.36	115.27
17	L	202	CLA	CBA-CAA-C2A	2.43	121.04	113.86
17	L	202	CLA	O2A-CGA-CBA	2.43	119.54	111.91
17	2	304	CLA	C4C-C3C-C2C	-2.43	103.36	106.90
17	B	833	CLA	C1-O2A-CGA	2.43	122.82	116.44
17	2	304	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
17	A	805	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
17	2	315	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
17	2	307	CLA	CHD-C4C-NC	2.43	128.03	124.20
17	3	308	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
20	A	846	BCR	C19-C18-C17	2.43	122.67	118.94
17	B	825	CLA	C1-O2A-CGA	2.43	122.81	116.44
17	B	823	CLA	CMB-C2B-C1B	2.42	129.06	125.37
17	A	852	CLA	C4-C3-C5	2.42	119.35	115.27
17	2	305	CLA	CHC-C4B-NB	-2.42	121.69	124.26
17	1	307	CLA	CHC-C4B-NB	-2.42	121.69	124.26
17	B	804	CLA	C16-C15-C13	2.42	123.75	115.92
17	B	838	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
20	A	844	BCR	C2-C1-C6	2.42	114.21	110.48
17	A	839	CLA	O2A-CGA-CBA	2.42	119.50	111.91
17	L	202	CLA	CHD-C4C-NC	2.42	128.02	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	838	CLA	C3B-C4B-NB	2.42	112.76	110.52
17	A	821	CLA	O2A-CGA-CBA	2.42	119.50	111.91
17	B	857	CLA	C1-C2-C3	-2.42	121.86	126.04
17	B	818	CLA	CHB-C1B-C2B	-2.42	120.41	127.24
25	1	313	5X6	C01-C02-C07	-2.42	109.88	114.36
17	5	312	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
17	1	304	CLA	CHB-C1B-C2B	-2.42	120.41	127.24
20	B	845	BCR	C15-C14-C13	2.42	130.76	127.31
16	A	801	CL0	C1-O2A-CGA	2.42	122.78	116.44
20	M	101	BCR	C10-C11-C12	2.42	130.76	123.22
17	A	829	CLA	CHD-C4C-NC	2.41	128.01	124.20
17	2	316	CLA	CHD-C4C-NC	2.41	128.01	124.20
17	A	802	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	A	828	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
17	2	306	CLA	CED-O2D-CGD	2.41	121.39	115.94
17	A	818	CLA	CHD-C4C-NC	2.41	128.01	124.20
17	L	202	CLA	CAC-C3C-C4C	2.41	127.94	124.81
17	B	823	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
17	2	308	CLA	CED-O2D-CGD	2.41	121.39	115.94
17	2	307	CLA	C4-C3-C2	-2.41	117.49	123.68
17	3	306	CLA	CHD-C4C-NC	2.41	128.00	124.20
17	5	303	CLA	CED-O2D-CGD	2.41	121.38	115.94
17	A	824	CLA	OBD-CAD-C3D	-2.41	122.73	128.52
17	A	856	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
17	B	816	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
17	A	831	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
17	2	315	CLA	C3B-C4B-NB	2.41	112.75	110.52
17	A	806	CLA	C4-C3-C5	2.41	119.32	115.27
17	A	822	CLA	CHD-C4C-NC	2.40	127.99	124.20
17	A	806	CLA	CHB-C1B-NB	-2.40	121.71	124.26
17	1	310	CLA	CHC-C4B-NB	-2.40	121.71	124.26
17	B	827	CLA	OBD-CAD-C3D	-2.40	122.74	128.52
17	B	822	CLA	CHB-C1B-C2B	-2.40	120.45	127.24
17	4	310	CLA	CMB-C2B-C1B	2.40	129.03	125.37
17	A	853	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
17	A	822	CLA	C1-O2A-CGA	2.40	122.74	116.44
17	A	815	CLA	C4-C3-C2	-2.40	117.52	123.68
17	2	311	CLA	CHC-C4B-NB	-2.40	121.72	124.26
25	5	301	5X6	C01-C02-C07	-2.40	109.91	114.36
17	A	811	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	2	311	CLA	CHC-C1C-C2C	-2.40	120.07	126.73
17	A	808	CLA	CHB-C1B-C2B	-2.40	120.47	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	825	CLA	CMB-C2B-C1B	2.40	129.02	125.37
17	B	806	CLA	C11-C10-C8	-2.40	108.18	115.92
25	2	317	5X6	C34-C29-C30	-2.40	119.24	122.61
17	4	303	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
17	A	852	CLA	O2D-CGD-CBD	2.39	115.52	111.27
17	B	831	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	B	835	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
17	1	306	CLA	C3B-C4B-NB	2.39	112.73	110.52
17	3	308	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	1	307	CLA	CHC-C1C-C2C	-2.39	120.09	126.73
17	J	103	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
17	A	855	CLA	O2A-CGA-CBA	2.39	119.41	111.91
17	O	205	CLA	CHD-C4C-NC	2.39	127.97	124.20
17	A	823	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
17	4	309	CLA	CHD-C4C-NC	2.39	127.97	124.20
17	A	829	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	A	817	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
17	5	305	CLA	C2A-C3A-C4A	-2.39	98.01	101.87
17	B	816	CLA	O2A-CGA-CBA	2.39	119.40	111.91
17	A	811	CLA	C5-C3-C2	-2.39	116.29	121.12
17	1	302	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
17	B	801	CLA	C2A-C1A-CHA	-2.39	119.69	123.86
17	B	814	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
17	L	203	CLA	C1-O2A-CGA	2.38	122.70	116.44
17	A	838	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
20	I	101	BCR	C15-C16-C17	2.38	128.36	123.47
17	A	837	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
17	F	204	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
17	3	315	CLA	CED-O2D-CGD	2.38	121.32	115.94
17	B	833	CLA	CED-O2D-CGD	2.38	121.32	115.94
17	B	831	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
17	1	305	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
17	B	801	CLA	C4A-NA-C1A	-2.38	105.64	106.71
17	B	827	CLA	CAC-C3C-C4C	2.38	127.89	124.81
25	5	317	5X6	C01-C02-C07	-2.38	109.95	114.36
20	L	205	BCR	C36-C18-C17	-2.38	119.59	122.92
25	5	317	5X6	C32-C31-C30	2.37	116.58	111.85
17	A	825	CLA	CMB-C2B-C1B	2.37	128.98	125.37
17	A	816	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
17	A	833	CLA	CED-O2D-CGD	2.37	121.30	115.94
17	1	306	CLA	CHD-C4C-NC	2.37	127.94	124.20
17	B	834	CLA	C3B-C4B-NB	2.37	112.71	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	104	BCR	C36-C18-C17	-2.37	119.60	122.92
17	L	202	CLA	CMC-C2C-C1C	2.37	128.65	125.04
17	2	306	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
17	A	819	CLA	C1-O2A-CGA	2.37	122.66	116.44
17	2	307	CLA	C4-C3-C5	2.37	119.26	115.27
17	1	307	CLA	CHB-C1B-C2B	-2.37	120.55	127.24
17	A	827	CLA	CED-O2D-CGD	2.37	121.29	115.94
17	5	307	CLA	CED-O2D-CGD	2.37	121.29	115.94
17	A	838	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
17	B	821	CLA	CMB-C2B-C1B	2.37	128.97	125.37
17	A	818	CLA	CHB-C4A-NA	2.37	127.78	124.51
20	B	848	BCR	C36-C18-C17	-2.37	119.61	122.92
17	5	311	CLA	CED-O2D-CGD	2.36	121.29	115.94
17	A	813	CLA	CMC-C2C-C1C	2.36	128.64	125.04
17	5	312	CLA	C3B-C4B-NB	2.36	112.71	110.52
17	1	307	CLA	O2A-CGA-CBA	2.36	119.32	111.91
17	A	834	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
17	4	306	CLA	C3B-C4B-NB	2.36	112.71	110.52
25	3	317	5X6	C06-C07-C02	2.36	116.56	111.85
17	B	828	CLA	O2A-CGA-CBA	2.36	119.32	111.91
17	1	302	CLA	CHD-C4C-NC	2.36	127.92	124.20
17	B	825	CLA	CMA-C3A-C4A	2.36	118.11	111.77
17	4	305	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
25	2	319	5X6	C14-C15-C16	-2.36	115.86	123.22
17	4	307	CLA	C3B-C4B-NB	2.36	112.70	110.52
17	3	307	CLA	C1-O2A-CGA	2.36	122.63	116.44
17	2	314	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
17	5	305	CLA	CAA-CBA-CGA	2.36	120.14	113.25
17	2	309	CLA	CED-O2D-CGD	2.35	121.26	115.94
17	B	805	CLA	C3B-C4B-NB	2.35	112.70	110.52
17	2	305	CLA	CHB-C1B-C2B	-2.35	120.59	127.24
17	A	834	CLA	CHD-C4C-NC	2.35	127.91	124.20
17	B	816	CLA	CHD-C4C-NC	2.35	127.91	124.20
17	A	820	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	L	202	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	A	839	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	B	830	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
25	2	321	5X6	C06-C07-C02	2.35	116.54	111.85
17	2	305	CLA	O2A-CGA-CBA	2.35	119.28	111.91
17	3	305	CLA	C4-C3-C5	2.35	119.22	115.27
24	B	849	DGD	O1G-C1A-C2A	2.35	119.28	111.91
17	3	311	CLA	CHB-C1B-C2B	-2.35	120.60	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	840	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
17	4	307	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
17	B	822	CLA	CED-O2D-CGD	2.35	121.25	115.94
17	B	807	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
20	A	844	BCR	C35-C13-C14	-2.35	119.64	122.92
20	A	857	BCR	C35-C13-C14	-2.35	119.64	122.92
24	B	849	DGD	C2G-O2G-C1B	-2.35	112.01	117.79
17	1	305	CLA	CHB-C1B-C2B	-2.35	120.61	127.24
17	1	310	CLA	CHD-C4C-NC	2.35	127.90	124.20
17	5	309	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
17	1	303	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	A	817	CLA	O2A-CGA-CBA	2.34	119.26	111.91
17	B	820	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
17	A	854	CLA	C3B-C4B-NB	2.34	112.69	110.52
17	O	204	CLA	C3B-C4B-NB	2.34	112.69	110.52
17	A	834	CLA	O2A-CGA-CBA	2.34	119.26	111.91
17	A	802	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
17	B	831	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
17	3	310	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	B	835	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
17	A	833	CLA	CAC-C3C-C4C	2.34	127.84	124.81
17	A	817	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
17	B	839	CLA	CHD-C4C-NC	2.34	127.88	124.20
17	J	103	CLA	CAA-C2A-C3A	-2.34	108.42	114.26
17	2	310	CLA	CHB-C4A-NA	2.34	127.74	124.51
17	B	806	CLA	C6-C5-C3	-2.34	107.33	113.45
17	3	314	CLA	CED-O2D-CGD	2.33	121.21	115.94
17	A	829	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
17	3	311	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
20	B	844	BCR	C15-C16-C17	2.33	128.25	123.47
17	A	826	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	B	829	CLA	CHD-C4C-NC	2.33	127.88	124.20
17	5	305	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
17	3	308	CLA	CHD-C4C-NC	2.33	127.87	124.20
17	3	305	CLA	CHC-C4B-NB	-2.33	121.79	124.26
20	A	843	BCR	C34-C9-C8	2.33	121.74	118.08
17	B	833	CLA	CAC-C3C-C4C	2.33	127.83	124.81
17	A	819	CLA	CHD-C4C-NC	2.33	127.87	124.20
17	1	304	CLA	CHC-C1C-C2C	-2.33	120.27	126.73
17	1	310	CLA	CHB-C1B-C2B	-2.32	120.67	127.24
17	5	308	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
17	A	831	CLA	C5-C3-C2	2.32	125.82	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	309	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	1	301	CLA	C3B-C4B-NB	2.32	112.67	110.52
17	B	824	CLA	C1-C2-C3	-2.32	122.03	126.04
17	B	817	CLA	C1-O2A-CGA	2.32	122.54	116.44
17	4	304	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
17	B	820	CLA	CHD-C4C-NC	2.32	127.86	124.20
17	A	823	CLA	C1-C2-C3	-2.32	122.03	126.04
17	A	813	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
17	A	838	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
25	2	321	5X6	C28-C29-C30	-2.32	115.85	121.46
17	3	305	CLA	CHB-C1B-C2B	-2.32	120.69	127.24
17	A	838	CLA	CHB-C4A-NA	2.32	127.71	124.51
17	1	307	CLA	C1-O2A-CGA	2.32	122.52	116.44
17	2	310	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
17	B	827	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
17	B	802	CLA	C6-C5-C3	2.31	119.52	113.45
17	4	307	CLA	CBA-CAA-C2A	2.31	120.69	113.86
17	B	811	CLA	CED-O2D-CGD	2.31	121.17	115.94
17	B	824	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
17	5	313	CLA	CMB-C2B-C1B	2.31	128.89	125.37
17	B	815	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
17	A	817	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
17	B	814	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	A	859	CLA	CHD-C4C-NC	2.31	127.84	124.20
17	A	834	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
17	B	816	CLA	CMC-C2C-C1C	2.31	128.55	125.04
17	4	306	CLA	CED-O2D-CGD	2.31	121.16	115.94
17	B	806	CLA	C4-C3-C5	2.31	119.15	115.27
17	O	204	CLA	CHB-C4A-NA	2.31	127.70	124.51
17	1	301	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
17	B	813	CLA	CED-O2D-CGD	2.30	121.15	115.94
17	B	831	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
17	4	307	CLA	CED-O2D-CGD	2.30	121.15	115.94
17	A	808	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	B	818	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
17	B	801	CLA	CED-O2D-CGD	2.30	121.13	115.94
17	B	840	CLA	O2A-CGA-CBA	2.30	119.12	111.91
17	B	821	CLA	CBA-CAA-C2A	2.30	120.64	113.86
17	B	828	CLA	CBA-CAA-C2A	2.30	120.64	113.86
17	B	818	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
17	A	820	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
17	A	854	CLA	CBC-CAC-C3C	-2.30	106.10	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	813	CLA	CHD-C4C-NC	2.30	127.82	124.20
17	B	805	CLA	CHD-C4C-NC	2.29	127.82	124.20
17	3	313	CLA	CED-O2D-CGD	2.29	121.13	115.94
17	A	823	CLA	CMB-C2B-C1B	2.29	128.86	125.37
17	A	830	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
25	1	315	5X6	C01-C02-C07	-2.29	110.11	114.36
17	B	804	CLA	C1-O2A-CGA	2.29	122.46	116.44
17	5	306	CLA	CHD-C4C-NC	2.29	127.82	124.20
17	A	833	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
17	B	811	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
17	A	852	CLA	O2A-CGA-CBA	2.29	119.09	111.91
25	2	319	5X6	C12-C13-C14	-2.29	115.43	118.94
17	1	311	CLA	CED-O2D-CGD	2.29	121.11	115.94
17	B	837	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
17	A	819	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
17	B	829	CLA	CMA-C3A-C2A	-2.29	104.61	113.83
17	B	802	CLA	CHD-C4C-NC	2.29	127.81	124.20
17	3	305	CLA	O2A-CGA-CBA	2.29	119.08	111.91
17	5	313	CLA	CHC-C4B-NB	-2.28	121.84	124.26
17	B	837	CLA	CMB-C2B-C1B	2.28	128.85	125.37
17	A	808	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
17	2	304	CLA	CED-O2D-CGD	2.28	121.10	115.94
17	A	853	CLA	C4A-NA-C1A	-2.28	105.68	106.71
17	2	308	CLA	CMB-C2B-C1B	2.28	128.85	125.37
17	B	832	CLA	CBA-CAA-C2A	2.28	120.60	113.86
25	1	312	5X6	C38-C30-C31	-2.28	110.13	114.36
17	5	314	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
17	B	838	CLA	CMB-C2B-C1B	2.28	128.84	125.37
17	B	831	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
17	3	312	CLA	CHD-C4C-NC	2.28	127.80	124.20
17	A	853	CLA	CMB-C2B-C1B	2.28	128.84	125.37
17	5	307	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
17	5	303	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
17	3	309	CLA	CHB-C1B-C2B	-2.28	120.80	127.24
17	1	309	CLA	CHB-C1B-C2B	-2.28	120.80	127.24
17	3	315	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
17	B	805	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	B	817	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
17	3	306	CLA	CED-O2D-CGD	2.28	121.09	115.94
17	B	857	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
17	A	856	CLA	CMB-C2B-C1B	2.28	128.84	125.37
17	A	852	CLA	CAA-C2A-C1A	-2.28	104.52	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	832	CLA	CHD-C4C-NC	2.28	127.79	124.20
17	A	854	CLA	C5-C3-C2	-2.27	116.51	121.12
17	A	808	CLA	C3B-C4B-NB	2.27	112.62	110.52
25	5	301	5X6	C42-C13-C12	-2.27	114.50	118.08
17	B	833	CLA	CHD-C4C-NC	2.27	127.78	124.20
17	2	306	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
17	A	808	CLA	CHD-C4C-NC	2.27	127.78	124.20
17	B	822	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
17	K	102	CLA	CED-O2D-CGD	2.27	121.07	115.94
17	A	856	CLA	C1-O2A-CGA	2.27	122.40	116.44
17	A	828	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
17	5	314	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	B	812	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
17	L	203	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
17	A	805	CLA	C4A-NA-C1A	-2.27	105.69	106.71
17	A	813	CLA	CED-O2D-CGD	2.27	121.07	115.94
17	A	831	CLA	O2A-CGA-CBA	2.27	119.03	111.91
17	A	826	CLA	CMB-C2B-C1B	2.27	128.82	125.37
17	3	307	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
17	B	830	CLA	O2A-CGA-CBA	2.27	119.02	111.91
25	2	320	5X6	C42-C13-C12	2.27	121.65	118.08
17	B	840	CLA	CGD-CBD-CAD	-2.27	103.39	110.73
16	A	801	CL0	CGD-CBD-CAD	-2.27	103.39	110.73
17	B	822	CLA	O2A-CGA-CBA	2.27	121.19	112.23
17	A	834	CLA	CHB-C1B-C2B	-2.27	120.84	127.24
17	A	806	CLA	CMA-C3A-C2A	-2.27	104.69	113.83
17	A	821	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
17	K	102	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
17	5	303	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	3	305	CLA	CED-O2D-CGD	2.26	121.05	115.94
17	2	310	CLA	CHC-C4B-NB	-2.26	121.86	124.26
17	A	824	CLA	CMB-C2B-C1B	2.26	128.81	125.37
25	1	316	5X6	C04-C03-C02	-2.26	119.43	122.61
17	5	313	CLA	CHC-C1C-NC	2.26	127.63	124.20
17	B	836	CLA	O2A-CGA-CBA	2.26	119.00	111.91
17	B	807	CLA	C4A-NA-C1A	-2.26	105.69	106.71
17	4	305	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
17	B	805	CLA	C4-C3-C2	-2.26	117.89	123.68
17	F	203	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	A	836	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
17	B	837	CLA	C4-C3-C5	2.26	119.07	115.27
17	5	303	CLA	O2D-CGD-O1D	-2.26	119.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	809	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
17	A	830	CLA	CED-O2D-CGD	2.26	121.04	115.94
17	B	833	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
17	A	853	CLA	CAC-C3C-C4C	2.26	127.74	124.81
17	4	304	CLA	C1-C2-C3	-2.25	122.14	126.04
17	B	832	CLA	C4-C3-C5	2.25	119.06	115.27
16	A	801	CL0	CBC-CAC-C3C	-2.25	106.22	112.43
17	A	807	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
20	M	101	BCR	C1-C6-C5	-2.25	119.44	122.61
17	A	833	CLA	C5-C3-C2	2.25	125.67	121.12
17	4	310	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
17	A	819	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	1	308	CLA	CAA-C2A-C3A	-2.25	110.84	116.10
17	A	833	CLA	CHD-C4C-NC	2.25	127.75	124.20
17	A	802	CLA	C1-O2A-CGA	2.25	122.35	116.44
17	2	313	CLA	CED-O2D-CGD	2.25	121.03	115.94
17	A	818	CLA	CAC-C3C-C4C	2.25	127.73	124.81
17	4	307	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
17	B	802	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	B	835	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	B	828	CLA	CHA-C1A-NA	-2.25	121.25	126.40
20	B	847	BCR	C16-C17-C18	2.25	130.52	127.31
17	B	832	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	A	811	CLA	CMB-C2B-C1B	2.25	128.79	125.37
17	K	102	CLA	CHD-C4C-NC	2.25	127.74	124.20
25	2	318	5X6	C19-C20-C21	-2.24	118.88	123.47
17	B	810	CLA	CED-O2D-CGD	2.24	121.01	115.94
17	2	305	CLA	CED-O2D-CGD	2.24	121.01	115.94
17	A	834	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
17	5	308	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
17	A	811	CLA	OBD-CAD-C3D	-2.24	123.12	128.52
17	5	314	CLA	CBD-CHA-C1A	2.24	131.02	127.43
17	B	821	CLA	CAC-C3C-C4C	2.24	127.72	124.81
25	4	313	5X6	C23-C22-C21	-2.24	115.50	118.94
17	1	309	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
17	A	821	CLA	C1-C2-C3	-2.24	122.17	126.04
17	A	837	CLA	CHD-C4C-NC	2.24	127.73	124.20
17	5	314	CLA	C3B-C4B-NB	2.24	112.59	110.52
17	B	810	CLA	C4-C3-C5	2.24	119.04	115.27
20	B	803	BCR	C7-C8-C9	2.24	129.62	126.23
17	3	306	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
17	1	304	CLA	CHC-C4B-NB	-2.24	121.89	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	857	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
17	B	808	CLA	C1-C2-C3	-2.24	122.17	126.04
17	4	307	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
17	B	819	CLA	OBD-CAD-C3D	-2.24	123.14	128.52
17	B	819	CLA	C1-C2-C3	-2.24	122.18	126.04
17	2	316	CLA	CHB-C4A-NA	2.24	127.60	124.51
17	F	203	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
25	1	316	5X6	C06-C07-C02	2.23	116.31	111.85
17	4	306	CLA	CHB-C1B-C2B	-2.23	120.92	127.24
17	B	824	CLA	CHC-C1C-C2C	-2.23	120.52	126.73
20	B	845	BCR	C16-C15-C14	2.23	128.05	123.47
20	L	206	BCR	C10-C11-C12	2.23	130.19	123.22
17	2	316	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
17	2	311	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
17	4	307	CLA	CHD-C4C-NC	2.23	127.72	124.20
17	2	313	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
17	B	828	CLA	CED-O2D-CGD	2.23	120.98	115.94
17	1	308	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
17	B	821	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
17	B	828	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
17	B	827	CLA	CMC-C2C-C1C	2.23	128.43	125.04
17	B	837	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
17	3	313	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
17	A	818	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
25	1	315	5X6	C32-C31-C30	2.23	116.29	111.85
17	B	806	CLA	C5-C3-C2	-2.23	116.61	121.12
17	A	825	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
17	B	818	CLA	C1-O2A-CGA	2.23	122.28	116.44
17	B	840	CLA	C4-C3-C2	-2.23	117.97	123.68
17	F	203	CLA	CHD-C4C-NC	2.22	127.71	124.20
17	B	802	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
17	3	306	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
17	A	818	CLA	C1-O2A-CGA	2.22	122.28	116.44
17	L	204	CLA	CHD-C4C-NC	2.22	127.71	124.20
17	B	813	CLA	C6-C5-C3	2.22	119.28	113.45
17	4	309	CLA	CED-O2D-CGD	2.22	120.96	115.94
17	A	813	CLA	CHB-C1B-C2B	-2.22	120.96	127.24
17	2	310	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
17	A	855	CLA	CBA-CAA-C2A	-2.22	107.31	113.86
17	5	308	CLA	CED-O2D-CGD	2.22	120.96	115.94
17	1	311	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	A	817	CLA	O1D-CGD-CBD	-2.22	119.94	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	854	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	K	102	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
17	A	804	CLA	CMB-C2B-C1B	2.22	128.75	125.37
17	A	821	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
17	5	303	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
20	J	104	BCR	C11-C10-C9	2.22	130.47	127.31
17	5	302	CLA	CED-O2D-CGD	2.22	120.95	115.94
17	O	203	CLA	CED-O2D-CGD	2.22	120.95	115.94
20	B	846	BCR	C37-C22-C23	2.22	121.57	118.08
17	4	311	CLA	CED-O2D-CGD	2.21	120.94	115.94
17	5	307	CLA	CHC-C1C-NC	2.21	127.56	124.20
17	A	806	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	4	311	CLA	CHB-C1B-C2B	-2.21	120.98	127.24
17	A	822	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	5	306	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
17	B	827	CLA	O2A-C1-C2	-2.21	102.82	108.64
17	1	309	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
17	1	302	CLA	C4C-C3C-C2C	-2.21	103.68	106.90
25	5	318	5X6	C12-C13-C14	-2.21	115.55	118.94
17	A	804	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
17	B	823	CLA	CED-O2D-CGD	2.21	120.93	115.94
17	5	313	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
25	1	312	5X6	C09-C04-C03	2.21	113.88	110.30
17	B	824	CLA	C4-C3-C5	2.21	118.98	115.27
17	4	304	CLA	CHC-C4B-NB	-2.21	121.92	124.26
17	F	204	CLA	CMA-C3A-C2A	-2.21	110.95	116.10
17	B	809	CLA	CHD-C4C-NC	2.21	127.68	124.20
17	A	818	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
17	A	809	CLA	C4-C3-C5	2.21	118.98	115.27
17	A	818	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
17	2	314	CLA	C3B-C4B-NB	2.20	112.56	110.52
25	F	205	5X6	C05-C06-C07	2.20	113.32	110.30
17	A	806	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	B	810	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
17	L	204	CLA	CHC-C4B-NB	-2.20	121.93	124.26
17	A	820	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
17	B	809	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
17	2	307	CLA	CHC-C4B-NB	-2.20	121.93	124.26
17	4	304	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
17	A	804	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
17	A	838	CLA	C4A-NA-C1A	-2.20	105.72	106.71
17	A	821	CLA	CHB-C4A-NA	2.20	127.55	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	308	CLA	CHB-C1B-C2B	-2.20	121.04	127.24
17	A	854	CLA	CHD-C4C-NC	2.20	127.66	124.20
17	B	837	CLA	CHD-C4C-NC	2.20	127.66	124.20
17	5	313	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
17	A	807	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
17	L	203	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
17	A	829	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
17	A	852	CLA	CGD-CBD-CAD	2.19	117.83	110.73
17	5	306	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
17	L	204	CLA	C3B-C4B-NB	2.19	112.55	110.52
17	4	308	CLA	C3B-C4B-NB	2.19	112.55	110.52
17	B	825	CLA	CED-O2D-CGD	2.19	120.89	115.94
17	A	826	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
17	1	301	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
17	1	306	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
17	O	205	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	L	203	CLA	CED-O2D-CGD	2.19	120.88	115.94
17	5	310	CLA	CED-O2D-CGD	2.19	120.88	115.94
17	5	314	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
17	B	826	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
17	A	815	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
17	1	301	CLA	CED-O2D-CGD	2.18	120.88	115.94
17	3	305	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
20	L	201	BCR	C34-C9-C8	2.18	121.52	118.08
25	F	205	5X6	C38-C30-C31	-2.18	110.31	114.36
17	2	305	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
17	A	814	CLA	CED-O2D-CGD	2.18	120.87	115.94
17	B	834	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
17	5	308	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
17	2	309	CLA	CHC-C1C-NC	2.18	127.51	124.20
16	A	801	CL0	CED-O2D-CGD	2.18	120.87	115.94
17	B	815	CLA	C4A-NA-C1A	-2.18	105.73	106.71
20	B	848	BCR	C16-C15-C14	2.18	127.94	123.47
20	A	845	BCR	C36-C18-C17	-2.18	119.87	122.92
20	B	843	BCR	C11-C10-C9	2.18	130.42	127.31
17	A	839	CLA	CHD-C4C-NC	2.18	127.64	124.20
17	B	820	CLA	O2A-CGA-CBA	2.18	118.75	111.91
17	A	835	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
17	A	817	CLA	CHD-C4C-NC	2.18	127.63	124.20
20	A	846	BCR	C16-C15-C14	2.18	127.93	123.47
17	B	819	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
17	2	307	CLA	CMD-C2D-C3D	-2.17	122.61	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	854	CLA	C1-C2-C3	-2.17	122.28	126.04
17	B	821	CLA	C3B-C4B-NB	2.17	112.53	110.52
17	A	827	CLA	CHD-C4C-NC	2.17	127.63	124.20
17	A	804	CLA	C4-C3-C5	2.17	118.92	115.27
17	L	202	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
17	B	813	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
17	4	305	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
17	B	831	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
17	2	316	CLA	CED-O2D-CGD	2.17	120.85	115.94
20	J	104	BCR	C35-C13-C14	-2.17	119.88	122.92
17	A	810	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
17	A	802	CLA	CHB-C1B-NB	-2.17	121.96	124.26
17	A	826	CLA	CHA-C1A-NA	-2.17	121.43	126.40
17	3	307	CLA	CHC-C4B-NB	-2.17	121.96	124.26
17	B	822	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
17	B	805	CLA	C6-C7-C8	-2.17	108.91	115.92
17	A	824	CLA	CMA-C3A-C2A	-2.17	105.09	113.83
17	B	828	CLA	C5-C3-C2	-2.17	116.73	121.12
17	A	804	CLA	CHB-C1B-NB	-2.17	121.97	124.26
17	A	839	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
17	A	833	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
17	B	835	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
17	2	306	CLA	O2A-CGA-CBA	2.16	120.97	114.03
17	A	832	CLA	C1-C2-C3	-2.16	122.31	126.04
25	3	318	5X6	C04-C03-C02	-2.16	119.57	122.61
17	1	303	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	A	807	CLA	C4A-NA-C1A	-2.16	105.73	106.71
17	5	309	CLA	C4-C3-C2	-2.16	118.14	123.68
17	A	836	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	A	816	CLA	CED-O2D-CGD	2.16	120.82	115.94
20	B	848	BCR	C15-C14-C13	2.16	130.39	127.31
17	2	307	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
17	B	811	CLA	CHD-C4C-NC	2.16	127.60	124.20
17	B	819	CLA	C7-C6-C5	-2.16	107.50	113.36
20	A	845	BCR	C16-C15-C14	2.16	127.89	123.47
17	5	312	CLA	CHB-C1B-C2B	-2.16	121.15	127.24
17	1	311	CLA	CHC-C4B-NB	-2.16	121.97	124.26
17	5	312	CLA	CED-O2D-CGD	2.16	120.81	115.94
22	A	848	LMT	C3'-C4'-C5'	-2.15	105.99	110.93
17	B	820	CLA	CMB-C2B-C1B	2.15	128.65	125.37
17	B	836	CLA	CMB-C2B-C1B	2.15	128.65	125.37
17	A	855	CLA	CHD-C4C-NC	2.15	127.59	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	306	CLA	CHB-C1B-C2B	-2.15	121.16	127.24
17	B	811	CLA	O2A-CGA-CBA	2.15	118.66	111.91
17	B	822	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
17	2	314	CLA	CED-O2D-CGD	2.15	120.80	115.94
17	2	315	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
25	4	313	5X6	C40-C22-C23	-2.15	114.69	118.08
17	O	205	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
17	2	315	CLA	CHB-C4A-NA	2.15	127.48	124.51
17	5	310	CLA	CHD-C4C-NC	2.15	127.59	124.20
20	L	206	BCR	C15-C14-C13	2.15	130.37	127.31
17	2	305	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
17	A	810	CLA	CHD-C4C-NC	2.14	127.58	124.20
17	A	825	CLA	CHB-C4A-NA	2.14	127.48	124.51
16	A	801	CL0	O2A-C1-C2	-2.14	103.00	108.64
17	B	821	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	B	835	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	A	827	CLA	CHA-C1A-NA	-2.14	121.49	126.40
17	B	810	CLA	C1-O2A-CGA	2.14	122.06	116.44
20	B	803	BCR	C15-C14-C13	2.14	130.37	127.31
17	A	810	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
17	A	811	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
17	5	305	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
20	A	846	BCR	C34-C9-C8	2.14	121.45	118.08
17	B	814	CLA	C1-O2A-CGA	2.14	122.05	116.44
17	B	829	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	A	830	CLA	C4A-NA-C1A	-2.14	105.75	106.71
17	A	832	CLA	C11-C12-C13	-2.14	109.01	115.92
17	A	812	CLA	O2A-C1-C2	2.14	114.25	108.64
17	F	203	CLA	O2A-CGA-CBA	2.14	120.89	114.03
20	B	843	BCR	C12-C13-C14	2.13	122.22	118.94
17	B	841	CLA	O2A-CGA-CBA	2.13	118.60	111.91
17	A	855	CLA	C4-C3-C5	2.13	118.86	115.27
17	2	308	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
17	B	809	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
17	A	856	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
17	3	306	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	A	837	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
17	A	833	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
17	A	811	CLA	CHD-C4C-NC	2.13	127.56	124.20
17	O	205	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
17	A	813	CLA	CHD-C4C-NC	2.13	127.56	124.20
17	2	305	CLA	O2D-CGD-O1D	-2.13	119.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	834	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
17	B	837	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
25	1	313	5X6	C05-C06-C07	2.13	113.22	110.30
25	5	316	5X6	C01-C02-C07	-2.13	110.42	114.36
17	A	806	CLA	CHD-C4C-NC	2.13	127.55	124.20
17	3	314	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
17	2	307	CLA	C1-O2A-CGA	2.13	122.02	116.44
17	O	204	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
17	1	311	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
25	2	321	5X6	C39-C26-C27	-2.12	114.73	118.08
17	1	305	CLA	O2D-CGD-O1D	-2.12	119.68	123.84
17	1	303	CLA	CED-O2D-CGD	2.12	120.74	115.94
17	A	814	CLA	O2A-CGA-CBA	2.12	120.86	114.03
17	A	859	CLA	CHB-C4A-NA	2.12	127.45	124.51
17	3	309	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
17	O	205	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
17	A	824	CLA	C1-O2A-CGA	2.12	122.01	116.44
17	A	823	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
17	B	810	CLA	C5-C3-C2	-2.12	116.83	121.12
17	B	820	CLA	C3B-C4B-NB	2.12	112.48	110.52
17	B	828	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
25	2	318	5X6	C04-C03-C02	-2.12	119.63	122.61
17	A	809	CLA	CAA-CBA-CGA	2.12	119.44	113.25
25	1	314	5X6	C38-C30-C31	-2.12	110.43	114.36
17	B	802	CLA	C4-C3-C5	2.12	118.83	115.27
17	A	853	CLA	C1-C2-C3	-2.12	122.38	126.04
17	1	304	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
17	B	804	CLA	CHB-C4A-NA	2.12	127.44	124.51
17	A	859	CLA	O2A-CGA-CBA	2.12	120.59	112.23
17	A	820	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
17	B	833	CLA	C4A-NA-C1A	-2.11	105.76	106.71
17	A	825	CLA	CHB-C1B-NB	-2.11	122.02	124.26
25	5	316	5X6	C28-C29-C30	-2.11	116.34	121.46
17	5	307	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
17	4	307	CLA	CHC-C4B-NB	-2.11	122.02	124.26
17	A	807	CLA	C1-O2A-CGA	2.11	121.98	116.44
17	B	805	CLA	CED-O2D-CGD	2.11	120.71	115.94
17	A	818	CLA	CMB-C2B-C1B	2.11	128.58	125.37
17	A	816	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
17	A	833	CLA	CMA-C3A-C2A	-2.11	105.33	113.83
17	3	310	CLA	CED-O2D-CGD	2.11	120.70	115.94
17	A	802	CLA	CHD-C4C-NC	2.11	127.52	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	845	BCR	C23-C22-C21	2.11	122.17	118.94
17	4	310	CLA	O2A-CGA-CBA	2.11	120.80	114.03
20	K	104	BCR	C11-C10-C9	2.11	130.31	127.31
17	A	828	CLA	O2A-CGA-CBA	2.10	118.51	111.91
17	1	308	CLA	CHD-C4C-NC	2.10	127.52	124.20
17	K	103	CLA	CHD-C4C-NC	2.10	127.52	124.20
17	B	812	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
20	A	843	BCR	C15-C14-C13	2.10	130.31	127.31
17	B	811	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
17	B	813	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
17	A	826	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
17	4	303	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
17	B	836	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
17	B	824	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
17	K	103	CLA	CHB-C4A-NA	2.10	127.42	124.51
17	A	821	CLA	CED-O2D-CGD	2.10	120.69	115.94
17	B	810	CLA	O2A-CGA-CBA	2.10	118.50	111.91
17	4	303	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	A	843	BCR	C30-C25-C24	2.10	121.72	115.78
17	5	305	CLA	O1A-CGA-CBA	-2.10	115.54	123.73
17	2	309	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	B	835	CLA	C3B-C4B-NB	2.10	112.46	110.52
17	2	307	CLA	C3B-C4B-NB	2.10	112.46	110.52
17	A	829	CLA	C5-C3-C4	2.10	119.24	114.60
17	A	810	CLA	CHB-C4A-NA	2.10	127.41	124.51
17	3	306	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
17	B	814	CLA	C4-C3-C5	2.10	118.80	115.27
17	4	308	CLA	CHB-C1B-C2B	-2.10	121.32	127.24
17	3	314	CLA	CBA-CAA-C2A	2.10	120.05	113.86
17	1	306	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
17	3	309	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
17	4	303	CLA	CED-O2D-CGD	2.09	120.67	115.94
17	B	829	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
17	2	308	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	A	838	CLA	CMB-C2B-C1B	2.09	128.56	125.37
17	B	829	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
17	3	307	CLA	CHB-C4A-NA	2.09	127.41	124.51
17	B	812	CLA	O2A-CGA-CBA	2.09	118.47	111.91
17	3	314	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
17	B	840	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
17	B	805	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	A	808	CLA	C5-C3-C2	-2.09	116.89	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	815	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
17	B	805	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
17	A	835	CLA	CMB-C2B-C1B	2.09	128.55	125.37
17	A	821	CLA	C3B-C4B-NB	2.09	112.45	110.52
17	B	827	CLA	CHB-C4A-NA	2.09	127.40	124.51
25	5	315	5X6	C40-C22-C23	-2.09	114.79	118.08
17	A	853	CLA	CED-O2D-CGD	2.09	120.66	115.94
17	A	816	CLA	CHA-C1A-NA	-2.09	121.62	126.40
17	2	304	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	O	203	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
17	1	302	CLA	O2A-CGA-CBA	2.08	118.45	111.91
17	5	304	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	4	305	CLA	CHC-C4B-NB	-2.08	122.05	124.26
17	B	802	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
17	B	806	CLA	O2A-CGA-CBA	2.08	118.44	111.91
17	B	836	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
17	B	811	CLA	CHA-C1A-NA	-2.08	121.63	126.40
17	A	838	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
17	A	831	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
17	B	840	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	B	804	CLA	C1-C2-C3	-2.08	122.45	126.04
17	A	826	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	B	814	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
17	2	316	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
17	O	203	CLA	CAA-C2A-C3A	-2.08	111.25	116.10
17	A	806	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
17	L	204	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
17	5	313	CLA	CHD-C4C-NC	2.08	127.47	124.20
17	A	829	CLA	C1-O2A-CGA	2.07	121.89	116.44
17	3	306	CLA	O2A-CGA-CBA	2.07	120.70	114.03
17	B	836	CLA	CHB-C4A-NA	2.07	127.38	124.51
17	B	806	CLA	CHB-C1B-NB	-2.07	122.06	124.26
20	A	843	BCR	C16-C15-C14	2.07	127.72	123.47
17	B	813	CLA	C4-C3-C2	-2.07	118.36	123.68
17	K	103	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
17	5	311	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
17	B	808	CLA	C4-C3-C5	2.07	118.76	115.27
17	1	306	CLA	CED-O2D-CGD	2.07	120.62	115.94
17	B	834	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
17	1	309	CLA	CHB-C4A-NA	2.07	127.38	124.51
17	F	204	CLA	CAA-C2A-C3A	-2.07	111.27	116.10
17	B	827	CLA	O2A-CGA-CBA	2.07	118.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	828	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
20	B	847	BCR	C29-C28-C27	2.07	116.00	111.38
17	B	831	CLA	CHD-C4C-NC	2.07	127.47	124.20
17	B	818	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
17	L	204	CLA	C1-C2-C3	-2.07	123.41	126.75
17	O	204	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
25	1	316	5X6	C23-C22-C21	-2.07	115.77	118.94
17	A	824	CLA	CHD-C4C-NC	2.07	127.46	124.20
17	A	820	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
17	A	829	CLA	O2A-CGA-CBA	2.07	118.39	111.91
17	A	831	CLA	CHB-C4A-NA	2.06	127.37	124.51
17	A	827	CLA	CMA-C3A-C2A	-2.06	105.50	113.83
20	A	843	BCR	C29-C30-C25	2.06	113.66	110.48
17	B	826	CLA	CMB-C2B-C1B	2.06	128.51	125.37
17	B	825	CLA	CAA-C2A-C3A	2.06	118.43	112.78
17	2	306	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	2	319	5X6	C01-C02-C07	-2.06	110.53	114.36
20	O	202	BCR	C12-C13-C14	2.06	122.11	118.94
17	B	827	CLA	C6-C7-C8	-2.06	109.25	115.92
17	J	103	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
17	4	303	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
17	B	832	CLA	O2A-CGA-CBA	2.06	118.38	111.91
17	A	816	CLA	C4-C3-C5	2.06	118.74	115.27
25	5	315	5X6	C34-C29-C30	-2.06	119.71	122.61
25	5	318	5X6	C32-C31-C30	2.06	115.96	111.85
17	A	855	CLA	O2D-CGD-CBD	2.06	114.93	111.27
17	A	853	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
17	A	830	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
17	A	853	CLA	C4-C3-C5	2.06	118.73	115.27
17	3	314	CLA	CHB-C4A-NA	2.06	127.36	124.51
17	B	812	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
17	A	821	CLA	CHD-C4C-NC	2.06	127.44	124.20
17	B	841	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
17	5	312	CLA	CHC-C4B-NB	-2.05	122.08	124.26
17	B	833	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	B	808	CLA	CHD-C4C-NC	2.05	127.44	124.20
17	B	805	CLA	CMB-C2B-C3B	2.05	131.56	126.59
20	A	845	BCR	C15-C14-C13	2.05	130.24	127.31
17	4	307	CLA	O2A-CGA-CBA	2.05	120.62	114.03
17	2	313	CLA	CAA-C2A-C1A	2.05	116.68	112.14
17	A	823	CLA	CHD-C4C-NC	2.05	127.43	124.20
17	B	838	CLA	CHD-C4C-NC	2.05	127.43	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	307	CLA	C3B-C4B-NB	2.05	112.42	110.52
17	1	306	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
17	B	819	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
17	B	813	CLA	C1-C2-C3	-2.05	122.50	126.04
17	J	103	CLA	CHD-C4C-NC	2.05	127.43	124.20
17	B	805	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
17	L	203	CLA	CHD-C4C-NC	2.05	127.43	124.20
17	3	305	CLA	CHB-C4A-NA	2.05	127.34	124.51
17	A	805	CLA	CHD-C4C-NC	2.04	127.43	124.20
17	K	102	CLA	CHB-C4A-NA	2.04	127.34	124.51
17	A	803	CLA	CMB-C2B-C1B	2.04	128.48	125.37
17	A	820	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
17	1	310	CLA	C3B-C4B-NB	2.04	112.41	110.52
17	A	834	CLA	CHB-C4A-NA	2.04	127.34	124.51
17	O	205	CLA	CED-O2D-CGD	2.04	120.56	115.94
20	A	844	BCR	C34-C9-C8	2.04	121.30	118.08
17	3	307	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
17	B	827	CLA	CHD-C4C-NC	2.04	127.42	124.20
17	A	835	CLA	CED-O2D-CGD	2.04	120.56	115.94
17	A	825	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
20	I	101	BCR	C16-C15-C14	2.04	127.66	123.47
20	A	843	BCR	C21-C20-C19	2.04	129.59	123.22
17	A	835	CLA	CBA-CAA-C2A	-2.04	107.84	113.86
17	B	812	CLA	CHD-C4C-NC	2.04	127.42	124.20
17	B	801	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
17	B	827	CLA	C4-C3-C5	2.04	118.70	115.27
17	B	813	CLA	C3B-C4B-NB	2.04	112.41	110.52
17	K	102	CLA	CHC-C4B-NB	-2.04	122.10	124.26
17	1	307	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
17	3	306	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
17	K	102	CLA	C1-C2-C3	-2.04	122.52	126.04
17	A	838	CLA	CHD-C4C-NC	2.04	127.41	124.20
17	A	830	CLA	CHB-C1B-NB	-2.04	122.10	124.26
17	F	204	CLA	CED-O2D-CGD	2.04	120.54	115.94
17	L	202	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	A	829	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
17	A	809	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
17	B	815	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
25	J	105	5X6	C28-C29-C30	-2.03	116.54	121.46
17	A	836	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
17	5	314	CLA	CHC-C4B-NB	-2.03	122.11	124.26
17	A	811	CLA	O2A-CGA-CBA	2.03	118.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	306	CLA	CHD-C4C-NC	2.03	127.40	124.20
17	O	204	CLA	CBA-CAA-C2A	2.03	119.85	113.86
20	K	104	BCR	C34-C9-C8	2.03	121.27	118.08
17	4	309	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
17	A	859	CLA	CMC-C2C-C1C	2.03	128.12	125.04
17	5	310	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
17	A	813	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
17	B	833	CLA	C6-C7-C8	-2.03	109.37	115.92
17	3	308	CLA	O2A-CGA-CBA	2.03	120.54	114.03
17	3	306	CLA	CMB-C2B-C1B	2.02	128.45	125.37
17	A	824	CLA	CHB-C1B-NB	-2.02	122.11	124.26
17	F	204	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	4	310	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	1	314	5X6	C40-C22-C23	-2.02	114.89	118.08
17	B	857	CLA	C3B-C4B-NB	2.02	112.39	110.52
17	B	819	CLA	CMB-C2B-C1B	2.02	128.44	125.37
20	L	201	BCR	C29-C30-C25	2.02	113.59	110.48
17	1	302	CLA	CMB-C2B-C1B	2.02	128.44	125.37
20	M	101	BCR	C15-C14-C13	2.02	130.19	127.31
17	2	312	CLA	CHB-C4A-NA	2.02	127.30	124.51
25	4	313	5X6	C39-C26-C27	-2.02	114.90	118.08
17	A	808	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
17	B	836	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
20	L	206	BCR	C12-C13-C14	2.02	122.04	118.94
17	5	313	CLA	O2A-CGA-CBA	2.02	120.51	114.03
17	A	809	CLA	CBC-CAC-C3C	-2.02	106.88	112.43
17	A	831	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
17	B	807	CLA	CHB-C1B-NB	-2.01	122.12	124.26
25	2	317	5X6	C39-C26-C27	-2.01	114.90	118.08
17	A	808	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
17	B	826	CLA	O2A-CGA-CBA	2.01	118.23	111.91
17	5	313	CLA	CED-O2D-CGD	2.01	120.49	115.94
17	2	312	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
17	2	309	CLA	C4C-C3C-C2C	-2.01	103.96	106.90
17	B	821	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
17	2	312	CLA	CHD-C4C-NC	2.01	127.37	124.20
17	B	805	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
17	A	832	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
17	5	302	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
17	4	309	CLA	CAA-C2A-C3A	-2.01	111.41	116.10
25	2	320	5X6	C31-C30-C29	-2.01	116.37	120.85
17	5	309	CLA	CHB-C1B-C2B	-2.01	121.56	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	314	CLA	O2A-CGA-CBA	2.01	120.17	112.23
17	A	852	CLA	C4A-NA-C1A	-2.01	105.80	106.71
17	K	103	CLA	CED-O2D-CGD	2.01	120.48	115.94
17	2	312	CLA	CHC-C1C-NC	2.01	127.25	124.20
17	F	203	CLA	CHA-C1A-NA	-2.01	121.80	126.40
17	A	859	CLA	CAC-C3C-C2C	2.01	130.96	127.53
17	3	310	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
17	2	313	CLA	CHD-C4C-NC	2.00	127.36	124.20
20	K	104	BCR	C10-C11-C12	2.00	129.47	123.22
17	B	816	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
20	O	202	BCR	C29-C30-C25	2.00	113.56	110.48
17	B	829	CLA	O2A-C1-C2	-2.00	103.37	108.64
17	2	308	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
17	O	203	CLA	CHC-C4B-NB	-2.00	122.14	124.26
17	B	818	CLA	CMA-C3A-C2A	-2.00	105.75	113.83
17	1	308	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
17	L	204	CLA	CAA-C2A-C1A	2.00	118.54	111.97
17	5	303	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
17	B	816	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
17	4	310	CLA	CHC-C4B-NB	-2.00	122.14	124.26
25	3	318	5X6	C39-C26-C27	-2.00	114.92	118.08
17	1	302	CLA	C1-O2A-CGA	2.00	121.69	116.44
17	1	305	CLA	CHC-C4B-NB	-2.00	122.14	124.26
17	5	309	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

There are no chirality outliers.

All (1869) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C11-C10-C8-C9
17	A	808	CLA	C2-C3-C5-C6
17	A	808	CLA	C4-C3-C5-C6
17	A	813	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	C3A-C2A-CAA-CBA
17	A	822	CLA	CHA-CBD-CGD-O1D
17	A	822	CLA	CHA-CBD-CGD-O2D
17	A	828	CLA	CHA-CBD-CGD-O1D
17	A	828	CLA	CHA-CBD-CGD-O2D
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	834	CLA	CHA-CBD-CGD-O2D
17	A	834	CLA	C4-C3-C5-C6
17	A	854	CLA	CHA-CBD-CGD-O1D
17	A	854	CLA	CHA-CBD-CGD-O2D
17	A	856	CLA	C1A-C2A-CAA-CBA
17	A	856	CLA	C3A-C2A-CAA-CBA
17	A	859	CLA	CBD-CGD-O2D-CED
17	B	805	CLA	C1A-C2A-CAA-CBA
17	B	805	CLA	C2-C3-C5-C6
17	B	805	CLA	C4-C3-C5-C6
17	B	806	CLA	C1A-C2A-CAA-CBA
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	812	CLA	C2-C3-C5-C6
17	B	812	CLA	C4-C3-C5-C6
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	813	CLA	C3A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C3A-C2A-CAA-CBA
17	B	824	CLA	CHA-CBD-CGD-O1D
17	B	824	CLA	CHA-CBD-CGD-O2D
17	B	831	CLA	C3A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	835	CLA	C1A-C2A-CAA-CBA
17	B	835	CLA	C3A-C2A-CAA-CBA
17	B	836	CLA	C6-C7-C8-C9
17	B	840	CLA	O1A-CGA-O2A-C1
17	B	840	CLA	C2-C3-C5-C6
17	B	840	CLA	C4-C3-C5-C6
17	K	102	CLA	C1A-C2A-CAA-CBA
17	L	203	CLA	C1A-C2A-CAA-CBA
17	L	203	CLA	C3A-C2A-CAA-CBA
17	O	204	CLA	C1A-C2A-CAA-CBA
17	O	204	CLA	C3A-C2A-CAA-CBA
17	O	205	CLA	CBD-CGD-O2D-CED
17	1	303	CLA	C2-C3-C5-C6
17	1	303	CLA	C4-C3-C5-C6
17	1	307	CLA	CBD-CGD-O2D-CED
17	2	304	CLA	CBD-CGD-O2D-CED
17	2	307	CLA	C1A-C2A-CAA-CBA
17	2	307	CLA	CHA-CBD-CGD-O1D
17	2	307	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	2	308	CLA	CBD-CGD-O2D-CED
17	2	312	CLA	CHA-CBD-CGD-O1D
17	2	312	CLA	CHA-CBD-CGD-O2D
17	2	313	CLA	C1A-C2A-CAA-CBA
17	2	313	CLA	CBD-CGD-O2D-CED
17	2	314	CLA	CBD-CGD-O2D-CED
17	2	316	CLA	CHA-CBD-CGD-O1D
17	2	316	CLA	CHA-CBD-CGD-O2D
17	2	316	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	C3A-C2A-CAA-CBA
17	3	313	CLA	C1A-C2A-CAA-CBA
17	3	313	CLA	C3A-C2A-CAA-CBA
17	3	314	CLA	CBA-CGA-O2A-C1
17	3	314	CLA	O1A-CGA-O2A-C1
17	4	306	CLA	CBD-CGD-O2D-CED
17	4	307	CLA	C1A-C2A-CAA-CBA
17	4	307	CLA	C3A-C2A-CAA-CBA
17	4	308	CLA	CBD-CGD-O2D-CED
17	4	309	CLA	CBD-CGD-O2D-CED
17	4	310	CLA	C1A-C2A-CAA-CBA
17	4	310	CLA	C3A-C2A-CAA-CBA
17	5	302	CLA	CBD-CGD-O2D-CED
17	5	310	CLA	CBD-CGD-O2D-CED
17	5	311	CLA	CBD-CGD-O2D-CED
17	5	312	CLA	CBD-CGD-O2D-CED
17	5	313	CLA	CBD-CGD-O2D-CED
19	A	841	LHG	C4-O6-P-O5
19	A	842	LHG	O1-C1-C2-C3
19	A	842	LHG	C3-O3-P-O5
19	J	102	LHG	C1-C2-C3-O3
19	J	102	LHG	C3-O3-P-O4
19	J	102	LHG	C3-O3-P-O5
19	J	102	LHG	C3-O3-P-O6
20	A	843	BCR	C5-C6-C7-C8
20	A	843	BCR	C21-C22-C23-C24
20	A	843	BCR	C37-C22-C23-C24
20	A	843	BCR	C23-C24-C25-C26
20	A	844	BCR	C17-C18-C19-C20
20	A	844	BCR	C36-C18-C19-C20
20	A	844	BCR	C18-C19-C20-C21
20	A	844	BCR	C20-C21-C22-C23
20	A	844	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
20	A	844	BCR	C22-C23-C24-C25
20	A	844	BCR	C23-C24-C25-C30
20	A	845	BCR	C21-C22-C23-C24
20	A	845	BCR	C37-C22-C23-C24
20	B	803	BCR	C7-C8-C9-C10
20	B	803	BCR	C7-C8-C9-C34
20	B	844	BCR	C7-C8-C9-C10
20	B	844	BCR	C7-C8-C9-C34
20	B	845	BCR	C6-C7-C8-C9
20	B	845	BCR	C7-C8-C9-C34
20	B	845	BCR	C11-C10-C9-C8
20	B	845	BCR	C11-C10-C9-C34
20	B	845	BCR	C10-C11-C12-C13
20	K	104	BCR	C17-C18-C19-C20
20	K	104	BCR	C36-C18-C19-C20
20	K	104	BCR	C22-C23-C24-C25
20	L	205	BCR	C21-C22-C23-C24
20	L	205	BCR	C37-C22-C23-C24
20	L	205	BCR	C23-C24-C25-C26
20	L	205	BCR	C23-C24-C25-C30
20	L	206	BCR	C22-C23-C24-C25
20	L	206	BCR	C23-C24-C25-C30
20	M	101	BCR	C7-C8-C9-C10
20	M	101	BCR	C22-C23-C24-C25
20	O	202	BCR	C7-C8-C9-C34
22	B	851	LMT	C2-C1-O1'-C1'
22	B	852	LMT	C2'-C1'-O1'-C1
24	B	849	DGD	C2B-C1B-O2G-C2G
25	F	205	5X6	C15-C16-C17-C41
25	F	205	5X6	C24-C25-C26-C39
25	F	205	5X6	C03-C11-C12-C13
25	F	205	5X6	C02-C03-C11-C12
25	F	205	5X6	C12-C13-C14-C15
25	F	205	5X6	C20-C21-C22-C40
25	J	105	5X6	C41-C17-C18-C19
25	J	105	5X6	C15-C16-C17-C18
25	J	105	5X6	C24-C25-C26-C39
25	J	105	5X6	C02-C03-C11-C12
25	J	105	5X6	C04-C03-C11-C12
25	J	105	5X6	C42-C13-C14-C15
25	J	105	5X6	C27-C28-C29-C30
25	J	105	5X6	C20-C21-C22-C40

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Mol	Chain	Res	Type	Atoms
25	J	105	5X6	C40-C22-C23-C24
25	J	105	5X6	C21-C22-C23-C24
25	1	312	5X6	C41-C17-C18-C19
25	1	312	5X6	C14-C15-C16-C17
25	1	312	5X6	C24-C25-C26-C39
25	1	312	5X6	C18-C19-C20-C21
25	1	312	5X6	C03-C11-C12-C13
25	1	312	5X6	C11-C12-C13-C14
25	1	312	5X6	C11-C12-C13-C42
25	1	312	5X6	C12-C13-C14-C15
25	1	312	5X6	C42-C13-C14-C15
25	1	312	5X6	C20-C21-C22-C40
25	1	312	5X6	C20-C21-C22-C23
25	1	312	5X6	C40-C22-C23-C24
25	1	313	5X6	C16-C17-C18-C19
25	1	313	5X6	C25-C26-C27-C28
25	1	313	5X6	C24-C25-C26-C39
25	1	313	5X6	C03-C11-C12-C13
25	1	313	5X6	C11-C12-C13-C42
25	1	313	5X6	C42-C13-C14-C15
25	1	313	5X6	C13-C14-C15-C16
25	1	313	5X6	C27-C28-C29-C30
25	1	313	5X6	C20-C21-C22-C40
25	1	314	5X6	C41-C17-C18-C19
25	1	314	5X6	C15-C16-C17-C18
25	1	314	5X6	C15-C16-C17-C41
25	1	314	5X6	C14-C15-C16-C17
25	1	314	5X6	C24-C25-C26-C27
25	1	314	5X6	C12-C13-C14-C15
25	1	314	5X6	C42-C13-C14-C15
25	1	314	5X6	C26-C27-C28-C29
25	1	314	5X6	C20-C21-C22-C40
25	1	314	5X6	C20-C21-C22-C23
25	1	314	5X6	C22-C23-C24-C25
25	1	315	5X6	C16-C17-C18-C19
25	1	315	5X6	C41-C17-C18-C19
25	1	315	5X6	C15-C16-C17-C18
25	1	315	5X6	C14-C15-C16-C17
25	1	315	5X6	C25-C26-C27-C28
25	1	315	5X6	C24-C25-C26-C27
25	1	315	5X6	C18-C19-C20-C21
25	1	315	5X6	C03-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	1	315	5X6	C02-C03-C11-C12
25	1	315	5X6	C12-C13-C14-C15
25	1	315	5X6	C42-C13-C14-C15
25	1	315	5X6	C26-C27-C28-C29
25	1	315	5X6	C20-C21-C22-C40
25	1	315	5X6	C20-C21-C22-C23
25	1	315	5X6	C40-C22-C23-C24
25	1	316	5X6	C41-C17-C18-C19
25	1	316	5X6	C17-C18-C19-C20
25	1	316	5X6	C25-C26-C27-C28
25	1	316	5X6	C24-C25-C26-C39
25	1	316	5X6	C18-C19-C20-C21
25	1	316	5X6	C03-C11-C12-C13
25	1	316	5X6	C42-C13-C14-C15
25	1	316	5X6	C20-C21-C22-C40
25	1	316	5X6	C20-C21-C22-C23
25	1	316	5X6	C21-C22-C23-C24
25	2	317	5X6	C16-C17-C18-C19
25	2	317	5X6	C41-C17-C18-C19
25	2	317	5X6	C15-C16-C17-C41
25	2	317	5X6	C17-C18-C19-C20
25	2	317	5X6	C14-C15-C16-C17
25	2	317	5X6	C39-C26-C27-C28
25	2	317	5X6	C24-C25-C26-C39
25	2	317	5X6	C18-C19-C20-C21
25	2	317	5X6	C02-C03-C11-C12
25	2	317	5X6	C11-C12-C13-C14
25	2	317	5X6	C12-C13-C14-C15
25	2	317	5X6	C42-C13-C14-C15
25	2	317	5X6	C19-C20-C21-C22
25	2	317	5X6	C20-C21-C22-C40
25	2	317	5X6	C20-C21-C22-C23
25	2	317	5X6	C40-C22-C23-C24
25	2	317	5X6	C22-C23-C24-C25
25	2	318	5X6	C41-C17-C18-C19
25	2	318	5X6	C15-C16-C17-C18
25	2	318	5X6	C15-C16-C17-C41
25	2	318	5X6	C25-C26-C27-C28
25	2	318	5X6	C24-C25-C26-C39
25	2	318	5X6	C24-C25-C26-C27
25	2	318	5X6	C11-C12-C13-C14
25	2	318	5X6	C42-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	2	318	5X6	C20-C21-C22-C23
25	2	318	5X6	C21-C22-C23-C24
25	2	318	5X6	C22-C23-C24-C25
25	2	319	5X6	C16-C17-C18-C19
25	2	319	5X6	C15-C16-C17-C18
25	2	319	5X6	C14-C15-C16-C17
25	2	319	5X6	C25-C26-C27-C28
25	2	319	5X6	C24-C25-C26-C39
25	2	319	5X6	C24-C25-C26-C27
25	2	319	5X6	C18-C19-C20-C21
25	2	319	5X6	C12-C13-C14-C15
25	2	319	5X6	C42-C13-C14-C15
25	2	319	5X6	C20-C21-C22-C40
25	2	319	5X6	C21-C22-C23-C24
25	2	319	5X6	C22-C23-C24-C25
25	2	320	5X6	C41-C17-C18-C19
25	2	320	5X6	C14-C15-C16-C17
25	2	320	5X6	C39-C26-C27-C28
25	2	320	5X6	C25-C26-C27-C28
25	2	320	5X6	C24-C25-C26-C27
25	2	320	5X6	C18-C19-C20-C21
25	2	320	5X6	C11-C12-C13-C42
25	2	320	5X6	C12-C13-C14-C15
25	2	320	5X6	C42-C13-C14-C15
25	2	320	5X6	C26-C27-C28-C29
25	2	320	5X6	C20-C21-C22-C40
25	2	320	5X6	C22-C23-C24-C25
25	2	321	5X6	C16-C17-C18-C19
25	2	321	5X6	C41-C17-C18-C19
25	2	321	5X6	C39-C26-C27-C28
25	2	321	5X6	C25-C26-C27-C28
25	2	321	5X6	C24-C25-C26-C39
25	2	321	5X6	C24-C25-C26-C27
25	2	321	5X6	C18-C19-C20-C21
25	2	321	5X6	C03-C11-C12-C13
25	2	321	5X6	C42-C13-C14-C15
25	2	321	5X6	C27-C28-C29-C34
25	2	321	5X6	C26-C27-C28-C29
25	2	321	5X6	C20-C21-C22-C40
25	2	321	5X6	C20-C21-C22-C23
25	2	321	5X6	C40-C22-C23-C24
25	2	321	5X6	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	3	316	5X6	C16-C17-C18-C19
25	3	316	5X6	C15-C16-C17-C41
25	3	316	5X6	C14-C15-C16-C17
25	3	316	5X6	C39-C26-C27-C28
25	3	316	5X6	C24-C25-C26-C39
25	3	316	5X6	C18-C19-C20-C21
25	3	316	5X6	C03-C11-C12-C13
25	3	316	5X6	C02-C03-C11-C12
25	3	316	5X6	C11-C12-C13-C14
25	3	316	5X6	C42-C13-C14-C15
25	3	316	5X6	C27-C28-C29-C30
25	3	316	5X6	C20-C21-C22-C40
25	3	316	5X6	C20-C21-C22-C23
25	3	316	5X6	C22-C23-C24-C25
25	3	317	5X6	C16-C17-C18-C19
25	3	317	5X6	C41-C17-C18-C19
25	3	317	5X6	C14-C15-C16-C17
25	3	317	5X6	C24-C25-C26-C39
25	3	317	5X6	C24-C25-C26-C27
25	3	317	5X6	C11-C12-C13-C14
25	3	317	5X6	C42-C13-C14-C15
25	3	317	5X6	C19-C20-C21-C22
25	3	317	5X6	C20-C21-C22-C40
25	3	317	5X6	C20-C21-C22-C23
25	3	317	5X6	C22-C23-C24-C25
25	3	317	5X6	C23-C24-C25-C26
25	3	318	5X6	C41-C17-C18-C19
25	3	318	5X6	C25-C26-C27-C28
25	3	318	5X6	C24-C25-C26-C39
25	3	318	5X6	C18-C19-C20-C21
25	3	318	5X6	C42-C13-C14-C15
25	3	318	5X6	C20-C21-C22-C40
25	3	318	5X6	C20-C21-C22-C23
25	3	318	5X6	C23-C24-C25-C26
25	4	312	5X6	C16-C17-C18-C19
25	4	312	5X6	C41-C17-C18-C19
25	4	312	5X6	C15-C16-C17-C41
25	4	312	5X6	C14-C15-C16-C17
25	4	312	5X6	C39-C26-C27-C28
25	4	312	5X6	C24-C25-C26-C39
25	4	312	5X6	C24-C25-C26-C27
25	4	312	5X6	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	4	312	5X6	C03-C11-C12-C13
25	4	312	5X6	C11-C12-C13-C42
25	4	312	5X6	C42-C13-C14-C15
25	4	312	5X6	C27-C28-C29-C34
25	4	312	5X6	C26-C27-C28-C29
25	4	312	5X6	C20-C21-C22-C40
25	4	312	5X6	C22-C23-C24-C25
25	4	313	5X6	C41-C17-C18-C19
25	4	313	5X6	C18-C19-C20-C21
25	4	313	5X6	C02-C03-C11-C12
25	4	313	5X6	C11-C12-C13-C14
25	4	313	5X6	C42-C13-C14-C15
25	4	313	5X6	C19-C20-C21-C22
25	4	313	5X6	C27-C28-C29-C30
25	4	313	5X6	C26-C27-C28-C29
25	4	313	5X6	C20-C21-C22-C23
25	4	313	5X6	C40-C22-C23-C24
25	4	313	5X6	C22-C23-C24-C25
25	4	314	5X6	C41-C17-C18-C19
25	4	314	5X6	C15-C16-C17-C18
25	4	314	5X6	C15-C16-C17-C41
25	4	314	5X6	C17-C18-C19-C20
25	4	314	5X6	C14-C15-C16-C17
25	4	314	5X6	C24-C25-C26-C39
25	4	314	5X6	C24-C25-C26-C27
25	4	314	5X6	C18-C19-C20-C21
25	4	314	5X6	C11-C12-C13-C14
25	4	314	5X6	C42-C13-C14-C15
25	4	314	5X6	C26-C27-C28-C29
25	4	314	5X6	C20-C21-C22-C40
25	4	314	5X6	C20-C21-C22-C23
25	4	314	5X6	C22-C23-C24-C25
25	5	301	5X6	C41-C17-C18-C19
25	5	301	5X6	C15-C16-C17-C18
25	5	301	5X6	C17-C18-C19-C20
25	5	301	5X6	C24-C25-C26-C39
25	5	301	5X6	C11-C12-C13-C42
25	5	301	5X6	C12-C13-C14-C15
25	5	301	5X6	C42-C13-C14-C15
25	5	301	5X6	C13-C14-C15-C16
25	5	301	5X6	C20-C21-C22-C40
25	5	301	5X6	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	5	301	5X6	C21-C22-C23-C24
25	5	301	5X6	C22-C23-C24-C25
25	5	315	5X6	C41-C17-C18-C19
25	5	315	5X6	C14-C15-C16-C17
25	5	315	5X6	C25-C26-C27-C28
25	5	315	5X6	C24-C25-C26-C39
25	5	315	5X6	C18-C19-C20-C21
25	5	315	5X6	C02-C03-C11-C12
25	5	315	5X6	C11-C12-C13-C14
25	5	315	5X6	C12-C13-C14-C15
25	5	315	5X6	C42-C13-C14-C15
25	5	315	5X6	C27-C28-C29-C34
25	5	315	5X6	C20-C21-C22-C40
25	5	315	5X6	C20-C21-C22-C23
25	5	315	5X6	C40-C22-C23-C24
25	5	315	5X6	C22-C23-C24-C25
25	5	316	5X6	C41-C17-C18-C19
25	5	316	5X6	C39-C26-C27-C28
25	5	316	5X6	C24-C25-C26-C39
25	5	316	5X6	C18-C19-C20-C21
25	5	316	5X6	C11-C12-C13-C14
25	5	316	5X6	C42-C13-C14-C15
25	5	316	5X6	C20-C21-C22-C40
25	5	316	5X6	C40-C22-C23-C24
25	5	317	5X6	C16-C17-C18-C19
25	5	317	5X6	C15-C16-C17-C18
25	5	317	5X6	C15-C16-C17-C41
25	5	317	5X6	C14-C15-C16-C17
25	5	317	5X6	C25-C26-C27-C28
25	5	317	5X6	C24-C25-C26-C39
25	5	317	5X6	C18-C19-C20-C21
25	5	317	5X6	C03-C11-C12-C13
25	5	317	5X6	C11-C12-C13-C14
25	5	317	5X6	C42-C13-C14-C15
25	5	317	5X6	C19-C20-C21-C22
25	5	317	5X6	C20-C21-C22-C40
25	5	317	5X6	C22-C23-C24-C25
25	5	318	5X6	C41-C17-C18-C19
25	5	318	5X6	C15-C16-C17-C41
25	5	318	5X6	C39-C26-C27-C28
25	5	318	5X6	C25-C26-C27-C28
25	5	318	5X6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	5	318	5X6	C18-C19-C20-C21
25	5	318	5X6	C11-C12-C13-C14
25	5	318	5X6	C42-C13-C14-C15
25	5	318	5X6	C26-C27-C28-C29
25	5	318	5X6	C20-C21-C22-C40
25	5	318	5X6	C22-C23-C24-C25
17	L	202	CLA	O1D-CGD-O2D-CED
17	1	307	CLA	O1D-CGD-O2D-CED
17	3	306	CLA	O1D-CGD-O2D-CED
17	4	308	CLA	O1D-CGD-O2D-CED
17	4	311	CLA	O1D-CGD-O2D-CED
17	A	859	CLA	C2C-C3C-CAC-CBC
17	A	859	CLA	C4C-C3C-CAC-CBC
17	J	103	CLA	O1D-CGD-O2D-CED
17	O	203	CLA	O1D-CGD-O2D-CED
17	O	204	CLA	O1D-CGD-O2D-CED
17	3	314	CLA	O1D-CGD-O2D-CED
17	5	304	CLA	O1D-CGD-O2D-CED
17	5	313	CLA	O1D-CGD-O2D-CED
17	B	816	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
17	J	103	CLA	CBD-CGD-O2D-CED
17	L	202	CLA	CBD-CGD-O2D-CED
17	O	203	CLA	CBD-CGD-O2D-CED
17	O	204	CLA	CBD-CGD-O2D-CED
17	1	301	CLA	CBD-CGD-O2D-CED
17	1	310	CLA	CBD-CGD-O2D-CED
17	1	311	CLA	CBD-CGD-O2D-CED
17	3	306	CLA	CBD-CGD-O2D-CED
17	3	308	CLA	CBD-CGD-O2D-CED
17	3	312	CLA	CBD-CGD-O2D-CED
17	3	314	CLA	CBD-CGD-O2D-CED
17	3	315	CLA	CBD-CGD-O2D-CED
17	4	311	CLA	CBD-CGD-O2D-CED
17	5	304	CLA	CBD-CGD-O2D-CED
17	5	307	CLA	CBD-CGD-O2D-CED
17	5	308	CLA	CBD-CGD-O2D-CED
17	B	805	CLA	O1A-CGA-O2A-C1
17	5	303	CLA	O1A-CGA-O2A-C1
17	A	859	CLA	O1D-CGD-O2D-CED
17	2	304	CLA	O1D-CGD-O2D-CED
17	4	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	5	311	CLA	O1D-CGD-O2D-CED
17	A	859	CLA	CBA-CGA-O2A-C1
22	A	848	LMT	O5B-C1B-O1B-C4'
17	1	310	CLA	O1D-CGD-O2D-CED
17	2	313	CLA	O1D-CGD-O2D-CED
17	2	314	CLA	O1D-CGD-O2D-CED
17	2	316	CLA	O1D-CGD-O2D-CED
17	5	302	CLA	O1D-CGD-O2D-CED
17	5	310	CLA	O1D-CGD-O2D-CED
17	5	312	CLA	O1D-CGD-O2D-CED
17	A	808	CLA	CBD-CGD-O2D-CED
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	CBD-CGD-O2D-CED
17	F	204	CLA	CBD-CGD-O2D-CED
17	1	303	CLA	CBD-CGD-O2D-CED
17	1	304	CLA	CBD-CGD-O2D-CED
17	2	307	CLA	CBD-CGD-O2D-CED
17	2	309	CLA	CBD-CGD-O2D-CED
17	2	312	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	CBD-CGD-O2D-CED
17	3	313	CLA	CBD-CGD-O2D-CED
17	4	307	CLA	CBD-CGD-O2D-CED
17	5	306	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	O1A-CGA-O2A-C1
17	B	831	CLA	O1A-CGA-O2A-C1
17	B	857	CLA	O1A-CGA-O2A-C1
17	O	205	CLA	O1D-CGD-O2D-CED
17	2	308	CLA	O1D-CGD-O2D-CED
17	4	309	CLA	O1D-CGD-O2D-CED
17	1	305	CLA	C4C-C3C-CAC-CBC
17	A	832	CLA	CBD-CGD-O2D-CED
17	1	305	CLA	CBD-CGD-O2D-CED
24	B	849	DGD	O1B-C1B-O2G-C2G
17	B	822	CLA	CBA-CGA-O2A-C1
17	1	305	CLA	C2C-C3C-CAC-CBC
17	A	804	CLA	C3-C5-C6-C7
17	A	812	CLA	C3-C5-C6-C7
17	A	818	CLA	C3-C5-C6-C7
17	A	819	CLA	C3-C5-C6-C7
17	A	833	CLA	C3-C5-C6-C7
17	B	810	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	B	812	CLA	C3-C5-C6-C7
17	B	813	CLA	C3-C5-C6-C7
17	K	102	CLA	C3-C5-C6-C7
17	2	307	CLA	C3-C5-C6-C7
17	5	305	CLA	C3-C5-C6-C7
17	A	810	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
17	B	832	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	CBD-CGD-O2D-CED
17	A	859	CLA	O1A-CGA-O2A-C1
22	B	852	LMT	O5'-C5'-C6'-O6'
22	F	201	LMT	O5'-C5'-C6'-O6'
17	B	818	CLA	CBD-CGD-O2D-CED
17	1	308	CLA	CBD-CGD-O2D-CED
17	4	305	CLA	CBD-CGD-O2D-CED
17	A	806	CLA	C2A-CAA-CBA-CGA
17	A	827	CLA	C2A-CAA-CBA-CGA
17	A	859	CLA	C2A-CAA-CBA-CGA
17	B	839	CLA	C2A-CAA-CBA-CGA
17	1	305	CLA	C2A-CAA-CBA-CGA
17	2	307	CLA	C2A-CAA-CBA-CGA
17	5	313	CLA	C2A-CAA-CBA-CGA
17	5	308	CLA	O1D-CGD-O2D-CED
22	A	848	LMT	C3'-C4'-O1B-C1B
17	B	822	CLA	O1A-CGA-O2A-C1
17	B	808	CLA	C3-C5-C6-C7
18	A	840	PQN	C13-C15-C16-C17
17	A	838	CLA	CBA-CGA-O2A-C1
17	B	805	CLA	CBA-CGA-O2A-C1
17	B	828	CLA	CBA-CGA-O2A-C1
17	B	831	CLA	CBA-CGA-O2A-C1
17	B	857	CLA	CBA-CGA-O2A-C1
17	3	315	CLA	CBA-CGA-O2A-C1
17	5	303	CLA	CBA-CGA-O2A-C1
17	1	301	CLA	O1D-CGD-O2D-CED
17	3	315	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	CBD-CGD-O2D-CED
17	A	813	CLA	CBD-CGD-O2D-CED
17	A	807	CLA	O1A-CGA-O2A-C1
17	A	836	CLA	O1A-CGA-O2A-C1
17	B	812	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	824	CLA	O1A-CGA-O2A-C1
17	B	828	CLA	O1A-CGA-O2A-C1
17	L	202	CLA	O1A-CGA-O2A-C1
17	3	308	CLA	O1D-CGD-O2D-CED
17	3	312	CLA	O1D-CGD-O2D-CED
25	J	105	5X6	C17-C18-C19-C20
25	1	315	5X6	C19-C20-C21-C22
25	1	316	5X6	C19-C20-C21-C22
25	2	318	5X6	C19-C20-C21-C22
25	2	318	5X6	C23-C24-C25-C26
25	2	319	5X6	C13-C14-C15-C16
25	2	319	5X6	C23-C24-C25-C26
25	2	320	5X6	C23-C24-C25-C26
25	3	316	5X6	C17-C18-C19-C20
25	4	312	5X6	C13-C14-C15-C16
25	4	314	5X6	C13-C14-C15-C16
25	5	301	5X6	C23-C24-C25-C26
25	5	317	5X6	C23-C24-C25-C26
25	5	318	5X6	C23-C24-C25-C26
17	F	204	CLA	C2C-C3C-CAC-CBC
17	1	301	CLA	C2C-C3C-CAC-CBC
17	B	810	CLA	CBD-CGD-O2D-CED
17	2	306	CLA	CBD-CGD-O2D-CED
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	838	CLA	CBA-CGA-O2A-C1
17	L	202	CLA	CBA-CGA-O2A-C1
17	L	204	CLA	CBA-CGA-O2A-C1
17	B	832	CLA	O1A-CGA-O2A-C1
17	B	816	CLA	O1D-CGD-O2D-CED
17	A	834	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	828	CLA	CBD-CGD-O2D-CED
17	L	204	CLA	CBD-CGD-O2D-CED
17	5	303	CLA	CBD-CGD-O2D-CED
22	B	852	LMT	O5B-C5B-C6B-O6B
22	F	201	LMT	O5B-C5B-C6B-O6B
17	1	309	CLA	CBD-CGD-O2D-CED
17	A	802	CLA	C3-C5-C6-C7
17	B	801	CLA	C3-C5-C6-C7
17	A	807	CLA	CBA-CGA-O2A-C1
17	B	824	CLA	CBA-CGA-O2A-C1
17	B	823	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	F	201	LMT	C4'-C5'-C6'-O6'
22	3	301	LMT	C4'-C5'-C6'-O6'
19	J	102	LHG	C2-C3-O3-P
17	A	838	CLA	O1A-CGA-O2A-C1
17	B	838	CLA	O1A-CGA-O2A-C1
17	L	204	CLA	O1A-CGA-O2A-C1
17	3	315	CLA	O1A-CGA-O2A-C1
17	A	806	CLA	C13-C15-C16-C17
22	B	851	LMT	O5'-C5'-C6'-O6'
17	A	815	CLA	C4-C3-C5-C6
17	B	802	CLA	C4-C3-C5-C6
17	B	807	CLA	C4-C3-C5-C6
17	B	813	CLA	C4-C3-C5-C6
17	B	815	CLA	C4-C3-C5-C6
17	B	817	CLA	C4-C3-C5-C6
22	B	852	LMT	C4'-C5'-C6'-O6'
17	A	815	CLA	C2-C3-C5-C6
17	A	834	CLA	C2-C3-C5-C6
17	B	802	CLA	C2-C3-C5-C6
17	B	807	CLA	C2-C3-C5-C6
17	B	813	CLA	C2-C3-C5-C6
17	B	815	CLA	C2-C3-C5-C6
17	B	817	CLA	C2-C3-C5-C6
17	A	808	CLA	O1D-CGD-O2D-CED
17	B	830	CLA	O1D-CGD-O2D-CED
17	1	311	CLA	O1D-CGD-O2D-CED
17	5	307	CLA	O1D-CGD-O2D-CED
22	B	852	LMT	O5'-C1'-O1'-C1
17	B	816	CLA	CBA-CGA-O2A-C1
17	4	307	CLA	O1D-CGD-O2D-CED
17	F	204	CLA	O1D-CGD-O2D-CED
17	2	312	CLA	O1D-CGD-O2D-CED
17	B	816	CLA	O1A-CGA-O2A-C1
17	5	306	CLA	O1D-CGD-O2D-CED
17	A	802	CLA	CBA-CGA-O2A-C1
17	A	808	CLA	CBA-CGA-O2A-C1
17	A	821	CLA	CBA-CGA-O2A-C1
17	A	822	CLA	CBA-CGA-O2A-C1
17	A	839	CLA	CBA-CGA-O2A-C1
17	B	802	CLA	CBA-CGA-O2A-C1
17	B	815	CLA	CBA-CGA-O2A-C1
17	B	835	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	F	205	5X6	C23-C24-C25-C26
25	J	105	5X6	C19-C20-C21-C22
17	1	308	CLA	C2C-C3C-CAC-CBC
17	5	305	CLA	C10-C11-C12-C13
17	2	308	CLA	C2C-C3C-CAC-CBC
17	A	826	CLA	C10-C11-C12-C13
17	A	827	CLA	C13-C15-C16-C17
17	B	820	CLA	C8-C10-C11-C12
17	B	826	CLA	C10-C11-C12-C13
17	B	828	CLA	C15-C16-C17-C18
17	B	841	CLA	C13-C15-C16-C17
19	J	102	LHG	O2-C2-C3-O3
19	J	102	LHG	C23-C24-C25-C26
17	A	828	CLA	CBA-CGA-O2A-C1
17	A	821	CLA	O1A-CGA-O2A-C1
17	A	822	CLA	O1A-CGA-O2A-C1
17	A	839	CLA	O1A-CGA-O2A-C1
22	3	301	LMT	O5'-C5'-C6'-O6'
17	B	837	CLA	C4-C3-C5-C6
22	L	207	LMT	C4B-C5B-C6B-O6B
17	A	839	CLA	C11-C10-C8-C9
17	B	804	CLA	C14-C13-C15-C16
17	B	807	CLA	C6-C7-C8-C9
17	B	808	CLA	C11-C10-C8-C9
17	B	809	CLA	C6-C7-C8-C9
17	B	810	CLA	C11-C12-C13-C14
17	B	811	CLA	C11-C10-C8-C9
17	B	812	CLA	C6-C7-C8-C9
17	B	814	CLA	C11-C10-C8-C9
17	B	818	CLA	C11-C10-C8-C9
17	B	830	CLA	C6-C7-C8-C9
17	B	812	CLA	O1D-CGD-O2D-CED
17	2	307	CLA	O1D-CGD-O2D-CED
17	2	309	CLA	O1D-CGD-O2D-CED
17	2	311	CLA	CBD-CGD-O2D-CED
17	A	818	CLA	C2A-CAA-CBA-CGA
20	A	857	BCR	C11-C12-C13-C35
20	B	844	BCR	C36-C18-C19-C20
20	L	201	BCR	C37-C22-C23-C24
20	L	206	BCR	C7-C8-C9-C34
20	M	101	BCR	C7-C8-C9-C34
25	J	105	5X6	C11-C12-C13-C42

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Mol	Chain	Res	Type	Atoms
25	1	312	5X6	C39-C26-C27-C28
25	1	313	5X6	C15-C16-C17-C41
25	1	313	5X6	C40-C22-C23-C24
25	1	314	5X6	C40-C22-C23-C24
25	1	315	5X6	C39-C26-C27-C28
25	1	316	5X6	C39-C26-C27-C28
25	1	316	5X6	C11-C12-C13-C42
25	2	319	5X6	C11-C12-C13-C42
25	2	320	5X6	C40-C22-C23-C24
25	2	321	5X6	C15-C16-C17-C41
25	3	316	5X6	C40-C22-C23-C24
25	3	317	5X6	C15-C16-C17-C41
25	3	317	5X6	C40-C22-C23-C24
25	3	318	5X6	C15-C16-C17-C41
25	3	318	5X6	C11-C12-C13-C42
25	3	318	5X6	C40-C22-C23-C24
25	4	312	5X6	C40-C22-C23-C24
25	4	313	5X6	C15-C16-C17-C41
25	4	313	5X6	C39-C26-C27-C28
25	4	313	5X6	C11-C12-C13-C42
25	4	314	5X6	C39-C26-C27-C28
25	4	314	5X6	C11-C12-C13-C42
25	5	301	5X6	C15-C16-C17-C41
25	5	301	5X6	C40-C22-C23-C24
25	5	315	5X6	C15-C16-C17-C41
25	5	315	5X6	C39-C26-C27-C28
25	5	316	5X6	C15-C16-C17-C41
25	5	317	5X6	C39-C26-C27-C28
25	5	317	5X6	C11-C12-C13-C42
25	5	317	5X6	C40-C22-C23-C24
25	5	318	5X6	C11-C12-C13-C42
20	B	845	BCR	C7-C8-C9-C10
20	L	206	BCR	C7-C8-C9-C10
25	F	205	5X6	C25-C26-C27-C28
25	F	205	5X6	C21-C22-C23-C24
25	J	105	5X6	C25-C26-C27-C28
25	1	314	5X6	C11-C12-C13-C14
25	1	315	5X6	C11-C12-C13-C14
25	1	315	5X6	C21-C22-C23-C24
25	2	320	5X6	C11-C12-C13-C14
25	4	312	5X6	C25-C26-C27-C28
22	B	850	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	B	851	LMT	C4'-C5'-C6'-O6'
17	B	802	CLA	O1A-CGA-O2A-C1
17	A	809	CLA	C10-C11-C12-C13
17	B	816	CLA	C10-C11-C12-C13
17	B	833	CLA	C15-C16-C17-C18
17	B	802	CLA	CBD-CGD-O2D-CED
22	3	301	LMT	C4B-C5B-C6B-O6B
17	A	820	CLA	C3-C5-C6-C7
17	B	820	CLA	C3-C5-C6-C7
17	A	855	CLA	C10-C11-C12-C13
17	B	808	CLA	C13-C15-C16-C17
17	B	812	CLA	C15-C16-C17-C18
17	B	839	CLA	C13-C15-C16-C17
24	B	849	DGD	O6E-C5E-C6E-O5E
17	3	310	CLA	O1D-CGD-O2D-CED
17	A	820	CLA	C15-C16-C17-C18
17	A	834	CLA	C8-C10-C11-C12
17	B	804	CLA	C15-C16-C17-C18
17	B	805	CLA	C13-C15-C16-C17
17	B	831	CLA	C5-C6-C7-C8
17	B	831	CLA	C10-C11-C12-C13
17	B	832	CLA	C5-C6-C7-C8
17	B	832	CLA	C8-C10-C11-C12
17	B	834	CLA	C10-C11-C12-C13
17	L	203	CLA	C13-C15-C16-C17
17	2	311	CLA	C5-C6-C7-C8
17	5	303	CLA	C15-C16-C17-C18
17	1	303	CLA	O1D-CGD-O2D-CED
19	A	842	LHG	O1-C1-C2-O2
17	A	808	CLA	O1A-CGA-O2A-C1
19	J	102	LHG	C7-C8-C9-C10
17	A	834	CLA	C15-C16-C17-C18
17	A	855	CLA	C8-C10-C11-C12
17	L	203	CLA	C8-C10-C11-C12
19	J	102	LHG	C24-C23-O8-C6
17	A	832	CLA	O1D-CGD-O2D-CED
17	1	305	CLA	O1D-CGD-O2D-CED
17	3	313	CLA	O1D-CGD-O2D-CED
17	A	812	CLA	C2-C1-O2A-CGA
17	B	802	CLA	C2-C1-O2A-CGA
17	4	304	CLA	C2-C1-O2A-CGA
17	A	804	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C10-C11-C12-C13
17	A	839	CLA	C10-C11-C12-C13
17	B	804	CLA	C8-C10-C11-C12
17	L	203	CLA	C5-C6-C7-C8
18	A	840	PQN	C18-C20-C21-C22
24	B	849	DGD	C1B-C2B-C3B-C4B
17	A	855	CLA	CBD-CGD-O2D-CED
17	L	202	CLA	C8-C10-C11-C12
17	1	301	CLA	C4C-C3C-CAC-CBC
17	A	804	CLA	C11-C12-C13-C15
17	A	817	CLA	C11-C10-C8-C7
17	B	819	CLA	C11-C10-C8-C7
17	5	308	CLA	C12-C13-C15-C16
17	B	827	CLA	C3-C5-C6-C7
25	1	314	5X6	C17-C18-C19-C20
25	4	314	5X6	C19-C20-C21-C22
25	5	318	5X6	C19-C20-C21-C22
17	K	103	CLA	CBD-CGD-O2D-CED
17	A	820	CLA	C2A-CAA-CBA-CGA
17	B	805	CLA	C2A-CAA-CBA-CGA
17	1	301	CLA	C2A-CAA-CBA-CGA
17	B	810	CLA	O1D-CGD-O2D-CED
17	1	304	CLA	O1D-CGD-O2D-CED
17	A	807	CLA	C5-C6-C7-C8
17	B	808	CLA	C10-C11-C12-C13
17	B	836	CLA	C8-C10-C11-C12
17	A	802	CLA	O1A-CGA-O2A-C1
17	B	815	CLA	O1A-CGA-O2A-C1
20	K	104	BCR	C18-C19-C20-C21
20	M	101	BCR	C10-C11-C12-C13
25	J	105	5X6	C14-C15-C16-C17
25	J	105	5X6	C22-C23-C24-C25
25	1	316	5X6	C14-C15-C16-C17
25	4	313	5X6	C14-C15-C16-C17
25	5	301	5X6	C14-C15-C16-C17
25	5	316	5X6	C22-C23-C24-C25
17	B	809	CLA	C3-C5-C6-C7
17	A	803	CLA	C5-C6-C7-C8
17	B	806	CLA	C15-C16-C17-C18
17	B	825	CLA	C15-C16-C17-C18
17	B	837	CLA	C5-C6-C7-C8
17	A	812	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	A	826	CLA	C13-C15-C16-C17
17	B	802	CLA	C8-C10-C11-C12
17	B	811	CLA	C13-C15-C16-C17
17	B	812	CLA	C10-C11-C12-C13
17	B	836	CLA	C5-C6-C7-C8
17	L	202	CLA	C5-C6-C7-C8
17	A	828	CLA	O1A-CGA-O2A-C1
19	J	102	LHG	O10-C23-O8-C6
19	A	842	LHG	C8-C7-O7-C5
17	A	826	CLA	C8-C10-C11-C12
17	A	856	CLA	C13-C15-C16-C17
17	B	840	CLA	C13-C15-C16-C17
17	5	305	CLA	C15-C16-C17-C18
17	B	814	CLA	C2C-C3C-CAC-CBC
17	A	834	CLA	CBA-CGA-O2A-C1
24	B	849	DGD	C2A-C1A-O1G-C1G
17	4	303	CLA	C2C-C3C-CAC-CBC
17	A	820	CLA	C10-C11-C12-C13
17	B	826	CLA	C13-C15-C16-C17
17	3	305	CLA	C13-C15-C16-C17
17	4	305	CLA	O1D-CGD-O2D-CED
19	A	842	LHG	O9-C7-O7-C5
17	B	814	CLA	C8-C10-C11-C12
17	5	302	CLA	C2C-C3C-CAC-CBC
17	A	831	CLA	C3-C5-C6-C7
17	A	804	CLA	O1D-CGD-O2D-CED
17	1	308	CLA	O1D-CGD-O2D-CED
17	B	839	CLA	CBA-CGA-O2A-C1
17	O	204	CLA	CBA-CGA-O2A-C1
17	5	314	CLA	CBA-CGA-O2A-C1
17	B	832	CLA	C13-C15-C16-C17
17	B	801	CLA	C15-C16-C17-C18
25	1	315	5X6	C17-C18-C19-C20
25	1	315	5X6	C23-C24-C25-C26
25	2	319	5X6	C17-C18-C19-C20
25	2	321	5X6	C17-C18-C19-C20
25	2	321	5X6	C19-C20-C21-C22
25	5	301	5X6	C19-C20-C21-C22
25	5	317	5X6	C17-C18-C19-C20
22	F	201	LMT	C4B-C5B-C6B-O6B
22	L	207	LMT	C5-C6-C7-C8
20	A	843	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
20	A	845	BCR	C20-C21-C22-C37
20	A	857	BCR	C20-C21-C22-C37
20	B	803	BCR	C11-C10-C9-C34
20	B	846	BCR	C11-C10-C9-C34
20	B	847	BCR	C11-C10-C9-C34
20	I	101	BCR	C16-C17-C18-C36
20	K	104	BCR	C16-C17-C18-C36
25	F	205	5X6	C41-C17-C18-C19
25	1	315	5X6	C24-C25-C26-C39
25	2	320	5X6	C24-C25-C26-C39
25	5	317	5X6	C41-C17-C18-C19
24	B	849	DGD	C4A-C5A-C6A-C7A
22	B	852	LMT	C4B-C5B-C6B-O6B
17	A	813	CLA	O1D-CGD-O2D-CED
17	2	307	CLA	C6-C7-C8-C9
17	A	829	CLA	CBA-CGA-O2A-C1
17	5	309	CLA	CBA-CGA-O2A-C1
24	B	849	DGD	C2A-C3A-C4A-C5A
17	B	818	CLA	O1D-CGD-O2D-CED
17	2	306	CLA	O1D-CGD-O2D-CED
20	A	843	BCR	C20-C21-C22-C23
20	B	803	BCR	C11-C10-C9-C8
20	B	846	BCR	C11-C10-C9-C8
20	B	847	BCR	C11-C10-C9-C8
20	B	848	BCR	C20-C21-C22-C23
20	I	101	BCR	C16-C17-C18-C19
20	K	104	BCR	C16-C17-C18-C19
25	F	205	5X6	C16-C17-C18-C19
25	J	105	5X6	C24-C25-C26-C27
25	1	316	5X6	C16-C17-C18-C19
25	1	316	5X6	C24-C25-C26-C27
25	2	321	5X6	C12-C13-C14-C15
25	3	316	5X6	C12-C13-C14-C15
25	3	317	5X6	C12-C13-C14-C15
25	3	318	5X6	C16-C17-C18-C19
25	3	318	5X6	C24-C25-C26-C27
25	4	312	5X6	C12-C13-C14-C15
25	4	313	5X6	C24-C25-C26-C27
25	4	314	5X6	C12-C13-C14-C15
25	5	301	5X6	C16-C17-C18-C19
25	5	316	5X6	C12-C13-C14-C15
25	5	316	5X6	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	5	318	5X6	C20-C21-C22-C23
17	A	816	CLA	C15-C16-C17-C18
17	B	815	CLA	C8-C10-C11-C12
17	5	305	CLA	C8-C10-C11-C12
18	A	840	PQN	C15-C16-C17-C18
17	B	839	CLA	O1A-CGA-O2A-C1
22	L	207	LMT	O5B-C5B-C6B-O6B
17	A	832	CLA	C4-C3-C5-C6
22	L	207	LMT	C6-C7-C8-C9
24	B	849	DGD	CAA-CBA-CCA-CDA
24	B	849	DGD	C9B-CAB-CBB-CCB
17	A	823	CLA	C11-C10-C8-C9
17	A	826	CLA	C14-C13-C15-C16
17	B	801	CLA	C11-C12-C13-C14
17	B	802	CLA	C11-C12-C13-C14
17	B	811	CLA	C11-C12-C13-C14
17	5	308	CLA	C14-C13-C15-C16
22	3	301	LMT	C7-C8-C9-C10
24	B	849	DGD	CEA-CFA-CGA-CHA
17	A	856	CLA	C8-C10-C11-C12
17	B	841	CLA	C15-C16-C17-C18
17	B	818	CLA	C2A-CAA-CBA-CGA
17	5	308	CLA	C2A-CAA-CBA-CGA
25	F	205	5X6	C11-C12-C13-C42
25	1	312	5X6	C15-C16-C17-C41
25	1	313	5X6	C39-C26-C27-C28
25	1	314	5X6	C39-C26-C27-C28
25	1	316	5X6	C15-C16-C17-C41
25	1	316	5X6	C40-C22-C23-C24
25	2	318	5X6	C40-C22-C23-C24
25	2	319	5X6	C15-C16-C17-C41
25	2	319	5X6	C40-C22-C23-C24
25	2	320	5X6	C15-C16-C17-C41
25	3	318	5X6	C39-C26-C27-C28
25	4	314	5X6	C40-C22-C23-C24
25	5	315	5X6	C11-C12-C13-C42
25	5	318	5X6	C40-C22-C23-C24
20	O	202	BCR	C7-C8-C9-C10
25	1	316	5X6	C11-C12-C13-C14
25	2	320	5X6	C21-C22-C23-C24
25	2	321	5X6	C11-C12-C13-C14
25	3	317	5X6	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	3	317	5X6	C21-C22-C23-C24
25	3	318	5X6	C21-C22-C23-C24
25	4	312	5X6	C11-C12-C13-C14
17	B	838	CLA	C2-C1-O2A-CGA
22	B	852	LMT	C6-C7-C8-C9
24	B	849	DGD	C7A-C8A-C9A-CAA
17	B	805	CLA	C16-C17-C18-C19
17	B	805	CLA	C16-C17-C18-C20
17	2	307	CLA	C6-C7-C8-C10
17	5	309	CLA	C13-C15-C16-C17
19	J	102	LHG	C25-C26-C27-C28
19	J	102	LHG	C26-C27-C28-C29
17	B	810	CLA	C15-C16-C17-C18
17	5	314	CLA	O1A-CGA-O2A-C1
17	F	204	CLA	C4C-C3C-CAC-CBC
17	A	834	CLA	O1D-CGD-O2D-CED
17	B	840	CLA	O1D-CGD-O2D-CED
17	A	831	CLA	C3A-C2A-CAA-CBA
17	B	806	CLA	C3A-C2A-CAA-CBA
17	1	311	CLA	C3A-C2A-CAA-CBA
17	2	307	CLA	C3A-C2A-CAA-CBA
17	2	309	CLA	C3A-C2A-CAA-CBA
17	3	315	CLA	C3A-C2A-CAA-CBA
17	4	305	CLA	C3A-C2A-CAA-CBA
17	4	311	CLA	C3A-C2A-CAA-CBA
17	5	311	CLA	C3A-C2A-CAA-CBA
22	F	201	LMT	C2-C1-O1'-C1'
17	1	308	CLA	C4C-C3C-CAC-CBC
19	J	102	LHG	C17-C18-C19-C20
17	A	834	CLA	O1A-CGA-O2A-C1
17	O	204	CLA	O1A-CGA-O2A-C1
17	2	313	CLA	C2C-C3C-CAC-CBC
19	J	102	LHG	C16-C17-C18-C19
22	A	848	LMT	C1-C2-C3-C4
25	1	313	5X6	C18-C19-C20-C21
19	A	841	LHG	C29-C30-C31-C32
17	B	827	CLA	CBA-CGA-O2A-C1
17	5	304	CLA	CBA-CGA-O2A-C1
17	A	825	CLA	C2-C3-C5-C6
22	3	301	LMT	C1-C2-C3-C4
17	5	312	CLA	C2A-CAA-CBA-CGA
24	B	849	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
17	A	833	CLA	C8-C10-C11-C12
24	B	849	DGD	CDA-CEA-CFA-CGA
22	3	301	LMT	O5B-C5B-C6B-O6B
22	F	201	LMT	C1-C2-C3-C4
17	A	829	CLA	O1A-CGA-O2A-C1
17	5	309	CLA	O1A-CGA-O2A-C1
19	A	841	LHG	C18-C19-C20-C21
19	A	842	LHG	C24-C25-C26-C27
17	A	820	CLA	C2-C1-O2A-CGA
17	B	828	CLA	C2-C1-O2A-CGA
17	B	857	CLA	C2-C1-O2A-CGA
17	2	308	CLA	C4C-C3C-CAC-CBC
19	A	841	LHG	C11-C12-C13-C14
22	A	848	LMT	O1'-C1-C2-C3
22	B	852	LMT	C3-C4-C5-C6
17	A	817	CLA	C15-C16-C17-C18
19	A	842	LHG	C7-C8-C9-C10
17	1	303	CLA	C3-C5-C6-C7
20	A	843	BCR	C1-C6-C7-C8
20	A	843	BCR	C23-C24-C25-C30
20	A	844	BCR	C23-C24-C25-C26
20	A	845	BCR	C23-C24-C25-C26
20	A	845	BCR	C23-C24-C25-C30
20	B	847	BCR	C23-C24-C25-C26
20	B	847	BCR	C23-C24-C25-C30
20	J	104	BCR	C23-C24-C25-C26
20	J	104	BCR	C23-C24-C25-C30
20	L	201	BCR	C1-C6-C7-C8
20	L	201	BCR	C5-C6-C7-C8
20	L	201	BCR	C23-C24-C25-C26
20	L	201	BCR	C23-C24-C25-C30
20	L	206	BCR	C23-C24-C25-C26
20	M	101	BCR	C5-C6-C7-C8
25	F	205	5X6	C04-C03-C11-C12
25	J	105	5X6	C27-C28-C29-C34
25	1	314	5X6	C02-C03-C11-C12
25	1	315	5X6	C04-C03-C11-C12
25	1	315	5X6	C27-C28-C29-C34
25	1	316	5X6	C04-C03-C11-C12
25	2	317	5X6	C27-C28-C29-C34
25	2	318	5X6	C02-C03-C11-C12
25	2	319	5X6	C04-C03-C11-C12

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Mol	Chain	Res	Type	Atoms
25	2	320	5X6	C04-C03-C11-C12
25	2	321	5X6	C27-C28-C29-C30
25	3	317	5X6	C02-C03-C11-C12
25	3	318	5X6	C02-C03-C11-C12
25	4	313	5X6	C27-C28-C29-C34
25	4	314	5X6	C27-C28-C29-C30
25	5	301	5X6	C02-C03-C11-C12
25	5	315	5X6	C27-C28-C29-C30
25	5	316	5X6	C27-C28-C29-C30
25	5	317	5X6	C02-C03-C11-C12
25	5	318	5X6	C02-C03-C11-C12
17	B	814	CLA	C4C-C3C-CAC-CBC
17	B	815	CLA	C13-C15-C16-C17
17	B	840	CLA	C8-C10-C11-C12
17	B	815	CLA	O1D-CGD-O2D-CED
17	4	303	CLA	CBD-CGD-O2D-CED
17	A	815	CLA	C10-C11-C12-C13
17	A	825	CLA	C4-C3-C5-C6
17	A	804	CLA	C11-C10-C8-C7
17	A	823	CLA	C11-C10-C8-C7
17	A	832	CLA	C2-C3-C5-C6
17	B	802	CLA	C11-C12-C13-C15
17	B	811	CLA	C11-C12-C13-C15
17	B	814	CLA	C11-C10-C8-C7
17	B	837	CLA	C2-C3-C5-C6
17	5	305	CLA	C12-C13-C15-C16
17	A	826	CLA	C15-C16-C17-C18
17	A	834	CLA	C13-C15-C16-C17
17	B	815	CLA	C10-C11-C12-C13
17	5	308	CLA	C10-C11-C12-C13
25	4	312	5X6	C19-C20-C21-C22
17	5	303	CLA	O1D-CGD-O2D-CED
17	A	825	CLA	CBA-CGA-O2A-C1
17	A	830	CLA	CBA-CGA-O2A-C1
17	L	203	CLA	C2A-CAA-CBA-CGA
17	A	855	CLA	C5-C6-C7-C8
22	3	301	LMT	C3-C4-C5-C6
24	B	849	DGD	C6A-C7A-C8A-C9A
17	1	309	CLA	O1D-CGD-O2D-CED
17	A	855	CLA	O1D-CGD-O2D-CED
17	L	204	CLA	O1D-CGD-O2D-CED
19	J	102	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	F	201	LMT	C7-C8-C9-C10
22	F	201	LMT	O1'-C1-C2-C3
25	1	313	5X6	C26-C27-C28-C29
25	1	314	5X6	C03-C11-C12-C13
25	3	317	5X6	C26-C27-C28-C29
25	4	313	5X6	C03-C11-C12-C13
17	5	304	CLA	O1A-CGA-O2A-C1
17	2	311	CLA	O1D-CGD-O2D-CED
17	3	305	CLA	CBD-CGD-O2D-CED
17	5	303	CLA	C3-C5-C6-C7
17	B	816	CLA	C13-C15-C16-C17
22	L	207	LMT	C3-C4-C5-C6
17	A	833	CLA	C10-C11-C12-C13
22	B	850	LMT	C7-C8-C9-C10
17	A	804	CLA	C11-C12-C13-C14
17	B	815	CLA	C11-C10-C8-C9
17	B	833	CLA	C14-C13-C15-C16
24	B	849	DGD	CEB-CFB-CGB-CHB
17	A	834	CLA	C3-C5-C6-C7
17	A	853	CLA	C2A-CAA-CBA-CGA
20	B	844	BCR	C37-C22-C23-C24
20	B	845	BCR	C11-C12-C13-C35
25	1	315	5X6	C11-C12-C13-C42
25	2	317	5X6	C11-C12-C13-C42
25	2	318	5X6	C11-C12-C13-C42
25	3	316	5X6	C11-C12-C13-C42
17	B	833	CLA	C5-C6-C7-C8
20	B	848	BCR	C7-C8-C9-C10
17	A	825	CLA	O1A-CGA-O2A-C1
17	B	827	CLA	O1A-CGA-O2A-C1
17	A	816	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	C1A-C2A-CAA-CBA
17	B	828	CLA	C1A-C2A-CAA-CBA
17	B	831	CLA	C1A-C2A-CAA-CBA
17	1	304	CLA	C1A-C2A-CAA-CBA
17	1	310	CLA	C1A-C2A-CAA-CBA
17	1	311	CLA	C1A-C2A-CAA-CBA
17	2	304	CLA	C1A-C2A-CAA-CBA
17	2	309	CLA	C1A-C2A-CAA-CBA
17	2	311	CLA	C1A-C2A-CAA-CBA
17	3	310	CLA	C1A-C2A-CAA-CBA
17	3	311	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	3	315	CLA	C1A-C2A-CAA-CBA
17	4	304	CLA	C1A-C2A-CAA-CBA
17	4	305	CLA	C1A-C2A-CAA-CBA
17	4	306	CLA	C1A-C2A-CAA-CBA
17	4	311	CLA	C1A-C2A-CAA-CBA
17	5	308	CLA	C1A-C2A-CAA-CBA
17	5	311	CLA	C1A-C2A-CAA-CBA
25	1	313	5X6	C23-C24-C25-C26
25	3	316	5X6	C19-C20-C21-C22
19	A	841	LHG	C4-O6-P-O3
17	A	837	CLA	C3-C5-C6-C7
17	B	828	CLA	O1D-CGD-O2D-CED
17	B	835	CLA	O1D-CGD-O2D-CED
24	B	849	DGD	C3B-C4B-C5B-C6B
17	B	807	CLA	C8-C10-C11-C12
17	A	831	CLA	CBA-CGA-O2A-C1
17	B	817	CLA	CBA-CGA-O2A-C1
17	4	304	CLA	CBA-CGA-O2A-C1
22	A	848	LMT	O5B-C5B-C6B-O6B
24	B	849	DGD	C3A-C4A-C5A-C6A
17	B	812	CLA	C8-C10-C11-C12
17	B	828	CLA	C13-C15-C16-C17
17	A	802	CLA	CBD-CGD-O2D-CED
19	A	842	LHG	C24-C23-O8-C6
17	A	813	CLA	C3A-C2A-CAA-CBA
17	A	830	CLA	O1A-CGA-O2A-C1
17	2	311	CLA	O1A-CGA-O2A-C1
17	1	302	CLA	C3-C5-C6-C7
17	A	812	CLA	C5-C6-C7-C8
17	5	305	CLA	CAA-CBA-CGA-O2A
17	B	830	CLA	C3-C5-C6-C7
17	B	817	CLA	O1A-CGA-O2A-C1
17	4	303	CLA	C4C-C3C-CAC-CBC
17	5	302	CLA	C4C-C3C-CAC-CBC
17	A	812	CLA	C15-C16-C17-C18
20	B	803	BCR	C16-C17-C18-C36
20	B	848	BCR	C20-C21-C22-C37
25	4	313	5X6	C20-C21-C22-C40
17	B	829	CLA	C4-C3-C5-C6
17	B	833	CLA	C4-C3-C5-C6
17	B	837	CLA	CBA-CGA-O2A-C1
17	2	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	5	305	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	C10-C11-C12-C13
22	B	851	LMT	O5B-C5B-C6B-O6B
17	B	820	CLA	C5-C6-C7-C8
17	B	833	CLA	C13-C15-C16-C17
17	A	829	CLA	C2-C1-O2A-CGA
17	A	853	CLA	C2-C1-O2A-CGA
17	B	824	CLA	C2-C1-O2A-CGA
17	B	832	CLA	C2-C1-O2A-CGA
17	1	303	CLA	C2-C1-O2A-CGA
17	5	304	CLA	C2-C1-O2A-CGA
17	B	809	CLA	C8-C10-C11-C12
17	5	305	CLA	C5-C6-C7-C8
17	1	307	CLA	CBA-CGA-O2A-C1
17	A	827	CLA	C5-C6-C7-C8
19	A	842	LHG	O10-C23-O8-C6
17	A	839	CLA	C3-C5-C6-C7
17	A	823	CLA	C10-C11-C12-C13
20	A	845	BCR	C20-C21-C22-C23
20	A	857	BCR	C20-C21-C22-C23
19	A	842	LHG	O7-C5-C6-O8
24	B	849	DGD	O2G-C2G-C3G-O3G
17	A	828	CLA	C10-C11-C12-C13
17	A	807	CLA	C4-C3-C5-C6
17	1	306	CLA	C4-C3-C5-C6
19	J	102	LHG	C29-C30-C31-C32
17	B	839	CLA	C15-C16-C17-C18
17	A	807	CLA	C12-C13-C15-C16
17	A	811	CLA	C11-C10-C8-C7
17	A	818	CLA	C11-C12-C13-C15
17	B	810	CLA	C11-C10-C8-C7
17	B	815	CLA	C11-C10-C8-C7
17	B	816	CLA	C6-C7-C8-C10
17	B	828	CLA	C6-C7-C8-C10
17	B	833	CLA	C2-C3-C5-C6
17	B	833	CLA	C12-C13-C15-C16
17	5	309	CLA	C6-C7-C8-C10
17	A	831	CLA	O1A-CGA-O2A-C1
17	A	818	CLA	C11-C12-C13-C14
17	B	816	CLA	C6-C7-C8-C9
17	5	305	CLA	C14-C13-C15-C16
17	5	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	5	309	CLA	C6-C7-C8-C9
20	B	847	BCR	C14-C15-C16-C17
19	A	841	LHG	C13-C14-C15-C16
17	B	830	CLA	CBA-CGA-O2A-C1
20	A	843	BCR	C7-C8-C9-C34
20	J	104	BCR	C37-C22-C23-C24
18	B	842	PQN	C15-C16-C17-C18
17	B	857	CLA	C10-C11-C12-C13
17	B	834	CLA	CBA-CGA-O2A-C1
19	A	841	LHG	C17-C18-C19-C20
25	2	317	5X6	C03-C11-C12-C13
17	A	807	CLA	C8-C10-C11-C12
17	B	815	CLA	C5-C6-C7-C8
17	B	826	CLA	C5-C6-C7-C8
22	A	848	LMT	C5-C6-C7-C8
17	A	819	CLA	CBA-CGA-O2A-C1
17	B	818	CLA	C4-C3-C5-C6
17	A	807	CLA	C2-C3-C5-C6
17	B	829	CLA	C2-C3-C5-C6
17	1	306	CLA	C2-C3-C5-C6
17	A	802	CLA	O1D-CGD-O2D-CED
17	4	303	CLA	O1D-CGD-O2D-CED
17	A	812	CLA	CBA-CGA-O2A-C1
17	B	806	CLA	CBA-CGA-O2A-C1
17	B	826	CLA	CBA-CGA-O2A-C1
22	A	848	LMT	C5'-C4'-O1B-C1B
17	B	828	CLA	C3A-C2A-CAA-CBA
17	K	102	CLA	C3A-C2A-CAA-CBA
22	B	852	LMT	C2-C1-O1'-C1'
22	L	207	LMT	C2-C3-C4-C5
17	A	824	CLA	CBA-CGA-O2A-C1
17	4	304	CLA	C11-C12-C13-C14
17	B	826	CLA	C15-C16-C17-C18
17	5	305	CLA	O1D-CGD-O2D-CED
19	A	842	LHG	C4-C5-C6-O8
17	A	810	CLA	C5-C6-C7-C8
17	B	837	CLA	O1A-CGA-O2A-C1
22	B	851	LMT	C3-C4-C5-C6
17	K	103	CLA	O1D-CGD-O2D-CED
17	5	309	CLA	C10-C11-C12-C13
17	4	304	CLA	O1A-CGA-O2A-C1
22	B	850	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
17	B	802	CLA	O1D-CGD-O2D-CED
17	B	816	CLA	C3-C5-C6-C7
17	B	825	CLA	C3-C5-C6-C7
17	4	303	CLA	C2A-CAA-CBA-CGA
17	5	313	CLA	C2C-C3C-CAC-CBC
17	B	830	CLA	O1A-CGA-O2A-C1
22	B	850	LMT	C6-C7-C8-C9
22	3	301	LMT	C2-C3-C4-C5
17	B	826	CLA	C3-C5-C6-C7
17	A	809	CLA	C16-C17-C18-C19
17	2	311	CLA	C3-C5-C6-C7
17	B	804	CLA	C2-C1-O2A-CGA
17	B	817	CLA	C2-C1-O2A-CGA
17	B	837	CLA	C2-C1-O2A-CGA
17	B	818	CLA	C2-C3-C5-C6
17	A	827	CLA	C15-C16-C17-C18
17	A	852	CLA	C15-C16-C17-C18
17	B	818	CLA	C5-C6-C7-C8
17	A	812	CLA	C11-C12-C13-C14
17	B	810	CLA	C11-C10-C8-C9
17	4	304	CLA	C6-C7-C8-C9
19	J	102	LHG	C35-C36-C37-C38
17	A	820	CLA	CBD-CGD-O2D-CED
22	B	850	LMT	C4'-C5'-C6'-O6'
17	A	833	CLA	C15-C16-C17-C18
17	B	814	CLA	C5-C6-C7-C8
17	B	834	CLA	O1A-CGA-O2A-C1
17	3	314	CLA	C2A-CAA-CBA-CGA
17	4	304	CLA	C2A-CAA-CBA-CGA
17	A	806	CLA	C16-C17-C18-C19
20	M	101	BCR	C1-C6-C7-C8
25	1	316	5X6	C27-C28-C29-C30
25	5	316	5X6	C04-C03-C11-C12
25	5	316	5X6	C27-C28-C29-C34
18	A	840	PQN	C20-C21-C22-C23
20	B	848	BCR	C7-C8-C9-C34
25	2	321	5X6	C15-C16-C17-C18
25	5	301	5X6	C25-C26-C27-C28
19	A	842	LHG	C13-C14-C15-C16
17	1	303	CLA	C6-C7-C8-C9
22	B	851	LMT	C11-C10-C9-C8
17	1	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	819	CLA	C4-C3-C5-C6
17	A	816	CLA	C12-C13-C15-C16
17	A	826	CLA	C6-C7-C8-C10
17	A	833	CLA	C11-C12-C13-C15
17	B	804	CLA	C12-C13-C15-C16
17	B	808	CLA	C11-C10-C8-C7
17	B	816	CLA	C11-C10-C8-C7
17	B	820	CLA	C11-C12-C13-C15
17	B	826	CLA	C6-C7-C8-C10
17	B	831	CLA	C11-C10-C8-C7
17	B	836	CLA	C6-C7-C8-C10
17	B	832	CLA	C15-C16-C17-C18
25	1	314	5X6	C19-C20-C21-C22
25	1	314	5X6	C13-C14-C15-C16
25	1	314	5X6	C23-C24-C25-C26
25	5	317	5X6	C13-C14-C15-C16
17	A	828	CLA	C16-C17-C18-C19
17	B	811	CLA	CBA-CGA-O2A-C1
17	K	102	CLA	C2A-CAA-CBA-CGA
19	A	841	LHG	C14-C15-C16-C17
22	3	301	LMT	C5-C6-C7-C8
20	B	847	BCR	C20-C21-C22-C37
20	J	104	BCR	C20-C21-C22-C37
20	M	101	BCR	C35-C13-C14-C15
20	M	101	BCR	C20-C21-C22-C37
24	B	849	DGD	CBA-CCA-CDA-CEA
22	B	850	LMT	C1-C2-C3-C4
18	B	842	PQN	C25-C26-C27-C28
17	B	804	CLA	C13-C15-C16-C17
17	B	834	CLA	C8-C10-C11-C12
17	4	306	CLA	C2C-C3C-CAC-CBC
17	A	810	CLA	CAD-CBD-CGD-O2D
17	A	812	CLA	CAD-CBD-CGD-O2D
17	A	813	CLA	CAD-CBD-CGD-O2D
17	A	815	CLA	CAD-CBD-CGD-O2D
17	A	829	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CAD-CBD-CGD-O2D
17	B	815	CLA	CAD-CBD-CGD-O2D
17	B	831	CLA	CAD-CBD-CGD-O2D
17	O	204	CLA	CAD-CBD-CGD-O2D
17	1	306	CLA	CAD-CBD-CGD-O2D
17	3	306	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	5	303	CLA	CAD-CBD-CGD-O2D
24	B	849	DGD	CCB-CDB-CEB-CFB
19	A	841	LHG	C30-C31-C32-C33
25	1	312	5X6	C26-C27-C28-C29
25	2	318	5X6	C03-C11-C12-C13
25	4	314	5X6	C03-C11-C12-C13
25	5	315	5X6	C03-C11-C12-C13
25	5	316	5X6	C03-C11-C12-C13
17	B	806	CLA	O1A-CGA-O2A-C1
22	F	201	LMT	O5'-C1'-O1'-C1
24	B	849	DGD	C1G-C2G-C3G-O3G
17	A	815	CLA	C3-C5-C6-C7
17	B	802	CLA	C16-C17-C18-C19
17	A	803	CLA	CHA-CBD-CGD-O1D
17	A	803	CLA	CHA-CBD-CGD-O2D
17	A	806	CLA	CHA-CBD-CGD-O1D
17	A	806	CLA	CHA-CBD-CGD-O2D
17	A	809	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	CHA-CBD-CGD-O2D
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	826	CLA	CHA-CBD-CGD-O1D
17	B	826	CLA	CHA-CBD-CGD-O2D
17	B	831	CLA	CHA-CBD-CGD-O1D
17	J	103	CLA	CHA-CBD-CGD-O1D
17	J	103	CLA	CHA-CBD-CGD-O2D
17	L	202	CLA	CHA-CBD-CGD-O1D
17	L	202	CLA	CHA-CBD-CGD-O2D
17	O	205	CLA	CHA-CBD-CGD-O1D
17	O	205	CLA	CHA-CBD-CGD-O2D
17	1	302	CLA	CHA-CBD-CGD-O1D
17	1	302	CLA	CHA-CBD-CGD-O2D
17	1	311	CLA	CHA-CBD-CGD-O1D
17	1	311	CLA	CHA-CBD-CGD-O2D
17	2	311	CLA	CHA-CBD-CGD-O1D
17	2	311	CLA	CHA-CBD-CGD-O2D
17	3	315	CLA	CHA-CBD-CGD-O1D
17	3	315	CLA	CHA-CBD-CGD-O2D
17	4	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	4	303	CLA	CHA-CBD-CGD-O2D
17	4	307	CLA	CHA-CBD-CGD-O1D
17	4	307	CLA	CHA-CBD-CGD-O2D
17	5	309	CLA	CHA-CBD-CGD-O1D
17	5	309	CLA	CHA-CBD-CGD-O2D
17	B	834	CLA	CBD-CGD-O2D-CED
17	A	819	CLA	O1A-CGA-O2A-C1
20	J	104	BCR	C20-C21-C22-C23
17	A	824	CLA	O1A-CGA-O2A-C1
17	B	811	CLA	O1A-CGA-O2A-C1
17	3	305	CLA	O1D-CGD-O2D-CED
22	B	850	LMT	C3-C4-C5-C6
17	A	803	CLA	C4-C3-C5-C6
17	A	818	CLA	C4-C3-C5-C6
17	A	812	CLA	O1A-CGA-O2A-C1
17	A	819	CLA	C2-C3-C5-C6
17	B	807	CLA	C11-C12-C13-C14
17	B	816	CLA	C11-C10-C8-C9
17	B	820	CLA	C11-C12-C13-C14
17	2	305	CLA	O1D-CGD-O2D-CED
17	2	305	CLA	CBD-CGD-O2D-CED
17	B	826	CLA	O1A-CGA-O2A-C1
17	A	810	CLA	C2A-CAA-CBA-CGA
20	M	101	BCR	C37-C22-C23-C24
25	2	321	5X6	C11-C12-C13-C42
25	3	317	5X6	C11-C12-C13-C42
20	A	857	BCR	C11-C12-C13-C14
17	A	834	CLA	C1A-C2A-CAA-CBA
17	B	817	CLA	C1A-C2A-CAA-CBA
17	1	302	CLA	C1A-C2A-CAA-CBA
17	3	309	CLA	C1A-C2A-CAA-CBA
17	5	309	CLA	C1A-C2A-CAA-CBA
17	1	303	CLA	C6-C7-C8-C10
17	A	831	CLA	C10-C11-C12-C13
17	A	837	CLA	C2-C1-O2A-CGA
17	B	840	CLA	C2-C1-O2A-CGA
19	J	102	LHG	C18-C19-C20-C21
17	A	810	CLA	C4-C3-C5-C6
17	A	854	CLA	C15-C16-C17-C18
17	A	809	CLA	C16-C17-C18-C20
17	B	820	CLA	C16-C17-C18-C19
17	1	307	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	B	806	CLA	C3-C5-C6-C7
17	A	829	CLA	O1D-CGD-O2D-CED
19	J	102	LHG	C30-C31-C32-C33
22	B	852	LMT	C11-C10-C9-C8
17	A	803	CLA	CAD-CBD-CGD-O1D
17	A	859	CLA	CAD-CBD-CGD-O1D
17	B	806	CLA	CAD-CBD-CGD-O1D
17	J	103	CLA	CAD-CBD-CGD-O1D
17	L	202	CLA	CAD-CBD-CGD-O1D
17	O	205	CLA	CAD-CBD-CGD-O1D
17	1	310	CLA	CAD-CBD-CGD-O1D
17	A	807	CLA	C15-C16-C17-C18
17	B	820	CLA	CBA-CGA-O2A-C1
17	4	303	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	C11-C12-C13-C15
17	A	815	CLA	C11-C10-C8-C7
17	B	802	CLA	C11-C10-C8-C7
17	B	806	CLA	C11-C10-C8-C7
17	B	807	CLA	C11-C12-C13-C15
17	B	809	CLA	C6-C7-C8-C10
17	B	818	CLA	C11-C10-C8-C7
17	B	837	CLA	C11-C10-C8-C7
17	A	804	CLA	C8-C10-C11-C12
17	5	309	CLA	C3-C5-C6-C7
17	B	806	CLA	C5-C6-C7-C8
17	A	814	CLA	C2A-CAA-CBA-CGA
19	J	102	LHG	C33-C34-C35-C36
19	A	841	LHG	C23-C24-C25-C26
25	F	205	5X6	C18-C19-C20-C21
17	A	828	CLA	C13-C15-C16-C17
17	A	833	CLA	C13-C15-C16-C17
17	4	303	CLA	O1A-CGA-O2A-C1
17	A	825	CLA	C15-C16-C17-C18
17	B	826	CLA	C4-C3-C5-C6
17	A	803	CLA	C2-C3-C5-C6
17	A	807	CLA	C11-C10-C8-C9
17	A	816	CLA	C14-C13-C15-C16
17	A	833	CLA	C11-C12-C13-C14
17	B	801	CLA	C11-C10-C8-C9
17	B	819	CLA	C11-C10-C8-C9
17	B	826	CLA	C6-C7-C8-C9
17	B	834	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B	837	CLA	C11-C10-C8-C9
25	3	317	5X6	C03-C11-C12-C13
25	5	316	5X6	C26-C27-C28-C29
20	B	844	BCR	C21-C22-C23-C24
25	5	317	5X6	C21-C22-C23-C24
19	A	842	LHG	C9-C10-C11-C12
25	1	314	5X6	C24-C25-C26-C39
17	A	818	CLA	C2-C3-C5-C6
17	B	827	CLA	C8-C10-C11-C12
22	F	201	LMT	C3-C4-C5-C6
17	A	818	CLA	C10-C11-C12-C13
17	5	308	CLA	C3-C5-C6-C7
17	A	807	CLA	C2-C1-O2A-CGA
17	5	303	CLA	C2-C1-O2A-CGA
17	B	820	CLA	C2C-C3C-CAC-CBC
20	K	104	BCR	C14-C15-C16-C17
22	B	851	LMT	C7-C8-C9-C10
17	A	816	CLA	CAA-CBA-CGA-O2A
17	B	820	CLA	O1A-CGA-O2A-C1
25	2	317	5X6	C04-C03-C11-C12
17	B	834	CLA	O1D-CGD-O2D-CED
17	B	818	CLA	CAA-CBA-CGA-O2A
17	4	306	CLA	C4C-C3C-CAC-CBC
19	A	842	LHG	C16-C17-C18-C19
17	A	822	CLA	C6-C7-C8-C10
17	A	837	CLA	C16-C17-C18-C19
17	B	807	CLA	C16-C17-C18-C19
17	L	203	CLA	C16-C17-C18-C19
20	B	803	BCR	C16-C17-C18-C19
22	F	201	LMT	C2'-C1'-O1'-C1
22	F	201	LMT	C11-C10-C9-C8
19	A	841	LHG	C3-O3-P-O6
19	A	842	LHG	C3-O3-P-O6
17	A	820	CLA	C8-C10-C11-C12
17	1	306	CLA	O1D-CGD-O2D-CED
17	A	802	CLA	C4-C3-C5-C6
17	A	812	CLA	C4-C3-C5-C6
17	A	829	CLA	CBD-CGD-O2D-CED
17	B	807	CLA	C6-C7-C8-C10
17	B	827	CLA	C11-C10-C8-C7
17	A	806	CLA	C11-C12-C13-C14
17	A	807	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	B	831	CLA	C11-C10-C8-C9
17	A	819	CLA	C13-C15-C16-C17
25	1	316	5X6	C23-C24-C25-C26
25	2	318	5X6	C13-C14-C15-C16
25	4	312	5X6	C23-C24-C25-C26
17	1	307	CLA	C11-C12-C13-C15
22	B	852	LMT	C2-C3-C4-C5
17	A	814	CLA	C2C-C3C-CAC-CBC
17	A	838	CLA	CBD-CGD-O2D-CED
17	L	204	CLA	C2A-CAA-CBA-CGA
17	2	305	CLA	C8-C10-C11-C12
22	L	207	LMT	C7-C8-C9-C10
20	B	846	BCR	C7-C8-C9-C34
17	A	815	CLA	CBA-CGA-O2A-C1
20	L	201	BCR	C21-C22-C23-C24
24	B	849	DGD	C4E-C5E-C6E-O5E
17	A	815	CLA	O1A-CGA-O2A-C1
25	2	317	5X6	C23-C24-C25-C26
25	3	316	5X6	C23-C24-C25-C26
25	4	313	5X6	C17-C18-C19-C20
18	B	842	PQN	C13-C15-C16-C17
17	B	836	CLA	C2C-C3C-CAC-CBC
25	1	313	5X6	C14-C15-C16-C17
17	A	806	CLA	C16-C17-C18-C20
17	B	815	CLA	C3-C5-C6-C7
17	A	852	CLA	C10-C11-C12-C13
17	2	305	CLA	C15-C16-C17-C18
17	1	311	CLA	CAA-CBA-CGA-O1A
17	A	804	CLA	C2-C1-O2A-CGA
17	A	834	CLA	C2-C1-O2A-CGA
17	B	812	CLA	C2-C1-O2A-CGA
17	L	204	CLA	C2-C1-O2A-CGA
17	2	311	CLA	C2-C1-O2A-CGA
17	B	814	CLA	C10-C11-C12-C13
17	5	309	CLA	C15-C16-C17-C18
17	5	306	CLA	CAA-CBA-CGA-O2A
17	5	313	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	C2A-CAA-CBA-CGA
17	4	307	CLA	C2A-CAA-CBA-CGA
17	B	830	CLA	C3A-C2A-CAA-CBA
17	5	308	CLA	C3A-C2A-CAA-CBA
17	2	309	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C6-C7-C8-C9
17	A	814	CLA	C4C-C3C-CAC-CBC
17	5	305	CLA	CAA-CBA-CGA-O1A
25	F	205	5X6	C19-C20-C21-C22
25	4	313	5X6	C13-C14-C15-C16
25	5	315	5X6	C17-C18-C19-C20
17	B	821	CLA	CAA-CBA-CGA-O2A
17	1	301	CLA	CAA-CBA-CGA-O1A
17	A	804	CLA	C6-C7-C8-C9
17	A	812	CLA	C14-C13-C15-C16
17	A	815	CLA	C11-C10-C8-C9
17	A	826	CLA	C6-C7-C8-C9
17	A	855	CLA	C11-C10-C8-C9
17	B	809	CLA	C14-C13-C15-C16
17	B	825	CLA	C11-C12-C13-C14
17	B	839	CLA	C11-C10-C8-C9
17	B	820	CLA	C16-C17-C18-C20
17	5	306	CLA	CAA-CBA-CGA-O1A
17	5	313	CLA	CAA-CBA-CGA-O1A
20	A	846	BCR	C11-C10-C9-C34
20	A	846	BCR	C16-C17-C18-C36
20	B	845	BCR	C20-C21-C22-C37
20	B	846	BCR	C35-C13-C14-C15
20	L	201	BCR	C11-C10-C9-C34
25	3	316	5X6	C41-C17-C18-C19
25	5	318	5X6	C24-C25-C26-C39
17	B	821	CLA	CAA-CBA-CGA-O1A
17	1	304	CLA	CAA-CBA-CGA-O2A
17	4	307	CLA	CAA-CBA-CGA-O1A
17	A	835	CLA	O1A-CGA-O2A-C1
19	A	841	LHG	C32-C33-C34-C35
17	B	811	CLA	O2A-C1-C2-C3
17	A	838	CLA	O1D-CGD-O2D-CED
17	A	837	CLA	C15-C16-C17-C18
17	1	311	CLA	CAA-CBA-CGA-O2A
17	4	305	CLA	CAA-CBA-CGA-O1A
17	4	311	CLA	CAA-CBA-CGA-O2A
20	I	101	BCR	C7-C8-C9-C34
17	B	833	CLA	C3-C5-C6-C7
17	A	837	CLA	C13-C15-C16-C17
19	A	841	LHG	C33-C34-C35-C36
17	5	307	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	A	838	CLA	C13-C15-C16-C17
17	3	305	CLA	C1A-C2A-CAA-CBA
17	5	302	CLA	C1A-C2A-CAA-CBA
17	A	812	CLA	C11-C10-C8-C7
17	A	831	CLA	C11-C12-C13-C15
17	B	837	CLA	C8-C10-C11-C12
17	4	311	CLA	CAA-CBA-CGA-O1A
25	2	321	5X6	C13-C14-C15-C16
25	3	317	5X6	C17-C18-C19-C20
25	5	316	5X6	C17-C18-C19-C20
17	B	822	CLA	CAA-CBA-CGA-O2A
17	A	822	CLA	C2A-CAA-CBA-CGA
17	A	823	CLA	C15-C16-C17-C18
17	2	307	CLA	C5-C6-C7-C8
19	A	842	LHG	O6-C4-C5-O7
17	1	301	CLA	CAA-CBA-CGA-O2A
17	1	304	CLA	CAA-CBA-CGA-O1A
17	3	308	CLA	CAA-CBA-CGA-O1A
17	B	818	CLA	C10-C11-C12-C13
22	B	852	LMT	C4-C5-C6-C7
17	B	807	CLA	C16-C17-C18-C20
17	2	309	CLA	CAA-CBA-CGA-O2A
17	A	830	CLA	C4-C3-C5-C6
17	A	812	CLA	C2-C3-C5-C6
17	O	205	CLA	CAA-CBA-CGA-O1A
17	4	305	CLA	CAA-CBA-CGA-O2A
17	5	307	CLA	CAA-CBA-CGA-O1A
17	A	820	CLA	C13-C15-C16-C17
17	A	824	CLA	C5-C6-C7-C8
20	A	846	BCR	C11-C10-C9-C8
20	A	846	BCR	C16-C17-C18-C19
20	B	845	BCR	C20-C21-C22-C23
20	B	846	BCR	C12-C13-C14-C15
25	2	320	5X6	C19-C20-C21-C22
17	5	312	CLA	CAA-CBA-CGA-O2A
17	2	313	CLA	C4C-C3C-CAC-CBC
17	O	205	CLA	CAA-CBA-CGA-O2A
17	5	312	CLA	CAA-CBA-CGA-O1A
17	A	820	CLA	O1D-CGD-O2D-CED
17	A	855	CLA	C4-C3-C5-C6
17	A	824	CLA	C2-C1-O2A-CGA
17	B	834	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	B	841	CLA	C2-C1-O2A-CGA
17	A	817	CLA	C2-C3-C5-C6
17	B	826	CLA	C2-C3-C5-C6
17	1	305	CLA	CAA-CBA-CGA-O1A
17	5	302	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	C11-C12-C13-C14
17	B	806	CLA	C14-C13-C15-C16
17	3	305	CLA	C6-C7-C8-C9
17	3	305	CLA	C14-C13-C15-C16
22	L	207	LMT	C1-C2-C3-C4
17	B	828	CLA	C3-C5-C6-C7
17	2	305	CLA	C3-C5-C6-C7
17	3	315	CLA	C4-C3-C5-C6
17	2	307	CLA	C2C-C3C-CAC-CBC
20	B	846	BCR	C23-C24-C25-C30
20	I	101	BCR	C23-C24-C25-C30
20	M	101	BCR	C23-C24-C25-C30
25	F	205	5X6	C27-C28-C29-C34
25	1	316	5X6	C27-C28-C29-C34
25	2	320	5X6	C27-C28-C29-C34
17	3	308	CLA	CAA-CBA-CGA-O2A
17	4	307	CLA	CAA-CBA-CGA-O2A
19	A	842	LHG	C10-C11-C12-C13
25	5	318	5X6	C13-C14-C15-C16
17	B	839	CLA	C4-C3-C5-C6
17	3	307	CLA	C4-C3-C5-C6
20	J	104	BCR	C21-C22-C23-C24
25	1	314	5X6	C25-C26-C27-C28
17	A	822	CLA	C6-C7-C8-C9
17	A	802	CLA	C2-C3-C5-C6
17	B	835	CLA	CAA-CBA-CGA-O2A
17	4	308	CLA	CAA-CBA-CGA-O2A
17	3	309	CLA	CAA-CBA-CGA-O2A
17	3	305	CLA	C8-C10-C11-C12
17	1	305	CLA	CAA-CBA-CGA-O2A
17	2	304	CLA	CAA-CBA-CGA-O2A
17	B	825	CLA	C13-C15-C16-C17
17	A	856	CLA	C15-C16-C17-C18
17	B	832	CLA	C4-C3-C5-C6
17	A	812	CLA	C11-C12-C13-C15
17	B	801	CLA	C11-C10-C8-C7
17	B	839	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	1	309	CLA	CAA-CBA-CGA-O2A
25	2	320	5X6	C17-C18-C19-C20
25	2	321	5X6	C23-C24-C25-C26
17	A	827	CLA	C10-C11-C12-C13
17	A	855	CLA	O1A-CGA-O2A-C1
17	A	806	CLA	CBA-CGA-O2A-C1
19	A	841	LHG	C31-C32-C33-C34
17	3	305	CLA	C3-C5-C6-C7
17	3	309	CLA	CAA-CBA-CGA-O1A
17	2	316	CLA	CAA-CBA-CGA-O2A
17	B	833	CLA	C8-C10-C11-C12
20	B	843	BCR	C20-C21-C22-C37
20	B	844	BCR	C11-C10-C9-C34
20	B	847	BCR	C35-C13-C14-C15
17	A	823	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	C4-C3-C5-C6
17	B	819	CLA	C4-C3-C5-C6
17	B	831	CLA	C4-C3-C5-C6
17	L	202	CLA	C4-C3-C5-C6
17	4	304	CLA	C4-C3-C5-C6
17	5	308	CLA	C4-C3-C5-C6
17	A	803	CLA	C15-C16-C17-C18
17	A	809	CLA	C8-C10-C11-C12
17	A	831	CLA	C13-C15-C16-C17
17	B	839	CLA	C5-C6-C7-C8
17	A	810	CLA	C2-C3-C5-C6
17	A	855	CLA	C2-C3-C5-C6
17	A	837	CLA	C16-C17-C18-C20
17	B	805	CLA	C10-C11-C12-C13
17	B	802	CLA	C11-C10-C8-C9
17	B	806	CLA	C11-C10-C8-C9
17	B	827	CLA	C11-C10-C8-C9
17	2	305	CLA	C11-C12-C13-C14
17	3	305	CLA	C11-C12-C13-C14
17	5	302	CLA	CAA-CBA-CGA-O1A
17	A	812	CLA	C3A-C2A-CAA-CBA
17	B	802	CLA	C3A-C2A-CAA-CBA
17	L	202	CLA	C3A-C2A-CAA-CBA
17	5	306	CLA	C3A-C2A-CAA-CBA
17	B	801	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	CAD-CBD-CGD-O2D
17	A	811	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	A	824	CLA	CAD-CBD-CGD-O2D
17	A	856	CLA	CAD-CBD-CGD-O2D
17	B	811	CLA	CAD-CBD-CGD-O2D
17	B	827	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	O	203	CLA	CAD-CBD-CGD-O2D
17	2	305	CLA	CAD-CBD-CGD-O2D
17	2	309	CLA	CAD-CBD-CGD-O2D
17	4	306	CLA	CAD-CBD-CGD-O2D
17	5	310	CLA	CAD-CBD-CGD-O2D
17	A	855	CLA	CBA-CGA-O2A-C1
17	L	203	CLA	C16-C17-C18-C20
17	3	310	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	CAA-CBA-CGA-O2A
25	J	105	5X6	C26-C27-C28-C29
17	A	836	CLA	C4-C3-C5-C6
17	B	808	CLA	C4-C3-C5-C6
17	B	835	CLA	CAA-CBA-CGA-O1A
17	2	304	CLA	CAA-CBA-CGA-O1A
17	A	830	CLA	C2-C3-C5-C6
17	3	315	CLA	CAA-CBA-CGA-O2A
20	B	845	BCR	C11-C12-C13-C14
25	1	313	5X6	C21-C22-C23-C24
25	2	319	5X6	C11-C12-C13-C14
25	3	317	5X6	C15-C16-C17-C18
17	3	306	CLA	CAA-CBA-CGA-O2A
19	A	842	LHG	O7-C7-C8-C9
17	2	316	CLA	CAA-CBA-CGA-O1A
17	A	805	CLA	O2A-C1-C2-C3
17	A	829	CLA	O2A-C1-C2-C3
17	B	817	CLA	O2A-C1-C2-C3
17	B	839	CLA	O2A-C1-C2-C3
17	L	202	CLA	O2A-C1-C2-C3
17	L	204	CLA	O2A-C1-C2-C3
17	1	303	CLA	C2A-CAA-CBA-CGA
17	A	810	CLA	CAA-CBA-CGA-O2A
17	5	308	CLA	CAA-CBA-CGA-O2A
17	A	854	CLA	O1A-CGA-O2A-C1
17	1	309	CLA	CAA-CBA-CGA-O1A
17	2	306	CLA	CAA-CBA-CGA-O2A
17	5	303	CLA	C8-C10-C11-C12
17	A	817	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	A	821	CLA	CHA-CBD-CGD-O2D
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	A	859	CLA	CHA-CBD-CGD-O1D
17	B	805	CLA	CHA-CBD-CGD-O1D
17	B	805	CLA	CHA-CBD-CGD-O2D
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	841	CLA	CHA-CBD-CGD-O1D
17	1	304	CLA	CHA-CBD-CGD-O1D
17	1	304	CLA	CHA-CBD-CGD-O2D
17	1	308	CLA	CHA-CBD-CGD-O1D
17	1	308	CLA	CHA-CBD-CGD-O2D
17	1	310	CLA	CHA-CBD-CGD-O1D
17	2	314	CLA	CHA-CBD-CGD-O1D
17	2	314	CLA	CHA-CBD-CGD-O2D
17	3	307	CLA	CHA-CBD-CGD-O2D
17	3	308	CLA	CHA-CBD-CGD-O1D
17	3	314	CLA	CHA-CBD-CGD-O2D
17	4	305	CLA	CHA-CBD-CGD-O1D
17	4	305	CLA	CHA-CBD-CGD-O2D
20	B	845	BCR	C9-C10-C11-C12
17	2	306	CLA	CAA-CBA-CGA-O1A
17	3	306	CLA	CAA-CBA-CGA-O1A
17	4	308	CLA	CAA-CBA-CGA-O1A
17	4	310	CLA	CAA-CBA-CGA-O1A
17	A	821	CLA	CAA-CBA-CGA-O2A
17	A	825	CLA	CAA-CBA-CGA-O2A
17	B	807	CLA	CAA-CBA-CGA-O2A
17	B	830	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	C2-C3-C5-C6
17	B	808	CLA	C2-C3-C5-C6
20	B	844	BCR	C11-C10-C9-C8
20	L	201	BCR	C11-C10-C9-C8
17	A	853	CLA	C15-C16-C17-C18
17	A	818	CLA	CAA-CBA-CGA-O2A
19	J	102	LHG	O8-C23-C24-C25
17	A	806	CLA	O1A-CGA-O2A-C1
17	A	811	CLA	C15-C16-C17-C18
17	5	311	CLA	CAA-CBA-CGA-O1A
17	B	818	CLA	C11-C12-C13-C14
17	A	828	CLA	C8-C10-C11-C12
17	A	803	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	1	306	CLA	CBD-CGD-O2D-CED
17	B	831	CLA	CAA-CBA-CGA-O2A
17	3	311	CLA	CAA-CBA-CGA-O2A
17	A	831	CLA	C4-C3-C5-C6
17	B	834	CLA	C4-C3-C5-C6
17	A	855	CLA	C11-C10-C8-C7
17	B	812	CLA	C6-C7-C8-C10
17	B	819	CLA	C2-C3-C5-C6
17	B	832	CLA	C2-C3-C5-C6
17	3	305	CLA	C6-C7-C8-C10
17	5	303	CLA	C11-C12-C13-C15
17	A	837	CLA	C10-C11-C12-C13
17	B	824	CLA	CAA-CBA-CGA-O2A
19	A	841	LHG	O8-C23-C24-C25
17	3	310	CLA	CAA-CBA-CGA-O1A
17	A	817	CLA	C11-C10-C8-C9
17	A	819	CLA	C6-C7-C8-C9
17	B	816	CLA	C11-C12-C13-C14
17	A	805	CLA	C2B-C3B-CAB-CBB
17	A	810	CLA	C2B-C3B-CAB-CBB
17	A	835	CLA	C2B-C3B-CAB-CBB
17	1	302	CLA	C2B-C3B-CAB-CBB
17	1	302	CLA	C10-C11-C12-C13
17	A	816	CLA	CBA-CGA-O2A-C1
17	A	802	CLA	C6-C7-C8-C10
17	2	304	CLA	C2A-CAA-CBA-CGA
16	A	801	CL0	C5-C6-C7-C8
17	A	823	CLA	CAA-CBA-CGA-O1A
20	A	843	BCR	C7-C8-C9-C10
19	J	102	LHG	C12-C13-C14-C15
17	A	832	CLA	C1A-C2A-CAA-CBA
17	B	802	CLA	C1A-C2A-CAA-CBA
17	L	202	CLA	C1A-C2A-CAA-CBA
17	1	307	CLA	C1A-C2A-CAA-CBA
17	2	314	CLA	C1A-C2A-CAA-CBA
17	5	306	CLA	C1A-C2A-CAA-CBA
17	A	810	CLA	CAA-CBA-CGA-O1A
16	A	801	CL0	CAA-CBA-CGA-O2A
17	A	835	CLA	CBA-CGA-O2A-C1
17	3	315	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	O10-C23-C24-C25
19	A	841	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	814	CLA	C16-C17-C18-C19
17	A	821	CLA	CAA-CBA-CGA-O1A
22	B	851	LMT	O1'-C1-C2-C3
17	4	310	CLA	CAA-CBA-CGA-O2A
17	A	815	CLA	C13-C15-C16-C17
17	A	817	CLA	C4-C3-C5-C6
17	O	203	CLA	C4B-C3B-CAB-CBB
17	2	312	CLA	C4B-C3B-CAB-CBB
17	3	308	CLA	C4B-C3B-CAB-CBB
17	4	309	CLA	C4B-C3B-CAB-CBB
17	5	302	CLA	C4B-C3B-CAB-CBB
17	5	306	CLA	C4B-C3B-CAB-CBB
17	5	310	CLA	C4B-C3B-CAB-CBB
17	5	311	CLA	C4B-C3B-CAB-CBB
19	A	841	LHG	C4-O6-P-O4
17	A	818	CLA	CAA-CBA-CGA-O1A
17	B	830	CLA	CAA-CBA-CGA-O1A
19	J	102	LHG	O10-C23-C24-C25
20	I	101	BCR	C23-C24-C25-C26
17	A	839	CLA	O1D-CGD-O2D-CED
17	A	825	CLA	C13-C15-C16-C17
17	5	304	CLA	C5-C6-C7-C8
17	A	804	CLA	CAA-CBA-CGA-O1A
17	A	825	CLA	CAA-CBA-CGA-O1A
17	B	801	CLA	CAA-CBA-CGA-O1A
17	B	805	CLA	CAA-CBA-CGA-O1A
17	B	807	CLA	CAA-CBA-CGA-O1A
17	A	859	CLA	CAA-CBA-CGA-O2A
17	5	311	CLA	CAA-CBA-CGA-O2A
17	5	311	CLA	C2A-CAA-CBA-CGA
19	A	842	LHG	O9-C7-C8-C9
19	J	102	LHG	C11-C12-C13-C14
22	3	301	LMT	C11-C10-C9-C8
17	B	809	CLA	C4-C3-C5-C6
17	A	836	CLA	CAD-CBD-CGD-O1D
17	B	817	CLA	CAD-CBD-CGD-O1D
17	B	841	CLA	CAD-CBD-CGD-O1D
17	F	204	CLA	CAD-CBD-CGD-O1D
17	3	308	CLA	CAD-CBD-CGD-O1D
17	3	311	CLA	CAA-CBA-CGA-O1A
17	B	810	CLA	CAA-CBA-CGA-O2A
17	K	102	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	B	849	DGD	O2G-C1B-C2B-C3B
17	A	811	CLA	C11-C10-C8-C9
17	A	812	CLA	C6-C7-C8-C9
17	A	812	CLA	C11-C10-C8-C9
17	A	831	CLA	C11-C12-C13-C14
17	A	836	CLA	C6-C7-C8-C9
17	5	303	CLA	C11-C12-C13-C14
17	5	304	CLA	C11-C12-C13-C14
17	A	811	CLA	CAA-CBA-CGA-O2A
17	5	303	CLA	CAA-CBA-CGA-O2A
17	B	810	CLA	CAA-CBA-CGA-O1A
17	A	820	CLA	CAA-CBA-CGA-O2A
17	A	839	CLA	CAA-CBA-CGA-O2A
17	A	852	CLA	CAA-CBA-CGA-O2A
17	3	307	CLA	CAA-CBA-CGA-O2A
17	A	803	CLA	CAA-CBA-CGA-O1A
17	A	811	CLA	C4-C3-C5-C6
17	A	839	CLA	C13-C15-C16-C17
17	A	807	CLA	C11-C10-C8-C7
17	A	852	CLA	C11-C10-C8-C7
17	A	854	CLA	C11-C10-C8-C7
17	B	805	CLA	C6-C7-C8-C10
17	B	810	CLA	C11-C12-C13-C15
17	B	816	CLA	C11-C12-C13-C15
17	B	825	CLA	C11-C12-C13-C15
17	B	832	CLA	C3A-C2A-CAA-CBA
17	5	305	CLA	C3A-C2A-CAA-CBA
17	A	811	CLA	CAA-CBA-CGA-O1A
17	3	314	CLA	CAA-CBA-CGA-O1A
17	A	808	CLA	C3-C5-C6-C7
20	B	844	BCR	C17-C18-C19-C20
20	I	101	BCR	C7-C8-C9-C10
20	M	101	BCR	C21-C22-C23-C24
25	4	313	5X6	C23-C24-C25-C26
17	A	826	CLA	CAA-CBA-CGA-O2A
17	5	314	CLA	CAA-CBA-CGA-O2A
17	A	839	CLA	C8-C10-C11-C12
17	B	833	CLA	C2C-C3C-CAC-CBC
17	K	102	CLA	CAA-CBA-CGA-O1A
17	B	816	CLA	C5-C6-C7-C8
17	B	811	CLA	CAA-CBA-CGA-O2A
17	3	314	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	F	201	LMT	C4-C5-C6-C7
17	K	102	CLA	C5-C6-C7-C8
17	B	831	CLA	CAA-CBA-CGA-O1A
17	3	307	CLA	CAA-CBA-CGA-O1A
17	A	827	CLA	C16-C17-C18-C19
17	A	854	CLA	CBA-CGA-O2A-C1
17	2	310	CLA	CAA-CBA-CGA-O1A
17	B	837	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

167 monomers are involved in 299 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	801	CLA	1	0
16	A	801	CL0	1	0
17	B	837	CLA	5	0
17	B	829	CLA	2	0
17	B	826	CLA	4	0
17	5	310	CLA	1	0
17	B	838	CLA	2	0
25	1	314	5X6	1	0
20	B	844	BCR	2	0
17	5	311	CLA	1	0
21	C	102	SF4	1	0
17	A	855	CLA	2	0
17	B	833	CLA	2	0
17	K	103	CLA	2	0
17	3	313	CLA	1	0
17	3	308	CLA	1	0
17	1	309	CLA	1	0
17	3	309	CLA	1	0
20	L	201	BCR	2	0
17	5	304	CLA	2	0
17	4	309	CLA	1	0
17	B	822	CLA	1	0
17	2	313	CLA	3	0
20	A	845	BCR	2	0
17	1	301	CLA	1	0
20	B	847	BCR	2	0
17	B	857	CLA	2	0
18	B	842	PQN	2	0
20	J	104	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	803	CLA	3	0
17	5	313	CLA	4	0
17	A	823	CLA	2	0
17	2	314	CLA	1	0
20	B	845	BCR	1	0
20	B	803	BCR	1	0
17	O	204	CLA	2	0
17	B	806	CLA	1	0
17	2	310	CLA	1	0
17	4	307	CLA	6	0
17	1	305	CLA	2	0
17	A	826	CLA	2	0
25	1	312	5X6	1	0
17	B	817	CLA	4	0
17	B	823	CLA	4	0
17	5	305	CLA	3	0
20	A	844	BCR	3	0
17	5	314	CLA	1	0
19	A	842	LHG	1	0
17	B	828	CLA	5	0
17	B	818	CLA	4	0
17	5	303	CLA	1	0
17	A	825	CLA	1	0
17	A	835	CLA	1	0
17	1	306	CLA	1	0
17	3	311	CLA	1	0
17	B	834	CLA	3	0
17	A	805	CLA	1	0
17	A	822	CLA	1	0
17	B	832	CLA	1	0
17	B	835	CLA	2	0
17	B	810	CLA	4	0
20	L	205	BCR	1	0
17	F	203	CLA	3	0
17	A	814	CLA	1	0
17	B	821	CLA	1	0
17	4	311	CLA	1	0
20	B	848	BCR	1	0
17	B	820	CLA	3	0
20	M	101	BCR	3	0
20	A	857	BCR	2	0
17	A	831	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	846	BCR	4	0
17	O	205	CLA	1	0
17	O	203	CLA	2	0
24	B	849	DGD	3	0
17	1	303	CLA	1	0
17	A	836	CLA	1	0
17	3	305	CLA	2	0
17	A	818	CLA	2	0
17	2	312	CLA	1	0
17	A	827	CLA	1	0
17	1	302	CLA	3	0
17	1	304	CLA	2	0
17	2	304	CLA	2	0
17	A	815	CLA	3	0
17	3	314	CLA	1	0
20	K	104	BCR	1	0
17	L	204	CLA	1	0
17	A	853	CLA	4	0
17	B	836	CLA	6	0
17	B	816	CLA	2	0
19	J	102	LHG	1	0
17	A	832	CLA	2	0
17	A	834	CLA	2	0
25	3	317	5X6	2	0
17	B	815	CLA	1	0
17	5	307	CLA	2	0
17	B	840	CLA	3	0
25	5	318	5X6	2	0
17	A	811	CLA	3	0
17	A	839	CLA	2	0
17	5	308	CLA	2	0
17	5	302	CLA	1	0
17	B	807	CLA	6	0
17	A	802	CLA	1	0
17	B	805	CLA	3	0
17	A	813	CLA	2	0
17	B	825	CLA	2	0
17	3	307	CLA	1	0
17	B	841	CLA	6	0
20	B	843	BCR	1	0
17	A	821	CLA	1	0
17	B	811	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	839	CLA	5	0
17	1	311	CLA	1	0
17	B	824	CLA	3	0
17	1	310	CLA	3	0
17	B	802	CLA	6	0
17	B	813	CLA	4	0
17	2	307	CLA	7	0
17	L	202	CLA	1	0
17	A	837	CLA	1	0
17	1	308	CLA	1	0
17	F	204	CLA	2	0
17	4	303	CLA	1	0
17	A	852	CLA	2	0
17	A	804	CLA	2	0
17	A	859	CLA	5	0
17	4	310	CLA	1	0
18	A	840	PQN	1	0
17	A	820	CLA	1	0
17	2	308	CLA	1	0
17	3	306	CLA	2	0
17	B	827	CLA	1	0
17	5	312	CLA	1	0
17	B	814	CLA	1	0
17	B	808	CLA	2	0
17	1	307	CLA	2	0
17	A	808	CLA	1	0
17	A	816	CLA	7	0
17	B	831	CLA	3	0
17	B	830	CLA	3	0
17	2	309	CLA	5	0
17	3	312	CLA	2	0
17	5	306	CLA	1	0
17	4	308	CLA	1	0
17	A	807	CLA	2	0
17	A	838	CLA	1	0
17	A	854	CLA	4	0
17	A	817	CLA	1	0
17	4	306	CLA	2	0
20	A	843	BCR	3	0
17	5	309	CLA	1	0
17	B	812	CLA	4	0
17	3	315	CLA	1	0

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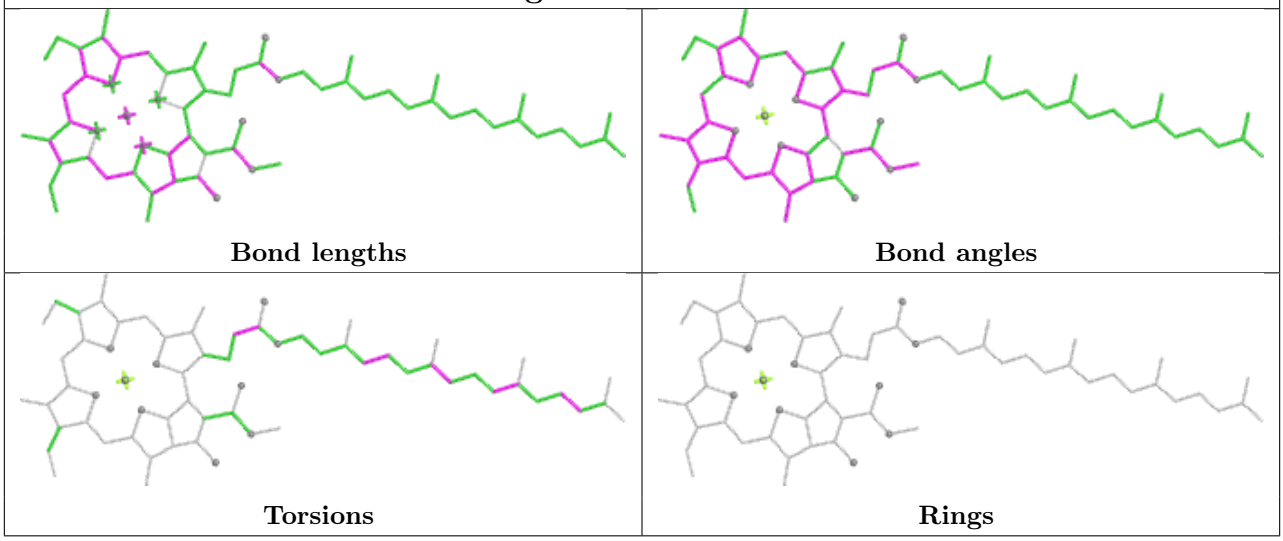
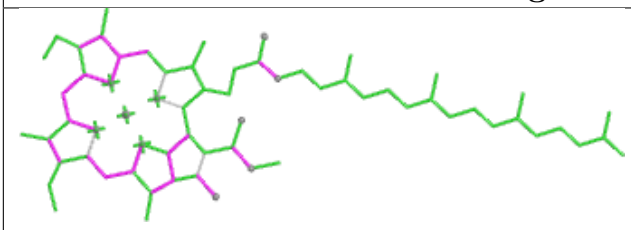
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	833	CLA	1	0
17	A	809	CLA	2	0
17	K	102	CLA	1	0
17	A	819	CLA	5	0
17	2	315	CLA	1	0
17	A	829	CLA	1	0
17	2	316	CLA	1	0
17	A	810	CLA	2	0
17	B	804	CLA	3	0
20	L	206	BCR	1	0
17	4	305	CLA	1	0
17	J	103	CLA	1	0

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

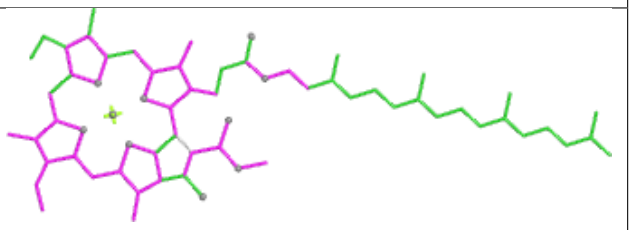
Ligand CLA B 801



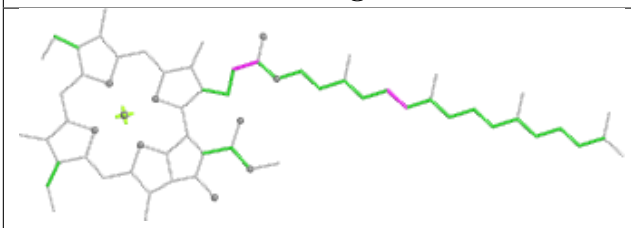
Ligand CL0 A 801



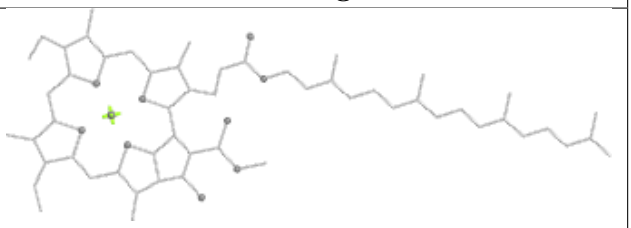
Bond lengths



Bond angles

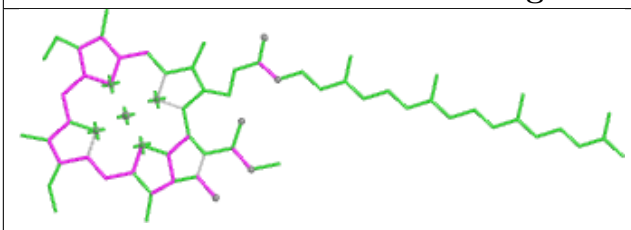


Torsions

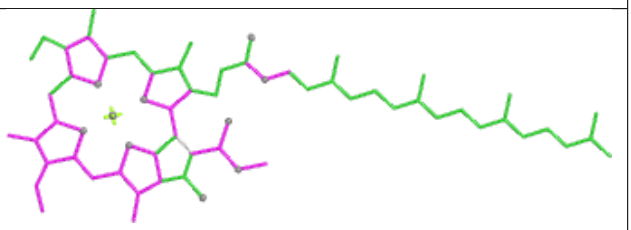


Rings

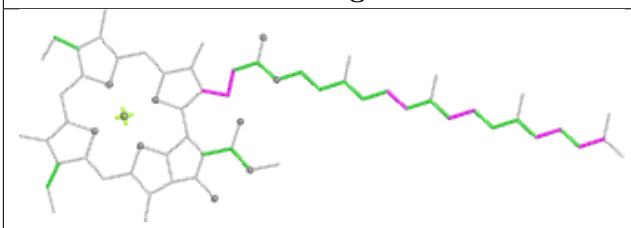
Ligand CLA L 203



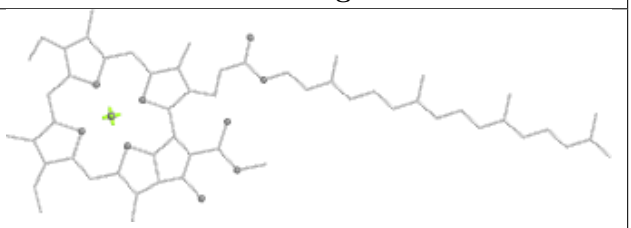
Bond lengths



Bond angles

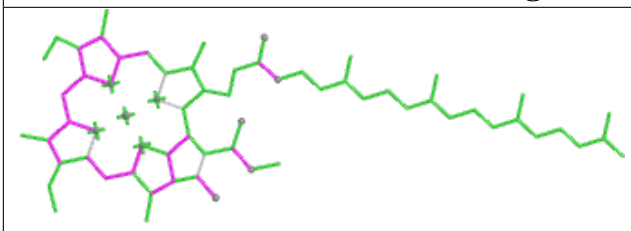


Torsions

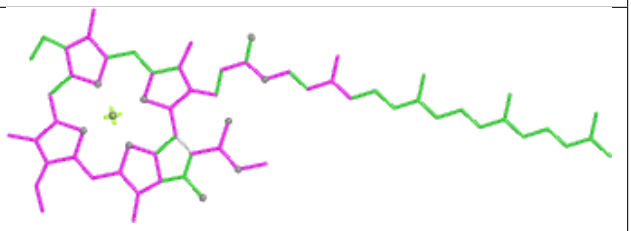


Rings

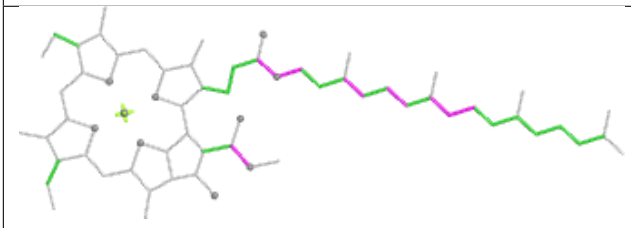
Ligand CLA B 837



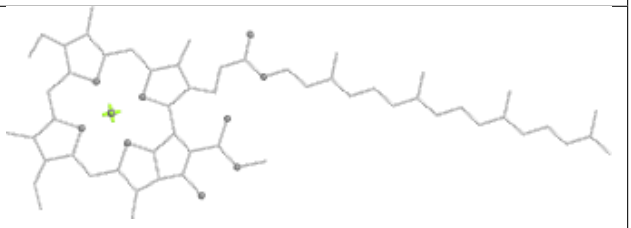
Bond lengths



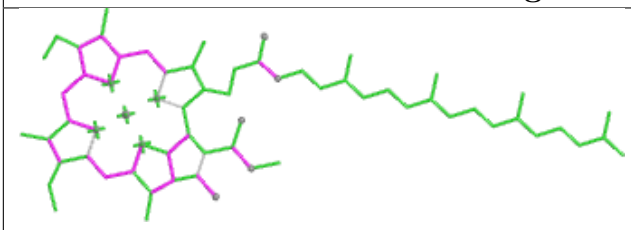
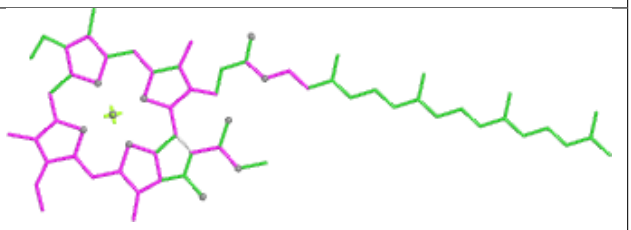
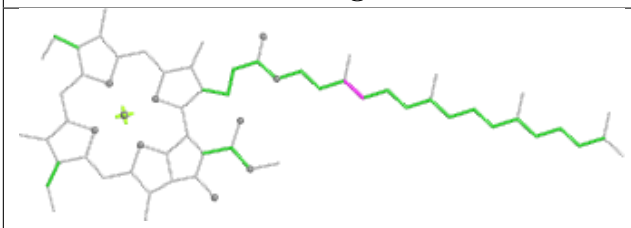
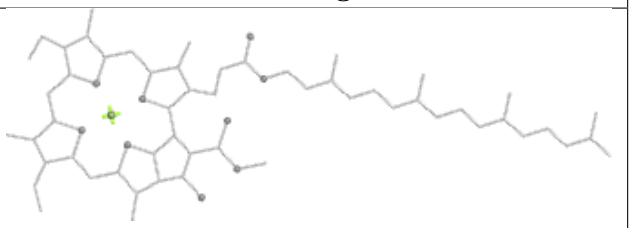
Bond angles

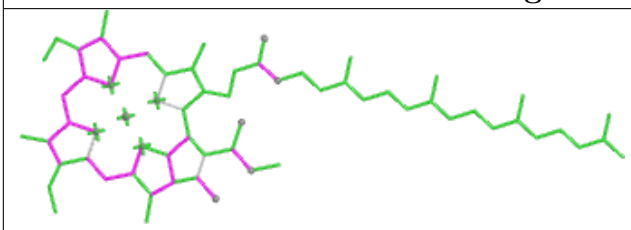
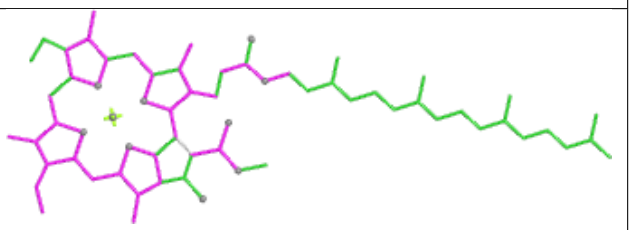
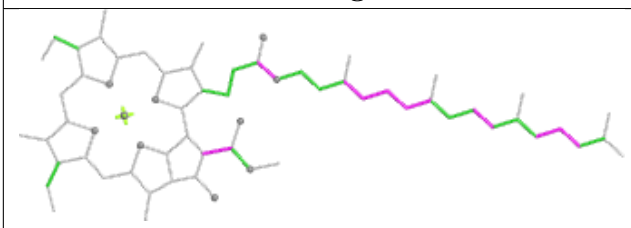
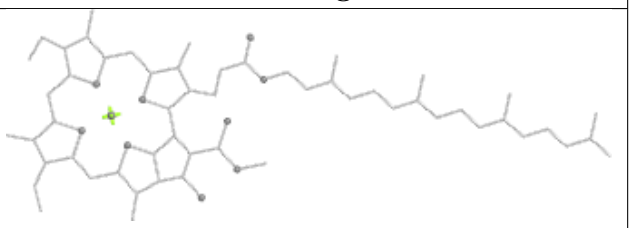


Torsions

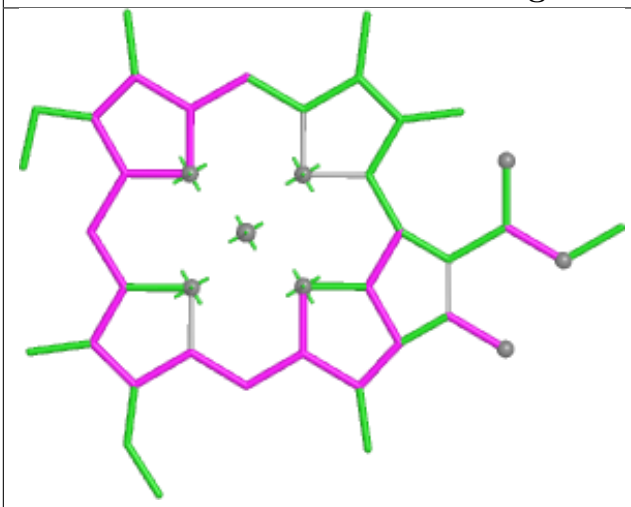


Rings

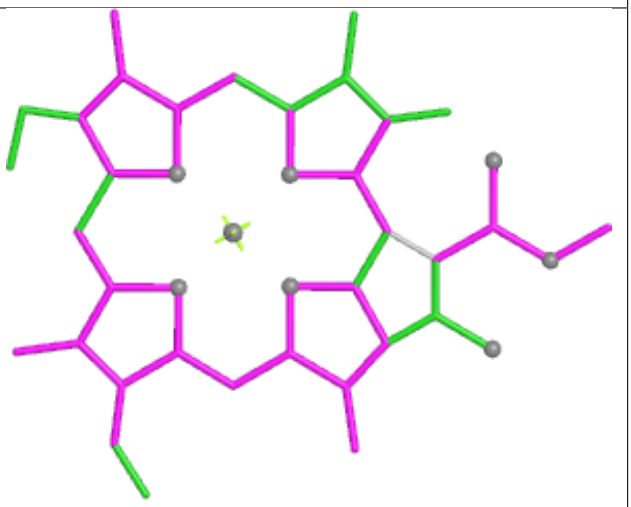
Ligand CLA B 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

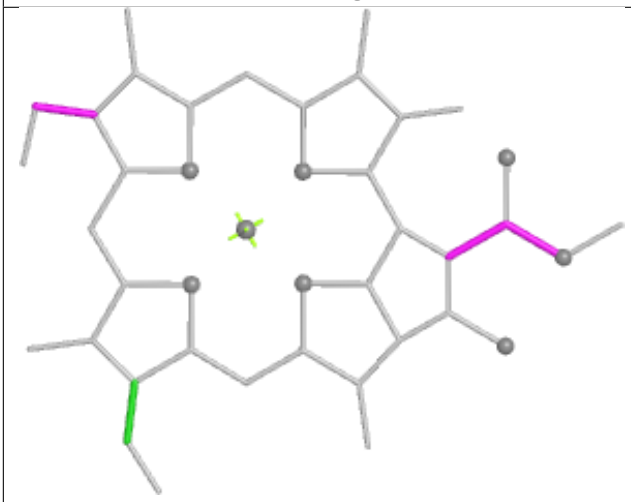
Ligand CLA 5 310



Bond lengths



Bond angles



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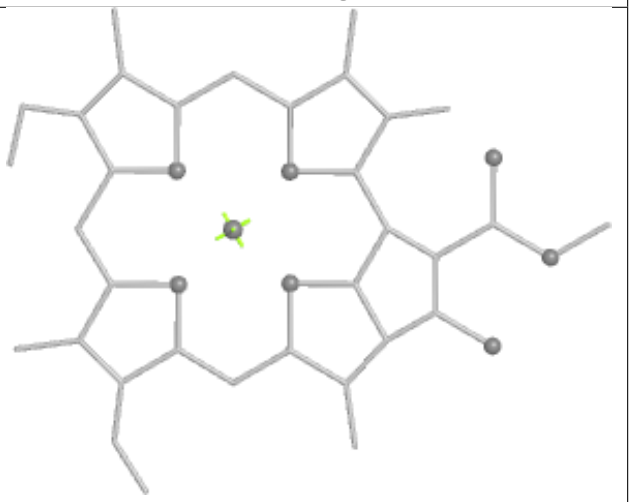
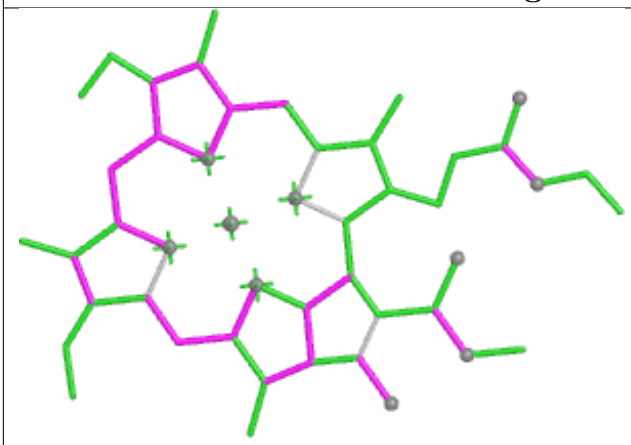
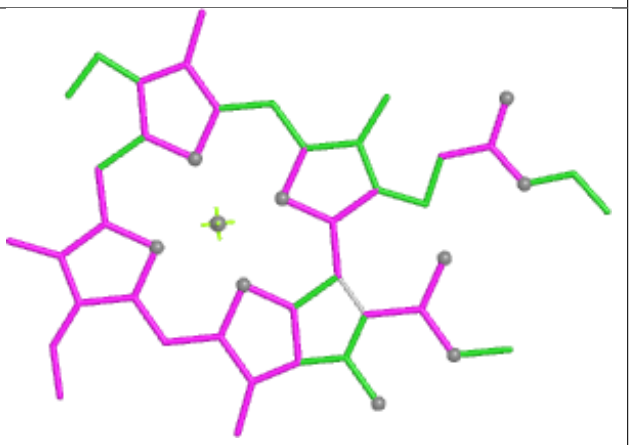


Rings

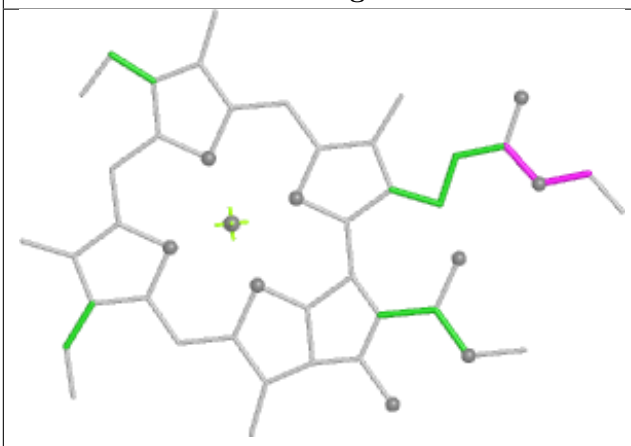
Ligand CLA B 838



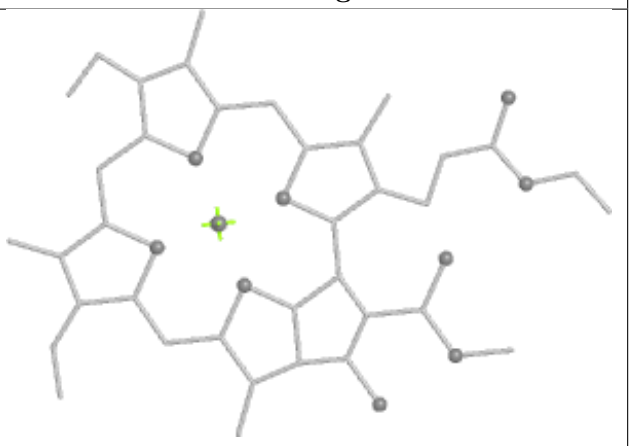
Bond lengths



Bond angles

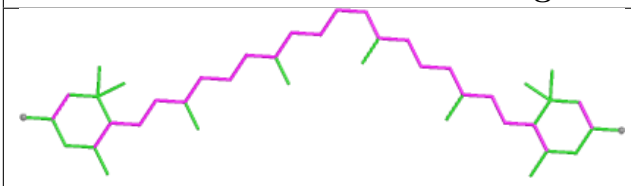


Torsions

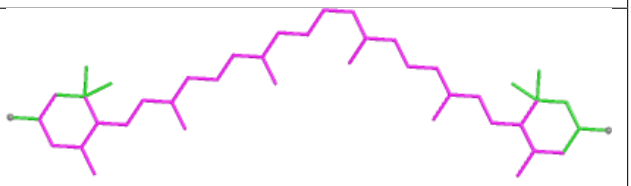


Rings

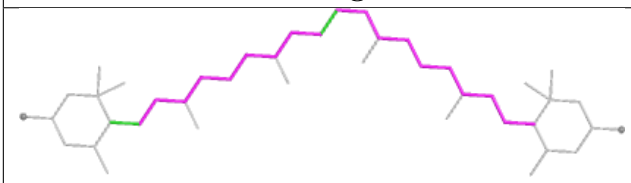
Ligand 5X6 1 314



Bond lengths



Bond angles



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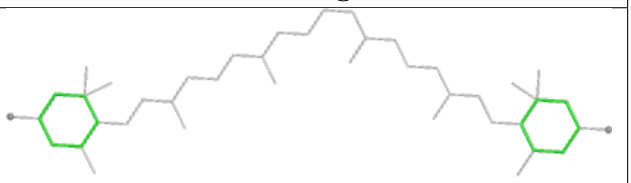
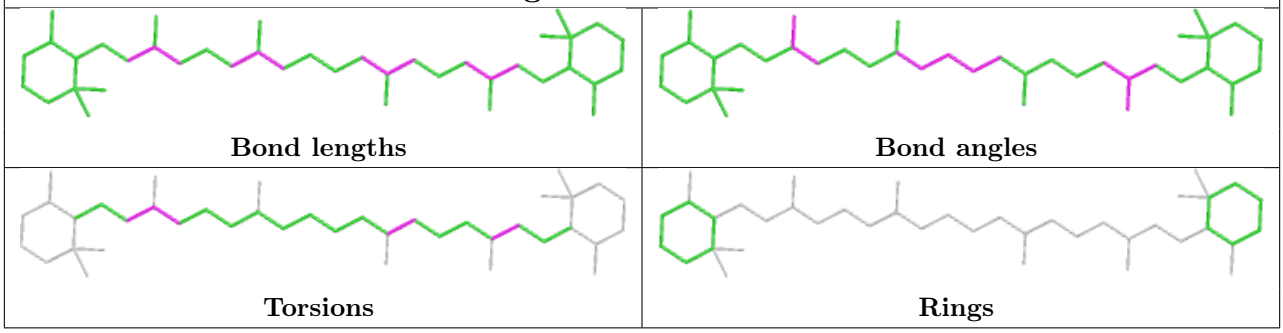
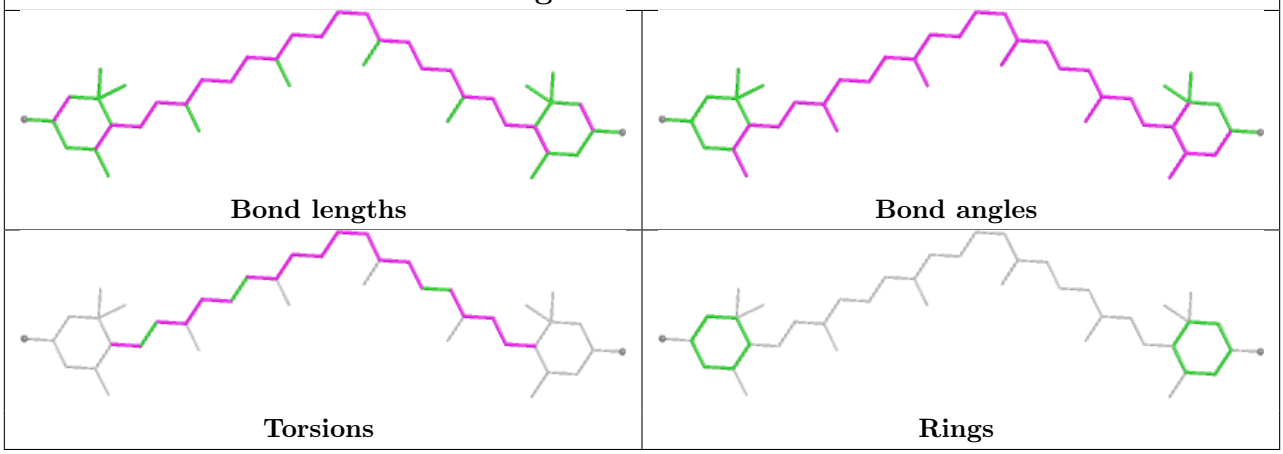


Rings

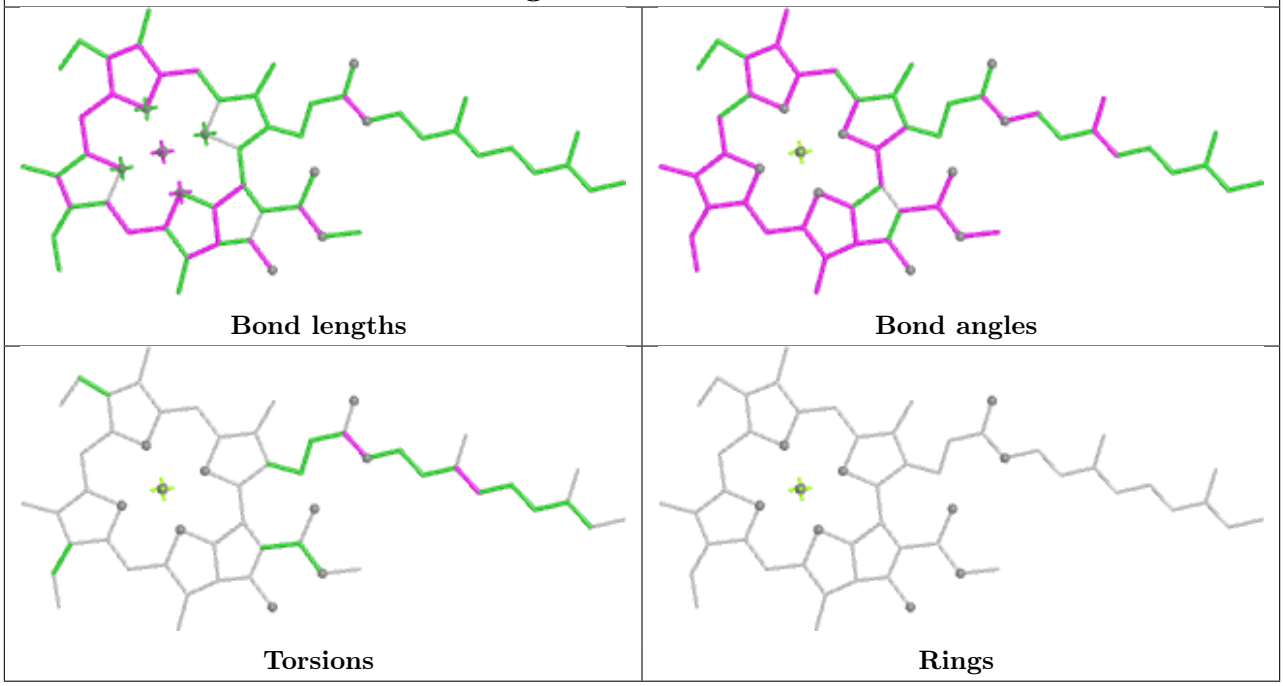
Ligand BCR B 844



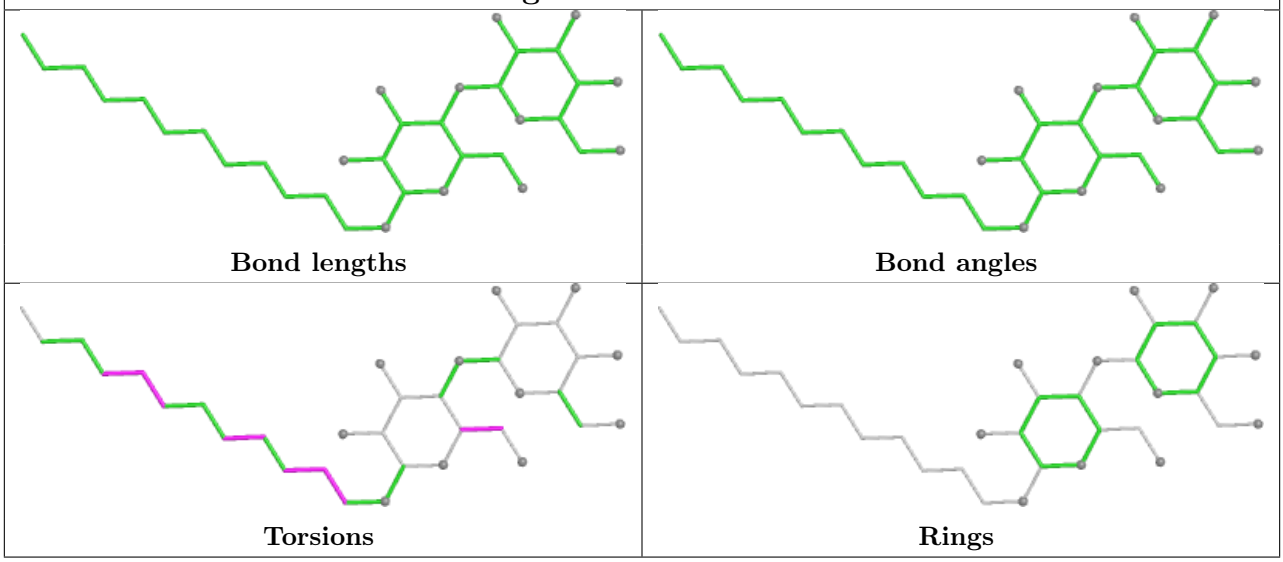
Ligand 5X6 1 316



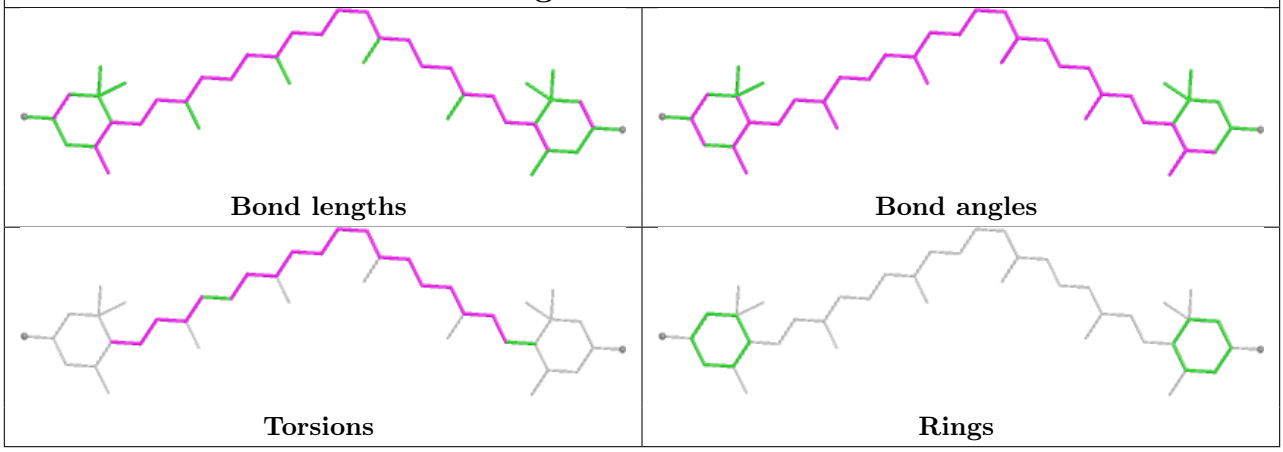
Ligand CLA A 830



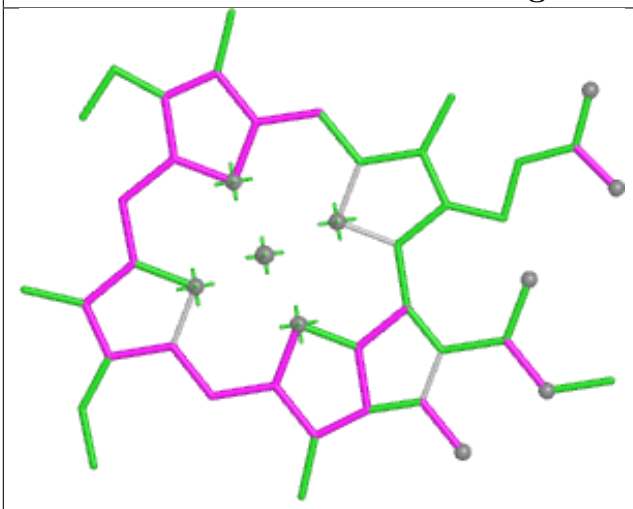
Ligand LMT B 850



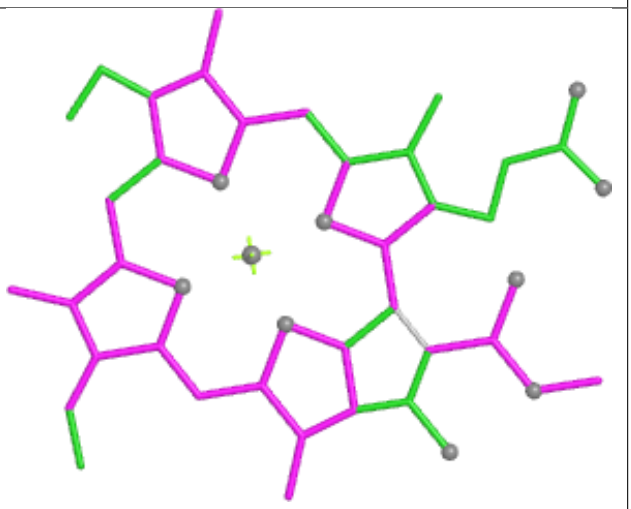
Ligand 5X6 4 314



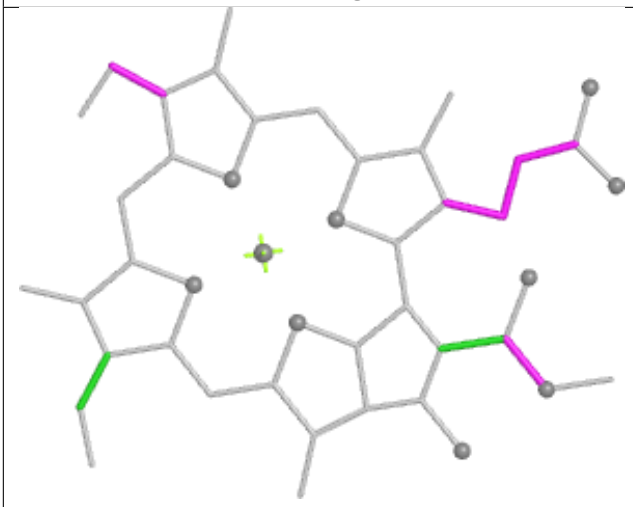
Ligand CLA 5 311



Bond lengths



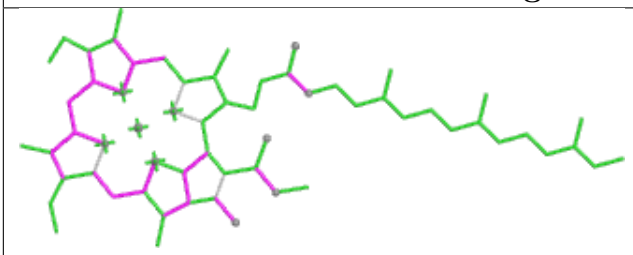
Bond angles



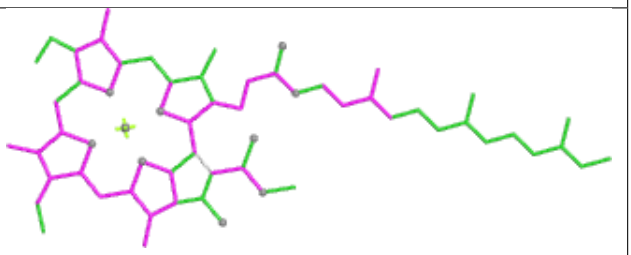
Torsions

Rings

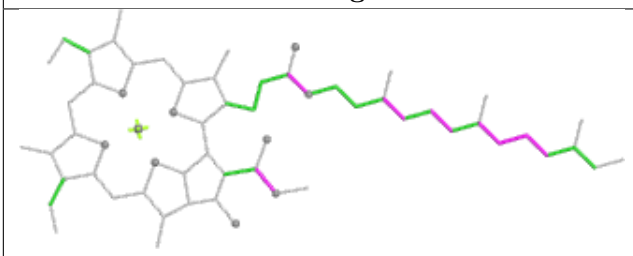
Ligand CLA A 855



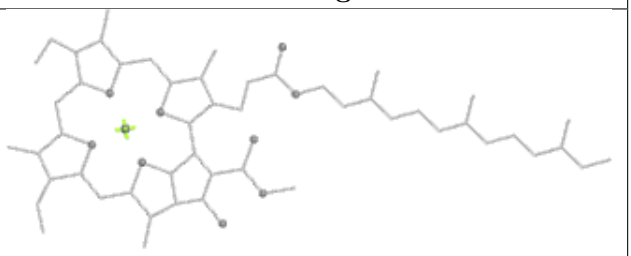
Bond lengths



Bond angles

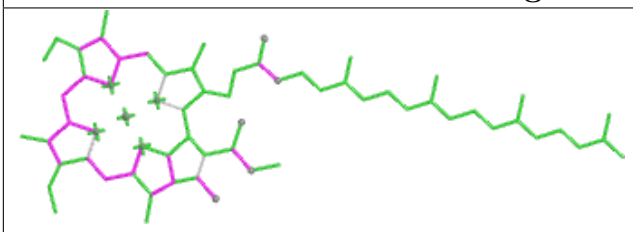


Torsions



Rings

Ligand CLA B 833



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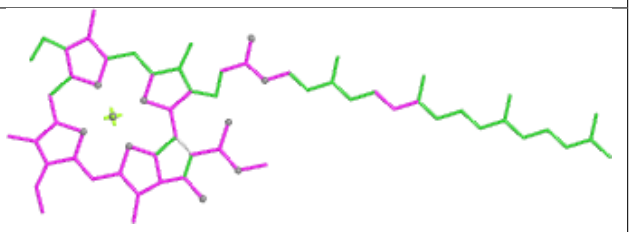
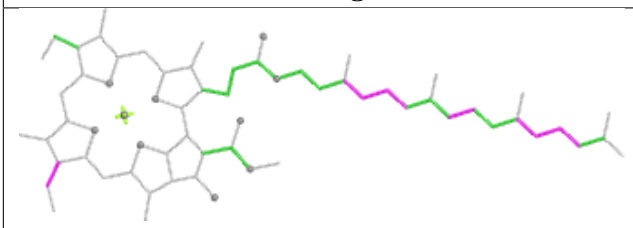


Bond angles



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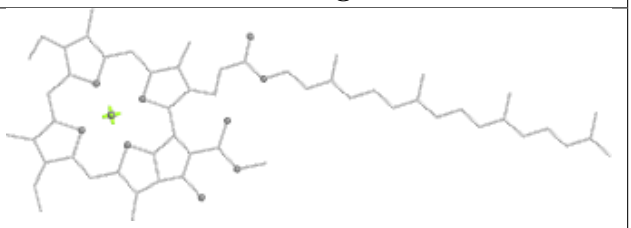
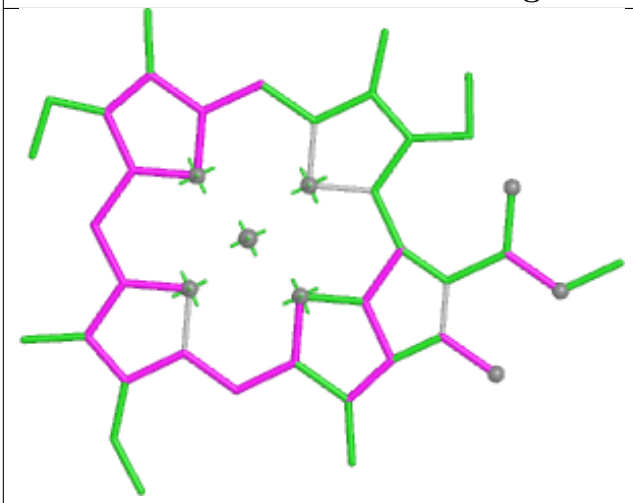


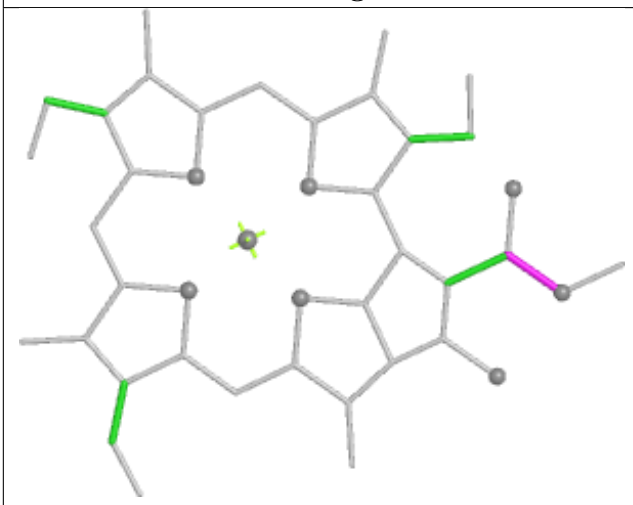
Rings

Ligand CLA K 103

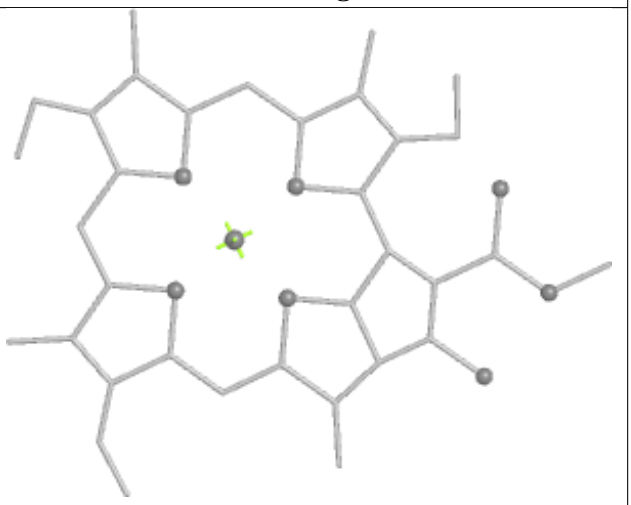


Bond lengths

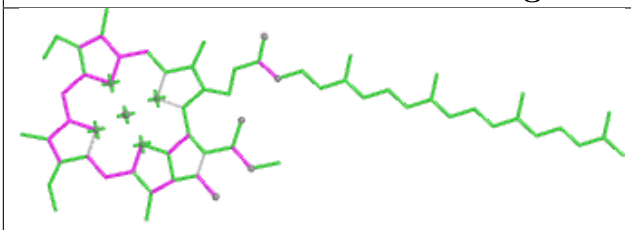
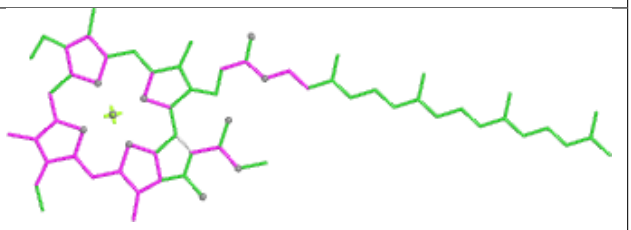
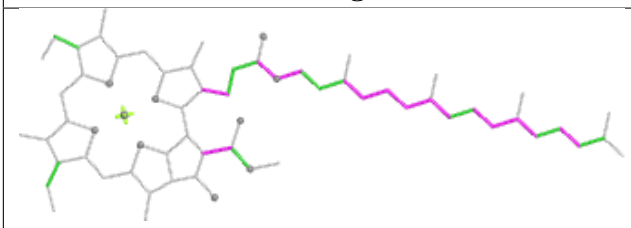
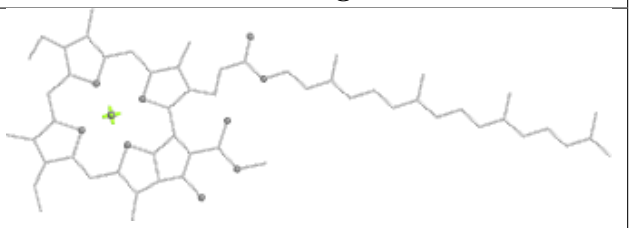
Bond angles

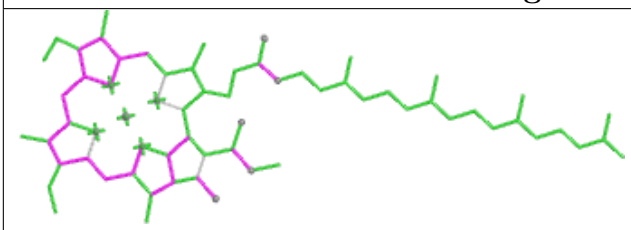
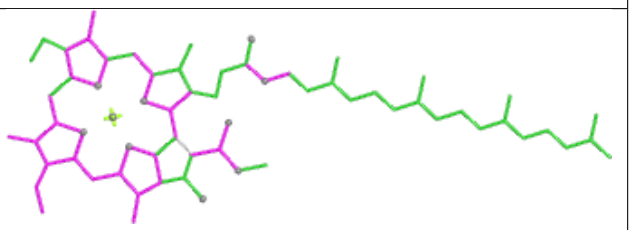
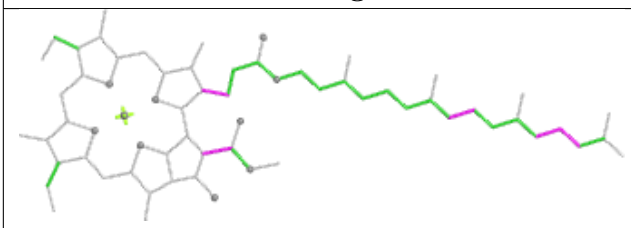
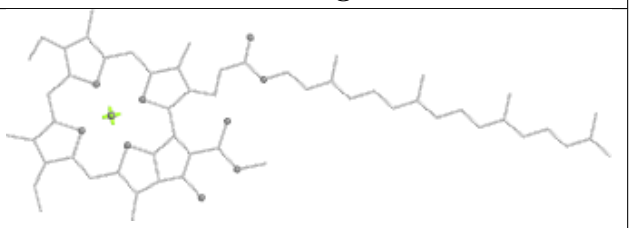


Torsions

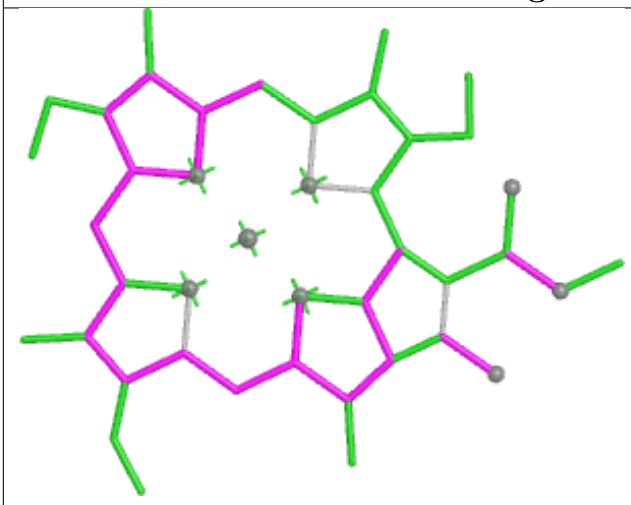


Rings

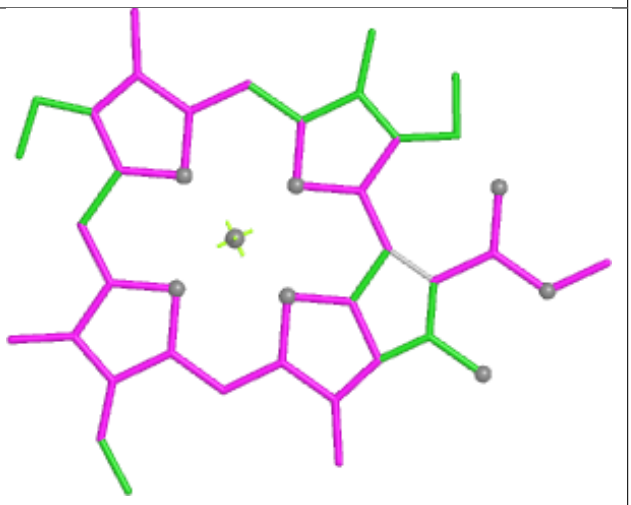
Ligand CLA A 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 856	
 Bond lengths	 Bond angles
 Torsions	 Rings

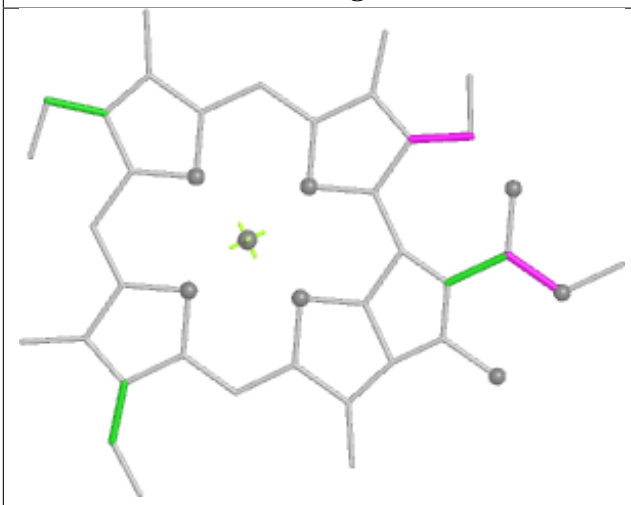
Ligand CLA 3 313



Bond lengths



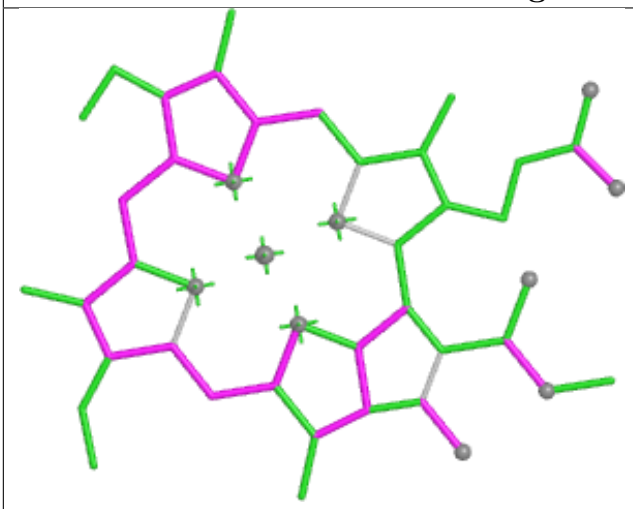
Bond angles



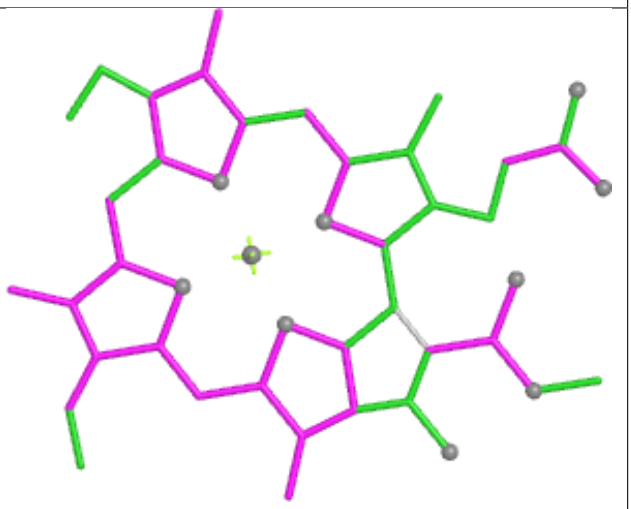
Torsions

Rings

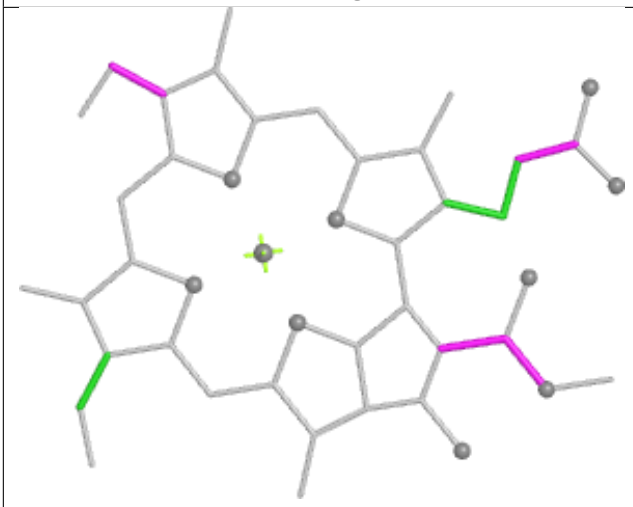
Ligand CLA 3 308



Bond lengths



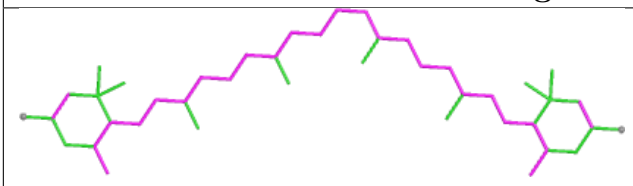
Bond angles



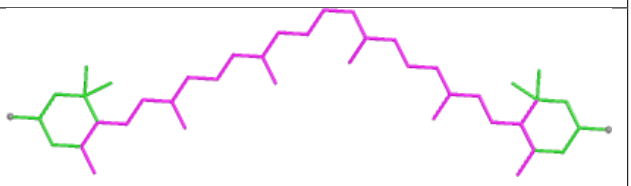
Torsions

Rings

Ligand 5X6 3 318

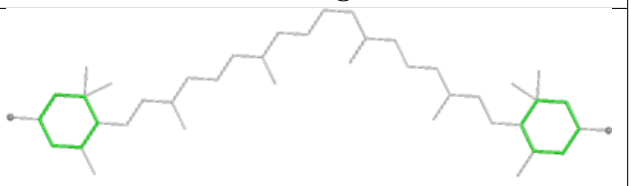


Bond lengths



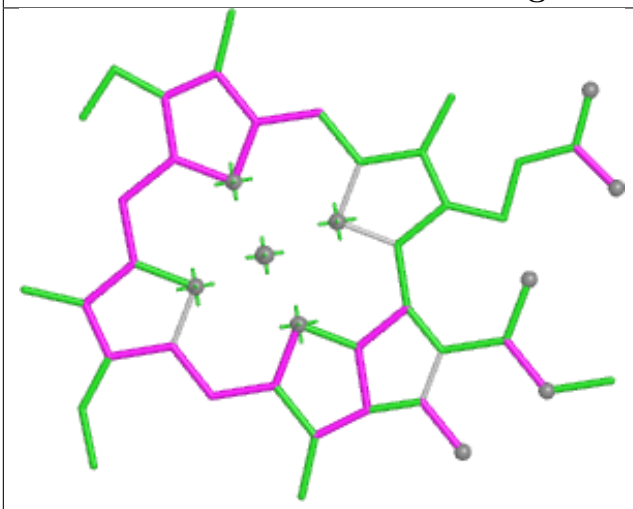
Bond angles

Torsions



Rings

Ligand CLA 1 309



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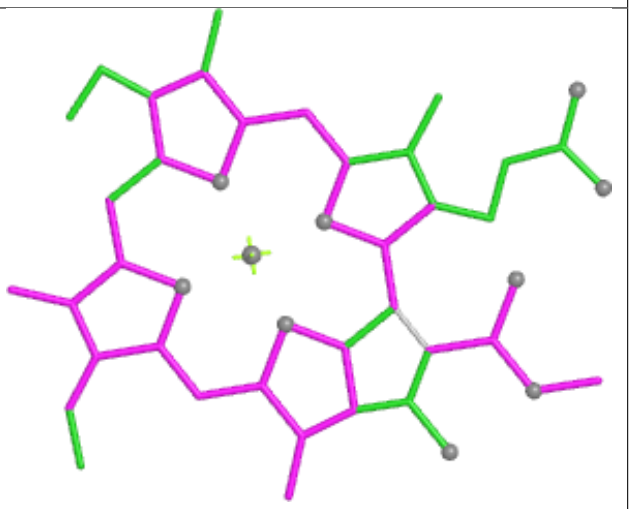

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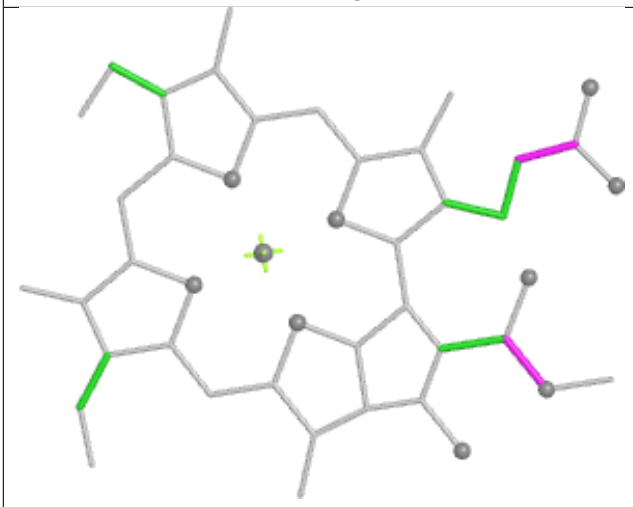
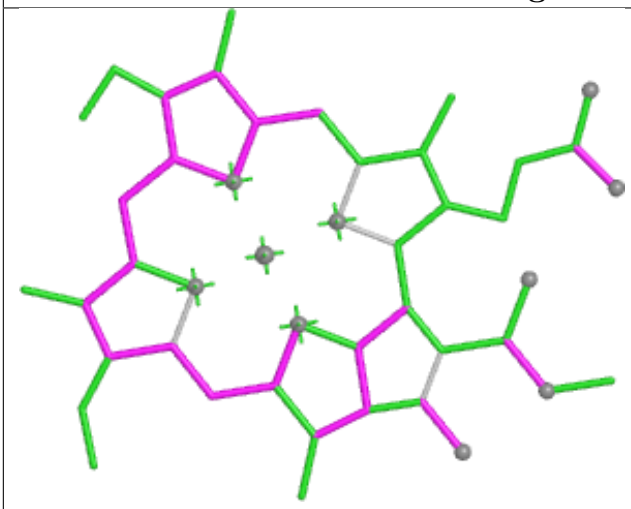


Torsions

Rings

Ligand CLA 3 309



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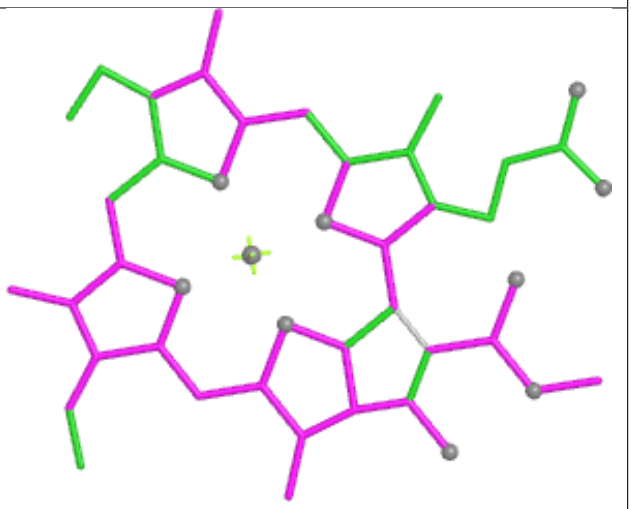

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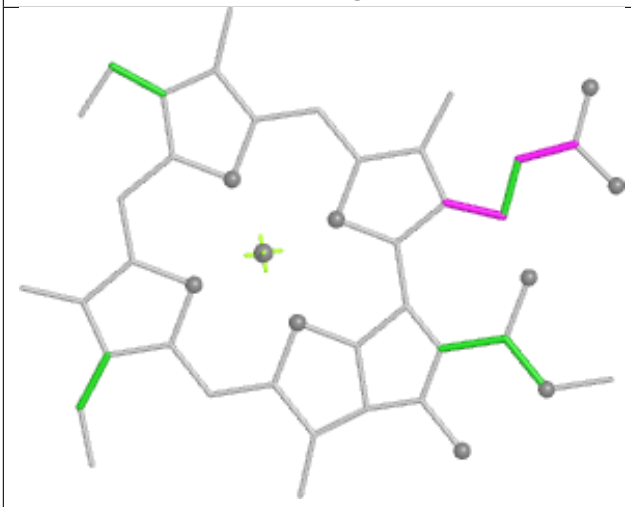
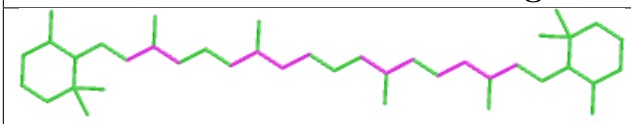


Torsions

Rings

Ligand BCR L 201



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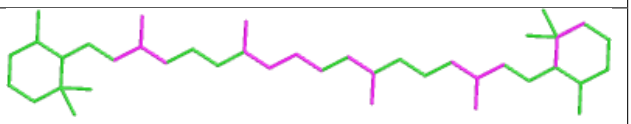

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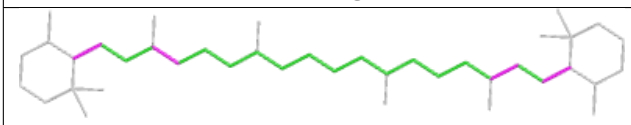

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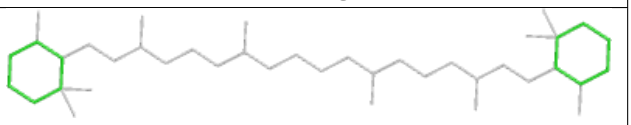
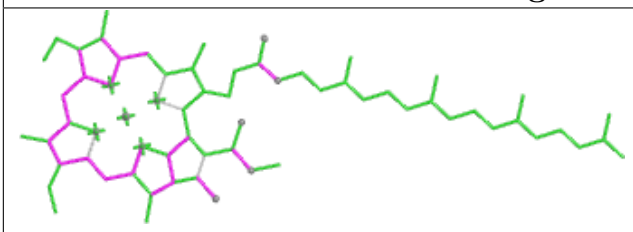


Rings

Ligand CLA 5 304



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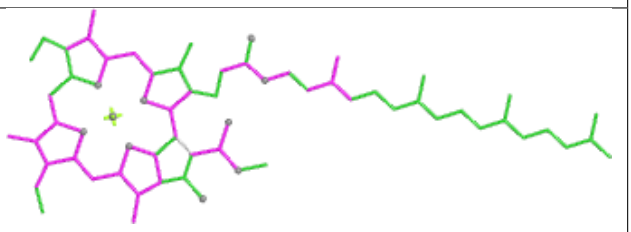

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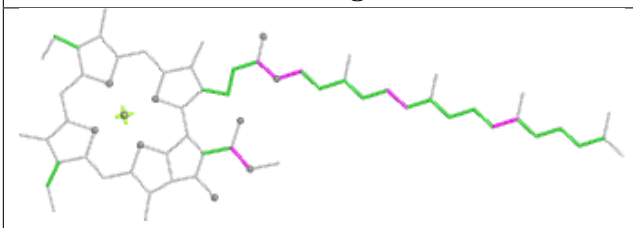

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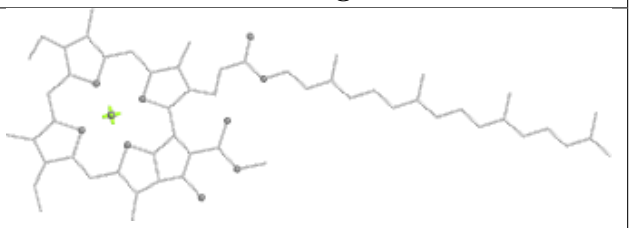
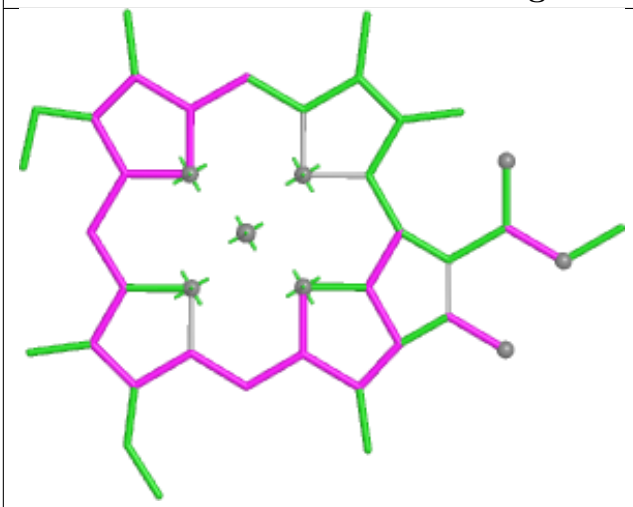


Rings

Ligand CLA 4 309



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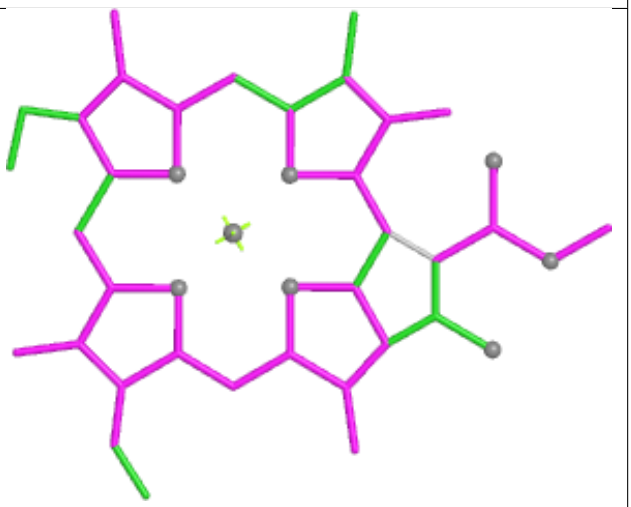

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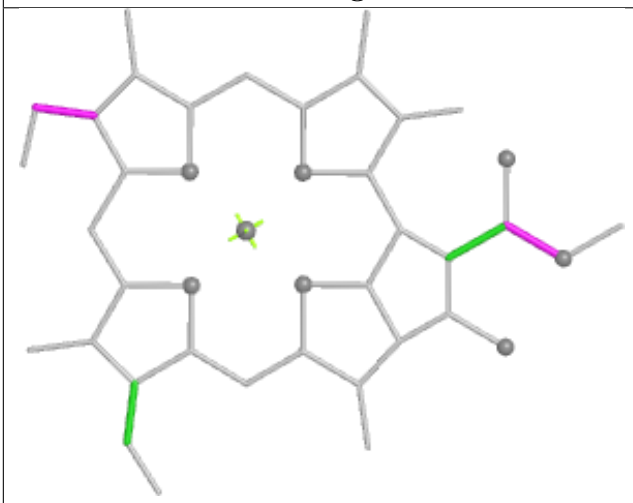

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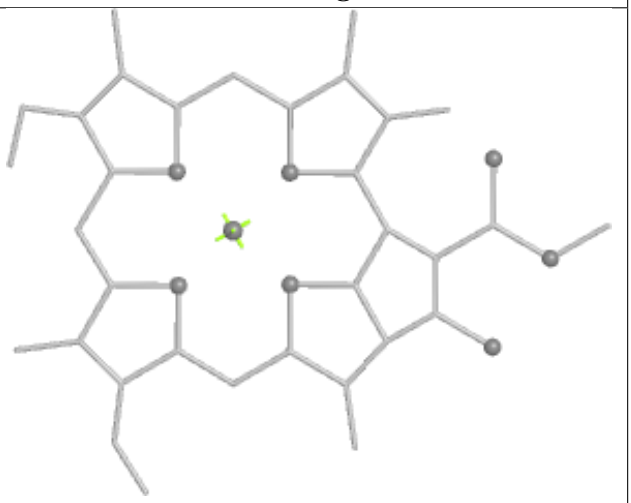
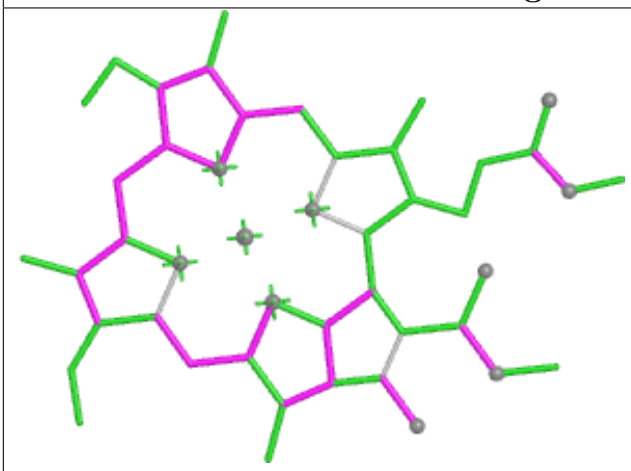
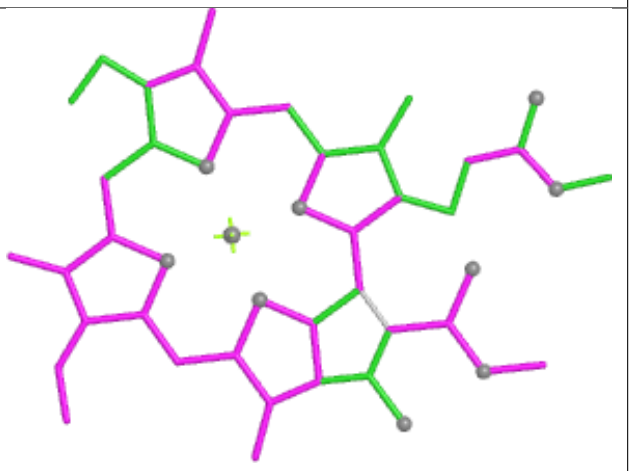
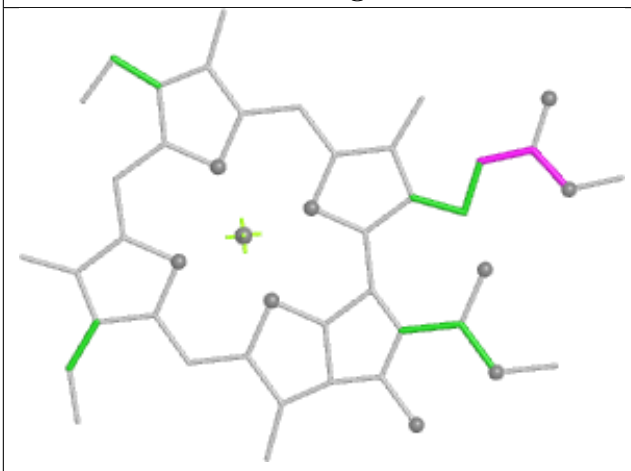
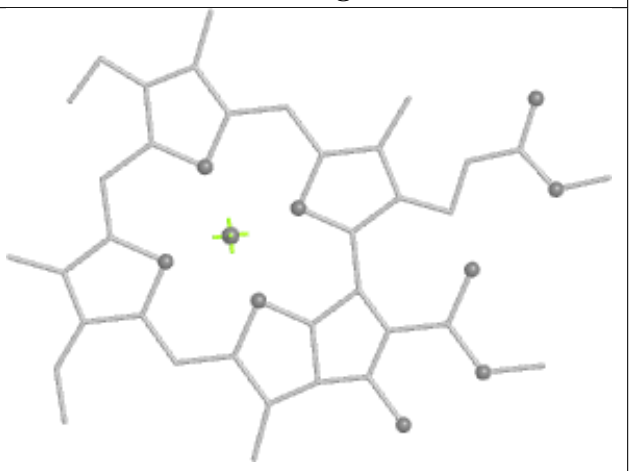
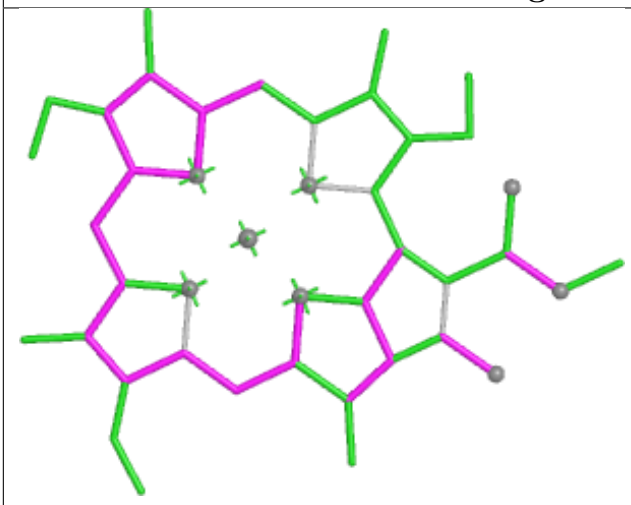


Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 313



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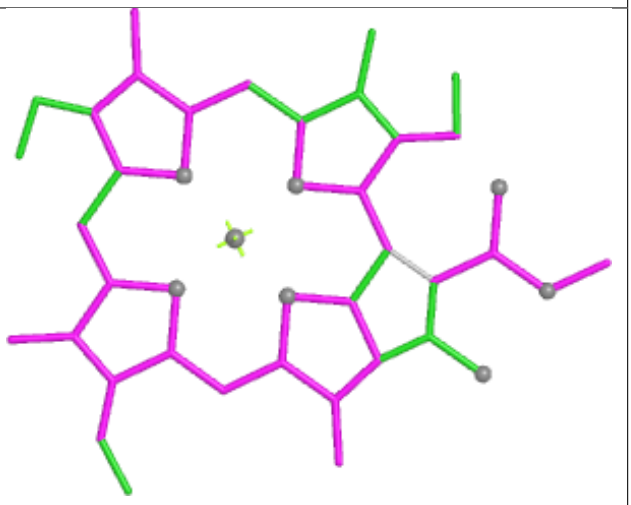

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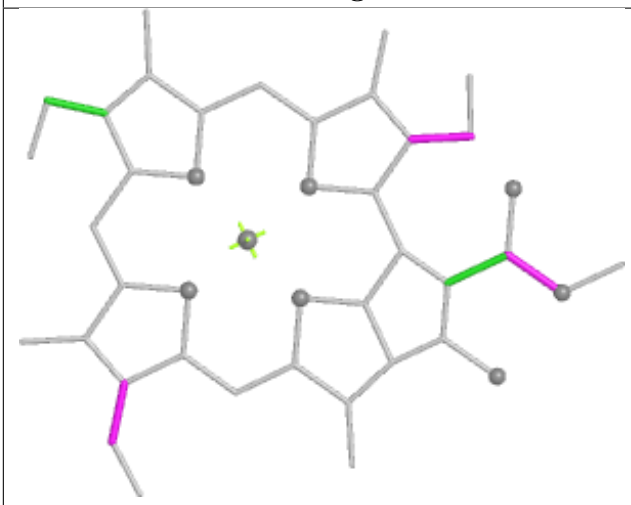
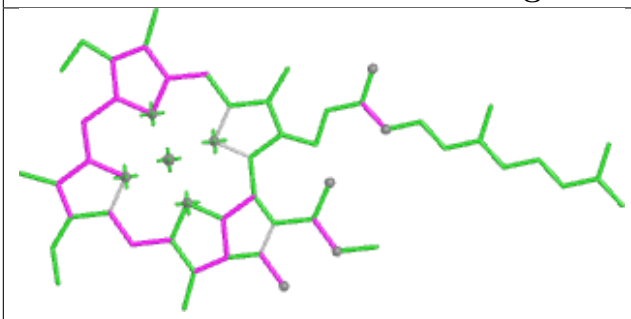


Torsions

Rings

Ligand CLA A 824



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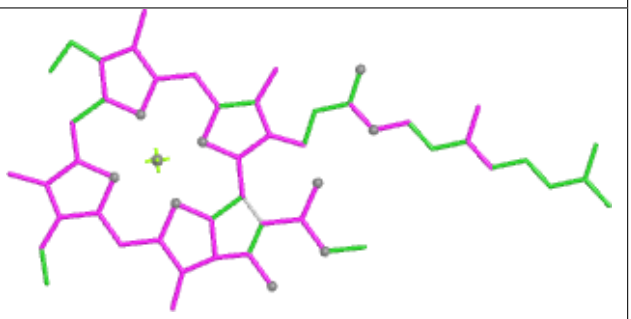

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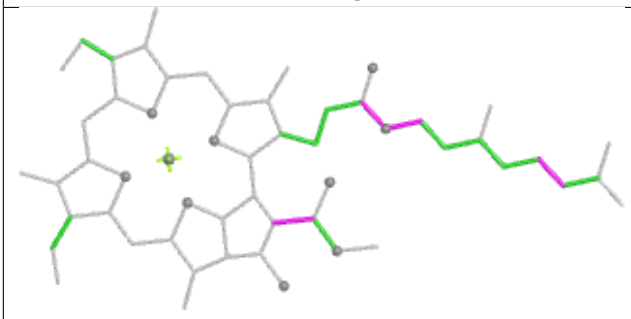

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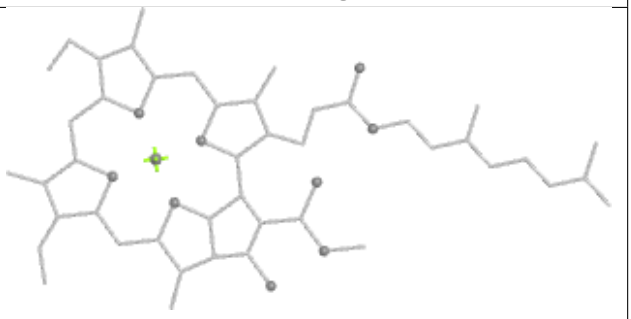
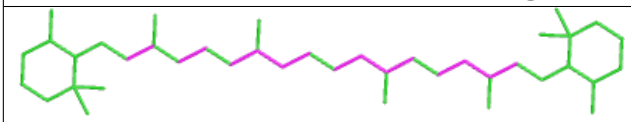


Rings

Ligand BCR A 845



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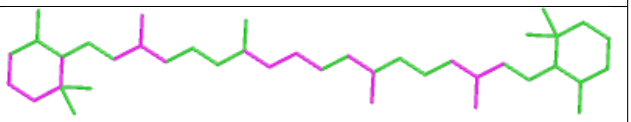
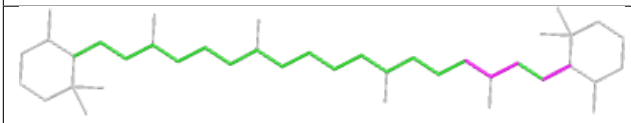


Bond angles



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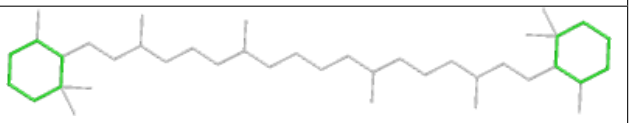
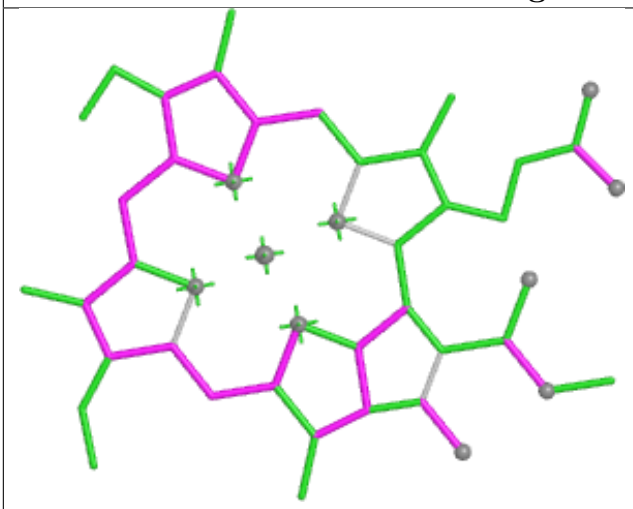


Rings

Ligand CLA 1 301



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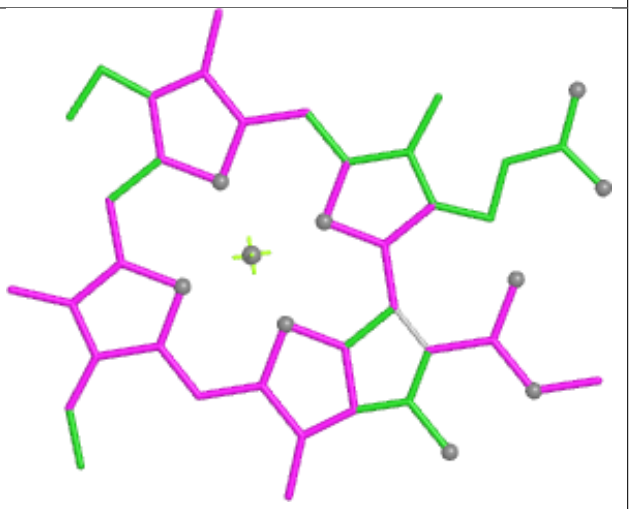

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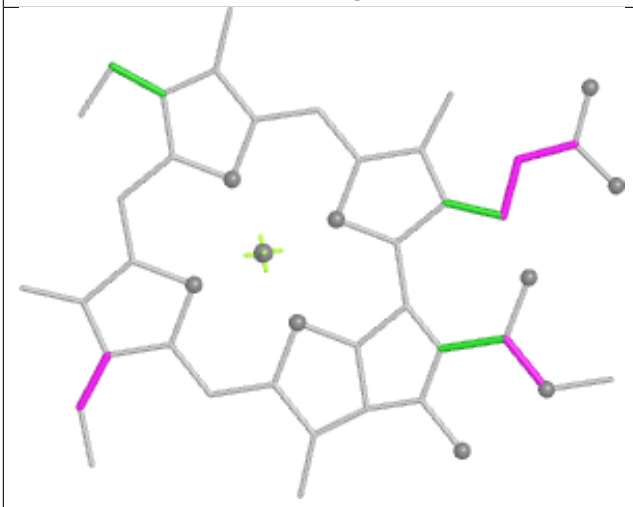
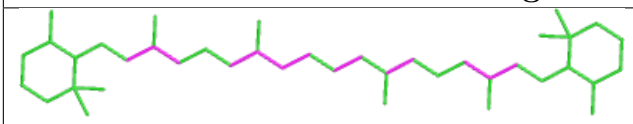


Torsions

Rings

Ligand BCR B 847



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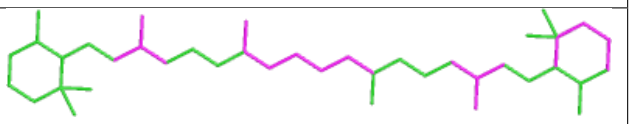
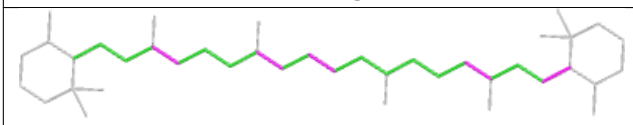


Bond angles



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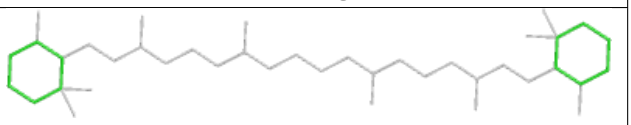
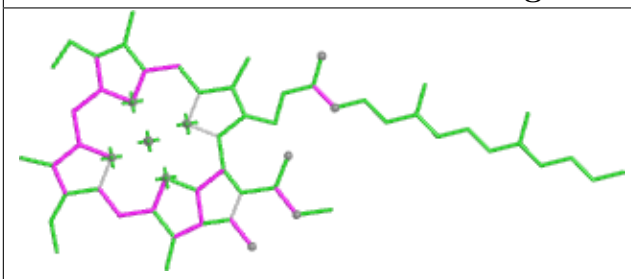


Rings

Ligand CLA B 857



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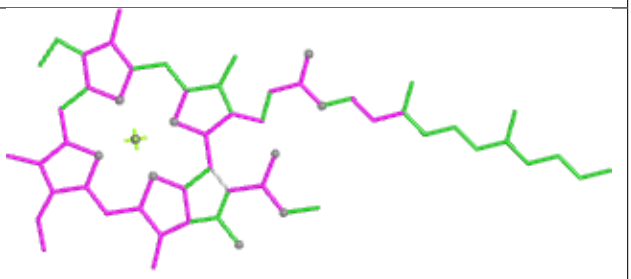

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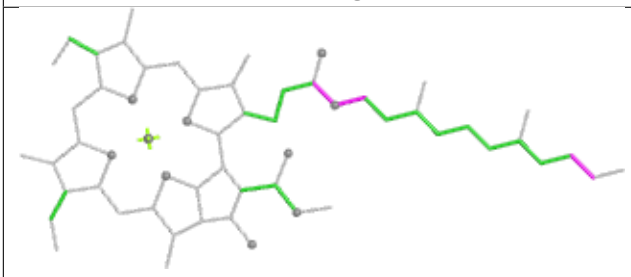

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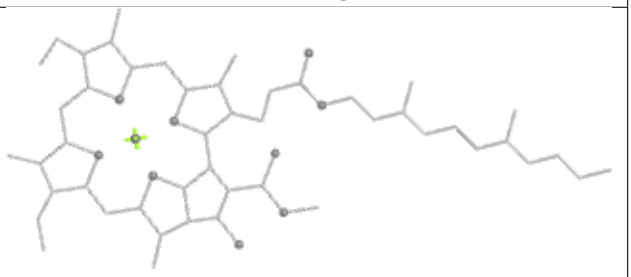
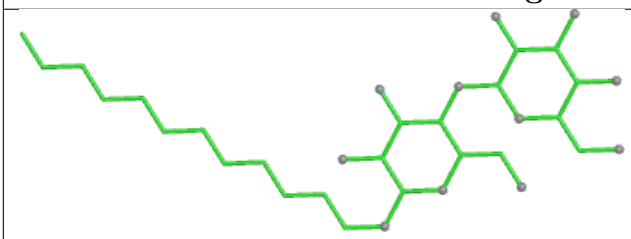


Rings

Ligand LMT 3 301



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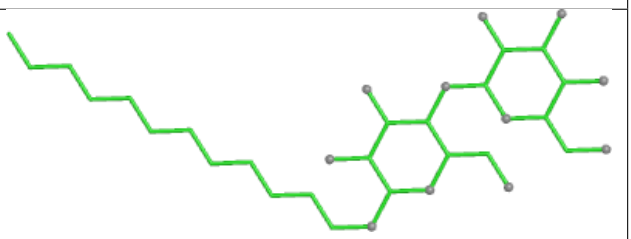
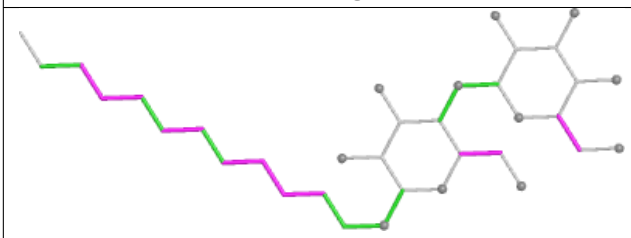


Bond angles



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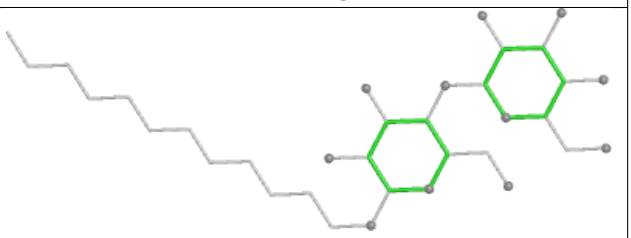
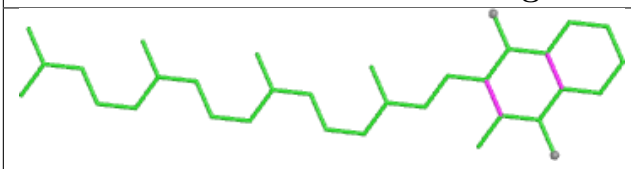
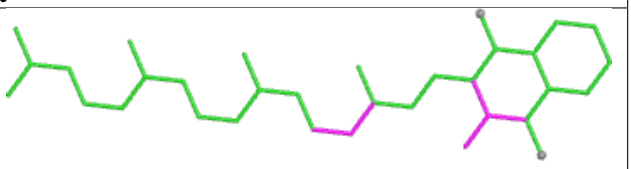


Rings

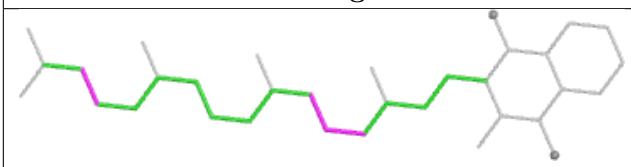
Ligand PQN B 842



Bond lengths



Bond angles



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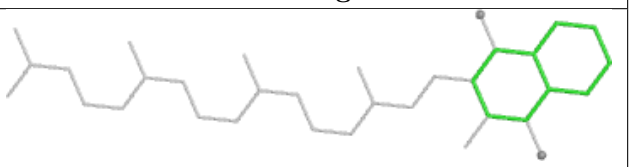
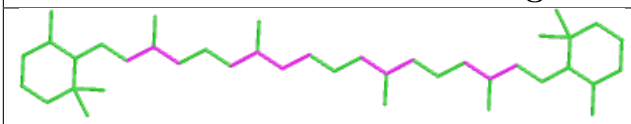
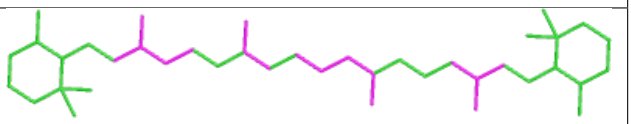


Rings

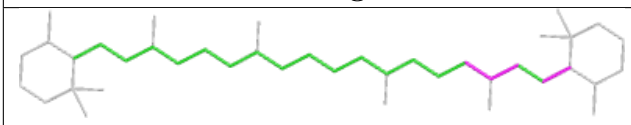
Ligand BCR J 104



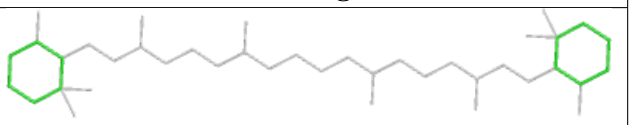
Bond lengths



Bond angles

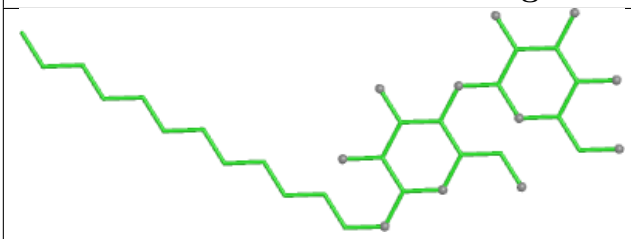


Torsions



Rings

Ligand LMT B 851



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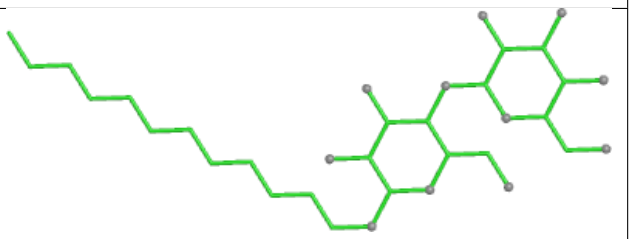

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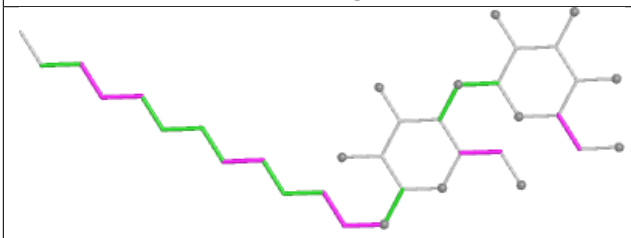
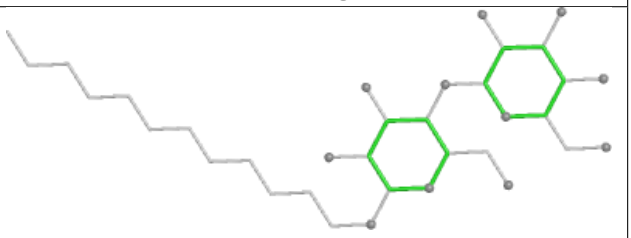
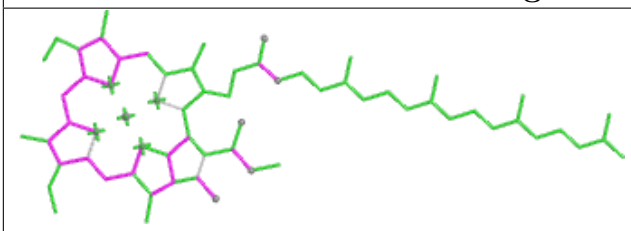


Torsions



Rings

Ligand CLA A 803



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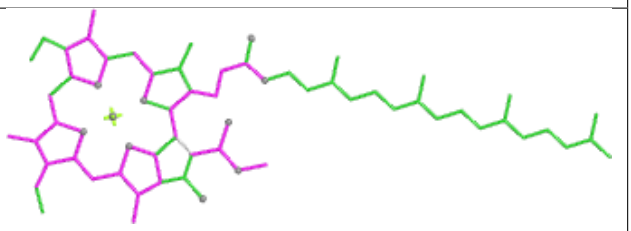

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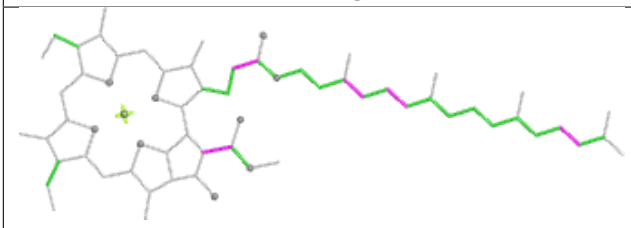

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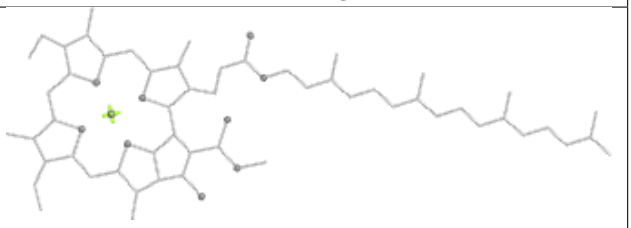
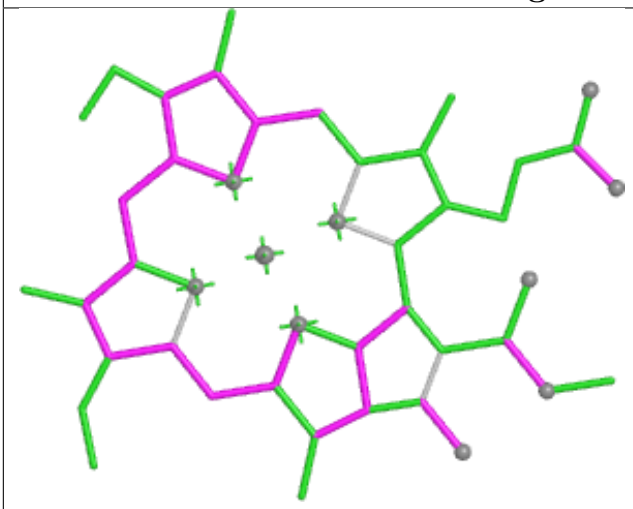


Rings

Ligand CLA 5 313



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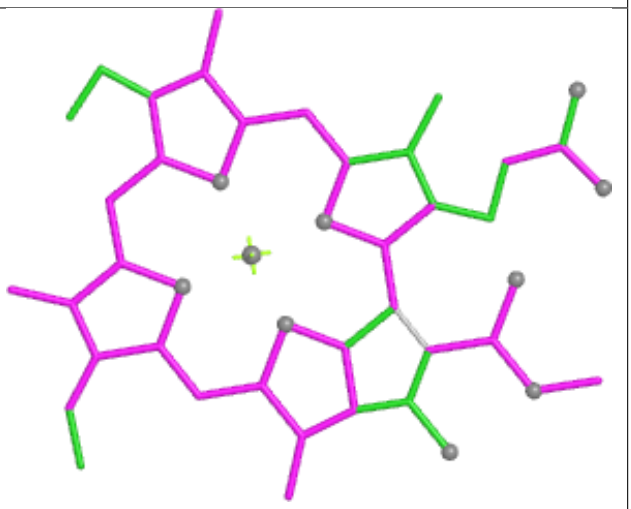

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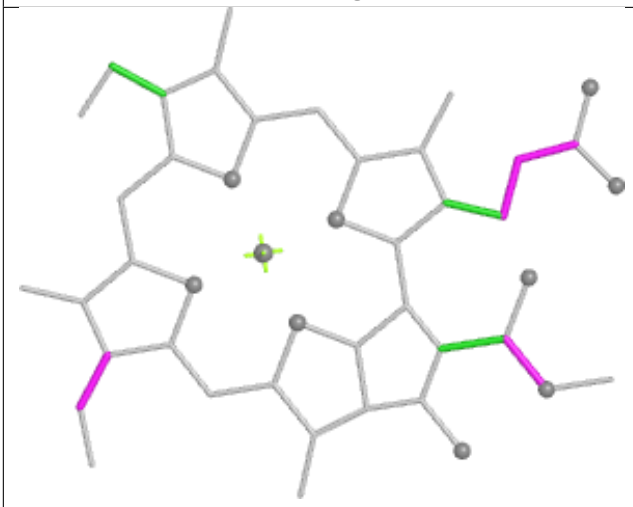
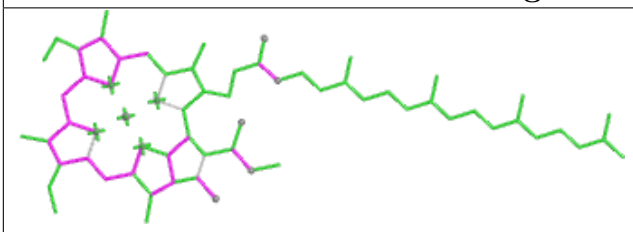


Torsions

Rings

Ligand CLA A 823



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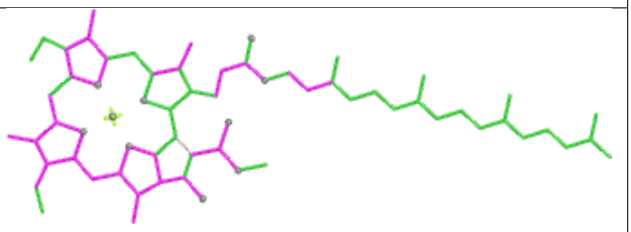

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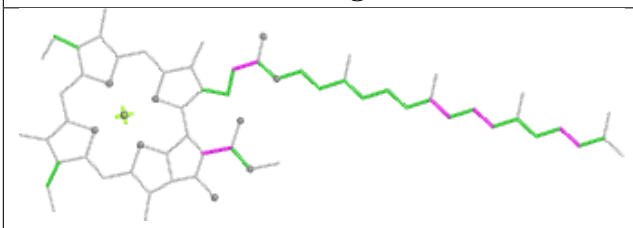

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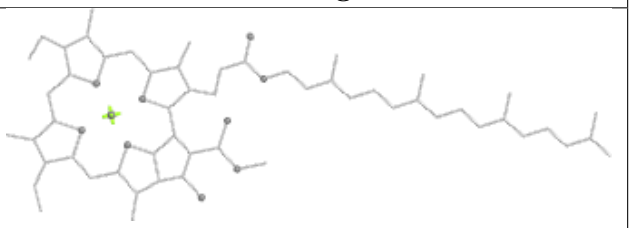
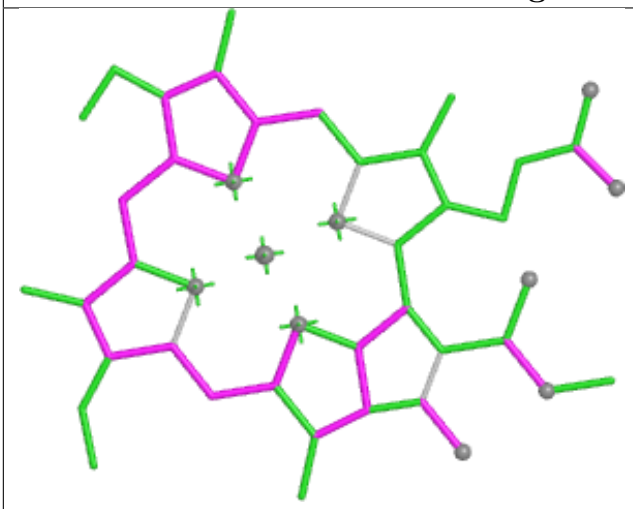


Rings

Ligand CLA 2 314



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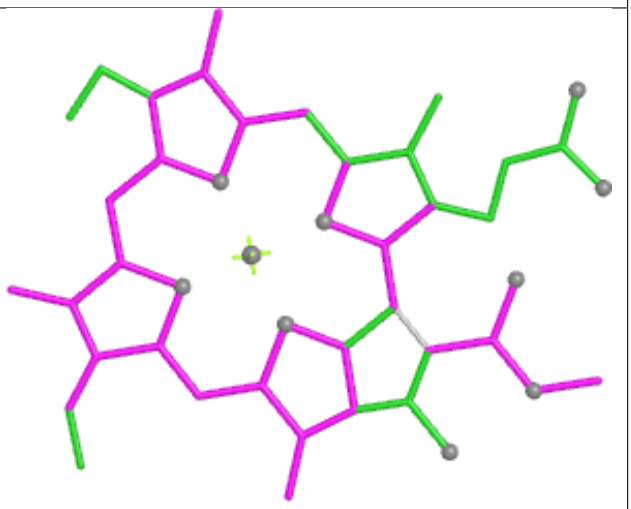

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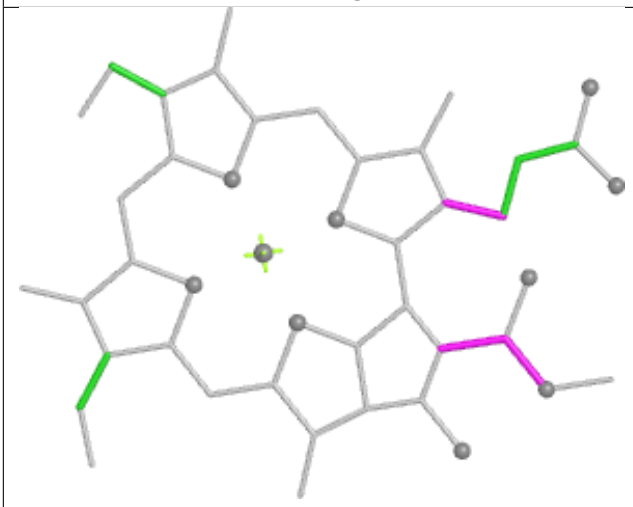
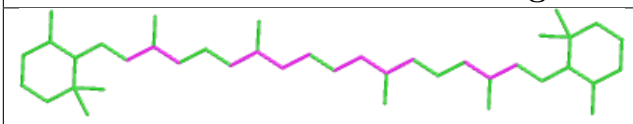


Torsions

Rings

Ligand BCR I 101



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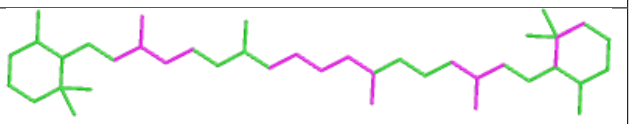
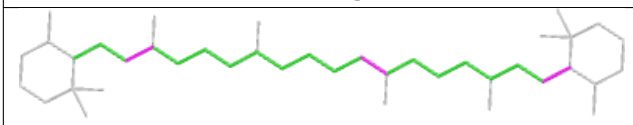


Bond angles



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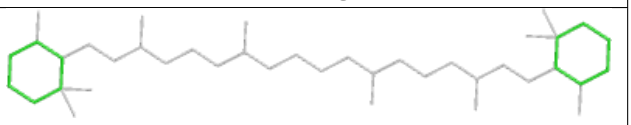
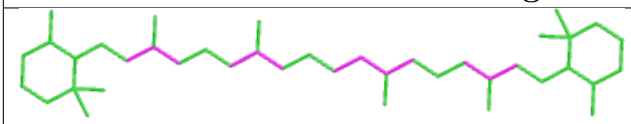


Rings

Ligand BCR B 845



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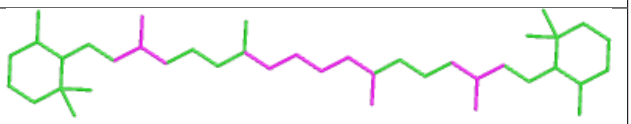
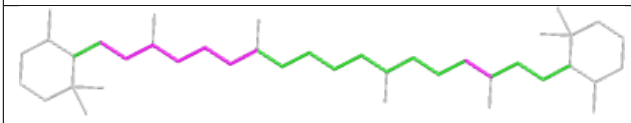


Bond angles



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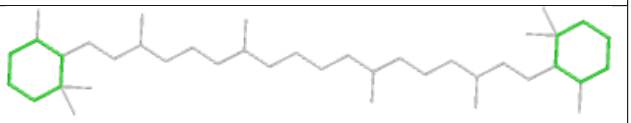
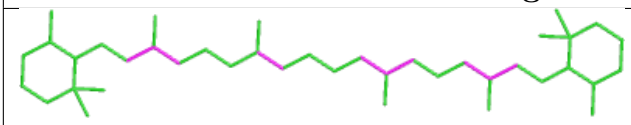


Rings

Ligand BCR B 803



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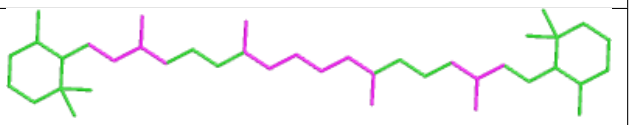
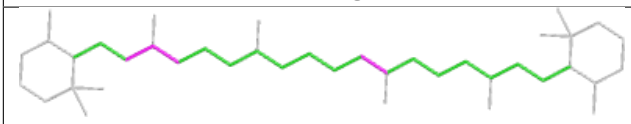


Bond angles



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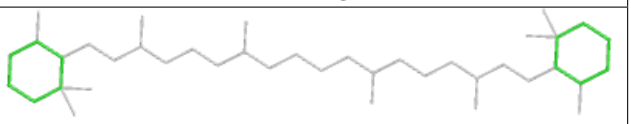
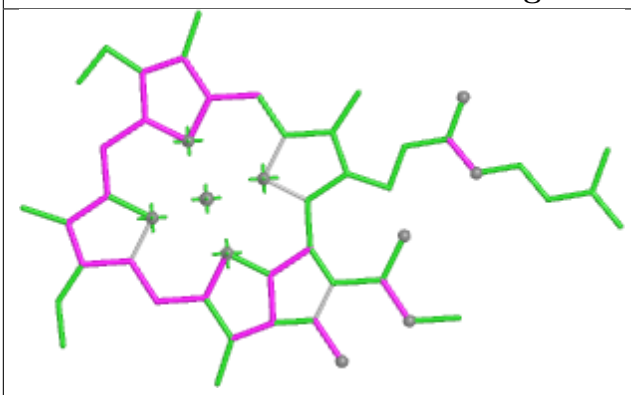


Rings

Ligand CLA O 204



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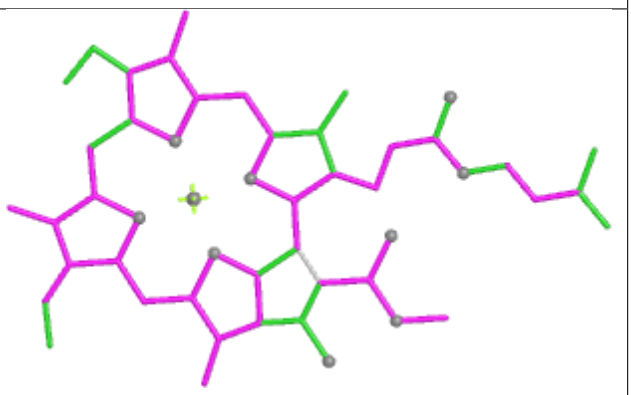

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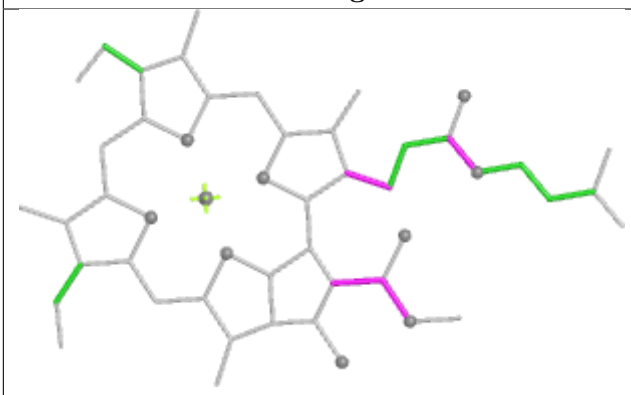

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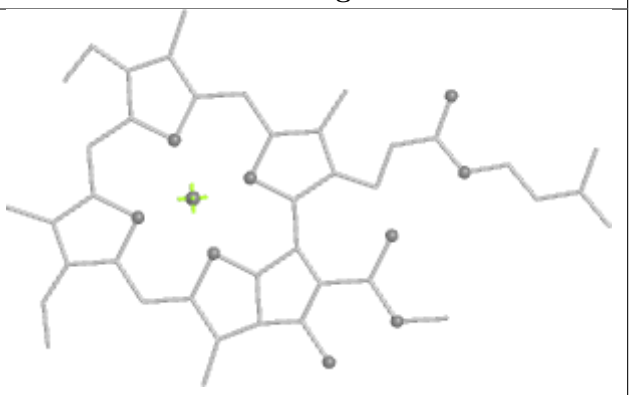
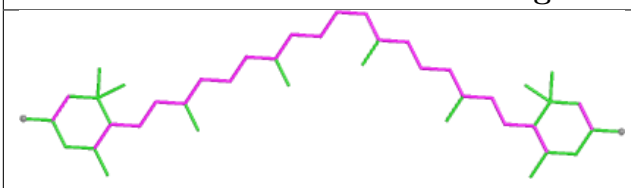
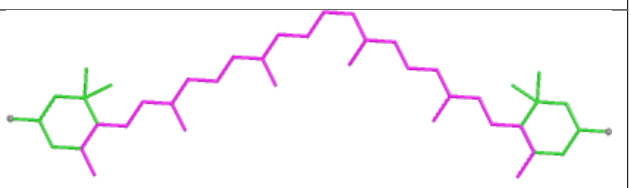
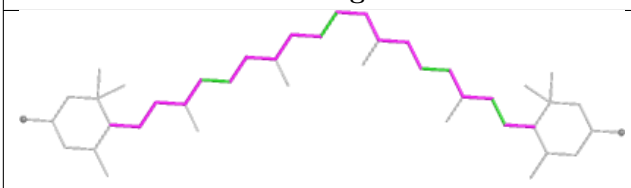
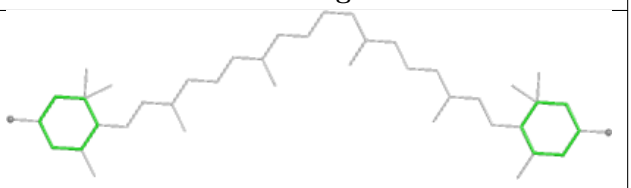
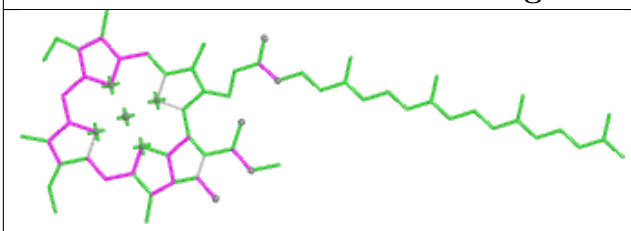
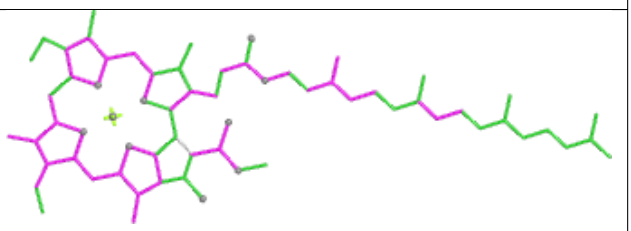
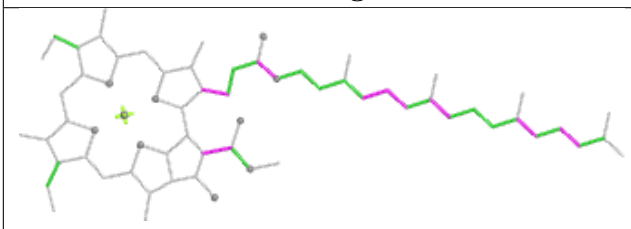
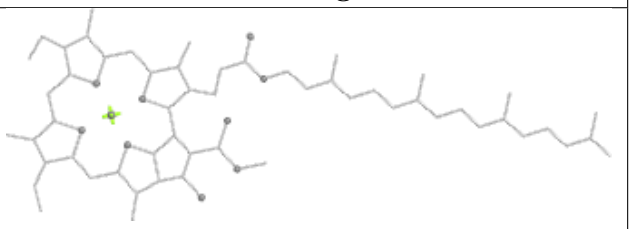
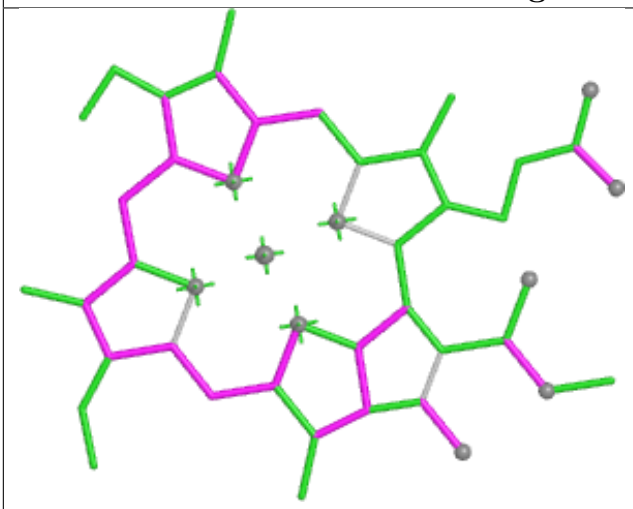


Rings

Ligand 5X6 J 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 310



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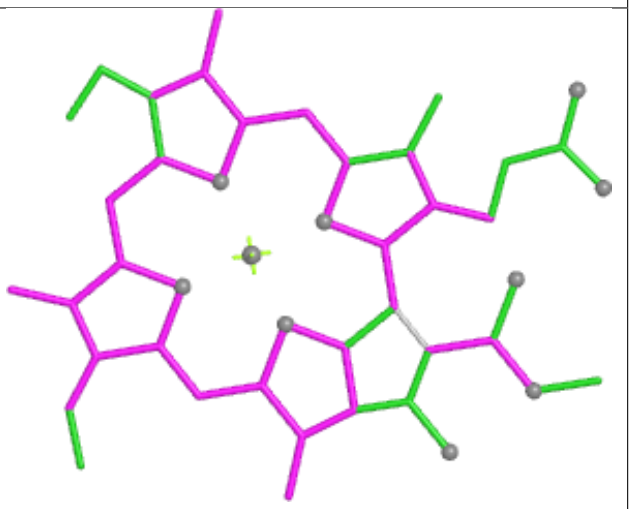
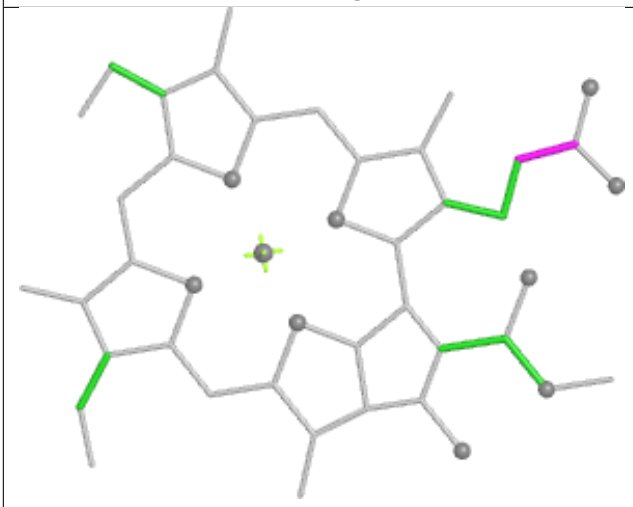


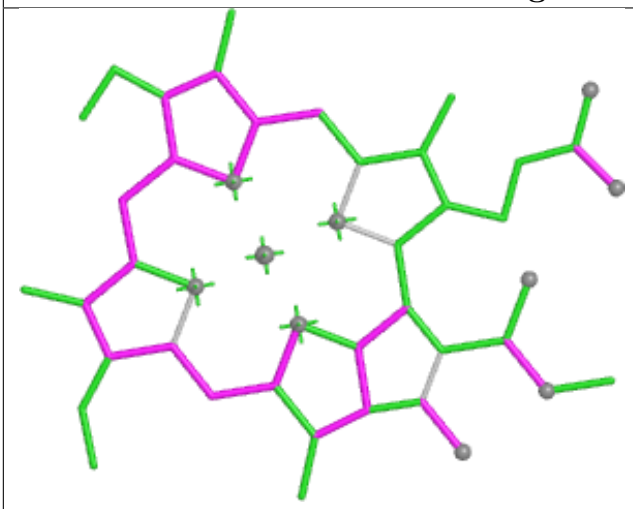
Bond angles



Torsions

Rings

Ligand CLA 4 307



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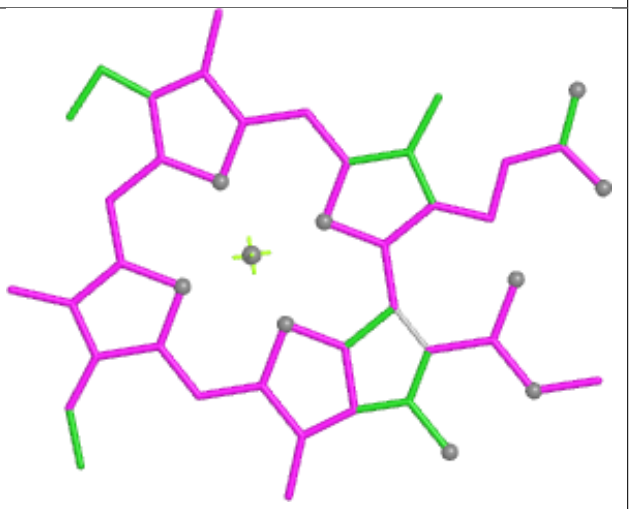
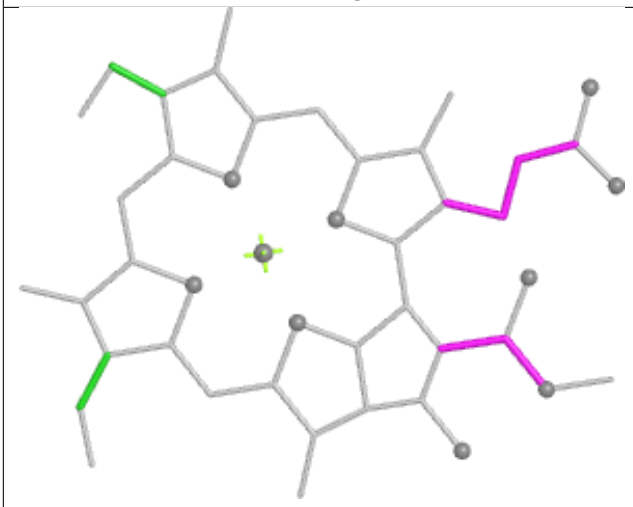


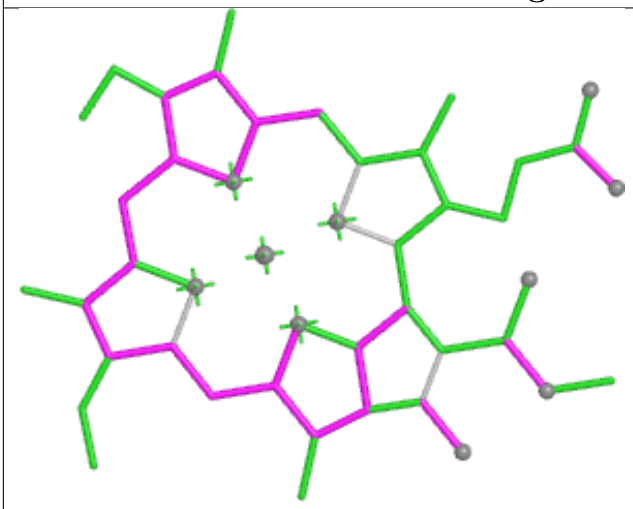
Bond angles



Torsions

Rings

Ligand CLA 1 305



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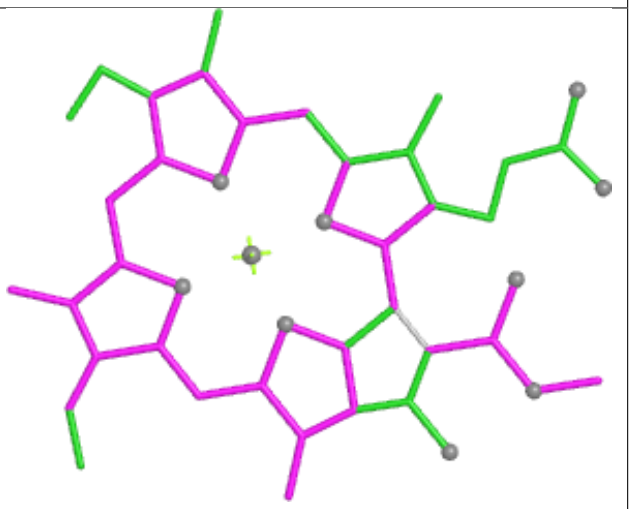
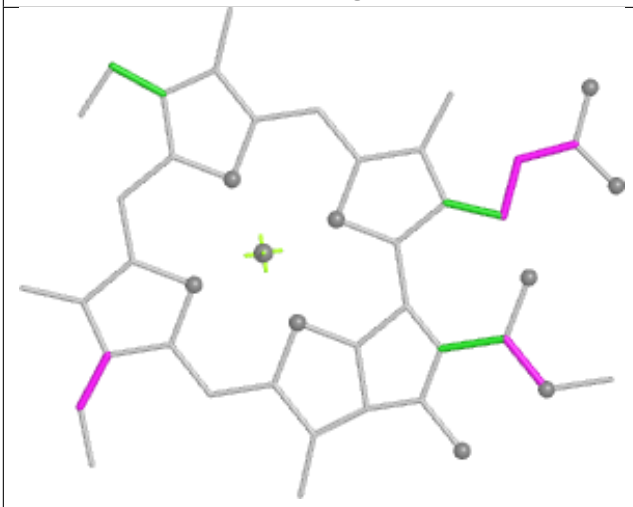


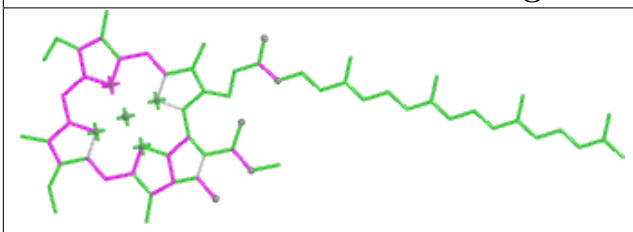
Bond angles



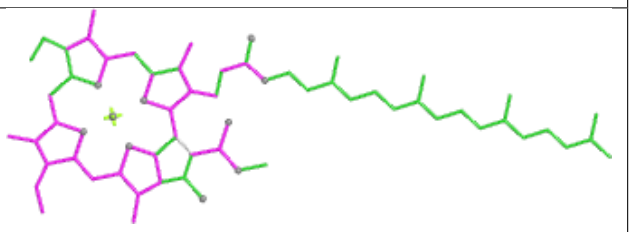
Torsions

Rings

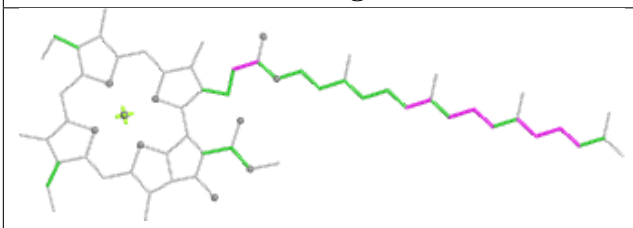
Ligand CLA A 826



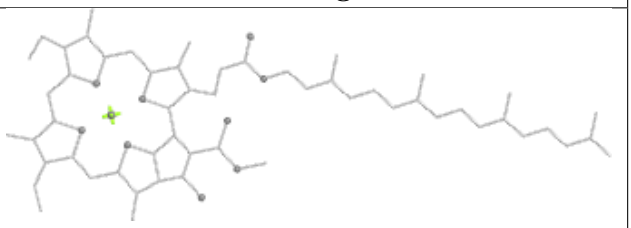
Bond lengths



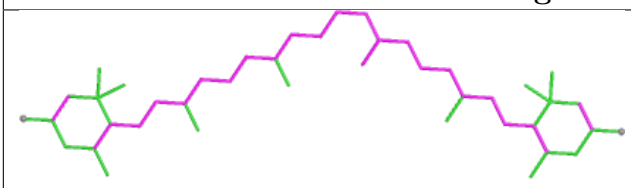
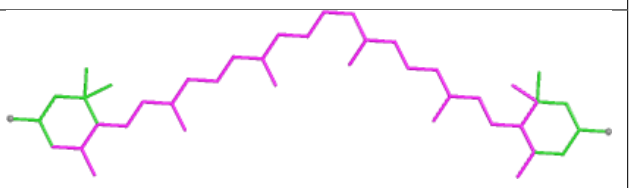
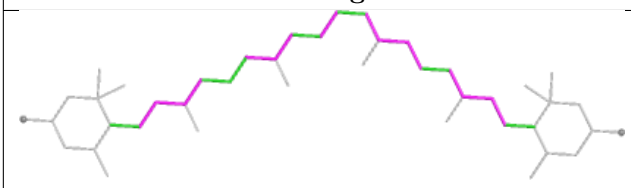
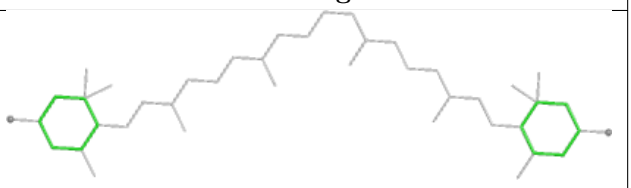
Bond angles

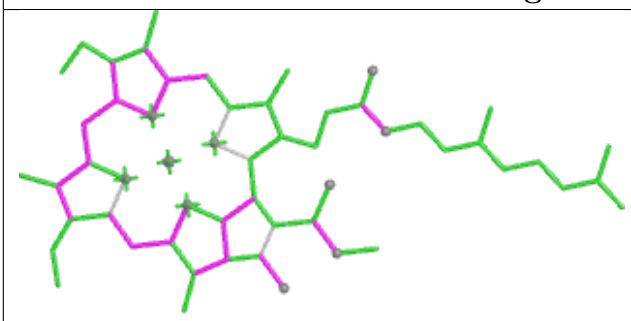
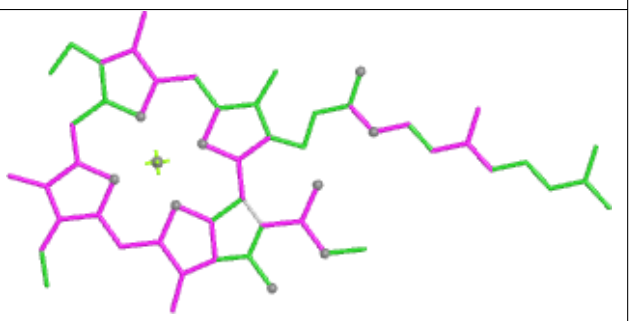
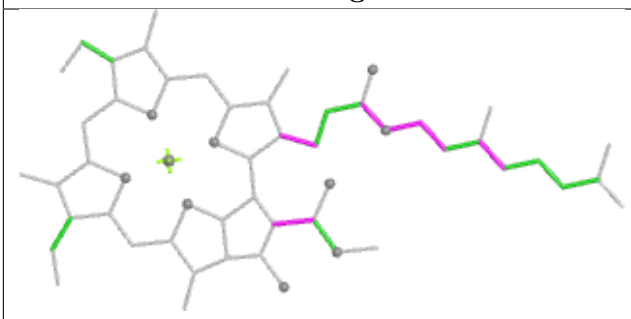
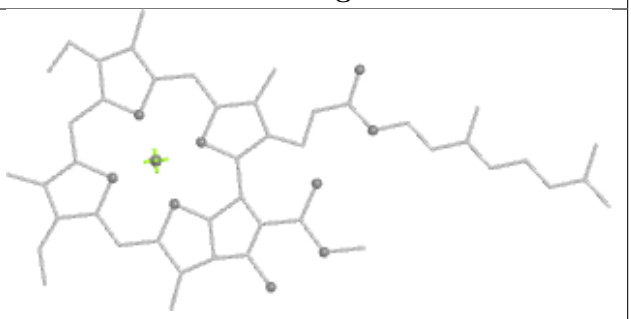


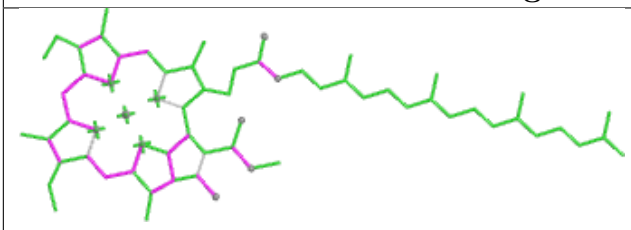
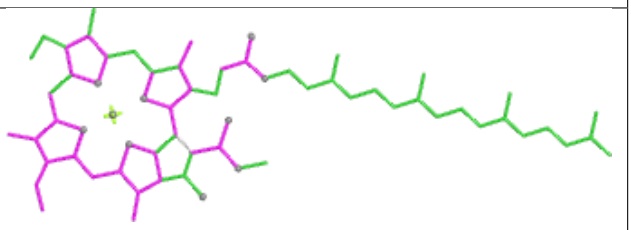
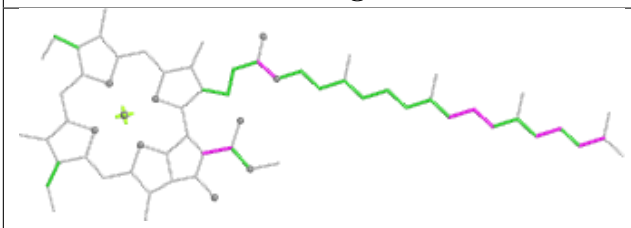
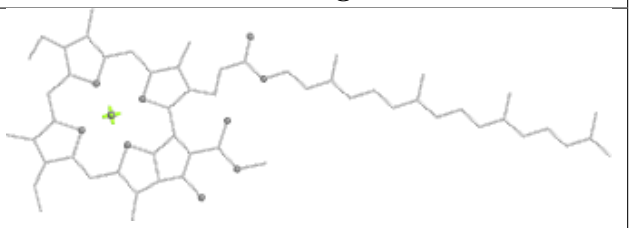
Torsions

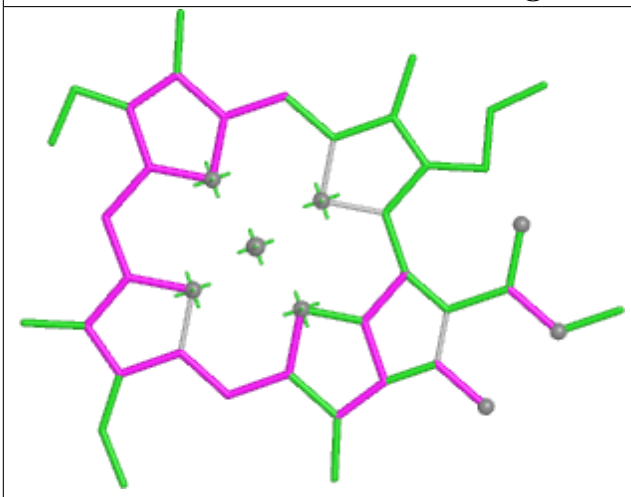
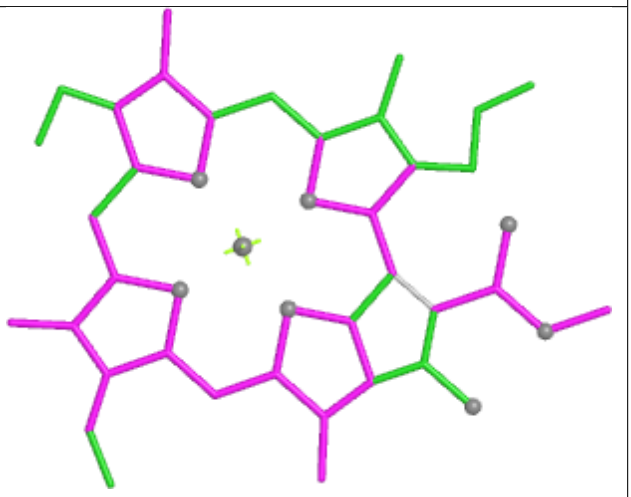
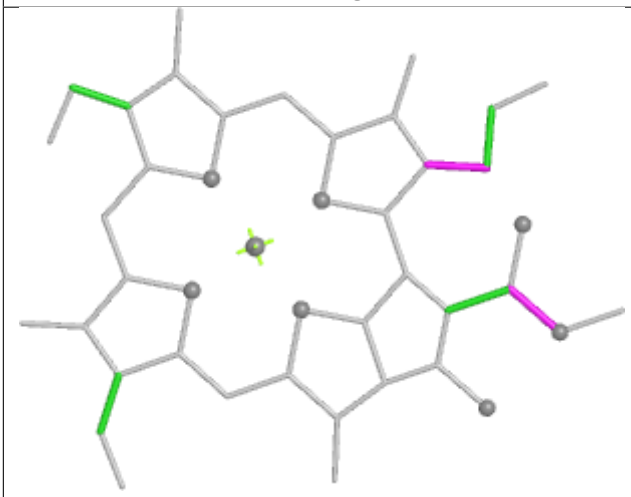
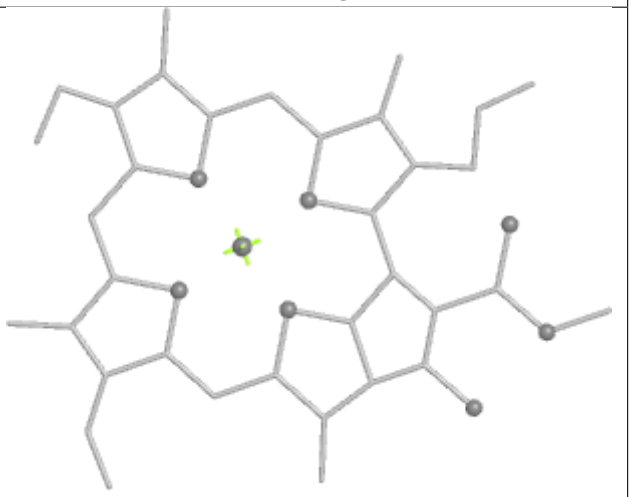


Rings

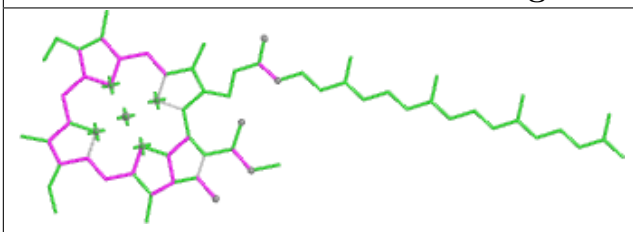
Ligand 5X6 1 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

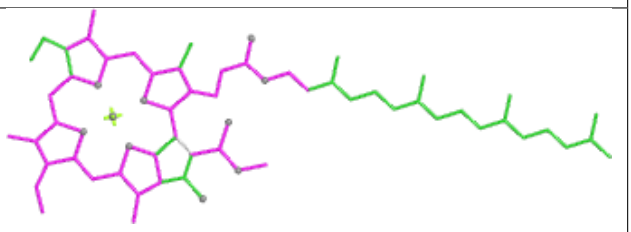
Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

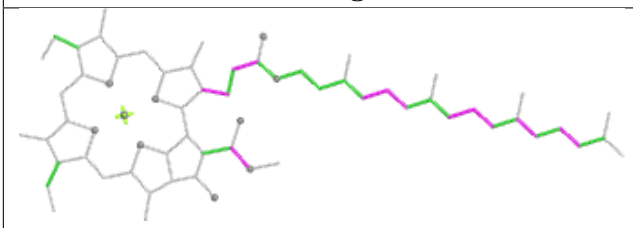
Ligand CLA 5 305



Bond lengths



Bond angles



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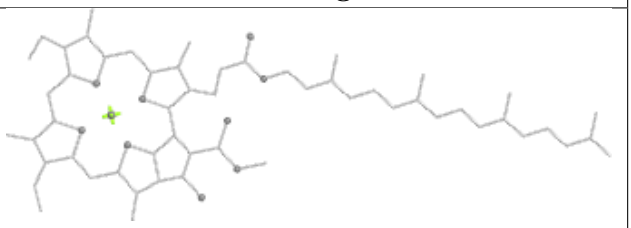
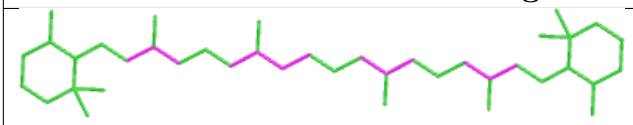


Rings

Ligand BCR A 844



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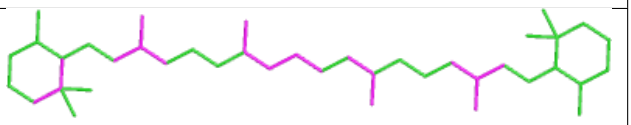
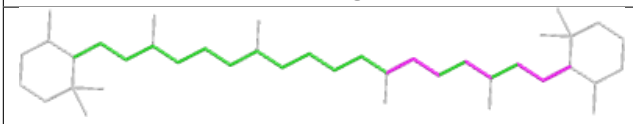


Bond angles



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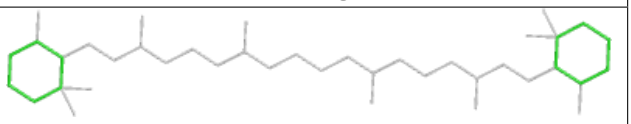
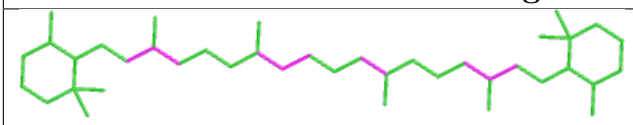
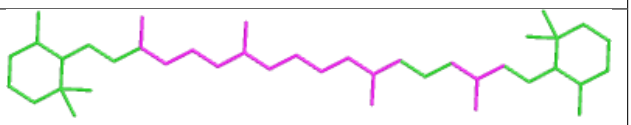


Rings

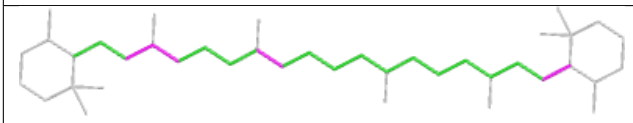
Ligand BCR B 846



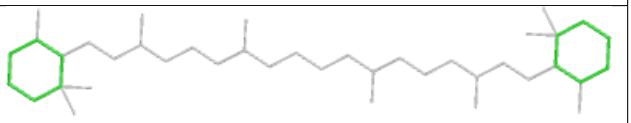
Bond lengths



Bond angles

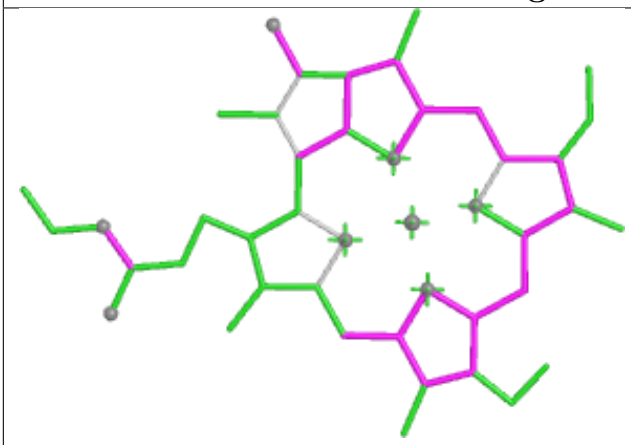


Torsions

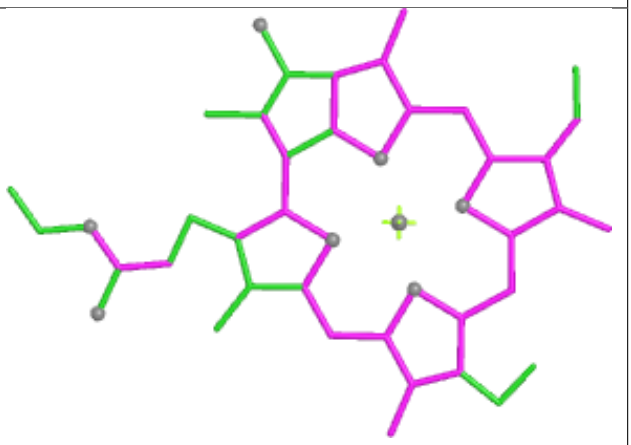


Rings

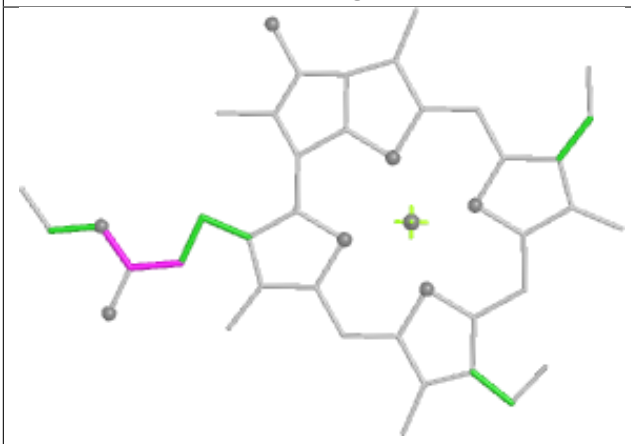
Ligand CLA 5 314



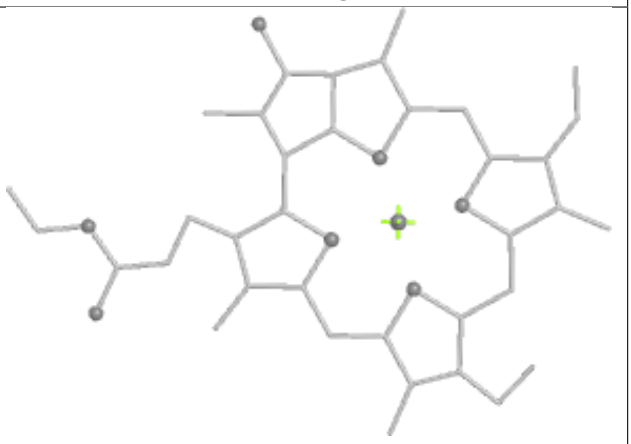
Bond lengths



Bond angles

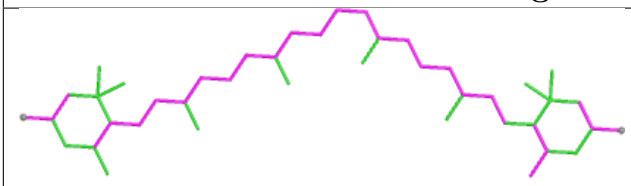


Torsions



Rings

Ligand 5X6 F 205



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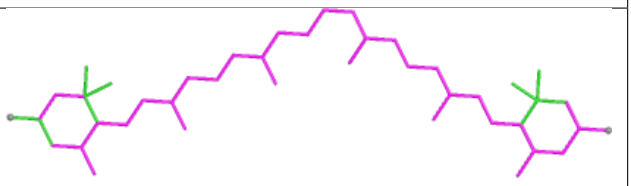
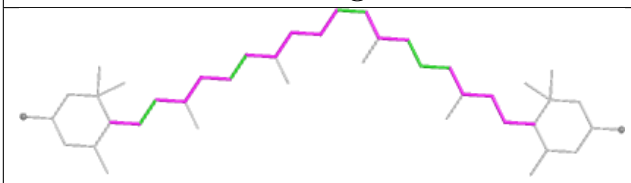
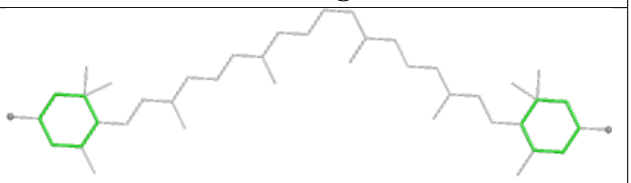


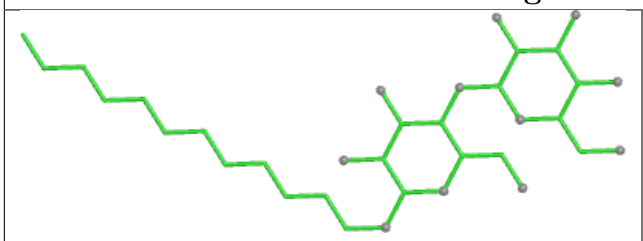
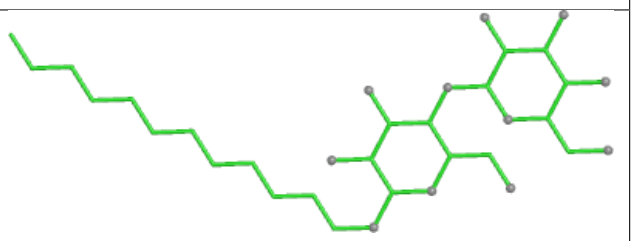
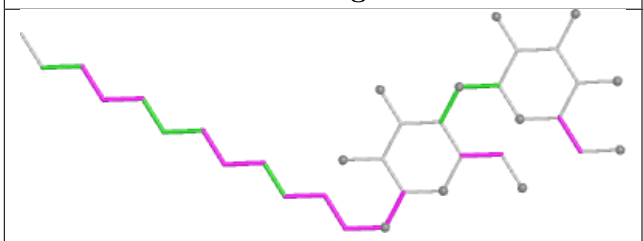
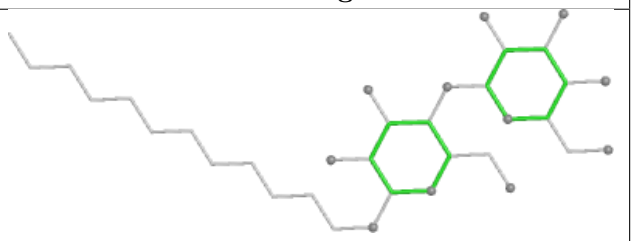
Bond angles

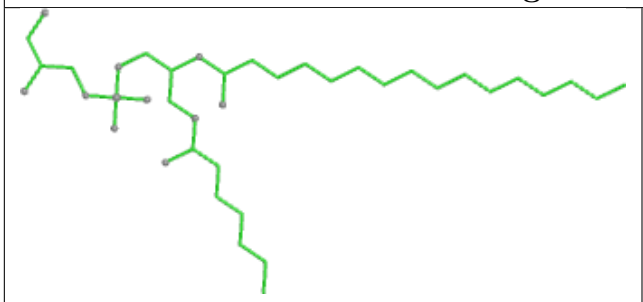
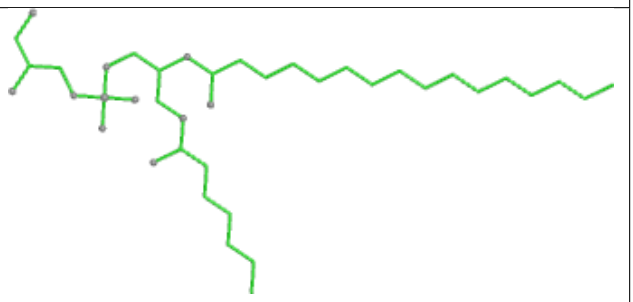
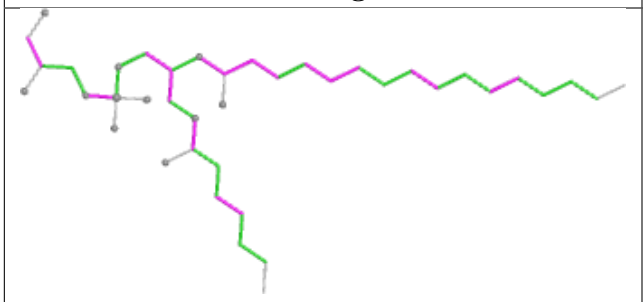
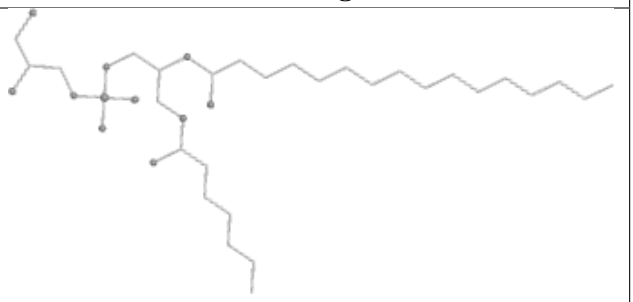


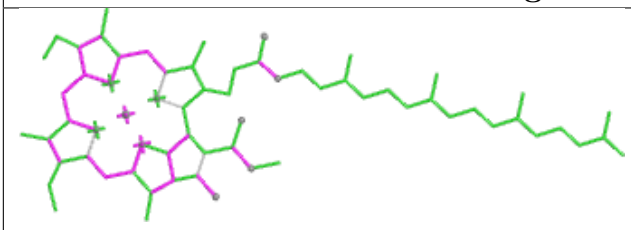
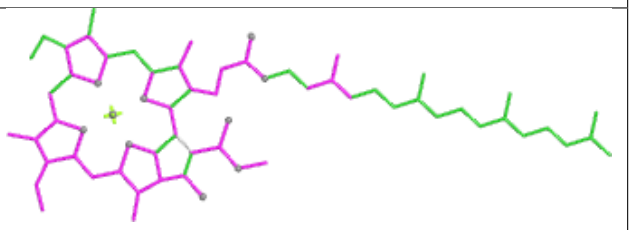
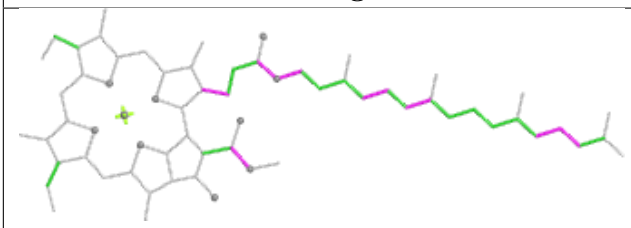
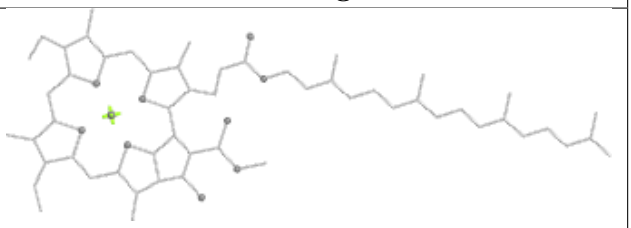
Torsions

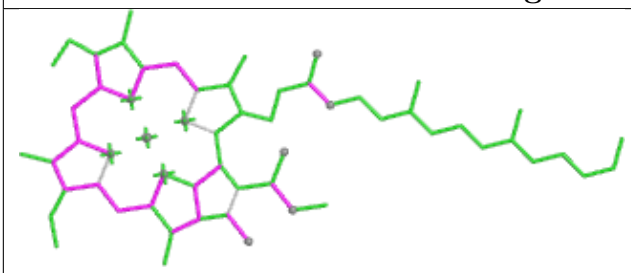
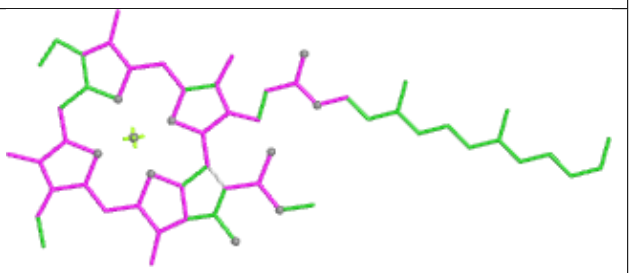
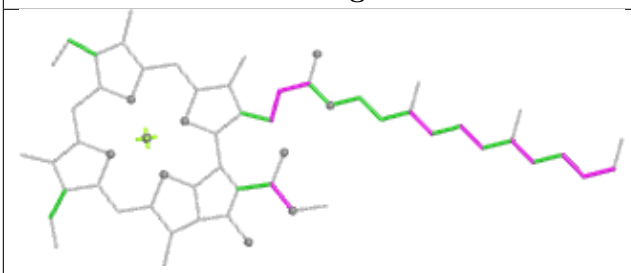
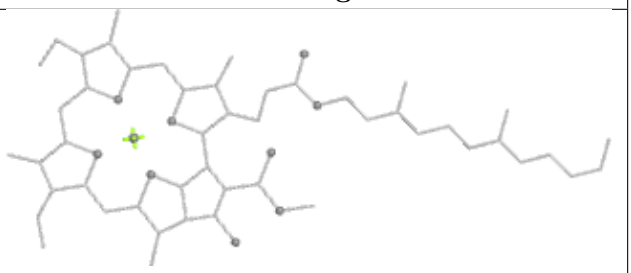


Rings

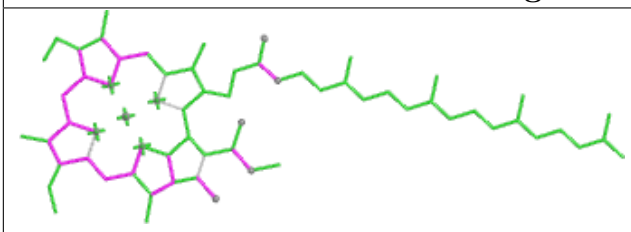
Ligand LMT F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

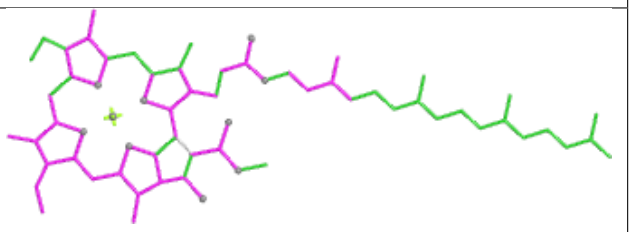
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

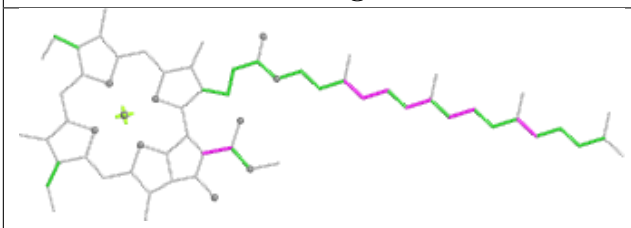
Ligand CLA B 809



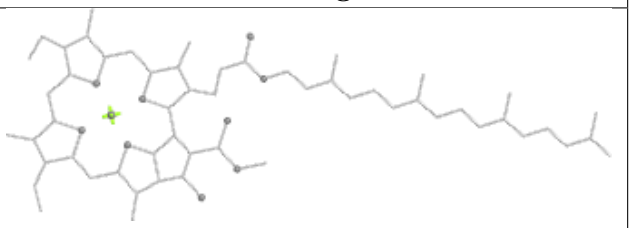
Bond lengths



Bond angles

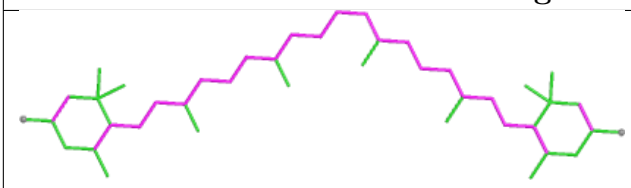


Torsions



Rings

Ligand 5X6 1 315



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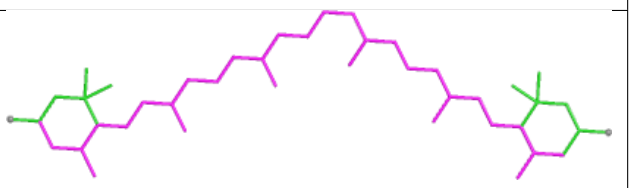

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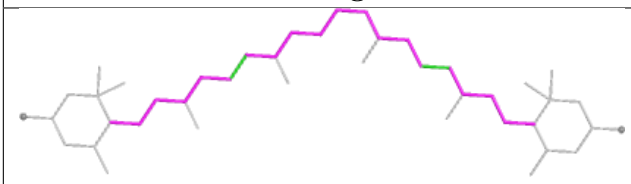

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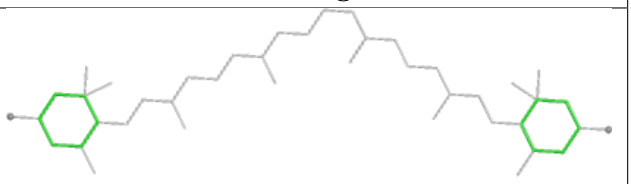
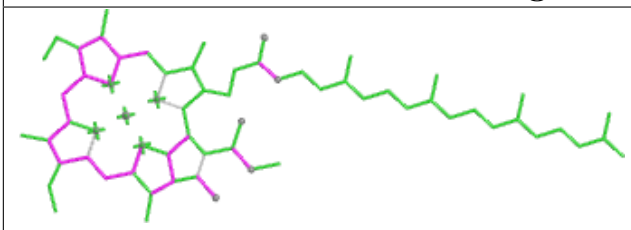


Rings

Ligand CLA 5 303



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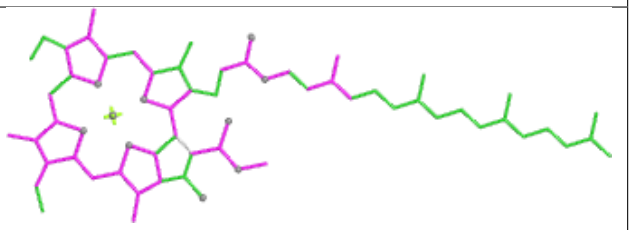
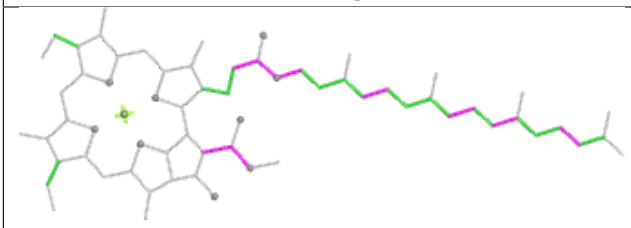


Bond angles



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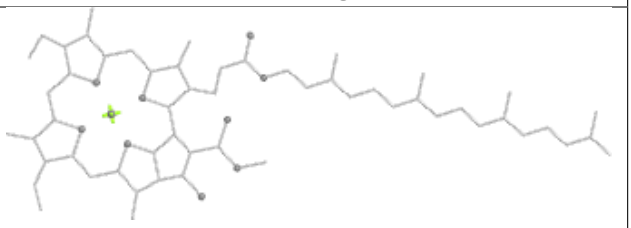
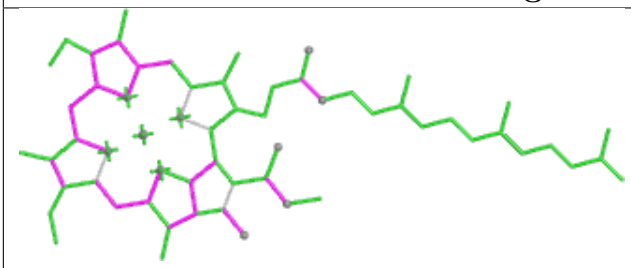


Rings

Ligand CLA B 819



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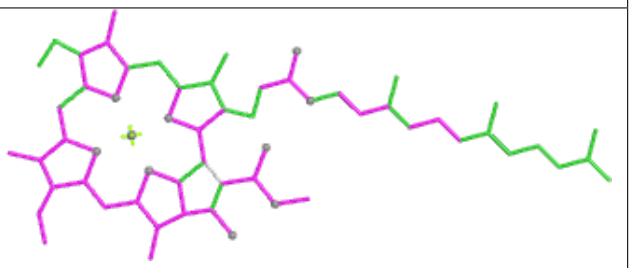
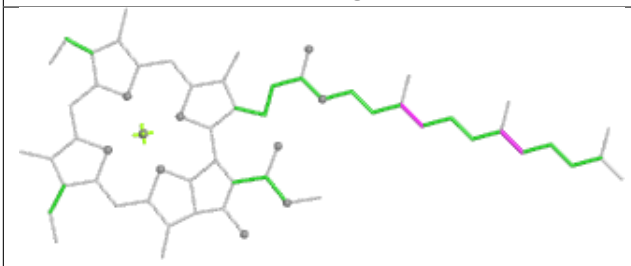


Bond angles



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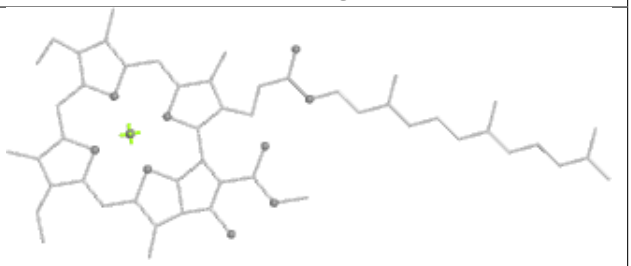
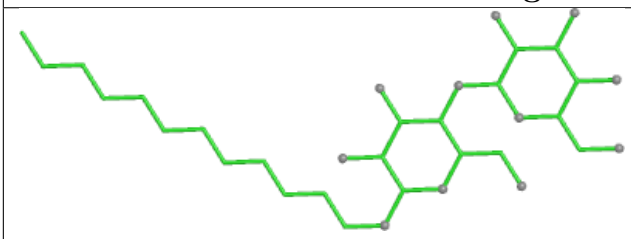


Rings

Ligand LMT L 207



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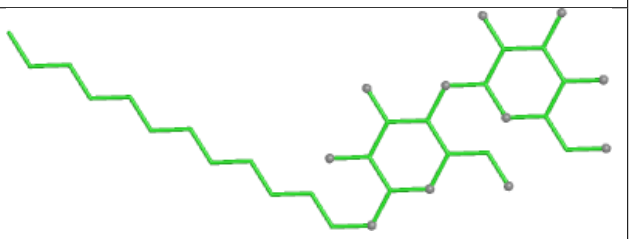
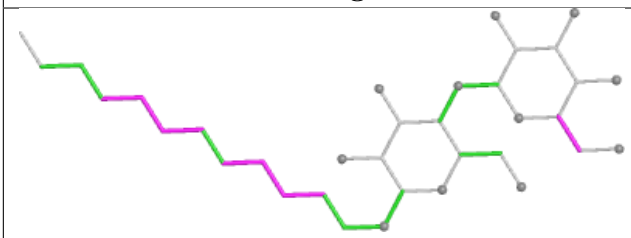


Bond angles



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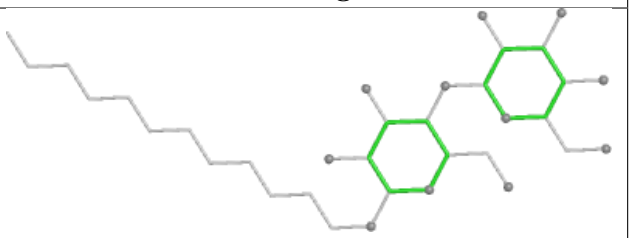
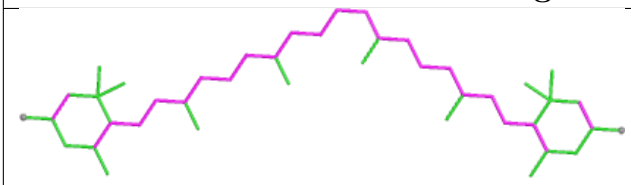


Rings

Ligand 5X6 2 321



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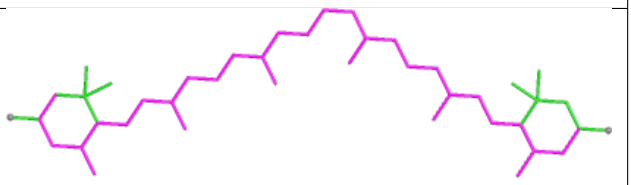
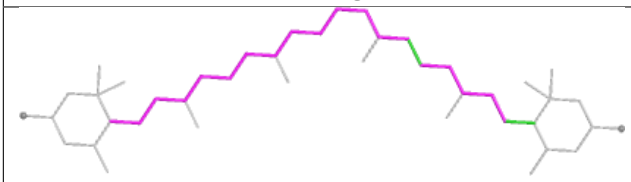


Bond angles



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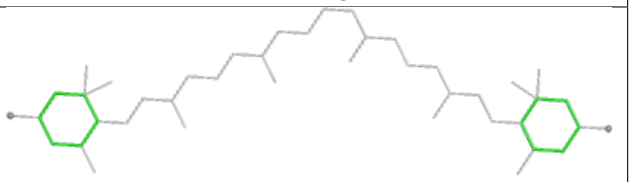
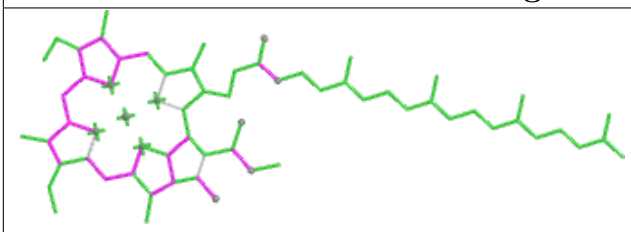
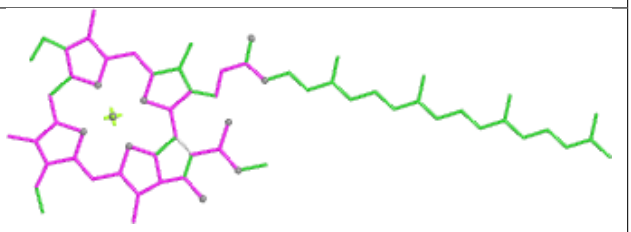
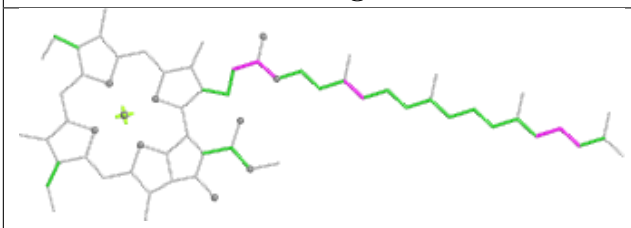
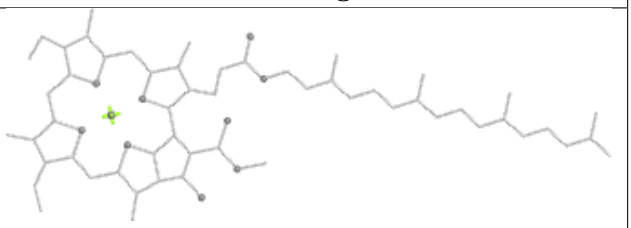


Rings

Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

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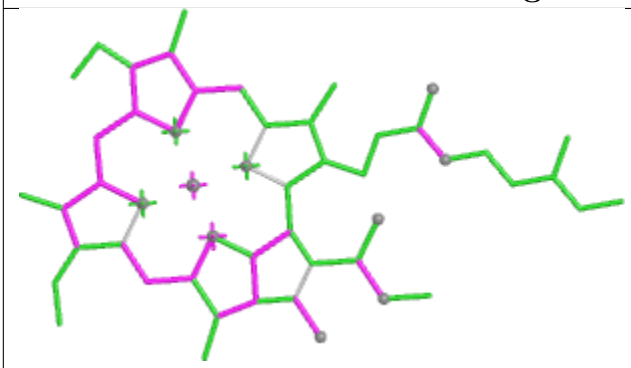
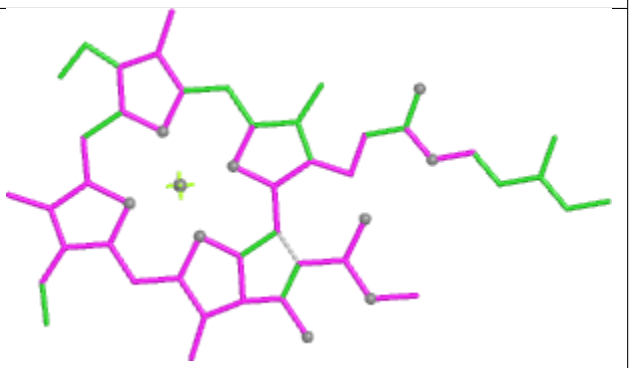
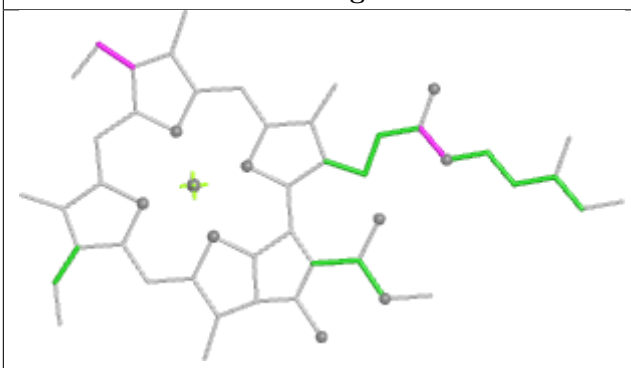
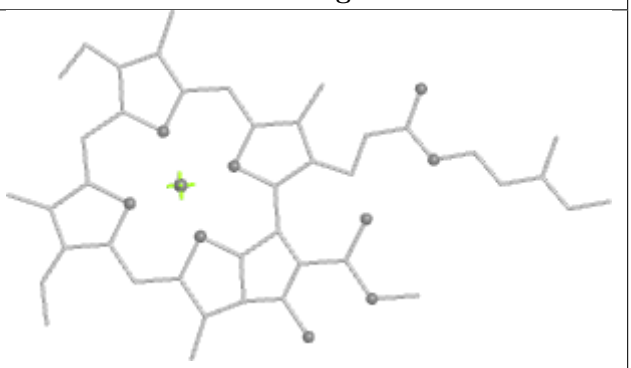
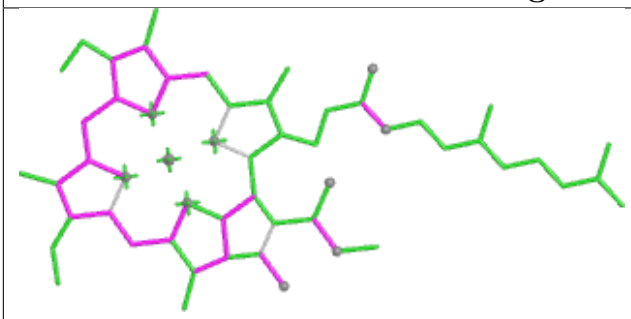
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 306



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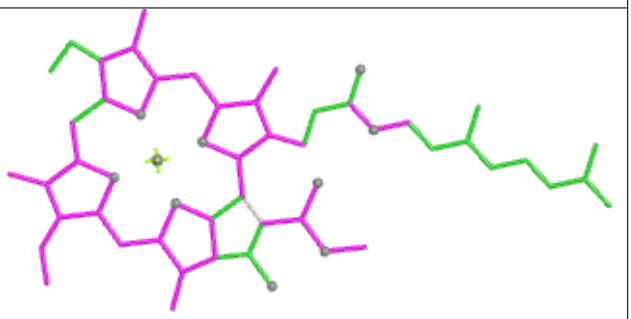
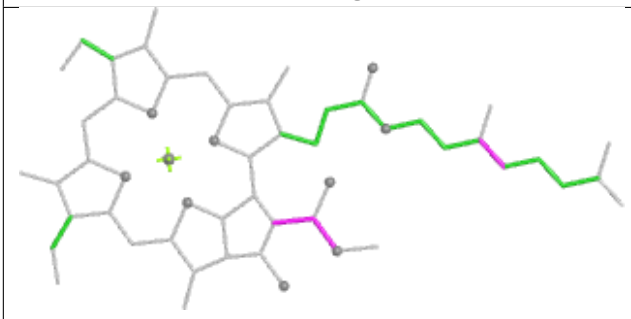


Bond angles



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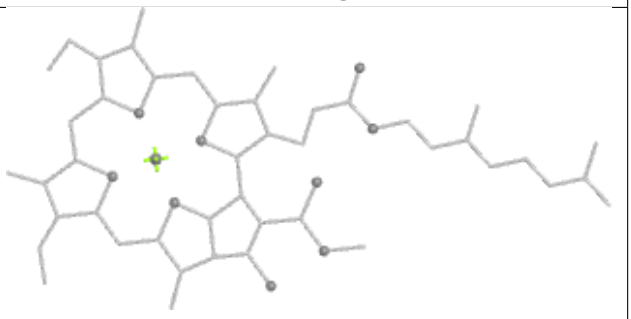
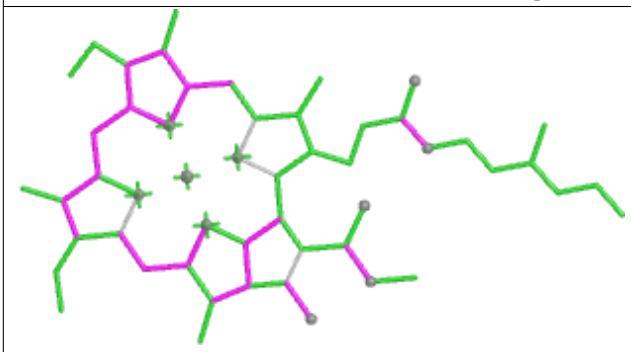


Rings

Ligand CLA 3 311



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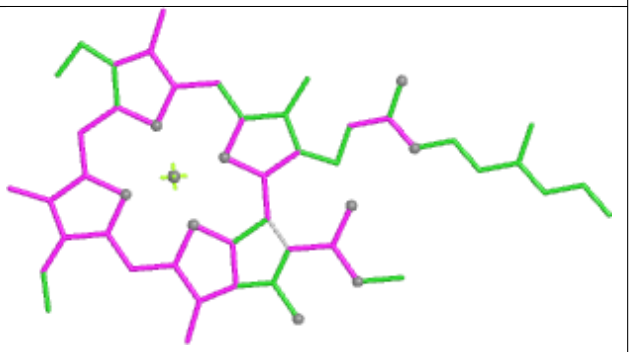
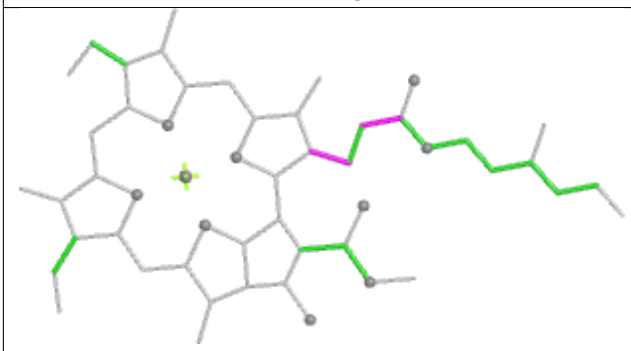


Bond angles



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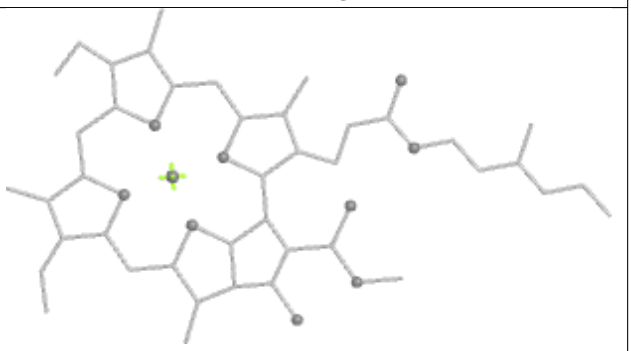
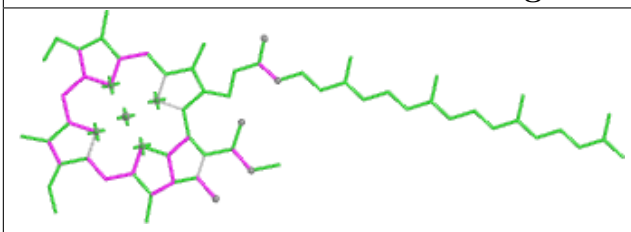
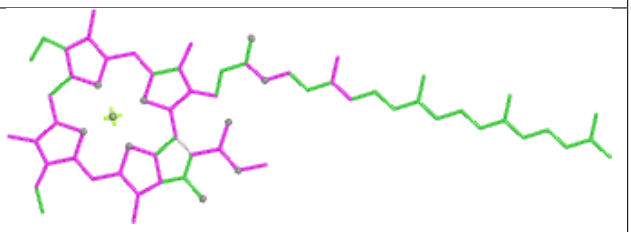
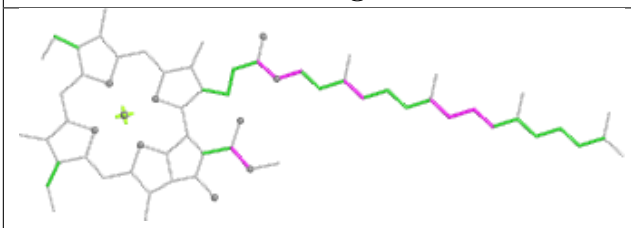
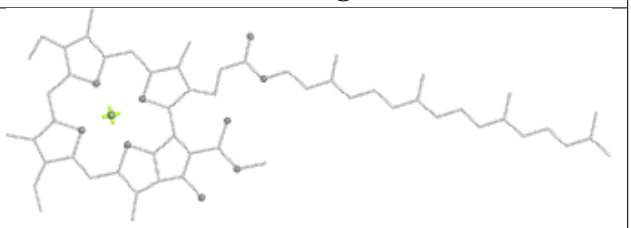
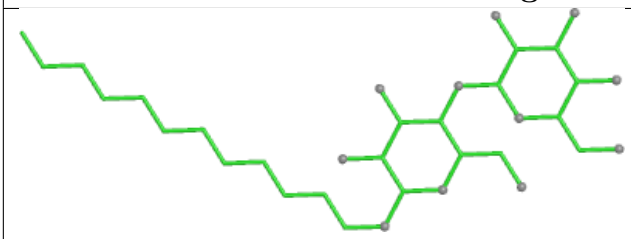
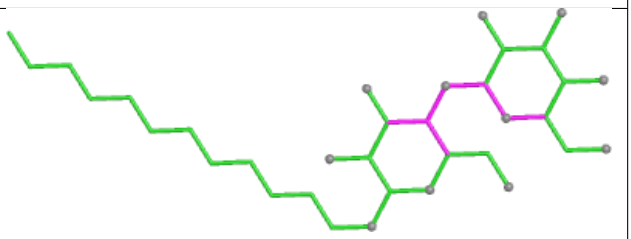
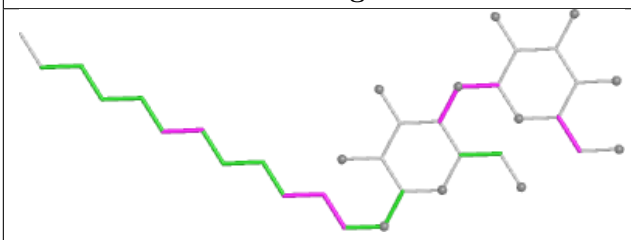
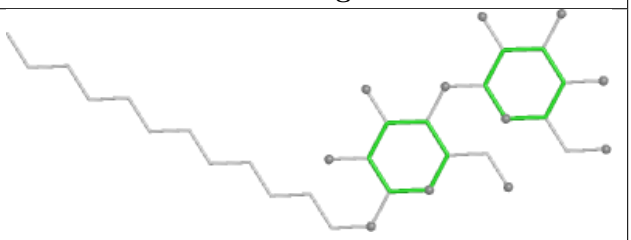
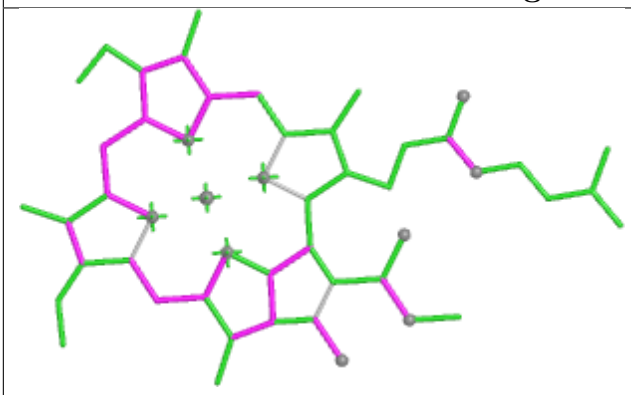
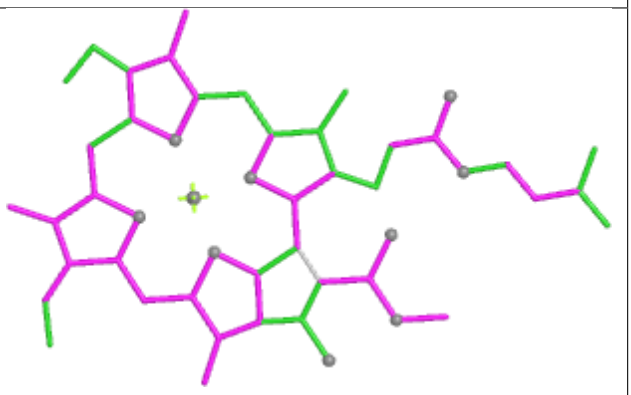
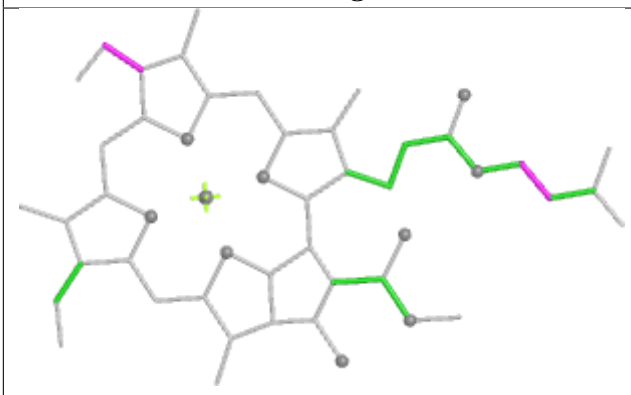
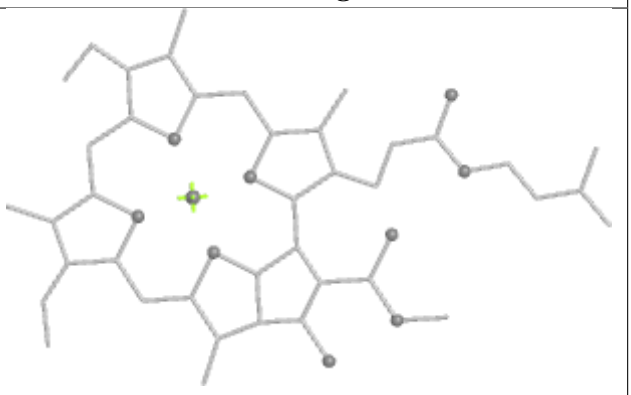
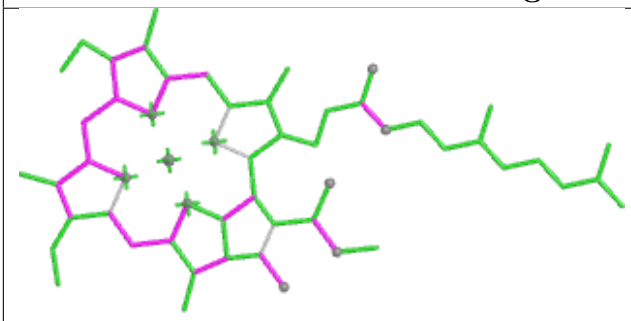
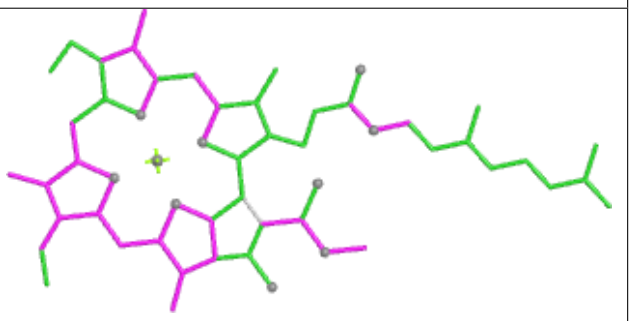
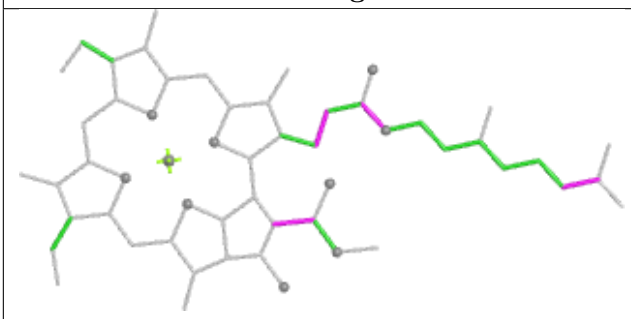
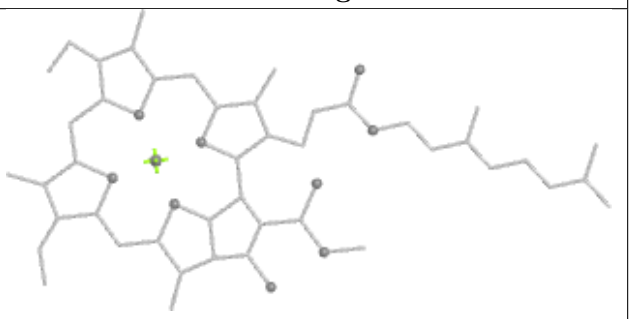


Rings

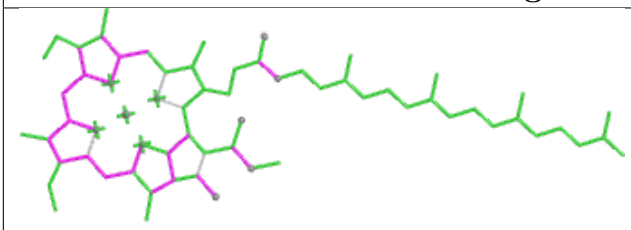
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 832



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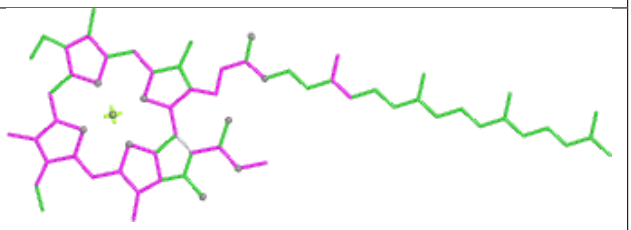

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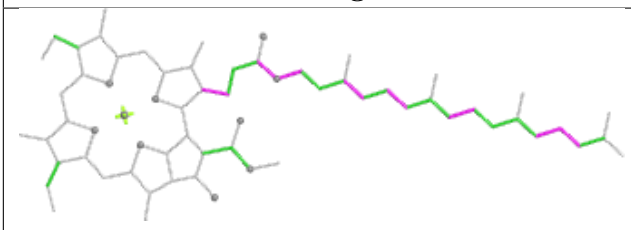

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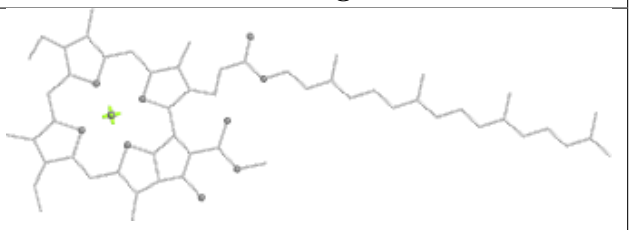
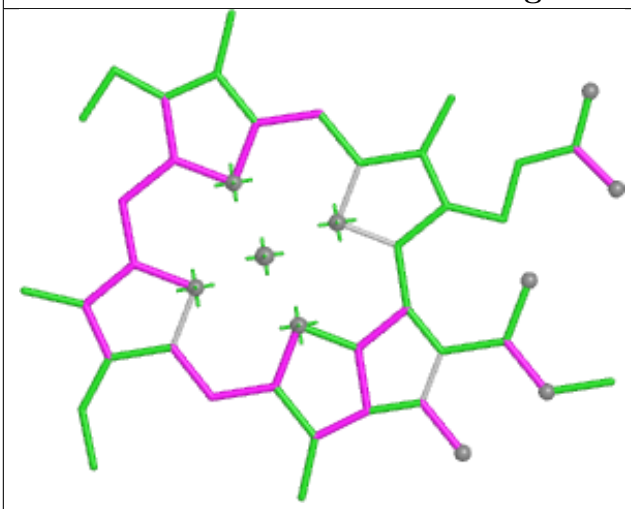


Rings

Ligand CLA B 835



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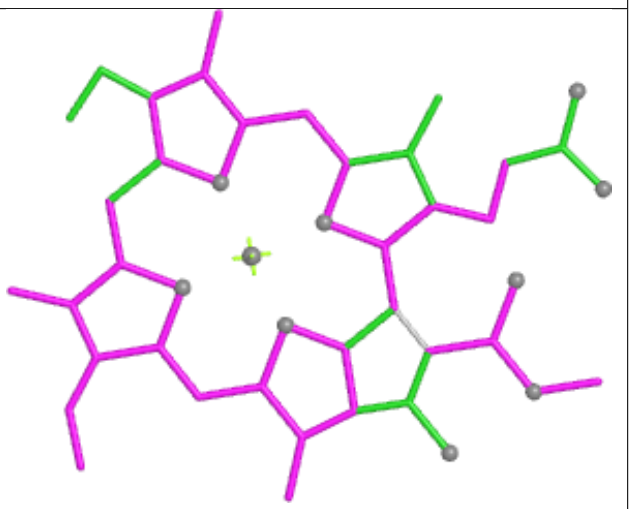

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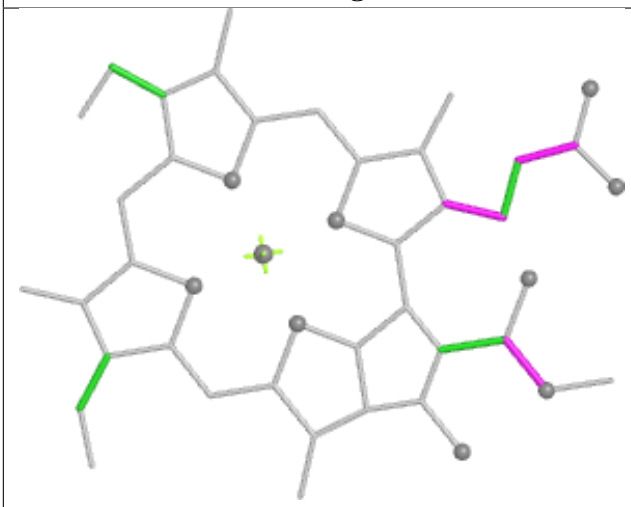

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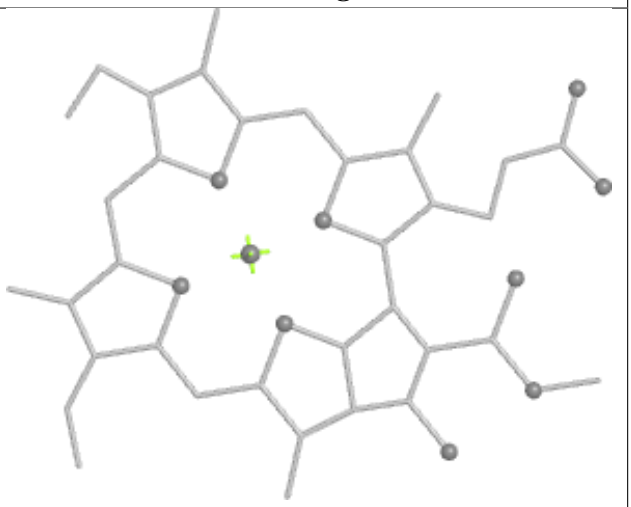
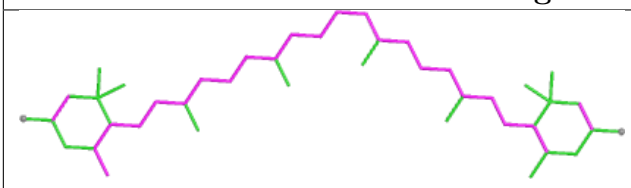


Rings

Ligand 5X6 5 317



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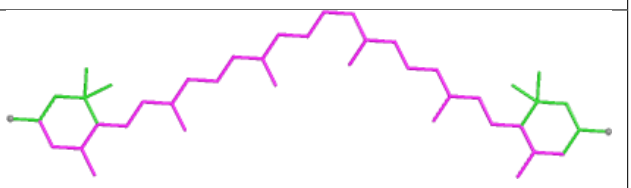

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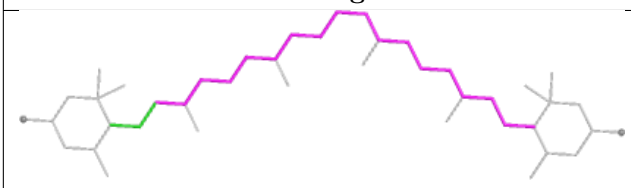

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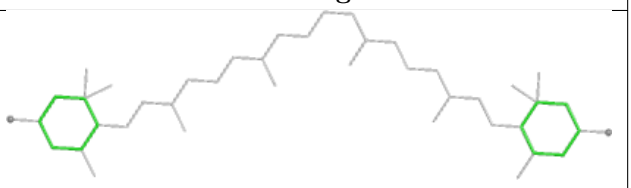
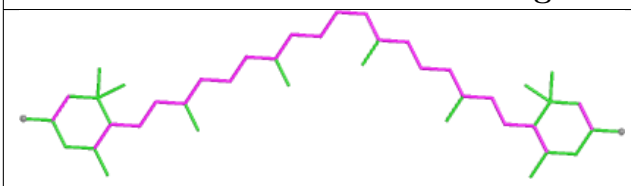


Rings

Ligand 5X6 4 312



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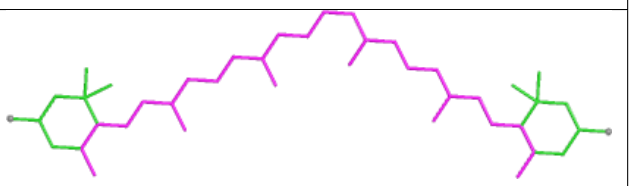
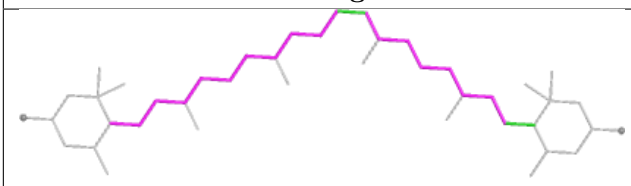


Bond angles



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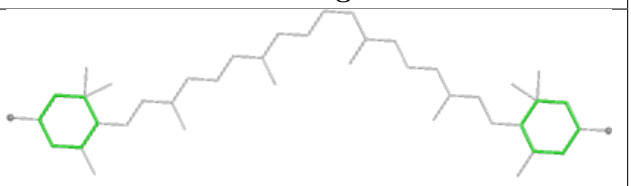
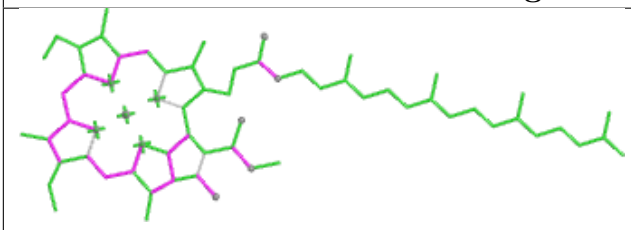


Rings

Ligand CLA B 810



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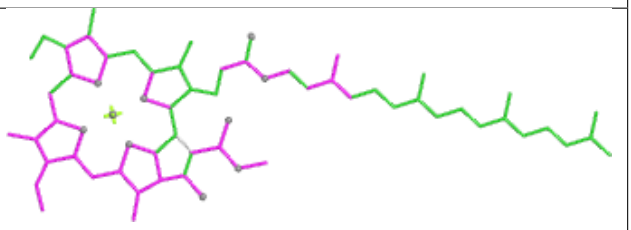
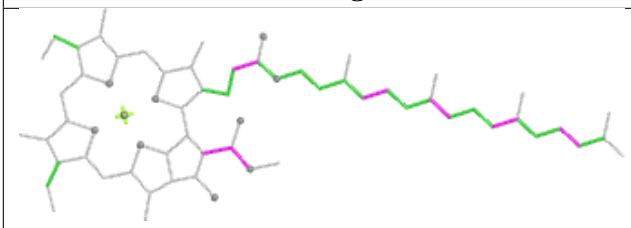


Bond angles



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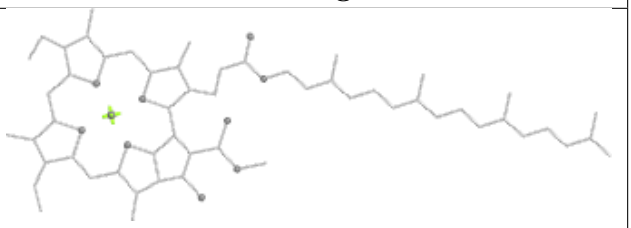
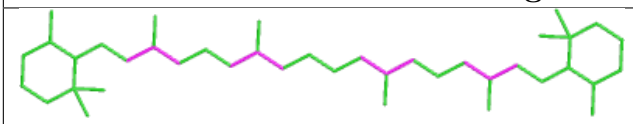


Rings

Ligand BCR L 205



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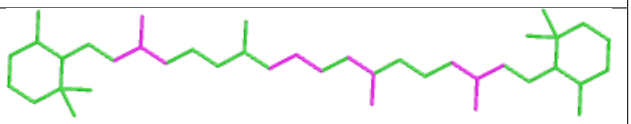
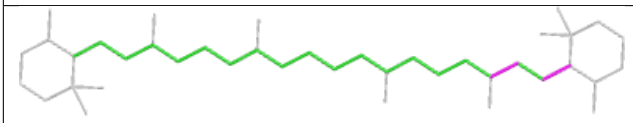


Bond angles



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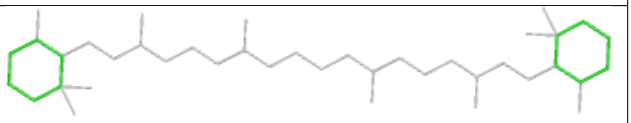
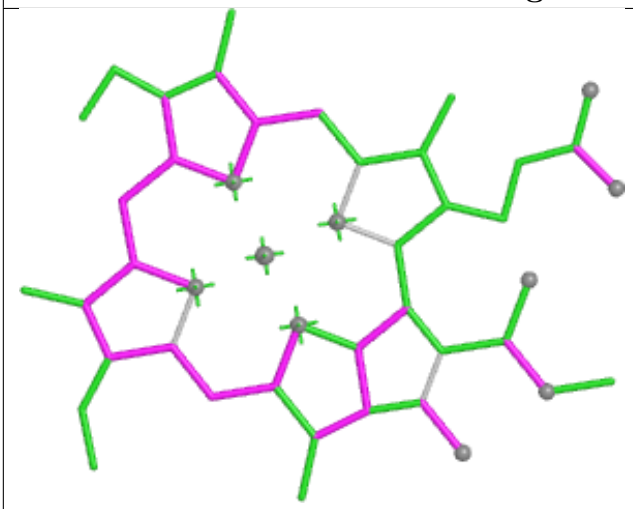


Rings

Ligand CLA F 203



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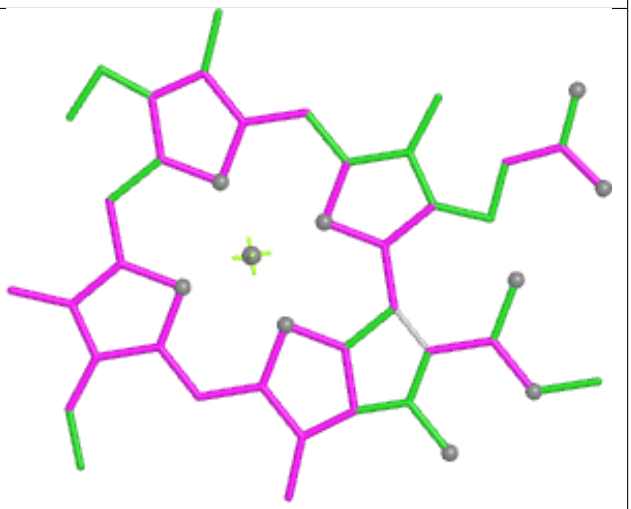
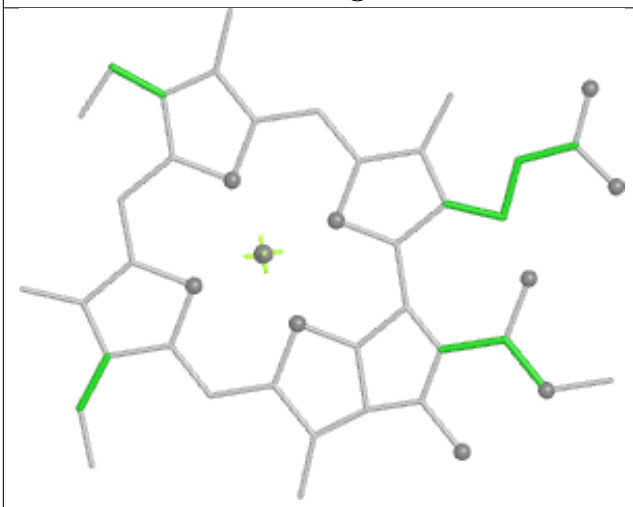


Bond angles



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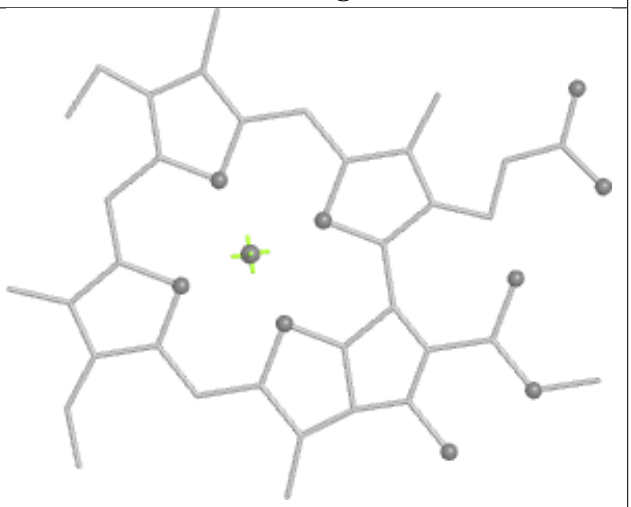
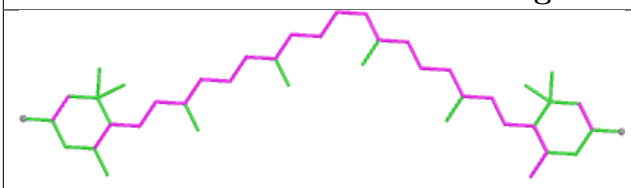
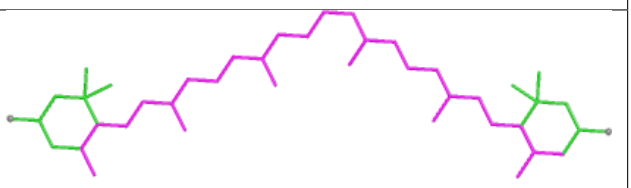
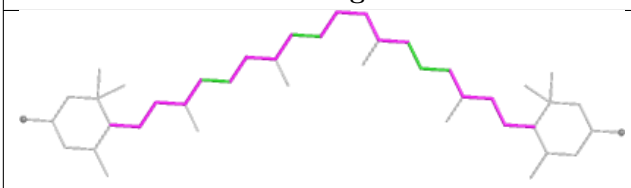
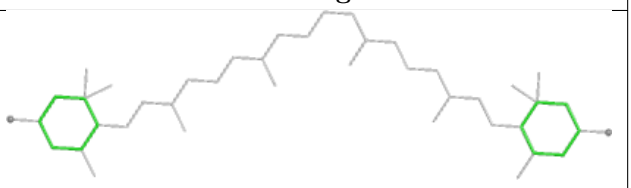
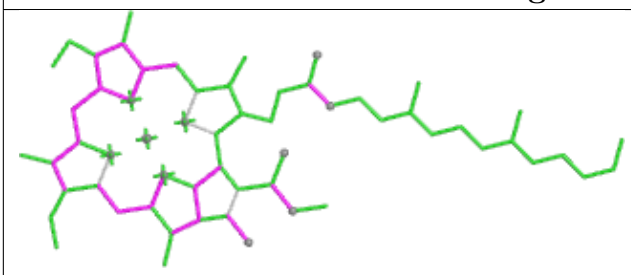
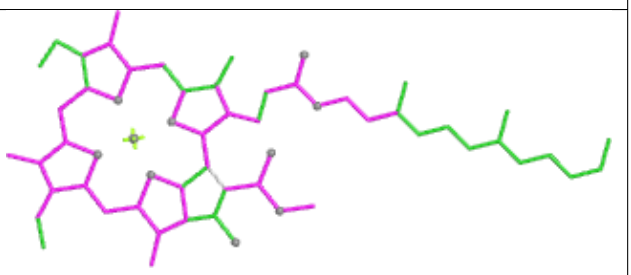
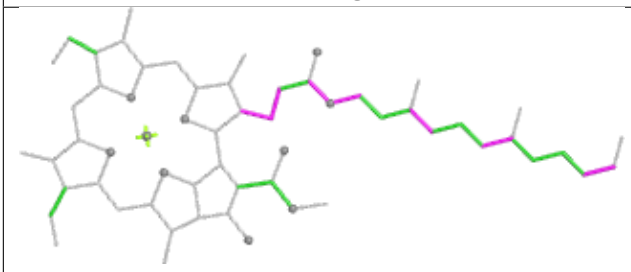
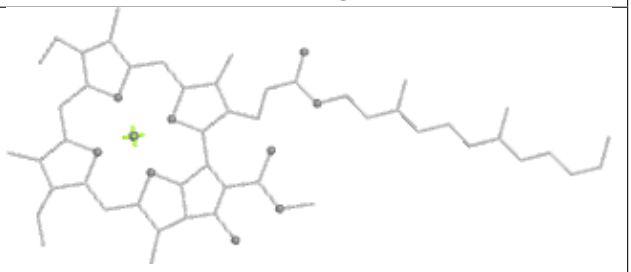
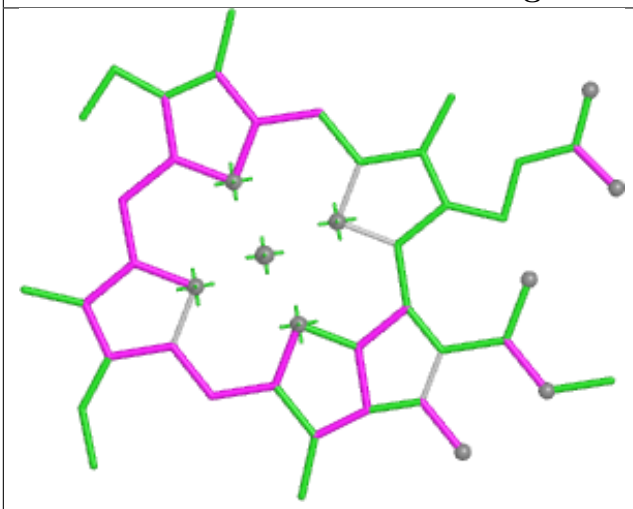


Rings

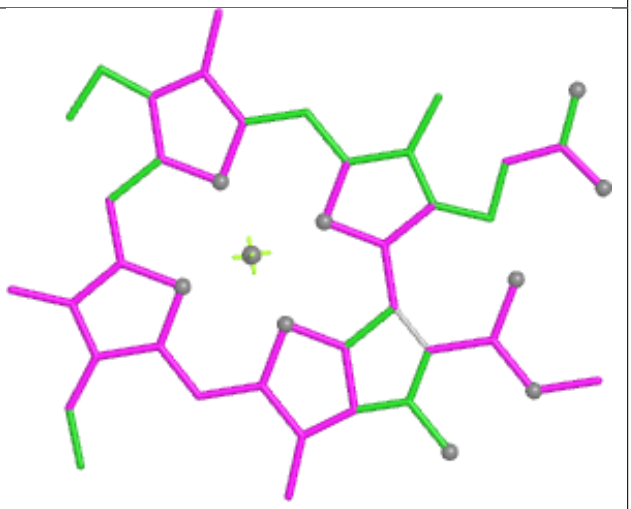
Ligand 5X6 5 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

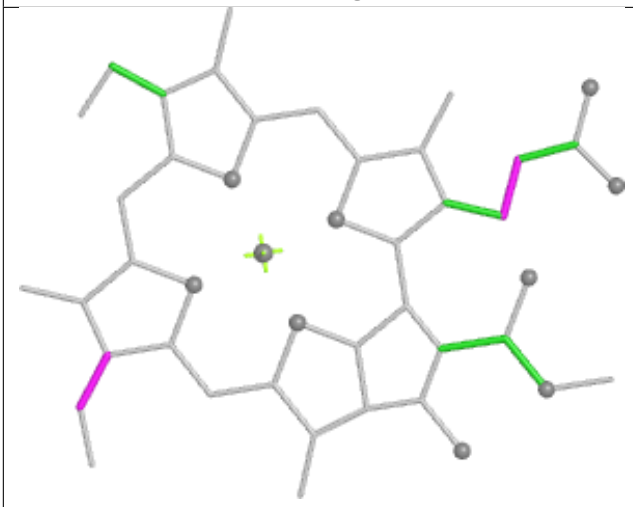
Ligand CLA A 814



Bond lengths



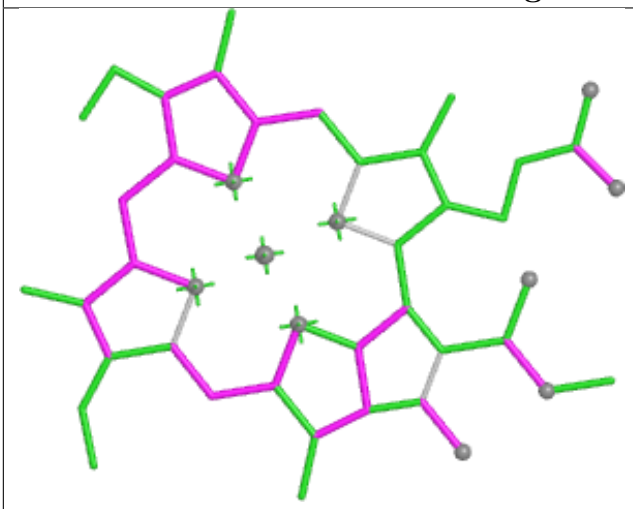
Bond angles



Torsions

Rings

Ligand CLA B 821



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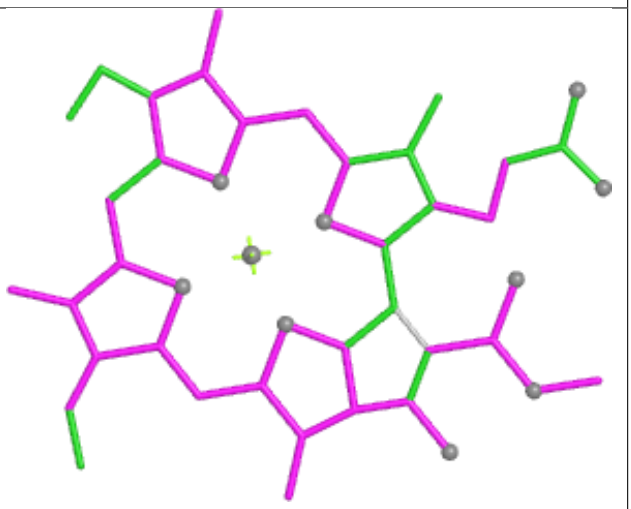
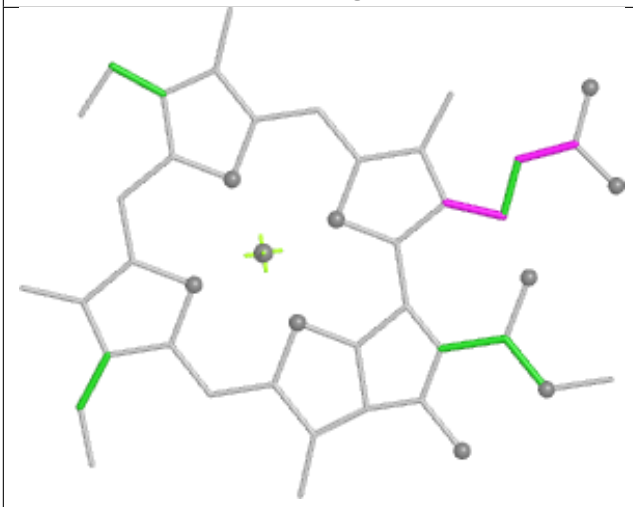


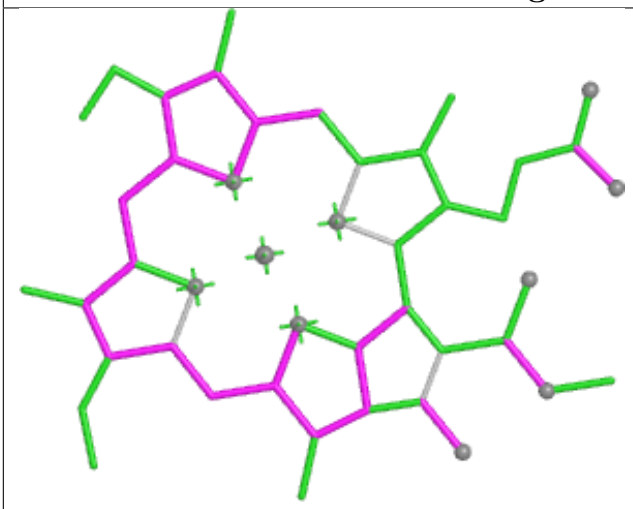
Bond angles



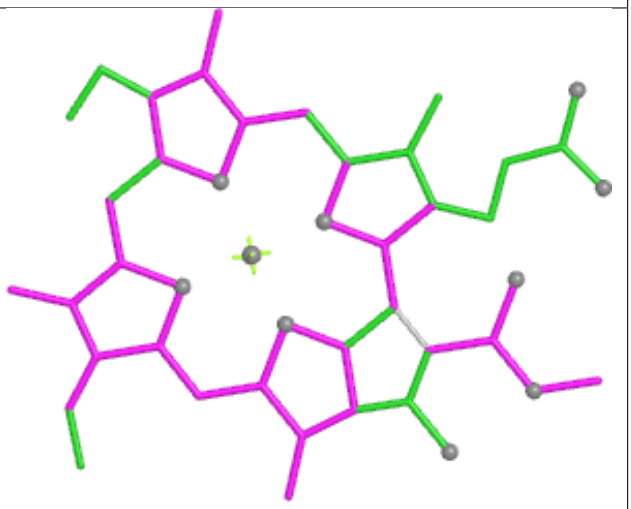
Torsions

Rings

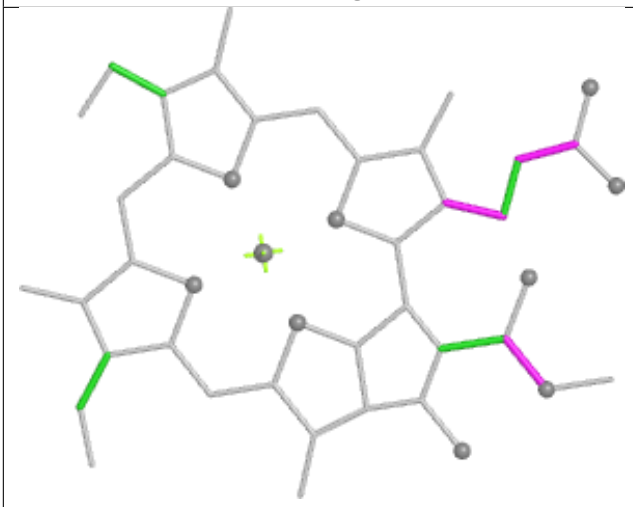
Ligand CLA 4 311



Bond lengths



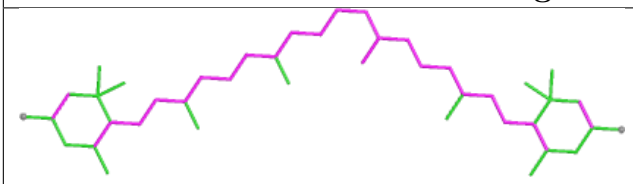
Bond angles



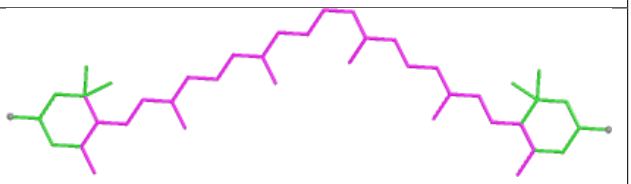
Torsions

Rings

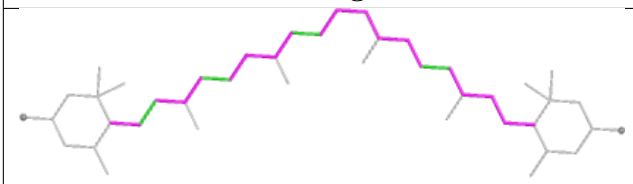
Ligand 5X6 5 315



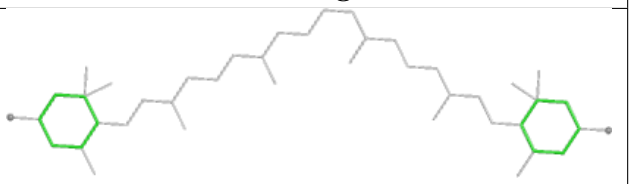
Bond lengths



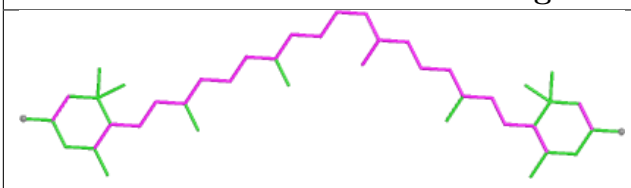
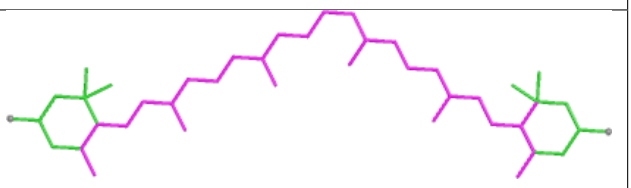
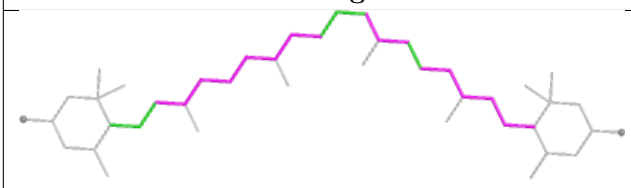
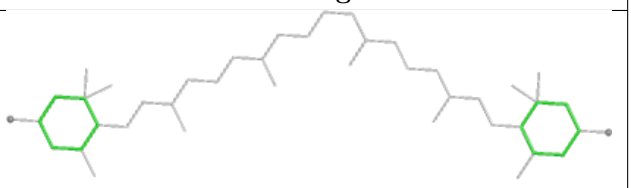
Bond angles

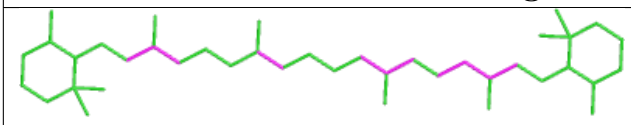
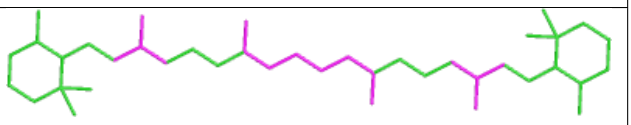
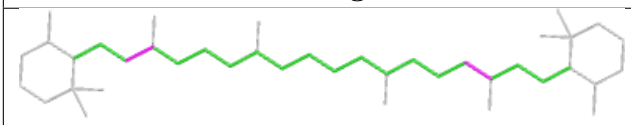
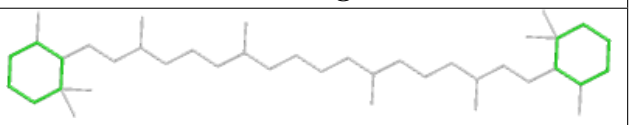


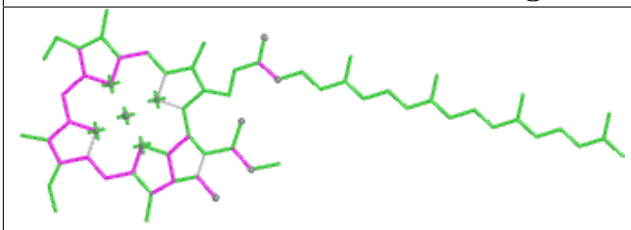
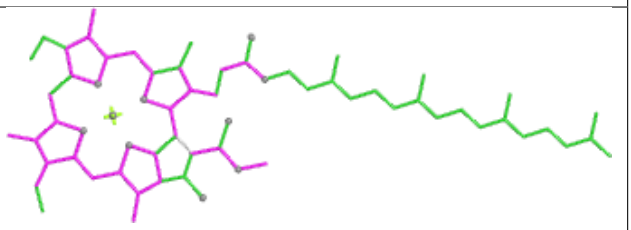
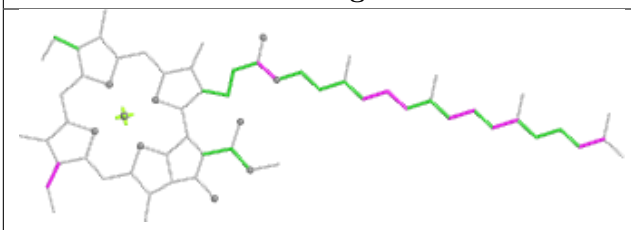
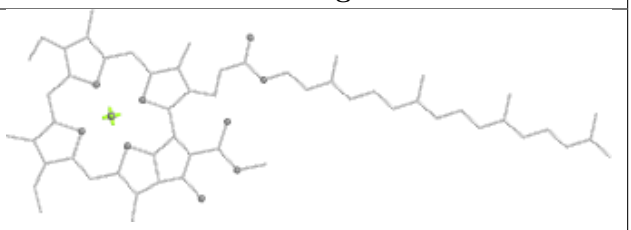
Torsions



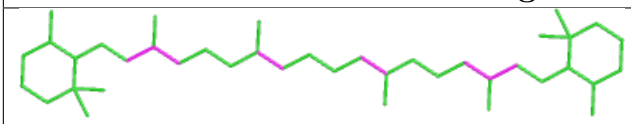
Rings

Ligand 5X6 2 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR M 101



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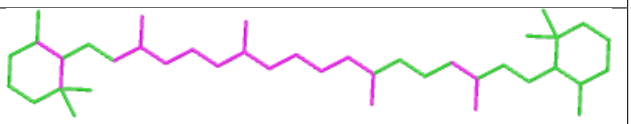
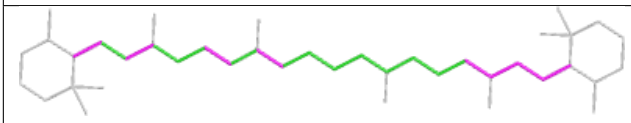


Bond angles



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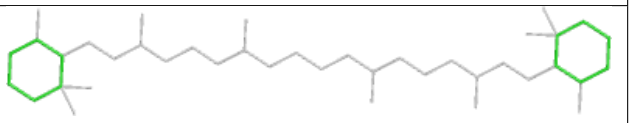
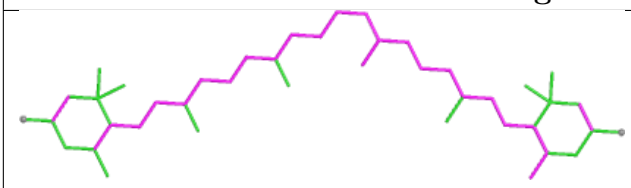


Rings

Ligand 5X6 2 320



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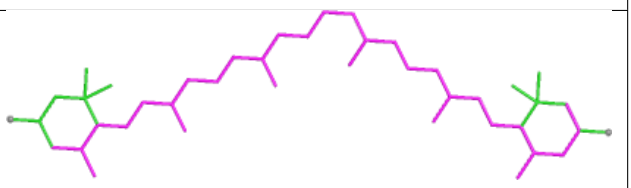
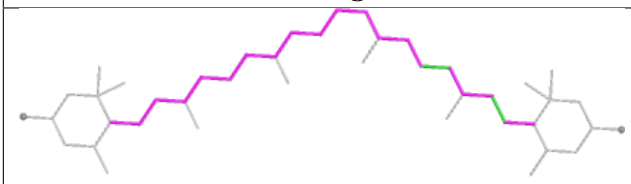


Bond angles



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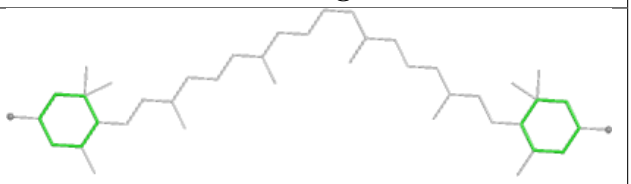
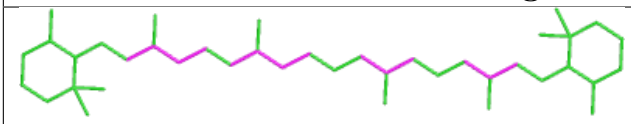


Rings

Ligand BCR A 857



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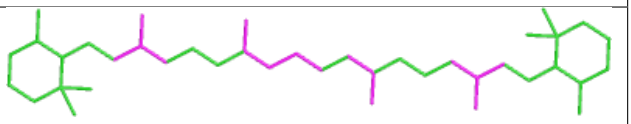
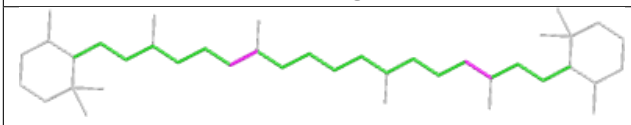


Bond angles



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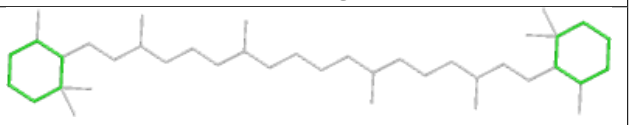
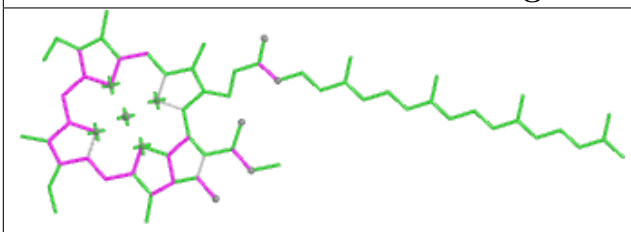
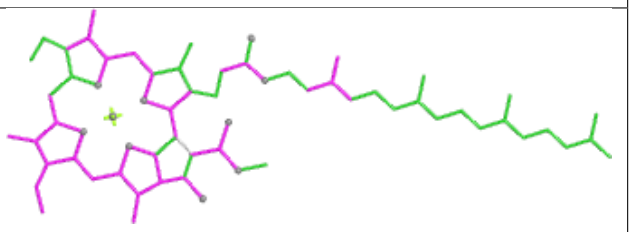
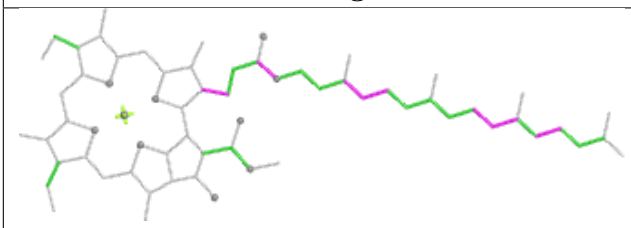
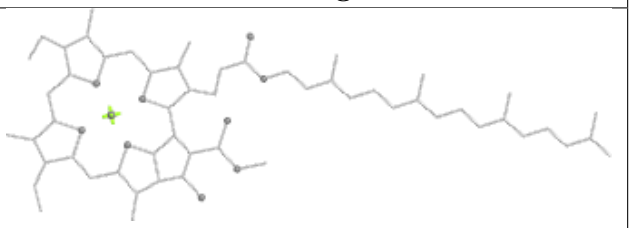
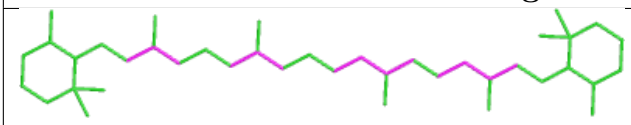
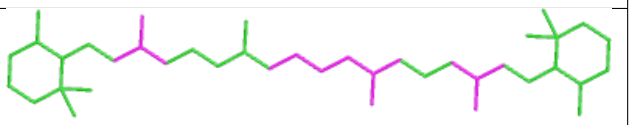
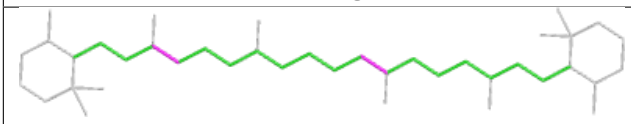
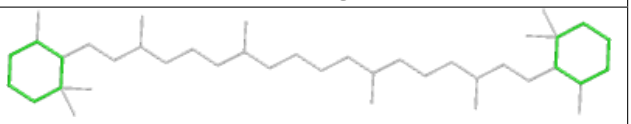
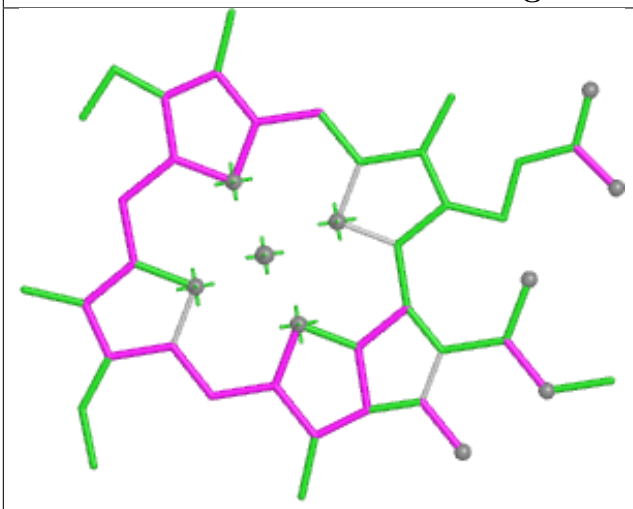


Rings

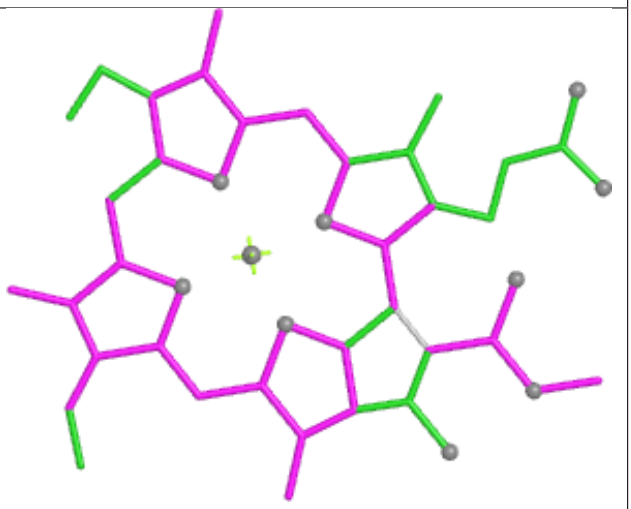
Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

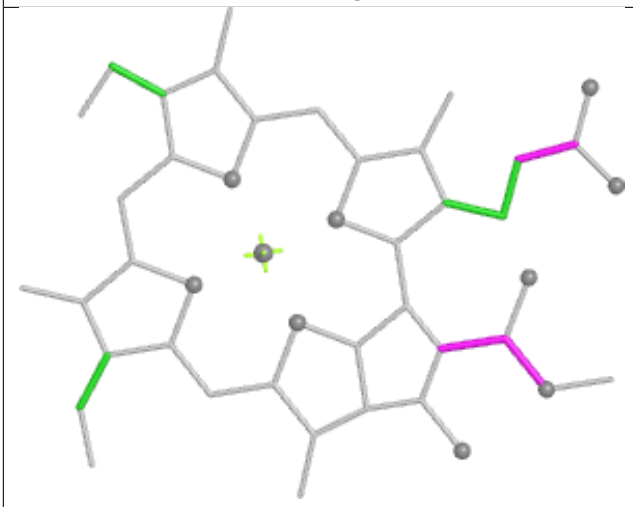
Ligand CLA O 205



Bond lengths



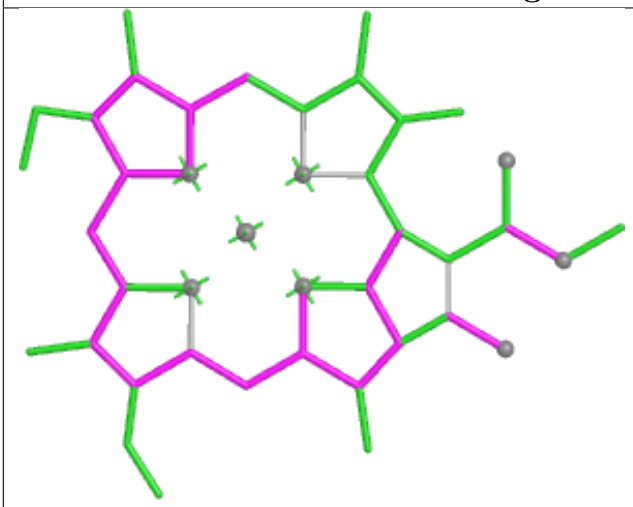
Bond angles



Torsions

Rings

Ligand CLA O 203



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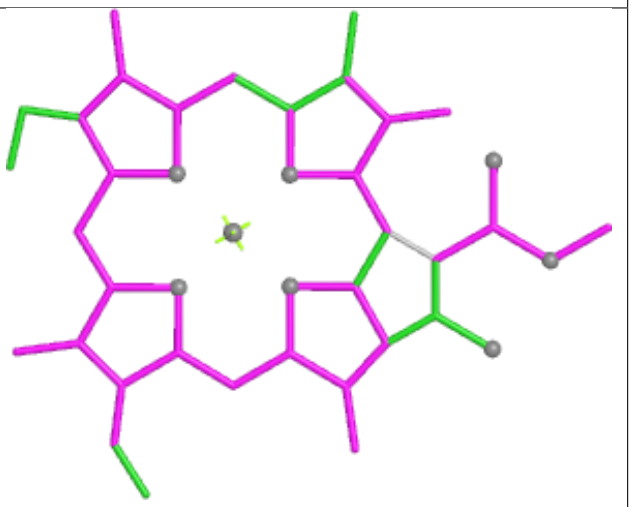
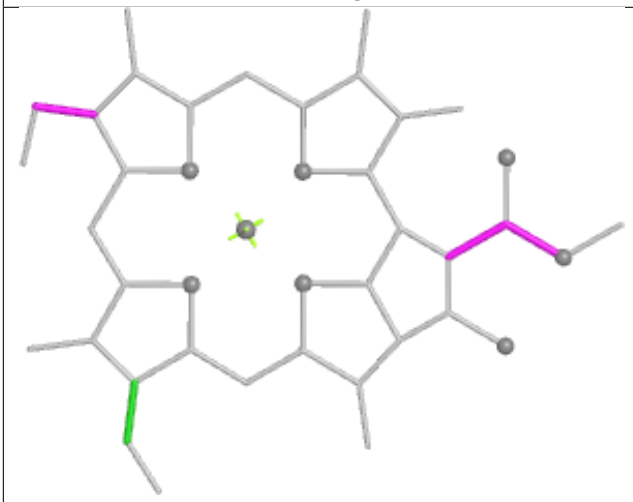
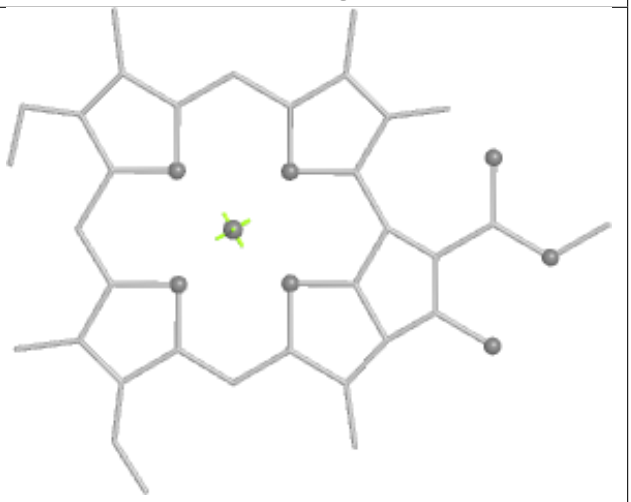


Bond angles

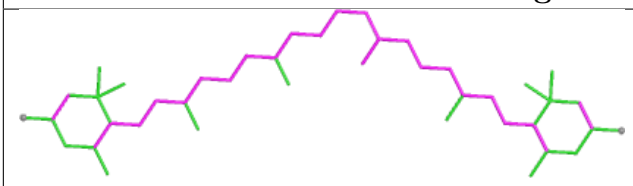


Torsions



Rings

Ligand 5X6 1 313



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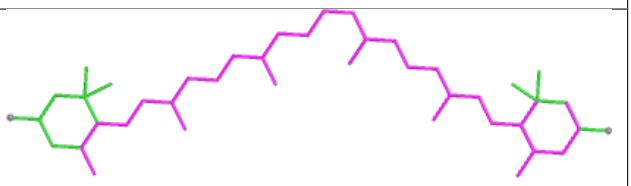
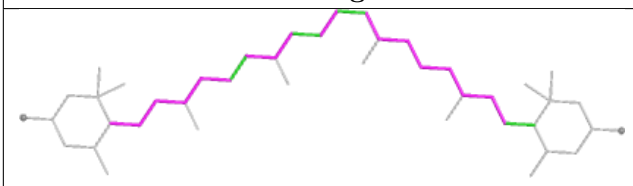
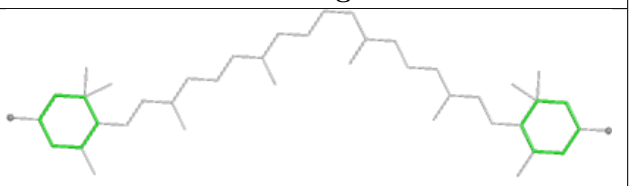


Bond angles

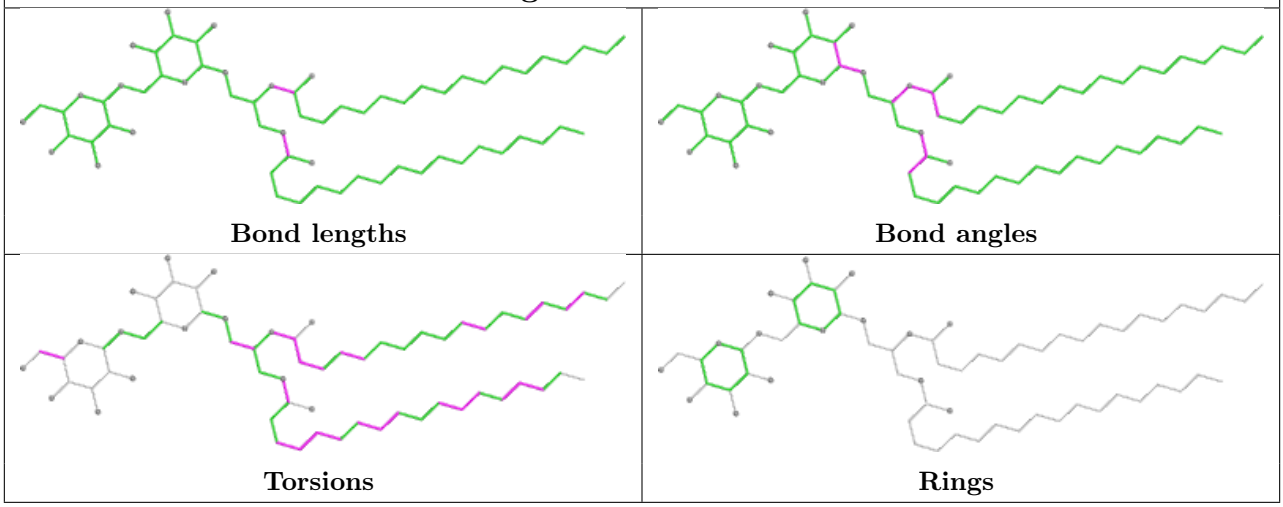


Torsions

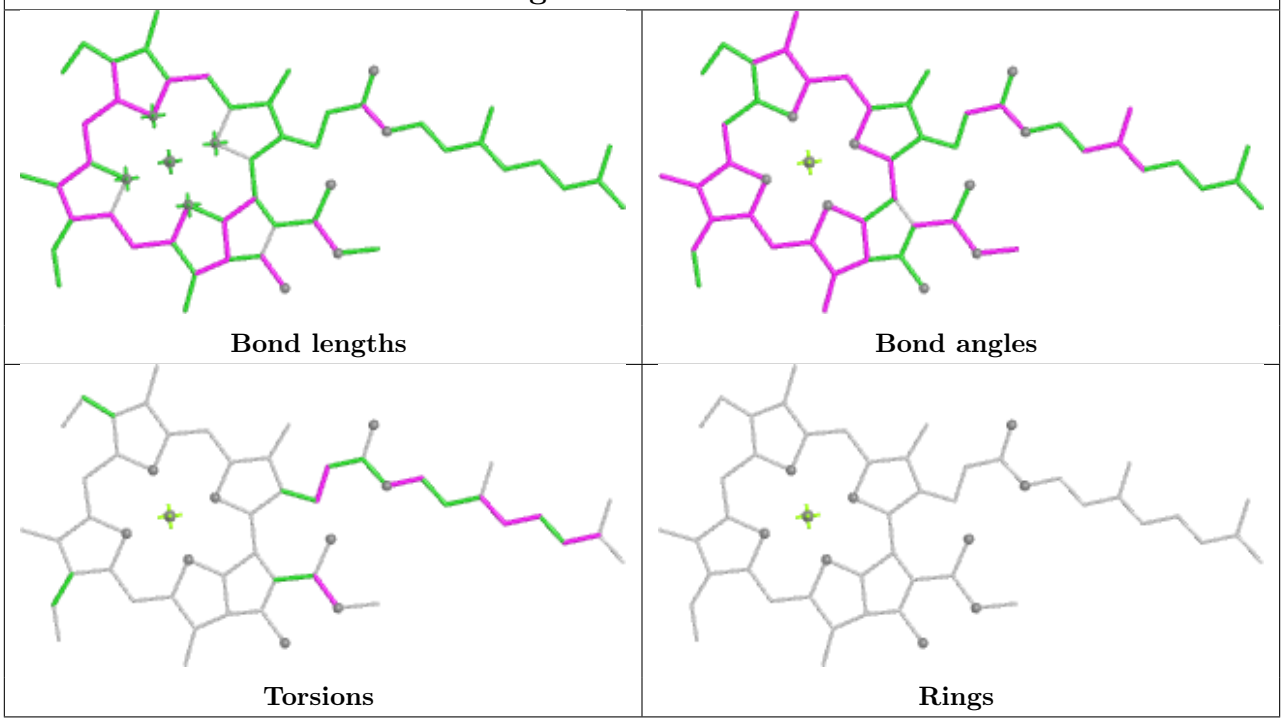


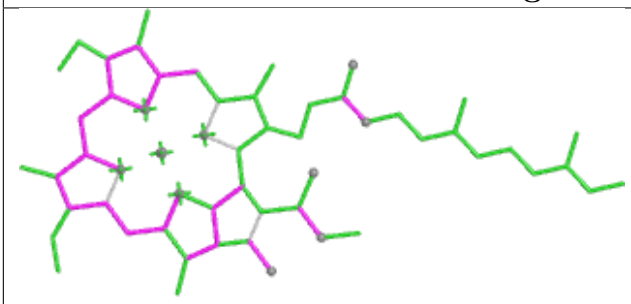
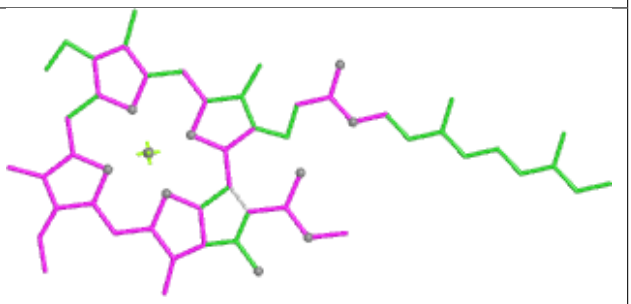
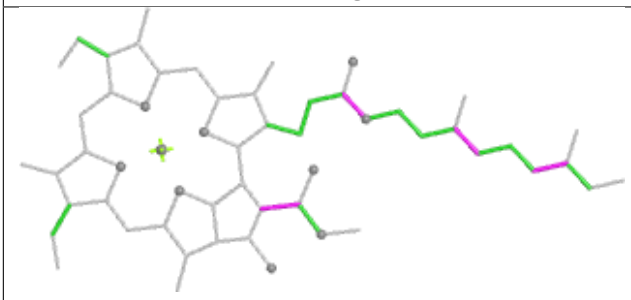
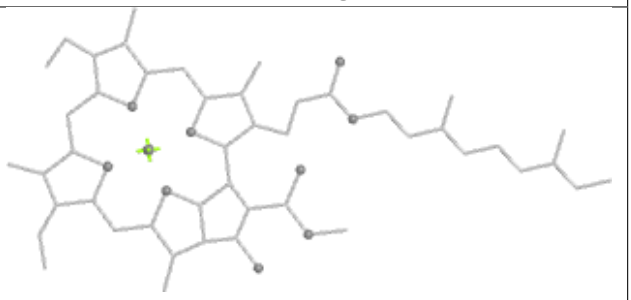
Rings

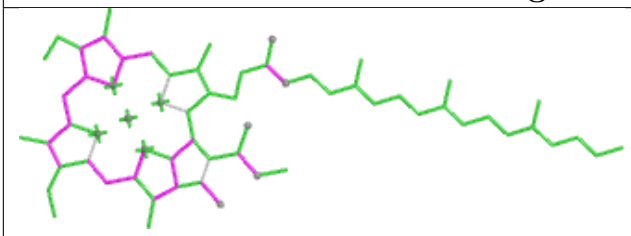
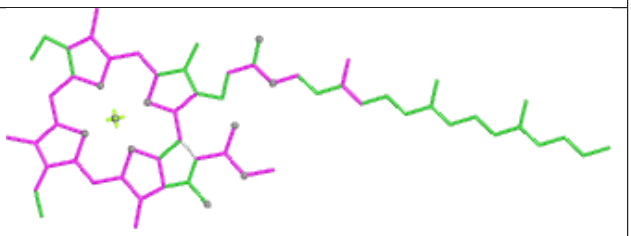
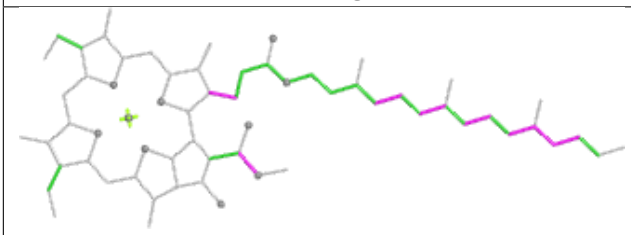
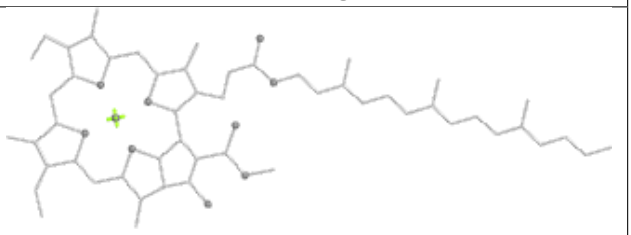
Ligand DGD B 849



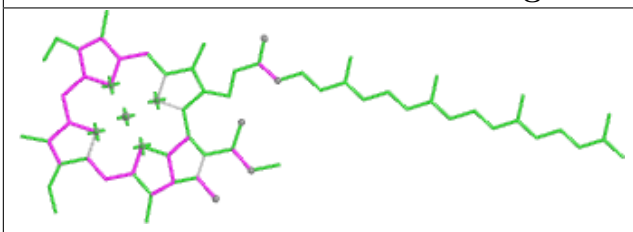
Ligand CLA 1 303



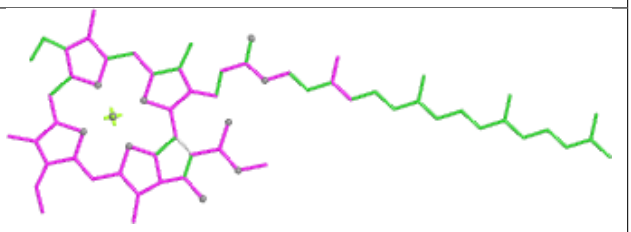
Ligand CLA A 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

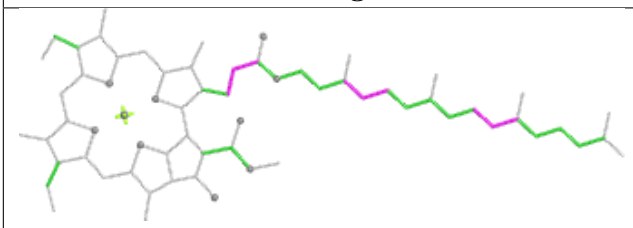
Ligand CLA A 818



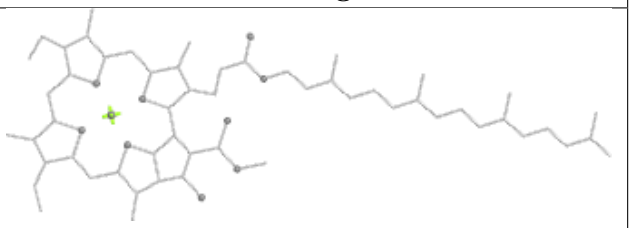
Bond lengths



Bond angles

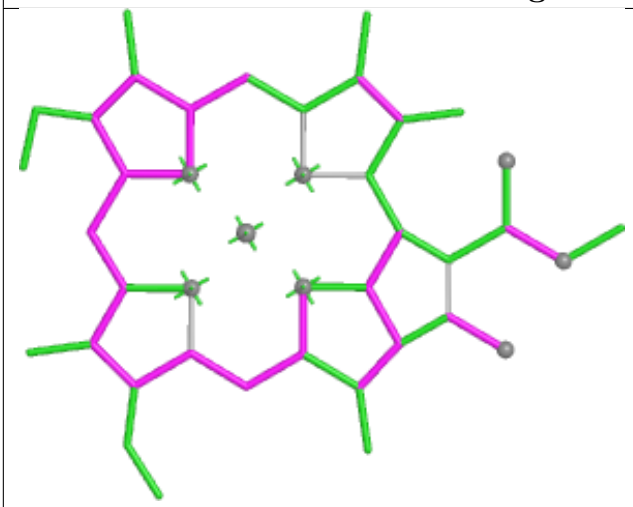


Torsions



Rings

Ligand CLA 2 312



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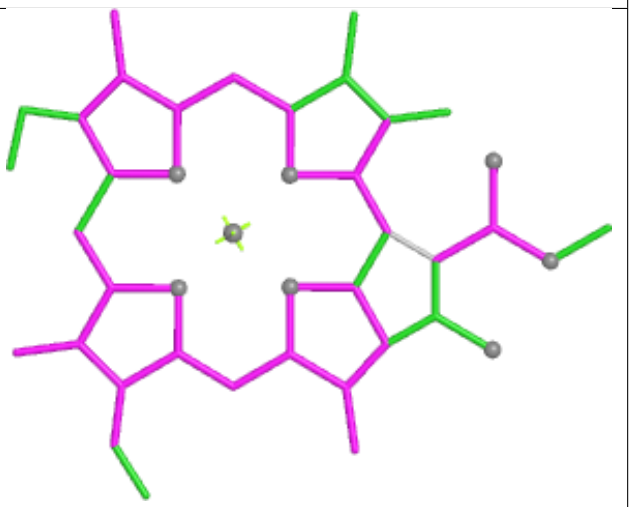
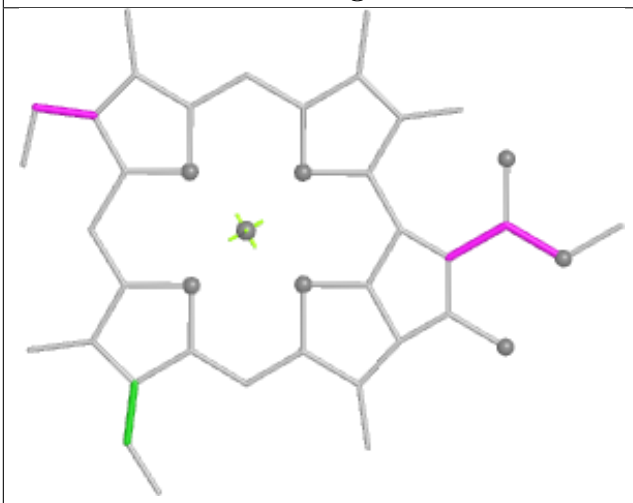


Bond angles



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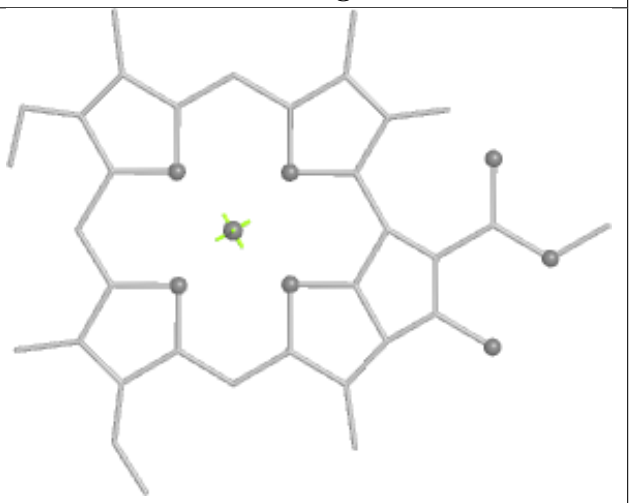
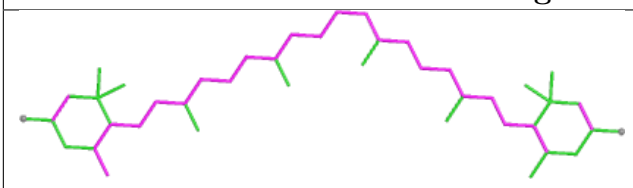


Rings

Ligand 5X6 4 313



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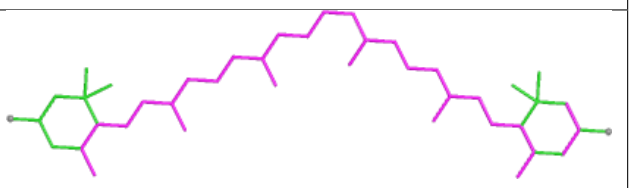

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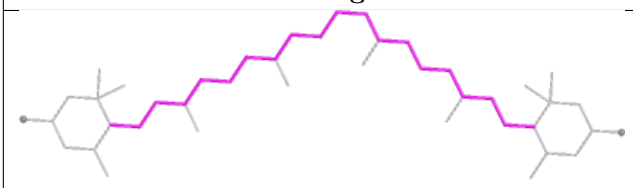

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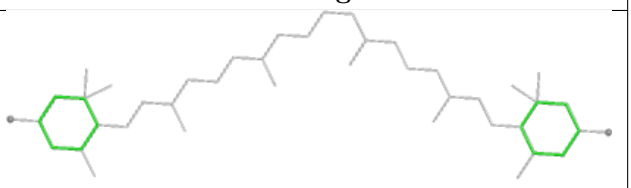
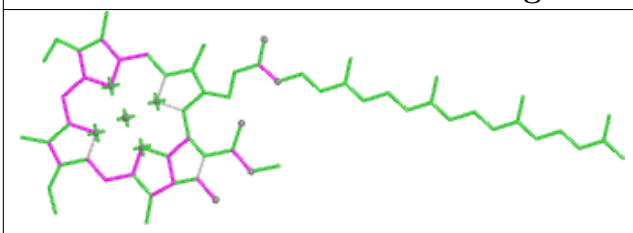


Rings

Ligand CLA A 827



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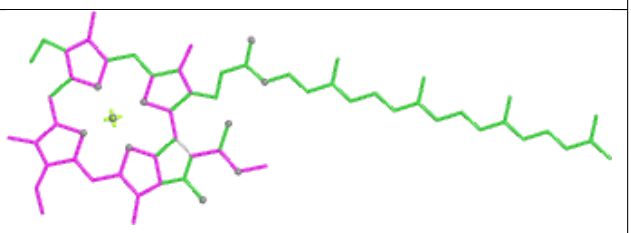
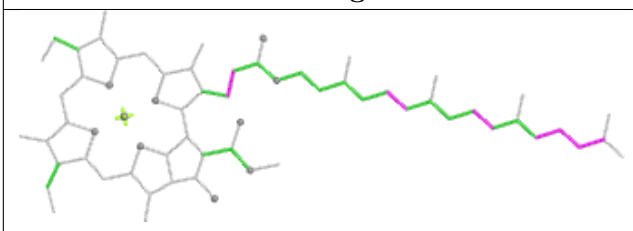


Bond angles



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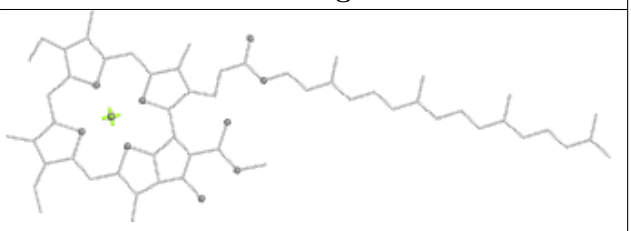
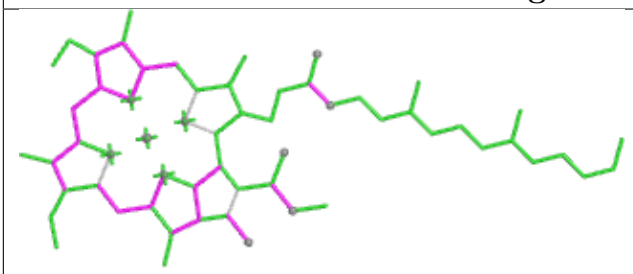


Rings

Ligand CLA 1 302



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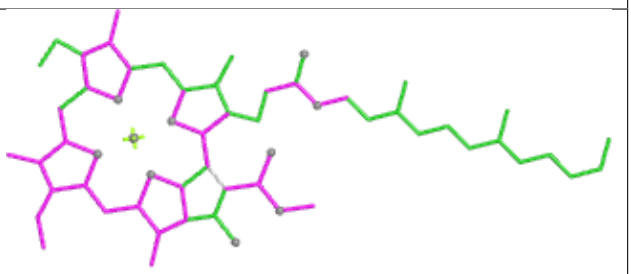

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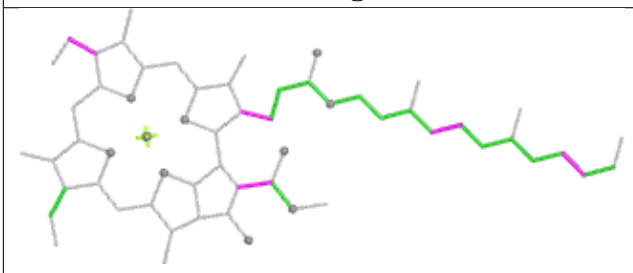

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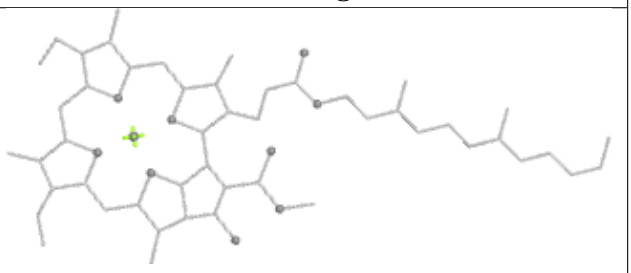
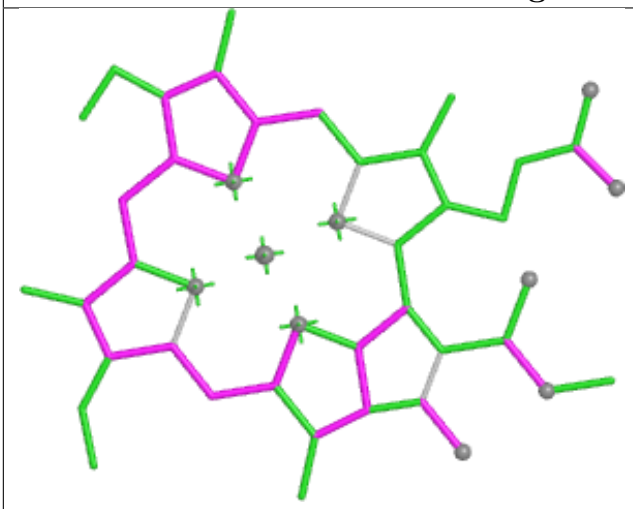


Rings

Ligand CLA 1 304



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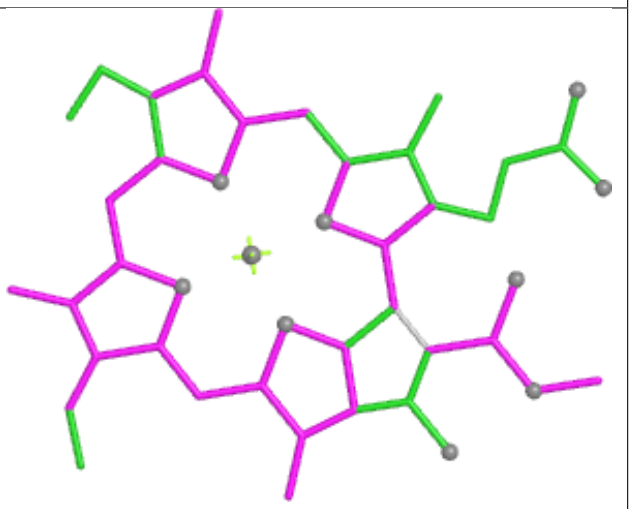
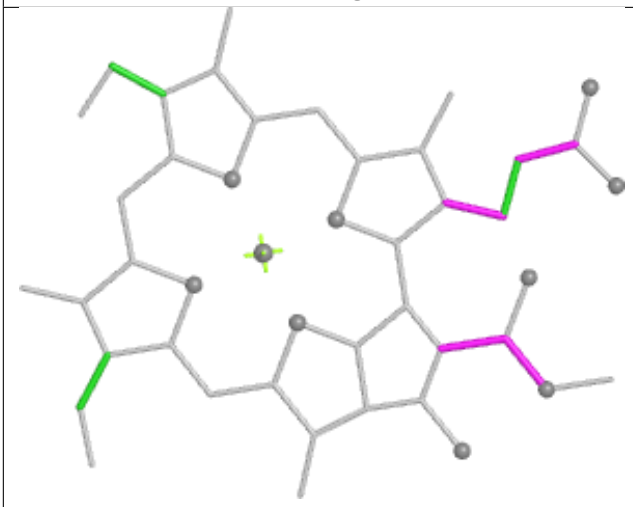


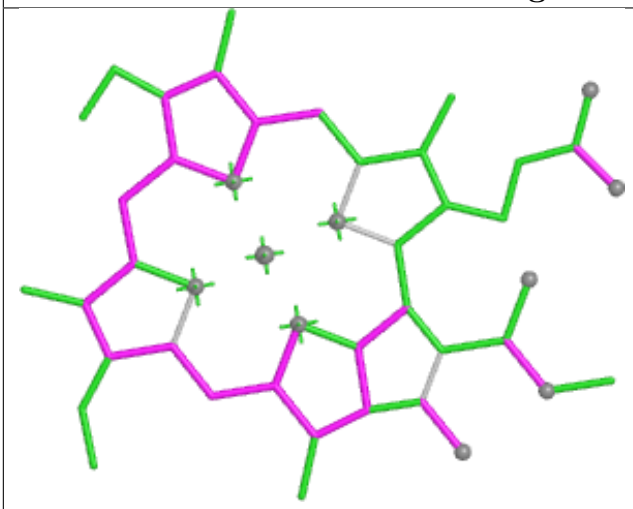
Bond angles



Torsions

Rings

Ligand CLA 2 304



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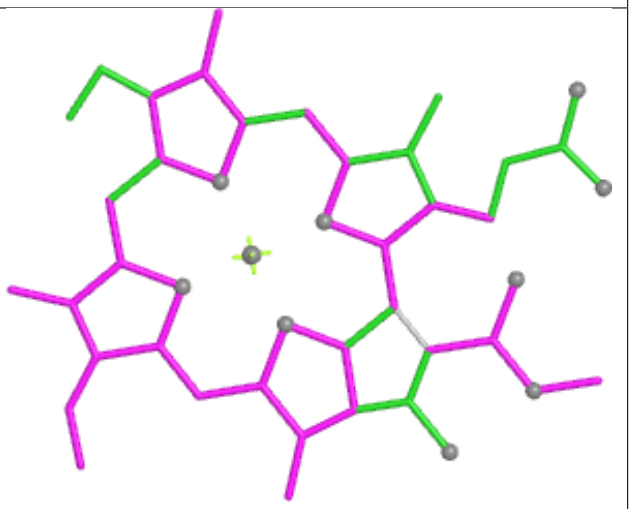

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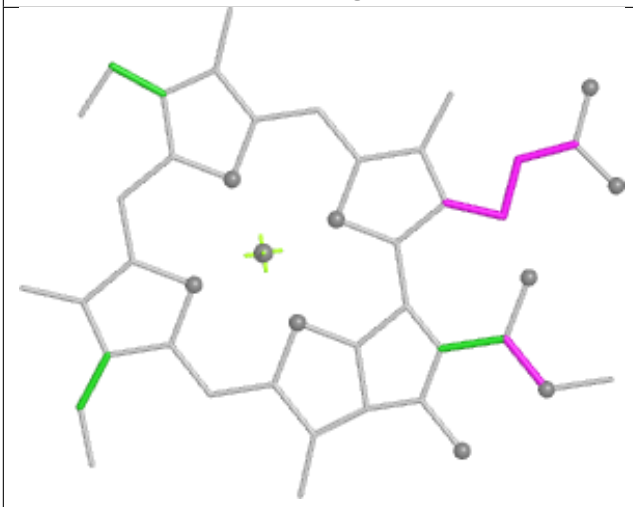
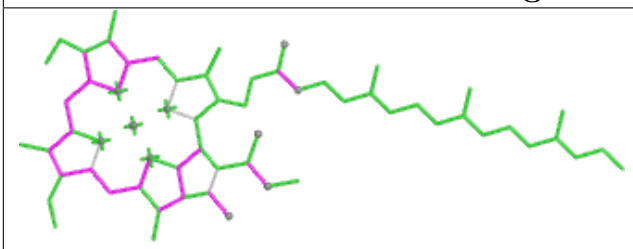


Torsions

Rings

Ligand CLA A 815



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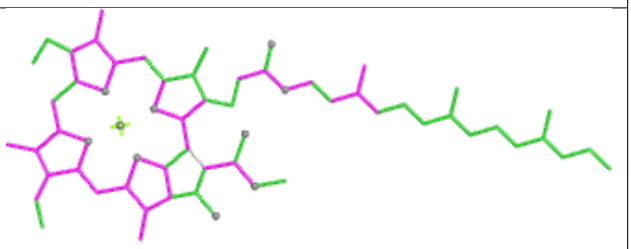
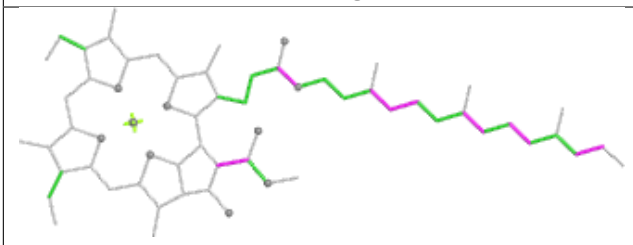


Bond angles



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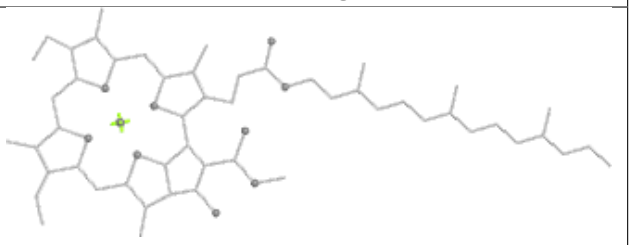
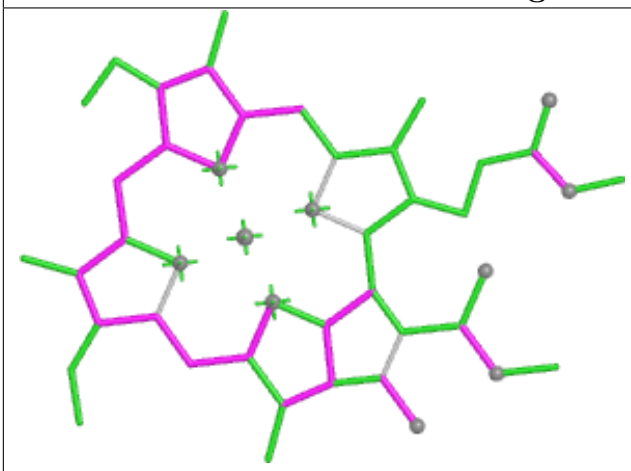


Rings

Ligand CLA 3 314



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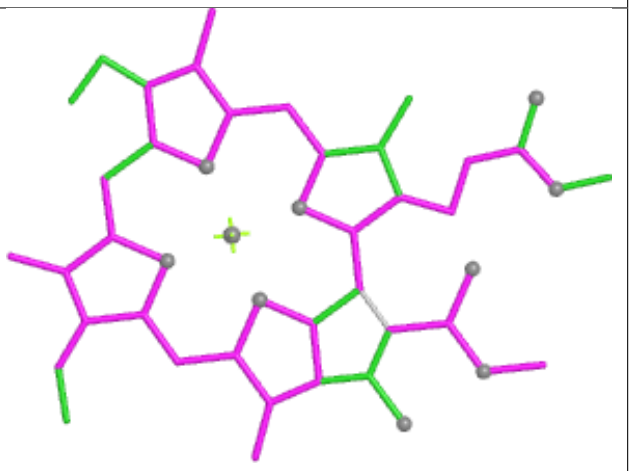
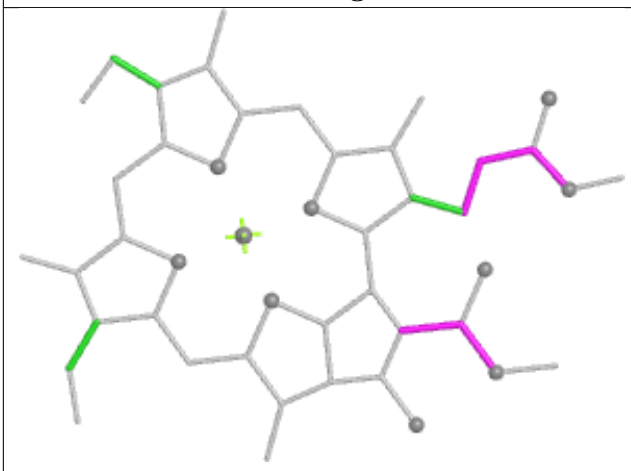


Bond angles



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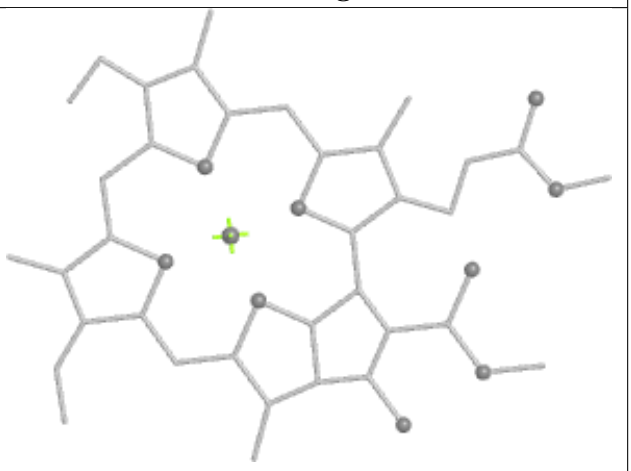
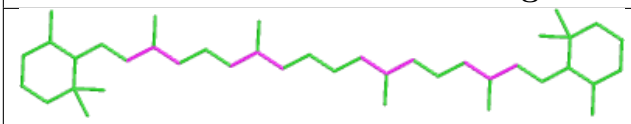


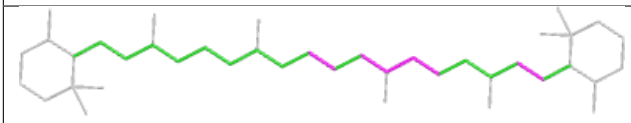
Rings

Ligand BCR K 104



Bond lengths

Bond angles



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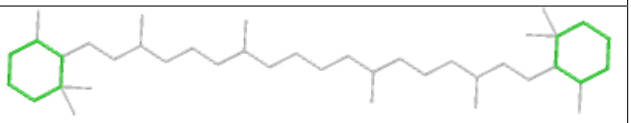
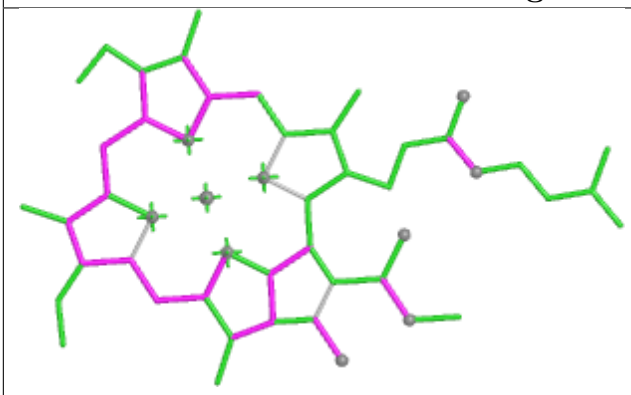


Rings

Ligand CLA L 204



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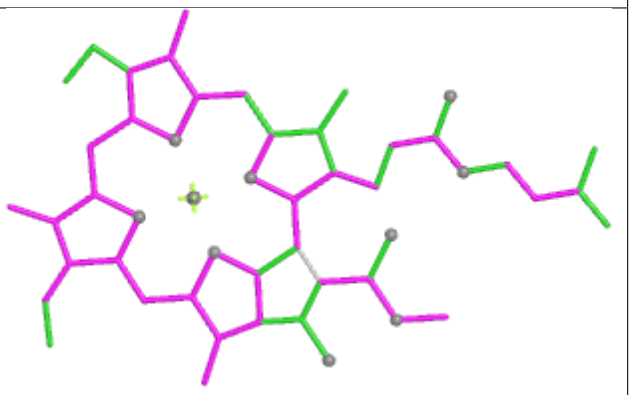
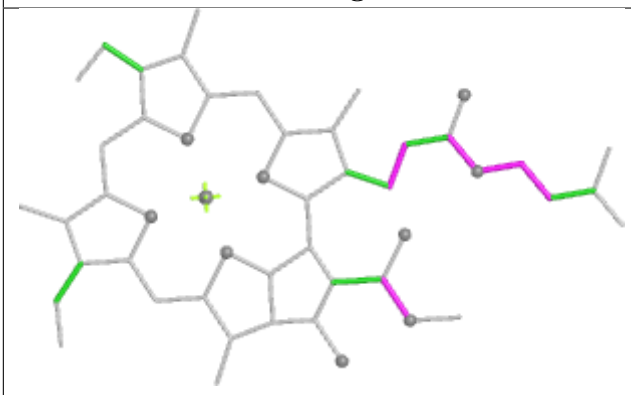


Bond angles



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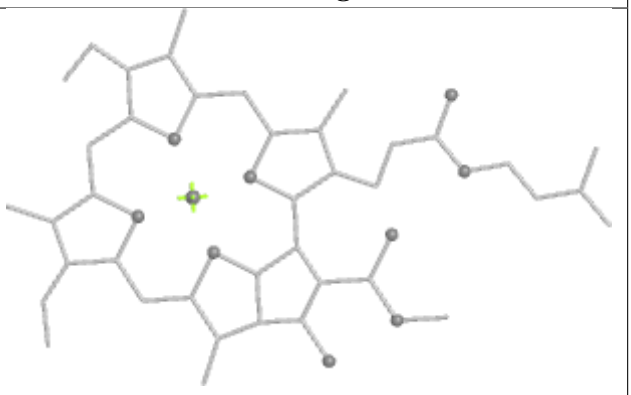
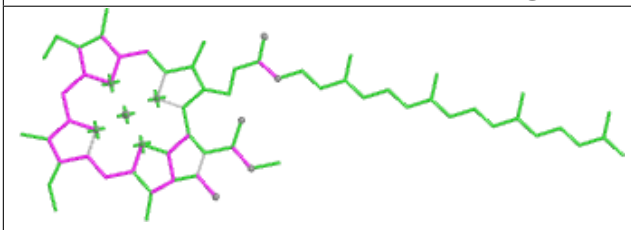


Rings

Ligand CLA A 853



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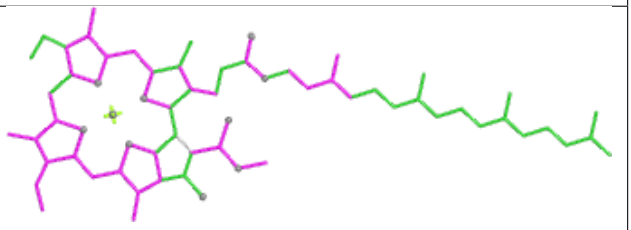
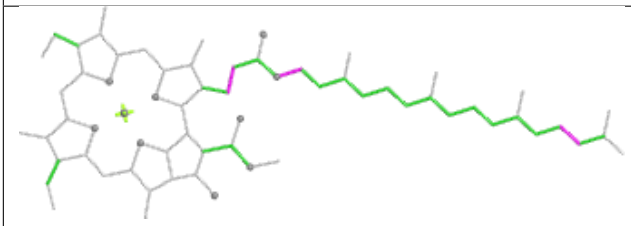


Bond angles



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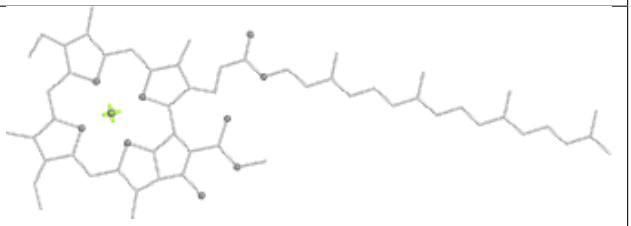
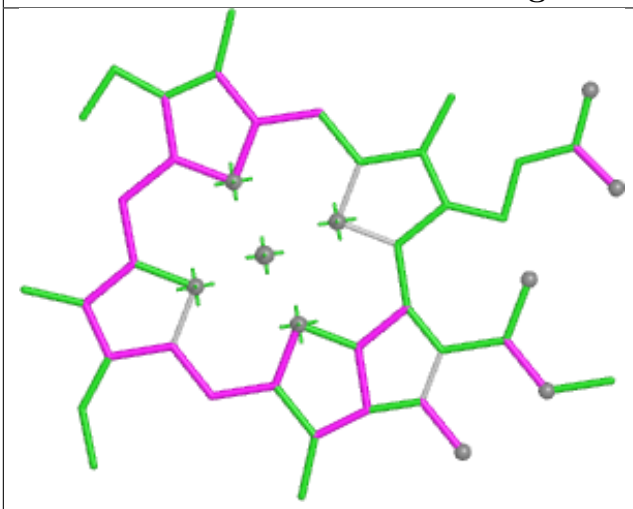


Rings

Ligand CLA 3 310



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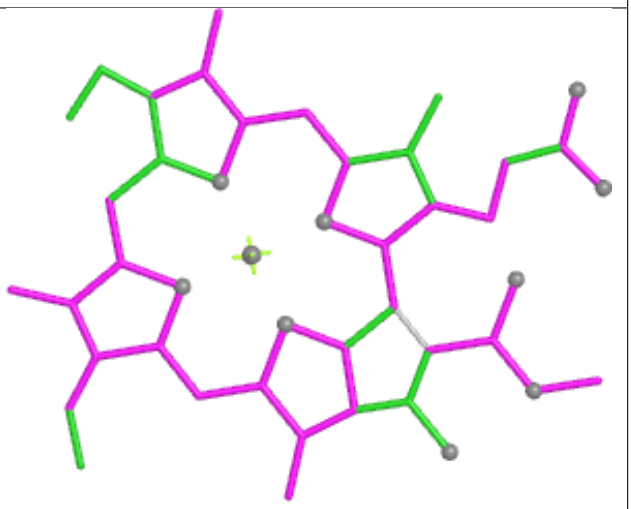
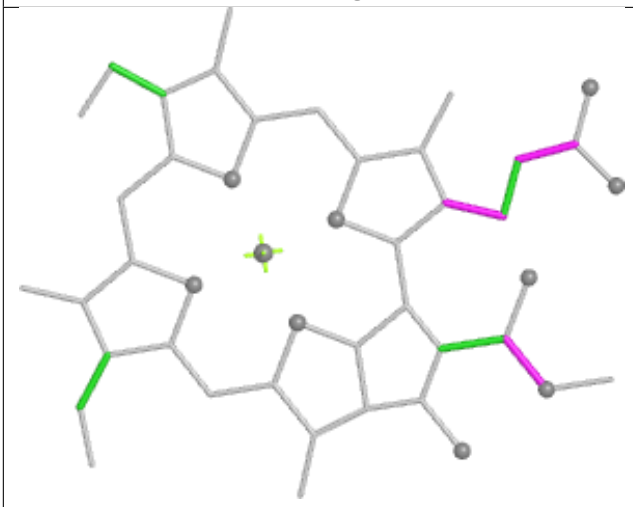


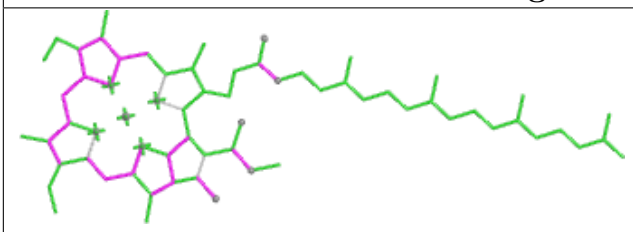
Bond angles



Torsions

Rings

Ligand CLA 2 305



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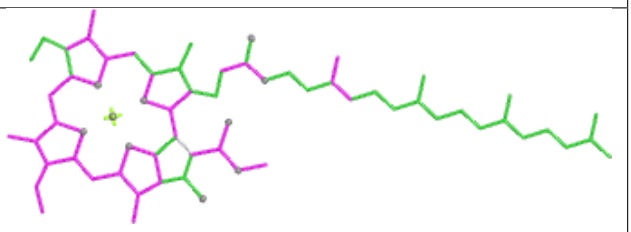
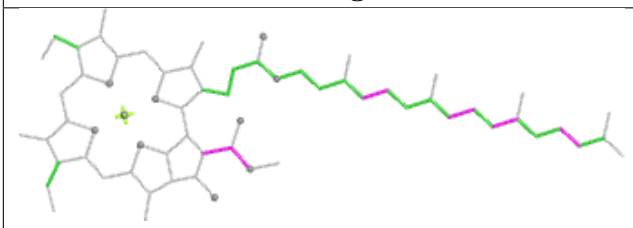
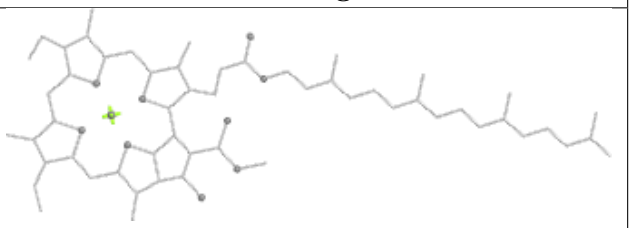


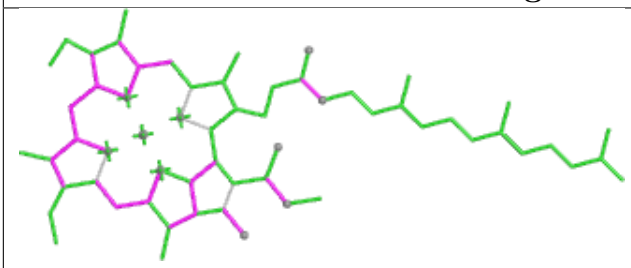
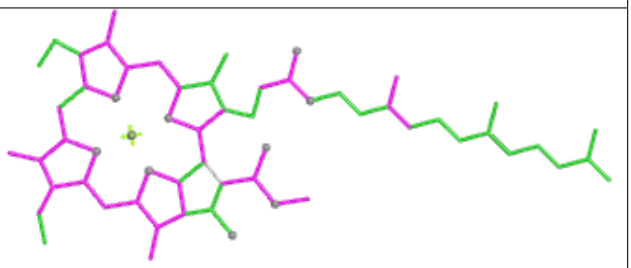
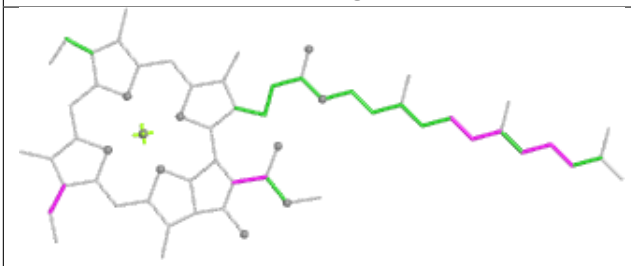
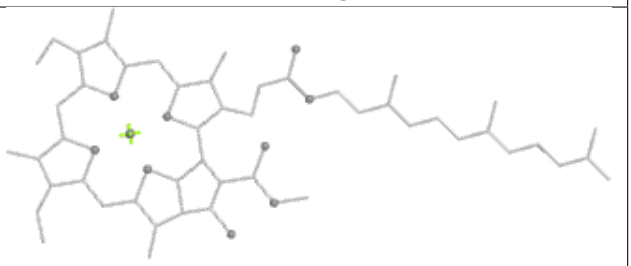
Bond angles

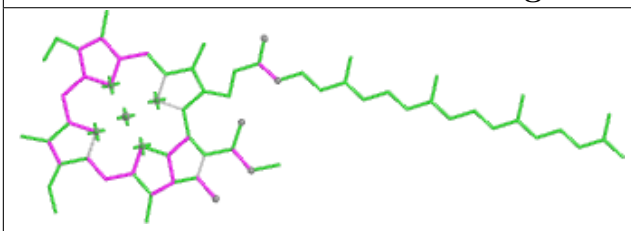
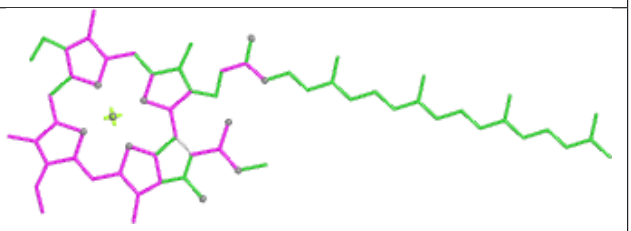
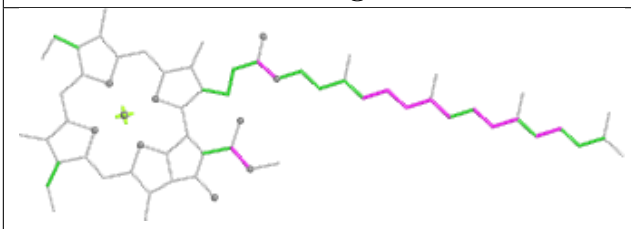
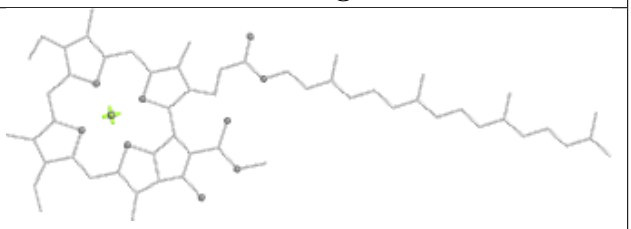


Torsions

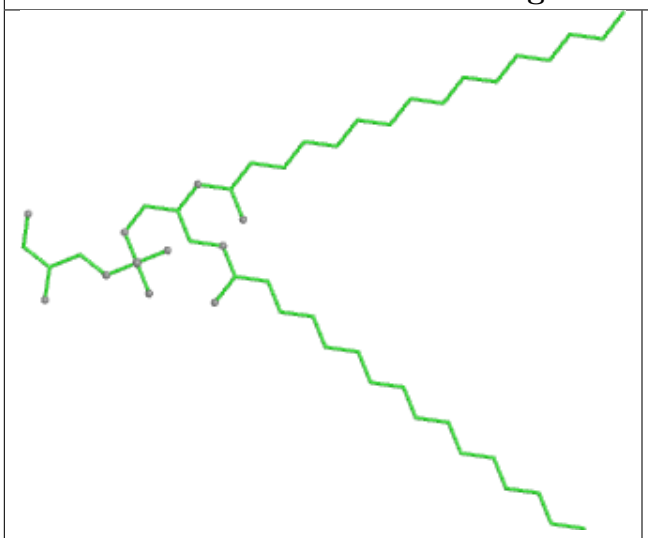


Rings

Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG J 102



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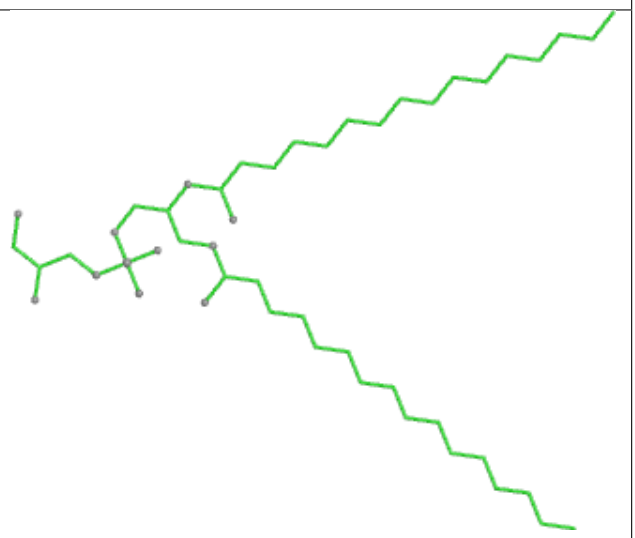

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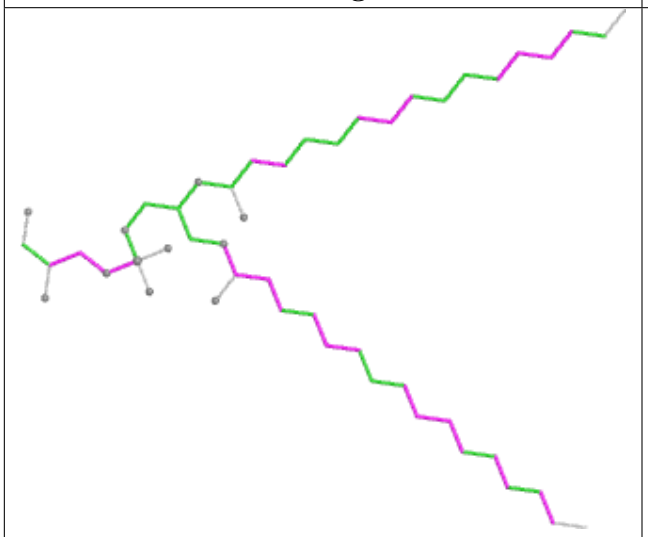

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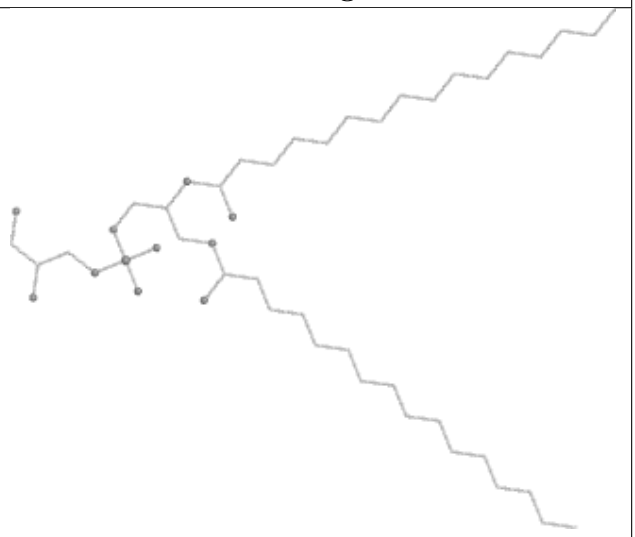
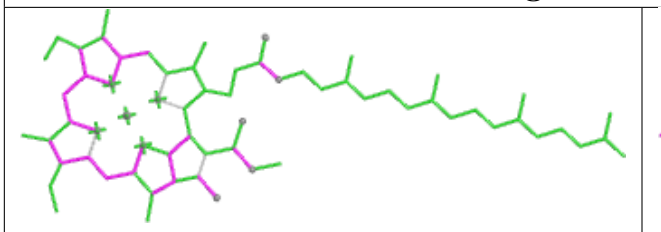


Rings

Ligand CLA A 832



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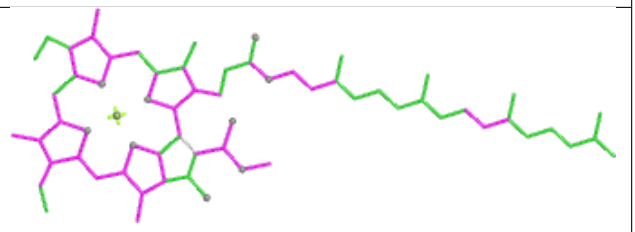

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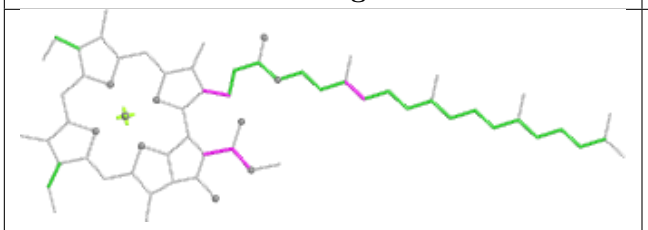

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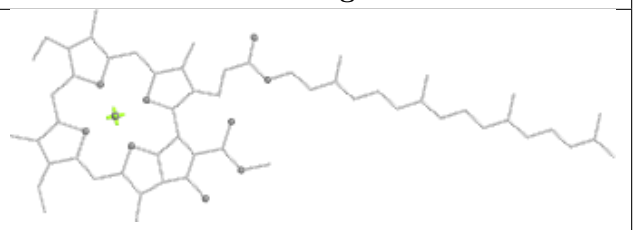
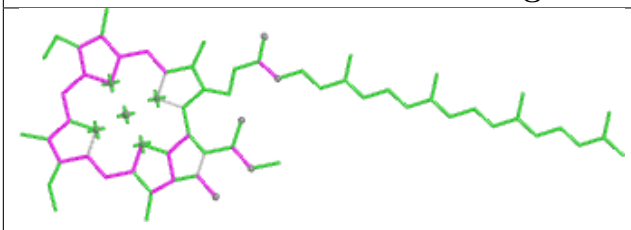


Rings

Ligand CLA A 834



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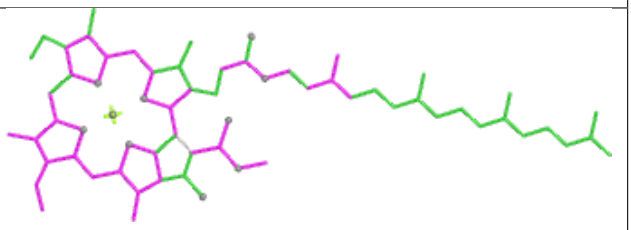

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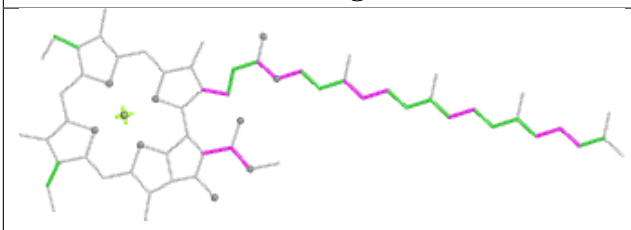

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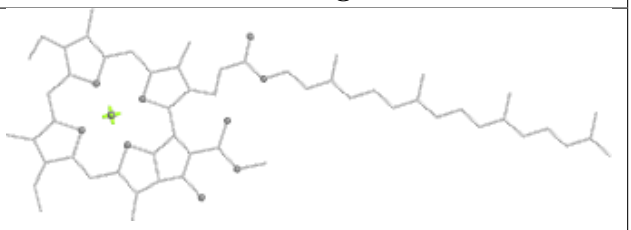
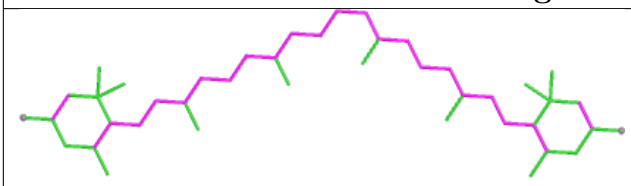


Rings

Ligand 5X6 3 317



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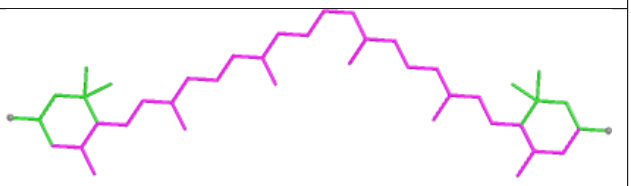

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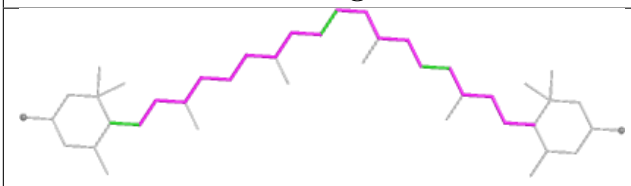

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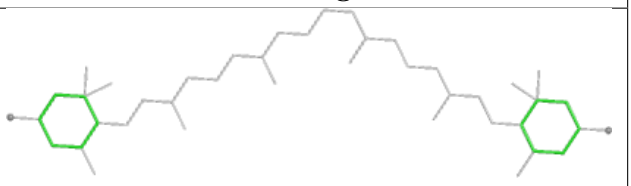
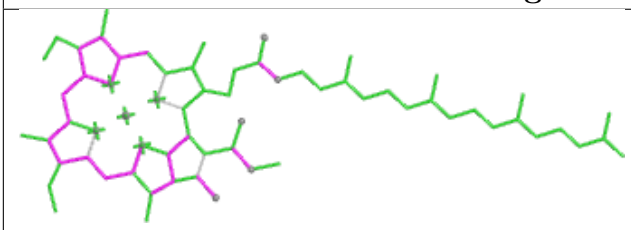


Rings

Ligand CLA B 815



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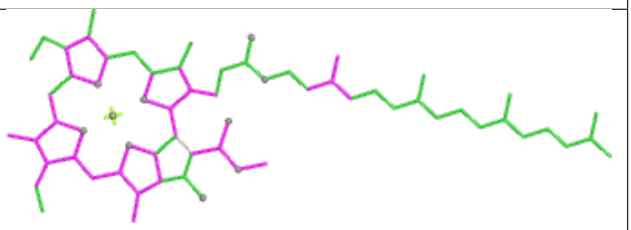

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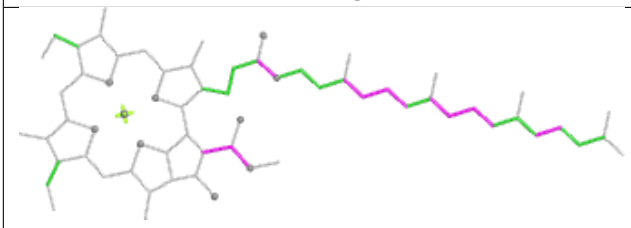

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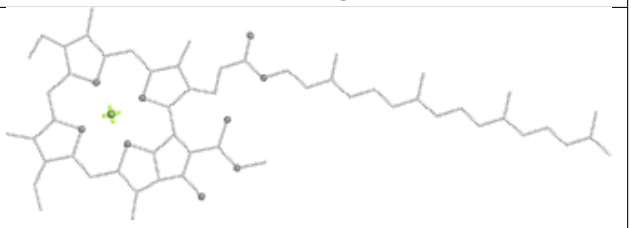
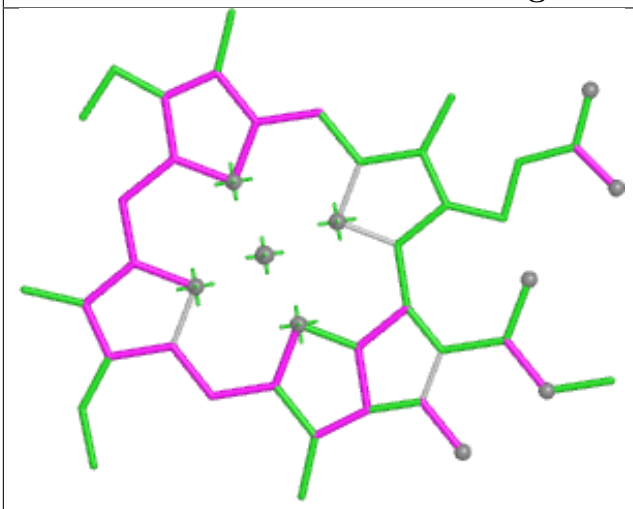


Rings

Ligand CLA 5 307



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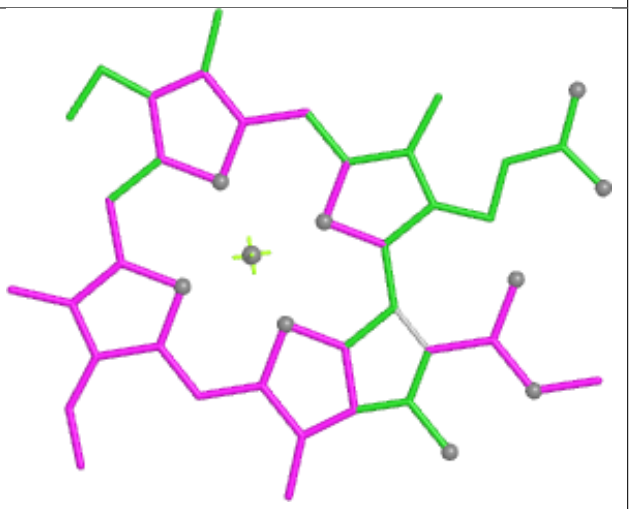

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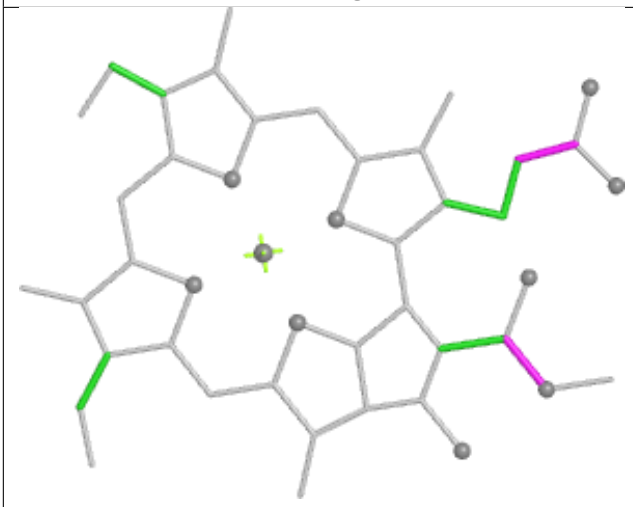
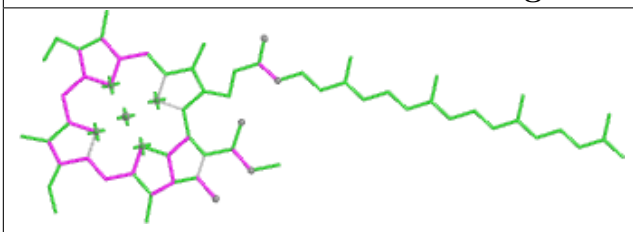


Torsions

Rings

Ligand CLA B 840



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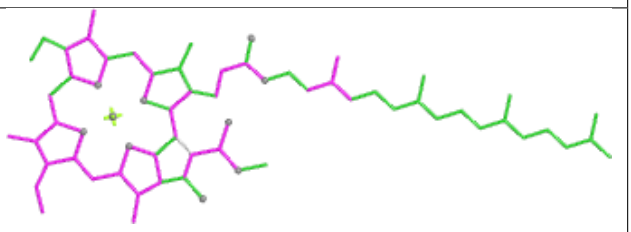

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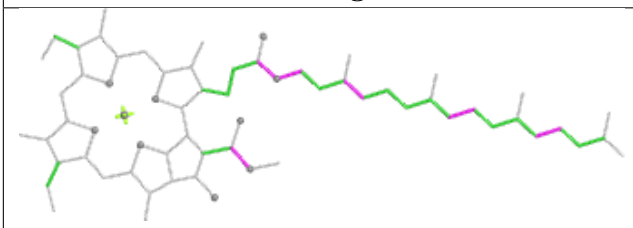

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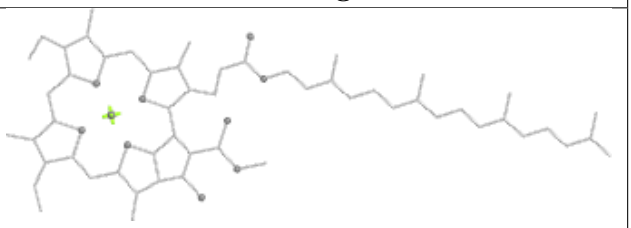
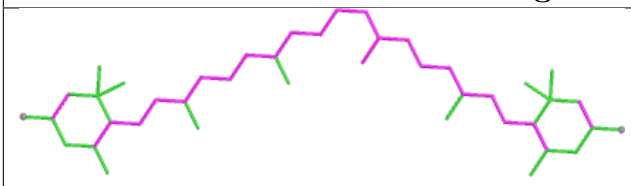


Rings

Ligand 5X6 5 318



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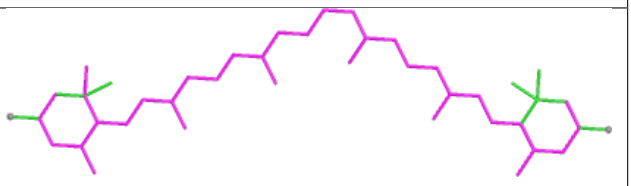

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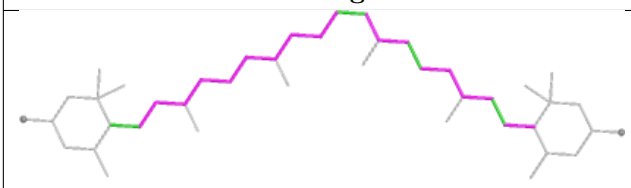

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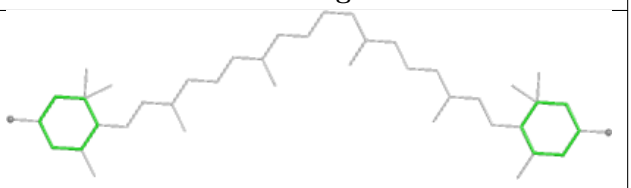
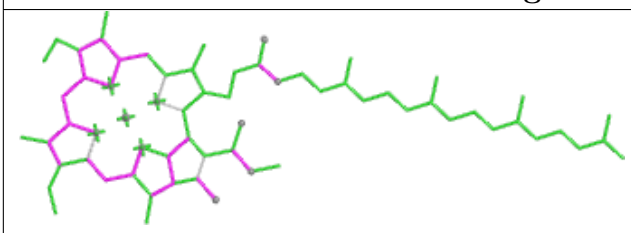


Rings

Ligand CLA A 811



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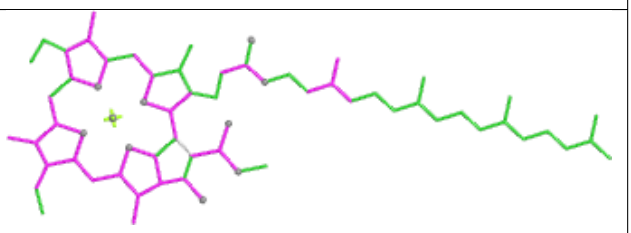

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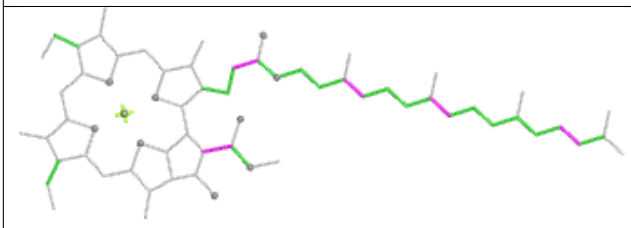

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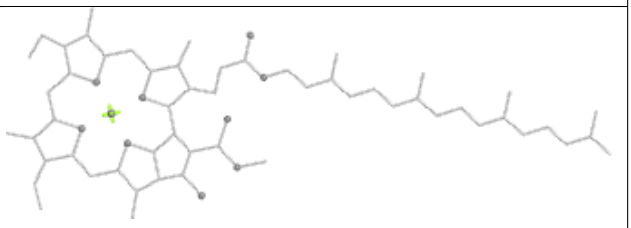
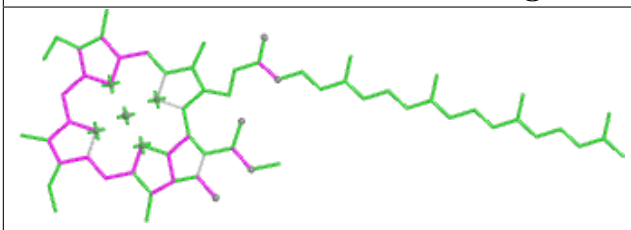


Rings

Ligand CLA A 839



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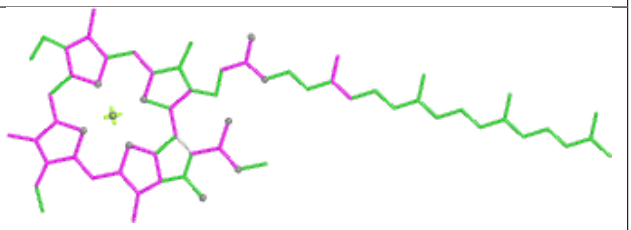

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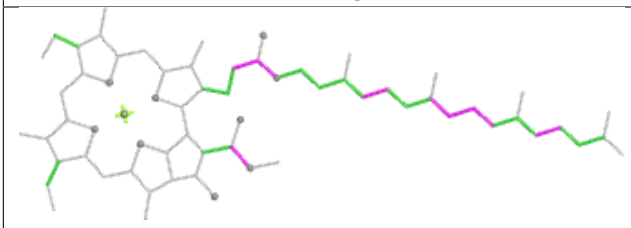

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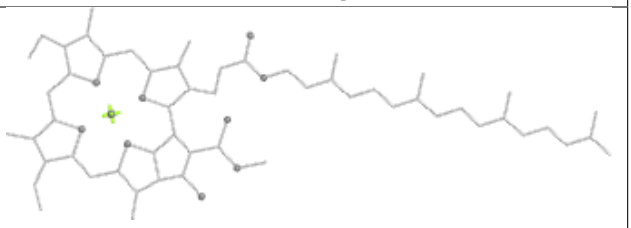
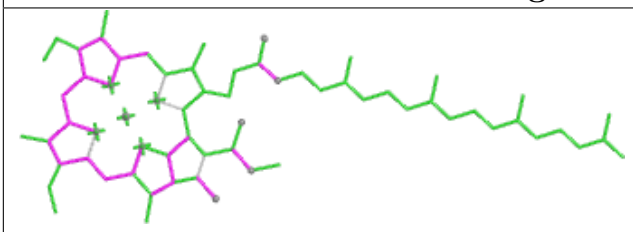


Rings

Ligand CLA 5 308



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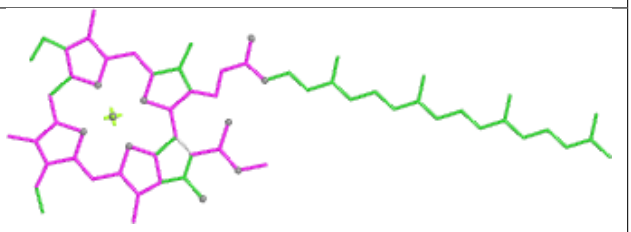

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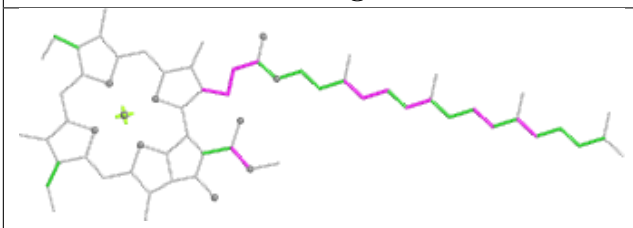

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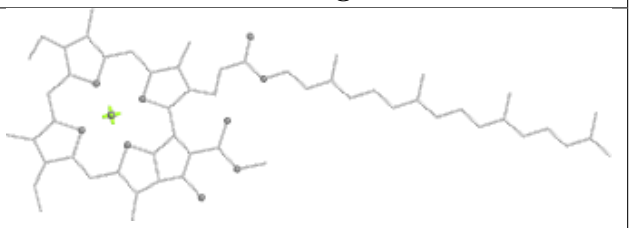
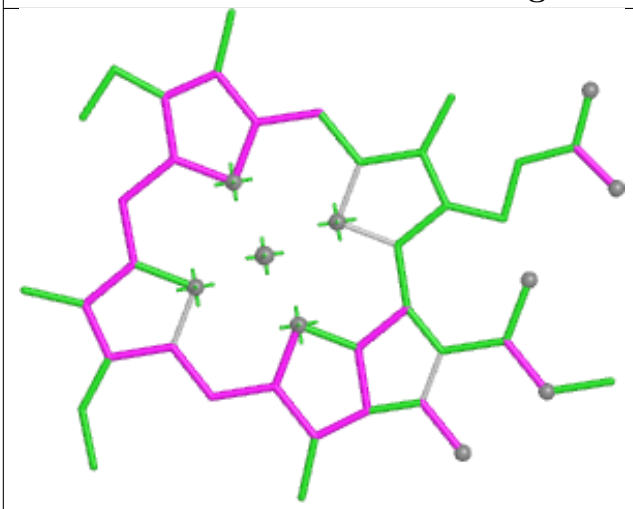


Rings

Ligand CLA 5 302



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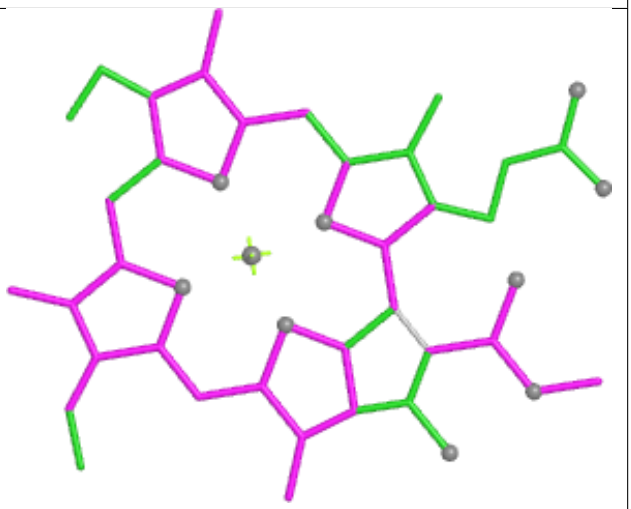
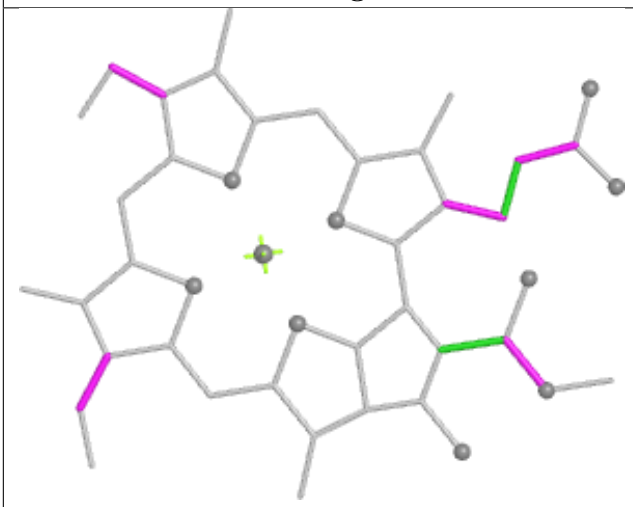


Bond angles



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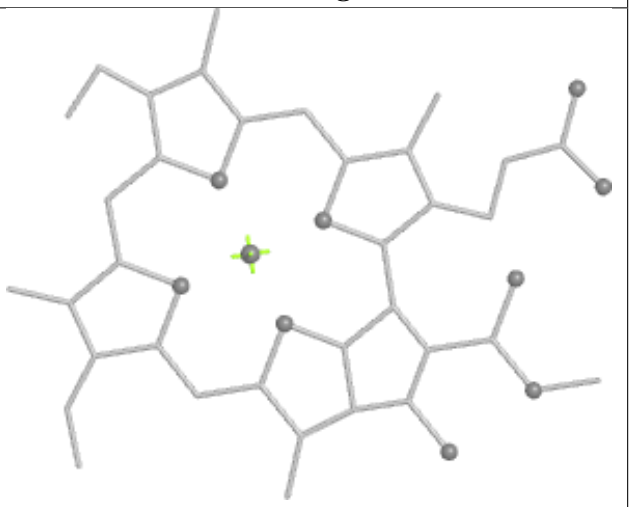
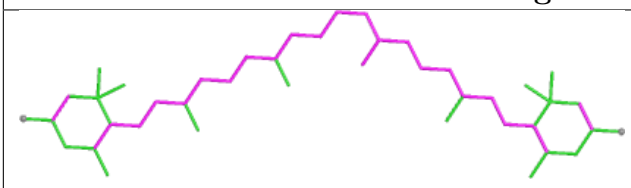
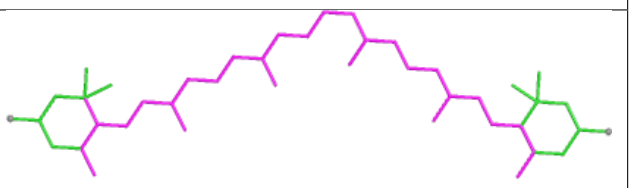
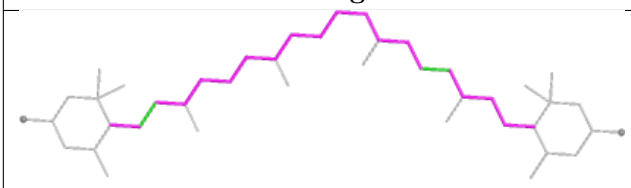
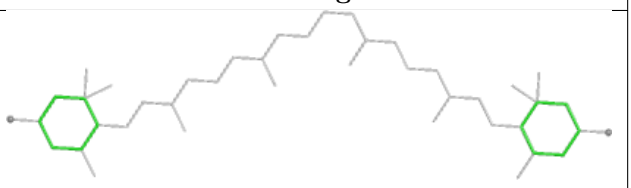
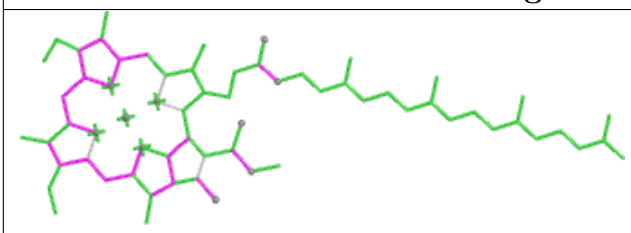
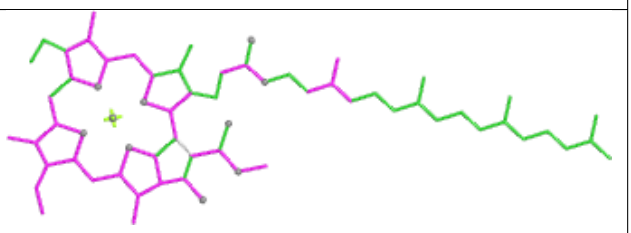
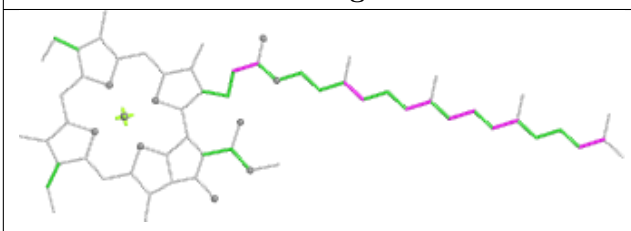
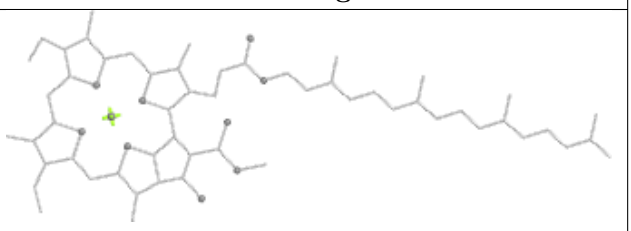
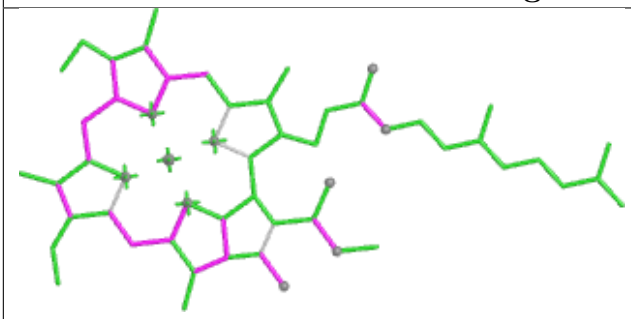


Rings

Ligand 5X6 2 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 802



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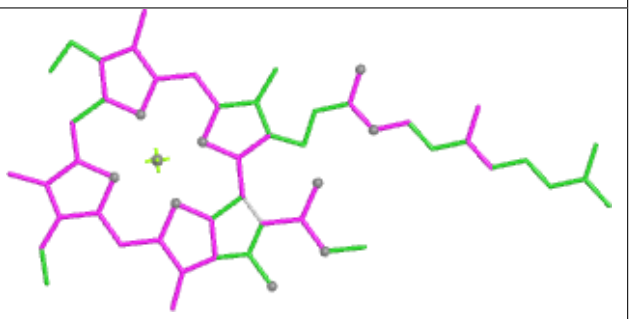

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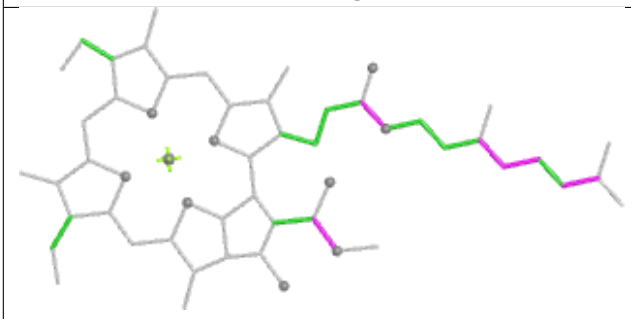

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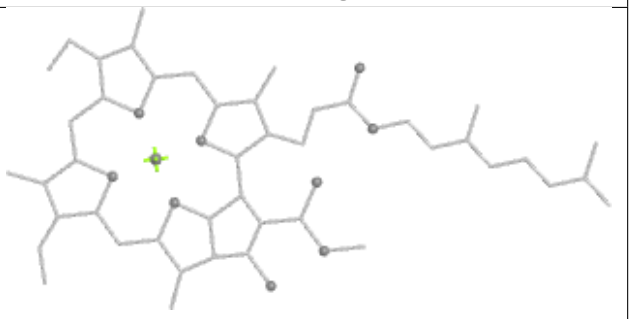
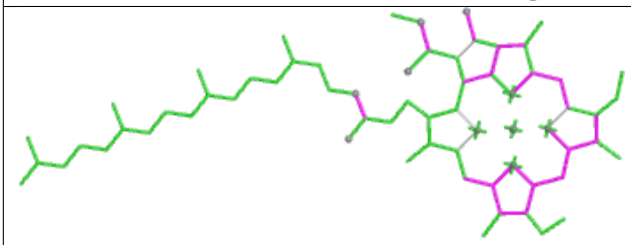


Rings

Ligand CLA B 805



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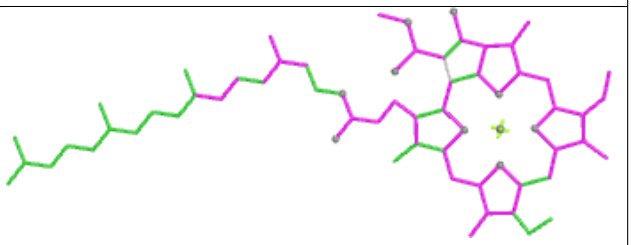

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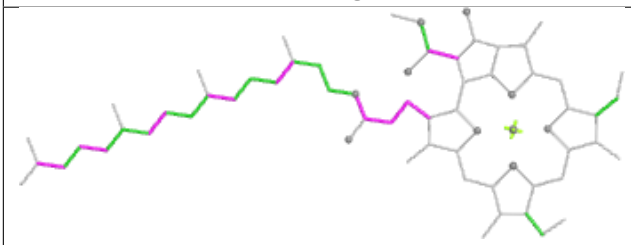
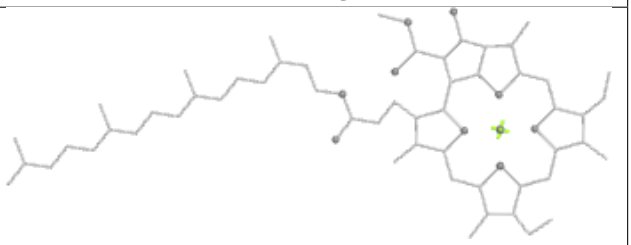
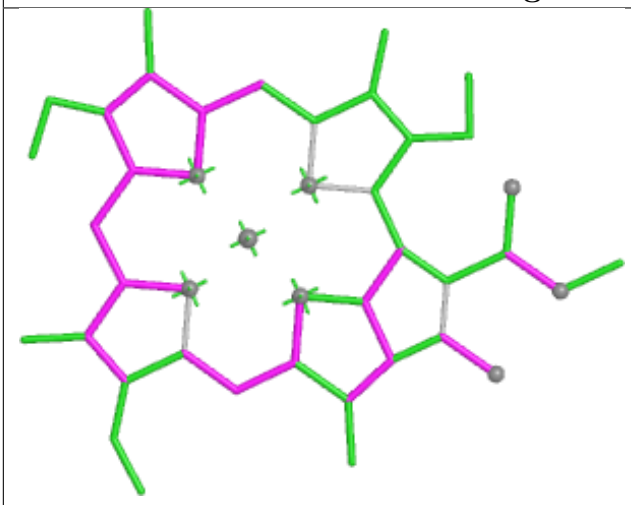


Torsions



Rings

Ligand CLA A 813



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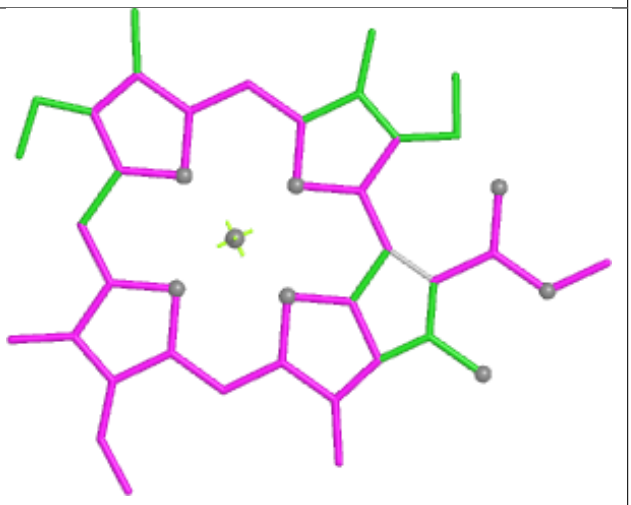

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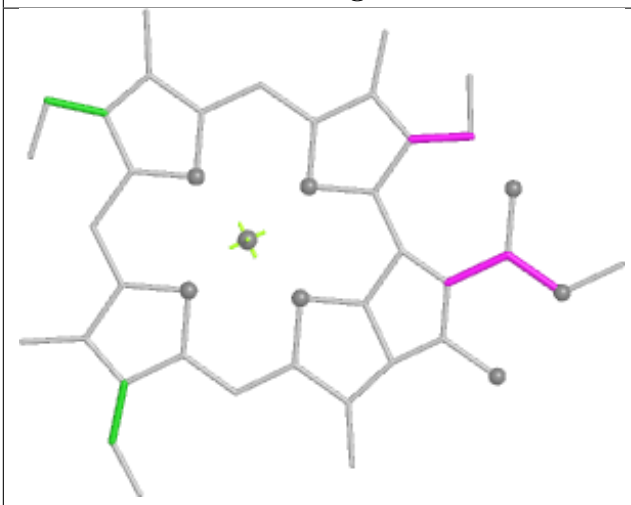
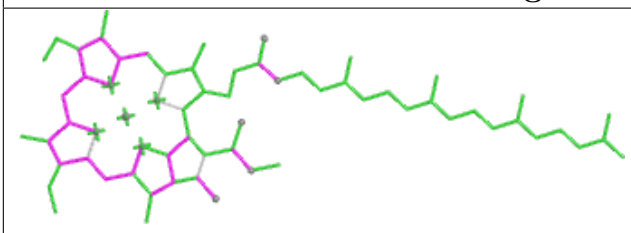


Torsions

Rings

Ligand CLA B 825



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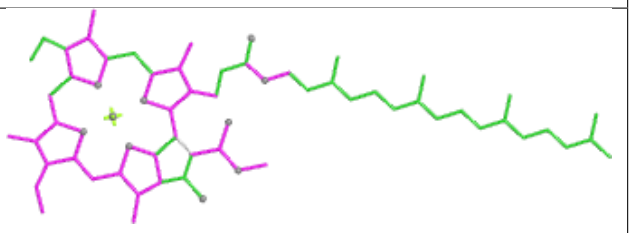

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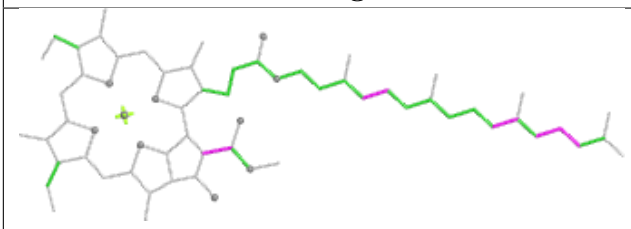

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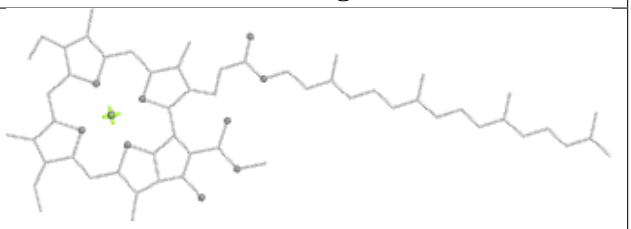
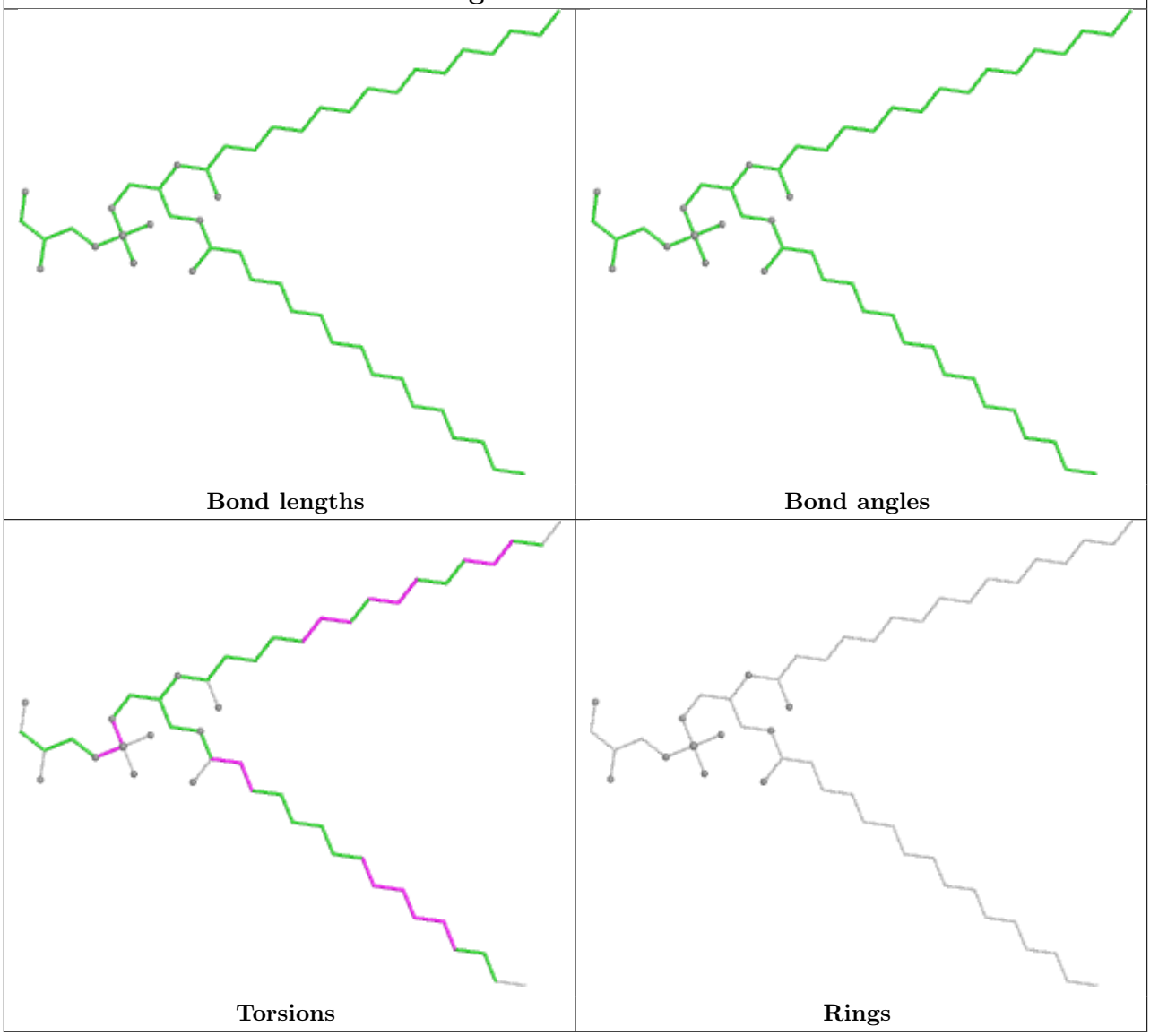
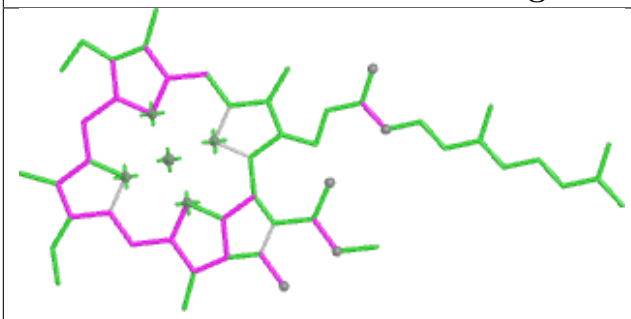


Rings

Ligand LHG A 841



Ligand CLA 3 307



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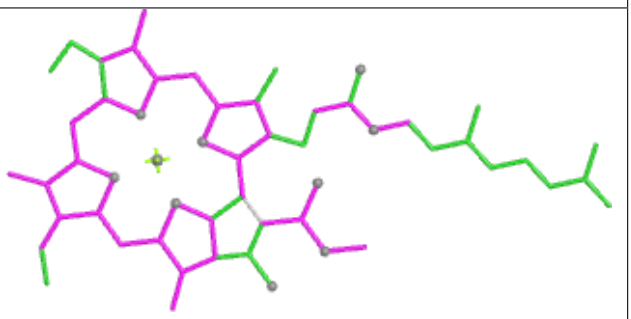
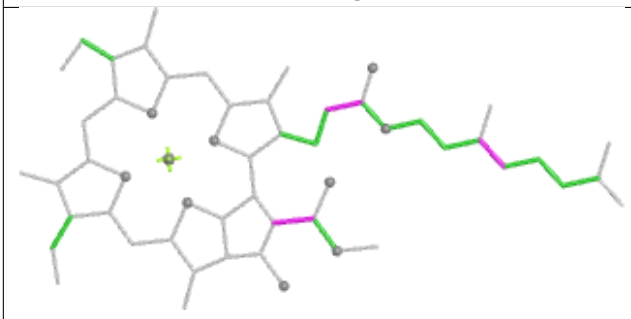


Bond angles



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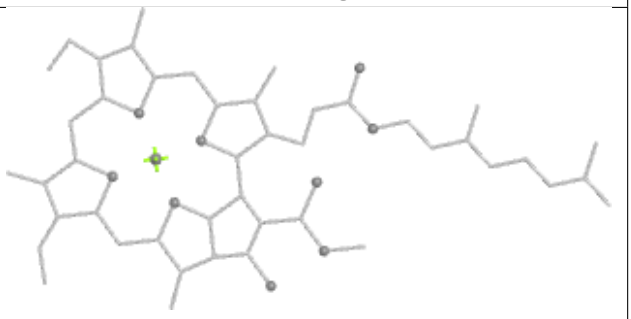
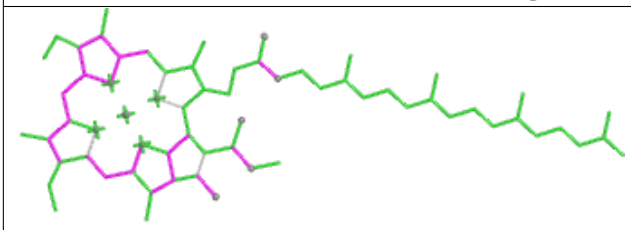


Rings

Ligand CLA B 841



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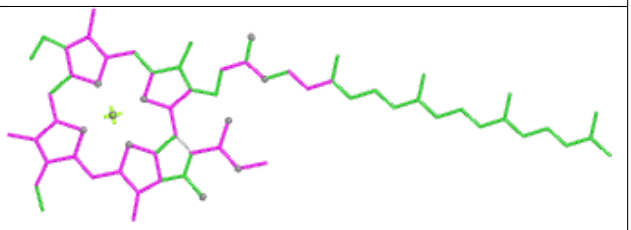
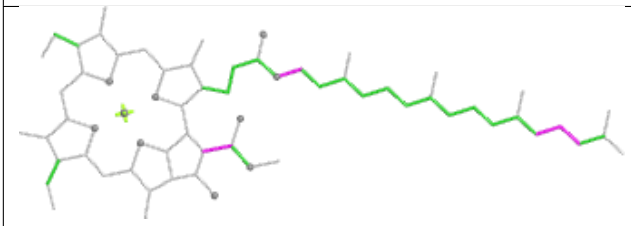


Bond angles



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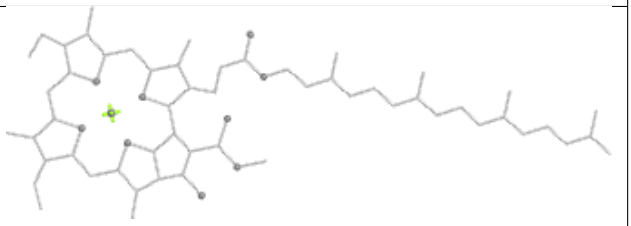
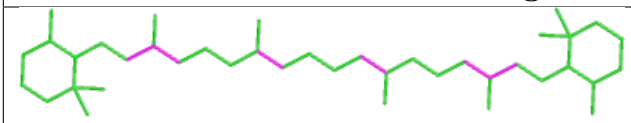


Rings

Ligand BCR B 843



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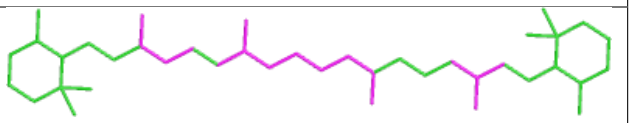
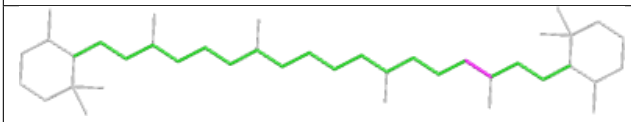


Bond angles



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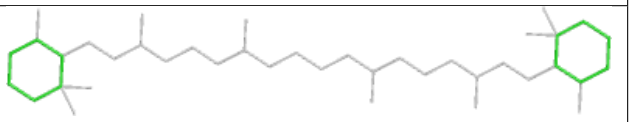
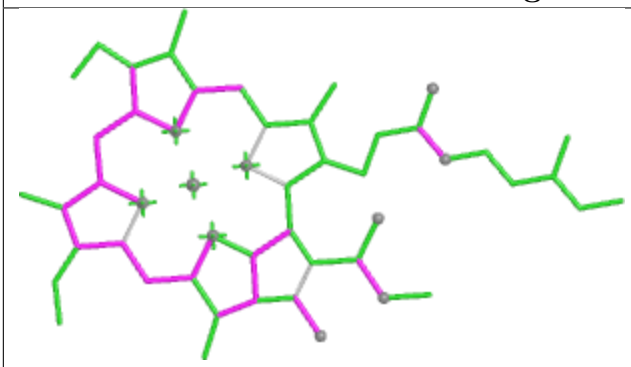
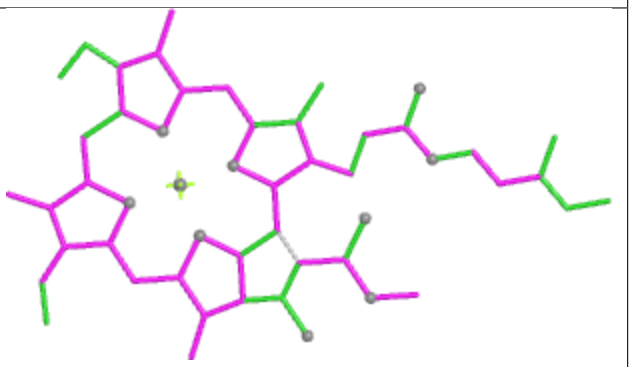
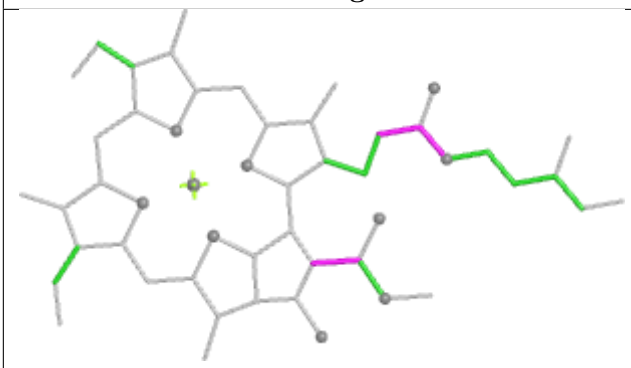
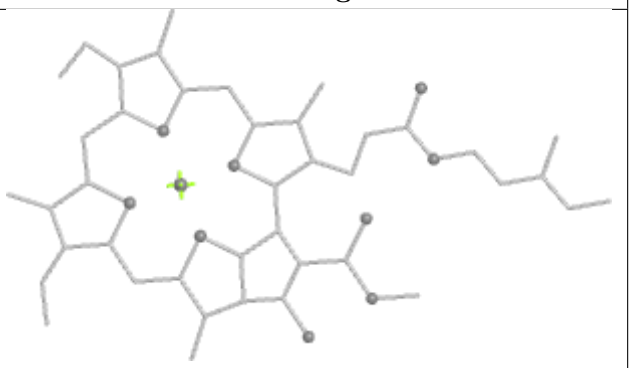
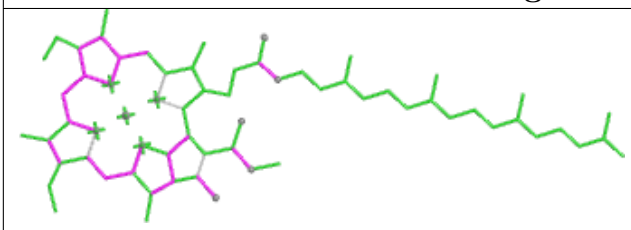
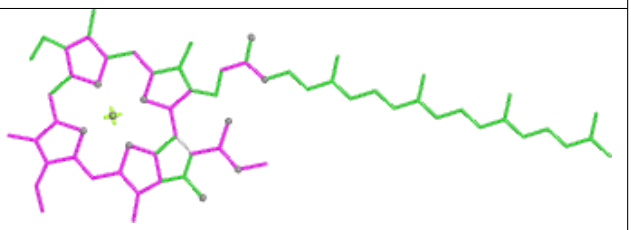
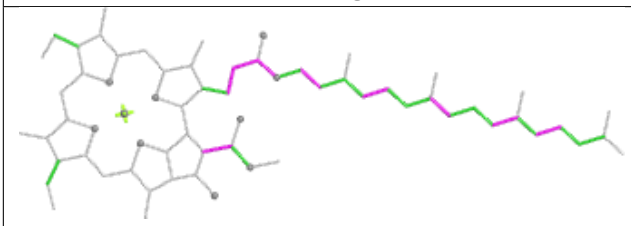
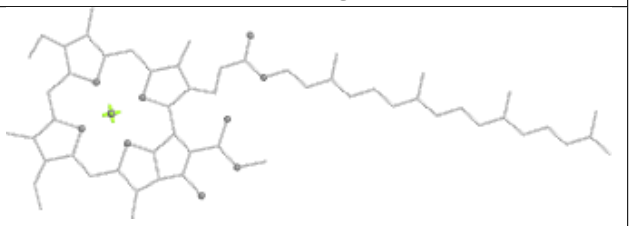
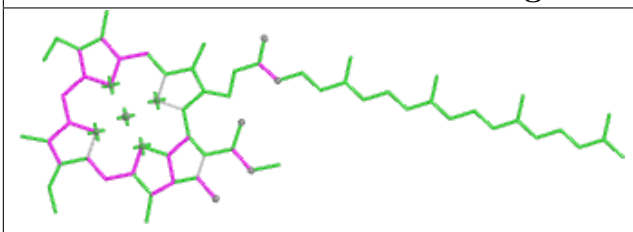


Rings

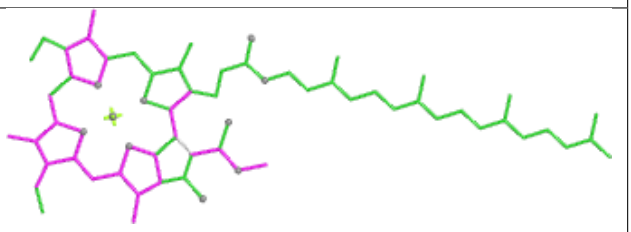
Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

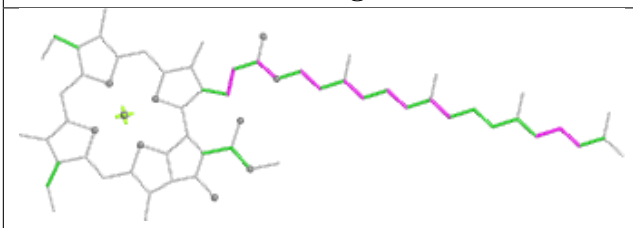
Ligand CLA B 839



Bond lengths



Bond angles



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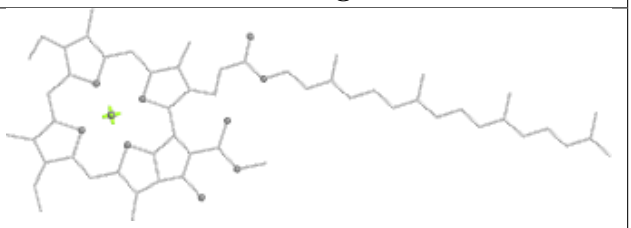
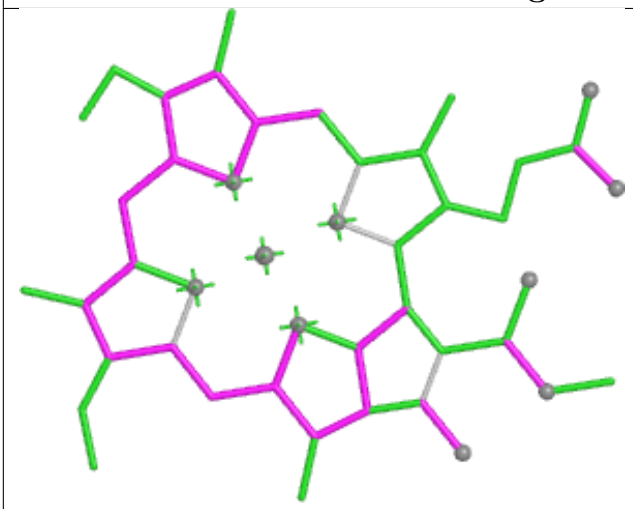


Rings

Ligand CLA 1 311



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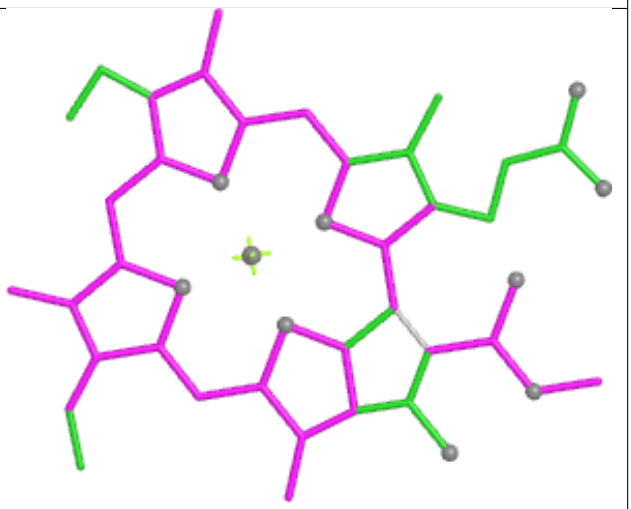

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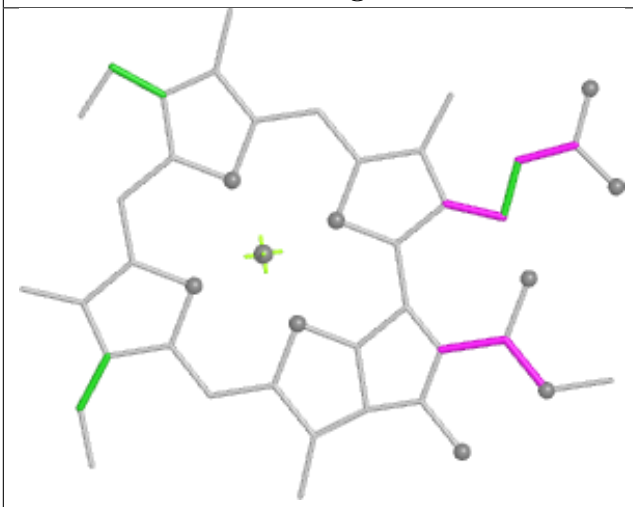

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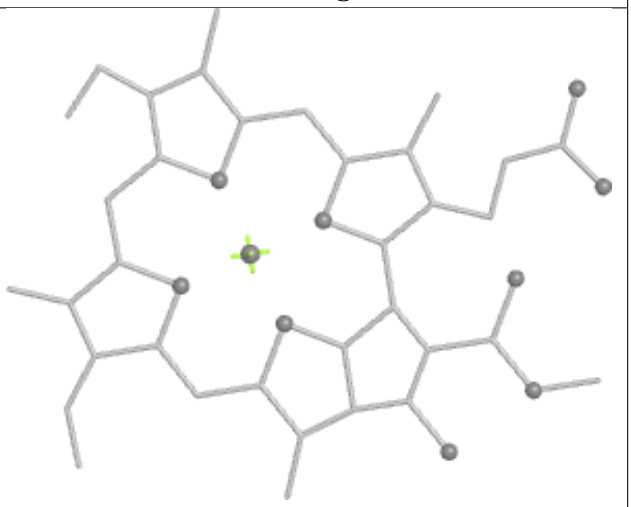
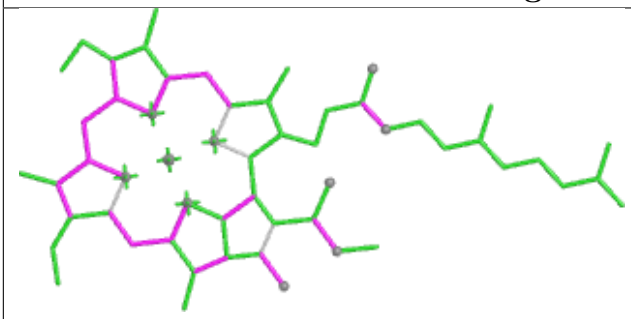
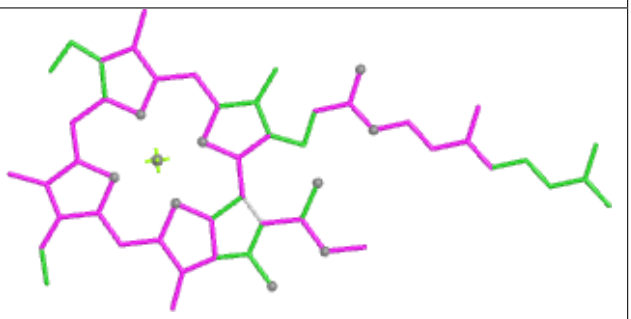
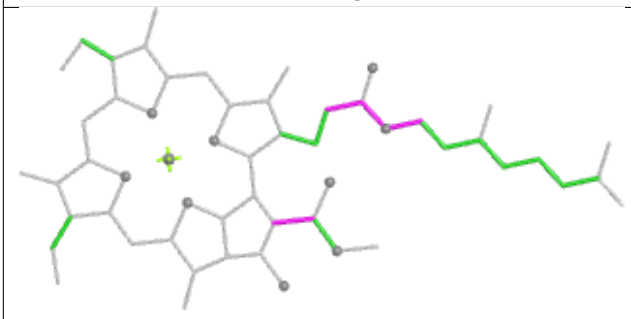
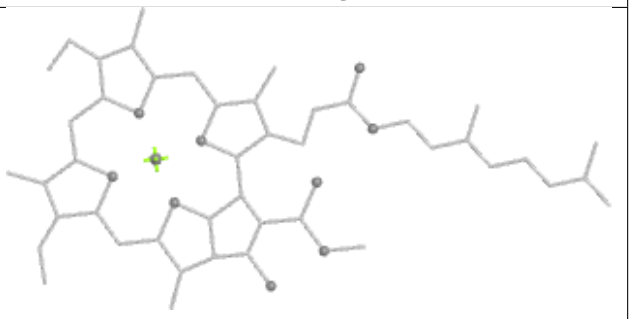
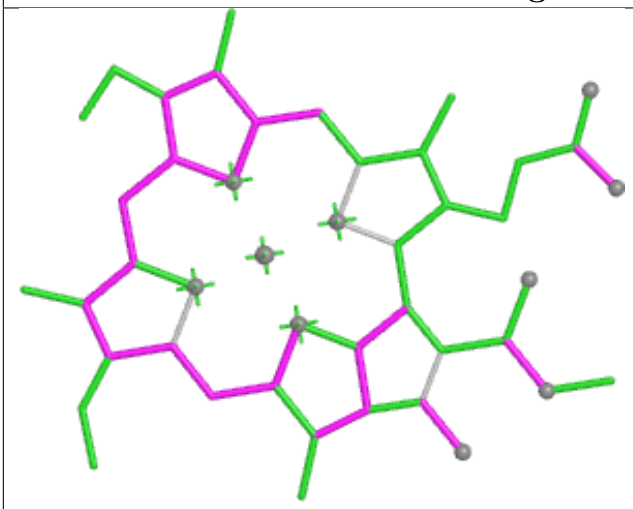


Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 310



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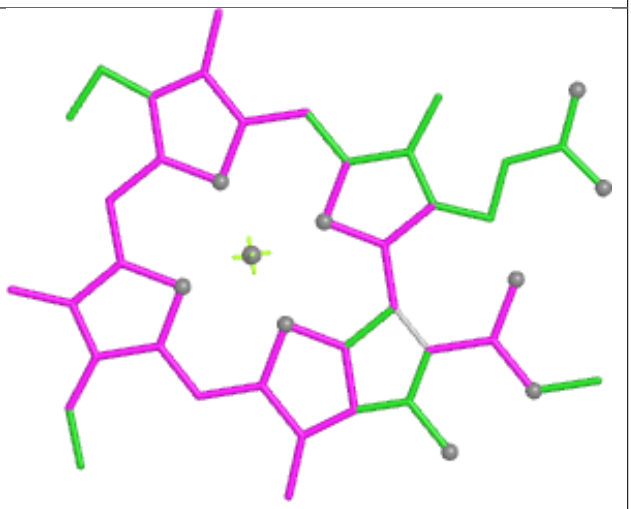

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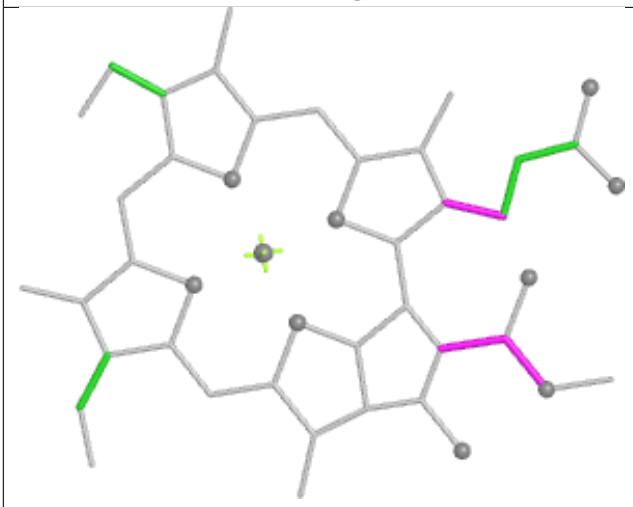
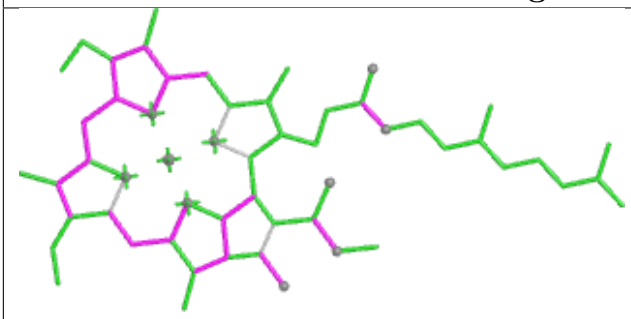


Torsions

Rings

Ligand CLA 2 311



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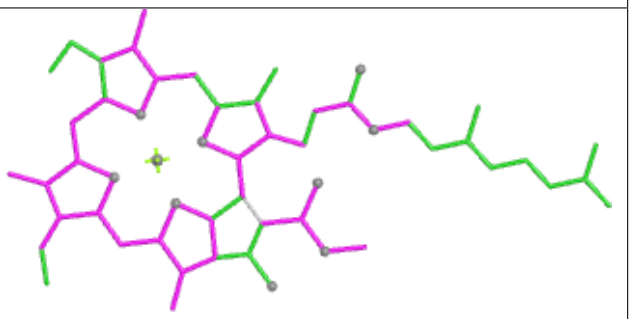

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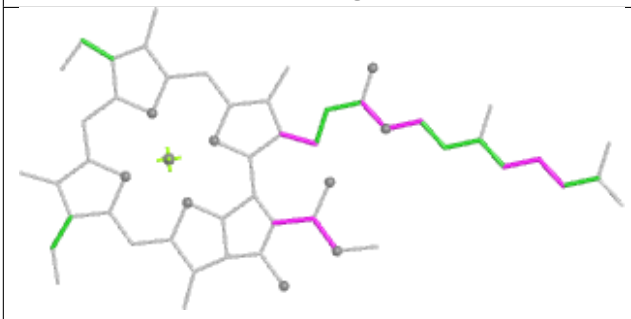

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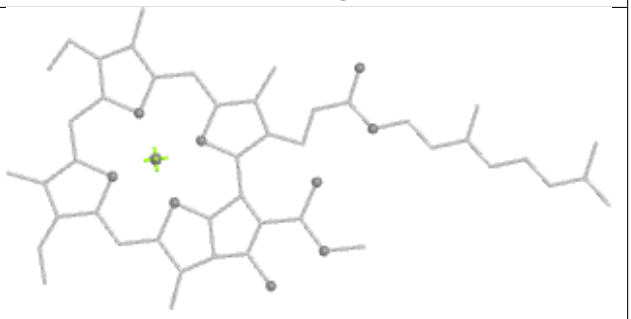
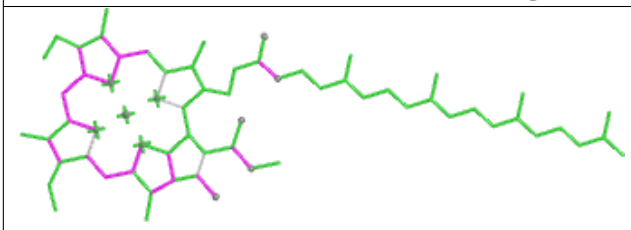


Rings

Ligand CLA B 802



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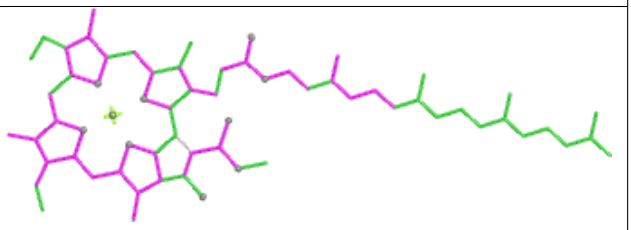

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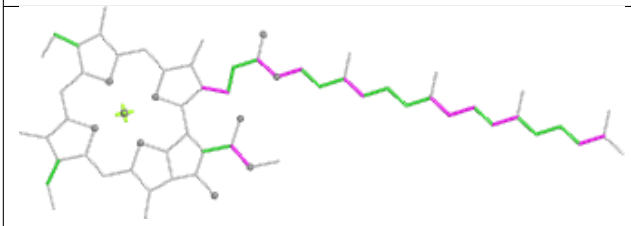

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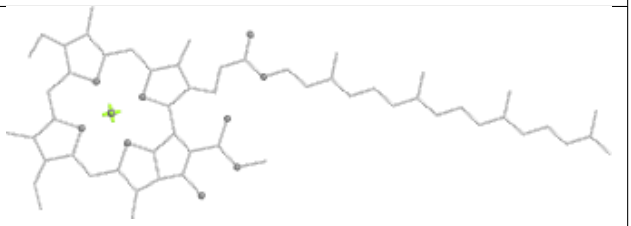
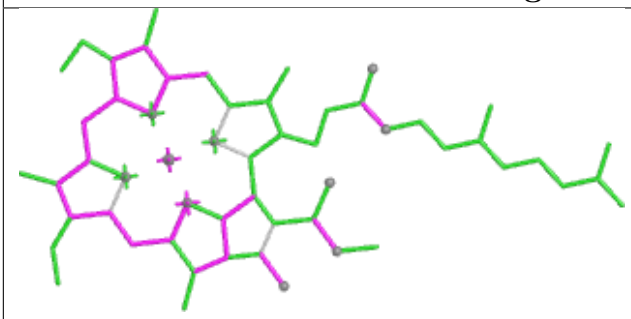


Rings

Ligand CLA B 813



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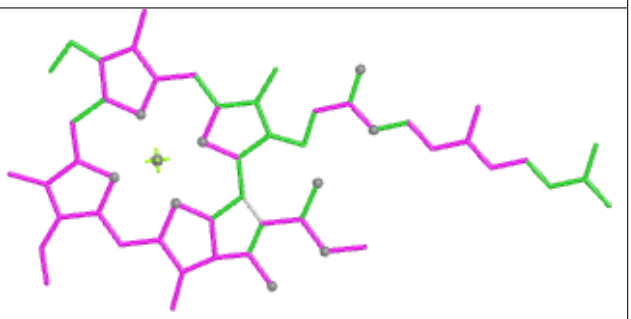

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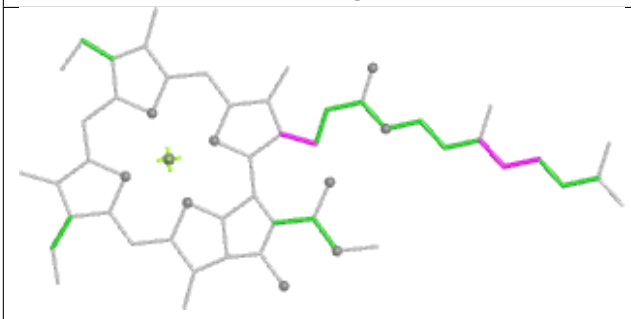

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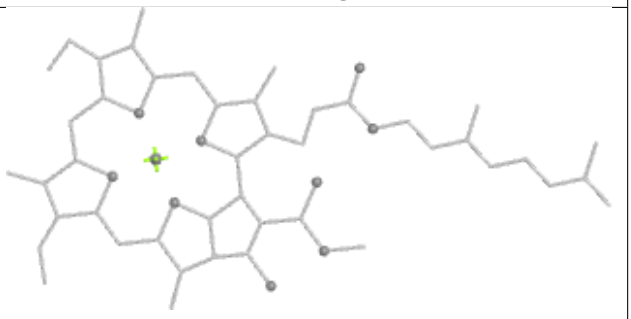
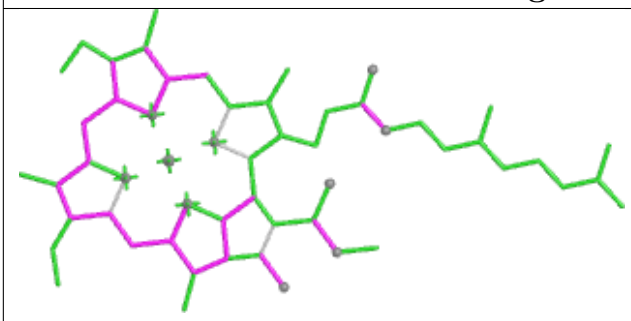


Rings

Ligand CLA 2 307



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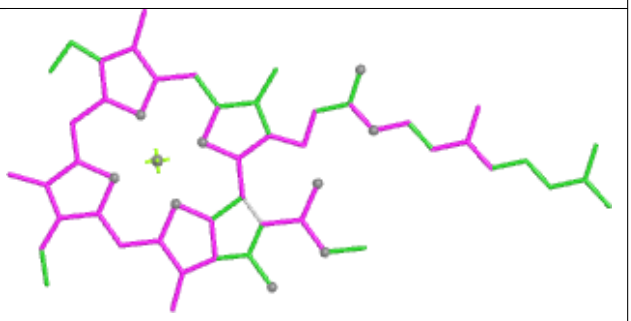

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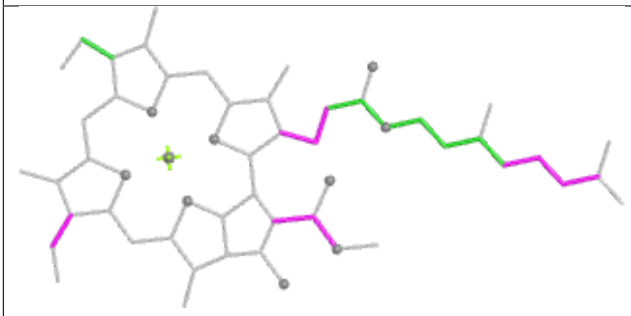

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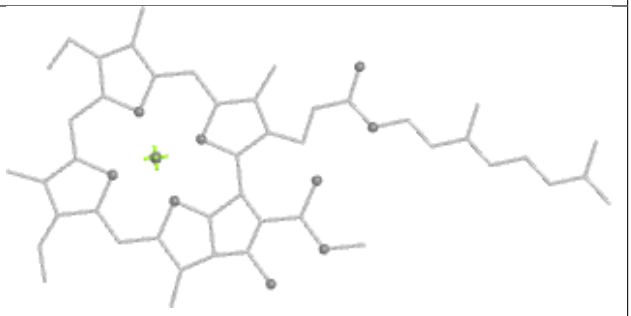
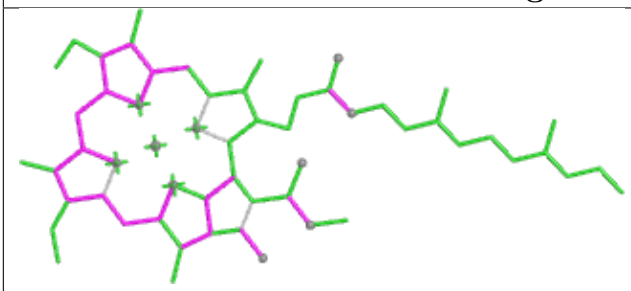
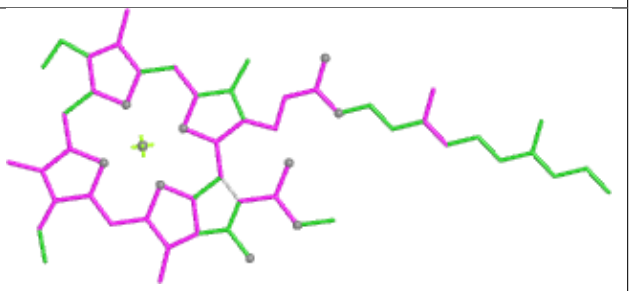
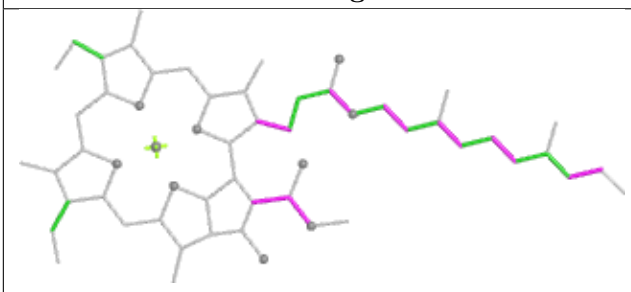
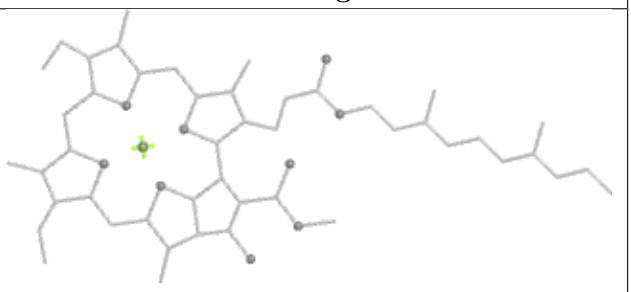
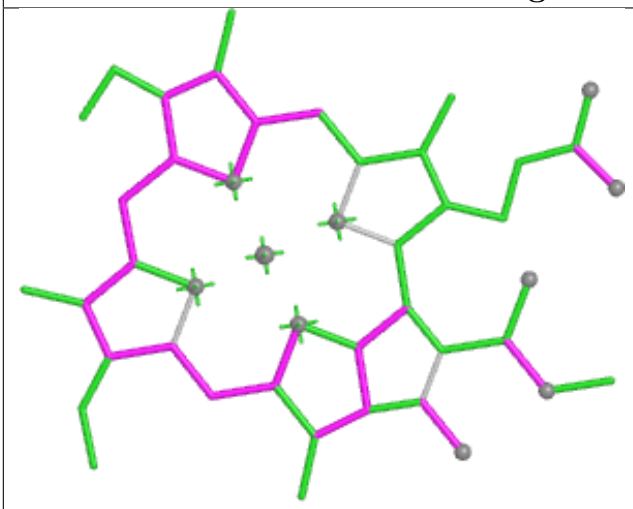


Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 306



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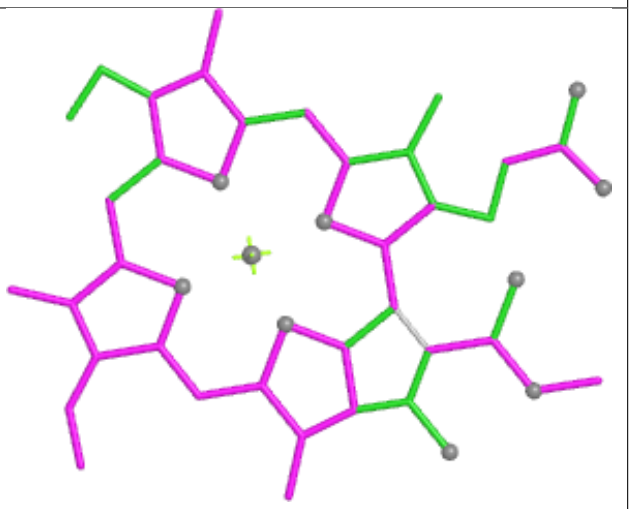

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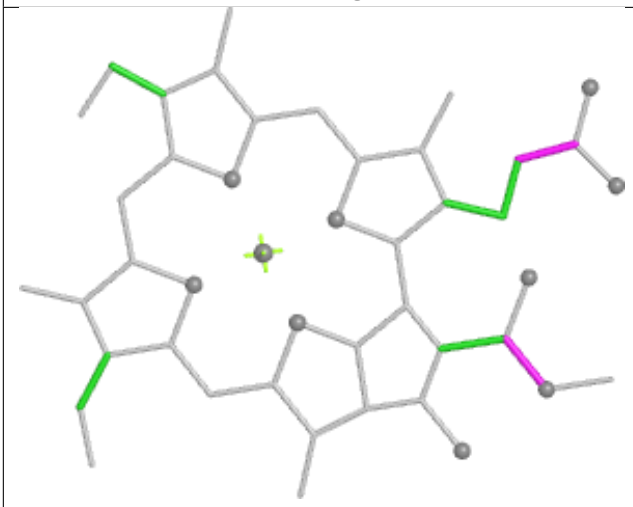
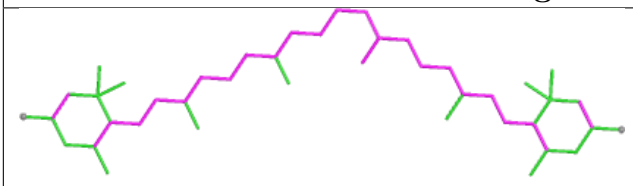


Torsions

Rings

Ligand 5X6 3 316



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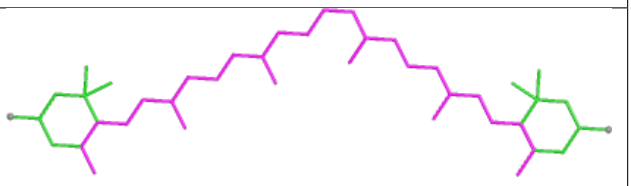
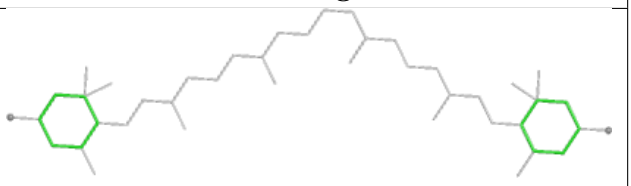


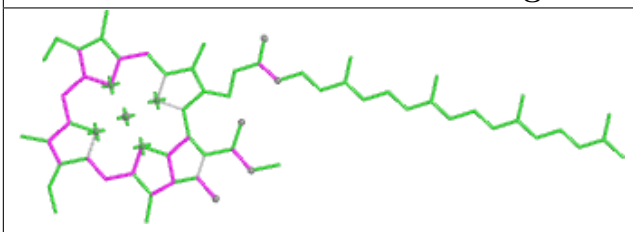
Bond angles

Torsions



Rings

Ligand CLA A 837



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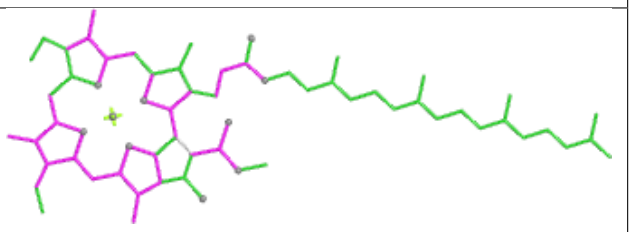

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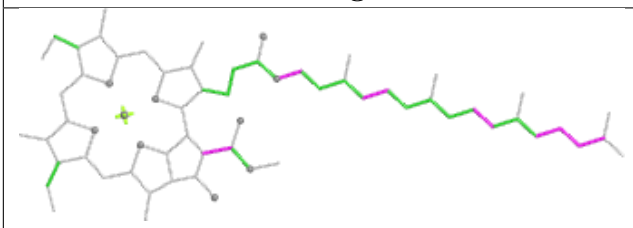

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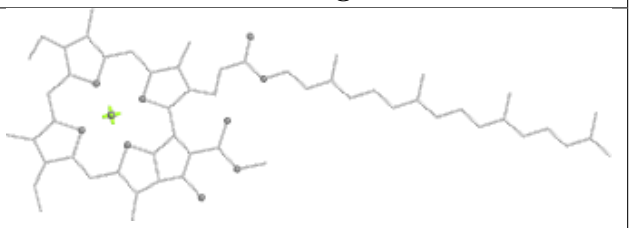
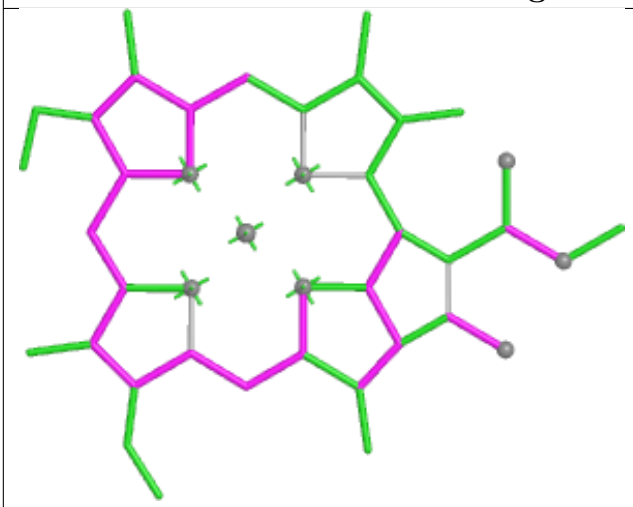


Rings

Ligand CLA 1 308



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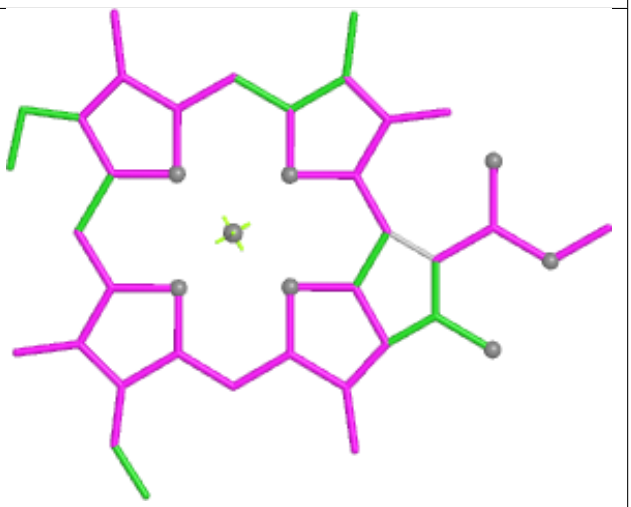

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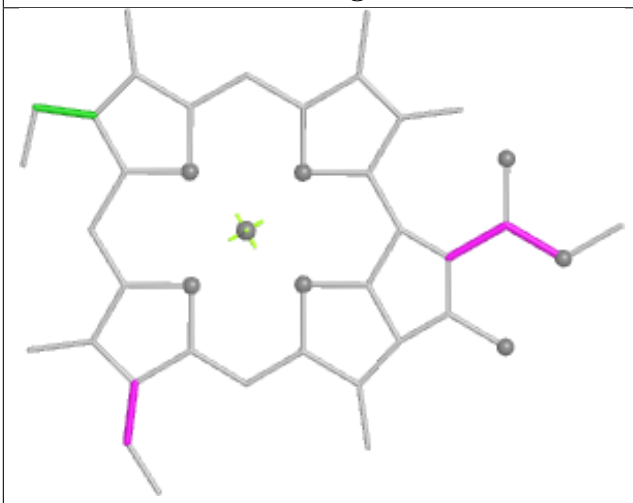

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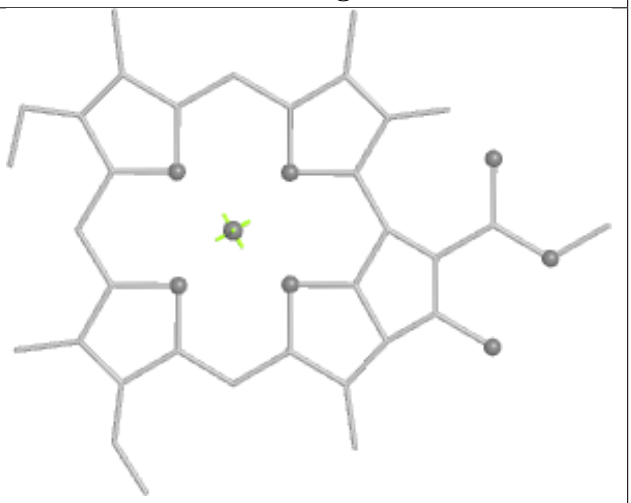
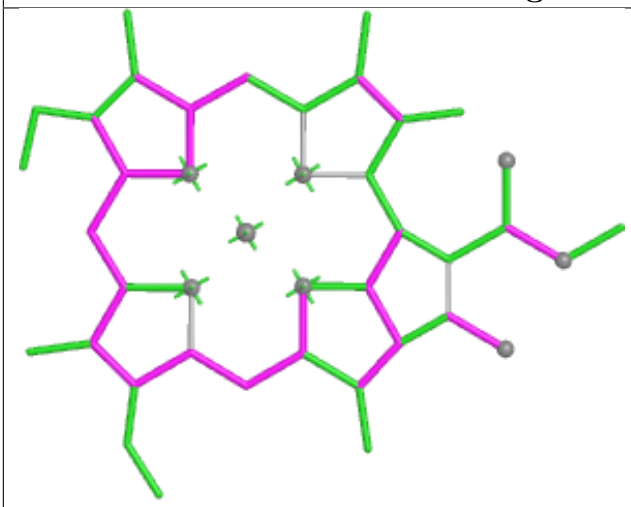


Rings

Ligand CLA F 204



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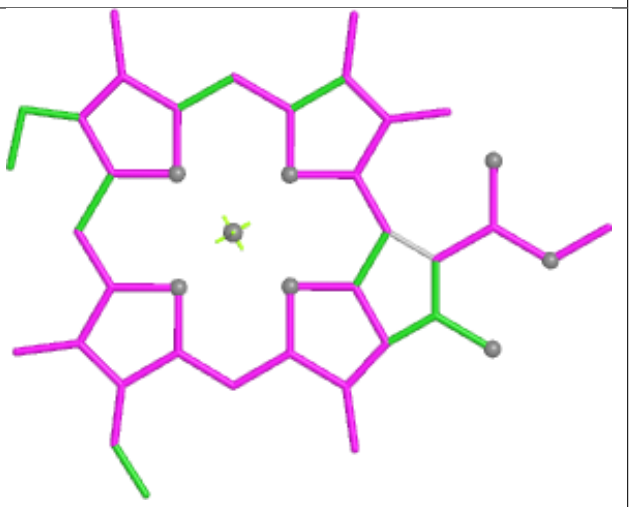

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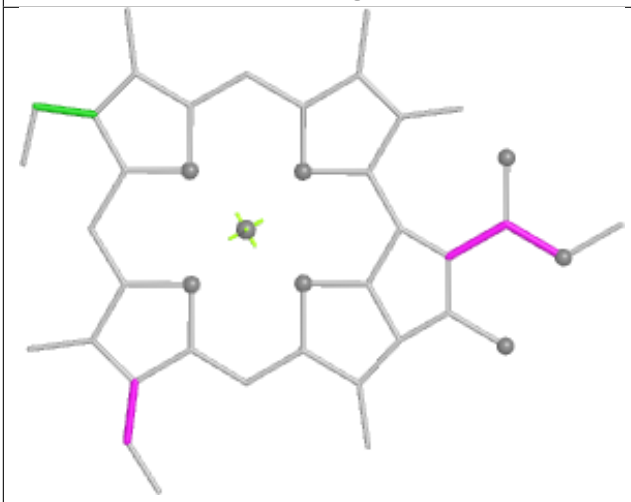

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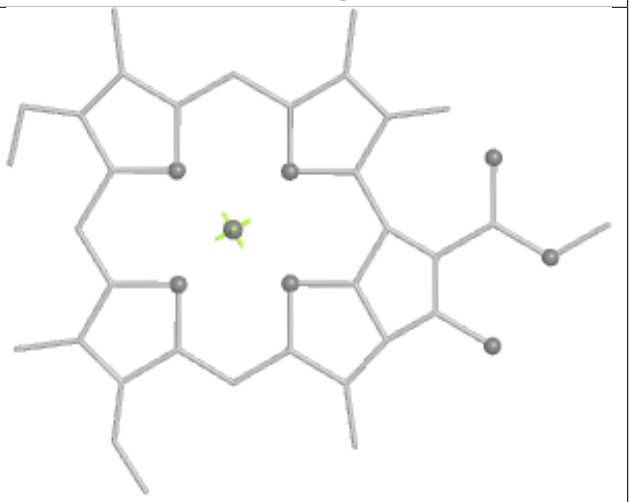
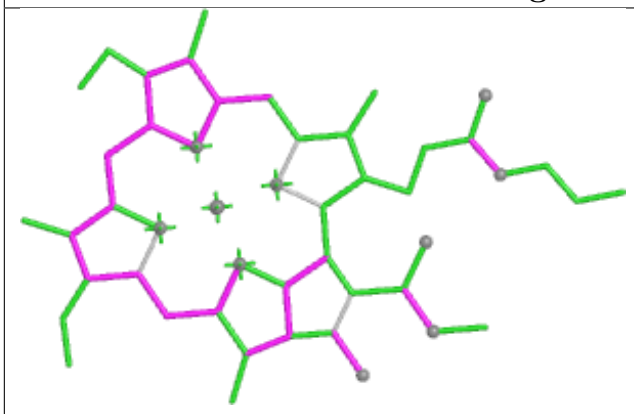


Rings

Ligand CLA 4 303



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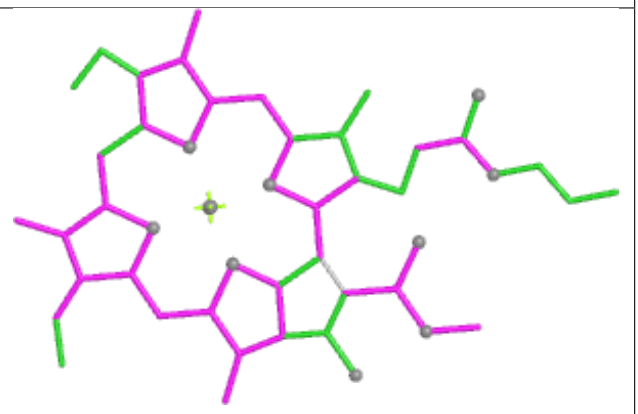
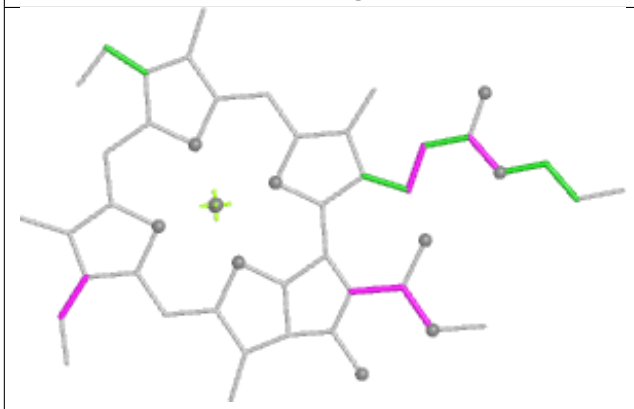


Bond angles



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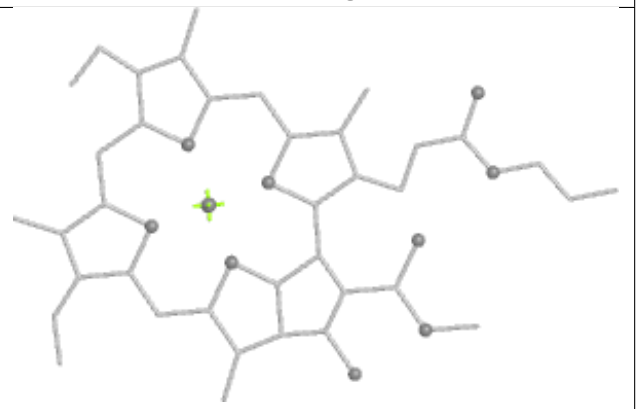
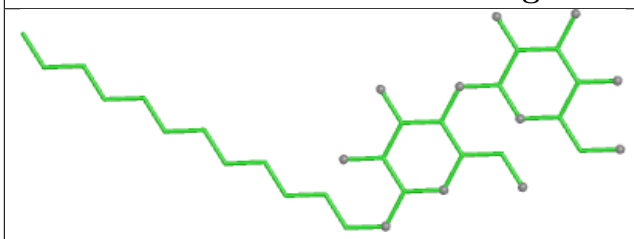


Rings

Ligand LMT B 852



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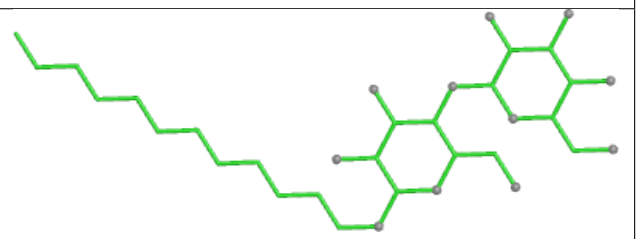
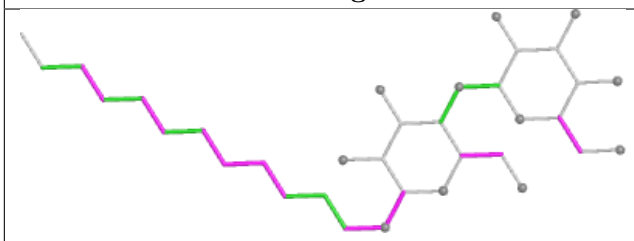
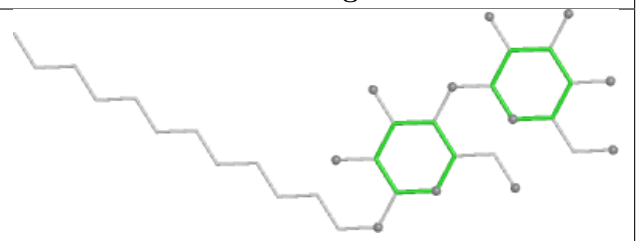


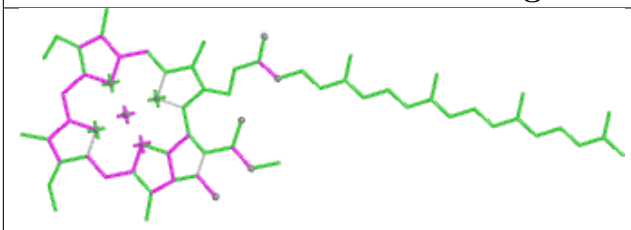
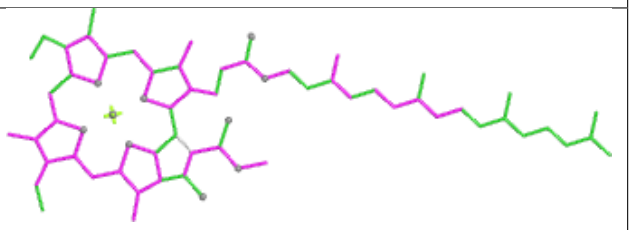
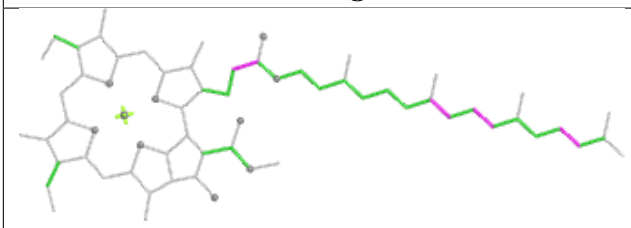
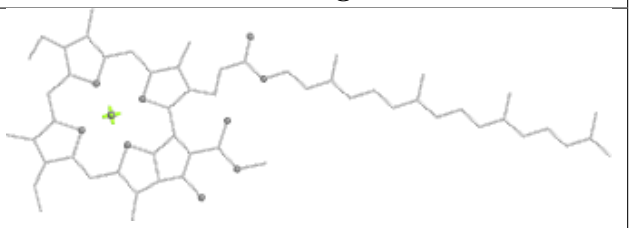
Bond angles

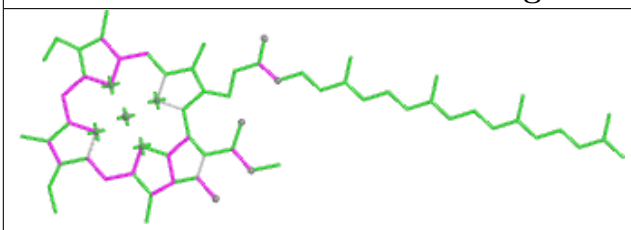
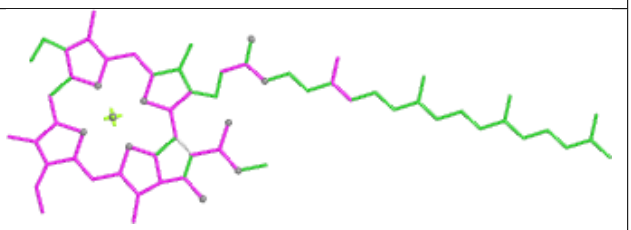
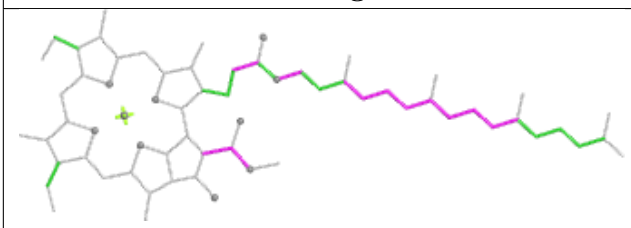
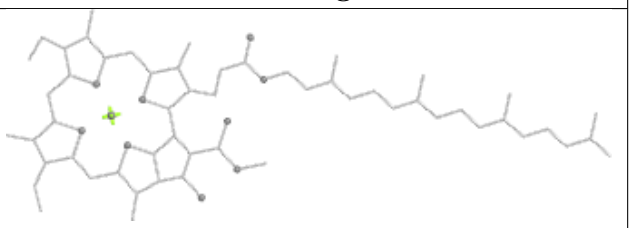


Torsions



Rings

Ligand CLA A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

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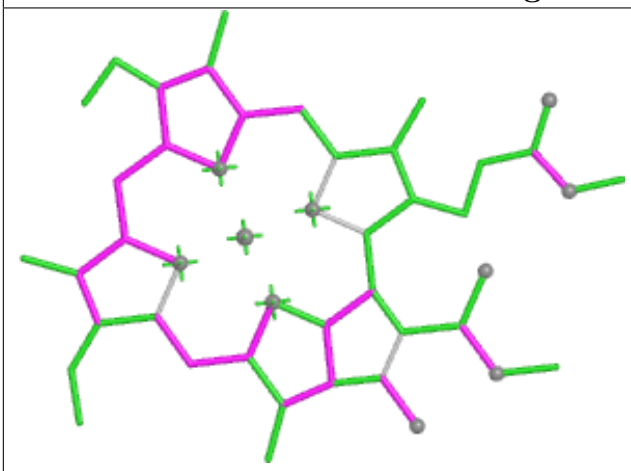
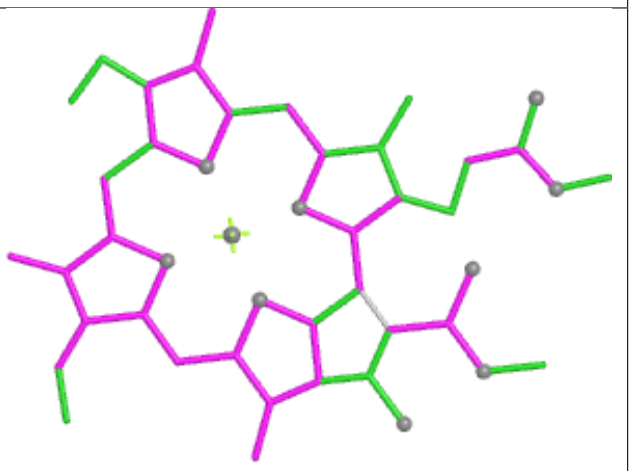
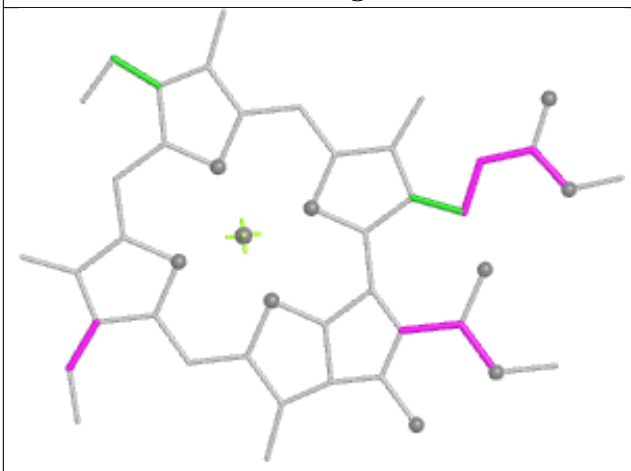
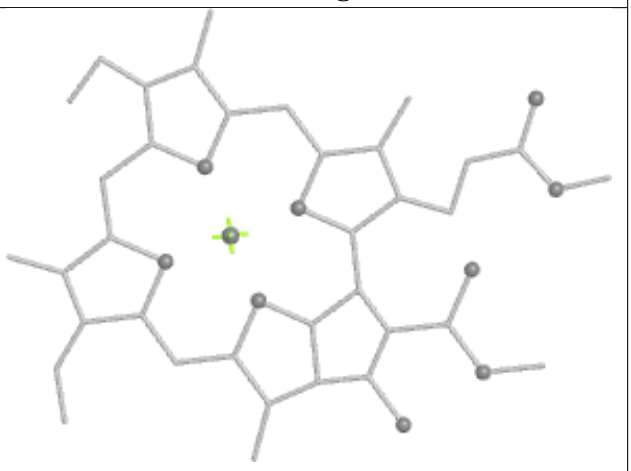
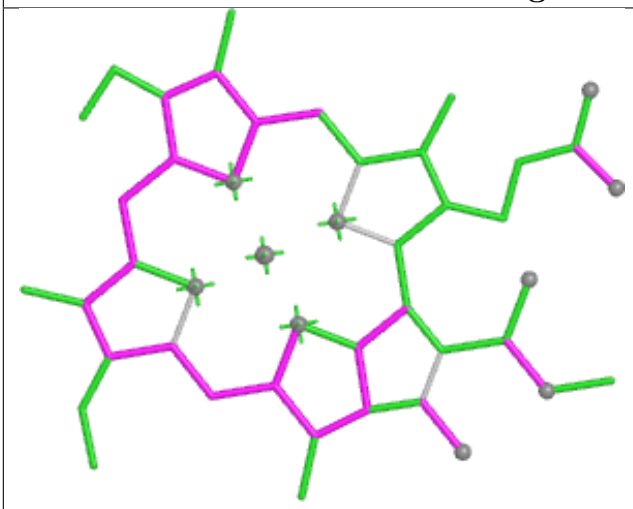
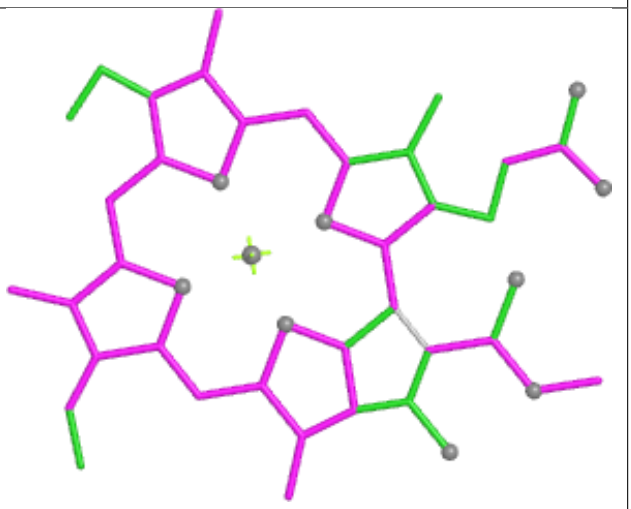
 Bond lengths	 Bond angles
 Torsions	 Rings

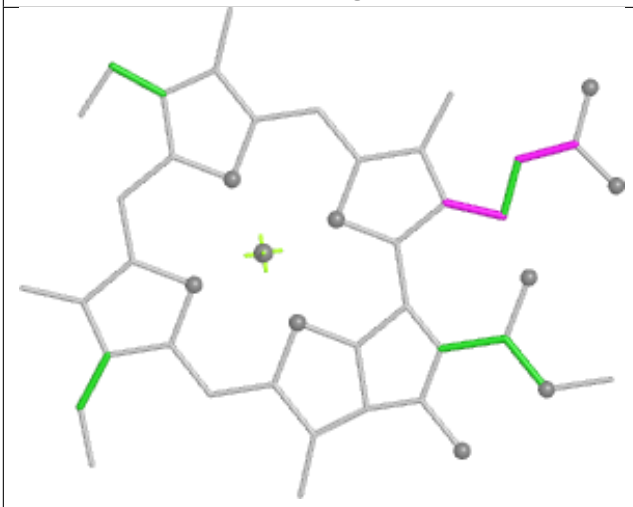
Ligand CLA 4 310



Bond lengths



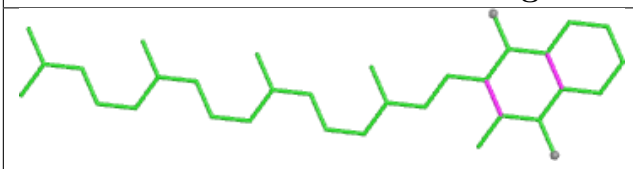
Bond angles



Torsions

Rings

Ligand PQN A 840



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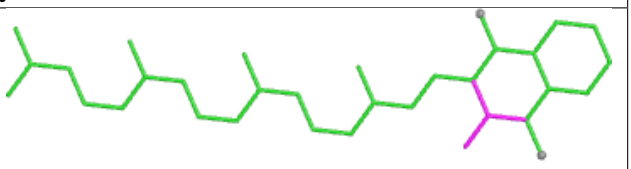
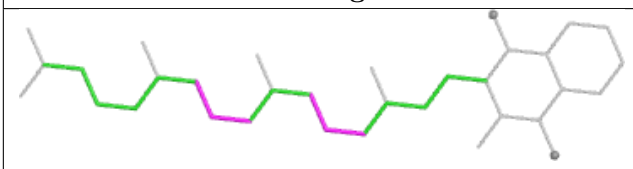


Bond angles



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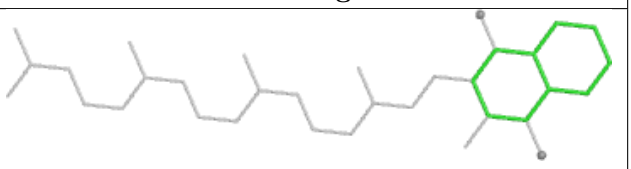
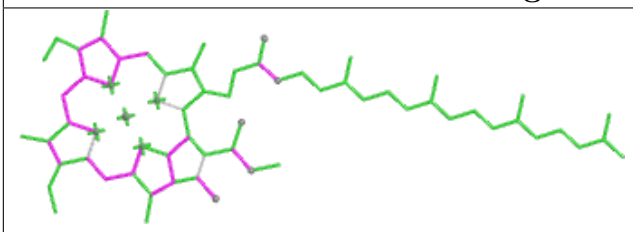


Rings

Ligand CLA A 820



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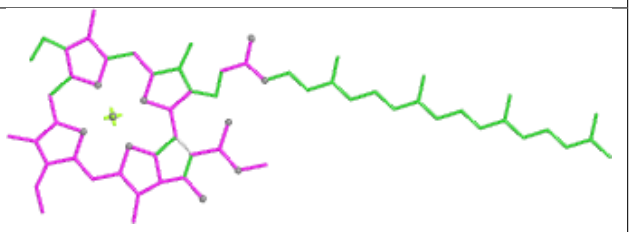
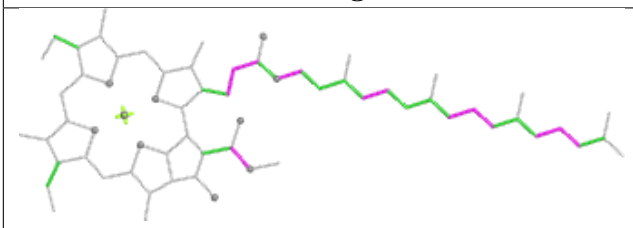


Bond angles



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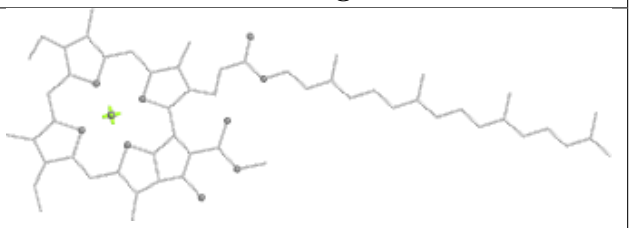
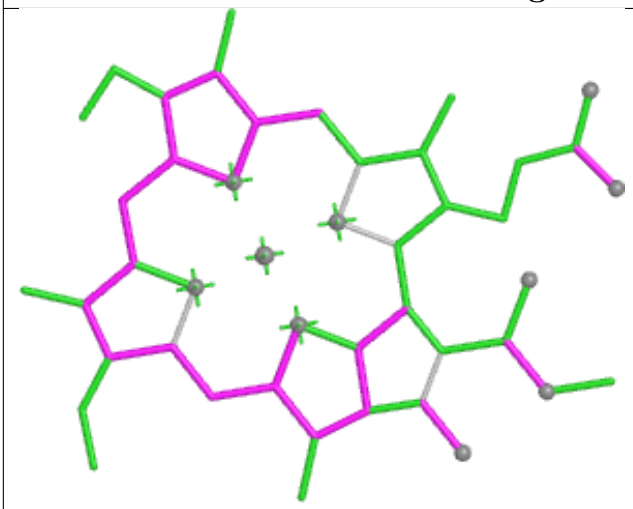


Rings

Ligand CLA 2 308



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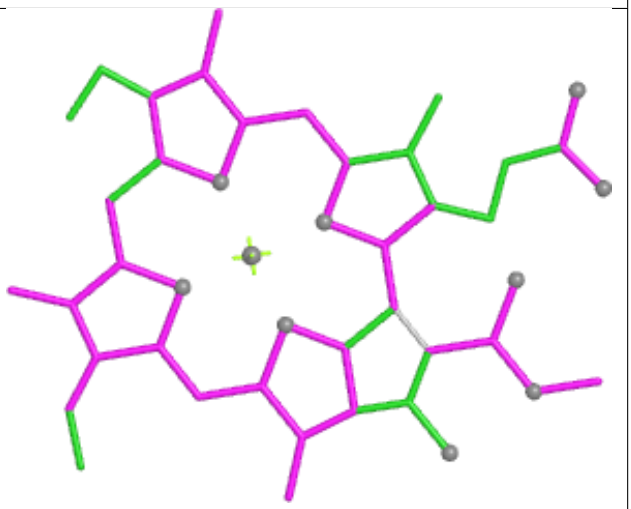

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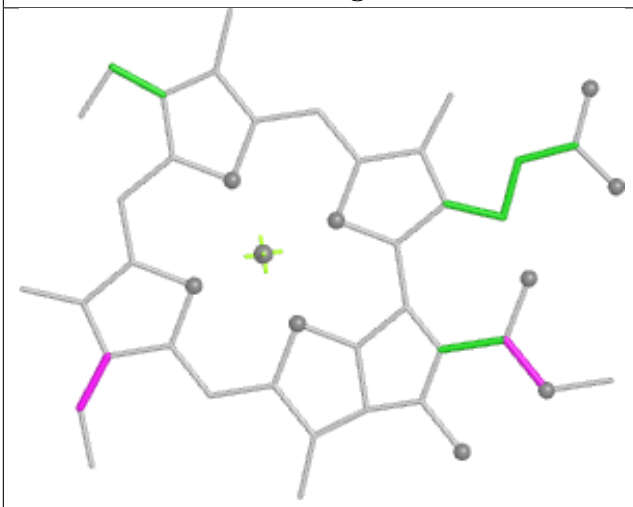

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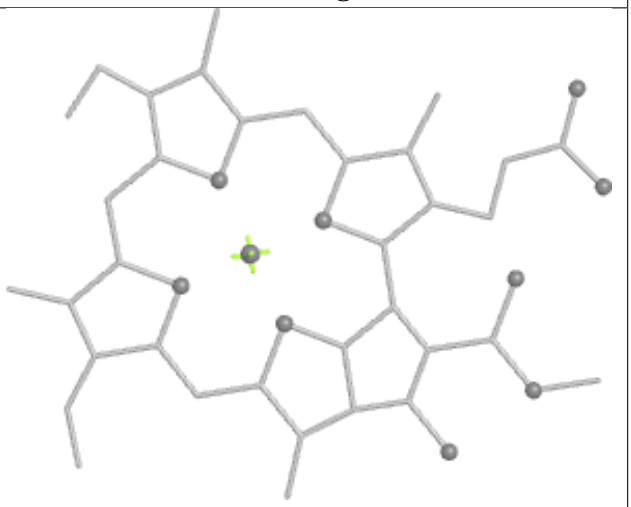
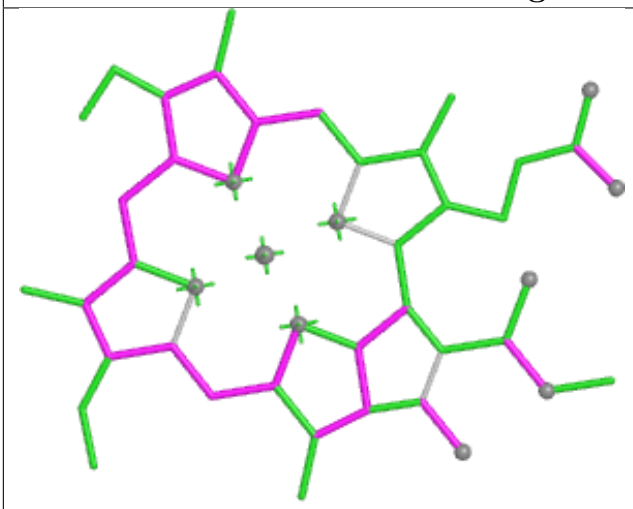


Rings

Ligand CLA 3 306



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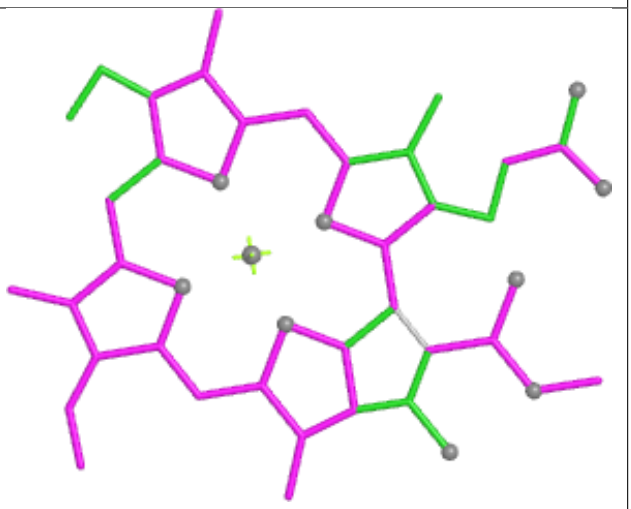

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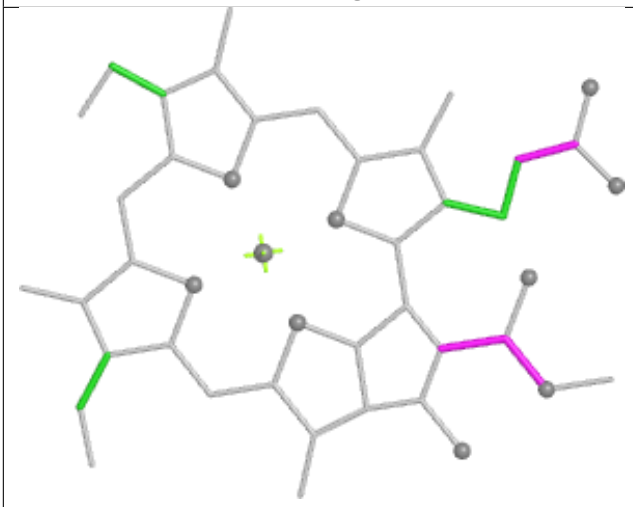
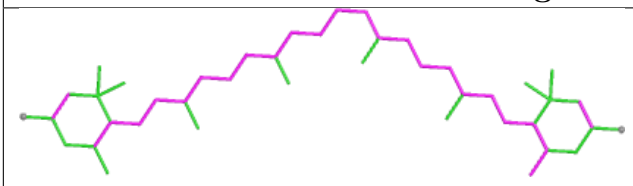


Torsions

Rings

Ligand 5X6 5 301



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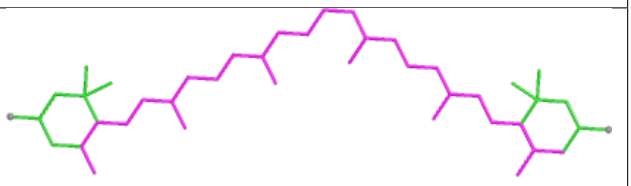

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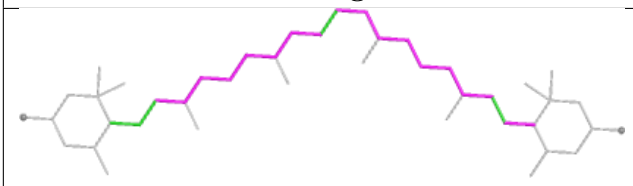

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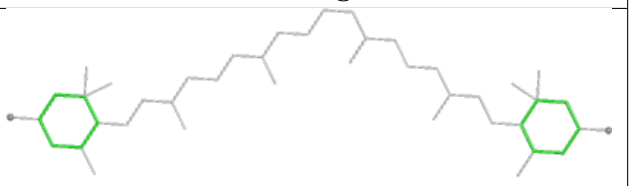
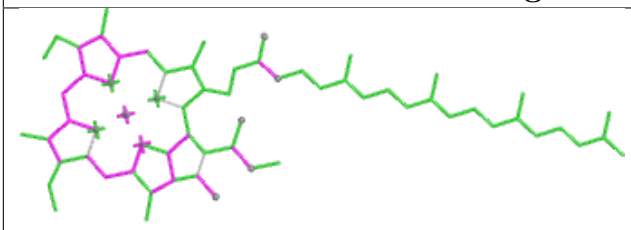


Rings

Ligand CLA B 827



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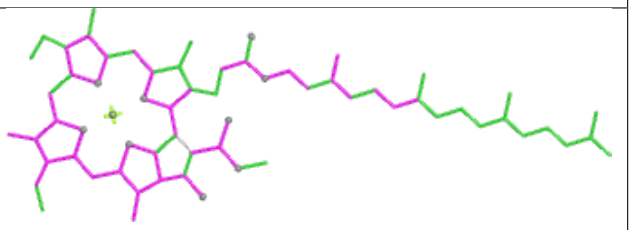
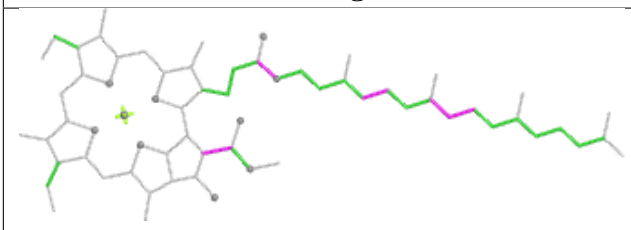


Bond angles



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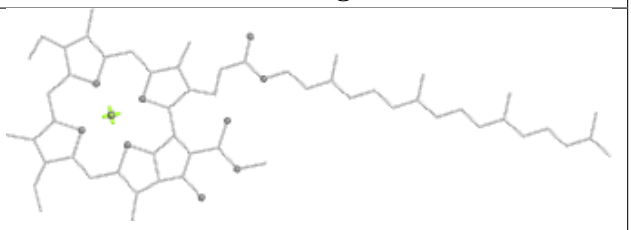
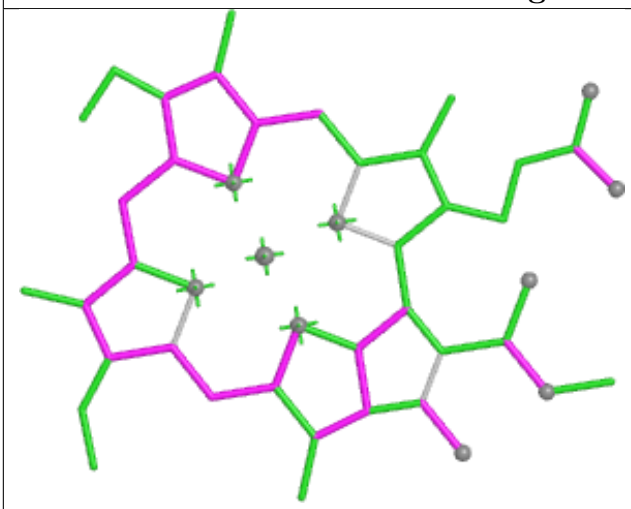


Rings

Ligand CLA 5 312



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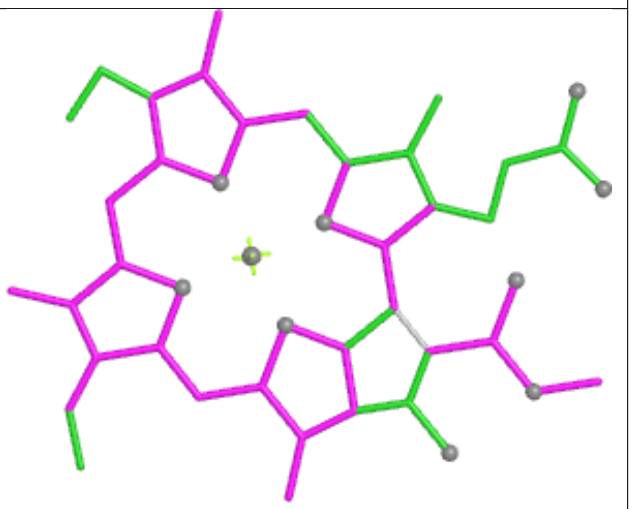
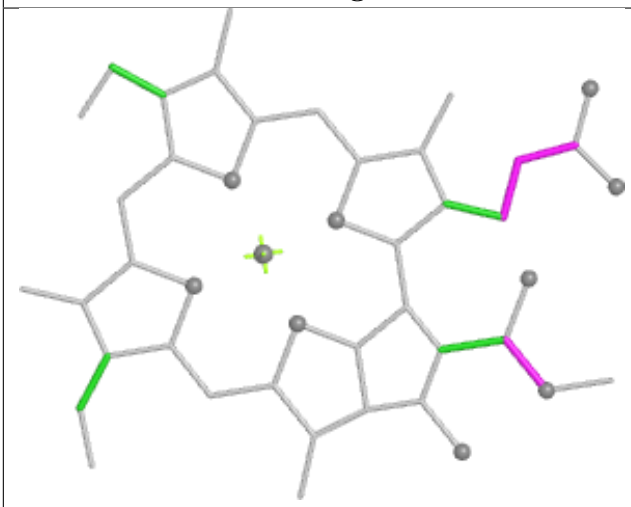


Bond angles



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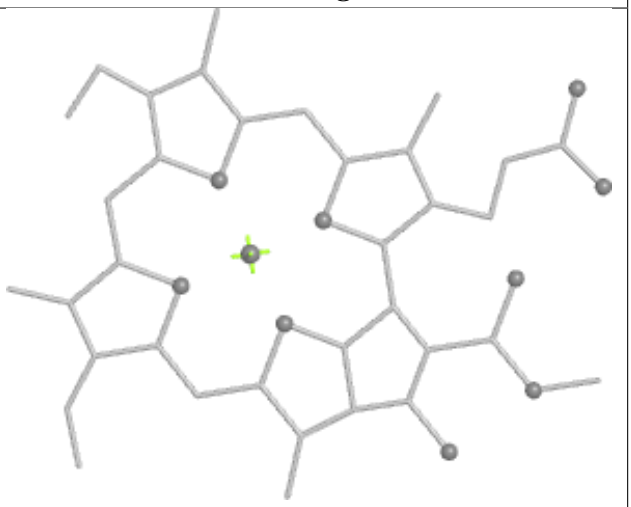
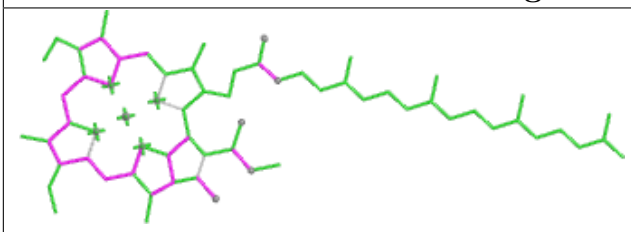
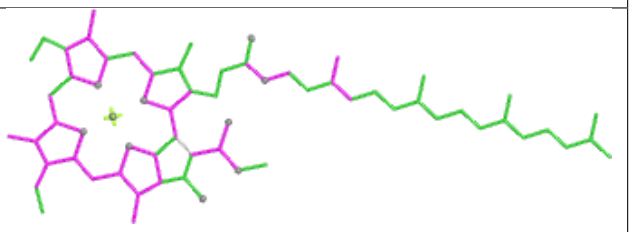
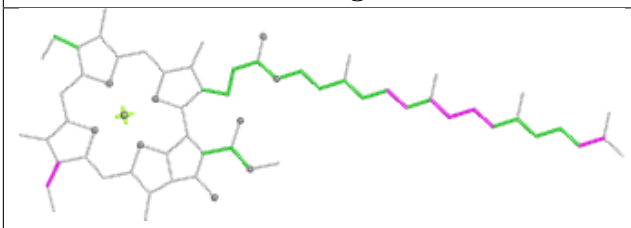
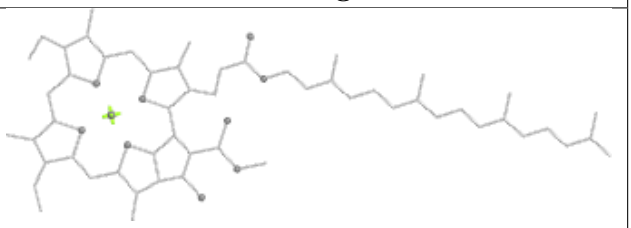
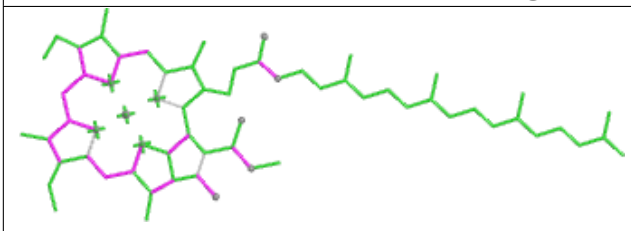
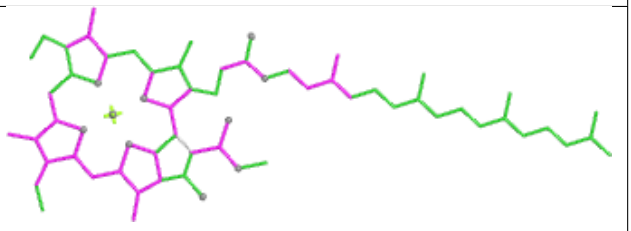
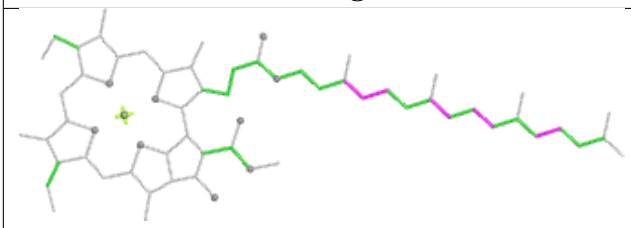
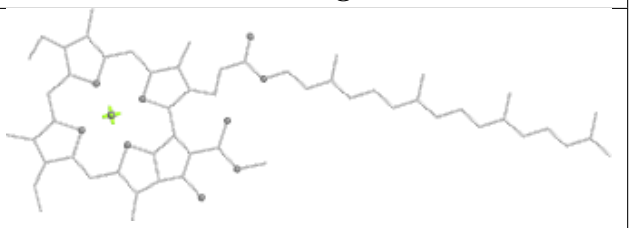
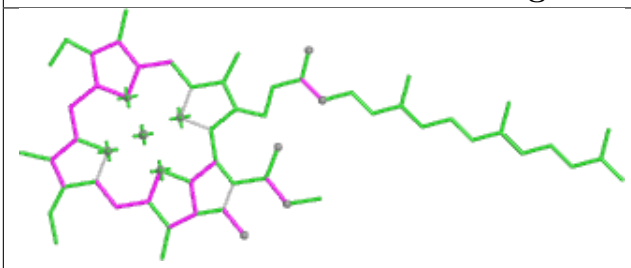
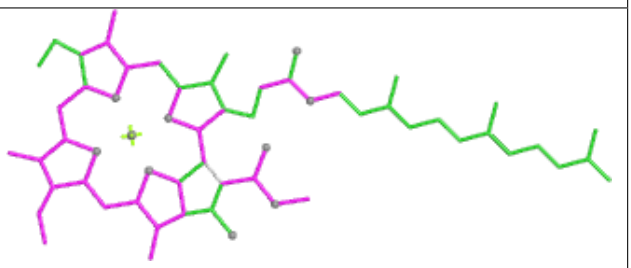
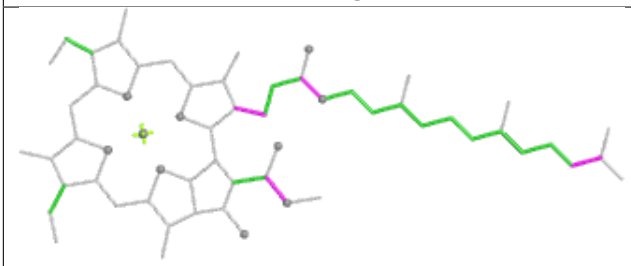
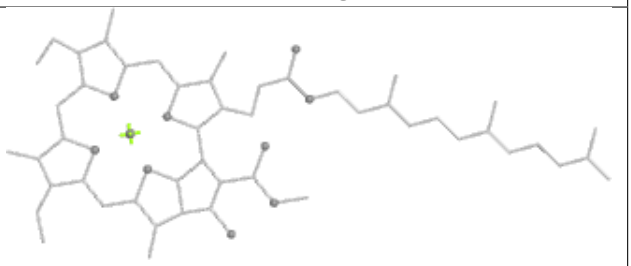
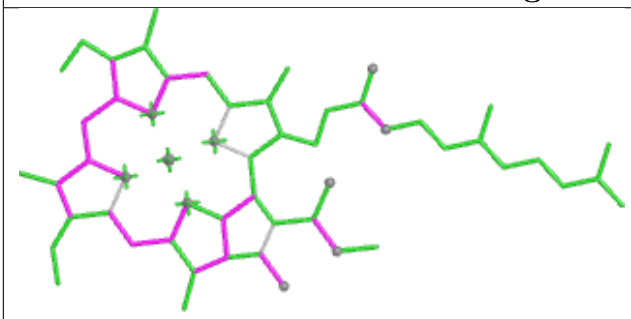
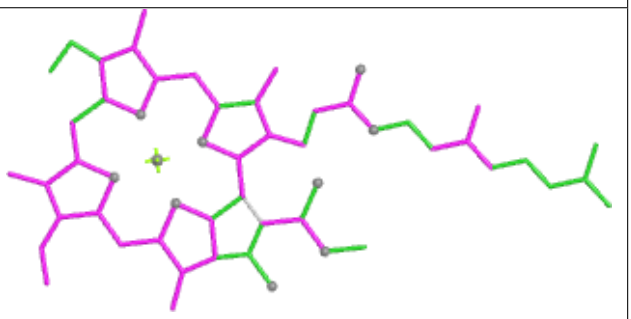
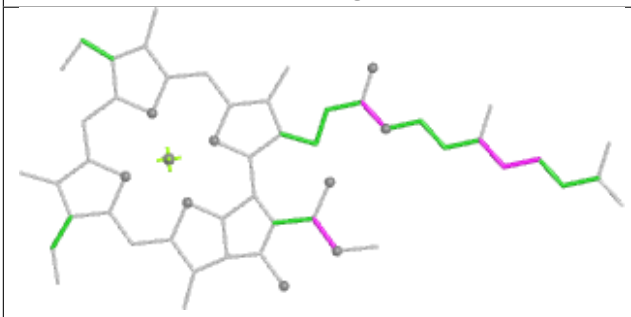
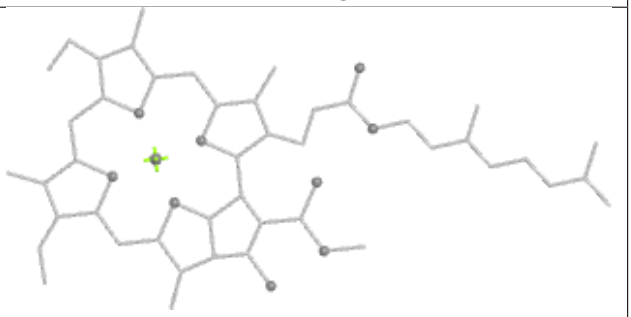


Rings

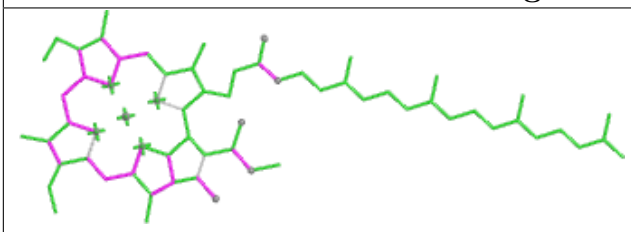
Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 806



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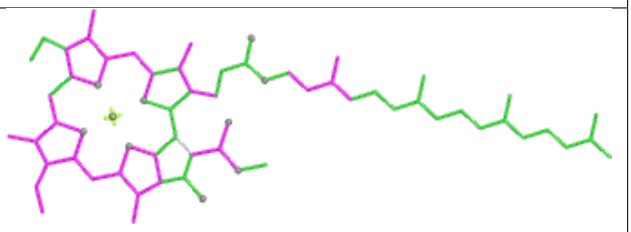

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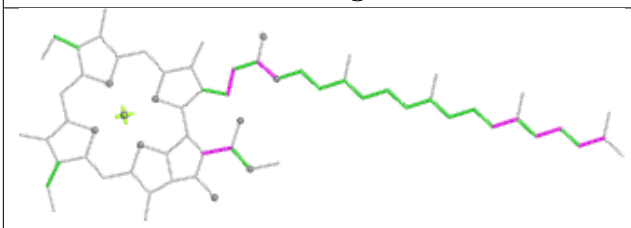
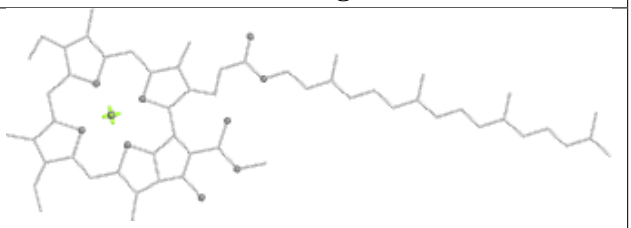
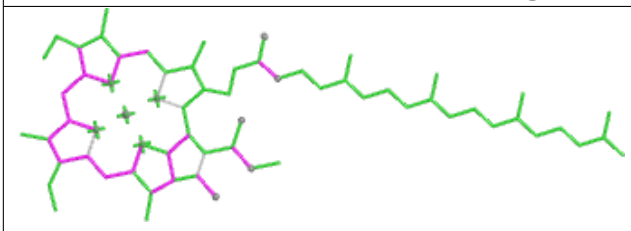


Torsions



Rings

Ligand CLA A 816



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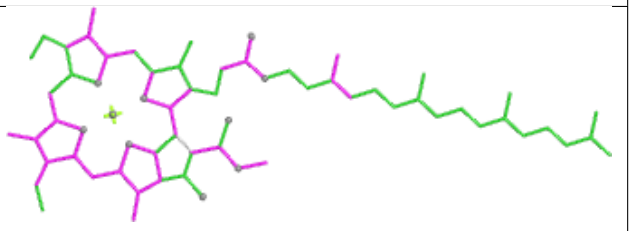

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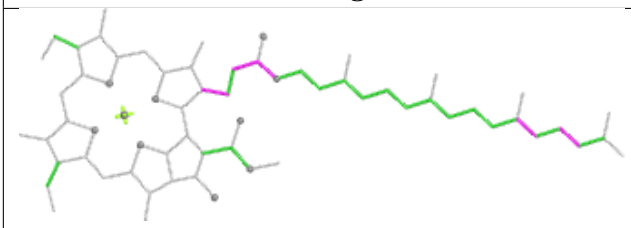

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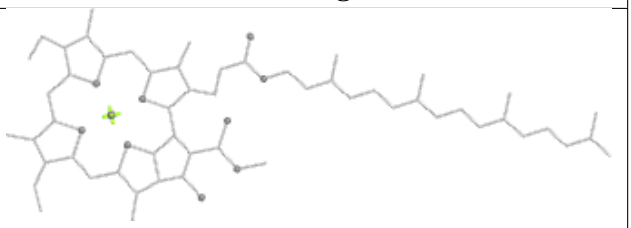
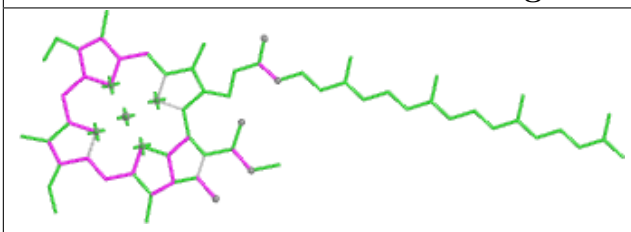


Rings

Ligand CLA B 831



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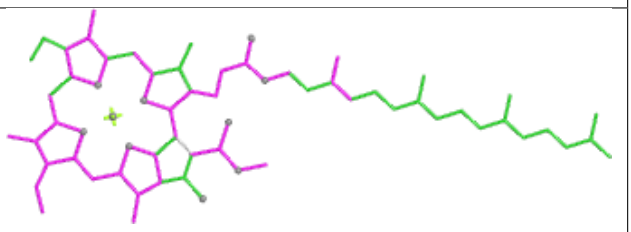

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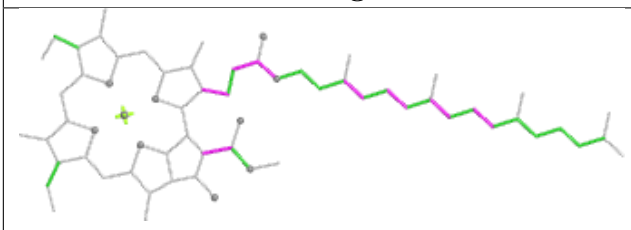

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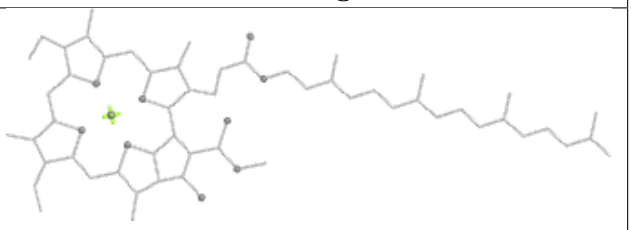
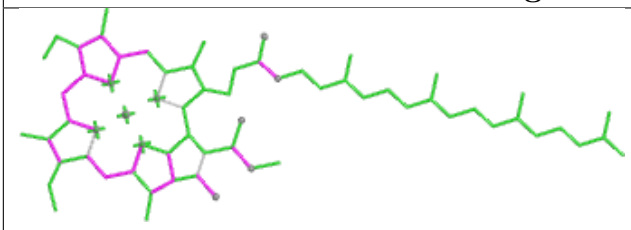


Rings

Ligand CLA B 830



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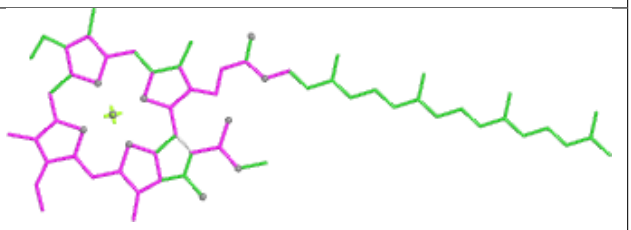

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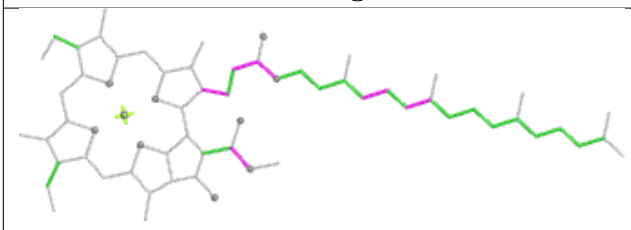

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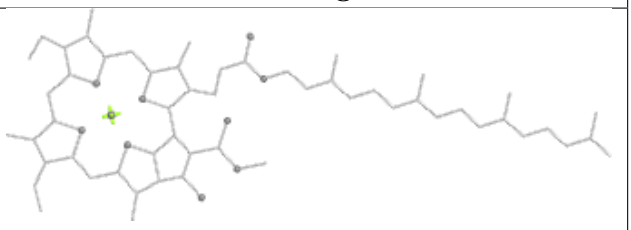
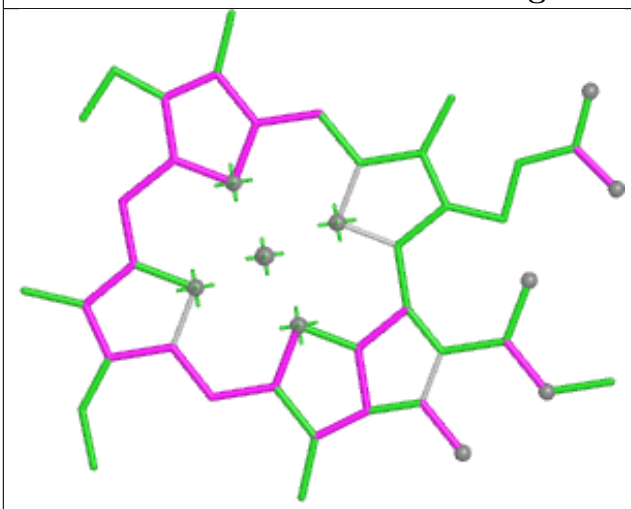


Rings

Ligand CLA 2 309



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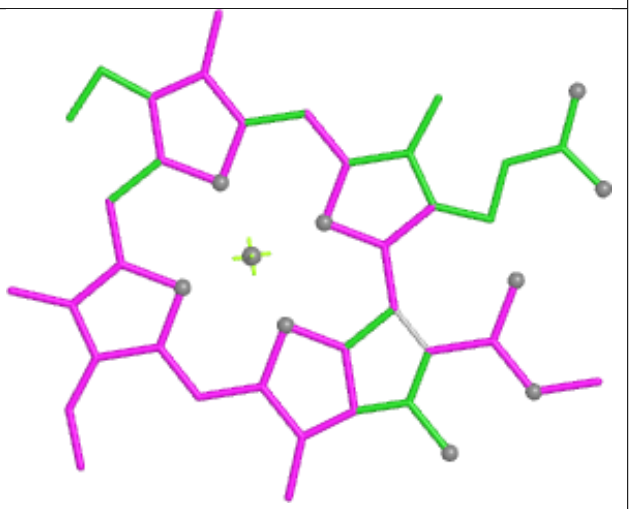

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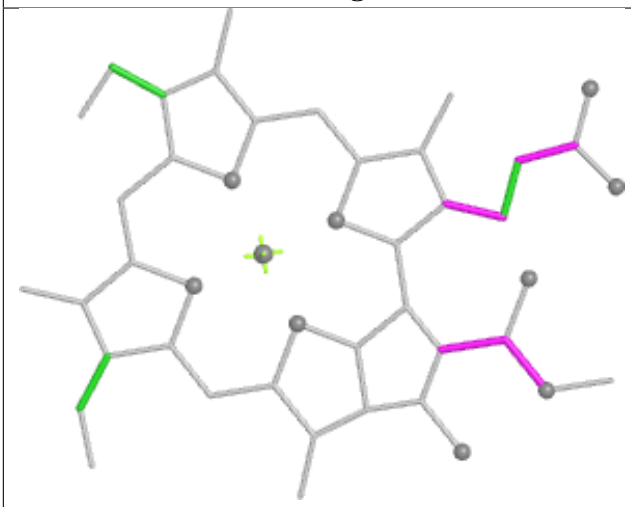

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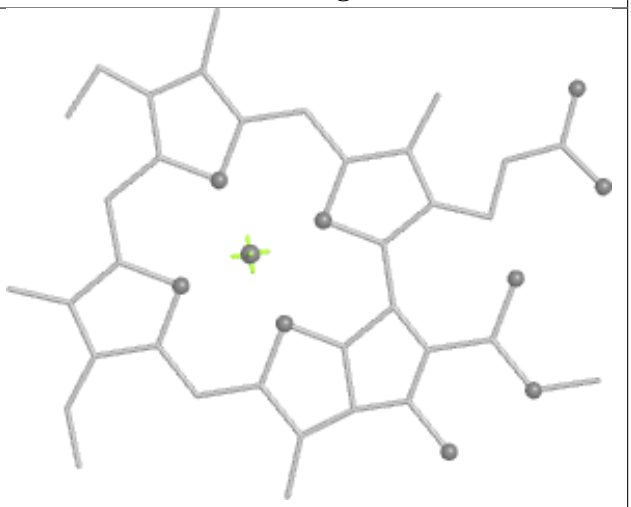
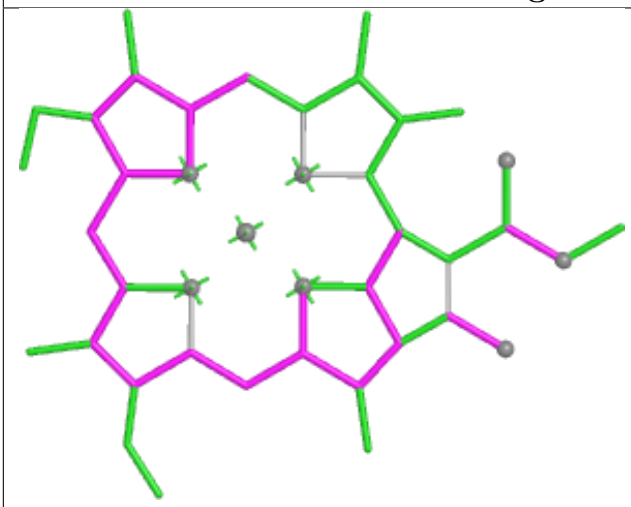


Rings

Ligand CLA 3 312



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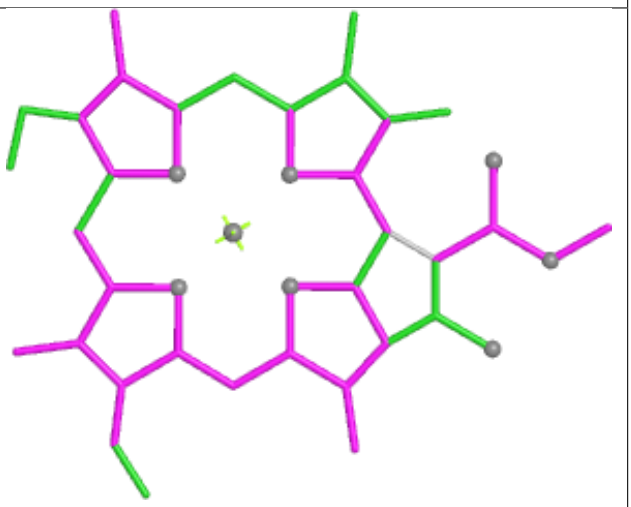

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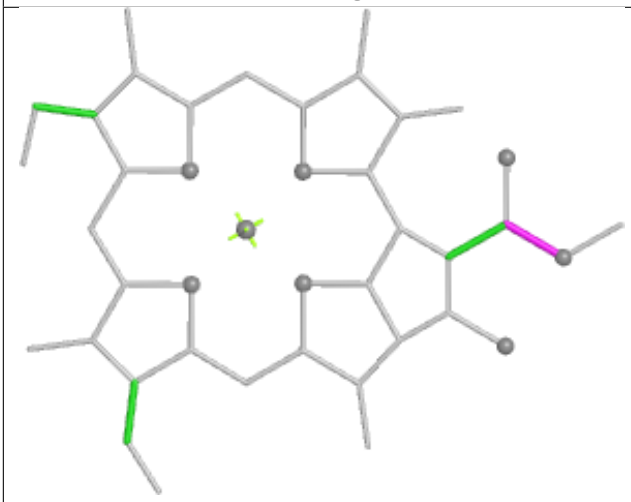

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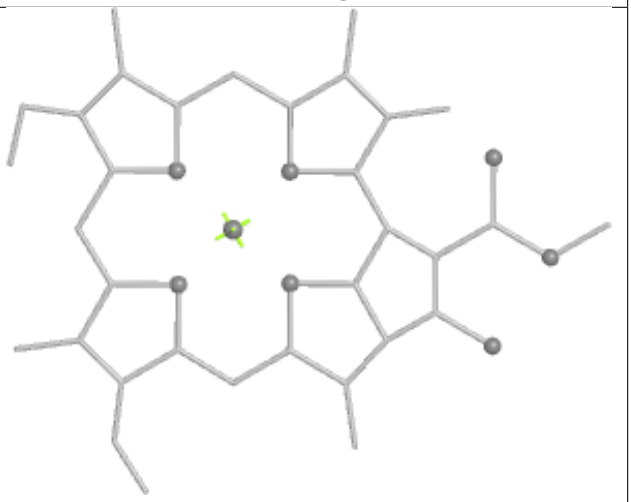
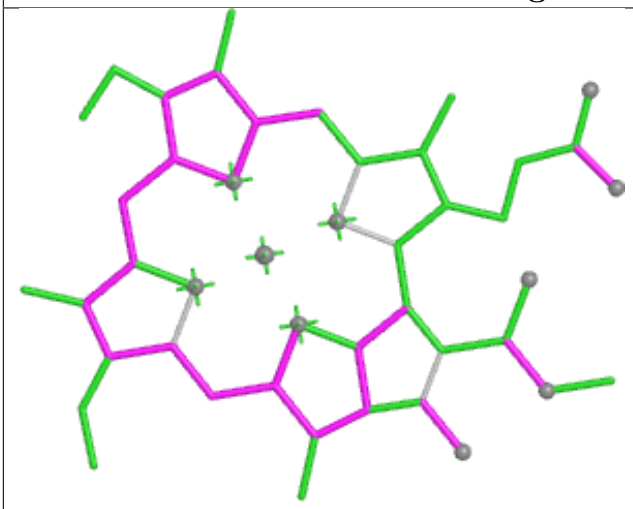


Rings

Ligand CLA 5 306



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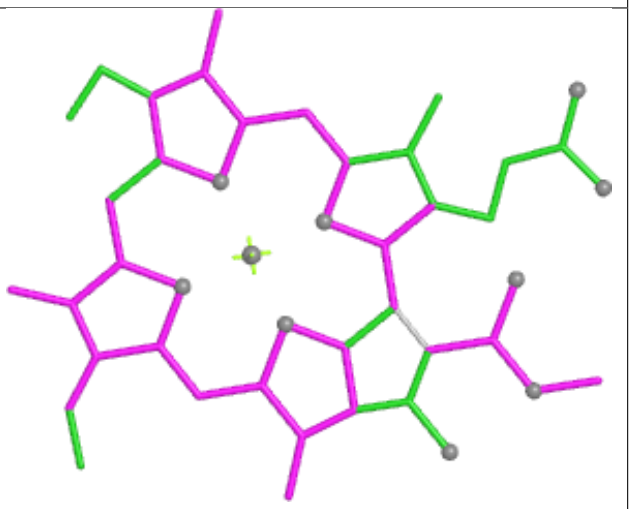

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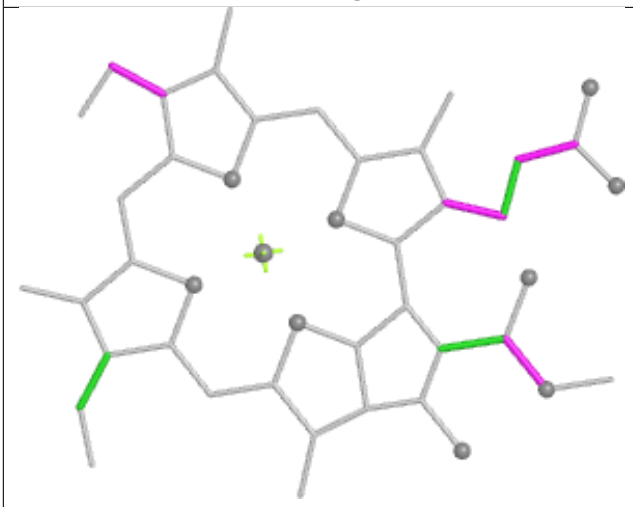
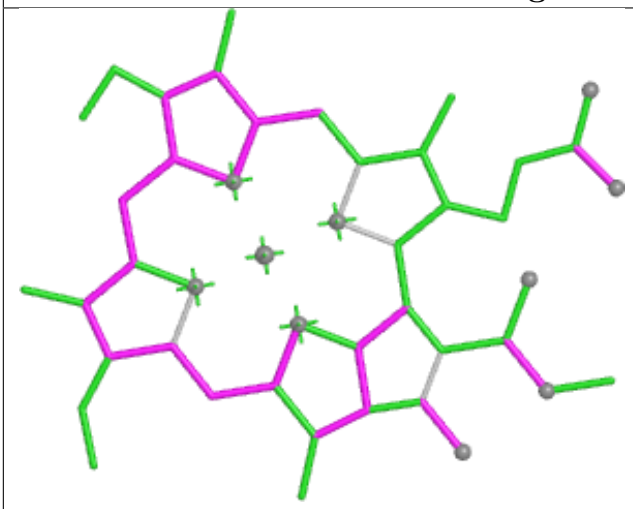


Torsions

Rings

Ligand CLA 4 308



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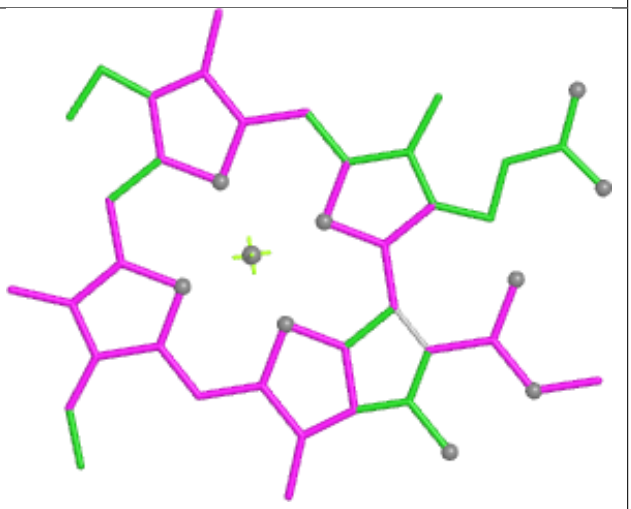

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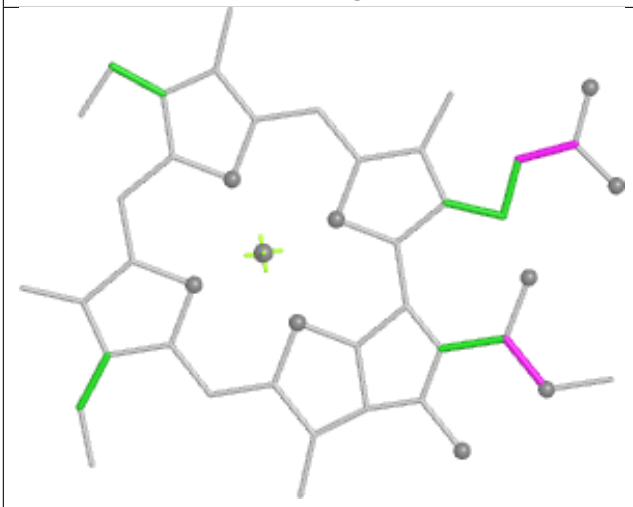
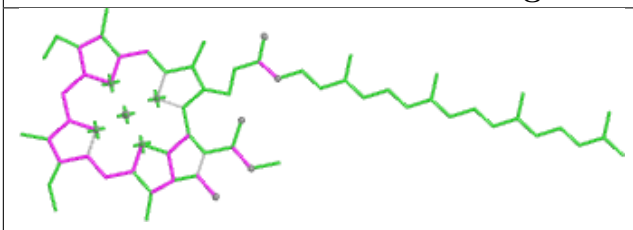


Torsions

Rings

Ligand CLA A 807



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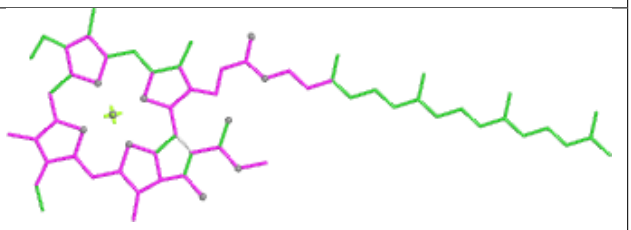

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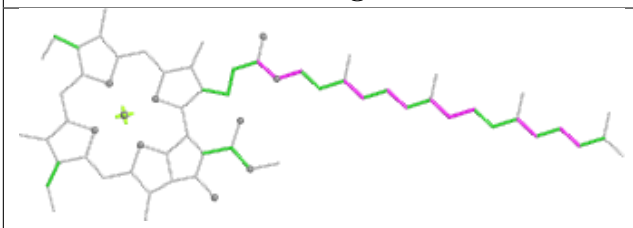

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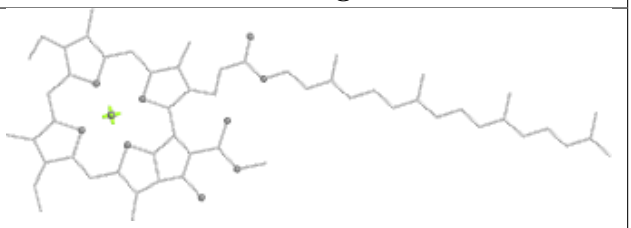
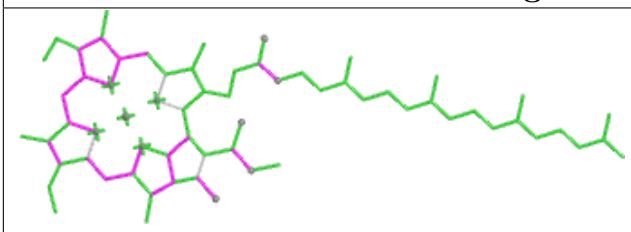


Rings

Ligand CLA A 838



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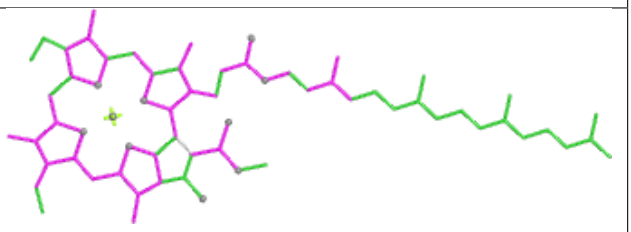

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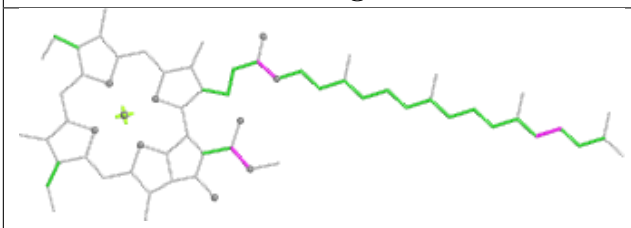

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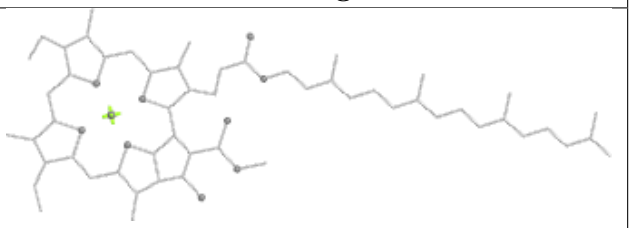
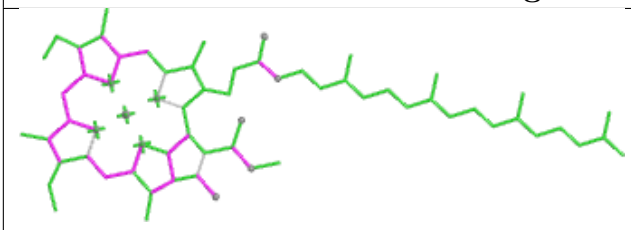


Rings

Ligand CLA A 854



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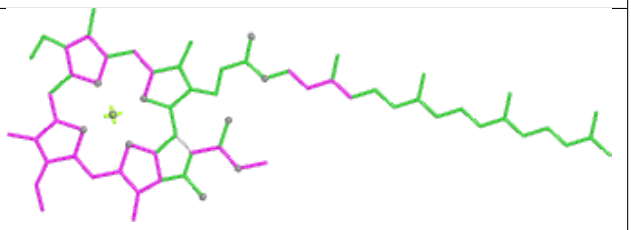

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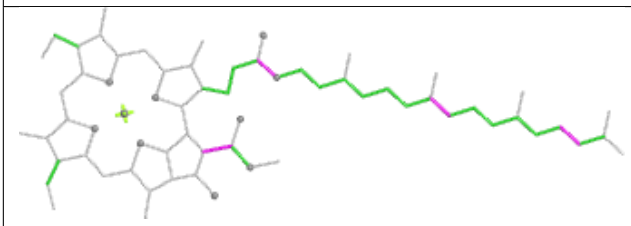

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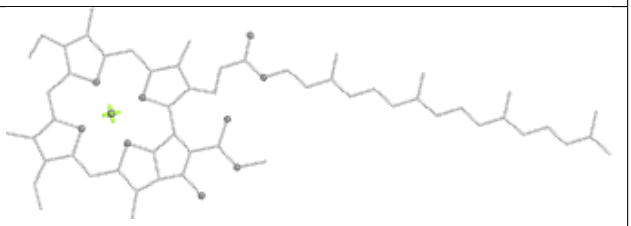
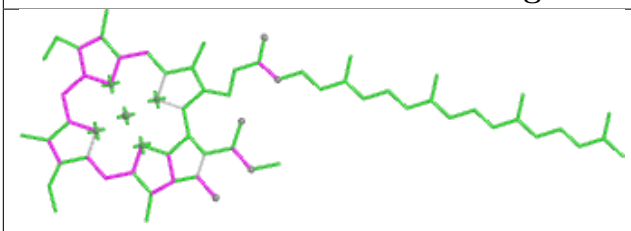


Rings

Ligand CLA A 817



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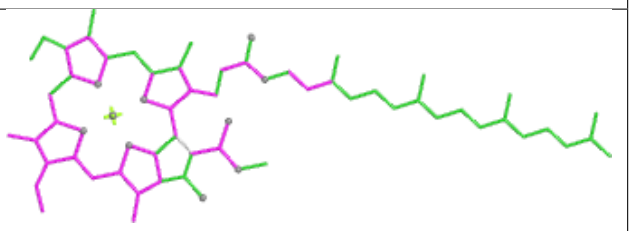
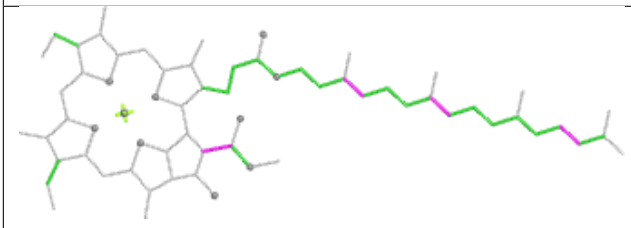


Bond angles



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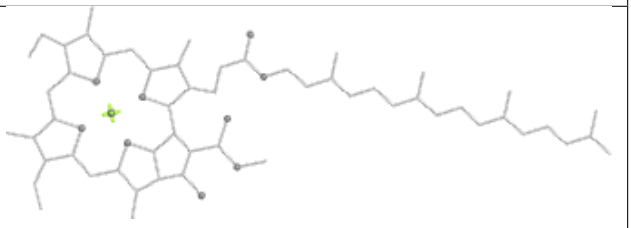
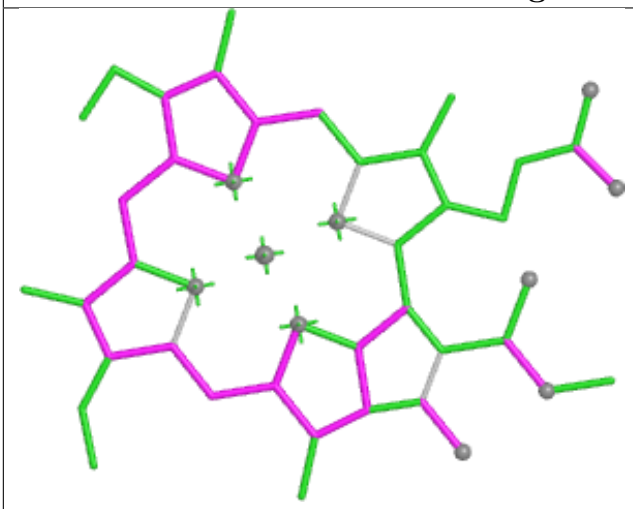


Rings

Ligand CLA 4 306



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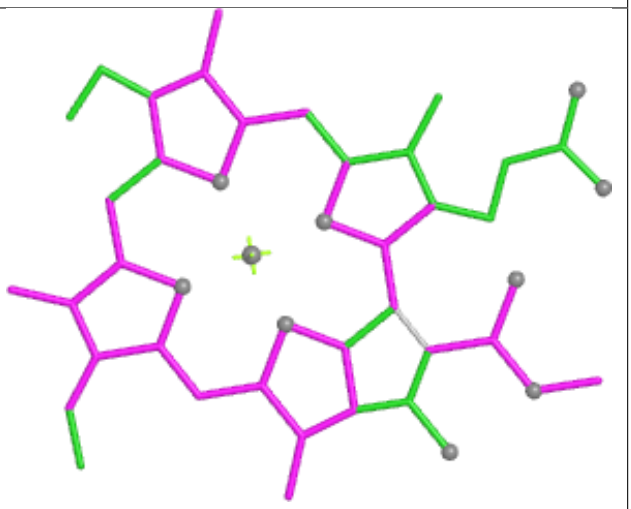
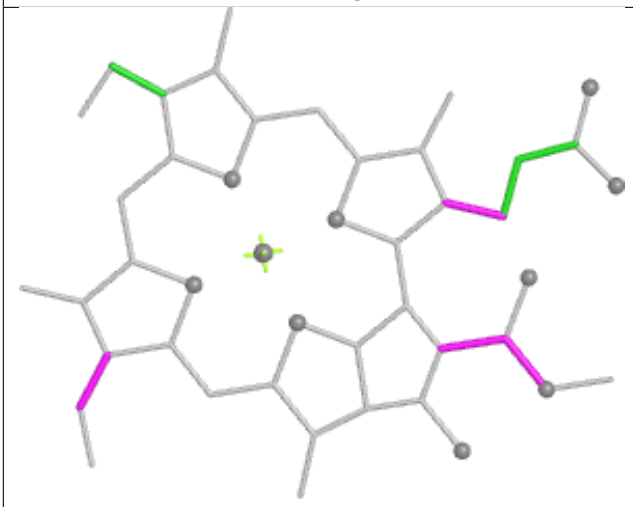


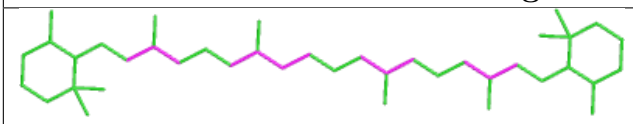
Bond angles



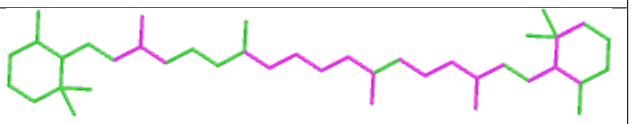
Torsions

Rings

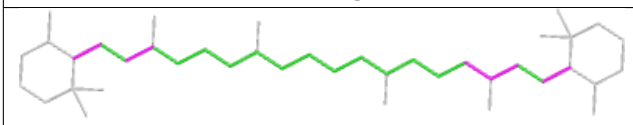
Ligand BCR A 843



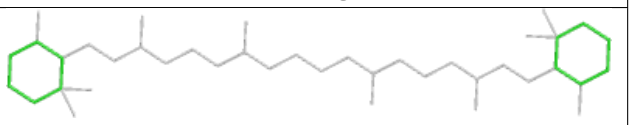
Bond lengths



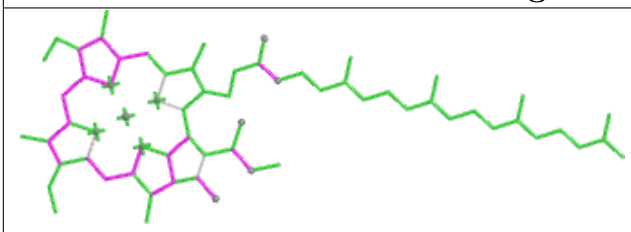
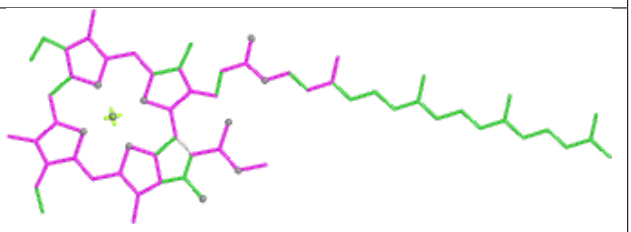
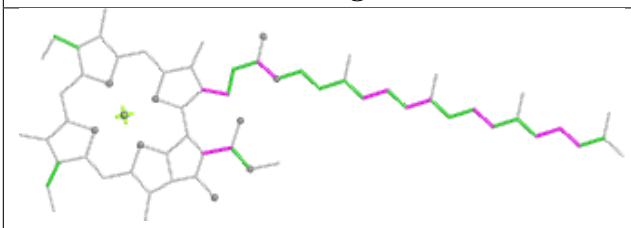
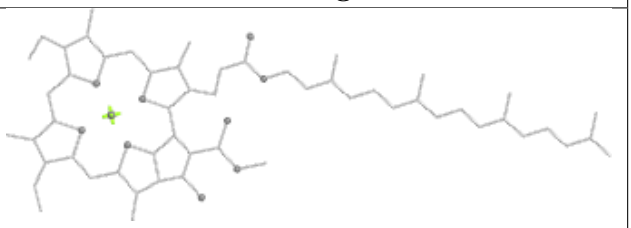
Bond angles

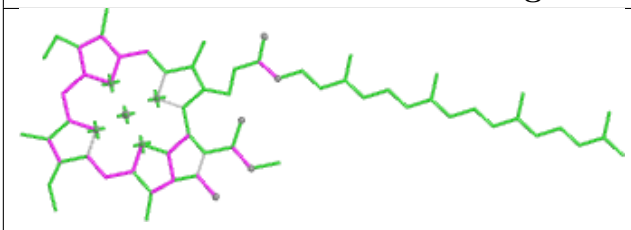
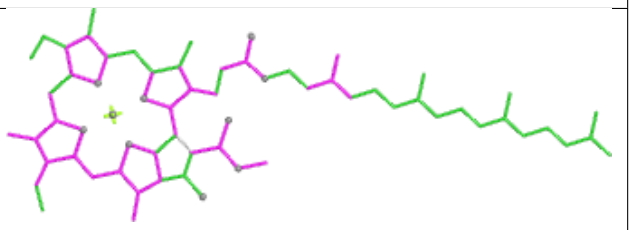
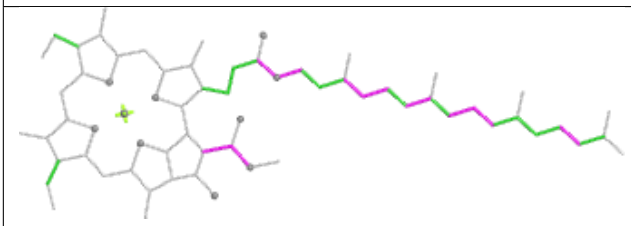
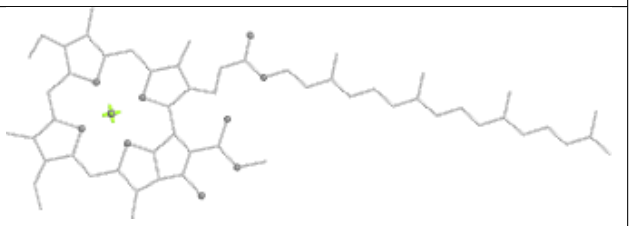


Torsions

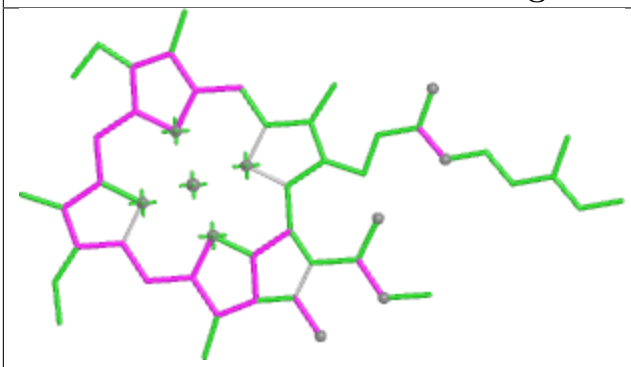


Rings

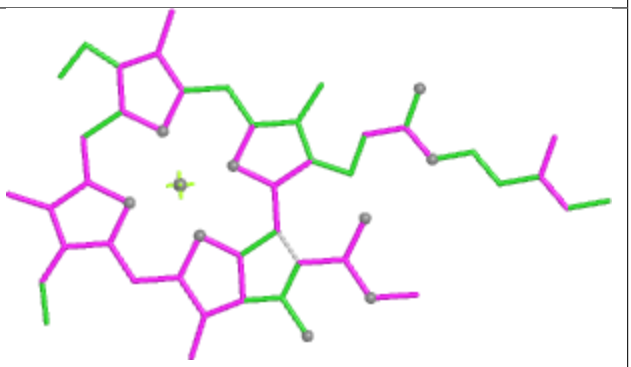
Ligand CLA 5 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

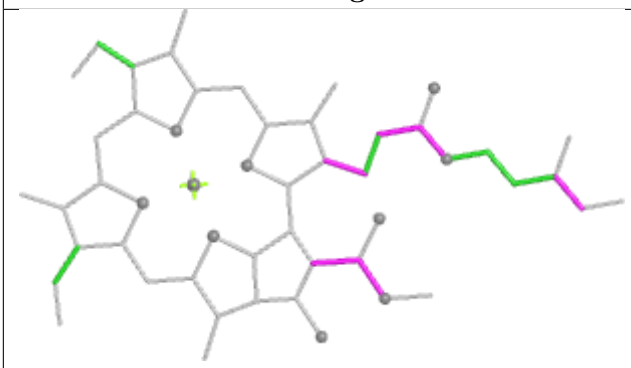
Ligand CLA 3 315



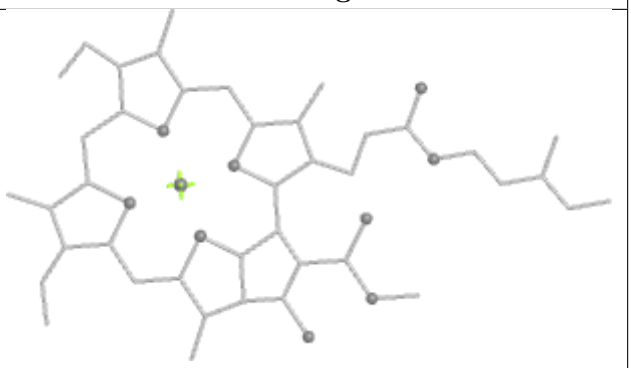
Bond lengths



Bond angles

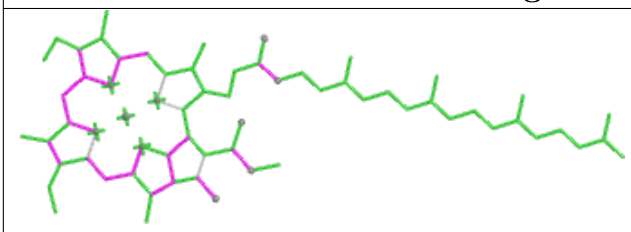


Torsions

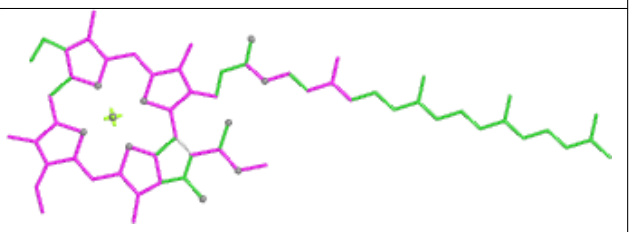


Rings

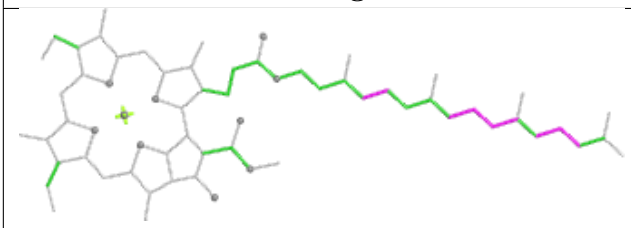
Ligand CLA A 833



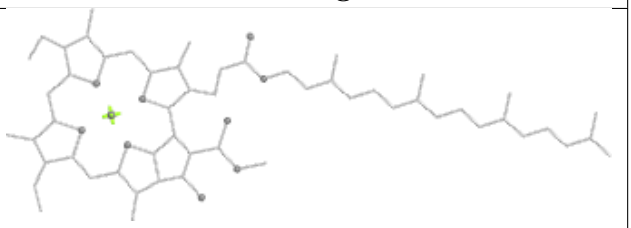
Bond lengths



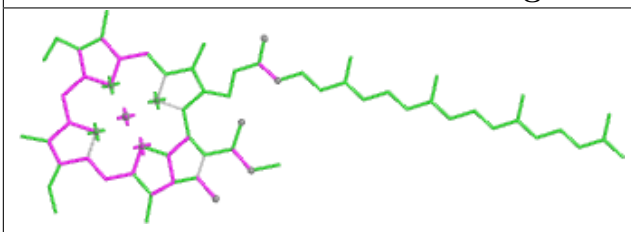
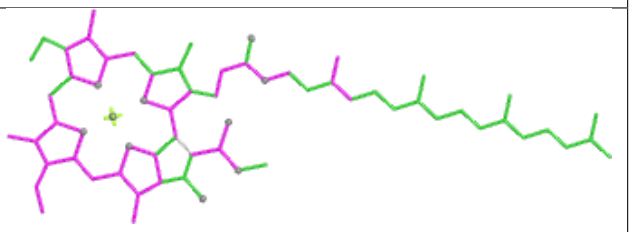
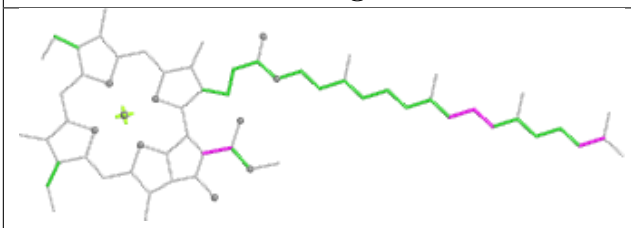
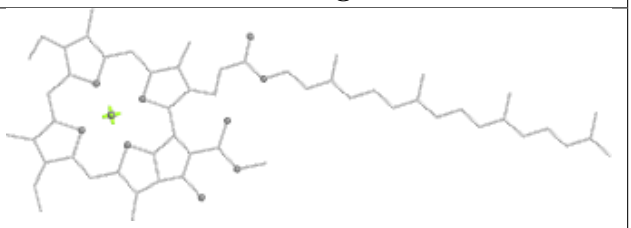
Bond angles

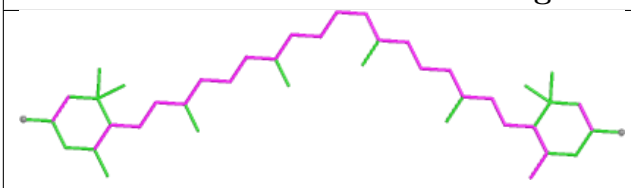
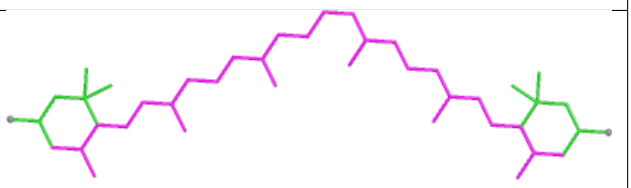
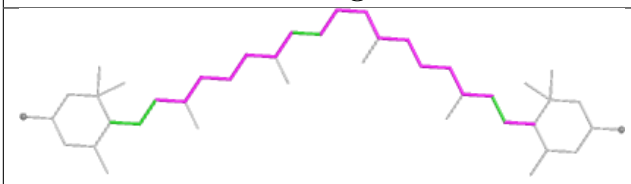
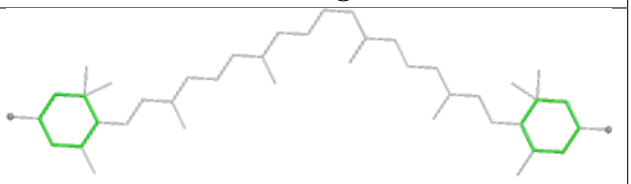


Torsions

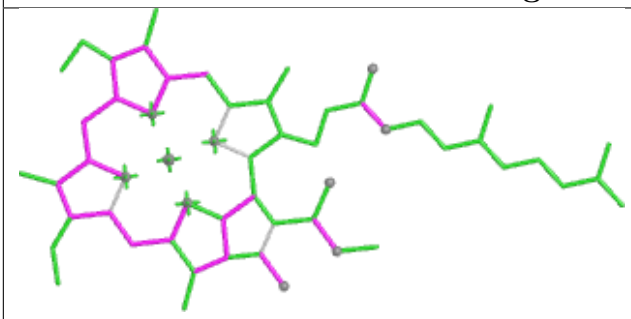


Rings

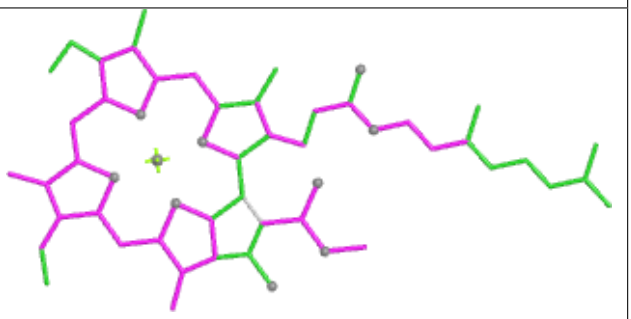
Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 5X6 2 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

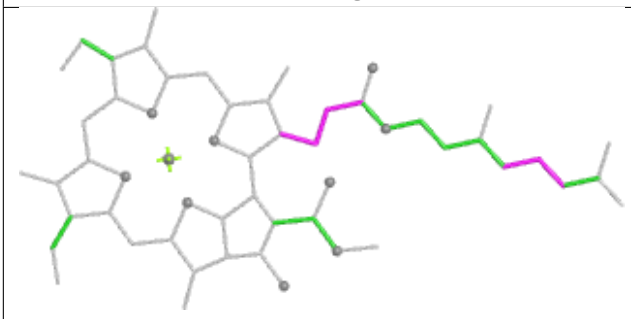
Ligand CLA K 102



Bond lengths



Bond angles



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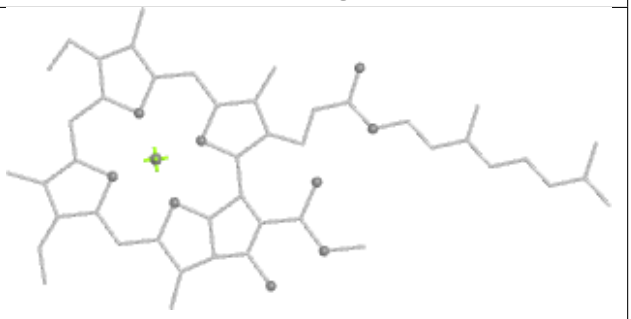
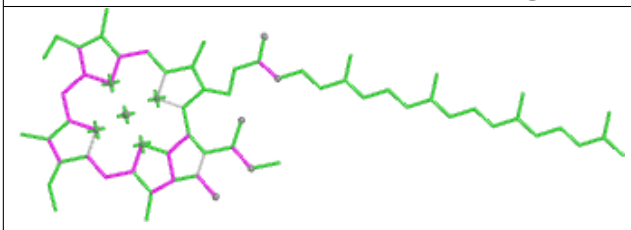
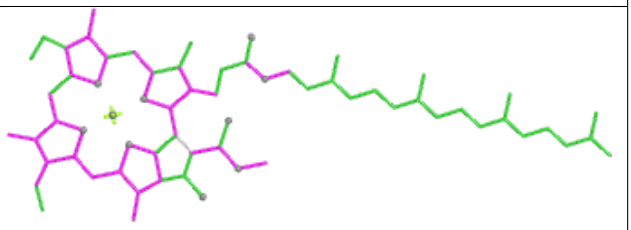


Rings

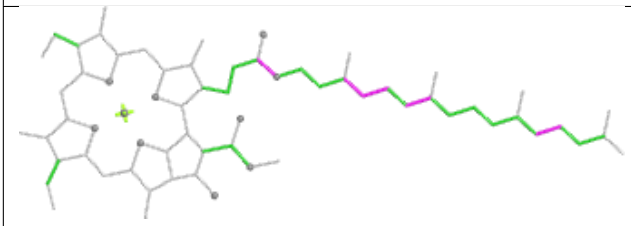
Ligand CLA A 819



Bond lengths



Bond angles



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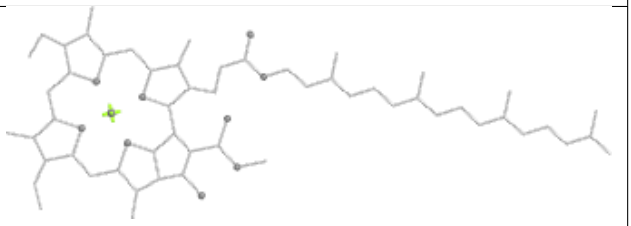
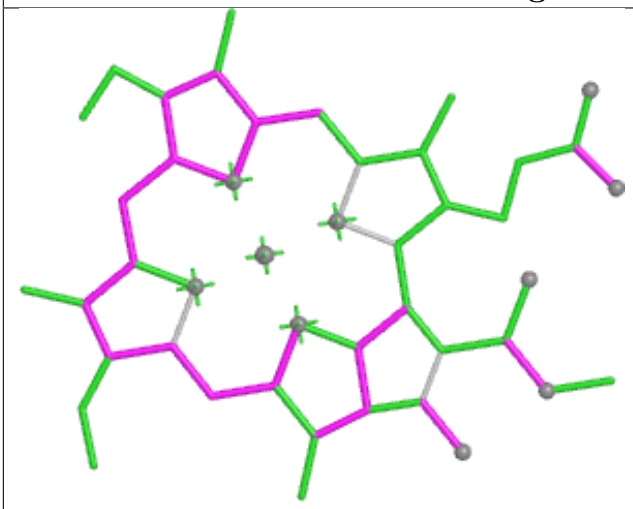


Rings

Ligand CLA 2 315



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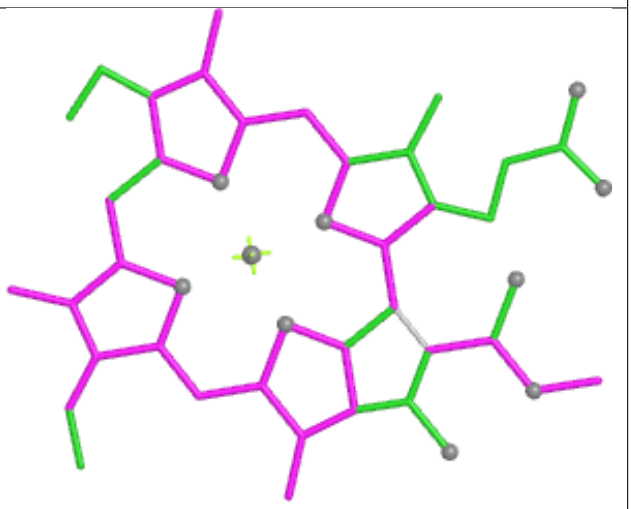
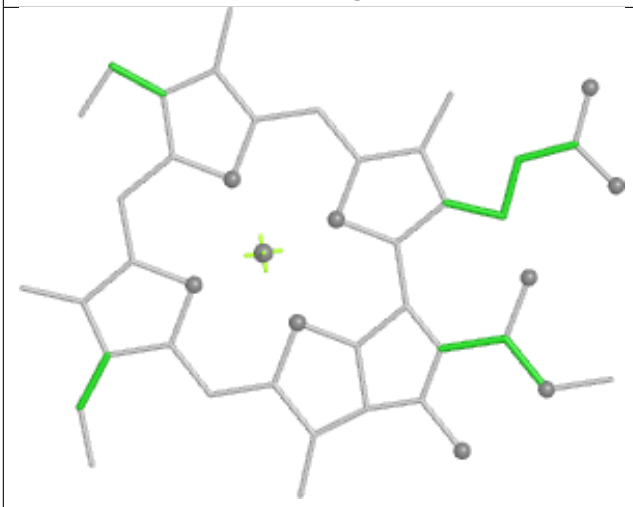
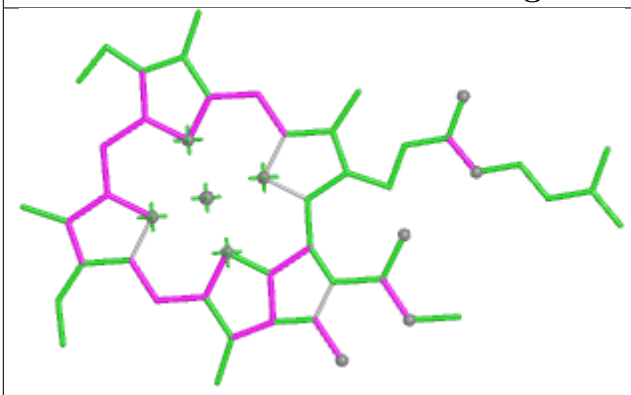
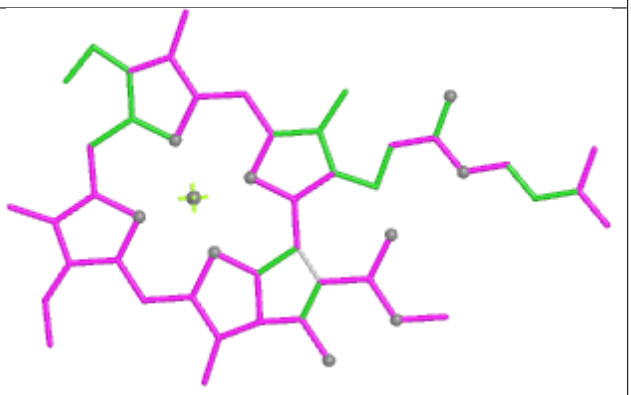
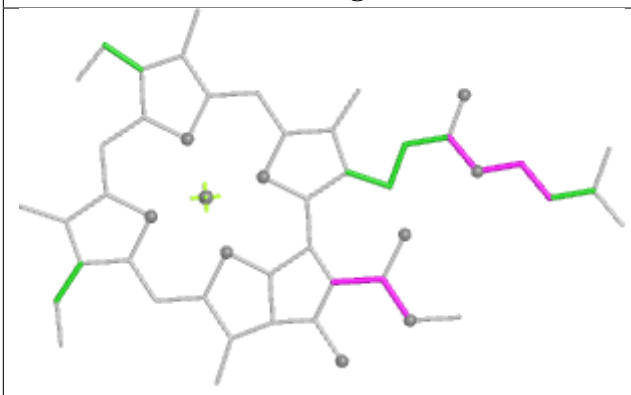
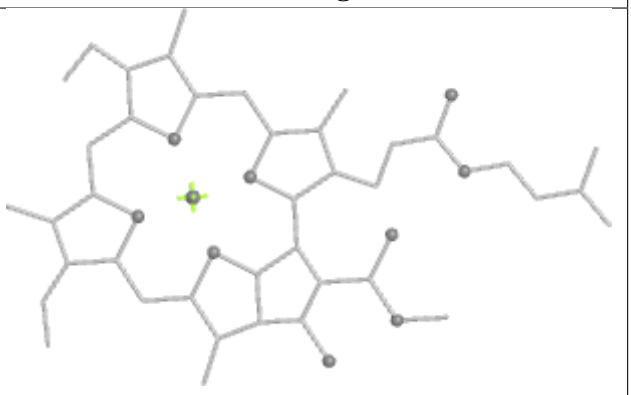


Bond angles

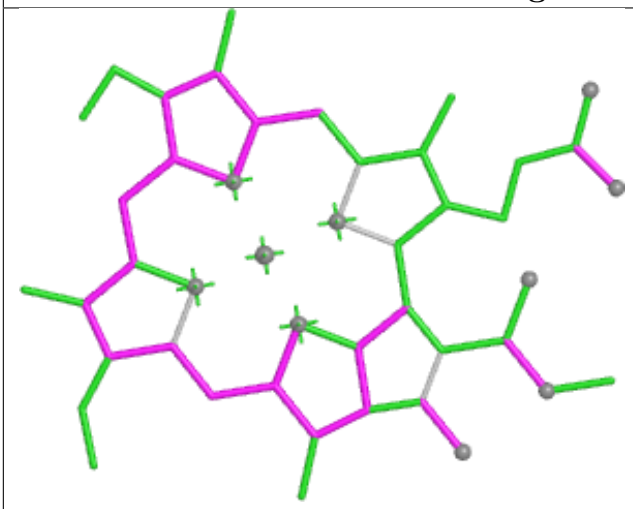


Torsions

Rings

Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 316



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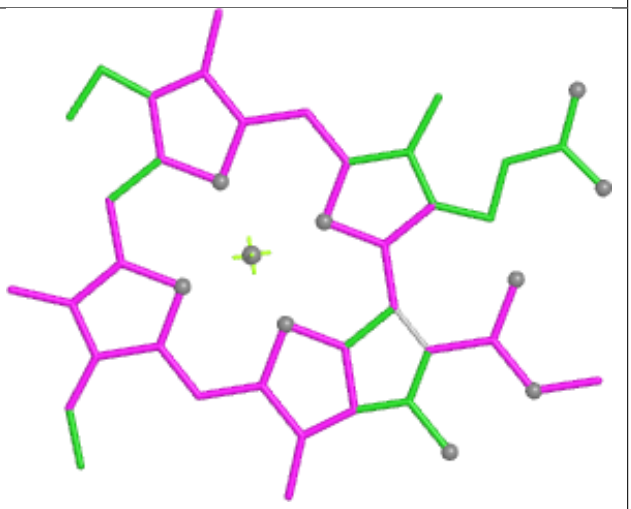
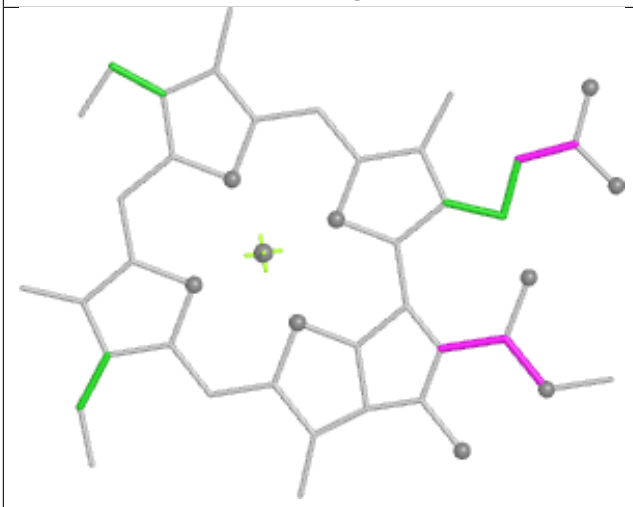


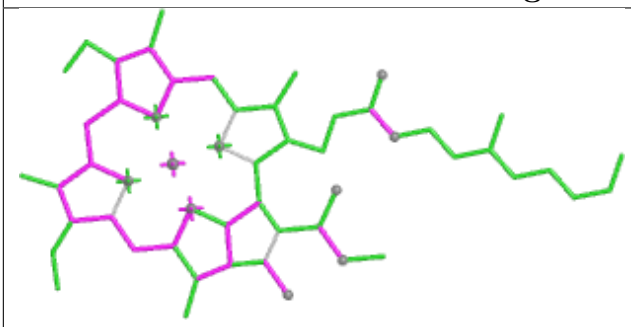
Bond angles



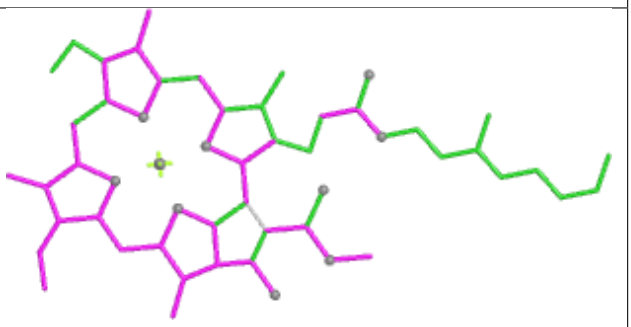
Torsions

Rings

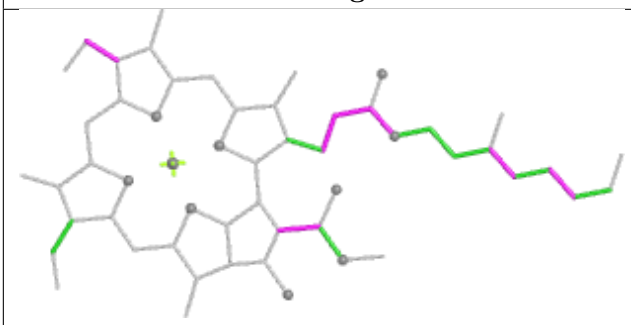
Ligand CLA A 810



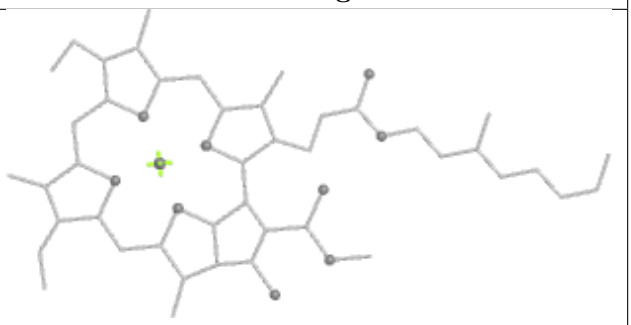
Bond lengths



Bond angles

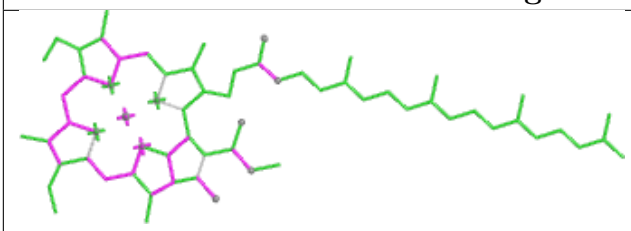


Torsions

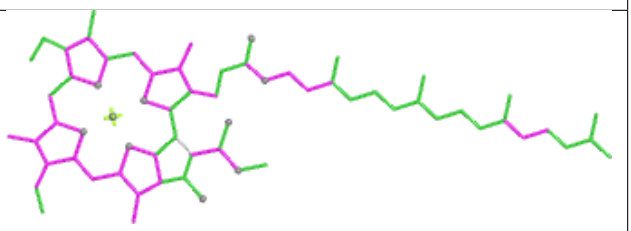


Rings

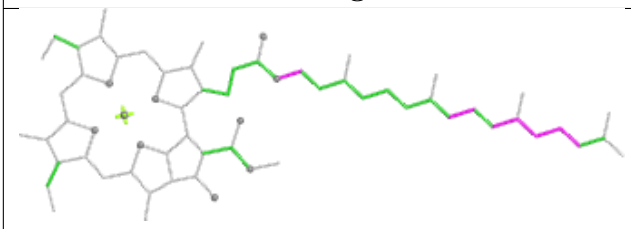
Ligand CLA B 804



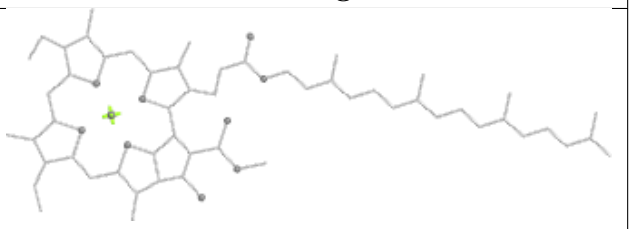
Bond lengths



Bond angles

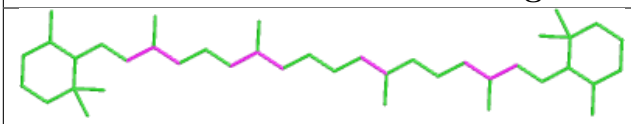


Torsions

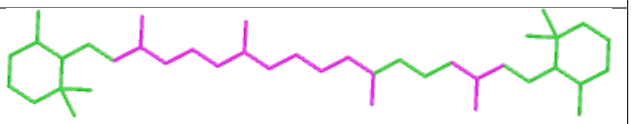


Rings

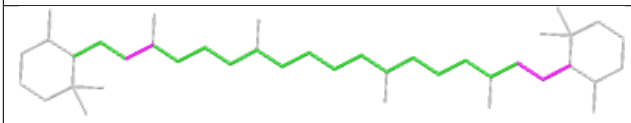
Ligand BCR L 206



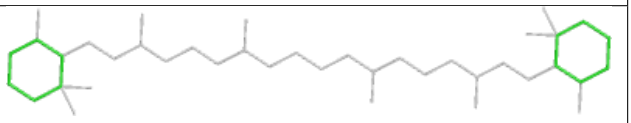
Bond lengths



Bond angles

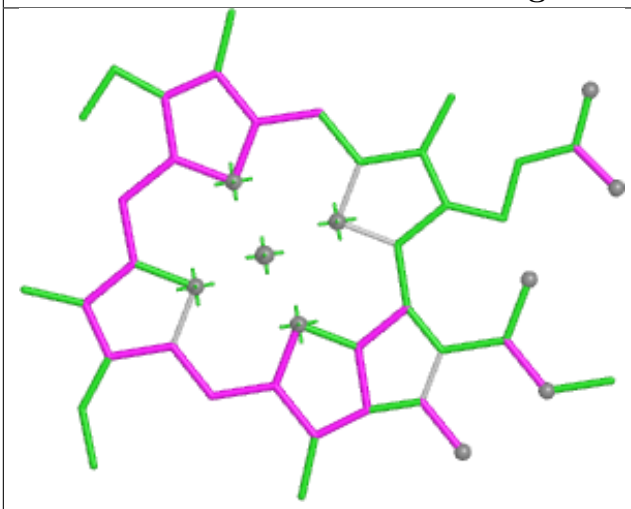


Torsions

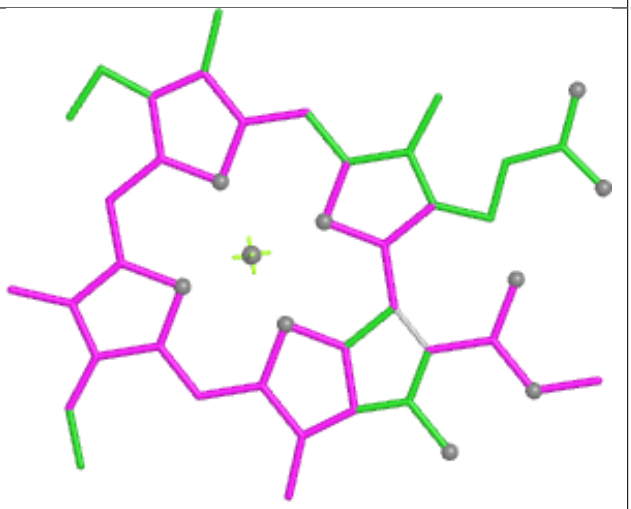


Rings

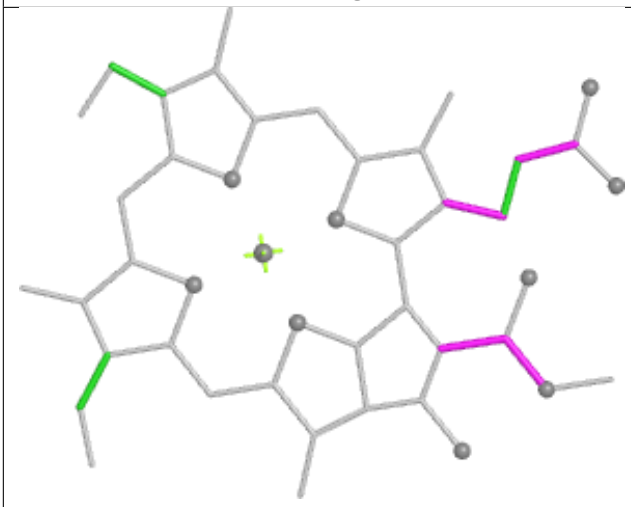
Ligand CLA 4 305



Bond lengths



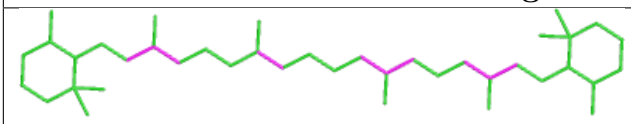
Bond angles



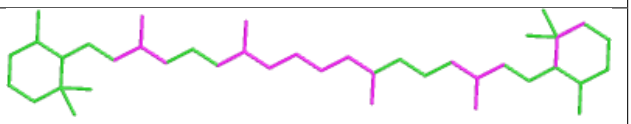
Torsions

Rings

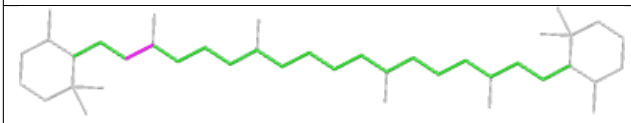
Ligand BCR O 202



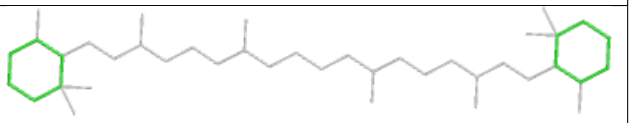
Bond lengths



Bond angles

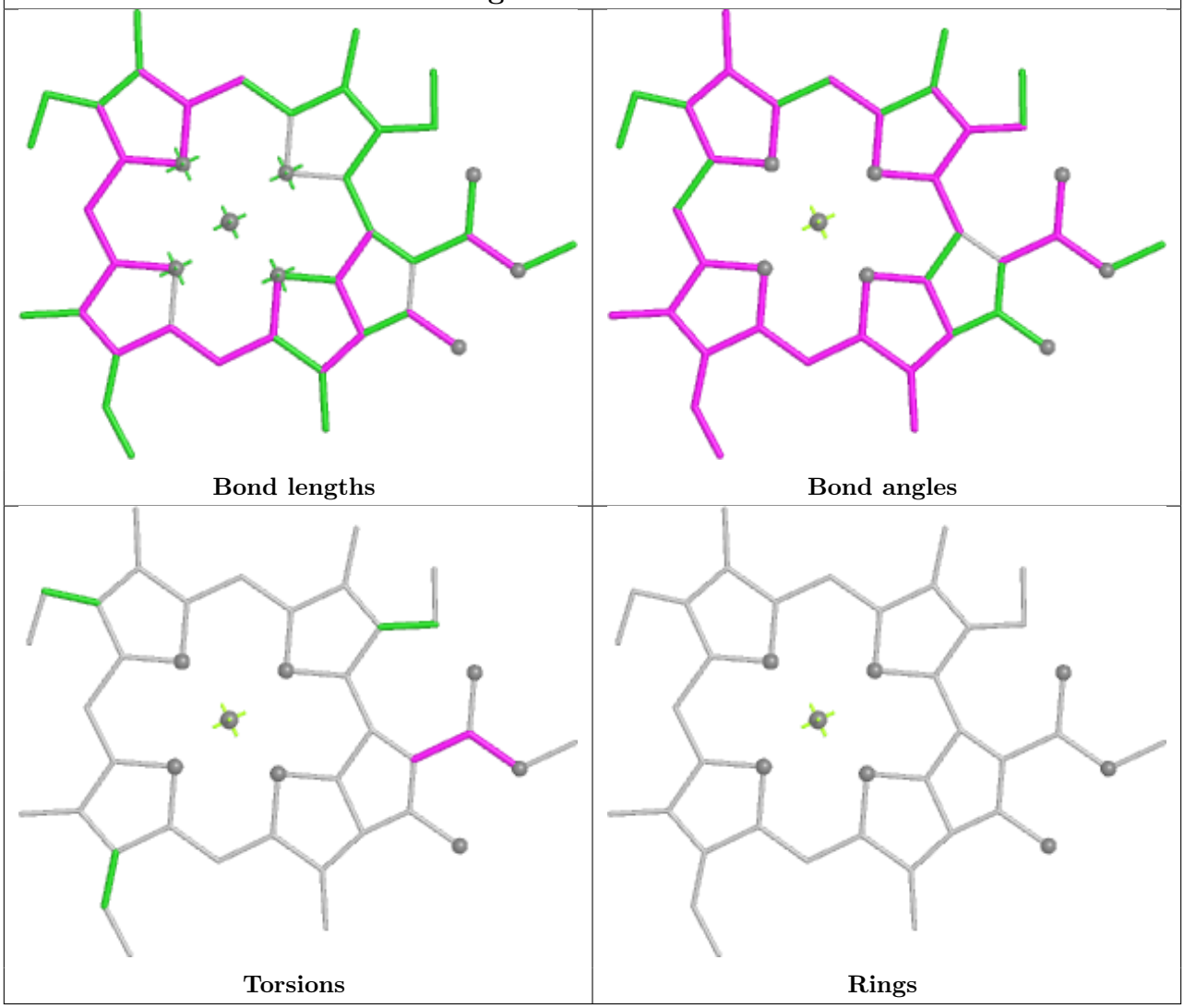


Torsions



Rings

Ligand CLA J 103



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.

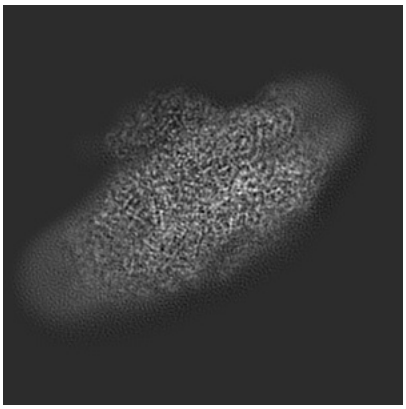
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37480. These allow visual inspection of the internal detail of the map and identification of artifacts.

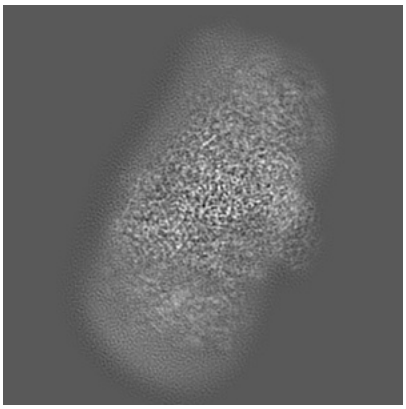
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

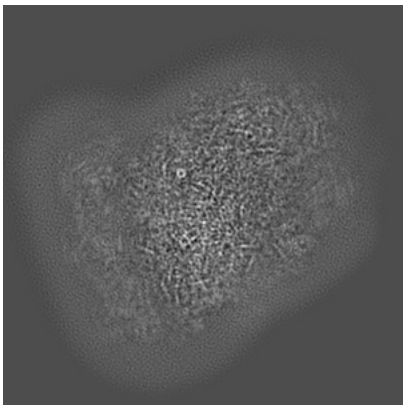
6.1.1 Primary map



X

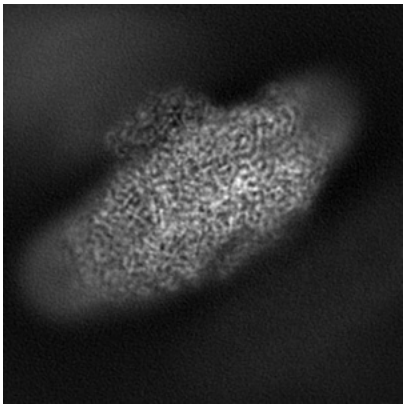


Y

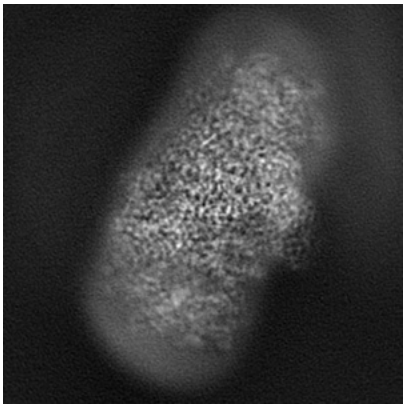


Z

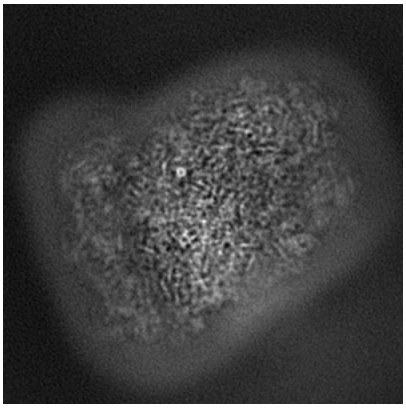
6.1.2 Raw map



X



Y

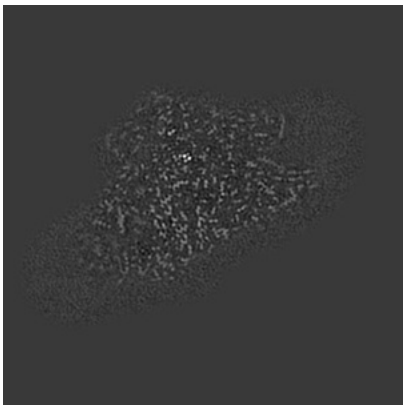


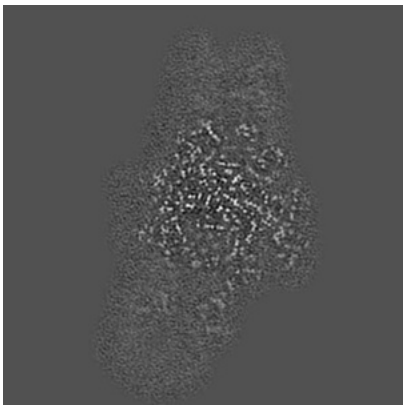
Z

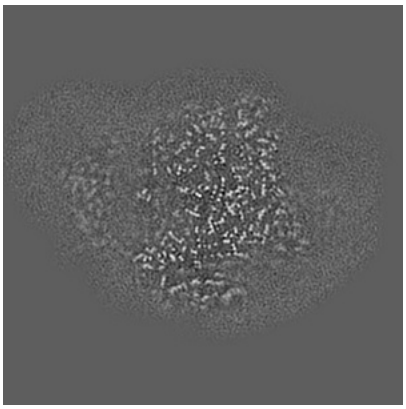
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

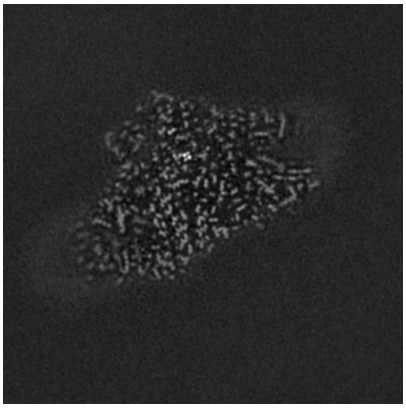
6.2.1 Primary map

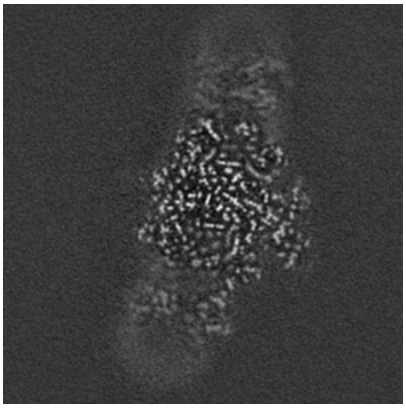

X Index: 128

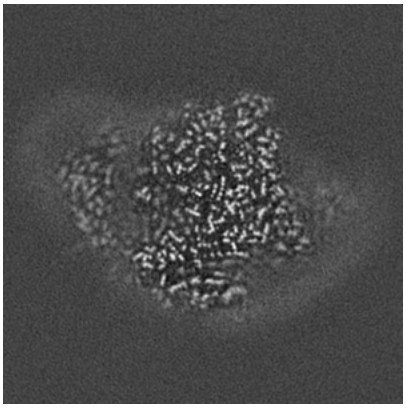

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

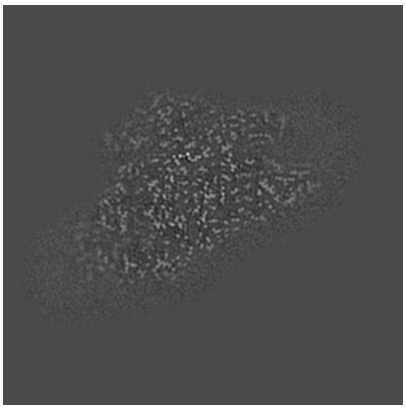

Y Index: 128

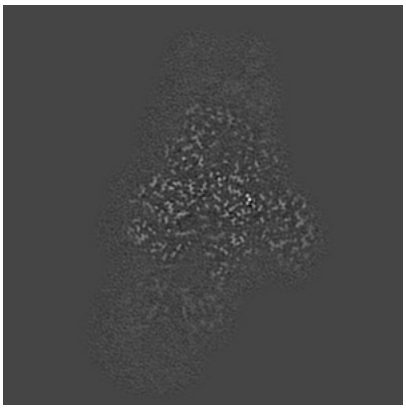

Z Index: 128

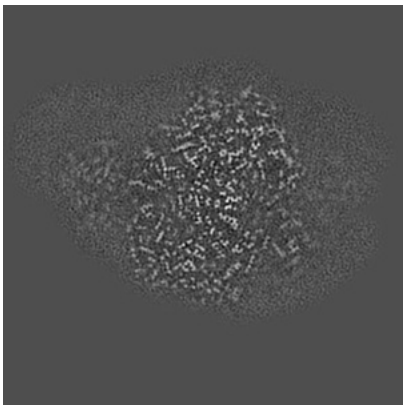
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

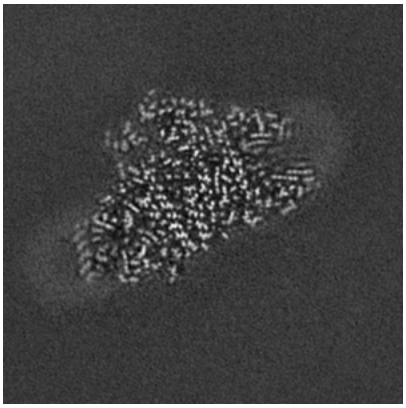
6.3.1 Primary map

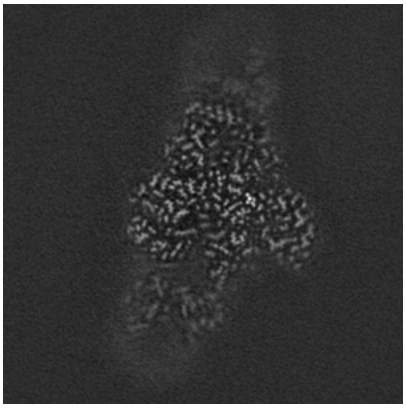

X Index: 127

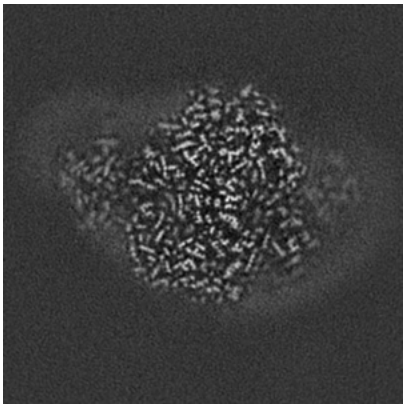

Y Index: 117


Z Index: 137

6.3.2 Raw map


X Index: 125

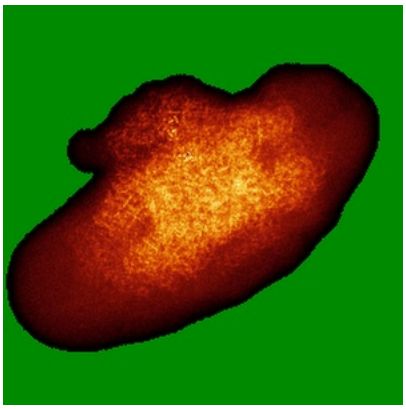

Y Index: 117

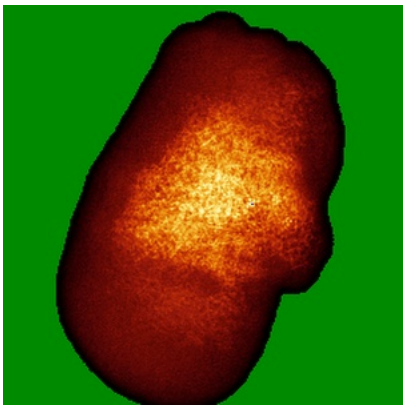

Z Index: 137

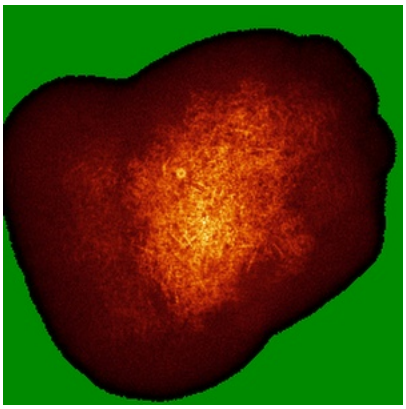
The images above show the largest variance slices of the map in three orthogonal directions.

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

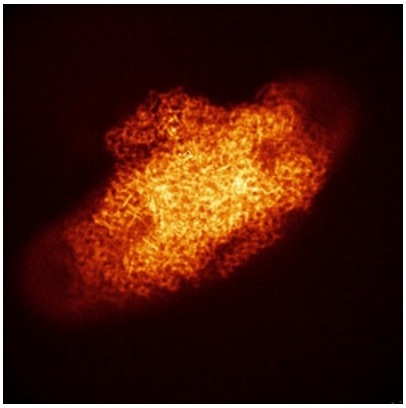
6.4.1 Primary map

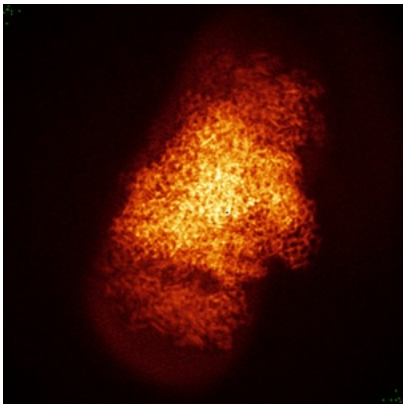

X

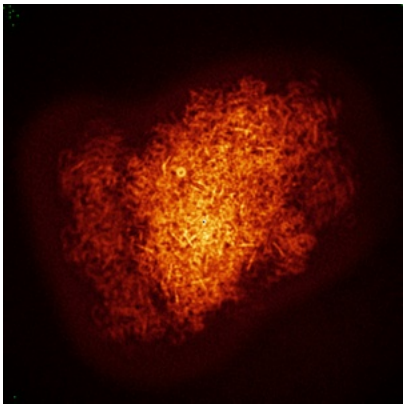

Y


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 0.016. 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.

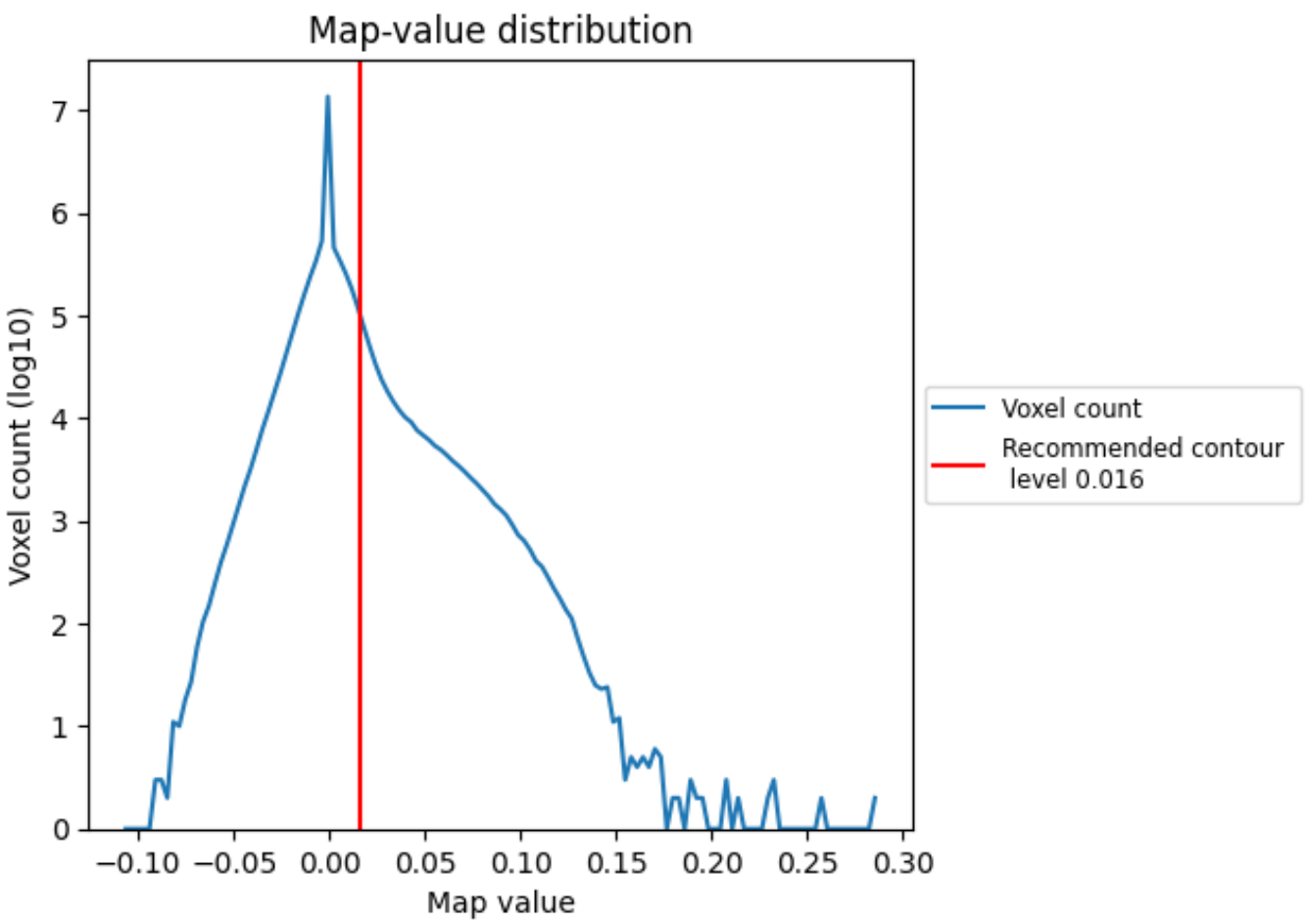
6.6 Mask visualisation (i)

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

7 Map analysis (i)

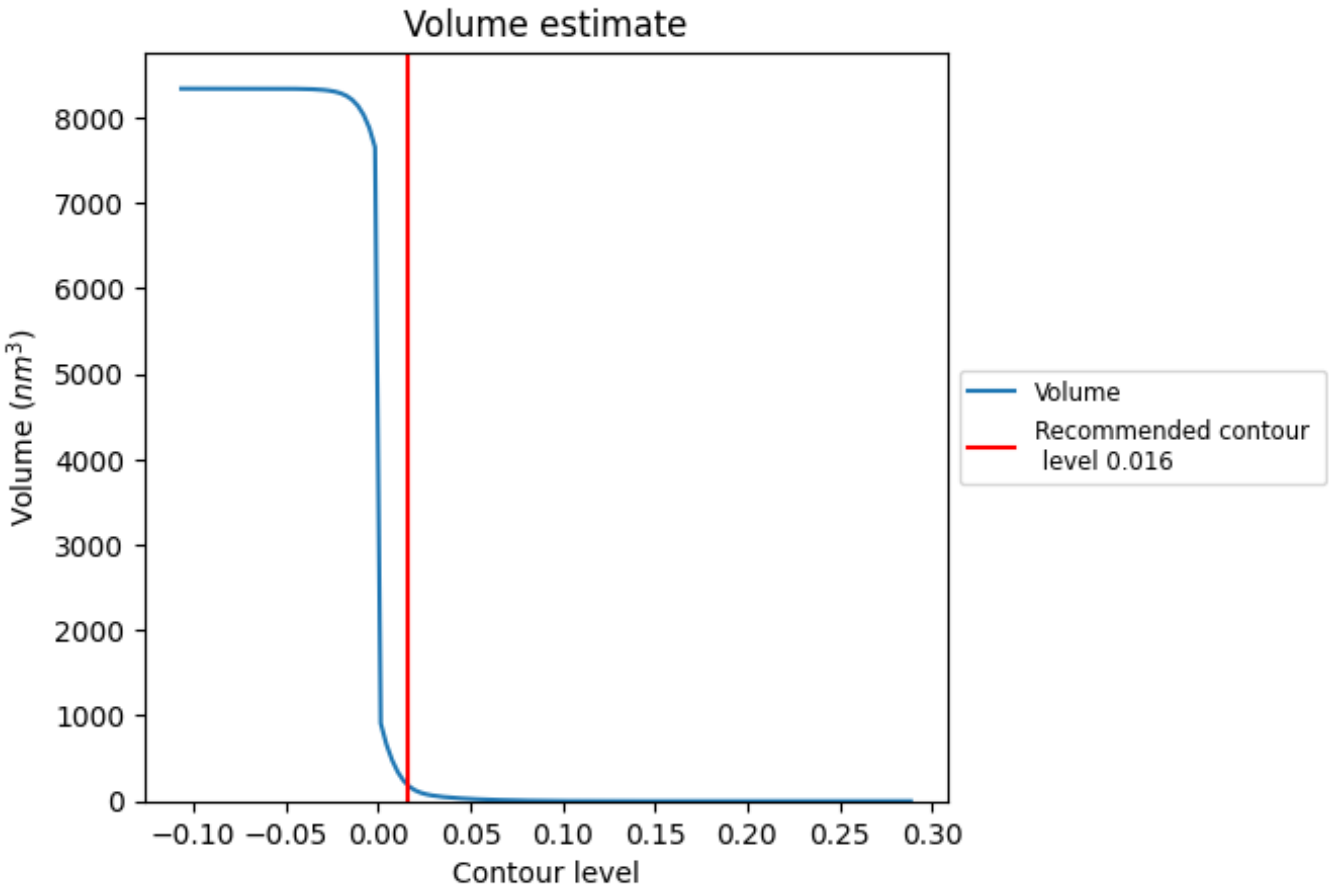
This section contains the results of statistical analysis of the map.

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.

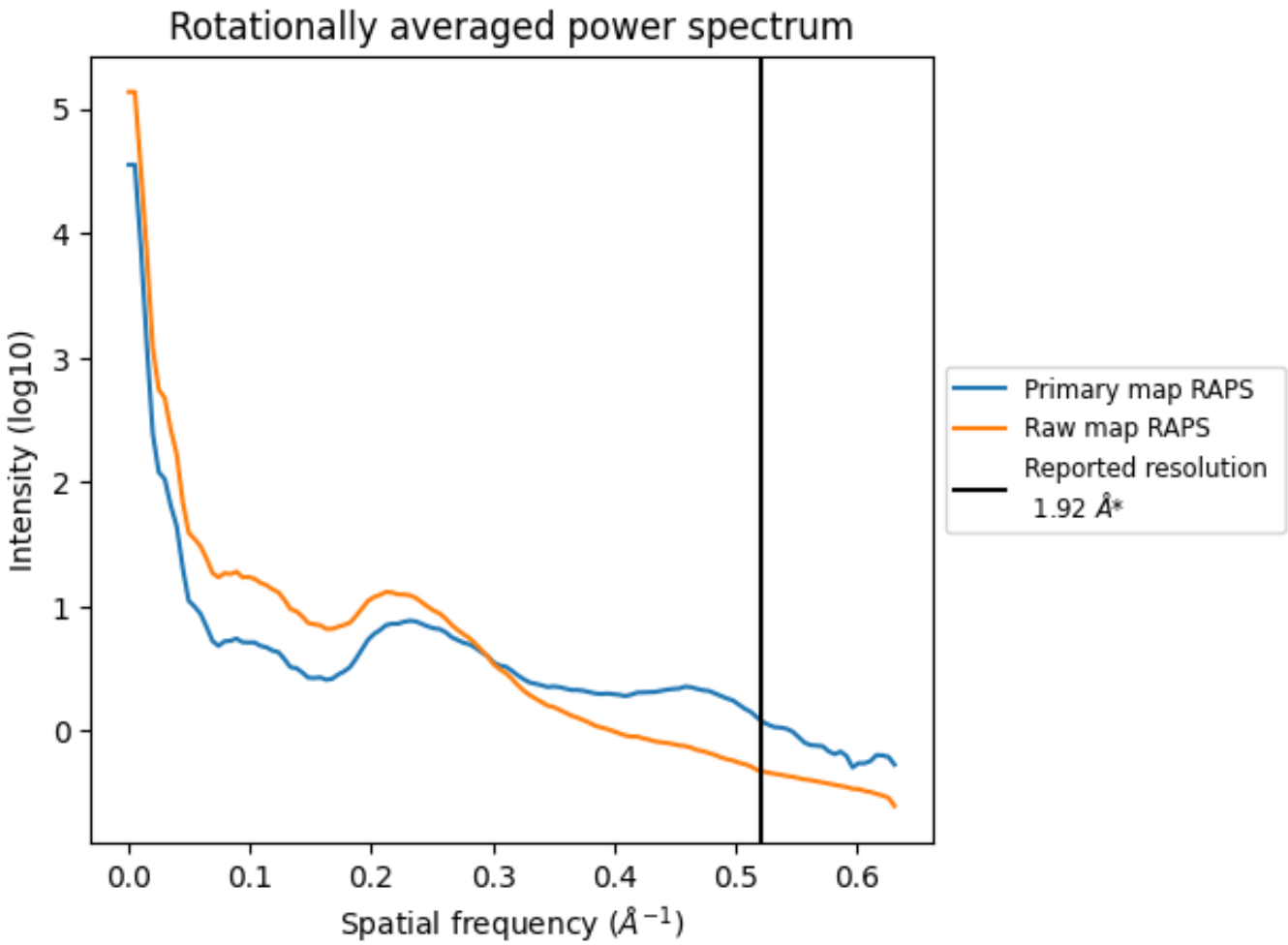
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

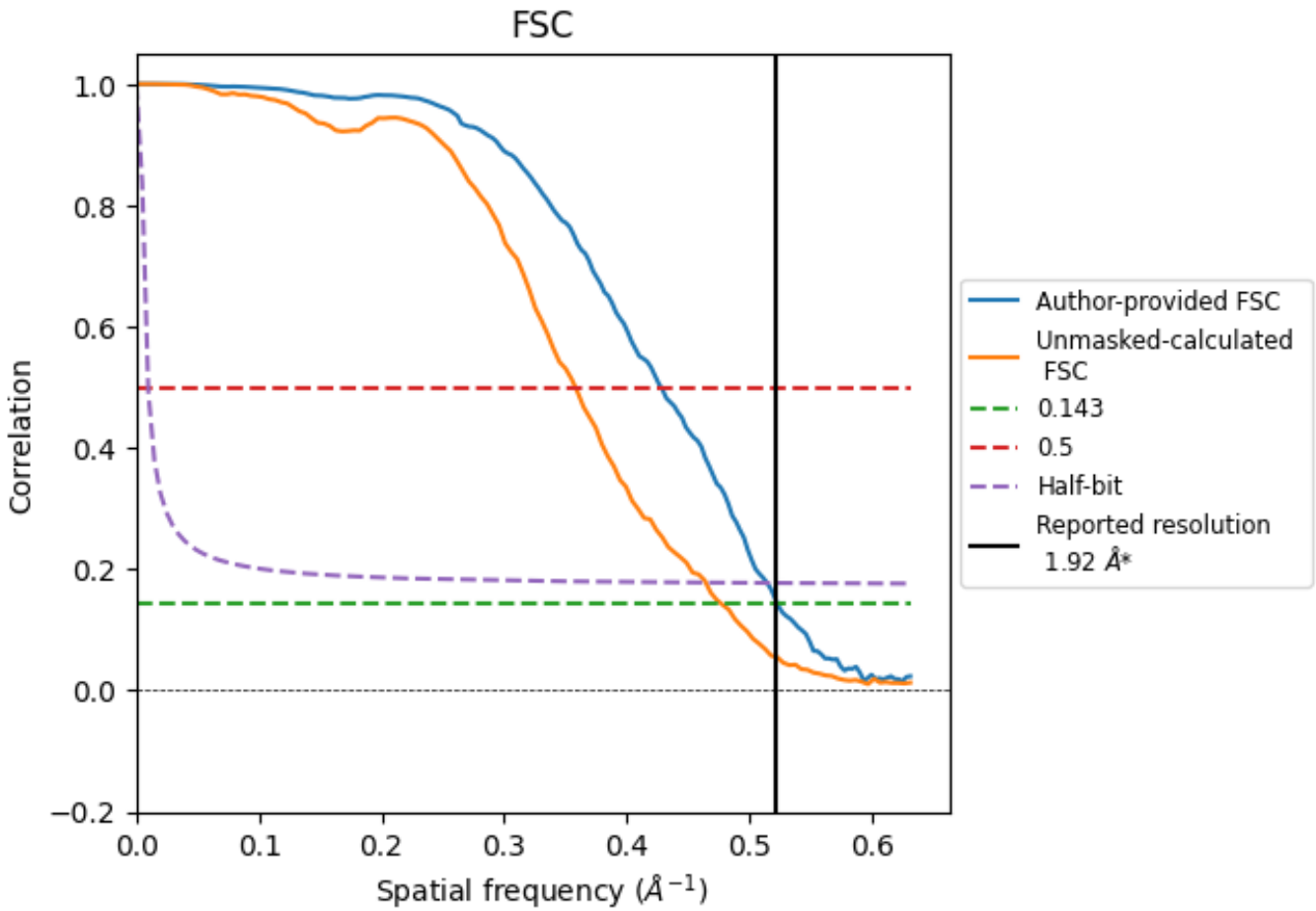


*Reported resolution corresponds to spatial frequency of 0.521 Å^{-1}

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 0.521 Å^{-1}

8.2 Resolution estimates (i)

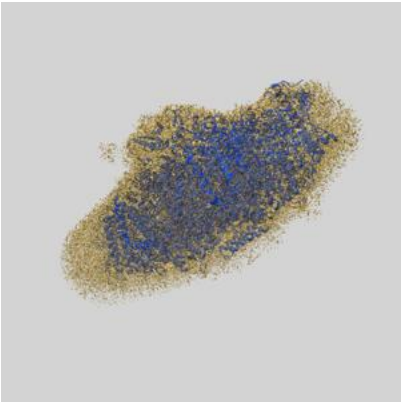
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.91	2.34	1.94
Unmasked-calculated*	2.10	2.79	2.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

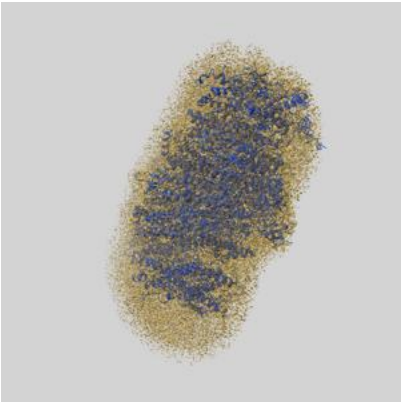
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37480 and PDB model 8WEY. Per-residue inclusion information can be found in section 3 on page 24.

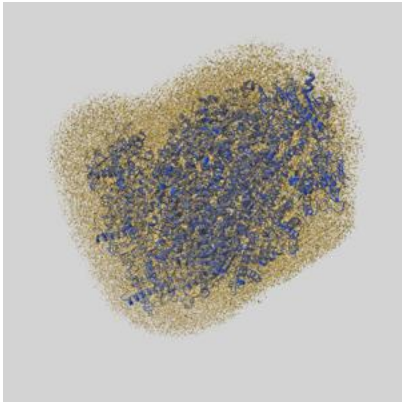
9.1 Map-model overlay (i)



X



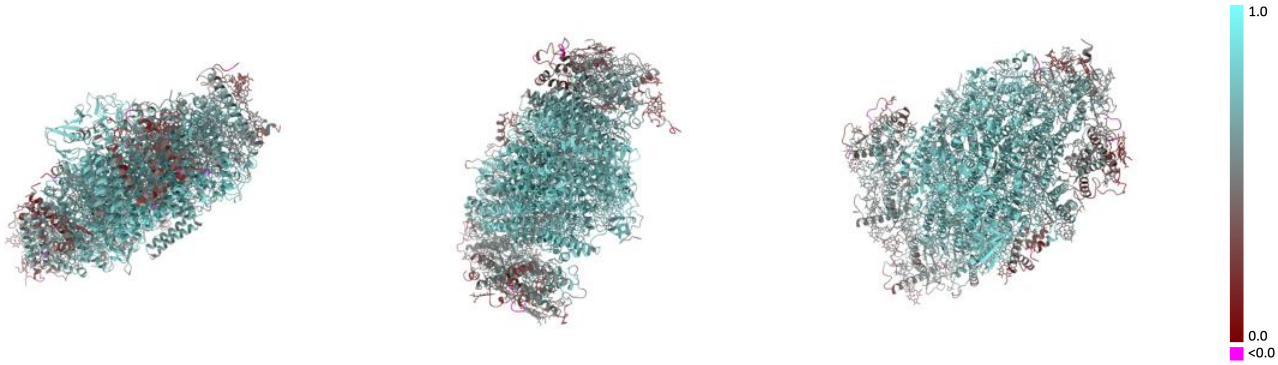
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

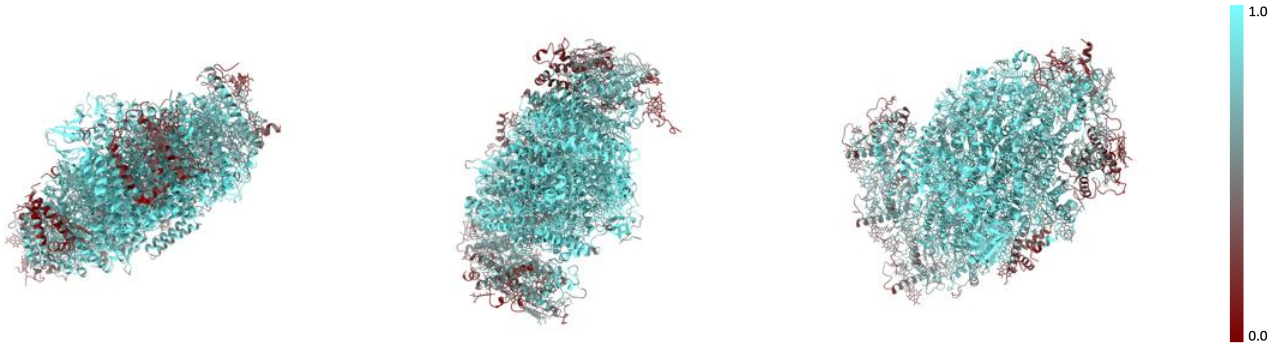
9.2 Q-score mapped to coordinate model (i)



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.

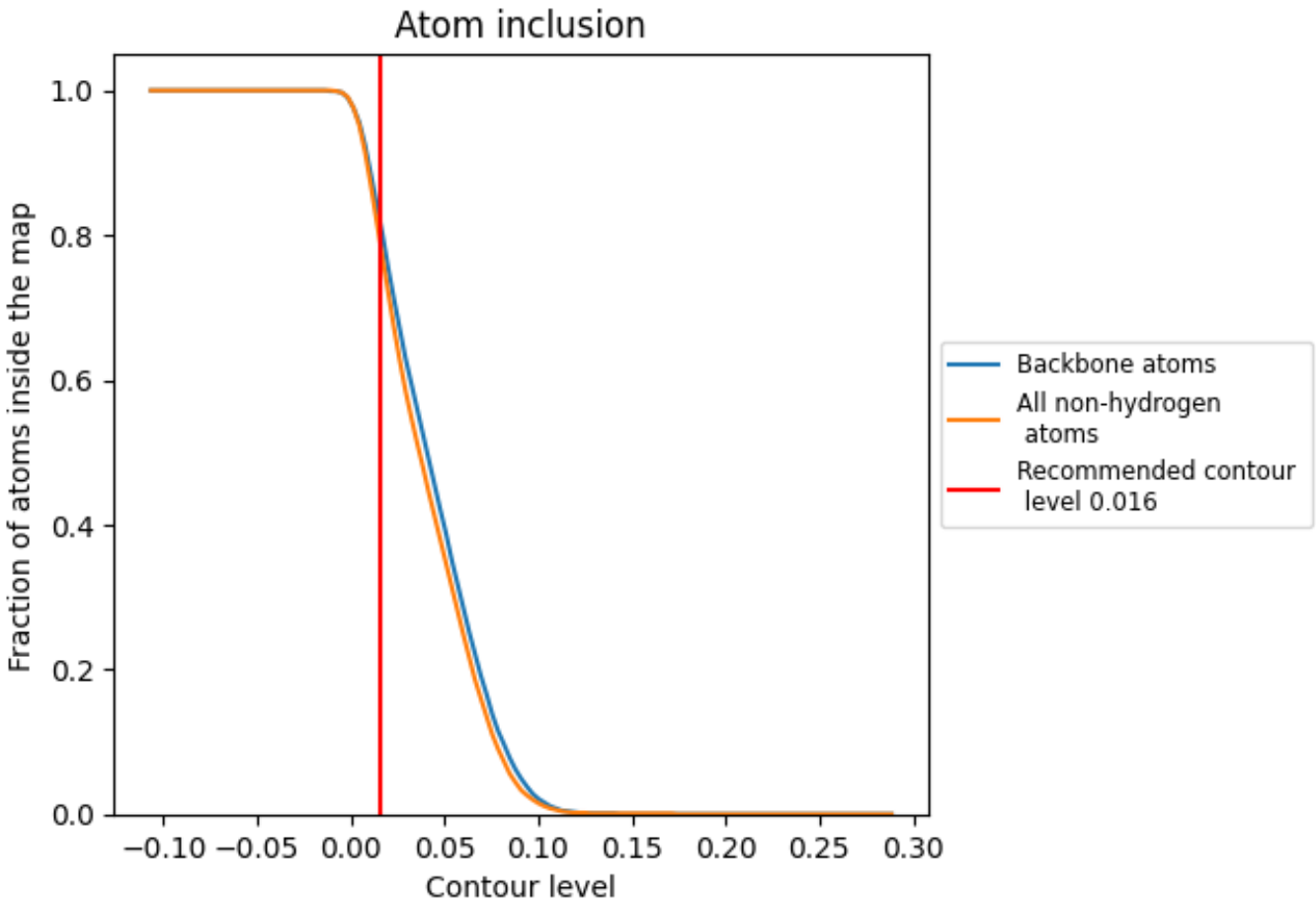
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.6620
1	0.5470	0.4670
2	0.5650	0.4990
3	0.4990	0.4530
4	0.3480	0.3730
5	0.6250	0.5340
A	0.9480	0.7870
B	0.9320	0.7720
C	0.9780	0.8100
D	0.8930	0.7170
E	0.8800	0.7220
F	0.8730	0.7150
I	0.8930	0.7250
J	0.8960	0.7440
K	0.7180	0.5880
L	0.7930	0.6310
M	0.8300	0.6850
O	0.2150	0.3110