Full wwPDB EM Validation Report (i)

Sep 9, 2026 – 08:10 PM JST

PDB ID	:	8HTU / pdb_00008htu
EMDB ID	:	EMD-35018
Title	:	Cryo-EM structure of PpPSI-L
Authors	:	Li, M.; Pan, X.W.; Sun, H.Y.
Deposited on	:	2022-12-21
Resolution	:	2.87 Å(reported)

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

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

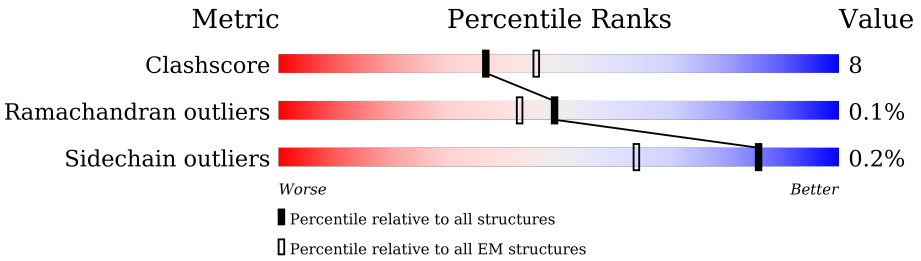
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

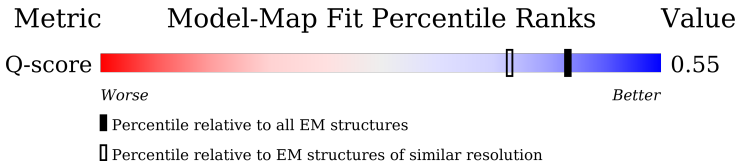
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	U	265	8% 70% 12% 17%
1	V	265	20% 69% 12% 19%
1	W	265	16% 72% 14% 14%
2	1	245	• 70% 9% 21%

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Mol	Chain	Length	Quality of chain
2	5	245	25% 55% 22% 22%
3	2	273	66% 11% 23%
3	6	273	26% 57% 18% 25%
4	3	323	61% 7% 31%
4	7	323	32% 51% 16% 32%
5	4	270	5% 66% 11% 24%
5	8	270	22% 61% 14% 24%
6	A	750	90% 9%
7	B	734	88% 12%
8	C	81	84% 15%
9	D	210	58% 10% 32%
10	E	132	44% 5% 52%
11	F	246	58% 7% 35%
12	G	155	53% 10% 37%
13	H	139	7% 60% 9% 32%
14	I	36	81% 14% 6%
15	J	41	95% 5%
16	K	132	60% 39%
17	L	223	67% 6% 27%
18	M	32	6% 84% 12%
19	O	143	5% 55% 8% 37%
20	9	311	17% 56% 15% 29%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 57715 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	S			
1	U	219	1659	1073	270	311	5		0	0
			Total	C	N	O	S			
1	V	215	1630	1052	265	308	5		0	0
			Total	C	N	O	P	S		
1	W	228	1734	1113	286	329	1	5	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	193	1478	964	248	265	1	0	0
			Total	C	N	O	S		
2	5	192	1473	961	247	264	1	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	211	1625	1055	273	293	4	0	0
			Total	C	N	O	S		
3	6	205	1583	1029	265	285	4	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	222	1719	1125	281	306	7	0	0
			Total	C	N	O	S		
4	7	219	1687	1105	274	301	7	0	0

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	206	1600	1040	267	288	5	0	0
5	8	204	1582	1028	265	284	5	0	0

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	742	5837	3827	993	998	19	0	0

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	733	5850	3839	996	999	16	0	0

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	80	595	365	103	116	11	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	142	1114	714	197	200	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	E	64	507	322	90	95	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	161	1251	808	217	223	3	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	G	97	740	478	127	135	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	95	736	472	125	138	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	34	266	181	35	48	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	J	41	325	222	48	54	1	0	0

- Molecule 16 is a protein called Photosystem I subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	K	81	565	356	98	108	3	0	0

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	163	1228	809	197	220	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	M	31	230	150	37	43	0	0

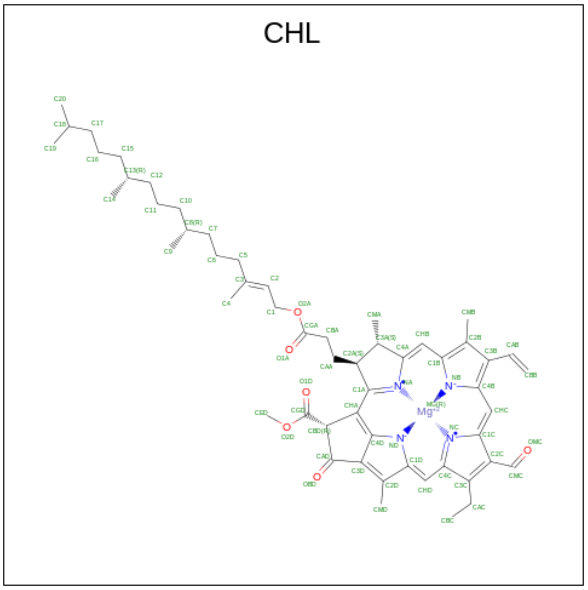
- Molecule 19 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	90	711	477	117	116	1	0	0

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	9	221	1713	1113	283	308	9	0	0

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	U	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
21	U	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
21	U	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
21	U	1	40	31	1	4	4	0
			Total	C	Mg	N	O	
21	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
21	V	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
21	V	1	42	33	1	4	4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	V	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
21	V	1	40	31	1	4	4	0
			Total	C	Mg	N	O	
21	V	1	40	31	1	4	4	0
			Total	C	Mg	N	O	
21	V	1	40	33	1	4	2	0
			Total	C	Mg	N	O	
21	W	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
21	W	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
21	W	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
21	W	1	40	31	1	4	4	0
			Total	C	Mg	N	O	
21	W	1	40	31	1	4	4	0
			Total	C	Mg	N	O	
21	W	1	40	33	1	4	2	0
			Total	C	Mg	N	O	
21	1	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
21	1	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	2	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
21	3	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
21	4	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	4	1	47	36	1	4	6	0

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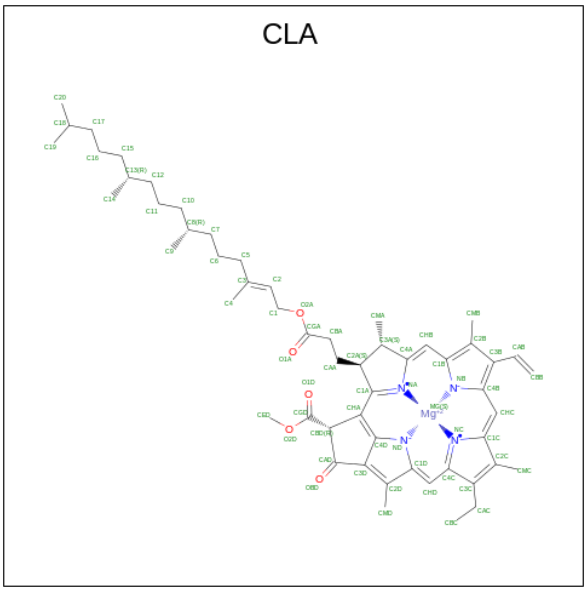
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	4	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
21	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
21	5	1	39	32	1	4	2	0
			Total	C	Mg	N	O	
21	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
21	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
21	6	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	6	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
21	6	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
21	6	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
21	7	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	8	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
21	8	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
21	8	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
21	9	1	39	32	1	4	2	0
			Total	C	Mg	N	O	
21	9	1	38	31	1	4	2	0
			Total	C	Mg	N	O	
21	9	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
21	9	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
21	9	1	43	34	1	4	4	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	U	1	65	55	1	4	5	0
22	U	1	65	55	1	4	5	0
22	U	1	52	42	1	4	5	0
22	U	1	65	55	1	4	5	0
22	U	1	45	35	1	4	5	0
22	U	1	65	55	1	4	5	0
22	U	1	65	55	1	4	5	0
22	U	1	42	34	1	4	3	0
22	V	1	59	49	1	4	5	0
22	V	1	60	50	1	4	5	0
22	V	1	50	40	1	4	5	0
22	V	1	39	31	1	4	3	0
22	V	1	40	32	1	4	3	0
22	V	1	38	30	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	V	1	56	47	1	4	4	0
			Total	C	Mg	N	O	
22	V	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	W	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	W	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
22	W	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	W	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	W	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
22	W	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
22	W	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	W	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	53	43	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	3	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	H	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
22	J	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	42	34	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	L	1	60	50	1	4	5	0
			Total	C	Mg	N		
22	O	1	27	22	1	4		0
			Total	C	Mg	N	O	
22	O	1	55	45	1	4	5	0
			Total	C	Mg	N		
22	O	1	27	22	1	4		0
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
22	5	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	6	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	46	36	1	4	5	0

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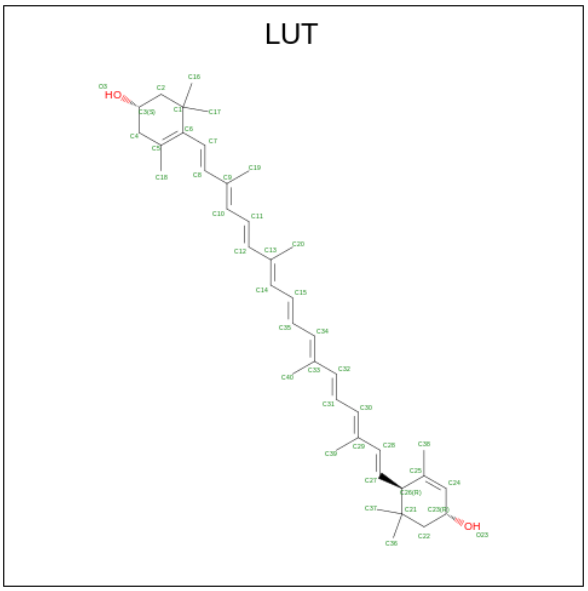
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	9	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
22	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	39	33	1	4	1	0
			Total	C	Mg	N	O	
22	9	1	52	42	1	4	5	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	U	1	42	40	2	0
			Total	C	O	
23	U	1	42	40	2	0
			Total	C	O	
23	V	1	42	40	2	0
			Total	C	O	
23	V	1	42	40	2	0
			Total	C	O	
23	W	1	42	40	2	0
			Total	C	O	
23	W	1	42	40	2	0
			Total	C	O	
23	1	1	42	40	2	0
			Total	C	O	
23	2	1	42	40	2	0
			Total	C	O	
23	3	1	42	40	2	0
			Total	C	O	
23	4	1	42	40	2	0
			Total	C	O	
23	5	1	42	40	2	0
			Total	C	O	
23	6	1	42	40	2	0
			Total	C	O	
23	7	1	42	40	2	0
			Total	C	O	
23	8	1	42	40	2	0

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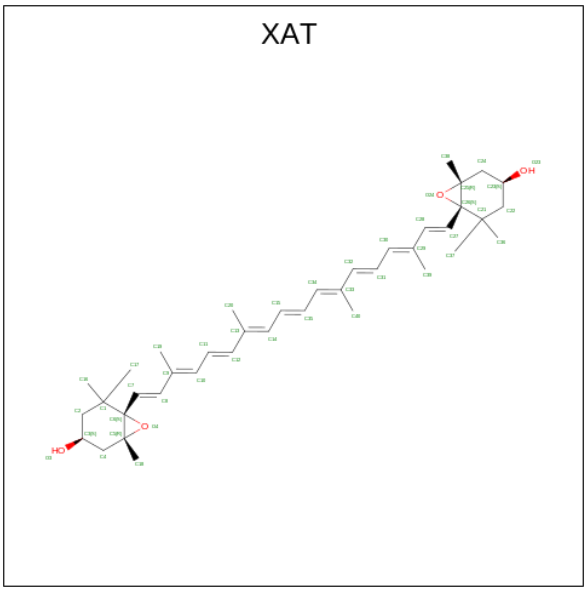
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	9	1	42	40	2	0
			Total	C	O	
23	9	1	42	40	2	0
			Total	C	O	
23	9	1	42	40	2	0

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	U	1	44	40	4	0
			Total	C	O	
24	V	1	44	40	4	0
			Total	C	O	
24	W	1	44	40	4	0
			Total	C	O	
24	1	1	44	40	4	0
			Total	C	O	
24	2	1	44	40	4	0
			Total	C	O	
24	3	1	44	40	4	0
			Total	C	O	
24	4	1	44	40	4	0
			Total	C	O	
24	5	1	44	40	4	0

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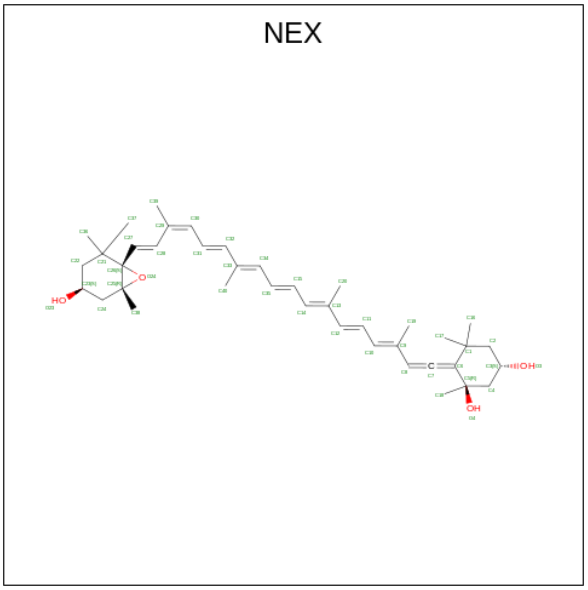
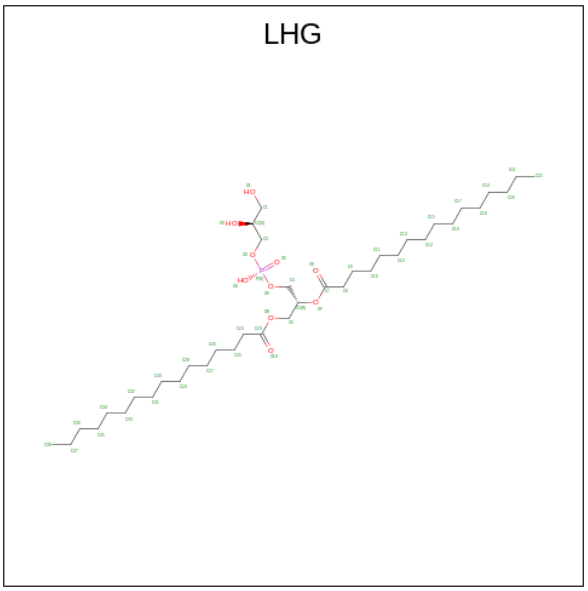
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	6	1	44	40	4	0
			Total	C	O	
24	7	1	44	40	4	0
			Total	C	O	
24	8	1	44	40	4	0

- Molecule 25 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	U	1	44	40	4	0
			Total	C	O	
25	V	1	44	40	4	0
			Total	C	O	
25	W	1	44	40	4	0
			Total	C	O	
25	9	1	44	40	4	0

- Molecule 26 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	
26	U	1	45	34	10	1	0
26	V	1	42	31	10	1	0
26	W	1	45	34	10	1	0
26	1	1	49	38	10	1	0
26	2	1	32	21	10	1	0
26	3	1	32	21	10	1	0
26	4	1	38	27	10	1	0
26	A	1	47	36	10	1	0
26	A	1	31	20	10	1	0
26	B	1	35	24	10	1	0
26	5	1	37	26	10	1	0
26	6	1	32	21	10	1	0
26	7	1	34	23	10	1	0
26	8	1	38	27	10	1	0

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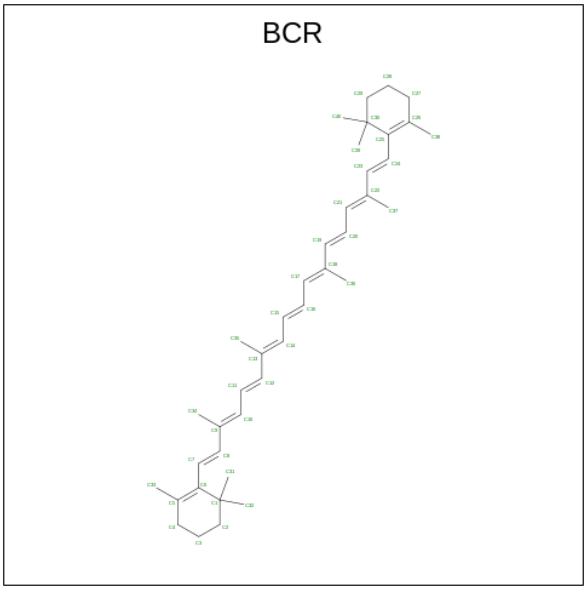
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	9	1	28	17	10	1	0

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	1	1	40	40	0
27	2	1	40	40	0
27	3	1	40	40	0
27	3	1	40	40	0
27	4	1	40	40	0
27	A	1	40	40	0
27	A	1	40	40	0
27	A	1	40	40	0
27	A	1	40	40	0
27	A	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	A	1	39	39	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	F	1	40	40	0
27	G	1	40	40	0
27	I	1	40	40	0
27	J	1	40	40	0
27	K	1	40	40	0
27	K	1	40	40	0
27	L	1	40	40	0
27	L	1	40	40	0
27	L	1	40	40	0
27	M	1	40	40	0
27	O	1	40	40	0
27	6	1	40	40	0
27	7	1	40	40	0

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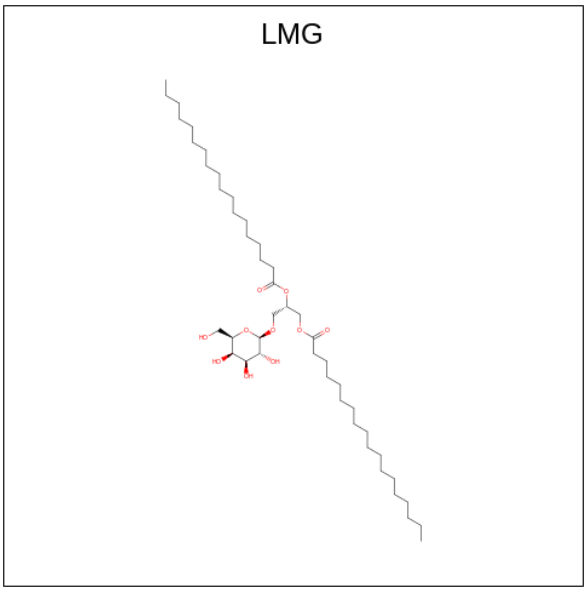
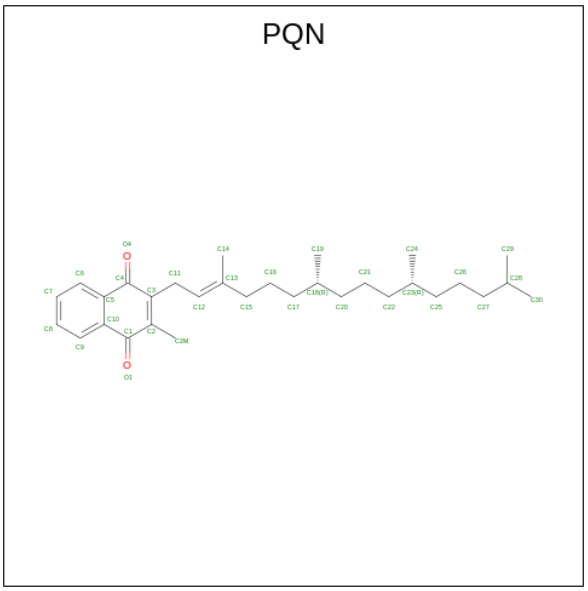
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	7	1	40	40	0
			Total	C	
27	8	1	40	40	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



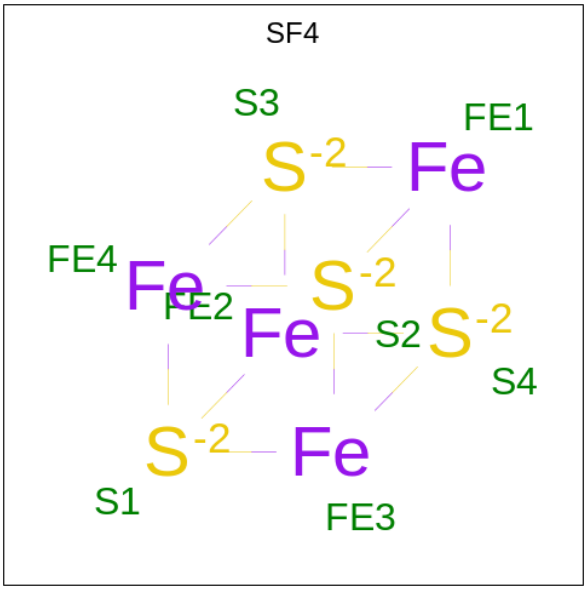
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	2	1	47	37	10	0
			Total	C	O	
28	A	1	34	24	10	0
			Total	C	O	
28	G	1	32	22	10	0
			Total	C	O	
28	J	1	55	45	10	0
			Total	C	O	
28	J	1	35	25	10	0
			Total	C	O	
28	L	1	44	34	10	0

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

Continued on next page...

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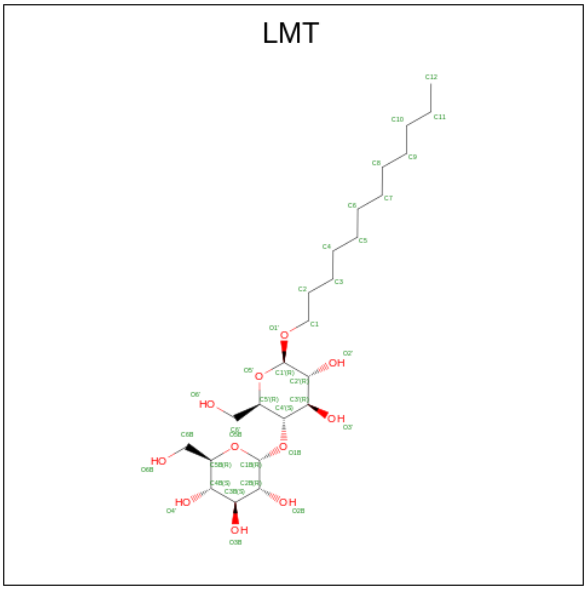
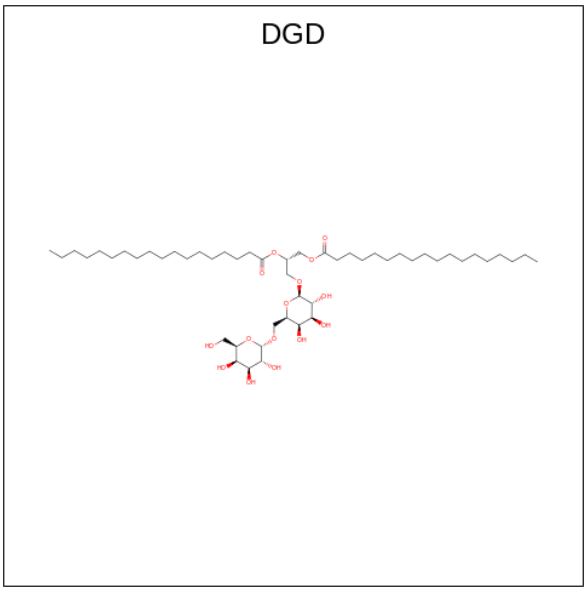
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
30	C	1	8	4	4	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	35	24	11	0
			Total	C	O	
31	B	1	31	20	11	0
			Total	C	O	
31	G	1	35	24	11	0
			Total	C	O	
31	K	1	35	24	11	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 33 is water.

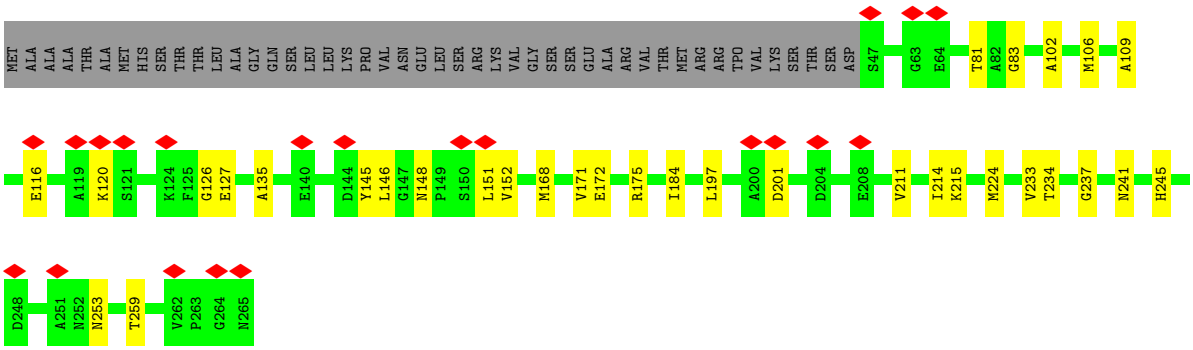
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
33	A	2	2	2	0

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.

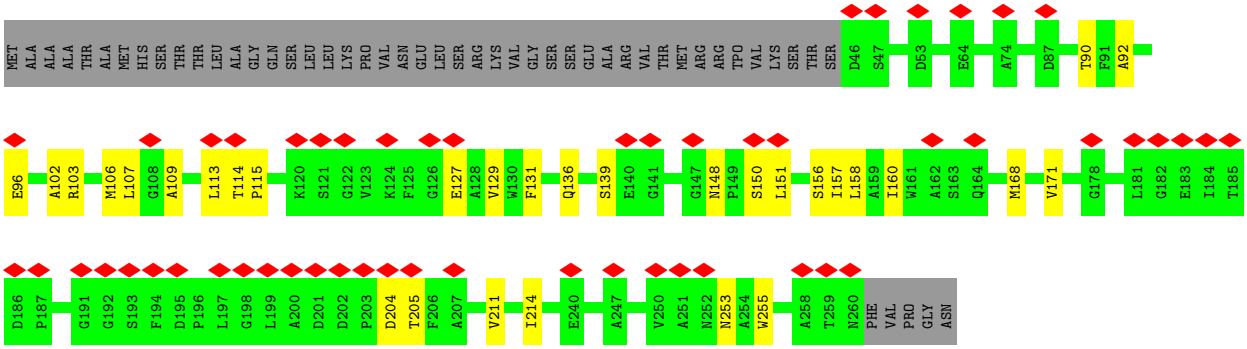
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain U:



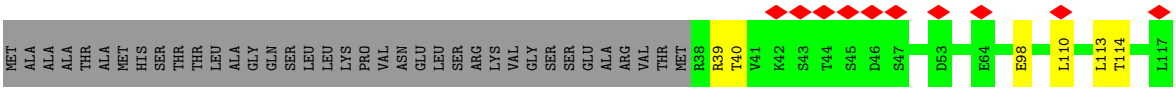
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

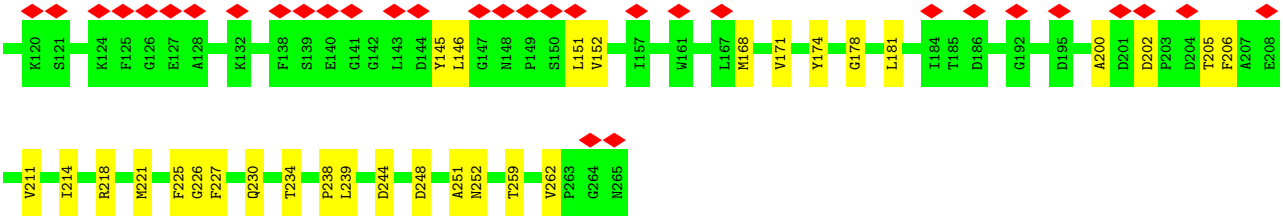
Chain V:



• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

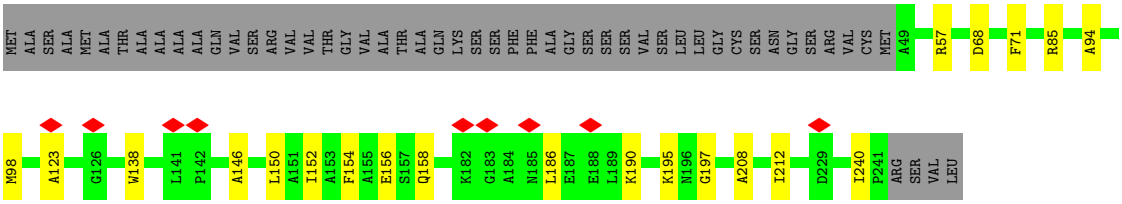
Chain W:





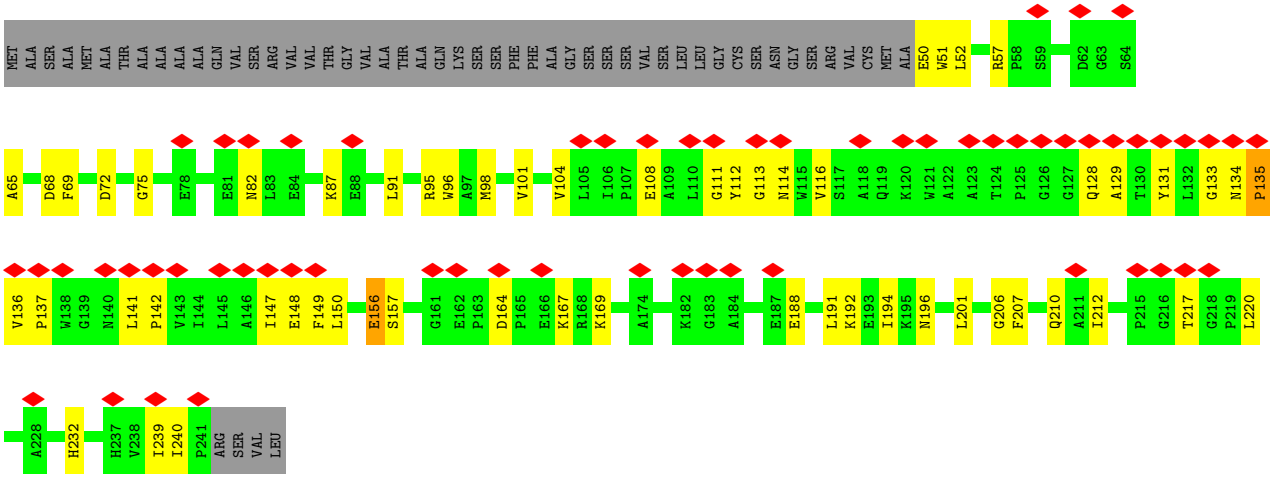
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



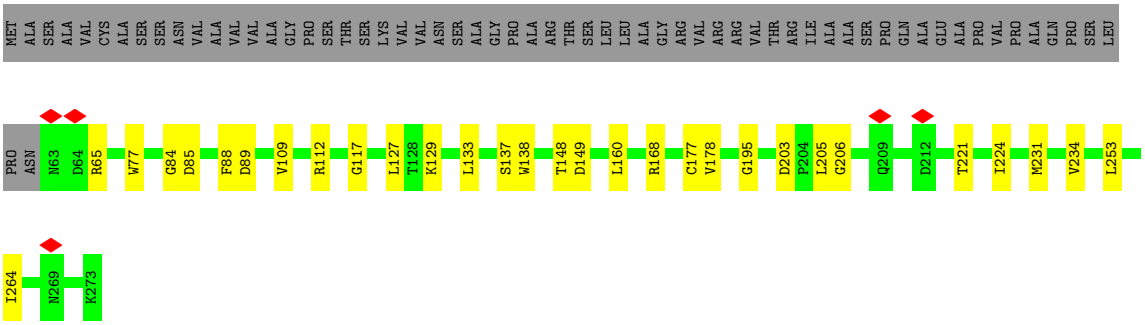
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



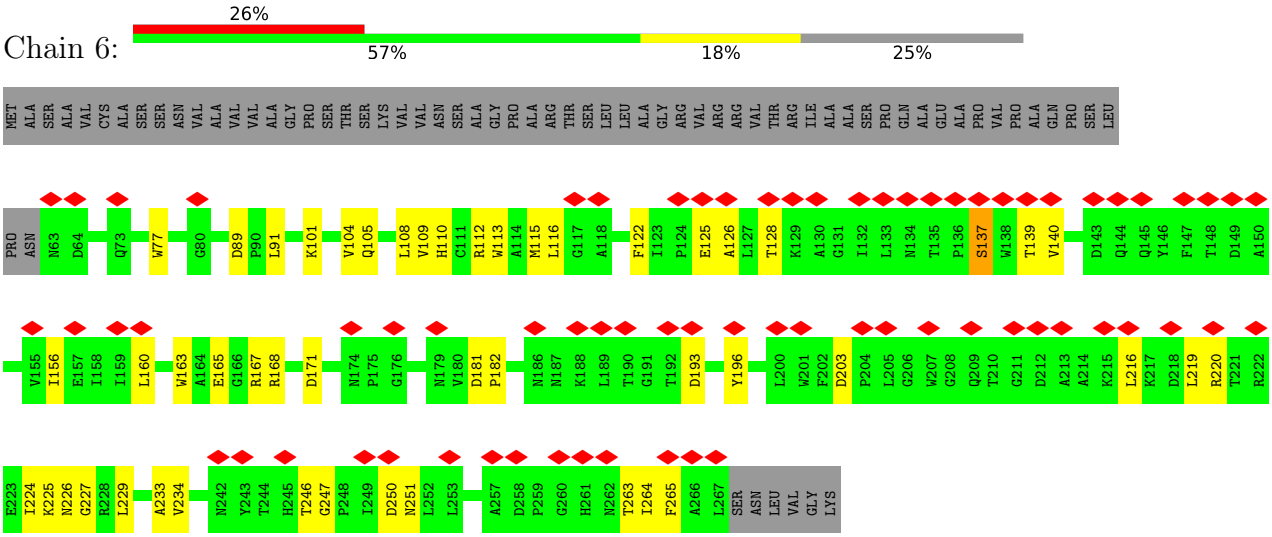
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



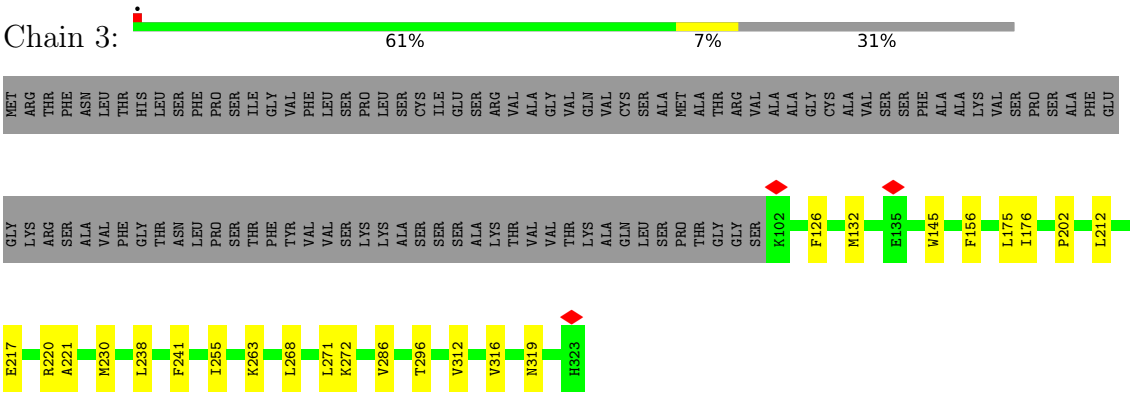
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



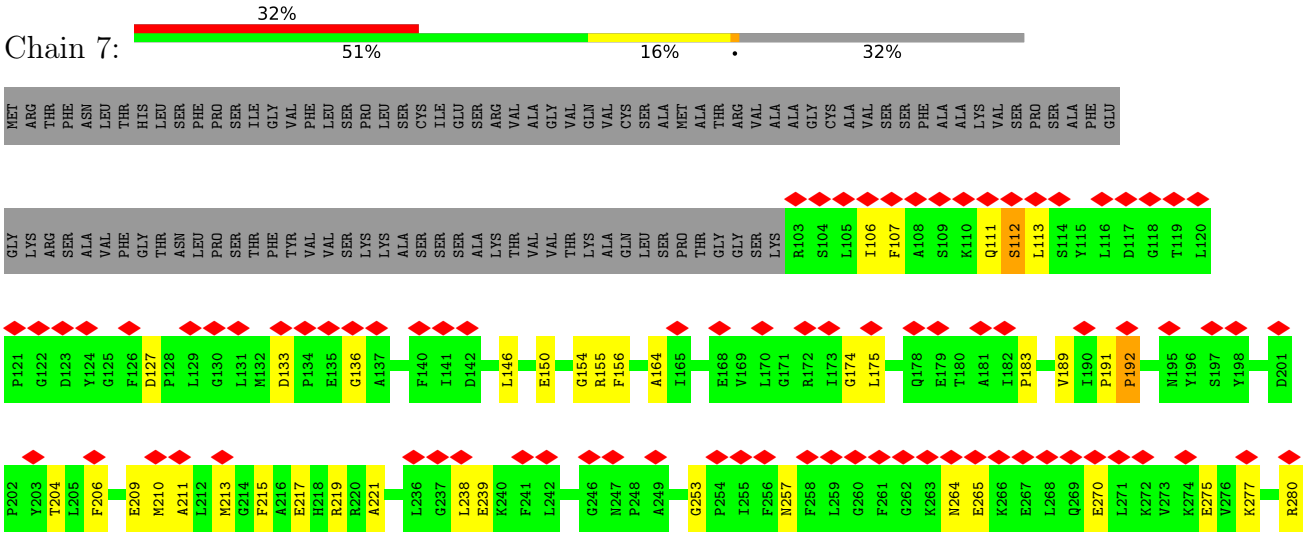
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

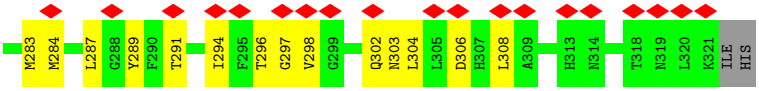
Chain 3:



- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

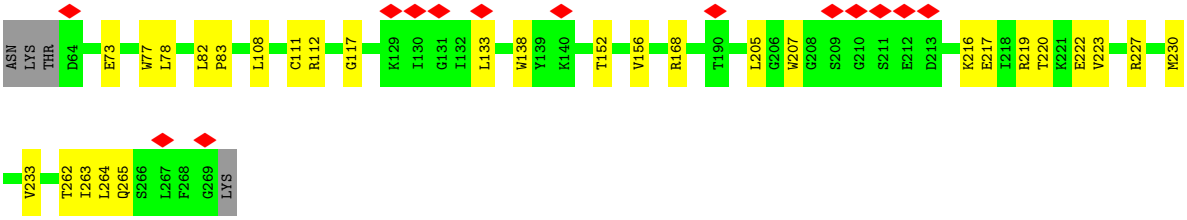
Chain 7:





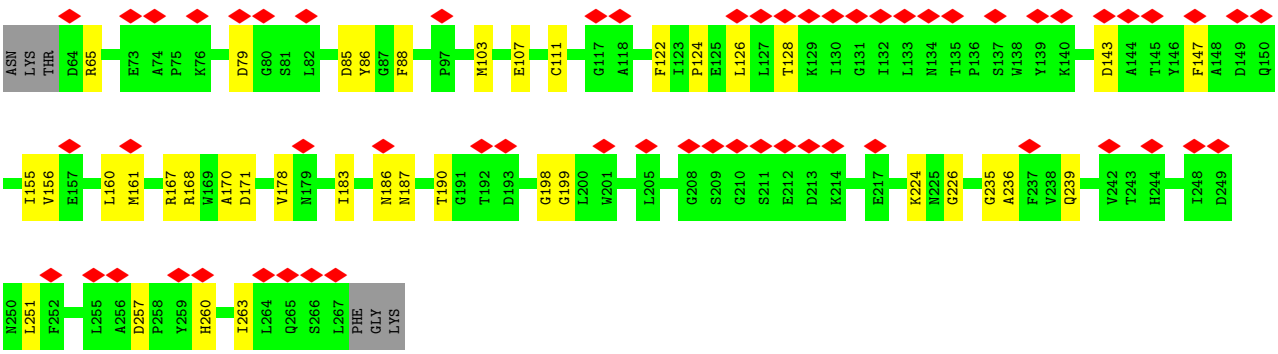
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



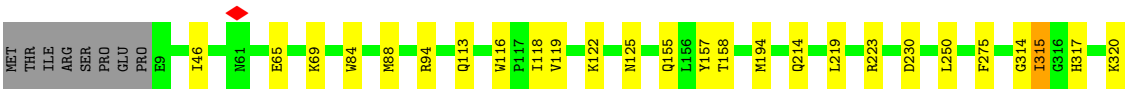
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

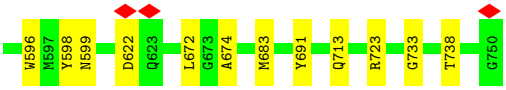
Chain 8:



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

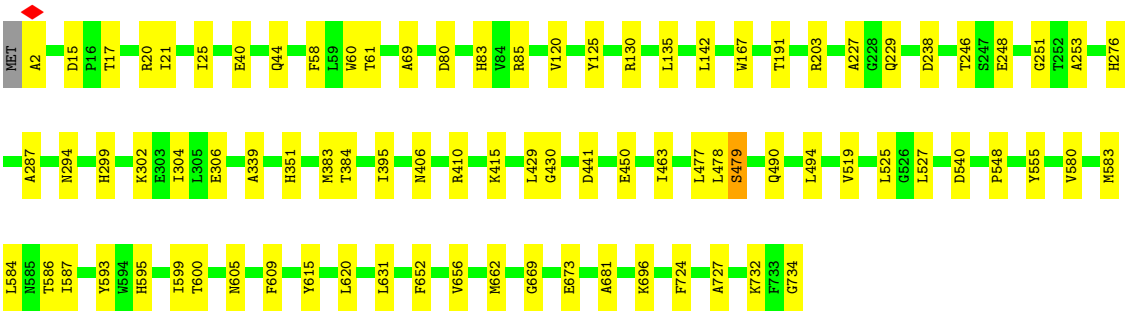
Chain A:





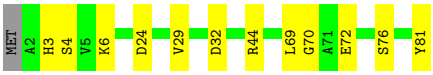
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 88% 12%



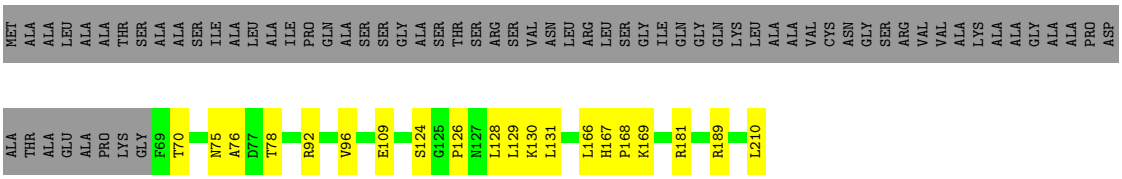
• Molecule 8: Photosystem I iron-sulfur center

Chain C: 84% 15%



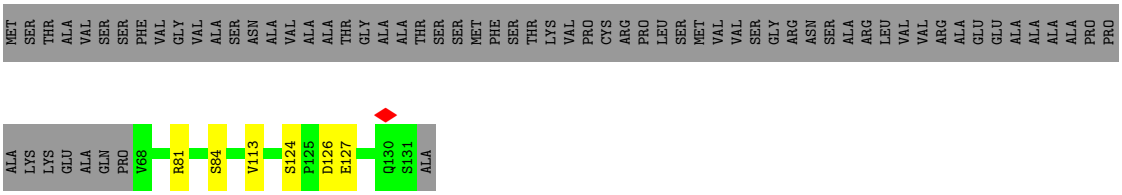
• Molecule 9: Photosystem I reaction center subunit II, chloroplastic

Chain D: 58% 10% 32%



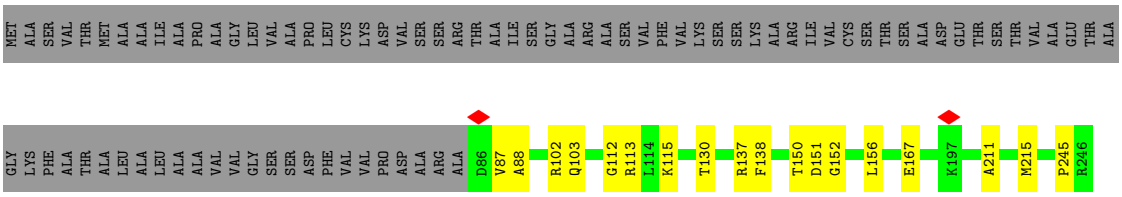
• Molecule 10: Photosystem I reaction center subunit IV, chloroplastic

Chain E: 44% 5% 52%



• Molecule 11: Photosystem I reaction center subunit III

Chain F: 58% 7% 35%



• Molecule 12: Photosystem I reaction center subunit V, chloroplastic

Chain G: 53% 10% 37%

MET ALA SER CYS ALA ALA SER MET THR GLY VAL ALA ALA SER SER LEU SER LEU LYS ALA ASN PHE SER GLY LEU ARG ARG GLY THR LYS VAL ASP SER ILE ALA MET SER ARG SER SER SER PHE ALA SER LYS THR ALA ILE ALA LYS SER SER GLY LYS VAL THR CYS GLU A59 N60

T61 G76 Q84 R85 V88 V95 T100 D103 Q110 E111 V112 K117 G123 F124 T125 I126 W132 T146 Q154 F155

- Molecule 13: Photosystem I reaction center subunit VI, chloroplastic

Chain H: 7% 60% 9% 32%

MET ALA ALA ALA SER ALA THR MET ALA VAL SER GLY LEU ALA GLY SER SER LEU ALA GLY GLN LYS PHE ALA ILE ALA PRO ALA LYS SER VAL SER VAL ARG SER PRO SER LYS VAL GLY ALA ILE SER ALA K45 Y46 G47 E48 F53 Y76 F84 F87 A88 G89 A90 F91

T92 K93 R94 G95 L96 G104 T108 L112 S116 D119 M133 G134 K139

- Molecule 14: Photosystem I reaction center subunit VIII

Chain I: 81% 14% 6%

M1 I9 L13 F18 P19 E34 ILE ILE

- Molecule 15: Photosystem I reaction center subunit IX

Chain J: 95% 5%

M1 E28 R31 L41

- Molecule 16: Photosystem I subunit X

Chain K: 60% 39%

MET ALA ALA MET ALA THR THR MET SER VAL ALA ALA THR VAL ARG GLN PHE GLU GLY LEU LYS ALA THR THR SER SER PHE SER LYS PRO LEU PRO SER LEU ALA LEU ARG LYS THR ALA GLY LYS GLY ALA LEU GLY ALA ARG CYS ASP Y50 M66 D92 V117 A130 GLY LEU

- Molecule 17: PSI subunit V

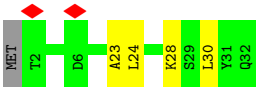
Chain L: 67% 6% 27%

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

E61 V65 I66 E67 P68 L69 E79 T80 P81 S85 E110 L125 R135 T148 M152 V222 K223

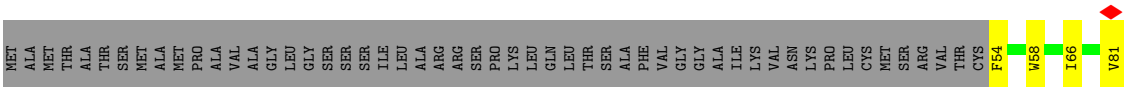
• Molecule 18: Photosystem I reaction center subunit XII

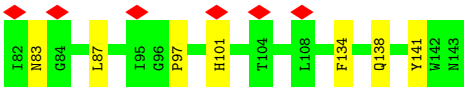
Chain M:



• Molecule 19: Photosystem I subunit O

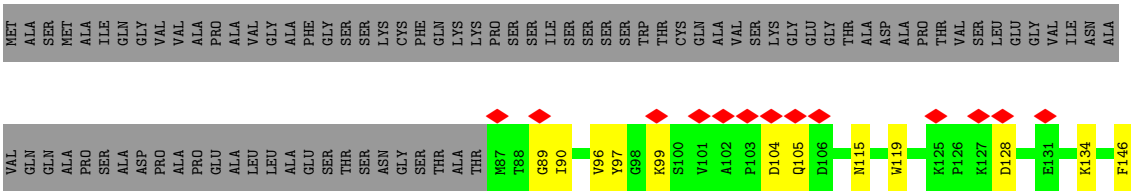
Chain O:

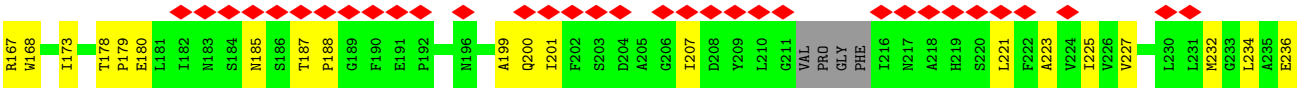




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: TPO, LMG, LHG, LUT, SF4, LMT, DGD, CHL, NEX, CLA, XAT, PQN, BCR

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	U	0.16	0/1708	0.32	0/2327
1	V	0.15	0/1677	0.28	0/2284
1	W	0.15	0/1770	0.30	0/2406
2	1	0.21	0/1527	0.39	0/2088
2	5	0.18	0/1522	0.47	2/2081 (0.1%)
3	2	0.15	0/1676	0.31	0/2296
3	6	0.21	0/1634	0.38	0/2240
4	3	0.16	0/1770	0.32	0/2400
4	7	0.27	1/1738 (0.1%)	0.50	4/2360 (0.2%)
5	4	0.15	0/1650	0.32	0/2255
5	8	0.13	0/1631	0.30	0/2230
6	A	0.19	0/6032	0.32	0/8227
7	B	0.16	0/6064	0.31	1/8274 (0.0%)
8	C	0.14	0/605	0.30	0/821
9	D	0.13	0/1142	0.31	0/1546
10	E	0.13	0/518	0.28	0/704
11	F	0.20	0/1277	0.36	0/1725
12	G	0.12	0/758	0.25	0/1034
13	H	0.16	0/753	0.28	0/1013
14	I	0.25	0/273	0.40	0/373
15	J	0.16	0/334	0.29	0/457
16	K	0.13	0/571	0.22	0/773
17	L	0.20	0/1263	0.33	0/1725
18	M	0.19	0/231	0.27	0/312
19	O	0.19	0/738	0.39	0/1009
20	9	0.18	0/1764	0.42	1/2397 (0.0%)
All	All	0.18	1/40626 (0.0%)	0.34	8/55357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7	183	PRO	CG-CD	-7.87	1.24	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	7	183	PRO	N-CD-CG	-11.22	86.37	103.20
4	7	183	PRO	CA-N-CD	-6.75	102.55	112.00
4	7	192	PRO	CA-N-CD	-5.89	103.75	112.00
7	B	479	SER	N-CA-C	-5.75	106.25	113.72
4	7	183	PRO	CA-CB-CG	-5.72	93.63	104.50
2	5	147	ILE	N-CA-C	-5.50	108.48	113.71
2	5	156	GLU	CA-CB-CG	5.40	124.90	114.10
20	9	200	GLN	CB-CG-CD	-5.14	103.86	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1659	0	1592	31	0
1	V	1630	0	1562	22	0
1	W	1734	0	1665	21	0
2	1	1478	0	1453	16	0
2	5	1473	0	1448	58	0
3	2	1625	0	1584	24	0
3	6	1583	0	1537	42	0
4	3	1719	0	1685	23	0
4	7	1687	0	1651	47	0
5	4	1600	0	1567	25	0
5	8	1582	0	1553	37	0
6	A	5837	0	5725	61	0
7	B	5850	0	5622	61	0
8	C	595	0	573	10	0
9	D	1114	0	1116	12	0
10	E	507	0	503	4	0
11	F	1251	0	1303	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	740	0	723	14	0
13	H	736	0	721	7	0
14	I	266	0	274	3	0
15	J	325	0	341	1	0
16	K	565	0	587	2	0
17	L	1228	0	1238	11	0
18	M	230	0	251	4	0
19	O	711	0	705	9	0
20	9	1713	0	1675	46	0
21	1	103	0	78	2	0
21	2	289	0	210	10	0
21	3	56	0	47	1	0
21	4	182	0	122	7	0
21	5	90	0	61	5	0
21	6	310	0	243	9	0
21	7	46	0	31	3	0
21	8	186	0	128	6	0
21	9	207	0	132	17	0
21	U	319	0	267	8	0
21	V	263	0	168	3	0
21	W	259	0	156	2	0
22	1	645	0	581	4	0
22	2	400	0	322	6	0
22	3	745	0	719	14	0
22	4	532	0	474	12	0
22	5	568	0	442	15	0
22	6	416	0	357	8	0
22	7	626	0	498	16	0
22	8	526	0	448	16	0
22	9	401	0	348	9	0
22	A	2769	0	2877	40	0
22	B	2419	0	2498	39	0
22	F	155	0	137	3	0
22	G	141	0	105	4	0
22	H	38	0	26	0	0
22	J	50	0	39	0	0
22	K	204	0	183	3	0
22	L	190	0	203	3	0
22	O	109	0	55	3	0
22	U	464	0	467	7	0
22	V	387	0	306	5	0
22	W	383	0	308	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	1	42	0	56	2	0
23	2	42	0	56	4	0
23	3	42	0	56	0	0
23	4	42	0	56	1	0
23	5	42	0	56	3	0
23	6	42	0	56	2	0
23	7	42	0	56	2	0
23	8	42	0	56	2	0
23	9	126	0	168	15	0
23	U	84	0	112	6	0
23	V	84	0	112	3	0
23	W	84	0	112	3	0
24	1	44	0	56	3	0
24	2	44	0	56	7	0
24	3	44	0	56	5	0
24	4	44	0	56	11	0
24	5	44	0	56	7	0
24	6	44	0	56	5	0
24	7	44	0	56	3	0
24	8	44	0	56	3	0
24	U	44	0	56	0	0
24	V	44	0	56	0	0
24	W	44	0	56	1	0
25	9	44	0	56	4	0
25	U	44	0	56	1	0
25	V	44	0	56	2	0
25	W	44	0	56	2	0
26	1	49	0	74	2	0
26	2	32	0	34	0	0
26	3	32	0	34	0	0
26	4	38	0	46	3	0
26	5	37	0	44	0	0
26	6	32	0	34	2	0
26	7	34	0	38	0	0
26	8	38	0	46	0	0
26	9	28	0	26	0	0
26	A	78	0	99	0	0
26	B	35	0	40	0	0
26	U	45	0	60	1	0
26	V	42	0	54	0	0
26	W	45	0	60	1	0
27	1	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	2	40	0	56	4	0
27	3	80	0	112	13	0
27	4	40	0	56	11	0
27	6	40	0	56	5	0
27	7	80	0	112	10	0
27	8	40	0	56	8	0
27	A	239	0	333	27	0
27	B	280	0	392	30	0
27	F	40	0	56	3	0
27	G	40	0	56	4	0
27	I	40	0	56	4	0
27	J	40	0	56	4	0
27	K	80	0	112	11	0
27	L	120	0	168	13	0
27	M	40	0	56	5	0
27	O	40	0	56	5	0
28	2	47	0	67	0	0
28	A	34	0	38	0	0
28	G	32	0	34	2	0
28	J	90	0	126	0	0
28	L	44	0	58	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	A	35	0	46	0	0
31	B	31	0	35	0	0
31	G	35	0	46	0	0
31	K	35	0	46	0	0
32	B	66	0	96	0	0
33	A	2	0	0	0	0
All	All	57715	0	56700	868	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 8.

All (868) 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)
27:L:305:BCR:HC8	27:L:305:BCR:H331	1.56	0.86
4:7:164:ALA:HB2	24:7:619:XAT:H163	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:823:CLA:CBC	27:B:1609:BCR:H343	2.11	0.81
2:5:108:GLU:HB3	2:5:220:LEU:HD21	1.63	0.79
2:5:52:LEU:HD21	21:5:601:CHL:HMA3	1.68	0.76
27:A:856:BCR:H331	27:A:856:BCR:HC8	1.68	0.76
27:3:620:BCR:H383	27:3:620:BCR:H23C	1.68	0.75
7:B:519:VAL:HG11	7:B:593:TYR:CE1	2.21	0.75
6:A:125:ASN:O	11:F:113:ARG:NH2	2.20	0.74
22:B:823:CLA:HBC3	27:B:1609:BCR:H343	1.68	0.74
4:7:284:MET:HE2	4:7:284:MET:HA	1.70	0.74
27:A:851:BCR:H23C	27:A:851:BCR:H403	1.68	0.73
2:5:114:ASN:ND2	2:5:217:THR:O	2.21	0.73
4:7:150:GLU:OE2	4:7:280:ARG:NH1	2.20	0.73
27:L:306:BCR:H321	27:L:306:BCR:HC8	1.71	0.72
22:B:815:CLA:HMA1	27:B:845:BCR:H343	1.72	0.71
27:B:801:BCR:H383	27:B:801:BCR:H23C	1.72	0.71
27:F:305:BCR:H383	27:F:305:BCR:H23C	1.72	0.71
20:9:119:TRP:O	21:9:601:CHL:ND	2.24	0.71
2:5:128:GLN:NE2	22:5:604:CLA:OBD	2.23	0.71
1:W:98:GLU:OE2	1:W:214:ILE:HD11	1.91	0.70
7:B:351:HIS:ND1	22:B:817:CLA:OBD	2.25	0.70
22:B:813:CLA:HMC1	22:B:813:CLA:HBC2	1.73	0.70
5:8:239:GLN:OE1	22:8:613:CLA:NA	2.25	0.69
20:9:232:MET:HE1	25:9:623:NEX:H30	1.75	0.69
2:1:195:LYS:NZ	26:1:630:LHG:O5	2.24	0.69
7:B:519:VAL:HG11	7:B:593:TYR:CD1	2.28	0.69
20:9:232:MET:HE3	21:9:606:CHL:CMB	2.23	0.69
2:5:91:LEU:HD12	2:5:169:LYS:CE	2.23	0.69
2:5:91:LEU:HD12	2:5:169:LYS:HE2	1.74	0.68
25:9:623:NEX:H192	25:9:623:NEX:H183	1.75	0.68
2:1:208:ALA:O	2:1:212:ILE:HD12	1.92	0.68
20:9:232:MET:HE3	21:9:606:CHL:HMB1	1.75	0.68
20:9:285:MET:HE3	22:9:602:CLA:HMC2	1.75	0.67
27:B:845:BCR:H383	27:B:845:BCR:H23C	1.75	0.67
27:7:621:BCR:H331	27:7:621:BCR:HC8	1.77	0.67
4:7:298:VAL:HG13	4:7:302:GLN:NE2	2.10	0.67
4:7:238:LEU:O	4:7:238:LEU:HD12	1.95	0.66
4:3:296:THR:HG22	4:3:319:ASN:OD1	1.95	0.66
27:7:620:BCR:H321	27:7:620:BCR:HC8	1.75	0.66
1:W:211:VAL:O	1:W:214:ILE:HG22	1.96	0.66
27:3:620:BCR:H331	27:3:620:BCR:HC8	1.77	0.66
22:4:611:CLA:NC	26:4:630:LHG:O5	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:174:GLY:O	4:7:175:LEU:HD12	1.96	0.66
1:U:259:THR:O	1:U:259:THR:HG22	1.95	0.65
22:4:604:CLA:C2B	27:4:621:BCR:H323	2.27	0.65
27:M:2001:BCR:H23C	27:M:2001:BCR:H382	1.79	0.65
4:7:221:ALA:HB2	22:7:609:CLA:HMA1	1.78	0.65
27:2:621:BCR:H382	27:2:621:BCR:H23C	1.79	0.65
5:4:133:LEU:HD23	5:4:133:LEU:O	1.97	0.64
2:5:239:ILE:HG21	5:8:155:ILE:HD11	1.80	0.64
22:7:606:CLA:H3A	27:7:620:BCR:C21	2.27	0.64
20:9:199:ALA:N	21:9:607:CHL:O1D	2.31	0.64
1:V:106:MET:HE1	22:V:610:CLA:CAB	2.28	0.64
4:7:302:GLN:NE2	4:7:303:ASN:OD1	2.30	0.64
22:A:829:CLA:HED1	22:A:830:CLA:H3A	1.80	0.64
22:3:606:CLA:H3A	27:3:620:BCR:C21	2.27	0.64
27:7:621:BCR:H331	27:7:621:BCR:C8	2.28	0.64
27:B:843:BCR:H382	27:B:843:BCR:H23C	1.79	0.64
27:K:205:BCR:H391	22:9:611:CLA:C2	2.28	0.63
20:9:285:MET:HE1	23:9:621:LUT:H391	1.81	0.63
6:A:122:LYS:NZ	11:F:130:THR:OG1	2.26	0.63
7:B:40:GLU:OE2	7:B:44:GLN:NE2	2.31	0.63
12:G:146:THR:HG21	28:G:202:LMG:HC91	1.80	0.63
24:5:618:XAT:H28	24:5:618:XAT:H361	1.79	0.63
5:8:186:ASN:OD1	5:8:187:ASN:N	2.31	0.63
5:4:111:CYS:SG	5:4:230:MET:HE2	2.38	0.63
1:V:106:MET:HE2	23:V:2620:LUT:C34	2.28	0.62
6:A:275:PHE:HD1	22:A:819:CLA:HMB2	1.64	0.62
1:W:225:PHE:CE1	1:W:225:PHE:CG	2.84	0.62
27:A:856:BCR:H331	27:A:856:BCR:C8	2.29	0.62
27:J:102:BCR:H383	27:J:102:BCR:H23C	1.81	0.62
21:U:607:CHL:HED1	1:W:262:VAL:HG21	1.80	0.62
3:6:263:THR:HG23	3:6:265:PHE:H	1.65	0.62
20:9:236:GLU:HG3	22:9:609:CLA:C4B	2.29	0.62
6:A:564:LYS:NZ	7:B:673:GLU:OE2	2.32	0.61
22:2:604:CLA:C3B	24:2:620:XAT:H183	2.30	0.61
6:A:399:VAL:HG13	27:A:851:BCR:H343	1.83	0.61
15:J:28:GLU:OE1	15:J:31:ARG:NH1	2.32	0.61
2:5:149:PHE:O	2:5:150:LEU:HD22	1.99	0.61
27:7:620:BCR:H321	27:7:620:BCR:C8	2.31	0.61
1:U:197:LEU:HD22	20:9:260:LEU:HD21	1.81	0.61
12:G:84:GLN:OE1	12:G:85:ARG:NH1	2.32	0.61
6:A:598:TYR:OH	22:A:801:CLA:HED2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:9:148:LEU:HD23	23:9:624:LUT:C24	2.31	0.61
6:A:371:MET:SD	6:A:504:SER:HB2	2.40	0.61
6:A:418:THR:HG23	6:A:419:GLN:HE21	1.66	0.61
5:8:65:ARG:NH2	5:8:85:ASP:OD1	2.34	0.60
2:5:87:LYS:HB3	2:5:169:LYS:NZ	2.16	0.60
27:L:306:BCR:H321	27:L:306:BCR:C8	2.32	0.60
27:1:619:BCR:H382	27:1:619:BCR:H23C	1.83	0.60
27:3:620:BCR:H331	27:3:620:BCR:C8	2.30	0.60
22:A:816:CLA:H3A	22:A:816:CLA:O2A	2.01	0.60
27:A:852:BCR:H362	22:A:854:CLA:H2	1.81	0.60
22:8:604:CLA:HMB3	24:8:620:XAT:H371	1.81	0.60
22:B:804:CLA:H3A	18:M:30:LEU:HD13	1.82	0.60
1:U:172:GLU:HG3	21:U:609:CHL:C4B	2.31	0.59
5:4:227:ARG:HA	5:4:230:MET:HE3	1.83	0.59
9:D:167:HIS:HB3	9:D:168:PRO:HD3	1.83	0.59
3:6:77:TRP:NE1	3:6:89:ASP:OD2	2.35	0.59
4:7:291:THR:HG21	22:7:613:CLA:HAC2	1.83	0.59
6:A:113:GLN:NE2	22:A:810:CLA:OBD	2.34	0.59
6:A:471:ASP:O	6:A:475:GLN:NE2	2.35	0.59
2:1:57:ARG:NH2	2:1:68:ASP:OD1	2.36	0.59
27:O:2004:BCR:H383	27:O:2004:BCR:H23C	1.85	0.59
6:A:403:ALA:HB2	27:A:851:BCR:H323	1.85	0.59
1:V:136:GLN:O	1:V:139:SER:OG	2.21	0.59
2:5:188:GLU:O	2:5:192:LYS:HG3	2.03	0.59
1:U:135:ALA:HB2	21:U:607:CHL:HED2	1.84	0.59
22:B:823:CLA:HBC2	27:B:1609:BCR:H343	1.84	0.59
5:4:112:ARG:NH1	21:4:608:CHL:OBD	2.35	0.59
2:5:108:GLU:CB	2:5:220:LEU:HD21	2.33	0.59
7:B:238:ASP:OD1	7:B:251:GLY:N	2.36	0.59
27:B:848:BCR:H383	27:B:848:BCR:H23C	1.84	0.59
6:A:495:THR:HG21	22:A:836:CLA:HMD1	1.85	0.58
7:B:61:THR:HG23	7:B:142:LEU:HD13	1.85	0.58
2:5:210:GLN:OE1	22:5:613:CLA:C4D	2.51	0.58
4:7:291:THR:HG21	22:7:613:CLA:CAC	2.33	0.58
5:8:161:MET:HE2	27:8:621:BCR:H352	1.84	0.58
3:6:216:LEU:O	3:6:220:ARG:HG2	2.04	0.58
7:B:696:LYS:NZ	8:C:81:TYR:O	2.35	0.58
5:4:112:ARG:NE	5:4:222:GLU:OE2	2.36	0.58
22:7:610:CLA:HMC2	23:7:618:LUT:C31	2.34	0.58
3:2:231:MET:HE1	21:2:602:CHL:CBB	2.33	0.58
3:6:101:LYS:O	3:6:104:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:237:GLY:O	1:U:241:ASN:ND2	2.32	0.58
4:3:217:GLU:OE1	4:3:220:ARG:NH2	2.36	0.58
7:B:294:ASN:ND2	12:G:110:GLN:O	2.35	0.58
2:5:50:GLU:N	2:5:69:PHE:O	2.37	0.58
2:5:128:GLN:HG2	2:5:129:ALA:H	1.68	0.58
3:6:122:PHE:O	3:6:126:ALA:N	2.32	0.58
1:W:113:LEU:HD22	1:W:239:LEU:HD21	1.86	0.58
3:2:112:ARG:NE	21:2:608:CHL:OBD	2.35	0.58
3:2:160:LEU:HD23	21:2:606:CHL:HMA2	1.86	0.58
22:5:603:CLA:HBC3	24:5:618:XAT:H391	1.86	0.58
12:G:85:ARG:NH2	12:G:123:GLY:O	2.37	0.57
19:O:134:PHE:O	19:O:138:GLN:NE2	2.36	0.57
19:O:97:PRO:O	19:O:101:HIS:ND1	2.37	0.57
7:B:339:ALA:HB2	27:B:847:BCR:H372	1.85	0.57
2:5:131:TYR:C	2:5:133:GLY:H	2.12	0.57
4:3:230:MET:HA	4:3:230:MET:HE2	1.86	0.57
22:B:824:CLA:H2A	22:B:824:CLA:O1A	2.02	0.57
22:U:604:CLA:CED	22:U:604:CLA:H2A	2.35	0.57
6:A:317:HIS:HB3	6:A:322:ILE:HD11	1.87	0.56
7:B:384:THR:HG21	7:B:583:MET:HG2	1.86	0.56
27:3:621:BCR:H331	27:3:621:BCR:C8	2.35	0.56
20:9:207:ILE:HG21	21:9:606:CHL:HMD3	1.87	0.56
20:9:285:MET:HE3	22:9:602:CLA:CMC	2.35	0.56
3:2:88:PHE:CE2	24:2:620:XAT:H383	2.39	0.56
22:2:610:CLA:H52	23:2:619:LUT:H10	1.87	0.56
5:4:216:LYS:O	5:4:219:ARG:N	2.39	0.56
6:A:320:LYS:NZ	6:A:340:GLU:OE2	2.38	0.56
2:5:108:GLU:HG2	2:5:113:GLY:O	2.04	0.56
4:7:111:GLN:O	4:7:113:LEU:N	2.38	0.56
9:D:109:GLU:OE2	9:D:124:SER:N	2.39	0.56
2:5:232:HIS:NE2	5:8:147:PHE:O	2.39	0.56
22:8:602:CLA:H2	24:8:620:XAT:H162	1.87	0.56
1:W:259:THR:O	1:W:259:THR:HG22	2.05	0.56
3:2:88:PHE:HE2	24:2:620:XAT:H383	1.71	0.56
6:A:379:THR:HG21	6:A:515:VAL:HB	1.87	0.56
17:L:125:LEU:HD12	22:L:304:CLA:HMB1	1.87	0.56
3:6:165:GLU:OE1	3:6:168:ARG:NH2	2.39	0.56
26:4:630:LHG:O5	26:4:630:LHG:O7	2.24	0.56
6:A:118:ILE:HG23	6:A:119:VAL:N	2.21	0.55
18:M:23:ALA:HB2	27:M:2001:BCR:H342	1.88	0.55
22:1:611:CLA:H2A	22:1:611:CLA:HED2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:617:CLA:C4B	22:3:617:CLA:C1C	2.84	0.55
2:5:87:LYS:HB3	2:5:169:LYS:HZ1	1.70	0.55
5:8:107:GLU:OE1	22:8:602:CLA:NA	2.39	0.55
26:W:2630:LHG:O3	26:W:2630:LHG:O1	2.18	0.55
3:6:108:LEU:HD22	3:6:196:TYR:OH	2.05	0.55
4:7:189:VAL:O	22:7:607:CLA:NB	2.39	0.55
5:8:235:GLY:O	5:8:239:GLN:N	2.31	0.55
21:8:618:CHL:HAB	27:8:621:BCR:H372	1.87	0.55
6:A:315:ILE:O	6:A:315:ILE:HG13	2.06	0.55
1:V:92:ALA:O	1:V:96:GLU:OE1	2.25	0.55
27:K:202:BCR:H383	27:K:202:BCR:H23C	1.88	0.55
3:6:163:TRP:O	3:6:167:ARG:HG2	2.06	0.55
22:2:604:CLA:C2B	24:2:620:XAT:H183	2.37	0.55
6:A:430:HIS:CE1	22:A:832:CLA:ND	2.76	0.54
20:9:104:ASP:OD1	20:9:105:GLN:N	2.39	0.54
11:F:103:GLN:HG2	11:F:138:PHE:CD2	2.42	0.54
17:L:67:GLU:OE1	19:O:54:PHE:N	2.40	0.54
27:B:845:BCR:H383	27:B:845:BCR:C23	2.38	0.54
3:6:167:ARG:HD2	22:8:601:CLA:OBD	2.07	0.54
5:8:190:THR:OG1	5:8:199:GLY:N	2.37	0.54
20:9:97:TYR:CE1	20:9:268:ILE:HD11	2.43	0.54
23:9:624:LUT:H181	23:9:624:LUT:H8	1.90	0.54
1:V:156:SER:O	1:V:160:ILE:HD12	2.07	0.54
5:8:257:ASP:OD2	5:8:260:HIS:HB2	2.08	0.54
1:U:145:TYR:O	1:U:146:LEU:HB2	2.06	0.54
22:A:802:CLA:CGA	22:A:802:CLA:H3A	2.38	0.54
12:G:112:VAL:HG23	12:G:112:VAL:O	2.08	0.54
27:A:852:BCR:C32	27:A:852:BCR:HC8	2.38	0.54
1:U:233:VAL:HG13	1:U:234:THR:HG23	1.90	0.53
1:V:109:ALA:O	1:V:113:LEU:HD23	2.07	0.53
4:3:126:PHE:HE2	24:3:619:XAT:H383	1.73	0.53
1:W:110:LEU:O	1:W:114:THR:HG23	2.09	0.53
27:O:2004:BCR:H321	27:O:2004:BCR:HC8	1.90	0.53
2:1:138:TRP:NE1	22:1:606:CLA:OBD	2.38	0.53
6:A:683:MET:HB3	22:A:802:CLA:C1C	2.38	0.53
17:L:148:THR:HG22	17:L:152:MET:HE3	1.90	0.53
27:O:2004:BCR:HC8	27:O:2004:BCR:C32	2.38	0.53
4:7:287:LEU:O	4:7:291:THR:HG22	2.08	0.53
4:7:296:THR:HG22	4:7:297:GLY:H	1.74	0.53
7:B:583:MET:SD	7:B:584:LEU:N	2.82	0.53
22:F:304:CLA:C1A	22:F:304:CLA:C4D	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:827:CLA:CHC	27:A:851:BCR:H342	2.39	0.53
7:B:302:LYS:O	7:B:306:GLU:HG2	2.09	0.53
27:G:205:BCR:H23C	27:G:205:BCR:H382	1.91	0.53
3:2:65:ARG:NH2	3:2:85:ASP:OD1	2.42	0.53
4:3:126:PHE:CE2	24:3:619:XAT:H383	2.44	0.53
3:6:171:ASP:OD2	21:6:608:CHL:HBC1	2.09	0.53
1:V:127:GLU:O	1:V:136:GLN:NE2	2.41	0.53
13:H:133:MET:SD	13:H:134:GLY:O	2.67	0.53
13:H:112:LEU:O	13:H:116:SER:OG	2.23	0.52
21:4:608:CHL:HBB1	21:4:608:CHL:HMB1	1.91	0.52
22:A:810:CLA:HAB	22:B:833:CLA:HMD2	1.91	0.52
24:5:618:XAT:H361	24:5:618:XAT:C28	2.38	0.52
5:8:263:ILE:N	22:8:613:CLA:O1A	2.42	0.52
20:9:234:LEU:HD23	25:9:623:NEX:H203	1.90	0.52
21:9:607:CHL:HHC	21:9:607:CHL:HBB1	1.90	0.52
27:B:801:BCR:H312	22:B:833:CLA:H61	1.90	0.52
5:8:103:MET:HE3	5:8:103:MET:HA	1.91	0.52
20:9:173:ILE:HG21	23:9:620:LUT:H12	1.92	0.52
20:9:180:GLU:HG3	20:9:302:LEU:HD12	1.91	0.52
3:2:117:GLY:HA2	24:2:620:XAT:H181	1.90	0.52
22:7:609:CLA:HBC1	24:7:619:XAT:C19	2.40	0.52
5:4:263:ILE:HG23	5:4:264:LEU:HD22	1.92	0.52
17:L:125:LEU:HD21	17:L:223:LYS:HA	1.91	0.52
27:7:620:BCR:C23	27:7:620:BCR:H383	2.38	0.52
20:9:99:LYS:NZ	20:9:271:GLU:OE1	2.42	0.52
5:4:233:VAL:HG11	24:4:620:XAT:H12	1.91	0.52
22:G:201:CLA:HMD1	28:G:202:LMG:O5	2.10	0.52
4:7:264:ASN:OD1	4:7:265:GLU:N	2.36	0.52
5:8:161:MET:HE1	27:8:621:BCR:H341	1.89	0.52
3:2:234:VAL:HG11	24:2:620:XAT:H12	1.91	0.52
22:7:602:CLA:CGA	22:7:602:CLA:H3A	2.40	0.52
5:8:86:TYR:N	22:8:602:CLA:OBD	2.36	0.52
5:8:161:MET:HG3	22:8:609:CLA:HMC3	1.92	0.52
5:4:262:THR:OG1	5:4:265:GLN:OE1	2.26	0.52
6:A:503:THR:HG21	22:A:828:CLA:HAB	1.92	0.52
22:B:813:CLA:HMC1	22:B:813:CLA:CBC	2.38	0.51
1:U:233:VAL:HG13	1:U:234:THR:N	2.24	0.51
5:4:152:THR:O	5:4:156:VAL:HG23	2.10	0.51
7:B:662:MET:HB2	22:B:803:CLA:C1C	2.39	0.51
20:9:285:MET:HE2	23:9:621:LUT:H402	1.93	0.51
2:1:186:LEU:HD21	2:1:190:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:608:CHL:O1A	22:8:610:CLA:HMD2	2.11	0.51
22:8:614:CLA:O1D	22:8:614:CLA:H2A	2.10	0.51
20:9:96:VAL:O	20:9:96:VAL:HG22	2.10	0.51
27:B:844:BCR:H23C	27:B:844:BCR:H403	1.92	0.51
27:L:306:BCR:H23C	27:L:306:BCR:C38	2.41	0.51
2:5:128:GLN:HG2	2:5:129:ALA:N	2.25	0.51
23:9:624:LUT:C24	23:9:624:LUT:H372	2.40	0.51
27:4:621:BCR:H402	27:4:621:BCR:H23C	1.93	0.51
18:M:24:LEU:HD11	18:M:28:LYS:HE2	1.92	0.51
2:5:116:VAL:HG12	2:5:116:VAL:O	2.10	0.51
5:8:251:LEU:HD22	23:8:619:LUT:H172	1.92	0.51
13:H:76:TYR:OH	17:L:110:GLU:OE1	2.25	0.51
4:7:156:PHE:CD2	22:7:609:CLA:HMD3	2.45	0.51
1:U:245:HIS:CE1	22:U:614:CLA:NC	2.78	0.51
22:O:2002:CLA:O1D	22:O:2002:CLA:H2A	2.11	0.51
5:8:88:PHE:HE2	24:8:620:XAT:H173	1.76	0.51
4:3:316:VAL:N	22:3:613:CLA:O1A	2.40	0.51
3:6:225:LYS:NZ	26:6:630:LHG:O10	2.21	0.51
2:1:71:PHE:HE2	24:1:618:XAT:H183	1.75	0.51
27:3:620:BCR:H383	27:3:620:BCR:C23	2.40	0.51
7:B:429:LEU:HD11	22:B:837:CLA:HMB1	1.93	0.51
2:5:65:ALA:N	2:5:68:ASP:OD2	2.42	0.51
22:A:803:CLA:CGA	22:A:803:CLA:H3A	2.41	0.50
27:A:849:BCR:H383	27:A:849:BCR:H23C	1.92	0.50
27:A:852:BCR:HC8	27:A:852:BCR:H321	1.94	0.50
9:D:70:THR:HG23	9:D:70:THR:O	2.11	0.50
1:U:127:GLU:N	1:U:127:GLU:OE1	2.43	0.50
1:U:135:ALA:CB	21:U:607:CHL:HED2	2.42	0.50
17:L:222:VAL:O	17:L:222:VAL:HG13	2.11	0.50
2:5:156:GLU:HG3	22:5:609:CLA:C4B	2.42	0.50
2:1:123:ALA:HB1	12:G:155:PHE:HB2	1.93	0.50
2:5:96:TRP:CD1	22:5:609:CLA:HMD3	2.47	0.50
2:5:240:ILE:HG23	2:5:240:ILE:O	2.11	0.50
1:W:168:MET:HA	1:W:171:VAL:HG22	1.93	0.50
4:3:156:PHE:CD2	22:3:609:CLA:HMD3	2.46	0.50
27:J:102:BCR:H383	27:J:102:BCR:C23	2.41	0.50
27:L:305:BCR:H392	27:L:305:BCR:H23C	1.93	0.50
3:6:234:VAL:HG11	24:6:620:XAT:H12	1.94	0.50
27:7:620:BCR:H383	27:7:620:BCR:H23C	1.94	0.50
22:3:604:CLA:C2B	24:3:619:XAT:H183	2.42	0.50
5:4:117:GLY:HA2	24:4:620:XAT:H181	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:827:CLA:H203	27:A:851:BCR:H381	1.93	0.50
27:B:801:BCR:H381	22:F:301:CLA:HMC1	1.93	0.50
20:9:223:ALA:HB3	21:9:605:CHL:HMC	1.93	0.50
1:V:253:ASN:OD1	1:V:255:TRP:N	2.44	0.50
22:3:606:CLA:H3A	27:3:620:BCR:H21C	1.93	0.50
27:F:305:BCR:H383	27:F:305:BCR:C23	2.41	0.50
6:A:713:GLN:NE2	10:E:113:VAL:O	2.43	0.50
1:V:168:MET:HA	1:V:171:VAL:HG12	1.93	0.49
6:A:436:SER:OG	7:B:681:ALA:HB2	2.12	0.49
22:A:836:CLA:HMD2	22:A:837:CLA:HBB1	1.94	0.49
22:B:828:CLA:H191	27:B:845:BCR:H351	1.94	0.49
8:C:32:ASP:OD1	8:C:32:ASP:N	2.44	0.49
22:6:604:CLA:C1B	27:6:621:BCR:H402	2.42	0.49
4:7:296:THR:HG22	4:7:297:GLY:N	2.27	0.49
3:6:116:LEU:CD2	22:6:610:CLA:HMC1	2.43	0.49
3:6:182:PRO:HB2	27:6:621:BCR:H322	1.93	0.49
22:A:803:CLA:OBD	22:B:802:CLA:HMB3	2.13	0.49
9:D:92:ARG:O	9:D:96:VAL:HG22	2.13	0.49
27:3:620:BCR:HC8	27:3:620:BCR:C33	2.43	0.49
20:9:128:ASP:OD1	20:9:128:ASP:N	2.46	0.49
6:A:738:THR:OG1	22:A:801:CLA:HED1	2.12	0.49
2:5:149:PHE:O	2:5:149:PHE:CD1	2.65	0.49
4:7:277:LYS:O	4:7:280:ARG:HB2	2.12	0.49
5:8:122:PHE:O	5:8:126:LEU:N	2.39	0.49
19:O:87:LEU:HD23	19:O:87:LEU:H	1.76	0.49
1:U:83:GLY:O	1:V:90:THR:HG22	2.13	0.49
3:2:129:LYS:HE2	3:2:253:LEU:HD12	1.94	0.49
6:A:582:CYS:O	7:B:669:GLY:N	2.37	0.49
2:5:156:GLU:HG3	22:5:609:CLA:C1B	2.43	0.49
4:7:150:GLU:OE2	4:7:280:ARG:NH2	2.46	0.49
23:9:624:LUT:H181	23:9:624:LUT:C8	2.43	0.49
3:6:225:LYS:HD2	26:6:630:LHG:C23	2.43	0.49
27:2:621:BCR:H11C	27:2:621:BCR:H341	1.68	0.49
22:A:837:CLA:O2D	22:A:837:CLA:H2A	2.13	0.49
20:9:201:ILE:HD12	21:9:606:CHL:CBC	2.42	0.49
22:B:814:CLA:H3A	27:B:845:BCR:H272	1.94	0.49
6:A:214:GLN:O	6:A:219:LEU:HD13	2.12	0.48
3:6:250:ASP:OD1	3:6:251:ASN:N	2.46	0.48
20:9:168:TRP:CE2	21:9:608:CHL:HED3	2.48	0.48
5:4:222:GLU:HG3	22:4:610:CLA:C4B	2.44	0.48
22:B:803:CLA:H142	27:I:101:BCR:H271	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:K:202:BCR:H23C	27:K:202:BCR:C38	2.43	0.48
20:9:232:MET:HE3	21:9:606:CHL:HMB2	1.95	0.48
3:2:203:ASP:OD1	3:2:206:GLY:N	2.46	0.48
6:A:503:THR:CG2	22:A:828:CLA:HAB	2.43	0.48
6:A:588:ASP:OD1	6:A:723:ARG:NH1	2.46	0.48
2:5:96:TRP:HD1	22:5:609:CLA:HMD3	1.79	0.48
1:U:245:HIS:HE1	22:U:614:CLA:NC	2.10	0.48
1:V:148:ASN:OD1	1:V:151:LEU:HD23	2.14	0.48
2:1:240:ILE:HG13	2:1:240:ILE:O	2.12	0.48
4:3:241:PHE:HD2	4:3:255:ILE:HD11	1.79	0.48
18:M:23:ALA:HB2	27:M:2001:BCR:C34	2.44	0.48
6:A:503:THR:HB	6:A:507:TRP:HE1	1.77	0.48
21:4:608:CHL:HMB3	27:4:621:BCR:C14	2.43	0.48
3:6:112:ARG:NH1	21:6:608:CHL:OBD	2.46	0.48
20:9:146:PHE:HB2	20:9:148:LEU:CD1	2.44	0.48
22:B:825:CLA:HMB2	22:B:838:CLA:H3A	1.95	0.48
7:B:477:LEU:O	7:B:478:LEU:HB2	2.14	0.48
22:8:610:CLA:H2A	22:8:610:CLA:O1D	2.13	0.48
21:U:606:CHL:OMC	23:U:2621:LUT:H163	2.13	0.48
1:V:129:VAL:HG11	1:V:131:PHE:CE1	2.49	0.48
6:A:599:ASN:OD1	22:A:803:CLA:CMC	2.62	0.48
7:B:450:GLU:OE2	11:F:137:ARG:NE	2.46	0.48
27:F:305:BCR:HC8	27:F:305:BCR:H311	1.96	0.48
27:A:856:BCR:H403	27:A:856:BCR:H23C	1.95	0.48
11:F:102:ARG:NE	11:F:152:GLY:O	2.46	0.48
2:5:101:VAL:HG11	23:5:617:LUT:H12	1.96	0.47
20:9:301:PRO:O	23:9:620:LUT:O3	2.32	0.47
3:6:246:THR:HG22	3:6:247:GLY:N	2.29	0.47
27:7:621:BCR:HC8	27:7:621:BCR:C33	2.42	0.47
5:8:161:MET:CE	27:8:621:BCR:H352	2.44	0.47
4:3:132:MET:O	4:3:132:MET:HG2	2.13	0.47
6:A:599:ASN:OD1	22:A:803:CLA:HMC1	2.15	0.47
11:F:150:THR:O	11:F:151:ASP:CG	2.57	0.47
2:5:148:GLU:OE1	22:5:606:CLA:C1C	2.61	0.47
21:6:618:CHL:HHC	21:6:618:CHL:HBB1	1.96	0.47
27:A:851:BCR:H331	27:A:851:BCR:C8	2.43	0.47
2:5:201:LEU:HD22	24:5:618:XAT:C15	2.45	0.47
4:7:111:GLN:O	4:7:112:SER:C	2.56	0.47
27:4:621:BCR:H23C	27:4:621:BCR:H393	1.97	0.47
6:A:574:ASP:OD2	6:A:578:ARG:NH1	2.38	0.47
6:A:672:LEU:HD21	7:B:620:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:101:LYS:O	3:6:105:GLN:HG2	2.14	0.47
3:6:137:SER:OG	3:6:140:VAL:HG22	2.15	0.47
1:U:126:GLY:C	1:U:127:GLU:OE1	2.58	0.47
21:W:609:CHL:HBB1	21:W:609:CHL:HMB1	1.95	0.47
3:2:77:TRP:NE1	3:2:89:ASP:OD2	2.40	0.47
2:5:134:ASN:O	2:5:135:PRO:C	2.58	0.47
4:7:239:GLU:N	4:7:239:GLU:OE1	2.46	0.47
20:9:258:ASP:OD2	20:9:263:SER:OG	2.24	0.47
22:A:809:CLA:C4	27:A:852:BCR:H331	2.45	0.47
2:5:51:TRP:O	21:5:601:CHL:ND	2.48	0.47
2:5:196:ASN:HB3	23:5:617:LUT:H201	1.96	0.47
5:8:168:ARG:NH1	22:8:609:CLA:O1D	2.37	0.47
3:2:148:THR:HG22	3:2:149:ASP:N	2.30	0.47
7:B:125:TYR:O	7:B:130:ARG:NH1	2.45	0.47
7:B:287:ALA:HB2	22:B:819:CLA:HBC2	1.97	0.47
7:B:662:MET:HG3	22:B:803:CLA:NC	2.29	0.47
8:C:29:VAL:HG12	9:D:181:ARG:HB3	1.97	0.47
10:E:124:SER:OG	10:E:126:ASP:OD1	2.30	0.47
4:7:146:LEU:HD12	22:7:602:CLA:H12	1.97	0.47
21:7:608:CHL:HHC	21:7:608:CHL:HBB1	1.96	0.47
1:U:184:ILE:HG23	1:U:184:ILE:O	2.15	0.47
22:B:839:CLA:H18	27:I:101:BCR:H362	1.95	0.47
27:I:101:BCR:H382	27:I:101:BCR:H23C	1.97	0.47
2:5:57:ARG:NH2	2:5:68:ASP:O	2.47	0.47
21:6:606:CHL:HHC	21:6:606:CHL:HBB1	1.97	0.47
5:4:77:TRP:CD1	5:4:78:LEU:HD12	2.49	0.46
22:B:806:CLA:CBB	22:B:828:CLA:HMC2	2.45	0.46
27:G:205:BCR:H11C	27:G:205:BCR:H341	1.76	0.46
14:I:9:ILE:O	14:I:13:LEU:HD13	2.14	0.46
23:9:621:LUT:H11	23:9:621:LUT:H191	1.78	0.46
6:A:672:LEU:HB2	22:A:854:CLA:H42	1.97	0.46
1:V:253:ASN:OD1	1:V:253:ASN:C	2.58	0.46
22:B:812:CLA:CGA	22:B:812:CLA:H3A	2.44	0.46
3:6:234:VAL:HG11	24:6:620:XAT:C12	2.46	0.46
1:V:160:ILE:HD12	1:V:160:ILE:H	1.80	0.46
27:4:621:BCR:H402	27:4:621:BCR:C23	2.45	0.46
22:A:854:CLA:HBA1	22:A:854:CLA:H3A	1.59	0.46
7:B:732:LYS:O	7:B:734:GLY:N	2.47	0.46
3:6:220:ARG:O	3:6:224:ILE:HG12	2.16	0.46
4:7:215:PHE:O	4:7:219:ARG:HG3	2.15	0.46
21:U:607:CHL:HHC	21:U:607:CHL:HBB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:607:CHL:HHC	21:1:607:CHL:HBB1	1.97	0.46
22:1:611:CLA:H2A	22:1:611:CLA:CED	2.44	0.46
3:2:127:LEU:HB2	3:2:133:LEU:HD12	1.97	0.46
3:2:231:MET:HE1	21:2:602:CHL:HBB1	1.97	0.46
6:A:738:THR:OG1	22:A:801:CLA:CED	2.63	0.46
27:M:2001:BCR:H321	27:M:2001:BCR:HC8	1.97	0.46
19:O:66:ILE:HG22	27:O:2004:BCR:H323	1.97	0.46
2:5:206:GLY:O	2:5:207:PHE:C	2.58	0.46
3:6:113:TRP:CE2	21:6:608:CHL:HED3	2.50	0.46
6:A:118:ILE:HG23	6:A:119:VAL:HG22	1.98	0.46
6:A:275:PHE:HE2	6:A:499:ALA:HB2	1.81	0.46
22:G:201:CLA:H3A	22:G:201:CLA:O2A	2.16	0.46
22:O:2002:CLA:H3A	22:O:2002:CLA:H11	1.97	0.46
27:O:2004:BCR:H383	27:O:2004:BCR:C23	2.45	0.46
1:W:230:GLN:O	1:W:234:THR:OG1	2.21	0.46
4:3:145:TRP:NE1	22:3:603:CLA:O1A	2.46	0.46
24:4:620:XAT:H181	24:4:620:XAT:C8	2.46	0.46
7:B:463:ILE:HD12	22:B:836:CLA:O2A	2.15	0.46
13:H:89:GLY:O	13:H:92:THR:OG1	2.31	0.46
3:6:193:ASP:OD1	3:6:193:ASP:O	2.34	0.46
1:W:174:TYR:O	1:W:178:GLY:N	2.49	0.46
5:4:73:GLU:OE1	5:4:73:GLU:HA	2.16	0.46
27:B:847:BCR:C23	27:B:847:BCR:H383	2.45	0.46
8:C:3:HIS:ND1	8:C:69:LEU:HA	2.31	0.46
8:C:3:HIS:CE1	8:C:76:SER:HG	2.34	0.46
27:L:301:BCR:H24C	22:L:303:CLA:C9	2.45	0.46
2:5:72:ASP:OD1	2:5:75:GLY:N	2.48	0.46
3:6:115:MET:HE3	3:6:227:GLY:CA	2.46	0.46
27:7:620:BCR:C23	27:7:620:BCR:C38	2.93	0.46
20:9:232:MET:HE1	25:9:623:NEX:C30	2.44	0.46
1:W:218:ARG:HA	1:W:221:MET:HE3	1.98	0.46
27:A:848:BCR:H11C	27:A:848:BCR:H341	1.69	0.46
8:C:70:GLY:O	8:C:72:GLU:N	2.46	0.46
2:5:164:ASP:O	2:5:167:LYS:N	2.49	0.46
1:U:197:LEU:HD12	23:U:2620:LUT:H222	1.98	0.45
27:B:843:BCR:H11C	27:B:843:BCR:H341	1.80	0.45
27:B:844:BCR:H11C	27:B:844:BCR:H341	1.84	0.45
27:B:1609:BCR:H341	27:B:1609:BCR:H11C	1.69	0.45
9:D:166:LEU:O	9:D:169:LYS:HE3	2.16	0.45
20:9:187:THR:HB	20:9:188:PRO:HD3	1.98	0.45
5:4:168:ARG:NH2	22:4:609:CLA:O1D	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:610:CLA:HBA2	22:4:610:CLA:H3A	1.80	0.45
19:O:81:VAL:HG12	19:O:83:ASN:H	1.81	0.45
5:4:117:GLY:HA2	24:4:620:XAT:C18	2.46	0.45
21:4:618:CHL:HHC	21:4:618:CHL:HBB1	1.97	0.45
6:A:455:HIS:O	6:A:459:MET:HG2	2.15	0.45
12:G:146:THR:HG23	22:G:201:CLA:OBD	2.17	0.45
5:8:85:ASP:OD1	5:8:85:ASP:C	2.58	0.45
1:W:226:GLY:O	1:W:227:PHE:C	2.57	0.45
9:D:128:LEU:HD21	13:H:53:PHE:HB3	1.98	0.45
3:6:115:MET:SD	22:6:610:CLA:HMC3	2.56	0.45
3:6:125:GLU:HA	3:6:128:THR:HG22	1.97	0.45
27:6:621:BCR:H11C	27:6:621:BCR:H341	1.73	0.45
5:8:251:LEU:HD13	23:8:619:LUT:H163	1.97	0.45
22:4:601:CLA:CAC	26:4:630:LHG:HC42	2.47	0.45
6:A:314:GLY:O	6:A:315:ILE:C	2.58	0.45
9:D:75:ASN:OD1	9:D:76:ALA:N	2.50	0.45
13:H:104:GLY:O	13:H:108:THR:OG1	2.27	0.45
22:5:611:CLA:HAB	27:8:621:BCR:H383	1.99	0.45
22:7:602:CLA:CGA	22:7:602:CLA:C3A	2.94	0.45
20:9:207:ILE:O	20:9:207:ILE:HG23	2.17	0.45
2:1:146:ALA:O	2:1:150:LEU:HD13	2.17	0.45
5:4:263:ILE:HG23	5:4:264:LEU:CD2	2.46	0.45
22:4:614:CLA:H3A	22:4:614:CLA:HBA2	1.84	0.45
8:C:4:SER:OG	8:C:6:LYS:NZ	2.50	0.45
21:U:609:CHL:HHC	21:U:609:CHL:HBB1	1.98	0.45
3:2:112:ARG:NH2	3:2:195:GLY:O	2.39	0.45
4:3:268:LEU:HD21	4:3:272:LYS:HE3	1.99	0.45
7:B:15:ASP:HB3	7:B:20:ARG:HB2	1.99	0.45
7:B:167:TRP:NE1	22:B:813:CLA:HBC3	2.32	0.45
22:F:303:CLA:O2A	22:F:303:CLA:H2A	2.17	0.45
4:7:154:GLY:N	4:7:283:MET:HE2	2.31	0.45
5:8:171:ASP:C	5:8:171:ASP:OD1	2.60	0.45
1:U:145:TYR:HD2	1:U:151:LEU:HD13	1.82	0.45
21:2:606:CHL:HHC	21:2:606:CHL:HBB1	1.97	0.45
6:A:223:ARG:NH1	6:A:250:LEU:O	2.49	0.45
11:F:151:ASP:OD1	11:F:151:ASP:C	2.60	0.45
21:V:609:CHL:HHC	21:V:609:CHL:HBB1	1.99	0.45
1:W:248:ASP:OD1	1:W:251:ALA:HB3	2.17	0.45
2:1:154:PHE:O	2:1:158:GLN:HG2	2.17	0.45
7:B:69:ALA:HB2	7:B:135:LEU:HB2	1.99	0.45
12:G:76:GLY:HA3	12:G:132:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:L:301:BCR:H392	27:L:301:BCR:H23C	1.98	0.45
21:5:607:CHL:HHC	21:5:607:CHL:HBB1	1.99	0.45
3:6:139:THR:HG23	3:6:140:VAL:HG13	1.99	0.45
21:8:618:CHL:HHC	21:8:618:CHL:HBB1	1.98	0.45
7:B:203:ARG:NH2	7:B:253:ALA:O	2.47	0.45
22:B:821:CLA:H3A	22:B:822:CLA:H11	1.99	0.45
3:6:203:ASP:OD1	3:6:203:ASP:O	2.35	0.45
5:8:156:VAL:O	5:8:160:LEU:HD13	2.16	0.45
21:V:605:CHL:HHC	21:V:605:CHL:HBB1	1.99	0.44
7:B:2:ALA:O	14:I:34:GLU:HB2	2.16	0.44
17:L:65:VAL:HG13	19:O:58:TRP:HB2	1.98	0.44
5:8:183:ILE:CD1	27:8:621:BCR:H382	2.48	0.44
20:9:299:VAL:HG12	20:9:300:SER:N	2.31	0.44
3:2:109:VAL:HG11	3:2:168:ARG:NH1	2.32	0.44
22:4:604:CLA:C3B	27:4:621:BCR:H323	2.47	0.44
27:A:852:BCR:H371	27:A:852:BCR:H24C	1.81	0.44
27:B:845:BCR:H351	27:B:845:BCR:H15C	1.82	0.44
21:8:607:CHL:HHC	21:8:607:CHL:HBB1	1.99	0.44
21:9:601:CHL:HHC	21:9:601:CHL:HBB1	1.99	0.44
25:W:2623:NEX:H11	25:W:2623:NEX:H191	1.74	0.44
24:4:620:XAT:H181	24:4:620:XAT:H8	1.99	0.44
6:A:194:MET:HE2	22:A:814:CLA:CHD	2.48	0.44
22:A:841:CLA:HAA2	22:B:831:CLA:HMB1	1.98	0.44
27:A:856:BCR:HC8	27:A:856:BCR:C33	2.43	0.44
7:B:227:ALA:O	12:G:61:THR:OG1	2.33	0.44
27:K:202:BCR:H331	27:K:202:BCR:C8	2.47	0.44
27:L:301:BCR:H11C	27:L:301:BCR:H341	1.86	0.44
2:5:112:TYR:CE2	2:5:131:TYR:HB2	2.52	0.44
3:6:196:TYR:CE2	3:6:220:ARG:NH2	2.86	0.44
21:9:605:CHL:HHC	21:9:605:CHL:HBB1	2.00	0.44
25:W:2623:NEX:H31	25:W:2623:NEX:H391	1.82	0.44
4:3:221:ALA:HB2	22:3:609:CLA:HMA1	2.00	0.44
22:4:602:CLA:HMC2	24:4:620:XAT:C31	2.47	0.44
27:4:621:BCR:H11C	27:4:621:BCR:H341	1.86	0.44
27:A:851:BCR:H11C	27:A:851:BCR:H341	1.85	0.44
21:5:601:CHL:OBD	5:8:167:ARG:NH1	2.50	0.44
3:2:264:ILE:N	22:2:613:CLA:O1A	2.48	0.44
4:3:312:VAL:HG11	20:9:309:LEU:O	2.17	0.44
7:B:299:HIS:HB3	7:B:304:ILE:HD11	1.98	0.44
10:E:81:ARG:NH2	10:E:127:GLU:OE2	2.51	0.44
22:K:204:CLA:HMC3	27:K:205:BCR:H311	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:602:CLA:HMC2	24:7:619:XAT:C31	2.48	0.44
22:3:612:CLA:CBB	27:3:621:BCR:H381	2.47	0.44
6:A:495:THR:O	22:A:837:CLA:ND	2.51	0.44
22:A:845:CLA:HMD3	19:O:141:TYR:CE2	2.53	0.44
27:A:852:BCR:H382	27:A:852:BCR:H23C	2.00	0.44
7:B:383:MET:HE1	27:B:847:BCR:H361	2.00	0.44
7:B:580:VAL:O	7:B:583:MET:HG3	2.17	0.44
7:B:583:MET:O	7:B:587:ILE:HG12	2.17	0.44
2:5:156:GLU:HG3	22:5:609:CLA:C2B	2.48	0.44
21:6:601:CHL:HHC	21:6:601:CHL:HBB1	2.00	0.44
21:6:608:CHL:HHC	21:6:608:CHL:HBB1	1.99	0.44
20:9:148:LEU:HD22	22:9:602:CLA:H12	1.99	0.44
1:W:244:ASP:OD1	1:W:252:ASN:OD1	2.35	0.44
5:4:220:THR:HA	5:4:223:VAL:HG12	2.00	0.44
7:B:430:GLY:HA2	7:B:525:LEU:HD22	2.00	0.44
7:B:631:LEU:HD22	7:B:724:PHE:HA	1.99	0.44
3:6:229:LEU:HD21	22:6:612:CLA:HBC3	2.00	0.44
27:6:621:BCR:H15C	27:6:621:BCR:H351	1.77	0.44
4:7:270:GLU:N	4:7:270:GLU:OE1	2.51	0.44
20:9:240:ILE:HG21	22:9:609:CLA:CMA	2.48	0.44
3:2:205:LEU:HD12	23:2:619:LUT:H22	1.98	0.44
4:3:212:LEU:HD12	22:3:606:CLA:HMA1	2.00	0.44
5:4:112:ARG:HG3	22:4:610:CLA:C3C	2.48	0.44
21:4:607:CHL:HHC	21:4:607:CHL:HBB1	1.99	0.44
22:A:809:CLA:H92	27:J:102:BCR:H372	1.98	0.44
2:5:91:LEU:HD12	2:5:169:LYS:HE3	1.97	0.44
4:7:156:PHE:CZ	21:7:608:CHL:HED3	2.53	0.44
1:U:168:MET:HA	1:U:171:VAL:HG22	2.00	0.44
3:2:160:LEU:HD11	27:2:621:BCR:C15	2.48	0.44
7:B:395:ILE:HD12	7:B:555:TYR:HD1	1.83	0.44
21:5:601:CHL:HHC	21:5:601:CHL:HBB1	1.99	0.44
5:4:205:LEU:HD12	23:4:619:LUT:H221	1.99	0.43
6:A:46:ILE:HD12	6:A:46:ILE:H	1.83	0.43
7:B:85:ARG:NH2	13:H:139:LYS:O	2.50	0.43
2:5:108:GLU:HB3	2:5:220:LEU:CD2	2.43	0.43
4:7:291:THR:O	4:7:294:ILE:HG22	2.17	0.43
22:9:609:CLA:HHC	22:9:609:CLA:HBB1	1.99	0.43
1:W:145:TYR:CD2	1:W:146:LEU:HD12	2.54	0.43
4:3:255:ILE:HD13	27:3:621:BCR:HC41	2.00	0.43
6:A:530:ASP:HA	6:A:533:VAL:HG12	1.99	0.43
22:B:804:CLA:HHC	22:B:806:CLA:OBD	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:3:HIS:NE2	8:C:76:SER:OG	2.44	0.43
21:6:607:CHL:HHC	21:6:607:CHL:HBB1	1.98	0.43
2:1:98:MET:HE3	2:1:197:GLY:CA	2.49	0.43
3:2:231:MET:HE2	24:2:620:XAT:C34	2.48	0.43
6:A:116:TRP:HB3	27:A:856:BCR:H333	1.99	0.43
7:B:490:GLN:HA	7:B:494:LEU:HB2	2.01	0.43
9:D:189:ARG:NH1	9:D:210:LEU:O	2.51	0.43
3:6:196:TYR:CE2	3:6:220:ARG:CZ	3.02	0.43
22:V:602:CLA:O1A	23:V:2621:LUT:H382	2.18	0.43
21:1:601:CHL:HHC	21:1:601:CHL:HBB1	2.00	0.43
21:2:601:CHL:HHC	21:2:601:CHL:HBB1	1.99	0.43
4:3:286:VAL:HG11	24:3:619:XAT:H12	2.00	0.43
7:B:441:ASP:OD1	7:B:615:TYR:HB2	2.18	0.43
2:5:133:GLY:HA3	2:5:136:VAL:HB	2.00	0.43
3:6:233:ALA:HB2	23:6:619:LUT:H392	2.00	0.43
23:6:619:LUT:H15	23:6:619:LUT:H201	1.85	0.43
4:7:155:ARG:NH1	4:7:275:GLU:OE2	2.52	0.43
20:9:260:LEU:HD22	23:9:620:LUT:H222	2.00	0.43
23:U:2620:LUT:H11	23:U:2620:LUT:H191	1.81	0.43
1:W:113:LEU:CD2	1:W:239:LEU:HD21	2.48	0.43
4:3:175:LEU:HD12	4:3:176:ILE:HG23	1.98	0.43
24:4:620:XAT:H35	24:4:620:XAT:H401	1.85	0.43
6:A:622:ASP:OD1	6:A:622:ASP:N	2.48	0.43
7:B:605:ASN:OD1	7:B:605:ASN:O	2.36	0.43
2:5:108:GLU:O	2:5:111:GLY:N	2.47	0.43
22:6:610:CLA:CGA	22:6:610:CLA:H3A	2.49	0.43
5:8:143:ASP:OD1	5:8:143:ASP:O	2.36	0.43
1:V:103:ARG:O	1:V:107:LEU:HD23	2.18	0.43
27:3:621:BCR:C23	27:3:621:BCR:H383	2.47	0.43
27:B:843:BCR:H15C	27:B:843:BCR:H351	1.88	0.43
2:5:212:ILE:HG22	2:5:212:ILE:O	2.18	0.43
24:6:620:XAT:H11	24:6:620:XAT:H191	1.93	0.43
21:8:608:CHL:HHC	21:8:608:CHL:HBB1	1.99	0.43
21:9:608:CHL:HHC	21:9:608:CHL:HBB1	2.01	0.43
6:A:155:GLN:HA	6:A:158:THR:HG22	2.01	0.43
27:A:852:BCR:H20C	27:A:852:BCR:H361	1.69	0.43
7:B:600:THR:HG21	7:B:609:PHE:HB2	2.01	0.43
5:8:65:ARG:NH1	5:8:79:ASP:O	2.50	0.43
2:1:71:PHE:CE2	24:1:618:XAT:H183	2.53	0.43
4:3:263:LYS:HE2	4:3:263:LYS:HA	2.01	0.43
6:A:543:VAL:HG11	6:A:596:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:21:ILE:O	7:B:25:ILE:HG13	2.19	0.43
22:B:810:CLA:H18	17:L:152:MET:HE1	2.00	0.43
2:5:156:GLU:HG3	22:5:609:CLA:C3B	2.49	0.43
23:9:624:LUT:H27	23:9:624:LUT:H371	1.74	0.43
3:2:84:GLY:HA3	3:2:224:ILE:HG21	2.01	0.43
4:3:241:PHE:HE1	2:5:82:ASN:OD1	2.01	0.43
4:3:271:LEU:HD23	22:3:610:CLA:H3A	2.01	0.43
6:A:423:LEU:HD13	22:A:825:CLA:C1C	2.49	0.43
27:A:851:BCR:H321	27:A:851:BCR:HC7	1.82	0.43
27:L:305:BCR:H15C	27:L:305:BCR:H351	1.81	0.43
2:5:104:VAL:O	2:5:104:VAL:HG12	2.18	0.43
4:7:150:GLU:OE1	22:7:602:CLA:HMA3	2.19	0.43
5:8:170:ALA:HB3	5:8:178:VAL:HG11	1.99	0.43
22:8:604:CLA:C1B	27:8:621:BCR:H323	2.49	0.43
23:V:2620:LUT:H11	23:V:2620:LUT:H191	1.77	0.43
2:1:156:GLU:OE2	22:1:609:CLA:C1C	2.66	0.43
22:4:604:CLA:H3A	22:4:604:CLA:HBA2	1.76	0.43
21:4:606:CHL:HHC	21:4:606:CHL:HBB1	2.00	0.43
27:4:621:BCR:H281	27:4:621:BCR:H403	1.73	0.43
12:G:125:THR:HG22	12:G:126:ILE:N	2.34	0.43
27:L:306:BCR:H23C	27:L:306:BCR:H382	2.01	0.43
1:V:107:LEU:CD2	22:V:610:CLA:HMC1	2.49	0.42
22:W:611:CLA:HMB2	19:O:66:ILE:HD11	2.01	0.42
24:1:618:XAT:H15	24:1:618:XAT:H201	1.92	0.42
6:A:84:TRP:O	6:A:88:MET:HG2	2.19	0.42
7:B:406:ASN:O	7:B:410:ARG:HG2	2.19	0.42
22:B:806:CLA:HBB2	22:B:828:CLA:HMC2	2.01	0.42
22:O:2002:CLA:H3A	22:O:2002:CLA:HBA2	1.84	0.42
3:6:219:LEU:HD21	22:6:610:CLA:O1A	2.19	0.42
3:6:264:ILE:O	3:6:264:ILE:HG13	2.19	0.42
4:7:191:PRO:N	4:7:192:PRO:HD3	2.34	0.42
23:9:624:LUT:H11	23:9:624:LUT:H191	1.94	0.42
1:U:116:GLU:O	1:U:120:LYS:HG2	2.19	0.42
1:U:215:LYS:NZ	26:U:2630:LHG:O4	2.47	0.42
1:W:202:ASP:HB3	1:W:205:THR:HG22	2.01	0.42
1:W:238:PRO:O	23:W:2620:LUT:O3	2.36	0.42
4:3:238:LEU:H	4:3:238:LEU:HD23	1.83	0.42
27:A:851:BCR:H331	27:A:851:BCR:HC8	2.02	0.42
7:B:662:MET:HG3	22:B:803:CLA:C4C	2.49	0.42
11:F:112:GLY:HA2	11:F:115:LYS:HE2	2.01	0.42
2:5:141:LEU:HB2	2:5:142:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:137:SER:HG	3:6:140:VAL:HG22	1.84	0.42
5:8:111:CYS:HB2	5:8:226:GLY:HA3	2.02	0.42
23:1:617:LUT:C8	23:1:617:LUT:H181	2.49	0.42
21:2:606:CHL:HBB2	21:2:607:CHL:CBB	2.49	0.42
27:2:621:BCR:H23C	27:2:621:BCR:C38	2.48	0.42
5:4:82:LEU:HD12	5:4:83:PRO:HD2	2.01	0.42
7:B:60:TRP:NE1	22:B:827:CLA:OBD	2.53	0.42
22:B:840:CLA:HBA1	22:B:840:CLA:H3A	1.91	0.42
27:B:1609:BCR:C33	27:B:1609:BCR:HC8	2.50	0.42
9:D:129:LEU:HD23	9:D:131:LEU:HD21	2.02	0.42
16:K:117:VAL:HA	27:K:205:BCR:H332	2.02	0.42
2:5:191:LEU:O	2:5:194:ILE:HG22	2.18	0.42
4:7:156:PHE:CE1	21:7:608:CHL:HED3	2.55	0.42
6:A:371:MET:SD	22:A:828:CLA:HMC2	2.59	0.42
21:U:606:CHL:HHC	21:U:606:CHL:HBB1	2.00	0.42
2:1:85:ARG:HG3	2:1:85:ARG:HH11	1.83	0.42
27:7:620:BCR:H15C	27:7:620:BCR:H351	1.88	0.42
21:8:606:CHL:HHC	21:8:606:CHL:HBB1	2.00	0.42
20:9:115:ASN:OD1	20:9:115:ASN:O	2.38	0.42
27:A:848:BCR:H382	27:A:848:BCR:H23C	2.01	0.42
7:B:276:HIS:HE2	22:B:818:CLA:C2B	2.32	0.42
12:G:146:THR:HG23	22:G:201:CLA:CAD	2.50	0.42
27:I:101:BCR:H402	27:L:301:BCR:H353	2.00	0.42
27:L:305:BCR:H331	27:L:305:BCR:C8	2.33	0.42
24:5:618:XAT:H15	24:5:618:XAT:H201	1.85	0.42
1:U:102:ALA:O	1:U:106:MET:HG3	2.19	0.42
24:W:2622:XAT:C28	24:W:2622:XAT:H381	2.48	0.42
2:1:94:ALA:O	2:1:98:MET:HG3	2.19	0.42
21:2:618:CHL:HHC	21:2:618:CHL:HBB1	2.01	0.42
6:A:122:LYS:CE	11:F:130:THR:OG1	2.68	0.42
7:B:631:LEU:HD13	7:B:727:ALA:CB	2.49	0.42
27:K:202:BCR:H11C	27:K:202:BCR:H341	1.81	0.42
4:7:106:ILE:HG12	4:7:107:PHE:H	1.83	0.42
1:U:109:ALA:HA	1:U:224:MET:SD	2.60	0.42
1:U:151:LEU:O	1:U:152:VAL:C	2.63	0.42
22:V:602:CLA:O1A	22:V:602:CLA:H43	2.20	0.42
22:A:809:CLA:CHC	22:A:810:CLA:HMD2	2.49	0.42
7:B:120:VAL:HG21	22:B:808:CLA:HED1	2.01	0.42
27:B:847:BCR:H351	27:B:847:BCR:H15C	1.81	0.42
8:C:3:HIS:HE2	8:C:76:SER:HG	1.57	0.42
11:F:211:ALA:O	11:F:215:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:2001:BCR:HC8	27:M:2001:BCR:H311	2.01	0.42
3:6:109:VAL:HG21	22:6:609:CLA:CAD	2.50	0.42
23:U:2621:LUT:H15	23:U:2621:LUT:H201	1.93	0.42
6:A:599:ASN:OD1	22:A:803:CLA:HBC2	2.20	0.42
27:A:851:BCR:HC8	27:A:851:BCR:C33	2.50	0.42
7:B:595:HIS:O	7:B:599:ILE:HG13	2.20	0.42
27:B:843:BCR:H401	12:G:132:TRP:CE2	2.55	0.42
17:L:125:LEU:HD12	22:L:304:CLA:HHB	2.02	0.42
2:5:95:ARG:HA	2:5:98:MET:HE3	2.02	0.42
3:6:156:ILE:O	3:6:160:LEU:HD23	2.20	0.42
21:9:606:CHL:HHC	21:9:606:CHL:HBB1	2.02	0.42
5:4:205:LEU:HD13	5:4:207:TRP:CZ2	2.54	0.42
6:A:495:THR:HG21	22:A:836:CLA:CMD	2.50	0.42
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.81	0.42
27:L:306:BCR:H20C	27:L:306:BCR:H361	1.85	0.42
2:5:240:ILE:O	2:5:240:ILE:CG2	2.67	0.42
1:V:211:VAL:O	1:V:214:ILE:HG22	2.20	0.41
22:2:611:CLA:O1A	2:5:157:SER:OG	2.28	0.41
22:2:614:CLA:CBB	22:2:614:CLA:HHC	2.50	0.41
4:3:238:LEU:HD22	22:5:603:CLA:CED	2.50	0.41
6:A:230:ASP:C	6:A:230:ASP:OD1	2.63	0.41
7:B:548:PRO:HB3	11:F:245:PRO:HG2	2.02	0.41
27:K:202:BCR:C33	27:K:202:BCR:HC8	2.49	0.41
27:6:621:BCR:H20C	27:6:621:BCR:H361	1.82	0.41
22:V:613:CLA:O1D	22:V:613:CLA:H2A	2.19	0.41
3:2:221:THR:HG22	3:2:221:THR:O	2.20	0.41
21:3:608:CHL:HBB1	21:3:608:CHL:HMB1	2.01	0.41
22:3:612:CLA:CBB	22:3:612:CLA:HHC	2.50	0.41
5:4:138:TRP:HB2	24:4:620:XAT:H3	2.03	0.41
6:A:691:TYR:OH	22:A:802:CLA:OBD	2.34	0.41
27:B:801:BCR:H371	27:B:801:BCR:H24C	1.92	0.41
22:B:807:CLA:HHB	22:B:808:CLA:HMB3	2.02	0.41
17:L:81:PRO:O	17:L:85:SER:HB2	2.19	0.41
4:7:150:GLU:OE2	4:7:280:ARG:CZ	2.68	0.41
4:7:213:MET:O	4:7:217:GLU:HG2	2.21	0.41
1:U:148:ASN:HB2	1:U:151:LEU:HD12	2.02	0.41
1:U:224:MET:HE2	23:U:2621:LUT:H10	2.01	0.41
21:2:607:CHL:HHC	21:2:607:CHL:HBB1	2.01	0.41
6:A:118:ILE:HG23	6:A:119:VAL:H	1.85	0.41
27:B:1609:BCR:C23	27:B:1609:BCR:H382	2.49	0.41
3:6:181:ASP:OD1	21:6:618:CHL:CHC	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:302:GLN:C	4:7:302:GLN:CD	2.89	0.41
4:7:302:GLN:OE1	4:7:306:ASP:OD2	2.38	0.41
5:8:183:ILE:HD13	27:8:621:BCR:C38	2.51	0.41
1:V:157:ILE:HG23	1:V:158:LEU:HD22	2.02	0.41
23:W:2621:LUT:H11	23:W:2621:LUT:H191	1.88	0.41
4:7:209:GLU:OE2	22:7:606:CLA:C3B	2.68	0.41
4:7:298:VAL:CG1	4:7:302:GLN:NE2	2.82	0.41
20:9:148:LEU:N	20:9:148:LEU:HD12	2.36	0.41
1:U:259:THR:O	1:U:259:THR:CG2	2.66	0.41
25:V:2623:NEX:H15	25:V:2623:NEX:H201	1.84	0.41
2:1:152:ILE:O	2:1:156:GLU:CG	2.68	0.41
8:C:24:ASP:O	8:C:44:ARG:HD2	2.20	0.41
3:6:263:THR:HG21	4:7:204:THR:OG1	2.20	0.41
4:7:206:PHE:CE1	4:7:210:MET:HE3	2.54	0.41
4:7:211:ALA:O	4:7:215:PHE:CD2	2.74	0.41
5:8:107:GLU:HB2	22:8:602:CLA:C1B	2.51	0.41
20:9:207:ILE:HG21	21:9:606:CHL:CMD	2.51	0.41
4:3:202:PRO:HB2	22:3:607:CLA:HMA2	2.02	0.41
22:4:602:CLA:HMC2	24:4:620:XAT:H31	2.01	0.41
6:A:395:GLY:O	6:A:399:VAL:HG23	2.20	0.41
22:A:809:CLA:HBA2	22:A:809:CLA:H3A	1.86	0.41
22:A:835:CLA:H2A	22:A:835:CLA:O2D	2.20	0.41
7:B:58:PHE:HA	7:B:61:THR:HG22	2.02	0.41
2:5:149:PHE:C	2:5:150:LEU:HD22	2.45	0.41
24:5:618:XAT:H11	24:5:618:XAT:H191	1.86	0.41
3:6:91:LEU:HD22	24:6:620:XAT:H363	2.02	0.41
5:8:124:PRO:O	5:8:128:THR:OG1	2.34	0.41
20:9:227:VAL:HG11	21:9:606:CHL:HED3	2.02	0.41
22:9:612:CLA:CHC	23:9:620:LUT:H203	2.50	0.41
22:U:604:CLA:H2A	22:U:604:CLA:HED3	2.00	0.41
22:U:610:CLA:CGA	22:U:610:CLA:C3A	2.99	0.41
3:2:137:SER:O	3:2:138:TRP:CD1	2.73	0.41
27:B:801:BCR:H331	27:B:801:BCR:C8	2.50	0.41
22:5:610:CLA:HBB1	22:5:612:CLA:H3A	2.02	0.41
23:5:617:LUT:H35	23:5:617:LUT:H401	1.88	0.41
1:U:175:ARG:O	1:U:184:ILE:HD12	2.20	0.41
1:U:211:VAL:O	1:U:214:ILE:HG22	2.21	0.41
1:U:253:ASN:HB2	22:U:614:CLA:HED1	2.02	0.41
25:V:2623:NEX:H11	25:V:2623:NEX:H191	1.77	0.41
1:W:151:LEU:O	1:W:152:VAL:C	2.63	0.41
23:2:619:LUT:H35	23:2:619:LUT:H401	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:619:XAT:H35	24:3:619:XAT:H401	1.88	0.41
5:4:108:LEU:O	5:4:112:ARG:HD3	2.20	0.41
9:D:78:THR:HG23	9:D:126:PRO:HB2	2.02	0.41
22:K:201:CLA:HBC3	22:9:611:CLA:O2A	2.20	0.41
20:9:221:LEU:O	20:9:225:ILE:HG12	2.20	0.41
22:U:610:CLA:CGA	22:U:610:CLA:H3A	2.51	0.41
1:V:102:ALA:O	1:V:106:MET:HG3	2.21	0.41
1:V:204:ASP:OD1	1:V:205:THR:N	2.54	0.41
3:2:177:CYS:O	3:2:178:VAL:HG22	2.21	0.41
6:A:674:ALA:HB1	6:A:733:GLY:O	2.21	0.41
7:B:80:ASP:OD2	7:B:83:HIS:HB2	2.21	0.41
22:B:805:CLA:HBA1	22:B:805:CLA:H3A	1.77	0.41
9:D:130:LYS:C	9:D:131:LEU:HD22	2.45	0.41
11:F:156:LEU:HD22	11:F:167:GLU:HG2	2.02	0.41
12:G:84:GLN:NE2	12:G:88:VAL:HG11	2.35	0.41
27:K:205:BCR:H383	27:K:205:BCR:C23	2.51	0.41
3:6:110:HIS:CE1	22:6:609:CLA:OBD	2.73	0.41
4:7:127:ASP:OD1	22:7:602:CLA:HBA2	2.21	0.41
4:7:213:MET:HG3	22:7:609:CLA:HMC3	2.03	0.41
5:8:190:THR:O	5:8:198:GLY:N	2.50	0.41
20:9:89:GLY:O	20:9:90:ILE:C	2.64	0.41
23:9:621:LUT:H35	23:9:621:LUT:H401	1.97	0.41
25:U:2623:NEX:H15	25:U:2623:NEX:H201	1.91	0.41
1:W:181:LEU:HD13	21:W:608:CHL:CAB	2.50	0.41
1:W:200:ALA:HB1	1:W:206:PHE:CD1	2.56	0.41
27:3:620:BCR:H23C	27:3:620:BCR:C38	2.42	0.41
12:G:95:VAL:HA	12:G:100:THR:HA	2.03	0.41
27:G:205:BCR:H15C	27:G:205:BCR:H351	1.81	0.41
16:K:66:MET:HE2	27:K:202:BCR:H402	2.02	0.41
24:5:618:XAT:H381	24:5:618:XAT:H27	1.71	0.41
4:7:304:LEU:O	4:7:308:LEU:HD23	2.21	0.41
5:8:235:GLY:O	5:8:236:ALA:C	2.64	0.41
1:U:81:THR:HG21	21:V:609:CHL:CBA	2.51	0.40
1:U:197:LEU:HD22	20:9:260:LEU:CD2	2.49	0.40
23:U:2621:LUT:H181	23:U:2621:LUT:C8	2.51	0.40
1:V:114:THR:OG1	1:V:115:PRO:HD3	2.22	0.40
23:1:617:LUT:H11	23:1:617:LUT:H191	1.91	0.40
21:4:606:CHL:CHB	27:4:621:BCR:H342	2.51	0.40
27:A:851:BCR:H20C	27:A:851:BCR:H361	1.97	0.40
27:B:1609:BCR:C33	27:B:1609:BCR:C8	2.99	0.40
27:B:1609:BCR:C8	27:B:1609:BCR:H331	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:81:ARG:HD2	10:E:84:SER:HB2	2.03	0.40
27:G:205:BCR:H24C	27:G:205:BCR:H371	1.85	0.40
2:5:136:VAL:N	2:5:137:PRO:CD	2.84	0.40
2:5:136:VAL:O	2:5:137:PRO:C	2.64	0.40
2:5:148:GLU:OE1	22:5:606:CLA:C4B	2.69	0.40
4:7:253:GLY:O	4:7:257:ASN:N	2.49	0.40
5:8:224:LYS:NZ	22:8:611:CLA:O1D	2.48	0.40
5:8:239:GLN:HG3	22:8:613:CLA:C4D	2.51	0.40
20:9:286:ALA:O	20:9:290:LEU:HD13	2.21	0.40
23:9:624:LUT:H8	23:9:624:LUT:C18	2.51	0.40
24:4:620:XAT:H11	24:4:620:XAT:H191	1.94	0.40
6:A:94:ARG:NH2	6:A:157:TYR:CE1	2.89	0.40
6:A:122:LYS:HE2	11:F:130:THR:OG1	2.22	0.40
7:B:15:ASP:OD1	7:B:17:THR:OG1	2.25	0.40
2:5:131:TYR:C	2:5:133:GLY:N	2.79	0.40
4:7:164:ALA:HB3	4:7:289:TYR:CE2	2.56	0.40
23:7:618:LUT:H11	23:7:618:LUT:H191	1.95	0.40
20:9:167:ARG:NH1	21:9:608:CHL:OBD	2.53	0.40
23:W:2620:LUT:H11	23:W:2620:LUT:H191	1.78	0.40
26:1:630:LHG:C24	27:4:621:BCR:H291	2.52	0.40
22:3:613:CLA:H2	22:3:614:CLA:HMD1	2.02	0.40
5:4:216:LYS:O	5:4:217:GLU:C	2.64	0.40
6:A:65:GLU:HG3	6:A:69:LYS:NZ	2.37	0.40
27:A:852:BCR:H15C	27:A:852:BCR:H351	1.96	0.40
7:B:191:THR:HG23	22:B:815:CLA:HMC2	2.02	0.40
7:B:246:THR:HG22	7:B:248:GLU:H	1.86	0.40
7:B:415:LYS:NZ	7:B:540:ASP:OD1	2.39	0.40
7:B:652:PHE:O	7:B:656:VAL:HG23	2.20	0.40
14:I:18:PHE:HB3	14:I:19:PRO:HD3	2.04	0.40
27:K:202:BCR:H331	27:K:202:BCR:HC8	2.02	0.40
24:6:620:XAT:H31	24:6:620:XAT:H391	1.96	0.40
20:9:178:THR:OG1	20:9:179:PRO:HD3	2.22	0.40
21:2:608:CHL:HHC	21:2:608:CHL:HBB1	2.03	0.40
27:3:620:BCR:C23	27:3:620:BCR:C38	2.98	0.40
22:A:843:CLA:HMC1	22:B:839:CLA:H11	2.04	0.40
7:B:527:LEU:HD12	7:B:586:THR:HG21	2.02	0.40
17:L:69:LEU:HD12	17:L:79:GLU:OE2	2.21	0.40
2:5:108:GLU:CG	2:5:220:LEU:HD21	2.51	0.40
1:V:148:ASN:OD1	1:V:150:SER:N	2.55	0.40
23:2:619:LUT:H11	23:2:619:LUT:H191	1.92	0.40
24:4:620:XAT:H31	24:4:620:XAT:H391	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:621:BCR:H361	27:4:621:BCR:H20C	1.86	0.40
7:B:229:GLN:O	7:B:229:GLN:HG3	2.21	0.40
22:K:204:CLA:HHD	22:K:204:CLA:HBC2	2.03	0.40
22:5:602:CLA:H3A	22:5:602:CLA:CGA	2.52	0.40
4:7:133:ASP:HB3	4:7:136:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	217/265 (82%)	208 (96%)	9 (4%)	0	100	100
1	V	213/265 (80%)	207 (97%)	6 (3%)	0	100	100
1	W	225/265 (85%)	215 (96%)	9 (4%)	1 (0%)	30	56
2	1	191/245 (78%)	183 (96%)	8 (4%)	0	100	100
2	5	190/245 (78%)	166 (87%)	23 (12%)	1 (0%)	24	51
3	2	209/273 (77%)	200 (96%)	9 (4%)	0	100	100
3	6	203/273 (74%)	190 (94%)	13 (6%)	0	100	100
4	3	220/323 (68%)	213 (97%)	7 (3%)	0	100	100
4	7	217/323 (67%)	203 (94%)	13 (6%)	1 (0%)	24	51
5	4	204/270 (76%)	192 (94%)	12 (6%)	0	100	100
5	8	202/270 (75%)	187 (93%)	15 (7%)	0	100	100
6	A	740/750 (99%)	716 (97%)	23 (3%)	1 (0%)	48	74
7	B	731/734 (100%)	714 (98%)	17 (2%)	0	100	100
8	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
9	D	140/210 (67%)	133 (95%)	7 (5%)	0	100	100
10	E	62/132 (47%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	F	159/246 (65%)	152 (96%)	6 (4%)	1 (1%)	21	48
12	G	95/155 (61%)	91 (96%)	4 (4%)	0	100	100
13	H	93/139 (67%)	90 (97%)	3 (3%)	0	100	100
14	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
15	J	39/41 (95%)	39 (100%)	0	0	100	100
16	K	79/132 (60%)	79 (100%)	0	0	100	100
17	L	161/223 (72%)	155 (96%)	6 (4%)	0	100	100
18	M	29/32 (91%)	29 (100%)	0	0	100	100
19	O	88/143 (62%)	81 (92%)	7 (8%)	0	100	100
20	9	217/311 (70%)	190 (88%)	26 (12%)	1 (0%)	24	51
All	All	5034/6382 (79%)	4800 (95%)	228 (4%)	6 (0%)	49	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	315	ILE
2	5	135	PRO
4	7	112	SER
11	F	88	ALA
1	W	39	ARG
20	9	185	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	U	166/203 (82%)	165 (99%)	1 (1%)	78	92
1	V	163/203 (80%)	163 (100%)	0	100	100
1	W	173/203 (85%)	173 (100%)	0	100	100
2	1	148/186 (80%)	148 (100%)	0	100	100
2	5	148/186 (80%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	167/213 (78%)	167 (100%)	0	100	100
3	6	162/213 (76%)	160 (99%)	2 (1%)	63	84
4	3	174/256 (68%)	174 (100%)	0	100	100
4	7	170/256 (66%)	170 (100%)	0	100	100
5	4	164/210 (78%)	164 (100%)	0	100	100
5	8	162/210 (77%)	162 (100%)	0	100	100
6	A	603/611 (99%)	602 (100%)	1 (0%)	87	96
7	B	595/596 (100%)	594 (100%)	1 (0%)	87	96
8	C	67/68 (98%)	67 (100%)	0	100	100
9	D	115/157 (73%)	115 (100%)	0	100	100
10	E	56/105 (53%)	56 (100%)	0	100	100
11	F	132/193 (68%)	131 (99%)	1 (1%)	73	89
12	G	77/121 (64%)	77 (100%)	0	100	100
13	H	75/103 (73%)	74 (99%)	1 (1%)	61	84
14	I	30/32 (94%)	30 (100%)	0	100	100
15	J	35/35 (100%)	35 (100%)	0	100	100
16	K	58/95 (61%)	58 (100%)	0	100	100
17	L	124/165 (75%)	123 (99%)	1 (1%)	73	89
18	M	26/27 (96%)	26 (100%)	0	100	100
19	O	74/115 (64%)	74 (100%)	0	100	100
20	9	174/243 (72%)	173 (99%)	1 (1%)	78	92
All	All	4038/5005 (81%)	4029 (100%)	9 (0%)	85	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	201	ASP
6	A	585	SER
7	B	479	SER
11	F	87	VAL
13	H	119	ASP
17	L	135	ARG
3	6	137	SER
3	6	226	ASN
20	9	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	136	GLN
1	U	148	ASN
1	U	245	HIS
1	U	260	ASN
2	1	55	ASN
2	1	128	GLN
2	1	140	ASN
2	1	232	HIS
5	4	134	ASN
5	4	187	ASN
6	A	419	GLN
6	A	422	ASN
6	A	628	HIS
7	B	114	ASN
7	B	158	GLN
7	B	170	ASN
7	B	368	GLN
7	B	502	ASN
7	B	630	GLN
9	D	188	ASN
10	E	98	GLN
11	F	128	ASN
11	F	240	ASN
12	G	152	ASN
19	O	85	ASN
2	5	140	ASN
3	6	73	GLN
4	7	302	GLN
5	8	187	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	W	40	1	8,10,11	1.58	1 (12%)	10,14,16	1.83	1 (10%)

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
1	TPO	W	40	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	40	TPO	P-O1P	3.35	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	40	TPO	P-OG1-CB	-5.15	107.66	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

366 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	1	606	-	49,53,73	1.49	7 (14%)	59,89,113	1.26	5 (8%)
22	CLA	B	822	7	64,68,73	1.30	7 (10%)	77,107,113	1.26	10 (12%)
26	LHG	B	851	22	34,34,48	1.11	2 (5%)	37,40,54	1.01	2 (5%)
22	CLA	1	613	2	54,58,73	1.41	8 (14%)	65,95,113	1.26	5 (7%)
27	BCR	B	843	-	41,41,41	0.74	0	56,56,56	2.18	22 (39%)
22	CLA	B	835	-	49,53,73	1.47	6 (12%)	59,89,113	1.29	6 (10%)
22	CLA	B	813	7	69,73,73	1.25	8 (11%)	83,113,113	1.19	8 (9%)
21	CHL	V	605	1	46,50,74	2.37	18 (39%)	51,85,114	3.56	24 (47%)
26	LHG	W	2630	22	44,44,48	0.97	2 (4%)	47,50,54	0.97	2 (4%)
22	CLA	3	617	4	57,63,73	1.78	8 (14%)	66,98,113	2.00	12 (18%)
22	CLA	9	609	20	49,53,73	2.34	18 (36%)	59,89,113	3.25	24 (40%)
22	CLA	1	616	2	49,53,73	1.49	5 (10%)	59,89,113	1.27	4 (6%)
27	BCR	B	844	-	41,41,41	0.70	0	56,56,56	2.02	23 (41%)
22	CLA	6	609	3	59,63,73	1.35	6 (10%)	71,101,113	1.19	8 (11%)
22	CLA	A	804	6	69,73,73	1.25	7 (10%)	83,113,113	1.21	7 (8%)
22	CLA	4	602	5	69,73,73	1.24	7 (10%)	83,113,113	1.11	7 (8%)
22	CLA	B	802	7	69,73,73	1.23	8 (11%)	83,113,113	1.12	5 (6%)
22	CLA	3	607	4	54,58,73	1.40	7 (12%)	65,95,113	1.27	7 (10%)
22	CLA	W	611	26	43,48,73	1.62	9 (20%)	54,83,113	1.30	8 (14%)
22	CLA	3	609	4	69,73,73	1.24	7 (10%)	83,113,113	1.25	7 (8%)
21	CHL	7	608	-	50,54,74	2.28	17 (34%)	56,90,114	3.33	24 (42%)
24	XAT	5	618	-	39,47,47	0.88	0	54,74,74	2.70	24 (44%)
21	CHL	9	601	20	42,47,74	2.35	16 (38%)	48,81,114	3.42	23 (47%)
21	CHL	V	607	-	44,48,74	2.38	18 (40%)	53,83,114	3.56	24 (45%)
22	CLA	U	604	-	56,60,73	1.38	8 (14%)	67,97,113	1.24	8 (11%)
21	CHL	U	605	1	41,46,74	2.47	17 (41%)	52,81,114	3.50	22 (42%)
26	LHG	U	2630	22	44,44,48	0.98	2 (4%)	47,50,54	0.96	2 (4%)
21	CHL	4	607	-	51,55,74	2.30	17 (33%)	57,91,114	3.21	23 (40%)
22	CLA	V	612	1	41,46,73	1.67	8 (19%)	52,81,113	1.43	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	LUT	3	618	-	42,43,43	0.77	1 (2%)	51,60,60	1.60	11 (21%)
21	CHL	4	608	-	50,54,74	2.33	18 (36%)	56,90,114	3.26	20 (35%)
22	CLA	A	811	6	59,63,73	1.34	8 (13%)	71,101,113	1.19	6 (8%)
22	CLA	4	611	26	49,53,73	1.50	7 (14%)	59,89,113	1.28	5 (8%)
22	CLA	5	603	2	49,53,73	1.50	6 (12%)	59,89,113	1.29	7 (11%)
22	CLA	2	603	3	50,54,73	1.46	8 (16%)	60,90,113	1.35	7 (11%)
22	CLA	7	612	4	49,53,73	1.49	7 (14%)	59,89,113	1.30	4 (6%)
24	XAT	7	619	-	39,47,47	1.22	3 (7%)	54,74,74	6.06	18 (33%)
22	CLA	V	603	1	64,68,73	1.30	6 (9%)	77,107,113	1.19	4 (5%)
23	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.81	14 (27%)
22	CLA	W	613	1	64,68,73	1.30	7 (10%)	77,107,113	1.16	5 (6%)
22	CLA	2	614	3	54,58,73	1.42	7 (12%)	65,95,113	1.26	7 (10%)
22	CLA	A	843	-	69,73,73	1.24	9 (13%)	83,113,113	1.16	5 (6%)
22	CLA	1	614	2	53,57,73	1.43	7 (13%)	64,94,113	1.20	5 (7%)
22	CLA	5	608	-	54,58,73	1.40	7 (12%)	65,95,113	1.30	6 (9%)
22	CLA	O	2002	-	59,63,73	1.36	7 (11%)	71,101,113	1.14	4 (5%)
21	CHL	V	601	1	66,71,74	1.96	18 (27%)	82,111,114	2.86	26 (31%)
22	CLA	A	826	-	69,73,73	1.24	7 (10%)	83,113,113	1.15	6 (7%)
22	CLA	B	815	7	49,53,73	1.47	8 (16%)	59,89,113	1.26	4 (6%)
27	BCR	M	2001	-	41,41,41	0.65	0	56,56,56	2.15	22 (39%)
22	CLA	V	613	1	60,64,73	1.34	6 (10%)	71,101,113	1.26	8 (11%)
22	CLA	V	610	1	43,47,73	1.63	7 (16%)	55,82,113	1.35	9 (16%)
22	CLA	A	820	6	69,73,73	1.23	7 (10%)	83,113,113	1.15	9 (10%)
22	CLA	A	809	6	60,64,73	1.33	7 (11%)	72,102,113	1.24	6 (8%)
22	CLA	B	810	7	69,73,73	1.23	8 (11%)	83,113,113	1.20	7 (8%)
22	CLA	4	612	5	49,53,73	1.48	7 (14%)	59,89,113	1.27	4 (6%)
22	CLA	B	834	7	69,73,73	1.24	8 (11%)	83,113,113	1.18	7 (8%)
22	CLA	B	819	-	64,68,73	1.30	8 (12%)	77,107,113	1.26	9 (11%)
22	CLA	2	610	3	64,68,73	1.29	8 (12%)	77,107,113	1.11	5 (6%)
22	CLA	5	612	2	50,54,73	1.50	7 (14%)	60,90,113	1.18	3 (5%)
21	CHL	2	606	-	50,54,74	2.28	18 (36%)	56,90,114	3.35	23 (41%)
22	CLA	F	304	11	45,51,73	1.49	9 (20%)	48,81,113	1.76	7 (14%)
22	CLA	B	837	7	69,73,73	1.24	8 (11%)	83,113,113	1.21	7 (8%)
24	XAT	U	2622	-	39,47,47	0.89	0	54,74,74	2.62	16 (29%)
27	BCR	G	205	-	41,41,41	0.76	0	56,56,56	1.92	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	5	614	2	47,51,73	1.48	6 (12%)	56,86,113	1.26	7 (12%)
21	CHL	V	608	-	43,48,74	2.31	17 (39%)	51,83,114	3.47	23 (45%)
27	BCR	B	848	-	41,41,41	0.73	0	56,56,56	1.97	17 (30%)
23	LUT	U	2620	-	42,43,43	0.73	0	51,60,60	1.72	14 (27%)
24	XAT	1	618	-	39,47,47	0.91	1 (2%)	54,74,74	2.52	24 (44%)
21	CHL	U	609	1	70,74,74	1.95	17 (24%)	80,114,114	2.83	24 (30%)
23	LUT	W	2621	-	42,43,43	0.76	0	51,60,60	1.66	9 (17%)
26	LHG	A	846	-	46,46,48	0.96	2 (4%)	49,52,54	0.99	3 (6%)
26	LHG	9	2630	22	27,27,48	1.30	2 (7%)	30,33,54	0.98	3 (10%)
22	CLA	B	805	7	69,73,73	1.24	8 (11%)	83,113,113	1.22	9 (10%)
22	CLA	G	204	12	50,54,73	1.47	6 (12%)	60,90,113	1.24	4 (6%)
22	CLA	6	614	3	54,58,73	1.42	7 (12%)	65,95,113	1.30	9 (13%)
22	CLA	U	610	1	69,73,73	1.24	7 (10%)	83,113,113	1.16	8 (9%)
22	CLA	6	611	26	49,53,73	1.47	6 (12%)	59,89,113	1.35	6 (10%)
22	CLA	K	201	16	46,50,73	1.51	8 (17%)	55,85,113	1.40	7 (12%)
22	CLA	A	834	6	69,73,73	1.26	8 (11%)	83,113,113	1.15	6 (7%)
23	LUT	6	619	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
23	LUT	2	619	-	42,43,43	1.60	8 (19%)	51,60,60	1.58	11 (21%)
22	CLA	2	611	26	49,53,73	1.48	7 (14%)	59,89,113	1.29	5 (8%)
23	LUT	5	617	-	42,43,43	1.71	8 (19%)	51,60,60	1.76	11 (21%)
30	SF4	C	102	8	0,12,12	-	-	-		
22	CLA	1	603	2	59,63,73	1.35	7 (11%)	71,101,113	1.32	8 (11%)
26	LHG	6	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.07	2 (5%)
22	CLA	2	609	3	50,54,73	1.43	6 (12%)	60,90,113	1.27	4 (6%)
23	LUT	9	624	-	42,43,43	0.81	0	51,60,60	3.48	25 (49%)
22	CLA	B	817	7	69,73,73	1.25	7 (10%)	83,113,113	1.20	6 (7%)
22	CLA	B	821	7	54,58,73	1.44	8 (14%)	65,95,113	1.22	5 (7%)
26	LHG	4	630	22	37,37,48	1.03	2 (5%)	40,43,54	1.21	6 (15%)
22	CLA	L	303	17	69,73,73	1.24	8 (11%)	83,113,113	1.15	8 (9%)
22	CLA	5	604	-	45,49,73	1.54	8 (17%)	54,84,113	1.23	3 (5%)
24	XAT	V	2622	-	39,47,47	1.06	1 (2%)	54,74,74	5.76	21 (38%)
22	CLA	A	808	6	64,68,73	1.30	7 (10%)	77,107,113	1.17	6 (7%)
21	CHL	6	608	-	52,56,74	2.24	17 (32%)	58,92,114	3.32	23 (39%)
22	CLA	B	808	7	69,73,73	1.25	9 (13%)	83,113,113	1.12	6 (7%)
27	BCR	B	847	-	41,41,41	0.75	0	56,56,56	2.14	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CHL	V	606	-	41,46,74	2.46	18 (43%)	52,81,114	3.38	23 (44%)
22	CLA	9	611	26	69,73,73	1.26	7 (10%)	83,113,113	1.17	6 (7%)
22	CLA	U	614	1	46,50,73	1.51	6 (13%)	55,85,113	1.17	4 (7%)
22	CLA	5	602	2	64,68,73	1.29	7 (10%)	77,107,113	1.18	7 (9%)
25	NEX	U	2623	-	38,46,46	1.06	3 (7%)	50,70,70	2.53	17 (34%)
22	CLA	B	825	-	69,73,73	1.24	7 (10%)	83,113,113	1.22	6 (7%)
22	CLA	5	609	2	45,49,73	1.54	7 (15%)	54,84,113	1.24	4 (7%)
22	CLA	A	802	-	69,73,73	1.24	8 (11%)	83,113,113	1.08	7 (8%)
22	CLA	J	101	15	54,58,73	1.41	8 (14%)	65,95,113	1.29	6 (9%)
22	CLA	7	610	4	59,63,73	1.38	6 (10%)	71,101,113	1.24	6 (8%)
22	CLA	B	840	7	69,73,73	1.23	7 (10%)	83,113,113	1.16	7 (8%)
22	CLA	8	609	5	59,63,73	1.36	8 (13%)	71,101,113	1.26	5 (7%)
27	BCR	A	856	-	40,40,41	0.70	0	54,54,56	1.68	13 (24%)
21	CHL	8	618	5	47,51,74	2.30	16 (34%)	52,86,114	3.38	23 (44%)
23	LUT	7	618	-	42,43,43	0.78	0	51,60,60	1.61	10 (19%)
21	CHL	3	608	-	60,64,74	2.09	18 (30%)	68,102,114	3.02	22 (32%)
22	CLA	6	612	3	49,53,73	1.49	6 (12%)	59,89,113	1.24	3 (5%)
22	CLA	7	613	4	59,63,73	1.36	7 (11%)	71,101,113	1.17	5 (7%)
25	NEX	9	623	-	38,46,46	1.04	2 (5%)	50,70,70	2.21	14 (28%)
27	BCR	6	621	-	41,41,41	0.81	0	56,56,56	2.42	21 (37%)
26	LHG	A	847	22	30,30,48	1.16	2 (6%)	33,36,54	1.23	3 (9%)
22	CLA	A	845	26	69,73,73	1.25	7 (10%)	83,113,113	1.10	4 (4%)
22	CLA	A	814	6	69,73,73	1.24	8 (11%)	83,113,113	1.24	6 (7%)
22	CLA	H	201	-	41,46,73	1.57	7 (17%)	51,80,113	1.24	4 (7%)
21	CHL	6	607	-	51,55,74	2.28	18 (35%)	57,91,114	3.30	23 (40%)
22	CLA	B	814	7	69,73,73	1.24	7 (10%)	83,113,113	1.26	10 (12%)
22	CLA	8	604	-	54,58,73	1.43	6 (11%)	65,95,113	1.24	7 (10%)
27	BCR	4	621	-	41,41,41	0.80	0	56,56,56	3.03	16 (28%)
27	BCR	3	621	-	41,41,41	0.79	1 (2%)	56,56,56	2.26	19 (33%)
22	CLA	6	604	-	54,58,73	1.43	8 (14%)	65,95,113	1.25	5 (7%)
22	CLA	K	206	16	46,50,73	1.51	8 (17%)	55,85,113	1.28	6 (10%)
27	BCR	K	205	-	41,41,41	0.81	1 (2%)	56,56,56	2.36	25 (44%)
22	CLA	W	612	1	41,46,73	1.65	7 (17%)	52,81,113	1.34	9 (17%)
22	CLA	4	604	-	59,63,73	1.35	7 (11%)	71,101,113	1.27	5 (7%)
22	CLA	7	606	-	50,54,73	1.45	6 (12%)	60,90,113	1.28	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	B	804	7	69,73,73	1.25	6 (8%)	83,113,113	1.19	7 (8%)
27	BCR	I	101	-	41,41,41	0.74	0	56,56,56	1.75	11 (19%)
22	CLA	8	603	5	59,63,73	1.37	8 (13%)	71,101,113	1.25	6 (8%)
21	CHL	4	606	-	50,54,74	2.29	19 (38%)	56,90,114	3.44	24 (42%)
22	CLA	L	304	-	64,68,73	1.29	6 (9%)	77,107,113	1.18	7 (9%)
21	CHL	5	607	2	42,47,74	2.36	17 (40%)	48,81,114	3.46	22 (45%)
22	CLA	W	602	1	64,68,73	1.30	7 (10%)	77,107,113	1.16	6 (7%)
27	BCR	B	845	-	41,41,41	0.73	0	56,56,56	2.51	22 (39%)
21	CHL	9	605	20	41,46,74	2.37	16 (39%)	48,80,114	3.56	22 (45%)
22	CLA	3	611	26	59,63,73	1.37	6 (10%)	71,101,113	1.16	4 (5%)
22	CLA	A	812	6	69,73,73	1.24	9 (13%)	83,113,113	1.12	5 (6%)
22	CLA	A	824	6	66,70,73	1.28	8 (12%)	79,109,113	1.19	9 (11%)
22	CLA	A	832	6	59,63,73	1.35	9 (15%)	71,101,113	1.29	5 (7%)
21	CHL	6	601	3	70,74,74	1.96	17 (24%)	80,114,114	2.83	25 (31%)
26	LHG	1	630	22	48,48,48	0.93	2 (4%)	51,54,54	0.95	3 (5%)
22	CLA	W	604	-	46,50,73	1.51	8 (17%)	55,85,113	1.28	4 (7%)
22	CLA	K	204	16	69,73,73	1.24	7 (10%)	83,113,113	1.23	5 (6%)
22	CLA	4	601	5	54,58,73	1.41	7 (12%)	65,95,113	1.28	7 (10%)
22	CLA	B	816	7	69,73,73	1.25	8 (11%)	83,113,113	1.16	5 (6%)
21	CHL	W	609	1	43,48,74	2.23	16 (37%)	49,82,114	3.48	21 (42%)
22	CLA	A	815	6	69,73,73	1.24	7 (10%)	83,113,113	1.14	7 (8%)
21	CHL	2	618	3	47,51,74	2.30	16 (34%)	52,86,114	3.41	24 (46%)
22	CLA	9	603	20	46,50,73	1.54	6 (13%)	55,85,113	1.31	5 (9%)
22	CLA	A	842	6	59,63,73	1.36	8 (13%)	71,101,113	1.25	6 (8%)
22	CLA	B	831	7	69,73,73	1.25	7 (10%)	83,113,113	1.24	7 (8%)
22	CLA	1	611	26	69,73,73	1.27	7 (10%)	83,113,113	1.18	8 (9%)
28	LMG	J	103	-	55,55,55	0.87	2 (3%)	63,63,63	1.00	3 (4%)
22	CLA	5	610	2	59,63,73	1.34	6 (10%)	71,101,113	1.14	5 (7%)
22	CLA	1	604	-	54,58,73	1.41	7 (12%)	65,95,113	1.28	7 (10%)
22	CLA	A	839	6	64,68,73	1.29	7 (10%)	77,107,113	1.20	7 (9%)
22	CLA	A	840	6	54,58,73	1.39	6 (11%)	65,95,113	1.31	6 (9%)
22	CLA	F	303	-	49,53,73	1.46	6 (12%)	59,89,113	1.31	7 (11%)
27	BCR	K	202	-	41,41,41	0.71	0	56,56,56	2.03	19 (33%)
21	CHL	W	607	-	44,48,74	2.38	18 (40%)	53,83,114	3.53	23 (43%)
22	CLA	B	824	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	5	613	2	54,58,73	1.41	7 (12%)	65,95,113	1.26	8 (12%)
25	NEX	V	2623	-	38,46,46	0.89	1 (2%)	50,70,70	2.56	18 (36%)
26	LHG	V	2630	22	41,41,48	1.02	2 (4%)	44,47,54	0.96	2 (4%)
22	CLA	L	302	17	69,73,73	1.26	8 (11%)	83,113,113	1.14	7 (8%)
30	SF4	A	853	6,7	0,12,12	-	-	-		
22	CLA	8	613	5	59,63,73	1.36	6 (10%)	71,101,113	1.23	6 (8%)
22	CLA	8	610	5	59,63,73	1.36	7 (11%)	71,101,113	1.17	8 (11%)
22	CLA	B	806	7	69,73,73	1.24	7 (10%)	83,113,113	1.18	6 (7%)
22	CLA	B	811	7	65,69,73	1.30	8 (12%)	78,108,113	1.12	7 (8%)
24	XAT	W	2622	-	39,47,47	0.90	0	54,74,74	2.64	19 (35%)
22	CLA	A	836	6	59,66,73	1.55	10 (16%)	69,99,113	1.66	10 (14%)
22	CLA	A	841	6	69,73,73	1.25	8 (11%)	83,113,113	1.12	5 (6%)
23	LUT	U	2621	-	42,43,43	0.78	0	51,60,60	1.70	11 (21%)
22	CLA	7	609	4	61,65,73	1.37	7 (11%)	73,103,113	1.18	5 (6%)
21	CHL	8	608	-	55,59,74	2.19	17 (30%)	62,96,114	3.25	26 (41%)
27	BCR	2	621	-	41,41,41	0.77	0	56,56,56	2.08	20 (35%)
22	CLA	U	603	1	69,73,73	1.26	7 (10%)	83,113,113	1.20	4 (4%)
22	CLA	A	819	6	66,70,73	1.26	7 (10%)	79,109,113	1.21	8 (10%)
22	CLA	5	606	2	49,53,73	1.50	8 (16%)	59,89,113	1.25	5 (8%)
22	CLA	B	841	26	69,73,73	1.25	7 (10%)	83,113,113	1.21	8 (9%)
27	BCR	A	850	-	41,41,41	0.74	0	56,56,56	1.80	15 (26%)
22	CLA	3	610	4	64,68,73	1.30	8 (12%)	77,107,113	1.16	7 (9%)
26	LHG	2	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.04	2 (5%)
23	LUT	8	619	-	42,43,43	0.75	1 (2%)	51,60,60	1.68	12 (23%)
22	CLA	A	821	6	59,63,73	1.35	8 (13%)	71,101,113	1.16	6 (8%)
22	CLA	8	611	26	59,63,73	1.37	7 (11%)	71,101,113	1.14	5 (7%)
22	CLA	V	611	26	43,48,73	1.62	7 (16%)	54,83,113	1.33	8 (14%)
22	CLA	A	827	33	69,73,73	1.25	7 (10%)	83,113,113	1.16	8 (9%)
22	CLA	B	827	7	60,64,73	1.31	7 (11%)	72,102,113	1.24	6 (8%)
22	CLA	W	603	1	42,47,73	1.58	7 (16%)	50,82,113	1.27	7 (14%)
22	CLA	U	613	1	69,73,73	1.26	7 (10%)	83,113,113	1.14	5 (6%)
29	PQN	B	842	-	34,34,34	0.63	1 (2%)	42,45,45	0.89	2 (4%)
24	XAT	4	620	-	39,47,47	0.99	1 (2%)	54,74,74	5.03	22 (40%)
25	NEX	W	2623	-	38,46,46	0.94	1 (2%)	50,70,70	2.78	19 (38%)
22	CLA	4	614	5	50,54,73	1.46	7 (14%)	60,90,113	1.24	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	G	203	12	54,58,73	1.42	7 (12%)	65,95,113	1.28	6 (9%)
27	BCR	3	620	-	41,41,41	0.73	0	56,56,56	2.08	19 (33%)
22	CLA	A	816	6	49,53,73	1.45	7 (14%)	59,89,113	1.34	7 (11%)
21	CHL	9	608	-	47,51,74	2.28	17 (36%)	52,86,114	3.30	23 (44%)
21	CHL	8	606	-	50,54,74	2.31	19 (38%)	56,90,114	3.31	25 (44%)
22	CLA	B	823	7	49,53,73	1.48	7 (14%)	59,89,113	1.34	7 (11%)
22	CLA	4	603	5	69,73,73	1.25	8 (11%)	83,113,113	1.21	8 (9%)
22	CLA	2	613	3	61,65,73	1.33	7 (11%)	73,103,113	1.27	7 (9%)
29	PQN	A	844	-	34,34,34	0.49	0	42,45,45	0.86	3 (7%)
22	CLA	B	818	7	68,72,73	1.25	8 (11%)	81,111,113	1.18	8 (9%)
22	CLA	8	612	5	50,54,73	1.48	6 (12%)	60,90,113	1.18	3 (5%)
31	LMT	G	206	-	36,36,36	0.65	0	47,47,47	1.26	6 (12%)
21	CHL	6	606	-	50,54,74	2.28	17 (34%)	56,90,114	3.33	23 (41%)
22	CLA	A	829	6	64,68,73	1.27	6 (9%)	77,107,113	1.25	7 (9%)
22	CLA	U	611	26	49,53,73	1.50	6 (12%)	59,89,113	1.21	4 (6%)
21	CHL	2	601	3	50,54,74	2.29	17 (34%)	56,90,114	3.35	24 (42%)
28	LMG	G	202	-	32,32,55	1.21	3 (9%)	40,40,63	1.15	2 (5%)
22	CLA	B	832	7	69,73,73	1.25	7 (10%)	83,113,113	1.22	9 (10%)
28	LMG	A	860	-	34,34,55	1.14	2 (5%)	42,42,63	1.10	2 (4%)
22	CLA	F	301	33	69,73,73	1.25	9 (13%)	83,113,113	1.11	5 (6%)
22	CLA	8	602	5	64,68,73	1.31	6 (9%)	77,107,113	1.15	6 (7%)
27	BCR	O	2004	-	41,41,41	0.75	0	56,56,56	2.10	18 (32%)
22	CLA	A	803	-	69,73,73	1.24	8 (11%)	83,113,113	1.19	4 (4%)
22	CLA	3	612	4	69,73,73	1.25	7 (10%)	83,113,113	1.12	6 (7%)
23	LUT	V	2621	-	42,43,43	0.78	0	51,60,60	1.68	11 (21%)
21	CHL	2	602	3	65,69,74	2.07	18 (27%)	74,108,114	3.02	26 (35%)
22	CLA	B	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.17	6 (7%)
22	CLA	W	610	1	69,73,73	1.26	7 (10%)	83,113,113	1.22	6 (7%)
22	CLA	A	801	6	69,73,73	1.24	7 (10%)	83,113,113	1.43	11 (13%)
21	CHL	W	606	-	41,46,74	2.47	18 (43%)	52,81,114	3.48	23 (44%)
27	BCR	J	102	-	41,41,41	0.71	0	56,56,56	2.24	17 (30%)
22	CLA	A	833	6	59,63,73	1.33	7 (11%)	71,101,113	1.21	6 (8%)
22	CLA	3	615	-	57,61,73	1.38	8 (14%)	68,98,113	1.26	5 (7%)
30	SF4	C	101	8	0,12,12	-	-	-		
24	XAT	8	620	-	39,47,47	1.76	6 (15%)	54,74,74	1.94	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	B	838	7	51,55,73	1.44	8 (15%)	61,91,113	1.31	9 (14%)
22	CLA	9	612	20	42,47,73	1.55	8 (19%)	52,81,113	1.21	3 (5%)
26	LHG	3	630	22	31,31,48	1.16	2 (6%)	34,37,54	1.05	2 (5%)
27	BCR	A	852	-	41,41,41	0.72	0	56,56,56	2.28	24 (42%)
22	CLA	B	829	7	69,73,73	1.26	7 (10%)	83,113,113	1.10	4 (4%)
22	CLA	4	610	5	65,69,73	1.32	8 (12%)	78,108,113	1.14	5 (6%)
22	CLA	7	614	4	45,49,73	1.53	6 (13%)	54,84,113	1.32	4 (7%)
22	CLA	U	602	1	69,73,73	1.25	6 (8%)	83,113,113	1.15	7 (8%)
22	CLA	7	611	26	45,49,73	1.53	8 (17%)	54,84,113	1.21	5 (9%)
24	XAT	6	620	-	39,47,47	1.23	2 (5%)	54,74,74	6.73	25 (46%)
31	LMT	B	849	-	32,32,36	0.66	0	43,43,47	1.32	7 (16%)
27	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.19	21 (37%)
22	CLA	4	613	5	59,63,73	1.35	6 (10%)	71,101,113	1.17	6 (8%)
22	CLA	7	615	-	43,48,73	1.56	6 (13%)	51,83,113	1.26	4 (7%)
22	CLA	A	830	6	69,73,73	1.24	7 (10%)	83,113,113	1.17	8 (9%)
27	BCR	1	619	-	41,41,41	0.74	0	56,56,56	2.55	27 (48%)
22	CLA	9	602	20	64,68,73	1.29	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	3	604	-	59,63,73	1.33	7 (11%)	71,101,113	1.22	8 (11%)
26	LHG	7	630	22	33,33,48	1.14	2 (6%)	36,39,54	1.08	3 (8%)
21	CHL	8	607	-	50,54,74	2.31	17 (34%)	56,90,114	3.34	23 (41%)
24	XAT	3	619	-	39,47,47	0.87	1 (2%)	54,74,74	2.76	21 (38%)
22	CLA	G	201	-	49,53,73	1.48	8 (16%)	59,89,113	1.21	5 (8%)
23	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
22	CLA	6	603	3	50,54,73	1.48	7 (14%)	60,90,113	1.34	7 (11%)
21	CHL	9	606	-	48,52,74	2.25	16 (33%)	53,87,114	3.40	24 (45%)
22	CLA	1	612	2	50,54,73	1.45	7 (14%)	60,90,113	1.23	4 (6%)
21	CHL	W	608	-	43,48,74	2.30	15 (34%)	51,83,114	3.44	22 (43%)
22	CLA	1	610	2	69,73,73	1.25	6 (8%)	83,113,113	1.13	6 (7%)
22	CLA	B	833	7	69,73,73	1.24	7 (10%)	83,113,113	1.19	6 (7%)
22	CLA	3	602	4	69,73,73	1.25	7 (10%)	83,113,113	1.12	7 (8%)
22	CLA	1	609	2	69,73,73	1.28	8 (11%)	83,113,113	1.13	6 (7%)
28	LMG	J	104	-	35,35,55	1.14	2 (5%)	43,43,63	1.01	2 (4%)
22	CLA	9	604	-	47,51,73	1.51	7 (14%)	56,86,113	1.19	4 (7%)
27	BCR	L	306	-	41,41,41	0.70	0	56,56,56	2.06	20 (35%)
21	CHL	U	606	-	50,54,74	2.28	18 (36%)	56,90,114	3.43	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	7	602	4	64,68,73	1.33	6 (9%)	77,107,113	1.34	9 (11%)
22	CLA	V	602	1	63,67,73	1.31	6 (9%)	75,105,113	1.19	7 (9%)
21	CHL	W	605	1	41,46,74	2.46	17 (41%)	52,81,114	3.47	22 (42%)
22	CLA	1	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.13	6 (7%)
21	CHL	1	601	2	60,64,74	2.11	18 (30%)	68,102,114	3.04	26 (38%)
22	CLA	A	806	6	69,73,73	1.24	7 (10%)	83,113,113	1.18	6 (7%)
27	BCR	F	305	-	41,41,41	0.69	0	56,56,56	2.13	19 (33%)
23	LUT	9	621	-	42,43,43	0.81	0	51,60,60	1.68	13 (25%)
21	CHL	U	607	-	70,74,74	1.95	17 (24%)	80,114,114	2.87	25 (31%)
22	CLA	A	831	6	69,73,73	1.24	6 (8%)	83,113,113	1.11	5 (6%)
21	CHL	5	601	2	55,59,74	2.20	18 (32%)	62,96,114	3.18	26 (41%)
22	CLA	W	614	1	42,47,73	1.62	9 (21%)	53,82,113	1.30	7 (13%)
22	CLA	7	617	4	50,54,73	1.46	6 (12%)	60,90,113	1.24	6 (10%)
27	BCR	B	801	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
21	CHL	U	608	-	43,48,74	2.32	17 (39%)	51,83,114	3.41	22 (43%)
22	CLA	B	807	7	69,73,73	1.25	8 (11%)	83,113,113	1.18	8 (9%)
21	CHL	9	607	-	47,51,74	2.29	16 (34%)	52,86,114	3.30	22 (42%)
22	CLA	B	826	7	69,73,73	1.26	8 (11%)	83,113,113	1.15	6 (7%)
22	CLA	B	839	-	69,73,73	1.24	6 (8%)	83,113,113	1.13	5 (6%)
22	CLA	7	604	-	54,58,73	1.41	6 (11%)	65,95,113	1.26	6 (9%)
32	DGD	B	850	-	67,67,67	0.89	2 (2%)	81,81,81	0.96	3 (3%)
22	CLA	V	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.27	6 (9%)
22	CLA	A	813	6	59,63,73	1.34	8 (13%)	71,101,113	1.27	6 (8%)
21	CHL	V	609	1	43,48,74	2.28	15 (34%)	49,82,114	3.43	21 (42%)
22	CLA	6	610	3	64,68,73	1.29	6 (9%)	77,107,113	1.14	5 (6%)
22	CLA	4	609	5	49,53,73	1.47	7 (14%)	59,89,113	1.26	8 (13%)
22	CLA	A	823	6	57,62,73	1.30	7 (12%)	67,99,113	1.26	7 (10%)
22	CLA	2	612	3	49,53,73	1.47	6 (12%)	59,89,113	1.28	3 (5%)
27	BCR	A	849	-	41,41,41	0.77	0	56,56,56	2.01	18 (32%)
22	CLA	B	809	7	69,73,73	1.25	8 (11%)	83,113,113	1.19	6 (7%)
22	CLA	A	810	6	69,73,73	1.24	6 (8%)	83,113,113	1.21	7 (8%)
22	CLA	A	828	6	69,73,73	1.26	9 (13%)	83,113,113	1.20	7 (8%)
22	CLA	B	828	7	69,73,73	1.24	8 (11%)	83,113,113	1.16	7 (8%)
27	BCR	L	301	-	41,41,41	0.72	0	56,56,56	2.29	19 (33%)
21	CHL	1	607	2	51,55,74	2.29	18 (35%)	57,91,114	3.21	23 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	5	611	26	50,54,73	1.47	7 (14%)	60,90,113	1.25	5 (8%)
22	CLA	8	614	5	49,53,73	1.49	6 (12%)	59,89,113	1.30	7 (11%)
21	CHL	6	618	3	51,55,74	2.24	17 (33%)	57,91,114	3.27	22 (38%)
22	CLA	V	614	1	49,53,73	1.49	7 (14%)	59,89,113	1.23	6 (10%)
21	CHL	U	601	1	66,71,74	1.96	18 (27%)	82,111,114	2.76	25 (30%)
22	CLA	A	805	6	69,73,73	1.25	7 (10%)	83,113,113	1.24	9 (10%)
22	CLA	8	601	5	54,58,73	1.44	9 (16%)	65,95,113	1.21	6 (9%)
22	CLA	B	820	7	59,63,73	1.34	8 (13%)	71,101,113	1.22	6 (8%)
31	LMT	A	857	-	36,36,36	0.77	0	47,47,47	1.36	7 (14%)
22	CLA	A	807	6	69,73,73	1.24	6 (8%)	83,113,113	1.15	5 (6%)
21	CHL	4	618	5	47,51,74	2.26	16 (34%)	52,86,114	3.34	22 (42%)
22	CLA	9	613	20	56,60,73	1.41	8 (14%)	67,97,113	1.24	7 (10%)
22	CLA	9	610	20	59,63,73	1.35	8 (13%)	71,101,113	1.18	7 (9%)
21	CHL	W	601	1	66,71,74	1.96	18 (27%)	82,111,114	2.77	25 (30%)
22	CLA	U	612	1	69,73,73	1.25	7 (10%)	83,113,113	1.09	4 (4%)
27	BCR	A	848	-	41,41,41	0.78	0	56,56,56	1.93	17 (30%)
26	LHG	5	630	22	36,36,48	1.08	2 (5%)	39,42,54	1.07	3 (7%)
22	CLA	A	838	6	59,63,73	1.34	7 (11%)	71,101,113	1.23	7 (9%)
23	LUT	W	2620	-	42,43,43	0.79	0	51,60,60	1.67	13 (25%)
22	CLA	O	2003	-	28,35,73	1.89	7 (25%)	32,60,113	1.40	3 (9%)
22	CLA	5	616	2	50,54,73	1.49	7 (14%)	60,90,113	1.18	3 (5%)
22	CLA	3	606	-	50,54,73	1.45	7 (14%)	60,90,113	1.28	4 (6%)
22	CLA	O	2001	19	28,35,73	1.88	7 (25%)	32,60,113	1.50	4 (12%)
24	XAT	2	620	-	39,47,47	0.91	2 (5%)	54,74,74	2.53	22 (40%)
26	LHG	8	630	22	37,37,48	1.07	2 (5%)	40,43,54	1.09	4 (10%)
22	CLA	6	613	3	69,73,73	1.26	5 (7%)	83,113,113	1.10	6 (7%)
22	CLA	1	608	-	49,53,73	1.49	8 (16%)	59,89,113	1.27	6 (10%)
22	CLA	A	818	6	69,73,73	1.25	7 (10%)	83,113,113	1.12	6 (7%)
22	CLA	A	822	-	69,73,73	1.24	7 (10%)	83,113,113	1.14	5 (6%)
22	CLA	7	603	4	49,53,73	1.52	7 (14%)	59,89,113	1.26	5 (8%)
28	LMG	L	307	-	44,44,55	1.00	2 (4%)	52,52,63	0.93	2 (3%)
22	CLA	A	854	-	64,68,73	1.29	8 (12%)	77,107,113	1.19	7 (9%)
22	CLA	3	613	4	69,73,73	1.25	7 (10%)	83,113,113	1.19	7 (8%)
22	CLA	A	817	-	69,73,73	1.26	7 (10%)	83,113,113	1.19	6 (7%)
22	CLA	B	830	7	49,53,73	1.50	7 (14%)	59,89,113	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	K	203	-	59,63,73	1.35	6 (10%)	71,101,113	1.20	8 (11%)
22	CLA	A	835	6	69,73,73	1.24	7 (10%)	83,113,113	1.13	7 (8%)
22	CLA	B	812	7	47,52,73	1.43	7 (14%)	55,87,113	1.34	5 (9%)
31	LMT	K	208	-	36,36,36	0.61	0	47,47,47	1.27	6 (12%)
28	LMG	2	631	-	47,47,55	0.98	2 (4%)	55,55,63	0.98	4 (7%)
22	CLA	3	603	4	69,73,73	1.26	7 (10%)	83,113,113	1.19	7 (8%)
22	CLA	7	607	4	49,53,73	1.49	6 (12%)	59,89,113	1.30	3 (5%)
23	LUT	9	620	-	42,43,43	0.75	0	51,60,60	1.79	13 (25%)
27	BCR	7	620	-	41,41,41	0.68	0	56,56,56	2.08	20 (35%)
21	CHL	2	608	-	50,54,74	2.34	17 (34%)	56,90,114	3.27	24 (42%)
27	BCR	L	305	-	41,41,41	0.70	0	56,56,56	1.98	21 (37%)
22	CLA	B	836	7	56,60,73	1.37	7 (12%)	67,97,113	1.26	7 (10%)
27	BCR	B	1609	-	41,41,41	0.75	0	56,56,56	3.14	26 (46%)
21	CHL	2	607	-	51,55,74	2.28	17 (33%)	57,91,114	3.33	24 (42%)
27	BCR	8	621	-	41,41,41	0.79	0	56,56,56	2.29	19 (33%)
22	CLA	A	825	6	69,73,73	1.25	6 (8%)	83,113,113	1.25	6 (7%)
22	CLA	2	604	-	54,58,73	1.40	6 (11%)	65,95,113	1.28	6 (9%)
22	CLA	A	837	6	69,73,73	1.26	8 (11%)	83,113,113	1.16	5 (6%)
21	CHL	6	602	3	60,64,74	2.13	16 (26%)	68,102,114	3.16	23 (33%)
22	CLA	3	614	4	49,53,73	1.49	8 (16%)	59,89,113	1.30	6 (10%)
27	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	2.14	24 (42%)
23	LUT	V	2620	-	42,43,43	0.76	0	51,60,60	1.73	16 (31%)

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
22	CLA	1	606	-	-	8/15/91/115	-
22	CLA	B	822	7	-	17/33/109/115	-
26	LHG	B	851	22	-	10/39/39/53	-
22	CLA	1	613	2	-	8/21/97/115	-
27	BCR	B	843	-	-	5/29/63/63	0/2/2/2
22	CLA	B	835	-	-	2/15/91/115	-
22	CLA	B	813	7	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	V	605	1	-	2/12/88/117	-
26	LHG	W	2630	22	-	13/49/49/53	-
22	CLA	3	617	4	-	13/29/102/115	-
22	CLA	9	609	20	-	4/15/91/115	-
22	CLA	1	616	2	-	9/15/91/115	-
27	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	CLA	6	609	3	-	2/27/103/115	-
22	CLA	A	804	6	-	20/39/115/115	-
22	CLA	4	602	5	-	19/39/115/115	-
22	CLA	B	802	7	-	10/39/115/115	-
22	CLA	3	607	4	-	10/21/97/115	-
22	CLA	W	611	26	-	1/8/84/115	-
22	CLA	3	609	4	-	12/39/115/115	-
21	CHL	7	608	-	-	5/17/93/117	-
24	XAT	5	618	-	-	4/31/93/93	0/4/4/4
21	CHL	9	601	20	-	0/6/82/117	-
21	CHL	V	607	-	-	0/8/84/117	-
22	CLA	U	604	-	-	10/24/100/115	-
21	CHL	U	605	1	-	0/4/80/117	-
26	LHG	U	2630	22	-	11/49/49/53	-
21	CHL	4	607	-	-	5/19/95/117	-
22	CLA	V	612	1	-	2/4/80/115	-
23	LUT	3	618	-	-	1/29/67/67	0/2/2/2
21	CHL	4	608	-	-	3/17/93/117	-
22	CLA	A	811	6	-	8/27/103/115	-
22	CLA	4	611	26	-	5/15/91/115	-
22	CLA	5	603	2	-	8/15/91/115	-
22	CLA	2	603	3	-	6/17/93/115	-
22	CLA	7	612	4	-	4/15/91/115	-
24	XAT	7	619	-	-	6/31/93/93	0/4/4/4
22	CLA	V	603	1	-	12/33/109/115	-
23	LUT	4	619	-	-	0/29/67/67	0/2/2/2
22	CLA	W	613	1	-	7/33/109/115	-
22	CLA	2	614	3	-	4/21/97/115	-
22	CLA	A	843	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	614	2	-	12/19/95/115	-
22	CLA	5	608	-	-	8/21/97/115	-
22	CLA	O	2002	-	-	14/27/103/115	-
21	CHL	V	601	1	-	18/35/111/117	-
22	CLA	A	826	-	-	10/39/115/115	-
22	CLA	B	815	7	-	3/15/91/115	-
27	BCR	M	2001	-	-	5/29/63/63	0/2/2/2
22	CLA	V	613	1	-	13/28/104/115	-
22	CLA	V	610	1	-	3/6/82/115	-
22	CLA	A	820	6	-	11/39/115/115	-
22	CLA	A	809	6	-	7/29/105/115	-
22	CLA	B	810	7	-	18/39/115/115	-
22	CLA	4	612	5	-	7/15/91/115	-
22	CLA	B	834	7	-	13/39/115/115	-
22	CLA	B	819	-	-	16/33/109/115	-
22	CLA	2	610	3	-	6/33/109/115	-
22	CLA	5	612	2	-	9/17/93/115	-
21	CHL	2	606	-	-	4/17/93/117	-
22	CLA	F	304	11	-	9/20/73/115	-
22	CLA	B	837	7	-	8/39/115/115	-
24	XAT	U	2622	-	-	1/31/93/93	0/4/4/4
27	BCR	G	205	-	-	4/29/63/63	0/2/2/2
22	CLA	5	614	2	-	4/13/89/115	-
21	CHL	V	608	-	-	3/8/84/117	-
27	BCR	B	848	-	-	3/29/63/63	0/2/2/2
23	LUT	U	2620	-	-	0/29/67/67	0/2/2/2
24	XAT	1	618	-	-	0/31/93/93	0/4/4/4
21	CHL	U	609	1	-	23/41/117/117	-
23	LUT	W	2621	-	-	2/29/67/67	0/2/2/2
26	LHG	A	846	-	-	12/51/51/53	-
26	LHG	9	2630	22	-	14/32/32/53	-
22	CLA	B	805	7	-	11/39/115/115	-
22	CLA	G	204	12	-	4/17/93/115	-
22	CLA	6	614	3	-	3/21/97/115	-
22	CLA	U	610	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	611	26	-	8/15/91/115	-
22	CLA	K	201	16	-	4/12/88/115	-
22	CLA	A	834	6	-	11/39/115/115	-
23	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	LUT	2	619	-	-	12/29/67/67	0/2/2/2
22	CLA	2	611	26	-	8/15/91/115	-
23	LUT	5	617	-	-	14/29/67/67	0/2/2/2
30	SF4	C	102	8	-	-	0/6/5/5
22	CLA	1	603	2	-	11/27/103/115	-
26	LHG	6	630	22	-	9/36/36/53	-
22	CLA	2	609	3	-	8/17/93/115	-
23	LUT	9	624	-	-	3/29/67/67	0/2/2/2
22	CLA	B	817	7	-	18/39/115/115	-
22	CLA	B	821	7	-	7/21/97/115	-
26	LHG	4	630	22	-	20/42/42/53	-
22	CLA	L	303	17	-	11/39/115/115	-
22	CLA	5	604	-	-	5/10/86/115	-
24	XAT	V	2622	-	-	2/31/93/93	0/4/4/4
22	CLA	A	808	6	-	8/33/109/115	-
21	CHL	6	608	-	-	5/20/96/117	-
22	CLA	B	808	7	-	13/39/115/115	-
27	BCR	B	847	-	-	2/29/63/63	0/2/2/2
21	CHL	V	606	-	-	2/4/80/117	-
22	CLA	9	611	26	-	16/39/115/115	-
22	CLA	U	614	1	-	4/12/88/115	-
22	CLA	5	602	2	-	14/33/109/115	-
25	NEX	U	2623	-	-	3/27/83/83	0/3/3/3
22	CLA	B	825	-	-	10/39/115/115	-
22	CLA	5	609	2	-	5/10/86/115	-
22	CLA	A	802	-	-	8/39/115/115	-
22	CLA	J	101	15	-	7/21/97/115	-
22	CLA	7	610	4	-	8/27/103/115	-
22	CLA	B	840	7	-	14/39/115/115	-
22	CLA	8	609	5	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	A	856	-	-	1/27/61/63	0/2/2/2
21	CHL	8	618	5	-	2/14/90/117	-
23	LUT	7	618	-	-	1/29/67/67	0/2/2/2
21	CHL	3	608	-	-	11/29/105/117	-
22	CLA	6	612	3	-	6/15/91/115	-
22	CLA	7	613	4	-	10/27/103/115	-
25	NEX	9	623	-	-	2/27/83/83	0/3/3/3
27	BCR	6	621	-	-	6/29/63/63	0/2/2/2
26	LHG	A	847	22	-	17/35/35/53	-
22	CLA	A	845	26	-	12/39/115/115	-
22	CLA	A	814	6	-	22/39/115/115	-
22	CLA	H	201	-	-	2/4/80/115	-
21	CHL	6	607	-	-	7/19/95/117	-
22	CLA	B	814	7	-	12/39/115/115	-
22	CLA	8	604	-	-	7/21/97/115	-
27	BCR	4	621	-	-	7/29/63/63	0/2/2/2
27	BCR	3	621	-	-	0/29/63/63	0/2/2/2
22	CLA	6	604	-	-	4/21/97/115	-
22	CLA	K	206	16	-	4/12/88/115	-
27	BCR	K	205	-	-	3/29/63/63	0/2/2/2
22	CLA	W	612	1	-	2/4/80/115	-
22	CLA	4	604	-	-	8/27/103/115	-
22	CLA	7	606	-	-	9/17/93/115	-
22	CLA	B	804	7	-	10/39/115/115	-
27	BCR	I	101	-	-	3/29/63/63	0/2/2/2
22	CLA	8	603	5	-	8/27/103/115	-
21	CHL	4	606	-	-	3/17/93/117	-
22	CLA	L	304	-	-	13/33/109/115	-
21	CHL	5	607	2	-	0/6/82/117	-
22	CLA	W	602	1	-	5/33/109/115	-
27	BCR	B	845	-	-	10/29/63/63	0/2/2/2
21	CHL	9	605	20	-	0/4/80/117	-
22	CLA	3	611	26	-	13/27/103/115	-
22	CLA	A	812	6	-	12/39/115/115	-
22	CLA	A	824	6	-	15/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	832	6	-	7/27/103/115	-
21	CHL	6	601	3	-	16/41/117/117	-
26	LHG	1	630	22	-	25/53/53/53	-
22	CLA	W	604	-	-	3/12/88/115	-
22	CLA	K	204	16	-	16/39/115/115	-
22	CLA	4	601	5	-	10/21/97/115	-
22	CLA	B	816	7	-	9/39/115/115	-
21	CHL	W	609	1	-	1/8/84/117	-
22	CLA	A	815	6	-	15/39/115/115	-
21	CHL	2	618	3	-	4/14/90/117	-
22	CLA	9	603	20	-	3/12/88/115	-
22	CLA	A	842	6	-	10/27/103/115	-
22	CLA	B	831	7	-	15/39/115/115	-
22	CLA	1	611	26	-	18/39/115/115	-
28	LMG	J	103	-	-	11/50/70/70	0/1/1/1
22	CLA	5	610	2	-	4/27/103/115	-
22	CLA	1	604	-	-	10/21/97/115	-
22	CLA	A	839	6	-	8/33/109/115	-
22	CLA	A	840	6	-	6/21/97/115	-
22	CLA	F	303	-	-	2/15/91/115	-
27	BCR	K	202	-	-	4/29/63/63	0/2/2/2
21	CHL	W	607	-	-	3/8/84/117	-
22	CLA	B	824	-	-	9/39/115/115	-
22	CLA	5	613	2	-	10/21/97/115	-
25	NEX	V	2623	-	-	2/27/83/83	0/3/3/3
26	LHG	V	2630	22	-	8/46/46/53	-
22	CLA	L	302	17	-	23/39/115/115	-
30	SF4	A	853	6,7	-	-	0/6/5/5
22	CLA	8	613	5	-	8/27/103/115	-
22	CLA	8	610	5	-	7/27/103/115	-
22	CLA	B	806	7	-	16/39/115/115	-
22	CLA	B	811	7	-	9/35/111/115	-
24	XAT	W	2622	-	-	1/31/93/93	0/4/4/4
22	CLA	A	836	6	-	13/37/105/115	-
22	CLA	A	841	6	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	U	2621	-	-	1/29/67/67	0/2/2/2
22	CLA	7	609	4	-	10/30/106/115	-
21	CHL	8	608	-	-	7/23/99/117	-
27	BCR	2	621	-	-	6/29/63/63	0/2/2/2
22	CLA	U	603	1	-	11/39/115/115	-
22	CLA	A	819	6	-	9/36/112/115	-
22	CLA	5	606	2	-	2/15/91/115	-
22	CLA	B	841	26	-	10/39/115/115	-
27	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	3	610	4	-	10/33/109/115	-
26	LHG	2	630	22	-	9/36/36/53	-
23	LUT	8	619	-	-	1/29/67/67	0/2/2/2
22	CLA	A	821	6	-	4/27/103/115	-
22	CLA	8	611	26	-	4/27/103/115	-
22	CLA	V	611	26	-	2/8/84/115	-
22	CLA	A	827	33	-	14/39/115/115	-
22	CLA	B	827	7	-	12/29/105/115	-
22	CLA	W	603	1	-	3/6/82/115	-
22	CLA	U	613	1	-	12/39/115/115	-
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
24	XAT	4	620	-	-	3/31/93/93	0/4/4/4
25	NEX	W	2623	-	-	7/27/83/83	0/3/3/3
22	CLA	4	614	5	-	9/17/93/115	-
22	CLA	G	203	12	-	8/21/97/115	-
27	BCR	3	620	-	-	2/29/63/63	0/2/2/2
22	CLA	A	816	6	-	5/15/91/115	-
21	CHL	9	608	-	-	2/14/90/117	-
21	CHL	8	606	-	-	3/17/93/117	-
22	CLA	B	823	7	-	6/15/91/115	-
22	CLA	4	603	5	-	15/39/115/115	-
22	CLA	2	613	3	-	14/30/106/115	-
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2
22	CLA	B	818	7	-	15/38/114/115	-
22	CLA	8	612	5	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	G	206	-	-	7/21/61/61	0/2/2/2
21	CHL	6	606	-	-	4/17/93/117	-
22	CLA	A	829	6	-	11/33/109/115	-
22	CLA	U	611	26	-	9/15/91/115	-
21	CHL	2	601	3	-	5/17/93/117	-
28	LMG	G	202	-	-	9/27/47/70	0/1/1/1
22	CLA	B	832	7	-	10/39/115/115	-
28	LMG	A	860	-	-	12/29/49/70	0/1/1/1
22	CLA	F	301	33	-	15/39/115/115	-
22	CLA	8	602	5	-	8/33/109/115	-
27	BCR	O	2004	-	-	5/29/63/63	0/2/2/2
22	CLA	A	803	-	-	8/39/115/115	-
22	CLA	3	612	4	-	16/39/115/115	-
23	LUT	V	2621	-	-	2/29/67/67	0/2/2/2
21	CHL	2	602	3	-	10/35/111/117	-
22	CLA	B	803	-	-	16/39/115/115	-
22	CLA	W	610	1	-	19/39/115/115	-
22	CLA	A	801	6	-	13/39/115/115	-
21	CHL	W	606	-	-	0/4/80/117	-
27	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	CLA	A	833	6	-	8/27/103/115	-
22	CLA	3	615	-	-	4/25/101/115	-
30	SF4	C	101	8	-	-	0/6/5/5
24	XAT	8	620	-	-	18/31/93/93	0/4/4/4
22	CLA	B	838	7	-	5/18/94/115	-
22	CLA	9	612	20	-	1/6/82/115	-
26	LHG	3	630	22	-	8/36/36/53	-
27	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	B	829	7	-	8/39/115/115	-
22	CLA	4	610	5	-	14/35/111/115	-
22	CLA	7	614	4	-	3/10/86/115	-
22	CLA	U	602	1	-	10/39/115/115	-
22	CLA	7	611	26	-	4/10/86/115	-
24	XAT	6	620	-	-	3/31/93/93	0/4/4/4
31	LMT	B	849	-	-	5/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	7	621	-	-	1/29/63/63	0/2/2/2
22	CLA	4	613	5	-	6/27/103/115	-
22	CLA	7	615	-	-	2/8/84/115	-
22	CLA	A	830	6	-	17/39/115/115	-
27	BCR	1	619	-	-	6/29/63/63	0/2/2/2
22	CLA	9	602	20	-	12/33/109/115	-
22	CLA	3	604	-	-	8/27/103/115	-
26	LHG	7	630	22	-	11/38/38/53	-
21	CHL	8	607	-	-	5/17/93/117	-
24	XAT	3	619	-	-	0/31/93/93	0/4/4/4
22	CLA	G	201	-	-	7/15/91/115	-
23	LUT	1	617	-	-	0/29/67/67	0/2/2/2
22	CLA	6	603	3	-	7/17/93/115	-
21	CHL	9	606	-	-	1/15/91/117	-
22	CLA	1	612	2	-	3/17/93/115	-
21	CHL	W	608	-	-	1/8/84/117	-
22	CLA	1	610	2	-	12/39/115/115	-
22	CLA	B	833	7	-	18/39/115/115	-
22	CLA	3	602	4	-	9/39/115/115	-
22	CLA	1	609	2	-	14/39/115/115	-
28	LMG	J	104	-	-	6/30/50/70	0/1/1/1
22	CLA	9	604	-	-	3/13/89/115	-
27	BCR	L	306	-	-	3/29/63/63	0/2/2/2
21	CHL	U	606	-	-	5/17/93/117	-
22	CLA	7	602	4	-	10/33/109/115	-
22	CLA	V	602	1	-	7/32/108/115	-
21	CHL	W	605	1	-	0/4/80/117	-
22	CLA	1	602	2	-	14/39/115/115	-
21	CHL	1	601	2	-	11/29/105/117	-
22	CLA	A	806	6	-	17/39/115/115	-
27	BCR	F	305	-	-	5/29/63/63	0/2/2/2
23	LUT	9	621	-	-	1/29/67/67	0/2/2/2
21	CHL	U	607	-	-	14/41/117/117	-
22	CLA	A	831	6	-	10/39/115/115	-
21	CHL	5	601	2	-	7/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	W	614	1	-	2/6/82/115	-
22	CLA	7	617	4	-	7/17/93/115	-
27	BCR	B	801	-	-	4/29/63/63	0/2/2/2
21	CHL	U	608	-	-	3/8/84/117	-
22	CLA	B	807	7	-	4/39/115/115	-
21	CHL	9	607	-	-	3/14/90/117	-
22	CLA	B	826	7	-	11/39/115/115	-
22	CLA	B	839	-	-	9/39/115/115	-
22	CLA	7	604	-	-	8/21/97/115	-
32	DGD	B	850	-	-	16/55/95/95	0/2/2/2
22	CLA	V	604	-	-	8/21/97/115	-
22	CLA	A	813	6	-	7/27/103/115	-
21	CHL	V	609	1	-	2/8/84/117	-
22	CLA	6	610	3	-	11/33/109/115	-
22	CLA	4	609	5	-	6/15/91/115	-
22	CLA	A	823	6	-	8/27/103/115	-
22	CLA	2	612	3	-	9/15/91/115	-
27	BCR	A	849	-	-	4/29/63/63	0/2/2/2
22	CLA	B	809	7	-	11/39/115/115	-
22	CLA	A	810	6	-	17/39/115/115	-
22	CLA	A	828	6	-	14/39/115/115	-
22	CLA	B	828	7	-	14/39/115/115	-
27	BCR	L	301	-	-	6/29/63/63	0/2/2/2
21	CHL	1	607	2	-	8/19/95/117	-
22	CLA	5	611	26	-	6/17/93/115	-
22	CLA	8	614	5	-	9/15/91/115	-
21	CHL	6	618	3	-	10/19/95/117	-
22	CLA	V	614	1	-	5/15/91/115	-
21	CHL	U	601	1	-	20/35/111/117	-
22	CLA	A	805	6	-	17/39/115/115	-
22	CLA	8	601	5	-	5/21/97/115	-
22	CLA	B	820	7	-	12/27/103/115	-
31	LMT	A	857	-	-	7/21/61/61	0/2/2/2
22	CLA	A	807	6	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	4	618	5	-	2/14/90/117	-
22	CLA	9	613	20	-	3/24/100/115	-
22	CLA	9	610	20	-	9/27/103/115	-
21	CHL	W	601	1	-	15/35/111/117	-
22	CLA	U	612	1	-	12/39/115/115	-
27	BCR	A	848	-	-	4/29/63/63	0/2/2/2
26	LHG	5	630	22	-	5/41/41/53	-
22	CLA	A	838	6	-	9/27/103/115	-
23	LUT	W	2620	-	-	2/29/67/67	0/2/2/2
22	CLA	5	616	2	-	4/17/93/115	-
22	CLA	3	606	-	-	10/17/93/115	-
26	LHG	8	630	22	-	9/42/42/53	-
24	XAT	2	620	-	-	0/31/93/93	0/4/4/4
22	CLA	6	613	3	-	12/39/115/115	-
22	CLA	1	608	-	-	7/15/91/115	-
22	CLA	A	818	6	-	5/39/115/115	-
22	CLA	A	822	-	-	12/39/115/115	-
22	CLA	7	603	4	-	6/15/91/115	-
28	LMG	L	307	-	-	14/39/59/70	0/1/1/1
22	CLA	A	854	-	-	17/33/109/115	-
22	CLA	3	613	4	-	13/39/115/115	-
22	CLA	A	817	-	-	12/39/115/115	-
22	CLA	B	830	7	-	8/15/91/115	-
22	CLA	K	203	-	-	10/27/103/115	-
22	CLA	A	835	6	-	14/39/115/115	-
22	CLA	B	812	7	-	4/15/91/115	-
31	LMT	K	208	-	-	7/21/61/61	0/2/2/2
28	LMG	2	631	-	-	12/42/62/70	0/1/1/1
22	CLA	3	603	4	-	8/39/115/115	-
22	CLA	7	607	4	-	3/15/91/115	-
23	LUT	9	620	-	-	2/29/67/67	0/2/2/2
27	BCR	7	620	-	-	1/29/63/63	0/2/2/2
21	CHL	2	608	-	-	0/17/93/117	-
27	BCR	L	305	-	-	2/29/63/63	0/2/2/2
22	CLA	B	836	7	-	10/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	1609	-	-	5/29/63/63	0/2/2/2
21	CHL	2	607	-	-	3/19/95/117	-
27	BCR	8	621	-	-	4/29/63/63	0/2/2/2
22	CLA	A	825	6	-	20/39/115/115	-
22	CLA	2	604	-	-	4/21/97/115	-
22	CLA	A	837	6	-	19/39/115/115	-
21	CHL	6	602	3	-	10/29/105/117	-
22	CLA	3	614	4	-	8/15/91/115	-
27	BCR	A	851	-	-	2/29/63/63	0/2/2/2
23	LUT	V	2620	-	-	1/29/67/67	0/2/2/2

All (2528) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	836	CLA	C4B-C3B	7.11	1.49	1.38
22	3	617	CLA	C4B-C3B	6.87	1.48	1.38
21	4	607	CHL	O2D-CGD	5.28	1.46	1.33
21	6	608	CHL	O2D-CGD	5.24	1.46	1.33
21	4	606	CHL	O2D-CGD	5.24	1.46	1.33
21	6	607	CHL	O2D-CGD	5.23	1.46	1.33
21	2	608	CHL	O2D-CGD	5.22	1.45	1.33
21	7	608	CHL	O2D-CGD	5.22	1.45	1.33
21	8	618	CHL	O2D-CGD	5.20	1.45	1.33
21	9	608	CHL	O2D-CGD	5.20	1.45	1.33
21	U	605	CHL	C3C-C2C	5.19	1.46	1.36
21	8	606	CHL	O2D-CGD	5.19	1.45	1.33
21	U	607	CHL	O2D-CGD	5.18	1.45	1.33
21	6	606	CHL	O2D-CGD	5.17	1.45	1.33
21	9	606	CHL	O2D-CGD	5.17	1.45	1.33
21	4	608	CHL	O2D-CGD	5.17	1.45	1.33
21	2	607	CHL	O2D-CGD	5.17	1.45	1.33
21	9	607	CHL	O2D-CGD	5.17	1.45	1.33
21	2	602	CHL	CHC-C1C	5.16	1.49	1.38
21	4	618	CHL	O2D-CGD	5.15	1.45	1.33
21	8	608	CHL	O2D-CGD	5.15	1.45	1.33
21	8	607	CHL	O2D-CGD	5.15	1.45	1.33
21	3	608	CHL	O2D-CGD	5.15	1.45	1.33
21	2	606	CHL	O2D-CGD	5.14	1.45	1.33
22	9	609	CLA	O2D-CGD	5.14	1.45	1.33
21	W	605	CHL	C3C-C2C	5.13	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	617	CLA	C2C-C3C	5.12	1.39	1.33
21	1	607	CHL	O2D-CGD	5.11	1.45	1.33
21	6	618	CHL	O2D-CGD	5.11	1.45	1.33
21	W	606	CHL	C3C-C2C	5.11	1.46	1.36
21	2	618	CHL	O2D-CGD	5.11	1.45	1.33
21	V	607	CHL	O2D-CGD	5.10	1.45	1.33
21	U	606	CHL	O2D-CGD	5.10	1.45	1.33
21	1	601	CHL	O2D-CGD	5.09	1.45	1.33
21	2	602	CHL	O2D-CGD	5.09	1.45	1.33
21	6	602	CHL	O2D-CGD	5.08	1.45	1.33
21	W	607	CHL	O2D-CGD	5.08	1.45	1.33
21	U	609	CHL	O2D-CGD	5.08	1.45	1.33
21	2	608	CHL	CHC-C1C	5.07	1.48	1.38
21	V	605	CHL	O2D-CGD	5.06	1.45	1.33
21	6	601	CHL	O2D-CGD	5.06	1.45	1.33
21	V	606	CHL	C3C-C2C	5.05	1.46	1.36
21	5	601	CHL	O2D-CGD	5.05	1.45	1.33
21	6	602	CHL	CHC-C1C	5.03	1.48	1.38
21	2	601	CHL	O2D-CGD	5.01	1.45	1.33
21	U	606	CHL	CHC-C1C	4.95	1.48	1.38
21	9	601	CHL	C3D-C4D	-4.93	1.33	1.44
21	7	608	CHL	C3D-C4D	-4.90	1.33	1.44
22	9	609	CLA	C3D-C4D	-4.90	1.33	1.44
21	3	608	CHL	C3D-C4D	-4.88	1.33	1.44
21	2	602	CHL	C3D-C4D	-4.88	1.33	1.44
21	W	606	CHL	C3D-C4D	-4.87	1.33	1.44
21	U	609	CHL	C3D-C4D	-4.87	1.33	1.44
22	3	617	CLA	C1C-C2C	-4.87	1.45	1.51
21	W	601	CHL	C3D-C4D	-4.87	1.33	1.44
21	9	608	CHL	C3D-C4D	-4.87	1.33	1.44
21	2	607	CHL	CHC-C1C	4.85	1.48	1.38
21	8	607	CHL	CHC-C1C	4.85	1.48	1.38
21	8	608	CHL	CHC-C1C	4.85	1.48	1.38
21	4	607	CHL	CHC-C1C	4.84	1.48	1.38
21	2	608	CHL	C3D-C4D	-4.84	1.33	1.44
21	U	608	CHL	C3D-C4D	-4.84	1.33	1.44
21	2	601	CHL	C3D-C4D	-4.84	1.33	1.44
21	W	607	CHL	C3D-C4D	-4.83	1.33	1.44
21	V	609	CHL	C3D-C4D	-4.83	1.33	1.44
21	9	606	CHL	C3D-C4D	-4.83	1.33	1.44
21	1	607	CHL	C3D-C4D	-4.83	1.33	1.44
21	2	618	CHL	C3D-C4D	-4.83	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	607	CHL	C3D-C4D	-4.82	1.33	1.44
21	1	601	CHL	CHC-C1C	4.82	1.48	1.38
21	2	606	CHL	C3D-C4D	-4.81	1.33	1.44
21	8	608	CHL	C3D-C4D	-4.81	1.33	1.44
21	6	601	CHL	CHC-C1C	4.80	1.48	1.38
21	4	606	CHL	C3D-C4D	-4.80	1.33	1.44
21	U	606	CHL	C3D-C4D	-4.80	1.33	1.44
21	4	607	CHL	C3D-C4D	-4.80	1.33	1.44
21	2	618	CHL	CHC-C1C	4.80	1.48	1.38
21	6	608	CHL	CHC-C1C	4.80	1.48	1.38
21	1	601	CHL	C3D-C4D	-4.80	1.33	1.44
21	U	601	CHL	C3D-C4D	-4.79	1.33	1.44
21	5	607	CHL	CHC-C1C	4.79	1.48	1.38
21	8	606	CHL	CHC-C1C	4.79	1.48	1.38
21	8	606	CHL	C3D-C4D	-4.79	1.33	1.44
21	W	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	9	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	U	605	CHL	C3D-C4D	-4.79	1.33	1.44
21	5	601	CHL	CHC-C1C	4.78	1.48	1.38
21	V	607	CHL	C3D-C4D	-4.78	1.33	1.44
21	V	608	CHL	C3D-C4D	-4.78	1.33	1.44
21	4	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	8	618	CHL	C3D-C4D	-4.77	1.33	1.44
21	6	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	5	607	CHL	C3D-C4D	-4.77	1.33	1.44
21	6	606	CHL	C3D-C4D	-4.77	1.33	1.44
21	1	607	CHL	CHC-C1C	4.77	1.48	1.38
21	W	608	CHL	C3D-C4D	-4.77	1.33	1.44
21	V	607	CHL	CHC-C1C	4.77	1.48	1.38
21	U	607	CHL	C3D-C4D	-4.76	1.33	1.44
21	V	601	CHL	C3D-C4D	-4.76	1.33	1.44
21	4	608	CHL	CHC-C1C	4.76	1.48	1.38
21	6	607	CHL	CHC-C1C	4.76	1.48	1.38
21	2	601	CHL	CHC-C1C	4.76	1.48	1.38
21	V	609	CHL	CHC-C1C	4.76	1.48	1.38
21	W	607	CHL	CHC-C1C	4.76	1.48	1.38
21	W	609	CHL	C3D-C4D	-4.76	1.33	1.44
21	V	605	CHL	C3D-C4D	-4.75	1.33	1.44
21	9	607	CHL	C3D-C4D	-4.75	1.33	1.44
21	8	607	CHL	C3D-C4D	-4.75	1.33	1.44
21	8	618	CHL	CHC-C1C	4.74	1.48	1.38
22	9	609	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	608	CHL	CHC-C1C	4.73	1.48	1.38
21	6	618	CHL	C3D-C4D	-4.73	1.33	1.44
21	6	607	CHL	C3D-C4D	-4.73	1.33	1.44
21	V	606	CHL	C3D-C4D	-4.73	1.33	1.44
21	6	601	CHL	C3D-C4D	-4.73	1.33	1.44
21	9	605	CHL	CHC-C1C	4.72	1.48	1.38
21	6	602	CHL	C3D-C4D	-4.72	1.33	1.44
21	5	601	CHL	C3D-C4D	-4.72	1.33	1.44
21	U	607	CHL	CHC-C1C	4.71	1.48	1.38
21	6	606	CHL	CHC-C1C	4.71	1.48	1.38
21	V	608	CHL	CHC-C1C	4.71	1.48	1.38
21	9	606	CHL	CHC-C1C	4.70	1.48	1.38
26	9	2630	LHG	O8-C23	4.69	1.47	1.33
21	V	605	CHL	CHC-C1C	4.69	1.48	1.38
21	4	606	CHL	CHC-C1C	4.68	1.48	1.38
21	W	605	CHL	O2D-CGD	4.68	1.45	1.30
21	V	606	CHL	O2D-CGD	4.68	1.45	1.30
21	4	618	CHL	C3D-C4D	-4.67	1.33	1.44
21	9	601	CHL	CHC-C1C	4.67	1.48	1.38
21	W	605	CHL	CHC-C1C	4.66	1.48	1.38
21	U	609	CHL	CHC-C1C	4.66	1.48	1.38
21	9	608	CHL	CHC-C1C	4.66	1.48	1.38
21	7	608	CHL	CHC-C1C	4.66	1.48	1.38
21	W	601	CHL	CHC-C1C	4.64	1.48	1.38
21	U	605	CHL	O2D-CGD	4.64	1.45	1.30
21	W	606	CHL	O2D-CGD	4.64	1.45	1.30
21	U	601	CHL	CHC-C1C	4.64	1.47	1.38
21	V	601	CHL	O2D-CGD	4.64	1.45	1.30
21	W	601	CHL	O2D-CGD	4.63	1.45	1.30
21	U	601	CHL	O2D-CGD	4.63	1.45	1.30
21	W	608	CHL	O2D-CGD	4.63	1.45	1.30
21	V	608	CHL	O2D-CGD	4.62	1.45	1.30
21	1	601	CHL	C2C-C3C	4.62	1.46	1.36
21	2	606	CHL	CHC-C1C	4.61	1.47	1.38
21	U	608	CHL	O2D-CGD	4.61	1.45	1.30
21	6	607	CHL	C2C-C3C	4.61	1.46	1.36
21	U	601	CHL	C3C-C2C	4.61	1.46	1.36
21	1	607	CHL	C2C-C3C	4.61	1.46	1.36
21	V	609	CHL	C2C-C3C	4.60	1.46	1.36
21	U	605	CHL	CHC-C1C	4.60	1.47	1.38
21	W	609	CHL	CHC-C1C	4.59	1.47	1.38
21	9	601	CHL	C2C-C3C	4.59	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	607	CHL	C2C-C3C	4.59	1.46	1.36
21	8	607	CHL	C2C-C3C	4.58	1.46	1.36
21	2	608	CHL	C2C-C3C	4.57	1.46	1.36
21	V	601	CHL	CHC-C1C	4.57	1.47	1.38
21	6	601	CHL	C2C-C3C	4.56	1.46	1.36
21	9	605	CHL	C2C-C3C	4.56	1.46	1.37
22	9	609	CLA	C3C-C2C	4.56	1.46	1.36
21	8	606	CHL	C2C-C3C	4.55	1.46	1.36
21	U	607	CHL	C2C-C3C	4.55	1.46	1.36
21	8	618	CHL	C2C-C3C	4.55	1.46	1.36
21	3	608	CHL	CHC-C1C	4.54	1.47	1.38
21	9	608	CHL	C2C-C3C	4.54	1.46	1.36
21	V	601	CHL	C3C-C2C	4.53	1.46	1.36
21	6	602	CHL	C2C-C3C	4.53	1.46	1.36
21	4	608	CHL	O2A-CGA	4.53	1.46	1.30
21	V	601	CHL	CHD-C1D	4.52	1.47	1.38
21	2	618	CHL	C2C-C3C	4.52	1.46	1.36
21	2	607	CHL	C2C-C3C	4.52	1.46	1.36
22	O	2003	CLA	C2B-C1B	4.52	1.49	1.40
21	W	601	CHL	C3C-C2C	4.52	1.46	1.36
21	4	606	CHL	O2A-CGA	4.52	1.45	1.30
21	2	602	CHL	O2A-CGA	4.51	1.46	1.33
21	2	608	CHL	O2A-CGA	4.51	1.45	1.30
21	V	605	CHL	C2C-C3C	4.51	1.46	1.36
21	4	607	CHL	C2C-C3C	4.50	1.46	1.36
21	2	601	CHL	O2A-CGA	4.50	1.45	1.30
21	7	608	CHL	O2A-CGA	4.50	1.45	1.30
21	6	618	CHL	CHC-C1C	4.50	1.47	1.38
21	W	607	CHL	C2C-C3C	4.50	1.46	1.37
21	2	601	CHL	C2C-C3C	4.49	1.46	1.36
21	5	601	CHL	C2C-C3C	4.49	1.46	1.36
21	1	607	CHL	CHD-C1D	4.49	1.47	1.38
22	O	2001	CLA	C2B-C1B	4.49	1.49	1.40
21	8	607	CHL	O2A-CGA	4.49	1.45	1.30
21	8	606	CHL	O2A-CGA	4.49	1.45	1.30
21	2	606	CHL	O2A-CGA	4.49	1.45	1.30
21	U	606	CHL	O2A-CGA	4.49	1.45	1.30
21	V	608	CHL	C2C-C3C	4.48	1.46	1.37
21	V	606	CHL	CHC-C1C	4.48	1.47	1.38
21	W	608	CHL	CHC-C1C	4.48	1.47	1.38
21	W	606	CHL	CHC-C1C	4.48	1.47	1.38
22	9	609	CLA	O2A-CGA	4.47	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	620	XAT	C30-C29	4.47	1.41	1.35
21	6	606	CHL	O2A-CGA	4.46	1.45	1.30
21	V	607	CHL	C2C-C3C	4.46	1.46	1.37
21	9	606	CHL	C2C-C3C	4.46	1.46	1.36
24	8	620	XAT	C14-C13	4.45	1.41	1.35
21	U	605	CHL	CHD-C1D	4.45	1.47	1.38
21	W	606	CHL	CHD-C1D	4.45	1.47	1.38
21	8	618	CHL	CHD-C1D	4.45	1.47	1.38
21	2	602	CHL	C2C-C3C	4.45	1.46	1.36
21	9	607	CHL	CHC-C1C	4.45	1.47	1.38
21	W	608	CHL	C2C-C3C	4.45	1.46	1.37
21	U	608	CHL	C2C-C3C	4.45	1.46	1.37
22	9	609	CLA	CHD-C1D	4.45	1.47	1.38
23	5	617	LUT	C34-C33	4.44	1.41	1.35
22	O	2003	CLA	C3B-C4B	4.43	1.49	1.40
21	U	608	CHL	CHD-C1D	4.43	1.47	1.38
21	4	607	CHL	CHD-C1D	4.43	1.47	1.38
21	6	618	CHL	CHD-C1D	4.42	1.47	1.38
24	8	620	XAT	C34-C33	4.42	1.41	1.35
21	5	601	CHL	O2A-CGA	4.42	1.46	1.33
21	V	606	CHL	CHD-C1D	4.42	1.47	1.38
21	4	606	CHL	C2C-C3C	4.41	1.46	1.36
21	W	605	CHL	CHD-C1D	4.41	1.47	1.38
21	9	601	CHL	CHD-C1D	4.41	1.47	1.38
21	U	609	CHL	C2C-C3C	4.41	1.46	1.36
22	O	2001	CLA	C3B-C4B	4.40	1.49	1.40
21	U	601	CHL	CHD-C1D	4.40	1.46	1.38
21	6	602	CHL	O2A-CGA	4.40	1.46	1.33
21	4	608	CHL	C2C-C3C	4.40	1.46	1.36
21	W	601	CHL	CHD-C1D	4.39	1.46	1.38
21	W	608	CHL	CHD-C1D	4.38	1.46	1.38
21	V	605	CHL	CHD-C1D	4.38	1.46	1.38
21	4	618	CHL	C2C-C3C	4.38	1.46	1.36
21	4	618	CHL	CHD-C1D	4.38	1.46	1.38
21	W	609	CHL	C2C-C3C	4.38	1.46	1.36
21	8	608	CHL	O2A-CGA	4.38	1.46	1.33
21	6	618	CHL	C2C-C3C	4.38	1.46	1.36
21	4	608	CHL	CHD-C1D	4.38	1.46	1.38
21	4	618	CHL	CHC-C1C	4.38	1.47	1.38
21	V	608	CHL	CHD-C1D	4.37	1.46	1.38
26	6	630	LHG	O8-C23	4.37	1.46	1.33
21	8	606	CHL	CHD-C1D	4.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	609	CHL	O2A-CGA	4.36	1.46	1.33
21	6	606	CHL	C2C-C3C	4.36	1.46	1.36
21	8	607	CHL	CHD-C1D	4.36	1.46	1.38
26	7	630	LHG	O8-C23	4.36	1.46	1.33
21	6	602	CHL	CHD-C1D	4.36	1.46	1.38
21	2	606	CHL	C2C-C3C	4.36	1.46	1.36
21	7	608	CHL	C2C-C3C	4.35	1.46	1.36
21	9	606	CHL	CHD-C1D	4.35	1.46	1.38
21	6	608	CHL	C2C-C3C	4.35	1.46	1.36
21	W	609	CHL	CHD-C1D	4.35	1.46	1.38
28	A	860	LMG	O8-C28	4.34	1.46	1.33
26	5	630	LHG	O8-C23	4.34	1.46	1.33
21	2	607	CHL	CHD-C1D	4.33	1.46	1.38
21	9	607	CHL	C2C-C3C	4.33	1.46	1.36
21	9	608	CHL	CHD-C1D	4.33	1.46	1.38
21	V	601	CHL	O2A-CGA	4.33	1.46	1.33
21	6	607	CHL	CHD-C1D	4.33	1.46	1.38
21	8	608	CHL	C2C-C3C	4.33	1.46	1.36
21	V	607	CHL	CHD-C1D	4.32	1.46	1.38
26	1	630	LHG	O8-C23	4.32	1.46	1.33
21	V	609	CHL	CHD-C1D	4.32	1.46	1.38
21	2	608	CHL	CHD-C1D	4.32	1.46	1.38
21	6	606	CHL	CHD-C1D	4.32	1.46	1.38
21	6	601	CHL	CHD-C1D	4.32	1.46	1.38
21	U	607	CHL	CHD-C1D	4.32	1.46	1.38
28	G	202	LMG	O8-C28	4.32	1.46	1.33
21	5	607	CHL	CHD-C1D	4.31	1.46	1.38
21	W	601	CHL	O2A-CGA	4.31	1.45	1.33
21	1	601	CHL	O2A-CGA	4.31	1.45	1.33
21	9	605	CHL	CHD-C1D	4.31	1.46	1.38
21	U	607	CHL	O2A-CGA	4.31	1.45	1.33
21	3	608	CHL	CHD-C1D	4.31	1.46	1.38
21	2	601	CHL	CHD-C1D	4.30	1.46	1.38
21	2	618	CHL	CHD-C1D	4.30	1.46	1.38
26	8	630	LHG	O8-C23	4.30	1.45	1.33
23	5	617	LUT	C14-C13	4.30	1.41	1.35
21	3	608	CHL	C2C-C3C	4.29	1.46	1.36
26	3	630	LHG	O8-C23	4.29	1.45	1.33
21	6	608	CHL	O2A-CGA	4.29	1.45	1.33
28	J	104	LMG	O7-C10	4.29	1.46	1.34
21	6	601	CHL	O2A-CGA	4.29	1.45	1.33
21	2	602	CHL	CHC-C4B	4.28	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	620	XAT	C10-C9	4.28	1.41	1.35
21	W	607	CHL	CHD-C1D	4.28	1.46	1.38
26	B	851	LHG	O8-C23	4.28	1.45	1.33
28	J	104	LMG	O8-C28	4.27	1.45	1.33
21	4	606	CHL	CHD-C1D	4.27	1.46	1.38
21	U	606	CHL	C2C-C3C	4.27	1.45	1.36
21	2	606	CHL	CHD-C1D	4.27	1.46	1.38
21	5	601	CHL	CHD-C1D	4.27	1.46	1.38
21	9	607	CHL	CHD-C1D	4.27	1.46	1.38
28	2	631	LMG	O8-C28	4.26	1.45	1.33
26	2	630	LHG	O8-C23	4.26	1.45	1.33
21	1	601	CHL	CHD-C1D	4.25	1.46	1.38
32	B	850	DGD	O1G-C1A	4.25	1.45	1.33
26	U	2630	LHG	O8-C23	4.25	1.45	1.33
21	U	601	CHL	O2A-CGA	4.25	1.45	1.33
21	2	602	CHL	CHD-C1D	4.24	1.46	1.38
32	B	850	DGD	O2G-C1B	4.24	1.46	1.34
26	V	2630	LHG	O8-C23	4.23	1.45	1.33
26	A	846	LHG	O8-C23	4.23	1.45	1.33
22	4	610	CLA	C1D-ND	4.22	1.43	1.37
26	2	630	LHG	O7-C7	4.22	1.46	1.34
26	4	630	LHG	O8-C23	4.22	1.45	1.33
23	5	617	LUT	C30-C29	4.21	1.41	1.35
22	7	609	CLA	C1D-ND	4.21	1.43	1.37
26	W	2630	LHG	O8-C23	4.21	1.45	1.33
21	3	608	CHL	O2A-CGA	4.21	1.45	1.33
28	J	103	LMG	O8-C28	4.20	1.45	1.33
21	U	609	CHL	CHD-C1D	4.20	1.46	1.38
28	L	307	LMG	O8-C28	4.20	1.45	1.33
21	7	608	CHL	CHD-C1D	4.20	1.46	1.38
26	V	2630	LHG	O7-C7	4.20	1.46	1.34
26	B	851	LHG	O7-C7	4.20	1.46	1.34
21	6	608	CHL	CHD-C1D	4.20	1.46	1.38
26	6	630	LHG	O7-C7	4.20	1.46	1.34
21	U	606	CHL	CHD-C1D	4.19	1.46	1.38
28	G	202	LMG	O7-C10	4.18	1.46	1.34
21	8	608	CHL	CHD-C1D	4.17	1.46	1.38
22	A	801	CLA	C1D-ND	4.15	1.42	1.37
22	5	609	CLA	C4B-NB	4.15	1.42	1.37
22	3	617	CLA	C1D-ND	4.15	1.42	1.37
26	A	847	LHG	O8-C23	4.14	1.45	1.33
21	4	607	CHL	CHD-C4C	4.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	617	LUT	C10-C9	4.14	1.41	1.35
22	7	609	CLA	C4B-NB	4.13	1.42	1.37
26	7	630	LHG	O7-C7	4.12	1.45	1.34
22	5	612	CLA	C4B-NB	4.12	1.42	1.37
26	3	630	LHG	O7-C7	4.12	1.45	1.34
22	5	616	CLA	C1D-ND	4.12	1.42	1.37
26	U	2630	LHG	O7-C7	4.11	1.45	1.34
21	W	606	CHL	C3A-C2A	-4.11	1.50	1.54
28	L	307	LMG	O7-C10	4.11	1.45	1.34
26	A	846	LHG	O7-C7	4.11	1.45	1.34
22	9	609	CLA	CHD-C4C	4.10	1.48	1.39
22	5	612	CLA	C1D-ND	4.10	1.42	1.37
26	A	847	LHG	O7-C7	4.10	1.45	1.34
21	U	605	CHL	C3A-C2A	-4.09	1.50	1.54
26	W	2630	LHG	O7-C7	4.09	1.45	1.34
21	9	605	CHL	C3A-C2A	-4.08	1.50	1.54
21	6	602	CHL	CHD-C4C	4.08	1.48	1.39
21	V	601	CHL	CHD-C4C	4.08	1.48	1.39
26	8	630	LHG	O7-C7	4.07	1.45	1.34
21	1	607	CHL	O2A-CGA	4.07	1.46	1.33
21	V	609	CHL	CHD-C4C	4.07	1.48	1.39
21	6	607	CHL	O2A-CGA	4.07	1.46	1.33
21	9	601	CHL	CHD-C4C	4.07	1.48	1.39
21	4	608	CHL	CHD-C4C	4.06	1.48	1.39
28	A	860	LMG	O7-C10	4.06	1.45	1.34
26	9	2630	LHG	O7-C7	4.06	1.45	1.34
22	6	612	CLA	C1D-ND	4.05	1.42	1.37
22	8	602	CLA	C1D-ND	4.05	1.42	1.37
22	3	609	CLA	C1D-ND	4.05	1.42	1.37
24	4	620	XAT	O4-C5	-4.05	1.40	1.46
22	5	609	CLA	C1D-ND	4.05	1.42	1.37
21	2	607	CHL	O2A-CGA	4.05	1.45	1.33
22	1	609	CLA	C1D-ND	4.04	1.42	1.37
22	3	611	CLA	C1D-ND	4.04	1.42	1.37
28	2	631	LMG	O7-C10	4.04	1.45	1.34
22	7	602	CLA	C1D-ND	4.04	1.42	1.37
21	2	608	CHL	CHD-C4C	4.04	1.48	1.39
26	5	630	LHG	O7-C7	4.03	1.45	1.34
21	9	606	CHL	CHD-C4C	4.03	1.48	1.39
21	V	607	CHL	C3A-C2A	-4.03	1.50	1.54
21	4	607	CHL	O2A-CGA	4.03	1.45	1.33
21	2	608	CHL	CHC-C4B	4.02	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	610	CLA	C1D-ND	4.02	1.42	1.37
25	9	623	NEX	C7-C8	-4.02	1.25	1.32
22	A	827	CLA	C1D-ND	4.02	1.42	1.37
21	U	606	CHL	CHC-C4B	4.02	1.48	1.39
21	V	606	CHL	C3A-C2A	-4.02	1.50	1.54
21	2	618	CHL	CHD-C4C	4.02	1.48	1.39
21	U	608	CHL	CHD-C4C	4.01	1.48	1.39
21	1	607	CHL	CHC-C4B	4.01	1.48	1.39
21	6	618	CHL	O2A-CGA	4.01	1.45	1.33
22	7	603	CLA	C1D-ND	4.01	1.42	1.37
21	W	609	CHL	CHD-C4C	4.01	1.48	1.39
21	8	618	CHL	CHD-C4C	4.00	1.48	1.39
21	9	601	CHL	C3A-C2A	-4.00	1.50	1.54
21	V	605	CHL	C3A-C2A	-4.00	1.50	1.54
21	2	607	CHL	CHD-C4C	4.00	1.48	1.39
21	8	607	CHL	CHD-C4C	3.99	1.48	1.39
21	1	607	CHL	CHD-C4C	3.99	1.48	1.39
21	6	601	CHL	CHD-C4C	3.98	1.48	1.39
21	W	601	CHL	CHD-C4C	3.98	1.48	1.39
21	W	607	CHL	C3A-C2A	-3.98	1.50	1.54
22	2	603	CLA	C1D-ND	3.98	1.42	1.37
21	9	607	CHL	CHD-C4C	3.98	1.48	1.39
22	1	609	CLA	C4B-NB	3.98	1.42	1.37
22	1	616	CLA	C1D-ND	3.97	1.42	1.37
21	7	608	CHL	CHD-C4C	3.97	1.48	1.39
21	W	606	CHL	CHD-C4C	3.97	1.48	1.39
21	5	607	CHL	C3A-C2A	-3.97	1.50	1.54
22	2	613	CLA	C1D-ND	3.97	1.42	1.37
21	W	605	CHL	CHD-C4C	3.97	1.48	1.39
22	8	604	CLA	C1D-ND	3.96	1.42	1.37
22	9	603	CLA	C4B-NB	3.96	1.42	1.37
21	U	609	CHL	CHD-C4C	3.96	1.48	1.39
21	U	601	CHL	CHD-C4C	3.96	1.48	1.39
21	6	618	CHL	CHD-C4C	3.96	1.48	1.39
21	V	605	CHL	CHD-C4C	3.95	1.48	1.39
22	5	603	CLA	C1D-ND	3.95	1.42	1.37
21	5	607	CHL	CHC-C4B	3.95	1.48	1.39
22	4	612	CLA	C1D-ND	3.95	1.42	1.37
21	9	608	CHL	CHD-C4C	3.95	1.48	1.39
22	7	612	CLA	C1D-ND	3.95	1.42	1.37
21	1	601	CHL	CHD-C4C	3.95	1.48	1.39
22	2	609	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	601	CHL	CHD-C4C	3.94	1.48	1.39
21	W	608	CHL	CHD-C4C	3.94	1.48	1.39
22	B	821	CLA	C1D-ND	3.94	1.42	1.37
21	6	607	CHL	CHD-C4C	3.94	1.48	1.39
21	5	607	CHL	CHD-C4C	3.94	1.48	1.39
22	1	603	CLA	C1D-ND	3.94	1.42	1.37
26	1	630	LHG	O7-C7	3.94	1.45	1.34
21	2	602	CHL	CHD-C4C	3.94	1.48	1.39
21	6	606	CHL	CHD-C4C	3.93	1.48	1.39
22	8	614	CLA	C1D-ND	3.93	1.42	1.37
22	4	610	CLA	C4B-NB	3.93	1.42	1.37
21	5	601	CHL	CHD-C4C	3.93	1.48	1.39
21	9	605	CHL	CHD-C4C	3.93	1.48	1.39
22	7	607	CLA	C1D-ND	3.93	1.42	1.37
22	4	603	CLA	C1D-ND	3.92	1.42	1.37
22	G	203	CLA	C1D-ND	3.92	1.42	1.37
21	U	605	CHL	CHD-C4C	3.92	1.48	1.39
21	2	618	CHL	CHC-C4B	3.92	1.48	1.39
22	H	201	CLA	C1D-ND	3.92	1.42	1.37
24	6	620	XAT	O24-C25	-3.92	1.40	1.46
22	7	604	CLA	C1D-ND	3.92	1.42	1.37
22	L	304	CLA	C1D-ND	3.91	1.42	1.37
22	8	603	CLA	C1D-ND	3.91	1.42	1.37
22	U	611	CLA	C1D-ND	3.91	1.42	1.37
21	5	601	CHL	CHC-C4B	3.91	1.48	1.39
22	3	612	CLA	C1D-ND	3.91	1.42	1.37
22	1	611	CLA	C1D-ND	3.91	1.42	1.37
22	4	604	CLA	C1D-ND	3.91	1.42	1.37
21	6	607	CHL	CHC-C4B	3.91	1.48	1.39
22	7	610	CLA	C1D-ND	3.91	1.42	1.37
22	1	614	CLA	C1D-ND	3.91	1.42	1.37
22	A	829	CLA	C1D-ND	3.91	1.42	1.37
22	7	615	CLA	C1D-ND	3.90	1.42	1.37
21	6	608	CHL	CHD-C4C	3.90	1.48	1.39
22	A	838	CLA	C1D-ND	3.90	1.42	1.37
22	U	614	CLA	C1D-ND	3.90	1.42	1.37
21	8	606	CHL	CHD-C4C	3.90	1.48	1.39
21	8	607	CHL	CHC-C4B	3.90	1.48	1.39
21	V	608	CHL	CHD-C4C	3.90	1.48	1.39
22	8	601	CLA	C1D-ND	3.89	1.42	1.37
22	2	614	CLA	C1D-ND	3.89	1.42	1.37
22	K	201	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	607	CHL	CHD-C4C	3.89	1.48	1.39
22	3	613	CLA	C1D-ND	3.89	1.42	1.37
21	2	607	CHL	CHC-C4B	3.89	1.48	1.39
21	V	606	CHL	CHD-C4C	3.88	1.48	1.39
22	6	614	CLA	C1D-ND	3.88	1.42	1.37
22	4	611	CLA	C1D-ND	3.88	1.42	1.37
22	8	612	CLA	C1D-ND	3.88	1.42	1.37
21	8	608	CHL	CHC-C4B	3.88	1.48	1.39
21	6	602	CHL	CHC-C4B	3.88	1.48	1.39
22	B	816	CLA	C1D-ND	3.88	1.42	1.37
21	3	608	CHL	CHD-C4C	3.88	1.48	1.39
22	B	826	CLA	C1D-ND	3.88	1.42	1.37
22	A	845	CLA	C1D-ND	3.87	1.42	1.37
22	B	823	CLA	C1D-ND	3.87	1.42	1.37
21	8	608	CHL	CHD-C4C	3.87	1.48	1.39
22	9	603	CLA	C1D-ND	3.87	1.42	1.37
22	6	604	CLA	C1D-ND	3.87	1.42	1.37
22	V	612	CLA	C1D-ND	3.87	1.42	1.37
21	9	607	CHL	CHC-C4B	3.87	1.48	1.39
22	W	602	CLA	C1D-ND	3.87	1.42	1.37
21	2	601	CHL	CHC-C4B	3.87	1.48	1.39
22	9	611	CLA	C1D-ND	3.86	1.42	1.37
22	5	606	CLA	C1D-ND	3.86	1.42	1.37
22	V	613	CLA	C1D-ND	3.86	1.42	1.37
21	2	606	CHL	CHD-C4C	3.86	1.48	1.39
21	W	607	CHL	CHD-C4C	3.85	1.48	1.39
22	1	604	CLA	C1D-ND	3.85	1.42	1.37
21	V	607	CHL	CHD-C4C	3.85	1.48	1.39
21	2	606	CHL	CHC-C4B	3.85	1.48	1.39
21	6	601	CHL	CHC-C4B	3.85	1.48	1.39
22	V	611	CLA	C1D-ND	3.84	1.42	1.37
22	6	603	CLA	C1D-ND	3.84	1.42	1.37
22	8	613	CLA	C1D-ND	3.84	1.42	1.37
21	4	607	CHL	CHC-C4B	3.84	1.48	1.39
22	V	602	CLA	C1D-ND	3.84	1.42	1.37
22	V	603	CLA	C1D-ND	3.84	1.42	1.37
21	1	601	CHL	CHC-C4B	3.84	1.48	1.39
22	2	611	CLA	C1D-ND	3.84	1.42	1.37
22	5	614	CLA	C1D-ND	3.84	1.42	1.37
21	4	618	CHL	CHD-C4C	3.84	1.48	1.39
22	6	613	CLA	C1D-ND	3.83	1.42	1.37
21	8	606	CHL	CHC-C4B	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	604	CLA	C1D-ND	3.83	1.42	1.37
22	5	604	CLA	C1D-ND	3.83	1.42	1.37
22	A	835	CLA	C1D-ND	3.83	1.42	1.37
22	G	204	CLA	C1D-ND	3.83	1.42	1.37
22	F	304	CLA	C1D-ND	3.83	1.43	1.37
22	J	101	CLA	C1D-ND	3.83	1.42	1.37
22	V	604	CLA	C1D-ND	3.83	1.42	1.37
21	W	605	CHL	C3A-C2A	-3.83	1.50	1.54
22	V	610	CLA	C1D-ND	3.83	1.42	1.37
22	5	608	CLA	C1D-ND	3.83	1.42	1.37
22	7	614	CLA	C1D-ND	3.83	1.42	1.37
22	A	818	CLA	C1D-ND	3.82	1.42	1.37
22	4	601	CLA	C1D-ND	3.82	1.42	1.37
22	A	842	CLA	C1D-ND	3.82	1.42	1.37
22	3	614	CLA	C1D-ND	3.82	1.42	1.37
22	9	602	CLA	C1D-ND	3.82	1.42	1.37
22	K	204	CLA	C1D-ND	3.82	1.42	1.37
21	6	608	CHL	CHC-C4B	3.82	1.48	1.39
21	9	605	CHL	CHC-C4B	3.82	1.48	1.39
22	K	206	CLA	C1D-ND	3.82	1.42	1.37
21	V	609	CHL	CHC-C4B	3.82	1.48	1.39
28	J	103	LMG	O7-C10	3.82	1.45	1.34
21	V	605	CHL	CHC-C4B	3.82	1.48	1.39
22	9	609	CLA	CHC-C4B	3.82	1.48	1.39
22	A	828	CLA	C1D-ND	3.81	1.42	1.37
22	5	610	CLA	C1D-ND	3.81	1.42	1.37
22	2	612	CLA	C1D-ND	3.81	1.42	1.37
22	3	611	CLA	C4B-NB	3.81	1.42	1.37
22	6	611	CLA	C1D-ND	3.81	1.42	1.37
22	9	610	CLA	C1D-ND	3.81	1.42	1.37
22	6	610	CLA	C1D-ND	3.81	1.42	1.37
21	U	606	CHL	CHD-C4C	3.81	1.47	1.39
22	W	612	CLA	C1D-ND	3.81	1.42	1.37
22	7	617	CLA	C1D-ND	3.81	1.42	1.37
22	G	201	CLA	C1D-ND	3.81	1.42	1.37
22	1	606	CLA	C1D-ND	3.81	1.42	1.37
22	F	303	CLA	C1D-ND	3.81	1.42	1.37
22	V	614	CLA	C1D-ND	3.80	1.42	1.37
22	B	804	CLA	C1D-ND	3.80	1.42	1.37
22	8	609	CLA	C1D-ND	3.80	1.42	1.37
22	3	602	CLA	C1D-ND	3.80	1.42	1.37
22	A	806	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	607	CLA	C1D-ND	3.80	1.42	1.37
22	A	815	CLA	C1D-ND	3.80	1.42	1.37
22	A	825	CLA	C1D-ND	3.80	1.42	1.37
22	1	610	CLA	C1D-ND	3.80	1.42	1.37
22	4	614	CLA	C1D-ND	3.80	1.42	1.37
22	9	604	CLA	C1D-ND	3.80	1.42	1.37
21	4	606	CHL	CHC-C4B	3.79	1.47	1.39
22	7	611	CLA	C1D-ND	3.79	1.42	1.37
22	A	817	CLA	C1D-ND	3.79	1.42	1.37
21	U	609	CHL	CHC-C4B	3.79	1.47	1.39
22	B	811	CLA	C1D-ND	3.79	1.42	1.37
22	8	611	CLA	C1D-ND	3.79	1.42	1.37
21	9	607	CHL	OBD-CAD	3.78	1.29	1.22
21	6	606	CHL	CHC-C4B	3.78	1.47	1.39
22	B	831	CLA	C1D-ND	3.78	1.42	1.37
21	9	601	CHL	CHC-C4B	3.78	1.47	1.39
21	4	608	CHL	CHB-C1B	3.78	1.47	1.39
21	U	607	CHL	CHC-C4B	3.78	1.47	1.39
22	A	804	CLA	C1D-ND	3.78	1.42	1.37
21	7	608	CHL	CHC-C4B	3.78	1.47	1.39
22	A	809	CLA	C1D-ND	3.78	1.42	1.37
22	O	2002	CLA	C1D-ND	3.78	1.42	1.37
22	U	602	CLA	C1D-ND	3.78	1.42	1.37
22	U	603	CLA	C1D-ND	3.78	1.42	1.37
22	U	604	CLA	C1D-ND	3.77	1.42	1.37
22	7	602	CLA	C4B-NB	3.77	1.42	1.37
21	6	606	CHL	OBD-CAD	3.77	1.29	1.22
22	B	841	CLA	C1D-ND	3.77	1.42	1.37
22	6	603	CLA	C4B-NB	3.77	1.42	1.37
22	A	807	CLA	C1D-ND	3.77	1.42	1.37
22	1	612	CLA	C1D-ND	3.77	1.42	1.37
22	K	203	CLA	C1D-ND	3.77	1.42	1.37
22	L	302	CLA	C1D-ND	3.77	1.42	1.37
22	A	808	CLA	C1D-ND	3.76	1.42	1.37
22	3	610	CLA	C1D-ND	3.76	1.42	1.37
22	B	836	CLA	C1D-ND	3.76	1.42	1.37
21	9	605	CHL	OBD-CAD	3.76	1.29	1.22
22	W	603	CLA	C1D-ND	3.76	1.42	1.37
22	2	610	CLA	C1D-ND	3.76	1.42	1.37
22	B	839	CLA	C1D-ND	3.76	1.42	1.37
22	A	840	CLA	C1D-ND	3.76	1.42	1.37
21	4	606	CHL	CHD-C4C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	603	CLA	C1D-ND	3.75	1.42	1.37
22	3	606	CLA	C1D-ND	3.75	1.42	1.37
22	4	613	CLA	C1D-ND	3.75	1.42	1.37
22	A	816	CLA	C1D-ND	3.75	1.42	1.37
22	5	611	CLA	C1D-ND	3.75	1.42	1.37
22	8	610	CLA	C1D-ND	3.75	1.42	1.37
22	W	613	CLA	C1D-ND	3.75	1.42	1.37
22	U	612	CLA	C1D-ND	3.75	1.42	1.37
22	2	604	CLA	C1D-ND	3.75	1.42	1.37
22	B	829	CLA	C1D-ND	3.75	1.42	1.37
21	U	605	CHL	OBD-CAD	3.75	1.28	1.22
22	A	834	CLA	C1D-ND	3.75	1.42	1.37
22	9	604	CLA	C4B-NB	3.74	1.42	1.37
26	4	630	LHG	O7-C7	3.74	1.44	1.34
21	W	608	CHL	OBD-CAD	3.74	1.28	1.22
21	4	607	CHL	OBD-CAD	3.74	1.28	1.22
22	9	613	CLA	C1D-ND	3.74	1.42	1.37
22	7	613	CLA	C1D-ND	3.74	1.42	1.37
21	8	618	CHL	OBD-CAD	3.74	1.28	1.22
22	A	831	CLA	C1D-ND	3.74	1.42	1.37
22	U	613	CLA	C1D-ND	3.74	1.42	1.37
22	B	832	CLA	C1D-ND	3.74	1.42	1.37
22	7	606	CLA	C1D-ND	3.74	1.42	1.37
22	B	807	CLA	C1D-ND	3.74	1.42	1.37
22	B	806	CLA	C1D-ND	3.73	1.42	1.37
22	W	614	CLA	C1D-ND	3.73	1.42	1.37
21	W	608	CHL	CHB-C1B	3.73	1.47	1.39
21	V	607	CHL	OBD-CAD	3.73	1.28	1.22
22	A	805	CLA	C1D-ND	3.73	1.42	1.37
22	5	613	CLA	C1D-ND	3.73	1.42	1.37
22	4	602	CLA	C1D-ND	3.72	1.42	1.37
22	7	610	CLA	C4B-NB	3.72	1.42	1.37
22	1	608	CLA	C1D-ND	3.72	1.42	1.37
21	8	607	CHL	OBD-CAD	3.72	1.28	1.22
22	A	837	CLA	C1D-ND	3.72	1.42	1.37
22	B	824	CLA	C1D-ND	3.72	1.42	1.37
22	8	601	CLA	C4B-NB	3.72	1.42	1.37
22	B	822	CLA	C1D-ND	3.71	1.42	1.37
22	B	819	CLA	C1D-ND	3.71	1.42	1.37
21	8	618	CHL	CHC-C4B	3.71	1.47	1.39
22	A	839	CLA	C1D-ND	3.71	1.42	1.37
22	A	810	CLA	C1D-ND	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	613	CLA	C1D-ND	3.71	1.42	1.37
22	4	609	CLA	C1D-ND	3.70	1.42	1.37
22	A	814	CLA	C1D-ND	3.70	1.42	1.37
22	A	826	CLA	C1D-ND	3.70	1.42	1.37
22	U	611	CLA	C4B-NB	3.70	1.42	1.37
22	1	602	CLA	C1D-ND	3.70	1.42	1.37
22	9	612	CLA	C1D-ND	3.70	1.42	1.37
22	B	803	CLA	C1D-ND	3.70	1.42	1.37
21	U	601	CHL	OBD-CAD	3.70	1.28	1.22
21	2	607	CHL	OBD-CAD	3.70	1.28	1.22
21	4	618	CHL	OBD-CAD	3.70	1.28	1.22
21	V	605	CHL	OBD-CAD	3.70	1.28	1.22
21	1	607	CHL	OBD-CAD	3.70	1.28	1.22
22	B	815	CLA	C1D-ND	3.69	1.42	1.37
22	O	2002	CLA	C4B-NB	3.69	1.42	1.37
22	6	609	CLA	C1D-ND	3.69	1.42	1.37
21	V	608	CHL	OBD-CAD	3.69	1.28	1.22
21	4	608	CHL	OBD-CAD	3.69	1.28	1.22
22	B	809	CLA	C1D-ND	3.69	1.42	1.37
22	5	611	CLA	C4B-NB	3.69	1.42	1.37
22	5	616	CLA	C4B-NB	3.69	1.42	1.37
21	9	608	CHL	CHC-C4B	3.69	1.47	1.39
21	9	601	CHL	OBD-CAD	3.69	1.28	1.22
22	A	832	CLA	C1D-ND	3.69	1.42	1.37
21	6	601	CHL	OBD-CAD	3.69	1.28	1.22
21	6	607	CHL	OBD-CAD	3.69	1.28	1.22
22	7	603	CLA	C4B-NB	3.69	1.42	1.37
21	2	618	CHL	OBD-CAD	3.68	1.28	1.22
22	U	610	CLA	C1D-ND	3.68	1.42	1.37
22	3	609	CLA	C4B-NB	3.68	1.42	1.37
21	9	606	CHL	CHC-C4B	3.68	1.47	1.39
23	2	619	LUT	C30-C29	3.68	1.40	1.35
22	A	837	CLA	C4B-NB	3.68	1.42	1.37
21	U	607	CHL	OBD-CAD	3.68	1.28	1.22
22	A	820	CLA	C1D-ND	3.68	1.42	1.37
22	5	602	CLA	C1D-ND	3.68	1.42	1.37
22	B	825	CLA	C1D-ND	3.68	1.42	1.37
21	W	605	CHL	OBD-CAD	3.68	1.28	1.22
23	2	619	LUT	C14-C13	3.67	1.40	1.35
21	5	601	CHL	OBD-CAD	3.67	1.28	1.22
22	9	609	CLA	OBD-CAD	3.67	1.28	1.22
22	A	803	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	606	CHL	OBD-CAD	3.67	1.28	1.22
21	W	609	CHL	OBD-CAD	3.67	1.28	1.22
22	B	835	CLA	C1D-ND	3.67	1.42	1.37
22	B	817	CLA	C1D-ND	3.67	1.42	1.37
22	B	818	CLA	C1D-ND	3.67	1.42	1.37
22	3	615	CLA	C1D-ND	3.67	1.42	1.37
22	V	610	CLA	C4B-NB	3.67	1.42	1.37
21	4	618	CHL	CHB-C1B	3.67	1.47	1.39
22	F	301	CLA	C1D-ND	3.67	1.42	1.37
22	A	824	CLA	C1D-ND	3.66	1.42	1.37
21	6	602	CHL	OBD-CAD	3.66	1.28	1.22
21	V	601	CHL	OBD-CAD	3.66	1.28	1.22
21	U	608	CHL	OBD-CAD	3.66	1.28	1.22
22	3	604	CLA	C1D-ND	3.66	1.42	1.37
22	B	830	CLA	C4B-NB	3.66	1.42	1.37
22	U	614	CLA	C4B-NB	3.65	1.42	1.37
22	3	603	CLA	C4B-NB	3.65	1.42	1.37
22	A	819	CLA	C1D-ND	3.65	1.42	1.37
21	V	606	CHL	OBD-CAD	3.65	1.28	1.22
21	U	606	CHL	OBD-CAD	3.65	1.28	1.22
22	B	811	CLA	C4B-NB	3.65	1.42	1.37
22	2	611	CLA	C4B-NB	3.64	1.42	1.37
22	8	612	CLA	C4B-NB	3.64	1.42	1.37
21	6	618	CHL	OBD-CAD	3.64	1.28	1.22
22	A	812	CLA	C1D-ND	3.64	1.42	1.37
22	4	611	CLA	C4B-NB	3.64	1.42	1.37
22	5	606	CLA	C4B-NB	3.64	1.42	1.37
21	2	606	CHL	OBD-CAD	3.64	1.28	1.22
21	9	607	CHL	CHB-C1B	3.63	1.47	1.39
22	7	613	CLA	C4B-NB	3.63	1.42	1.37
21	V	609	CHL	OBD-CAD	3.63	1.28	1.22
22	F	304	CLA	C4B-NB	3.63	1.42	1.37
21	2	601	CHL	OBD-CAD	3.63	1.28	1.22
21	9	608	CHL	OBD-CAD	3.63	1.28	1.22
22	A	842	CLA	C4B-NB	3.63	1.42	1.37
22	B	834	CLA	C1D-ND	3.63	1.42	1.37
21	W	607	CHL	OBD-CAD	3.63	1.28	1.22
22	A	822	CLA	C1D-ND	3.62	1.42	1.37
22	B	837	CLA	C1D-ND	3.62	1.42	1.37
22	9	613	CLA	C4B-NB	3.62	1.42	1.37
21	W	605	CHL	CHC-C4B	3.62	1.47	1.39
22	5	613	CLA	C4B-NB	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	827	CLA	C1D-ND	3.61	1.42	1.37
22	A	811	CLA	C1D-ND	3.61	1.42	1.37
22	B	813	CLA	C1D-ND	3.61	1.42	1.37
22	B	838	CLA	C1D-ND	3.61	1.42	1.37
22	W	603	CLA	C4B-NB	3.61	1.42	1.37
21	V	606	CHL	CHB-C1B	3.61	1.47	1.39
21	8	608	CHL	OBD-CAD	3.61	1.28	1.22
21	U	601	CHL	CHC-C4B	3.61	1.47	1.39
24	V	2622	XAT	O4-C5	-3.61	1.41	1.46
21	U	609	CHL	OBD-CAD	3.61	1.28	1.22
22	A	833	CLA	C1D-ND	3.61	1.42	1.37
22	6	612	CLA	C4B-NB	3.60	1.42	1.37
25	U	2623	NEX	C7-C8	-3.60	1.26	1.32
24	7	619	XAT	O24-C25	-3.60	1.41	1.46
21	9	606	CHL	OBD-CAD	3.60	1.28	1.22
21	6	618	CHL	CHC-C4B	3.60	1.47	1.39
21	2	608	CHL	CHB-C1B	3.60	1.47	1.39
22	B	814	CLA	C1D-ND	3.60	1.42	1.37
22	8	610	CLA	C4B-NB	3.60	1.42	1.37
21	3	608	CHL	OBD-CAD	3.60	1.28	1.22
21	4	608	CHL	CHC-C4B	3.60	1.47	1.39
22	B	802	CLA	C1D-ND	3.60	1.42	1.37
22	W	610	CLA	C4B-NB	3.60	1.42	1.37
22	B	828	CLA	C1D-ND	3.60	1.42	1.37
22	7	611	CLA	C4B-NB	3.60	1.42	1.37
22	B	805	CLA	C1D-ND	3.59	1.42	1.37
22	W	611	CLA	C1D-ND	3.59	1.42	1.37
22	A	813	CLA	C1D-ND	3.59	1.42	1.37
21	2	608	CHL	OBD-CAD	3.59	1.28	1.22
22	A	802	CLA	C1D-ND	3.59	1.42	1.37
22	A	821	CLA	C1D-ND	3.59	1.42	1.37
22	6	613	CLA	C4B-NB	3.59	1.42	1.37
23	2	619	LUT	C34-C33	3.59	1.40	1.35
22	5	604	CLA	C4B-NB	3.59	1.42	1.37
21	5	607	CHL	OBD-CAD	3.58	1.28	1.22
22	G	201	CLA	C4B-NB	3.58	1.42	1.37
21	2	602	CHL	OBD-CAD	3.58	1.28	1.22
22	B	821	CLA	C4B-NB	3.58	1.42	1.37
22	8	613	CLA	C4B-NB	3.58	1.42	1.37
22	V	613	CLA	C4B-NB	3.57	1.42	1.37
21	8	606	CHL	OBD-CAD	3.57	1.28	1.22
22	7	612	CLA	C4B-NB	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	601	CHL	OBD-CAD	3.57	1.28	1.22
21	4	606	CHL	OBD-CAD	3.57	1.28	1.22
22	A	830	CLA	C1D-ND	3.57	1.42	1.37
22	1	616	CLA	C4B-NB	3.57	1.42	1.37
21	V	609	CHL	CHB-C1B	3.57	1.47	1.39
22	8	614	CLA	C4B-NB	3.57	1.42	1.37
21	9	608	CHL	CHB-C1B	3.57	1.47	1.39
22	B	833	CLA	C1D-ND	3.57	1.42	1.37
22	8	611	CLA	C4B-NB	3.56	1.42	1.37
21	4	618	CHL	CHC-C4B	3.56	1.47	1.39
21	U	605	CHL	CHC-C4B	3.56	1.47	1.39
21	6	601	CHL	CHB-C1B	3.56	1.47	1.39
22	5	603	CLA	C4B-NB	3.56	1.42	1.37
22	B	838	CLA	C4B-NB	3.56	1.42	1.37
21	U	601	CHL	CHB-C1B	3.55	1.47	1.39
22	L	303	CLA	C1D-ND	3.55	1.42	1.37
21	W	601	CHL	CHC-C4B	3.55	1.47	1.39
22	G	204	CLA	C4B-NB	3.55	1.42	1.37
22	7	617	CLA	C4B-NB	3.55	1.42	1.37
22	1	606	CLA	C4B-NB	3.55	1.42	1.37
21	9	601	CHL	CHB-C1B	3.55	1.47	1.39
21	W	607	CHL	CHB-C1B	3.55	1.47	1.39
22	5	610	CLA	C4B-NB	3.55	1.42	1.37
21	7	608	CHL	CHB-C1B	3.55	1.47	1.39
21	1	601	CHL	OBD-CAD	3.54	1.28	1.22
22	B	810	CLA	C1D-ND	3.54	1.42	1.37
21	6	608	CHL	CHB-C1B	3.54	1.47	1.39
22	A	841	CLA	C1D-ND	3.54	1.42	1.37
21	6	608	CHL	OBD-CAD	3.54	1.28	1.22
21	W	609	CHL	CHB-C1B	3.54	1.47	1.39
21	3	608	CHL	CHB-C1B	3.54	1.47	1.39
22	B	820	CLA	C1D-ND	3.54	1.42	1.37
22	H	201	CLA	C4B-NB	3.54	1.42	1.37
21	W	607	CHL	CHC-C4B	3.54	1.47	1.39
21	U	605	CHL	CHB-C1B	3.53	1.47	1.39
22	8	603	CLA	C4B-NB	3.53	1.42	1.37
21	U	609	CHL	CHB-C1B	3.53	1.47	1.39
22	B	822	CLA	C4B-NB	3.53	1.42	1.37
21	4	607	CHL	CHB-C1B	3.53	1.47	1.39
22	4	613	CLA	C4B-NB	3.53	1.42	1.37
21	W	605	CHL	CHB-C1B	3.53	1.47	1.39
21	6	606	CHL	CHB-C1B	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	607	CHL	CHB-C1B	3.52	1.47	1.39
21	V	606	CHL	CHC-C4B	3.52	1.47	1.39
22	W	611	CLA	C4B-NB	3.52	1.42	1.37
22	6	609	CLA	C4B-NB	3.52	1.42	1.37
22	B	831	CLA	C4B-NB	3.52	1.42	1.37
21	W	606	CHL	CHC-C4B	3.52	1.47	1.39
21	V	608	CHL	CHB-C1B	3.52	1.47	1.39
21	W	601	CHL	CHB-C1B	3.52	1.47	1.39
22	B	808	CLA	C1D-ND	3.52	1.42	1.37
22	2	614	CLA	C4B-NB	3.52	1.42	1.37
21	2	601	CHL	CHB-C1B	3.52	1.47	1.39
22	3	610	CLA	C4B-NB	3.52	1.42	1.37
22	A	854	CLA	C1D-ND	3.52	1.42	1.37
22	3	613	CLA	C4B-NB	3.51	1.42	1.37
22	9	611	CLA	C4B-NB	3.51	1.42	1.37
21	6	602	CHL	C3B-C4B	3.51	1.51	1.42
22	1	611	CLA	C4B-NB	3.51	1.42	1.37
21	W	606	CHL	CHB-C1B	3.51	1.47	1.39
22	A	843	CLA	C1D-ND	3.51	1.42	1.37
22	B	832	CLA	C4B-NB	3.51	1.42	1.37
21	2	602	CHL	C3B-C4B	3.51	1.51	1.42
22	V	611	CLA	C4B-NB	3.50	1.42	1.37
21	1	607	CHL	CHB-C1B	3.50	1.47	1.39
22	9	612	CLA	C4B-NB	3.50	1.42	1.37
21	2	607	CHL	CHB-C1B	3.50	1.47	1.39
21	5	601	CHL	CHB-C1B	3.50	1.47	1.39
22	U	612	CLA	C4B-NB	3.50	1.42	1.37
21	V	601	CHL	CHC-C4B	3.50	1.47	1.39
22	2	609	CLA	C4B-NB	3.50	1.42	1.37
21	V	607	CHL	CHC-C4B	3.50	1.47	1.39
21	V	607	CHL	CHB-C1B	3.50	1.47	1.39
21	V	605	CHL	CHB-C1B	3.50	1.47	1.39
22	6	604	CLA	C4B-NB	3.49	1.42	1.37
21	U	607	CHL	CHB-C1B	3.49	1.47	1.39
22	A	808	CLA	C4B-NB	3.49	1.42	1.37
21	U	608	CHL	CHB-C1B	3.49	1.47	1.39
22	B	826	CLA	C4B-NB	3.49	1.42	1.37
22	7	614	CLA	C4B-NB	3.49	1.42	1.37
22	4	614	CLA	C4B-NB	3.49	1.42	1.37
22	B	830	CLA	C1D-ND	3.49	1.42	1.37
22	K	206	CLA	C4B-NB	3.48	1.42	1.37
21	W	609	CHL	CHC-C4B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	605	CHL	CHB-C1B	3.48	1.47	1.39
22	1	614	CLA	C4B-NB	3.48	1.42	1.37
21	7	608	CHL	OBD-CAD	3.48	1.28	1.22
22	5	608	CLA	C4B-NB	3.48	1.42	1.37
21	8	618	CHL	CHB-C1B	3.47	1.47	1.39
22	A	802	CLA	C4B-NB	3.47	1.42	1.37
21	2	618	CHL	CHB-C1B	3.47	1.47	1.39
22	7	615	CLA	C4B-NB	3.47	1.42	1.37
22	A	845	CLA	C4B-NB	3.47	1.42	1.37
21	U	608	CHL	CHC-C4B	3.47	1.47	1.39
21	8	608	CHL	CHB-C1B	3.47	1.47	1.39
22	B	814	CLA	C4B-NB	3.47	1.42	1.37
22	W	612	CLA	C4B-NB	3.46	1.42	1.37
22	2	610	CLA	C4B-NB	3.46	1.42	1.37
22	A	841	CLA	C4B-NB	3.46	1.42	1.37
22	8	602	CLA	C4B-NB	3.46	1.42	1.37
21	V	608	CHL	CHC-C4B	3.46	1.47	1.39
22	B	804	CLA	C4B-NB	3.46	1.42	1.37
21	6	602	CHL	CHB-C1B	3.46	1.47	1.39
22	9	609	CLA	CHB-C1B	3.46	1.47	1.39
22	B	808	CLA	C4B-NB	3.46	1.42	1.37
22	1	610	CLA	C4B-NB	3.46	1.42	1.37
22	8	604	CLA	C4B-NB	3.46	1.42	1.37
22	9	602	CLA	C4B-NB	3.46	1.42	1.37
21	6	607	CHL	CHB-C1B	3.46	1.47	1.39
22	1	608	CLA	C4B-NB	3.45	1.42	1.37
22	B	840	CLA	C1D-ND	3.45	1.42	1.37
21	2	602	CHL	CHB-C1B	3.45	1.47	1.39
21	3	608	CHL	CHC-C4B	3.45	1.47	1.39
22	V	614	CLA	C4B-NB	3.45	1.42	1.37
22	L	302	CLA	C4B-NB	3.44	1.42	1.37
22	A	805	CLA	C4B-NB	3.44	1.42	1.37
22	6	614	CLA	C4B-NB	3.43	1.42	1.37
22	4	612	CLA	C4B-NB	3.43	1.42	1.37
22	A	834	CLA	C4B-NB	3.43	1.42	1.37
24	7	619	XAT	O4-C5	-3.43	1.41	1.46
22	3	614	CLA	C4B-NB	3.43	1.42	1.37
22	4	604	CLA	C4B-NB	3.43	1.42	1.37
21	6	618	CHL	CHB-C1B	3.43	1.47	1.39
22	4	602	CLA	C4B-NB	3.43	1.42	1.37
22	5	614	CLA	C4B-NB	3.43	1.42	1.37
21	1	601	CHL	CHB-C1B	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	606	CHL	C3B-C4B	3.43	1.50	1.42
22	3	615	CLA	C4B-NB	3.43	1.42	1.37
22	1	613	CLA	C4B-NB	3.42	1.42	1.37
22	A	854	CLA	C4B-NB	3.42	1.42	1.37
21	8	607	CHL	CHB-C1B	3.42	1.47	1.39
22	K	203	CLA	C4B-NB	3.42	1.42	1.37
24	6	620	XAT	O4-C5	-3.42	1.41	1.46
22	A	814	CLA	C4B-NB	3.42	1.42	1.37
22	W	614	CLA	C4B-NB	3.42	1.42	1.37
22	4	601	CLA	C4B-NB	3.41	1.42	1.37
22	A	831	CLA	C4B-NB	3.41	1.42	1.37
22	U	610	CLA	C4B-NB	3.41	1.42	1.37
22	B	816	CLA	C4B-NB	3.41	1.42	1.37
22	U	603	CLA	C4B-NB	3.41	1.42	1.37
22	7	604	CLA	C4B-NB	3.41	1.42	1.37
22	V	603	CLA	C4B-NB	3.40	1.42	1.37
22	A	828	CLA	C4B-NB	3.40	1.42	1.37
22	B	819	CLA	C4B-NB	3.40	1.42	1.37
22	U	602	CLA	C4B-NB	3.40	1.42	1.37
21	V	601	CHL	CHB-C1B	3.40	1.47	1.39
22	B	829	CLA	C4B-NB	3.40	1.42	1.37
22	J	101	CLA	C4B-NB	3.40	1.42	1.37
22	V	602	CLA	C4B-NB	3.40	1.42	1.37
22	U	613	CLA	C4B-NB	3.40	1.42	1.37
22	2	612	CLA	C4B-NB	3.40	1.42	1.37
22	4	603	CLA	C4B-NB	3.40	1.42	1.37
22	A	810	CLA	C4B-NB	3.39	1.42	1.37
22	1	612	CLA	C4B-NB	3.39	1.42	1.37
21	8	606	CHL	CHB-C1B	3.39	1.47	1.39
21	9	606	CHL	CHB-C1B	3.39	1.47	1.39
22	G	203	CLA	C4B-NB	3.39	1.42	1.37
22	W	613	CLA	C4B-NB	3.39	1.42	1.37
22	3	606	CLA	C4B-NB	3.39	1.41	1.37
21	2	606	CHL	CHB-C1B	3.39	1.47	1.39
22	A	826	CLA	C4B-NB	3.38	1.41	1.37
25	W	2623	NEX	C7-C8	-3.38	1.26	1.32
22	2	603	CLA	C4B-NB	3.38	1.41	1.37
22	A	836	CLA	C1D-ND	3.38	1.41	1.37
22	B	833	CLA	C4B-NB	3.38	1.41	1.37
22	B	841	CLA	C4B-NB	3.38	1.41	1.37
22	V	604	CLA	C4B-NB	3.38	1.41	1.37
22	8	609	CLA	C4B-NB	3.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	803	CLA	C4B-NB	3.37	1.41	1.37
22	F	301	CLA	C4B-NB	3.37	1.41	1.37
22	5	602	CLA	C4B-NB	3.37	1.41	1.37
22	U	604	CLA	C4B-NB	3.37	1.41	1.37
22	A	818	CLA	C4B-NB	3.37	1.41	1.37
22	A	835	CLA	C4B-NB	3.36	1.41	1.37
22	B	824	CLA	C4B-NB	3.36	1.41	1.37
21	U	606	CHL	CHB-C1B	3.36	1.46	1.39
22	9	610	CLA	C4B-NB	3.36	1.41	1.37
22	6	610	CLA	C4B-NB	3.36	1.41	1.37
22	A	843	CLA	C4B-NB	3.36	1.41	1.37
22	1	604	CLA	C4B-NB	3.36	1.41	1.37
22	B	820	CLA	C4B-NB	3.35	1.41	1.37
22	A	809	CLA	C4B-NB	3.35	1.41	1.37
22	4	609	CLA	C4B-NB	3.35	1.41	1.37
22	B	837	CLA	C4B-NB	3.35	1.41	1.37
22	A	822	CLA	C4B-NB	3.35	1.41	1.37
22	A	825	CLA	C4B-NB	3.34	1.41	1.37
22	W	604	CLA	C4B-NB	3.34	1.41	1.37
22	B	815	CLA	C4B-NB	3.34	1.41	1.37
22	A	811	CLA	C4B-NB	3.34	1.41	1.37
22	A	813	CLA	C4B-NB	3.34	1.41	1.37
21	W	608	CHL	CHC-C4B	3.33	1.46	1.39
22	L	303	CLA	C4B-NB	3.33	1.41	1.37
21	1	601	CHL	C3B-C4B	3.33	1.50	1.42
22	A	824	CLA	C4B-NB	3.33	1.41	1.37
22	B	813	CLA	C4B-NB	3.33	1.41	1.37
22	7	607	CLA	C4B-NB	3.33	1.41	1.37
22	A	823	CLA	C4B-NB	3.32	1.41	1.37
22	B	809	CLA	C4B-NB	3.32	1.41	1.37
21	5	601	CHL	C3B-C4B	3.32	1.50	1.42
22	1	602	CLA	C4B-NB	3.32	1.41	1.37
22	B	805	CLA	C4B-NB	3.32	1.41	1.37
21	8	608	CHL	C3B-C4B	3.31	1.50	1.42
22	A	815	CLA	C4B-NB	3.31	1.41	1.37
22	7	606	CLA	C4B-NB	3.31	1.41	1.37
22	B	821	CLA	C4D-ND	-3.31	1.33	1.37
22	2	613	CLA	C4B-NB	3.31	1.41	1.37
22	A	840	CLA	C4B-NB	3.31	1.41	1.37
21	2	608	CHL	C3B-C4B	3.31	1.50	1.42
22	3	607	CLA	C4B-NB	3.31	1.41	1.37
21	V	605	CHL	C3B-C4B	3.31	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	604	CLA	C4B-NB	3.30	1.41	1.37
21	6	608	CHL	C3B-C4B	3.30	1.50	1.42
22	A	833	CLA	C4B-NB	3.30	1.41	1.37
21	2	618	CHL	C3B-C4B	3.30	1.50	1.42
21	8	606	CHL	C3B-C4B	3.30	1.50	1.42
22	B	812	CLA	C2D-C1D	3.30	1.48	1.42
22	A	839	CLA	C4B-NB	3.29	1.41	1.37
23	2	619	LUT	C10-C9	3.29	1.40	1.35
22	V	612	CLA	C4B-NB	3.29	1.41	1.37
22	3	602	CLA	C4B-NB	3.29	1.41	1.37
22	B	803	CLA	C4B-NB	3.29	1.41	1.37
21	2	607	CHL	C3B-C4B	3.29	1.50	1.42
21	6	601	CHL	C3B-C4B	3.28	1.50	1.42
21	1	607	CHL	C3B-C4B	3.28	1.50	1.42
21	9	605	CHL	C3B-C4B	3.28	1.50	1.42
22	A	801	CLA	C4B-NB	3.28	1.41	1.37
22	3	612	CLA	C4B-NB	3.28	1.41	1.37
21	4	606	CHL	CHB-C1B	3.28	1.46	1.39
22	A	817	CLA	C4B-NB	3.27	1.41	1.37
21	6	607	CHL	C3B-C4B	3.27	1.50	1.42
22	6	611	CLA	C4B-NB	3.27	1.41	1.37
21	5	607	CHL	C3B-C4B	3.26	1.50	1.42
22	A	821	CLA	C4B-NB	3.26	1.41	1.37
22	1	603	CLA	C4B-NB	3.26	1.41	1.37
22	A	804	CLA	C4B-NB	3.26	1.41	1.37
22	A	806	CLA	C4B-NB	3.26	1.41	1.37
22	B	834	CLA	C4B-NB	3.26	1.41	1.37
22	O	2003	CLA	C2D-C1D	3.25	1.48	1.42
22	W	602	CLA	C4B-NB	3.25	1.41	1.37
22	K	204	CLA	C4B-NB	3.25	1.41	1.37
21	U	607	CHL	C3B-C4B	3.24	1.50	1.42
22	A	830	CLA	C4B-NB	3.24	1.41	1.37
22	B	812	CLA	C4B-NB	3.24	1.41	1.37
22	A	812	CLA	C4B-NB	3.24	1.41	1.37
21	8	607	CHL	C3B-C4B	3.24	1.50	1.42
21	4	607	CHL	C3B-C4B	3.23	1.50	1.42
22	A	827	CLA	C4B-NB	3.23	1.41	1.37
21	2	601	CHL	C3B-C4B	3.23	1.50	1.42
22	9	609	CLA	C3B-C4B	3.23	1.50	1.42
22	K	201	CLA	C4B-NB	3.23	1.41	1.37
22	B	830	CLA	C4D-ND	-3.23	1.33	1.37
22	8	601	CLA	C4D-ND	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	606	CHL	C3B-C4B	3.22	1.50	1.42
21	9	606	CHL	C3B-C4B	3.22	1.50	1.42
22	B	828	CLA	C4B-NB	3.22	1.41	1.37
21	7	608	CHL	C3B-C4B	3.21	1.50	1.42
22	B	807	CLA	C4B-NB	3.21	1.41	1.37
21	V	609	CHL	C3B-C4B	3.21	1.50	1.42
22	O	2001	CLA	C2D-C1D	3.21	1.48	1.42
22	B	817	CLA	C4B-NB	3.21	1.41	1.37
22	3	604	CLA	C4B-NB	3.21	1.41	1.37
21	U	609	CHL	C3B-C4B	3.21	1.50	1.42
22	F	303	CLA	C4B-NB	3.20	1.41	1.37
22	A	832	CLA	C4B-NB	3.20	1.41	1.37
22	A	823	CLA	C2D-C1D	3.20	1.48	1.42
22	B	839	CLA	C4B-NB	3.20	1.41	1.37
22	A	819	CLA	C4B-NB	3.20	1.41	1.37
22	V	610	CLA	CAB-C3B	-3.19	1.44	1.50
21	4	606	CHL	C3B-C4B	3.19	1.50	1.42
22	A	807	CLA	C4B-NB	3.18	1.41	1.37
22	B	802	CLA	C4B-NB	3.18	1.41	1.37
22	B	827	CLA	C4B-NB	3.18	1.41	1.37
22	A	812	CLA	C4D-ND	-3.18	1.33	1.37
22	B	838	CLA	C4D-ND	-3.17	1.33	1.37
22	A	803	CLA	C4D-ND	-3.17	1.33	1.37
22	L	304	CLA	C4B-NB	3.17	1.41	1.37
22	A	820	CLA	C4D-ND	-3.17	1.33	1.37
21	9	601	CHL	C3B-C4B	3.17	1.50	1.42
22	B	810	CLA	C4B-NB	3.17	1.41	1.37
21	2	606	CHL	C3B-C4B	3.17	1.50	1.42
22	6	613	CLA	C4D-ND	-3.16	1.33	1.37
22	A	811	CLA	C4D-ND	-3.16	1.33	1.37
22	A	809	CLA	C4D-ND	-3.15	1.33	1.37
22	9	609	CLA	C1D-C2D	3.15	1.51	1.45
22	A	821	CLA	C4D-ND	-3.15	1.33	1.37
22	B	840	CLA	C4B-NB	3.15	1.41	1.37
21	9	607	CHL	C3B-C4B	3.15	1.50	1.42
21	9	605	CHL	C1D-C2D	3.14	1.51	1.45
22	B	806	CLA	C4D-ND	-3.14	1.33	1.37
22	7	610	CLA	C3B-C4B	3.14	1.50	1.42
22	A	829	CLA	C4B-NB	3.14	1.41	1.37
22	A	836	CLA	C4D-ND	-3.13	1.33	1.37
22	B	819	CLA	C4D-ND	-3.13	1.33	1.37
22	A	807	CLA	C4D-ND	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	608	CHL	C3B-C4B	3.12	1.50	1.42
22	A	838	CLA	C4B-NB	3.12	1.41	1.37
22	B	835	CLA	C4D-ND	-3.12	1.33	1.37
22	B	823	CLA	C4B-NB	3.12	1.41	1.37
22	A	833	CLA	C4D-ND	-3.12	1.33	1.37
22	3	602	CLA	C4D-ND	-3.11	1.33	1.37
22	B	836	CLA	C4B-NB	3.11	1.41	1.37
22	A	818	CLA	C4D-ND	-3.11	1.33	1.37
22	B	835	CLA	C4B-NB	3.11	1.41	1.37
22	9	604	CLA	C3B-C4B	3.11	1.50	1.42
22	B	829	CLA	C4D-ND	-3.10	1.33	1.37
22	A	816	CLA	C4B-NB	3.10	1.41	1.37
22	W	614	CLA	CAB-C3B	-3.10	1.44	1.50
22	B	818	CLA	C4B-NB	3.10	1.41	1.37
21	6	602	CHL	C1D-C2D	3.10	1.51	1.45
22	9	612	CLA	C4D-ND	-3.10	1.33	1.37
22	A	824	CLA	C4D-ND	-3.09	1.33	1.37
22	A	823	CLA	C4D-ND	-3.09	1.33	1.37
22	3	607	CLA	C4D-ND	-3.09	1.33	1.37
22	F	301	CLA	C4D-ND	-3.09	1.33	1.37
22	U	613	CLA	C4D-ND	-3.09	1.33	1.37
22	B	840	CLA	C4D-ND	-3.09	1.33	1.37
21	6	601	CHL	C1D-C2D	3.09	1.51	1.45
22	2	613	CLA	C4D-ND	-3.09	1.33	1.37
21	4	607	CHL	C1D-C2D	3.09	1.51	1.45
22	U	610	CLA	C3B-C4B	3.08	1.50	1.42
22	B	806	CLA	C4B-NB	3.08	1.41	1.37
22	B	812	CLA	C4D-ND	-3.08	1.33	1.37
22	8	611	CLA	C3B-C4B	3.08	1.50	1.42
22	B	818	CLA	C4D-ND	-3.08	1.33	1.37
21	8	618	CHL	C3B-C4B	3.08	1.50	1.42
22	A	808	CLA	C4D-ND	-3.07	1.33	1.37
22	B	822	CLA	C4D-ND	-3.07	1.33	1.37
22	B	826	CLA	C4D-ND	-3.07	1.33	1.37
21	8	607	CHL	C1D-C2D	3.07	1.51	1.45
22	1	610	CLA	C4D-ND	-3.07	1.33	1.37
22	A	854	CLA	C4D-ND	-3.07	1.33	1.37
22	A	810	CLA	C4D-ND	-3.07	1.33	1.37
22	A	840	CLA	C4D-ND	-3.07	1.33	1.37
22	5	606	CLA	C4D-ND	-3.07	1.33	1.37
21	2	607	CHL	C1D-C2D	3.07	1.51	1.45
22	B	811	CLA	C3B-C4B	3.07	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	604	CLA	C4D-ND	-3.07	1.33	1.37
22	A	822	CLA	C4D-ND	-3.07	1.33	1.37
21	V	609	CHL	C1D-C2D	3.07	1.51	1.45
21	W	609	CHL	C1D-C2D	3.07	1.51	1.45
22	V	612	CLA	C4D-ND	-3.07	1.33	1.37
21	W	606	CHL	C1D-C2D	3.07	1.51	1.45
22	2	604	CLA	C4D-ND	-3.07	1.33	1.37
23	2	619	LUT	C8-C9	-3.06	1.39	1.45
22	W	612	CLA	CAB-C3B	-3.06	1.44	1.50
22	1	602	CLA	C4D-ND	-3.06	1.33	1.37
22	1	613	CLA	C4D-ND	-3.06	1.33	1.37
22	O	2002	CLA	C4D-ND	-3.06	1.33	1.37
22	A	819	CLA	C4D-ND	-3.06	1.33	1.37
21	V	601	CHL	C1D-C2D	3.06	1.51	1.45
22	B	814	CLA	C4D-ND	-3.06	1.33	1.37
21	4	618	CHL	C1D-C2D	3.06	1.51	1.45
22	W	613	CLA	C4D-ND	-3.06	1.33	1.37
22	A	834	CLA	C4D-ND	-3.06	1.33	1.37
22	B	831	CLA	C4D-ND	-3.06	1.33	1.37
22	B	824	CLA	C4D-ND	-3.05	1.33	1.37
21	2	618	CHL	C1D-C2D	3.05	1.51	1.45
22	7	602	CLA	C4D-ND	-3.05	1.33	1.37
22	A	820	CLA	C4B-NB	3.05	1.41	1.37
22	A	806	CLA	C4D-ND	-3.05	1.33	1.37
22	B	805	CLA	C4D-ND	-3.05	1.33	1.37
22	K	203	CLA	C4D-ND	-3.05	1.33	1.37
22	2	614	CLA	C4D-ND	-3.05	1.33	1.37
22	A	831	CLA	C4D-ND	-3.05	1.33	1.37
22	B	817	CLA	C4D-ND	-3.05	1.33	1.37
22	V	611	CLA	CAB-C3B	-3.05	1.44	1.50
22	1	608	CLA	C4D-ND	-3.05	1.33	1.37
22	A	805	CLA	C4D-ND	-3.05	1.33	1.37
22	B	815	CLA	C4D-ND	-3.05	1.33	1.37
22	A	816	CLA	C4D-ND	-3.04	1.33	1.37
22	B	807	CLA	C4D-ND	-3.04	1.33	1.37
22	L	304	CLA	C4D-ND	-3.04	1.33	1.37
22	B	825	CLA	C4D-ND	-3.04	1.33	1.37
22	4	609	CLA	C4D-ND	-3.04	1.33	1.37
22	B	837	CLA	C4D-ND	-3.04	1.33	1.37
22	L	303	CLA	C4D-ND	-3.04	1.33	1.37
22	3	614	CLA	C4D-ND	-3.04	1.33	1.37
22	9	603	CLA	C4D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	612	CLA	C3B-C4B	3.03	1.49	1.42
21	W	605	CHL	C1D-C2D	3.03	1.51	1.45
22	A	830	CLA	C4D-ND	-3.03	1.33	1.37
22	W	611	CLA	CAB-C3B	-3.03	1.44	1.50
22	V	611	CLA	C4D-ND	-3.03	1.33	1.37
22	A	817	CLA	C4D-ND	-3.03	1.33	1.37
22	5	603	CLA	C4D-ND	-3.03	1.33	1.37
22	8	610	CLA	C3B-C4B	3.03	1.49	1.42
21	5	607	CHL	C1D-C2D	3.03	1.51	1.45
22	A	839	CLA	C4D-ND	-3.03	1.33	1.37
22	V	612	CLA	CAB-C3B	-3.03	1.44	1.50
22	5	609	CLA	C3B-C4B	3.03	1.49	1.42
22	A	841	CLA	C4D-ND	-3.03	1.33	1.37
22	4	602	CLA	C4D-ND	-3.02	1.33	1.37
22	B	837	CLA	C3B-C4B	3.02	1.49	1.42
22	B	808	CLA	C4D-ND	-3.02	1.33	1.37
22	2	614	CLA	C3B-C4B	3.02	1.49	1.42
22	W	612	CLA	C4D-ND	-3.02	1.33	1.37
22	7	603	CLA	C3B-C4B	3.02	1.49	1.42
22	B	836	CLA	C4D-ND	-3.02	1.33	1.37
22	8	611	CLA	C4D-ND	-3.02	1.33	1.37
22	9	610	CLA	C4D-ND	-3.02	1.33	1.37
22	4	604	CLA	C3B-C4B	3.02	1.49	1.42
22	4	613	CLA	C4D-ND	-3.02	1.33	1.37
22	A	802	CLA	C4D-ND	-3.02	1.33	1.37
22	B	804	CLA	C4D-ND	-3.01	1.33	1.37
22	A	815	CLA	C4D-ND	-3.01	1.33	1.37
22	2	611	CLA	C4D-ND	-3.01	1.33	1.37
22	F	303	CLA	C4D-ND	-3.01	1.33	1.37
21	U	609	CHL	C1D-C2D	3.01	1.51	1.45
22	1	611	CLA	C3B-C4B	3.01	1.49	1.42
22	7	606	CLA	C4D-ND	-3.01	1.33	1.37
22	A	842	CLA	C4D-ND	-3.01	1.33	1.37
22	6	610	CLA	C4D-ND	-3.01	1.33	1.37
21	8	618	CHL	C1D-C2D	3.00	1.51	1.45
22	B	841	CLA	C4D-ND	-3.00	1.33	1.37
22	V	602	CLA	C4D-ND	-3.00	1.33	1.37
22	A	825	CLA	C4D-ND	-3.00	1.33	1.37
21	9	607	CHL	C1D-C2D	3.00	1.51	1.45
22	3	604	CLA	C4D-ND	-3.00	1.33	1.37
22	A	826	CLA	C4D-ND	-3.00	1.33	1.37
22	B	828	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	839	CLA	C4D-ND	-3.00	1.33	1.37
22	7	614	CLA	C4D-ND	-3.00	1.33	1.37
21	V	605	CHL	C1D-C2D	3.00	1.51	1.45
22	7	613	CLA	C4D-ND	-3.00	1.33	1.37
22	6	603	CLA	C3B-C4B	3.00	1.49	1.42
22	9	612	CLA	C3B-C4B	3.00	1.49	1.42
22	7	610	CLA	C4D-ND	-3.00	1.33	1.37
22	A	837	CLA	C4D-ND	-3.00	1.33	1.37
21	2	601	CHL	C1D-C2D	3.00	1.51	1.45
22	7	609	CLA	C3B-C4B	2.99	1.49	1.42
22	A	828	CLA	C3B-C4B	2.99	1.49	1.42
21	2	608	CHL	C1D-C2D	2.99	1.51	1.45
22	9	602	CLA	C4D-ND	-2.99	1.33	1.37
22	B	833	CLA	C4D-ND	-2.99	1.33	1.37
22	6	604	CLA	C4D-ND	-2.99	1.33	1.37
22	B	827	CLA	C4D-ND	-2.99	1.33	1.37
22	6	613	CLA	C1B-C2B	2.99	1.50	1.43
22	7	617	CLA	C4D-ND	-2.99	1.33	1.37
22	8	612	CLA	C4D-ND	-2.99	1.33	1.37
22	A	832	CLA	C4D-ND	-2.99	1.33	1.37
21	4	608	CHL	C1D-C2D	2.99	1.51	1.45
22	8	601	CLA	C3B-C4B	2.99	1.49	1.42
21	U	608	CHL	C1D-C2D	2.99	1.51	1.45
22	B	820	CLA	C4D-ND	-2.98	1.33	1.37
22	3	611	CLA	C4D-ND	-2.98	1.33	1.37
22	5	611	CLA	C4D-ND	-2.98	1.33	1.37
22	4	601	CLA	C4D-ND	-2.98	1.33	1.37
22	4	604	CLA	C4D-ND	-2.98	1.33	1.37
21	U	601	CHL	C1D-C2D	2.98	1.51	1.45
21	U	605	CHL	C1D-C2D	2.98	1.51	1.45
21	W	601	CHL	C1D-C2D	2.98	1.51	1.45
22	B	830	CLA	C3B-C4B	2.98	1.49	1.42
22	8	612	CLA	C3B-C4B	2.98	1.49	1.42
22	A	813	CLA	C4D-ND	-2.98	1.33	1.37
21	6	618	CHL	C3B-C4B	2.98	1.49	1.42
22	V	614	CLA	C4D-ND	-2.98	1.33	1.37
21	W	608	CHL	C1D-C2D	2.98	1.51	1.45
22	G	201	CLA	C4D-ND	-2.98	1.33	1.37
22	3	606	CLA	C4D-ND	-2.97	1.33	1.37
22	1	614	CLA	C4D-ND	-2.97	1.33	1.37
22	B	825	CLA	C4B-NB	2.97	1.41	1.37
22	4	612	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	611	CLA	C4D-ND	-2.97	1.33	1.37
22	9	603	CLA	C3B-C4B	2.97	1.49	1.42
22	U	610	CLA	C4D-ND	-2.97	1.33	1.37
22	B	813	CLA	C4D-ND	-2.97	1.33	1.37
22	8	610	CLA	C4D-ND	-2.97	1.33	1.37
22	9	613	CLA	C3B-C4B	2.97	1.49	1.42
21	6	618	CHL	C1D-C2D	2.97	1.51	1.45
22	7	615	CLA	C4D-ND	-2.97	1.33	1.37
22	5	602	CLA	C4D-ND	-2.97	1.33	1.37
21	6	607	CHL	C1D-C2D	2.97	1.51	1.45
22	8	604	CLA	C1B-C2B	2.97	1.50	1.43
22	3	612	CLA	C4D-ND	-2.97	1.33	1.37
22	V	613	CLA	C4D-ND	-2.96	1.33	1.37
21	6	606	CHL	C1D-C2D	2.96	1.51	1.45
21	8	606	CHL	C1D-C2D	2.96	1.51	1.45
21	9	606	CHL	C1D-C2D	2.96	1.51	1.45
22	B	810	CLA	C4D-ND	-2.96	1.33	1.37
22	W	610	CLA	C4D-ND	-2.96	1.33	1.37
22	V	604	CLA	C4D-ND	-2.96	1.33	1.37
22	A	843	CLA	C4D-ND	-2.96	1.33	1.37
22	G	203	CLA	C4D-ND	-2.96	1.33	1.37
22	A	828	CLA	C4D-ND	-2.96	1.33	1.37
22	B	809	CLA	C4D-ND	-2.96	1.33	1.37
22	B	816	CLA	C4D-ND	-2.96	1.33	1.37
22	9	610	CLA	C3B-C4B	2.96	1.49	1.42
22	8	604	CLA	C4D-ND	-2.95	1.33	1.37
22	4	614	CLA	C4D-ND	-2.95	1.33	1.37
22	A	805	CLA	C3B-C4B	2.95	1.49	1.42
22	5	611	CLA	C3B-C4B	2.95	1.49	1.42
22	U	602	CLA	C4D-ND	-2.95	1.33	1.37
21	1	601	CHL	C1D-C2D	2.95	1.51	1.45
22	W	602	CLA	C4D-ND	-2.94	1.33	1.37
22	U	612	CLA	C3B-C4B	2.94	1.49	1.42
22	7	611	CLA	C3B-C4B	2.94	1.49	1.42
22	A	804	CLA	C4D-ND	-2.94	1.33	1.37
22	A	836	CLA	C4C-C3C	2.94	1.46	1.41
21	2	606	CHL	C1D-C2D	2.94	1.51	1.45
22	4	610	CLA	C3B-C4B	2.94	1.49	1.42
21	W	607	CHL	C1D-C2D	2.94	1.51	1.45
22	W	602	CLA	C3B-C4B	2.94	1.49	1.42
21	V	607	CHL	C1D-C2D	2.94	1.51	1.45
22	3	610	CLA	C3B-C4B	2.94	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	C3B-C4B	2.94	1.49	1.42
22	J	101	CLA	C4D-ND	-2.94	1.33	1.37
22	O	2001	CLA	C4D-ND	-2.94	1.33	1.37
22	9	613	CLA	C4D-ND	-2.94	1.33	1.37
22	9	604	CLA	C4D-ND	-2.94	1.33	1.37
22	8	613	CLA	C4D-ND	-2.94	1.33	1.37
22	U	611	CLA	C3B-C4B	2.94	1.49	1.42
21	2	602	CHL	C1D-C2D	2.94	1.51	1.45
22	G	204	CLA	C4D-ND	-2.94	1.33	1.37
22	L	302	CLA	C4D-ND	-2.93	1.33	1.37
22	W	603	CLA	C4D-ND	-2.93	1.33	1.37
22	3	613	CLA	C4D-ND	-2.93	1.33	1.37
22	B	832	CLA	C4D-ND	-2.93	1.33	1.37
22	A	814	CLA	C4D-ND	-2.93	1.33	1.37
22	W	611	CLA	C4D-ND	-2.93	1.33	1.37
22	7	612	CLA	C3B-C4B	2.93	1.49	1.42
22	U	611	CLA	C4D-ND	-2.93	1.33	1.37
21	5	601	CHL	C1D-C2D	2.93	1.51	1.45
22	W	603	CLA	C3B-C4B	2.93	1.49	1.42
22	B	834	CLA	C4D-ND	-2.93	1.33	1.37
22	5	614	CLA	C4D-ND	-2.93	1.33	1.37
22	A	829	CLA	C3B-C4B	2.93	1.49	1.42
22	3	615	CLA	C4D-ND	-2.92	1.33	1.37
21	8	608	CHL	C1D-C2D	2.92	1.51	1.45
22	W	604	CLA	C4D-ND	-2.92	1.33	1.37
22	K	204	CLA	C4D-ND	-2.92	1.33	1.37
22	1	606	CLA	C4D-ND	-2.92	1.33	1.37
21	4	618	CHL	C3B-C4B	2.92	1.49	1.42
22	W	610	CLA	C3B-C4B	2.92	1.49	1.42
21	V	608	CHL	C1D-C2D	2.92	1.51	1.45
22	A	845	CLA	C4D-ND	-2.92	1.33	1.37
21	V	606	CHL	C1D-C2D	2.92	1.51	1.45
22	V	610	CLA	C4D-ND	-2.92	1.33	1.37
22	B	823	CLA	C4D-ND	-2.92	1.33	1.37
22	A	827	CLA	C4D-ND	-2.92	1.33	1.37
22	7	614	CLA	C3B-C4B	2.92	1.49	1.42
21	1	607	CHL	C1D-C2D	2.92	1.51	1.45
22	5	612	CLA	C4D-ND	-2.91	1.33	1.37
22	H	201	CLA	C4D-ND	-2.91	1.33	1.37
22	7	604	CLA	C4D-ND	-2.91	1.33	1.37
21	6	608	CHL	C1D-C2D	2.91	1.51	1.45
21	U	606	CHL	C1D-C2D	2.91	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	603	CLA	C4D-ND	-2.91	1.33	1.37
22	A	813	CLA	C3B-C4B	2.91	1.49	1.42
22	6	609	CLA	C3B-C4B	2.91	1.49	1.42
22	B	802	CLA	C4D-ND	-2.91	1.33	1.37
22	B	803	CLA	C4D-ND	-2.91	1.33	1.37
22	O	2002	CLA	C3B-C4B	2.91	1.49	1.42
22	V	602	CLA	C3B-C4B	2.90	1.49	1.42
22	L	303	CLA	C3B-C4B	2.90	1.49	1.42
22	5	610	CLA	C4D-ND	-2.90	1.33	1.37
22	3	603	CLA	C3B-C4B	2.90	1.49	1.42
22	8	602	CLA	C4D-ND	-2.90	1.33	1.37
22	8	603	CLA	C3B-C4B	2.90	1.49	1.42
22	6	603	CLA	C4D-ND	-2.90	1.33	1.37
22	9	611	CLA	C3B-C4B	2.90	1.49	1.42
21	7	608	CHL	C1D-C2D	2.90	1.51	1.45
22	A	808	CLA	C3B-C4B	2.90	1.49	1.42
22	8	603	CLA	C4D-ND	-2.89	1.33	1.37
22	3	602	CLA	C3B-C4B	2.89	1.49	1.42
22	W	614	CLA	C4D-ND	-2.89	1.33	1.37
22	1	604	CLA	C4D-ND	-2.89	1.33	1.37
21	9	601	CHL	C1D-C2D	2.89	1.51	1.45
22	9	611	CLA	C4D-ND	-2.89	1.33	1.37
22	1	616	CLA	C4D-ND	-2.89	1.33	1.37
22	U	612	CLA	C4D-ND	-2.89	1.33	1.37
22	A	838	CLA	C4D-ND	-2.89	1.33	1.37
21	V	606	CHL	C3D-C2D	2.89	1.47	1.39
22	A	835	CLA	C4D-ND	-2.88	1.33	1.37
22	K	206	CLA	C4D-ND	-2.88	1.33	1.37
22	2	603	CLA	C4D-ND	-2.88	1.33	1.37
22	3	610	CLA	C4D-ND	-2.88	1.33	1.37
22	A	823	CLA	C3B-C4B	2.88	1.49	1.42
22	6	604	CLA	C3B-C4B	2.88	1.49	1.42
22	U	614	CLA	C4D-ND	-2.88	1.33	1.37
22	8	609	CLA	C4D-ND	-2.88	1.33	1.37
22	7	617	CLA	C3B-C4B	2.88	1.49	1.42
21	9	608	CHL	C1D-C2D	2.88	1.51	1.45
22	B	813	CLA	C3B-C4B	2.88	1.49	1.42
22	O	2003	CLA	C4D-ND	-2.87	1.33	1.37
22	6	614	CLA	C3B-C4B	2.87	1.49	1.42
22	B	811	CLA	C4D-ND	-2.87	1.33	1.37
22	2	610	CLA	C4D-ND	-2.87	1.33	1.37
22	3	611	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	613	CLA	C3B-C4B	2.87	1.49	1.42
22	8	614	CLA	C3B-C4B	2.87	1.49	1.42
22	8	614	CLA	C4D-ND	-2.87	1.33	1.37
22	5	614	CLA	C3B-C4B	2.87	1.49	1.42
22	K	206	CLA	C3B-C4B	2.87	1.49	1.42
22	2	611	CLA	C3B-C4B	2.86	1.49	1.42
22	B	805	CLA	C3B-C4B	2.86	1.49	1.42
22	A	829	CLA	C4D-ND	-2.86	1.33	1.37
22	7	607	CLA	C4D-ND	-2.86	1.33	1.37
22	1	609	CLA	C4D-ND	-2.86	1.33	1.37
21	U	607	CHL	C1D-C2D	2.86	1.51	1.45
22	4	603	CLA	C4D-ND	-2.86	1.33	1.37
22	V	603	CLA	C4D-ND	-2.86	1.33	1.37
22	B	822	CLA	C3B-C4B	2.86	1.49	1.42
22	7	604	CLA	C3B-C4B	2.86	1.49	1.42
22	5	608	CLA	C4D-ND	-2.86	1.33	1.37
22	8	609	CLA	C3B-C4B	2.86	1.49	1.42
22	9	602	CLA	C3B-C4B	2.86	1.49	1.42
22	1	612	CLA	C4D-ND	-2.86	1.33	1.37
22	6	610	CLA	C3B-C4B	2.86	1.49	1.42
22	1	608	CLA	C3B-C4B	2.85	1.49	1.42
22	G	204	CLA	C3B-C4B	2.85	1.49	1.42
22	5	606	CLA	C3B-C4B	2.85	1.49	1.42
22	2	612	CLA	C3B-C4B	2.85	1.49	1.42
22	A	843	CLA	C3B-C4B	2.85	1.49	1.42
22	2	609	CLA	C4D-ND	-2.85	1.33	1.37
22	3	615	CLA	C3B-C4B	2.85	1.49	1.42
22	K	203	CLA	C3B-C4B	2.85	1.49	1.42
22	A	854	CLA	C3B-C4B	2.85	1.49	1.42
22	B	821	CLA	C3B-C4B	2.84	1.49	1.42
22	5	610	CLA	C3B-C4B	2.84	1.49	1.42
22	U	604	CLA	C3B-C4B	2.84	1.49	1.42
22	3	604	CLA	C3B-C4B	2.84	1.49	1.42
22	3	613	CLA	C3B-C4B	2.84	1.49	1.42
22	A	821	CLA	C3B-C4B	2.84	1.49	1.42
22	3	614	CLA	C3B-C4B	2.84	1.49	1.42
22	7	611	CLA	C4D-ND	-2.84	1.33	1.37
21	W	608	CHL	C1B-C2B	2.84	1.49	1.43
22	A	814	CLA	C3B-C4B	2.84	1.49	1.42
21	9	607	CHL	C3D-C2D	2.84	1.46	1.39
22	B	814	CLA	C3B-C4B	2.84	1.49	1.42
22	7	612	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	819	CLA	C3B-C4B	2.84	1.49	1.42
22	5	616	CLA	C3B-C4B	2.84	1.49	1.42
22	B	804	CLA	C3B-C4B	2.84	1.49	1.42
22	B	824	CLA	C3B-C4B	2.84	1.49	1.42
22	A	809	CLA	C3B-C4B	2.84	1.49	1.42
22	3	607	CLA	C3B-C4B	2.83	1.49	1.42
22	L	302	CLA	C3B-C4B	2.83	1.49	1.42
22	V	614	CLA	C3B-C4B	2.83	1.49	1.42
22	4	611	CLA	C3B-C4B	2.83	1.49	1.42
22	4	611	CLA	C4D-ND	-2.83	1.33	1.37
21	4	606	CHL	C1D-C2D	2.83	1.50	1.45
22	B	838	CLA	C3B-C4B	2.83	1.49	1.42
22	1	611	CLA	C4D-ND	-2.83	1.33	1.37
22	6	609	CLA	C4D-ND	-2.83	1.33	1.37
22	B	832	CLA	C3B-C4B	2.83	1.49	1.42
21	4	618	CHL	C3D-C2D	2.83	1.46	1.39
22	A	806	CLA	C3B-C4B	2.83	1.49	1.42
22	U	602	CLA	C3B-C4B	2.83	1.49	1.42
22	1	606	CLA	C3B-C4B	2.83	1.49	1.42
22	1	610	CLA	C3B-C4B	2.83	1.49	1.42
22	7	607	CLA	C3B-C4B	2.82	1.49	1.42
22	A	837	CLA	C3B-C4B	2.82	1.49	1.42
22	6	612	CLA	C4D-ND	-2.82	1.33	1.37
22	U	604	CLA	C4D-ND	-2.82	1.33	1.37
22	4	614	CLA	C3B-C4B	2.82	1.49	1.42
22	K	201	CLA	C4D-ND	-2.82	1.33	1.37
22	A	817	CLA	C3B-C4B	2.82	1.49	1.42
22	5	603	CLA	C3B-C4B	2.82	1.49	1.42
22	1	603	CLA	C4D-ND	-2.82	1.33	1.37
22	5	616	CLA	C4D-ND	-2.82	1.33	1.37
22	A	832	CLA	C3B-C4B	2.82	1.49	1.42
22	1	612	CLA	C3B-C4B	2.81	1.49	1.42
22	A	842	CLA	C3B-C4B	2.81	1.49	1.42
22	5	609	CLA	C1B-C2B	2.81	1.49	1.43
22	A	810	CLA	C3B-C4B	2.81	1.49	1.42
22	B	802	CLA	C1B-C2B	2.81	1.49	1.43
22	7	603	CLA	C4D-ND	-2.80	1.33	1.37
22	A	827	CLA	C3B-C4B	2.80	1.49	1.42
22	B	817	CLA	C3B-C4B	2.80	1.49	1.42
22	6	614	CLA	C4D-ND	-2.80	1.33	1.37
22	G	203	CLA	C3B-C4B	2.80	1.49	1.42
22	A	801	CLA	C4D-ND	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	610	CLA	C3B-C4B	2.79	1.49	1.42
21	3	608	CHL	C1D-C2D	2.79	1.50	1.45
22	2	612	CLA	C4D-ND	-2.79	1.33	1.37
22	3	606	CLA	C3B-C4B	2.79	1.49	1.42
22	F	301	CLA	C3B-C4B	2.79	1.49	1.42
22	B	836	CLA	C3B-C4B	2.79	1.49	1.42
22	A	825	CLA	C3B-C4B	2.79	1.49	1.42
22	3	612	CLA	C3B-C4B	2.79	1.49	1.42
22	1	604	CLA	C3B-C4B	2.79	1.49	1.42
21	6	618	CHL	C3D-C2D	2.79	1.46	1.39
22	B	819	CLA	C3B-C4B	2.79	1.49	1.42
22	U	603	CLA	C4D-ND	-2.79	1.33	1.37
21	2	602	CHL	MG-NA	-2.78	1.99	2.06
22	8	604	CLA	C3B-C4B	2.78	1.49	1.42
22	2	609	CLA	C3B-C4B	2.78	1.49	1.42
22	J	101	CLA	C3B-C4B	2.78	1.49	1.42
22	H	201	CLA	C3B-C4B	2.78	1.49	1.42
21	2	602	CHL	C3D-C2D	2.77	1.46	1.39
22	1	614	CLA	C3B-C4B	2.77	1.49	1.42
22	B	807	CLA	C3B-C4B	2.77	1.49	1.42
22	7	613	CLA	C3B-C4B	2.77	1.49	1.42
22	B	829	CLA	C3B-C4B	2.77	1.49	1.42
22	A	804	CLA	C3B-C4B	2.77	1.49	1.42
22	V	604	CLA	C3B-C4B	2.76	1.49	1.42
22	4	609	CLA	C3B-C4B	2.76	1.49	1.42
22	8	613	CLA	C1B-C2B	2.76	1.49	1.43
21	4	607	CHL	C3D-C2D	2.76	1.46	1.39
21	W	605	CHL	C3D-C2D	2.76	1.46	1.39
22	B	826	CLA	C3B-C4B	2.76	1.49	1.42
22	A	820	CLA	C3B-C4B	2.76	1.49	1.42
21	4	608	CHL	C1B-C2B	2.76	1.49	1.43
22	6	613	CLA	C3B-C4B	2.76	1.49	1.42
21	5	607	CHL	C3D-C2D	2.76	1.46	1.39
22	V	613	CLA	C3B-C4B	2.75	1.49	1.42
22	5	602	CLA	C3B-C4B	2.75	1.49	1.42
22	1	603	CLA	C3B-C4B	2.75	1.49	1.42
22	A	831	CLA	C3B-C4B	2.75	1.49	1.42
21	5	601	CHL	C3D-C2D	2.75	1.46	1.39
22	1	602	CLA	C3B-C4B	2.75	1.49	1.42
22	B	820	CLA	C3B-C4B	2.75	1.49	1.42
22	5	613	CLA	C1B-C2B	2.74	1.49	1.43
22	A	815	CLA	C3B-C4B	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	614	CLA	C3B-C4B	2.74	1.49	1.42
22	4	601	CLA	C3B-C4B	2.74	1.49	1.42
21	9	607	CHL	MG-NA	-2.74	1.99	2.06
22	4	602	CLA	C3B-C4B	2.74	1.49	1.42
22	6	604	CLA	C1B-C2B	2.74	1.49	1.43
21	4	608	CHL	MG-NA	-2.74	1.99	2.06
22	7	615	CLA	C3B-C4B	2.74	1.49	1.42
22	A	838	CLA	C3B-C4B	2.74	1.49	1.42
22	B	808	CLA	C3B-C4B	2.74	1.49	1.42
22	1	616	CLA	C3B-C4B	2.74	1.49	1.42
22	K	201	CLA	C3B-C4B	2.74	1.49	1.42
22	A	801	CLA	C3B-C4B	2.73	1.49	1.42
22	B	823	CLA	C3B-C4B	2.73	1.49	1.42
22	6	612	CLA	C3B-C4B	2.73	1.49	1.42
22	B	827	CLA	C3B-C4B	2.73	1.49	1.42
22	7	609	CLA	C1B-C2B	2.73	1.49	1.43
22	4	612	CLA	C3B-C4B	2.73	1.49	1.42
22	B	834	CLA	C3B-C4B	2.73	1.49	1.42
22	A	830	CLA	C3B-C4B	2.73	1.49	1.42
22	U	603	CLA	C3B-C4B	2.73	1.49	1.42
22	A	834	CLA	C3B-C4B	2.73	1.49	1.42
21	6	602	CHL	C3D-C2D	2.73	1.46	1.39
22	A	802	CLA	C3B-C4B	2.72	1.49	1.42
22	F	304	CLA	C3B-C4B	2.72	1.49	1.42
23	2	619	LUT	C28-C29	-2.72	1.40	1.45
22	G	201	CLA	C3B-C4B	2.72	1.49	1.42
22	A	845	CLA	C3B-C4B	2.72	1.49	1.42
22	7	602	CLA	C3B-C4B	2.72	1.49	1.42
22	8	602	CLA	C3B-C4B	2.72	1.49	1.42
21	U	605	CHL	C3D-C2D	2.72	1.46	1.39
22	B	815	CLA	C3B-C4B	2.72	1.49	1.42
22	A	818	CLA	C3B-C4B	2.72	1.49	1.42
22	5	604	CLA	C3B-C4B	2.71	1.49	1.42
21	4	608	CHL	C3D-C2D	2.71	1.46	1.39
22	W	604	CLA	C3B-C4B	2.71	1.49	1.42
22	4	613	CLA	C3B-C4B	2.71	1.49	1.42
22	2	603	CLA	C3B-C4B	2.71	1.49	1.42
22	8	613	CLA	C3B-C4B	2.71	1.49	1.42
22	K	204	CLA	C3B-C4B	2.71	1.49	1.42
22	A	803	CLA	C3B-C4B	2.71	1.49	1.42
21	8	618	CHL	C3D-C2D	2.71	1.46	1.39
22	V	612	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	204	CLA	C1B-C2B	2.71	1.49	1.43
21	V	607	CHL	C3D-C2D	2.70	1.46	1.39
21	U	607	CHL	C3D-C2D	2.70	1.46	1.39
22	B	825	CLA	C3B-C4B	2.70	1.49	1.42
22	1	613	CLA	C3B-C4B	2.70	1.49	1.42
22	A	826	CLA	C3B-C4B	2.70	1.49	1.42
22	6	611	CLA	C1B-C2B	2.70	1.49	1.43
21	V	601	CHL	C3D-C2D	2.70	1.46	1.39
22	A	833	CLA	C3B-C4B	2.70	1.49	1.42
21	W	609	CHL	C3D-C2D	2.70	1.46	1.39
22	W	613	CLA	C3B-C4B	2.70	1.49	1.42
22	B	806	CLA	C3B-C4B	2.70	1.49	1.42
21	8	607	CHL	C3D-C2D	2.70	1.46	1.39
22	7	613	CLA	C1B-C2B	2.69	1.49	1.43
22	7	615	CLA	C1B-C2B	2.69	1.49	1.43
21	6	607	CHL	C3D-C2D	2.69	1.46	1.39
22	V	603	CLA	C3B-C4B	2.69	1.49	1.42
22	U	613	CLA	C1B-C2B	2.69	1.49	1.43
22	V	611	CLA	C4B-C3B	2.69	1.49	1.43
21	W	601	CHL	C3D-C2D	2.69	1.46	1.39
21	8	606	CHL	C3D-C2D	2.69	1.46	1.39
22	5	616	CLA	C1B-C2B	2.69	1.49	1.43
22	B	803	CLA	C3B-C4B	2.69	1.49	1.42
22	H	201	CLA	C1B-C2B	2.68	1.49	1.43
22	B	833	CLA	C3B-C4B	2.68	1.49	1.42
22	A	822	CLA	C3B-C4B	2.68	1.49	1.42
21	U	601	CHL	C3D-C2D	2.68	1.46	1.39
22	L	304	CLA	C3B-C4B	2.68	1.49	1.42
22	A	811	CLA	C3B-C4B	2.68	1.49	1.42
22	B	818	CLA	C3B-C4B	2.68	1.49	1.42
22	A	824	CLA	C3B-C4B	2.68	1.49	1.42
22	2	613	CLA	C3B-C4B	2.67	1.49	1.42
22	A	835	CLA	C3B-C4B	2.67	1.49	1.42
22	5	608	CLA	C3B-C4B	2.67	1.49	1.42
22	B	831	CLA	C3B-C4B	2.67	1.49	1.42
22	B	809	CLA	C3B-C4B	2.67	1.49	1.42
21	4	606	CHL	C3D-C2D	2.67	1.46	1.39
22	F	303	CLA	C3B-C4B	2.67	1.49	1.42
21	W	608	CHL	C3D-C2D	2.67	1.46	1.39
22	B	816	CLA	C3B-C4B	2.67	1.49	1.42
22	8	602	CLA	C1B-C2B	2.67	1.49	1.43
22	2	604	CLA	C3B-C4B	2.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	839	CLA	C3B-C4B	2.67	1.49	1.42
22	1	609	CLA	C3B-C4B	2.67	1.49	1.42
21	2	607	CHL	C3D-C2D	2.66	1.46	1.39
21	W	601	CHL	MG-NA	-2.66	1.99	2.06
22	U	603	CLA	C1B-C2B	2.66	1.49	1.43
22	A	812	CLA	C3B-C4B	2.66	1.49	1.42
22	4	603	CLA	C3B-C4B	2.66	1.49	1.42
22	5	613	CLA	C3B-C4B	2.66	1.49	1.42
22	W	613	CLA	C1B-C2B	2.66	1.49	1.43
21	V	605	CHL	C3D-C2D	2.66	1.46	1.39
21	W	606	CHL	C3D-C2D	2.66	1.46	1.39
22	U	602	CLA	C1B-C2B	2.66	1.49	1.43
22	G	203	CLA	C1B-C2B	2.66	1.49	1.43
22	A	834	CLA	C1B-C2B	2.66	1.49	1.43
22	7	612	CLA	C1B-C2B	2.66	1.49	1.43
22	4	610	CLA	C4D-ND	-2.66	1.34	1.37
22	A	839	CLA	C3B-C4B	2.65	1.49	1.42
22	A	842	CLA	C1B-C2B	2.65	1.49	1.43
21	1	607	CHL	C3D-C2D	2.65	1.46	1.39
21	U	605	CHL	C1B-C2B	2.65	1.49	1.43
22	A	836	CLA	C2C-C3C	2.65	1.39	1.34
22	A	807	CLA	C3B-C4B	2.65	1.49	1.42
22	A	840	CLA	C3B-C4B	2.65	1.49	1.42
22	6	611	CLA	C3B-C4B	2.65	1.49	1.42
21	1	601	CHL	C3D-C2D	2.65	1.46	1.39
21	9	605	CHL	C3D-C2D	2.65	1.46	1.39
21	V	601	CHL	C4C-C3C	2.65	1.49	1.45
21	W	607	CHL	C1B-C2B	2.65	1.49	1.43
21	U	608	CHL	C3D-C2D	2.65	1.46	1.39
22	B	841	CLA	C3B-C4B	2.65	1.49	1.42
22	B	828	CLA	C3B-C4B	2.64	1.49	1.42
22	4	612	CLA	C1B-C2B	2.64	1.49	1.43
21	6	606	CHL	C3D-C2D	2.64	1.46	1.39
22	3	606	CLA	C1B-C2B	2.64	1.49	1.43
21	2	608	CHL	C3D-C2D	2.64	1.46	1.39
22	4	604	CLA	C1B-C2B	2.64	1.49	1.43
22	4	614	CLA	C1B-C2B	2.64	1.49	1.43
22	B	840	CLA	C1B-C2B	2.64	1.49	1.43
22	B	841	CLA	C1B-C2B	2.64	1.49	1.43
22	8	612	CLA	C1B-C2B	2.64	1.49	1.43
22	1	602	CLA	C1B-C2B	2.64	1.49	1.43
22	B	802	CLA	C3B-C4B	2.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	607	CHL	C3D-C2D	2.64	1.46	1.39
22	3	617	CLA	C4D-ND	-2.64	1.34	1.37
22	V	603	CLA	C1B-C2B	2.64	1.49	1.43
22	2	613	CLA	C1B-C2B	2.64	1.49	1.43
21	2	606	CHL	C3D-C2D	2.64	1.46	1.39
22	5	612	CLA	C1B-C2B	2.64	1.49	1.43
22	1	616	CLA	C1B-C2B	2.64	1.49	1.43
22	3	611	CLA	C1B-C2B	2.64	1.49	1.43
22	A	825	CLA	C1B-C2B	2.64	1.49	1.43
22	3	617	CLA	C1B-C2B	2.64	1.49	1.43
22	O	2001	CLA	CAD-C3D	-2.64	1.45	1.50
22	7	602	CLA	C1B-C2B	2.63	1.49	1.43
22	8	603	CLA	C1B-C2B	2.63	1.49	1.43
22	5	613	CLA	C4D-ND	-2.63	1.34	1.37
21	V	607	CHL	C1B-C2B	2.63	1.49	1.43
22	B	804	CLA	C1B-C2B	2.63	1.49	1.43
21	W	605	CHL	C1B-C2B	2.63	1.49	1.43
22	L	304	CLA	C1B-C2B	2.63	1.49	1.43
22	B	840	CLA	C3B-C4B	2.63	1.48	1.42
21	6	618	CHL	C4C-C3C	2.63	1.49	1.45
22	1	613	CLA	C1B-C2B	2.62	1.49	1.43
22	5	602	CLA	C1B-C2B	2.62	1.49	1.43
22	8	609	CLA	C1B-C2B	2.62	1.49	1.43
22	W	612	CLA	C4B-C3B	2.62	1.49	1.43
22	3	617	CLA	CMC-C2C	-2.62	1.46	1.50
22	B	829	CLA	C1B-C2B	2.62	1.49	1.43
22	7	614	CLA	C1B-C2B	2.62	1.49	1.43
21	2	618	CHL	C3D-C2D	2.62	1.46	1.39
22	3	609	CLA	C1B-C2B	2.62	1.49	1.43
22	4	601	CLA	C1B-C2B	2.62	1.49	1.43
22	4	613	CLA	C1B-C2B	2.62	1.49	1.43
22	3	609	CLA	C4D-ND	-2.62	1.34	1.37
21	U	606	CHL	C3D-C2D	2.62	1.46	1.39
21	V	609	CHL	C3D-C2D	2.62	1.46	1.39
22	U	604	CLA	C1B-C2B	2.62	1.49	1.43
22	V	610	CLA	C4B-C3B	2.62	1.49	1.43
22	7	607	CLA	C1B-C2B	2.62	1.49	1.43
21	V	608	CHL	C3D-C2D	2.61	1.46	1.39
21	V	608	CHL	C1B-C2B	2.61	1.49	1.43
23	5	617	LUT	C8-C9	-2.61	1.40	1.45
22	B	808	CLA	C1B-C2B	2.61	1.49	1.43
22	5	603	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	609	CLA	C4C-C3C	2.61	1.49	1.45
21	3	608	CHL	MG-NA	-2.61	2.00	2.06
21	W	601	CHL	C1B-C2B	2.61	1.49	1.43
21	9	608	CHL	C3D-C2D	2.61	1.46	1.39
22	B	810	CLA	C1B-C2B	2.60	1.49	1.43
22	W	614	CLA	C4B-C3B	2.60	1.49	1.43
22	7	611	CLA	C1B-C2B	2.60	1.49	1.43
22	K	206	CLA	C1B-C2B	2.60	1.49	1.43
22	7	604	CLA	C1B-C2B	2.60	1.49	1.43
22	8	601	CLA	C1B-C2B	2.60	1.49	1.43
22	W	611	CLA	C4B-C3B	2.60	1.49	1.43
22	3	614	CLA	C1B-C2B	2.60	1.49	1.43
22	4	602	CLA	C1B-C2B	2.60	1.49	1.43
22	9	611	CLA	C1B-C2B	2.60	1.49	1.43
22	B	823	CLA	C1B-C2B	2.60	1.49	1.43
22	5	614	CLA	C1B-C2B	2.60	1.49	1.43
22	B	825	CLA	C1B-C2B	2.60	1.49	1.43
22	B	833	CLA	C1B-C2B	2.60	1.49	1.43
22	4	603	CLA	C1B-C2B	2.60	1.49	1.43
22	B	832	CLA	C1B-C2B	2.60	1.49	1.43
22	6	614	CLA	C1B-C2B	2.59	1.49	1.43
22	7	606	CLA	C1B-C2B	2.59	1.49	1.43
22	B	810	CLA	C3B-C4B	2.59	1.48	1.42
22	2	610	CLA	C1B-C2B	2.59	1.49	1.43
22	W	612	CLA	C1B-C2B	2.59	1.49	1.43
21	2	601	CHL	C3D-C2D	2.59	1.46	1.39
21	V	609	CHL	MG-NA	-2.59	2.00	2.06
22	U	614	CLA	C1B-C2B	2.59	1.49	1.43
22	W	604	CLA	C1B-C2B	2.59	1.49	1.43
22	1	614	CLA	C1B-C2B	2.59	1.49	1.43
22	4	611	CLA	C1B-C2B	2.59	1.49	1.43
21	2	608	CHL	MG-NA	-2.59	2.00	2.06
22	9	602	CLA	C1B-C2B	2.59	1.49	1.43
22	1	609	CLA	C1B-C2B	2.59	1.49	1.43
22	B	822	CLA	C1B-C2B	2.59	1.49	1.43
22	7	603	CLA	C1B-C2B	2.59	1.49	1.43
22	V	612	CLA	C4B-C3B	2.59	1.49	1.43
22	A	837	CLA	C1B-C2B	2.59	1.49	1.43
22	V	602	CLA	C1B-C2B	2.58	1.49	1.43
22	6	612	CLA	C1B-C2B	2.58	1.49	1.43
21	U	609	CHL	C3D-C2D	2.58	1.46	1.39
22	B	812	CLA	C3B-C4B	2.58	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	2003	CLA	CAD-C3D	-2.58	1.45	1.50
22	3	613	CLA	C1B-C2B	2.58	1.49	1.43
22	1	612	CLA	C1B-C2B	2.58	1.49	1.43
22	4	609	CLA	C1B-C2B	2.58	1.49	1.43
21	W	609	CHL	C3B-C4B	2.58	1.48	1.42
21	1	607	CHL	MG-NA	-2.58	2.00	2.06
22	5	604	CLA	C1B-C2B	2.58	1.49	1.43
21	4	618	CHL	C4C-C3C	2.58	1.49	1.45
22	5	608	CLA	C1B-C2B	2.58	1.49	1.43
22	V	611	CLA	C1B-C2B	2.58	1.49	1.43
21	8	608	CHL	C3D-C2D	2.58	1.46	1.39
22	7	617	CLA	C1B-C2B	2.58	1.49	1.43
22	V	614	CLA	C1B-C2B	2.58	1.49	1.43
22	5	606	CLA	C1B-C2B	2.58	1.49	1.43
22	V	613	CLA	C1B-C2B	2.58	1.49	1.43
22	B	826	CLA	C1B-C2B	2.58	1.49	1.43
22	B	816	CLA	C1B-C2B	2.58	1.49	1.43
22	8	614	CLA	C1B-C2B	2.58	1.49	1.43
22	A	843	CLA	C1B-C2B	2.57	1.49	1.43
22	6	603	CLA	C1B-C2B	2.57	1.49	1.43
22	9	603	CLA	C1B-C2B	2.57	1.49	1.43
22	K	201	CLA	C1B-C2B	2.57	1.49	1.43
22	1	611	CLA	C1B-C2B	2.57	1.49	1.43
22	B	815	CLA	C1B-C2B	2.57	1.49	1.43
22	3	612	CLA	C1B-C2B	2.57	1.49	1.43
22	F	303	CLA	C1B-C2B	2.57	1.49	1.43
22	1	603	CLA	C1B-C2B	2.57	1.49	1.43
22	A	840	CLA	C1B-C2B	2.57	1.49	1.43
22	B	812	CLA	C1B-C2B	2.57	1.49	1.43
21	1	601	CHL	MG-NA	-2.57	2.00	2.06
22	G	204	CLA	C1B-C2B	2.57	1.49	1.43
21	U	601	CHL	C1B-C2B	2.57	1.49	1.43
22	F	301	CLA	C1B-C2B	2.57	1.49	1.43
21	6	601	CHL	C3D-C2D	2.57	1.46	1.39
22	A	801	CLA	C1B-C2B	2.56	1.49	1.43
22	A	824	CLA	C1B-C2B	2.56	1.49	1.43
22	B	831	CLA	C1B-C2B	2.56	1.49	1.43
22	A	818	CLA	C1B-C2B	2.56	1.49	1.43
22	V	610	CLA	C1B-C2B	2.56	1.49	1.43
22	7	606	CLA	C3B-C4B	2.56	1.48	1.42
22	1	610	CLA	C1B-C2B	2.56	1.49	1.43
21	6	602	CHL	C4C-C3C	2.56	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	608	CHL	C3D-C2D	2.56	1.46	1.39
22	B	805	CLA	C1B-C2B	2.56	1.49	1.43
22	F	304	CLA	C1B-C2B	2.56	1.49	1.43
21	W	609	CHL	C1B-C2B	2.56	1.49	1.43
22	A	807	CLA	C1B-C2B	2.56	1.49	1.43
22	A	816	CLA	C1B-C2B	2.55	1.49	1.43
22	J	101	CLA	C1B-C2B	2.55	1.49	1.43
22	W	603	CLA	C1B-C2B	2.55	1.49	1.43
22	1	604	CLA	C1B-C2B	2.55	1.49	1.43
21	9	601	CHL	C4C-C3C	2.55	1.49	1.45
22	B	835	CLA	C3B-C4B	2.55	1.48	1.42
21	W	609	CHL	C4C-C3C	2.55	1.49	1.45
21	2	607	CHL	MG-NA	-2.55	2.00	2.06
22	A	841	CLA	C1B-C2B	2.55	1.49	1.43
22	2	604	CLA	C1B-C2B	2.55	1.49	1.43
22	3	609	CLA	C3B-C4B	2.54	1.48	1.42
22	A	831	CLA	C1B-C2B	2.54	1.49	1.43
22	U	611	CLA	C1B-C2B	2.54	1.49	1.43
22	B	835	CLA	C1B-C2B	2.54	1.49	1.43
22	A	839	CLA	C1B-C2B	2.54	1.49	1.43
22	2	611	CLA	C1B-C2B	2.54	1.49	1.43
22	A	806	CLA	C1B-C2B	2.54	1.49	1.43
22	W	610	CLA	C1B-C2B	2.54	1.49	1.43
22	U	612	CLA	C1B-C2B	2.54	1.49	1.43
22	W	614	CLA	C1B-C2B	2.54	1.49	1.43
21	V	601	CHL	C1B-C2B	2.54	1.49	1.43
22	1	608	CLA	C1B-C2B	2.53	1.49	1.43
22	2	612	CLA	C1B-C2B	2.53	1.49	1.43
21	4	607	CHL	C4C-C3C	2.53	1.49	1.45
21	U	609	CHL	MG-NA	-2.53	2.00	2.06
22	A	836	CLA	C1B-C2B	2.53	1.49	1.43
22	2	609	CLA	C1B-C2B	2.53	1.49	1.43
21	U	601	CHL	MG-NA	-2.53	2.00	2.06
22	B	821	CLA	C1B-C2B	2.53	1.49	1.43
21	8	618	CHL	C4C-C3C	2.53	1.49	1.45
22	A	845	CLA	C1B-C2B	2.53	1.49	1.43
22	A	816	CLA	C3B-C4B	2.53	1.48	1.42
22	9	609	CLA	C3D-C2D	2.52	1.46	1.39
22	B	811	CLA	C1B-C2B	2.52	1.49	1.43
22	A	813	CLA	C1B-C2B	2.52	1.49	1.43
23	2	619	LUT	C12-C13	-2.52	1.40	1.45
22	B	818	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	610	CLA	C1B-C2B	2.52	1.49	1.43
22	B	820	CLA	C1B-C2B	2.52	1.49	1.43
22	A	828	CLA	C1B-C2B	2.52	1.49	1.43
22	A	812	CLA	C1B-C2B	2.52	1.49	1.43
21	V	606	CHL	C1B-C2B	2.52	1.49	1.43
21	W	606	CHL	C1B-C2B	2.52	1.49	1.43
22	A	826	CLA	C1B-C2B	2.52	1.49	1.43
22	A	829	CLA	C1B-C2B	2.51	1.49	1.43
22	A	817	CLA	C1B-C2B	2.51	1.49	1.43
22	A	814	CLA	C1B-C2B	2.51	1.49	1.43
22	B	809	CLA	C1B-C2B	2.51	1.49	1.43
21	5	601	CHL	MG-NA	-2.51	2.00	2.06
22	A	808	CLA	C1B-C2B	2.50	1.49	1.43
22	A	811	CLA	C1B-C2B	2.50	1.49	1.43
21	9	606	CHL	C3D-C2D	2.50	1.46	1.39
21	3	608	CHL	C4B-NB	-2.50	1.34	1.37
22	B	827	CLA	C1B-C2B	2.50	1.49	1.43
22	A	809	CLA	C1B-C2B	2.50	1.49	1.43
21	V	609	CHL	C4C-C3C	2.50	1.49	1.45
22	W	602	CLA	C1B-C2B	2.49	1.49	1.43
22	V	604	CLA	C1B-C2B	2.49	1.49	1.43
22	2	603	CLA	C1B-C2B	2.49	1.49	1.43
22	B	814	CLA	C1B-C2B	2.49	1.49	1.43
21	6	602	CHL	MG-NA	-2.49	2.00	2.06
22	3	615	CLA	C1B-C2B	2.49	1.49	1.43
21	3	608	CHL	C3D-C2D	2.49	1.45	1.39
21	U	607	CHL	C4C-C3C	2.49	1.49	1.45
22	7	610	CLA	C1B-C2B	2.49	1.49	1.43
22	U	610	CLA	C1B-C2B	2.49	1.49	1.43
22	A	835	CLA	C1B-C2B	2.49	1.49	1.43
21	U	601	CHL	C4C-C3C	2.49	1.49	1.45
22	2	614	CLA	C1B-C2B	2.49	1.49	1.43
22	G	201	CLA	C1B-C2B	2.49	1.49	1.43
22	4	610	CLA	C1B-C2B	2.48	1.49	1.43
21	4	618	CHL	MG-NA	-2.48	2.00	2.06
21	6	601	CHL	MG-NA	-2.48	2.00	2.06
22	A	804	CLA	C1B-C2B	2.48	1.49	1.43
22	B	819	CLA	C1B-C2B	2.48	1.49	1.43
22	3	604	CLA	C1B-C2B	2.48	1.49	1.43
21	4	607	CHL	MG-NA	-2.48	2.00	2.06
22	5	610	CLA	C1B-C2B	2.48	1.49	1.43
22	K	203	CLA	C1B-C2B	2.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	2002	CLA	C1B-C2B	2.47	1.49	1.43
22	A	827	CLA	C1B-C2B	2.47	1.49	1.43
21	U	607	CHL	C1B-NB	-2.47	1.34	1.37
22	A	805	CLA	C1B-C2B	2.47	1.49	1.43
22	8	611	CLA	C1B-C2B	2.47	1.49	1.43
22	B	803	CLA	C1B-C2B	2.47	1.49	1.43
22	B	807	CLA	C1B-C2B	2.47	1.49	1.43
21	4	608	CHL	C3B-C4B	2.47	1.48	1.42
22	9	613	CLA	C1B-C2B	2.47	1.49	1.43
22	A	833	CLA	C1B-C2B	2.46	1.49	1.43
21	V	606	CHL	C4C-C3C	2.46	1.49	1.44
22	B	806	CLA	C1B-C2B	2.46	1.49	1.43
21	W	606	CHL	C4C-C3C	2.46	1.49	1.44
22	6	609	CLA	C1B-C2B	2.46	1.49	1.43
22	5	611	CLA	C1B-C2B	2.46	1.49	1.43
21	7	608	CHL	C3D-C2D	2.45	1.45	1.39
22	B	828	CLA	C1B-C2B	2.45	1.49	1.43
21	U	608	CHL	C1B-C2B	2.45	1.49	1.43
22	1	606	CLA	C1B-C2B	2.45	1.49	1.43
21	3	608	CHL	C3B-C4B	2.45	1.48	1.42
21	W	605	CHL	C4C-C3C	2.45	1.49	1.44
22	9	604	CLA	C1B-C2B	2.45	1.49	1.43
21	3	608	CHL	C1B-NB	-2.45	1.34	1.37
22	L	302	CLA	C1B-C2B	2.44	1.49	1.43
21	6	608	CHL	C4C-C3C	2.44	1.49	1.45
21	9	606	CHL	C4C-C3C	2.44	1.49	1.45
21	W	607	CHL	MG-NA	-2.44	2.00	2.06
21	9	606	CHL	C1B-NB	-2.44	1.34	1.37
22	3	603	CLA	C1B-C2B	2.44	1.49	1.43
22	9	612	CLA	C1B-C2B	2.44	1.49	1.43
22	A	823	CLA	C1B-C2B	2.43	1.49	1.43
21	V	606	CHL	MG-NA	-2.43	2.00	2.06
22	B	836	CLA	C1B-C2B	2.43	1.49	1.43
21	2	606	CHL	MG-NA	-2.43	2.00	2.06
22	A	820	CLA	C1B-C2B	2.43	1.49	1.43
22	B	839	CLA	C1B-C2B	2.42	1.49	1.43
23	2	619	LUT	C32-C33	-2.42	1.40	1.45
22	A	815	CLA	C1B-C2B	2.42	1.49	1.43
21	W	606	CHL	MG-NA	-2.42	2.00	2.06
22	W	611	CLA	C1B-C2B	2.42	1.49	1.43
22	B	830	CLA	C1B-C2B	2.42	1.48	1.43
21	V	601	CHL	MG-NA	-2.41	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	618	CHL	MG-NA	-2.41	2.00	2.06
22	B	817	CLA	C1B-C2B	2.41	1.48	1.43
22	B	824	CLA	C1B-C2B	2.41	1.48	1.43
21	U	606	CHL	MG-NA	-2.41	2.00	2.06
22	3	610	CLA	C1B-C2B	2.41	1.48	1.43
21	4	606	CHL	C1B-C2B	2.41	1.48	1.43
22	3	602	CLA	C1B-C2B	2.41	1.48	1.43
25	V	2623	NEX	C7-C8	-2.41	1.28	1.32
22	A	822	CLA	C1B-C2B	2.40	1.48	1.43
21	V	607	CHL	MG-NA	-2.40	2.00	2.06
21	7	608	CHL	MG-NA	-2.40	2.00	2.06
21	U	609	CHL	C4C-C3C	2.40	1.49	1.45
22	B	813	CLA	C1B-C2B	2.40	1.48	1.43
22	F	304	CLA	C4D-C3D	-2.40	1.47	1.50
22	A	803	CLA	C1B-C2B	2.40	1.48	1.43
21	U	605	CHL	C4C-C3C	2.40	1.49	1.44
22	3	607	CLA	C1B-C2B	2.40	1.48	1.43
21	9	608	CHL	C1B-NB	-2.40	1.34	1.37
21	6	618	CHL	MG-NA	-2.39	2.00	2.06
21	4	608	CHL	C4B-NB	-2.39	1.34	1.37
21	5	607	CHL	MG-NA	-2.39	2.00	2.06
21	9	601	CHL	C3D-C2D	2.39	1.45	1.39
22	B	834	CLA	C1B-C2B	2.39	1.48	1.43
22	A	810	CLA	C1B-C2B	2.39	1.48	1.43
22	L	303	CLA	C1B-C2B	2.38	1.48	1.43
21	8	608	CHL	C4C-C3C	2.38	1.49	1.45
21	U	605	CHL	MG-NA	-2.38	2.00	2.06
21	8	606	CHL	C1B-NB	-2.38	1.34	1.37
21	2	618	CHL	MG-NA	-2.38	2.00	2.06
22	A	802	CLA	C1B-C2B	2.38	1.48	1.43
21	9	608	CHL	MG-NA	-2.38	2.00	2.06
22	1	611	CLA	CHC-C1C	2.38	1.43	1.38
22	F	304	CLA	MG-NA	2.38	2.11	2.06
21	U	609	CHL	C1B-NB	-2.38	1.34	1.37
21	8	608	CHL	MG-NA	-2.38	2.00	2.06
21	8	607	CHL	MG-NA	-2.37	2.00	2.06
21	3	608	CHL	C1B-C2B	2.37	1.48	1.43
21	U	607	CHL	MG-NA	-2.37	2.00	2.06
22	9	610	CLA	C1B-C2B	2.37	1.48	1.43
21	W	605	CHL	MG-NA	-2.37	2.00	2.06
22	8	610	CLA	C1B-C2B	2.37	1.48	1.43
21	6	607	CHL	MG-NA	-2.37	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	854	CLA	C1B-C2B	2.37	1.48	1.43
22	7	610	CLA	CHC-C1C	2.36	1.43	1.38
22	1	611	CLA	CMC-C2C	-2.36	1.45	1.50
22	5	609	CLA	C4D-ND	-2.36	1.34	1.37
21	V	601	CHL	C1B-NB	-2.36	1.34	1.37
22	A	838	CLA	C1B-C2B	2.36	1.48	1.43
21	7	608	CHL	C4C-C3C	2.36	1.49	1.45
22	4	604	CLA	CHC-C1C	2.36	1.43	1.38
22	A	821	CLA	C1B-C2B	2.36	1.48	1.43
21	U	608	CHL	MG-NA	-2.36	2.00	2.06
21	1	601	CHL	C1B-NB	-2.35	1.34	1.37
21	W	608	CHL	C4C-C3C	2.35	1.49	1.44
22	9	609	CLA	MG-NA	-2.35	2.00	2.06
22	A	832	CLA	C1B-C2B	2.35	1.48	1.43
23	5	617	LUT	C12-C13	-2.34	1.40	1.45
22	A	843	CLA	CMD-C2D	-2.34	1.45	1.50
21	W	609	CHL	MG-NA	-2.34	2.00	2.06
21	4	618	CHL	C1B-C2B	2.34	1.48	1.43
21	9	606	CHL	C1B-C2B	2.34	1.48	1.43
21	W	601	CHL	C4C-C3C	2.34	1.49	1.45
21	2	618	CHL	C4C-C3C	2.34	1.49	1.45
21	4	606	CHL	MG-NA	-2.33	2.00	2.06
21	7	608	CHL	C1B-C2B	2.33	1.48	1.43
27	K	205	BCR	C30-C25	-2.33	1.50	1.53
21	4	606	CHL	C1B-NB	-2.33	1.34	1.37
21	6	608	CHL	MG-NA	-2.32	2.00	2.06
21	U	608	CHL	C4C-C3C	2.32	1.49	1.44
22	9	602	CLA	CMC-C2C	-2.32	1.45	1.50
21	V	605	CHL	MG-NA	-2.32	2.00	2.06
29	B	842	PQN	C11-C3	-2.31	1.47	1.51
21	6	608	CHL	C1B-C2B	2.31	1.48	1.43
21	9	605	CHL	MG-NA	-2.31	2.00	2.06
21	2	607	CHL	C4C-C3C	2.31	1.49	1.45
21	W	608	CHL	MG-NA	-2.31	2.00	2.06
21	8	607	CHL	C4C-C3C	2.31	1.49	1.45
22	8	611	CLA	CHC-C1C	2.31	1.43	1.38
21	V	608	CHL	C4C-C3C	2.30	1.49	1.44
22	B	838	CLA	C1B-C2B	2.30	1.48	1.43
21	6	606	CHL	C1B-C2B	2.30	1.48	1.43
21	V	608	CHL	MG-NA	-2.30	2.00	2.06
21	6	602	CHL	C1B-C2B	2.30	1.48	1.43
21	4	608	CHL	C4C-C3C	2.30	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	830	CLA	C1B-C2B	2.30	1.48	1.43
21	6	606	CHL	C4C-C3C	2.30	1.49	1.45
22	B	808	CLA	CMD-C2D	-2.30	1.45	1.50
22	8	609	CLA	CHC-C1C	2.29	1.43	1.38
22	A	819	CLA	C1B-C2B	2.29	1.48	1.43
22	V	611	CLA	CHC-C1C	2.29	1.43	1.38
22	A	821	CLA	CMB-C2B	-2.29	1.45	1.50
22	B	830	CLA	CHC-C1C	2.29	1.43	1.38
21	6	606	CHL	C1B-NB	-2.29	1.35	1.37
21	6	601	CHL	C4C-C3C	2.29	1.49	1.45
25	U	2623	NEX	O24-C25	-2.28	1.42	1.46
21	8	618	CHL	C1B-C2B	2.28	1.48	1.43
21	9	608	CHL	C4C-C3C	2.28	1.49	1.45
22	L	303	CLA	CHC-C1C	2.28	1.43	1.38
21	2	608	CHL	C1B-C2B	2.28	1.48	1.43
22	B	837	CLA	C1B-C2B	2.28	1.48	1.43
21	6	601	CHL	C1B-C2B	2.28	1.48	1.43
21	9	607	CHL	C1B-C2B	2.27	1.48	1.43
21	6	607	CHL	C4C-C3C	2.27	1.49	1.45
21	6	606	CHL	MG-NA	-2.27	2.00	2.06
27	A	851	BCR	C1-C6	-2.27	1.50	1.53
21	W	609	CHL	C1B-NB	-2.27	1.35	1.37
22	9	613	CLA	CMB-C2B	-2.27	1.46	1.50
22	3	602	CLA	CHC-C1C	2.26	1.43	1.38
21	5	607	CHL	C4C-C3C	2.26	1.48	1.45
21	2	606	CHL	C1B-NB	-2.26	1.35	1.37
22	B	811	CLA	CHC-C1C	2.26	1.43	1.38
21	8	606	CHL	C4C-C3C	2.26	1.48	1.45
22	7	609	CLA	C4D-ND	-2.26	1.34	1.37
21	V	605	CHL	C4C-C3C	2.26	1.48	1.45
22	B	829	CLA	CMB-C2B	-2.26	1.46	1.50
21	6	618	CHL	C1B-C2B	2.26	1.48	1.43
21	4	606	CHL	C4C-C3C	2.26	1.48	1.45
22	L	302	CLA	CMB-C2B	-2.25	1.46	1.50
21	9	601	CHL	C1B-C2B	2.25	1.48	1.43
21	4	618	CHL	C1B-NB	-2.25	1.35	1.37
21	W	608	CHL	C4B-NB	-2.25	1.35	1.37
21	2	618	CHL	C1B-NB	-2.25	1.35	1.37
21	V	605	CHL	C1B-C2B	2.25	1.48	1.43
22	B	813	CLA	CHC-C1C	2.25	1.43	1.38
21	2	601	CHL	C1B-C2B	2.25	1.48	1.43
22	9	611	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	608	CHL	C4B-NB	-2.25	1.35	1.37
22	A	832	CLA	CMB-C2B	-2.24	1.46	1.50
21	8	608	CHL	C1B-C2B	2.24	1.48	1.43
21	9	605	CHL	C1B-C2B	2.24	1.48	1.43
21	U	608	CHL	C1B-NB	-2.24	1.35	1.37
21	5	607	CHL	C1B-C2B	2.24	1.48	1.43
22	A	832	CLA	CHC-C1C	2.24	1.43	1.38
22	A	821	CLA	CMD-C2D	-2.24	1.46	1.50
22	B	830	CLA	CMB-C2B	-2.24	1.46	1.50
21	V	605	CHL	C1B-NB	-2.24	1.35	1.37
21	8	608	CHL	C1B-NB	-2.24	1.35	1.37
22	A	805	CLA	CHC-C1C	2.24	1.43	1.38
21	2	608	CHL	C4C-C3C	2.24	1.48	1.45
22	8	610	CLA	CHC-C1C	2.24	1.43	1.38
21	2	601	CHL	MG-NA	-2.23	2.01	2.06
22	7	611	CLA	CMD-C2D	-2.23	1.46	1.50
21	6	607	CHL	C1B-C2B	2.23	1.48	1.43
22	U	603	CLA	CMB-C2B	-2.23	1.46	1.50
22	9	609	CLA	C1B-C2B	2.23	1.48	1.43
21	5	601	CHL	C1B-C2B	2.23	1.48	1.43
21	W	607	CHL	C4B-NB	-2.23	1.35	1.37
21	1	607	CHL	C4C-C3C	2.23	1.48	1.45
22	B	827	CLA	CMD-C2D	-2.23	1.46	1.50
22	5	611	CLA	CMD-C2D	-2.23	1.46	1.50
22	B	814	CLA	CHC-C1C	2.22	1.43	1.38
22	W	611	CLA	CMB-C2B	-2.22	1.46	1.50
21	6	601	CHL	C1B-NB	-2.22	1.35	1.37
21	8	606	CHL	MG-NA	-2.22	2.01	2.06
21	V	606	CHL	C4B-NB	-2.22	1.35	1.37
22	A	841	CLA	CHC-C1C	2.22	1.43	1.38
21	V	607	CHL	C4B-NB	-2.22	1.35	1.37
22	A	836	CLA	MG-NB	-2.22	2.01	2.05
22	B	840	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	808	CLA	CMB-C2B	-2.22	1.46	1.50
21	W	606	CHL	C4B-NB	-2.21	1.35	1.37
22	B	808	CLA	CMC-C2C	-2.21	1.46	1.50
22	W	611	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	854	CLA	CMD-C2D	-2.21	1.46	1.50
21	8	607	CHL	C1B-C2B	2.21	1.48	1.43
22	A	801	CLA	CMD-C2D	-2.21	1.46	1.50
22	1	609	CLA	MG-NC	2.21	2.11	2.06
21	U	606	CHL	C1B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	607	CHL	C1B-C2B	2.21	1.48	1.43
22	A	828	CLA	CHC-C1C	2.21	1.43	1.38
22	7	603	CLA	CHC-C1C	2.21	1.43	1.38
22	B	803	CLA	CHC-C1C	2.21	1.43	1.38
22	B	817	CLA	CHC-C1C	2.21	1.43	1.38
21	2	602	CHL	C2C-C1C	2.21	1.49	1.44
21	U	601	CHL	C4B-C3B	2.21	1.48	1.43
22	6	603	CLA	CHC-C1C	2.21	1.43	1.38
23	5	617	LUT	C28-C29	-2.21	1.41	1.45
22	A	802	CLA	CMB-C2B	-2.20	1.46	1.50
21	1	607	CHL	C1B-C2B	2.20	1.48	1.43
21	V	607	CHL	C4C-C3C	2.20	1.48	1.44
21	W	607	CHL	C4B-C3B	2.20	1.48	1.43
22	5	613	CLA	CMB-C2B	-2.20	1.46	1.50
22	3	607	CLA	CHC-C1C	2.20	1.43	1.38
22	B	826	CLA	CHC-C1C	2.20	1.43	1.38
21	V	609	CHL	C1B-NB	-2.20	1.35	1.37
22	3	610	CLA	CHC-C1C	2.20	1.43	1.38
21	9	601	CHL	MG-NA	-2.20	2.01	2.06
22	V	602	CLA	CHC-C1C	2.20	1.43	1.38
22	7	617	CLA	CHC-C1C	2.20	1.43	1.38
22	B	838	CLA	CMD-C2D	-2.20	1.46	1.50
22	1	606	CLA	CHC-C1C	2.20	1.43	1.38
21	2	601	CHL	C4C-C3C	2.19	1.48	1.45
22	V	604	CLA	CMB-C2B	-2.19	1.46	1.50
21	U	601	CHL	C4B-NB	-2.19	1.35	1.37
21	9	607	CHL	C1B-NB	-2.19	1.35	1.37
22	W	611	CLA	CHC-C1C	2.19	1.43	1.38
22	A	822	CLA	CMB-C2B	-2.19	1.46	1.50
22	B	828	CLA	CMB-C2B	-2.19	1.46	1.50
22	7	611	CLA	CHC-C1C	2.19	1.43	1.38
22	2	611	CLA	CHC-C1C	2.19	1.43	1.38
21	4	607	CHL	C1B-NB	-2.19	1.35	1.37
21	6	607	CHL	C1B-NB	-2.19	1.35	1.37
22	4	614	CLA	CHC-C1C	2.19	1.43	1.38
21	W	607	CHL	C4C-C3C	2.19	1.48	1.44
22	9	609	CLA	C1C-C2C	2.19	1.48	1.44
22	3	615	CLA	CHC-C1C	2.19	1.43	1.38
22	U	602	CLA	CHC-C1C	2.19	1.43	1.38
22	B	820	CLA	CMD-C2D	-2.19	1.46	1.50
22	9	612	CLA	CMD-C2D	-2.18	1.46	1.50
21	W	601	CHL	C4B-NB	-2.18	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	604	CLA	CHC-C1C	2.18	1.43	1.38
21	V	601	CHL	C4B-C3B	2.18	1.48	1.43
22	A	843	CLA	CHC-C1C	2.18	1.43	1.38
22	3	609	CLA	CMB-C2B	-2.18	1.46	1.50
22	B	823	CLA	CHC-C1C	2.18	1.43	1.38
22	A	830	CLA	CMD-C2D	-2.18	1.46	1.50
22	B	819	CLA	CMB-C2B	-2.18	1.46	1.50
22	A	814	CLA	CHC-C1C	2.18	1.43	1.38
22	B	837	CLA	CHC-C1C	2.18	1.43	1.38
22	A	841	CLA	CMD-C2D	-2.18	1.46	1.50
22	V	614	CLA	CMD-C2D	-2.18	1.46	1.50
21	2	602	CHL	C4C-C3C	2.18	1.48	1.45
21	U	608	CHL	C4B-NB	-2.18	1.35	1.37
22	9	610	CLA	CHC-C1C	2.17	1.42	1.38
21	W	605	CHL	C4B-C3B	2.17	1.48	1.43
22	1	604	CLA	CMB-C2B	-2.17	1.46	1.50
22	O	2002	CLA	CHC-C1C	2.17	1.42	1.38
22	U	610	CLA	CHC-C1C	2.17	1.42	1.38
28	G	202	LMG	O1-C1	2.17	1.43	1.40
22	A	810	CLA	CHC-C1C	2.17	1.42	1.38
22	7	614	CLA	CHC-C1C	2.17	1.42	1.38
22	B	802	CLA	CHC-C1C	2.17	1.42	1.38
21	U	601	CHL	C1B-NB	-2.17	1.35	1.37
21	4	607	CHL	C1B-C2B	2.17	1.48	1.43
22	A	828	CLA	CMC-C2C	-2.17	1.46	1.50
22	B	809	CLA	CMB-C2B	-2.17	1.46	1.50
21	2	601	CHL	C1B-NB	-2.17	1.35	1.37
21	U	608	CHL	C4B-C3B	2.17	1.48	1.43
22	K	206	CLA	CHC-C1C	2.16	1.42	1.38
21	W	606	CHL	C4B-C3B	2.16	1.48	1.43
21	V	607	CHL	C4B-C3B	2.16	1.48	1.43
22	3	615	CLA	CMB-C2B	-2.16	1.46	1.50
22	A	830	CLA	CHC-C1C	2.16	1.42	1.38
22	B	809	CLA	CMD-C2D	-2.16	1.46	1.50
22	9	609	CLA	C1B-NB	-2.16	1.35	1.37
22	B	825	CLA	CMD-C2D	-2.16	1.46	1.50
21	V	609	CHL	C1B-C2B	2.16	1.48	1.43
21	5	607	CHL	C1B-NB	-2.16	1.35	1.37
22	A	824	CLA	CMD-C2D	-2.16	1.46	1.50
21	8	606	CHL	C1B-C2B	2.16	1.48	1.43
22	A	837	CLA	CHC-C1C	2.16	1.42	1.38
22	A	826	CLA	CMB-C2B	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	601	CHL	C4B-NB	-2.16	1.35	1.37
21	V	608	CHL	C4B-C3B	2.16	1.48	1.43
22	U	613	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	825	CLA	CHC-C1C	2.16	1.42	1.38
22	6	609	CLA	CHC-C1C	2.16	1.42	1.38
22	5	611	CLA	CHC-C1C	2.16	1.42	1.38
23	3	618	LUT	C22-C21	-2.16	1.52	1.54
21	9	606	CHL	MG-NA	-2.16	2.01	2.06
21	8	618	CHL	C1B-NB	-2.16	1.35	1.37
22	1	609	CLA	CHC-C1C	2.16	1.42	1.38
24	8	620	XAT	C12-C13	-2.16	1.41	1.45
22	5	612	CLA	CMD-C2D	-2.15	1.46	1.50
21	6	618	CHL	C1B-NB	-2.15	1.35	1.37
21	5	601	CHL	C4C-C3C	2.15	1.48	1.45
21	5	601	CHL	C1B-NB	-2.15	1.35	1.37
22	5	603	CLA	CMB-C2B	-2.15	1.46	1.50
22	8	613	CLA	CMB-C2B	-2.15	1.46	1.50
22	A	801	CLA	CMB-C2B	-2.15	1.46	1.50
21	W	609	CHL	C4B-NB	-2.15	1.35	1.37
21	2	606	CHL	C1B-C2B	2.15	1.48	1.43
22	W	602	CLA	CHC-C1C	2.15	1.42	1.38
21	1	601	CHL	C1B-C2B	2.15	1.48	1.43
22	B	824	CLA	CMD-C2D	-2.15	1.46	1.50
22	7	607	CLA	CHC-C1C	2.15	1.42	1.38
24	8	620	XAT	C8-C9	-2.14	1.41	1.45
22	J	101	CLA	CHC-C1C	2.14	1.42	1.38
22	B	802	CLA	CMD-C2D	-2.14	1.46	1.50
22	5	604	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	811	CLA	CMB-C2B	-2.14	1.46	1.50
22	6	614	CLA	CHC-C1C	2.14	1.42	1.38
22	7	609	CLA	CHC-C1C	2.14	1.42	1.38
24	1	618	XAT	O4-C5	-2.14	1.43	1.46
22	B	819	CLA	CHC-C1C	2.14	1.42	1.38
21	2	618	CHL	C1B-C2B	2.14	1.48	1.43
21	2	602	CHL	CHB-C4A	-2.14	1.32	1.37
22	B	814	CLA	CMD-C2D	-2.14	1.46	1.50
21	7	608	CHL	C1B-NB	-2.14	1.35	1.37
22	A	802	CLA	CMD-C2D	-2.14	1.46	1.50
22	5	614	CLA	CHC-C1C	2.14	1.42	1.38
22	3	606	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	831	CLA	CMB-C2B	-2.14	1.46	1.50
22	A	806	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	614	CLA	CHC-C1C	2.14	1.42	1.38
21	1	601	CHL	C4C-C3C	2.14	1.48	1.45
22	W	604	CLA	CMB-C2B	-2.13	1.46	1.50
22	9	610	CLA	CMB-C2B	-2.13	1.46	1.50
22	A	824	CLA	CHC-C1C	2.13	1.42	1.38
22	A	845	CLA	CMD-C2D	-2.13	1.46	1.50
22	2	610	CLA	CHC-C1C	2.13	1.42	1.38
22	A	819	CLA	CHC-C1C	2.13	1.42	1.38
22	6	612	CLA	CMB-C2B	-2.13	1.46	1.50
21	U	605	CHL	C4B-C3B	2.13	1.48	1.43
22	7	613	CLA	CMB-C2B	-2.13	1.46	1.50
22	4	610	CLA	CMD-C2D	-2.13	1.46	1.50
22	K	204	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	824	CLA	CMB-C2B	-2.13	1.46	1.50
22	5	602	CLA	CMD-C2D	-2.13	1.46	1.50
22	9	612	CLA	CHC-C1C	2.13	1.42	1.38
23	5	617	LUT	C32-C33	-2.13	1.41	1.45
22	A	837	CLA	CMB-C2B	-2.13	1.46	1.50
22	V	612	CLA	CHC-C1C	2.13	1.42	1.38
22	4	611	CLA	CHC-C1C	2.12	1.42	1.38
22	B	816	CLA	CMB-C2B	-2.12	1.46	1.50
22	8	603	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	808	CLA	CHC-C1C	2.12	1.42	1.38
22	B	811	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	836	CLA	CMD-C2D	-2.12	1.46	1.50
21	2	606	CHL	C4C-C3C	2.12	1.48	1.45
21	9	605	CHL	C4C-C3C	2.12	1.48	1.44
22	3	614	CLA	CHC-C1C	2.12	1.42	1.38
22	7	604	CLA	CHC-C1C	2.12	1.42	1.38
22	F	304	CLA	C2A-C3A	-2.12	1.54	1.57
22	3	615	CLA	CMD-C2D	-2.12	1.46	1.50
22	W	614	CLA	CMD-C2D	-2.12	1.46	1.50
22	4	610	CLA	CMB-C2B	-2.12	1.46	1.50
22	5	606	CLA	CHC-C1C	2.12	1.42	1.38
21	W	606	CHL	C1B-NB	-2.12	1.35	1.37
22	B	835	CLA	CMB-C2B	-2.12	1.46	1.50
22	W	614	CLA	CHC-C1C	2.12	1.42	1.38
22	1	608	CLA	CHC-C1C	2.12	1.42	1.38
22	B	822	CLA	CHC-C1C	2.12	1.42	1.38
21	8	606	CHL	C2C-C1C	2.12	1.49	1.44
22	4	613	CLA	CMB-C2B	-2.12	1.46	1.50
21	6	607	CHL	C2C-C1C	2.12	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	2001	CLA	CHC-C1C	2.12	1.42	1.38
22	B	825	CLA	CHC-C1C	2.12	1.42	1.38
22	B	820	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	823	CLA	CHC-C1C	2.12	1.42	1.38
22	1	613	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	805	CLA	CMD-C2D	-2.12	1.46	1.50
22	5	613	CLA	CMD-C2D	-2.12	1.46	1.50
22	7	602	CLA	CHC-C1C	2.12	1.42	1.38
22	9	611	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	819	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	833	CLA	CMD-C2D	-2.11	1.46	1.50
24	3	619	XAT	O4-C5	-2.11	1.43	1.46
21	V	606	CHL	C1B-NB	-2.11	1.35	1.37
21	2	607	CHL	C1B-NB	-2.11	1.35	1.37
22	3	606	CLA	CHC-C1C	2.11	1.42	1.38
22	1	602	CLA	CMD-C2D	-2.11	1.46	1.50
22	U	611	CLA	CHC-C1C	2.11	1.42	1.38
22	A	832	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	828	CLA	CHC-C1C	2.11	1.42	1.38
22	G	204	CLA	CHC-C1C	2.11	1.42	1.38
22	L	304	CLA	CMB-C2B	-2.11	1.46	1.50
22	A	836	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	832	CLA	CMB-C2B	-2.11	1.46	1.50
22	K	206	CLA	CMB-C2B	-2.11	1.46	1.50
21	W	601	CHL	C4B-C3B	2.11	1.48	1.43
22	U	610	CLA	CMD-C2D	-2.11	1.46	1.50
22	U	613	CLA	CHC-C1C	2.11	1.42	1.38
21	6	608	CHL	C1B-NB	-2.11	1.35	1.37
22	2	604	CLA	CMB-C2B	-2.11	1.46	1.50
22	B	833	CLA	CMB-C2B	-2.11	1.46	1.50
22	V	612	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	820	CLA	CHC-C1C	2.11	1.42	1.38
22	F	301	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	806	CLA	CHC-C1C	2.10	1.42	1.38
22	7	609	CLA	MG-NC	2.10	2.11	2.06
22	A	815	CLA	CHC-C1C	2.10	1.42	1.38
21	9	605	CHL	C1B-NB	-2.10	1.35	1.37
22	A	835	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	818	CLA	CHC-C1C	2.10	1.42	1.38
22	O	2003	CLA	CHC-C1C	2.10	1.42	1.38
21	9	601	CHL	C1B-NB	-2.10	1.35	1.37
22	A	842	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	605	CHL	C4B-NB	-2.10	1.35	1.37
22	A	824	CLA	CMB-C2B	-2.10	1.46	1.50
22	6	604	CLA	CHC-C1C	2.10	1.42	1.38
22	1	603	CLA	CMB-C2B	-2.10	1.46	1.50
22	U	604	CLA	CHC-C1C	2.10	1.42	1.38
22	V	614	CLA	CHC-C1C	2.10	1.42	1.38
22	3	603	CLA	CMB-C2B	-2.10	1.46	1.50
22	B	836	CLA	CHC-C1C	2.10	1.42	1.38
21	U	606	CHL	C2C-C1C	2.10	1.49	1.44
22	A	840	CLA	CMB-C2B	-2.09	1.46	1.50
21	9	607	CHL	C4C-C3C	2.09	1.48	1.45
21	W	601	CHL	C1B-NB	-2.09	1.35	1.37
22	4	601	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	803	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	805	CLA	CHC-C1C	2.09	1.42	1.38
22	U	603	CLA	CMD-C2D	-2.09	1.46	1.50
22	1	613	CLA	CMD-C2D	-2.09	1.46	1.50
22	4	603	CLA	CHC-C1C	2.09	1.42	1.38
22	A	813	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	608	CHL	C4C-C3C	2.09	1.48	1.45
21	8	607	CHL	C2C-C1C	2.09	1.49	1.44
22	9	612	CLA	CMC-C2C	-2.09	1.46	1.50
22	V	610	CLA	CHC-C1C	2.09	1.42	1.38
22	2	614	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	817	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	834	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	838	CLA	CHC-C1C	2.09	1.42	1.38
27	3	621	BCR	C30-C25	-2.09	1.50	1.53
25	U	2623	NEX	C1-C6	-2.09	1.51	1.54
22	2	611	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	833	CLA	CMB-C2B	-2.09	1.46	1.50
22	3	604	CLA	CMB-C2B	-2.09	1.46	1.50
22	B	809	CLA	CHC-C1C	2.09	1.42	1.38
22	A	812	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	829	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	836	CLA	CAC-C3C	-2.09	1.47	1.51
22	A	834	CLA	CMD-C2D	-2.09	1.46	1.50
22	K	201	CLA	CMD-C2D	-2.09	1.46	1.50
21	5	607	CHL	C2C-C1C	2.09	1.49	1.44
22	W	610	CLA	CHC-C1C	2.09	1.42	1.38
22	B	821	CLA	CHC-C1C	2.09	1.42	1.38
22	B	812	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	603	CLA	CMB-C2B	-2.09	1.46	1.50
21	1	607	CHL	C1B-NB	-2.09	1.35	1.37
22	A	842	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	854	CLA	CHC-C1C	2.09	1.42	1.38
22	B	815	CLA	CHC-C1C	2.09	1.42	1.38
22	A	826	CLA	CMD-C2D	-2.08	1.46	1.50
22	7	603	CLA	CMB-C2B	-2.08	1.46	1.50
22	W	613	CLA	CMB-C2B	-2.08	1.46	1.50
21	U	607	CHL	C1B-C2B	2.08	1.48	1.43
22	B	823	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	812	CLA	CMC-C2C	-2.08	1.46	1.50
22	1	602	CLA	CHC-C1C	2.08	1.42	1.38
22	B	807	CLA	CHC-C1C	2.08	1.42	1.38
22	A	807	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	828	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	833	CLA	CHC-C1C	2.08	1.42	1.38
22	A	834	CLA	CHC-C1C	2.08	1.42	1.38
22	L	303	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	839	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	835	CLA	CMB-C2B	-2.08	1.46	1.50
22	G	203	CLA	CHC-C1C	2.08	1.42	1.38
22	1	604	CLA	CHC-C1C	2.08	1.42	1.38
21	V	606	CHL	C4B-C3B	2.08	1.48	1.43
22	8	602	CLA	CMB-C2B	-2.08	1.46	1.50
22	V	604	CLA	CHC-C1C	2.08	1.42	1.38
22	5	616	CLA	CHC-C1C	2.08	1.42	1.38
21	U	606	CHL	C1B-C2B	2.08	1.48	1.43
22	A	812	CLA	CMB-C2B	-2.08	1.46	1.50
24	2	620	XAT	O4-C5	-2.08	1.43	1.46
22	3	613	CLA	CHC-C1C	2.08	1.42	1.38
22	K	203	CLA	CHC-C1C	2.08	1.42	1.38
22	2	610	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	807	CLA	CMD-C2D	-2.08	1.46	1.50
22	4	609	CLA	CHC-C1C	2.08	1.42	1.38
22	B	834	CLA	CHC-C1C	2.08	1.42	1.38
22	7	615	CLA	CHC-C1C	2.08	1.42	1.38
22	A	838	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	612	CLA	CMC-C2C	-2.07	1.46	1.50
22	4	609	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	818	CLA	CMB-C2B	-2.07	1.46	1.50
22	3	611	CLA	CHC-C1C	2.07	1.42	1.38
22	3	609	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	610	CLA	CMB-C2B	-2.07	1.46	1.50
22	4	602	CLA	CHC-C1C	2.07	1.42	1.38
22	A	820	CLA	CMB-C2B	-2.07	1.46	1.50
22	9	602	CLA	CMD-C2D	-2.07	1.46	1.50
22	2	614	CLA	CMB-C2B	-2.07	1.46	1.50
22	5	602	CLA	CHC-C1C	2.07	1.42	1.38
22	2	603	CLA	CMB-C2B	-2.07	1.46	1.50
22	6	603	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	838	CLA	CHC-C1C	2.07	1.42	1.38
22	3	610	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	829	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	813	CLA	CHC-C1C	2.07	1.42	1.38
22	5	610	CLA	CHC-C1C	2.07	1.42	1.38
22	A	808	CLA	CMB-C2B	-2.07	1.46	1.50
22	9	613	CLA	CMD-C2D	-2.07	1.46	1.50
21	U	605	CHL	C4B-NB	-2.07	1.35	1.37
22	1	612	CLA	CMD-C2D	-2.07	1.46	1.50
22	5	612	CLA	CMC-C2C	-2.07	1.46	1.50
22	9	604	CLA	CMB-C2B	-2.07	1.46	1.50
22	4	601	CLA	CHC-C1C	2.07	1.42	1.38
22	A	809	CLA	CHC-C1C	2.07	1.42	1.38
24	7	619	XAT	C8-C9	2.06	1.50	1.45
22	1	610	CLA	CHC-C1C	2.06	1.42	1.38
22	4	604	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	815	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	806	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	834	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	822	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	837	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	817	CLA	CMB-C2B	-2.06	1.46	1.50
22	L	302	CLA	CHC-C1C	2.06	1.42	1.38
22	8	604	CLA	CHC-C1C	2.06	1.42	1.38
22	4	611	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	840	CLA	CMB-C2B	-2.06	1.46	1.50
21	V	608	CHL	C1B-NB	-2.06	1.35	1.37
22	1	606	CLA	CMB-C2B	-2.06	1.46	1.50
22	9	613	CLA	CHC-C1C	2.06	1.42	1.38
22	1	609	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	806	CLA	CMB-C2B	-2.06	1.46	1.50
22	3	603	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	822	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	811	CLA	CHC-C1C	2.06	1.42	1.38
22	B	807	CLA	CMB-C2B	-2.06	1.46	1.50
22	H	201	CLA	CHC-C1C	2.06	1.42	1.38
22	A	805	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
22	8	612	CLA	CHC-C1C	2.05	1.42	1.38
22	1	603	CLA	CHC-C1C	2.05	1.42	1.38
22	B	826	CLA	CMB-C2B	-2.05	1.46	1.50
23	8	619	LUT	C22-C21	-2.05	1.52	1.54
21	2	602	CHL	C1B-C2B	2.05	1.48	1.43
22	1	614	CLA	CHC-C1C	2.05	1.42	1.38
22	3	613	CLA	CMD-C2D	-2.05	1.46	1.50
22	O	2003	CLA	C3C-C2C	2.05	1.39	1.35
22	B	838	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	814	CLA	CMC-C2C	-2.05	1.46	1.50
22	G	203	CLA	CMB-C2B	-2.05	1.46	1.50
22	8	603	CLA	CHC-C1C	2.05	1.42	1.38
22	F	304	CLA	MG-NC	2.05	2.11	2.06
22	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	818	CLA	CMD-C2D	-2.05	1.46	1.50
21	V	605	CHL	C2C-C1C	2.05	1.49	1.44
21	1	607	CHL	C2C-C1C	2.05	1.49	1.44
22	6	614	CLA	CMD-C2D	-2.05	1.46	1.50
22	U	604	CLA	CMB-C2B	-2.05	1.46	1.50
22	2	610	CLA	CMB-C2B	-2.05	1.46	1.50
22	8	601	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	832	CLA	CHC-C1C	2.05	1.42	1.38
22	V	613	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	854	CLA	CMB-C2B	-2.05	1.46	1.50
22	6	604	CLA	CMB-C2B	-2.05	1.46	1.50
22	W	603	CLA	CHC-C1C	2.05	1.42	1.38
22	3	607	CLA	CMB-C2B	-2.05	1.46	1.50
22	2	603	CLA	CHC-C1C	2.05	1.42	1.38
25	9	623	NEX	O24-C25	-2.04	1.43	1.46
22	A	827	CLA	CMB-C2B	-2.04	1.46	1.50
22	V	603	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	810	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	841	CLA	CMB-C2B	-2.04	1.46	1.50
21	9	608	CHL	C1B-C2B	2.04	1.48	1.43
21	4	606	CHL	C2C-C1C	2.04	1.49	1.44
22	A	817	CLA	CHC-C1C	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	841	CLA	CMD-C2D	-2.04	1.46	1.50
22	J	101	CLA	CMB-C2B	-2.04	1.46	1.50
22	W	603	CLA	CMB-C2B	-2.04	1.46	1.50
22	F	301	CLA	CMB-C2B	-2.04	1.46	1.50
22	7	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
22	W	602	CLA	CMB-C2B	-2.04	1.46	1.50
22	5	604	CLA	CHC-C1C	2.04	1.42	1.38
22	O	2001	CLA	C3C-C2C	2.04	1.39	1.35
22	8	609	CLA	CMC-C2C	-2.04	1.46	1.50
22	U	612	CLA	CMB-C2B	-2.04	1.46	1.50
22	F	301	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	827	CLA	CHC-C1C	2.04	1.42	1.38
22	A	815	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	823	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	839	CLA	CMD-C2D	-2.04	1.46	1.50
22	K	204	CLA	CMD-C2D	-2.04	1.46	1.50
22	7	612	CLA	CHC-C1C	2.04	1.42	1.38
21	8	606	CHL	CHB-C4A	-2.04	1.32	1.37
22	W	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	803	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	841	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
21	5	601	CHL	C2C-C1C	2.04	1.48	1.44
22	4	612	CLA	CMC-C2C	-2.04	1.46	1.50
22	5	608	CLA	CMB-C2B	-2.04	1.46	1.50
22	1	612	CLA	CHC-C1C	2.04	1.42	1.38
22	3	602	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	804	CLA	CMB-C2B	-2.04	1.46	1.50
22	1	602	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	843	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	802	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	803	CLA	CMD-C2D	-2.03	1.46	1.50
22	K	201	CLA	CMB-C2B	-2.03	1.46	1.50
22	3	612	CLA	CMB-C2B	-2.03	1.46	1.50
22	3	614	CLA	CMD-C2D	-2.03	1.46	1.50
21	U	609	CHL	C1B-C2B	2.03	1.48	1.43
22	A	809	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	836	CLA	CMB-C2B	-2.03	1.46	1.50
22	5	604	CLA	CMB-C2B	-2.03	1.46	1.50
22	7	612	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	810	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	812	CLA	CHC-C1C	2.03	1.42	1.38
22	A	828	CLA	CMD-C2D	-2.03	1.46	1.50
22	W	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	F	303	CLA	CMD-C2D	-2.03	1.46	1.50
21	1	601	CHL	C2C-C1C	2.03	1.48	1.44
22	A	828	CLA	CMB-C2B	-2.03	1.46	1.50
22	2	609	CLA	CHC-C1C	2.03	1.42	1.38
22	B	808	CLA	CHC-C1C	2.03	1.42	1.38
22	B	827	CLA	CHC-C1C	2.03	1.42	1.38
22	F	301	CLA	CHC-C1C	2.03	1.42	1.38
22	B	834	CLA	CMB-C2B	-2.03	1.46	1.50
22	9	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	8	603	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	832	CLA	CMC-C2C	-2.03	1.46	1.50
22	G	201	CLA	CMB-C2B	-2.03	1.46	1.50
22	K	206	CLA	CMD-C2D	-2.03	1.46	1.50
22	O	2002	CLA	CMD-C2D	-2.03	1.46	1.50
21	4	606	CHL	CHB-C4A	-2.03	1.32	1.37
22	B	826	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	824	CLA	CHC-C1C	2.03	1.42	1.38
21	W	607	CHL	C1B-NB	-2.02	1.35	1.37
22	J	101	CLA	CMD-C2D	-2.02	1.46	1.50
22	L	303	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	842	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	831	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	804	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	802	CLA	CMC-C2C	-2.02	1.46	1.50
22	2	613	CLA	CMB-C2B	-2.02	1.46	1.50
22	G	201	CLA	CHC-C1C	2.02	1.42	1.38
22	1	608	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	804	CLA	CHC-C1C	2.02	1.42	1.38
22	B	813	CLA	CMD-C2D	-2.02	1.46	1.50
22	6	611	CLA	CHC-C1C	2.02	1.42	1.38
22	V	604	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	5	609	CLA	MG-NA	2.02	2.11	2.06
22	B	813	CLA	CMB-C2B	-2.02	1.46	1.50
22	2	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	8	601	CLA	CHC-C1C	2.02	1.42	1.38
22	4	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	839	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	602	CLA	CMB-C2B	-2.02	1.46	1.50
22	4	603	CLA	CMB-C2B	-2.02	1.46	1.50
22	H	201	CLA	CMB-C2B	-2.02	1.46	1.50
21	U	606	CHL	C4C-C3C	2.02	1.48	1.45
22	7	611	CLA	CMB-C2B	-2.02	1.46	1.50
22	W	614	CLA	CMB-C2B	-2.02	1.46	1.50
22	5	606	CLA	CMC-C2C	-2.02	1.46	1.50
22	5	609	CLA	CMB-C2B	-2.02	1.46	1.50
22	3	612	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	821	CLA	CMB-C2B	-2.01	1.46	1.50
22	2	613	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	614	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	803	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	820	CLA	CHC-C1C	2.01	1.42	1.38
22	A	821	CLA	CHC-C1C	2.01	1.42	1.38
22	4	610	CLA	CHC-C1C	2.01	1.42	1.38
22	1	614	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	819	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	845	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	803	CLA	CMB-C2B	-2.01	1.46	1.50
22	K	201	CLA	CHC-C1C	2.01	1.42	1.38
22	G	201	CLA	CMD-C2D	-2.01	1.46	1.50
22	7	606	CLA	CHC-C1C	2.01	1.42	1.38
22	A	814	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	815	CLA	CMD-C2D	-2.01	1.46	1.50
22	2	612	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	805	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	816	CLA	CMD-C2D	-2.01	1.46	1.50
22	5	606	CLA	CMB-C2B	-2.01	1.46	1.50
22	6	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	8	601	CLA	CMB-C2B	-2.01	1.46	1.50
22	8	611	CLA	CMB-C2B	-2.01	1.46	1.50
22	5	608	CLA	CHC-C1C	2.01	1.42	1.38
22	W	604	CLA	CMD-C2D	-2.01	1.46	1.50
21	4	608	CHL	C1B-NB	-2.01	1.35	1.37
22	U	612	CLA	CMC-C2C	-2.01	1.46	1.50
22	U	614	CLA	CMB-C2B	-2.01	1.46	1.50
22	3	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	610	CLA	CMD-C2D	-2.01	1.46	1.50
22	9	602	CLA	CHC-C1C	2.01	1.42	1.38
22	A	843	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	302	CLA	CMD-C2D	-2.01	1.46	1.50
22	6	610	CLA	CMB-C2B	-2.01	1.46	1.50
22	W	604	CLA	CHC-C1C	2.01	1.42	1.38
21	9	608	CHL	C2C-C1C	2.01	1.48	1.44
22	A	813	CLA	CMB-C2B	-2.01	1.46	1.50
22	8	601	CLA	CMC-C2C	-2.01	1.46	1.50
22	B	831	CLA	CMD-C2D	-2.01	1.46	1.50
22	5	616	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	816	CLA	CMB-C2B	-2.01	1.46	1.50
21	2	606	CHL	C2C-C1C	2.01	1.48	1.44
22	1	613	CLA	CHC-C1C	2.01	1.42	1.38
22	8	609	CLA	CMB-C2B	-2.00	1.46	1.50
22	F	304	CLA	CMD-C2D	-2.00	1.46	1.50
22	1	608	CLA	CMB-C2B	-2.00	1.46	1.50
21	V	607	CHL	C1B-NB	-2.00	1.35	1.37
22	A	818	CLA	CMB-C2B	-2.00	1.46	1.50
22	3	617	CLA	C4C-NC	2.00	1.40	1.37
22	B	837	CLA	CMB-C2B	-2.00	1.46	1.50
24	2	620	XAT	O24-C25	-2.00	1.43	1.46
22	U	604	CLA	CMD-C2D	-2.00	1.46	1.50
21	2	608	CHL	C2C-C1C	2.00	1.48	1.44
22	4	612	CLA	CMB-C2B	-2.00	1.46	1.50
22	A	812	CLA	CHC-C1C	2.00	1.42	1.38
22	B	816	CLA	CHC-C1C	2.00	1.42	1.38

All (3774) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	V	2622	XAT	O4-C5-C4	-29.06	91.55	113.38
24	4	620	XAT	O4-C5-C4	-27.98	92.37	113.38
24	6	620	XAT	O4-C5-C4	-26.00	93.85	113.38
24	7	619	XAT	O24-C25-C24	-25.27	94.40	113.38
24	6	620	XAT	O24-C25-C24	-22.02	96.84	113.38
24	7	619	XAT	O4-C5-C4	-21.43	97.29	113.38
24	7	619	XAT	O4-C5-C18	-20.33	90.69	115.06
24	6	620	XAT	O4-C5-C18	-18.63	92.74	115.06
24	6	620	XAT	O24-C25-C38	-18.60	92.77	115.06
24	7	619	XAT	O24-C25-C38	-17.52	94.06	115.06
24	4	620	XAT	O4-C5-C18	-17.24	94.41	115.06
24	V	2622	XAT	O4-C5-C18	-16.18	95.67	115.06
23	9	624	LUT	C37-C21-C36	-14.07	87.15	107.89
24	V	2622	XAT	C17-C1-C16	-13.85	86.95	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	620	XAT	C37-C21-C36	-13.44	87.54	107.37
22	3	617	CLA	C1C-C2C-C3C	-12.59	105.61	110.89
24	6	620	XAT	C37-C21-C22	-12.46	87.34	108.98
24	V	2622	XAT	C17-C1-C2	-12.35	87.52	108.98
27	B	1609	BCR	C40-C30-C25	-12.32	90.31	110.30
25	U	2623	NEX	O24-C25-C24	12.24	122.58	113.38
27	4	621	BCR	C40-C30-C25	-11.75	91.23	110.30
24	U	2622	XAT	O4-C5-C4	11.36	121.91	113.38
24	3	619	XAT	O4-C5-C4	10.71	121.42	113.38
25	V	2623	NEX	O24-C25-C24	10.43	121.22	113.38
24	W	2622	XAT	O4-C5-C4	10.36	121.17	113.38
24	2	620	XAT	O4-C5-C4	10.20	121.04	113.38
21	4	606	CHL	C2B-C1B-NB	9.98	116.92	110.23
27	4	621	BCR	C39-C30-C25	9.89	126.34	110.30
21	2	602	CHL	C2B-C1B-NB	9.58	116.66	110.23
23	9	624	LUT	C37-C21-C22	-9.55	91.35	109.44
21	U	606	CHL	C2B-C1B-NB	9.50	116.60	110.23
21	6	602	CHL	C2B-C1B-NB	9.40	116.53	110.23
24	V	2622	XAT	O24-C25-C24	9.36	120.41	113.38
21	V	605	CHL	C2B-C1B-NB	9.34	116.50	110.23
21	6	607	CHL	C2B-C1B-NB	9.34	116.49	110.23
21	8	608	CHL	C2B-C1B-NB	9.32	116.48	110.23
21	9	605	CHL	C2B-C1B-NB	9.31	116.47	110.23
21	V	601	CHL	C2B-C1B-NB	9.31	116.47	110.23
21	8	606	CHL	C2B-C1B-NB	9.28	116.45	110.23
21	1	601	CHL	C2B-C1B-NB	9.24	116.43	110.23
21	8	607	CHL	C2B-C1B-NB	9.24	116.42	110.23
21	2	606	CHL	C2B-C1B-NB	9.22	116.41	110.23
21	6	608	CHL	C2B-C1B-NB	9.16	116.37	110.23
22	9	609	CLA	CMD-C2D-C1D	9.15	140.84	124.71
21	5	607	CHL	C2B-C1B-NB	9.15	116.36	110.23
21	6	601	CHL	C2B-C1B-NB	9.14	116.36	110.23
21	U	607	CHL	C2B-C1B-NB	9.13	116.35	110.23
21	2	618	CHL	C2B-C1B-NB	9.11	116.34	110.23
21	2	601	CHL	C2B-C1B-NB	9.10	116.33	110.23
22	9	609	CLA	C2B-C1B-NB	9.10	116.33	110.23
21	9	606	CHL	C2B-C1B-NB	9.09	116.33	110.23
21	9	605	CHL	C1D-ND-C4D	-9.09	99.88	106.33
21	3	608	CHL	C2B-C1B-NB	9.09	116.32	110.23
21	6	618	CHL	C2B-C1B-NB	9.08	116.32	110.23
21	5	601	CHL	C2B-C1B-NB	9.08	116.32	110.23
21	6	606	CHL	C2B-C1B-NB	9.08	116.32	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	U	606	CHL	C1D-ND-C4D	-9.04	99.91	106.33
21	8	618	CHL	C2B-C1B-NB	9.04	116.29	110.23
21	2	607	CHL	C2B-C1B-NB	9.02	116.28	110.23
21	W	609	CHL	C2B-C1B-NB	8.98	116.25	110.23
23	9	624	LUT	C37-C21-C26	-8.94	96.00	109.55
21	6	602	CHL	C1D-ND-C4D	-8.94	99.99	106.33
21	W	605	CHL	C2B-C1B-NB	8.93	116.22	110.23
25	9	623	NEX	O24-C25-C24	8.92	120.08	113.38
21	V	607	CHL	C2B-C1B-NB	8.92	116.21	110.23
21	U	601	CHL	C2B-C1B-NB	8.88	116.19	110.23
21	7	608	CHL	C2B-C1B-NB	8.88	116.19	110.23
21	U	605	CHL	C2B-C1B-NB	8.88	116.18	110.23
21	1	607	CHL	C2B-C1B-NB	8.87	116.18	110.23
21	W	607	CHL	C2B-C1B-NB	8.85	116.17	110.23
21	W	606	CHL	C2B-C1B-NB	8.85	116.17	110.23
21	V	608	CHL	C2B-C1B-NB	8.85	116.16	110.23
21	V	605	CHL	C1D-ND-C4D	-8.84	100.05	106.33
21	U	609	CHL	C1D-ND-C4D	-8.84	100.05	106.33
21	2	606	CHL	C1D-ND-C4D	-8.84	100.06	106.33
21	7	608	CHL	CMD-C2D-C1D	8.83	140.28	124.71
21	6	606	CHL	C1D-ND-C4D	-8.83	100.06	106.33
21	6	608	CHL	C1D-ND-C4D	-8.79	100.09	106.33
21	2	601	CHL	CMD-C2D-C1D	8.79	140.20	124.71
21	9	601	CHL	CMD-C2D-C1D	8.77	140.17	124.71
21	U	608	CHL	C2B-C1B-NB	8.77	116.11	110.23
21	9	601	CHL	C2B-C1B-NB	8.76	116.10	110.23
21	U	609	CHL	CMD-C2D-C1D	8.75	140.14	124.71
21	9	606	CHL	CMD-C2D-C1D	8.75	140.13	124.71
21	V	609	CHL	C1D-ND-C4D	-8.74	100.12	106.33
21	V	609	CHL	C2B-C1B-NB	8.74	116.09	110.23
21	2	602	CHL	C1D-ND-C4D	-8.74	100.13	106.33
21	9	605	CHL	CMD-C2D-C1D	8.73	140.09	124.71
24	V	2622	XAT	C16-C1-C2	8.72	124.13	108.98
21	4	607	CHL	C2B-C1B-NB	8.69	116.06	110.23
21	W	609	CHL	C1D-ND-C4D	-8.69	100.16	106.33
21	9	607	CHL	C2B-C1B-NB	8.69	116.06	110.23
21	7	608	CHL	C1D-ND-C4D	-8.68	100.17	106.33
21	2	607	CHL	CMD-C2D-C1D	8.67	139.99	124.71
21	8	607	CHL	C1D-ND-C4D	-8.66	100.19	106.33
22	9	609	CLA	C1D-ND-C4D	-8.65	100.19	106.33
21	8	608	CHL	C1D-ND-C4D	-8.64	100.20	106.33
21	V	607	CHL	C1D-ND-C4D	-8.64	100.20	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	601	CHL	C2B-C1B-NB	8.64	116.02	110.23
21	5	607	CHL	C1D-ND-C4D	-8.63	100.20	106.33
21	2	618	CHL	CMD-C2D-C1D	8.62	139.91	124.71
21	4	606	CHL	C1D-ND-C4D	-8.62	100.21	106.33
21	2	608	CHL	C2B-C1B-NB	8.62	116.01	110.23
21	6	601	CHL	C1D-ND-C4D	-8.61	100.22	106.33
21	V	609	CHL	CMD-C2D-C1D	8.61	139.88	124.71
21	6	607	CHL	C1D-ND-C4D	-8.60	100.23	106.33
21	2	607	CHL	C1D-ND-C4D	-8.58	100.24	106.33
21	W	607	CHL	C1D-ND-C4D	-8.54	100.27	106.33
21	U	607	CHL	C1D-ND-C4D	-8.53	100.27	106.33
21	6	601	CHL	CMD-C2D-C1D	8.52	139.74	124.71
21	W	608	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	2	601	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	9	608	CHL	C1D-ND-C4D	-8.52	100.28	106.33
21	3	608	CHL	CMD-C2D-C1D	8.52	139.72	124.71
21	W	601	CHL	C1D-ND-C4D	-8.51	100.29	106.33
21	W	606	CHL	CMD-C2D-C1D	8.51	139.71	124.71
21	8	608	CHL	CMD-C2D-C1D	8.51	139.71	124.71
21	U	609	CHL	C2B-C1B-NB	8.49	115.93	110.23
21	U	606	CHL	CMD-C2D-C1D	8.49	139.68	124.71
21	2	618	CHL	C1D-ND-C4D	-8.49	100.31	106.33
21	8	607	CHL	CMD-C2D-C1D	8.49	139.67	124.71
21	U	605	CHL	C1D-ND-C4D	-8.48	100.31	106.33
21	5	601	CHL	C1D-ND-C4D	-8.47	100.32	106.33
21	4	607	CHL	CMD-C2D-C1D	8.46	139.62	124.71
21	6	608	CHL	CMD-C2D-C1D	8.45	139.60	124.71
21	9	606	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	8	618	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	4	607	CHL	C1D-ND-C4D	-8.44	100.34	106.33
21	8	606	CHL	C1D-ND-C4D	-8.42	100.35	106.33
21	2	608	CHL	CMD-C2D-C1D	8.41	139.54	124.71
21	4	608	CHL	C2B-C1B-NB	8.41	115.87	110.23
21	9	601	CHL	C1D-ND-C4D	-8.40	100.37	106.33
21	1	601	CHL	CMD-C2D-C1D	8.40	139.51	124.71
21	V	606	CHL	C2B-C1B-NB	8.40	115.86	110.23
21	W	607	CHL	CMD-C2D-C1D	8.39	139.50	124.71
21	W	606	CHL	C1D-ND-C4D	-8.39	100.38	106.33
21	V	601	CHL	CMD-C2D-C1D	8.37	139.47	124.71
21	4	618	CHL	C1D-ND-C4D	-8.37	100.39	106.33
21	V	608	CHL	CMD-C2D-C1D	8.37	139.46	124.71
21	W	609	CHL	CMD-C2D-C1D	8.36	139.46	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	608	CHL	CMD-C2D-C1D	8.36	139.45	124.71
21	4	608	CHL	CMD-C2D-C1D	8.36	139.45	124.71
21	8	606	CHL	CMD-C2D-C1D	8.35	139.43	124.71
21	W	601	CHL	CMD-C2D-C1D	8.34	139.41	124.71
21	4	606	CHL	CMD-C2D-C1D	8.34	139.41	124.71
21	9	607	CHL	C1D-ND-C4D	-8.34	100.41	106.33
21	W	605	CHL	C1D-ND-C4D	-8.33	100.41	106.33
21	U	605	CHL	CMD-C2D-C1D	8.33	139.40	124.71
21	2	606	CHL	CMD-C2D-C1D	8.33	139.40	124.71
21	2	608	CHL	C1D-ND-C4D	-8.33	100.42	106.33
21	1	607	CHL	CMD-C2D-C1D	8.33	139.39	124.71
21	W	605	CHL	CMD-C2D-C1D	8.33	139.39	124.71
21	V	608	CHL	C1D-ND-C4D	-8.32	100.42	106.33
21	U	601	CHL	CMD-C2D-C1D	8.32	139.38	124.71
21	6	618	CHL	C1D-ND-C4D	-8.32	100.43	106.33
21	V	605	CHL	CMD-C2D-C1D	8.31	139.36	124.71
21	6	607	CHL	CMD-C2D-C1D	8.30	139.35	124.71
21	6	606	CHL	CMD-C2D-C1D	8.28	139.30	124.71
21	8	618	CHL	CMD-C2D-C1D	8.27	139.28	124.71
21	U	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
21	V	607	CHL	CMD-C2D-C1D	8.26	139.27	124.71
21	1	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
21	6	602	CHL	CMD-C2D-C1D	8.26	139.26	124.71
21	4	608	CHL	C1D-ND-C4D	-8.25	100.47	106.33
21	U	608	CHL	CMD-C2D-C1D	8.22	139.21	124.71
21	9	608	CHL	CMD-C2D-C1D	8.18	139.14	124.71
21	U	607	CHL	CMD-C2D-C1D	8.17	139.12	124.71
21	9	608	CHL	C2B-C1B-NB	8.17	115.71	110.23
21	V	606	CHL	C1D-ND-C4D	-8.16	100.53	106.33
21	5	607	CHL	CMD-C2D-C1D	8.16	139.10	124.71
24	6	620	XAT	C36-C21-C22	8.14	123.13	108.98
21	V	601	CHL	C1D-ND-C4D	-8.14	100.55	106.33
21	1	607	CHL	C1D-ND-C4D	-8.13	100.56	106.33
21	U	608	CHL	C1D-ND-C4D	-8.13	100.56	106.33
21	6	618	CHL	CMD-C2D-C1D	8.10	138.99	124.71
21	5	601	CHL	CMD-C2D-C1D	8.10	138.98	124.71
21	4	618	CHL	C2B-C1B-NB	8.03	115.62	110.23
21	2	602	CHL	CMD-C2D-C1D	7.99	138.80	124.71
24	3	619	XAT	C18-C5-C6	-7.90	109.02	122.26
21	6	608	CHL	C2C-C3C-C4C	-7.90	100.86	106.49
21	4	618	CHL	CMD-C2D-C1D	7.90	138.64	124.71
21	9	607	CHL	CMD-C2D-C1D	7.87	138.58	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	608	CHL	C1D-ND-C4D	-7.83	100.77	106.33
21	8	608	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
22	F	304	CLA	C4D-ND-C1D	-7.74	103.37	112.85
21	6	602	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
21	W	608	CHL	C2B-C1B-NB	7.71	115.40	110.23
21	U	607	CHL	C2C-C3C-C4C	-7.71	101.00	106.49
21	4	606	CHL	C2C-C3C-C4C	-7.69	101.01	106.49
21	V	606	CHL	CMD-C2D-C1D	7.67	138.24	124.71
21	4	618	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
21	2	602	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
27	3	621	BCR	C38-C26-C25	-7.52	116.08	124.53
21	U	606	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
21	2	608	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
21	2	607	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
21	2	601	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
23	9	624	LUT	C36-C21-C26	7.39	120.75	109.55
21	6	618	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
27	B	1609	BCR	C39-C30-C25	7.33	122.19	110.30
27	L	301	BCR	C37-C22-C21	-7.33	112.66	122.92
24	W	2622	XAT	O24-C25-C24	7.32	118.88	113.38
21	6	607	CHL	C2C-C3C-C4C	-7.30	101.29	106.49
21	5	607	CHL	C2C-C3C-C4C	-7.29	101.30	106.49
27	6	621	BCR	C7-C8-C9	-7.28	115.23	126.23
27	8	621	BCR	C7-C8-C9	-7.26	115.27	126.23
21	2	618	CHL	C2C-C3C-C4C	-7.26	101.32	106.49
21	6	606	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
21	V	607	CHL	C2C-C3C-C4C	-7.24	101.11	106.49
21	8	607	CHL	C2C-C3C-C4C	-7.23	101.34	106.49
21	6	601	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
21	W	609	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
21	V	605	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
21	W	607	CHL	C2C-C3C-C4C	-7.20	101.14	106.49
21	8	618	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	U	609	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	1	607	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
21	9	608	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
21	V	609	CHL	C2C-C3C-C4C	-7.17	101.38	106.49
21	1	601	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
21	U	606	CHL	C2D-C1D-ND	7.12	115.35	110.10
21	2	606	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
21	U	608	CHL	C2C-C3C-C4C	-7.10	101.22	106.49
21	9	606	CHL	C2C-C3C-C4C	-7.10	101.43	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	606	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
21	4	608	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	5	601	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	9	601	CHL	C2C-C3C-C4C	-7.09	101.43	106.49
21	7	608	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
21	V	608	CHL	C2C-C3C-C4C	-7.04	101.26	106.49
27	B	1609	BCR	C40-C30-C39	-7.04	86.93	108.53
21	9	605	CHL	C2C-C3C-C4C	-7.03	101.27	106.49
24	U	2622	XAT	O24-C25-C24	7.03	118.66	113.38
24	2	620	XAT	O24-C25-C24	7.02	118.66	113.38
21	6	602	CHL	C2D-C1D-ND	6.99	115.26	110.10
21	4	607	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
21	W	608	CHL	C2C-C3C-C4C	-6.95	101.33	106.49
21	6	608	CHL	C2D-C1D-ND	6.90	115.19	110.10
21	2	606	CHL	C2D-C1D-ND	6.87	115.17	110.10
21	9	605	CHL	C2D-C1D-ND	6.86	115.16	110.10
21	V	601	CHL	C1B-C2B-C3B	-6.86	100.52	107.03
24	5	618	XAT	O4-C5-C4	6.85	118.53	113.38
21	8	608	CHL	C2D-C1D-ND	6.83	115.14	110.10
21	4	618	CHL	C2D-C1D-ND	6.83	115.14	110.10
27	1	619	BCR	C27-C26-C25	-6.79	112.87	122.73
21	5	601	CHL	C2D-C1D-ND	6.79	115.11	110.10
21	V	607	CHL	C2D-C1D-ND	6.77	115.09	110.10
21	V	605	CHL	C2D-C1D-ND	6.77	115.09	110.10
21	U	605	CHL	C4C-C3C-C2C	-6.76	100.87	107.07
21	W	605	CHL	C1B-C2B-C3B	-6.76	100.61	107.03
21	4	606	CHL	C2D-C1D-ND	6.74	115.07	110.10
21	U	601	CHL	C1B-C2B-C3B	-6.73	100.64	107.03
21	6	606	CHL	C2D-C1D-ND	6.73	115.06	110.10
21	W	607	CHL	C1B-C2B-C3B	-6.72	100.65	107.03
21	U	605	CHL	C1B-C2B-C3B	-6.72	100.65	107.03
21	W	605	CHL	C4C-C3C-C2C	-6.71	100.91	107.07
21	2	602	CHL	C2D-C1D-ND	6.71	115.05	110.10
21	W	607	CHL	C2D-C1D-ND	6.70	115.04	110.10
21	W	609	CHL	C2D-C1D-ND	6.70	115.04	110.10
21	V	607	CHL	C1B-C2B-C3B	-6.70	100.67	107.03
21	U	609	CHL	C2D-C1D-ND	6.69	115.03	110.10
21	V	606	CHL	C4C-C3C-C2C	-6.69	100.94	107.07
21	6	607	CHL	C2D-C1D-ND	6.68	115.03	110.10
21	3	608	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
21	U	607	CHL	C2D-C1D-ND	6.67	115.02	110.10
21	2	607	CHL	C2D-C1D-ND	6.67	115.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	608	CHL	C1B-C2B-C3B	-6.67	100.70	107.03
21	2	601	CHL	C2D-C1D-ND	6.66	115.01	110.10
21	V	609	CHL	C2D-C1D-ND	6.65	115.01	110.10
21	6	601	CHL	C2D-C1D-ND	6.65	115.00	110.10
21	8	607	CHL	C2D-C1D-ND	6.64	114.99	110.10
21	W	601	CHL	C1B-C2B-C3B	-6.63	100.73	107.03
21	W	606	CHL	C4C-C3C-C2C	-6.63	100.99	107.07
21	9	607	CHL	C2D-C1D-ND	6.63	114.99	110.10
21	5	607	CHL	C2D-C1D-ND	6.62	114.98	110.10
24	4	620	XAT	O24-C25-C24	6.62	118.36	113.38
21	9	605	CHL	CHD-C1D-ND	-6.59	118.40	124.45
21	U	605	CHL	C2D-C1D-ND	6.59	114.96	110.10
21	7	608	CHL	C2D-C1D-ND	6.59	114.96	110.10
21	W	601	CHL	C2D-C1D-ND	6.58	114.95	110.10
27	K	205	BCR	C33-C5-C6	-6.57	117.14	124.53
25	W	2623	NEX	C35-C34-C33	-6.56	117.95	127.31
21	V	608	CHL	C2D-C1D-ND	6.56	114.94	110.10
21	6	618	CHL	C2D-C1D-ND	6.54	114.93	110.10
21	9	606	CHL	C2D-C1D-ND	6.54	114.92	110.10
21	8	606	CHL	C2D-C1D-ND	6.52	114.91	110.10
21	W	606	CHL	C1B-C2B-C3B	-6.51	100.85	107.03
21	V	605	CHL	O2D-CGD-CBD	6.50	122.83	111.27
21	4	608	CHL	C2D-C1D-ND	6.50	114.90	110.10
21	U	601	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	V	606	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	W	608	CHL	C2D-C1D-ND	6.50	114.89	110.10
21	2	608	CHL	C2D-C1D-ND	6.48	114.88	110.10
21	2	618	CHL	C2D-C1D-ND	6.48	114.88	110.10
27	A	852	BCR	C32-C1-C6	6.47	120.80	110.30
21	1	601	CHL	C2D-C1D-ND	6.46	114.86	110.10
21	8	618	CHL	C2D-C1D-ND	6.45	114.86	110.10
21	V	609	CHL	CHD-C1D-ND	-6.43	118.54	124.45
21	W	605	CHL	C2D-C1D-ND	6.43	114.84	110.10
21	2	607	CHL	CHD-C1D-ND	-6.42	118.55	124.45
21	V	606	CHL	C1B-C2B-C3B	-6.40	100.95	107.03
21	9	608	CHL	C2D-C1D-ND	6.39	114.81	110.10
21	4	607	CHL	C2D-C1D-ND	6.38	114.81	110.10
27	L	301	BCR	C23-C24-C25	-6.38	109.28	127.20
21	2	602	CHL	CHD-C1D-ND	-6.36	118.61	124.45
27	7	621	BCR	C28-C27-C26	-6.36	102.73	114.08
21	W	606	CHL	CHD-C1D-ND	-6.35	118.61	124.45
21	9	607	CHL	CHD-C1D-ND	-6.35	118.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	607	CHL	CHD-C1D-ND	-6.35	118.62	124.45
21	W	601	CHL	CHD-C1D-ND	-6.34	118.63	124.45
21	U	608	CHL	C1B-C2B-C3B	-6.33	101.02	107.03
21	6	601	CHL	CHD-C1D-ND	-6.32	118.64	124.45
21	4	618	CHL	CHD-C1D-ND	-6.31	118.65	124.45
21	8	607	CHL	CHD-C1D-ND	-6.29	118.67	124.45
21	V	601	CHL	C2D-C1D-ND	6.29	114.74	110.10
21	U	605	CHL	CHD-C1D-ND	-6.28	118.69	124.45
21	U	606	CHL	CHD-C1D-ND	-6.27	118.69	124.45
21	W	606	CHL	C2D-C1D-ND	6.27	114.72	110.10
27	B	845	BCR	C37-C22-C21	-6.26	114.15	122.92
21	W	605	CHL	CHD-C1D-ND	-6.26	118.70	124.45
22	9	609	CLA	CHD-C1D-ND	-6.26	118.70	124.45
21	9	607	CHL	C2C-C3C-C4C	-6.26	102.03	106.49
21	6	602	CHL	CHD-C1D-ND	-6.25	118.71	124.45
25	W	2623	NEX	O24-C25-C24	6.25	118.08	113.38
21	4	608	CHL	CHD-C1D-ND	-6.25	118.71	124.45
22	A	832	CLA	C4A-NA-C1A	6.25	109.51	106.71
21	U	609	CHL	CHD-C1D-ND	-6.24	118.72	124.45
21	U	608	CHL	C2D-C1D-ND	6.22	114.69	110.10
21	1	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
22	9	609	CLA	C2D-C1D-ND	6.21	114.68	110.10
21	W	608	CHL	C1B-C2B-C3B	-6.20	101.14	107.03
25	W	2623	NEX	C31-C30-C29	-6.19	118.47	127.31
21	1	607	CHL	C2D-C1D-ND	6.19	114.66	110.10
21	V	607	CHL	CHD-C1D-ND	-6.19	118.77	124.45
21	2	608	CHL	CHD-C1D-ND	-6.18	118.77	124.45
21	3	608	CHL	C2D-C1D-ND	6.18	114.66	110.10
27	4	621	BCR	C24-C23-C22	-6.18	116.90	126.23
24	1	618	XAT	O24-C25-C24	6.15	118.00	113.38
21	8	606	CHL	CHD-C1D-ND	-6.15	118.80	124.45
21	5	601	CHL	CHD-C1D-ND	-6.15	118.81	124.45
21	W	609	CHL	CHD-C1D-ND	-6.14	118.81	124.45
21	V	606	CHL	CHD-C1D-ND	-6.14	118.81	124.45
27	6	621	BCR	C33-C5-C6	-6.13	117.64	124.53
23	9	624	LUT	C36-C21-C22	6.13	121.05	109.44
21	W	607	CHL	CHD-C1D-ND	-6.13	118.82	124.45
21	5	607	CHL	CHD-C1D-ND	-6.13	118.82	124.45
21	2	606	CHL	CHD-C1D-ND	-6.12	118.83	124.45
21	2	601	CHL	CHD-C1D-ND	-6.12	118.83	124.45
21	V	601	CHL	CHD-C1D-ND	-6.11	118.84	124.45
21	8	618	CHL	CHD-C1D-ND	-6.11	118.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	605	CHL	CHD-C1D-ND	-6.11	118.84	124.45
21	W	608	CHL	CHD-C1D-ND	-6.10	118.85	124.45
21	U	601	CHL	CHD-C1D-ND	-6.09	118.86	124.45
21	V	608	CHL	CHD-C1D-ND	-6.08	118.86	124.45
21	6	607	CHL	CHD-C1D-ND	-6.08	118.87	124.45
21	6	606	CHL	CHD-C1D-ND	-6.06	118.88	124.45
21	7	608	CHL	CHD-C1D-ND	-6.05	118.89	124.45
24	1	618	XAT	C38-C25-C26	-6.05	112.12	122.26
21	U	608	CHL	CHD-C1D-ND	-6.05	118.90	124.45
27	B	1609	BCR	C3-C4-C5	-6.03	103.30	114.08
21	1	607	CHL	CHD-C1D-ND	-6.03	118.91	124.45
25	W	2623	NEX	C38-C25-C26	-6.03	112.16	122.26
22	B	809	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	V	612	CLA	C4A-NA-C1A	6.02	109.41	106.71
21	2	618	CHL	CHD-C1D-ND	-5.99	118.95	124.45
22	B	825	CLA	C4A-NA-C1A	5.98	109.40	106.71
21	9	608	CHL	CHD-C1D-ND	-5.97	118.96	124.45
21	U	607	CHL	CHD-C1D-ND	-5.95	118.99	124.45
21	8	608	CHL	CHD-C1D-ND	-5.94	118.99	124.45
21	9	606	CHL	CHD-C1D-ND	-5.94	119.00	124.45
27	8	621	BCR	C24-C23-C22	-5.94	117.27	126.23
21	6	618	CHL	CHD-C1D-ND	-5.92	119.01	124.45
24	5	618	XAT	O24-C25-C38	5.90	122.12	115.06
21	4	606	CHL	CHD-C1D-ND	-5.90	119.03	124.45
21	6	608	CHL	CHD-C1D-ND	-5.89	119.05	124.45
24	5	618	XAT	C18-C5-C6	-5.88	112.40	122.26
27	4	621	BCR	C40-C30-C39	-5.85	90.56	108.53
24	1	618	XAT	C18-C5-C6	-5.79	112.55	122.26
27	K	202	BCR	C3-C4-C5	-5.79	103.75	114.08
22	K	204	CLA	C4A-NA-C1A	5.78	109.31	106.71
22	7	602	CLA	C4A-NA-C1A	5.77	109.30	106.71
21	3	608	CHL	CHD-C1D-ND	-5.77	119.15	124.45
22	4	604	CLA	C4A-NA-C1A	5.77	109.30	106.71
27	B	845	BCR	C3-C4-C5	-5.76	103.79	114.08
22	U	603	CLA	C4A-NA-C1A	5.74	109.29	106.71
27	J	102	BCR	C3-C4-C5	-5.74	103.83	114.08
21	V	607	CHL	O2D-CGD-CBD	5.73	121.45	111.27
21	9	601	CHL	CHD-C1D-ND	-5.71	119.21	124.45
25	W	2623	NEX	O24-C25-C38	5.71	121.89	115.06
22	A	836	CLA	CAC-C3C-C4C	5.70	125.17	117.97
21	W	608	CHL	C3B-C4B-NB	5.69	114.05	110.23
22	3	606	CLA	C4A-NA-C1A	5.67	109.26	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	205	BCR	C38-C26-C25	-5.65	118.19	124.53
21	9	601	CHL	C2D-C1D-ND	5.64	114.26	110.10
22	J	101	CLA	C4A-NA-C1A	5.63	109.24	106.71
27	K	205	BCR	C8-C7-C6	-5.63	111.40	127.20
22	7	607	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	8	609	CLA	C4A-NA-C1A	5.62	109.23	106.71
27	6	621	BCR	C24-C23-C22	-5.58	117.80	126.23
25	W	2623	NEX	C15-C14-C13	-5.57	119.36	127.31
22	2	603	CLA	C4A-NA-C1A	5.57	109.21	106.71
22	3	615	CLA	C4A-NA-C1A	5.56	109.21	106.71
25	V	2623	NEX	C38-C25-C26	-5.56	112.94	122.26
27	3	620	BCR	C28-C27-C26	-5.55	104.16	114.08
27	J	102	BCR	C8-C7-C6	-5.54	111.64	127.20
22	8	613	CLA	C4A-NA-C1A	5.51	109.19	106.71
21	9	605	CHL	C3D-C4D-ND	5.51	119.16	110.24
27	A	851	BCR	C28-C27-C26	-5.51	104.23	114.08
24	U	2622	XAT	C38-C25-C26	-5.51	113.03	122.26
24	W	2622	XAT	C18-C5-C6	-5.50	113.04	122.26
22	A	836	CLA	C4A-NA-C1A	5.49	109.17	106.71
27	B	845	BCR	C15-C14-C13	-5.49	119.48	127.31
22	A	836	CLA	C2C-C3C-C4C	-5.48	107.53	119.42
27	7	620	BCR	C23-C24-C25	-5.48	111.82	127.20
27	O	2004	BCR	C32-C1-C6	5.48	119.18	110.30
21	2	602	CHL	C3D-C4D-ND	5.47	119.09	110.24
22	A	814	CLA	C4A-NA-C1A	5.45	109.16	106.71
24	4	620	XAT	C38-C25-C26	-5.45	113.13	122.26
22	6	611	CLA	C4A-NA-C1A	5.44	109.15	106.71
21	6	618	CHL	O2D-CGD-CBD	5.44	120.93	111.27
25	9	623	NEX	C38-C25-C26	-5.44	113.15	122.26
22	1	603	CLA	C4A-NA-C1A	5.43	109.15	106.71
21	9	601	CHL	C3D-C4D-ND	5.43	119.02	110.24
21	U	609	CHL	C3D-C4D-ND	5.42	119.01	110.24
21	V	607	CHL	C3B-C4B-NB	5.41	113.86	110.23
21	5	607	CHL	C3D-C4D-ND	5.41	118.98	110.24
24	W	2622	XAT	C38-C25-C26	-5.40	113.20	122.26
22	A	828	CLA	C4A-NA-C1A	5.40	109.14	106.71
22	B	826	CLA	C4A-NA-C1A	5.40	109.13	106.71
21	U	606	CHL	O2D-CGD-CBD	5.39	120.85	111.27
21	V	609	CHL	C3D-C4D-ND	5.39	118.95	110.24
21	8	607	CHL	C3D-C4D-ND	5.38	118.95	110.24
21	V	605	CHL	C3D-C4D-ND	5.38	118.94	110.24
22	9	609	CLA	C3D-C4D-ND	5.38	118.94	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	601	CHL	O2D-CGD-CBD	5.38	120.83	111.27
21	4	607	CHL	C3D-C4D-ND	5.38	118.94	110.24
21	6	606	CHL	C3D-C4D-ND	5.38	118.94	110.24
21	U	608	CHL	C3B-C4B-NB	5.38	113.84	110.23
21	6	602	CHL	C3D-C4D-ND	5.37	118.93	110.24
21	U	606	CHL	C3D-C4D-ND	5.37	118.92	110.24
21	2	606	CHL	C3D-C4D-ND	5.35	118.90	110.24
21	9	608	CHL	C3D-C4D-ND	5.35	118.89	110.24
21	2	607	CHL	O2D-CGD-CBD	5.35	120.77	111.27
22	B	810	CLA	C4A-NA-C1A	5.34	109.11	106.71
22	7	612	CLA	C4A-NA-C1A	5.34	109.11	106.71
21	W	609	CHL	C3D-C4D-ND	5.33	118.87	110.24
22	1	611	CLA	C4A-NA-C1A	5.33	109.10	106.71
22	9	609	CLA	O2D-CGD-CBD	5.33	120.74	111.27
21	W	601	CHL	C3D-C4D-ND	5.33	118.86	110.24
21	W	606	CHL	C3D-C4D-ND	5.32	118.85	110.24
27	B	847	BCR	C28-C27-C26	-5.32	104.57	114.08
21	V	607	CHL	C3D-C4D-ND	5.32	118.85	110.24
22	B	840	CLA	C4A-NA-C1A	5.32	109.10	106.71
27	K	205	BCR	C7-C8-C9	-5.32	118.20	126.23
22	K	201	CLA	C4A-NA-C1A	5.31	109.09	106.71
21	V	608	CHL	C3B-C4B-NB	5.31	113.79	110.23
22	B	832	CLA	C4A-NA-C1A	5.30	109.09	106.71
21	8	618	CHL	C3D-C4D-ND	5.30	118.82	110.24
21	W	608	CHL	C3D-C4D-ND	5.30	118.81	110.24
27	7	621	BCR	C3-C4-C5	-5.30	104.61	114.08
21	9	607	CHL	C3D-C4D-ND	5.30	118.81	110.24
21	W	606	CHL	C3B-C4B-NB	5.30	113.78	110.23
21	2	607	CHL	C3D-C4D-ND	5.29	118.80	110.24
27	F	305	BCR	C28-C27-C26	-5.29	104.63	114.08
24	U	2622	XAT	C18-C5-C6	-5.29	113.39	122.26
21	W	605	CHL	C3D-C4D-ND	5.29	118.79	110.24
21	U	605	CHL	C3D-C4D-ND	5.29	118.79	110.24
21	6	606	CHL	O2D-CGD-CBD	5.28	120.65	111.27
22	A	834	CLA	C4A-NA-C1A	5.28	109.08	106.71
21	4	606	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
22	A	806	CLA	C4A-NA-C1A	5.27	109.08	106.71
22	8	603	CLA	C4A-NA-C1A	5.27	109.08	106.71
27	J	102	BCR	C28-C27-C26	-5.27	104.66	114.08
21	V	608	CHL	C3C-C4C-NC	5.27	116.33	110.57
21	6	608	CHL	CAC-C3C-C4C	5.27	131.64	124.81
21	4	618	CHL	C3D-C4D-ND	5.26	118.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	607	CHL	C3D-C4D-ND	5.26	118.75	110.24
21	V	606	CHL	C3D-C4D-ND	5.26	118.75	110.24
21	W	607	CHL	C3D-C4D-ND	5.24	118.72	110.24
21	U	607	CHL	C3D-C4D-ND	5.24	118.71	110.24
21	6	608	CHL	C3D-C4D-ND	5.23	118.70	110.24
22	B	824	CLA	C4A-NA-C1A	5.22	109.05	106.71
21	2	618	CHL	C3D-C4D-ND	5.22	118.68	110.24
21	4	606	CHL	C3D-C4D-ND	5.22	118.68	110.24
21	8	606	CHL	C3D-C4D-ND	5.22	118.68	110.24
22	4	603	CLA	C4A-NA-C1A	5.22	109.05	106.71
22	B	841	CLA	C4A-NA-C1A	5.22	109.05	106.71
21	3	608	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
21	6	618	CHL	C3D-C4D-ND	5.21	118.67	110.24
21	6	601	CHL	C3D-C4D-ND	5.21	118.66	110.24
21	W	607	CHL	C3C-C4C-NC	5.20	116.25	110.57
21	7	608	CHL	C3D-C4D-ND	5.20	118.66	110.24
22	A	803	CLA	C4A-NA-C1A	5.20	109.05	106.71
21	U	605	CHL	C3B-C4B-NB	5.20	113.72	110.23
21	5	601	CHL	C3D-C4D-ND	5.20	118.65	110.24
21	U	608	CHL	C3D-C4D-ND	5.19	118.64	110.24
21	U	605	CHL	C3C-C4C-NC	5.19	116.24	110.57
21	4	618	CHL	CAC-C3C-C4C	5.18	131.53	124.81
21	5	601	CHL	O2D-CGD-CBD	5.18	120.47	111.27
21	9	607	CHL	O2D-CGD-CBD	5.17	120.46	111.27
21	V	601	CHL	C3D-C4D-ND	5.17	118.60	110.24
21	W	607	CHL	C3B-C4B-NB	5.17	113.70	110.23
21	1	601	CHL	O2D-CGD-CBD	5.16	120.45	111.27
21	W	607	CHL	O2D-CGD-CBD	5.16	120.44	111.27
21	4	608	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
21	V	607	CHL	C3C-C4C-NC	5.16	116.21	110.57
22	B	817	CLA	C4A-NA-C1A	5.16	109.03	106.71
22	B	829	CLA	C4A-NA-C1A	5.16	109.03	106.71
21	9	606	CHL	O2D-CGD-CBD	5.16	120.44	111.27
21	8	606	CHL	O2D-CGD-CBD	5.16	120.44	111.27
22	A	813	CLA	C4A-NA-C1A	5.16	109.03	106.71
21	V	606	CHL	C3C-C4C-NC	5.16	116.20	110.57
21	2	608	CHL	C3D-C4D-ND	5.16	118.58	110.24
21	2	601	CHL	C3D-C4D-ND	5.15	118.58	110.24
27	4	621	BCR	C7-C8-C9	-5.15	118.45	126.23
21	1	607	CHL	C3D-C4D-ND	5.15	118.56	110.24
22	A	854	CLA	C4A-NA-C1A	5.14	109.02	106.71
21	8	608	CHL	C3D-C4D-ND	5.14	118.56	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	2001	BCR	C11-C10-C9	-5.14	119.98	127.31
21	1	601	CHL	C3D-C4D-ND	5.13	118.54	110.24
24	3	619	XAT	O24-C25-C24	5.13	117.24	113.38
22	A	807	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	6	603	CLA	C4A-NA-C1A	5.12	109.01	106.71
21	4	608	CHL	C3D-C4D-ND	5.12	118.52	110.24
25	W	2623	NEX	C11-C10-C9	-5.12	120.01	127.31
25	W	2623	NEX	C27-C28-C29	-5.11	117.59	125.53
23	5	617	LUT	C15-C35-C34	5.11	133.95	123.47
21	V	608	CHL	C3D-C4D-ND	5.11	118.50	110.24
24	1	618	XAT	O4-C5-C18	5.11	121.18	115.06
22	5	608	CLA	C4A-NA-C1A	5.11	109.00	106.71
21	U	601	CHL	C3D-C4D-ND	5.11	118.50	110.24
22	A	816	CLA	C4A-NA-C1A	5.11	109.00	106.71
22	9	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
22	B	807	CLA	C4A-NA-C1A	5.10	109.00	106.71
21	W	605	CHL	C3C-C4C-NC	5.10	116.14	110.57
22	B	820	CLA	C4A-NA-C1A	5.09	109.00	106.71
27	8	621	BCR	C33-C5-C6	-5.09	118.81	124.53
21	4	606	CHL	C3C-C4C-NC	5.08	116.27	110.57
21	U	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
22	A	840	CLA	C4A-NA-C1A	5.08	108.99	106.71
22	V	603	CLA	C4A-NA-C1A	5.08	108.99	106.71
27	L	301	BCR	C3-C4-C5	-5.08	105.01	114.08
21	8	608	CHL	C3D-C2D-C1D	-5.08	98.91	105.83
21	W	605	CHL	C3B-C4B-NB	5.07	113.63	110.23
22	B	827	CLA	C4A-NA-C1A	5.07	108.99	106.71
27	A	852	BCR	C31-C1-C6	-5.07	102.08	110.30
21	W	601	CHL	C3B-C4B-NB	5.07	113.63	110.23
21	9	606	CHL	C3D-C4D-ND	5.07	118.43	110.24
21	6	607	CHL	O2D-CGD-CBD	5.06	120.27	111.27
21	V	601	CHL	C3B-C4B-NB	5.06	113.62	110.23
21	6	602	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
27	M	2001	BCR	C28-C27-C26	-5.05	105.06	114.08
21	V	606	CHL	C3B-C4B-NB	5.04	113.61	110.23
22	A	833	CLA	C4A-NA-C1A	5.04	108.97	106.71
21	2	606	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
21	2	602	CHL	C3B-C2B-C1B	-5.04	101.08	107.16
22	U	613	CLA	C4A-NA-C1A	5.03	108.97	106.71
27	L	305	BCR	C28-C27-C26	-5.03	105.09	114.08
21	W	608	CHL	C3C-C4C-NC	5.02	116.06	110.57
27	B	1609	BCR	C40-C30-C29	-5.02	88.81	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	618	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
22	A	825	CLA	C4A-NA-C1A	5.02	108.96	106.71
22	8	604	CLA	C4A-NA-C1A	5.02	108.96	106.71
21	U	608	CHL	C3C-C4C-NC	5.02	116.05	110.57
21	2	601	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
21	6	602	CHL	O2D-CGD-CBD	5.02	120.18	111.27
21	U	606	CHL	C3C-C4C-NC	5.01	116.19	110.57
21	2	607	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
21	6	608	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
22	A	826	CLA	C4A-NA-C1A	5.00	108.96	106.71
21	U	609	CHL	O2D-CGD-CBD	5.00	120.16	111.27
22	6	604	CLA	C4A-NA-C1A	5.00	108.95	106.71
21	W	607	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
27	2	621	BCR	C11-C10-C9	-4.99	120.19	127.31
21	8	618	CHL	O2D-CGD-CBD	4.99	120.14	111.27
22	B	813	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	2	620	XAT	C38-C25-C26	-4.99	113.90	122.26
21	W	606	CHL	C3C-C4C-NC	4.98	116.01	110.57
21	2	606	CHL	O2D-CGD-CBD	4.98	120.12	111.27
21	9	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
22	4	601	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	F	303	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	1	616	CLA	C4A-NA-C1A	4.97	108.94	106.71
22	A	842	CLA	C4A-NA-C1A	4.97	108.94	106.71
27	B	848	BCR	C24-C23-C22	-4.97	118.73	126.23
21	6	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
21	5	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
21	V	607	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
21	U	609	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
21	9	606	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
22	A	804	CLA	C4A-NA-C1A	4.95	108.93	106.71
27	7	620	BCR	C28-C27-C26	-4.95	105.24	114.08
22	1	613	CLA	C4A-NA-C1A	4.95	108.93	106.71
22	A	837	CLA	C4A-NA-C1A	4.95	108.93	106.71
21	W	609	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
22	G	204	CLA	C4A-NA-C1A	4.94	108.93	106.71
22	9	609	CLA	CAC-C3C-C4C	4.94	131.22	124.81
22	3	614	CLA	C4A-NA-C1A	4.94	108.93	106.71
22	A	823	CLA	C4A-NA-C1A	4.94	108.93	106.71
21	W	609	CHL	C3B-C2B-C1B	-4.94	101.20	107.16
22	1	606	CLA	C4A-NA-C1A	4.94	108.92	106.71
21	U	605	CHL	C3D-C2D-C1D	-4.93	99.10	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	618	XAT	C38-C25-C26	-4.93	113.99	122.26
22	A	819	CLA	C4A-NA-C1A	4.93	108.92	106.71
22	6	614	CLA	C4A-NA-C1A	4.93	108.92	106.71
21	9	605	CHL	C3C-C4C-NC	4.93	115.95	110.57
21	U	601	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
21	8	607	CHL	O2D-CGD-CBD	4.93	120.03	111.27
21	6	607	CHL	C3C-C4C-NC	4.92	116.09	110.57
22	A	805	CLA	C4A-NA-C1A	4.92	108.92	106.71
21	6	618	CHL	CAC-C3C-C4C	4.92	131.19	124.81
22	2	611	CLA	C4A-NA-C1A	4.92	108.92	106.71
21	7	608	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
21	6	618	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
21	W	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
21	2	601	CHL	C3C-C4C-NC	4.91	116.08	110.57
21	4	606	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
21	U	607	CHL	C3C-C4C-NC	4.91	116.08	110.57
22	B	808	CLA	C4A-NA-C1A	4.91	108.91	106.71
23	8	619	LUT	C17-C1-C6	-4.91	102.34	110.30
21	V	609	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	V	608	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	9	607	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
21	2	602	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
24	5	618	XAT	O4-C5-C18	4.90	120.92	115.06
21	2	608	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
21	W	605	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
21	5	607	CHL	C3C-C4C-NC	4.89	116.06	110.57
21	8	606	CHL	C3C-C4C-NC	4.89	116.06	110.57
21	4	606	CHL	O2D-CGD-CBD	4.89	119.95	111.27
21	2	618	CHL	O2D-CGD-CBD	4.89	119.95	111.27
21	6	608	CHL	C3C-C4C-NC	4.89	116.05	110.57
21	5	607	CHL	C3D-C2D-C1D	-4.88	99.16	105.83
27	I	101	BCR	C33-C5-C6	-4.88	119.04	124.53
21	V	605	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
21	1	601	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
22	L	302	CLA	C4A-NA-C1A	4.88	108.90	106.71
21	W	609	CHL	CAC-C3C-C4C	4.88	131.14	124.81
21	6	607	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
21	U	601	CHL	C3B-C4B-NB	4.88	113.50	110.23
21	8	607	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
22	U	604	CLA	C4A-NA-C1A	4.87	108.90	106.71
22	O	2001	CLA	C4A-NA-C1A	4.87	108.90	106.71
21	2	618	CHL	C3D-C2D-C1D	-4.87	99.18	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	808	CLA	C4A-NA-C1A	4.87	108.89	106.71
21	4	608	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
22	1	604	CLA	C4A-NA-C1A	4.86	108.89	106.71
21	6	606	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
27	F	305	BCR	C35-C13-C14	-4.86	116.11	122.92
22	A	843	CLA	C4A-NA-C1A	4.86	108.89	106.71
21	3	608	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
27	7	621	BCR	C38-C26-C25	-4.86	119.07	124.53
21	8	608	CHL	C3C-C4C-NC	4.86	116.02	110.57
21	4	618	CHL	O2D-CGD-CBD	4.85	119.89	111.27
21	V	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
21	6	606	CHL	C3C-C4C-NC	4.85	116.01	110.57
21	U	607	CHL	O2D-CGD-CBD	4.85	119.88	111.27
22	A	824	CLA	C4A-NA-C1A	4.84	108.88	106.71
22	7	606	CLA	C4A-NA-C1A	4.84	108.88	106.71
21	W	608	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
21	8	606	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
22	7	610	CLA	C4A-NA-C1A	4.84	108.88	106.71
21	8	618	CHL	C3B-C2B-C1B	-4.83	101.33	107.16
21	6	618	CHL	C3B-C2B-C1B	-4.83	101.33	107.16
22	A	822	CLA	C4A-NA-C1A	4.83	108.88	106.71
21	U	607	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
21	8	608	CHL	CAC-C3C-C4C	4.83	131.07	124.81
21	3	608	CHL	C3D-C4D-ND	4.82	118.04	110.24
21	W	606	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
21	V	605	CHL	C3C-C4C-NC	4.82	115.98	110.57
23	4	619	LUT	C17-C1-C6	-4.82	102.48	110.30
22	B	806	CLA	C4A-NA-C1A	4.82	108.87	106.71
27	O	2004	BCR	C20-C21-C22	-4.82	120.43	127.31
21	V	606	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
22	B	831	CLA	C4A-NA-C1A	4.81	108.87	106.71
21	9	608	CHL	C3C-C4C-NC	4.81	115.97	110.57
27	1	619	BCR	C28-C27-C26	-4.81	105.49	114.08
21	U	606	CHL	C3B-C2B-C1B	-4.81	101.36	107.16
27	B	845	BCR	C35-C13-C12	-4.80	110.51	118.08
21	8	607	CHL	C3B-C2B-C1B	-4.80	101.36	107.16
21	V	601	CHL	CAC-C3C-C4C	4.80	131.04	124.81
22	A	839	CLA	C4A-NA-C1A	4.80	108.86	106.71
27	6	621	BCR	C11-C10-C9	-4.79	120.47	127.31
21	2	606	CHL	C3C-C4C-NC	4.79	115.94	110.57
21	4	607	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
22	B	805	CLA	C4A-NA-C1A	4.78	108.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	836	CLA	C4A-NA-C1A	4.78	108.85	106.71
21	8	618	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
22	U	602	CLA	C4A-NA-C1A	4.77	108.85	106.71
27	B	847	BCR	C23-C24-C25	-4.77	113.80	127.20
21	U	601	CHL	C3C-C4C-NC	4.77	115.92	110.57
22	A	801	CLA	O2D-CGD-CBD	4.77	119.75	111.27
21	U	608	CHL	C3D-C2D-C1D	-4.77	99.33	105.83
21	9	607	CHL	C3B-C2B-C1B	-4.76	101.41	107.16
21	4	618	CHL	C3C-C4C-NC	4.76	115.91	110.57
22	B	823	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	8	601	CLA	C4A-NA-C1A	4.76	108.84	106.71
27	O	2004	BCR	C24-C23-C22	-4.76	119.05	126.23
21	1	607	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
21	5	601	CHL	C3C-C4C-NC	4.75	115.90	110.57
21	7	608	CHL	CAC-C3C-C4C	4.75	130.97	124.81
22	9	609	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
21	2	606	CHL	C3B-C2B-C1B	-4.75	101.43	107.16
22	K	206	CLA	C4A-NA-C1A	4.74	108.84	106.71
21	4	608	CHL	CAC-C3C-C4C	4.73	130.95	124.81
21	8	607	CHL	C3C-C4C-NC	4.73	115.88	110.57
21	W	609	CHL	C3C-C4C-NC	4.73	115.88	110.57
21	9	606	CHL	C3C-C4C-NC	4.73	115.87	110.57
22	2	604	CLA	C4A-NA-C1A	4.72	108.83	106.71
22	B	816	CLA	C4A-NA-C1A	4.72	108.83	106.71
21	6	601	CHL	C3C-C4C-NC	4.72	115.86	110.57
21	2	602	CHL	C3C-C4C-NC	4.72	115.86	110.57
27	1	619	BCR	C37-C22-C23	4.72	125.51	118.08
21	6	607	CHL	C3B-C2B-C1B	-4.71	101.47	107.16
21	1	607	CHL	C3B-C2B-C1B	-4.70	101.48	107.16
22	B	812	CLA	C4A-NA-C1A	4.70	108.82	106.71
22	9	613	CLA	C4A-NA-C1A	4.69	108.82	106.71
21	9	608	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
25	U	2623	NEX	C38-C25-C26	-4.69	114.40	122.26
21	W	601	CHL	C3C-C4C-NC	4.69	115.83	110.57
27	B	847	BCR	C38-C26-C25	-4.69	119.26	124.53
22	1	602	CLA	C4A-NA-C1A	4.69	108.81	106.71
24	V	2622	XAT	C38-C25-C26	-4.69	114.41	122.26
27	B	801	BCR	C28-C27-C26	-4.68	105.72	114.08
22	3	613	CLA	C4A-NA-C1A	4.68	108.81	106.71
21	8	608	CHL	C3B-C2B-C1B	-4.68	101.51	107.16
27	O	2004	BCR	C38-C26-C25	-4.67	119.28	124.53
21	2	601	CHL	C3B-C2B-C1B	-4.67	101.52	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	621	BCR	C3-C4-C5	-4.67	105.74	114.08
21	5	607	CHL	C3B-C2B-C1B	-4.67	101.53	107.16
22	4	612	CLA	C4A-NA-C1A	4.66	108.80	106.71
21	7	608	CHL	C3C-C4C-NC	4.66	115.79	110.57
21	1	601	CHL	C3B-C2B-C1B	-4.66	101.54	107.16
21	2	602	CHL	O2D-CGD-CBD	4.65	119.54	111.27
21	6	602	CHL	CAC-C3C-C4C	4.65	130.85	124.81
21	2	607	CHL	C3C-C4C-NC	4.65	115.79	110.57
22	W	604	CLA	C4A-NA-C1A	4.65	108.80	106.71
21	9	601	CHL	C3C-C4C-NC	4.64	115.78	110.57
21	2	618	CHL	C3C-C4C-NC	4.64	115.78	110.57
25	W	2623	NEX	C5-C6-C1	4.64	124.30	119.70
21	2	618	CHL	C3B-C2B-C1B	-4.64	101.56	107.16
21	1	601	CHL	C3C-C4C-NC	4.64	115.77	110.57
21	6	608	CHL	C3B-C2B-C1B	-4.64	101.57	107.16
21	5	601	CHL	C3B-C2B-C1B	-4.63	101.57	107.16
21	9	605	CHL	C3B-C2B-C1B	-4.62	101.58	107.16
22	4	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	B	834	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	B	804	CLA	C4A-NA-C1A	4.62	108.78	106.71
21	6	601	CHL	C3B-C2B-C1B	-4.61	101.59	107.16
22	B	839	CLA	C4A-NA-C1A	4.61	108.78	106.71
21	1	607	CHL	C3C-C4C-NC	4.61	115.74	110.57
21	V	601	CHL	C4-C3-C5	4.61	123.02	115.27
21	2	608	CHL	C3B-C2B-C1B	-4.61	101.60	107.16
21	2	607	CHL	C3B-C2B-C1B	-4.61	101.60	107.16
23	3	618	LUT	C8-C7-C6	-4.60	114.29	127.20
22	O	2003	CLA	C4A-NA-C1A	4.60	108.77	106.71
22	6	613	CLA	C4A-NA-C1A	4.60	108.77	106.71
21	U	609	CHL	CAC-C3C-C4C	4.59	130.77	124.81
22	G	203	CLA	C4A-NA-C1A	4.59	108.77	106.71
22	5	614	CLA	C4A-NA-C1A	4.59	108.77	106.71
21	V	601	CHL	C3C-C4C-NC	4.58	115.71	110.57
22	B	833	CLA	C4A-NA-C1A	4.58	108.76	106.71
21	U	609	CHL	C3C-C4C-NC	4.58	115.70	110.57
21	V	605	CHL	C3B-C2B-C1B	-4.57	101.64	107.16
21	6	602	CHL	C3C-C4C-NC	4.57	115.70	110.57
21	7	608	CHL	C3B-C2B-C1B	-4.57	101.65	107.16
24	3	619	XAT	C38-C25-C26	-4.57	114.60	122.26
21	3	608	CHL	C3C-C4C-NC	4.57	115.69	110.57
21	8	618	CHL	C3C-C4C-NC	4.57	115.69	110.57
22	5	606	CLA	C4A-NA-C1A	4.56	108.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	827	CLA	C4A-NA-C1A	4.56	108.76	106.71
22	4	613	CLA	C4A-NA-C1A	4.56	108.76	106.71
21	8	606	CHL	C3B-C2B-C1B	-4.56	101.66	107.16
21	6	606	CHL	C3B-C2B-C1B	-4.55	101.67	107.16
21	6	618	CHL	C3C-C4C-NC	4.55	115.67	110.57
22	2	614	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	A	812	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	7	613	CLA	C4A-NA-C1A	4.54	108.75	106.71
21	U	607	CHL	CAC-C3C-C4C	4.53	130.69	124.81
22	F	301	CLA	C4A-NA-C1A	4.53	108.74	106.71
21	V	609	CHL	C3C-C4C-NC	4.53	115.65	110.57
21	6	602	CHL	C3B-C2B-C1B	-4.53	101.70	107.16
22	7	614	CLA	C4A-NA-C1A	4.52	108.74	106.71
21	2	608	CHL	C3C-C4C-NC	4.52	115.64	110.57
27	6	621	BCR	C20-C21-C22	-4.52	120.86	127.31
27	3	620	BCR	C31-C1-C6	-4.52	102.97	110.30
22	5	602	CLA	C4A-NA-C1A	4.52	108.74	106.71
22	L	304	CLA	C4A-NA-C1A	4.51	108.73	106.71
22	4	611	CLA	C4A-NA-C1A	4.51	108.73	106.71
22	A	841	CLA	C4A-NA-C1A	4.51	108.73	106.71
24	5	618	XAT	O24-C25-C24	4.51	116.77	113.38
24	8	620	XAT	C35-C15-C14	4.50	132.70	123.47
22	3	609	CLA	O2D-CGD-CBD	4.50	119.26	111.27
27	A	849	BCR	C7-C8-C9	-4.49	119.45	126.23
22	B	819	CLA	C4A-NA-C1A	4.49	108.72	106.71
21	4	608	CHL	C3C-C4C-NC	4.49	115.60	110.57
21	9	606	CHL	C3B-C2B-C1B	-4.49	101.74	107.16
21	V	601	CHL	C2C-C1C-NC	4.49	114.18	109.97
21	V	606	CHL	C2C-C1C-NC	4.49	114.17	109.97
22	7	615	CLA	C4A-NA-C1A	4.49	108.72	106.71
22	9	609	CLA	C3C-C4C-NC	4.48	115.60	110.57
22	9	609	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
21	U	606	CHL	CHD-C4C-C3C	-4.48	118.26	124.84
27	A	856	BCR	C28-C27-C26	-4.47	106.09	114.08
22	A	818	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	W	613	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	A	835	CLA	C4A-NA-C1A	4.46	108.71	106.71
21	1	607	CHL	O2D-CGD-CBD	4.46	119.20	111.27
21	9	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
21	U	605	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	A	850	BCR	C7-C8-C9	-4.46	119.50	126.23
21	3	608	CHL	CAC-C3C-C4C	4.46	130.59	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	829	CLA	C4A-NA-C1A	4.46	108.71	106.71
27	B	844	BCR	C33-C5-C6	-4.45	119.53	124.53
21	U	607	CHL	C3B-C2B-C1B	-4.45	101.79	107.16
22	B	802	CLA	C4A-NA-C1A	4.45	108.71	106.71
22	B	830	CLA	C4A-NA-C1A	4.44	108.70	106.71
27	B	801	BCR	C20-C21-C22	-4.43	120.98	127.31
21	9	607	CHL	C3C-C4C-NC	4.43	115.54	110.57
21	9	601	CHL	C3B-C2B-C1B	-4.43	101.81	107.16
22	B	837	CLA	C4A-NA-C1A	4.43	108.70	106.71
21	W	606	CHL	C2C-C1C-NC	4.43	114.12	109.97
21	4	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27
27	1	619	BCR	C30-C25-C26	-4.42	116.39	122.61
27	B	843	BCR	C28-C27-C26	-4.42	106.19	114.08
21	V	609	CHL	C3B-C2B-C1B	-4.41	101.83	107.16
22	3	604	CLA	C4A-NA-C1A	4.41	108.69	106.71
22	V	604	CLA	C4A-NA-C1A	4.41	108.69	106.71
27	3	621	BCR	C8-C7-C6	-4.40	114.84	127.20
21	4	607	CHL	C3B-C2B-C1B	-4.40	101.85	107.16
27	A	849	BCR	C38-C26-C25	-4.40	119.59	124.53
22	V	614	CLA	C4A-NA-C1A	4.40	108.68	106.71
22	8	612	CLA	C4A-NA-C1A	4.40	108.68	106.71
27	4	621	BCR	C29-C30-C25	4.40	117.25	110.48
27	A	851	BCR	C30-C25-C24	4.40	128.21	115.78
24	V	2622	XAT	C17-C1-C6	-4.39	98.18	110.05
22	7	604	CLA	C4A-NA-C1A	4.39	108.68	106.71
22	9	603	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	A	848	BCR	C11-C10-C9	-4.39	121.05	127.31
22	2	613	CLA	C4A-NA-C1A	4.38	108.68	106.71
32	B	850	DGD	O2G-C1B-C2B	4.38	120.95	111.50
22	B	818	CLA	C4A-NA-C1A	4.38	108.67	106.71
27	B	1609	BCR	C11-C10-C9	-4.38	121.07	127.31
22	3	607	CLA	C4A-NA-C1A	4.37	108.67	106.71
24	3	619	XAT	O24-C25-C38	4.37	120.29	115.06
27	A	850	BCR	C24-C23-C22	-4.37	119.64	126.23
21	2	608	CHL	CAC-C3C-C4C	4.37	130.48	124.81
21	4	607	CHL	CAC-C3C-C4C	4.36	130.47	124.81
22	5	613	CLA	C4A-NA-C1A	4.35	108.66	106.71
21	4	618	CHL	C3B-C2B-C1B	-4.35	101.91	107.16
22	3	603	CLA	C4A-NA-C1A	4.35	108.66	106.71
22	H	201	CLA	C4A-NA-C1A	4.35	108.66	106.71
27	L	306	BCR	C20-C21-C22	-4.34	121.11	127.31
21	W	605	CHL	C2C-C1C-NC	4.34	114.04	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	620	XAT	C39-C29-C30	-4.34	116.84	122.92
23	V	2620	LUT	C17-C1-C6	-4.34	103.27	110.30
21	6	601	CHL	O2D-CGD-CBD	4.33	118.97	111.27
21	9	606	CHL	CAC-C3C-C4C	4.33	130.43	124.81
27	7	620	BCR	C3-C4-C5	-4.32	106.36	114.08
21	U	601	CHL	C2C-C1C-NC	4.32	114.02	109.97
22	B	815	CLA	C4A-NA-C1A	4.31	108.64	106.71
21	8	608	CHL	O2D-CGD-CBD	4.31	118.92	111.27
26	A	847	LHG	O7-C7-C8	4.30	120.77	111.50
21	8	618	CHL	CAC-C3C-C4C	4.30	130.39	124.81
27	A	850	BCR	C38-C26-C25	-4.30	119.70	124.53
27	A	851	BCR	C34-C9-C8	4.30	124.85	118.08
22	W	602	CLA	C4A-NA-C1A	4.30	108.64	106.71
27	A	852	BCR	C34-C9-C10	-4.30	116.90	122.92
23	9	620	LUT	C17-C1-C6	-4.29	103.34	110.30
22	B	811	CLA	C4A-NA-C1A	4.28	108.63	106.71
27	A	849	BCR	C20-C21-C22	-4.28	121.20	127.31
22	A	810	CLA	C4A-NA-C1A	4.28	108.63	106.71
22	B	819	CLA	C4-C3-C5	4.28	122.47	115.27
22	7	617	CLA	C4A-NA-C1A	4.28	108.63	106.71
21	4	607	CHL	C3C-C4C-NC	4.27	115.36	110.57
27	M	2001	BCR	C27-C26-C25	-4.27	116.53	122.73
27	6	621	BCR	C38-C26-C25	-4.27	119.73	124.53
21	W	601	CHL	C2C-C1C-NC	4.27	113.97	109.97
22	V	611	CLA	C4A-NA-C1A	4.27	108.62	106.71
27	4	621	BCR	C11-C10-C9	-4.26	121.22	127.31
22	L	303	CLA	C4A-NA-C1A	4.26	108.62	106.71
21	U	601	CHL	CAC-C3C-C4C	4.26	130.34	124.81
22	A	811	CLA	C4A-NA-C1A	4.26	108.62	106.71
21	2	618	CHL	CAC-C3C-C4C	4.26	130.33	124.81
22	A	838	CLA	C4A-NA-C1A	4.26	108.62	106.71
22	5	603	CLA	C4A-NA-C1A	4.26	108.62	106.71
21	W	608	CHL	CMB-C2B-C1B	4.25	131.85	125.37
22	F	304	CLA	C4D-C3D-CAD	-4.25	109.18	121.60
27	3	621	BCR	C33-C5-C6	4.25	129.30	124.53
22	1	608	CLA	C4A-NA-C1A	4.25	108.61	106.71
28	2	631	LMG	O7-C10-C11	4.24	120.64	111.50
22	B	814	CLA	C4A-NA-C1A	4.24	108.61	106.71
27	B	845	BCR	C24-C23-C22	-4.24	119.83	126.23
27	G	205	BCR	C11-C10-C9	-4.24	121.26	127.31
23	5	617	LUT	C39-C29-C30	-4.23	116.99	122.92
21	9	601	CHL	C3D-C2D-C1D	-4.23	100.06	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	609	CHL	C3B-C4B-NB	4.23	114.44	110.52
27	I	101	BCR	C24-C23-C22	-4.23	119.84	126.23
27	B	845	BCR	C15-C16-C17	-4.23	114.81	123.47
22	1	610	CLA	C4A-NA-C1A	4.22	108.60	106.71
23	5	617	LUT	C19-C9-C10	-4.22	117.01	122.92
22	3	609	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
22	B	803	CLA	C4A-NA-C1A	4.22	108.60	106.71
22	9	604	CLA	C4A-NA-C1A	4.21	108.60	106.71
21	9	601	CHL	CAC-C3C-C4C	4.21	130.27	124.81
22	3	609	CLA	C4A-NA-C1A	4.21	108.60	106.71
23	7	618	LUT	C17-C1-C6	-4.20	103.49	110.30
21	3	608	CHL	C4-C3-C5	4.20	122.33	115.27
22	O	2002	CLA	C4A-NA-C1A	4.20	108.59	106.71
22	A	809	CLA	C4A-NA-C1A	4.19	108.59	106.71
28	A	860	LMG	O7-C10-C11	4.19	120.53	111.50
21	4	606	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
22	V	602	CLA	C4A-NA-C1A	4.18	108.59	106.71
22	A	821	CLA	C4A-NA-C1A	4.18	108.59	106.71
27	1	619	BCR	C16-C17-C18	-4.18	121.35	127.31
27	I	101	BCR	C38-C26-C25	-4.17	119.84	124.53
27	B	843	BCR	C20-C21-C22	-4.17	121.35	127.31
21	2	602	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
24	1	618	XAT	C26-C27-C28	-4.17	117.18	125.99
21	8	606	CHL	CHD-C4C-C3C	-4.17	118.72	124.84
21	U	609	CHL	C3B-C2B-C1B	-4.16	102.14	107.16
21	6	606	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
24	8	620	XAT	C19-C9-C10	-4.16	117.10	122.92
22	3	612	CLA	C4A-NA-C1A	4.15	108.57	106.71
21	2	606	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
23	2	619	LUT	C19-C9-C10	-4.15	117.11	122.92
22	W	603	CLA	C4A-NA-C1A	4.15	108.57	106.71
22	8	602	CLA	C4A-NA-C1A	4.15	108.57	106.71
21	V	607	CHL	CHD-C4C-C3C	-4.15	118.50	124.98
21	W	607	CHL	CHD-C4C-C3C	-4.14	118.51	124.98
21	7	608	CHL	O2D-CGD-CBD	4.14	118.63	111.27
27	4	621	BCR	C20-C21-C22	-4.14	121.40	127.31
21	6	607	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
22	3	610	CLA	C4A-NA-C1A	4.14	108.57	106.71
27	4	621	BCR	C33-C5-C6	-4.13	119.89	124.53
27	K	205	BCR	C3-C4-C5	-4.13	106.70	114.08
27	3	621	BCR	C23-C24-C25	-4.13	115.61	127.20
23	V	2620	LUT	C11-C10-C9	-4.13	121.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	306	BCR	C7-C8-C9	-4.12	120.01	126.23
22	B	838	CLA	C4A-NA-C1A	4.11	108.56	106.71
27	B	845	BCR	C28-C27-C26	-4.11	106.73	114.08
21	V	609	CHL	CAC-C3C-C4C	4.11	130.14	124.81
24	4	620	XAT	C35-C34-C33	-4.11	121.45	127.31
23	W	2620	LUT	C11-C10-C9	-4.10	121.45	127.31
27	3	620	BCR	C37-C22-C23	4.10	124.54	118.08
27	3	620	BCR	C7-C8-C9	-4.10	120.04	126.23
27	2	621	BCR	C30-C25-C26	-4.10	116.84	122.61
23	8	619	LUT	C3-C4-C5	-4.10	103.69	111.85
21	U	607	CHL	C4-C3-C5	4.09	122.16	115.27
22	B	835	CLA	C4A-NA-C1A	4.09	108.55	106.71
21	V	605	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	B	843	BCR	C37-C22-C23	4.08	124.51	118.08
27	A	849	BCR	C33-C5-C6	-4.08	119.95	124.53
22	B	828	CLA	C4A-NA-C1A	4.08	108.54	106.71
21	9	605	CHL	CHD-C4C-C3C	-4.07	118.62	124.98
22	5	616	CLA	C4A-NA-C1A	4.07	108.53	106.71
24	1	618	XAT	O24-C25-C38	4.07	119.93	115.06
22	A	815	CLA	C4A-NA-C1A	4.06	108.53	106.71
27	L	301	BCR	C37-C22-C23	4.06	124.47	118.08
27	1	619	BCR	C11-C10-C9	-4.06	121.52	127.31
27	B	1609	BCR	C30-C25-C26	-4.06	116.90	122.61
22	4	609	CLA	C4A-NA-C1A	4.05	108.53	106.71
21	5	607	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
22	3	602	CLA	C4A-NA-C1A	4.05	108.53	106.71
27	J	102	BCR	C32-C1-C6	-4.05	103.74	110.30
23	W	2620	LUT	C17-C1-C6	-4.04	103.74	110.30
27	O	2004	BCR	C31-C1-C6	-4.04	103.74	110.30
22	2	610	CLA	C4A-NA-C1A	4.03	108.52	106.71
27	F	305	BCR	C7-C8-C9	-4.03	120.14	126.23
21	8	607	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
23	4	619	LUT	C7-C8-C9	-4.02	120.16	126.23
23	W	2621	LUT	C17-C1-C6	-4.01	103.79	110.30
21	2	601	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
22	7	603	CLA	C4A-NA-C1A	4.01	108.51	106.71
25	V	2623	NEX	C11-C10-C9	-4.01	121.59	127.31
27	K	202	BCR	C20-C21-C22	-4.01	121.59	127.31
22	7	609	CLA	C1D-ND-C4D	-4.01	103.49	106.33
22	A	831	CLA	C4A-NA-C1A	4.01	108.51	106.71
27	3	621	BCR	C20-C21-C22	-4.01	121.59	127.31
21	V	608	CHL	CHD-C4C-C3C	-4.01	118.72	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	306	BCR	C30-C25-C26	-4.01	116.97	122.61
23	9	620	LUT	C3-C4-C5	-4.00	103.88	111.85
24	6	620	XAT	C15-C14-C13	-4.00	121.60	127.31
27	2	621	BCR	C27-C26-C25	-4.00	116.92	122.73
21	U	601	CHL	C4C-C3C-C2C	-4.00	101.07	106.90
23	1	617	LUT	C17-C1-C6	-3.99	103.82	110.30
21	2	602	CHL	CAC-C3C-C4C	3.99	129.99	124.81
22	9	612	CLA	C4A-NA-C1A	3.99	108.50	106.71
22	9	609	CLA	C2C-C1C-NC	3.98	113.70	109.97
22	A	817	CLA	C4A-NA-C1A	3.98	108.50	106.71
22	A	801	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
21	2	607	CHL	CAC-C3C-C4C	3.98	129.97	124.81
23	V	2621	LUT	C17-C1-C6	-3.98	103.84	110.30
27	B	845	BCR	C12-C13-C14	3.98	125.04	118.94
22	U	611	CLA	C4A-NA-C1A	3.97	108.49	106.71
23	U	2620	LUT	C17-C1-C6	-3.97	103.86	110.30
27	B	843	BCR	C11-C10-C9	-3.97	121.64	127.31
25	9	623	NEX	C26-C27-C28	-3.97	117.60	125.99
24	5	618	XAT	C35-C34-C33	-3.97	121.65	127.31
27	3	620	BCR	C3-C4-C5	-3.97	107.00	114.08
21	9	608	CHL	C3B-C2B-C1B	-3.96	102.38	107.16
27	G	205	BCR	C38-C26-C25	-3.96	120.08	124.53
24	U	2622	XAT	O24-C25-C38	3.96	119.80	115.06
24	V	2622	XAT	O24-C25-C38	3.96	119.80	115.06
21	8	608	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
27	K	202	BCR	C37-C22-C23	3.95	124.30	118.08
22	A	845	CLA	C4A-NA-C1A	3.95	108.48	106.71
23	2	619	LUT	C35-C15-C14	3.95	131.56	123.47
22	9	611	CLA	C4A-NA-C1A	3.94	108.48	106.71
21	5	601	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
21	6	601	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
22	1	614	CLA	C4A-NA-C1A	3.93	108.47	106.71
21	6	606	CHL	CAC-C3C-C4C	3.93	129.91	124.81
21	W	601	CHL	CAC-C3C-C4C	3.93	129.91	124.81
21	9	608	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
28	J	104	LMG	O7-C10-C11	3.93	119.96	111.50
22	4	602	CLA	C4A-NA-C1A	3.93	108.47	106.71
21	2	608	CHL	O2D-CGD-CBD	3.92	118.24	111.27
27	J	102	BCR	C38-C26-C25	-3.91	120.13	124.53
21	1	601	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
21	V	601	CHL	C4C-C3C-C2C	-3.91	101.20	106.90
22	A	829	CLA	O2D-CGD-O1D	-3.90	116.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	2001	BCR	C37-C22-C23	3.90	124.22	118.08
21	4	608	CHL	C3B-C4B-NB	3.90	114.13	110.52
21	W	601	CHL	C4C-C3C-C2C	-3.90	101.22	106.90
27	B	848	BCR	C28-C27-C26	-3.89	107.13	114.08
27	8	621	BCR	C16-C17-C18	-3.89	121.76	127.31
27	B	845	BCR	C38-C26-C25	-3.89	120.17	124.53
23	7	618	LUT	C7-C8-C9	-3.88	120.37	126.23
21	3	608	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
26	A	846	LHG	O7-C7-C8	3.86	119.83	111.50
22	8	614	CLA	C4A-NA-C1A	3.86	108.44	106.71
27	F	305	BCR	C33-C5-C6	-3.86	120.19	124.53
21	1	607	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
21	6	608	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
21	W	608	CHL	CHD-C4C-C3C	-3.86	118.95	124.98
25	V	2623	NEX	C17-C1-C6	-3.85	107.02	110.47
21	U	605	CHL	CHD-C4C-C3C	-3.85	118.97	124.98
21	3	608	CHL	O2D-CGD-CBD	3.85	118.10	111.27
21	2	607	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
22	5	604	CLA	C4A-NA-C1A	3.84	108.43	106.71
27	B	801	BCR	C16-C17-C18	-3.84	121.84	127.31
22	1	609	CLA	C4A-NA-C1A	3.83	108.43	106.71
21	3	608	CHL	C3B-C4B-NB	3.83	114.07	110.52
27	L	306	BCR	C33-C5-C6	-3.83	120.23	124.53
27	B	847	BCR	C3-C4-C5	-3.82	107.25	114.08
21	U	608	CHL	CHD-C4C-C3C	-3.82	119.01	124.98
26	3	630	LHG	O7-C7-C8	3.82	119.73	111.50
24	5	618	XAT	C31-C30-C29	-3.81	121.87	127.31
22	9	609	CLA	C4C-C3C-C2C	-3.81	101.34	106.90
21	9	607	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
21	4	606	CHL	CAC-C3C-C4C	3.81	129.75	124.81
27	F	305	BCR	C3-C4-C5	-3.80	107.29	114.08
27	J	102	BCR	C11-C10-C9	-3.79	121.89	127.31
27	A	852	BCR	C24-C23-C22	-3.79	120.50	126.23
22	A	820	CLA	C4A-NA-C1A	3.79	108.41	106.71
24	1	618	XAT	O4-C5-C4	3.79	116.23	113.38
27	A	848	BCR	C38-C26-C25	-3.78	120.29	124.53
27	A	848	BCR	C7-C8-C9	-3.78	120.53	126.23
24	W	2622	XAT	O24-C25-C38	3.77	119.58	115.06
23	3	618	LUT	C7-C8-C9	-3.77	120.53	126.23
21	2	602	CHL	O2A-CGA-CBA	3.77	123.75	111.91
21	7	608	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
21	W	605	CHL	CHD-C4C-C3C	-3.77	119.09	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	621	LUT	C3-C4-C5	-3.77	104.34	111.85
21	W	601	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
21	9	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
27	7	620	BCR	C11-C10-C9	-3.77	121.94	127.31
27	3	621	BCR	C28-C27-C26	-3.76	107.36	114.08
23	U	2621	LUT	C7-C8-C9	-3.76	120.55	126.23
27	B	1609	BCR	C24-C23-C22	-3.76	120.55	126.23
22	W	610	CLA	C4-C3-C5	3.76	121.59	115.27
27	K	205	BCR	C20-C21-C22	-3.76	121.95	127.31
27	1	619	BCR	C23-C22-C21	-3.75	113.18	118.94
28	J	103	LMG	O7-C10-C11	3.75	119.59	111.50
22	K	203	CLA	C4A-NA-C1A	3.75	108.39	106.71
21	V	606	CHL	CHD-C4C-C3C	-3.75	119.12	124.98
23	V	2621	LUT	C11-C10-C9	-3.75	121.96	127.31
21	U	607	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	V	2623	NEX	C26-C27-C28	-3.74	118.08	125.99
24	3	619	XAT	C26-C27-C28	-3.74	118.09	125.99
28	G	202	LMG	O7-C10-C11	3.74	119.56	111.50
27	B	1609	BCR	C23-C24-C25	-3.73	116.72	127.20
25	V	2623	NEX	C2-C1-C6	3.72	112.83	109.21
27	2	621	BCR	C33-C5-C6	-3.72	120.35	124.53
27	B	845	BCR	C36-C18-C19	3.72	123.94	118.08
21	U	606	CHL	CAC-C3C-C4C	3.72	129.64	124.81
21	2	601	CHL	CAC-C3C-C4C	3.72	129.63	124.81
25	9	623	NEX	C39-C29-C30	-3.72	117.72	122.92
27	B	843	BCR	C24-C23-C22	-3.71	120.62	126.23
27	G	205	BCR	C15-C14-C13	-3.71	122.01	127.31
27	B	844	BCR	C38-C26-C25	-3.71	120.36	124.53
21	1	607	CHL	CAC-C3C-C4C	3.71	129.62	124.81
24	8	620	XAT	C12-C13-C14	3.71	124.63	118.94
21	9	606	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
23	4	619	LUT	C3-C4-C5	-3.71	104.47	111.85
21	6	608	CHL	O2D-CGD-CBD	3.71	117.85	111.27
22	U	612	CLA	C4A-NA-C1A	3.71	108.37	106.71
27	A	848	BCR	C16-C17-C18	-3.70	122.02	127.31
27	J	102	BCR	C15-C14-C13	-3.70	122.03	127.31
21	4	608	CHL	O2D-CGD-CBD	3.70	117.84	111.27
21	U	609	CHL	CHD-C4C-C3C	-3.70	119.41	124.84
26	7	630	LHG	O7-C7-C8	3.70	119.47	111.50
27	B	1609	BCR	C29-C30-C25	3.69	116.17	110.48
24	4	620	XAT	O24-C25-C38	3.69	119.48	115.06
23	2	619	LUT	C39-C29-C30	-3.69	117.75	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	825	CLA	C4-C3-C5	3.69	121.47	115.27
24	5	618	XAT	C15-C14-C13	-3.68	122.05	127.31
21	U	601	CHL	CHD-C4C-C3C	-3.68	119.42	124.84
27	4	621	BCR	C40-C30-C29	-3.68	94.17	108.91
22	B	822	CLA	C4A-NA-C1A	3.68	108.36	106.71
27	M	2001	BCR	C33-C5-C6	-3.68	120.40	124.53
23	5	617	LUT	C32-C33-C34	3.68	124.59	118.94
26	1	630	LHG	O7-C7-C8	3.68	119.43	111.50
24	4	620	XAT	C5-C4-C3	-3.67	105.48	112.75
27	B	848	BCR	C32-C1-C6	-3.67	104.34	110.30
24	3	619	XAT	C35-C15-C14	-3.67	115.95	123.47
24	6	620	XAT	O24-C25-C26	-3.67	55.92	58.96
23	V	2620	LUT	C7-C8-C9	-3.67	120.69	126.23
27	B	848	BCR	C11-C10-C9	-3.67	122.08	127.31
24	3	619	XAT	C35-C34-C33	-3.67	122.08	127.31
27	L	305	BCR	C35-C13-C12	3.66	123.85	118.08
23	7	618	LUT	C3-C4-C5	-3.66	104.56	111.85
23	9	621	LUT	C11-C10-C9	-3.66	122.09	127.31
22	W	614	CLA	C4A-NA-C1A	3.66	108.35	106.71
27	1	619	BCR	C36-C18-C19	3.66	123.84	118.08
22	G	201	CLA	C4A-NA-C1A	3.66	108.35	106.71
21	2	608	CHL	CHD-C4C-C3C	-3.66	119.47	124.84
21	2	618	CHL	CHD-C4C-C3C	-3.65	119.47	124.84
27	2	621	BCR	C20-C21-C22	-3.65	122.10	127.31
25	U	2623	NEX	C26-C27-C28	-3.65	118.28	125.99
27	1	619	BCR	C7-C8-C9	-3.65	120.72	126.23
26	8	630	LHG	O7-C7-C8	3.65	119.36	111.50
26	B	851	LHG	O7-C7-C8	3.64	119.36	111.50
21	4	608	CHL	CHD-C4C-C3C	-3.64	119.48	124.84
21	6	601	CHL	CAC-C3C-C4C	3.64	129.54	124.81
24	8	620	XAT	C15-C35-C34	3.64	130.94	123.47
27	K	202	BCR	C37-C22-C21	-3.64	117.82	122.92
21	W	609	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
24	8	620	XAT	C20-C13-C14	-3.64	117.83	122.92
21	4	606	CHL	CMB-C2B-C1B	3.64	130.91	125.37
26	5	630	LHG	O7-C7-C8	3.63	119.33	111.50
23	5	617	LUT	C40-C33-C34	-3.63	117.84	122.92
27	7	620	BCR	C37-C22-C23	3.62	123.79	118.08
21	W	606	CHL	CHD-C4C-C3C	-3.62	119.33	124.98
27	L	306	BCR	C37-C22-C21	-3.62	117.86	122.92
27	F	305	BCR	C20-C21-C22	-3.62	122.15	127.31
22	2	609	CLA	O2D-CGD-O1D	-3.61	116.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	609	CLA	C1D-ND-C4D	-3.61	103.77	106.33
21	2	606	CHL	CAC-C3C-C4C	3.60	129.49	124.81
22	W	612	CLA	C4A-NA-C1A	3.60	108.33	106.71
23	U	2620	LUT	C11-C10-C9	-3.60	122.18	127.31
23	W	2620	LUT	C7-C8-C9	-3.60	120.80	126.23
21	V	609	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
27	3	621	BCR	C16-C17-C18	-3.60	122.18	127.31
26	2	630	LHG	O7-C7-C8	3.59	119.25	111.50
21	8	607	CHL	CAC-C3C-C4C	3.59	129.47	124.81
24	7	619	XAT	O4-C5-C6	-3.59	55.99	58.96
24	6	620	XAT	C37-C21-C26	-3.58	100.37	110.05
27	2	621	BCR	C24-C23-C22	-3.58	120.82	126.23
21	6	602	CHL	CHC-C4B-NB	-3.58	120.47	124.26
23	9	621	LUT	C17-C1-C6	-3.58	104.49	110.30
27	7	621	BCR	C32-C1-C6	-3.58	104.50	110.30
25	9	623	NEX	O24-C25-C38	3.58	119.34	115.06
22	9	610	CLA	C4A-NA-C1A	3.58	108.31	106.71
27	B	847	BCR	C38-C26-C27	3.58	120.48	113.62
21	6	602	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
27	B	844	BCR	C30-C25-C24	3.57	125.87	115.78
24	8	620	XAT	C28-C29-C30	3.57	124.42	118.94
27	B	847	BCR	C15-C14-C13	-3.57	122.22	127.31
26	U	2630	LHG	O7-C7-C8	3.56	119.18	111.50
24	6	620	XAT	C36-C21-C26	3.56	119.65	110.05
27	B	1609	BCR	C34-C9-C10	-3.56	117.94	122.92
22	W	611	CLA	C4A-NA-C1A	3.56	108.31	106.71
22	B	821	CLA	C4A-NA-C1A	3.55	108.30	106.71
27	B	845	BCR	C10-C11-C12	-3.55	112.14	123.22
27	7	621	BCR	C37-C22-C23	3.54	123.66	118.08
27	J	102	BCR	C20-C21-C22	-3.54	122.25	127.31
23	V	2621	LUT	C3-C4-C5	-3.54	104.80	111.85
25	V	2623	NEX	C4-C3-C2	-3.54	103.94	110.77
27	L	306	BCR	C3-C4-C5	-3.54	107.76	114.08
21	9	601	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
26	W	2630	LHG	O7-C7-C8	3.53	119.12	111.50
27	B	843	BCR	C37-C22-C21	-3.53	117.98	122.92
27	L	306	BCR	C27-C26-C25	-3.53	117.61	122.73
27	A	848	BCR	C24-C23-C22	-3.53	120.91	126.23
21	5	601	CHL	CAC-C3C-C4C	3.53	129.38	124.81
24	1	618	XAT	C28-C29-C30	-3.52	113.53	118.94
22	A	809	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	6	619	LUT	C15-C14-C13	-3.52	122.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	620	XAT	C40-C33-C34	-3.52	117.99	122.92
27	K	202	BCR	C32-C1-C6	-3.52	104.59	110.30
27	B	845	BCR	C33-C5-C6	-3.52	120.58	124.53
22	8	611	CLA	C4A-NA-C1A	3.50	108.28	106.71
22	4	610	CLA	C1D-ND-C4D	-3.50	103.85	106.33
21	2	602	CHL	CHC-C4B-NB	-3.50	120.55	124.26
22	5	611	CLA	C4A-NA-C1A	3.49	108.28	106.71
22	V	610	CLA	C4A-NA-C1A	3.49	108.28	106.71
22	9	609	CLA	CHD-C4C-C3C	-3.49	119.71	124.84
27	3	620	BCR	C2-C1-C6	3.49	115.85	110.48
27	M	2001	BCR	C29-C30-C25	3.49	115.85	110.48
21	9	605	CHL	C2A-C1A-CHA	-3.48	117.77	123.85
27	A	852	BCR	C20-C21-C22	-3.48	122.34	127.31
22	5	611	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	2	612	CLA	C4A-NA-C1A	3.48	108.27	106.71
23	V	2620	LUT	C3-C4-C5	-3.48	104.92	111.85
27	1	619	BCR	C24-C23-C22	-3.48	120.98	126.23
21	8	618	CHL	CHD-C4C-C3C	-3.48	119.73	124.84
27	A	849	BCR	C11-C10-C9	-3.47	122.35	127.31
27	B	843	BCR	C1-C6-C5	-3.47	117.72	122.61
24	4	620	XAT	C11-C10-C9	-3.47	122.35	127.31
24	5	618	XAT	C28-C29-C30	-3.47	113.61	118.94
22	3	611	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
27	B	1609	BCR	C38-C26-C25	-3.47	120.63	124.53
22	K	203	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
27	L	305	BCR	C15-C14-C13	-3.47	122.36	127.31
27	B	1609	BCR	C4-C5-C6	-3.47	117.70	122.73
27	K	202	BCR	C11-C10-C9	-3.46	122.36	127.31
22	A	825	CLA	CHD-C1D-ND	-3.46	121.27	124.45
27	A	849	BCR	C37-C22-C23	3.46	123.53	118.08
23	W	2620	LUT	C3-C4-C5	-3.46	104.97	111.85
26	6	630	LHG	O7-C7-C8	3.46	118.95	111.50
27	L	305	BCR	C24-C23-C22	-3.46	121.01	126.23
27	L	301	BCR	C16-C17-C18	-3.46	122.38	127.31
22	6	612	CLA	C4A-NA-C1A	3.45	108.26	106.71
26	V	2630	LHG	O7-C7-C8	3.45	118.94	111.50
21	W	609	CHL	CHB-C4A-NA	3.45	129.28	124.51
24	4	620	XAT	C6-C7-C8	-3.45	118.70	125.99
21	9	601	CHL	C2A-C1A-CHA	-3.45	117.83	123.85
27	B	847	BCR	C8-C7-C6	-3.45	117.52	127.20
22	U	610	CLA	C4A-NA-C1A	3.45	108.26	106.71
22	B	822	CLA	O2D-CGD-O1D	-3.45	117.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	620	XAT	O24-C25-C38	3.45	119.18	115.06
27	A	848	BCR	C34-C9-C10	-3.44	118.10	122.92
21	6	618	CHL	CHD-C4C-C3C	-3.44	119.78	124.84
27	M	2001	BCR	C3-C4-C5	-3.44	107.94	114.08
22	V	613	CLA	C4A-NA-C1A	3.43	108.25	106.71
26	4	630	LHG	O7-C7-C8	3.43	118.89	111.50
22	6	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
27	1	619	BCR	C38-C26-C25	3.42	128.37	124.53
23	U	2621	LUT	C11-C10-C9	-3.42	122.43	127.31
27	8	621	BCR	C11-C10-C9	-3.42	122.43	127.31
21	4	607	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
21	9	601	CHL	CMD-C2D-C3D	-3.41	119.76	127.61
23	1	617	LUT	C8-C7-C6	-3.41	117.62	127.20
22	1	612	CLA	C4A-NA-C1A	3.41	108.24	106.71
22	B	822	CLA	C4-C3-C5	3.41	121.00	115.27
23	5	617	LUT	C20-C13-C14	-3.41	118.15	122.92
27	I	101	BCR	C20-C21-C22	-3.40	122.45	127.31
22	W	610	CLA	C4A-NA-C1A	3.40	108.24	106.71
22	A	829	CLA	O2D-CGD-CBD	3.40	117.31	111.27
27	A	848	BCR	C20-C21-C22	-3.40	122.45	127.31
27	1	619	BCR	C3-C4-C5	-3.40	108.00	114.08
27	L	306	BCR	C38-C26-C25	3.40	128.34	124.53
27	B	844	BCR	C11-C10-C9	-3.40	122.46	127.31
23	1	617	LUT	C7-C8-C9	-3.40	121.10	126.23
27	L	301	BCR	C38-C26-C25	-3.39	120.72	124.53
24	7	619	XAT	O24-C25-C26	-3.39	56.15	58.96
22	9	609	CLA	CMD-C2D-C3D	-3.39	119.81	127.61
23	U	2621	LUT	C17-C1-C6	-3.39	104.80	110.30
27	B	848	BCR	C34-C9-C8	3.39	123.42	118.08
27	G	205	BCR	C30-C25-C26	-3.39	117.84	122.61
24	1	618	XAT	C18-C5-C4	3.38	118.09	114.28
27	A	850	BCR	C20-C21-C22	-3.38	122.49	127.31
27	B	843	BCR	C15-C14-C13	-3.38	122.49	127.31
21	6	607	CHL	CAC-C3C-C4C	3.38	129.19	124.81
23	9	621	LUT	C1-C6-C5	-3.37	117.86	122.61
27	8	621	BCR	C36-C18-C19	3.37	123.39	118.08
24	V	2622	XAT	C16-C1-C6	3.37	119.15	110.05
27	G	205	BCR	C24-C23-C22	-3.37	121.14	126.23
24	6	620	XAT	O4-C5-C6	-3.37	56.17	58.96
21	5	607	CHL	CAC-C3C-C4C	3.37	129.18	124.81
22	B	805	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
25	V	2623	NEX	C39-C29-C30	-3.37	118.21	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	608	CHL	CHB-C4A-NA	3.36	129.16	124.51
27	B	801	BCR	C37-C22-C23	3.36	123.38	118.08
27	B	801	BCR	C37-C22-C21	-3.36	118.21	122.92
23	U	2621	LUT	C19-C9-C8	3.36	123.37	118.08
23	U	2621	LUT	C1-C6-C5	-3.36	117.88	122.61
22	B	807	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
21	V	605	CHL	CAC-C3C-C4C	3.36	129.17	124.81
22	6	609	CLA	C4A-NA-C1A	3.35	108.21	106.71
27	A	849	BCR	C3-C4-C5	-3.35	108.09	114.08
23	5	617	LUT	C12-C13-C14	3.35	124.08	118.94
22	A	801	CLA	C1D-ND-C4D	-3.35	103.96	106.33
21	W	608	CHL	C2A-C1A-CHA	-3.34	118.01	123.86
22	3	611	CLA	C4A-NA-C1A	3.34	108.21	106.71
24	5	618	XAT	C11-C10-C9	-3.34	122.54	127.31
25	U	2623	NEX	C27-C28-C29	-3.34	120.35	125.53
21	W	606	CHL	CHB-C4A-NA	3.34	129.13	124.51
24	5	618	XAT	C39-C29-C28	3.34	123.34	118.08
24	2	620	XAT	C18-C5-C6	-3.34	116.67	122.26
27	7	621	BCR	C23-C24-C25	-3.34	117.83	127.20
21	1	601	CHL	CHC-C4B-NB	-3.34	120.73	124.26
27	B	1609	BCR	C20-C21-C22	-3.33	122.55	127.31
24	7	619	XAT	C16-C1-C2	-3.33	103.20	108.98
21	V	601	CHL	CHD-C4C-C3C	-3.32	119.95	124.84
22	B	810	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
27	F	305	BCR	C37-C22-C23	3.32	123.31	118.08
27	A	849	BCR	C36-C18-C19	3.32	123.31	118.08
27	6	621	BCR	C33-C5-C4	3.32	119.99	113.62
24	W	2622	XAT	O4-C5-C18	3.31	119.03	115.06
27	B	847	BCR	C20-C21-C22	-3.31	122.58	127.31
22	7	602	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
27	3	620	BCR	C1-C6-C5	-3.31	117.95	122.61
27	3	621	BCR	C11-C10-C9	-3.31	122.58	127.31
23	2	619	LUT	C40-C33-C34	-3.31	118.29	122.92
22	A	820	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
21	4	618	CHL	CHD-C4C-C3C	-3.30	119.98	124.84
21	W	606	CHL	C2A-C1A-CHA	-3.30	118.09	123.85
27	B	843	BCR	C27-C26-C25	-3.30	117.94	122.73
22	8	610	CLA	C4A-NA-C1A	3.30	108.19	106.71
21	6	602	CHL	CHB-C4A-NA	3.30	129.08	124.51
23	2	619	LUT	C20-C13-C14	-3.30	118.30	122.92
27	7	621	BCR	C38-C26-C27	3.30	119.96	113.62
22	B	831	CLA	C4-C3-C5	3.30	120.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	805	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	U	2620	LUT	C3-C4-C5	-3.30	105.29	111.85
23	9	621	LUT	C19-C9-C8	3.30	123.27	118.08
27	B	843	BCR	C36-C18-C19	3.29	123.27	118.08
24	V	2622	XAT	O4-C5-C6	-3.29	56.23	58.96
21	U	606	CHL	CHC-C4B-NB	-3.29	120.77	124.26
25	U	2623	NEX	C39-C29-C30	-3.29	118.32	122.92
21	8	608	CHL	CHC-C4B-NB	-3.29	120.78	124.26
27	A	852	BCR	C30-C25-C26	-3.29	117.98	122.61
27	A	852	BCR	C38-C26-C25	-3.28	120.84	124.53
22	B	808	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
27	6	621	BCR	C15-C14-C13	-3.28	122.63	127.31
21	V	605	CHL	C2A-C1A-CHA	-3.28	118.13	123.85
21	4	608	CHL	CHB-C4A-NA	3.27	129.04	124.51
27	B	848	BCR	C8-C7-C6	-3.27	118.01	127.20
27	8	621	BCR	C8-C7-C6	-3.27	118.02	127.20
27	7	621	BCR	C4-C5-C6	-3.27	117.98	122.73
23	W	2621	LUT	C3-C4-C5	-3.27	105.34	111.85
23	9	620	LUT	C11-C10-C9	-3.26	122.65	127.31
27	B	848	BCR	C20-C21-C22	-3.26	122.65	127.31
22	A	804	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	9	621	LUT	C36-C21-C26	3.26	114.48	109.55
21	U	601	CHL	CHB-C4A-NA	3.26	129.02	124.51
27	B	845	BCR	C23-C22-C21	3.26	123.94	118.94
28	L	307	LMG	O7-C10-C11	3.25	118.51	111.50
27	G	205	BCR	C15-C16-C17	-3.25	116.82	123.47
27	3	621	BCR	C38-C26-C27	3.25	119.85	113.62
27	2	621	BCR	C7-C8-C9	-3.25	121.33	126.23
27	B	843	BCR	C34-C9-C8	3.25	123.19	118.08
27	B	801	BCR	C36-C18-C19	3.24	123.19	118.08
21	U	605	CHL	C2A-C1A-CHA	-3.24	118.20	123.85
23	6	619	LUT	C15-C35-C34	-3.24	116.84	123.47
21	2	607	CHL	CHC-C4B-NB	-3.24	120.83	124.26
21	6	608	CHL	CHC-C4B-NB	-3.23	120.83	124.26
27	A	848	BCR	C30-C25-C26	-3.23	118.07	122.61
22	A	824	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
21	U	607	CHL	CHC-C4B-NB	-3.23	120.84	124.26
24	1	618	XAT	C6-C7-C8	-3.22	119.18	125.99
27	K	202	BCR	C34-C9-C8	3.22	123.15	118.08
27	M	2001	BCR	C20-C21-C22	-3.22	122.72	127.31
24	5	618	XAT	C31-C32-C33	-3.22	117.38	126.42
22	V	602	CLA	O2D-CGD-O1D	-3.22	117.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	8	606	CHL	CAC-C3C-C4C	3.22	128.98	124.81
27	A	851	BCR	C30-C25-C26	-3.21	118.08	122.61
21	V	601	CHL	O2A-CGA-CBA	3.21	122.00	111.91
27	B	844	BCR	C1-C6-C7	3.21	124.87	115.78
27	7	620	BCR	C33-C5-C6	-3.21	120.92	124.53
22	V	613	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
27	B	843	BCR	C29-C30-C25	3.21	115.42	110.48
24	7	619	XAT	C39-C29-C28	3.21	123.14	118.08
27	L	301	BCR	C16-C15-C14	-3.21	116.90	123.47
21	W	607	CHL	CHB-C4A-NA	3.21	128.95	124.51
21	9	606	CHL	CHB-C4A-NA	3.21	128.94	124.51
27	A	851	BCR	C24-C25-C26	-3.21	113.70	121.46
21	1	601	CHL	CAC-C3C-C4C	3.20	128.97	124.81
27	A	851	BCR	C38-C26-C27	3.20	119.77	113.62
21	V	609	CHL	CHC-C4B-NB	-3.20	120.87	124.26
21	6	601	CHL	CHC-C4B-NB	-3.20	120.87	124.26
23	9	620	LUT	C19-C9-C8	3.20	123.12	118.08
27	L	305	BCR	C36-C18-C19	3.20	123.12	118.08
24	6	620	XAT	C27-C28-C29	-3.20	120.56	125.53
22	9	609	CLA	CHC-C4B-NB	-3.20	120.87	124.26
23	3	618	LUT	C17-C1-C6	-3.20	105.11	110.30
21	6	602	CHL	CMB-C2B-C1B	3.20	130.24	125.37
22	9	609	CLA	C2A-C1A-CHA	-3.20	118.27	123.86
23	6	619	LUT	C7-C8-C9	-3.20	121.40	126.23
27	B	801	BCR	C24-C23-C22	-3.20	121.40	126.23
27	A	849	BCR	C16-C17-C18	-3.20	122.75	127.31
22	A	834	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
21	3	608	CHL	CHB-C4A-NA	3.19	128.93	124.51
22	A	803	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	7	611	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
22	B	818	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	831	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	A	835	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
27	A	852	BCR	C7-C8-C9	-3.19	121.42	126.23
21	W	608	CHL	CHB-C4A-NA	3.19	128.92	124.51
27	L	301	BCR	C11-C10-C9	-3.19	122.76	127.31
21	W	605	CHL	C2A-C1A-CHA	-3.18	118.30	123.85
22	B	802	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
24	8	620	XAT	C32-C33-C34	3.18	123.82	118.94
24	2	620	XAT	C35-C15-C14	-3.18	116.97	123.47
27	B	847	BCR	C11-C10-C9	-3.18	122.78	127.31
23	W	2621	LUT	C7-C8-C9	-3.18	121.44	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	816	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
27	K	202	BCR	C28-C27-C26	-3.17	108.41	114.08
24	2	620	XAT	C6-C7-C8	-3.17	119.29	125.99
22	A	801	CLA	C4A-NA-C1A	3.17	108.13	106.71
21	U	608	CHL	CHB-C4A-NA	3.17	128.90	124.51
27	8	621	BCR	C30-C25-C24	3.17	124.74	115.78
21	U	605	CHL	CHB-C4A-NA	3.16	128.89	124.51
22	5	610	CLA	C4A-NA-C1A	3.16	108.13	106.71
22	A	845	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
27	K	205	BCR	C16-C17-C18	-3.16	122.80	127.31
21	V	605	CHL	CHB-C4A-NA	3.16	128.88	124.51
26	8	630	LHG	O8-C23-C24	3.16	121.82	111.91
21	4	606	CHL	CHC-C4B-NB	-3.16	120.91	124.26
24	5	618	XAT	C6-C7-C8	-3.16	119.31	125.99
22	L	303	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
22	8	602	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
21	4	607	CHL	CHC-C4B-NB	-3.15	120.92	124.26
22	3	607	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
21	V	607	CHL	CHB-C4A-NA	3.15	128.87	124.51
27	G	205	BCR	C33-C5-C6	-3.15	120.99	124.53
23	9	621	LUT	C7-C8-C9	-3.15	121.47	126.23
22	9	609	CLA	CHB-C4A-NA	3.15	128.87	124.51
24	6	620	XAT	C19-C9-C8	3.15	123.04	118.08
21	2	618	CHL	CHC-C4B-NB	-3.15	120.92	124.26
22	B	833	CLA	C4-C3-C5	3.15	120.56	115.27
24	2	620	XAT	C26-C27-C28	-3.15	119.34	125.99
22	O	2003	CLA	C3A-C4A-CHB	-3.14	120.06	123.91
21	6	607	CHL	CHB-C4A-NA	3.14	128.86	124.51
22	B	834	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
27	B	1609	BCR	C39-C30-C29	3.14	121.48	108.91
21	V	607	CHL	C2A-C1A-CHA	-3.14	118.37	123.85
21	5	601	CHL	CHC-C4B-NB	-3.14	120.93	124.26
21	1	607	CHL	CHC-C4B-NB	-3.14	120.93	124.26
23	W	2621	LUT	C19-C9-C8	3.14	123.02	118.08
23	4	619	LUT	C36-C21-C26	3.14	114.29	109.55
22	A	840	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
24	U	2622	XAT	C26-C27-C28	-3.13	119.38	125.99
22	1	611	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
27	A	850	BCR	C33-C5-C6	-3.13	121.02	124.53
22	U	614	CLA	C4A-NA-C1A	3.13	108.11	106.71
27	2	621	BCR	C32-C1-C6	-3.13	105.23	110.30
22	A	842	CLA	O2D-CGD-O1D	-3.13	117.73	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	847	BCR	C15-C16-C17	-3.13	117.07	123.47
22	5	612	CLA	C4A-NA-C1A	3.13	108.11	106.71
22	8	611	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
27	J	102	BCR	C38-C26-C27	3.12	119.62	113.62
21	U	609	CHL	CHC-C4B-NB	-3.12	120.95	124.26
22	2	609	CLA	O2D-CGD-CBD	3.12	116.81	111.27
22	B	824	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	A	827	CLA	CHD-C1D-ND	-3.12	121.59	124.45
21	2	601	CHL	CHC-C4B-NB	-3.12	120.96	124.26
21	V	606	CHL	CAC-C3C-C4C	3.12	129.78	125.04
27	O	2004	BCR	C1-C6-C7	3.11	124.59	115.78
24	7	619	XAT	C15-C14-C13	-3.11	122.87	127.31
22	B	804	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
21	6	606	CHL	CHC-C4B-NB	-3.11	120.97	124.26
27	B	848	BCR	C37-C22-C23	3.11	122.98	118.08
21	U	608	CHL	CAC-C3C-C4C	3.11	129.77	125.04
27	A	851	BCR	C11-C10-C9	-3.11	122.88	127.31
22	1	603	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
23	U	2620	LUT	C36-C21-C26	3.10	114.25	109.55
25	U	2623	NEX	C15-C14-C13	-3.10	122.88	127.31
22	A	839	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	1	608	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
22	A	816	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
21	W	605	CHL	CHB-C4A-NA	3.10	128.80	124.51
21	9	607	CHL	C1C-C2C-C3C	-3.10	104.65	107.11
21	6	601	CHL	CHB-C4A-NA	3.10	128.80	124.51
27	B	848	BCR	C16-C17-C18	-3.10	122.89	127.31
27	F	305	BCR	C11-C10-C9	-3.10	122.89	127.31
22	A	802	CLA	C4A-NA-C1A	3.10	108.10	106.71
22	1	612	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
21	2	608	CHL	CMB-C2B-C1B	3.09	130.08	125.37
22	5	613	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
27	1	619	BCR	C16-C15-C14	-3.09	117.14	123.47
21	W	601	CHL	CHB-C4A-NA	3.09	128.79	124.51
24	4	620	XAT	O4-C5-C6	-3.09	56.40	58.96
22	B	813	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
21	2	608	CHL	CHC-C4B-NB	-3.09	120.99	124.26
27	A	852	BCR	C36-C18-C17	-3.09	118.60	122.92
21	W	606	CHL	CAC-C3C-C4C	3.08	129.74	125.04
21	W	608	CHL	CAC-C3C-C4C	3.08	129.74	125.04
21	U	607	CHL	CHB-C4A-NA	3.08	128.78	124.51
21	6	618	CHL	C3B-C4B-NB	3.08	113.37	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	604	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	4	620	XAT	C31-C30-C29	-3.08	122.91	127.31
23	1	617	LUT	C3-C4-C5	-3.08	105.72	111.85
22	B	837	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
21	6	618	CHL	CHB-C4A-NA	3.08	128.77	124.51
22	A	810	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
21	2	618	CHL	CHB-C4A-NA	3.08	128.76	124.51
23	9	624	LUT	C39-C29-C28	3.07	122.92	118.08
27	A	856	BCR	C23-C22-C21	-3.07	117.97	124.81
27	1	619	BCR	C20-C21-C22	-3.07	122.92	127.31
21	6	607	CHL	CHC-C4B-NB	-3.07	121.01	124.26
24	7	619	XAT	C18-C5-C4	-3.07	110.83	114.28
23	U	2621	LUT	C3-C4-C5	-3.07	105.74	111.85
22	A	830	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
27	K	205	BCR	C33-C5-C4	3.06	119.50	113.62
22	B	812	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	U	607	CHL	C4-C3-C2	-3.06	115.82	123.68
21	V	605	CHL	C3B-C4B-NB	3.06	113.36	110.52
22	V	610	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
21	9	606	CHL	C3B-C4B-NB	3.06	113.36	110.52
22	A	833	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	V	2622	XAT	C31-C30-C29	-3.06	122.94	127.31
21	8	608	CHL	CHB-C4A-NA	3.06	128.74	124.51
31	A	857	LMT	C1'-C2'-C3'	-3.06	103.62	110.00
22	2	611	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
21	5	601	CHL	C1-C2-C3	-3.06	121.80	126.75
27	A	848	BCR	C16-C15-C14	-3.06	117.21	123.47
24	1	618	XAT	C32-C33-C34	-3.06	114.25	118.94
21	5	607	CHL	C2A-C1A-CHA	-3.05	118.52	123.85
22	3	617	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
21	9	605	CHL	CHC-C4B-NB	-3.05	121.03	124.26
24	4	620	XAT	C27-C28-C29	-3.05	120.80	125.53
22	B	820	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
27	B	847	BCR	C24-C23-C22	-3.05	121.62	126.23
21	W	605	CHL	CAC-C3C-C4C	3.05	129.69	125.04
21	7	608	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
27	2	621	BCR	C15-C14-C13	-3.05	122.96	127.31
22	A	814	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	4	620	XAT	C39-C29-C28	3.05	122.88	118.08
21	6	606	CHL	C2A-C1A-CHA	-3.05	118.53	123.86
21	V	605	CHL	CHC-C4B-NB	-3.05	121.03	124.26
21	6	608	CHL	CHB-C4A-NA	3.05	128.73	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	U	2620	LUT	C7-C8-C9	-3.05	121.63	126.23
22	B	823	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
21	7	608	CHL	CHC-C4B-NB	-3.05	121.03	124.26
21	V	601	CHL	CHB-C4A-NA	3.05	128.72	124.51
21	4	606	CHL	CHB-C4A-NA	3.05	128.72	124.51
21	7	608	CHL	CHB-C4A-NA	3.05	128.72	124.51
21	W	607	CHL	C2A-C1A-CHA	-3.05	118.54	123.85
22	A	801	CLA	CGD-CBD-CAD	3.05	120.60	110.73
22	A	828	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	2	612	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	6	601	CHL	O2A-CGA-CBA	3.04	121.45	111.91
21	W	601	CHL	CMB-C2B-C1B	3.04	130.00	125.37
27	3	620	BCR	C29-C30-C25	3.04	115.16	110.48
22	4	609	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	7	620	BCR	C15-C14-C13	-3.04	122.98	127.31
27	A	849	BCR	C38-C26-C27	3.03	119.44	113.62
21	5	607	CHL	CHC-C4B-NB	-3.03	121.05	124.26
27	J	102	BCR	C34-C9-C8	3.03	122.85	118.08
31	K	208	LMT	C1'-O5'-C5'	-3.03	107.74	113.69
22	A	808	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	8	607	CHL	CHC-C4B-NB	-3.03	121.05	124.26
21	U	606	CHL	C2A-C1A-CHA	-3.03	118.56	123.86
27	B	848	BCR	C7-C8-C9	-3.03	121.66	126.23
22	W	610	CLA	C4-C3-C2	-3.03	115.91	123.68
22	B	803	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	9	611	CLA	CAA-C2A-C3A	-3.03	104.49	112.78
24	1	618	XAT	C39-C29-C28	3.03	122.85	118.08
22	A	811	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	A	843	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	A	812	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
27	8	621	BCR	C33-C5-C4	3.02	119.42	113.62
21	2	602	CHL	C4A-NA-C1A	-3.02	105.35	106.71
21	V	606	CHL	CHB-C4A-NA	3.02	128.69	124.51
22	A	826	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	4	620	XAT	C35-C15-C14	-3.02	117.28	123.47
22	A	831	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	9	623	NEX	C15-C35-C34	-3.02	117.29	123.47
27	G	205	BCR	C36-C18-C19	3.02	122.83	118.08
27	B	801	BCR	C32-C1-C6	-3.02	105.40	110.30
23	U	2621	LUT	C36-C21-C26	3.02	114.12	109.55
21	8	606	CHL	CHC-C4B-NB	-3.02	121.06	124.26
22	B	814	CLA	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	851	BCR	C33-C5-C6	-3.02	121.14	124.53
22	4	612	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	5	608	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	W	2623	NEX	C26-C27-C28	-3.01	119.62	125.99
27	8	621	BCR	C38-C26-C25	-3.01	121.14	124.53
23	V	2621	LUT	C7-C8-C9	-3.01	121.68	126.23
21	2	606	CHL	CHC-C4B-NB	-3.01	121.07	124.26
21	9	607	CHL	CHC-C4B-NB	-3.01	121.07	124.26
27	A	850	BCR	C11-C10-C9	-3.01	123.01	127.31
23	5	617	LUT	C35-C15-C14	3.01	129.64	123.47
22	B	826	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	4	620	XAT	C38-C25-C24	3.01	117.67	114.28
24	7	619	XAT	C26-C27-C28	-3.01	119.63	125.99
27	B	844	BCR	C30-C25-C26	-3.01	118.38	122.61
22	W	604	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
21	V	608	CHL	CAC-C3C-C4C	3.01	129.62	125.04
24	5	618	XAT	C24-C23-C22	-3.01	104.97	110.77
21	W	607	CHL	CAC-C3C-C4C	3.01	129.62	125.04
27	B	843	BCR	C7-C8-C9	-3.00	121.69	126.23
21	7	608	CHL	C3B-C4B-NB	3.00	113.30	110.52
21	9	601	CHL	C3B-C4B-NB	3.00	113.30	110.52
21	2	601	CHL	CHB-C4A-NA	3.00	128.66	124.51
22	7	617	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	9	609	CLA	CMC-C2C-C1C	3.00	129.60	125.04
21	8	608	CHL	C1-C2-C3	-3.00	121.90	126.75
27	6	621	BCR	C3-C4-C5	-3.00	108.72	114.08
27	A	850	BCR	C30-C25-C26	-3.00	118.39	122.61
25	U	2623	NEX	C2-C1-C6	3.00	112.12	109.21
23	U	2620	LUT	C8-C7-C6	-2.99	118.79	127.20
22	V	613	CLA	C1-C2-C3	-2.99	120.87	126.04
21	4	608	CHL	CHB-C1B-NB	-2.99	121.09	124.26
22	4	601	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	8	607	CHL	CHB-C4A-NA	2.99	128.65	124.51
22	A	817	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	L	301	BCR	C39-C30-C25	2.99	115.15	110.30
27	L	306	BCR	C37-C22-C23	2.99	122.78	118.08
27	3	621	BCR	C32-C1-C6	-2.99	105.45	110.30
22	8	614	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	3	615	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
21	V	606	CHL	CMB-C2B-C1B	2.98	129.91	125.37
22	A	823	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	U	606	CHL	CHB-C4A-NA	2.98	128.63	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	3	619	XAT	C18-C5-C4	2.98	117.63	114.28
21	4	618	CHL	C3B-C4B-NB	2.98	113.28	110.52
24	W	2622	XAT	C26-C27-C28	-2.98	119.70	125.99
22	B	824	CLA	C4-C3-C5	2.98	120.28	115.27
24	1	618	XAT	C15-C14-C13	-2.98	123.06	127.31
22	A	832	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
27	A	852	BCR	C16-C17-C18	-2.98	123.06	127.31
27	M	2001	BCR	C8-C9-C10	2.97	123.51	118.94
22	A	813	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	V	2623	NEX	C15-C14-C13	-2.97	123.07	127.31
27	I	101	BCR	C8-C7-C6	-2.97	118.85	127.20
27	B	844	BCR	C28-C27-C26	-2.97	108.77	114.08
22	4	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	A	806	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	9	605	CHL	C3B-C4B-NB	2.97	113.27	110.52
22	B	840	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	2	607	CHL	CHB-C4A-NA	2.97	128.62	124.51
27	A	851	BCR	C15-C14-C13	-2.97	123.07	127.31
21	2	606	CHL	CHB-C4A-NA	2.97	128.62	124.51
21	8	618	CHL	CHB-C4A-NA	2.97	128.62	124.51
22	B	829	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	V	608	CHL	C2A-C1A-CHA	-2.97	118.67	123.86
22	3	613	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
27	A	851	BCR	C7-C8-C9	-2.97	121.75	126.23
22	7	611	CLA	C4A-NA-C1A	2.97	108.04	106.71
23	5	617	LUT	C8-C9-C10	2.97	123.49	118.94
22	U	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
27	K	205	BCR	C38-C26-C27	2.97	119.31	113.62
21	U	609	CHL	CMD-C2D-C3D	-2.97	120.79	127.61
23	9	624	LUT	C22-C23-C24	2.96	115.11	111.74
22	1	613	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	5	609	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	6	609	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
27	K	205	BCR	C37-C22-C23	2.96	122.74	118.08
22	B	838	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	7	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	9	606	CHL	CMD-C2D-C3D	-2.96	120.80	127.61
27	B	843	BCR	C16-C17-C18	-2.96	123.08	127.31
27	6	621	BCR	C35-C13-C12	2.96	122.74	118.08
21	W	607	CHL	CMB-C2B-C1B	2.96	129.88	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	605	CHL	CHB-C4A-NA	2.96	128.60	124.51
21	U	607	CHL	C2A-C1A-CHA	-2.96	118.69	123.86
21	2	606	CHL	C2A-C1A-CHA	-2.96	118.69	123.86
23	9	620	LUT	C36-C21-C26	2.96	114.03	109.55
27	4	621	BCR	C15-C16-C17	-2.96	117.42	123.47
22	O	2001	CLA	C3A-C4A-CHB	-2.96	120.29	123.91
22	3	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
21	2	601	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
21	W	608	CHL	CHB-C1B-NB	-2.95	121.13	124.26
21	V	607	CHL	CAC-C3C-C4C	2.95	129.54	125.04
27	A	851	BCR	C38-C26-C25	-2.95	121.21	124.53
27	A	849	BCR	C24-C23-C22	-2.95	121.77	126.23
22	B	814	CLA	C1-C2-C3	-2.95	120.94	126.04
27	B	848	BCR	C29-C30-C25	2.95	115.02	110.48
22	U	612	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	7	621	BCR	C30-C25-C26	-2.95	118.46	122.61
27	8	621	BCR	C15-C14-C13	-2.95	123.10	127.31
21	U	605	CHL	CAC-C3C-C4C	2.95	129.53	125.04
22	6	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	F	305	BCR	C16-C17-C18	-2.95	123.10	127.31
22	K	206	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	5	608	CLA	C1-C2-C3	-2.95	121.98	126.75
21	U	605	CHL	CMB-C2B-C1B	2.94	129.85	125.37
22	3	611	CLA	O2D-CGD-CBD	2.94	116.50	111.27
27	7	621	BCR	C20-C21-C22	-2.94	123.11	127.31
21	6	602	CHL	O2A-CGA-CBA	2.94	121.14	111.91
22	3	610	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	B	841	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	9	602	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
21	V	606	CHL	C2A-C1A-CHA	-2.94	118.72	123.85
23	V	2621	LUT	C19-C9-C8	2.94	122.71	118.08
22	4	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	W	612	CLA	CMA-C3A-C2A	-2.94	109.24	116.10
22	V	603	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
27	3	620	BCR	C16-C17-C18	-2.94	123.12	127.31
27	4	621	BCR	C36-C18-C19	2.93	122.70	118.08
22	4	610	CLA	C4A-NA-C1A	2.93	108.03	106.71
21	9	605	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
23	5	617	LUT	C28-C29-C30	2.93	123.44	118.94
21	6	608	CHL	C3B-C4B-NB	2.93	113.23	110.52
22	3	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	9	601	CHL	CHB-C4A-NA	2.93	128.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	850	BCR	C38-C26-C27	2.93	119.24	113.62
24	8	620	XAT	C8-C9-C10	2.93	123.43	118.94
21	5	601	CHL	CHB-C4A-NA	2.93	128.56	124.51
21	U	607	CHL	C3B-C4B-NB	2.93	113.23	110.52
22	A	836	CLA	C4B-C3B-CAB	-2.93	122.54	129.25
27	1	619	BCR	C21-C20-C19	-2.92	114.09	123.22
27	I	101	BCR	C30-C25-C26	-2.92	118.50	122.61
22	7	614	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	7	630	LHG	O8-C23-C24	2.92	121.07	111.91
21	8	606	CHL	CHB-C4A-NA	2.92	128.55	124.51
22	8	610	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
21	V	607	CHL	CMB-C2B-C1B	2.92	129.81	125.37
21	2	602	CHL	CMB-C2B-C1B	2.92	129.81	125.37
21	2	618	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
22	A	830	CLA	C4A-NA-C1A	2.92	108.02	106.71
22	B	832	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
21	9	607	CHL	CAC-C3C-C4C	2.92	128.59	124.81
27	1	619	BCR	C33-C5-C4	2.92	119.22	113.62
22	3	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	9	624	LUT	C38-C25-C24	-2.91	117.32	123.56
21	U	609	CHL	C2A-C1A-CHA	-2.91	118.77	123.86
22	4	614	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	L	303	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	9	611	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	2	619	LUT	C12-C13-C14	2.91	123.41	118.94
22	G	204	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	6	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	W	605	CHL	CMB-C2B-C1B	2.91	129.80	125.37
22	8	613	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	9	606	CHL	CHC-C4B-NB	-2.91	121.18	124.26
27	1	619	BCR	C11-C12-C13	-2.91	118.24	126.42
27	L	306	BCR	C11-C10-C9	-2.91	123.16	127.31
27	B	1609	BCR	C30-C25-C24	2.91	124.00	115.78
22	4	604	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
27	B	844	BCR	C7-C8-C9	-2.90	121.85	126.23
21	W	609	CHL	C2A-C1A-CHA	-2.90	118.78	123.86
24	3	619	XAT	C6-C7-C8	-2.90	119.86	125.99
27	B	844	BCR	C15-C16-C17	-2.90	117.53	123.47
22	1	604	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
21	4	618	CHL	CHB-C4A-NA	2.90	128.52	124.51
27	J	102	BCR	C37-C22-C23	2.90	122.65	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	U	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	7	619	XAT	C15-C35-C34	-2.90	117.54	123.47
22	9	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
27	G	205	BCR	C7-C8-C9	-2.90	121.86	126.23
22	B	825	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
27	1	619	BCR	C40-C30-C25	-2.89	105.60	110.30
22	A	821	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
21	W	601	CHL	O2A-CGA-CBA	2.89	120.99	111.91
27	A	848	BCR	C32-C1-C6	-2.89	105.61	110.30
27	1	619	BCR	C33-C5-C6	-2.89	121.28	124.53
22	1	616	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	2	613	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
21	V	608	CHL	CMB-C2B-C1B	2.89	129.77	125.37
27	B	1609	BCR	C2-C1-C6	2.89	114.93	110.48
21	7	608	CHL	C2A-C1A-CHA	-2.89	118.81	123.86
22	A	822	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	A	825	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
21	6	606	CHL	C3B-C4B-NB	2.89	113.19	110.52
23	6	619	LUT	C32-C33-C34	-2.88	114.51	118.94
21	9	601	CHL	CHC-C4B-NB	-2.88	121.20	124.26
31	A	857	LMT	C1'-O5'-C5'	-2.88	108.03	113.69
21	V	609	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
21	U	607	CHL	O2A-CGA-CBA	2.88	120.96	111.91
22	9	609	CLA	C3B-C4B-NB	2.88	113.19	110.52
27	J	102	BCR	C4-C5-C6	-2.88	118.55	122.73
24	8	620	XAT	C27-C28-C29	2.88	130.00	125.53
22	G	201	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	8	612	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	2	613	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
26	4	630	LHG	O8-C23-C24	2.88	120.95	111.91
21	6	602	CHL	OMC-CMC-C2C	-2.88	119.17	125.69
21	9	607	CHL	CHB-C4A-NA	2.88	128.49	124.51
22	F	301	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	806	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
21	V	609	CHL	C3B-C4B-NB	2.88	113.18	110.52
22	B	833	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	L	304	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	U	2622	XAT	O4-C5-C18	2.88	118.50	115.06
24	8	620	XAT	C38-C25-C26	-2.88	117.44	122.26
22	1	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	5	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	616	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	3	620	BCR	C11-C10-C9	-2.87	123.21	127.31
22	W	611	CLA	O2D-CGD-O1D	-2.87	117.57	124.09
21	1	607	CHL	CHB-C4A-NA	2.87	128.48	124.51
27	4	621	BCR	C30-C25-C26	-2.87	118.57	122.61
21	9	608	CHL	C3B-C4B-NB	2.87	113.18	110.52
21	9	606	CHL	CMB-C2B-C1B	2.87	129.74	125.37
21	5	607	CHL	CHB-C4A-NA	2.87	128.48	124.51
21	2	607	CHL	CMD-C2D-C3D	-2.87	121.02	127.61
22	B	830	CLA	CHD-C1D-ND	-2.87	121.82	124.45
27	A	851	BCR	C15-C16-C17	-2.87	117.60	123.47
22	4	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	A	842	CLA	CHD-C1D-ND	-2.87	121.82	124.45
27	L	305	BCR	C11-C10-C9	-2.87	123.22	127.31
27	A	849	BCR	C37-C22-C21	-2.86	118.91	122.92
22	6	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
21	6	602	CHL	C3B-C4B-NB	2.86	113.17	110.52
24	4	620	XAT	C15-C14-C13	-2.86	123.22	127.31
21	8	607	CHL	CMB-C2B-C1B	2.86	129.73	125.37
21	W	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
23	W	2621	LUT	C15-C14-C13	-2.86	123.23	127.31
27	K	202	BCR	C7-C8-C9	-2.86	121.91	126.23
22	U	602	CLA	C4-C3-C5	2.86	120.08	115.27
22	L	302	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	K	204	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	3	617	CLA	C4B-C3B-CAB	-2.86	122.69	129.25
21	2	602	CHL	CHB-C4A-NA	2.86	128.47	124.51
22	7	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	2	620	XAT	O4-C5-C18	2.86	118.48	115.06
28	A	860	LMG	O8-C28-C29	2.86	120.88	111.91
23	8	619	LUT	C7-C8-C9	-2.86	121.92	126.23
21	1	601	CHL	CHB-C4A-NA	2.86	128.46	124.51
27	B	844	BCR	C37-C22-C23	2.85	122.58	118.08
22	A	819	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	9	624	LUT	C7-C8-C9	-2.85	121.92	126.23
27	B	1609	BCR	C33-C5-C4	2.85	119.10	113.62
27	A	852	BCR	C3-C4-C5	-2.85	108.98	114.08
24	6	620	XAT	C18-C5-C6	-2.85	117.48	122.26
22	F	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	5	614	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
31	G	206	LMT	C1'-C2'-C3'	-2.85	104.06	110.00
27	B	848	BCR	C16-C15-C14	-2.85	117.64	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
21	6	601	CHL	C3B-C4B-NB	2.85	113.16	110.52
27	A	856	BCR	C7-C8-C9	-2.85	121.93	126.23
22	A	818	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	2	621	BCR	C8-C7-C6	-2.85	119.21	127.20
24	4	620	XAT	C8-C9-C10	-2.85	114.58	118.94
21	4	607	CHL	CHB-C4A-NA	2.84	128.44	124.51
22	4	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	9	602	CLA	C4-C3-C5	2.84	120.05	115.27
22	4	613	CLA	CHD-C1D-ND	-2.84	121.84	124.45
27	J	102	BCR	C15-C16-C17	-2.84	117.65	123.47
25	U	2623	NEX	C38-C25-C24	2.84	117.48	114.28
21	3	608	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
21	4	607	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
28	J	103	LMG	O8-C28-C29	2.84	120.81	111.91
21	V	601	CHL	CAA-C2A-C3A	2.84	120.54	112.78
27	B	844	BCR	C3-C4-C5	-2.84	109.01	114.08
21	V	609	CHL	CHB-C4A-NA	2.83	128.43	124.51
24	6	620	XAT	C6-C7-C8	-2.83	120.00	125.99
21	U	609	CHL	O2A-CGA-CBA	2.83	120.80	111.91
24	7	619	XAT	C31-C30-C29	-2.83	123.27	127.31
24	W	2622	XAT	C35-C34-C33	-2.83	123.27	127.31
24	3	619	XAT	O4-C5-C18	2.83	118.45	115.06
21	V	605	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
22	8	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	9	620	LUT	C35-C15-C14	-2.83	117.68	123.47
22	B	815	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	A	851	BCR	C37-C22-C23	2.83	122.53	118.08
25	9	623	NEX	C15-C14-C13	-2.83	123.27	127.31
23	9	621	LUT	C19-C9-C10	-2.83	118.96	122.92
24	6	620	XAT	C11-C10-C9	-2.83	123.27	127.31
21	5	601	CHL	O2A-CGA-CBA	2.83	120.78	111.91
22	V	602	CLA	CHD-C1D-ND	-2.83	121.86	124.45
21	5	601	CHL	O2D-CGD-O1D	-2.83	118.31	123.84
25	V	2623	NEX	O24-C25-C38	2.83	118.44	115.06
22	5	611	CLA	O2D-CGD-CBD	2.82	116.29	111.27
24	W	2622	XAT	C31-C30-C29	-2.82	123.28	127.31
21	U	601	CHL	CMB-C2B-C1B	2.82	129.67	125.37
27	L	305	BCR	C16-C17-C18	-2.82	123.29	127.31
22	B	830	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	5	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	8	621	BCR	C36-C18-C17	-2.82	118.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	608	CHL	CHB-C4A-NA	2.82	128.41	124.51
21	W	601	CHL	CHB-C1B-NB	-2.81	121.28	124.26
21	V	601	CHL	C2A-C1A-CHA	-2.81	118.94	123.86
21	5	607	CHL	C3B-C4B-NB	2.81	113.12	110.52
21	8	607	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
22	3	603	CLA	CHB-C1B-NB	2.81	127.23	124.26
21	6	607	CHL	C2A-C1A-CHA	-2.81	118.95	123.86
22	5	612	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
24	1	618	XAT	C4-C3-C2	-2.80	105.36	110.77
28	J	104	LMG	O8-C28-C29	2.80	120.71	111.91
21	1	601	CHL	O2A-CGA-CBA	2.80	120.71	111.91
22	A	841	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	2	620	XAT	C8-C9-C10	-2.80	114.64	118.94
27	K	205	BCR	C1-C6-C7	2.80	123.71	115.78
27	K	205	BCR	C23-C24-C25	-2.80	119.33	127.20
27	K	202	BCR	C24-C23-C22	-2.80	122.00	126.23
22	3	606	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	V	2623	NEX	C15-C35-C34	-2.80	117.74	123.47
21	8	608	CHL	C3B-C4B-NB	2.80	113.11	110.52
22	B	811	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	V	2621	LUT	C15-C14-C13	-2.80	123.31	127.31
27	A	848	BCR	C35-C13-C12	2.80	122.49	118.08
22	U	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
27	2	621	BCR	C40-C30-C25	-2.80	105.76	110.30
24	W	2622	XAT	C35-C15-C14	-2.80	117.75	123.47
22	8	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	835	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	B	847	BCR	C29-C30-C25	2.80	114.78	110.48
21	W	609	CHL	CHB-C1B-NB	-2.80	121.30	124.26
22	8	601	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	U	601	CHL	C1-C2-C3	-2.79	121.21	126.04
21	8	618	CHL	CHC-C4B-NB	-2.79	121.30	124.26
22	7	609	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	2	608	CHL	CHB-C4A-NA	2.79	128.37	124.51
27	O	2004	BCR	C2-C1-C6	2.79	114.78	110.48
22	2	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	L	306	BCR	C28-C27-C26	-2.79	109.10	114.08
22	7	606	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	6	601	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
22	A	838	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	B	801	BCR	C29-C30-C25	2.79	114.77	110.48
27	7	620	BCR	C40-C30-C25	-2.79	105.78	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	620	XAT	C26-C27-C28	-2.79	120.10	125.99
27	2	621	BCR	C34-C9-C10	-2.78	119.02	122.92
21	V	601	CHL	CMB-C2B-C1B	2.78	129.61	125.37
24	6	620	XAT	C8-C9-C10	-2.78	114.67	118.94
27	A	851	BCR	C24-C23-C22	-2.78	122.03	126.23
27	A	848	BCR	C34-C9-C8	2.78	122.46	118.08
22	7	613	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
27	3	621	BCR	C37-C22-C23	2.78	122.46	118.08
22	B	837	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	U	2623	NEX	C19-C9-C10	-2.78	119.03	122.92
22	8	611	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	B	827	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	2	614	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	6	602	CHL	C2A-C1A-CHA	-2.78	119.00	123.86
25	9	623	NEX	C11-C10-C9	-2.78	123.35	127.31
24	7	619	XAT	C8-C9-C10	2.77	123.19	118.94
27	3	620	BCR	C23-C22-C21	-2.77	114.69	118.94
21	9	608	CHL	CHC-C4B-NB	-2.77	121.32	124.26
22	7	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	A	805	CLA	CHD-C1D-ND	-2.77	121.91	124.45
24	1	618	XAT	C15-C35-C34	-2.76	117.81	123.47
27	F	305	BCR	C36-C18-C19	2.76	122.43	118.08
21	2	618	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
22	K	201	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
25	W	2623	NEX	C11-C12-C13	-2.76	118.65	126.42
23	9	624	LUT	C40-C33-C32	2.76	122.43	118.08
27	I	101	BCR	C7-C8-C9	-2.76	122.06	126.23
27	A	851	BCR	C8-C9-C10	-2.76	114.70	118.94
21	9	608	CHL	C2A-C1A-CHA	-2.76	119.03	123.86
22	6	614	CLA	C1-C2-C3	-2.76	122.28	126.75
22	V	611	CLA	C3B-C4B-NB	-2.76	108.38	110.23
22	2	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
21	1	607	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
22	A	827	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	7	602	CLA	CHC-C4B-NB	2.76	127.18	124.26
22	G	203	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	2	619	LUT	C32-C33-C34	2.76	123.17	118.94
21	U	609	CHL	C3B-C4B-NB	2.76	113.07	110.52
21	W	601	CHL	C1-C2-C3	-2.76	121.28	126.04
21	6	607	CHL	C3B-C4B-NB	2.75	113.07	110.52
21	8	618	CHL	C3B-C4B-NB	2.75	113.07	110.52
21	W	606	CHL	CMB-C2B-C1B	2.75	129.56	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	618	CHL	O2D-CGD-O1D	-2.75	118.45	123.84
21	U	608	CHL	C2A-C1A-CHA	-2.75	119.05	123.86
27	M	2001	BCR	C30-C25-C26	-2.75	118.74	122.61
24	V	2622	XAT	C11-C10-C9	-2.75	123.38	127.31
22	B	828	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	2	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	K	202	BCR	C36-C18-C19	2.75	122.41	118.08
22	A	854	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	A	852	BCR	C19-C18-C17	2.75	123.16	118.94
22	A	801	CLA	C4D-C3D-CAD	-2.75	104.86	108.10
22	A	818	CLA	CHD-C1D-ND	-2.75	121.93	124.45
27	A	856	BCR	C21-C20-C19	-2.75	117.81	124.67
23	U	2620	LUT	C19-C9-C8	2.75	122.40	118.08
22	1	606	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	V	2620	LUT	C19-C9-C8	2.74	122.40	118.08
22	B	806	CLA	CHD-C1D-ND	-2.74	121.93	124.45
22	W	602	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
21	V	605	CHL	O1D-CGD-CBD	-2.74	118.87	124.48
27	6	621	BCR	C35-C13-C14	-2.74	119.08	122.92
22	B	819	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	V	611	CLA	O2D-CGD-O1D	-2.74	117.86	124.09
22	W	611	CLA	CMB-C2B-C3B	2.74	130.69	123.59
21	U	601	CHL	CHB-C1B-NB	-2.74	121.36	124.26
21	2	601	CHL	C3B-C4B-NB	2.74	113.06	110.52
22	8	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	2	608	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
27	7	621	BCR	C34-C9-C8	2.74	122.39	118.08
24	V	2622	XAT	C27-C28-C29	-2.74	121.28	125.53
27	B	801	BCR	C16-C15-C14	-2.74	117.86	123.47
21	1	601	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
22	6	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	U	614	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	B	835	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
27	G	205	BCR	C28-C27-C26	-2.74	109.19	114.08
27	2	621	BCR	C16-C17-C18	-2.74	123.40	127.31
24	5	618	XAT	C7-C8-C9	-2.74	121.28	125.53
23	7	618	LUT	C18-C5-C4	2.74	119.42	114.36
21	V	601	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
27	F	305	BCR	C29-C30-C25	2.74	114.69	110.48
22	1	609	CLA	C4-C3-C5	2.74	119.87	115.27
27	B	1609	BCR	C32-C1-C6	-2.73	105.86	110.30
22	A	802	CLA	O2D-CGD-O1D	-2.73	118.49	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	608	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
22	A	810	CLA	C4-C3-C5	2.73	119.87	115.27
24	W	2622	XAT	C7-C8-C9	-2.73	121.29	125.53
22	B	817	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	1	602	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	4	621	BCR	C30-C25-C24	2.73	123.50	115.78
21	8	607	CHL	C2A-C1A-CHA	-2.73	119.08	123.86
21	U	609	CHL	CHB-C4A-NA	2.73	128.29	124.51
27	7	621	BCR	C11-C10-C9	-2.73	123.42	127.31
21	W	601	CHL	C2A-C1A-CHA	-2.73	119.09	123.86
22	6	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	8	606	CHL	CMD-C2D-C3D	-2.73	121.34	127.61
21	4	607	CHL	C3B-C4B-NB	2.73	113.05	110.52
22	7	602	CLA	C3B-C4B-NB	-2.73	107.99	110.52
24	1	618	XAT	C30-C31-C32	-2.73	114.71	123.22
25	U	2623	NEX	C11-C10-C9	-2.72	123.42	127.31
27	J	102	BCR	C37-C22-C21	-2.72	119.11	122.92
21	8	606	CHL	C3B-C4B-NB	2.72	113.04	110.52
21	4	606	CHL	C3B-C4B-NB	2.72	113.04	110.52
22	B	838	CLA	C3B-C4B-NB	-2.72	107.99	110.52
27	L	306	BCR	C15-C14-C13	-2.72	123.43	127.31
27	6	621	BCR	C16-C17-C18	-2.72	123.43	127.31
22	9	602	CLA	C4-C3-C2	-2.72	116.70	123.68
22	A	809	CLA	CHD-C1D-ND	-2.72	121.96	124.45
21	4	608	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	9	604	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
21	U	601	CHL	O2A-CGA-CBA	2.72	120.43	111.91
27	A	852	BCR	C1-C6-C7	2.72	123.46	115.78
22	3	607	CLA	CHD-C1D-ND	-2.71	121.96	124.45
27	B	845	BCR	C33-C5-C4	2.71	118.83	113.62
22	A	819	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	7	610	CLA	C3B-C4B-NB	-2.71	108.00	110.52
23	7	618	LUT	C18-C5-C6	-2.71	121.48	124.53
21	8	608	CHL	O2A-CGA-CBA	2.71	120.42	111.91
22	A	836	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
21	8	606	CHL	C2A-C1A-CHA	-2.71	119.12	123.86
21	6	608	CHL	C2A-C1A-CHA	-2.71	119.12	123.86
21	8	608	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
22	B	805	CLA	CHD-C1D-ND	-2.71	121.97	124.45
22	L	302	CLA	CHD-C1D-ND	-2.71	121.97	124.45
24	6	620	XAT	C20-C13-C12	2.71	122.34	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	V	608	CHL	CMD-C2D-C3D	-2.70	121.39	127.61
21	2	606	CHL	CMB-C2B-C1B	2.70	129.49	125.37
27	B	844	BCR	C38-C26-C27	2.70	118.81	113.62
24	W	2622	XAT	C11-C10-C9	-2.70	123.45	127.31
21	8	618	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
22	B	806	CLA	C1-C2-C3	-2.70	121.37	126.04
23	9	624	LUT	C28-C29-C30	-2.70	114.80	118.94
27	L	301	BCR	C7-C8-C9	-2.70	122.16	126.23
21	6	608	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
32	B	850	DGD	O1G-C1A-C2A	2.70	120.37	111.91
22	B	802	CLA	CHC-C4B-NB	2.70	127.11	124.26
25	V	2623	NEX	C27-C28-C29	-2.70	121.34	125.53
22	3	602	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
22	A	821	CLA	C3B-C4B-NB	-2.70	108.01	110.52
24	6	620	XAT	C26-C27-C28	-2.70	120.29	125.99
25	V	2623	NEX	C5-C6-C1	2.69	122.37	119.70
24	4	620	XAT	C19-C9-C8	2.69	122.32	118.08
24	3	619	XAT	C12-C13-C14	-2.69	114.81	118.94
24	3	619	XAT	C20-C13-C12	2.69	122.32	118.08
26	V	2630	LHG	O8-C23-C24	2.69	120.36	111.91
27	B	844	BCR	C34-C9-C8	2.69	122.32	118.08
27	O	2004	BCR	C36-C18-C19	2.69	122.32	118.08
22	B	821	CLA	CHD-C1D-ND	-2.69	121.98	124.45
21	2	601	CHL	O2D-CGD-O1D	-2.69	118.58	123.84
27	3	621	BCR	C4-C5-C6	-2.69	118.82	122.73
21	U	606	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
25	V	2623	NEX	C20-C13-C12	2.69	122.32	118.08
23	9	624	LUT	C32-C33-C34	-2.69	114.81	118.94
22	W	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	7	620	BCR	C34-C9-C8	2.69	122.31	118.08
22	B	807	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	B	821	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	6	630	LHG	O8-C23-C24	2.69	120.34	111.91
22	B	803	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	U	2630	LHG	O8-C23-C24	2.69	120.34	111.91
22	O	2002	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
21	9	608	CHL	CMD-C2D-C3D	-2.69	121.44	127.61
27	B	844	BCR	C15-C14-C13	-2.69	123.48	127.31
22	A	803	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
21	6	608	CHL	OMC-CMC-C2C	-2.68	119.62	125.69
27	B	845	BCR	C40-C30-C25	-2.68	105.95	110.30
24	W	2622	XAT	C25-C24-C23	2.68	118.06	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	V	2623	NEX	C31-C30-C29	-2.68	123.48	127.31
26	A	847	LHG	O8-C23-C24	2.68	120.33	111.91
27	L	301	BCR	C35-C13-C12	2.68	122.30	118.08
22	G	203	CLA	C1-C2-C3	-2.68	122.41	126.75
22	A	801	CLA	CBA-CAA-C2A	-2.68	105.95	113.86
21	4	606	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
26	5	630	LHG	O8-C23-C24	2.68	120.31	111.91
23	9	620	LUT	C7-C8-C9	-2.68	122.19	126.23
27	A	852	BCR	C16-C15-C14	-2.68	117.99	123.47
21	9	605	CHL	CAC-C3C-C4C	2.68	129.12	125.04
27	B	847	BCR	C34-C9-C8	2.68	122.30	118.08
22	5	613	CLA	CHC-C4B-NB	2.68	127.09	124.26
21	W	601	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
21	W	605	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
22	J	101	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
24	1	618	XAT	C38-C25-C24	2.68	117.29	114.28
27	B	847	BCR	C40-C30-C25	-2.68	105.96	110.30
22	A	806	CLA	CHD-C1D-ND	-2.67	122.00	124.45
23	2	619	LUT	C15-C35-C34	2.67	128.95	123.47
27	A	850	BCR	C16-C17-C18	-2.67	123.49	127.31
21	3	608	CHL	O2A-CGA-CBA	2.67	120.30	111.91
21	W	609	CHL	CMD-C2D-C3D	-2.67	121.46	127.61
22	2	614	CLA	CHD-C1D-ND	-2.67	122.00	124.45
22	6	610	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	B	847	BCR	C33-C5-C6	-2.67	121.53	124.53
21	1	601	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
23	U	2620	LUT	C22-C23-C24	2.67	114.78	111.74
21	U	608	CHL	CMD-C2D-C3D	-2.67	121.47	127.61
27	M	2001	BCR	C37-C22-C21	-2.67	119.18	122.92
21	3	608	CHL	CMB-C2B-C3B	2.67	133.06	126.59
23	W	2621	LUT	C11-C10-C9	-2.67	123.50	127.31
22	H	201	CLA	CBD-CHA-C1A	2.67	131.71	127.43
27	A	849	BCR	C15-C14-C13	-2.67	123.50	127.31
22	U	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	V	605	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
21	6	607	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
21	W	607	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
22	U	610	CLA	O2A-CGA-O1A	-2.67	116.87	123.59
28	G	202	LMG	O8-C28-C29	2.67	120.27	111.91
27	B	847	BCR	C36-C18-C19	2.66	122.28	118.08
22	V	610	CLA	C3B-C4B-NB	-2.66	108.45	110.23
22	5	606	CLA	O2D-CGD-O1D	-2.66	118.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	607	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	2	609	CLA	C4A-NA-C1A	2.66	107.90	106.71
27	F	305	BCR	C1-C6-C7	2.66	123.31	115.78
23	4	619	LUT	C8-C7-C6	-2.66	119.72	127.20
27	L	305	BCR	C19-C18-C17	-2.66	114.86	118.94
21	8	608	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
31	G	206	LMT	C1B-O1B-C4'	-2.66	111.38	117.96
26	3	630	LHG	O8-C23-C24	2.66	120.25	111.91
22	3	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	7	617	CLA	CHD-C1D-ND	-2.66	122.01	124.45
21	U	605	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
21	6	606	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
27	B	801	BCR	C36-C18-C17	-2.66	119.20	122.92
21	U	606	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
21	1	601	CHL	C3B-C4B-NB	2.66	112.98	110.52
22	K	203	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	K	204	CLA	C4-C3-C5	2.65	119.73	115.27
24	8	620	XAT	C37-C21-C22	-2.65	104.38	108.98
21	6	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
21	U	601	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
24	3	619	XAT	C24-C23-C22	-2.65	105.65	110.77
27	K	202	BCR	C2-C1-C6	2.65	114.56	110.48
22	V	602	CLA	O2D-CGD-CBD	2.65	115.98	111.27
27	8	621	BCR	C30-C25-C26	-2.65	118.88	122.61
21	6	618	CHL	CHC-C4B-NB	-2.65	121.45	124.26
22	V	614	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
27	A	856	BCR	C30-C25-C24	2.65	123.27	115.78
23	9	624	LUT	C19-C9-C8	2.65	122.25	118.08
22	9	609	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	W	2630	LHG	O8-C23-C24	2.65	120.21	111.91
27	B	845	BCR	C21-C20-C19	-2.65	114.96	123.22
23	6	619	LUT	C28-C29-C30	-2.65	114.88	118.94
23	4	619	LUT	C16-C1-C6	2.64	114.59	110.30
22	3	603	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	9	2630	LHG	C9-C8-C7	-2.64	104.01	113.62
22	3	614	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	814	CLA	CHD-C1D-ND	-2.64	122.03	124.45
27	K	205	BCR	C28-C27-C26	-2.64	109.36	114.08
23	W	2621	LUT	C1-C6-C5	-2.64	118.89	122.61
27	3	621	BCR	C36-C18-C17	-2.64	119.22	122.92
22	B	835	CLA	CHC-C4B-NB	2.64	127.05	124.26
23	U	2621	LUT	C19-C9-C10	-2.64	119.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	619	BCR	C15-C14-C13	-2.64	123.54	127.31
22	A	837	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	7	604	CLA	CHD-C1D-ND	-2.64	122.03	124.45
22	B	839	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	A	837	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	A	850	BCR	C28-C27-C26	-2.64	109.37	114.08
22	1	610	CLA	C1-C2-C3	-2.64	121.48	126.04
23	9	624	LUT	C20-C13-C12	2.64	122.23	118.08
21	2	606	CHL	C3B-C4B-NB	2.64	112.96	110.52
23	9	620	LUT	C28-C29-C30	-2.64	114.90	118.94
21	1	601	CHL	C1-C2-C3	-2.63	121.49	126.04
27	L	306	BCR	C1-C6-C5	-2.63	118.91	122.61
23	6	619	LUT	C11-C10-C9	-2.63	123.55	127.31
22	9	611	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	1	617	LUT	C11-C10-C9	-2.63	123.56	127.31
22	A	815	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	1	604	CLA	CHD-C1D-ND	-2.63	122.04	124.45
27	B	845	BCR	C38-C26-C27	2.63	118.67	113.62
22	7	602	CLA	O2D-CGD-CBD	2.63	115.94	111.27
27	7	620	BCR	C20-C21-C22	-2.63	123.56	127.31
22	A	839	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	5	602	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	B	814	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	4	608	CHL	CMB-C2B-C1B	2.63	129.37	125.37
27	L	305	BCR	C8-C9-C10	-2.63	114.91	118.94
27	B	801	BCR	C7-C8-C9	-2.63	122.27	126.23
22	5	613	CLA	C1-C2-C3	-2.63	122.50	126.75
22	1	609	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
27	L	306	BCR	C8-C7-C6	-2.63	119.83	127.20
22	7	610	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	7	604	CLA	C1-C2-C3	-2.63	122.50	126.75
22	7	607	CLA	CHD-C1D-ND	-2.62	122.04	124.45
27	O	2004	BCR	C1-C6-C5	-2.62	118.92	122.61
22	B	812	CLA	CHD-C1D-ND	-2.62	121.98	124.52
22	4	614	CLA	CHD-C1D-ND	-2.62	122.04	124.45
22	U	610	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	1	630	LHG	O8-C23-C24	2.62	120.13	111.91
23	9	624	LUT	C35-C34-C33	-2.62	123.57	127.31
22	7	615	CLA	O2D-CGD-O1D	-2.62	118.14	124.09
22	K	203	CLA	O2D-CGD-CBD	2.62	115.92	111.27
21	2	607	CHL	C3B-C4B-NB	2.62	112.94	110.52
27	6	621	BCR	C23-C24-C25	-2.62	119.85	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	606	CHL	CHB-C1B-NB	-2.62	121.48	124.26
21	V	608	CHL	CHB-C1B-NB	-2.62	121.49	124.26
22	W	614	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
23	1	617	LUT	C36-C21-C26	2.62	113.51	109.55
27	A	849	BCR	C28-C27-C26	-2.62	109.41	114.08
22	B	836	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	U	2621	LUT	C15-C14-C13	-2.61	123.58	127.31
27	7	621	BCR	C1-C6-C5	-2.61	118.93	122.61
22	U	610	CLA	C1-C2-C3	-2.61	121.52	126.04
23	9	624	LUT	C15-C14-C13	-2.61	123.58	127.31
27	1	619	BCR	C19-C18-C17	-2.61	114.93	118.94
27	G	205	BCR	C3-C4-C5	-2.61	109.42	114.08
27	1	619	BCR	C38-C26-C27	2.61	118.63	113.62
22	7	603	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	B	834	CLA	CHD-C1D-ND	-2.61	122.06	124.45
22	V	613	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	V	2622	XAT	C18-C5-C6	-2.61	117.89	122.26
25	U	2623	NEX	C35-C15-C14	-2.61	118.13	123.47
21	V	607	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
27	3	620	BCR	C27-C26-C25	-2.61	118.94	122.73
22	V	612	CLA	CAB-C3B-C2B	2.61	130.35	123.59
27	M	2001	BCR	C15-C16-C17	-2.61	118.13	123.47
21	V	601	CHL	CHB-C1B-NB	-2.61	121.50	124.26
22	A	817	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
27	1	619	BCR	C1-C6-C5	-2.61	118.94	122.61
27	1	619	BCR	C29-C30-C25	2.60	114.49	110.48
23	7	618	LUT	C11-C10-C9	-2.60	123.59	127.31
31	A	857	LMT	C1-O1'-C1'	-2.60	109.52	113.84
27	K	205	BCR	C24-C23-C22	-2.60	122.30	126.23
21	5	601	CHL	C3B-C4B-NB	2.60	112.93	110.52
22	9	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	A	835	CLA	CHD-C1D-ND	-2.60	122.06	124.45
23	9	624	LUT	C11-C10-C9	-2.60	123.60	127.31
27	L	305	BCR	C20-C21-C22	-2.60	123.60	127.31
27	O	2004	BCR	C37-C22-C21	-2.60	119.28	122.92
22	A	836	CLA	CHD-C1D-ND	-2.60	122.07	124.45
22	B	827	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	2	613	CLA	C1-C2-C3	-2.60	121.55	126.04
22	8	604	CLA	C1-C2-C3	-2.60	122.55	126.75
27	G	205	BCR	C33-C5-C4	2.60	118.61	113.62
25	U	2623	NEX	C31-C30-C29	-2.60	123.60	127.31
21	U	607	CHL	CMD-C2D-C3D	-2.60	121.64	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	606	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
21	9	601	CHL	CMB-C2B-C1B	2.60	129.32	125.37
22	W	612	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
22	B	821	CLA	C1-C2-C3	-2.59	122.56	126.75
31	G	206	LMT	C1'-O5'-C5'	-2.59	108.60	113.69
22	B	802	CLA	C3B-C4B-NB	-2.59	108.11	110.52
21	8	618	CHL	C2A-C1A-CHA	-2.59	119.33	123.86
25	W	2623	NEX	C2-C1-C6	2.59	111.72	109.21
22	7	602	CLA	CHD-C1D-ND	-2.59	122.08	124.45
27	B	845	BCR	C34-C9-C10	-2.59	119.30	122.92
22	6	614	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
27	K	205	BCR	C36-C18-C19	2.59	122.15	118.08
22	7	602	CLA	C1-C2-C3	-2.58	121.57	126.04
27	G	205	BCR	C38-C26-C27	2.58	118.58	113.62
21	V	607	CHL	CMD-C2D-C3D	-2.58	121.67	127.61
22	G	204	CLA	CHD-C1D-ND	-2.58	122.08	124.45
22	A	854	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
27	6	621	BCR	C30-C25-C26	-2.58	118.98	122.61
22	1	612	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	804	CLA	CHB-C4A-NA	2.58	128.08	124.51
27	B	1609	BCR	C8-C7-C6	-2.58	119.96	127.20
27	4	621	BCR	C11-C12-C13	-2.58	119.17	126.42
22	9	604	CLA	CHD-C1D-ND	-2.58	122.08	124.45
27	3	620	BCR	C23-C24-C25	-2.58	119.96	127.20
22	1	609	CLA	C1D-ND-C4D	-2.58	104.50	106.33
22	L	303	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	V	612	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
24	5	618	XAT	C20-C13-C12	2.57	122.13	118.08
21	U	606	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
22	A	830	CLA	C3B-C4B-NB	-2.57	108.13	110.52
23	4	619	LUT	C35-C34-C33	-2.57	123.64	127.31
23	2	619	LUT	C8-C9-C10	2.57	122.89	118.94
21	2	607	CHL	CMB-C2B-C1B	2.57	129.29	125.37
21	V	607	CHL	CHB-C1B-NB	-2.57	121.53	124.26
27	O	2004	BCR	C15-C14-C13	-2.57	123.64	127.31
22	A	811	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	B	832	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	8	621	BCR	C15-C16-C17	-2.57	118.21	123.47
22	A	808	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	6	608	CHL	O2A-CGA-CBA	2.57	119.97	111.91
21	U	609	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
25	U	2623	NEX	C20-C13-C12	2.57	122.12	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	607	CHL	C2A-C1A-CHA	-2.57	119.37	123.86
22	W	610	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	6	611	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	F	305	BCR	C16-C15-C14	-2.57	118.22	123.47
21	V	609	CHL	C2A-C1A-CHA	-2.57	119.37	123.86
22	3	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	A	814	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	W	2622	XAT	C6-C7-C8	-2.57	120.57	125.99
22	B	836	CLA	CMB-C2B-C1B	-2.56	121.46	125.37
27	B	845	BCR	C19-C18-C17	-2.56	115.01	118.94
27	K	202	BCR	C11-C12-C13	-2.56	119.21	126.42
22	A	813	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
22	9	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
24	U	2622	XAT	C31-C30-C29	-2.56	123.66	127.31
22	2	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	7	619	XAT	C31-C32-C33	-2.56	119.22	126.42
21	W	607	CHL	CHB-C1B-NB	-2.56	121.55	124.26
22	B	828	CLA	CHC-C4B-NB	2.56	126.97	124.26
21	6	606	CHL	O2D-CGD-O1D	-2.56	118.83	123.84
27	A	851	BCR	C27-C26-C25	-2.56	119.02	122.73
21	4	606	CHL	C2A-C1A-CHA	-2.56	119.39	123.86
21	4	606	CHL	OMC-CMC-C2C	-2.56	119.90	125.69
27	A	852	BCR	C35-C13-C12	2.56	122.11	118.08
22	B	817	CLA	CHD-C1D-ND	-2.56	122.10	124.45
22	8	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
21	U	605	CHL	CHB-C1B-NB	-2.56	121.55	124.26
27	A	852	BCR	C20-C19-C18	-2.56	119.23	126.42
22	B	837	CLA	C3B-C4B-NB	-2.56	108.14	110.52
27	L	301	BCR	C23-C22-C21	2.56	122.86	118.94
21	5	607	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
27	3	620	BCR	C40-C30-C25	-2.56	106.15	110.30
21	W	605	CHL	CHB-C1B-NB	-2.56	121.55	124.26
27	K	205	BCR	C16-C15-C14	-2.56	118.24	123.47
22	B	831	CLA	CHD-C1D-ND	-2.55	122.11	124.45
31	A	857	LMT	O3B-C3B-C4B	-2.55	104.44	110.35
22	2	603	CLA	CHC-C4B-NB	2.55	126.96	124.26
27	2	621	BCR	C38-C26-C25	2.55	127.39	124.53
23	9	620	LUT	C39-C29-C28	2.55	122.10	118.08
23	4	619	LUT	C35-C15-C14	-2.55	118.25	123.47
27	L	305	BCR	C30-C25-C24	2.55	123.00	115.78
27	B	844	BCR	C31-C1-C6	2.55	114.44	110.30
22	W	612	CLA	CAB-C3B-C2B	2.55	130.20	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	618	XAT	C19-C9-C8	2.55	122.09	118.08
22	3	602	CLA	CHD-C1D-ND	-2.55	122.11	124.45
27	2	621	BCR	C34-C9-C8	2.55	122.09	118.08
22	W	611	CLA	CAB-C3B-C2B	2.55	130.19	123.59
22	U	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	A	816	CLA	CHD-C1D-ND	-2.55	122.11	124.45
21	4	618	CHL	CMB-C2B-C1B	2.54	129.24	125.37
27	G	205	BCR	C1-C6-C5	-2.54	119.03	122.61
22	7	614	CLA	CHD-C1D-ND	-2.54	122.12	124.45
21	2	618	CHL	C3B-C4B-NB	2.54	112.87	110.52
22	B	807	CLA	O2D-CGD-CBD	2.54	115.78	111.27
31	B	849	LMT	C1'-C2'-C3'	-2.54	104.71	110.00
22	V	611	CLA	CMB-C2B-C3B	2.54	130.17	123.59
21	U	601	CHL	C4-C3-C5	2.54	119.54	115.27
27	3	621	BCR	C34-C9-C8	2.54	122.08	118.08
22	1	608	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	8	609	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	B	814	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
27	M	2001	BCR	C15-C14-C13	-2.54	123.69	127.31
27	G	205	BCR	C34-C9-C8	2.54	122.07	118.08
22	W	611	CLA	C3B-C4B-NB	-2.53	108.53	110.23
27	7	620	BCR	C30-C25-C26	-2.53	119.04	122.61
27	3	620	BCR	C4-C5-C6	-2.53	119.05	122.73
27	A	852	BCR	C28-C27-C26	-2.53	109.55	114.08
27	7	621	BCR	C16-C17-C18	-2.53	123.70	127.31
22	B	815	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	W	2623	NEX	C19-C9-C10	-2.53	119.38	122.92
22	A	833	CLA	CHD-C1D-ND	-2.53	122.13	124.45
21	6	602	CHL	CMD-C2D-C3D	-2.53	121.79	127.61
22	7	606	CLA	CHD-C1D-ND	-2.53	122.13	124.45
28	J	103	LMG	C8-O7-C10	-2.53	111.56	117.79
21	2	601	CHL	C2A-C1A-CHA	-2.53	119.44	123.86
22	3	615	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	B	813	CLA	C3B-C4B-NB	-2.53	108.17	110.52
21	6	606	CHL	CMB-C2B-C1B	2.53	129.22	125.37
21	4	618	CHL	CHC-C4B-NB	-2.53	121.58	124.26
27	O	2004	BCR	C3-C4-C5	-2.53	109.56	114.08
24	5	618	XAT	C19-C9-C8	2.53	122.06	118.08
22	3	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	A	807	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	B	838	CLA	CHC-C4B-NB	2.53	126.93	124.26
27	O	2004	BCR	C11-C10-C9	-2.52	123.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	810	CLA	CHD-C1D-ND	-2.52	122.13	124.45
22	A	813	CLA	CHD-C1D-ND	-2.52	122.13	124.45
21	U	608	CHL	CMB-C2B-C3B	2.52	130.13	123.59
22	6	609	CLA	CHD-C1D-ND	-2.52	122.14	124.45
23	3	618	LUT	C21-C26-C27	-2.52	109.51	112.70
22	5	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
31	B	849	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
27	L	305	BCR	C3-C4-C5	-2.52	109.58	114.08
22	U	603	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	8	608	CHL	C2A-C1A-CHA	-2.52	119.45	123.86
27	B	848	BCR	C34-C9-C10	-2.52	119.40	122.92
22	1	613	CLA	CHD-C1D-ND	-2.52	122.14	124.45
27	A	852	BCR	C38-C26-C27	2.52	118.45	113.62
21	1	607	CHL	O2D-CGD-O1D	-2.52	118.92	123.84
27	A	856	BCR	C29-C30-C25	2.52	114.35	110.48
22	2	604	CLA	C1-C2-C3	-2.51	122.68	126.75
22	A	828	CLA	CHD-C1D-ND	-2.51	122.14	124.45
22	A	816	CLA	CHC-C4B-NB	2.51	126.92	124.26
26	4	630	LHG	O4-P-O6	2.51	119.42	107.75
21	W	606	CHL	CHB-C1B-NB	-2.51	121.60	124.26
22	3	613	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	3	618	LUT	C3-C4-C5	-2.51	106.85	111.85
22	6	604	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	8	611	CLA	CHB-C1B-NB	2.51	126.91	124.26
21	4	607	CHL	C2A-C1A-CHA	-2.51	119.47	123.86
22	7	603	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	5	604	CLA	CHD-C1D-ND	-2.51	122.15	124.45
24	7	619	XAT	C17-C1-C16	2.51	111.07	107.37
27	K	202	BCR	C4-C5-C6	-2.50	119.10	122.73
22	A	841	CLA	C3B-C4B-NB	-2.50	108.19	110.52
22	5	606	CLA	CHD-C1D-ND	-2.50	122.15	124.45
21	1	601	CHL	C4-C3-C5	2.50	119.48	115.27
27	L	301	BCR	C4-C5-C6	-2.50	119.10	122.73
22	4	601	CLA	C1-C2-C3	-2.50	122.70	126.75
24	2	620	XAT	C35-C34-C33	-2.50	123.74	127.31
22	6	613	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	8	614	CLA	CHD-C1D-ND	-2.50	122.16	124.45
27	7	621	BCR	C15-C14-C13	-2.50	123.75	127.31
22	3	617	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	V	604	CLA	C1-C2-C3	-2.50	122.71	126.75
31	A	857	LMT	O5'-C1'-C2'	-2.50	105.06	110.35
22	1	604	CLA	C1-C2-C3	-2.50	122.71	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	844	BCR	C33-C5-C4	2.49	118.41	113.62
22	W	614	CLA	CMB-C2B-C3B	2.49	130.05	123.59
24	V	2622	XAT	C35-C34-C33	-2.49	123.75	127.31
21	6	618	CHL	CMD-C2D-C3D	-2.49	121.88	127.61
27	O	2004	BCR	C38-C26-C27	2.49	118.40	113.62
27	B	847	BCR	C37-C22-C23	2.49	122.00	118.08
22	A	831	CLA	CHD-C1D-ND	-2.49	122.17	124.45
24	5	618	XAT	C35-C15-C14	-2.49	118.37	123.47
22	V	611	CLA	CAB-C3B-C2B	2.49	130.04	123.59
22	A	828	CLA	C3B-C4B-NB	-2.49	108.20	110.52
27	A	856	BCR	C11-C10-C9	-2.49	123.76	127.31
22	W	613	CLA	C1-C2-C3	-2.49	121.74	126.04
22	6	603	CLA	CHB-C1B-NB	2.49	126.89	124.26
22	8	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	W	603	CLA	O2D-CGD-O1D	-2.48	118.45	124.09
22	A	814	CLA	CHD-C1D-ND	-2.48	122.17	124.45
27	B	844	BCR	C19-C18-C17	-2.48	115.13	118.94
22	B	837	CLA	CHB-C4A-NA	2.48	127.95	124.51
27	A	848	BCR	C38-C26-C27	2.48	118.39	113.62
24	U	2622	XAT	C11-C10-C9	-2.48	123.77	127.31
22	B	816	CLA	O2D-CGD-CBD	2.48	115.68	111.27
22	O	2001	CLA	CHD-C1D-ND	-2.48	122.12	124.52
23	8	619	LUT	C11-C10-C9	-2.48	123.77	127.31
21	5	601	CHL	CMB-C2B-C1B	2.48	129.15	125.37
22	B	822	CLA	CHD-C1D-ND	-2.48	122.17	124.45
27	O	2004	BCR	C16-C17-C18	-2.48	123.77	127.31
23	V	2620	LUT	C1-C6-C5	-2.48	119.12	122.61
27	8	621	BCR	C20-C21-C22	-2.48	123.77	127.31
22	2	613	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	B	810	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	841	CLA	C1-C2-C3	-2.48	121.76	126.04
23	V	2620	LUT	C31-C30-C29	-2.48	123.78	127.31
22	W	602	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	L	303	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
22	W	614	CLA	CAB-C3B-C2B	2.48	130.01	123.59
21	6	601	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
23	6	619	LUT	C40-C33-C32	2.48	121.98	118.08
27	2	621	BCR	C36-C18-C19	2.48	121.98	118.08
31	G	206	LMT	O3B-C3B-C4B	-2.48	104.63	110.35
27	A	856	BCR	C2-C1-C6	2.47	114.29	110.48
22	B	834	CLA	C3B-C4B-NB	-2.47	108.22	110.52
21	2	602	CHL	OMC-CMC-C2C	-2.47	120.10	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M	2001	BCR	C36-C18-C19	2.47	121.97	118.08
21	6	618	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
22	U	610	CLA	CAA-C2A-C1A	-2.47	103.88	111.97
21	6	608	CHL	CMB-C2B-C1B	2.47	129.13	125.37
21	9	607	CHL	C3B-C4B-NB	2.47	112.81	110.52
22	9	610	CLA	CHD-C1D-ND	-2.47	122.19	124.45
21	U	608	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
21	8	607	CHL	C3B-C4B-NB	2.47	112.80	110.52
27	7	620	BCR	C7-C8-C9	-2.47	122.51	126.23
28	2	631	LMG	O8-C28-C29	2.47	119.65	111.91
22	4	609	CLA	CHD-C1D-ND	-2.47	122.19	124.45
22	7	603	CLA	CHB-C1B-NB	2.47	126.87	124.26
27	6	621	BCR	C31-C1-C6	2.46	114.30	110.30
22	8	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	V	612	CLA	CMB-C2B-C3B	2.46	129.97	123.59
22	5	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	K	205	BCR	C32-C1-C6	-2.46	106.30	110.30
25	V	2623	NEX	C28-C29-C30	2.46	122.72	118.94
21	3	608	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
22	A	840	CLA	CHC-C4B-NB	2.46	126.86	124.26
22	4	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	K	202	BCR	C16-C17-C18	-2.46	123.80	127.31
21	9	608	CHL	CMB-C2B-C1B	2.46	129.12	125.37
21	5	601	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
24	6	620	XAT	C38-C25-C24	-2.46	111.51	114.28
22	W	612	CLA	CMB-C2B-C3B	2.46	129.96	123.59
22	A	840	CLA	CHD-C1D-ND	-2.46	122.19	124.45
22	B	823	CLA	CHD-C1D-ND	-2.46	122.19	124.45
21	2	606	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
27	B	1609	BCR	C8-C9-C10	2.46	122.71	118.94
27	L	305	BCR	C7-C8-C9	-2.46	122.52	126.23
22	1	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	3	621	BCR	C30-C25-C24	2.46	122.73	115.78
22	A	822	CLA	CHD-C1D-ND	-2.46	122.20	124.45
22	U	602	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	9	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	B	842	PQN	C11-C12-C13	-2.45	122.71	126.79
22	J	101	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	U	613	CLA	C1-C2-C3	-2.45	121.80	126.04
21	W	607	CHL	OMC-CMC-C2C	-2.45	120.14	125.69
22	A	823	CLA	CMB-C2B-C1B	-2.45	121.63	125.37
22	B	839	CLA	CHD-C1D-ND	-2.45	122.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	303	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	W	614	CLA	C3B-C4B-NB	-2.45	108.59	110.23
22	F	304	CLA	C2B-C1B-NB	2.45	111.88	110.23
22	7	609	CLA	O2D-CGD-CBD	2.45	115.62	111.27
22	2	613	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
21	2	608	CHL	OMC-CMC-C2C	-2.45	120.14	125.69
21	V	608	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
21	2	601	CHL	CMB-C2B-C1B	2.45	129.10	125.37
22	4	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	K	205	BCR	C37-C22-C21	-2.45	119.49	122.92
22	B	833	CLA	CHD-C1D-ND	-2.45	122.20	124.45
27	A	852	BCR	C1-C6-C5	-2.45	119.17	122.61
22	B	803	CLA	C3B-C4B-NB	-2.45	108.24	110.52
23	W	2621	LUT	C18-C5-C4	2.45	118.89	114.36
22	A	807	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	B	813	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	5	614	CLA	CHD-C1D-ND	-2.45	122.20	124.45
27	A	849	BCR	C33-C5-C4	2.45	118.32	113.62
22	A	823	CLA	CHD-C1D-ND	-2.45	122.15	124.52
21	6	608	CHL	CED-O2D-CGD	2.45	121.47	115.94
27	L	301	BCR	C34-C9-C8	2.45	121.93	118.08
22	U	604	CLA	CHD-C1D-ND	-2.45	122.21	124.45
21	2	602	CHL	C4-C3-C5	2.44	119.38	115.27
27	M	2001	BCR	C1-C6-C7	2.44	122.69	115.78
22	A	820	CLA	O2D-CGD-CBD	2.44	115.61	111.27
22	4	604	CLA	CHD-C1D-ND	-2.44	122.21	124.45
21	9	607	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
22	B	825	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	2	607	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
27	O	2004	BCR	C7-C8-C9	-2.44	122.54	126.23
25	9	623	NEX	C5-C4-C3	2.44	114.64	111.75
22	A	820	CLA	CHD-C1D-ND	-2.44	122.21	124.45
27	A	856	BCR	C15-C16-C17	-2.44	118.47	123.47
22	A	839	CLA	C1-C2-C3	-2.44	121.82	126.04
31	K	208	LMT	C1'-C2'-C3'	-2.44	104.91	110.00
22	V	602	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	A	834	CLA	CHD-C1D-ND	-2.44	122.21	124.45
31	B	849	LMT	O3B-C3B-C4B	-2.44	104.71	110.35
22	A	807	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	A	804	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	6	619	LUT	C30-C31-C32	-2.44	115.61	123.22
22	A	804	CLA	O2D-CGD-CBD	2.44	115.60	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	V	2622	XAT	C35-C15-C14	-2.44	118.48	123.47
24	1	618	XAT	C8-C9-C10	-2.44	115.20	118.94
22	A	816	CLA	O2A-CGA-O1A	-2.43	117.23	123.30
22	3	602	CLA	C3B-C4B-NB	-2.43	108.26	110.52
24	7	619	XAT	C6-C7-C8	-2.43	120.85	125.99
31	K	208	LMT	C4B-C3B-C2B	-2.43	106.58	110.82
27	F	305	BCR	C12-C13-C14	2.43	122.67	118.94
23	V	2621	LUT	C36-C21-C26	2.43	113.23	109.55
22	8	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	B	845	BCR	C37-C22-C23	2.43	121.91	118.08
22	4	612	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	4	603	CLA	CHC-C4B-NB	2.43	126.83	124.26
21	6	607	CHL	CMB-C2B-C1B	2.43	129.07	125.37
22	A	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	840	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	4	630	LHG	P-O6-C4	-2.43	107.45	121.68
22	8	604	CLA	CHD-C1D-ND	-2.43	122.22	124.45
27	3	620	BCR	C20-C21-C22	-2.43	123.85	127.31
22	W	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	834	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	V	601	CHL	CMB-C2B-C3B	2.42	129.87	123.59
27	M	2001	BCR	C24-C23-C22	-2.42	122.57	126.23
22	7	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	6	618	CHL	CMB-C2B-C1B	2.42	129.06	125.37
21	1	607	CHL	C3B-C4B-NB	2.42	112.76	110.52
21	8	606	CHL	C1C-C2C-C3C	-2.42	105.19	107.11
22	B	813	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	3	607	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	2	610	CLA	C1-C2-C3	-2.42	121.86	126.04
21	6	607	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
24	2	620	XAT	C20-C13-C12	2.42	121.89	118.08
21	6	606	CHL	OMC-CMC-C2C	-2.42	120.21	125.69
22	K	204	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	B	844	BCR	C7-C6-C5	-2.42	115.60	121.46
26	B	851	LHG	O8-C23-C24	2.42	119.50	111.91
21	7	608	CHL	CMB-C2B-C1B	2.42	129.05	125.37
21	2	602	CHL	CMD-C2D-C3D	-2.42	122.05	127.61
22	7	606	CLA	CHC-C4B-NB	2.42	126.82	124.26
22	3	612	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
21	5	601	CHL	C2A-C1A-CHA	-2.42	119.63	123.86
22	6	610	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
22	V	610	CLA	CHD-C1D-ND	-2.42	122.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	613	CLA	CHD-C1D-ND	-2.42	122.23	124.45
21	6	601	CHL	CMB-C2B-C1B	2.42	129.05	125.37
22	9	603	CLA	CHB-C4A-NA	2.42	127.85	124.51
21	2	602	CHL	C2A-C3A-C4A	-2.41	97.97	101.87
22	B	809	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	7	615	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	4	610	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	A	815	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	8	612	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	A	846	LHG	O8-C23-C24	2.41	119.48	111.91
23	9	624	LUT	C16-C1-C6	-2.41	106.39	110.30
22	3	603	CLA	CHC-C4B-NB	2.41	126.81	124.26
27	A	852	BCR	C2-C1-C6	2.41	114.19	110.48
22	B	838	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	2	608	CHL	CED-O2D-CGD	2.41	121.38	115.94
22	K	204	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	4	608	CHL	OMC-CMC-C2C	-2.41	120.25	125.69
21	2	608	CHL	C4A-NA-C1A	-2.41	105.62	106.71
24	U	2622	XAT	C6-C7-C8	-2.41	120.91	125.99
22	B	829	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	3	608	CHL	CHB-C1B-NB	-2.41	121.71	124.26
22	B	840	CLA	CHC-C4B-NB	2.41	126.80	124.26
22	9	610	CLA	C3B-C4B-NB	-2.40	108.28	110.52
24	3	619	XAT	C4-C3-C2	-2.40	106.14	110.77
22	B	828	CLA	C3B-C4B-NB	-2.40	108.29	110.52
27	6	621	BCR	C40-C30-C25	2.40	114.19	110.30
27	3	621	BCR	C16-C15-C14	-2.40	118.56	123.47
21	6	601	CHL	C2A-C1A-CHA	-2.40	119.67	123.86
22	V	611	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	K	206	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	2	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
23	W	2620	LUT	C36-C21-C26	2.40	113.18	109.55
22	1	616	CLA	CHD-C1D-ND	-2.40	122.25	124.45
27	8	621	BCR	C39-C30-C25	2.40	114.19	110.30
23	9	624	LUT	C30-C31-C32	-2.39	115.74	123.22
22	B	803	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
21	9	601	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
22	2	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	I	101	BCR	C11-C10-C9	-2.39	123.89	127.31
21	8	608	CHL	CMB-C2B-C1B	2.39	129.01	125.37
22	L	304	CLA	CHD-C1D-ND	-2.39	122.26	124.45
21	U	606	CHL	CHB-C1B-C2B	-2.39	120.48	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	836	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	3	619	XAT	C38-C25-C24	2.39	116.97	114.28
22	H	201	CLA	CHD-C1D-ND	-2.39	122.26	124.45
21	8	618	CHL	CMB-C2B-C1B	2.39	129.01	125.37
27	L	305	BCR	C16-C15-C14	-2.39	118.58	123.47
22	B	818	CLA	C3B-C4B-NB	-2.39	108.30	110.52
22	A	814	CLA	C4-C3-C5	2.39	119.29	115.27
22	B	819	CLA	CHD-C1D-ND	-2.39	122.26	124.45
21	U	601	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
21	2	618	CHL	C2A-C1A-CHA	-2.39	119.68	123.86
31	K	208	LMT	O2'-C2'-C3'	-2.39	104.83	110.35
24	8	620	XAT	O24-C25-C24	-2.39	111.59	113.38
22	A	819	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
22	B	841	CLA	CHD-C1D-ND	-2.39	122.26	124.45
31	B	849	LMT	C1-O1'-C1'	-2.39	109.88	113.84
27	B	845	BCR	C1-C6-C5	-2.39	119.25	122.61
21	9	605	CHL	CMB-C2B-C1B	2.39	129.00	125.37
31	K	208	LMT	O3B-C3B-C4B	-2.39	104.83	110.35
22	L	303	CLA	O2D-CGD-CBD	2.38	115.50	111.27
24	6	620	XAT	C35-C34-C33	-2.38	123.91	127.31
26	8	630	LHG	C5-O7-C7	-2.38	111.93	117.79
23	8	619	LUT	C28-C29-C30	-2.38	115.29	118.94
24	2	620	XAT	C12-C13-C14	-2.38	115.29	118.94
22	7	612	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	8	610	CLA	CHB-C4A-NA	2.38	127.81	124.51
21	2	602	CHL	CHB-C1B-C2B	-2.38	120.51	127.24
22	O	2003	CLA	CHD-C1D-ND	-2.38	122.22	124.52
22	B	818	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	A	838	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	L	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	9	612	CLA	CBD-CHA-C1A	2.38	131.24	127.43
27	B	847	BCR	C37-C22-C21	-2.38	119.59	122.92
22	8	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	W	607	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
21	6	602	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
27	F	305	BCR	C37-C22-C21	-2.38	119.59	122.92
24	6	620	XAT	C35-C15-C14	-2.38	118.60	123.47
24	2	620	XAT	C4-C3-C2	-2.38	106.18	110.77
22	A	805	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
22	2	604	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	A	819	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	6	612	CLA	CHB-C4A-NA	2.38	127.80	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	805	CLA	C3B-C4B-NB	-2.37	108.31	110.52
24	U	2622	XAT	C7-C8-C9	-2.37	121.85	125.53
21	7	608	CHL	CED-O2D-CGD	2.37	121.31	115.94
22	V	603	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	A	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	3	612	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	B	826	CLA	C3B-C4B-NB	-2.37	108.32	110.52
21	5	607	CHL	CMB-C2B-C1B	2.37	128.98	125.37
22	A	809	CLA	O2D-CGD-CBD	2.37	115.48	111.27
22	B	802	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	1	618	XAT	C24-C23-C22	-2.37	106.20	110.77
22	A	841	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	5	608	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	K	201	CLA	CAA-C2A-C3A	-2.37	108.34	114.26
21	2	606	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
24	7	619	XAT	C38-C25-C26	-2.37	118.29	122.26
27	A	848	BCR	C37-C22-C21	-2.37	119.61	122.92
22	8	601	CLA	C1-C2-C3	-2.37	122.92	126.75
22	W	604	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	W	603	CLA	CHD-C1D-ND	-2.37	122.28	124.45
23	W	2620	LUT	C31-C30-C29	-2.36	123.94	127.31
22	B	825	CLA	CHD-C1D-ND	-2.36	122.28	124.45
22	4	611	CLA	C3B-C4B-NB	-2.36	108.32	110.52
22	7	615	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	7	606	CLA	C3B-C4B-NB	-2.36	108.32	110.52
22	3	617	CLA	C1-C2-C3	-2.36	121.96	126.04
22	B	804	CLA	CHD-C1D-ND	-2.36	122.28	124.45
21	9	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
27	B	844	BCR	C24-C23-C22	-2.36	122.67	126.23
21	8	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
21	V	607	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
22	3	609	CLA	C1D-ND-C4D	-2.36	104.66	106.33
21	U	608	CHL	C4B-C3B-C2B	-2.36	104.79	107.03
22	B	811	CLA	CHD-C1D-ND	-2.36	122.29	124.45
22	B	817	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	B	844	BCR	C24-C25-C26	-2.36	115.75	121.46
22	A	837	CLA	CHB-C1B-NB	2.36	126.75	124.26
22	B	805	CLA	C3B-C4B-NB	-2.36	108.33	110.52
27	L	306	BCR	C24-C23-C22	-2.36	122.67	126.23
22	A	813	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	1	601	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
22	4	611	CLA	CHC-C4B-NB	2.36	126.75	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	610	CLA	CMB-C2B-C3B	2.36	129.70	123.59
22	B	822	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
22	A	826	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	F	304	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	V	604	CLA	CHD-C1D-ND	-2.36	122.29	124.45
22	B	841	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	7	620	BCR	C33-C5-C4	2.35	118.14	113.62
27	L	305	BCR	C37-C22-C23	2.35	121.79	118.08
22	B	814	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
21	U	601	CHL	CMB-C2B-C3B	2.35	129.69	123.59
27	2	621	BCR	C1-C6-C5	-2.35	119.30	122.61
22	G	203	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	1	607	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
27	A	849	BCR	C30-C25-C26	-2.35	119.30	122.61
21	W	609	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
22	6	609	CLA	C3B-C4B-NB	-2.35	108.33	110.52
27	3	621	BCR	C36-C18-C19	2.35	121.78	118.08
22	K	201	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	W	614	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	A	816	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	4	619	LUT	C31-C30-C29	-2.35	123.96	127.31
22	A	854	CLA	CMB-C2B-C3B	2.35	132.27	126.59
21	8	607	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
27	1	619	BCR	C4-C5-C6	-2.35	119.32	122.73
21	V	606	CHL	CHB-C1B-NB	-2.35	121.77	124.26
27	A	851	BCR	C35-C13-C12	2.35	121.77	118.08
27	A	848	BCR	C33-C5-C6	-2.34	121.89	124.53
27	A	856	BCR	C22-C23-C24	-2.34	118.82	124.67
27	3	621	BCR	C15-C14-C13	-2.34	123.96	127.31
23	8	619	LUT	C15-C35-C34	-2.34	118.67	123.47
21	V	608	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
27	B	844	BCR	C36-C18-C19	2.34	121.77	118.08
22	1	611	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	3	619	XAT	C10-C11-C12	-2.34	115.91	123.22
22	A	837	CLA	CHC-C4B-NB	2.34	126.74	124.26
22	3	617	CLA	C1D-ND-C4D	-2.34	104.67	106.33
22	V	602	CLA	C3B-C4B-NB	-2.34	108.34	110.52
27	L	305	BCR	C15-C16-C17	-2.34	118.68	123.47
24	1	618	XAT	C40-C33-C32	2.34	121.77	118.08
22	B	827	CLA	CHD-C1D-ND	-2.34	122.30	124.45
23	4	619	LUT	C22-C23-C24	2.34	114.41	111.74
22	1	610	CLA	CHD-C1D-ND	-2.34	122.30	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	B	831	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	3	618	LUT	C15-C14-C13	-2.34	123.97	127.31
21	9	608	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
27	M	2001	BCR	C34-C9-C8	-2.34	114.39	118.08
22	3	602	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	9	620	LUT	C35-C34-C33	-2.34	123.97	127.31
22	B	830	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	3	608	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
23	3	618	LUT	C35-C34-C33	-2.34	123.97	127.31
22	B	821	CLA	CHB-C4A-NA	2.34	127.74	124.51
21	U	607	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
25	W	2623	NEX	C25-C24-C23	-2.34	108.13	112.75
22	A	806	CLA	CHB-C4A-NA	2.34	127.74	124.51
31	B	849	LMT	O2'-C2'-C3'	-2.33	104.95	110.35
27	B	843	BCR	C35-C13-C12	2.33	121.75	118.08
22	V	604	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	B	805	CLA	O2D-CGD-CBD	2.33	115.41	111.27
22	3	617	CLA	C2B-C1B-NB	2.33	111.80	110.23
22	F	304	CLA	CHD-C1D-ND	-2.33	122.33	124.45
24	V	2622	XAT	C7-C8-C9	-2.33	121.91	125.53
22	6	610	CLA	CHB-C4A-NA	2.33	127.73	124.51
21	2	602	CHL	O2A-CGA-O1A	-2.33	117.71	123.59
27	B	843	BCR	C33-C5-C6	-2.33	121.91	124.53
22	6	603	CLA	C3B-C4B-NB	-2.33	108.35	110.52
24	5	618	XAT	C4-C3-C2	-2.33	106.27	110.77
25	W	2623	NEX	C38-C25-C24	2.33	116.90	114.28
22	4	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	A	827	CLA	CHB-C4A-NA	2.33	127.73	124.51
21	1	607	CHL	CMB-C2B-C1B	2.33	128.91	125.37
22	G	201	CLA	CHD-C1D-ND	-2.33	122.31	124.45
21	8	618	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
21	9	605	CHL	OMC-CMC-C2C	-2.33	120.43	125.69
25	W	2623	NEX	O24-C25-C26	-2.33	57.03	58.96
21	W	608	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
22	W	611	CLA	CHB-C1B-NB	2.32	126.72	124.26
22	W	604	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	B	822	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	A	808	CLA	C3B-C4B-NB	-2.32	108.36	110.52
22	A	843	CLA	C3B-C4B-NB	-2.32	108.36	110.52
27	7	620	BCR	C27-C26-C25	-2.32	119.36	122.73
23	W	2620	LUT	C35-C34-C33	-2.32	123.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	3	606	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	A	834	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	U	610	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	4	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	821	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	5	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
21	W	608	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
22	5	608	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
22	U	614	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	B	827	CLA	CHC-C4B-NB	2.32	126.71	124.26
22	1	608	CLA	C3B-C4B-NB	-2.32	108.36	110.52
31	B	849	LMT	C1B-O1B-C4'	-2.32	112.22	117.96
21	U	608	CHL	CHB-C1B-NB	-2.32	121.80	124.26
22	A	830	CLA	CHC-C4B-NB	2.32	126.71	124.26
22	5	614	CLA	CHC-C4B-NB	2.32	126.71	124.26
22	O	2002	CLA	CHD-C1D-ND	-2.32	122.32	124.45
21	9	607	CHL	CMD-C2D-C3D	-2.32	122.28	127.61
22	A	835	CLA	O2D-CGD-CBD	2.32	115.39	111.27
24	V	2622	XAT	C26-C27-C28	-2.32	121.09	125.99
27	I	101	BCR	C15-C16-C17	-2.32	118.73	123.47
27	B	843	BCR	C16-C15-C14	-2.32	118.73	123.47
22	B	836	CLA	CMB-C2B-C3B	2.32	132.20	126.59
22	V	613	CLA	CHB-C4A-NA	2.32	127.71	124.51
27	A	852	BCR	C12-C13-C14	-2.31	115.39	118.94
27	A	856	BCR	C24-C25-C26	-2.31	115.86	121.46
22	U	602	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	K	205	BCR	C15-C14-C13	-2.31	124.01	127.31
21	W	605	CHL	CMB-C2B-C3B	2.31	129.59	123.59
22	A	817	CLA	CHB-C4A-NA	2.31	127.71	124.51
27	B	843	BCR	C19-C18-C17	-2.31	115.39	118.94
21	6	601	CHL	C4-C3-C5	2.31	119.16	115.27
21	1	607	CHL	O2A-CGA-CBA	2.31	121.37	112.23
24	2	620	XAT	C38-C25-C24	2.31	116.88	114.28
21	W	606	CHL	CMB-C2B-C3B	2.31	129.58	123.59
22	B	804	CLA	C1-C2-C3	-2.31	122.04	126.04
27	7	620	BCR	C1-C6-C7	2.31	122.32	115.78
22	B	818	CLA	CHC-C4B-NB	2.31	126.70	124.26
23	9	620	LUT	C8-C7-C6	-2.31	120.71	127.20
27	A	852	BCR	C8-C9-C10	2.31	122.49	118.94
22	A	821	CLA	CHB-C1B-NB	2.31	126.70	124.26
21	9	606	CHL	C2A-C1A-CHA	-2.31	119.82	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	830	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	5	613	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	B	839	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	4	606	CHL	O2A-CGA-CBA	2.31	121.45	114.03
22	B	820	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	5	602	CLA	C1-C2-C3	-2.31	122.05	126.04
22	8	609	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	A	829	CLA	CMB-C2B-C1B	-2.31	121.86	125.37
27	A	850	BCR	C32-C1-C6	-2.31	106.56	110.30
22	9	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
22	3	607	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	B	830	CLA	C3B-C4B-NB	-2.30	108.38	110.52
27	K	202	BCR	C29-C30-C25	2.30	114.03	110.48
31	A	857	LMT	C1B-O1B-C4'	-2.30	112.26	117.96
22	A	814	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	9	624	LUT	C8-C9-C10	-2.30	115.41	118.94
22	A	801	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	L	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	B	838	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	2	630	LHG	O8-C23-C24	2.30	119.13	111.91
23	V	2621	LUT	C31-C30-C29	-2.30	124.03	127.31
27	L	305	BCR	C29-C30-C25	2.30	114.02	110.48
22	U	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	W	613	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	B	812	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	2	603	CLA	CHB-C1B-NB	2.30	126.69	124.26
27	L	301	BCR	C36-C18-C19	2.30	121.70	118.08
27	B	844	BCR	C1-C6-C5	-2.30	119.38	122.61
22	1	602	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	5	602	CLA	CHD-C1D-ND	-2.30	122.34	124.45
27	7	621	BCR	C36-C18-C19	2.30	121.70	118.08
22	7	609	CLA	C1-C2-C3	-2.30	122.07	126.04
21	W	601	CHL	O2D-CGD-O1D	-2.30	118.87	124.09
21	V	605	CHL	CMB-C2B-C1B	2.30	128.87	125.37
22	A	817	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
21	9	607	CHL	C2A-C1A-CHA	-2.30	119.84	123.86
23	4	619	LUT	C1-C6-C5	-2.30	119.38	122.61
22	A	819	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	6	614	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	W	614	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	B	838	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	6	603	CLA	CHB-C4A-NA	2.30	127.69	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	3	612	CLA	CHD-C1D-ND	-2.29	122.34	124.45
22	A	840	CLA	C3B-C4B-NB	-2.29	108.39	110.52
23	7	618	LUT	C8-C7-C6	-2.29	120.76	127.20
21	V	605	CHL	C1C-C2C-C3C	-2.29	105.29	107.11
22	6	614	CLA	CHC-C4B-NB	2.29	126.69	124.26
28	2	631	LMG	C8-O7-C10	-2.29	112.14	117.79
22	B	814	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	7	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	A	823	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	O	2002	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	V	613	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	A	802	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	5	614	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	V	612	CLA	CHD-C1D-ND	-2.29	122.35	124.45
22	F	301	CLA	C1-C2-C3	-2.29	122.08	126.04
21	V	608	CHL	CMB-C2B-C3B	2.29	129.52	123.59
22	2	614	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	U	604	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	1	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	U	2622	XAT	C35-C15-C14	-2.29	118.79	123.47
22	9	609	CLA	CMB-C2B-C1B	2.29	128.85	125.37
23	W	2620	LUT	C19-C9-C8	2.29	121.68	118.08
22	3	610	CLA	C3B-C4B-NB	-2.29	108.39	110.52
21	V	607	CHL	O1D-CGD-CBD	-2.29	119.80	124.48
22	6	611	CLA	CHC-C4B-NB	2.29	126.68	124.26
22	2	604	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	B	818	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	7	613	CLA	C1-C2-C3	-2.29	122.09	126.04
22	1	613	CLA	C1-C2-C3	-2.29	123.05	126.75
21	9	606	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
22	A	804	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	V	607	CHL	CMB-C2B-C3B	2.28	129.51	123.59
22	G	203	CLA	CHD-C1D-ND	-2.28	122.36	124.45
21	U	608	CHL	CMB-C2B-C1B	2.28	128.85	125.37
27	6	621	BCR	C8-C7-C6	-2.28	120.79	127.20
27	G	205	BCR	C32-C1-C6	-2.28	106.60	110.30
22	6	613	CLA	CHB-C4A-NA	2.28	127.67	124.51
27	6	621	BCR	C39-C30-C25	-2.28	106.60	110.30
27	A	856	BCR	C15-C14-C13	-2.28	124.06	127.31
27	L	306	BCR	C40-C30-C25	-2.28	106.60	110.30
21	W	609	CHL	CBD-CHA-C1A	2.28	131.08	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	W	606	CHL	O2D-CGD-O1D	-2.28	118.91	124.09
22	K	206	CLA	C3B-C4B-NB	-2.28	108.40	110.52
23	2	619	LUT	C39-C29-C28	2.28	121.67	118.08
22	K	201	CLA	CHD-C1D-ND	-2.28	122.36	124.45
21	U	605	CHL	CMB-C2B-C3B	2.28	129.49	123.59
22	6	611	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	A	820	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
27	M	2001	BCR	C8-C7-C6	-2.28	120.81	127.20
21	2	618	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
22	B	836	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	A	849	BCR	C15-C16-C17	-2.28	118.81	123.47
24	4	620	XAT	C24-C23-C22	-2.28	106.38	110.77
22	B	832	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	7	613	CLA	CHD-C1D-ND	-2.28	122.36	124.45
31	A	857	LMT	O2'-C2'-C3'	-2.28	105.09	110.35
22	V	614	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	3	609	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	A	820	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	8	603	CLA	CHB-C4A-NA	2.27	127.66	124.51
21	4	618	CHL	CMD-C2D-C3D	-2.27	122.39	127.61
21	V	609	CHL	OMC-CMC-C2C	-2.27	120.55	125.69
23	4	619	LUT	C15-C14-C13	-2.27	124.07	127.31
21	6	607	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
21	W	607	CHL	CMB-C2B-C3B	2.27	129.47	123.59
27	L	305	BCR	C34-C9-C10	2.27	126.10	122.92
22	A	829	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	A	845	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	W	602	CLA	C3B-C4B-NB	-2.27	108.41	110.52
27	B	1609	BCR	C15-C14-C13	-2.27	124.07	127.31
24	8	620	XAT	C10-C11-C12	2.27	130.30	123.22
27	4	621	BCR	C20-C19-C18	-2.27	120.04	126.42
22	2	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	A	832	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	1	603	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	4	601	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	2	610	CLA	C3B-C4B-NB	-2.27	108.41	110.52
23	8	619	LUT	C39-C29-C28	2.27	121.65	118.08
22	K	201	CLA	C3B-C4B-NB	-2.27	108.41	110.52
24	6	620	XAT	C7-C8-C9	-2.27	122.01	125.53
22	5	610	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	B	812	CLA	O2A-CGA-O1A	-2.27	117.65	123.30
21	9	608	CHL	OMC-CMC-C2C	-2.27	120.56	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	610	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	2	614	CLA	C3B-C4B-NB	-2.26	108.41	110.52
22	A	835	CLA	CHB-C4A-NA	2.26	127.64	124.51
21	V	601	CHL	CHC-C1C-C2C	-2.26	120.44	126.73
27	K	205	BCR	C35-C13-C12	2.26	121.64	118.08
22	1	606	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	5	603	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	V	610	CLA	CAB-C3B-C2B	2.26	129.45	123.59
27	A	850	BCR	C16-C15-C14	-2.26	118.84	123.47
21	V	609	CHL	CBD-CHA-C1A	2.26	131.05	127.43
22	1	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	B	831	CLA	CHC-C4B-NB	2.26	126.65	124.26
22	B	808	CLA	C3B-C4B-NB	-2.26	108.42	110.52
27	3	620	BCR	C30-C25-C26	-2.26	119.43	122.61
22	2	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
21	4	606	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
22	A	843	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	A	822	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	A	852	BCR	C11-C10-C9	-2.26	124.09	127.31
21	2	608	CHL	C3B-C4B-NB	2.26	112.61	110.52
23	9	621	LUT	C38-C25-C24	-2.26	118.73	123.56
27	2	621	BCR	C3-C4-C5	-2.26	110.05	114.08
22	3	607	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
23	8	619	LUT	C8-C7-C6	-2.26	120.87	127.20
21	4	608	CHL	CED-O2D-CGD	2.25	121.04	115.94
22	A	819	CLA	CHB-C1B-NB	2.25	126.64	124.26
22	K	201	CLA	CHC-C4B-NB	2.25	126.64	124.26
27	7	620	BCR	C29-C30-C25	2.25	113.95	110.48
22	A	812	CLA	CHD-C1D-ND	-2.25	122.38	124.45
21	V	606	CHL	O2D-CGD-O1D	-2.25	118.97	124.09
22	A	827	CLA	O1D-CGD-CBD	2.25	129.09	124.48
27	K	202	BCR	C15-C14-C13	-2.25	124.09	127.31
22	A	805	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	B	815	CLA	CHB-C4A-NA	2.25	127.63	124.51
31	G	206	LMT	O2'-C2'-C3'	-2.25	105.14	110.35
23	9	624	LUT	C15-C35-C34	-2.25	118.86	123.47
27	A	851	BCR	C23-C22-C21	-2.25	115.49	118.94
22	W	610	CLA	C6-C5-C3	2.25	119.36	113.45
22	B	806	CLA	C3B-C4B-NB	-2.25	108.43	110.52
27	J	102	BCR	C30-C25-C26	-2.25	119.44	122.61
22	3	606	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	9	624	LUT	C35-C15-C14	-2.25	118.87	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	851	BCR	C31-C1-C6	-2.25	106.65	110.30
27	L	306	BCR	C31-C1-C6	2.25	113.94	110.30
22	3	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	V	613	CLA	O2D-CGD-CBD	2.25	115.26	111.27
27	B	848	BCR	C15-C14-C13	-2.25	124.11	127.31
22	B	822	CLA	C3B-C4B-NB	-2.24	108.43	110.52
21	1	601	CHL	CHB-C1B-C2B	-2.24	120.90	127.24
22	B	823	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	A	832	CLA	C3B-C4B-NB	-2.24	108.43	110.52
27	L	306	BCR	C15-C16-C17	-2.24	118.88	123.47
21	4	607	CHL	CED-O2D-CGD	2.24	121.01	115.94
22	A	832	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	6	604	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	9	624	LUT	C12-C13-C14	-2.24	115.50	118.94
21	U	605	CHL	O2D-CGD-O1D	-2.24	119.00	124.09
22	U	614	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	A	810	CLA	C3B-C4B-NB	-2.24	108.44	110.52
22	B	836	CLA	C3B-C4B-NB	-2.24	108.44	110.52
22	1	611	CLA	O2D-CGD-CBD	2.24	115.25	111.27
22	W	612	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	F	303	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	V	605	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
22	4	602	CLA	C1-C2-C3	-2.24	122.17	126.04
21	8	606	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
21	2	606	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
27	K	205	BCR	C7-C6-C5	-2.24	116.04	121.46
22	B	832	CLA	C3B-C4B-NB	-2.24	108.44	110.52
24	U	2622	XAT	C15-C14-C13	-2.24	124.11	127.31
22	B	822	CLA	O2D-CGD-CBD	2.24	115.25	111.27
22	B	819	CLA	CHB-C4A-NA	2.24	127.61	124.51
21	U	609	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	B	814	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
22	B	810	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
21	U	607	CHL	CHB-C1B-C2B	-2.24	120.92	127.24
22	5	602	CLA	CHB-C4A-NA	2.24	127.60	124.51
21	5	607	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	A	826	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	V	2620	LUT	C21-C26-C27	-2.23	109.88	112.70
27	L	306	BCR	C1-C6-C7	2.23	122.10	115.78
27	J	102	BCR	C2-C1-C6	2.23	113.92	110.48
21	4	607	CHL	CMB-C2B-C1B	2.23	128.77	125.37
25	V	2623	NEX	C19-C9-C10	-2.23	119.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	U	606	CHL	C3B-C4B-NB	2.23	112.59	110.52
22	B	828	CLA	CHD-C1D-ND	-2.23	122.40	124.45
27	A	852	BCR	C15-C14-C13	-2.23	124.12	127.31
24	2	620	XAT	C10-C11-C12	-2.23	116.25	123.22
21	9	601	CHL	OMC-CMC-C2C	-2.23	120.64	125.69
22	B	816	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	9	602	CLA	CHB-C4A-NA	2.23	127.60	124.51
27	B	1609	BCR	C16-C17-C18	-2.23	124.13	127.31
22	A	810	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	8	618	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
23	4	619	LUT	C11-C10-C9	-2.23	124.13	127.31
22	U	613	CLA	CHB-C4A-NA	2.23	127.59	124.51
27	M	2001	BCR	C19-C18-C17	-2.23	115.52	118.94
21	9	607	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
21	5	601	CHL	C1C-C2C-C3C	-2.23	105.35	107.11
24	5	618	XAT	C37-C21-C26	-2.23	104.03	110.05
22	3	603	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	A	812	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	1	601	CHL	OMC-CMC-C2C	-2.23	120.66	125.69
24	V	2622	XAT	C6-C7-C8	-2.23	121.29	125.99
22	A	808	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	7	608	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
24	V	2622	XAT	C15-C14-C13	-2.22	124.14	127.31
23	9	621	LUT	C35-C15-C14	-2.22	118.92	123.47
21	5	607	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
21	V	606	CHL	CMD-C2D-C3D	-2.22	122.50	127.61
21	5	601	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
22	A	816	CLA	C3B-C4B-NB	-2.22	108.45	110.52
27	A	851	BCR	C20-C21-C22	-2.22	124.14	127.31
27	M	2001	BCR	C16-C17-C18	-2.22	124.14	127.31
22	5	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
27	B	843	BCR	C15-C16-C17	-2.22	118.93	123.47
22	B	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	1	614	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	3	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	9	606	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
22	B	840	CLA	C3B-C4B-NB	-2.22	108.46	110.52
27	A	851	BCR	C12-C13-C14	-2.22	115.54	118.94
25	9	623	NEX	C31-C30-C29	-2.22	124.14	127.31
22	B	806	CLA	CHB-C4A-NA	2.22	127.58	124.51
21	U	609	CHL	C4-C3-C5	2.22	119.00	115.27
22	6	603	CLA	CHD-C1D-ND	-2.22	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	611	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	8	602	CLA	O2D-CGD-CBD	2.22	115.21	111.27
21	2	607	CHL	OMC-CMC-C2C	-2.22	120.68	125.69
21	2	606	CHL	CHB-C1B-C2B	-2.22	120.98	127.24
22	V	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	2	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	L	302	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	A	844	PQN	C11-C12-C13	-2.21	123.11	126.79
21	W	605	CHL	O2D-CGD-O1D	-2.21	119.06	124.09
22	2	603	CLA	C3B-C4B-NB	-2.21	108.46	110.52
22	B	820	CLA	C3B-C4B-NB	-2.21	108.46	110.52
22	4	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
21	4	607	CHL	OMC-CMC-C2C	-2.21	120.68	125.69
22	A	802	CLA	C3B-C4B-NB	-2.21	108.46	110.52
21	7	608	CHL	C1C-C2C-C3C	-2.21	105.36	107.11
22	G	201	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
22	4	603	CLA	CHB-C1B-NB	2.21	126.60	124.26
22	5	611	CLA	CHB-C1B-NB	2.21	126.60	124.26
23	V	2621	LUT	C1-C6-C5	-2.21	119.50	122.61
21	8	607	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
27	A	850	BCR	C15-C14-C13	-2.21	124.15	127.31
22	A	815	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
22	U	610	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	U	2622	XAT	C35-C34-C33	-2.21	124.16	127.31
21	2	602	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
22	9	603	CLA	CHB-C1B-NB	2.21	126.60	124.26
23	9	621	LUT	C35-C34-C33	-2.21	124.16	127.31
22	B	823	CLA	C3B-C4B-NB	-2.21	108.47	110.52
25	V	2623	NEX	C35-C34-C33	-2.21	124.16	127.31
27	K	202	BCR	C15-C16-C17	-2.21	118.95	123.47
22	B	826	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	7	606	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	A	824	CLA	C3B-C4B-NB	-2.21	108.47	110.52
22	B	838	CLA	CHB-C1B-NB	2.21	126.59	124.26
22	A	840	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	2	604	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	7	618	LUT	C38-C25-C24	-2.20	118.84	123.56
22	J	101	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	U	2620	LUT	C19-C9-C10	-2.20	119.83	122.92
22	5	611	CLA	C3B-C4B-NB	-2.20	108.47	110.52
22	3	617	CLA	CMC-C2C-C1C	2.20	125.25	118.85
21	W	608	CHL	O2D-CGD-O1D	-2.20	119.09	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	621	BCR	C34-C9-C10	-2.20	119.84	122.92
21	6	607	CHL	OMC-CMC-C2C	-2.20	120.71	125.69
22	5	609	CLA	CMA-C3A-C2A	-2.20	110.96	116.10
27	L	305	BCR	C24-C25-C26	-2.20	116.13	121.46
23	2	619	LUT	C7-C8-C9	-2.20	122.91	126.23
24	4	620	XAT	C28-C29-C30	-2.20	115.57	118.94
27	7	621	BCR	C30-C25-C24	2.20	122.00	115.78
22	9	602	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	A	820	CLA	CHB-C1B-NB	2.20	126.58	124.26
23	V	2620	LUT	C36-C21-C26	2.20	112.88	109.55
24	W	2622	XAT	C15-C14-C13	-2.20	124.17	127.31
21	2	601	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
27	L	301	BCR	C2-C1-C6	2.20	113.86	110.48
22	A	834	CLA	C3B-C4B-NB	-2.20	108.48	110.52
22	6	614	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
21	V	609	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
22	3	604	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	B	807	CLA	CHC-C4B-NB	2.20	126.58	124.26
22	U	611	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	K	206	CLA	CHB-C4A-NA	2.20	127.55	124.51
27	L	305	BCR	C12-C13-C14	-2.20	115.57	118.94
22	3	613	CLA	O2D-CGD-CBD	2.20	115.17	111.27
21	9	607	CHL	CMB-C2B-C1B	2.19	128.71	125.37
22	B	825	CLA	C3B-C4B-NB	-2.19	108.48	110.52
22	H	201	CLA	CHB-C4A-NA	2.19	127.55	124.51
26	1	630	LHG	C5-O7-C7	-2.19	112.39	117.79
22	A	815	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	A	823	CLA	CHB-C4A-NA	2.19	127.54	124.51
27	L	301	BCR	C33-C5-C4	2.19	117.83	113.62
23	W	2620	LUT	C19-C9-C10	-2.19	119.85	122.92
24	4	620	XAT	C30-C31-C32	-2.19	116.38	123.22
22	A	801	CLA	CHC-C4B-NB	2.19	126.58	124.26
22	4	601	CLA	CHD-C1D-ND	-2.19	122.44	124.45
25	9	623	NEX	C24-C23-C22	-2.19	106.54	110.77
23	V	2620	LUT	C8-C7-C6	-2.19	121.05	127.20
21	U	608	CHL	O2D-CGD-O1D	-2.19	119.12	124.09
22	B	827	CLA	C3B-C4B-NB	-2.19	108.48	110.52
22	8	610	CLA	C3B-C4B-NB	-2.19	108.48	110.52
21	V	601	CHL	O2D-CGD-O1D	-2.19	119.12	124.09
21	W	601	CHL	CMB-C2B-C3B	2.19	129.26	123.59
22	V	610	CLA	CMA-C3A-C2A	-2.19	110.99	116.10
22	2	614	CLA	CHB-C4A-NA	2.19	127.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	C3B-C4B-NB	-2.19	108.48	110.52
22	B	825	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
21	2	618	CHL	CMB-C2B-C1B	2.19	128.70	125.37
23	6	619	LUT	C38-C25-C24	-2.19	118.88	123.56
27	F	305	BCR	C7-C6-C5	-2.19	116.16	121.46
22	B	809	CLA	CHB-C4A-NA	2.19	127.54	124.51
27	3	621	BCR	C3-C4-C5	-2.19	110.17	114.08
22	7	612	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	9	611	CLA	C3B-C4B-NB	-2.19	108.49	110.52
22	B	817	CLA	CHB-C1B-NB	2.19	126.57	124.26
22	B	818	CLA	O2D-CGD-CBD	2.19	115.15	111.27
22	A	817	CLA	CHD-C1D-ND	-2.19	122.45	124.45
26	5	630	LHG	C5-O7-C7	-2.18	112.41	117.79
23	3	618	LUT	C11-C10-C9	-2.18	124.19	127.31
23	5	617	LUT	C30-C31-C32	2.18	130.03	123.22
22	1	604	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	5	618	XAT	C15-C35-C34	-2.18	119.00	123.47
27	1	619	BCR	C12-C13-C14	-2.18	115.59	118.94
22	A	830	CLA	CHB-C1B-NB	2.18	126.57	124.26
22	6	609	CLA	CHB-C1B-NB	2.18	126.57	124.26
26	9	2630	LHG	O7-C7-C8	2.18	116.20	111.50
23	9	621	LUT	C31-C30-C29	-2.18	124.20	127.31
21	4	618	CHL	C2A-C1A-CHA	-2.18	120.04	123.86
26	A	846	LHG	C5-O7-C7	-2.18	112.42	117.79
23	W	2620	LUT	C1-C6-C5	-2.18	119.54	122.61
22	A	828	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	3	604	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	A	824	CLA	CHC-C4B-NB	2.18	126.56	124.26
22	9	613	CLA	CHB-C1B-NB	2.18	126.56	124.26
22	A	842	CLA	CHB-C4A-NA	2.18	127.53	124.51
22	A	806	CLA	C3B-C4B-NB	-2.18	108.49	110.52
22	A	833	CLA	C3B-C4B-NB	-2.18	108.49	110.52
24	3	619	XAT	C39-C29-C28	2.18	121.51	118.08
21	8	606	CHL	CHB-C1B-C2B	-2.18	121.08	127.24
27	7	620	BCR	C8-C7-C6	-2.18	121.08	127.20
22	A	802	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	8	608	CHL	CHB-C1B-C2B	-2.18	121.09	127.24
27	A	851	BCR	C40-C30-C25	2.18	113.83	110.30
21	1	601	CHL	CMB-C2B-C1B	2.18	128.68	125.37
22	A	824	CLA	CHD-C1D-ND	-2.18	122.45	124.45
27	A	851	BCR	C36-C18-C19	2.18	121.50	118.08
21	5	601	CHL	C5-C3-C4	2.18	119.41	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	828	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	V	2620	LUT	C11-C12-C13	-2.17	120.31	126.42
22	6	613	CLA	C1-C2-C3	-2.17	122.28	126.04
27	G	205	BCR	C21-C20-C19	-2.17	116.43	123.22
22	V	611	CLA	CHB-C1B-NB	2.17	126.56	124.26
22	6	603	CLA	CHC-C4B-NB	2.17	126.56	124.26
21	8	608	CHL	C5-C3-C4	2.17	119.40	114.60
22	U	604	CLA	O2D-CGD-CBD	2.17	115.13	111.27
22	F	304	CLA	CHB-C1B-NB	2.17	126.56	124.26
21	2	618	CHL	CHB-C1B-C2B	-2.17	121.10	127.24
22	A	842	CLA	C7-C6-C5	-2.17	107.46	113.36
27	A	848	BCR	C36-C18-C19	2.17	121.50	118.08
22	B	819	CLA	C3B-C4B-NB	-2.17	108.50	110.52
22	1	614	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
27	7	620	BCR	C37-C22-C21	-2.17	119.88	122.92
21	9	601	CHL	CBD-CHA-C1A	2.17	130.91	127.43
21	V	601	CHL	C1-C2-C3	-2.17	122.29	126.04
21	W	609	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
24	2	620	XAT	C19-C9-C8	2.17	121.50	118.08
22	7	617	CLA	CHB-C4A-NA	2.17	127.51	124.51
21	6	601	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
27	A	850	BCR	C1-C6-C5	-2.17	119.56	122.61
22	3	604	CLA	C3B-C4B-NB	-2.17	108.50	110.52
22	2	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	5	601	CHL	CHB-C1B-C2B	-2.17	121.11	127.24
22	5	609	CLA	CHB-C4A-NA	2.17	127.51	124.51
22	J	101	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
21	8	607	CHL	CHB-C1B-C2B	-2.17	121.12	127.24
22	4	614	CLA	C3B-C4B-NB	-2.17	108.50	110.52
22	B	840	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	6	607	CHL	CHB-C1B-C2B	-2.17	121.12	127.24
22	5	608	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	3	618	LUT	C31-C30-C29	-2.17	124.22	127.31
23	1	617	LUT	C38-C25-C24	-2.16	118.93	123.56
22	B	810	CLA	C3B-C4B-NB	-2.16	108.51	110.52
24	W	2622	XAT	C12-C13-C14	-2.16	115.62	118.94
22	W	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	A	820	CLA	C3B-C4B-NB	-2.16	108.51	110.52
22	B	813	CLA	O2D-CGD-CBD	2.16	115.11	111.27
22	7	610	CLA	CHB-C1B-NB	2.16	126.55	124.26
27	B	848	BCR	C33-C5-C6	-2.16	122.10	124.53
27	7	620	BCR	C16-C17-C18	-2.16	124.22	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	604	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
22	3	609	CLA	C4-C3-C5	2.16	118.91	115.27
22	W	603	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
22	4	609	CLA	C3B-C4B-NB	-2.16	108.51	110.52
27	8	621	BCR	C11-C12-C13	-2.16	120.35	126.42
22	3	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	K	203	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	832	CLA	C4-C3-C5	2.16	118.90	115.27
22	8	610	CLA	C1-C2-C3	-2.16	122.31	126.04
22	A	809	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
27	L	305	BCR	C2-C3-C4	-2.16	106.56	111.38
22	A	830	CLA	O2D-CGD-CBD	2.16	115.10	111.27
22	2	614	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	V	2620	LUT	C19-C9-C10	-2.16	119.90	122.92
27	A	848	BCR	C28-C27-C26	-2.16	110.22	114.08
22	B	807	CLA	C3B-C4B-NB	-2.16	108.51	110.52
23	1	617	LUT	C31-C30-C29	-2.16	124.23	127.31
27	A	849	BCR	C36-C18-C17	-2.16	119.90	122.92
21	9	605	CHL	CHB-C1B-C2B	-2.16	121.15	127.24
22	3	602	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
22	B	822	CLA	C1-C2-C3	-2.15	122.32	126.04
21	U	607	CHL	CAA-C2A-C3A	2.15	118.67	112.78
21	1	601	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
21	8	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
23	W	2621	LUT	C38-C25-C24	-2.15	118.95	123.56
23	8	619	LUT	C36-C21-C26	2.15	112.81	109.55
21	6	602	CHL	CHB-C1B-C2B	-2.15	121.16	127.24
21	1	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
24	W	2622	XAT	O4-C5-C6	-2.15	57.18	58.96
22	A	824	CLA	O2D-CGD-CBD	2.15	115.09	111.27
21	W	601	CHL	C4-C3-C5	2.15	118.89	115.27
22	A	806	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
22	B	820	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
22	A	835	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	A	842	CLA	C3B-C4B-NB	-2.15	108.52	110.52
24	2	620	XAT	C27-C28-C29	-2.15	122.19	125.53
22	A	836	CLA	CAC-C3C-C2C	2.15	127.30	123.22
22	A	805	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
27	G	205	BCR	C19-C18-C17	-2.15	115.64	118.94
22	3	610	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	V	610	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	W	2620	LUT	C35-C15-C14	-2.15	119.07	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	617	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	7	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	3	614	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	B	828	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	U	2620	LUT	C35-C34-C33	-2.15	124.25	127.31
22	O	2001	CLA	CHB-C4A-NA	2.15	127.62	124.34
27	L	301	BCR	C28-C27-C26	-2.15	110.25	114.08
25	W	2623	NEX	C35-C15-C14	-2.15	119.08	123.47
22	2	603	CLA	CHD-C1D-ND	-2.14	122.48	124.45
22	A	805	CLA	CHB-C1B-NB	2.14	126.53	124.26
27	B	1609	BCR	C1-C6-C5	-2.14	119.59	122.61
23	V	2621	LUT	C18-C5-C4	2.14	118.33	114.36
21	4	618	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
22	3	617	CLA	CHB-C1B-NB	2.14	126.52	124.26
21	9	601	CHL	C4D-C3D-CAD	2.14	110.62	108.10
21	V	606	CHL	CMB-C2B-C3B	2.14	129.14	123.59
22	B	808	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	1	611	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	A	818	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	7	618	LUT	C40-C33-C32	2.14	121.45	118.08
22	A	838	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	B	801	BCR	C38-C26-C27	2.14	117.72	113.62
23	3	618	LUT	C1-C6-C5	-2.14	119.60	122.61
31	K	208	LMT	C1B-O1B-C4'	-2.14	112.67	117.96
22	9	613	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	A	804	CLA	C3B-C4B-NB	-2.14	108.53	110.52
22	6	609	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	B	808	CLA	CHD-C1D-ND	-2.13	122.49	124.45
22	1	608	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	A	823	CLA	CMB-C2B-C3B	2.13	131.76	126.59
21	W	606	CHL	CHC-C1C-C2C	-2.13	120.80	126.73
26	4	630	LHG	O8-C23-O10	-2.13	118.21	123.59
21	6	601	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
24	3	619	XAT	C28-C29-C30	-2.13	115.67	118.94
21	W	606	CHL	C4B-C3B-C2B	-2.13	105.00	107.03
22	4	610	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
22	B	826	CLA	O2D-CGD-CBD	2.13	115.06	111.27
22	B	824	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	V	603	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	4	603	CLA	C3B-C4B-NB	-2.13	108.54	110.52
24	2	620	XAT	C15-C35-C34	-2.13	119.11	123.47
21	W	608	CHL	C4B-C3B-C2B	-2.13	105.01	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	843	BCR	C33-C5-C4	2.13	117.71	113.62
22	8	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	A	854	CLA	C2B-C1B-NB	2.13	111.66	110.23
22	8	604	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	8	601	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	8	603	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	A	812	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	B	842	PQN	C11-C3-C4	-2.13	116.22	118.50
22	B	832	CLA	O2D-CGD-CBD	2.13	115.05	111.27
27	6	621	BCR	C37-C22-C21	-2.13	119.94	122.92
22	B	832	CLA	CHC-C4B-NB	2.13	126.51	124.26
22	1	606	CLA	C3B-C4B-NB	-2.13	108.54	110.52
27	8	621	BCR	C24-C25-C26	-2.12	116.31	121.46
22	1	616	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	A	826	CLA	C3B-C4B-NB	-2.12	108.54	110.52
22	B	819	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	L	303	CLA	CHB-C1B-NB	2.12	126.51	124.26
22	8	610	CLA	CHB-C1B-NB	2.12	126.51	124.26
24	U	2622	XAT	O4-C5-C6	-2.12	57.20	58.96
22	4	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	U	2620	LUT	C31-C30-C29	-2.12	124.28	127.31
27	B	801	BCR	C11-C10-C9	-2.12	124.28	127.31
22	7	617	CLA	C3B-C4B-NB	-2.12	108.55	110.52
22	B	833	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	9	623	NEX	C16-C1-C6	2.12	112.37	110.47
21	8	606	CHL	CMB-C2B-C1B	2.12	128.60	125.37
22	1	602	CLA	C3B-C4B-NB	-2.12	108.55	110.52
22	A	838	CLA	C3B-C4B-NB	-2.12	108.55	110.52
21	8	618	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
21	V	605	CHL	CHB-C1B-C2B	-2.12	121.24	127.24
21	V	606	CHL	CHC-C1C-C2C	-2.12	120.84	126.73
27	B	1609	BCR	C35-C13-C12	2.12	121.42	118.08
23	1	617	LUT	C35-C15-C14	-2.12	119.13	123.47
22	B	819	CLA	C6-C5-C3	2.12	119.02	113.45
27	7	621	BCR	C8-C7-C6	-2.12	121.25	127.20
22	F	303	CLA	CHC-C4B-NB	2.12	126.50	124.26
22	B	835	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
22	A	825	CLA	C3B-C4B-NB	-2.12	108.55	110.52
22	A	813	CLA	CMB-C2B-C3B	2.12	131.72	126.59
22	A	802	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	B	811	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	W	2620	LUT	C38-C25-C24	-2.12	119.03	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	613	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	3	620	BCR	C15-C14-C13	-2.12	124.29	127.31
22	B	840	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	1	611	CLA	CAC-C3C-C4C	2.12	127.56	124.81
27	7	621	BCR	C2-C1-C6	2.12	113.74	110.48
21	U	605	CHL	CHC-C1C-C2C	-2.12	120.85	126.73
22	1	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	V	611	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	L	302	CLA	CHB-C1B-NB	2.12	126.50	124.26
21	8	618	CHL	CHB-C1B-C2B	-2.12	121.26	127.24
22	B	814	CLA	CBA-CAA-C2A	2.12	120.11	113.86
22	F	301	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	L	304	CLA	CHC-C4B-NB	2.11	126.50	124.26
22	4	614	CLA	CHB-C4A-NA	2.11	127.44	124.51
22	A	836	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	A	851	BCR	C19-C18-C17	-2.11	115.70	118.94
32	B	850	DGD	O3E-C3E-C4E	-2.11	105.46	110.35
22	V	614	CLA	C3B-C4B-NB	-2.11	108.55	110.52
22	B	835	CLA	CHB-C4A-NA	2.11	127.44	124.51
21	U	601	CHL	CHC-C1C-C2C	-2.11	120.86	126.73
23	W	2620	LUT	C11-C12-C13	-2.11	120.48	126.42
27	K	205	BCR	C30-C25-C26	-2.11	119.64	122.61
22	4	610	CLA	CHB-C4A-NA	2.11	127.43	124.51
27	L	301	BCR	C38-C26-C27	2.11	117.67	113.62
22	5	602	CLA	C3B-C4B-NB	-2.11	108.56	110.52
31	G	206	LMT	C4B-C3B-C2B	-2.11	107.14	110.82
22	A	836	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	9	623	NEX	C28-C29-C30	2.11	122.18	118.94
22	F	303	CLA	O2A-CGA-O1A	-2.11	118.03	123.30
22	B	824	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
21	5	607	CHL	CHB-C1B-C2B	-2.11	121.27	127.24
22	A	835	CLA	CHC-C4B-NB	2.11	126.49	124.26
22	A	805	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	U	604	CLA	C3B-C4B-NB	-2.11	108.56	110.52
27	B	848	BCR	C36-C18-C19	2.11	121.40	118.08
22	1	602	CLA	CHB-C4A-NA	2.11	127.43	124.51
21	2	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
21	9	605	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
22	A	811	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	A	830	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	W	603	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	4	613	CLA	CHB-C4A-NA	2.11	127.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	2623	NEX	C35-C34-C33	-2.11	124.30	127.31
22	1	608	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
27	J	102	BCR	C34-C9-C10	-2.11	119.97	122.92
22	U	610	CLA	C3B-C4B-NB	-2.11	108.56	110.52
22	L	302	CLA	C3B-C4B-NB	-2.11	108.56	110.52
22	V	613	CLA	C5-C3-C2	2.11	125.38	121.12
22	B	837	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	B	805	CLA	C5-C3-C2	2.11	125.38	121.12
22	V	610	CLA	CHB-C4A-NA	2.11	127.42	124.51
22	A	803	CLA	CHD-C1D-ND	-2.11	122.52	124.45
21	U	609	CHL	CHB-C1B-C2B	-2.11	121.29	127.24
21	4	606	CHL	CED-O2D-CGD	2.11	120.70	115.94
26	4	630	LHG	O7-C7-O9	-2.11	118.61	123.70
22	A	808	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	1	617	LUT	C1-C6-C5	-2.10	119.65	122.61
22	A	838	CLA	CMB-C2B-C1B	-2.10	122.16	125.37
21	4	618	CHL	O2D-CGD-O1D	-2.10	119.72	123.84
27	F	305	BCR	C27-C26-C25	-2.10	119.68	122.73
27	O	2004	BCR	C7-C6-C5	-2.10	116.37	121.46
22	6	609	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	U	602	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
28	L	307	LMG	O8-C28-C29	2.10	118.50	111.91
22	5	616	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	9	2630	LHG	C6-O8-C23	2.10	124.90	117.12
22	7	602	CLA	CHB-C1B-NB	2.10	126.48	124.26
31	B	849	LMT	C4B-C3B-C2B	-2.10	107.15	110.82
21	6	606	CHL	CHB-C1B-C2B	-2.10	121.30	127.24
22	B	811	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	G	201	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	W	612	CLA	C3B-C4B-NB	-2.10	108.82	110.23
21	2	601	CHL	CHB-C1B-C2B	-2.10	121.31	127.24
21	4	607	CHL	CHB-C1B-C2B	-2.10	121.31	127.24
21	2	602	CHL	CED-O2D-CGD	2.10	120.69	115.94
21	2	608	CHL	O2A-CGA-CBA	2.10	120.78	114.03
22	B	818	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	4	613	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	7	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	1	614	CLA	CHB-C4A-NA	2.10	127.41	124.51
23	8	619	LUT	C15-C14-C13	-2.10	124.32	127.31
22	B	832	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	9	609	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
22	3	610	CLA	CHB-C1B-NB	2.10	126.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	203	CLA	C3B-C4B-NB	-2.10	108.57	110.52
22	B	810	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	B	1609	BCR	C12-C13-C14	-2.10	115.72	118.94
23	6	619	LUT	C39-C29-C28	2.10	121.38	118.08
22	1	613	CLA	CHB-C4A-NA	2.10	127.41	124.51
27	3	620	BCR	C36-C18-C19	2.10	121.38	118.08
23	7	618	LUT	C35-C34-C33	-2.10	124.32	127.31
22	6	614	CLA	CHB-C4A-NA	2.09	127.41	124.51
22	8	613	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	B	824	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	8	601	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	A	826	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	3	614	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
24	1	618	XAT	O4-C5-C6	-2.09	57.23	58.96
21	W	601	CHL	CHC-C1C-C2C	-2.09	120.92	126.73
22	A	807	CLA	C3B-C4B-NB	-2.09	108.58	110.52
21	U	601	CHL	O2D-CGD-O1D	-2.09	119.34	124.09
23	9	621	LUT	C15-C14-C13	-2.09	124.33	127.31
23	V	2620	LUT	C16-C1-C6	2.09	113.69	110.30
27	F	305	BCR	C38-C26-C27	2.09	117.63	113.62
22	A	811	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	4	601	CLA	O2D-CGD-CBD	2.09	114.98	111.27
22	W	610	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
22	B	820	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	1	603	CLA	C3B-C4B-NB	-2.09	108.58	110.52
21	2	607	CHL	CHB-C1B-C2B	-2.09	121.34	127.24
22	1	603	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	A	839	CLA	CHB-C4A-NA	2.09	127.40	124.51
27	B	843	BCR	C3-C4-C5	-2.09	110.35	114.08
21	9	608	CHL	CED-O2D-CGD	2.09	120.66	115.94
22	A	833	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	V	612	CLA	CMA-C3A-C2A	-2.09	111.23	116.10
22	B	822	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	6	613	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	A	824	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	6	608	CHL	CHB-C1B-C2B	-2.09	121.34	127.24
22	6	610	CLA	CHD-C1D-ND	-2.09	122.54	124.45
22	B	838	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	1	609	CLA	C4-C3-C2	-2.09	118.33	123.68
23	U	2620	LUT	C35-C15-C14	-2.09	119.20	123.47
21	6	618	CHL	CHB-C1B-C2B	-2.09	121.34	127.24
21	7	608	CHL	CBC-CAC-C3C	-2.09	106.68	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	203	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	3	607	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	A	839	CLA	C3B-C4B-NB	-2.08	108.58	110.52
22	V	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
27	B	847	BCR	C8-C9-C10	-2.08	115.74	118.94
22	8	609	CLA	C3B-C4B-NB	-2.08	108.58	110.52
24	1	618	XAT	C35-C34-C33	-2.08	124.34	127.31
21	V	608	CHL	O2D-CGD-O1D	-2.08	119.36	124.09
21	V	607	CHL	C4B-C3B-C2B	-2.08	105.05	107.03
22	7	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	6	614	CLA	CHB-C1B-NB	2.08	126.46	124.26
22	F	303	CLA	C3B-C4B-NB	-2.08	108.58	110.52
22	A	821	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	3	611	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	3	603	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	A	825	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	2	620	XAT	C15-C14-C13	-2.08	124.34	127.31
22	6	614	CLA	C3B-C4B-NB	-2.08	108.59	110.52
22	U	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	G	204	CLA	CHB-C4A-NA	2.08	127.38	124.51
29	A	844	PQN	C21-C20-C18	-2.08	109.21	115.92
23	9	620	LUT	C18-C5-C4	2.08	118.20	114.36
22	1	609	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	V	614	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	4	603	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	A	824	CLA	CHB-C1B-NB	2.08	126.45	124.26
22	J	101	CLA	C3B-C4B-NB	-2.07	108.59	110.52
22	B	837	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	4	611	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	U	2623	NEX	C28-C29-C30	2.07	122.12	118.94
22	B	808	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	B	804	CLA	O2D-CGD-CBD	2.07	114.95	111.27
22	B	813	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	5	603	CLA	CHC-C4B-NB	2.07	126.45	124.26
21	6	601	CHL	CHB-C1B-C2B	-2.07	121.39	127.24
22	3	615	CLA	C3B-C4B-NB	-2.07	108.59	110.52
22	F	301	CLA	C3B-C4B-NB	-2.07	108.59	110.52
23	V	2621	LUT	C19-C9-C10	-2.07	120.02	122.92
23	V	2620	LUT	C15-C14-C13	-2.07	124.36	127.31
27	B	801	BCR	C34-C9-C8	2.07	121.34	118.08
22	B	826	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	B	810	CLA	CHC-C4B-NB	2.07	126.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	602	CLA	CHC-C4B-NB	2.07	126.45	124.26
27	B	843	BCR	C11-C12-C13	-2.07	120.61	126.42
22	B	811	CLA	C3B-C4B-NB	-2.07	108.60	110.52
22	A	829	CLA	CMB-C2B-C3B	2.07	131.59	126.59
22	5	603	CLA	CHB-C1B-NB	2.07	126.44	124.26
22	7	613	CLA	CHB-C4A-NA	2.07	127.37	124.51
21	8	606	CHL	O2A-CGA-CBA	2.07	120.67	114.03
22	B	823	CLA	CAC-C3C-C4C	2.07	127.49	124.81
21	W	605	CHL	CHC-C1C-C2C	-2.07	120.99	126.73
22	V	614	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
22	9	604	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	9	612	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	4	612	CLA	CHD-C1D-ND	-2.07	122.56	124.45
23	4	619	LUT	C39-C29-C28	2.07	121.33	118.08
22	A	822	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
27	M	2001	BCR	C33-C5-C4	2.06	117.58	113.62
22	4	613	CLA	O2D-CGD-CBD	2.06	114.94	111.27
21	5	607	CHL	CBD-CHA-C1A	2.06	130.73	127.43
22	1	606	CLA	CHB-C4A-NA	2.06	127.37	124.51
22	8	603	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	B	805	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
22	A	824	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	L	302	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	2	608	CHL	C2A-C3A-C4A	-2.06	98.54	101.87
22	G	203	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	9	610	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	9	623	NEX	C10-C11-C12	-2.06	116.78	123.22
23	1	617	LUT	C39-C29-C28	2.06	121.32	118.08
21	V	609	CHL	CHB-C1B-C2B	-2.06	121.42	127.24
22	A	819	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
21	V	608	CHL	C4B-C3B-C2B	-2.06	105.07	107.03
22	B	823	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	1	603	CLA	O2D-CGD-CBD	2.06	114.93	111.27
21	6	618	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
25	U	2623	NEX	C12-C13-C14	-2.06	115.78	118.94
22	1	603	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	U	2620	LUT	C39-C29-C28	2.06	121.32	118.08
22	3	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	A	839	CLA	CHC-C4B-NB	2.06	126.44	124.26
27	B	848	BCR	C10-C11-C12	-2.06	116.80	123.22
22	A	831	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	3	609	CLA	CHC-C4B-NB	2.06	126.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	601	CLA	CHB-C4A-NA	2.06	127.36	124.51
21	V	606	CHL	C4B-C3B-C2B	-2.06	105.08	107.03
21	9	601	CHL	CHB-C1B-C2B	-2.06	121.43	127.24
27	K	205	BCR	C1-C6-C5	-2.06	119.72	122.61
22	4	609	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
27	1	619	BCR	C15-C16-C17	-2.05	119.27	123.47
22	A	801	CLA	C3B-C4B-NB	-2.05	108.61	110.52
22	3	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	9	624	LUT	C31-C30-C29	-2.05	124.38	127.31
26	8	630	LHG	O8-C23-O10	-2.05	118.41	123.59
29	A	844	PQN	C17-C16-C15	-2.05	107.78	113.36
22	B	805	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	1	617	LUT	C16-C1-C6	2.05	113.63	110.30
27	6	621	BCR	C38-C26-C27	2.05	117.56	113.62
22	A	818	CLA	C3B-C4B-NB	-2.05	108.61	110.52
24	U	2622	XAT	C39-C29-C28	2.05	121.31	118.08
22	A	828	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	8	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	A	838	CLA	CMB-C2B-C3B	2.05	131.56	126.59
24	1	618	XAT	C11-C10-C9	-2.05	124.38	127.31
22	A	810	CLA	O2D-CGD-CBD	2.05	114.91	111.27
28	2	631	LMG	O7-C10-O9	-2.05	118.75	123.70
22	A	820	CLA	CMB-C2B-C3B	2.05	131.55	126.59
24	2	620	XAT	O4-C5-C6	-2.05	57.26	58.96
22	B	831	CLA	O2D-CGD-CBD	2.05	114.91	111.27
27	K	205	BCR	C36-C18-C17	-2.05	120.05	122.92
22	B	803	CLA	CHC-C4B-NB	2.05	126.42	124.26
21	9	608	CHL	CHB-C1B-C2B	-2.05	121.45	127.24
22	7	609	CLA	CAC-C3C-C4C	2.05	127.47	124.81
22	B	819	CLA	CHB-C1B-NB	2.05	126.42	124.26
22	5	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	3	612	CLA	C1-C2-C3	-2.05	122.50	126.04
27	2	621	BCR	C24-C25-C26	2.05	126.42	121.46
21	2	618	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
22	B	841	CLA	CHC-C4B-NB	2.05	126.42	124.26
22	7	603	CLA	C3B-C4B-NB	-2.05	108.62	110.52
22	A	834	CLA	CHC-C4B-NB	2.05	126.42	124.26
22	B	807	CLA	CHB-C1B-NB	2.05	126.42	124.26
27	A	856	BCR	C8-C9-C10	-2.04	115.80	118.94
22	K	203	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
27	B	801	BCR	C33-C5-C6	-2.04	122.23	124.53
22	A	811	CLA	O2A-CGA-O1A	-2.04	118.43	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	619	LUT	C38-C25-C24	-2.04	119.19	123.56
27	I	101	BCR	C16-C15-C14	-2.04	119.29	123.47
21	7	608	CHL	CHB-C1B-C2B	-2.04	121.46	127.24
22	U	602	CLA	C3B-C4B-NB	-2.04	108.62	110.52
22	5	606	CLA	CHB-C4A-NA	2.04	127.34	124.51
22	9	613	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
21	W	609	CHL	CMB-C2B-C1B	2.04	128.48	125.37
22	B	813	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	W	612	CLA	CAA-C2A-C3A	-2.04	111.33	116.10
22	4	609	CLA	CHC-C4B-NB	2.04	126.42	124.26
22	A	827	CLA	CHC-C4B-NB	2.04	126.42	124.26
21	9	605	CHL	CBD-CHA-C1A	2.04	130.70	127.43
26	A	847	LHG	C5-O7-C7	-2.04	112.77	117.79
23	V	2620	LUT	C15-C35-C34	-2.04	119.29	123.47
22	A	802	CLA	CHC-C4B-NB	2.04	126.42	124.26
22	6	604	CLA	C1-C2-C3	-2.04	123.45	126.75
27	K	205	BCR	C11-C10-C9	-2.04	124.40	127.31
21	1	607	CHL	CHB-C1B-C2B	-2.04	121.48	127.24
22	9	610	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	B	845	BCR	C29-C30-C25	2.04	113.62	110.48
27	A	850	BCR	C20-C19-C18	-2.04	120.69	126.42
22	B	839	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
24	6	620	XAT	C15-C35-C34	-2.04	119.30	123.47
22	5	614	CLA	CHB-C1B-NB	2.04	126.41	124.26
27	7	621	BCR	C16-C15-C14	-2.04	119.30	123.47
22	B	811	CLA	CHB-C1B-NB	2.04	126.41	124.26
23	U	2620	LUT	C38-C25-C24	-2.04	119.20	123.56
21	U	607	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
22	B	809	CLA	C4-C3-C2	-2.04	118.46	123.68
27	L	306	BCR	C16-C17-C18	-2.04	124.41	127.31
22	A	833	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	B	809	CLA	C3B-C4B-NB	-2.04	108.63	110.52
22	8	614	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
22	8	603	CLA	CHB-C1B-NB	2.03	126.41	124.26
21	8	608	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
22	L	304	CLA	C1-C2-C3	-2.03	122.53	126.04
21	2	618	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
27	M	2001	BCR	C31-C1-C6	2.03	113.60	110.30
22	8	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	8	614	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	1	602	CLA	C1-C2-C3	-2.03	122.53	126.04
25	W	2623	NEX	C30-C31-C32	-2.03	116.87	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	604	CLA	CHC-C4B-NB	2.03	126.41	124.26
23	3	618	LUT	C36-C21-C26	2.03	112.62	109.55
27	2	621	BCR	C15-C16-C17	-2.03	119.31	123.47
23	9	620	LUT	C30-C31-C32	-2.03	116.88	123.22
22	5	603	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
22	B	841	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	B	805	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
22	5	603	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	L	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	854	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	816	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	4	607	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
26	7	630	LHG	O8-C23-O10	-2.03	118.47	123.59
27	I	101	BCR	C28-C27-C26	-2.03	110.45	114.08
22	A	801	CLA	CHA-C4D-ND	2.03	136.75	132.50
22	A	845	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	3	619	XAT	C19-C9-C8	2.03	121.27	118.08
21	8	608	CHL	CED-O2D-CGD	2.03	120.53	115.94
22	9	613	CLA	C3B-C4B-NB	-2.03	108.63	110.52
21	9	606	CHL	CHB-C1B-C2B	-2.03	121.51	127.24
22	8	604	CLA	CHC-C4B-NB	2.03	126.40	124.26
27	B	844	BCR	C20-C21-C22	-2.03	124.42	127.31
27	O	2004	BCR	C15-C16-C17	-2.03	119.32	123.47
27	F	305	BCR	C15-C14-C13	-2.03	124.42	127.31
23	V	2620	LUT	C38-C25-C24	-2.03	119.22	123.56
21	8	606	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
21	9	606	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
22	W	603	CLA	CAA-C2A-C3A	-2.03	111.37	116.10
21	U	609	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
25	U	2623	NEX	C24-C23-C22	-2.03	106.86	110.77
22	7	617	CLA	O2D-CGD-CBD	2.02	114.87	111.27
24	2	620	XAT	C36-C21-C22	-2.02	105.47	108.98
22	W	611	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
22	A	827	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	3	604	CLA	O2D-CGD-CBD	2.02	114.86	111.27
21	2	601	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
22	3	602	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	3	617	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	3	617	CLA	C4B-C3B-C2B	-2.02	106.05	107.45
22	2	611	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	5	613	CLA	O2D-CGD-CBD	2.02	114.86	111.27
24	W	2622	XAT	C27-C28-C29	-2.02	122.39	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	834	CLA	CHC-C4B-NB	2.02	126.40	124.26
21	U	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
22	1	612	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	3	610	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	A	818	CLA	CHC-C4B-NB	2.02	126.40	124.26
22	A	836	CLA	CHD-C4C-NC	2.02	125.98	122.91
22	A	804	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	1	604	CLA	CHB-C1B-NB	2.02	126.39	124.26
23	6	619	LUT	C20-C13-C12	2.02	121.26	118.08
24	5	618	XAT	O4-C5-C6	-2.02	57.29	58.96
22	9	609	CLA	C4D-CHA-C1A	-2.02	118.79	121.25
21	W	607	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
22	W	613	CLA	CHB-C4A-NA	2.02	127.30	124.51
21	2	607	CHL	O2A-CGA-CBA	2.02	120.21	112.23
22	4	609	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	6	609	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	8	614	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
22	W	602	CLA	CHB-C1B-NB	2.02	126.39	124.26
27	7	620	BCR	C35-C13-C12	2.02	121.26	118.08
25	W	2623	NEX	C31-C32-C33	-2.02	120.75	126.42
22	7	611	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	4	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	804	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	841	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	5	606	CLA	O2A-CGA-O1A	-2.02	118.28	123.30
23	9	624	LUT	C21-C26-C27	-2.02	110.15	112.70
23	U	2621	LUT	C35-C15-C14	-2.02	119.35	123.47
24	5	618	XAT	C11-C12-C13	-2.02	120.75	126.42
22	1	604	CLA	CHC-C4B-NB	2.01	126.39	124.26
22	W	603	CLA	C3B-C4B-NB	-2.01	108.65	110.52
22	A	827	CLA	C3B-C4B-NB	-2.01	108.65	110.52
22	1	611	CLA	C1-C2-C3	-2.01	122.56	126.04
27	7	621	BCR	C23-C22-C21	-2.01	115.85	118.94
22	7	611	CLA	O2D-CGD-CBD	2.01	114.85	111.27
22	A	841	CLA	CHB-C4A-NA	2.01	127.30	124.51
21	2	608	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
22	U	612	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	A	854	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	8	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	4	602	CLA	C3B-C4B-NB	-2.01	108.65	110.52
22	U	604	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	B	833	CLA	O2D-CGD-CBD	2.01	114.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	843	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	5	613	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	K	202	BCR	C24-C25-C26	2.01	126.33	121.46
24	3	619	XAT	O24-C25-C26	-2.01	57.30	58.96
21	U	606	CHL	CMB-C2B-C1B	2.01	128.43	125.37
22	F	304	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
23	8	619	LUT	C35-C34-C33	-2.01	124.45	127.31
22	K	206	CLA	CHB-C1B-NB	2.01	126.38	124.26
24	W	2622	XAT	C20-C13-C12	2.01	121.24	118.08
22	B	828	CLA	CHB-C4A-NA	2.01	127.29	124.51
22	B	834	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	3	603	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
21	4	618	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
21	2	601	CHL	O2A-CGA-O1A	-2.01	118.30	123.30
22	6	611	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
27	B	801	BCR	C27-C26-C25	-2.00	119.82	122.73
22	8	601	CLA	CHB-C4A-NA	2.00	127.28	124.51
21	6	606	CHL	C1C-C2C-C3C	-2.00	105.52	107.11
27	G	205	BCR	C40-C30-C25	-2.00	107.05	110.30
23	U	2621	LUT	C31-C30-C29	-2.00	124.45	127.31
22	W	611	CLA	CHB-C4A-NA	2.00	127.28	124.51
22	B	807	CLA	CHB-C4A-NA	2.00	127.28	124.51

There are no chirality outliers.

All (2845) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	U	601	CHL	CAD-CBD-CGD-O2D
21	U	607	CHL	C1A-C2A-CAA-CBA
21	U	607	CHL	C3A-C2A-CAA-CBA
21	U	608	CHL	CHA-CBD-CGD-O2D
21	U	609	CHL	C1A-C2A-CAA-CBA
21	U	609	CHL	CHA-CBD-CGD-O1D
21	U	609	CHL	CHA-CBD-CGD-O2D
21	V	601	CHL	C1A-C2A-CAA-CBA
21	V	601	CHL	C3A-C2A-CAA-CBA
21	V	601	CHL	CAD-CBD-CGD-O2D
21	V	601	CHL	C4-C3-C5-C6
21	V	605	CHL	CHA-CBD-CGD-O2D
21	V	608	CHL	C1A-C2A-CAA-CBA
21	W	608	CHL	C1A-C2A-CAA-CBA
21	W	609	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	1	601	CHL	CHA-CBD-CGD-O1D
21	1	601	CHL	CHA-CBD-CGD-O2D
21	1	601	CHL	CAD-CBD-CGD-O1D
21	1	601	CHL	CAD-CBD-CGD-O2D
21	1	607	CHL	C1A-C2A-CAA-CBA
21	1	607	CHL	C3A-C2A-CAA-CBA
21	1	607	CHL	CAD-CBD-CGD-O1D
21	1	607	CHL	CAD-CBD-CGD-O2D
21	2	601	CHL	CHA-CBD-CGD-O1D
21	2	601	CHL	CHA-CBD-CGD-O2D
21	2	601	CHL	CAD-CBD-CGD-O1D
21	2	607	CHL	CHA-CBD-CGD-O1D
21	2	607	CHL	CHA-CBD-CGD-O2D
21	2	618	CHL	CAD-CBD-CGD-O1D
21	2	618	CHL	CAD-CBD-CGD-O2D
21	3	608	CHL	C1A-C2A-CAA-CBA
21	3	608	CHL	C2-C3-C5-C6
21	3	608	CHL	C4-C3-C5-C6
21	4	606	CHL	CHA-CBD-CGD-O1D
21	4	606	CHL	CHA-CBD-CGD-O2D
21	4	607	CHL	CHA-CBD-CGD-O1D
21	4	607	CHL	CHA-CBD-CGD-O2D
21	5	601	CHL	CHA-CBD-CGD-O1D
21	5	601	CHL	CHA-CBD-CGD-O2D
21	5	601	CHL	CAD-CBD-CGD-O1D
21	5	601	CHL	CAD-CBD-CGD-O2D
21	6	601	CHL	CHA-CBD-CGD-O1D
21	6	601	CHL	CHA-CBD-CGD-O2D
21	6	601	CHL	CAD-CBD-CGD-O1D
21	6	601	CHL	CAD-CBD-CGD-O2D
21	6	607	CHL	CHA-CBD-CGD-O1D
21	6	607	CHL	CHA-CBD-CGD-O2D
21	6	608	CHL	CHA-CBD-CGD-O1D
21	6	608	CHL	CHA-CBD-CGD-O2D
21	7	608	CHL	CHA-CBD-CGD-O1D
21	7	608	CHL	CHA-CBD-CGD-O2D
21	8	606	CHL	CHA-CBD-CGD-O1D
21	8	606	CHL	CHA-CBD-CGD-O2D
21	8	607	CHL	CHA-CBD-CGD-O1D
21	8	607	CHL	CHA-CBD-CGD-O2D
21	8	608	CHL	CHA-CBD-CGD-O1D
21	8	608	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	8	618	CHL	CHA-CBD-CGD-O1D
21	8	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	C1A-C2A-CAA-CBA
22	U	602	CLA	C4-C3-C5-C6
22	U	610	CLA	C3A-C2A-CAA-CBA
22	U	611	CLA	CHA-CBD-CGD-O1D
22	U	611	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	C14-C13-C15-C16
22	V	611	CLA	C1A-C2A-CAA-CBA
22	V	613	CLA	CHA-CBD-CGD-O1D
22	V	613	CLA	CHA-CBD-CGD-O2D
22	V	614	CLA	C1A-C2A-CAA-CBA
22	V	614	CLA	C3A-C2A-CAA-CBA
22	W	610	CLA	C2-C3-C5-C6
22	W	610	CLA	C4-C3-C5-C6
22	W	610	CLA	C6-C7-C8-C9
22	W	610	CLA	C11-C10-C8-C9
22	1	602	CLA	C1A-C2A-CAA-CBA
22	1	602	CLA	C3A-C2A-CAA-CBA
22	1	604	CLA	C1A-C2A-CAA-CBA
22	1	604	CLA	C3A-C2A-CAA-CBA
22	1	606	CLA	C2B-C3B-CAB-CBB
22	1	606	CLA	C4B-C3B-CAB-CBB
22	1	606	CLA	CHA-CBD-CGD-O1D
22	1	606	CLA	CHA-CBD-CGD-O2D
22	1	606	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	C1A-C2A-CAA-CBA
22	1	609	CLA	C1A-C2A-CAA-CBA
22	1	609	CLA	C3A-C2A-CAA-CBA
22	1	609	CLA	C2B-C3B-CAB-CBB
22	1	609	CLA	C4B-C3B-CAB-CBB
22	1	609	CLA	C2-C3-C5-C6
22	1	609	CLA	C4-C3-C5-C6
22	1	610	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C3A-C2A-CAA-CBA
22	1	614	CLA	C1A-C2A-CAA-CBA
22	1	614	CLA	C2A-CAA-CBA-CGA
22	1	616	CLA	CHA-CBD-CGD-O1D
22	2	609	CLA	C1A-C2A-CAA-CBA
22	2	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	2	611	CLA	C2B-C3B-CAB-CBB
22	2	611	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	C1A-C2A-CAA-CBA
22	2	612	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	CHA-CBD-CGD-O1D
22	3	602	CLA	C1A-C2A-CAA-CBA
22	3	602	CLA	C3A-C2A-CAA-CBA
22	3	604	CLA	C2A-CAA-CBA-CGA
22	3	606	CLA	C1A-C2A-CAA-CBA
22	3	606	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C1A-C2A-CAA-CBA
22	3	607	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C1A-C2A-CAA-CBA
22	3	609	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C4-C3-C5-C6
22	3	610	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C3A-C2A-CAA-CBA
22	3	611	CLA	C2B-C3B-CAB-CBB
22	3	611	CLA	C4B-C3B-CAB-CBB
22	3	614	CLA	C2B-C3B-CAB-CBB
22	3	614	CLA	C4B-C3B-CAB-CBB
22	3	617	CLA	C1A-C2A-CAA-CBA
22	3	617	CLA	C3A-C2A-CAA-CBA
22	4	601	CLA	CHA-CBD-CGD-O1D
22	4	601	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	C3A-C2A-CAA-CBA
22	4	603	CLA	CBD-CGD-O2D-CED
22	4	604	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C1A-C2A-CAA-CBA
22	4	609	CLA	C3A-C2A-CAA-CBA
22	4	610	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	C1A-C2A-CAA-CBA
22	4	614	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	CBA-CGA-O2A-C1
22	4	614	CLA	O1A-CGA-O2A-C1
22	A	801	CLA	CAD-CBD-CGD-O1D
22	A	801	CLA	CAD-CBD-CGD-O2D
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	810	CLA	C2B-C3B-CAB-CBB
22	A	810	CLA	C4B-C3B-CAB-CBB
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	811	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	815	CLA	C1A-C2A-CAA-CBA
22	A	817	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	821	CLA	C1A-C2A-CAA-CBA
22	A	821	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	825	CLA	CHA-CBD-CGD-O1D
22	A	825	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	CHA-CBD-CGD-O1D
22	A	828	CLA	CHA-CBD-CGD-O2D
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C3A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C3A-C2A-CAA-CBA
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	C1A-C2A-CAA-CBA
22	A	835	CLA	C3A-C2A-CAA-CBA
22	A	837	CLA	C4B-C3B-CAB-CBB
22	A	839	CLA	C2B-C3B-CAB-CBB
22	A	839	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	CHA-CBD-CGD-O1D
22	A	841	CLA	CHA-CBD-CGD-O2D
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C3A-C2A-CAA-CBA
22	A	845	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	854	CLA	C1A-C2A-CAA-CBA
22	A	854	CLA	C3A-C2A-CAA-CBA
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	803	CLA	CBD-CGD-O2D-CED
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	805	CLA	CHA-CBD-CGD-O2D
22	B	806	CLA	C2B-C3B-CAB-CBB
22	B	806	CLA	C4B-C3B-CAB-CBB
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C2B-C3B-CAB-CBB
22	B	811	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	813	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	817	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C4B-C3B-CAB-CBB
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C4B-C3B-CAB-CBB
22	B	819	CLA	O2A-C1-C2-C3
22	B	822	CLA	C2A-CAA-CBA-CGA
22	B	822	CLA	C2B-C3B-CAB-CBB
22	B	822	CLA	C4B-C3B-CAB-CBB
22	B	824	CLA	C2-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
22	B	826	CLA	C2B-C3B-CAB-CBB
22	B	826	CLA	C4B-C3B-CAB-CBB
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C4B-C3B-CAB-CBB
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C4-C3-C5-C6
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	C4-C3-C5-C6
22	B	835	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	C1A-C2A-CAA-CBA
22	B	836	CLA	C3A-C2A-CAA-CBA
22	B	836	CLA	C2A-CAA-CBA-CGA
22	B	837	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C3A-C2A-CAA-CBA
22	F	304	CLA	C2B-C3B-CAB-CBB
22	F	304	CLA	C4B-C3B-CAB-CBB
22	G	201	CLA	CBD-CGD-O2D-CED
22	J	101	CLA	C2B-C3B-CAB-CBB
22	J	101	CLA	C4B-C3B-CAB-CBB
22	K	201	CLA	C1A-C2A-CAA-CBA
22	K	201	CLA	C3A-C2A-CAA-CBA
22	K	204	CLA	C2A-CAA-CBA-CGA
22	K	204	CLA	C2-C3-C5-C6
22	K	204	CLA	C4-C3-C5-C6
22	L	302	CLA	CHA-CBD-CGD-O1D
22	L	302	CLA	CHA-CBD-CGD-O2D
22	L	302	CLA	CAD-CBD-CGD-O1D
22	L	302	CLA	C11-C12-C13-C14
22	L	304	CLA	C1A-C2A-CAA-CBA
22	L	304	CLA	C2A-CAA-CBA-CGA
22	O	2002	CLA	C3A-C2A-CAA-CBA
22	O	2002	CLA	C2B-C3B-CAB-CBB
22	O	2002	CLA	C4B-C3B-CAB-CBB
22	O	2002	CLA	CAD-CBD-CGD-O1D
22	O	2002	CLA	CAD-CBD-CGD-O2D
22	5	603	CLA	CBD-CGD-O2D-CED
22	5	608	CLA	CHA-CBD-CGD-O1D
22	5	608	CLA	CHA-CBD-CGD-O2D
22	5	610	CLA	C1A-C2A-CAA-CBA
22	5	611	CLA	CHA-CBD-CGD-O1D
22	5	611	CLA	CHA-CBD-CGD-O2D
22	5	611	CLA	CAD-CBD-CGD-O1D
22	5	612	CLA	CBD-CGD-O2D-CED
22	5	613	CLA	C1A-C2A-CAA-CBA
22	5	613	CLA	C3A-C2A-CAA-CBA
22	5	613	CLA	CHA-CBD-CGD-O1D
22	5	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	603	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	C1A-C2A-CAA-CBA
22	6	610	CLA	C3A-C2A-CAA-CBA
22	6	613	CLA	CHA-CBD-CGD-O1D
22	6	613	CLA	CHA-CBD-CGD-O2D
22	7	603	CLA	C1A-C2A-CAA-CBA
22	7	603	CLA	C3A-C2A-CAA-CBA
22	7	604	CLA	CHA-CBD-CGD-O1D
22	7	604	CLA	CHA-CBD-CGD-O2D
22	7	604	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	C1A-C2A-CAA-CBA
22	7	609	CLA	C1A-C2A-CAA-CBA
22	7	609	CLA	C3A-C2A-CAA-CBA
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C3A-C2A-CAA-CBA
22	7	610	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	C4B-C3B-CAB-CBB
22	7	614	CLA	CBD-CGD-O2D-CED
22	7	617	CLA	C1A-C2A-CAA-CBA
22	7	617	CLA	C3A-C2A-CAA-CBA
22	7	617	CLA	CBA-CGA-O2A-C1
22	7	617	CLA	O1A-CGA-O2A-C1
22	8	602	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	CHA-CBD-CGD-O1D
22	8	612	CLA	CHA-CBD-CGD-O2D
22	8	613	CLA	CHA-CBD-CGD-O1D
22	8	613	CLA	CHA-CBD-CGD-O2D
22	8	614	CLA	C1A-C2A-CAA-CBA
22	8	614	CLA	CAD-CBD-CGD-O1D
22	8	614	CLA	CAD-CBD-CGD-O2D
22	8	614	CLA	CBD-CGD-O2D-CED
22	9	604	CLA	CBD-CGD-O2D-CED
22	9	610	CLA	C1A-C2A-CAA-CBA
22	9	612	CLA	C1A-C2A-CAA-CBA
23	2	619	LUT	C7-C8-C9-C10
23	2	619	LUT	C7-C8-C9-C19
23	2	619	LUT	C11-C12-C13-C20
23	2	619	LUT	C28-C29-C30-C31
23	2	619	LUT	C39-C29-C30-C31
23	2	619	LUT	C30-C31-C32-C33
23	5	617	LUT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	5	617	LUT	C26-C27-C28-C29
24	U	2622	XAT	O4-C6-C7-C8
24	V	2622	XAT	C25-C26-C27-C28
24	V	2622	XAT	O24-C26-C27-C28
24	4	620	XAT	C1-C6-C7-C8
24	4	620	XAT	C5-C6-C7-C8
24	4	620	XAT	O4-C6-C7-C8
24	5	618	XAT	C21-C26-C27-C28
24	5	618	XAT	C25-C26-C27-C28
24	5	618	XAT	C31-C32-C33-C34
24	5	618	XAT	C31-C32-C33-C40
24	6	620	XAT	C21-C26-C27-C28
24	6	620	XAT	C25-C26-C27-C28
24	6	620	XAT	O24-C26-C27-C28
24	7	619	XAT	C1-C6-C7-C8
24	7	619	XAT	C5-C6-C7-C8
24	7	619	XAT	O4-C6-C7-C8
24	8	620	XAT	C6-C7-C8-C9
24	8	620	XAT	C31-C32-C33-C34
24	8	620	XAT	C31-C32-C33-C40
25	U	2623	NEX	O24-C26-C27-C28
25	W	2623	NEX	C13-C14-C15-C35
25	W	2623	NEX	C27-C28-C29-C30
25	W	2623	NEX	C27-C28-C29-C39
25	W	2623	NEX	C31-C32-C33-C34
25	W	2623	NEX	C31-C32-C33-C40
26	U	2630	LHG	C4-O6-P-O5
26	V	2630	LHG	C4-O6-P-O5
26	W	2630	LHG	C3-O3-P-O6
26	W	2630	LHG	C4-O6-P-O5
26	1	630	LHG	O1-C1-C2-C3
26	1	630	LHG	C4-O6-P-O5
26	2	630	LHG	C4-O6-P-O4
26	4	630	LHG	O1-C1-C2-O2
26	4	630	LHG	O1-C1-C2-C3
26	4	630	LHG	O9-C7-O7-C5
26	A	847	LHG	C3-O3-P-O6
26	A	847	LHG	O6-C4-C5-O7
26	B	851	LHG	C4-O6-P-O4
26	5	630	LHG	C3-O3-P-O6
26	5	630	LHG	C4-O6-P-O5
26	6	630	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
26	6	630	LHG	C4-O6-P-O4
26	6	630	LHG	C4-O6-P-O5
26	7	630	LHG	C3-O3-P-O4
26	7	630	LHG	C3-O3-P-O5
26	8	630	LHG	C3-O3-P-O6
26	8	630	LHG	C4-O6-P-O5
27	1	619	BCR	C5-C6-C7-C8
27	4	621	BCR	C7-C8-C9-C10
27	4	621	BCR	C7-C8-C9-C34
27	4	621	BCR	C21-C22-C23-C24
27	4	621	BCR	C37-C22-C23-C24
27	A	848	BCR	C23-C24-C25-C26
27	A	849	BCR	C23-C24-C25-C26
27	A	850	BCR	C23-C24-C25-C26
27	A	852	BCR	C5-C6-C7-C8
27	A	852	BCR	C23-C24-C25-C26
27	A	852	BCR	C23-C24-C25-C30
27	B	801	BCR	C23-C24-C25-C26
27	B	843	BCR	C23-C24-C25-C26
27	B	843	BCR	C23-C24-C25-C30
27	B	845	BCR	C7-C8-C9-C10
27	B	845	BCR	C7-C8-C9-C34
27	B	845	BCR	C11-C12-C13-C14
27	B	847	BCR	C21-C22-C23-C24
27	B	848	BCR	C23-C24-C25-C26
27	B	848	BCR	C23-C24-C25-C30
27	B	1609	BCR	C7-C8-C9-C10
27	B	1609	BCR	C7-C8-C9-C34
27	G	205	BCR	C5-C6-C7-C8
27	G	205	BCR	C23-C24-C25-C26
27	G	205	BCR	C23-C24-C25-C30
27	K	202	BCR	C23-C24-C25-C26
27	L	305	BCR	C1-C6-C7-C8
27	L	305	BCR	C5-C6-C7-C8
27	M	2001	BCR	C7-C8-C9-C10
27	M	2001	BCR	C7-C8-C9-C34
27	M	2001	BCR	C23-C24-C25-C26
27	6	621	BCR	C7-C8-C9-C10
27	6	621	BCR	C7-C8-C9-C34
27	6	621	BCR	C21-C22-C23-C24
27	6	621	BCR	C37-C22-C23-C24
27	8	621	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	8	621	BCR	C7-C8-C9-C34
27	8	621	BCR	C21-C22-C23-C24
27	8	621	BCR	C37-C22-C23-C24
28	A	860	LMG	O6-C1-O1-C7
28	A	860	LMG	C11-C10-O7-C8
28	G	202	LMG	O6-C1-O1-C7
28	J	103	LMG	C11-C10-O7-C8
31	A	857	LMT	C2-C1-O1'-C1'
31	K	208	LMT	O5'-C1'-O1'-C1
22	B	813	CLA	C4C-C3C-CAC-CBC
22	U	614	CLA	O1D-CGD-O2D-CED
22	V	603	CLA	O1D-CGD-O2D-CED
22	7	614	CLA	O1D-CGD-O2D-CED
22	8	604	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	C2C-C3C-CAC-CBC
22	4	603	CLA	O1D-CGD-O2D-CED
22	A	827	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	O1D-CGD-O2D-CED
22	5	603	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1D-CGD-O2D-CED
21	4	608	CHL	CBD-CGD-O2D-CED
22	U	604	CLA	CBD-CGD-O2D-CED
22	U	614	CLA	CBD-CGD-O2D-CED
22	V	603	CLA	CBD-CGD-O2D-CED
22	W	604	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	CBD-CGD-O2D-CED
22	3	610	CLA	CBD-CGD-O2D-CED
22	4	602	CLA	CBD-CGD-O2D-CED
22	4	604	CLA	CBD-CGD-O2D-CED
22	4	614	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	CBD-CGD-O2D-CED
22	B	827	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	G	203	CLA	CBD-CGD-O2D-CED
22	K	204	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	5	604	CLA	CBD-CGD-O2D-CED
22	5	610	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	CBD-CGD-O2D-CED
22	8	604	CLA	CBD-CGD-O2D-CED
22	8	610	CLA	CBD-CGD-O2D-CED
22	9	602	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	O1A-CGA-O2A-C1
22	2	604	CLA	O1A-CGA-O2A-C1
22	3	607	CLA	O1A-CGA-O2A-C1
22	3	612	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	O1A-CGA-O2A-C1
22	A	806	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	O1A-CGA-O2A-C1
22	B	810	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	L	303	CLA	O1A-CGA-O2A-C1
22	6	609	CLA	O1A-CGA-O2A-C1
22	8	613	CLA	O1A-CGA-O2A-C1
22	3	606	CLA	O1A-CGA-O2A-C1
22	3	606	CLA	CBA-CGA-O2A-C1
22	F	304	CLA	CBD-CGD-O2D-CED
22	U	612	CLA	O1D-CGD-O2D-CED
22	1	606	CLA	O1D-CGD-O2D-CED
22	A	845	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	G	201	CLA	O1D-CGD-O2D-CED
22	5	612	CLA	O1D-CGD-O2D-CED
22	9	604	CLA	O1D-CGD-O2D-CED
22	3	607	CLA	CBA-CGA-O2A-C1
22	3	612	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	CBA-CGA-O2A-C1
22	B	810	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	L	303	CLA	CBA-CGA-O2A-C1
22	6	609	CLA	CBA-CGA-O2A-C1
22	8	613	CLA	CBA-CGA-O2A-C1
21	3	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	U	603	CLA	CBD-CGD-O2D-CED
22	U	610	CLA	CBD-CGD-O2D-CED
22	V	614	CLA	CBD-CGD-O2D-CED
22	1	604	CLA	CBD-CGD-O2D-CED
22	1	608	CLA	CBD-CGD-O2D-CED
22	1	611	CLA	CBD-CGD-O2D-CED
22	3	603	CLA	CBD-CGD-O2D-CED
22	4	610	CLA	CBD-CGD-O2D-CED
22	4	611	CLA	CBD-CGD-O2D-CED
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED
22	A	840	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	CBD-CGD-O2D-CED
22	B	809	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	CBD-CGD-O2D-CED
22	B	840	CLA	CBD-CGD-O2D-CED
22	K	206	CLA	CBD-CGD-O2D-CED
22	6	610	CLA	CBD-CGD-O2D-CED
22	6	611	CLA	CBD-CGD-O2D-CED
22	7	602	CLA	CBD-CGD-O2D-CED
22	7	606	CLA	CBD-CGD-O2D-CED
22	8	611	CLA	CBD-CGD-O2D-CED
22	9	610	CLA	CBD-CGD-O2D-CED
22	1	603	CLA	O1A-CGA-O2A-C1
22	1	613	CLA	O1A-CGA-O2A-C1
22	2	614	CLA	O1A-CGA-O2A-C1
22	3	604	CLA	O1A-CGA-O2A-C1
22	4	601	CLA	O1A-CGA-O2A-C1
22	4	603	CLA	O1A-CGA-O2A-C1
22	4	604	CLA	O1A-CGA-O2A-C1
22	4	613	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
22	A	821	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	O1A-CGA-O2A-C1
22	A	833	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	O1A-CGA-O2A-C1
22	A	845	CLA	O1A-CGA-O2A-C1
22	B	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	839	CLA	O1A-CGA-O2A-C1
22	B	841	CLA	O1A-CGA-O2A-C1
22	J	101	CLA	O1A-CGA-O2A-C1
22	O	2002	CLA	O1A-CGA-O2A-C1
22	5	608	CLA	O1A-CGA-O2A-C1
28	A	860	LMG	O10-C28-O8-C9
22	F	304	CLA	O1D-CGD-O2D-CED
22	U	611	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	B	835	CLA	O1D-CGD-O2D-CED
22	7	604	CLA	O1D-CGD-O2D-CED
22	1	610	CLA	O1D-CGD-O2D-CED
22	5	614	CLA	O1D-CGD-O2D-CED
22	7	610	CLA	O1D-CGD-O2D-CED
22	8	614	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	CBD-CGD-O2D-CED
22	O	2002	CLA	CBD-CGD-O2D-CED
22	7	611	CLA	CBD-CGD-O2D-CED
22	W	604	CLA	O1D-CGD-O2D-CED
22	4	602	CLA	O1D-CGD-O2D-CED
22	4	604	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1D-CGD-O2D-CED
22	A	804	CLA	O1A-CGA-O2A-C1
22	5	611	CLA	O1A-CGA-O2A-C1
21	U	609	CHL	C3-C5-C6-C7
22	U	602	CLA	C3-C5-C6-C7
22	V	613	CLA	C3-C5-C6-C7
22	3	604	CLA	C3-C5-C6-C7
22	A	807	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	A	811	CLA	C3-C5-C6-C7
22	A	820	CLA	C3-C5-C6-C7
22	A	822	CLA	C3-C5-C6-C7
22	A	823	CLA	C3-C5-C6-C7
22	A	824	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	837	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	K	204	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	7	610	CLA	C3-C5-C6-C7
22	1	603	CLA	CBA-CGA-O2A-C1
22	1	614	CLA	CBA-CGA-O2A-C1
22	2	604	CLA	CBA-CGA-O2A-C1
22	3	604	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	836	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	CBA-CGA-O2A-C1
22	5	608	CLA	CBA-CGA-O2A-C1
22	8	603	CLA	CBA-CGA-O2A-C1
28	A	860	LMG	C29-C28-O8-C9
26	4	630	LHG	C8-C7-O7-C5
22	U	604	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	O1D-CGD-O2D-CED
22	G	203	CLA	O1D-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	5	611	CLA	CBA-CGA-O2A-C1
22	6	603	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	C4-C3-C5-C6
22	U	602	CLA	C2-C3-C5-C6
22	3	609	CLA	C2-C3-C5-C6
22	B	831	CLA	C2-C3-C5-C6
22	9	602	CLA	C2-C3-C5-C6
22	V	610	CLA	CBD-CGD-O2D-CED
22	2	603	CLA	CBD-CGD-O2D-CED
22	9	613	CLA	CBD-CGD-O2D-CED
21	U	606	CHL	C2A-CAA-CBA-CGA
21	U	609	CHL	C2A-CAA-CBA-CGA
21	1	601	CHL	C2A-CAA-CBA-CGA
21	2	607	CHL	C2A-CAA-CBA-CGA
21	4	607	CHL	C2A-CAA-CBA-CGA
21	5	601	CHL	C2A-CAA-CBA-CGA
21	6	602	CHL	C2A-CAA-CBA-CGA
21	6	608	CHL	C2A-CAA-CBA-CGA
21	7	608	CHL	C2A-CAA-CBA-CGA
22	4	601	CLA	C2A-CAA-CBA-CGA
22	A	811	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C2A-CAA-CBA-CGA
22	A	854	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	804	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	825	CLA	C2A-CAA-CBA-CGA
22	L	302	CLA	C2A-CAA-CBA-CGA
22	6	611	CLA	C2A-CAA-CBA-CGA
22	3	617	CLA	O1A-CGA-O2A-C1
22	F	301	CLA	O1A-CGA-O2A-C1
22	L	304	CLA	O1A-CGA-O2A-C1
22	A	843	CLA	C3-C5-C6-C7
22	B	827	CLA	C3-C5-C6-C7
22	F	301	CLA	C3-C5-C6-C7
22	L	303	CLA	C3-C5-C6-C7
22	7	602	CLA	C3-C5-C6-C7
22	U	604	CLA	CBA-CGA-O2A-C1
22	U	612	CLA	CBA-CGA-O2A-C1
22	V	603	CLA	CBA-CGA-O2A-C1
22	1	602	CLA	CBA-CGA-O2A-C1
22	1	613	CLA	CBA-CGA-O2A-C1
22	2	614	CLA	CBA-CGA-O2A-C1
22	3	602	CLA	CBA-CGA-O2A-C1
22	3	603	CLA	CBA-CGA-O2A-C1
22	4	601	CLA	CBA-CGA-O2A-C1
22	4	603	CLA	CBA-CGA-O2A-C1
22	4	604	CLA	CBA-CGA-O2A-C1
22	4	613	CLA	CBA-CGA-O2A-C1
22	A	804	CLA	CBA-CGA-O2A-C1
22	A	829	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
22	A	845	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	CBA-CGA-O2A-C1
22	B	820	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	CBA-CGA-O2A-C1
22	B	841	CLA	CBA-CGA-O2A-C1
22	F	301	CLA	CBA-CGA-O2A-C1
22	J	101	CLA	CBA-CGA-O2A-C1
22	O	2002	CLA	CBA-CGA-O2A-C1
22	8	609	CLA	CBA-CGA-O2A-C1
21	4	608	CHL	O1D-CGD-O2D-CED
21	6	602	CHL	CBD-CGD-O2D-CED
22	W	610	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	F	303	CLA	CBD-CGD-O2D-CED
22	1	614	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	O1D-CGD-O2D-CED
22	K	204	CLA	O1D-CGD-O2D-CED
22	5	604	CLA	O1D-CGD-O2D-CED
22	9	602	CLA	O1D-CGD-O2D-CED
22	9	609	CLA	O1D-CGD-O2D-CED
28	A	860	LMG	O9-C10-O7-C8
28	J	103	LMG	O9-C10-O7-C8
22	U	604	CLA	O1A-CGA-O2A-C1
22	V	603	CLA	O1A-CGA-O2A-C1
22	1	602	CLA	O1A-CGA-O2A-C1
22	3	602	CLA	O1A-CGA-O2A-C1
22	A	836	CLA	O1A-CGA-O2A-C1
22	A	854	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	O1A-CGA-O2A-C1
22	7	604	CLA	O1A-CGA-O2A-C1
22	8	603	CLA	O1A-CGA-O2A-C1
22	8	609	CLA	O1A-CGA-O2A-C1
21	W	607	CHL	CBD-CGD-O2D-CED
22	U	613	CLA	CBD-CGD-O2D-CED
22	1	616	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	CBD-CGD-O2D-CED
22	3	606	CLA	CBD-CGD-O2D-CED
22	4	613	CLA	CBD-CGD-O2D-CED
22	A	802	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	CBD-CGD-O2D-CED
22	J	101	CLA	CBD-CGD-O2D-CED
22	7	612	CLA	CBD-CGD-O2D-CED
22	8	613	CLA	CBD-CGD-O2D-CED
22	9	603	CLA	CBD-CGD-O2D-CED
22	9	611	CLA	CBD-CGD-O2D-CED
22	6	604	CLA	O1D-CGD-O2D-CED
22	W	610	CLA	C3-C5-C6-C7
22	A	854	CLA	C3-C5-C6-C7
22	3	615	CLA	CBA-CGA-O2A-C1
22	B	811	CLA	CBA-CGA-O2A-C1
22	L	302	CLA	CBA-CGA-O2A-C1
22	L	304	CLA	CBA-CGA-O2A-C1
22	7	604	CLA	CBA-CGA-O2A-C1
28	J	104	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	B	811	CLA	O1A-CGA-O2A-C1
22	B	836	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	O1D-CGD-O2D-CED
22	5	610	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	C11-C10-O7-C8
22	1	612	CLA	CBA-CGA-O2A-C1
22	5	612	CLA	CBA-CGA-O2A-C1
21	6	607	CHL	CBD-CGD-O2D-CED
22	V	613	CLA	CBD-CGD-O2D-CED
22	2	612	CLA	CBD-CGD-O2D-CED
22	4	601	CLA	CBD-CGD-O2D-CED
22	L	304	CLA	CBD-CGD-O2D-CED
22	5	602	CLA	CBD-CGD-O2D-CED
22	5	608	CLA	CBD-CGD-O2D-CED
22	3	602	CLA	O1D-CGD-O2D-CED
22	3	610	CLA	O1D-CGD-O2D-CED
31	B	849	LMT	O5'-C5'-C6'-O6'
22	A	820	CLA	CBD-CGD-O2D-CED
22	8	602	CLA	CBD-CGD-O2D-CED
22	L	302	CLA	C3-C5-C6-C7
22	3	617	CLA	CBA-CGA-O2A-C1
22	8	604	CLA	CBA-CGA-O2A-C1
22	A	854	CLA	O1D-CGD-O2D-CED
22	8	610	CLA	O1D-CGD-O2D-CED
31	G	206	LMT	O5B-C5B-C6B-O6B
22	3	603	CLA	O1A-CGA-O2A-C1
22	B	826	CLA	O1A-CGA-O2A-C1
22	L	302	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	C4-C3-C5-C6
22	B	819	CLA	C4-C3-C5-C6
31	B	849	LMT	C4'-C5'-C6'-O6'
21	V	601	CHL	C2-C3-C5-C6
22	A	825	CLA	C2-C3-C5-C6
22	B	819	CLA	C2-C3-C5-C6
22	B	806	CLA	C2A-CAA-CBA-CGA
22	G	203	CLA	C2A-CAA-CBA-CGA
22	U	612	CLA	O1A-CGA-O2A-C1
22	3	615	CLA	O1A-CGA-O2A-C1
28	L	307	LMG	O6-C1-O1-C7
22	4	614	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	O1D-CGD-O2D-CED
22	6	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	827	CLA	C3-C5-C6-C7
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	840	CLA	CBA-CGA-O2A-C1
22	5	616	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	O1D-CGD-O2D-CED
22	U	603	CLA	O1D-CGD-O2D-CED
22	V	614	CLA	O1D-CGD-O2D-CED
22	B	840	CLA	O1D-CGD-O2D-CED
28	J	104	LMG	O10-C28-O8-C9
31	G	206	LMT	C4B-C5B-C6B-O6B
22	1	611	CLA	O1D-CGD-O2D-CED
22	3	603	CLA	O1D-CGD-O2D-CED
22	4	611	CLA	O1D-CGD-O2D-CED
22	B	809	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
22	1	613	CLA	CBD-CGD-O2D-CED
26	9	2630	LHG	C1-C2-C3-O3
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	O1A-CGA-O2A-C1
22	8	604	CLA	O1A-CGA-O2A-C1
22	7	606	CLA	O1D-CGD-O2D-CED
22	8	611	CLA	O1D-CGD-O2D-CED
21	U	601	CHL	CBA-CGA-O2A-C1
22	V	602	CLA	CBA-CGA-O2A-C1
22	V	604	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	B	828	CLA	CBA-CGA-O2A-C1
22	5	613	CLA	CBA-CGA-O2A-C1
22	7	609	CLA	CBA-CGA-O2A-C1
22	8	611	CLA	CBA-CGA-O2A-C1
22	2	611	CLA	CBD-CGD-O2D-CED
22	3	614	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	CBD-CGD-O2D-CED
22	5	612	CLA	O1A-CGA-O2A-C1
22	1	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	1	630	LHG	C30-C31-C32-C33
21	U	609	CHL	C8-C10-C11-C12
21	6	601	CHL	C8-C10-C11-C12
22	1	611	CLA	C8-C10-C11-C12
22	A	830	CLA	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	B	840	CLA	C15-C16-C17-C18
26	9	2630	LHG	O2-C2-C3-O3
31	K	208	LMT	C2'-C1'-O1'-C1
22	A	840	CLA	O1A-CGA-O2A-C1
22	B	805	CLA	O1A-CGA-O2A-C1
22	7	609	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	C4-C3-C5-C6
21	U	607	CHL	C14-C13-C15-C16
21	U	609	CHL	C11-C10-C8-C9
21	U	609	CHL	C11-C12-C13-C14
21	6	601	CHL	C11-C12-C13-C14
22	U	603	CLA	C11-C10-C8-C9
22	A	828	CLA	C14-C13-C15-C16
22	A	845	CLA	C11-C10-C8-C9
22	B	831	CLA	C6-C7-C8-C9
22	6	610	CLA	C6-C7-C8-C9
22	B	836	CLA	O1D-CGD-O2D-CED
22	6	611	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	C15-C16-C17-C18
22	B	832	CLA	C15-C16-C17-C18
22	L	302	CLA	C5-C6-C7-C8
23	5	617	LUT	C11-C12-C13-C20
23	5	617	LUT	C27-C28-C29-C39
24	7	619	XAT	C7-C8-C9-C19
24	8	620	XAT	C7-C8-C9-C19
27	B	845	BCR	C11-C12-C13-C35
27	B	847	BCR	C37-C22-C23-C24
23	5	617	LUT	C27-C28-C29-C30
24	7	619	XAT	C7-C8-C9-C10
24	8	620	XAT	C7-C8-C9-C10
32	B	850	DGD	C1B-C2B-C3B-C4B
21	U	601	CHL	O1A-CGA-O2A-C1
22	4	602	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	828	CLA	O1A-CGA-O2A-C1
22	3	603	CLA	C13-C15-C16-C17
22	A	828	CLA	C8-C10-C11-C12
22	B	803	CLA	C10-C11-C12-C13
22	B	811	CLA	C5-C6-C7-C8
22	A	824	CLA	O1D-CGD-O2D-CED
22	6	610	CLA	O1D-CGD-O2D-CED
22	5	613	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBA-CGA-O2A-C1
26	7	630	LHG	C24-C23-O8-C6
22	1	610	CLA	C5-C6-C7-C8
22	1	610	CLA	C15-C16-C17-C18
22	4	602	CLA	C8-C10-C11-C12
22	A	803	CLA	C10-C11-C12-C13
22	A	819	CLA	C8-C10-C11-C12
22	B	804	CLA	C13-C15-C16-C17
22	B	837	CLA	C5-C6-C7-C8
22	B	840	CLA	C8-C10-C11-C12
22	6	613	CLA	C5-C6-C7-C8
29	A	844	PQN	C20-C21-C22-C23
29	A	844	PQN	C23-C25-C26-C27
28	A	860	LMG	C10-C11-C12-C13
31	K	208	LMT	C4'-C5'-C6'-O6'
31	K	208	LMT	O5B-C5B-C6B-O6B
21	U	601	CHL	C13-C15-C16-C17
22	W	613	CLA	C8-C10-C11-C12
22	1	610	CLA	C13-C15-C16-C17
22	A	802	CLA	C15-C16-C17-C18
22	A	820	CLA	C13-C15-C16-C17
22	A	828	CLA	C13-C15-C16-C17
22	A	829	CLA	C8-C10-C11-C12
22	B	808	CLA	C5-C6-C7-C8
22	B	822	CLA	C5-C6-C7-C8
22	B	828	CLA	C10-C11-C12-C13
22	K	203	CLA	C5-C6-C7-C8
22	U	610	CLA	O1D-CGD-O2D-CED
22	1	604	CLA	O1D-CGD-O2D-CED
26	1	630	LHG	C23-C24-C25-C26
26	7	630	LHG	C7-C8-C9-C10
26	9	2630	LHG	C7-C8-C9-C10
22	4	610	CLA	O1D-CGD-O2D-CED
22	A	840	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	808	CLA	O1D-CGD-O2D-CED
22	W	610	CLA	C8-C10-C11-C12
22	4	604	CLA	C5-C6-C7-C8
22	A	804	CLA	C13-C15-C16-C17
22	A	810	CLA	C15-C16-C17-C18
22	B	813	CLA	C13-C15-C16-C17
22	B	828	CLA	C5-C6-C7-C8
22	F	301	CLA	C10-C11-C12-C13
22	9	611	CLA	C15-C16-C17-C18
22	B	822	CLA	O1D-CGD-O2D-CED
22	9	610	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	O9-C10-O7-C8
22	5	608	CLA	C2-C1-O2A-CGA
21	W	601	CHL	C8-C10-C11-C12
22	U	610	CLA	C5-C6-C7-C8
22	1	611	CLA	C10-C11-C12-C13
22	A	806	CLA	C15-C16-C17-C18
22	B	816	CLA	C13-C15-C16-C17
22	K	204	CLA	C8-C10-C11-C12
22	V	604	CLA	CBD-CGD-O2D-CED
31	A	857	LMT	O1'-C1-C2-C3
26	1	630	LHG	C11-C12-C13-C14
22	A	845	CLA	C5-C6-C7-C8
21	V	601	CHL	C6-C7-C8-C10
22	1	602	CLA	C6-C7-C8-C10
22	3	617	CLA	C11-C10-C8-C7
22	A	803	CLA	C11-C10-C8-C7
22	A	822	CLA	C11-C12-C13-C15
22	A	825	CLA	C6-C7-C8-C10
22	B	810	CLA	C11-C12-C13-C15
22	B	818	CLA	C11-C10-C8-C7
22	A	815	CLA	C3-C5-C6-C7
22	B	825	CLA	C3-C5-C6-C7
22	V	604	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	8	611	CLA	O1A-CGA-O2A-C1
21	6	607	CHL	C2A-CAA-CBA-CGA
21	6	618	CHL	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	823	CLA	C2A-CAA-CBA-CGA
22	A	825	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	G	204	CLA	C2A-CAA-CBA-CGA
22	9	611	CLA	C2A-CAA-CBA-CGA
21	3	608	CHL	O1D-CGD-O2D-CED
22	1	608	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	O1D-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
22	K	206	CLA	O1D-CGD-O2D-CED
22	O	2002	CLA	O1D-CGD-O2D-CED
21	6	601	CHL	C13-C15-C16-C17
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	839	CLA	CBD-CGD-O2D-CED
22	A	836	CLA	C10-C11-C12-C13
23	2	619	LUT	C10-C11-C12-C13
23	5	617	LUT	C10-C11-C12-C13
23	5	617	LUT	C30-C31-C32-C33
24	8	620	XAT	C10-C11-C12-C13
31	K	208	LMT	O5'-C5'-C6'-O6'
22	1	610	CLA	C8-C10-C11-C12
22	A	803	CLA	C8-C10-C11-C12
22	A	805	CLA	C5-C6-C7-C8
22	B	806	CLA	C8-C10-C11-C12
22	B	828	CLA	C13-C15-C16-C17
22	9	602	CLA	C8-C10-C11-C12
22	A	801	CLA	CBA-CGA-O2A-C1
22	7	611	CLA	O1D-CGD-O2D-CED
22	V	602	CLA	O1A-CGA-O2A-C1
22	A	830	CLA	O1A-CGA-O2A-C1
22	5	613	CLA	O1A-CGA-O2A-C1
22	G	204	CLA	CBA-CGA-O2A-C1
22	7	606	CLA	CBA-CGA-O2A-C1
21	U	607	CHL	C8-C10-C11-C12
21	U	609	CHL	C13-C15-C16-C17
22	V	603	CLA	C5-C6-C7-C8
22	2	610	CLA	C10-C11-C12-C13
22	A	815	CLA	C10-C11-C12-C13
22	B	824	CLA	C5-C6-C7-C8
22	A	815	CLA	O1D-CGD-O2D-CED
22	A	836	CLA	CBD-CGD-O2D-CED
22	L	302	CLA	CBD-CGD-O2D-CED
22	3	609	CLA	C15-C16-C17-C18
22	A	804	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	A	806	CLA	C10-C11-C12-C13
22	A	841	CLA	C13-C15-C16-C17
22	B	810	CLA	C8-C10-C11-C12
22	B	837	CLA	C15-C16-C17-C18
26	U	2630	LHG	C4-O6-P-O3
26	V	2630	LHG	C4-O6-P-O3
26	W	2630	LHG	C4-O6-P-O3
26	2	630	LHG	C4-O6-P-O3
26	3	630	LHG	C4-O6-P-O3
26	B	851	LHG	C4-O6-P-O3
26	7	630	LHG	C3-O3-P-O6
26	7	630	LHG	C4-O6-P-O3
26	9	2630	LHG	C3-O3-P-O6
22	4	610	CLA	CBA-CGA-O2A-C1
22	A	842	CLA	CBA-CGA-O2A-C1
22	U	603	CLA	C8-C10-C11-C12
22	4	603	CLA	C15-C16-C17-C18
22	A	814	CLA	C15-C16-C17-C18
22	A	835	CLA	C15-C16-C17-C18
22	B	833	CLA	O1D-CGD-O2D-CED
22	9	613	CLA	O1D-CGD-O2D-CED
21	U	601	CHL	C8-C10-C11-C12
21	W	601	CHL	C2A-CAA-CBA-CGA
21	2	602	CHL	C2A-CAA-CBA-CGA
21	3	608	CHL	C2A-CAA-CBA-CGA
22	3	612	CLA	C2A-CAA-CBA-CGA
22	3	615	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C2A-CAA-CBA-CGA
22	5	608	CLA	C2A-CAA-CBA-CGA
22	L	304	CLA	C11-C12-C13-C15
22	4	610	CLA	C3-C5-C6-C7
22	U	610	CLA	CBA-CGA-O2A-C1
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	CBA-CGA-O2A-C1
26	1	630	LHG	C24-C23-O8-C6
22	V	613	CLA	CAA-CBA-CGA-O2A
22	2	603	CLA	O1D-CGD-O2D-CED
22	A	828	CLA	C5-C6-C7-C8
23	2	619	LUT	C20-C13-C14-C15
23	5	617	LUT	C20-C13-C14-C15
23	5	617	LUT	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	8	620	XAT	C11-C10-C9-C19
24	8	620	XAT	C40-C33-C34-C35
26	U	2630	LHG	C14-C15-C16-C17
22	A	801	CLA	O1A-CGA-O2A-C1
22	A	801	CLA	O1D-CGD-O2D-CED
22	W	613	CLA	C11-C12-C13-C14
22	6	613	CLA	C16-C17-C18-C20
22	A	817	CLA	CBA-CGA-O2A-C1
22	A	831	CLA	CBA-CGA-O2A-C1
22	A	832	CLA	CBA-CGA-O2A-C1
26	A	846	LHG	C13-C14-C15-C16
31	G	206	LMT	C5-C6-C7-C8
22	V	610	CLA	O1D-CGD-O2D-CED
21	U	607	CHL	CBD-CGD-O2D-CED
22	3	613	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	CBD-CGD-O2D-CED
22	A	822	CLA	CBD-CGD-O2D-CED
28	L	307	LMG	C16-C17-C18-C19
22	W	610	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	O1D-CGD-O2D-CED
22	F	303	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1A-CGA-O2A-C1
26	7	630	LHG	O10-C23-O8-C6
26	1	630	LHG	C33-C34-C35-C36
28	2	631	LMG	C29-C30-C31-C32
22	B	813	CLA	C5-C6-C7-C8
26	1	630	LHG	C32-C33-C34-C35
28	2	631	LMG	C23-C24-C25-C26
32	B	850	DGD	C7A-C8A-C9A-CAA
22	3	606	CLA	O1D-CGD-O2D-CED
23	2	619	LUT	C12-C13-C14-C15
23	5	617	LUT	C12-C13-C14-C15
23	5	617	LUT	C28-C29-C30-C31
24	8	620	XAT	C11-C10-C9-C8
24	8	620	XAT	C32-C33-C34-C35
22	B	838	CLA	CBA-CGA-O2A-C1
26	4	630	LHG	C9-C10-C11-C12
21	U	609	CHL	C16-C17-C18-C20
22	1	603	CLA	C6-C7-C8-C10
22	A	818	CLA	C16-C17-C18-C20
22	A	823	CLA	C6-C7-C8-C9
22	A	825	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	A	837	CLA	C16-C17-C18-C19
22	B	820	CLA	C6-C7-C8-C10
22	8	603	CLA	C6-C7-C8-C10
22	8	609	CLA	C6-C7-C8-C10
22	A	838	CLA	O1D-CGD-O2D-CED
22	V	613	CLA	C4-C3-C5-C6
22	2	613	CLA	C4-C3-C5-C6
22	6	613	CLA	C4-C3-C5-C6
22	8	609	CLA	C4-C3-C5-C6
21	U	607	CHL	C11-C10-C8-C9
22	V	613	CLA	C11-C10-C8-C9
22	1	611	CLA	C11-C12-C13-C14
22	A	804	CLA	C14-C13-C15-C16
22	A	805	CLA	C6-C7-C8-C9
22	A	824	CLA	C6-C7-C8-C9
22	A	827	CLA	C14-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C14
22	B	803	CLA	C11-C12-C13-C14
22	B	810	CLA	C14-C13-C15-C16
22	B	818	CLA	C6-C7-C8-C9
22	B	833	CLA	C14-C13-C15-C16
22	6	613	CLA	C11-C10-C8-C9
22	7	602	CLA	C6-C7-C8-C9
22	2	613	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	O1D-CGD-O2D-CED
22	A	824	CLA	C13-C15-C16-C17
26	A	846	LHG	C23-C24-C25-C26
26	A	847	LHG	C11-C10-C9-C8
28	A	860	LMG	C29-C30-C31-C32
32	B	850	DGD	C8B-C9B-CAB-CBB
21	V	601	CHL	C13-C15-C16-C17
22	A	815	CLA	C15-C16-C17-C18
22	F	304	CLA	CBA-CGA-O2A-C1
22	1	616	CLA	C2A-CAA-CBA-CGA
22	2	609	CLA	C2A-CAA-CBA-CGA
22	A	808	CLA	C2A-CAA-CBA-CGA
27	2	621	BCR	C21-C22-C23-C24
27	L	306	BCR	C7-C8-C9-C10
22	B	833	CLA	C3-C5-C6-C7
22	6	613	CLA	C3-C5-C6-C7
29	B	842	PQN	C15-C16-C17-C18
28	L	307	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	4	630	LHG	C7-C8-C9-C10
26	2	630	LHG	C11-C10-C9-C8
26	3	630	LHG	C11-C10-C9-C8
32	B	850	DGD	CAA-CBA-CCA-CDA
22	1	603	CLA	C4B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C4B-C3B-CAB-CBB
22	B	802	CLA	C4B-C3B-CAB-CBB
22	B	808	CLA	C4B-C3B-CAB-CBB
22	B	810	CLA	C4B-C3B-CAB-CBB
22	B	821	CLA	C4B-C3B-CAB-CBB
22	B	840	CLA	C4B-C3B-CAB-CBB
22	K	206	CLA	C4B-C3B-CAB-CBB
22	L	302	CLA	C4B-C3B-CAB-CBB
22	6	610	CLA	C4B-C3B-CAB-CBB
22	W	613	CLA	C11-C12-C13-C15
22	2	610	CLA	C11-C12-C13-C15
22	A	804	CLA	C16-C17-C18-C20
22	L	304	CLA	C11-C12-C13-C14
22	6	613	CLA	C16-C17-C18-C19
21	6	601	CHL	C5-C6-C7-C8
22	B	826	CLA	C13-C15-C16-C17
22	L	303	CLA	C8-C10-C11-C12
22	9	611	CLA	C13-C15-C16-C17
22	6	612	CLA	CBD-CGD-O2D-CED
21	W	607	CHL	O1D-CGD-O2D-CED
21	6	602	CHL	O1D-CGD-O2D-CED
22	4	613	CLA	O1D-CGD-O2D-CED
22	8	613	CLA	O1D-CGD-O2D-CED
21	V	601	CHL	C15-C16-C17-C18
22	2	610	CLA	C5-C6-C7-C8
22	U	610	CLA	O1A-CGA-O2A-C1
28	2	631	LMG	C19-C20-C21-C22
22	A	822	CLA	CBA-CGA-O2A-C1
22	B	825	CLA	CBA-CGA-O2A-C1
22	K	203	CLA	CBA-CGA-O2A-C1
26	U	2630	LHG	C15-C16-C17-C18
22	7	612	CLA	O1D-CGD-O2D-CED
22	9	603	CLA	O1D-CGD-O2D-CED
21	U	606	CHL	C3A-C2A-CAA-CBA
21	6	606	CHL	C3A-C2A-CAA-CBA
21	6	618	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	V	603	CLA	C3A-C2A-CAA-CBA
22	3	610	CLA	C3A-C2A-CAA-CBA
22	3	612	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	810	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	831	CLA	C3A-C2A-CAA-CBA
22	B	809	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	821	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	830	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	837	CLA	C3A-C2A-CAA-CBA
22	G	203	CLA	C3A-C2A-CAA-CBA
22	K	203	CLA	C3A-C2A-CAA-CBA
22	K	204	CLA	C3A-C2A-CAA-CBA
22	5	603	CLA	C3A-C2A-CAA-CBA
22	5	610	CLA	C3A-C2A-CAA-CBA
22	5	612	CLA	C3A-C2A-CAA-CBA
22	5	616	CLA	C3A-C2A-CAA-CBA
22	7	606	CLA	C3A-C2A-CAA-CBA
22	8	603	CLA	C3A-C2A-CAA-CBA
22	9	610	CLA	C3A-C2A-CAA-CBA
21	3	608	CHL	C5-C6-C7-C8
22	4	603	CLA	C5-C6-C7-C8
28	L	307	LMG	C11-C12-C13-C14
22	1	616	CLA	O1D-CGD-O2D-CED
22	4	610	CLA	O1A-CGA-O2A-C1
26	1	630	LHG	O10-C23-O8-C6
21	V	601	CHL	C16-C17-C18-C19
22	A	825	CLA	C16-C17-C18-C19
22	A	845	CLA	C16-C17-C18-C20
22	L	302	CLA	C16-C17-C18-C20
22	8	603	CLA	C6-C7-C8-C9
26	1	630	LHG	C28-C29-C30-C31
22	J	101	CLA	O1D-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
26	W	2630	LHG	C9-C10-C11-C12
26	1	630	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	K	208	LMT	C2-C3-C4-C5
22	9	611	CLA	O1D-CGD-O2D-CED
22	U	613	CLA	C3-C5-C6-C7
22	B	805	CLA	C3-C5-C6-C7
26	4	630	LHG	C26-C27-C28-C29
22	3	617	CLA	C4-C3-C5-C6
22	A	807	CLA	C4-C3-C5-C6
22	A	854	CLA	C4-C3-C5-C6
22	B	804	CLA	C4-C3-C5-C6
22	B	820	CLA	C4-C3-C5-C6
22	L	302	CLA	C4-C3-C5-C6
31	A	857	LMT	O5B-C1B-O1B-C4'
22	A	824	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	CBA-CGA-O2A-C1
22	U	613	CLA	C2-C3-C5-C6
22	V	613	CLA	C2-C3-C5-C6
22	3	617	CLA	C2-C3-C5-C6
22	A	826	CLA	C2-C3-C5-C6
22	A	854	CLA	C2-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	B	836	CLA	C2-C3-C5-C6
22	6	613	CLA	C2-C3-C5-C6
28	G	202	LMG	C11-C10-O7-C8
22	K	203	CLA	C2A-CAA-CBA-CGA
26	1	630	LHG	O1-C1-C2-O2
22	1	609	CLA	C15-C16-C17-C18
26	4	630	LHG	C13-C14-C15-C16
22	5	602	CLA	O1D-CGD-O2D-CED
22	A	838	CLA	C6-C7-C8-C10
22	1	603	CLA	C2B-C3B-CAB-CBB
22	2	613	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	837	CLA	C2B-C3B-CAB-CBB
22	A	843	CLA	C2B-C3B-CAB-CBB
22	B	802	CLA	C2B-C3B-CAB-CBB
22	B	808	CLA	C2B-C3B-CAB-CBB
22	B	810	CLA	C2B-C3B-CAB-CBB
22	B	817	CLA	C2B-C3B-CAB-CBB
22	B	821	CLA	C2B-C3B-CAB-CBB
22	B	830	CLA	C2B-C3B-CAB-CBB
22	B	840	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	K	206	CLA	C2B-C3B-CAB-CBB
22	L	302	CLA	C2B-C3B-CAB-CBB
22	6	610	CLA	C2B-C3B-CAB-CBB
22	7	611	CLA	C2B-C3B-CAB-CBB
26	2	630	LHG	O2-C2-C3-O3
22	3	611	CLA	C5-C6-C7-C8
22	A	815	CLA	C5-C6-C7-C8
22	A	813	CLA	O1A-CGA-O2A-C1
22	A	831	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	O1A-CGA-O2A-C1
22	A	841	CLA	O1A-CGA-O2A-C1
26	3	630	LHG	C23-C24-C25-C26
22	4	602	CLA	C10-C11-C12-C13
28	G	202	LMG	O9-C10-O7-C8
22	3	604	CLA	C2-C1-O2A-CGA
22	3	612	CLA	C2-C1-O2A-CGA
22	A	817	CLA	C2-C1-O2A-CGA
22	B	810	CLA	C2-C1-O2A-CGA
22	B	814	CLA	C2-C1-O2A-CGA
22	4	603	CLA	C10-C11-C12-C13
22	A	823	CLA	C5-C6-C7-C8
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	837	CLA	C16-C17-C18-C20
22	A	829	CLA	C3-C5-C6-C7
22	B	807	CLA	C3-C5-C6-C7
23	U	2621	LUT	C5-C6-C7-C8
23	V	2620	LUT	C5-C6-C7-C8
23	V	2621	LUT	C5-C6-C7-C8
23	W	2620	LUT	C5-C6-C7-C8
23	W	2621	LUT	C1-C6-C7-C8
23	W	2621	LUT	C5-C6-C7-C8
23	6	619	LUT	C5-C6-C7-C8
23	7	618	LUT	C5-C6-C7-C8
23	8	619	LUT	C5-C6-C7-C8
23	9	620	LUT	C5-C6-C7-C8
23	9	621	LUT	C5-C6-C7-C8
23	9	624	LUT	C1-C6-C7-C8
23	9	624	LUT	C5-C6-C7-C8
27	1	619	BCR	C1-C6-C7-C8
27	1	619	BCR	C23-C24-C25-C26
27	2	621	BCR	C23-C24-C25-C26
27	4	621	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	4	621	BCR	C23-C24-C25-C26
27	A	848	BCR	C1-C6-C7-C8
27	A	848	BCR	C5-C6-C7-C8
27	A	848	BCR	C23-C24-C25-C30
27	A	849	BCR	C1-C6-C7-C8
27	A	849	BCR	C5-C6-C7-C8
27	A	849	BCR	C23-C24-C25-C30
27	A	850	BCR	C5-C6-C7-C8
27	A	850	BCR	C23-C24-C25-C30
27	A	851	BCR	C5-C6-C7-C8
27	A	852	BCR	C1-C6-C7-C8
27	B	801	BCR	C1-C6-C7-C8
27	B	801	BCR	C5-C6-C7-C8
27	B	801	BCR	C23-C24-C25-C30
27	B	843	BCR	C1-C6-C7-C8
27	B	843	BCR	C5-C6-C7-C8
27	B	845	BCR	C1-C6-C7-C8
27	B	845	BCR	C5-C6-C7-C8
27	B	845	BCR	C23-C24-C25-C26
27	B	1609	BCR	C5-C6-C7-C8
27	F	305	BCR	C23-C24-C25-C26
27	G	205	BCR	C1-C6-C7-C8
27	I	101	BCR	C23-C24-C25-C26
27	I	101	BCR	C23-C24-C25-C30
27	J	102	BCR	C23-C24-C25-C26
27	J	102	BCR	C23-C24-C25-C30
27	K	202	BCR	C5-C6-C7-C8
27	K	202	BCR	C23-C24-C25-C30
27	K	205	BCR	C23-C24-C25-C26
27	L	301	BCR	C5-C6-C7-C8
27	L	301	BCR	C23-C24-C25-C26
27	L	301	BCR	C23-C24-C25-C30
27	M	2001	BCR	C23-C24-C25-C30
27	O	2004	BCR	C1-C6-C7-C8
27	O	2004	BCR	C5-C6-C7-C8
27	O	2004	BCR	C23-C24-C25-C26
27	O	2004	BCR	C23-C24-C25-C30
27	6	621	BCR	C5-C6-C7-C8
27	6	621	BCR	C23-C24-C25-C26
27	7	621	BCR	C23-C24-C25-C26
21	9	606	CHL	C2A-CAA-CBA-CGA
22	A	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	V	601	CHL	C8-C10-C11-C12
22	B	819	CLA	C8-C10-C11-C12
22	K	204	CLA	C5-C6-C7-C8
22	U	613	CLA	O1D-CGD-O2D-CED
22	A	822	CLA	O1A-CGA-O2A-C1
22	B	838	CLA	O1A-CGA-O2A-C1
26	9	2630	LHG	C9-C10-C11-C12
31	A	857	LMT	C4-C5-C6-C7
21	2	602	CHL	C4-C3-C5-C6
22	A	826	CLA	C4-C3-C5-C6
22	A	843	CLA	C4-C3-C5-C6
22	L	304	CLA	C4-C3-C5-C6
21	U	607	CHL	C11-C10-C8-C7
21	U	607	CHL	C12-C13-C15-C16
21	W	601	CHL	C6-C7-C8-C10
21	6	601	CHL	C11-C12-C13-C15
22	V	613	CLA	C11-C10-C8-C7
22	W	602	CLA	C11-C10-C8-C7
22	2	613	CLA	C2-C3-C5-C6
22	A	804	CLA	C6-C7-C8-C10
22	A	805	CLA	C6-C7-C8-C10
22	A	805	CLA	C12-C13-C15-C16
22	A	807	CLA	C2-C3-C5-C6
22	A	810	CLA	C11-C10-C8-C7
22	A	812	CLA	C12-C13-C15-C16
22	A	827	CLA	C11-C10-C8-C7
22	A	827	CLA	C12-C13-C15-C16
22	A	828	CLA	C12-C13-C15-C16
22	A	835	CLA	C2-C3-C5-C6
22	A	843	CLA	C2-C3-C5-C6
22	A	854	CLA	C6-C7-C8-C10
22	B	803	CLA	C11-C12-C13-C15
22	B	810	CLA	C6-C7-C8-C10
22	B	810	CLA	C12-C13-C15-C16
22	B	814	CLA	C2-C3-C5-C6
22	B	818	CLA	C6-C7-C8-C10
22	B	833	CLA	C12-C13-C15-C16
22	B	841	CLA	C12-C13-C15-C16
22	L	302	CLA	C2-C3-C5-C6
22	L	302	CLA	C6-C7-C8-C10
22	L	304	CLA	C2-C3-C5-C6
22	6	610	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	6	613	CLA	C11-C10-C8-C7
22	7	602	CLA	C6-C7-C8-C10
22	8	609	CLA	C2-C3-C5-C6
22	9	602	CLA	C6-C7-C8-C10
29	A	844	PQN	C21-C22-C23-C25
22	3	615	CLA	C3-C5-C6-C7
22	A	824	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1A-CGA-O2A-C1
22	K	203	CLA	O1A-CGA-O2A-C1
22	9	602	CLA	O1A-CGA-O2A-C1
21	6	601	CHL	C15-C16-C17-C18
22	B	814	CLA	C8-C10-C11-C12
22	B	817	CLA	C13-C15-C16-C17
22	1	603	CLA	C6-C7-C8-C9
22	A	823	CLA	C6-C7-C8-C10
22	B	826	CLA	C16-C17-C18-C19
22	5	608	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	CBA-CGA-O2A-C1
22	U	604	CLA	C2A-CAA-CBA-CGA
22	3	617	CLA	C2A-CAA-CBA-CGA
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C2A-CAA-CBA-CGA
22	F	301	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C5-C6-C7-C8
31	A	857	LMT	C2B-C1B-O1B-C4'
31	A	857	LMT	C6-C7-C8-C9
22	4	601	CLA	O1D-CGD-O2D-CED
22	2	612	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	O6D-C5D-C6D-O5D
22	L	304	CLA	O1D-CGD-O2D-CED
22	A	814	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	CBA-CGA-O2A-C1
22	U	610	CLA	C16-C17-C18-C19
22	A	833	CLA	C6-C7-C8-C9
22	B	820	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C12-C13-C15
31	K	208	LMT	C4B-C5B-C6B-O6B
21	U	607	CHL	C13-C15-C16-C17
22	W	610	CLA	C13-C15-C16-C17
22	A	801	CLA	C5-C6-C7-C8
22	A	834	CLA	C8-C10-C11-C12
31	G	206	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	V	613	CLA	O1D-CGD-O2D-CED
26	A	846	LHG	C8-C7-O7-C5
26	A	847	LHG	C8-C7-O7-C5
26	9	2630	LHG	C8-C7-O7-C5
22	A	814	CLA	CBD-CGD-O2D-CED
31	G	206	LMT	C2-C3-C4-C5
31	G	206	LMT	C2'-C1'-O1'-C1
21	U	601	CHL	C5-C6-C7-C8
26	1	630	LHG	C27-C28-C29-C30
28	L	307	LMG	C32-C33-C34-C35
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	O1A-CGA-O2A-C1
21	U	609	CHL	C16-C17-C18-C19
22	A	818	CLA	C16-C17-C18-C19
22	8	609	CLA	C6-C7-C8-C9
22	3	603	CLA	C15-C16-C17-C18
22	B	814	CLA	C15-C16-C17-C18
21	6	607	CHL	O1D-CGD-O2D-CED
22	U	613	CLA	C4-C3-C5-C6
22	A	835	CLA	C4-C3-C5-C6
22	B	814	CLA	C4-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6
21	4	607	CHL	CBA-CGA-O2A-C1
21	6	607	CHL	CBA-CGA-O2A-C1
21	2	602	CHL	C2-C3-C5-C6
22	B	804	CLA	C2-C3-C5-C6
22	B	809	CLA	C2-C3-C5-C6
22	B	822	CLA	C2-C3-C5-C6
21	V	601	CHL	C6-C7-C8-C9
22	W	602	CLA	C11-C10-C8-C9
22	1	602	CLA	C6-C7-C8-C9
22	1	609	CLA	C6-C7-C8-C9
22	1	611	CLA	C11-C10-C8-C9
22	3	613	CLA	C11-C12-C13-C14
22	3	617	CLA	C11-C10-C8-C9
22	A	803	CLA	C11-C10-C8-C9
22	A	805	CLA	C14-C13-C15-C16
22	A	810	CLA	C11-C10-C8-C9
22	A	810	CLA	C11-C12-C13-C14
22	A	812	CLA	C14-C13-C15-C16
22	A	817	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	825	CLA	C6-C7-C8-C9
22	A	827	CLA	C6-C7-C8-C9
22	A	827	CLA	C11-C10-C8-C9
22	A	836	CLA	C11-C10-C8-C9
22	A	839	CLA	C6-C7-C8-C9
22	B	810	CLA	C6-C7-C8-C9
22	B	810	CLA	C11-C12-C13-C14
22	B	832	CLA	C14-C13-C15-C16
22	L	302	CLA	C6-C7-C8-C9
22	6	610	CLA	C11-C10-C8-C9
29	B	842	PQN	C16-C17-C18-C19
22	B	816	CLA	C3-C5-C6-C7
21	1	607	CHL	C2A-CAA-CBA-CGA
21	8	607	CHL	C2A-CAA-CBA-CGA
22	3	611	CLA	C2A-CAA-CBA-CGA
22	B	808	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
22	6	612	CLA	C2A-CAA-CBA-CGA
22	A	820	CLA	O1D-CGD-O2D-CED
22	5	616	CLA	O1D-CGD-O2D-CED
29	B	842	PQN	C20-C21-C22-C23
21	6	618	CHL	CBA-CGA-O2A-C1
21	U	606	CHL	C1A-C2A-CAA-CBA
21	6	606	CHL	C1A-C2A-CAA-CBA
21	6	618	CHL	C1A-C2A-CAA-CBA
22	U	610	CLA	C1A-C2A-CAA-CBA
22	V	602	CLA	C1A-C2A-CAA-CBA
22	V	603	CLA	C1A-C2A-CAA-CBA
22	V	604	CLA	C1A-C2A-CAA-CBA
22	1	613	CLA	C1A-C2A-CAA-CBA
22	2	611	CLA	C1A-C2A-CAA-CBA
22	2	614	CLA	C1A-C2A-CAA-CBA
22	3	604	CLA	C1A-C2A-CAA-CBA
22	3	612	CLA	C1A-C2A-CAA-CBA
22	4	602	CLA	C1A-C2A-CAA-CBA
22	4	610	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	G	203	CLA	C1A-C2A-CAA-CBA
22	K	203	CLA	C1A-C2A-CAA-CBA
22	K	204	CLA	C1A-C2A-CAA-CBA
22	L	303	CLA	C1A-C2A-CAA-CBA
22	O	2002	CLA	C1A-C2A-CAA-CBA
22	5	603	CLA	C1A-C2A-CAA-CBA
22	5	612	CLA	C1A-C2A-CAA-CBA
22	5	616	CLA	C1A-C2A-CAA-CBA
22	8	603	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C6-C7-C8-C10
22	A	838	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C12-C13-C14
22	8	610	CLA	C6-C7-C8-C10
26	A	846	LHG	O9-C7-O7-C5
26	A	847	LHG	O9-C7-O7-C5
26	9	2630	LHG	O9-C7-O7-C5
26	1	630	LHG	C8-C7-O7-C5
22	1	613	CLA	O1D-CGD-O2D-CED
22	8	602	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	C10-C11-C12-C13
22	F	301	CLA	C15-C16-C17-C18
26	V	2630	LHG	C3-O3-P-O6
22	3	614	CLA	O1D-CGD-O2D-CED
21	2	602	CHL	C8-C10-C11-C12
22	2	611	CLA	O1D-CGD-O2D-CED
32	B	850	DGD	C4D-C5D-C6D-O5D
32	B	850	DGD	CCA-CDA-CEA-CFA
22	K	204	CLA	C10-C11-C12-C13
22	U	604	CLA	C3-C5-C6-C7
22	2	610	CLA	C11-C12-C13-C14
22	B	832	CLA	C3-C5-C6-C7
22	A	829	CLA	C10-C11-C12-C13
26	4	630	LHG	C24-C23-O8-C6
22	V	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	834	CLA	C15-C16-C17-C18
22	7	606	CLA	O1A-CGA-O2A-C1
32	B	850	DGD	C6B-C7B-C8B-C9B
26	8	630	LHG	C8-C7-O7-C5
22	A	825	CLA	O1A-CGA-O2A-C1
21	6	601	CHL	C2A-CAA-CBA-CGA
22	2	604	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C2A-CAA-CBA-CGA
21	V	601	CHL	C16-C17-C18-C20
22	B	813	CLA	C16-C17-C18-C19
21	W	601	CHL	C3-C5-C6-C7
26	1	630	LHG	C4-C5-C6-O8
26	4	630	LHG	C4-C5-C6-O8
26	A	847	LHG	C4-C5-C6-O8
26	B	851	LHG	C4-C5-C6-O8
28	G	202	LMG	O1-C7-C8-C9
28	J	104	LMG	O1-C7-C8-C9
22	B	832	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C15-C16-C17-C18
22	B	832	CLA	C13-C15-C16-C17
28	L	307	LMG	C8-C7-O1-C1
26	A	846	LHG	C16-C17-C18-C19
22	7	609	CLA	CBD-CGD-O2D-CED
21	U	601	CHL	C15-C16-C17-C18
21	U	607	CHL	C5-C6-C7-C8
22	A	804	CLA	C8-C10-C11-C12
22	B	825	CLA	C10-C11-C12-C13
26	3	630	LHG	C9-C10-C11-C12
26	9	2630	LHG	C23-C24-C25-C26
22	A	814	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C3-C5-C6-C7
22	B	834	CLA	C13-C15-C16-C17
22	B	809	CLA	C13-C15-C16-C17
22	5	613	CLA	O1D-CGD-O2D-CED
28	2	631	LMG	O6-C5-C6-O5
22	A	837	CLA	C4-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
21	1	601	CHL	C6-C7-C8-C9
22	B	826	CLA	C16-C17-C18-C20
22	W	610	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	CBA-CGA-O2A-C1
22	9	610	CLA	CBA-CGA-O2A-C1
22	7	613	CLA	CBD-CGD-O2D-CED
22	B	834	CLA	C8-C10-C11-C12
22	G	204	CLA	O1A-CGA-O2A-C1
21	8	608	CHL	C2A-CAA-CBA-CGA
22	4	603	CLA	C2A-CAA-CBA-CGA
22	4	612	CLA	C2A-CAA-CBA-CGA
22	2	604	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C2-C1-O2A-CGA
22	5	602	CLA	C2-C1-O2A-CGA
22	A	826	CLA	C3-C5-C6-C7
26	1	630	LHG	C24-C25-C26-C27
22	A	825	CLA	O1D-CGD-O2D-CED
21	U	609	CHL	CBA-CGA-O2A-C1
22	3	610	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	O1A-CGA-O2A-C1
22	9	610	CLA	O1A-CGA-O2A-C1
26	2	630	LHG	O6-C4-C5-O7
22	8	610	CLA	C6-C7-C8-C9
26	4	630	LHG	C11-C12-C13-C14
22	B	839	CLA	C5-C6-C7-C8
22	B	840	CLA	C10-C11-C12-C13
22	A	808	CLA	O1A-CGA-O2A-C1
26	4	630	LHG	O10-C23-O8-C6
22	A	818	CLA	C13-C15-C16-C17
21	2	602	CHL	CAA-CBA-CGA-O2A
28	L	307	LMG	O7-C8-C9-O8
22	B	828	CLA	C15-C16-C17-C18
22	A	823	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
22	A	830	CLA	C4-C3-C5-C6
22	A	836	CLA	C8-C10-C11-C12
21	U	601	CHL	C11-C12-C13-C15
21	U	609	CHL	C6-C7-C8-C10
21	U	609	CHL	C11-C12-C13-C15
21	U	609	CHL	C12-C13-C15-C16
21	W	601	CHL	C12-C13-C15-C16
22	1	609	CLA	C6-C7-C8-C10
22	1	611	CLA	C11-C10-C8-C7
22	3	609	CLA	C12-C13-C15-C16
22	3	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	801	CLA	C11-C10-C8-C7
22	A	802	CLA	C12-C13-C15-C16
22	A	810	CLA	C11-C12-C13-C15
22	A	814	CLA	C11-C12-C13-C15
22	A	817	CLA	C12-C13-C15-C16
22	A	827	CLA	C6-C7-C8-C10
22	A	836	CLA	C11-C10-C8-C7
22	A	837	CLA	C2-C3-C5-C6
22	A	839	CLA	C6-C7-C8-C10
22	A	843	CLA	C12-C13-C15-C16
22	B	808	CLA	C11-C10-C8-C7
22	B	811	CLA	C11-C12-C13-C15
22	B	816	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C12-C13-C15
22	B	818	CLA	C12-C13-C15-C16
22	B	827	CLA	C2-C3-C5-C6
22	B	831	CLA	C6-C7-C8-C10
22	B	832	CLA	C12-C13-C15-C16
22	B	840	CLA	C11-C12-C13-C15
22	B	841	CLA	C11-C10-C8-C7
22	6	610	CLA	C6-C7-C8-C10
29	B	842	PQN	C16-C17-C18-C20
21	U	601	CHL	C11-C10-C8-C9
21	U	601	CHL	C11-C12-C13-C14
21	U	609	CHL	C6-C7-C8-C9
21	U	609	CHL	C14-C13-C15-C16
21	W	601	CHL	C14-C13-C15-C16
22	3	609	CLA	C14-C13-C15-C16
22	A	801	CLA	C11-C10-C8-C9
22	A	805	CLA	C11-C10-C8-C9
22	A	806	CLA	C14-C13-C15-C16
22	A	814	CLA	C11-C12-C13-C14
22	A	825	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C10-C8-C9
22	A	843	CLA	C14-C13-C15-C16
22	B	811	CLA	C11-C12-C13-C14
22	B	816	CLA	C6-C7-C8-C9
22	B	817	CLA	C11-C12-C13-C14
22	B	818	CLA	C14-C13-C15-C16
22	B	829	CLA	C14-C13-C15-C16
22	B	831	CLA	C11-C12-C13-C14
22	B	834	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	840	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
22	B	841	CLA	C14-C13-C15-C16
29	A	844	PQN	C21-C22-C23-C24
22	L	302	CLA	O1D-CGD-O2D-CED
22	B	822	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	C2A-CAA-CBA-CGA
22	8	613	CLA	C2A-CAA-CBA-CGA
22	5	609	CLA	CBD-CGD-O2D-CED
24	8	620	XAT	C27-C28-C29-C39
27	K	205	BCR	C7-C8-C9-C34
21	W	601	CHL	C16-C17-C18-C19
22	B	813	CLA	C16-C17-C18-C20
22	V	604	CLA	O1D-CGD-O2D-CED
23	2	619	LUT	C11-C12-C13-C14
24	8	620	XAT	C27-C28-C29-C30
27	1	619	BCR	C21-C22-C23-C24
27	K	205	BCR	C7-C8-C9-C10
22	A	807	CLA	C8-C10-C11-C12
22	A	828	CLA	C15-C16-C17-C18
22	B	820	CLA	C5-C6-C7-C8
22	A	835	CLA	CBA-CGA-O2A-C1
26	6	630	LHG	C24-C23-O8-C6
22	2	613	CLA	C4B-C3B-CAB-CBB
22	3	606	CLA	C4B-C3B-CAB-CBB
22	3	613	CLA	C4B-C3B-CAB-CBB
22	4	603	CLA	C4B-C3B-CAB-CBB
22	4	609	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	F	301	CLA	C4B-C3B-CAB-CBB
22	G	201	CLA	C4B-C3B-CAB-CBB
22	H	201	CLA	C4B-C3B-CAB-CBB
26	2	630	LHG	O6-C4-C5-C6
26	A	847	LHG	O6-C4-C5-C6
22	V	603	CLA	C3-C5-C6-C7
22	A	839	CLA	O1D-CGD-O2D-CED
22	4	603	CLA	C4-C3-C5-C6
22	A	823	CLA	C2-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	W	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	O1A-CGA-O2A-C1
22	F	304	CLA	O1A-CGA-O2A-C1
22	7	602	CLA	C11-C12-C13-C14
22	J	101	CLA	C2A-CAA-CBA-CGA
21	3	608	CHL	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
22	8	610	CLA	CBA-CGA-O2A-C1
28	L	307	LMG	C29-C28-O8-C9
26	2	630	LHG	C2-C3-O3-P
22	A	813	CLA	O1D-CGD-O2D-CED
21	U	609	CHL	C3A-C2A-CAA-CBA
22	1	608	CLA	C3A-C2A-CAA-CBA
22	1	614	CLA	C3A-C2A-CAA-CBA
22	4	604	CLA	C3A-C2A-CAA-CBA
22	A	817	CLA	C3A-C2A-CAA-CBA
22	A	830	CLA	C3A-C2A-CAA-CBA
22	A	842	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	814	CLA	C3A-C2A-CAA-CBA
23	5	617	LUT	C9-C10-C11-C12
24	8	620	XAT	C9-C10-C11-C12
22	1	610	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	O1D-CGD-O2D-CED
22	6	612	CLA	O1D-CGD-O2D-CED
26	U	2630	LHG	C23-C24-C25-C26
22	3	610	CLA	O1A-CGA-O2A-C1
22	9	613	CLA	O2A-C1-C2-C3
22	A	841	CLA	O1D-CGD-O2D-CED
22	9	611	CLA	C3-C5-C6-C7
22	A	814	CLA	C4-C3-C5-C6
21	1	601	CHL	C6-C7-C8-C10
22	U	610	CLA	C16-C17-C18-C20
22	A	822	CLA	O1D-CGD-O2D-CED
22	3	606	CLA	C2A-CAA-CBA-CGA
22	A	832	CLA	C2A-CAA-CBA-CGA
22	L	303	CLA	C2A-CAA-CBA-CGA
22	8	601	CLA	C2A-CAA-CBA-CGA
22	8	614	CLA	C2A-CAA-CBA-CGA
22	3	610	CLA	C8-C10-C11-C12
22	B	832	CLA	C5-C6-C7-C8
26	4	630	LHG	O6-C4-C5-O7
22	7	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	U	609	CHL	O1A-CGA-O2A-C1
32	B	850	DGD	C1A-C2A-C3A-C4A
21	W	601	CHL	C16-C17-C18-C20
22	3	613	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C2B-C3B-CAB-CBB
22	F	301	CLA	C2B-C3B-CAB-CBB
22	H	201	CLA	C2B-C3B-CAB-CBB
26	4	630	LHG	C11-C10-C9-C8
22	B	822	CLA	O1A-CGA-O2A-C1
26	4	630	LHG	O7-C5-C6-O8
26	7	630	LHG	O7-C5-C6-O8
22	B	819	CLA	C5-C6-C7-C8
22	A	804	CLA	C16-C17-C18-C19
22	A	841	CLA	C10-C11-C12-C13
26	A	847	LHG	C1-C2-C3-O3
26	1	630	LHG	O9-C7-O7-C5
26	8	630	LHG	O9-C7-O7-C5
21	8	608	CHL	C2-C1-O2A-CGA
22	A	832	CLA	C2-C1-O2A-CGA
22	4	603	CLA	C2-C3-C5-C6
21	V	609	CHL	C2C-C3C-CAC-CBC
21	V	601	CHL	C11-C12-C13-C14
22	U	603	CLA	C14-C13-C15-C16
22	4	610	CLA	C6-C7-C8-C9
22	A	807	CLA	C11-C12-C13-C14
22	A	831	CLA	C6-C7-C8-C9
22	A	831	CLA	C11-C12-C13-C14
22	A	836	CLA	C6-C7-C8-C9
22	A	837	CLA	C6-C7-C8-C9
22	B	819	CLA	C6-C7-C8-C9
22	B	828	CLA	C11-C10-C8-C9
32	B	850	DGD	C4A-C5A-C6A-C7A
31	B	849	LMT	O5B-C5B-C6B-O6B
22	1	611	CLA	C5-C6-C7-C8
21	4	606	CHL	C2A-CAA-CBA-CGA
22	4	613	CLA	C2A-CAA-CBA-CGA
22	A	845	CLA	C16-C17-C18-C19
22	L	302	CLA	C16-C17-C18-C19
22	3	609	CLA	C3-C5-C6-C7
22	A	814	CLA	C3-C5-C6-C7
23	V	2621	LUT	C1-C6-C7-C8
23	6	619	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	2	621	BCR	C5-C6-C7-C8
27	3	620	BCR	C23-C24-C25-C26
27	A	850	BCR	C1-C6-C7-C8
27	F	305	BCR	C23-C24-C25-C30
27	K	202	BCR	C1-C6-C7-C8
27	L	301	BCR	C1-C6-C7-C8
22	1	610	CLA	C10-C11-C12-C13
22	B	807	CLA	C8-C10-C11-C12
23	5	617	LUT	C11-C12-C13-C14
27	B	848	BCR	C21-C22-C23-C24
27	B	1609	BCR	C21-C22-C23-C24
22	B	805	CLA	C15-C16-C17-C18
22	U	602	CLA	C15-C16-C17-C18
22	2	613	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	O1D-CGD-O2D-CED
22	U	603	CLA	C11-C10-C8-C7
22	U	612	CLA	C12-C13-C15-C16
22	V	603	CLA	C11-C10-C8-C7
22	W	610	CLA	C11-C10-C8-C7
22	W	610	CLA	C12-C13-C15-C16
22	1	602	CLA	C11-C10-C8-C7
22	1	609	CLA	C11-C12-C13-C15
22	1	611	CLA	C11-C12-C13-C15
22	3	612	CLA	C11-C10-C8-C7
22	3	617	CLA	C6-C7-C8-C10
22	A	805	CLA	C11-C10-C8-C7
22	A	807	CLA	C11-C12-C13-C15
22	A	822	CLA	C11-C10-C8-C7
22	A	825	CLA	C11-C12-C13-C15
22	A	826	CLA	C11-C10-C8-C7
22	A	828	CLA	C11-C10-C8-C7
22	A	830	CLA	C12-C13-C15-C16
22	A	831	CLA	C11-C12-C13-C15
22	A	837	CLA	C6-C7-C8-C10
22	A	854	CLA	C11-C10-C8-C7
22	B	806	CLA	C6-C7-C8-C10
22	B	819	CLA	C6-C7-C8-C10
22	B	826	CLA	C12-C13-C15-C16
22	B	827	CLA	C6-C7-C8-C10
22	B	829	CLA	C12-C13-C15-C16
22	B	831	CLA	C11-C12-C13-C15
22	B	834	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	837	CLA	C6-C7-C8-C10
22	B	839	CLA	C6-C7-C8-C10
22	L	302	CLA	C11-C12-C13-C15
22	5	602	CLA	C11-C10-C8-C7
22	9	611	CLA	C11-C12-C13-C15
29	A	844	PQN	C17-C18-C20-C21
21	U	601	CHL	C3-C5-C6-C7
22	U	610	CLA	C8-C10-C11-C12
22	A	805	CLA	C10-C11-C12-C13
24	8	620	XAT	C29-C30-C31-C32
25	W	2623	NEX	C33-C34-C35-C15
22	6	604	CLA	CBA-CGA-O2A-C1
21	6	602	CHL	C5-C6-C7-C8
22	U	612	CLA	C10-C11-C12-C13
22	B	822	CLA	CAA-CBA-CGA-O2A
22	A	835	CLA	O1A-CGA-O2A-C1
21	2	601	CHL	C2A-CAA-CBA-CGA
26	V	2630	LHG	C23-C24-C25-C26
22	A	832	CLA	C3-C5-C6-C7
26	1	630	LHG	C18-C19-C20-C21
21	6	608	CHL	CBA-CGA-O2A-C1
22	5	602	CLA	CBA-CGA-O2A-C1
22	4	610	CLA	C12-C13-C15-C16
22	2	613	CLA	C5-C6-C7-C8
22	B	813	CLA	C10-C11-C12-C13
21	2	601	CHL	CAD-CBD-CGD-O2D
22	W	602	CLA	CAD-CBD-CGD-O2D
22	W	604	CLA	CAD-CBD-CGD-O2D
22	1	608	CLA	CAD-CBD-CGD-O2D
22	1	610	CLA	CAD-CBD-CGD-O2D
22	1	614	CLA	CAD-CBD-CGD-O2D
22	2	603	CLA	CAD-CBD-CGD-O2D
22	2	610	CLA	CAD-CBD-CGD-O2D
22	2	611	CLA	CAD-CBD-CGD-O2D
22	3	602	CLA	CAD-CBD-CGD-O2D
22	3	606	CLA	CAD-CBD-CGD-O2D
22	3	607	CLA	CAD-CBD-CGD-O2D
22	3	611	CLA	CAD-CBD-CGD-O2D
22	4	610	CLA	CAD-CBD-CGD-O2D
22	4	611	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	809	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	838	CLA	CAD-CBD-CGD-O2D
22	B	802	CLA	CAD-CBD-CGD-O2D
22	B	804	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D
22	G	203	CLA	CAD-CBD-CGD-O2D
22	5	602	CLA	CAD-CBD-CGD-O2D
22	6	612	CLA	CAD-CBD-CGD-O2D
22	7	607	CLA	CAD-CBD-CGD-O2D
22	7	617	CLA	CAD-CBD-CGD-O2D
22	9	611	CLA	CAD-CBD-CGD-O2D
22	A	854	CLA	C8-C10-C11-C12
22	B	816	CLA	CBD-CGD-O2D-CED
22	G	203	CLA	CBA-CGA-O2A-C1
28	J	103	LMG	C29-C28-O8-C9
22	3	611	CLA	C6-C7-C8-C10
22	7	602	CLA	C11-C12-C13-C15
26	U	2630	LHG	C4-C5-C6-O8
26	4	630	LHG	C5-C4-O6-P
26	A	847	LHG	C2-C3-O3-P
22	5	602	CLA	O1A-CGA-O2A-C1
22	6	604	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	C15-C16-C17-C18
22	A	826	CLA	CAA-CBA-CGA-O2A
22	3	603	CLA	C2A-CAA-CBA-CGA
24	8	620	XAT	C14-C15-C35-C34
22	B	806	CLA	C16-C17-C18-C19
22	A	814	CLA	O1D-CGD-O2D-CED
21	V	605	CHL	CHA-CBD-CGD-O1D
21	2	618	CHL	CHA-CBD-CGD-O1D
21	6	618	CHL	CHA-CBD-CGD-O1D
21	6	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	CHA-CBD-CGD-O1D
22	U	604	CLA	CHA-CBD-CGD-O1D
22	U	604	CLA	CHA-CBD-CGD-O2D
22	U	611	CLA	CHA-CBD-CGD-O2D
22	U	612	CLA	CHA-CBD-CGD-O1D
22	U	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	V	603	CLA	CHA-CBD-CGD-O1D
22	V	603	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	611	CLA	CHA-CBD-CGD-O1D
22	1	611	CLA	CHA-CBD-CGD-O2D
22	1	616	CLA	CHA-CBD-CGD-O2D
22	2	612	CLA	CHA-CBD-CGD-O1D
22	2	612	CLA	CHA-CBD-CGD-O2D
22	2	613	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	CHA-CBD-CGD-O1D
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O1D
22	A	845	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	CHA-CBD-CGD-O1D
22	B	822	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	5	613	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	CHA-CBD-CGD-O1D
22	8	602	CLA	CHA-CBD-CGD-O1D
22	1	610	CLA	O1A-CGA-O2A-C1
22	B	827	CLA	O1A-CGA-O2A-C1
22	7	610	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	O1A-CGA-O2A-C1
26	6	630	LHG	O10-C23-O8-C6
26	U	2630	LHG	O7-C5-C6-O8
26	B	851	LHG	O7-C5-C6-O8
28	J	104	LMG	O1-C7-C8-O7
21	3	608	CHL	O1A-CGA-O2A-C1
28	L	307	LMG	O10-C28-O8-C9
32	B	850	DGD	CDA-CEA-CFA-CGA
22	F	304	CLA	OBD-CAD-CBD-CGD
22	A	801	CLA	C3-C5-C6-C7
22	A	836	CLA	C3-C5-C6-C7
22	A	804	CLA	O1D-CGD-O2D-CED
22	7	609	CLA	O1D-CGD-O2D-CED
22	1	609	CLA	C13-C15-C16-C17
22	U	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	U	610	CLA	C11-C12-C13-C14
22	V	603	CLA	C11-C10-C8-C9
22	4	610	CLA	C11-C10-C8-C9
22	A	802	CLA	C11-C10-C8-C9
22	A	817	CLA	C11-C10-C8-C9
22	A	819	CLA	C14-C13-C15-C16
22	B	806	CLA	C11-C12-C13-C14
22	B	827	CLA	C6-C7-C8-C9
22	B	839	CLA	C6-C7-C8-C9
21	6	608	CHL	O1A-CGA-O2A-C1
22	G	203	CLA	O1A-CGA-O2A-C1
31	B	849	LMT	C4-C5-C6-C7
22	A	816	CLA	CBD-CGD-O2D-CED
26	9	2630	LHG	C11-C10-C9-C8
27	2	621	BCR	C37-C22-C23-C24
27	L	306	BCR	C7-C8-C9-C34
27	O	2004	BCR	C21-C22-C23-C24
22	W	613	CLA	C3-C5-C6-C7
21	2	606	CHL	C1A-C2A-CAA-CBA
22	W	603	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	806	CLA	C16-C17-C18-C20
22	A	842	CLA	C2-C1-O2A-CGA
26	5	630	LHG	C26-C27-C28-C29
25	W	2623	NEX	C29-C30-C31-C32
26	2	630	LHG	C3-O3-P-O6
26	A	846	LHG	C3-O3-P-O6
26	B	851	LHG	C3-O3-P-O6
26	9	2630	LHG	C24-C25-C26-C27
22	5	609	CLA	O1D-CGD-O2D-CED
22	2	603	CLA	CBA-CGA-O2A-C1
22	U	611	CLA	C4B-C3B-CAB-CBB
22	1	611	CLA	C4B-C3B-CAB-CBB
22	3	607	CLA	C4B-C3B-CAB-CBB
22	A	842	CLA	C4B-C3B-CAB-CBB
22	7	603	CLA	C4B-C3B-CAB-CBB
22	9	611	CLA	C4B-C3B-CAB-CBB
26	U	2630	LHG	C4-O6-P-O4
26	V	2630	LHG	C3-O3-P-O4
26	V	2630	LHG	C4-O6-P-O4
26	W	2630	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
26	W	2630	LHG	C4-O6-P-O4
26	3	630	LHG	C4-O6-P-O5
26	5	630	LHG	C3-O3-P-O4
26	7	630	LHG	C4-O6-P-O4
26	8	630	LHG	C3-O3-P-O4
26	9	2630	LHG	C3-O3-P-O4
22	A	829	CLA	C11-C12-C13-C14
22	4	603	CLA	C13-C15-C16-C17
22	3	611	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1
22	7	609	CLA	C8-C10-C11-C12
22	B	834	CLA	C5-C6-C7-C8
22	B	837	CLA	C8-C10-C11-C12
22	A	831	CLA	C2A-CAA-CBA-CGA
22	3	611	CLA	C3-C5-C6-C7
26	A	846	LHG	C10-C11-C12-C13
21	6	602	CHL	CAD-CBD-CGD-O1D
21	6	618	CHL	CAD-CBD-CGD-O1D
22	U	611	CLA	CAD-CBD-CGD-O1D
22	V	613	CLA	CAD-CBD-CGD-O1D
22	4	601	CLA	CAD-CBD-CGD-O1D
22	4	602	CLA	CAD-CBD-CGD-O1D
22	A	815	CLA	CAD-CBD-CGD-O1D
22	A	824	CLA	CAD-CBD-CGD-O1D
22	A	845	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	822	CLA	CAD-CBD-CGD-O1D
22	5	613	CLA	CAD-CBD-CGD-O1D
22	6	614	CLA	CAD-CBD-CGD-O1D
22	7	604	CLA	CAD-CBD-CGD-O1D
22	7	614	CLA	CAD-CBD-CGD-O1D
22	8	601	CLA	CAD-CBD-CGD-O1D
22	7	606	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C15-C16-C17-C18
22	A	831	CLA	C8-C10-C11-C12
22	8	613	CLA	C5-C6-C7-C8
22	B	831	CLA	O1A-CGA-O2A-C1
21	1	601	CHL	C5-C6-C7-C8
21	U	607	CHL	O1D-CGD-O2D-CED
26	W	2630	LHG	C15-C16-C17-C18
22	B	831	CLA	CBA-CGA-O2A-C1
22	7	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	8	612	CLA	CBA-CGA-O2A-C1
21	4	607	CHL	O1A-CGA-O2A-C1
21	U	601	CHL	C16-C17-C18-C20
22	O	2002	CLA	C4-C3-C5-C6
21	U	608	CHL	CHA-CBD-CGD-O1D
21	V	601	CHL	C11-C12-C13-C15
21	V	601	CHL	C12-C13-C15-C16
22	U	602	CLA	C6-C7-C8-C10
22	U	610	CLA	C11-C12-C13-C15
22	W	612	CLA	CAD-CBD-CGD-O2D
22	A	802	CLA	C11-C10-C8-C7
22	A	807	CLA	C11-C10-C8-C7
22	A	814	CLA	C6-C7-C8-C10
22	A	815	CLA	C3A-C2A-CAA-CBA
22	A	817	CLA	C11-C10-C8-C7
22	A	819	CLA	C12-C13-C15-C16
22	A	843	CLA	C11-C10-C8-C7
22	B	805	CLA	C6-C7-C8-C10
22	B	806	CLA	C11-C12-C13-C15
22	F	301	CLA	C12-C13-C15-C16
22	L	303	CLA	C11-C12-C13-C15
22	L	304	CLA	C3A-C2A-CAA-CBA
22	7	615	CLA	CAD-CBD-CGD-O2D
23	9	624	LUT	C25-C26-C27-C28
26	1	630	LHG	C16-C17-C18-C19
22	3	613	CLA	CAA-CBA-CGA-O2A
22	1	603	CLA	C5-C6-C7-C8
22	A	827	CLA	C13-C15-C16-C17
22	B	813	CLA	C8-C10-C11-C12
22	L	303	CLA	C10-C11-C12-C13
22	2	610	CLA	C8-C10-C11-C12
22	A	837	CLA	C10-C11-C12-C13
21	6	607	CHL	O1A-CGA-O2A-C1
22	4	602	CLA	C2A-CAA-CBA-CGA
22	A	822	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C2A-CAA-CBA-CGA
22	9	602	CLA	C11-C12-C13-C15
21	U	601	CHL	CAD-CBD-CGD-O1D
21	V	601	CHL	CAD-CBD-CGD-O1D
21	V	608	CHL	CAD-CBD-CGD-O1D
22	V	612	CLA	CAD-CBD-CGD-O1D
22	W	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	W	614	CLA	CAD-CBD-CGD-O1D
22	7	615	CLA	CAD-CBD-CGD-O1D
28	L	307	LMG	C7-C8-C9-O8
26	W	2630	LHG	O7-C5-C6-O8
26	A	847	LHG	O7-C5-C6-O8
28	G	202	LMG	O1-C7-C8-O7
28	L	307	LMG	C29-C30-C31-C32
22	A	825	CLA	C10-C11-C12-C13
22	V	602	CLA	C11-C12-C13-C14
22	A	837	CLA	O1A-CGA-O2A-C1
22	3	611	CLA	C6-C7-C8-C9
21	W	601	CHL	C10-C11-C12-C13
28	J	103	LMG	C37-C38-C39-C40
22	3	611	CLA	O1A-CGA-O2A-C1
28	J	103	LMG	O10-C28-O8-C9
21	6	618	CHL	CBD-CGD-O2D-CED
21	2	602	CHL	CBA-CGA-O2A-C1
22	A	814	CLA	C2-C3-C5-C6
22	B	833	CLA	CAA-CBA-CGA-O2A
22	W	610	CLA	C11-C12-C13-C14
22	W	610	CLA	C14-C13-C15-C16
22	1	602	CLA	C11-C10-C8-C9
22	3	612	CLA	C11-C10-C8-C9
22	3	617	CLA	C6-C7-C8-C9
22	A	812	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C10-C8-C9
22	A	830	CLA	C14-C13-C15-C16
22	A	854	CLA	C11-C10-C8-C9
22	B	808	CLA	C14-C13-C15-C16
22	B	810	CLA	C11-C10-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	B	826	CLA	C14-C13-C15-C16
22	B	833	CLA	C6-C7-C8-C9
22	B	837	CLA	C6-C7-C8-C9
22	5	602	CLA	C11-C10-C8-C9
22	9	611	CLA	C11-C10-C8-C9
29	A	844	PQN	C16-C17-C18-C19
29	A	844	PQN	C19-C18-C20-C21
21	2	602	CHL	O1A-CGA-O2A-C1
22	K	203	CLA	CBD-CGD-O2D-CED
21	6	618	CHL	O1A-CGA-O2A-C1
28	L	307	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	1	619	BCR	C37-C22-C23-C24
22	A	833	CLA	C5-C6-C7-C8
22	B	816	CLA	O1D-CGD-O2D-CED
21	1	607	CHL	CAA-CBA-CGA-O2A
22	A	810	CLA	C8-C10-C11-C12
22	U	611	CLA	C2B-C3B-CAB-CBB
22	1	604	CLA	C2B-C3B-CAB-CBB
22	1	614	CLA	C2B-C3B-CAB-CBB
22	3	606	CLA	C2B-C3B-CAB-CBB
22	3	607	CLA	C2B-C3B-CAB-CBB
22	3	610	CLA	C2B-C3B-CAB-CBB
22	4	603	CLA	C2B-C3B-CAB-CBB
22	4	609	CLA	C2B-C3B-CAB-CBB
22	A	812	CLA	C2B-C3B-CAB-CBB
22	A	832	CLA	C2B-C3B-CAB-CBB
22	A	835	CLA	C2B-C3B-CAB-CBB
22	B	812	CLA	C2B-C3B-CAB-CBB
22	B	820	CLA	C2B-C3B-CAB-CBB
22	B	841	CLA	C2B-C3B-CAB-CBB
22	G	201	CLA	C2B-C3B-CAB-CBB
22	7	606	CLA	C2B-C3B-CAB-CBB
22	V	613	CLA	C2A-CAA-CBA-CGA
22	3	612	CLA	C4-C3-C5-C6
22	A	810	CLA	C4-C3-C5-C6
22	7	613	CLA	C4-C3-C5-C6
26	9	2630	LHG	O7-C7-C8-C9
22	U	613	CLA	C15-C16-C17-C18
28	G	202	LMG	O6-C5-C6-O5
22	B	825	CLA	C5-C6-C7-C8
22	U	602	CLA	O1A-CGA-O2A-C1
26	W	2630	LHG	C23-C24-C25-C26
28	L	307	LMG	O8-C28-C29-C30
28	A	860	LMG	C9-C8-O7-C10
22	W	613	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	C2A-CAA-CBA-CGA
22	2	613	CLA	C2A-CAA-CBA-CGA
22	B	828	CLA	C2A-CAA-CBA-CGA
22	6	613	CLA	C2A-CAA-CBA-CGA
22	A	801	CLA	C2-C1-O2A-CGA
22	A	804	CLA	C2-C1-O2A-CGA
22	A	806	CLA	C2-C1-O2A-CGA
28	J	103	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
22	A	816	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	C3-C5-C6-C7
22	U	613	CLA	C8-C10-C11-C12
22	A	805	CLA	C8-C10-C11-C12
22	A	817	CLA	C8-C10-C11-C12
26	7	630	LHG	C25-C26-C27-C28
28	J	103	LMG	C29-C30-C31-C32
27	L	306	BCR	C5-C6-C7-C8
22	O	2002	CLA	C2-C3-C5-C6
22	A	807	CLA	C10-C11-C12-C13
22	U	602	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C8-C10-C11-C12
22	A	829	CLA	C11-C12-C13-C15
22	V	604	CLA	C2A-CAA-CBA-CGA
28	A	860	LMG	C2-C1-O1-C7
26	1	630	LHG	O7-C5-C6-O8
22	K	201	CLA	CBD-CGD-O2D-CED
26	U	2630	LHG	C3-O3-P-O6
26	1	630	LHG	C3-O3-P-O6
26	1	630	LHG	C4-O6-P-O3
26	3	630	LHG	C3-O3-P-O6
26	A	846	LHG	C4-O6-P-O3
26	A	847	LHG	C4-O6-P-O3
26	5	630	LHG	C4-O6-P-O3
26	6	630	LHG	C3-O3-P-O6
26	8	630	LHG	C4-O6-P-O3
26	9	2630	LHG	C4-O6-P-O3
32	B	850	DGD	C7B-C8B-C9B-CAB
21	U	601	CHL	C16-C17-C18-C19
22	W	602	CLA	C11-C12-C13-C15
26	W	2630	LHG	C4-C5-C6-O8
21	U	601	CHL	C11-C10-C8-C7
22	W	610	CLA	C11-C12-C13-C15
22	A	804	CLA	C12-C13-C15-C16
22	A	806	CLA	C12-C13-C15-C16
22	A	812	CLA	C11-C10-C8-C7
22	B	833	CLA	C6-C7-C8-C10
22	1	609	CLA	C11-C12-C13-C14
22	A	802	CLA	C14-C13-C15-C16
22	A	806	CLA	C11-C12-C13-C14
22	A	822	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	843	CLA	C11-C10-C8-C9
22	B	808	CLA	C11-C10-C8-C9
22	B	817	CLA	C11-C10-C8-C9
22	F	301	CLA	C14-C13-C15-C16
22	L	303	CLA	C11-C12-C13-C14
28	J	103	LMG	C13-C14-C15-C16
22	W	610	CLA	C15-C16-C17-C18
21	V	609	CHL	C4C-C3C-CAC-CBC
22	A	808	CLA	C5-C6-C7-C8
22	A	837	CLA	C5-C6-C7-C8
31	G	206	LMT	C6-C7-C8-C9
28	J	103	LMG	C39-C40-C41-C42
22	K	203	CLA	O1D-CGD-O2D-CED
29	B	842	PQN	C14-C13-C15-C16
26	A	846	LHG	C7-C8-C9-C10
22	7	613	CLA	C2-C3-C5-C6
22	A	841	CLA	C16-C17-C18-C20
21	6	601	CHL	CBA-CGA-O2A-C1
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	839	CLA	CBA-CGA-O2A-C1
22	B	809	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	8	602	CLA	CBA-CGA-O2A-C1
28	2	631	LMG	C29-C28-O8-C9
21	6	601	CHL	O1A-CGA-O2A-C1
22	B	809	CLA	O1A-CGA-O2A-C1
22	K	201	CLA	O1D-CGD-O2D-CED
22	U	613	CLA	C10-C11-C12-C13
22	A	814	CLA	C5-C6-C7-C8
22	A	819	CLA	O1A-CGA-O2A-C1
22	1	604	CLA	C4B-C3B-CAB-CBB
22	1	608	CLA	C4B-C3B-CAB-CBB
22	1	610	CLA	C4B-C3B-CAB-CBB
22	1	614	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	C4B-C3B-CAB-CBB
22	3	610	CLA	C4B-C3B-CAB-CBB
22	4	601	CLA	C4B-C3B-CAB-CBB
22	4	612	CLA	C4B-C3B-CAB-CBB
22	A	801	CLA	C4B-C3B-CAB-CBB
22	A	812	CLA	C4B-C3B-CAB-CBB
22	A	832	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	818	CLA	C4B-C3B-CAB-CBB
22	B	841	CLA	C4B-C3B-CAB-CBB
22	K	203	CLA	C4B-C3B-CAB-CBB
22	5	613	CLA	C4B-C3B-CAB-CBB
22	6	611	CLA	C4B-C3B-CAB-CBB
22	7	606	CLA	C4B-C3B-CAB-CBB
22	8	604	CLA	C4B-C3B-CAB-CBB
22	U	613	CLA	C2A-CAA-CBA-CGA
22	3	613	CLA	C2A-CAA-CBA-CGA
31	B	849	LMT	O5'-C1'-O1'-C1
23	5	617	LUT	C29-C30-C31-C32
24	8	620	XAT	C33-C34-C35-C15
32	B	850	DGD	C3A-C4A-C5A-C6A
22	W	602	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	829	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	C2C-C3C-CAC-CBC
22	V	602	CLA	C5-C6-C7-C8
22	F	301	CLA	C13-C15-C16-C17
22	A	830	CLA	C3-C5-C6-C7
32	B	850	DGD	C2A-C3A-C4A-C5A
29	B	842	PQN	C12-C13-C15-C16
22	B	838	CLA	C2C-C3C-CAC-CBC
22	U	610	CLA	C10-C11-C12-C13
22	3	609	CLA	C8-C10-C11-C12
22	6	613	CLA	C8-C10-C11-C12
26	A	847	LHG	O2-C2-C3-O3
22	W	610	CLA	C2-C1-O2A-CGA
22	A	805	CLA	C2-C1-O2A-CGA
22	A	837	CLA	C2-C1-O2A-CGA
22	L	303	CLA	C2-C1-O2A-CGA
22	B	817	CLA	C8-C10-C11-C12
22	B	834	CLA	C10-C11-C12-C13
22	8	602	CLA	C11-C12-C13-C15
28	G	202	LMG	C2-C1-O1-C7
22	U	611	CLA	CAA-CBA-CGA-O1A
22	U	602	CLA	C2A-CAA-CBA-CGA
22	3	607	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	B	834	CLA	C2A-CAA-CBA-CGA
26	B	851	LHG	C10-C11-C12-C13
22	1	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	606	CHL	C3A-C2A-CAA-CBA
22	A	826	CLA	C3A-C2A-CAA-CBA
22	B	803	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	825	CLA	C3A-C2A-CAA-CBA
22	8	614	CLA	C3A-C2A-CAA-CBA
22	9	611	CLA	C3A-C2A-CAA-CBA
22	B	817	CLA	C16-C17-C18-C20
22	7	613	CLA	C6-C7-C8-C9
22	A	822	CLA	C13-C15-C16-C17
21	W	601	CHL	C6-C7-C8-C9
22	U	603	CLA	C6-C7-C8-C9
22	3	612	CLA	C6-C7-C8-C9
22	A	807	CLA	C11-C10-C8-C9
22	A	808	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	A	825	CLA	C11-C10-C8-C9
22	A	854	CLA	C6-C7-C8-C9
22	9	602	CLA	C11-C12-C13-C14
22	9	610	CLA	C5-C6-C7-C8
26	1	630	LHG	C15-C16-C17-C18
25	U	2623	NEX	C39-C29-C30-C31
25	V	2623	NEX	C39-C29-C30-C31
25	9	623	NEX	C39-C29-C30-C31
26	7	630	LHG	C4-C5-C6-O8
27	A	852	BCR	C11-C10-C9-C34
27	A	852	BCR	C16-C17-C18-C36
27	B	845	BCR	C20-C21-C22-C37
27	F	305	BCR	C35-C13-C14-C15
27	L	301	BCR	C20-C21-C22-C37
26	4	630	LHG	C10-C11-C12-C13
22	1	609	CLA	O2A-C1-C2-C3
22	A	805	CLA	O2A-C1-C2-C3
22	A	810	CLA	O2A-C1-C2-C3
22	B	804	CLA	O2A-C1-C2-C3
22	8	601	CLA	O2A-C1-C2-C3
21	2	606	CHL	CAA-CBA-CGA-O2A
22	7	612	CLA	CAA-CBA-CGA-O1A
22	7	612	CLA	CAA-CBA-CGA-O2A
22	8	602	CLA	O1A-CGA-O2A-C1
28	A	860	LMG	C7-C8-O7-C10
21	6	602	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	3	613	CLA	C1A-C2A-CAA-CBA
22	B	803	CLA	C1A-C2A-CAA-CBA
22	B	825	CLA	C1A-C2A-CAA-CBA
21	6	601	CHL	C12-C13-C15-C16
22	4	610	CLA	C6-C7-C8-C10
22	A	830	CLA	C11-C10-C8-C7
22	A	843	CLA	C11-C12-C13-C15
22	B	824	CLA	C6-C7-C8-C10
22	B	810	CLA	O1D-CGD-O2D-CED
22	7	602	CLA	C10-C11-C12-C13
21	2	606	CHL	CAA-CBA-CGA-O1A
22	A	839	CLA	O1A-CGA-O2A-C1
28	2	631	LMG	O10-C28-O8-C9
22	4	609	CLA	CAA-CBA-CGA-O1A
26	A	846	LHG	C24-C25-C26-C27
22	A	854	CLA	C11-C12-C13-C15
22	B	807	CLA	C2A-CAA-CBA-CGA
22	6	603	CLA	C2A-CAA-CBA-CGA
22	8	612	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C13-C15-C16-C17
22	A	822	CLA	C5-C6-C7-C8
22	8	609	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	C13-C15-C16-C17
26	3	630	LHG	C26-C27-C28-C29
26	4	630	LHG	O6-C4-C5-C6
22	1	603	CLA	O1D-CGD-O2D-CED
22	W	613	CLA	C4-C3-C5-C6
22	W	613	CLA	C2-C3-C5-C6
22	3	612	CLA	C2-C3-C5-C6
22	U	612	CLA	C2B-C3B-CAB-CBB
22	1	610	CLA	C2B-C3B-CAB-CBB
22	1	611	CLA	C2B-C3B-CAB-CBB
22	1	616	CLA	C2B-C3B-CAB-CBB
22	2	609	CLA	C2B-C3B-CAB-CBB
22	4	601	CLA	C2B-C3B-CAB-CBB
22	4	602	CLA	C2B-C3B-CAB-CBB
22	A	808	CLA	C2B-C3B-CAB-CBB
22	A	842	CLA	C2B-C3B-CAB-CBB
22	K	203	CLA	C2B-C3B-CAB-CBB
22	7	609	CLA	C2B-C3B-CAB-CBB
22	8	604	CLA	C2B-C3B-CAB-CBB
22	9	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	U	609	CHL	C2C-C3C-CAC-CBC
22	K	204	CLA	C2C-C3C-CAC-CBC
25	U	2623	NEX	C28-C29-C30-C31
25	V	2623	NEX	C28-C29-C30-C31
25	9	623	NEX	C28-C29-C30-C31
27	A	852	BCR	C11-C10-C9-C8
27	A	852	BCR	C16-C17-C18-C19
27	B	845	BCR	C20-C21-C22-C23
27	F	305	BCR	C12-C13-C14-C15
27	L	301	BCR	C20-C21-C22-C23
26	V	2630	LHG	C11-C10-C9-C8
26	V	2630	LHG	O7-C5-C6-O8
21	2	602	CHL	CAA-CBA-CGA-O1A
23	2	619	LUT	C33-C34-C35-C15
22	9	611	CLA	C8-C10-C11-C12
26	B	851	LHG	C9-C10-C11-C12
22	4	602	CLA	C15-C16-C17-C18
22	A	825	CLA	C5-C6-C7-C8
22	U	611	CLA	CAA-CBA-CGA-O2A
21	5	601	CHL	C2-C1-O2A-CGA
21	6	602	CHL	C2-C1-O2A-CGA
22	4	602	CLA	C2-C1-O2A-CGA
22	B	819	CLA	C2-C1-O2A-CGA
22	B	829	CLA	C2-C1-O2A-CGA
22	B	839	CLA	C2-C1-O2A-CGA
22	7	617	CLA	O1D-CGD-O2D-CED
28	A	860	LMG	C11-C12-C13-C14
22	4	610	CLA	C11-C12-C13-C14
22	A	804	CLA	C6-C7-C8-C9
22	A	822	CLA	C11-C12-C13-C14
22	A	829	CLA	C6-C7-C8-C9
22	B	833	CLA	O1A-CGA-O2A-C1
26	1	630	LHG	C19-C20-C21-C22
26	W	2630	LHG	C5-C4-O6-P
22	A	819	CLA	CAA-CBA-CGA-O2A
22	U	612	CLA	C2A-CAA-CBA-CGA
22	7	603	CLA	C2A-CAA-CBA-CGA
22	B	802	CLA	O1A-CGA-O2A-C1
27	1	619	BCR	C23-C24-C25-C30
27	2	621	BCR	C23-C24-C25-C30
27	4	621	BCR	C23-C24-C25-C30
27	A	851	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	A	856	BCR	C5-C6-C7-C8
27	B	1609	BCR	C1-C6-C7-C8
27	M	2001	BCR	C5-C6-C7-C8
22	9	609	CLA	C2C-C3C-CAC-CBC
22	1	611	CLA	CAA-CBA-CGA-O2A
22	A	817	CLA	CAA-CBA-CGA-O2A
26	8	630	LHG	C10-C11-C12-C13
22	A	835	CLA	O1D-CGD-O2D-CED
22	8	614	CLA	CAA-CBA-CGA-O2A
22	3	602	CLA	C8-C10-C11-C12
22	B	802	CLA	CBA-CGA-O2A-C1
21	U	607	CHL	C4-C3-C5-C6
21	6	601	CHL	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	W	611	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	C16-C17-C18-C19
22	5	602	CLA	C10-C11-C12-C13
22	A	804	CLA	C5-C6-C7-C8
22	4	611	CLA	CAA-CBA-CGA-O2A
22	6	611	CLA	CAA-CBA-CGA-O2A
22	5	614	CLA	C2A-CAA-CBA-CGA
28	L	307	LMG	C30-C31-C32-C33
22	1	606	CLA	CAA-CBA-CGA-O2A
26	B	851	LHG	C13-C14-C15-C16
22	B	808	CLA	CAA-CBA-CGA-O2A
22	B	833	CLA	CBA-CGA-O2A-C1
26	U	2630	LHG	C29-C30-C31-C32
22	B	828	CLA	C3-C5-C6-C7
22	4	609	CLA	CAA-CBA-CGA-O2A
22	6	611	CLA	CAA-CBA-CGA-O1A
22	1	616	CLA	C4B-C3B-CAB-CBB
22	2	603	CLA	C4B-C3B-CAB-CBB
22	2	609	CLA	C4B-C3B-CAB-CBB
22	3	603	CLA	C4B-C3B-CAB-CBB
22	4	602	CLA	C4B-C3B-CAB-CBB
22	4	614	CLA	C4B-C3B-CAB-CBB
22	7	609	CLA	C4B-C3B-CAB-CBB
22	8	610	CLA	C4B-C3B-CAB-CBB
22	3	612	CLA	C5-C6-C7-C8
22	F	301	CLA	C4-C3-C5-C6
22	3	612	CLA	C6-C7-C8-C10
22	A	828	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	829	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C10-C8-C7
22	9	611	CLA	C11-C10-C8-C7
21	7	608	CHL	CAA-CBA-CGA-O2A
21	8	607	CHL	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O2A
26	B	851	LHG	C24-C23-O8-C6
26	A	847	LHG	O1-C1-C2-O2
22	7	617	CLA	CBD-CGD-O2D-CED
26	A	847	LHG	C24-C23-O8-C6
22	K	204	CLA	C15-C16-C17-C18
22	5	606	CLA	CAA-CBA-CGA-O2A
22	7	607	CLA	CAA-CBA-CGA-O2A
21	6	602	CHL	CAA-CBA-CGA-O2A
22	5	612	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C15-C16-C17-C18
22	L	302	CLA	C10-C11-C12-C13
22	B	817	CLA	C16-C17-C18-C19
22	B	819	CLA	C11-C12-C13-C15
22	B	825	CLA	C16-C17-C18-C20
22	4	612	CLA	CAA-CBA-CGA-O1A
22	6	612	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	CBA-CGA-O2A-C1
23	2	619	LUT	C40-C33-C34-C35
24	8	620	XAT	C20-C13-C14-C15
21	U	601	CHL	CAA-CBA-CGA-O2A
22	V	602	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	CAA-CBA-CGA-O2A
22	9	610	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C4-C3-C5-C6
22	B	831	CLA	C15-C16-C17-C18
22	7	603	CLA	CAA-CBA-CGA-O2A
22	A	809	CLA	O1A-CGA-O2A-C1
22	B	821	CLA	O1A-CGA-O2A-C1
22	A	810	CLA	C2-C3-C5-C6
22	B	832	CLA	C2-C3-C5-C6
22	A	814	CLA	C16-C17-C18-C20
21	W	601	CHL	CBA-CGA-O2A-C1
26	4	630	LHG	C24-C25-C26-C27
21	V	601	CHL	C14-C13-C15-C16
22	1	602	CLA	C11-C12-C13-C14
22	A	804	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	A	814	CLA	C6-C7-C8-C9
22	A	843	CLA	C11-C12-C13-C14
22	B	805	CLA	C6-C7-C8-C9
22	B	806	CLA	C6-C7-C8-C9
22	K	204	CLA	C14-C13-C15-C16
22	9	611	CLA	C11-C12-C13-C14
22	1	616	CLA	CAA-CBA-CGA-O2A
21	6	602	CHL	C3A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
21	W	601	CHL	O1A-CGA-O2A-C1
22	8	612	CLA	CAA-CBA-CGA-O2A
26	6	630	LHG	O8-C23-C24-C25
21	2	602	CHL	CAD-CBD-CGD-O2D
22	V	604	CLA	CAD-CBD-CGD-O2D
22	V	610	CLA	CAD-CBD-CGD-O2D
22	V	614	CLA	CAD-CBD-CGD-O2D
22	2	609	CLA	CAD-CBD-CGD-O2D
22	2	614	CLA	CAD-CBD-CGD-O2D
22	3	610	CLA	CAD-CBD-CGD-O2D
22	3	614	CLA	CAD-CBD-CGD-O2D
22	4	614	CLA	CAD-CBD-CGD-O2D
22	A	813	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	CAD-CBD-CGD-O2D
22	B	833	CLA	CAD-CBD-CGD-O2D
22	B	834	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	B	841	CLA	CAD-CBD-CGD-O2D
22	G	201	CLA	CAD-CBD-CGD-O2D
22	K	204	CLA	CAD-CBD-CGD-O2D
22	5	611	CLA	CAD-CBD-CGD-O2D
22	5	614	CLA	CAD-CBD-CGD-O2D
22	7	610	CLA	CAD-CBD-CGD-O2D
21	U	609	CHL	C4C-C3C-CAC-CBC
22	B	831	CLA	C10-C11-C12-C13
26	3	630	LHG	O9-C7-O7-C5
22	A	831	CLA	C2-C1-O2A-CGA
22	A	835	CLA	C2-C1-O2A-CGA
21	6	606	CHL	CAA-CBA-CGA-O2A
26	4	630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	2	609	CLA	CAA-CBA-CGA-O2A
22	3	604	CLA	CAA-CBA-CGA-O2A
22	L	304	CLA	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O1A
22	3	613	CLA	C2-C3-C5-C6
26	8	630	LHG	O7-C7-C8-C9
26	A	847	LHG	C10-C11-C12-C13
21	1	601	CHL	O1A-CGA-O2A-C1
23	3	618	LUT	C7-C8-C9-C10
27	2	621	BCR	C7-C8-C9-C10
27	3	620	BCR	C7-C8-C9-C10
24	W	2622	XAT	O4-C6-C7-C8
24	7	619	XAT	O24-C26-C27-C28
21	U	606	CHL	CAA-CBA-CGA-O2A
21	8	607	CHL	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O2A
22	8	614	CLA	CAA-CBA-CGA-O1A
22	A	835	CLA	CBD-CGD-O2D-CED
22	4	603	CLA	CAA-CBA-CGA-O2A
22	B	834	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
22	B	818	CLA	C15-C16-C17-C18
22	6	612	CLA	CAA-CBA-CGA-O1A
21	U	601	CHL	O2A-C1-C2-C3
21	W	601	CHL	O2A-C1-C2-C3
21	1	601	CHL	O2A-C1-C2-C3
21	5	601	CHL	O2A-C1-C2-C3
21	8	608	CHL	O2A-C1-C2-C3
22	U	602	CLA	O2A-C1-C2-C3
22	1	611	CLA	O2A-C1-C2-C3
22	4	604	CLA	O2A-C1-C2-C3
22	A	814	CLA	O2A-C1-C2-C3
22	A	830	CLA	O2A-C1-C2-C3
22	B	817	CLA	O2A-C1-C2-C3
22	B	824	CLA	O2A-C1-C2-C3
22	B	841	CLA	O2A-C1-C2-C3
21	1	601	CHL	CBA-CGA-O2A-C1
22	5	602	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C10-C11-C12-C13
22	B	817	CLA	C10-C11-C12-C13
22	3	607	CLA	CAA-CBA-CGA-O2A
22	A	836	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	2	631	LMG	O8-C28-C29-C30
32	B	850	DGD	O1G-C1A-C2A-C3A
21	U	606	CHL	CAA-CBA-CGA-O1A
21	6	606	CHL	CAA-CBA-CGA-O1A
22	2	611	CLA	CAA-CBA-CGA-O1A
22	4	611	CLA	CAA-CBA-CGA-O1A
28	J	103	LMG	C22-C23-C24-C25
21	6	618	CHL	O1D-CGD-O2D-CED
22	U	603	CLA	C16-C17-C18-C20
22	8	602	CLA	C11-C12-C13-C14
31	A	857	LMT	C9-C10-C11-C12
22	2	603	CLA	O1A-CGA-O2A-C1
28	J	103	LMG	C38-C39-C40-C41
21	1	607	CHL	CHA-CBD-CGD-O1D
21	1	607	CHL	CHA-CBD-CGD-O2D
21	2	602	CHL	CHA-CBD-CGD-O2D
21	2	618	CHL	CHA-CBD-CGD-O2D
21	4	618	CHL	CHA-CBD-CGD-O2D
21	9	607	CHL	CHA-CBD-CGD-O2D
21	9	608	CHL	CHA-CBD-CGD-O1D
21	9	608	CHL	CHA-CBD-CGD-O2D
22	U	613	CLA	CHA-CBD-CGD-O1D
22	U	613	CLA	CHA-CBD-CGD-O2D
22	U	614	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	3	612	CLA	CHA-CBD-CGD-O1D
22	3	612	CLA	CHA-CBD-CGD-O2D
22	3	617	CLA	CHA-CBD-CGD-O1D
22	3	617	CLA	CHA-CBD-CGD-O2D
22	4	602	CLA	CHA-CBD-CGD-O2D
22	A	801	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	843	CLA	CHA-CBD-CGD-O2D
22	B	819	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	826	CLA	CHA-CBD-CGD-O1D
22	B	826	CLA	CHA-CBD-CGD-O2D
22	B	830	CLA	CHA-CBD-CGD-O1D
22	O	2002	CLA	CHA-CBD-CGD-O1D
22	O	2002	CLA	CHA-CBD-CGD-O2D
22	5	604	CLA	CHA-CBD-CGD-O1D
22	5	604	CLA	CHA-CBD-CGD-O2D
22	5	609	CLA	CHA-CBD-CGD-O1D
22	5	609	CLA	CHA-CBD-CGD-O2D
22	6	611	CLA	CHA-CBD-CGD-O1D
22	6	611	CLA	CHA-CBD-CGD-O2D
22	7	602	CLA	CHA-CBD-CGD-O1D
22	7	602	CLA	CHA-CBD-CGD-O2D
22	7	613	CLA	CHA-CBD-CGD-O1D
22	7	613	CLA	CHA-CBD-CGD-O2D
22	8	601	CLA	CHA-CBD-CGD-O2D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	8	604	CLA	CHA-CBD-CGD-O2D
22	1	606	CLA	CAA-CBA-CGA-O1A
22	1	616	CLA	CAA-CBA-CGA-O1A
22	U	604	CLA	CAA-CBA-CGA-O2A
22	L	302	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	C2-C3-C5-C6
22	9	609	CLA	C4C-C3C-CAC-CBC
22	5	603	CLA	CAA-CBA-CGA-O2A
22	U	603	CLA	C10-C11-C12-C13
22	B	804	CLA	C15-C16-C17-C18
22	8	612	CLA	O1A-CGA-O2A-C1
22	1	614	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O2A
22	A	824	CLA	CAA-CBA-CGA-O2A
28	G	202	LMG	O8-C28-C29-C30
26	A	847	LHG	O10-C23-O8-C6
22	A	818	CLA	C15-C16-C17-C18
22	A	827	CLA	C5-C6-C7-C8
21	7	608	CHL	CAA-CBA-CGA-O1A
22	3	614	CLA	CAA-CBA-CGA-O1A
21	U	609	CHL	CAA-CBA-CGA-O2A
22	A	830	CLA	CAA-CBA-CGA-O2A
28	2	631	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	3	609	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	CAA-CBA-CGA-O2A
22	A	842	CLA	CAA-CBA-CGA-O2A
22	A	841	CLA	C8-C10-C11-C12
21	U	601	CHL	C12-C13-C15-C16
22	3	612	CLA	C12-C13-C15-C16
22	A	836	CLA	C6-C7-C8-C10
28	A	860	LMG	C12-C13-C14-C15
26	W	2630	LHG	O9-C7-O7-C5
22	G	204	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	CAA-CBA-CGA-O2A
22	5	602	CLA	CAA-CBA-CGA-O2A
22	A	816	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C11-C10-C8-C9
22	B	811	CLA	C11-C10-C8-C9
22	F	301	CLA	C11-C10-C8-C9
22	9	602	CLA	C6-C7-C8-C9
21	3	608	CHL	C2B-C3B-CAB-CBB
22	1	608	CLA	C2B-C3B-CAB-CBB
22	4	612	CLA	C2B-C3B-CAB-CBB
22	4	614	CLA	C2B-C3B-CAB-CBB
22	B	818	CLA	C2B-C3B-CAB-CBB
22	5	603	CLA	C2B-C3B-CAB-CBB
22	4	612	CLA	CAA-CBA-CGA-O2A
22	5	606	CLA	CAA-CBA-CGA-O1A
22	B	821	CLA	CBA-CGA-O2A-C1
22	6	614	CLA	CBA-CGA-O2A-C1
22	4	602	CLA	CAA-CBA-CGA-O2A
22	4	603	CLA	CAA-CBA-CGA-O1A
22	A	854	CLA	C11-C12-C13-C14
22	A	810	CLA	O1A-CGA-O2A-C1
22	7	603	CLA	CAA-CBA-CGA-O1A
22	7	607	CLA	CAA-CBA-CGA-O1A
22	A	818	CLA	C2A-CAA-CBA-CGA
22	7	613	CLA	C2A-CAA-CBA-CGA
22	3	604	CLA	CAA-CBA-CGA-O1A
28	J	104	LMG	O7-C10-C11-C12
21	U	607	CHL	C10-C11-C12-C13
21	6	602	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	6	603	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	C16-C17-C18-C19
22	7	613	CLA	C6-C7-C8-C10
22	A	815	CLA	C4-C3-C5-C6
26	A	847	LHG	O1-C1-C2-C3
21	8	608	CHL	CAA-CBA-CGA-O2A
22	1	609	CLA	C10-C11-C12-C13
27	B	843	BCR	C11-C12-C13-C14
27	I	101	BCR	C21-C22-C23-C24
22	1	604	CLA	CBA-CGA-O2A-C1
21	V	601	CHL	C10-C11-C12-C13
21	V	606	CHL	CHA-CBD-CGD-O2D
21	4	608	CHL	C1A-C2A-CAA-CBA
21	6	601	CHL	C1A-C2A-CAA-CBA
21	8	606	CHL	C1A-C2A-CAA-CBA
22	2	613	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C1A-C2A-CAA-CBA
22	G	201	CLA	C1A-C2A-CAA-CBA
22	9	604	CLA	C1A-C2A-CAA-CBA
26	2	630	LHG	C1-C2-C3-O3
21	U	601	CHL	CAA-CBA-CGA-O1A
22	V	602	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	C5-C6-C7-C8
22	5	603	CLA	CAA-CBA-CGA-O1A
22	U	603	CLA	C2-C1-O2A-CGA
22	A	807	CLA	C2-C1-O2A-CGA
22	B	828	CLA	C2-C1-O2A-CGA
22	7	604	CLA	C2-C1-O2A-CGA
22	A	827	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	CAA-CBA-CGA-O1A
22	A	836	CLA	CAA-CBA-CGA-O1A
22	B	834	CLA	CAA-CBA-CGA-O1A
22	9	610	CLA	CAA-CBA-CGA-O1A
26	8	630	LHG	O9-C7-C8-C9
22	7	609	CLA	CAA-CBA-CGA-O2A
28	G	202	LMG	O10-C28-C29-C30
22	1	602	CLA	C8-C10-C11-C12
22	U	603	CLA	C4B-C3B-CAB-CBB
22	U	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	W	603	CLA	C4B-C3B-CAB-CBB
22	A	808	CLA	C4B-C3B-CAB-CBB
22	A	840	CLA	C4B-C3B-CAB-CBB
22	5	603	CLA	C4B-C3B-CAB-CBB
22	5	609	CLA	C4B-C3B-CAB-CBB
22	5	612	CLA	C4B-C3B-CAB-CBB
22	7	613	CLA	C4B-C3B-CAB-CBB
22	8	612	CLA	C4B-C3B-CAB-CBB
26	6	630	LHG	C3-O3-P-O5
26	9	2630	LHG	C4-O6-P-O5
22	B	840	CLA	C4C-C3C-CAC-CBC
22	3	607	CLA	CAA-CBA-CGA-O1A
22	4	602	CLA	CAA-CBA-CGA-O1A
22	A	824	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CAA-CBA-CGA-O1A
22	L	302	CLA	CAA-CBA-CGA-O1A
22	L	304	CLA	CAA-CBA-CGA-O1A
26	6	630	LHG	O10-C23-C24-C25
28	J	104	LMG	O9-C10-C11-C12
32	B	850	DGD	O1A-C1A-C2A-C3A
22	1	604	CLA	O1A-CGA-O2A-C1
22	3	614	CLA	CAA-CBA-CGA-O2A
23	W	2620	LUT	C1-C6-C7-C8
23	9	620	LUT	C1-C6-C7-C8
27	B	845	BCR	C23-C24-C25-C30
27	F	305	BCR	C5-C6-C7-C8
27	7	620	BCR	C5-C6-C7-C8
22	1	611	CLA	C15-C16-C17-C18
22	8	612	CLA	CAA-CBA-CGA-O1A
22	A	811	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	O1A-CGA-O2A-C1
22	5	612	CLA	CAA-CBA-CGA-O2A
22	B	803	CLA	C8-C10-C11-C12
22	9	611	CLA	C10-C11-C12-C13
22	A	810	CLA	CBA-CGA-O2A-C1
22	U	604	CLA	CAA-CBA-CGA-O1A
22	1	614	CLA	CAA-CBA-CGA-O1A
22	2	609	CLA	CAA-CBA-CGA-O1A
22	2	613	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	CAA-CBA-CGA-O1A
22	5	602	CLA	CAA-CBA-CGA-O1A
28	2	631	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	A	824	CLA	C5-C6-C7-C8
22	V	604	CLA	CAA-CBA-CGA-O2A
22	8	609	CLA	CAA-CBA-CGA-O2A
22	4	613	CLA	C5-C6-C7-C8
22	L	303	CLA	C15-C16-C17-C18
26	U	2630	LHG	C7-C8-C9-C10
21	U	609	CHL	CAA-CBA-CGA-O1A
22	B	822	CLA	CAA-CBA-CGA-O1A
22	1	602	CLA	C4-C3-C5-C6
22	B	817	CLA	C4-C3-C5-C6
22	A	816	CLA	CAA-CBA-CGA-O1A
21	W	607	CHL	CAD-CBD-CGD-O1D
21	4	618	CHL	CAD-CBD-CGD-O1D
22	U	613	CLA	CAD-CBD-CGD-O1D
22	U	614	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	819	CLA	CAD-CBD-CGD-O1D
22	A	829	CLA	CAD-CBD-CGD-O1D
22	B	823	CLA	CAD-CBD-CGD-O1D
22	B	830	CLA	CAD-CBD-CGD-O1D
22	K	204	CLA	CAD-CBD-CGD-O1D
22	5	604	CLA	CAD-CBD-CGD-O1D
22	9	602	CLA	CAD-CBD-CGD-O1D
22	6	614	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	CAA-CBA-CGA-O2A
21	U	601	CHL	C14-C13-C15-C16
22	4	602	CLA	C14-C13-C15-C16
22	A	805	CLA	C11-C12-C13-C14
22	A	815	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C10-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	802	CLA	C5-C6-C7-C8
21	W	601	CHL	CAA-CBA-CGA-O2A
22	1	613	CLA	CAA-CBA-CGA-O2A
26	W	2630	LHG	C16-C17-C18-C19
22	3	613	CLA	C10-C11-C12-C13
22	A	834	CLA	C13-C15-C16-C17
22	B	802	CLA	C8-C10-C11-C12
26	B	851	LHG	O10-C23-O8-C6
22	A	816	CLA	C2A-CAA-CBA-CGA
22	1	604	CLA	CAA-CBA-CGA-O2A
22	1	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	A	846	LHG	O8-C23-C24-C25
22	A	812	CLA	C15-C16-C17-C18
26	1	630	LHG	C7-C8-C9-C10
21	8	608	CHL	CAA-CBA-CGA-O1A
22	B	810	CLA	C4-C3-C5-C6
21	U	607	CHL	C2-C3-C5-C6
21	U	608	CHL	CAD-CBD-CGD-O2D
21	V	606	CHL	CAD-CBD-CGD-O2D
21	V	608	CHL	CAD-CBD-CGD-O2D
21	3	608	CHL	C3A-C2A-CAA-CBA
22	V	612	CLA	CAD-CBD-CGD-O2D
22	V	613	CLA	C3A-C2A-CAA-CBA
22	W	603	CLA	CHA-CBD-CGD-O1D
22	W	614	CLA	CAD-CBD-CGD-O2D
22	1	613	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	C11-C12-C13-C15
22	4	610	CLA	C11-C10-C8-C7
22	A	805	CLA	C11-C12-C13-C15
22	A	808	CLA	C6-C7-C8-C10
22	A	815	CLA	C6-C7-C8-C10
22	A	820	CLA	C11-C10-C8-C7
22	A	838	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C12-C13-C15-C16
22	B	809	CLA	C11-C10-C8-C7
22	B	811	CLA	C11-C10-C8-C7
22	B	816	CLA	C11-C12-C13-C15
22	B	838	CLA	C3A-C2A-CAA-CBA
22	G	201	CLA	C3A-C2A-CAA-CBA
22	9	603	CLA	C3A-C2A-CAA-CBA
22	3	609	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	CAA-CBA-CGA-O1A
22	B	823	CLA	CAA-CBA-CGA-O2A
22	B	839	CLA	CAA-CBA-CGA-O2A
22	F	304	CLA	CAA-CBA-CGA-O2A
22	1	602	CLA	C15-C16-C17-C18
28	2	631	LMG	C17-C18-C19-C20
22	B	806	CLA	C10-C11-C12-C13
24	8	620	XAT	C11-C12-C13-C14
22	1	613	CLA	CAA-CBA-CGA-O1A
22	B	828	CLA	CAA-CBA-CGA-O1A
22	3	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	CAA-CBA-CGA-O2A
22	B	825	CLA	CAA-CBA-CGA-O2A
22	6	610	CLA	CAA-CBA-CGA-O2A
22	W	610	CLA	C10-C11-C12-C13
22	A	842	CLA	CAA-CBA-CGA-O1A
22	B	803	CLA	CAA-CBA-CGA-O1A
22	F	304	CLA	CAA-CBA-CGA-O1A
22	A	838	CLA	C5-C6-C7-C8
22	A	815	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C13-C15-C16-C17
22	B	806	CLA	C5-C6-C7-C8
26	A	846	LHG	O10-C23-C24-C25
22	3	614	CLA	C2A-CAA-CBA-CGA
22	2	612	CLA	CAA-CBA-CGA-O2A
21	W	601	CHL	CAA-CBA-CGA-O1A
22	2	612	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

226 monomers are involved in 491 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	606	CLA	1	0
22	B	822	CLA	1	0
27	B	843	BCR	4	0
22	B	813	CLA	3	0
21	V	605	CHL	1	0
26	W	2630	LHG	1	0
22	3	617	CLA	1	0
22	9	609	CLA	3	0
27	B	844	BCR	2	0
22	6	609	CLA	2	0
22	4	602	CLA	2	0
22	B	802	CLA	1	0
22	3	607	CLA	1	0
22	W	611	CLA	1	0
22	3	609	CLA	2	0
21	7	608	CHL	3	0
24	5	618	XAT	7	0
21	9	601	CHL	2	0
22	U	604	CLA	2	0
26	U	2630	LHG	1	0
21	4	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4	608	CHL	3	0
22	4	611	CLA	1	0
22	5	603	CLA	2	0
24	7	619	XAT	3	0
23	4	619	LUT	1	0
22	2	614	CLA	1	0
22	A	843	CLA	1	0
22	O	2002	CLA	3	0
22	B	815	CLA	2	0
27	M	2001	BCR	5	0
22	V	613	CLA	1	0
22	V	610	CLA	2	0
22	A	809	CLA	4	0
22	B	810	CLA	1	0
22	B	819	CLA	1	0
22	2	610	CLA	1	0
22	5	612	CLA	1	0
21	2	606	CHL	3	0
22	F	304	CLA	1	0
22	B	837	CLA	1	0
27	G	205	BCR	4	0
27	B	848	BCR	1	0
23	U	2620	LUT	2	0
24	1	618	XAT	3	0
21	U	609	CHL	2	0
23	W	2621	LUT	1	0
22	B	805	CLA	1	0
22	U	610	CLA	2	0
22	K	201	CLA	1	0
23	6	619	LUT	2	0
23	2	619	LUT	4	0
22	2	611	CLA	1	0
23	5	617	LUT	3	0
26	6	630	LHG	2	0
23	9	624	LUT	7	0
22	B	817	CLA	1	0
22	B	821	CLA	1	0
26	4	630	LHG	3	0
22	L	303	CLA	1	0
22	5	604	CLA	1	0
21	6	608	CHL	4	0
22	B	808	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	847	BCR	4	0
22	9	611	CLA	2	0
22	U	614	CLA	3	0
22	5	602	CLA	1	0
25	U	2623	NEX	1	0
22	B	825	CLA	1	0
22	5	609	CLA	6	0
22	A	802	CLA	3	0
22	7	610	CLA	1	0
22	B	840	CLA	1	0
22	8	609	CLA	2	0
27	A	856	BCR	5	0
21	8	618	CHL	2	0
23	7	618	LUT	2	0
21	3	608	CHL	1	0
22	6	612	CLA	1	0
22	7	613	CLA	2	0
25	9	623	NEX	4	0
27	6	621	BCR	5	0
22	A	845	CLA	1	0
22	A	814	CLA	1	0
21	6	607	CHL	1	0
22	B	814	CLA	1	0
22	8	604	CLA	2	0
27	4	621	BCR	11	0
27	3	621	BCR	4	0
22	6	604	CLA	1	0
27	K	205	BCR	4	0
22	4	604	CLA	3	0
22	7	606	CLA	2	0
22	B	804	CLA	2	0
27	I	101	BCR	4	0
21	4	606	CHL	2	0
22	L	304	CLA	2	0
21	5	607	CHL	1	0
27	B	845	BCR	6	0
21	9	605	CHL	2	0
22	A	832	CLA	1	0
21	6	601	CHL	1	0
26	1	630	LHG	2	0
22	K	204	CLA	2	0
22	4	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	W	609	CHL	1	0
21	2	618	CHL	1	0
22	B	831	CLA	1	0
22	1	611	CLA	2	0
22	5	610	CLA	1	0
22	F	303	CLA	1	0
27	K	202	BCR	7	0
22	B	824	CLA	1	0
22	5	613	CLA	1	0
25	V	2623	NEX	2	0
22	8	613	CLA	3	0
22	8	610	CLA	2	0
22	B	806	CLA	3	0
24	W	2622	XAT	1	0
22	A	836	CLA	3	0
22	A	841	CLA	1	0
23	U	2621	LUT	4	0
22	7	609	CLA	4	0
21	8	608	CHL	2	0
27	2	621	BCR	4	0
22	A	819	CLA	1	0
22	5	606	CLA	2	0
22	3	610	CLA	1	0
23	8	619	LUT	2	0
22	8	611	CLA	1	0
22	A	827	CLA	2	0
22	B	827	CLA	1	0
24	4	620	XAT	11	0
25	W	2623	NEX	2	0
22	4	614	CLA	1	0
27	3	620	BCR	9	0
22	A	816	CLA	1	0
21	9	608	CHL	3	0
21	8	606	CHL	1	0
22	B	823	CLA	3	0
22	2	613	CLA	1	0
22	B	818	CLA	1	0
21	6	606	CHL	1	0
22	A	829	CLA	1	0
21	2	601	CHL	1	0
28	G	202	LMG	2	0
22	F	301	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	602	CLA	4	0
27	O	2004	BCR	5	0
22	A	803	CLA	5	0
22	3	612	CLA	2	0
23	V	2621	LUT	1	0
21	2	602	CHL	2	0
22	B	803	CLA	4	0
22	A	801	CLA	3	0
27	J	102	BCR	4	0
24	8	620	XAT	3	0
22	B	838	CLA	1	0
22	9	612	CLA	1	0
27	A	852	BCR	8	0
22	4	610	CLA	3	0
24	6	620	XAT	5	0
27	7	621	BCR	3	0
22	A	830	CLA	1	0
27	1	619	BCR	1	0
22	9	602	CLA	3	0
22	3	604	CLA	1	0
21	8	607	CHL	1	0
24	3	619	XAT	5	0
22	G	201	CLA	4	0
23	1	617	LUT	2	0
21	9	606	CHL	8	0
21	W	608	CHL	1	0
22	B	833	CLA	2	0
22	1	609	CLA	1	0
27	L	306	BCR	5	0
21	U	606	CHL	2	0
22	7	602	CLA	6	0
22	V	602	CLA	2	0
21	1	601	CHL	1	0
27	F	305	BCR	3	0
23	9	621	LUT	4	0
21	U	607	CHL	4	0
21	5	601	CHL	4	0
27	B	801	BCR	5	0
22	B	807	CLA	1	0
21	9	607	CHL	2	0
22	B	839	CLA	2	0
21	V	609	CHL	2	0

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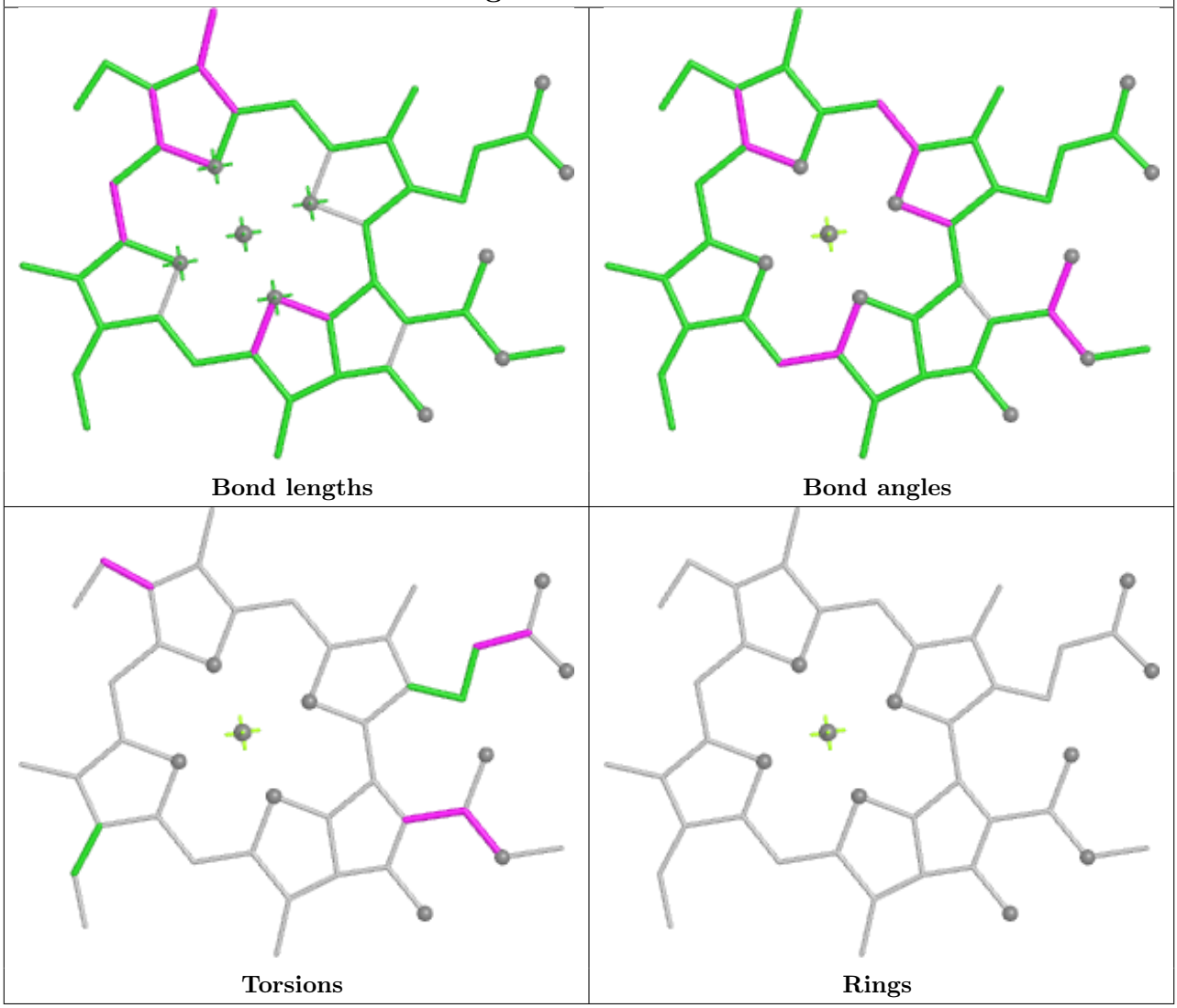
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	610	CLA	4	0
22	4	609	CLA	1	0
27	A	849	BCR	1	0
22	A	810	CLA	3	0
22	A	828	CLA	3	0
22	B	828	CLA	3	0
27	L	301	BCR	4	0
21	1	607	CHL	1	0
22	5	611	CLA	1	0
22	8	614	CLA	1	0
21	6	618	CHL	2	0
22	8	601	CLA	1	0
21	4	618	CHL	1	0
27	A	848	BCR	2	0
23	W	2620	LUT	2	0
22	3	606	CLA	3	0
24	2	620	XAT	7	0
22	A	854	CLA	3	0
22	3	613	CLA	2	0
22	A	835	CLA	1	0
22	B	812	CLA	1	0
22	3	603	CLA	1	0
22	7	607	CLA	1	0
23	9	620	LUT	4	0
27	7	620	BCR	7	0
21	2	608	CHL	2	0
27	L	305	BCR	4	0
22	B	836	CLA	1	0
27	B	1609	BCR	8	0
21	2	607	CHL	2	0
27	8	621	BCR	8	0
22	A	825	CLA	1	0
22	2	604	CLA	2	0
22	A	837	CLA	3	0
22	3	614	CLA	1	0
27	A	851	BCR	11	0
23	V	2620	LUT	2	0

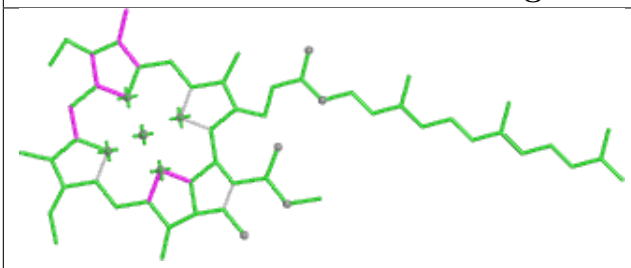
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

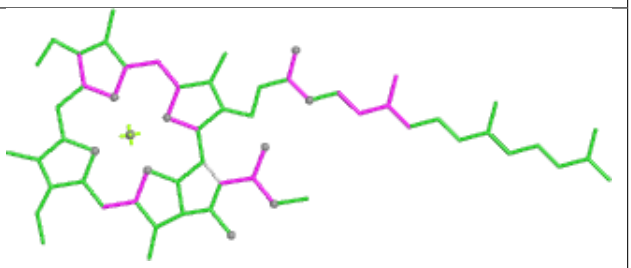
Ligand CLA 1 606



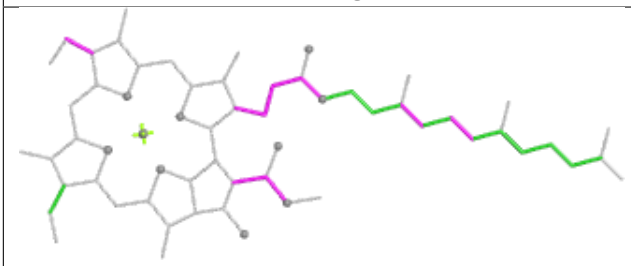
Ligand CLA B 822



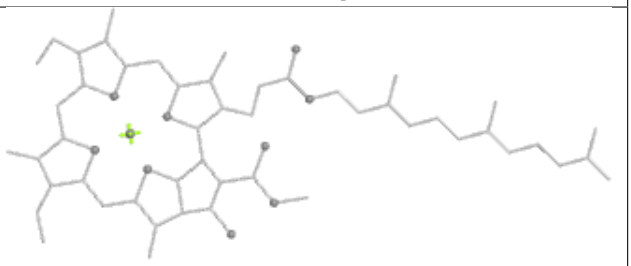
Bond lengths



Bond angles

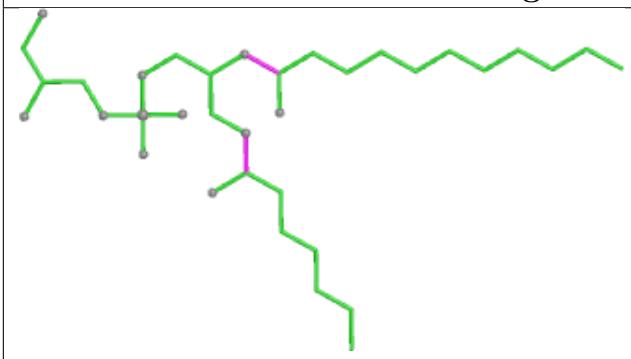


Torsions

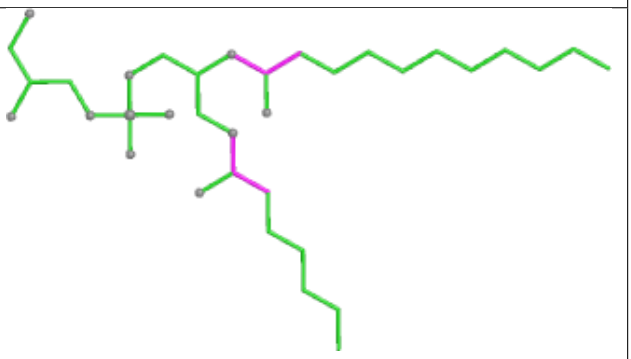


Rings

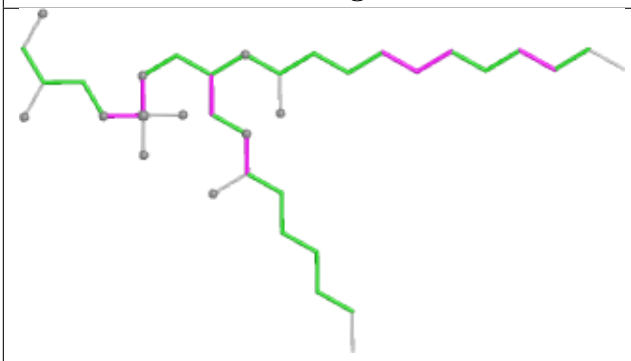
Ligand LHG B 851



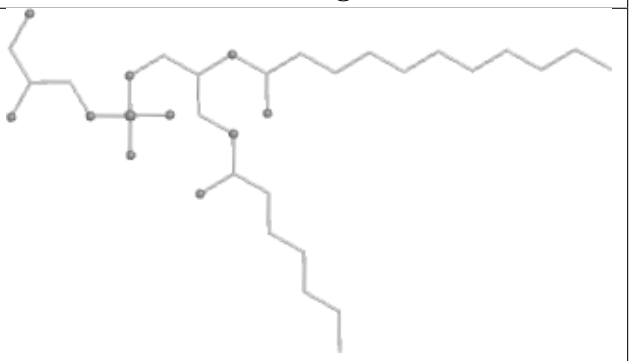
Bond lengths



Bond angles

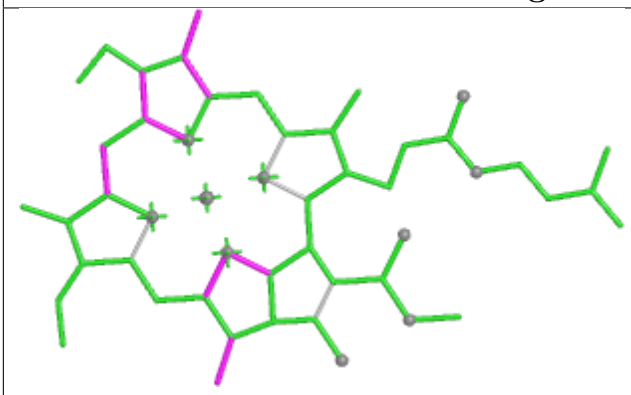


Torsions

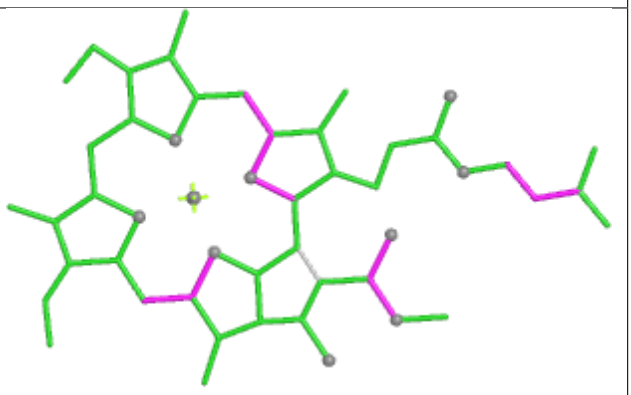


Rings

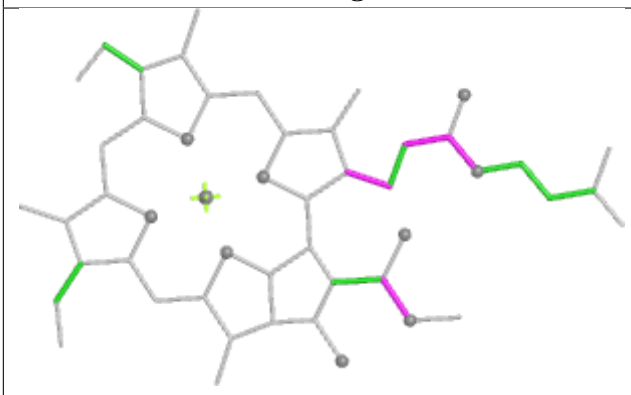
Ligand CLA 1 613



Bond lengths



Bond angles



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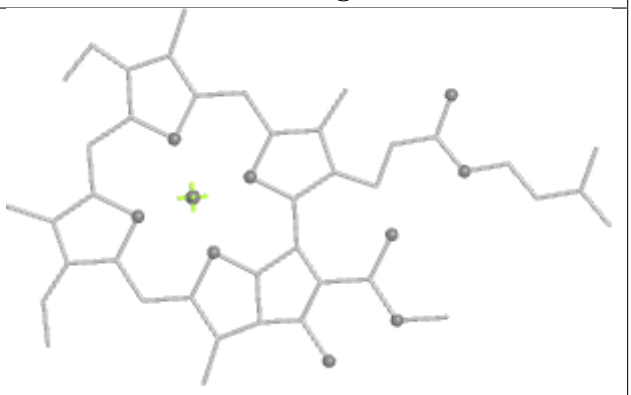
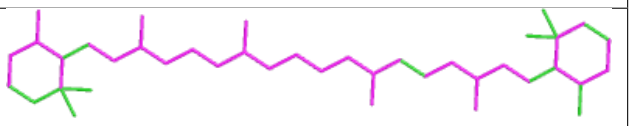


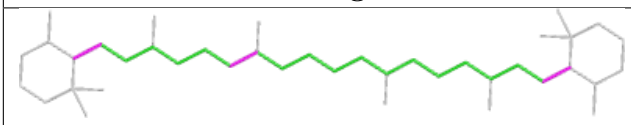
Rings

Ligand BCR B 843

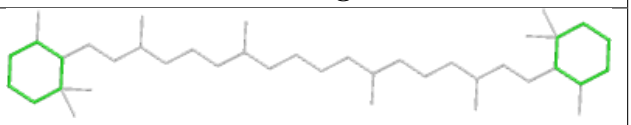
Bond lengths



Bond angles

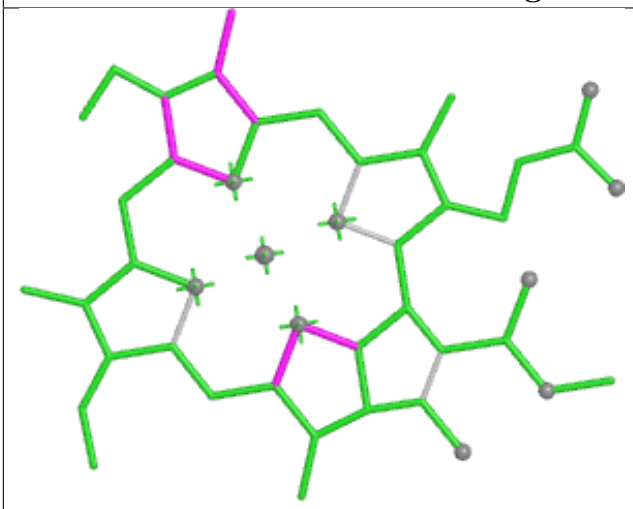


Torsions

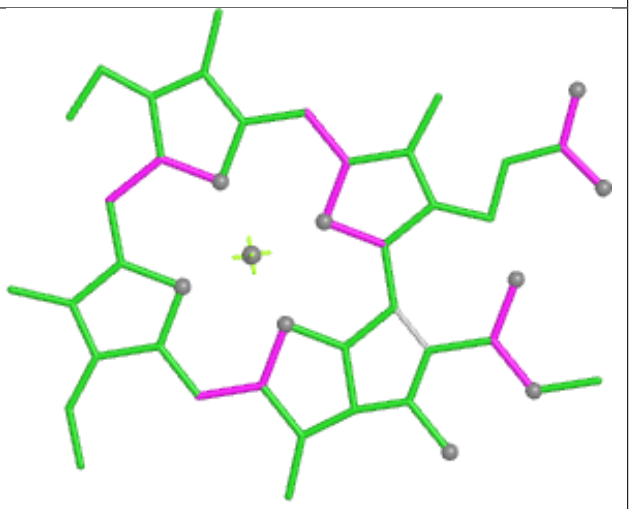


Rings

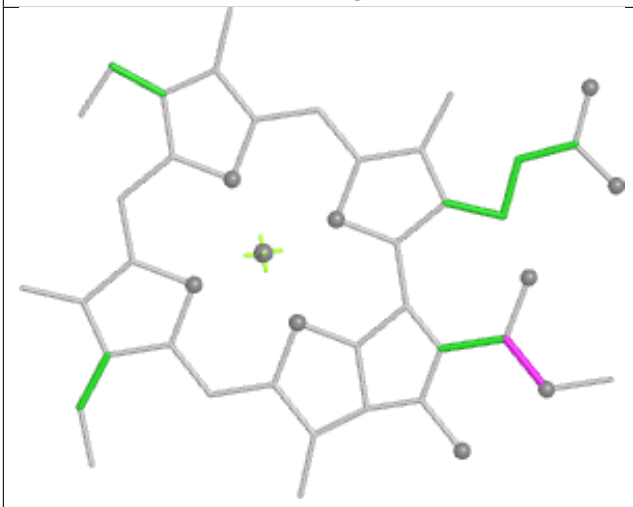
Ligand CLA B 835



Bond lengths



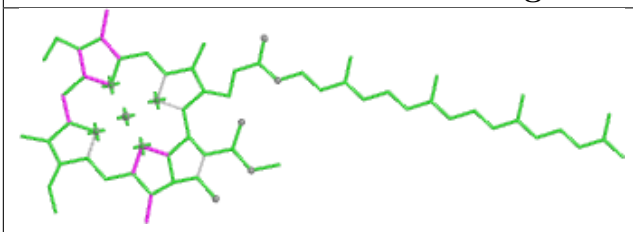
Bond angles



Torsions

Rings

Ligand CLA B 813



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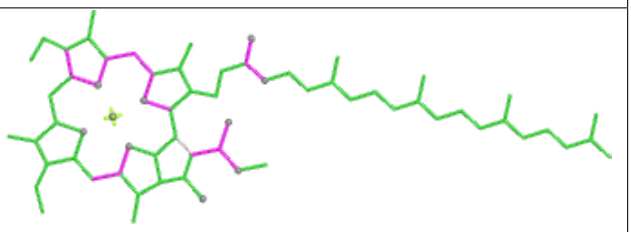
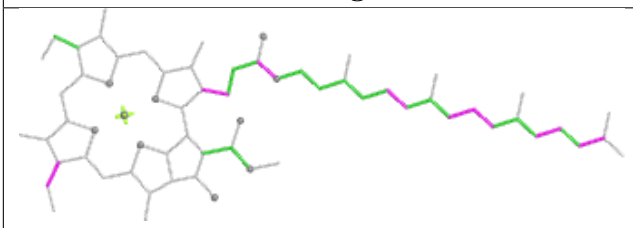


Bond angles



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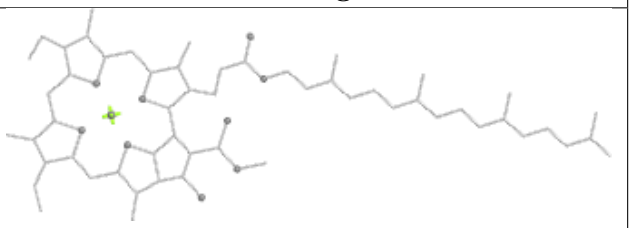
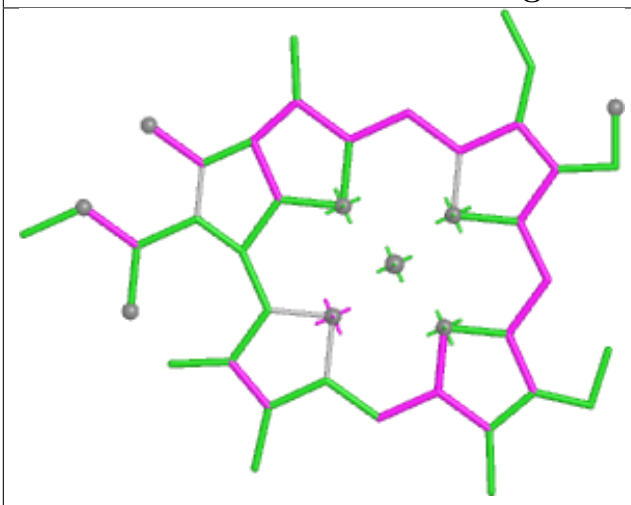


Rings

Ligand CHL V 605



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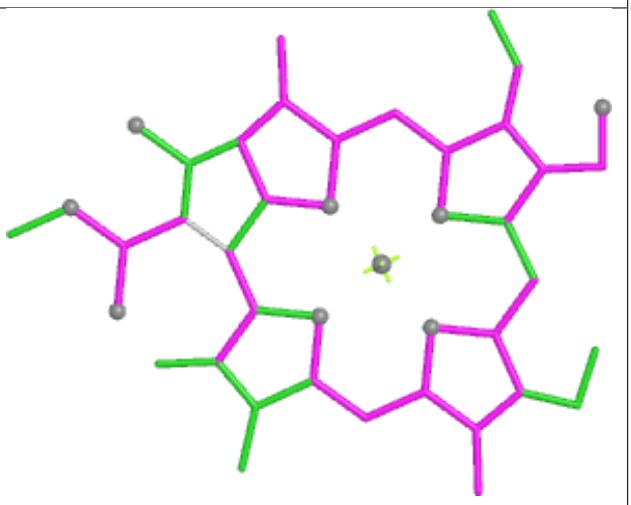

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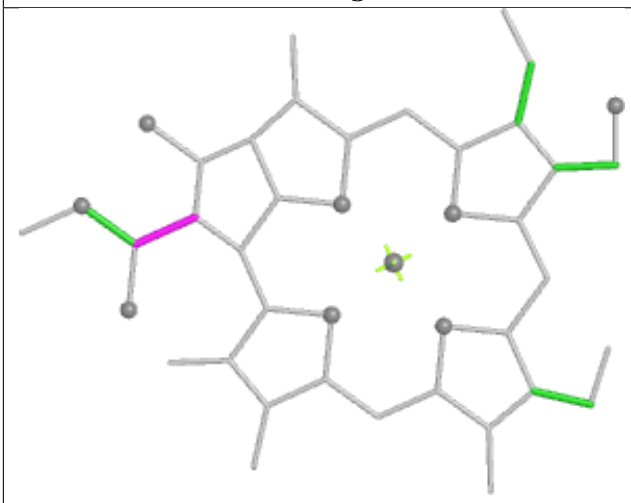

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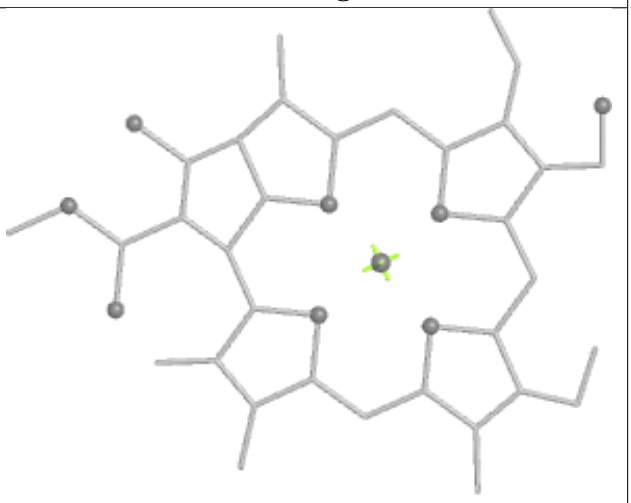
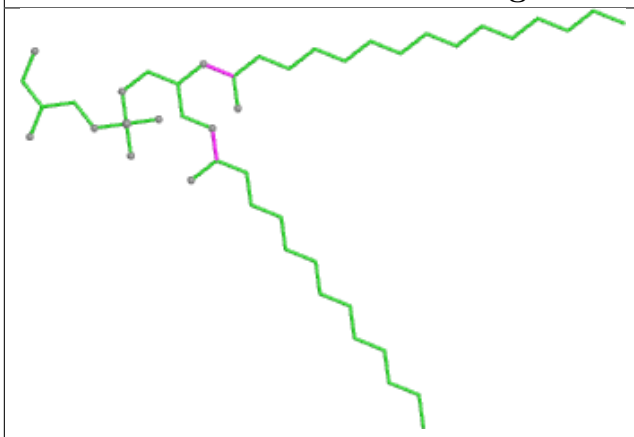


Rings

Ligand LHG W 2630



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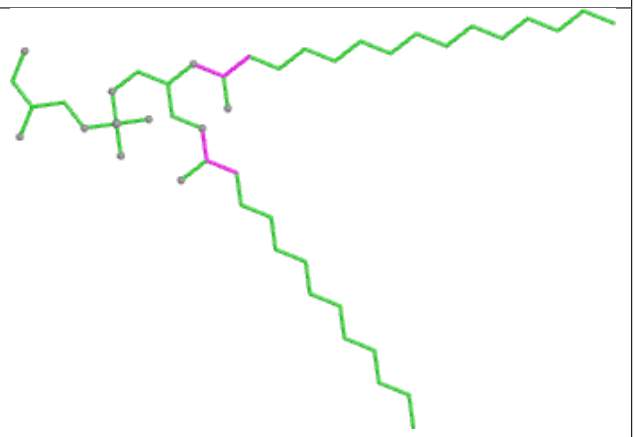
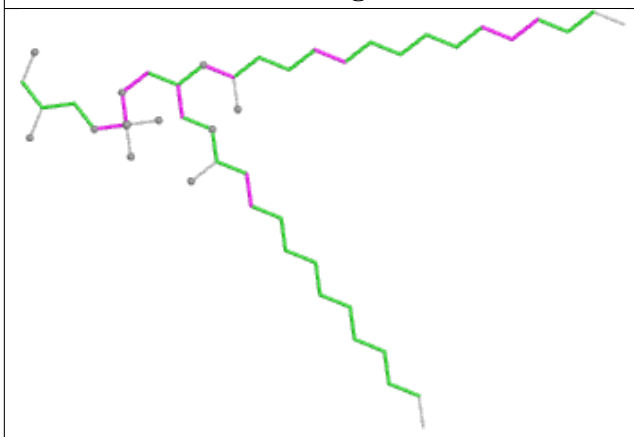


Bond angles



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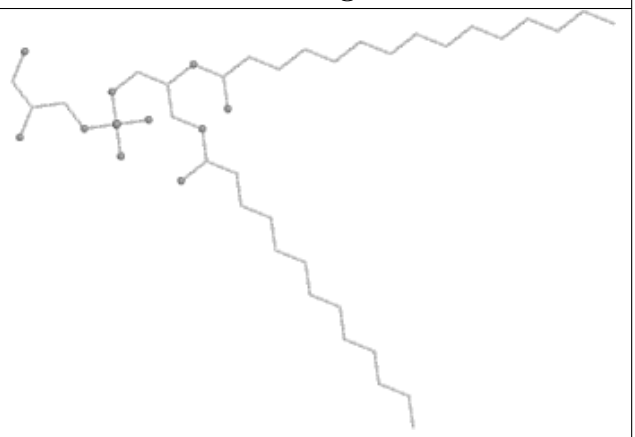
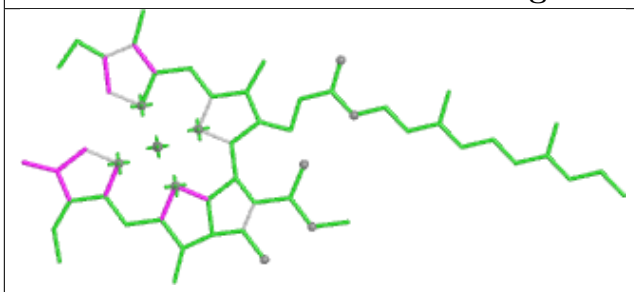
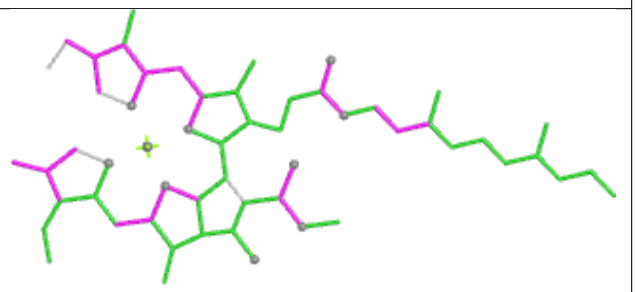


Rings

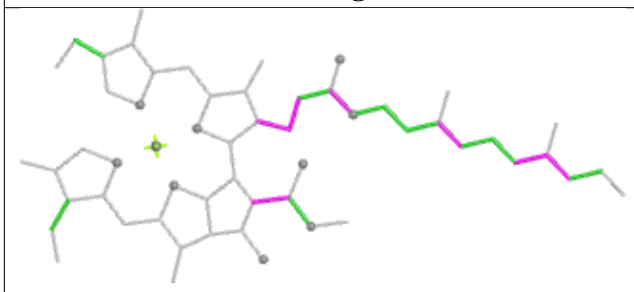
Ligand CLA 3 617



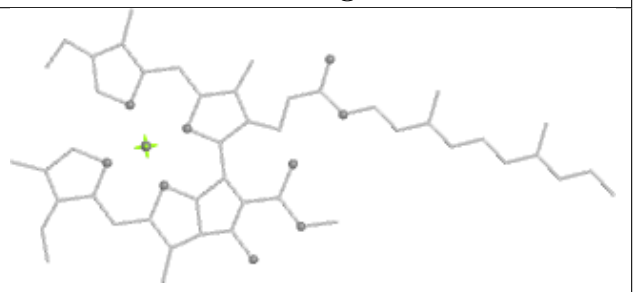
Bond lengths



Bond angles

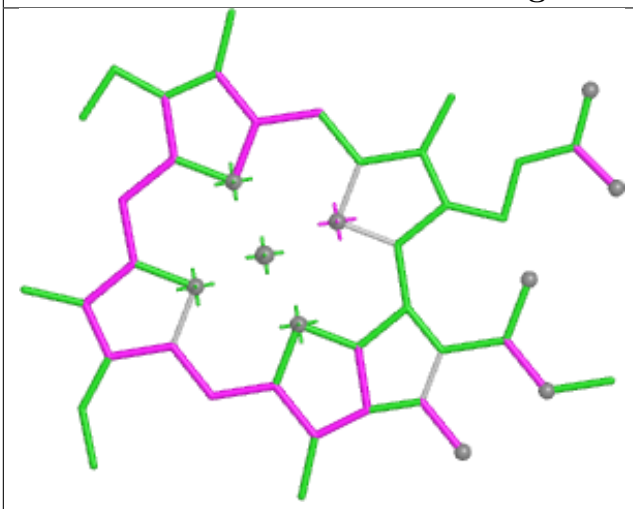


Torsions



Rings

Ligand CLA 9 609



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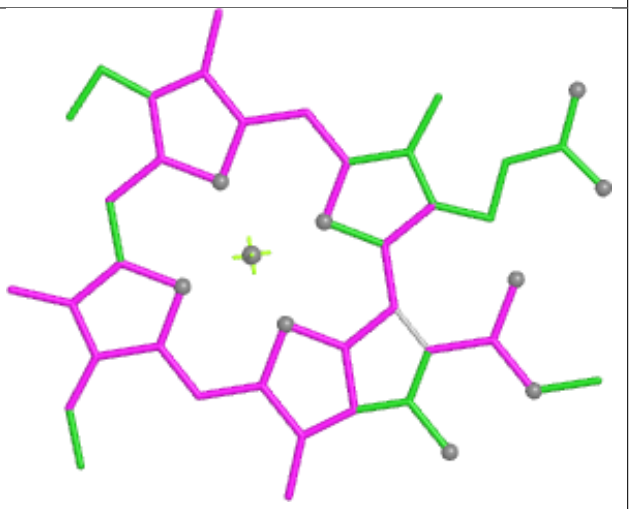
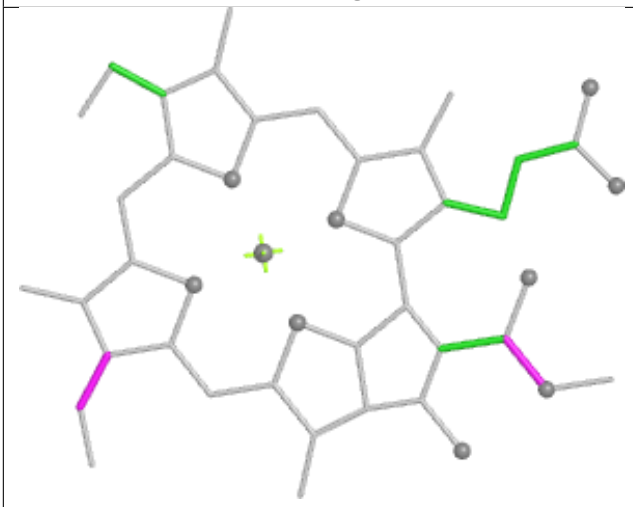


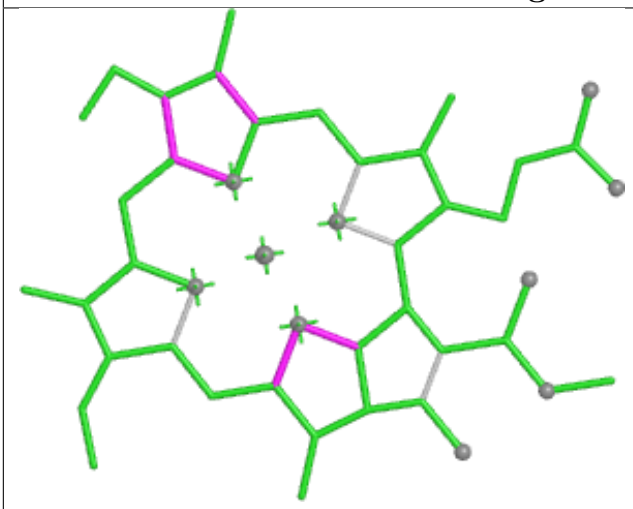
Bond angles



Torsions

Rings

Ligand CLA 1 616



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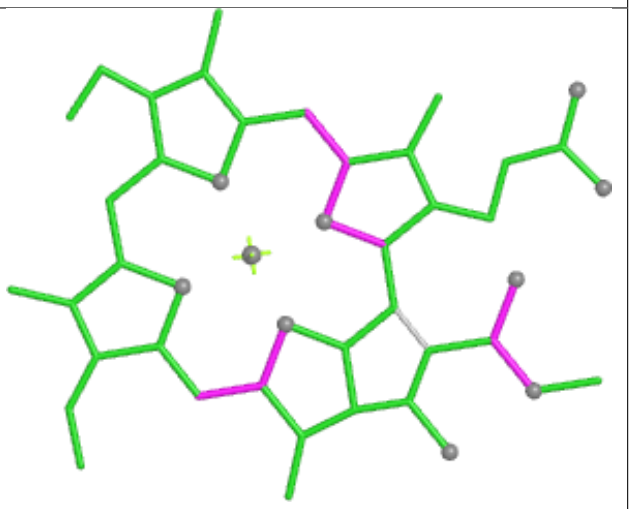

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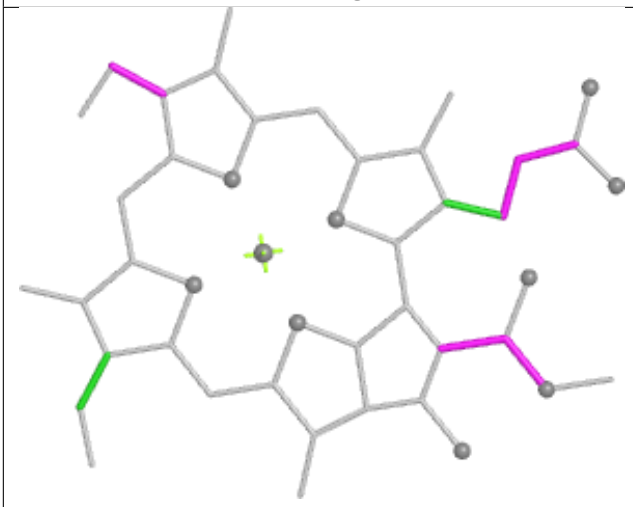
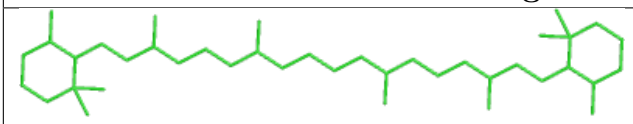


Torsions

Rings

Ligand BCR B 844



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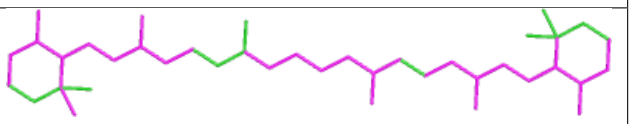

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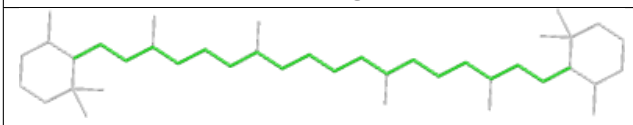

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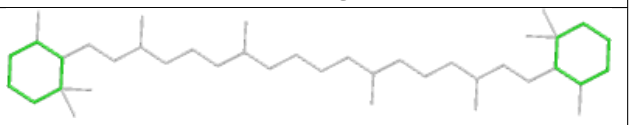
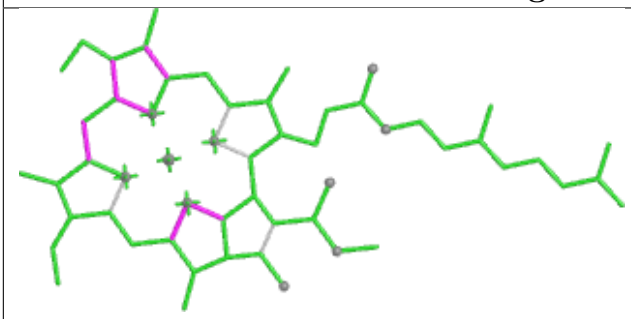


Rings

Ligand CLA 6 609



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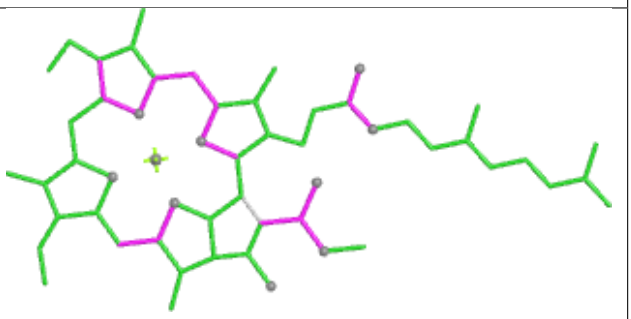

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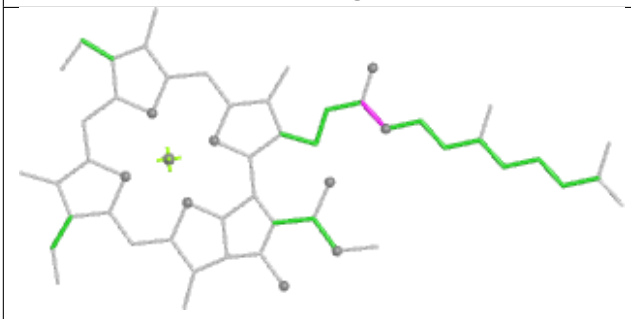

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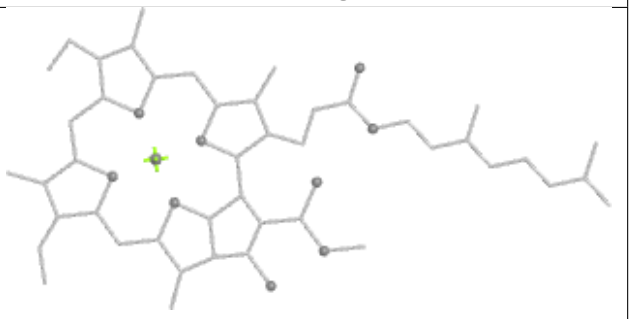
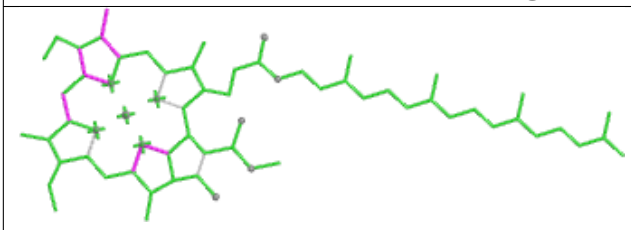


Rings

Ligand CLA A 804



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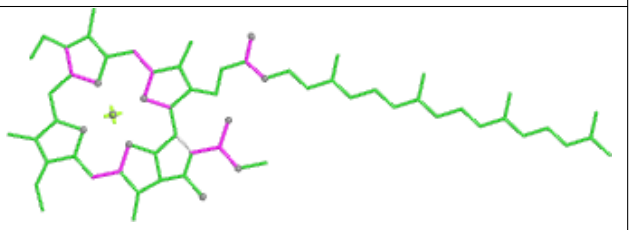

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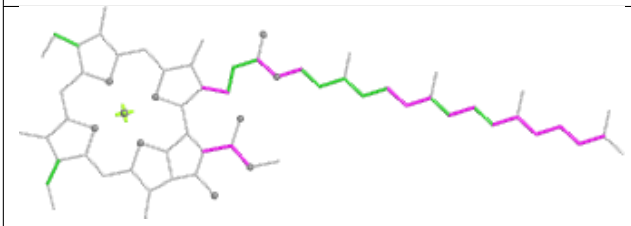

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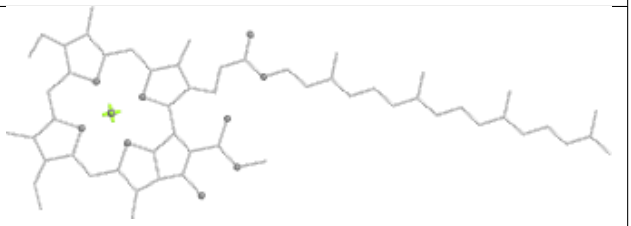
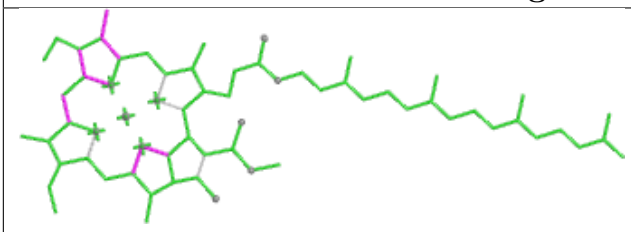
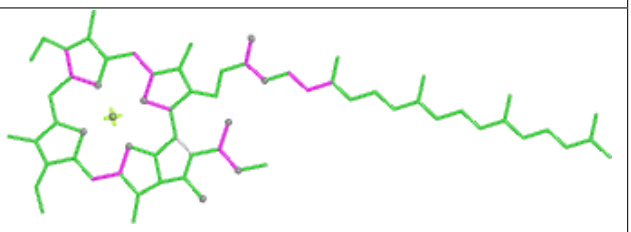
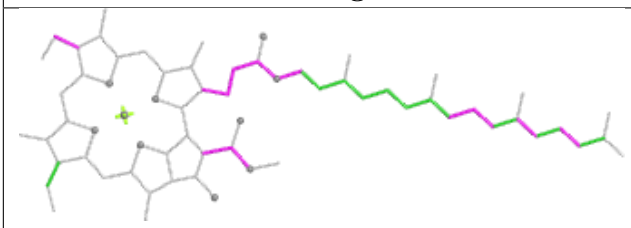
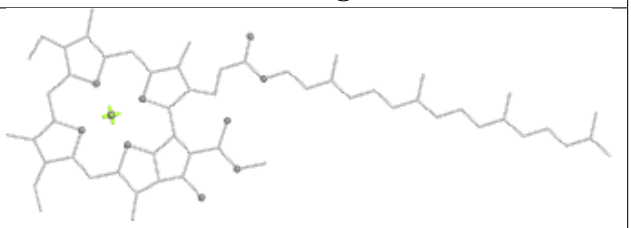


Rings

Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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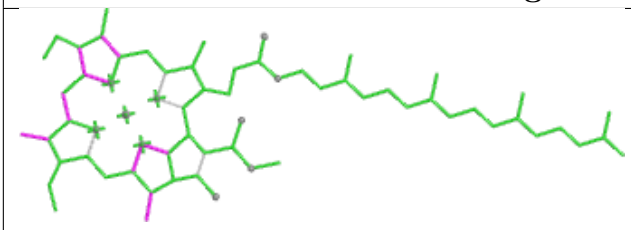
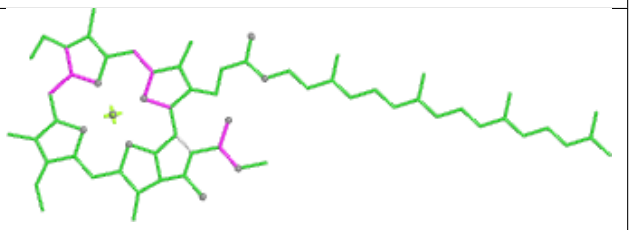
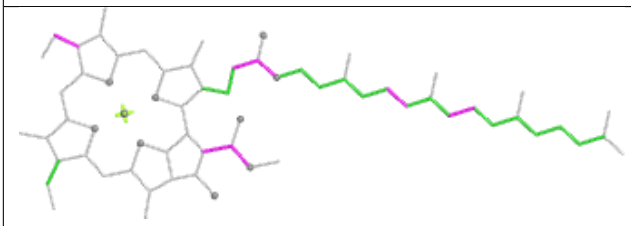
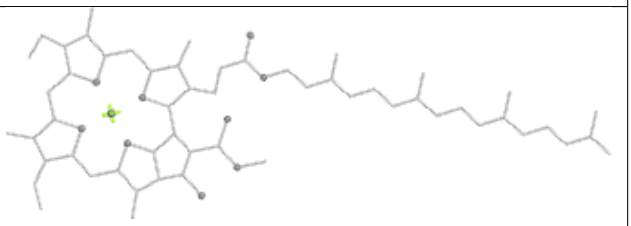
 Bond lengths	 Bond angles
 Torsions	 Rings

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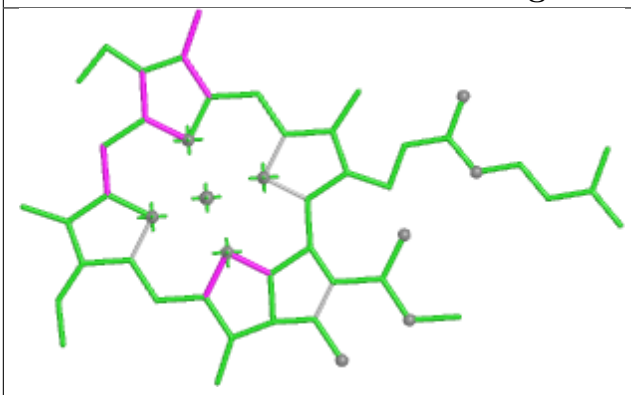
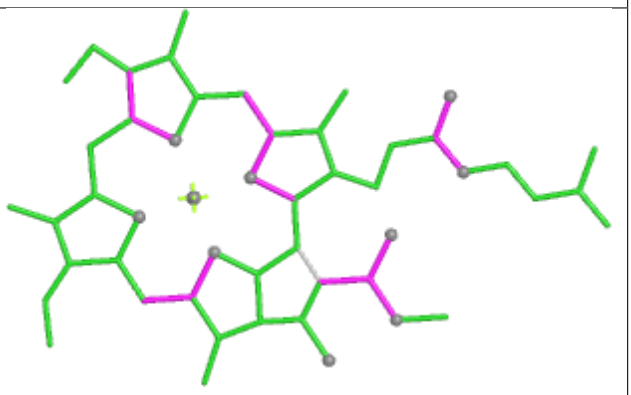
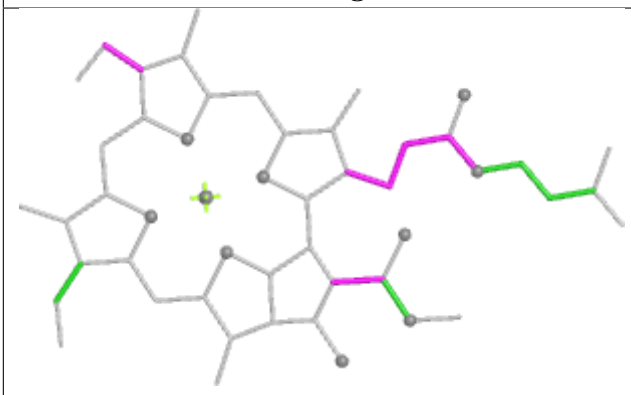
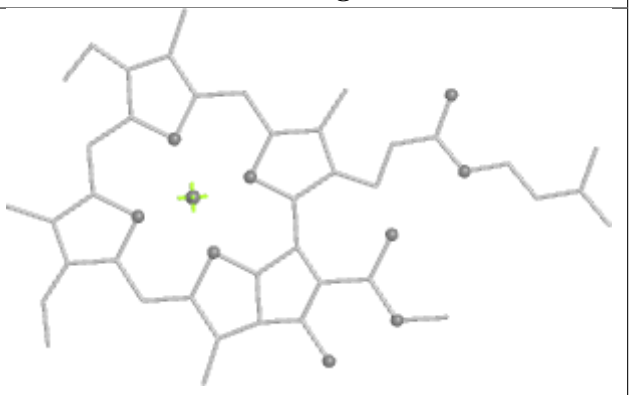
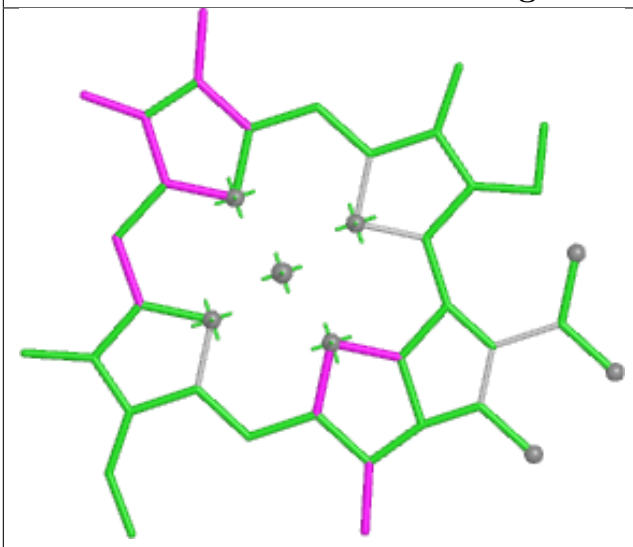
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 611



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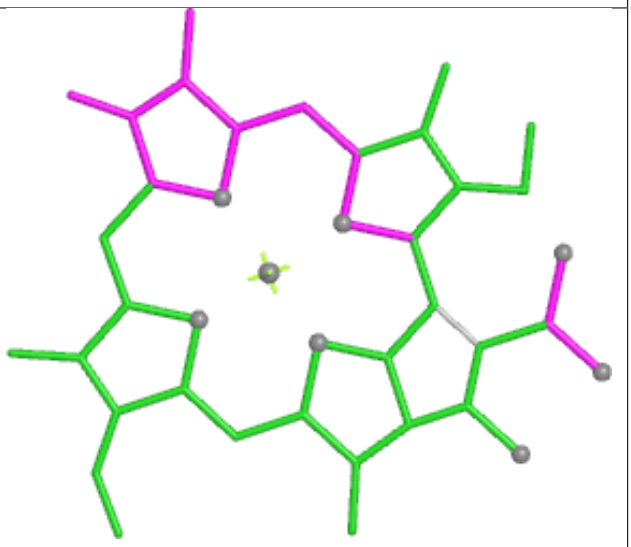
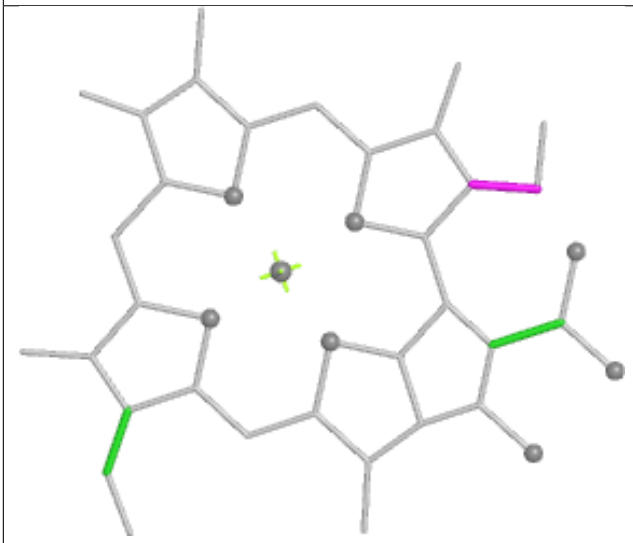


Bond angles



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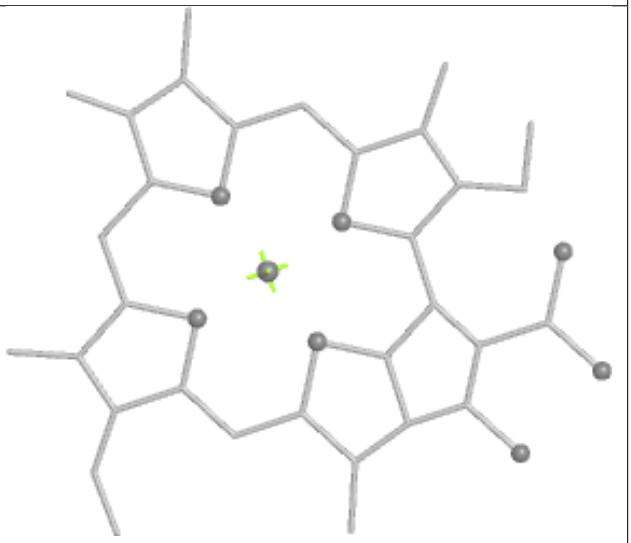

Rings

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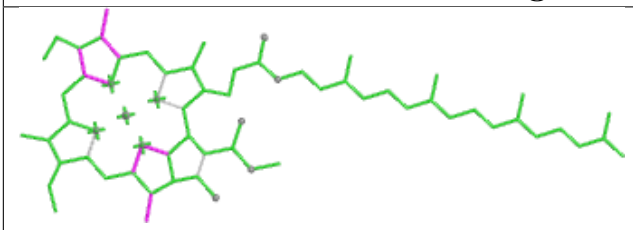

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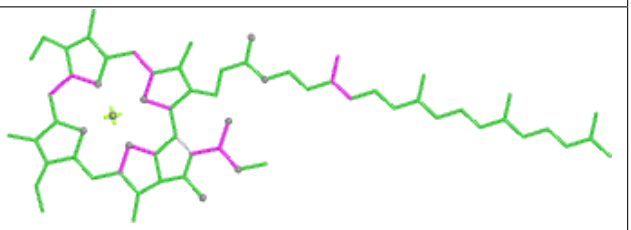

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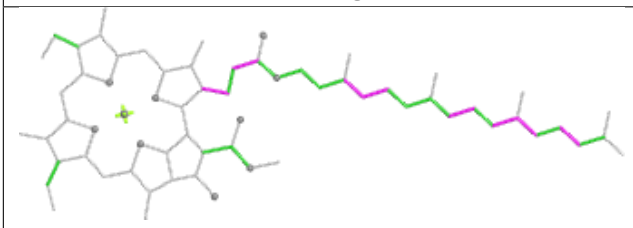

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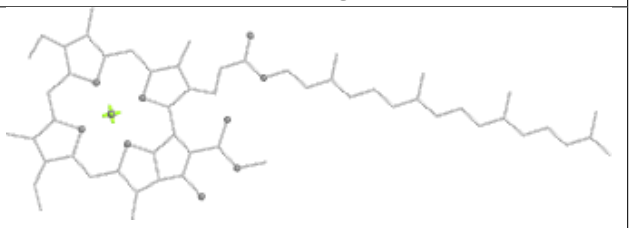
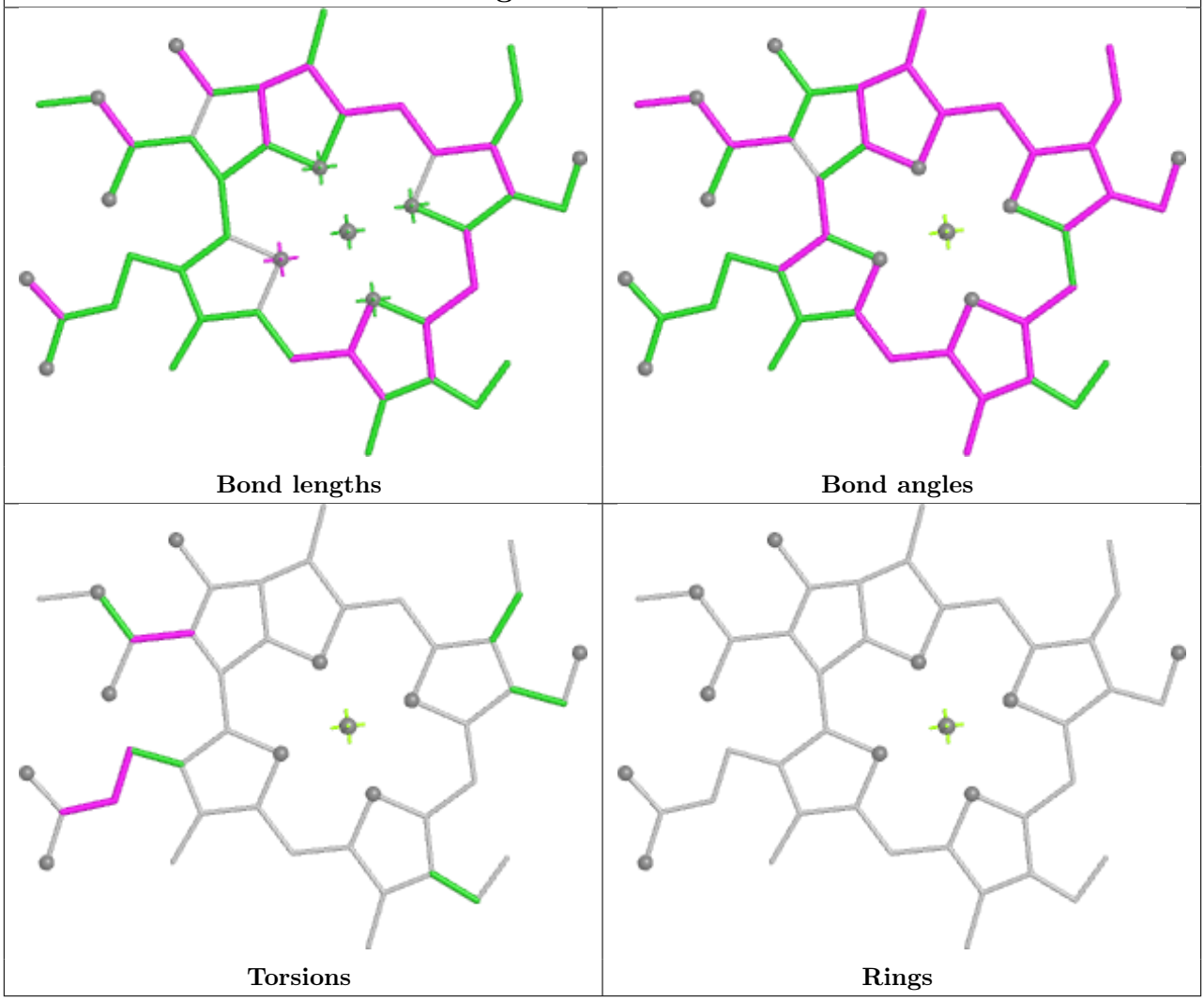


Rings

Ligand CHL 7 608



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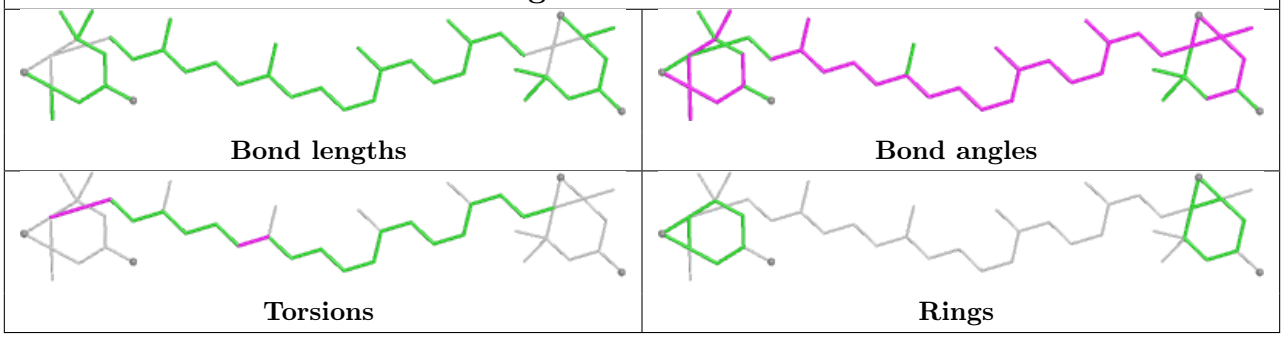

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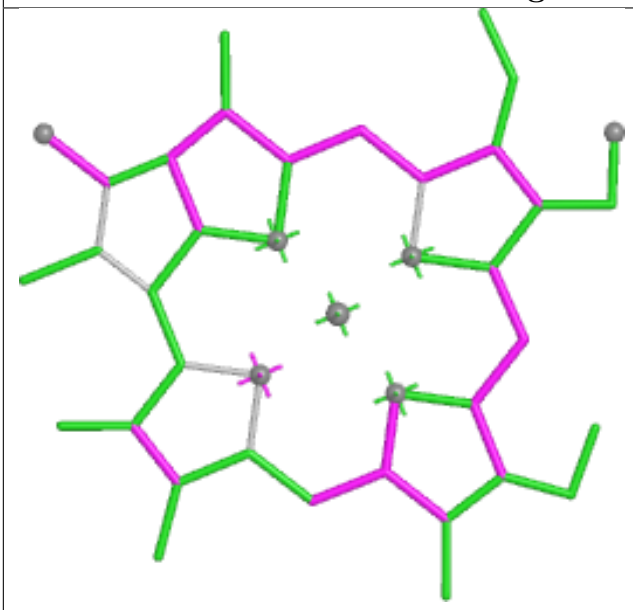
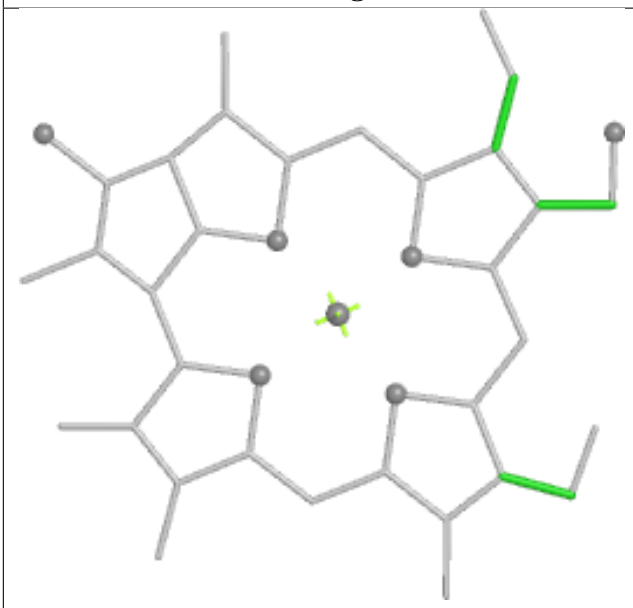


Bond lengths

Bond angles



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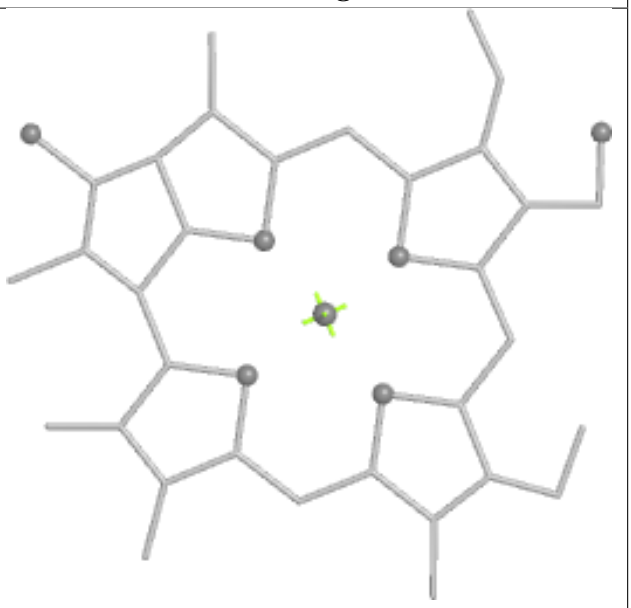
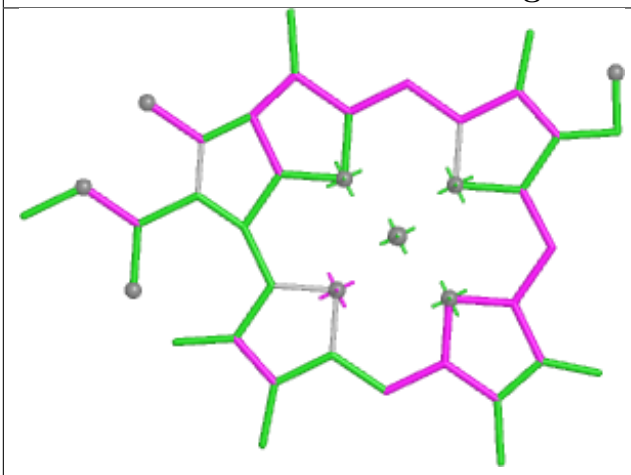


Rings

Ligand CHL V 607



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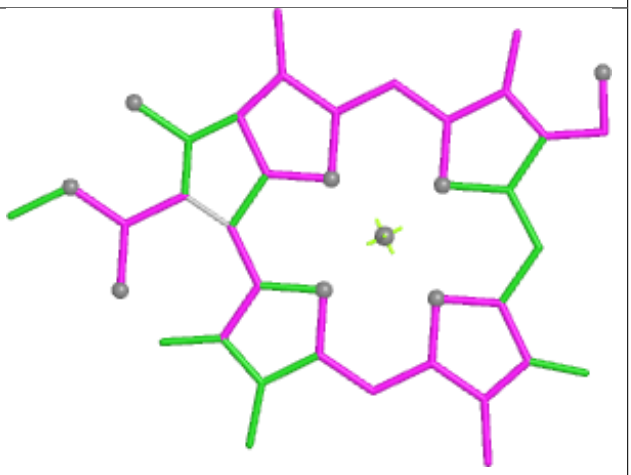
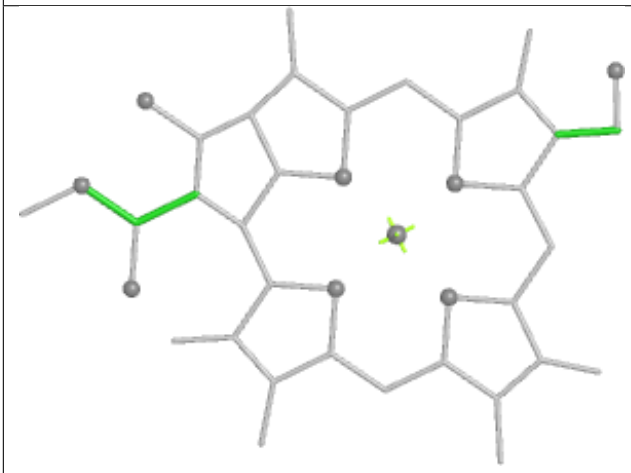


Bond angles



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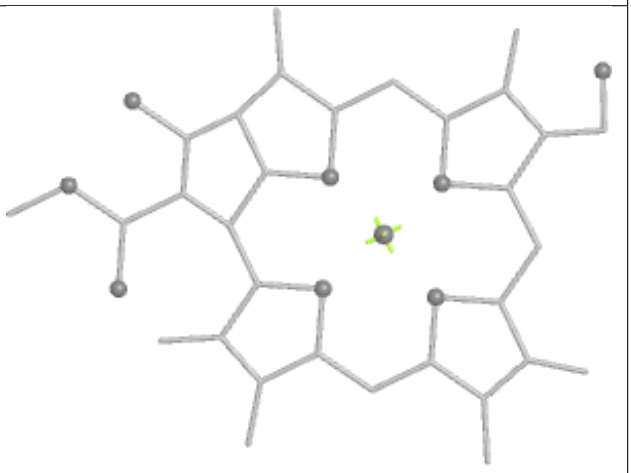
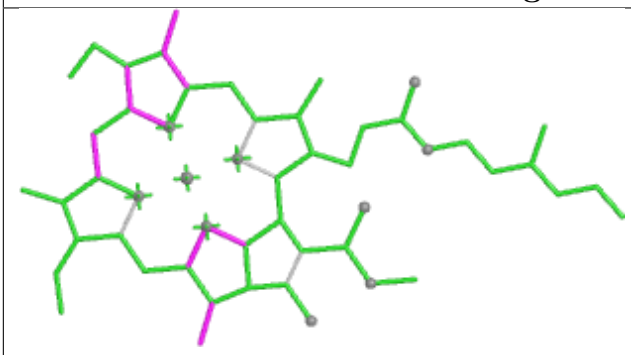
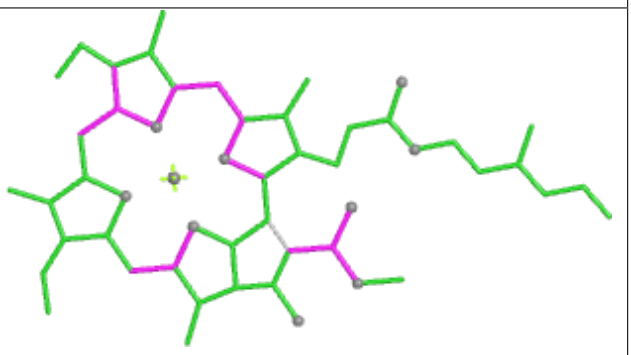
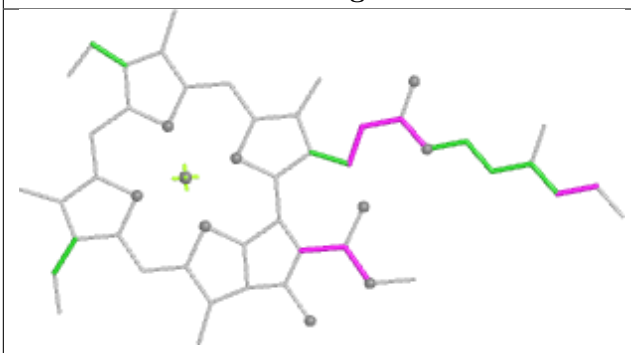
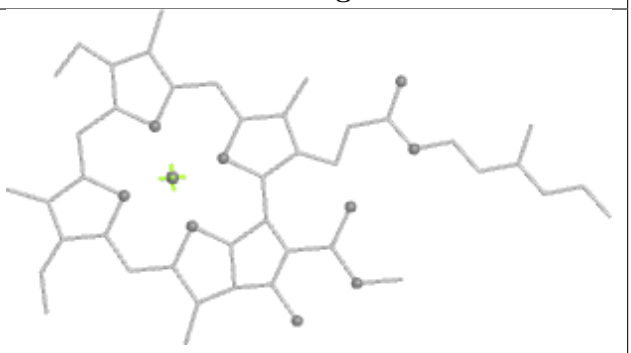
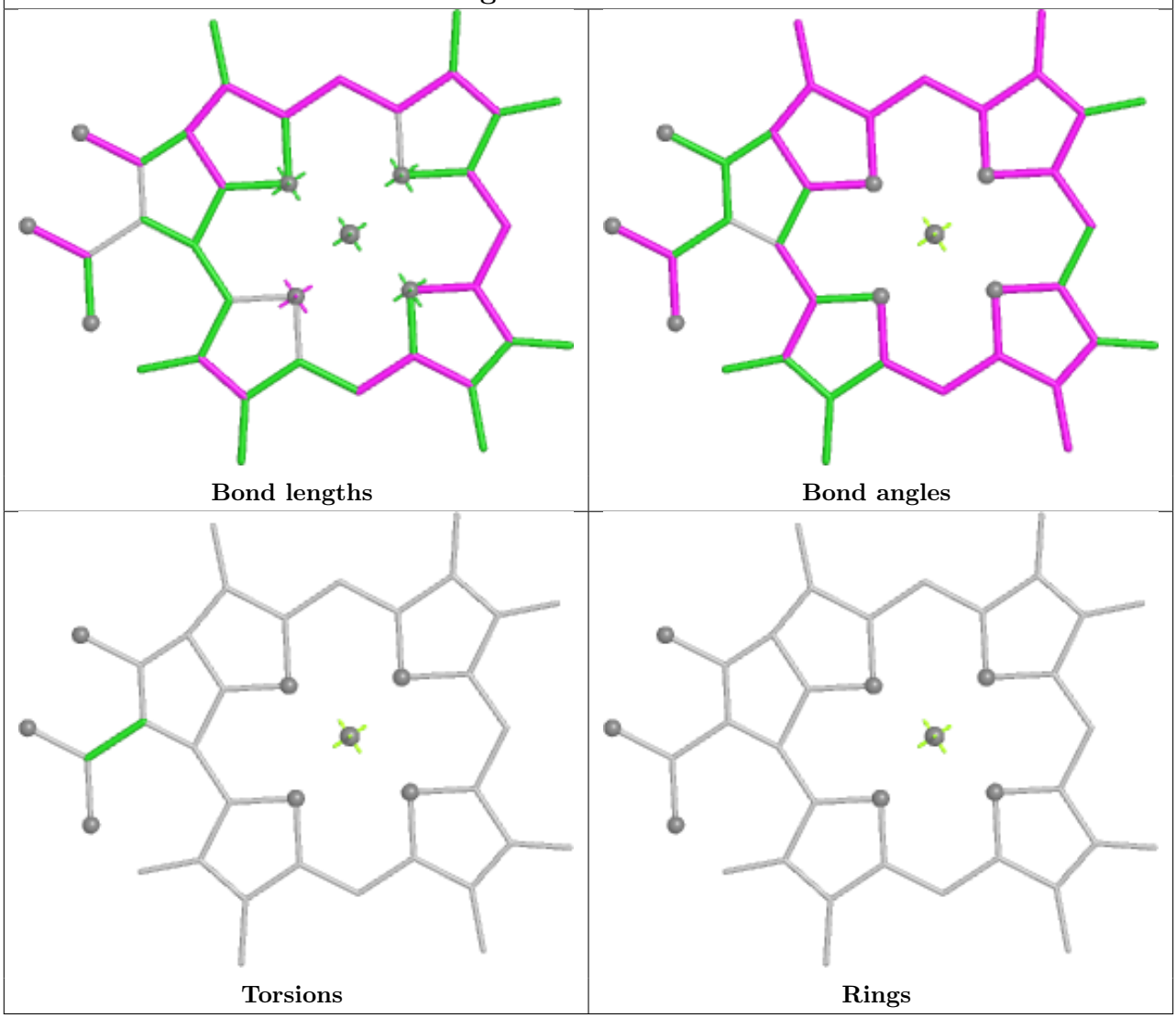


Rings

Ligand CLA U 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL U 605



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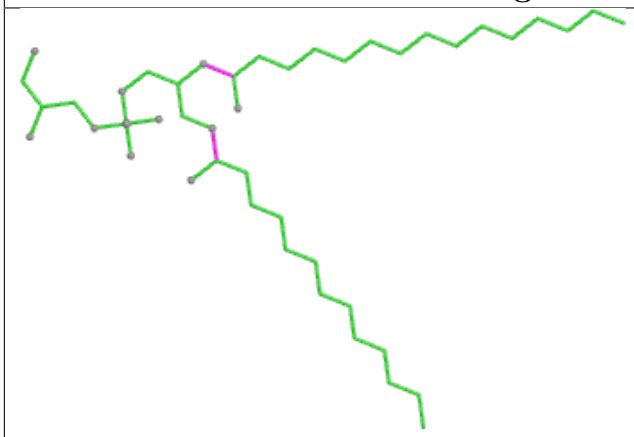
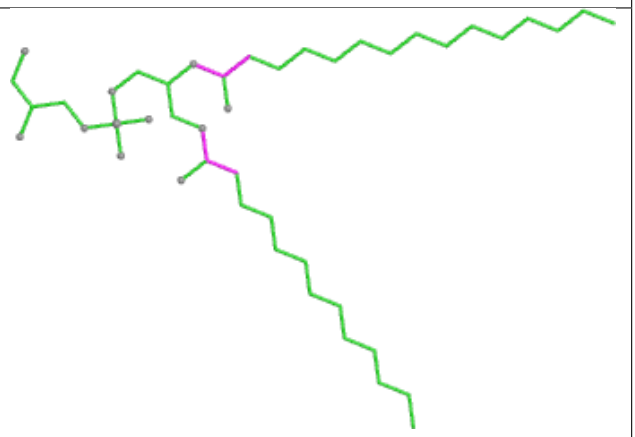
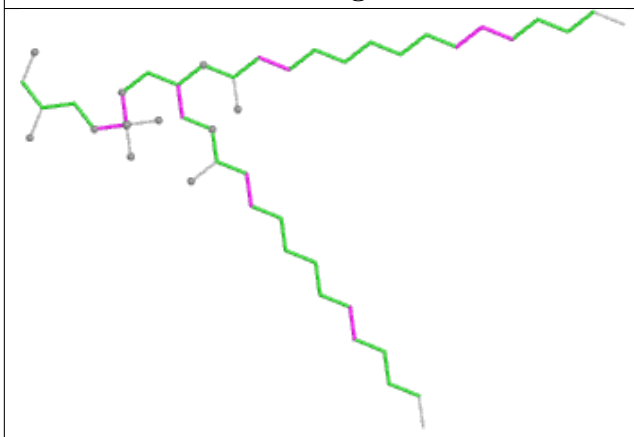
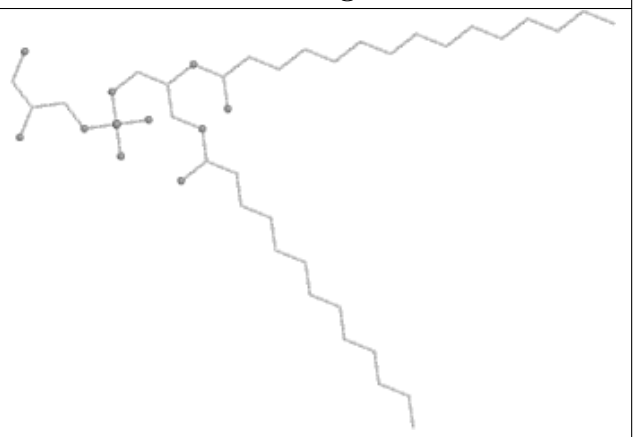
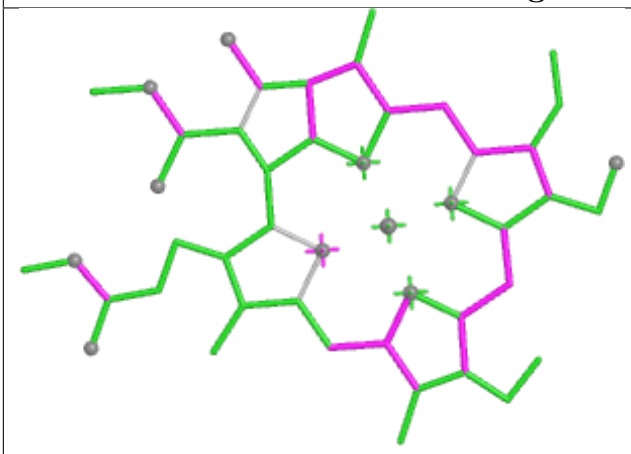
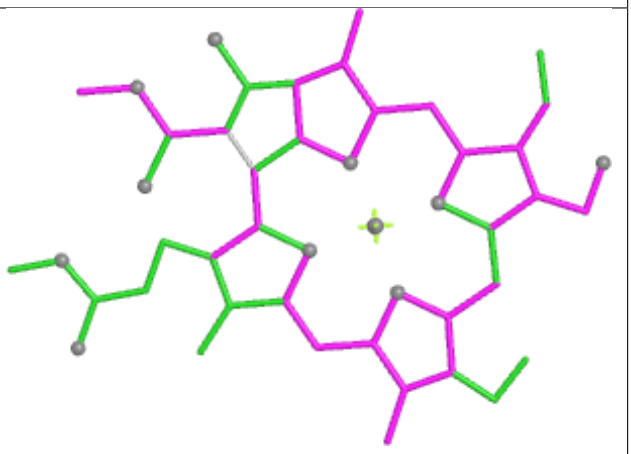
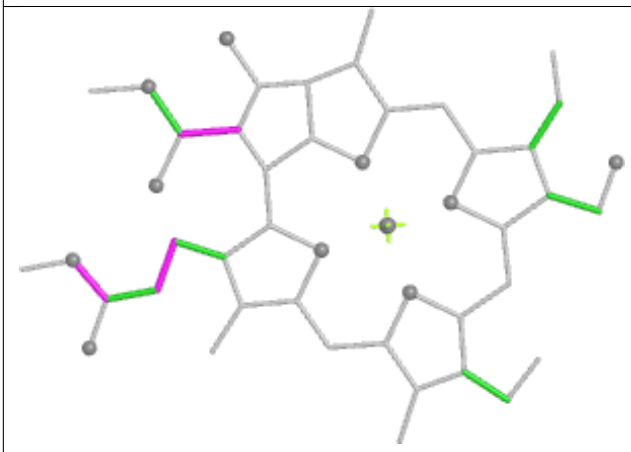
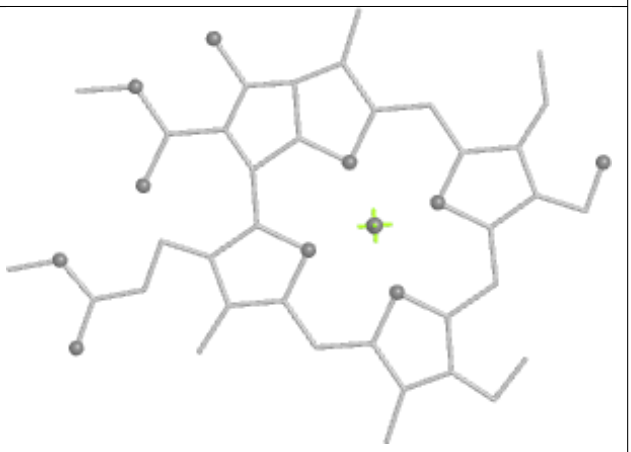
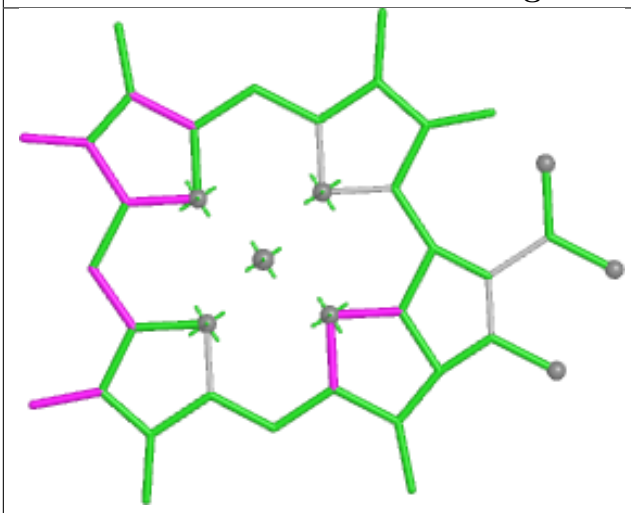
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CHL 4 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 612



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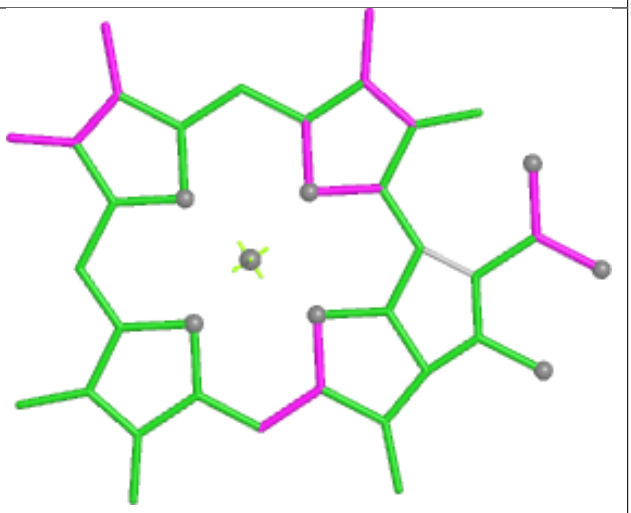

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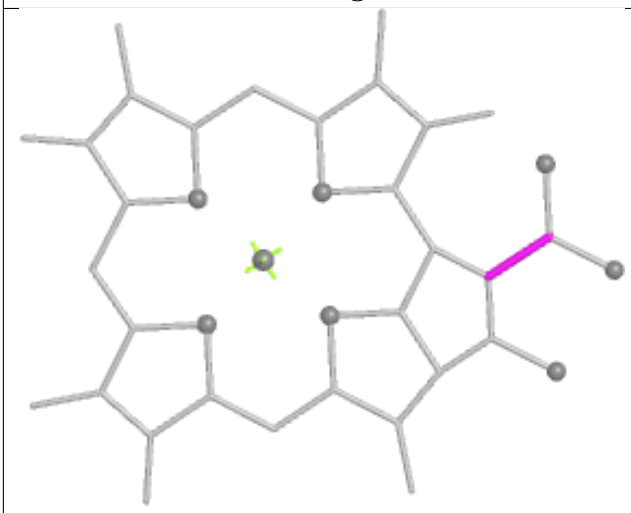

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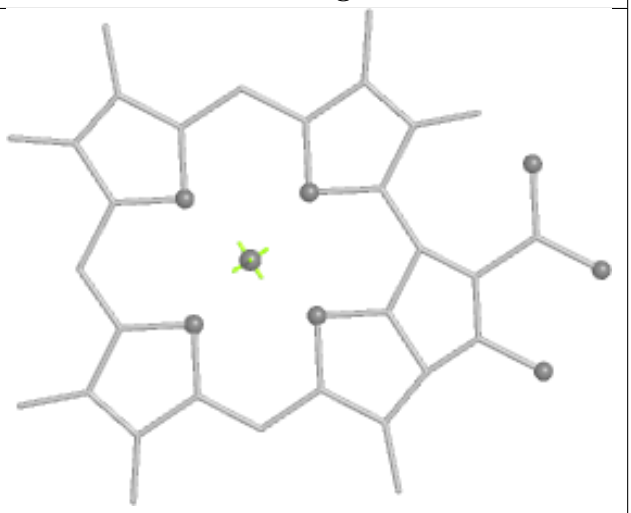
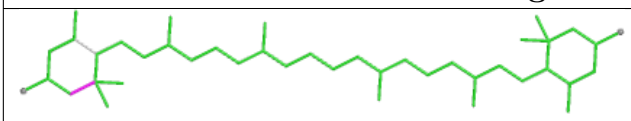


Rings

Ligand LUT 3 618



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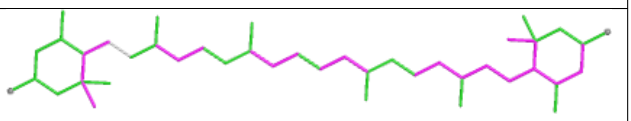

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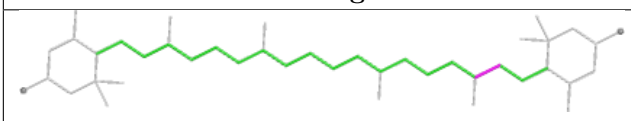

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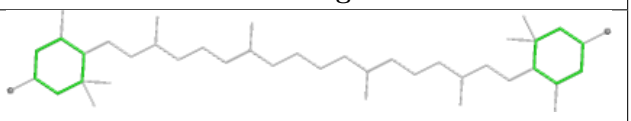
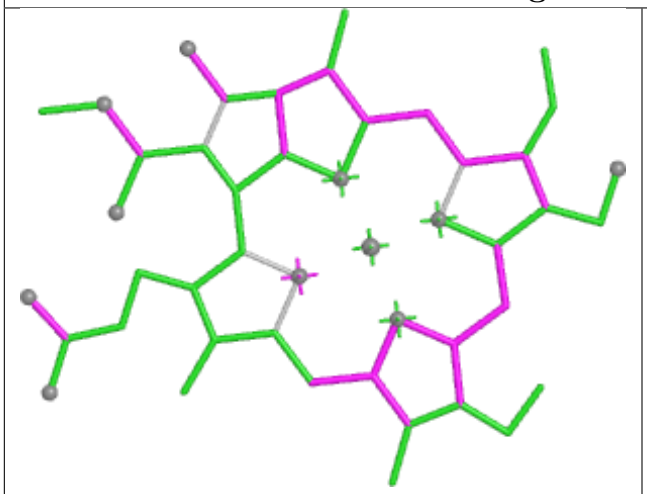


Rings

Ligand CHL 4 608



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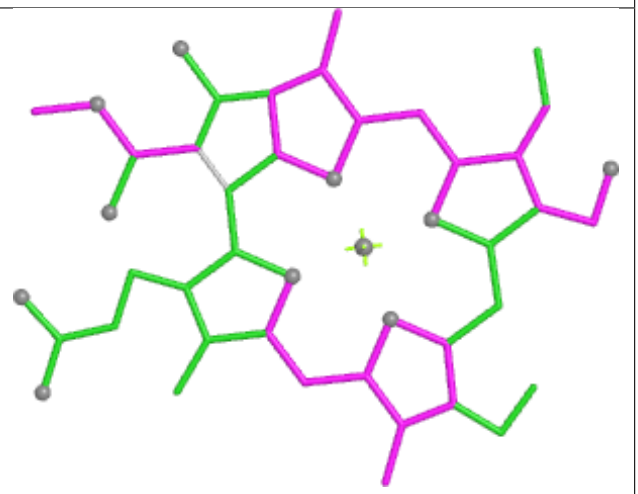

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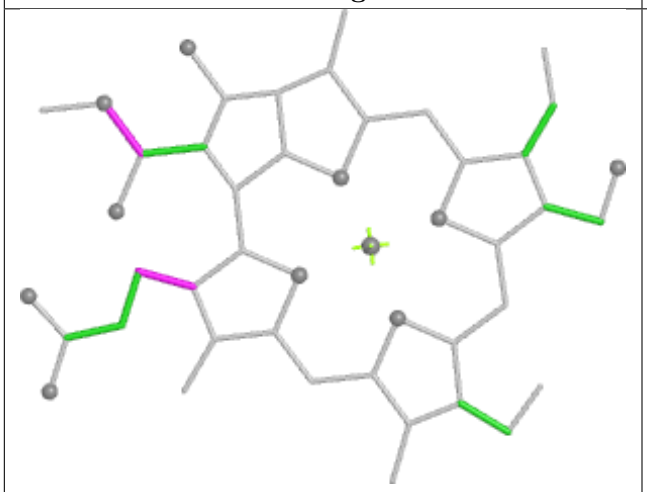

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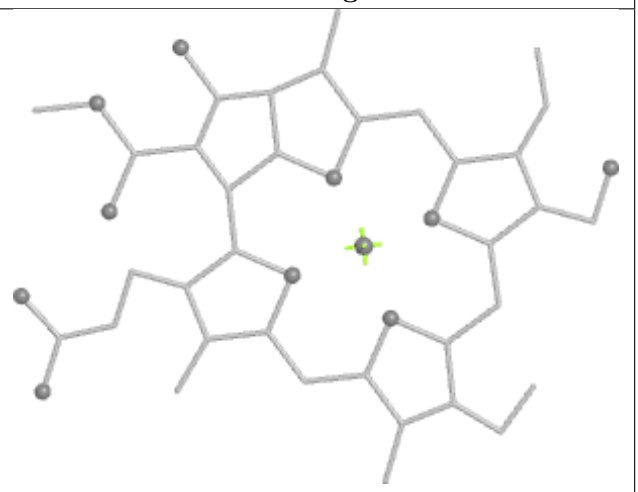
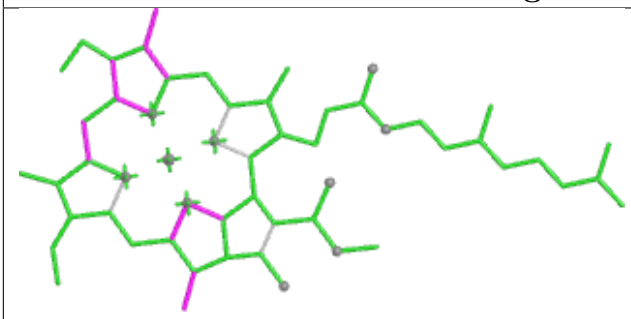
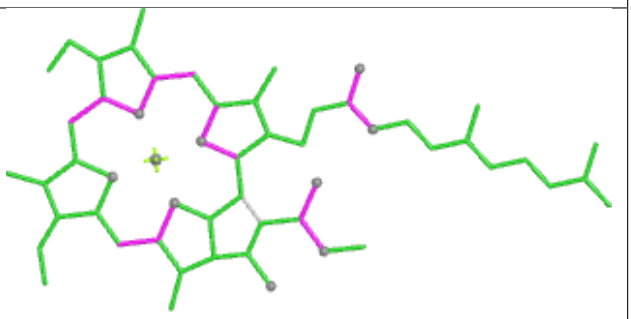
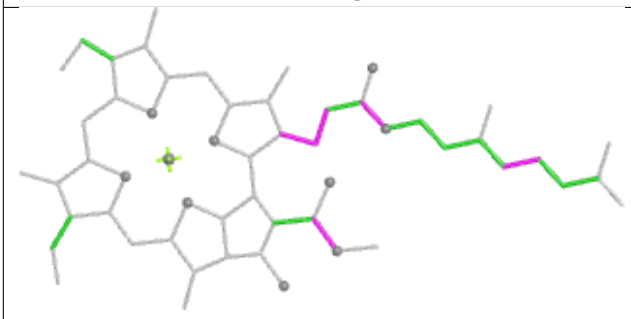
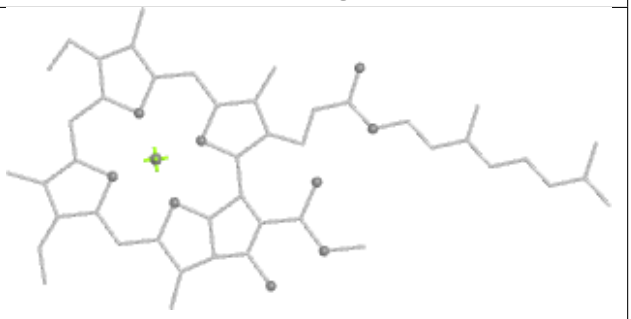


Rings

Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

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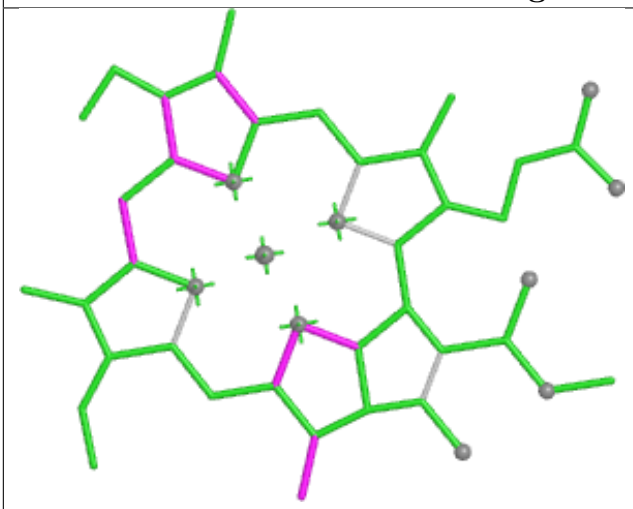

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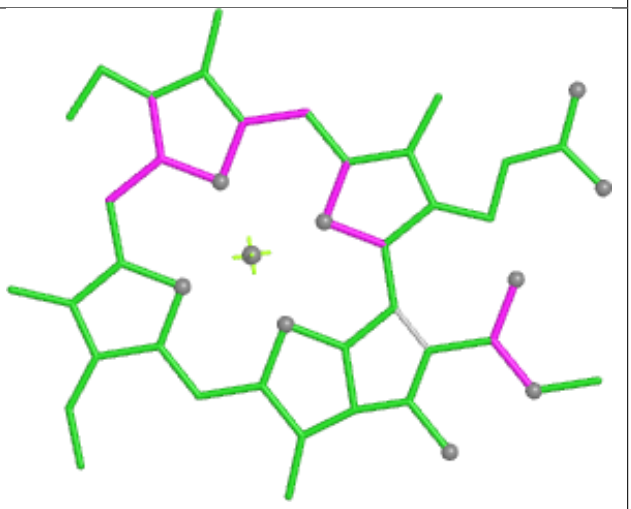
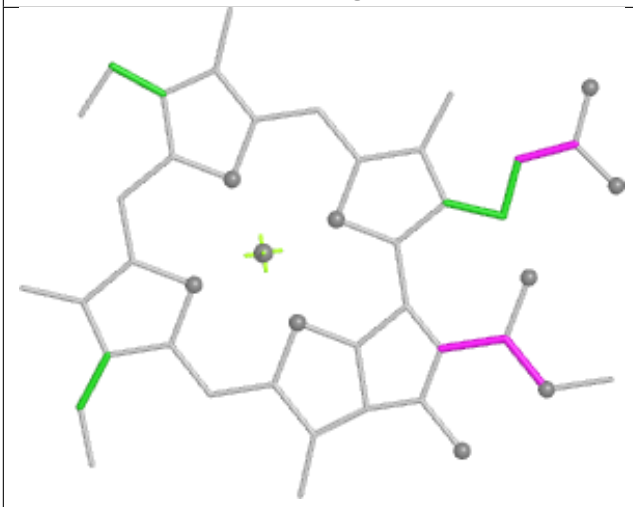


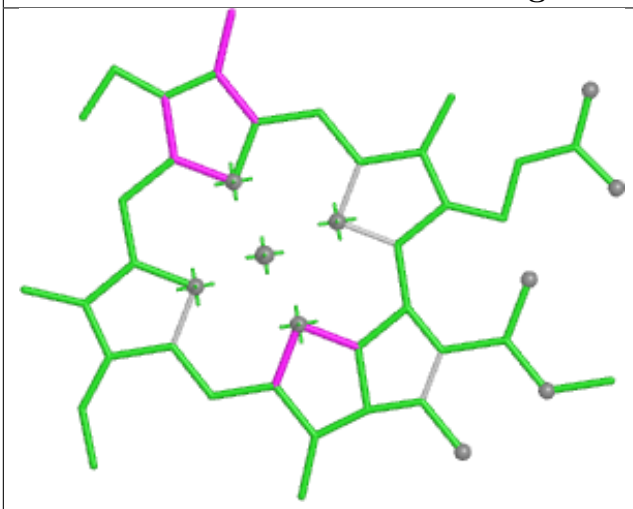
Bond angles



Torsions

Rings

Ligand CLA 5 603



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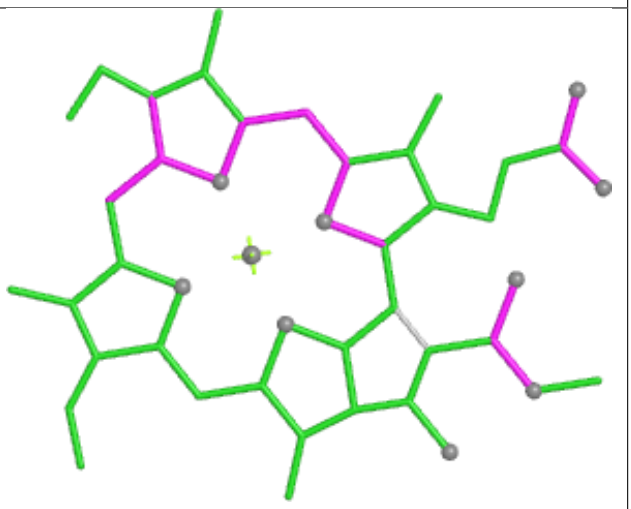

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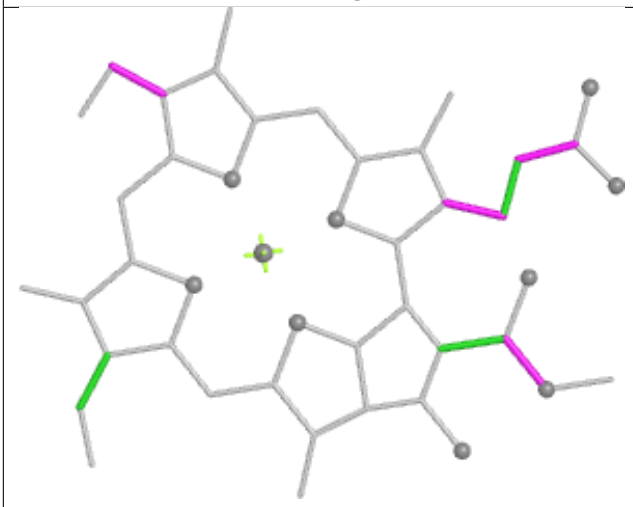

Torsions

Rings

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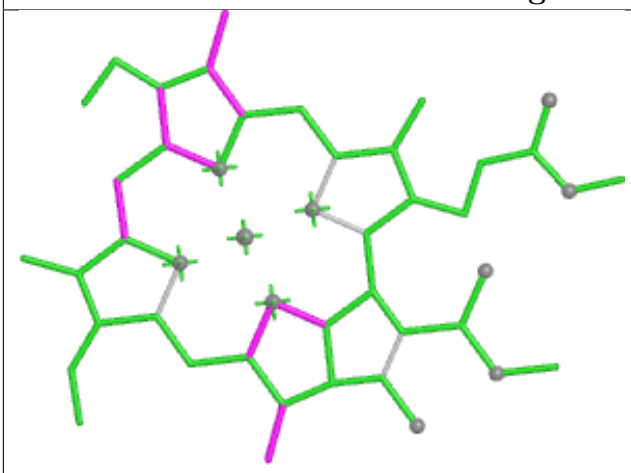

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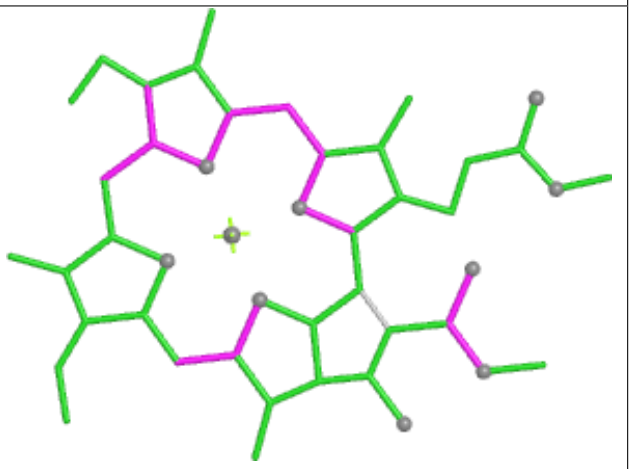

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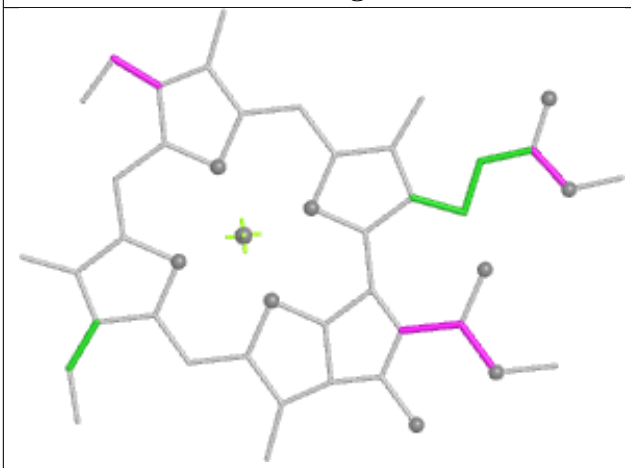

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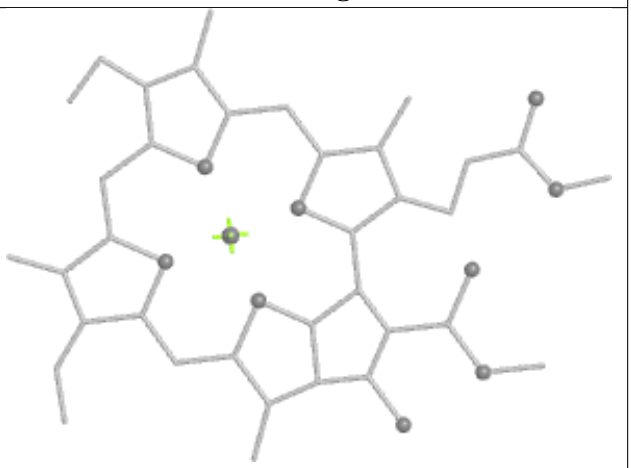
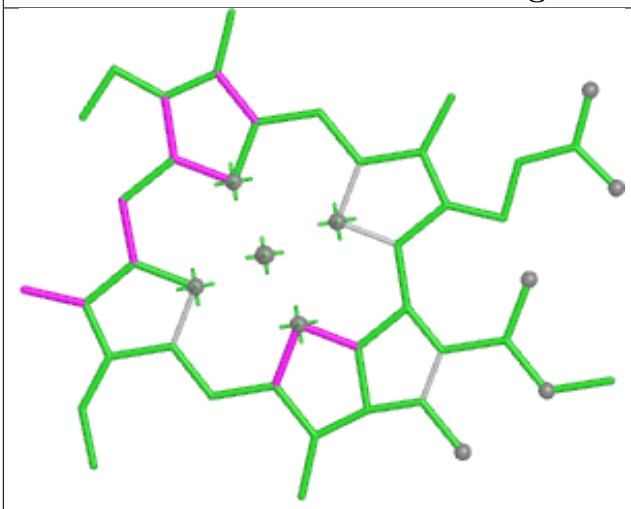


Rings

Ligand CLA 7 612



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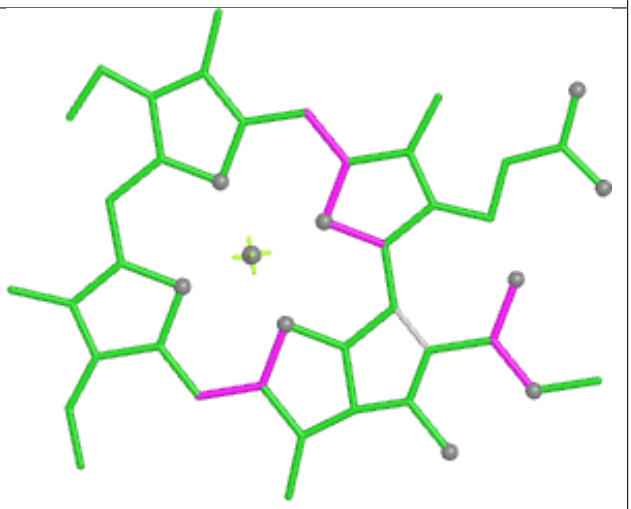

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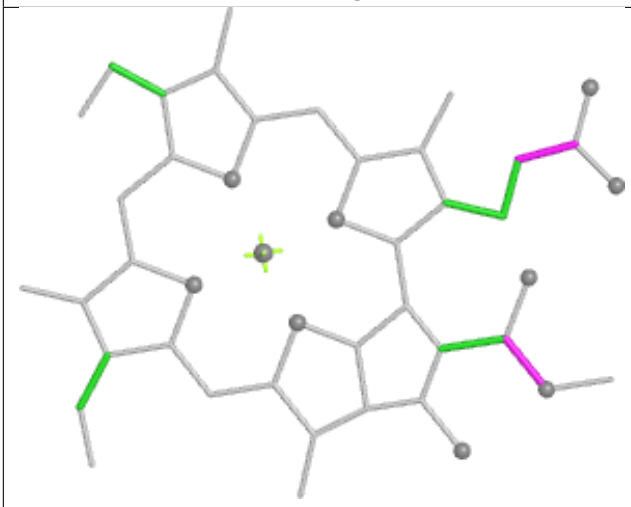

Torsions

Rings

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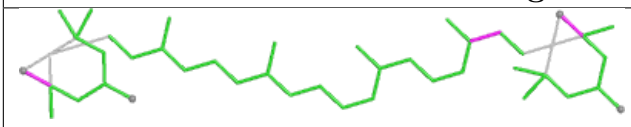

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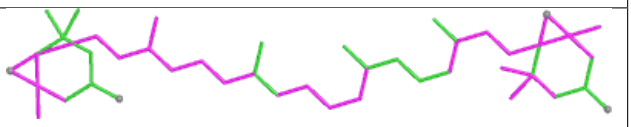

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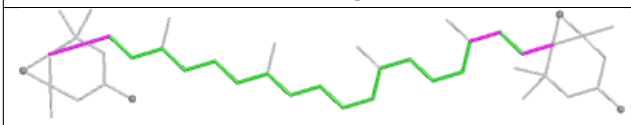

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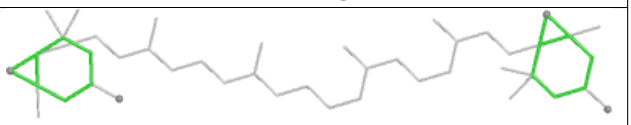
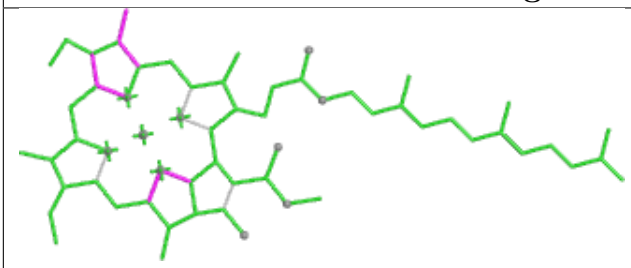


Rings

Ligand CLA V 603



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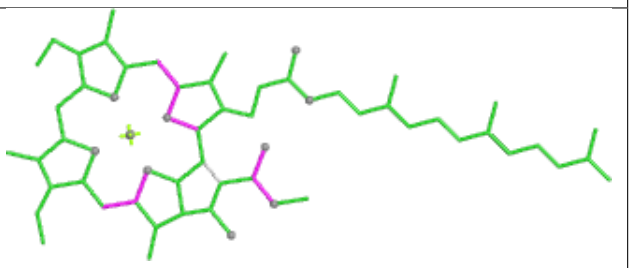

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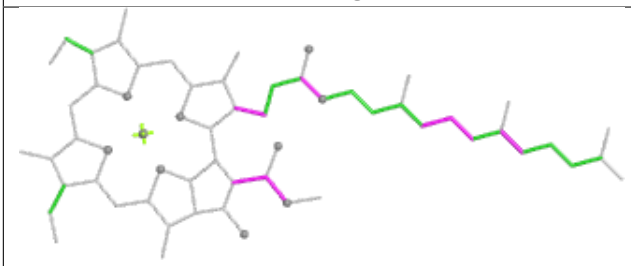

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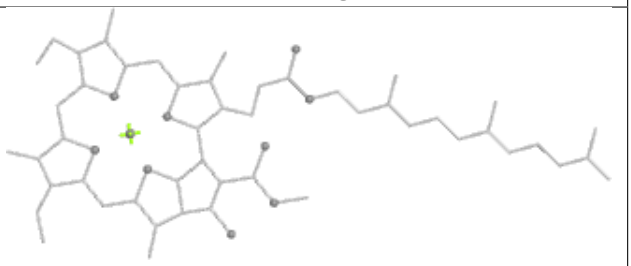
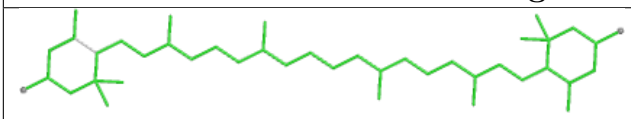


Rings

Ligand LUT 4 619



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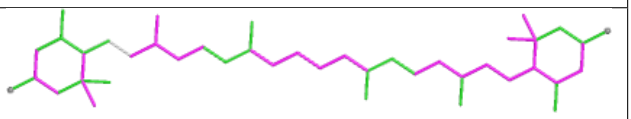

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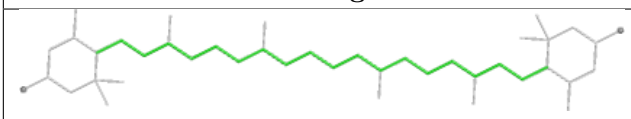

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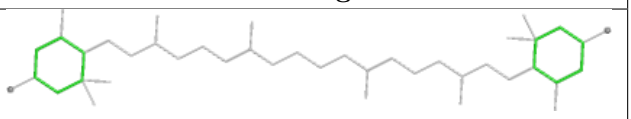
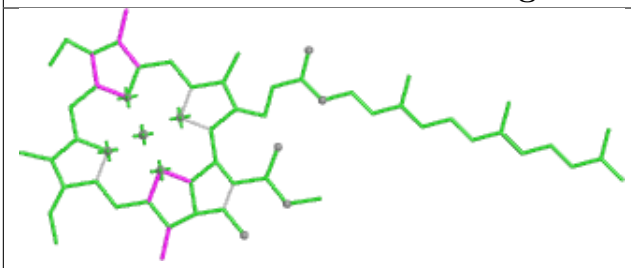


Rings

Ligand CLA W 613



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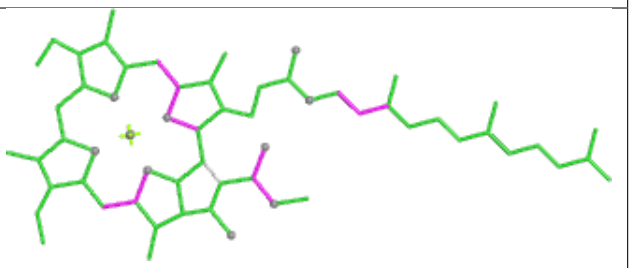

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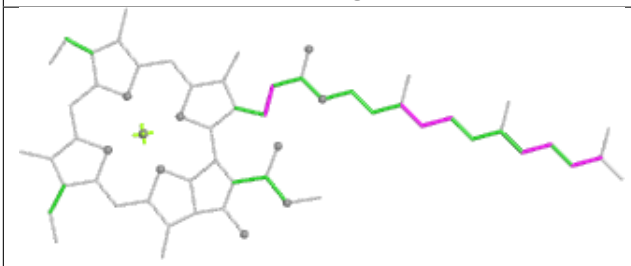

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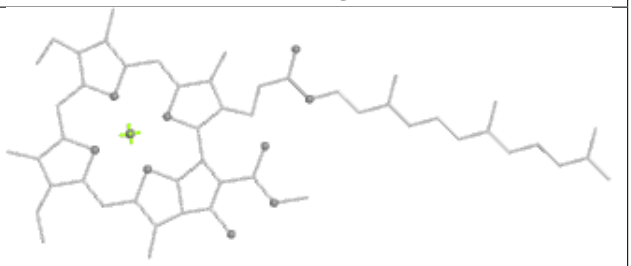
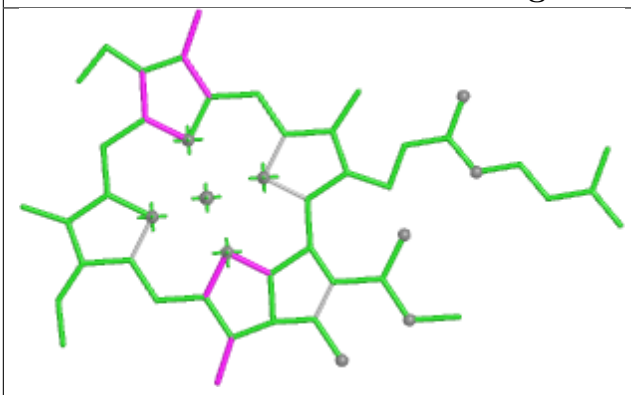
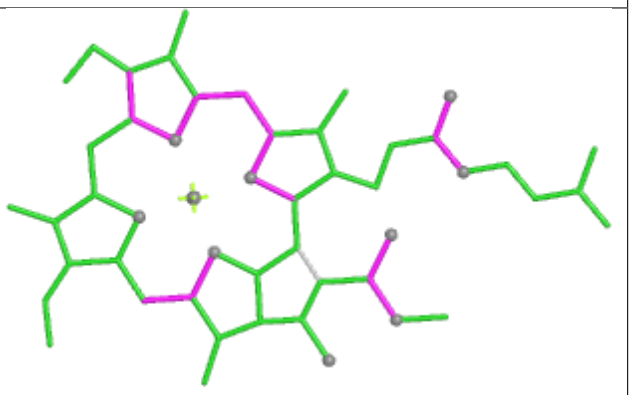
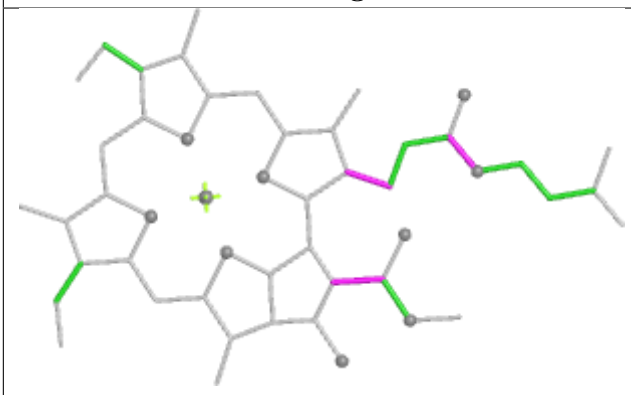
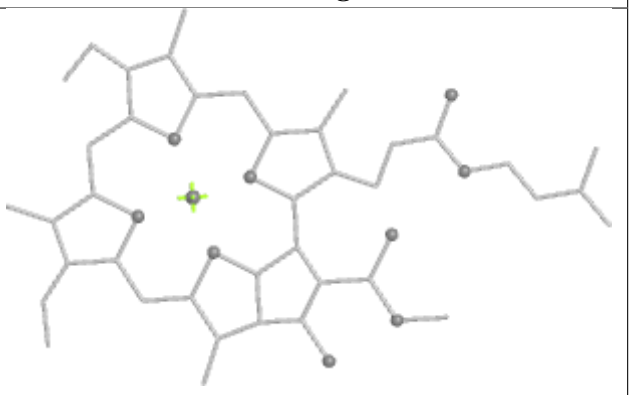


Rings

Ligand CLA 2 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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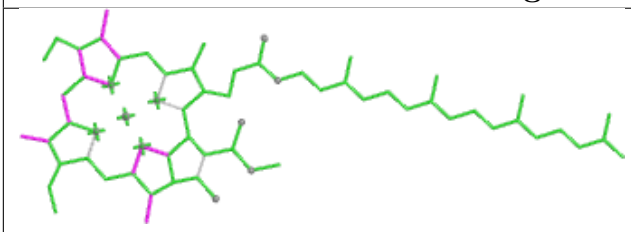
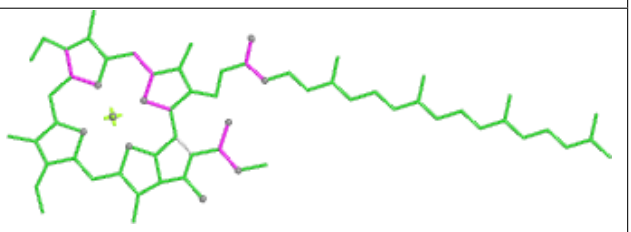
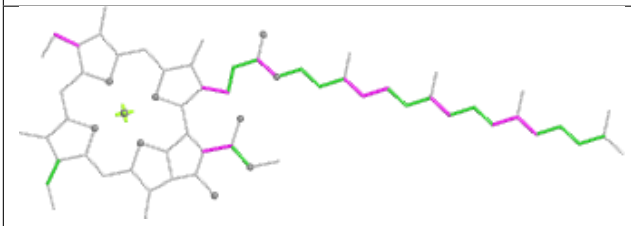
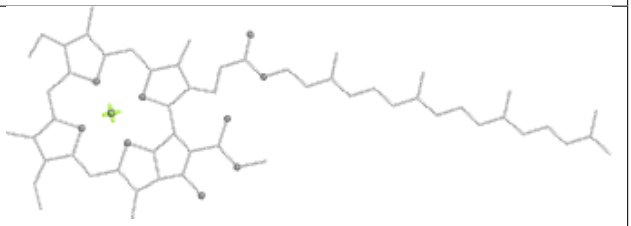
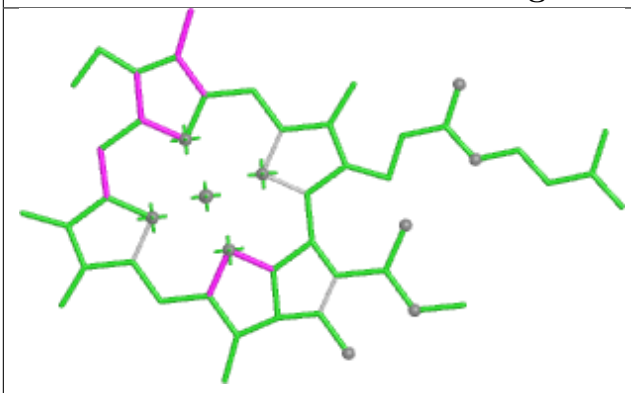
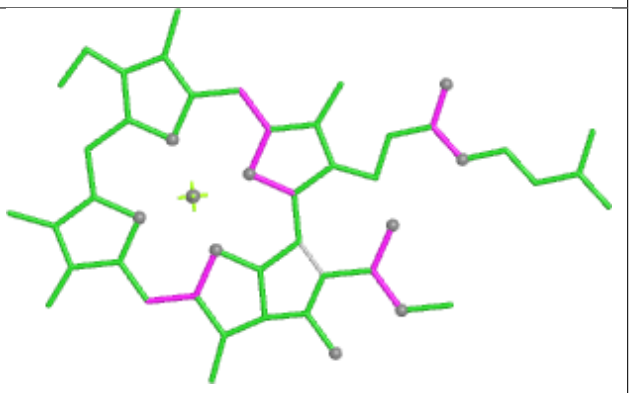
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 614



Bond lengths



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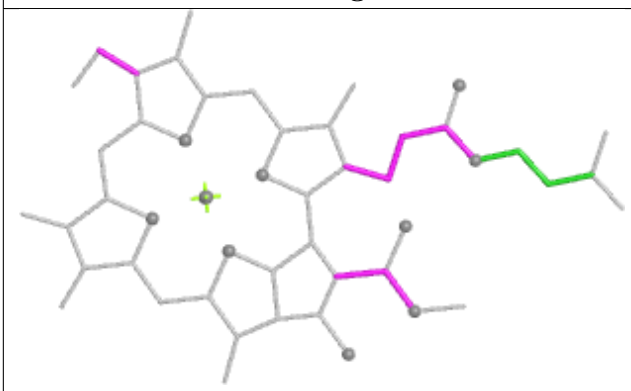

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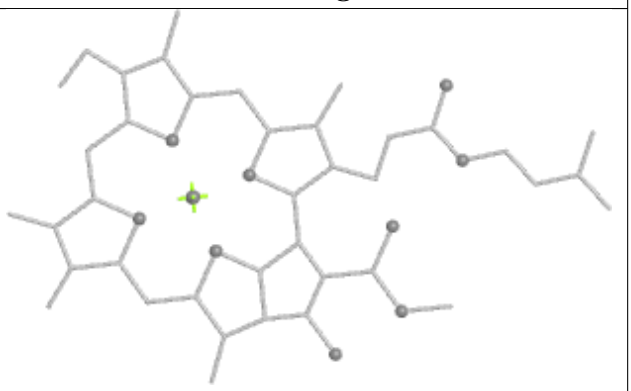
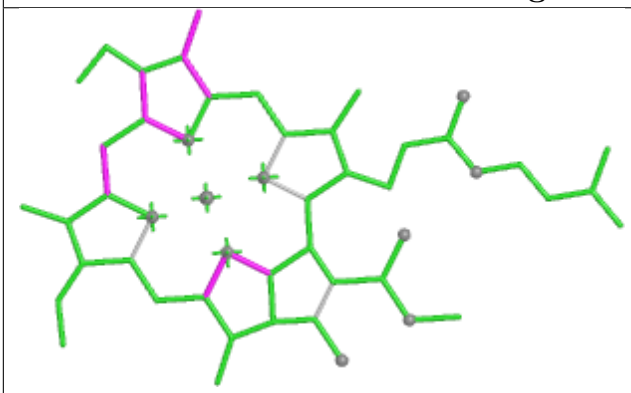


Rings

Ligand CLA 5 608



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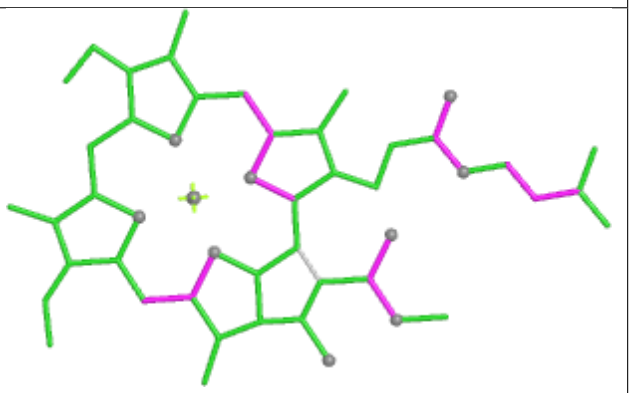

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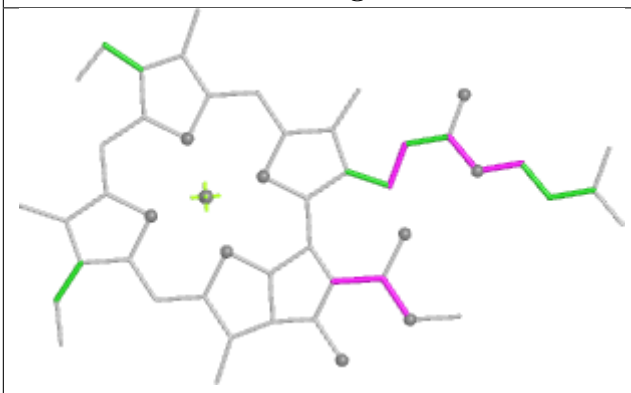

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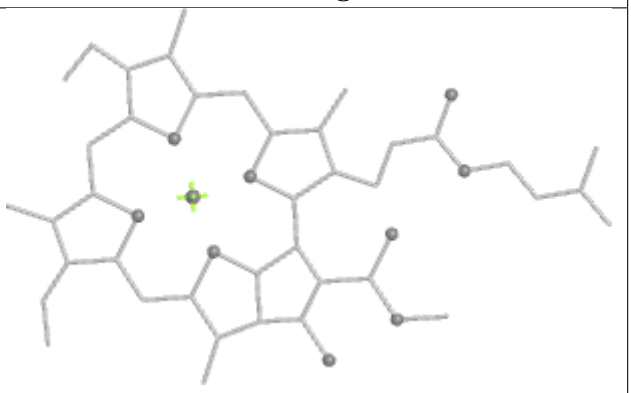
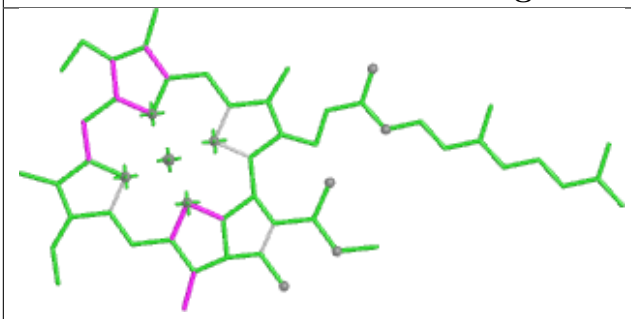


Rings

Ligand CLA O 2002



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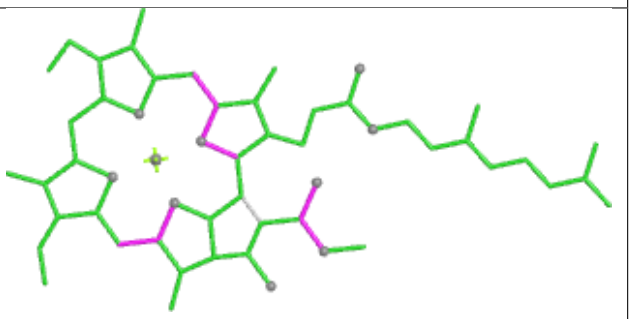

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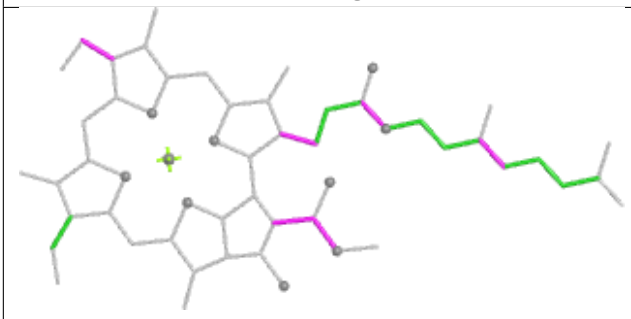

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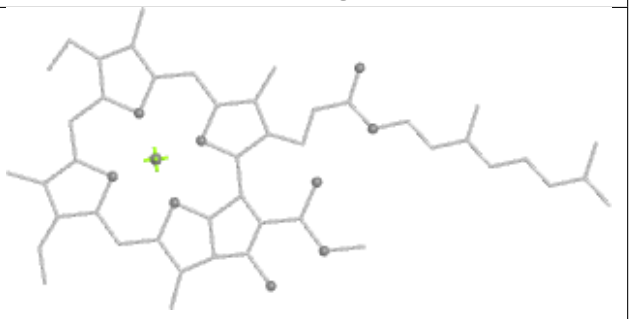
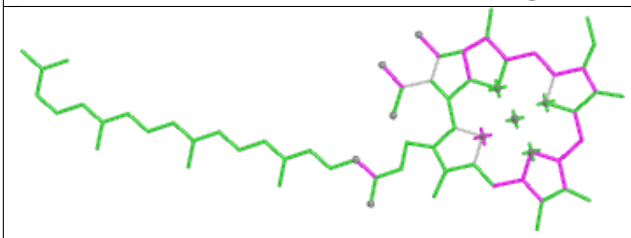


Rings

Ligand CHL V 601



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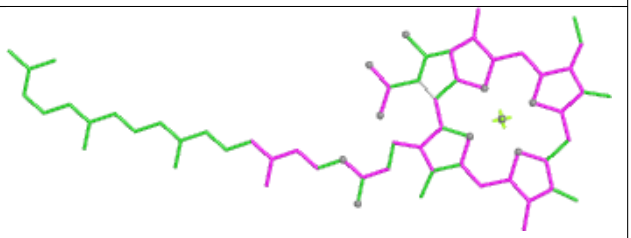

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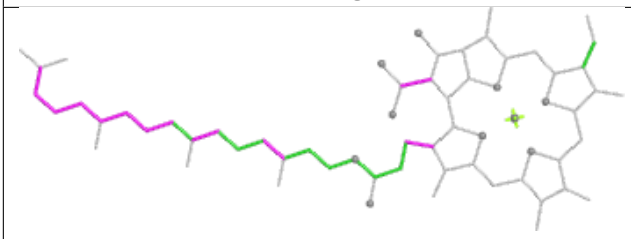

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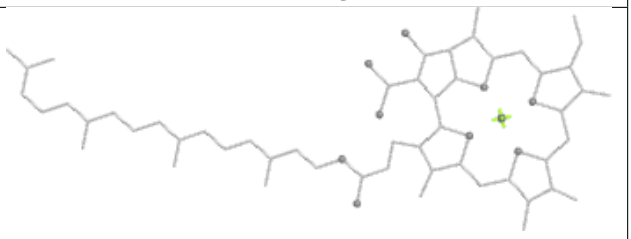
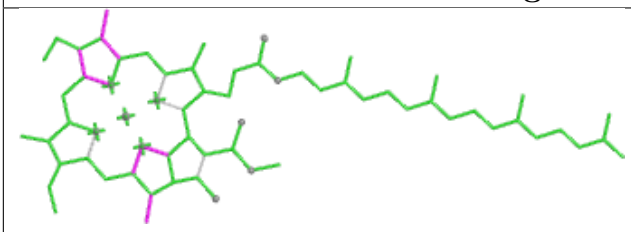


Rings

Ligand CLA A 826



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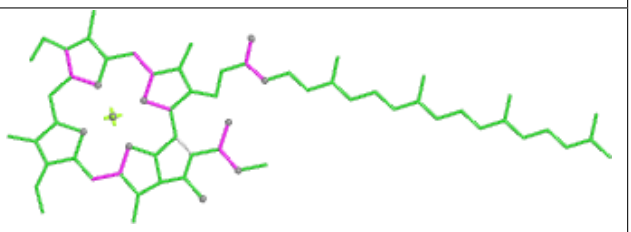

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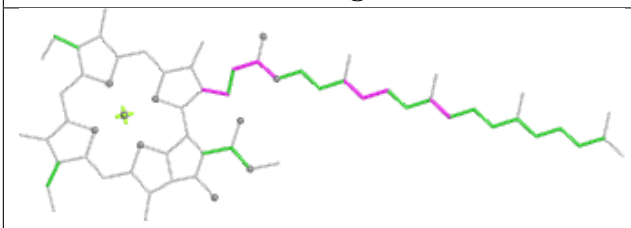

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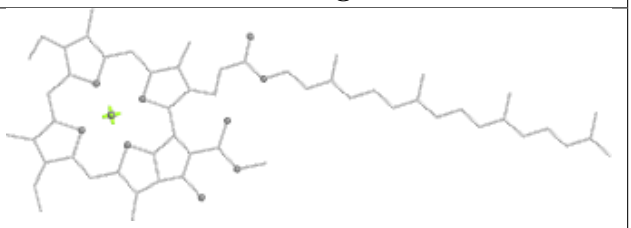
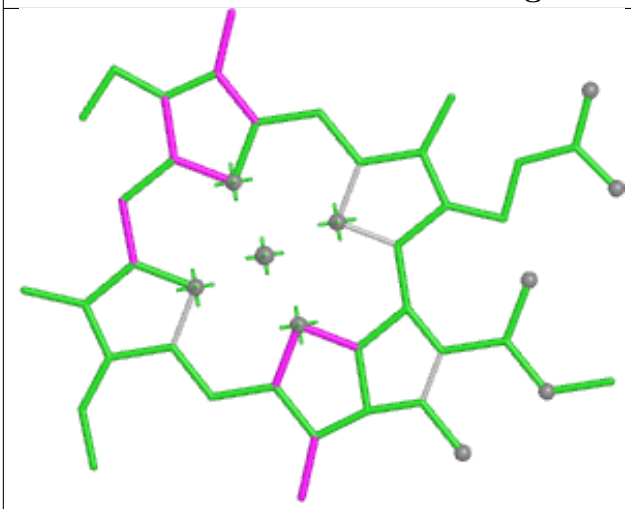


Rings

Ligand CLA B 815



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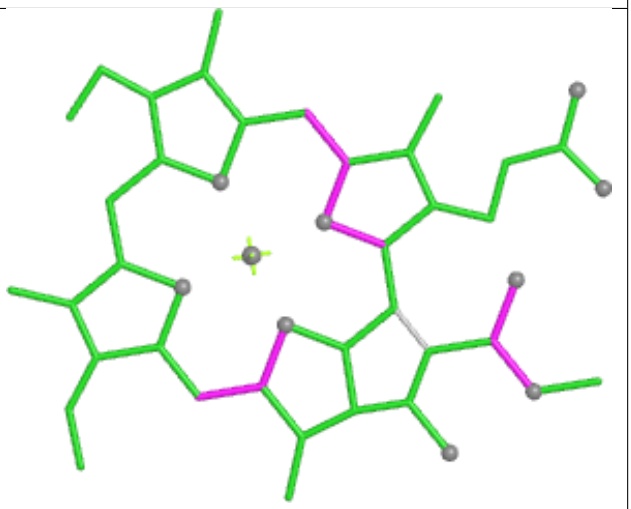

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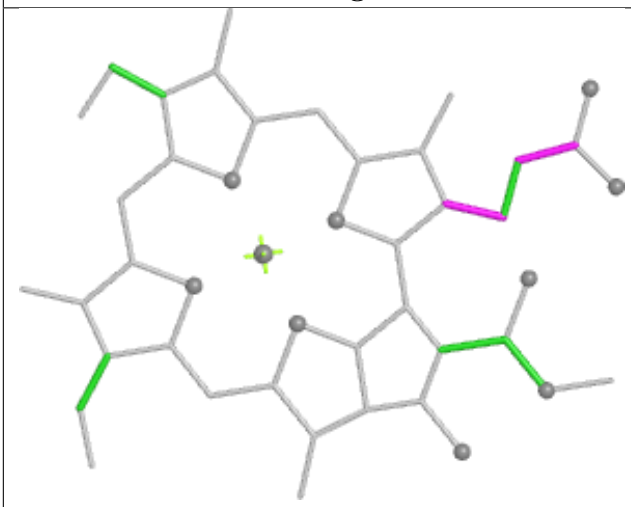

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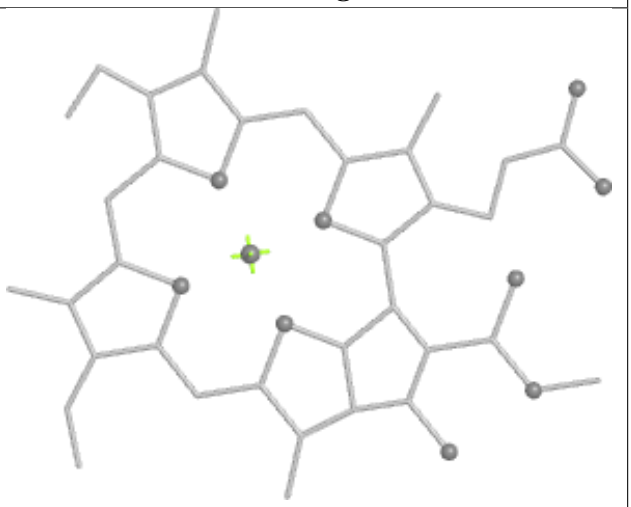
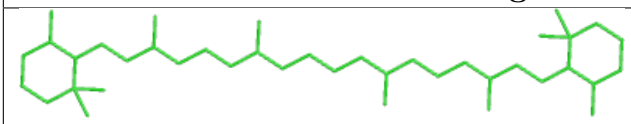
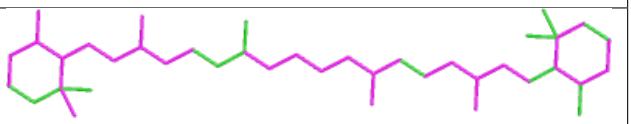
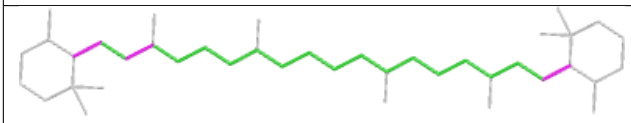
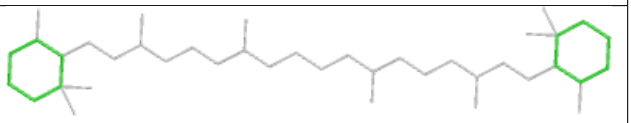


Rings

Ligand BCR M 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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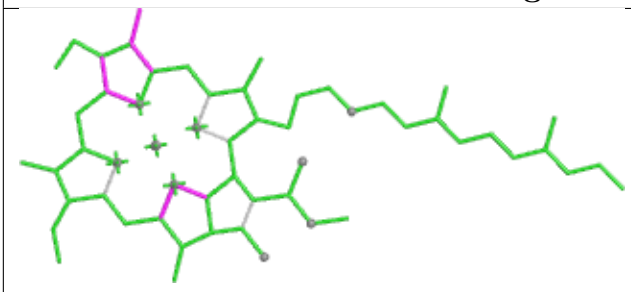
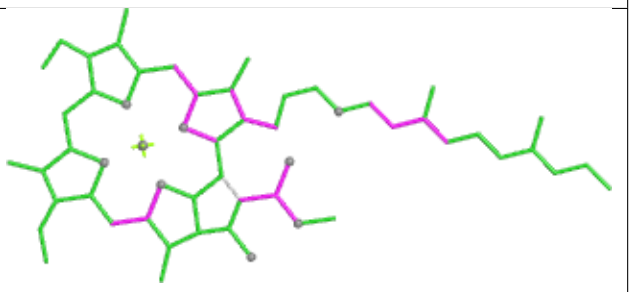
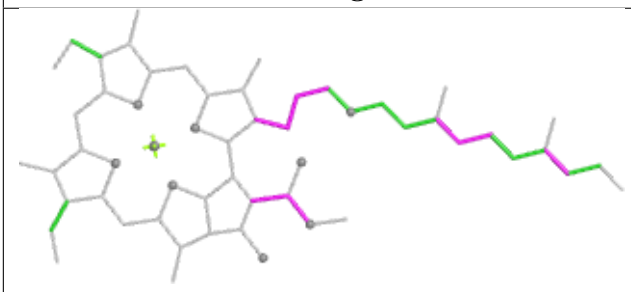
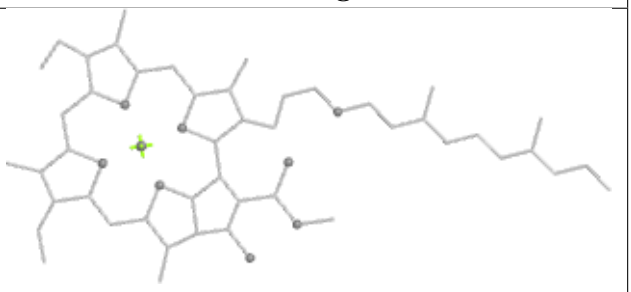
 Bond lengths	 Bond angles
 Torsions	 Rings

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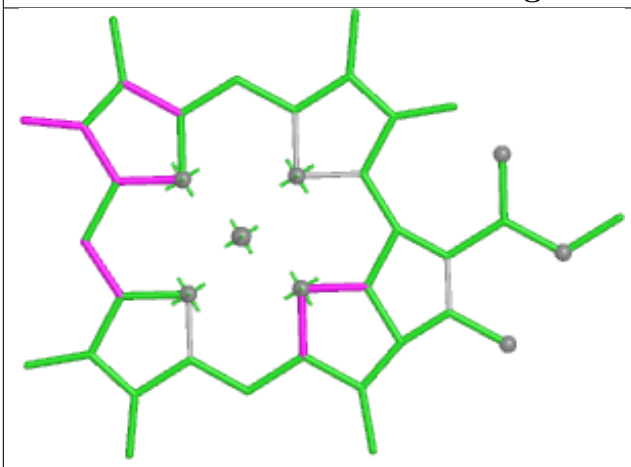
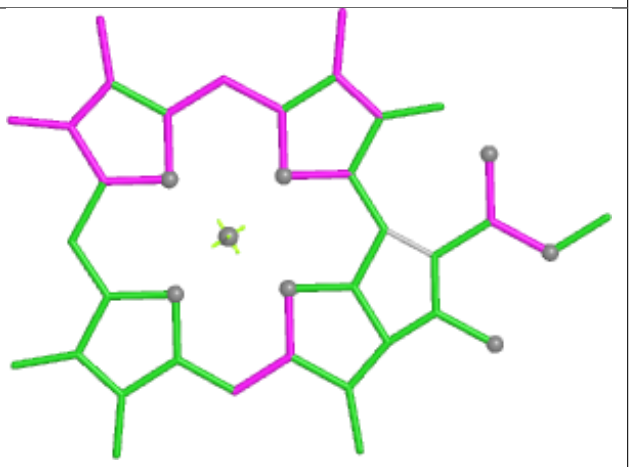
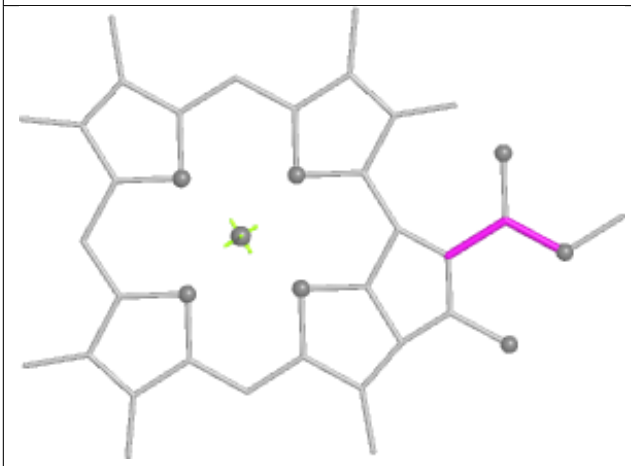
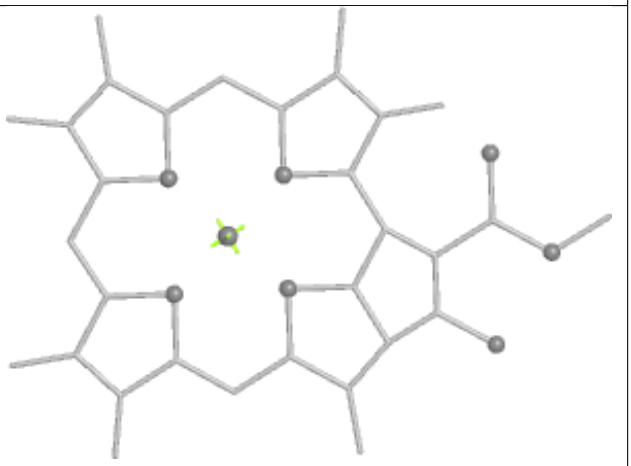
 Bond lengths	 Bond angles
 Torsions	 Rings

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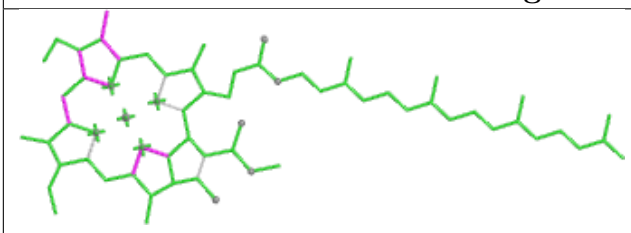
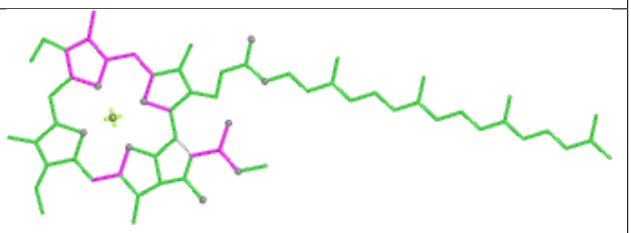
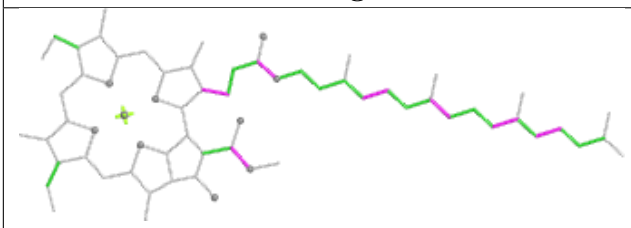
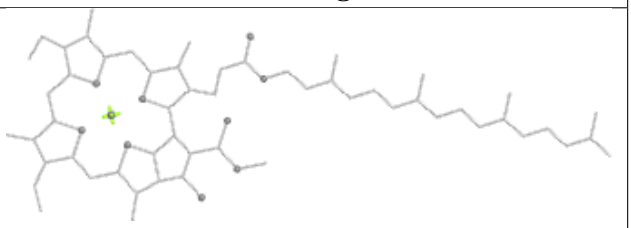
 Bond lengths	 Bond angles
 Torsions	 Rings

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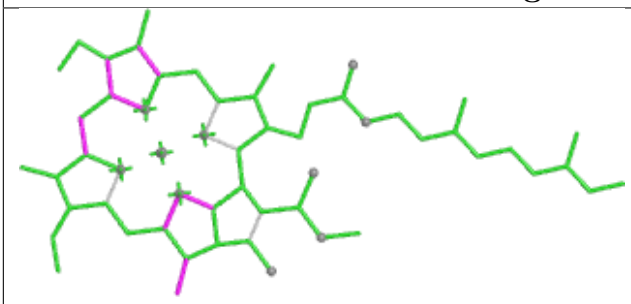
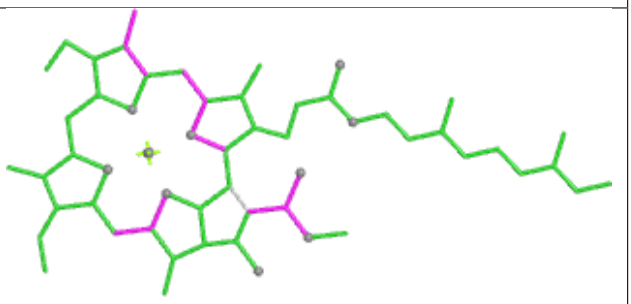
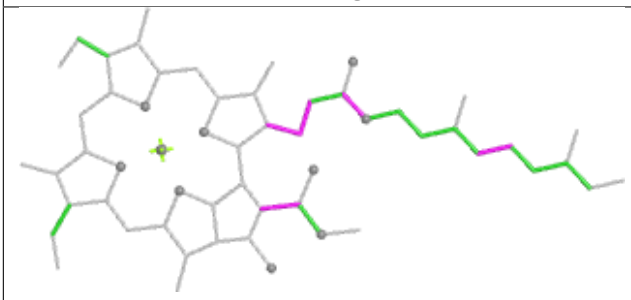
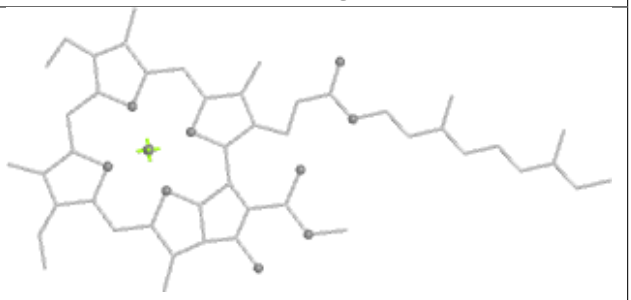
 Bond lengths	 Bond angles
 Torsions	 Rings

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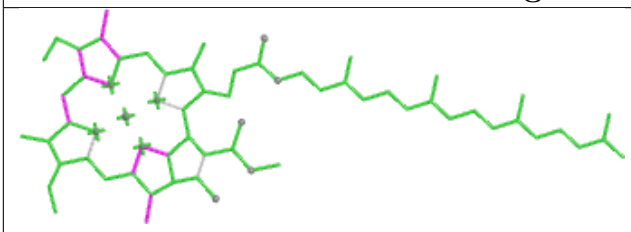
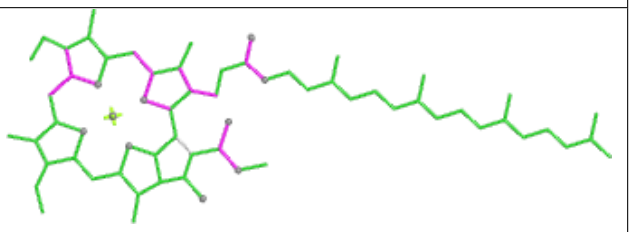
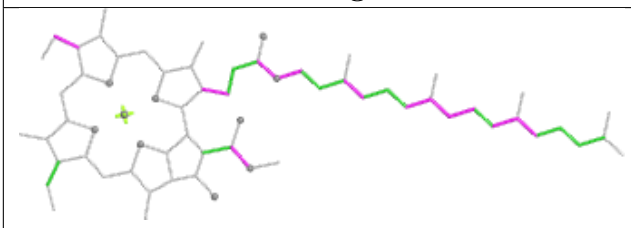
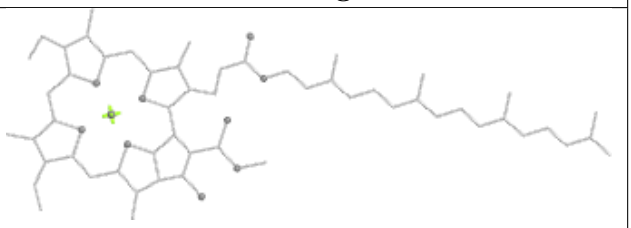
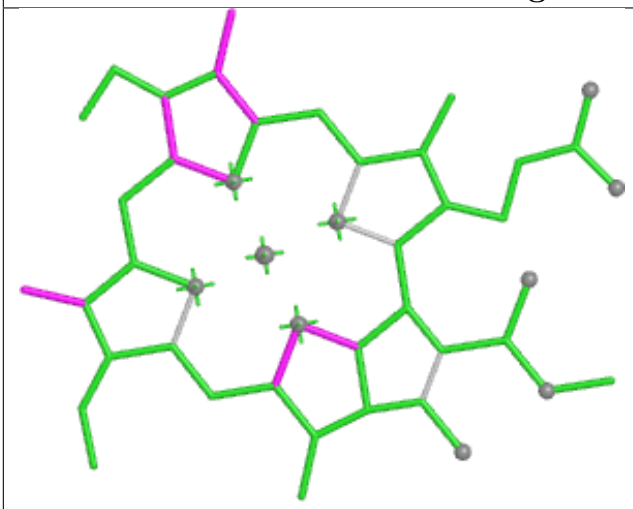
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 612



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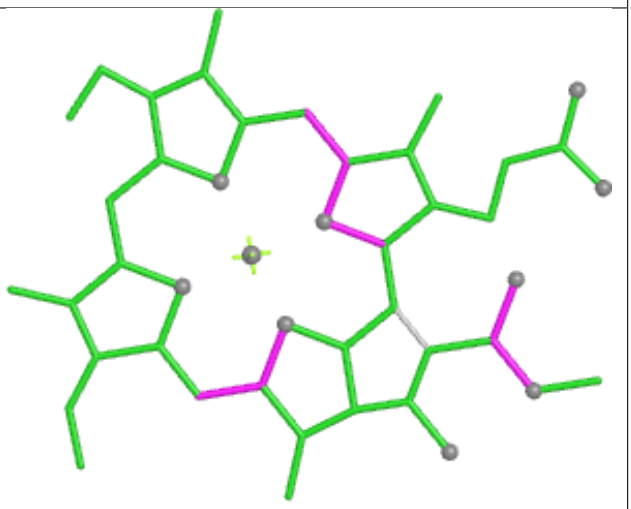
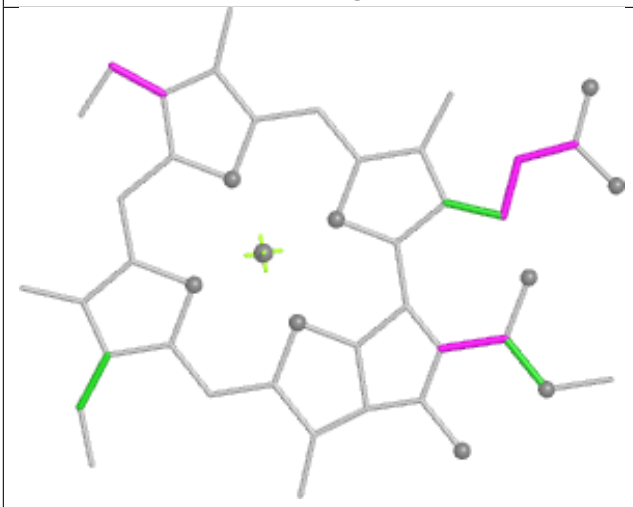


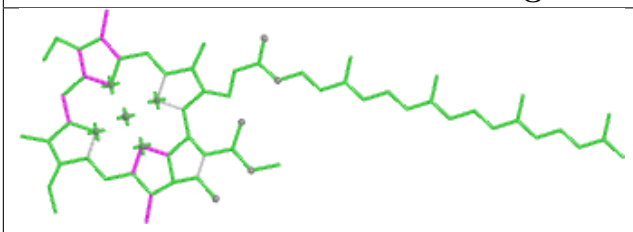
Bond angles



Torsions

Rings

Ligand CLA B 834



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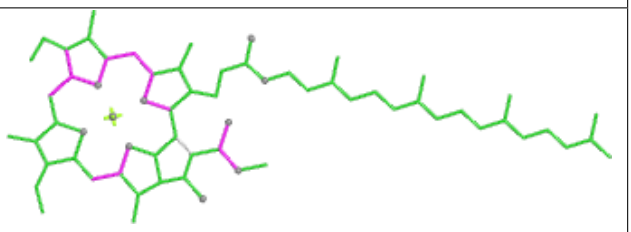
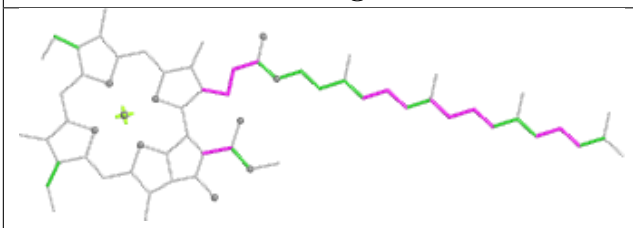


Bond angles



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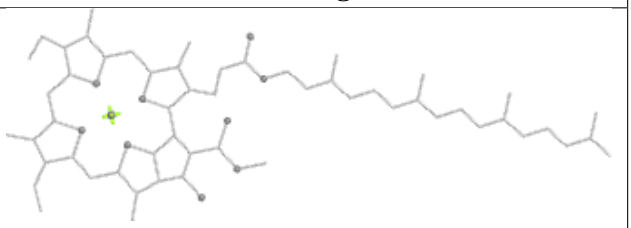

Rings

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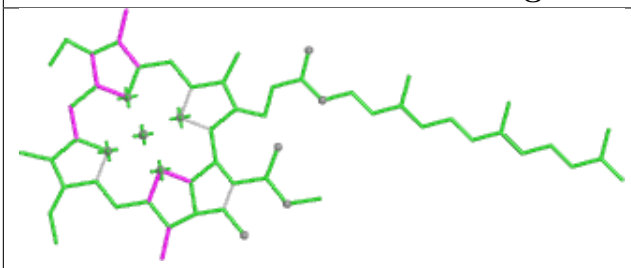
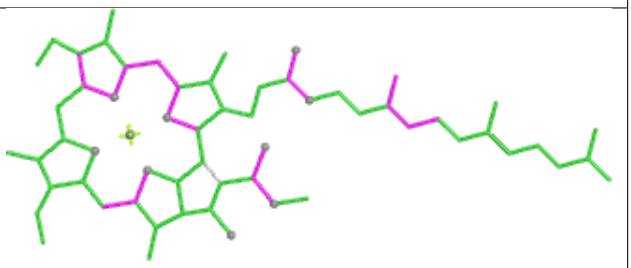
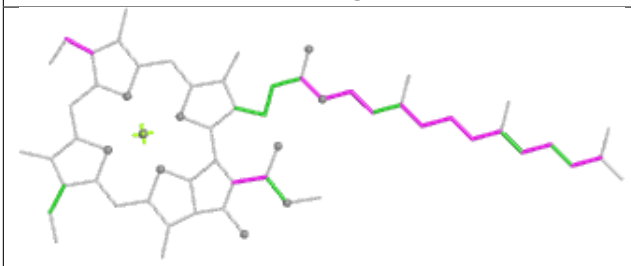
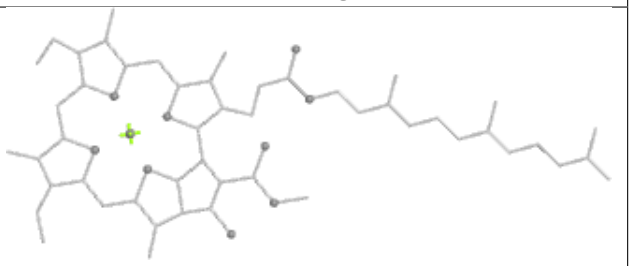
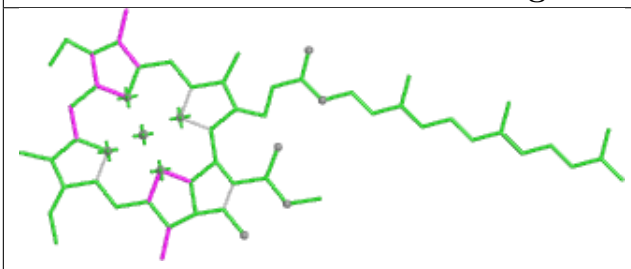
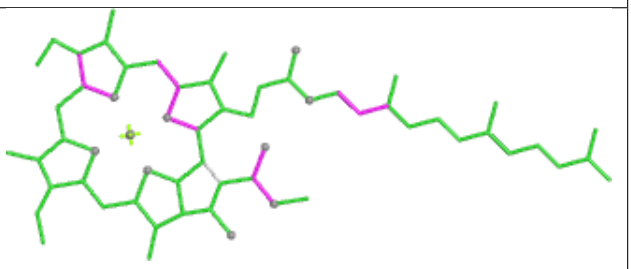
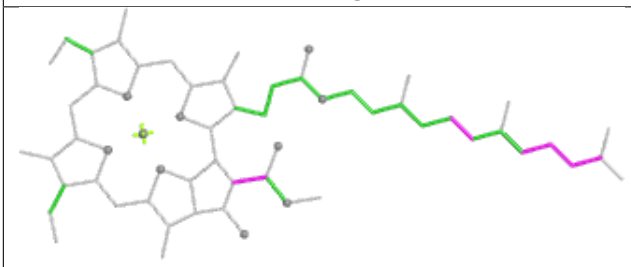
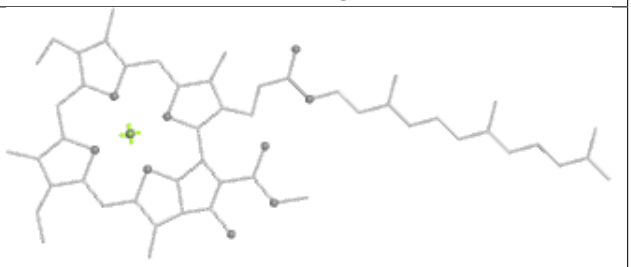
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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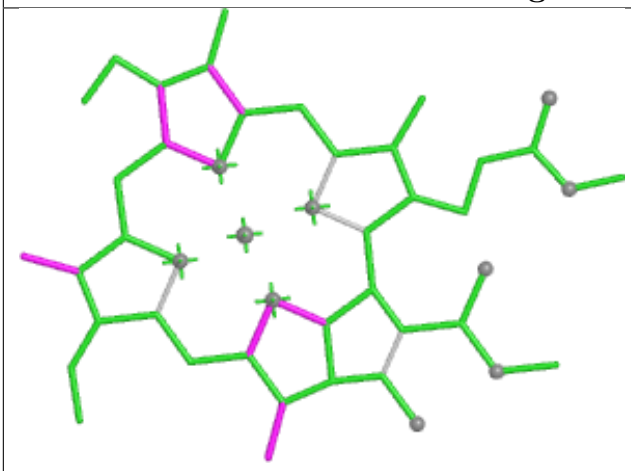
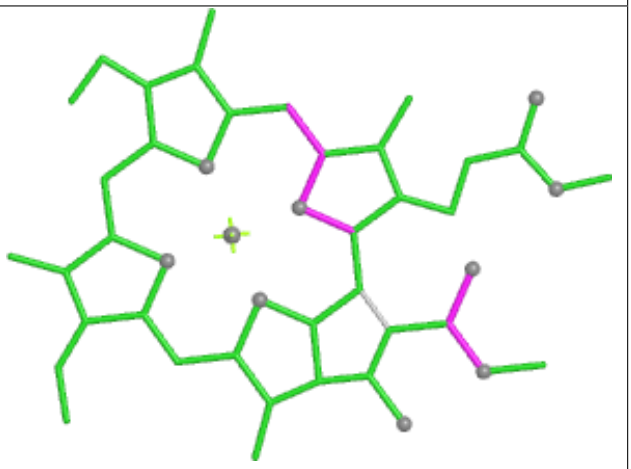
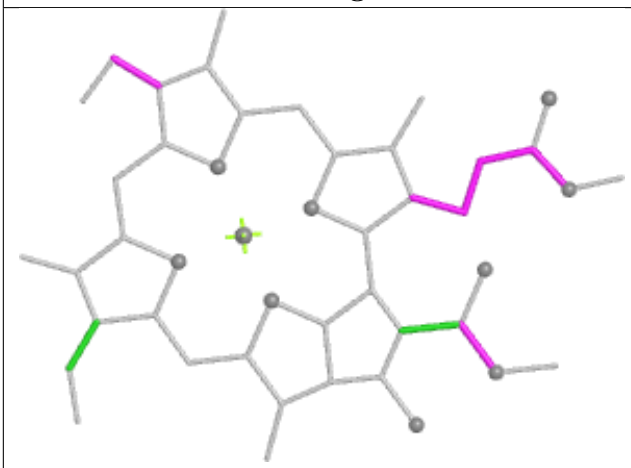
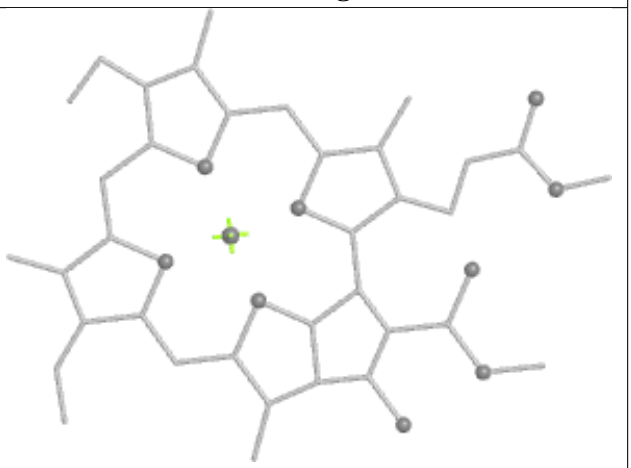
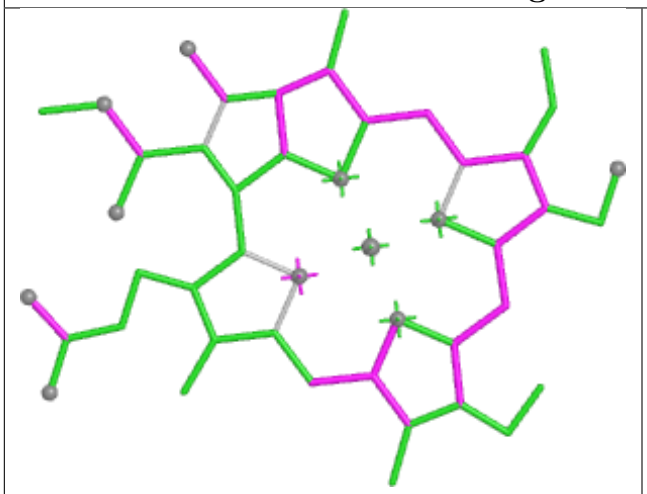
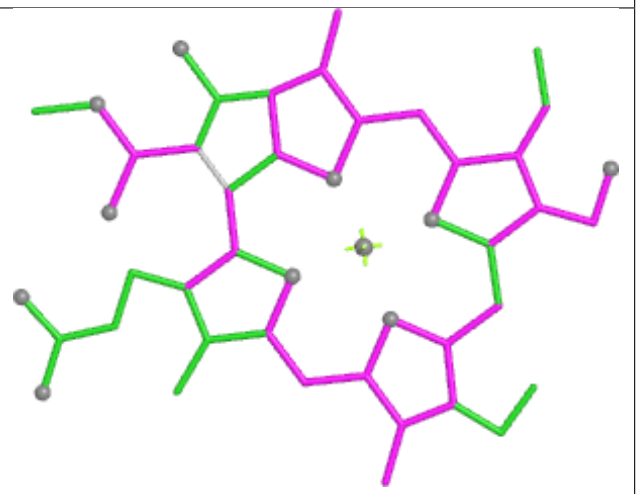
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 606



Bond lengths



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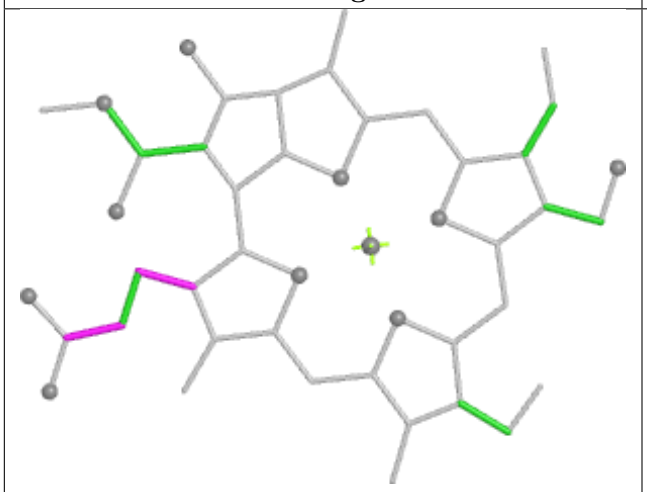

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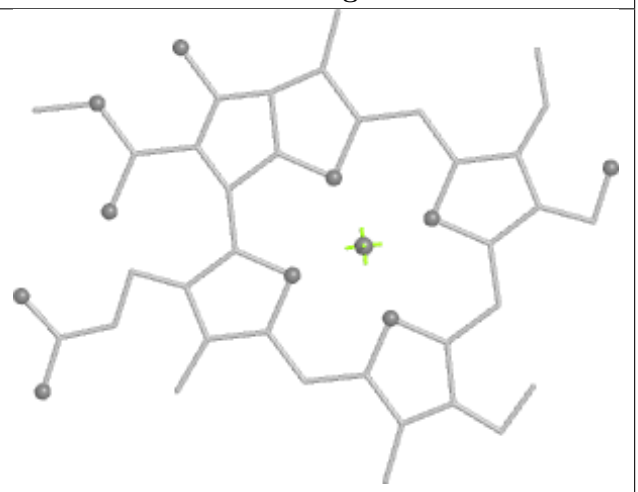
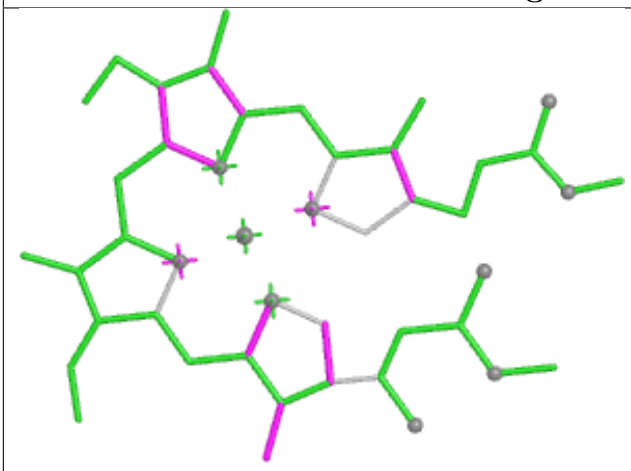
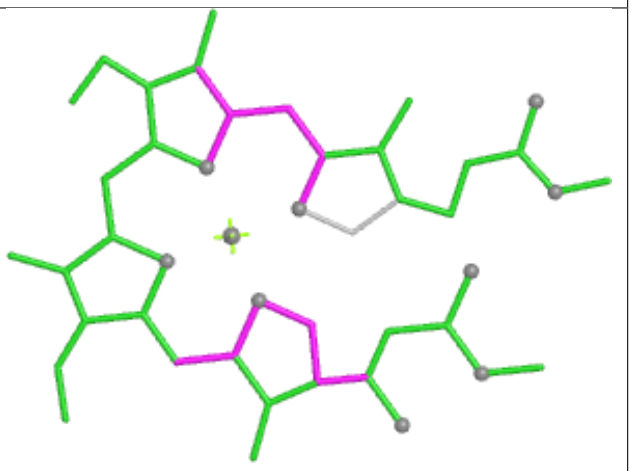


Rings

Ligand CLA F 304



Bond lengths



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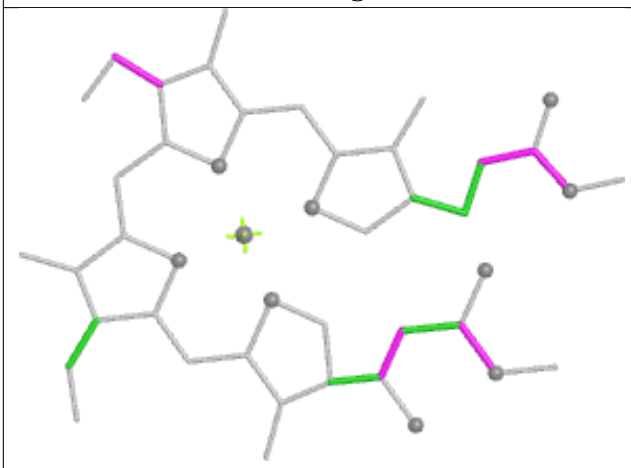

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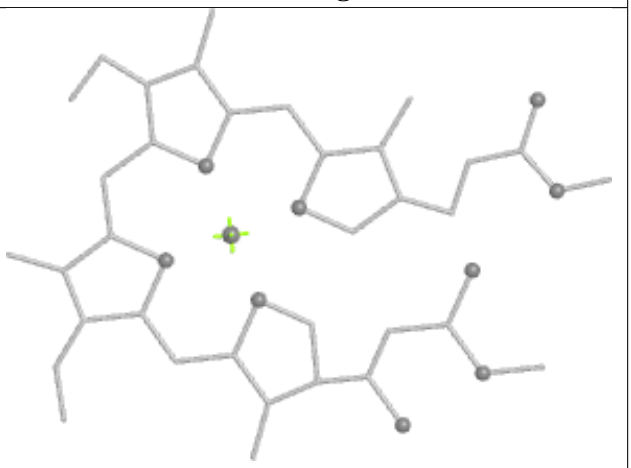
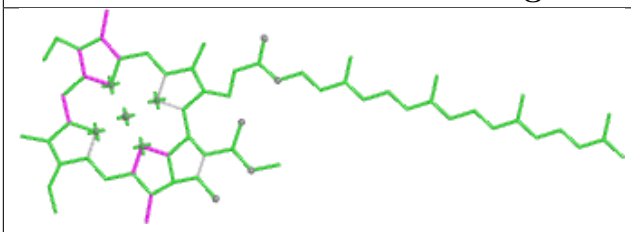


Rings

Ligand CLA B 837



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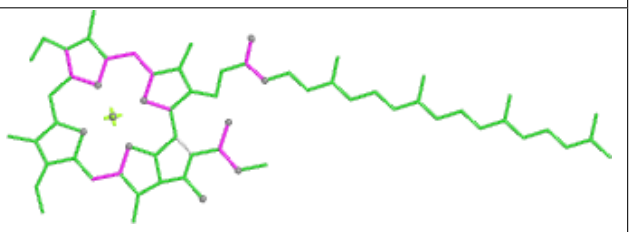

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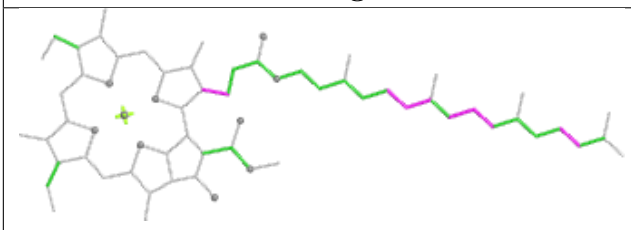

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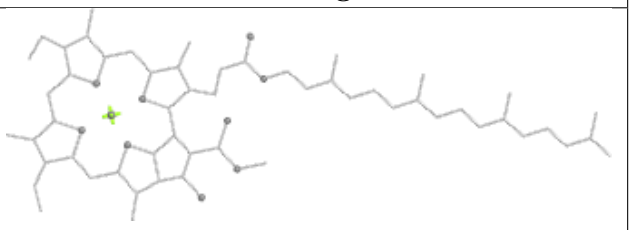
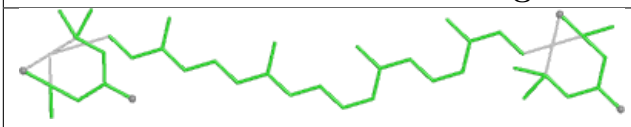
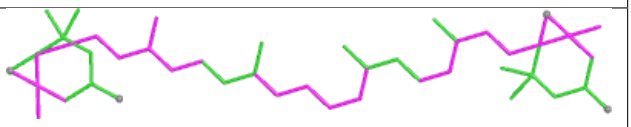
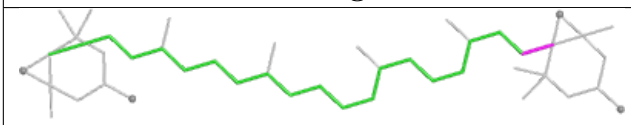
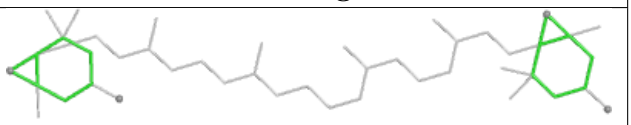
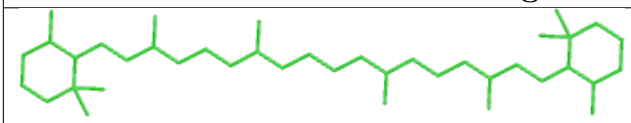
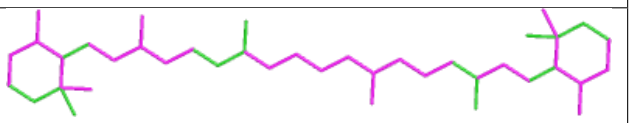
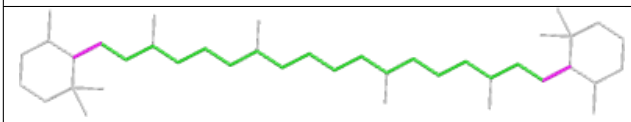
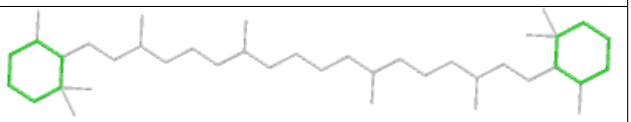
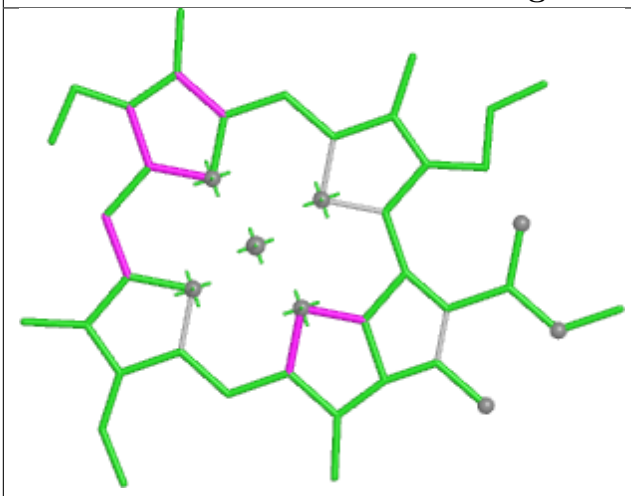
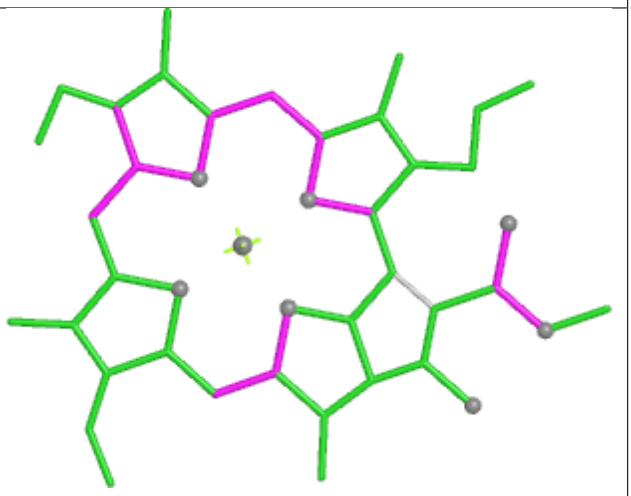
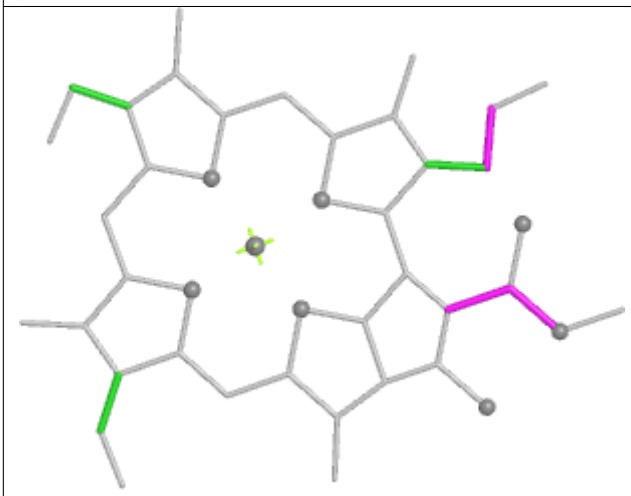
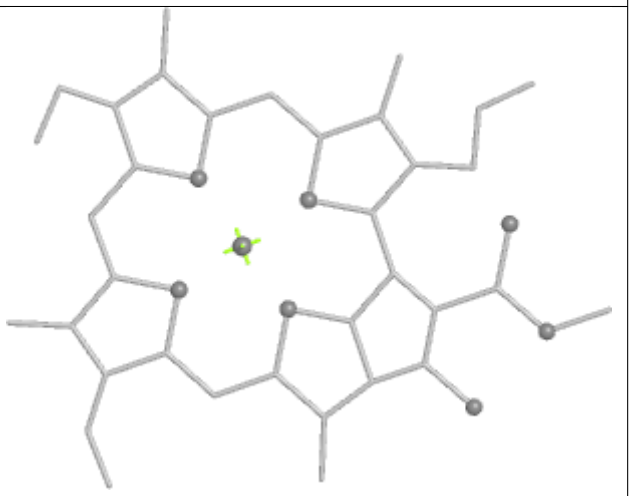


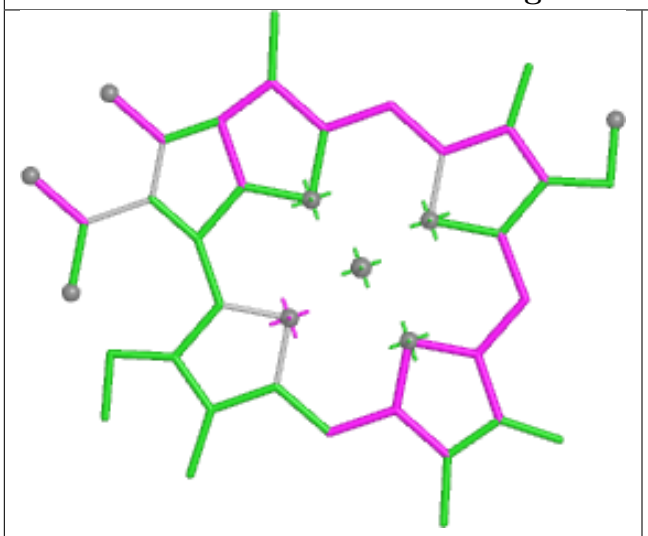
Rings

Ligand XAT U 2622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR G 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

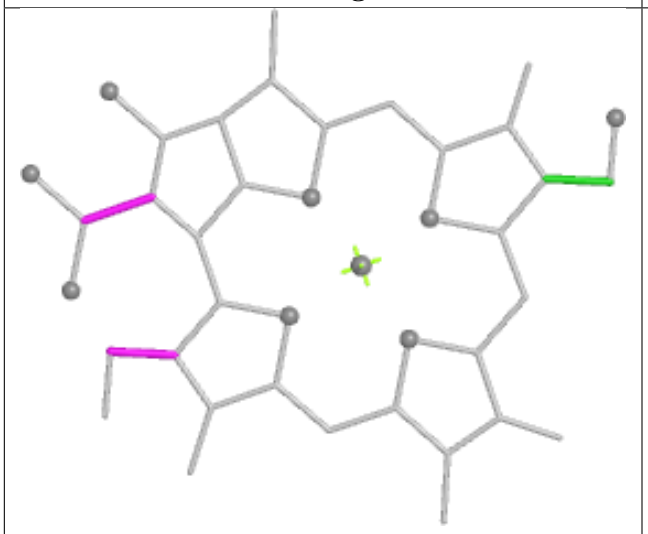
Ligand CLA 5 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL V 608



Bond lengths

Bond angles



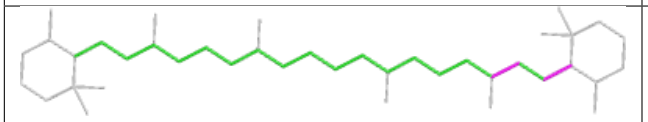
Torsions

Rings

Ligand BCR B 848

Bond lengths

Bond angles



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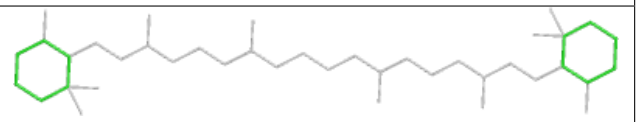
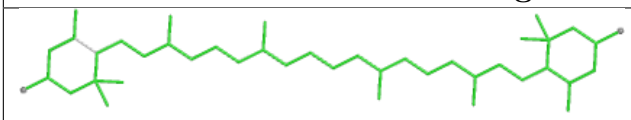
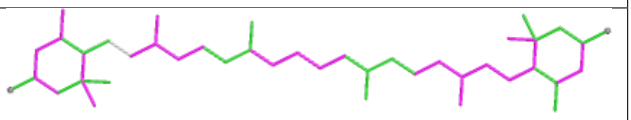


Rings

Ligand LUT U 2620



Bond lengths



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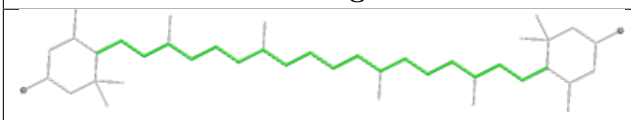

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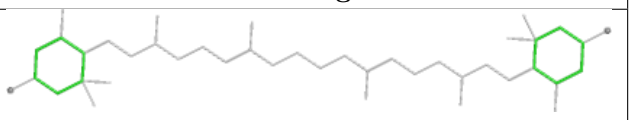
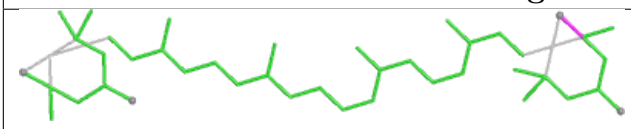


Rings

Ligand XAT 1 618



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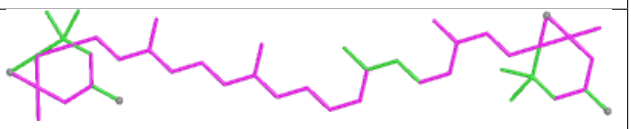
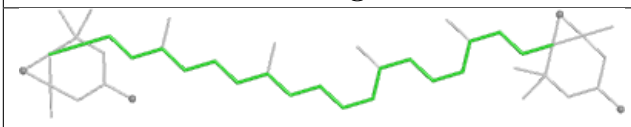


Bond angles



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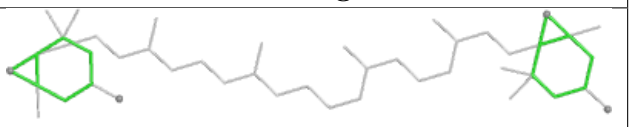
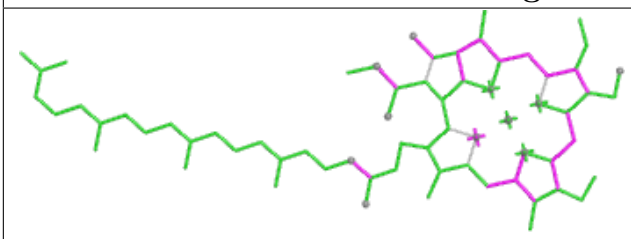


Rings

Ligand CHL U 609



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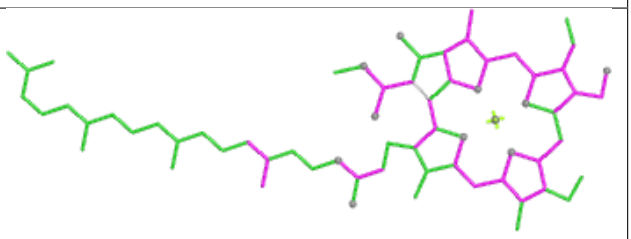
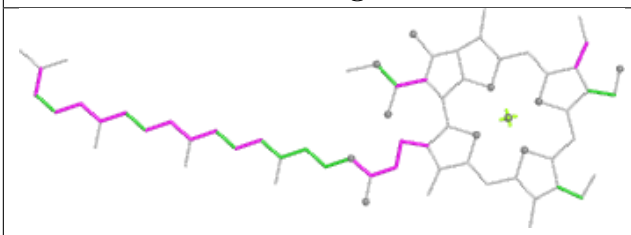


Bond angles



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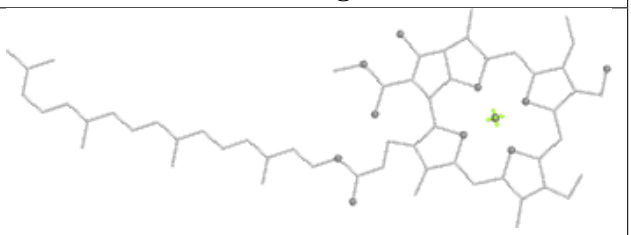
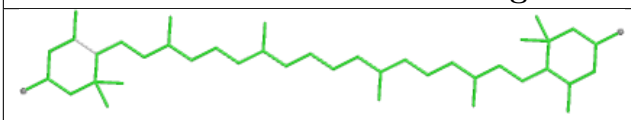
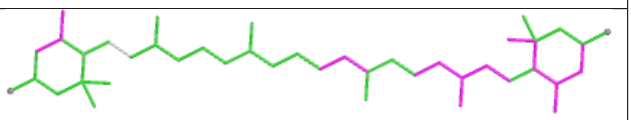


Rings

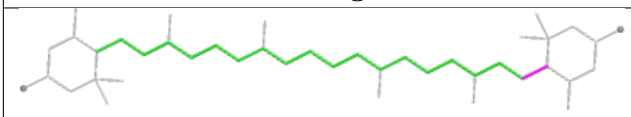
Ligand LUT W 2621



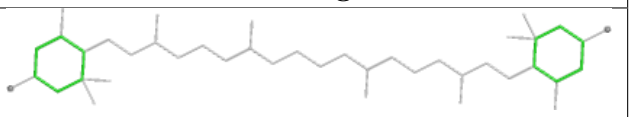
Bond lengths



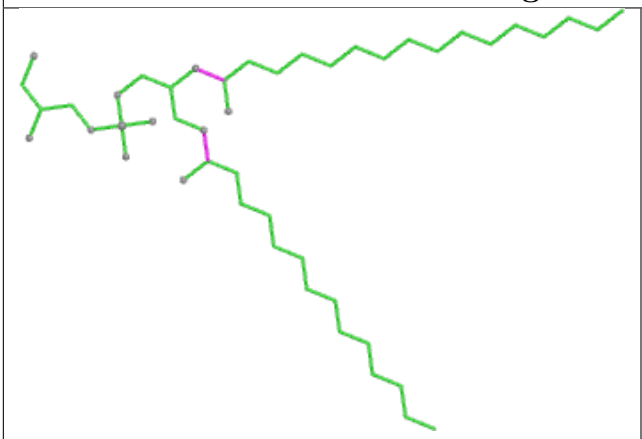
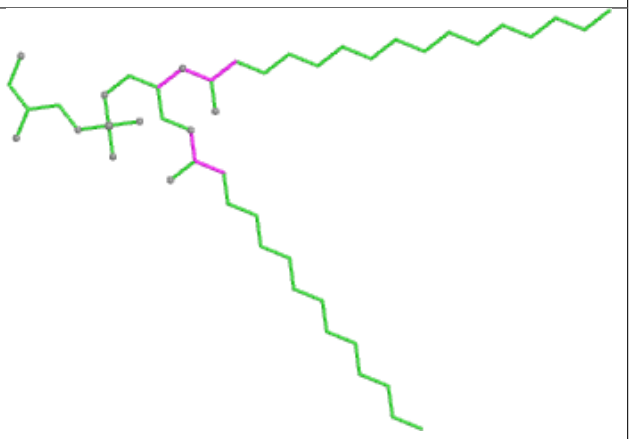
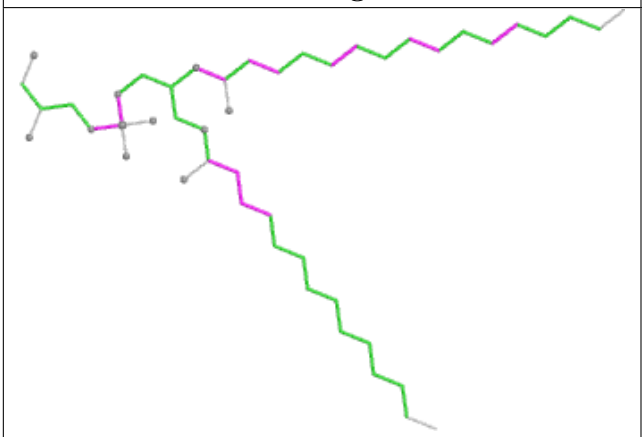
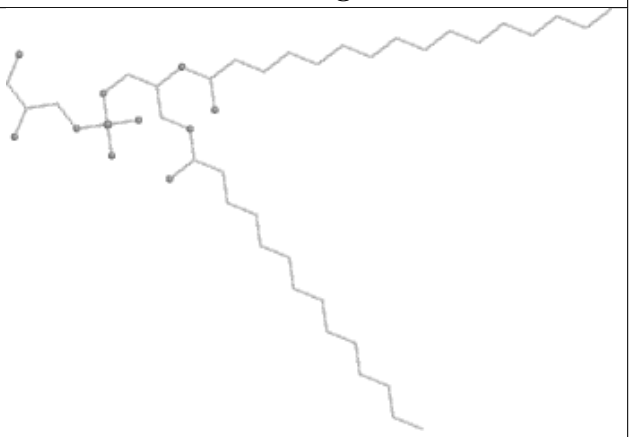
Bond angles



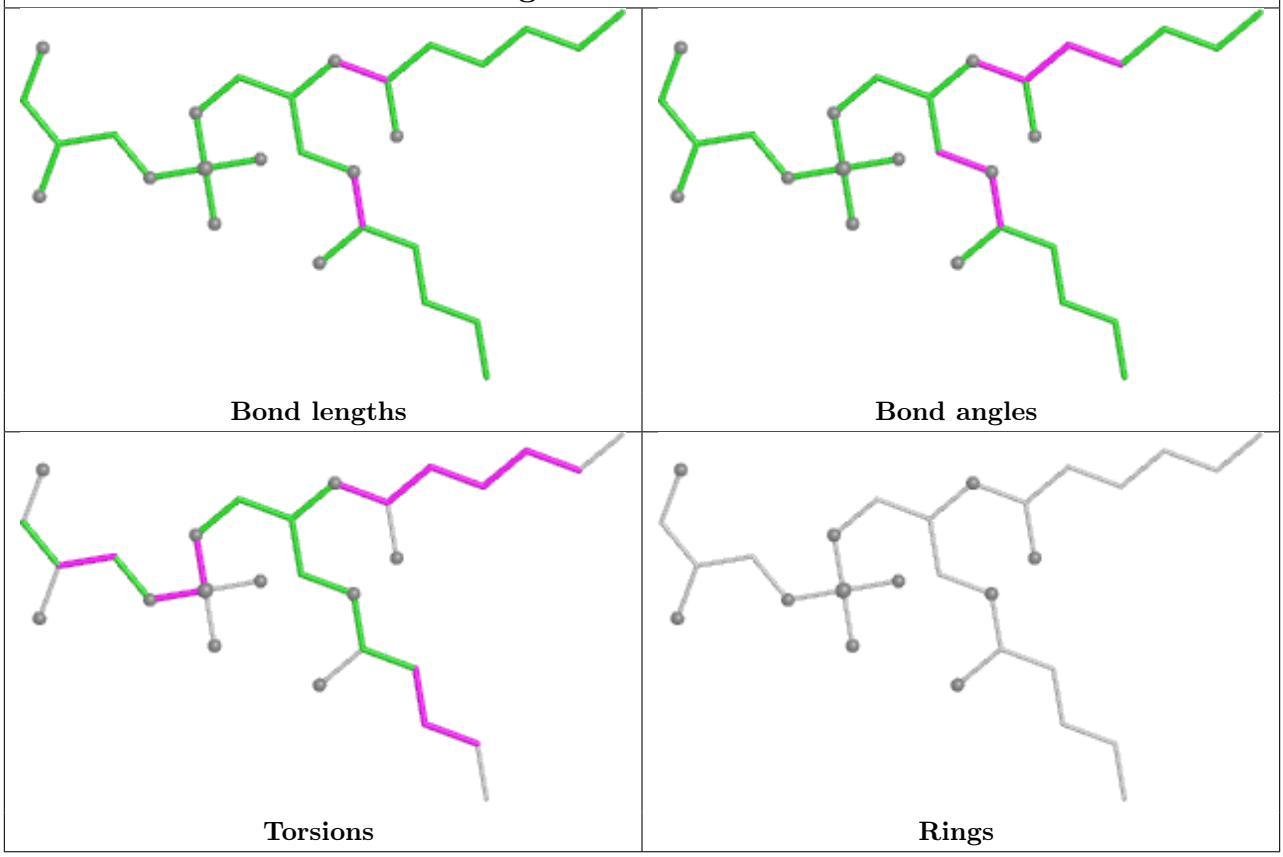
Torsions



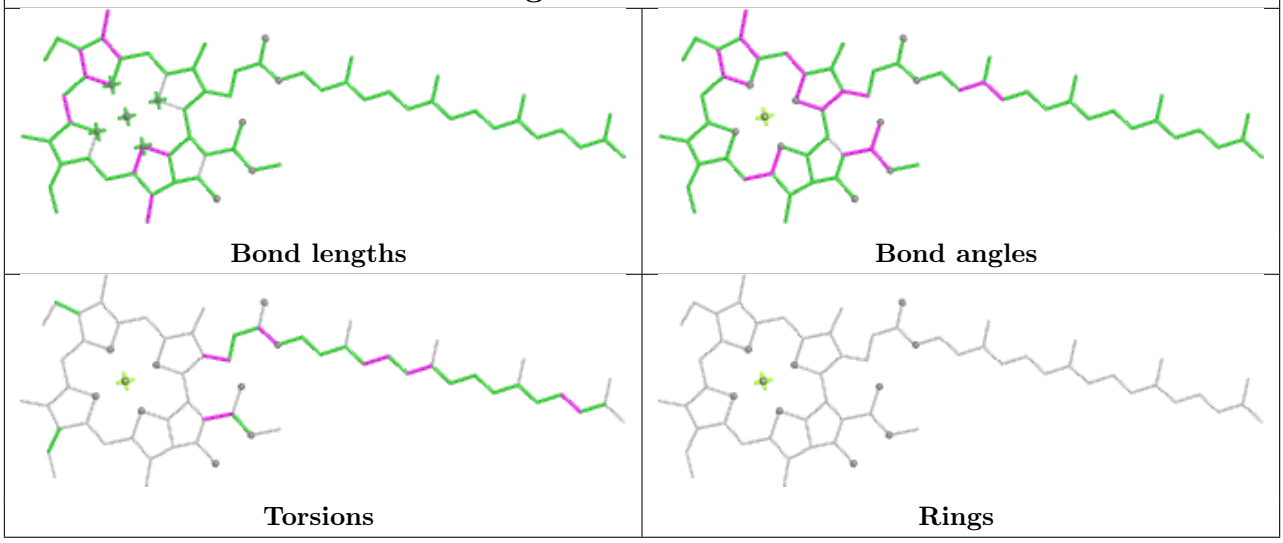
Rings

Ligand LHG A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 9 2630



Ligand CLA B 805



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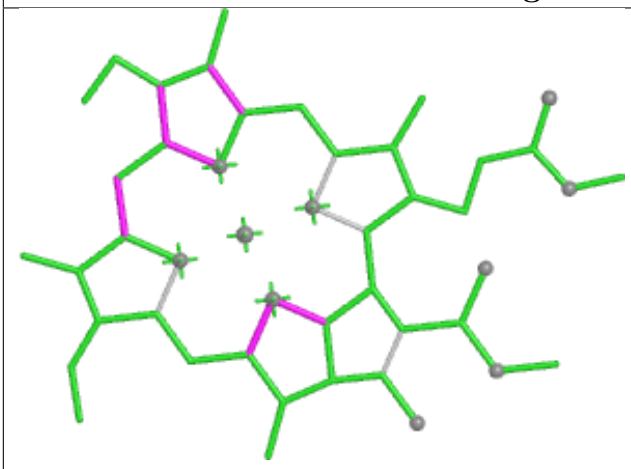
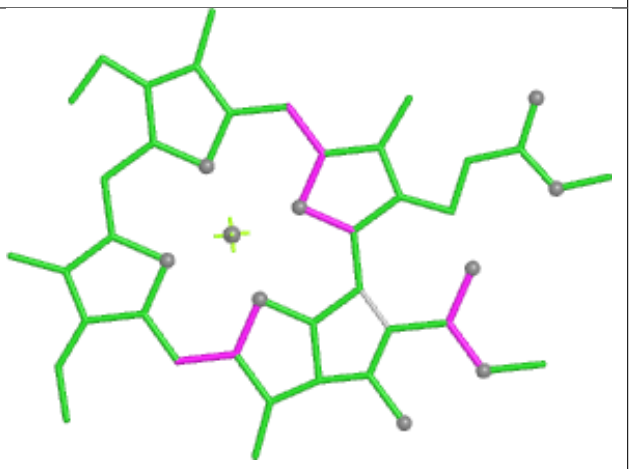
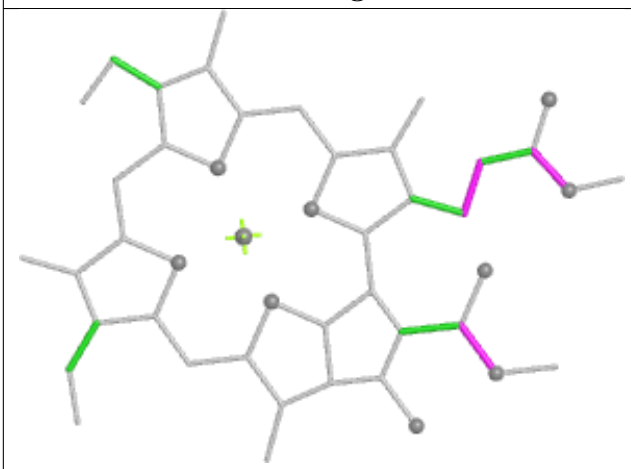
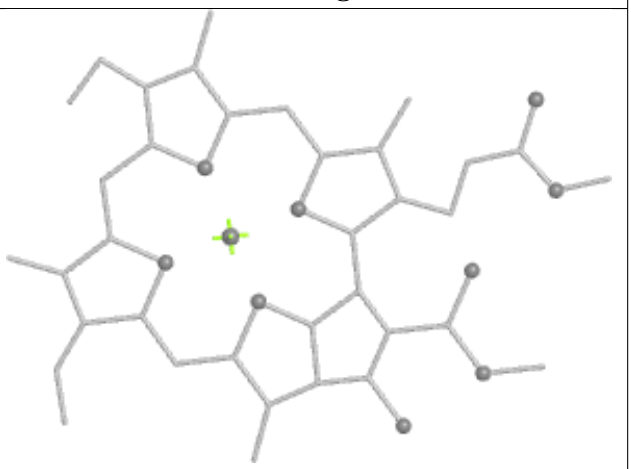
 Bond lengths	 Bond angles
 Torsions	 Rings

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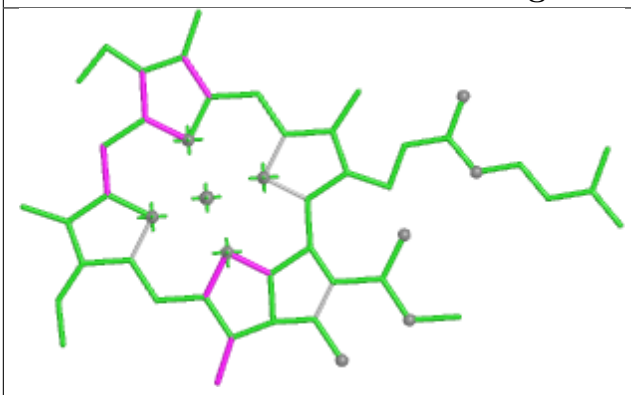
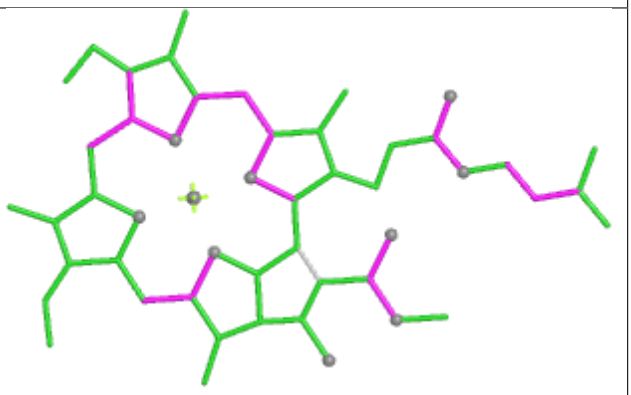
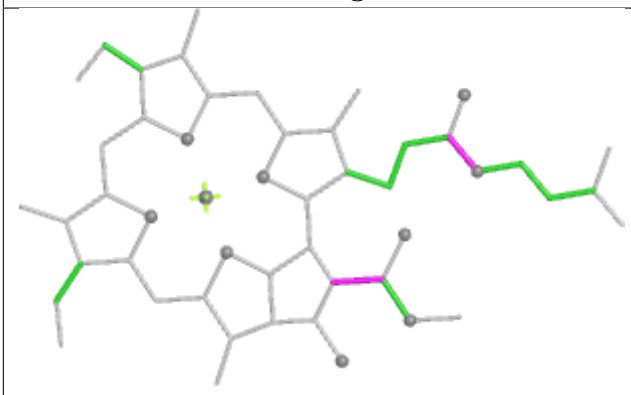
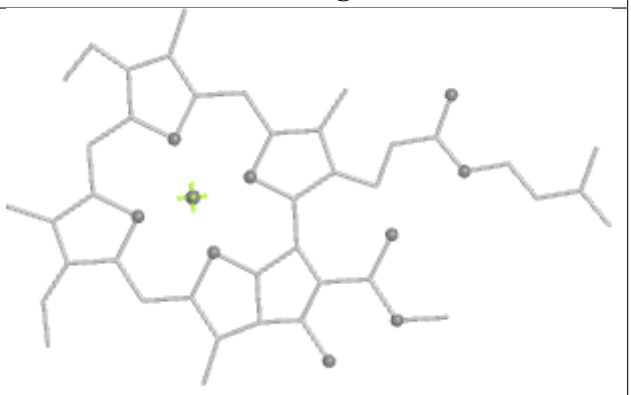
 Bond lengths	 Bond angles
 Torsions	 Rings

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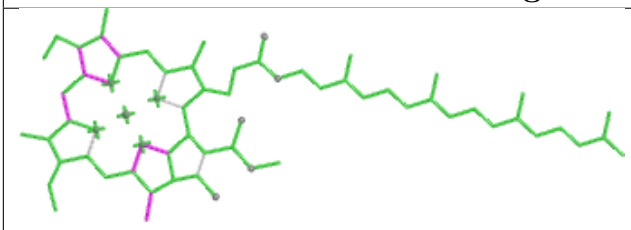
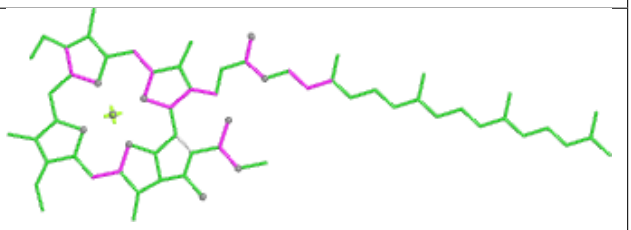
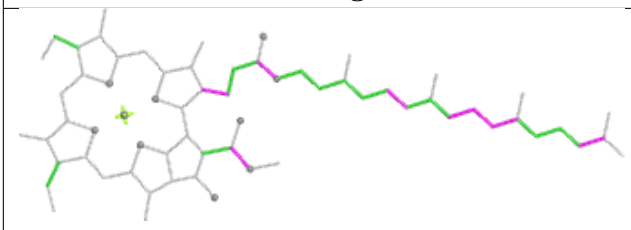
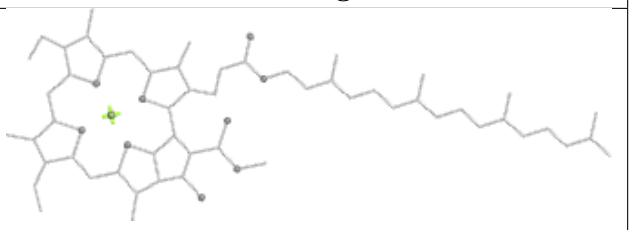
 Bond lengths	 Bond angles
 Torsions	 Rings

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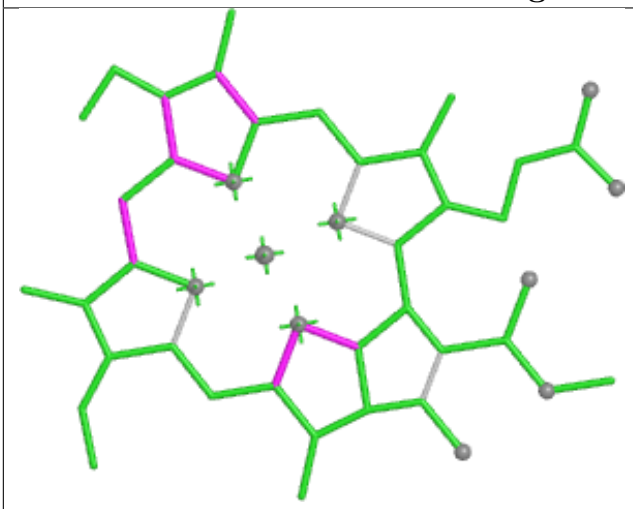

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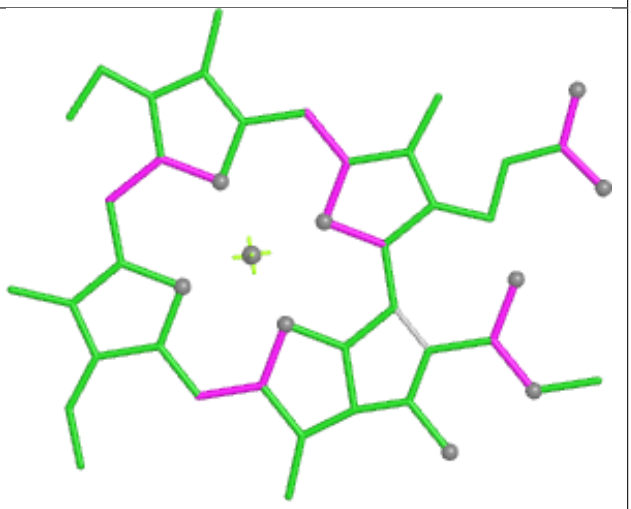
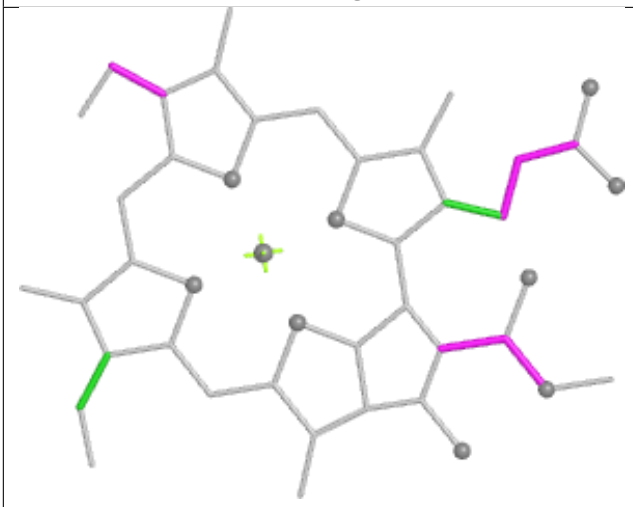


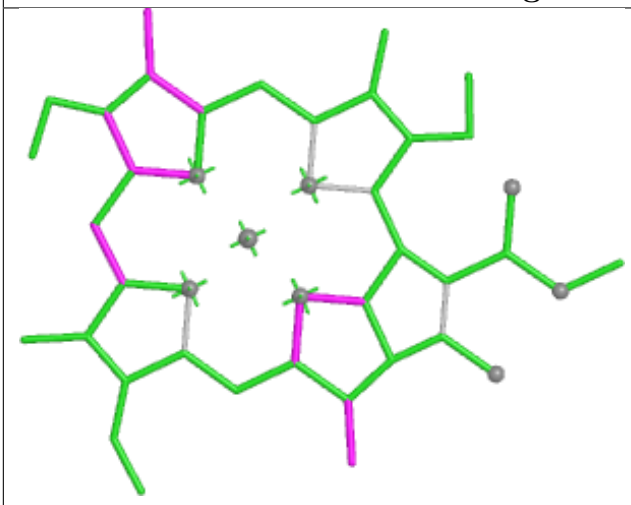
Bond angles



Torsions

Rings

Ligand CLA K 201



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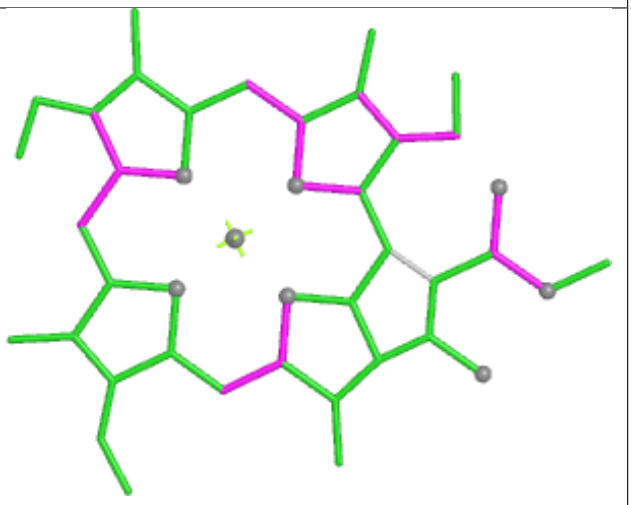

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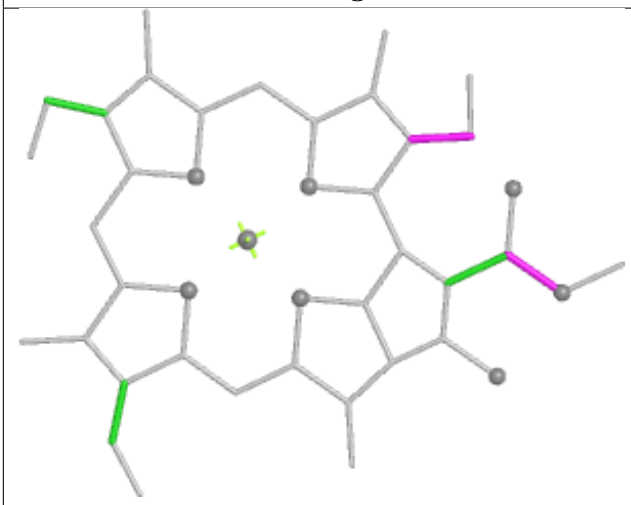

Torsions

Rings

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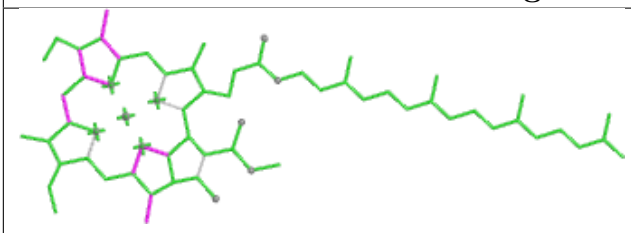

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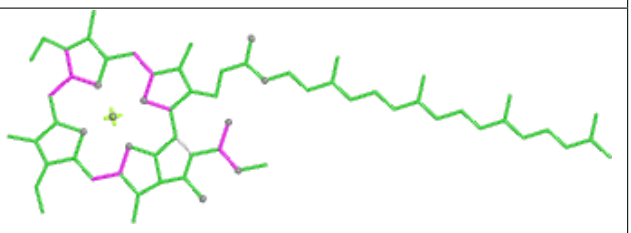

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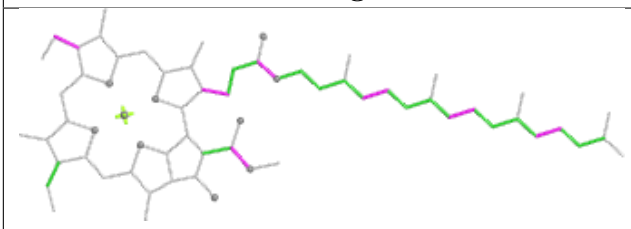

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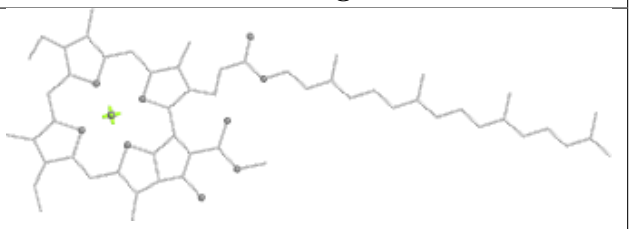
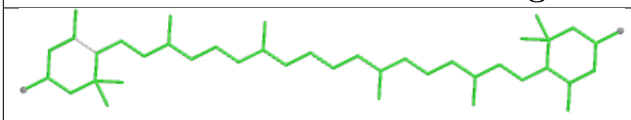


Rings

Ligand LUT 6 619



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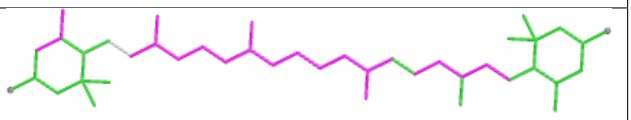

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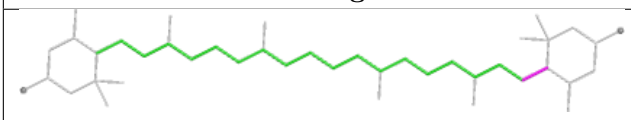

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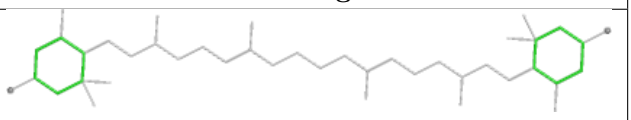
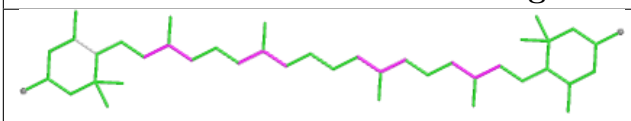


Rings

Ligand LUT 2 619



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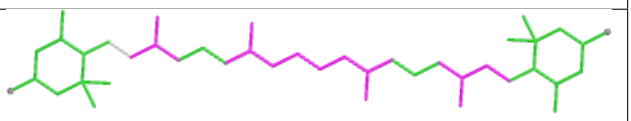

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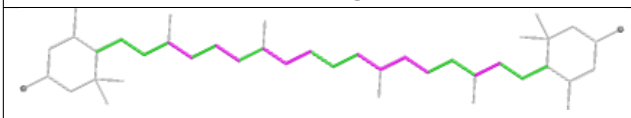

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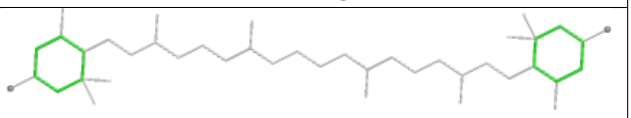
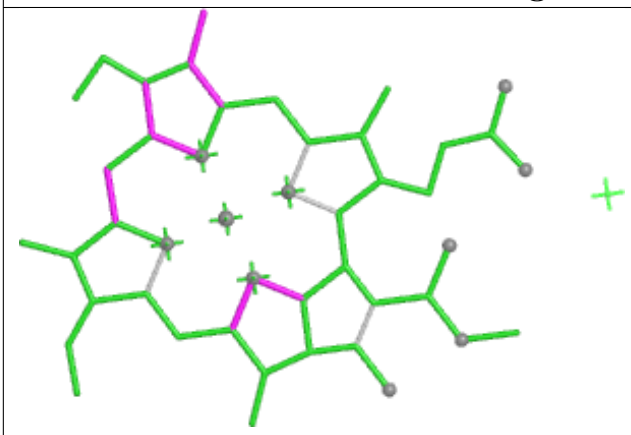


Rings

Ligand CLA 2 611



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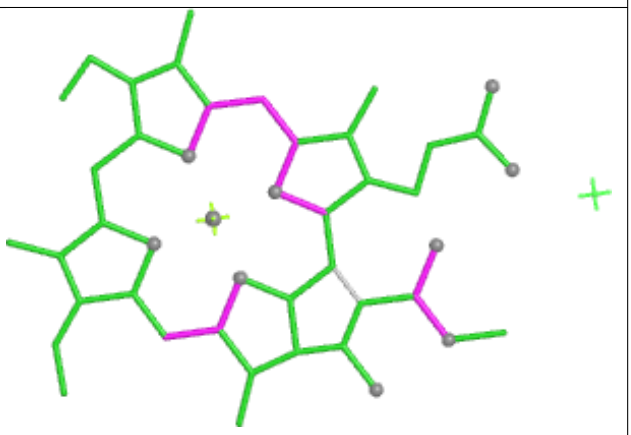

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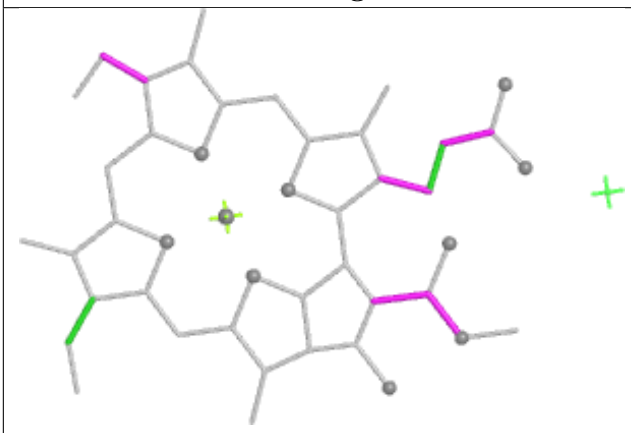

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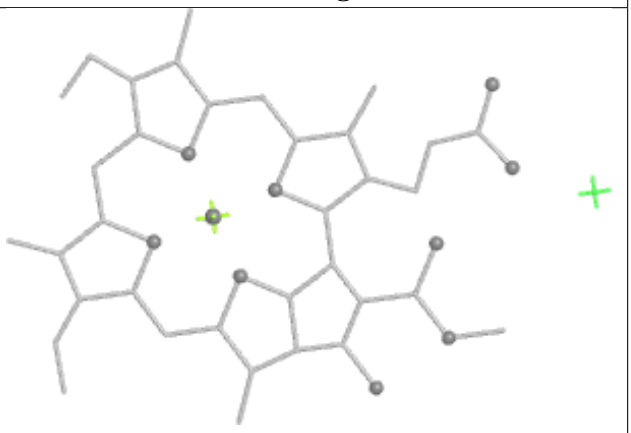
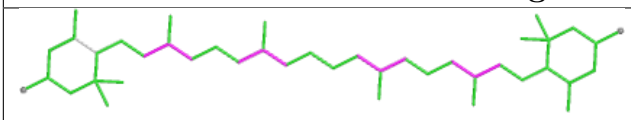
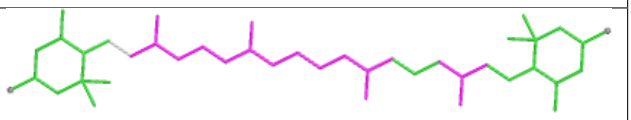
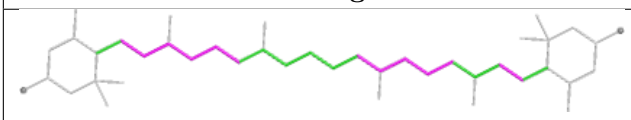
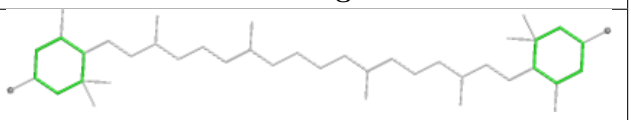


Rings

Ligand LUT 5 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

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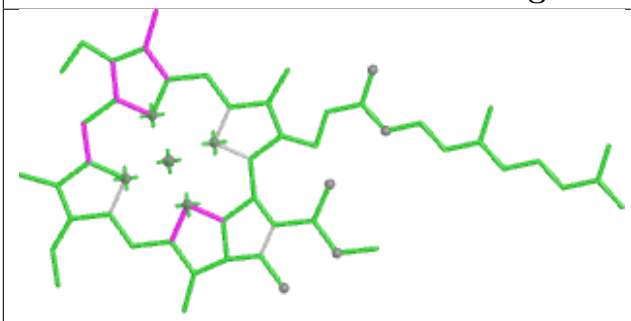
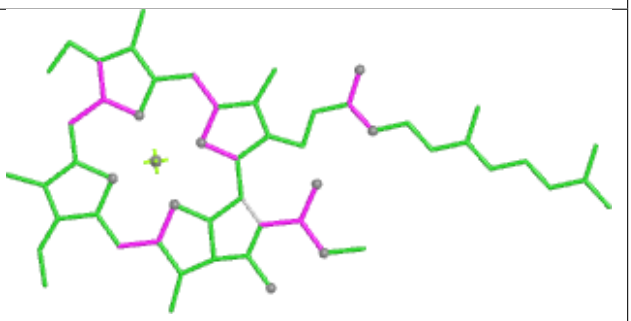
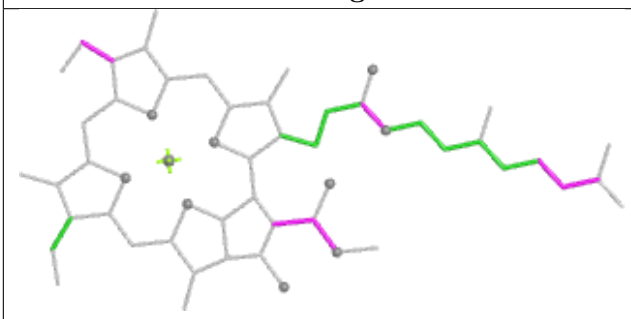
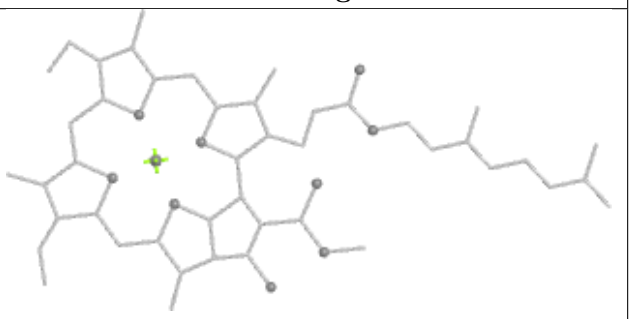
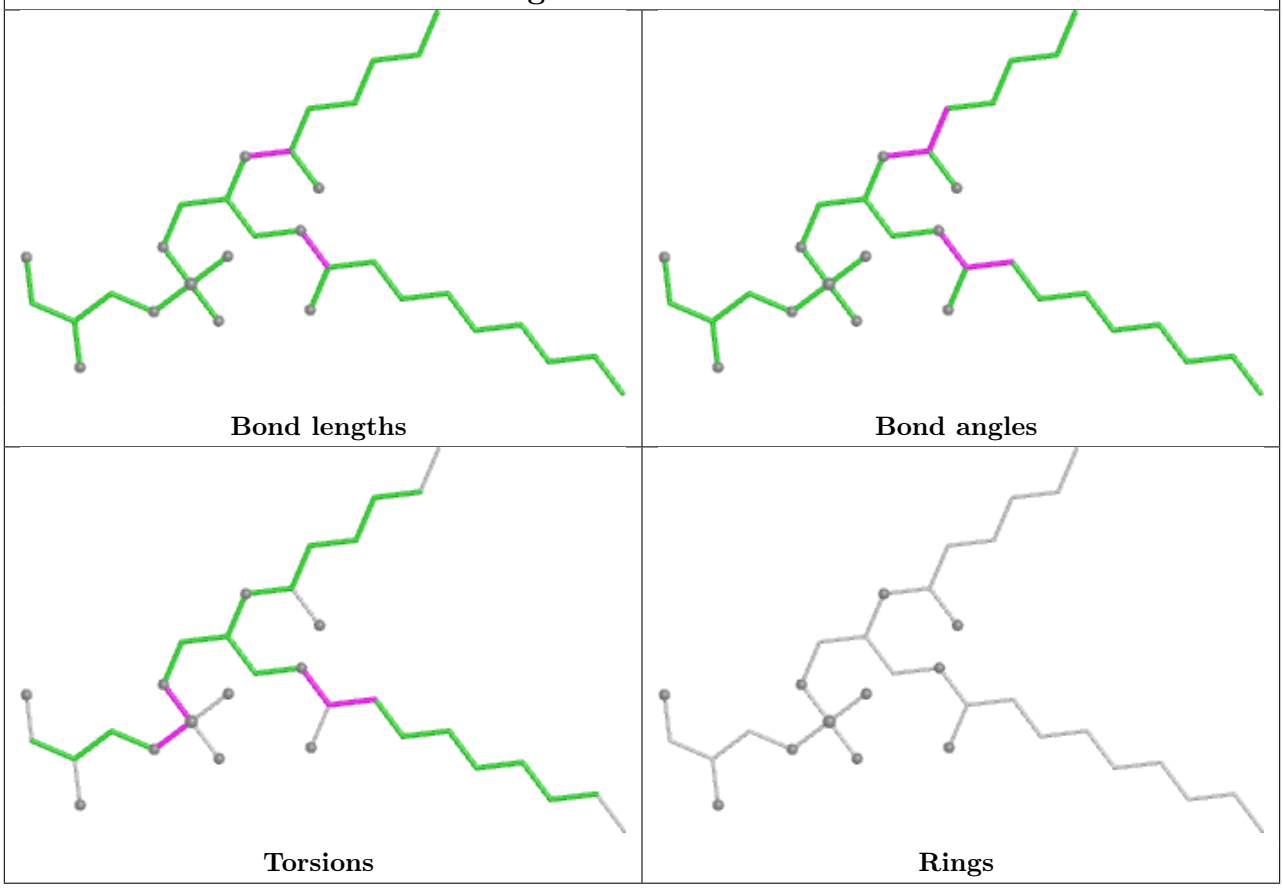
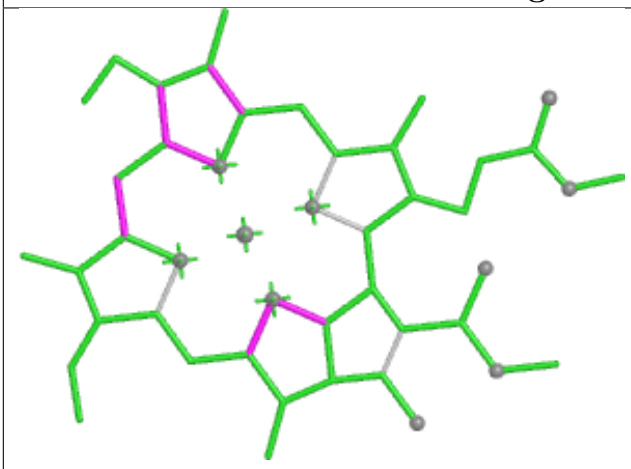
 Bond lengths	 Bond angles
 Torsions	 Rings

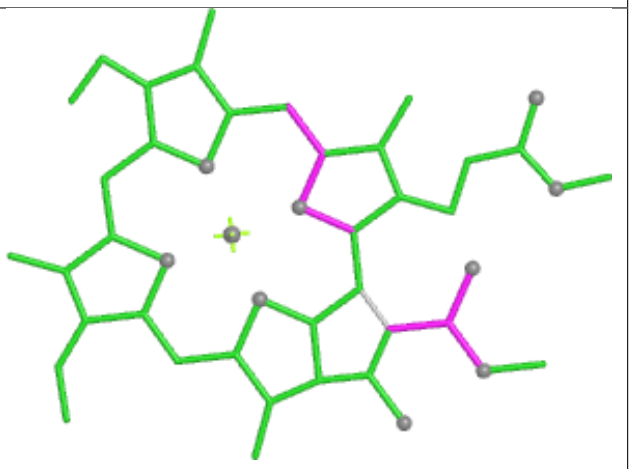
Ligand LHG 6 630



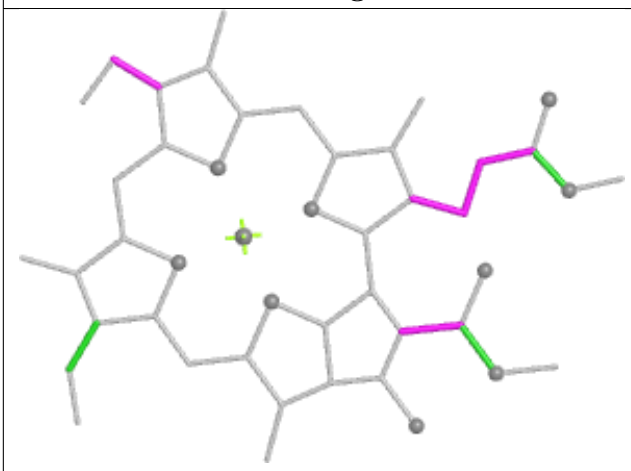
Ligand CLA 2 609



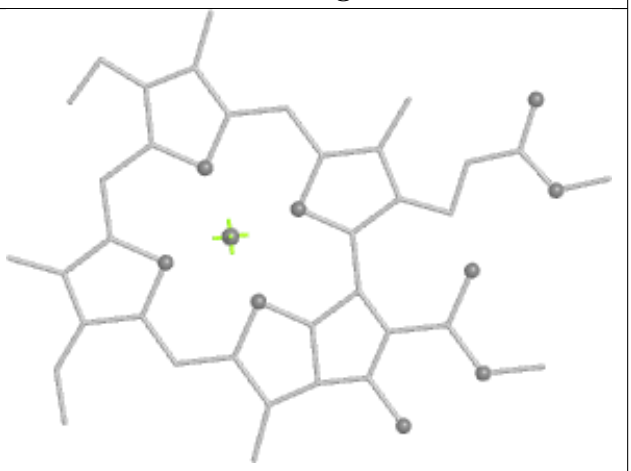
Bond lengths



Bond angles



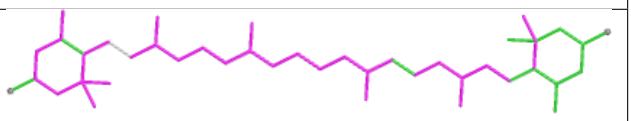
Torsions



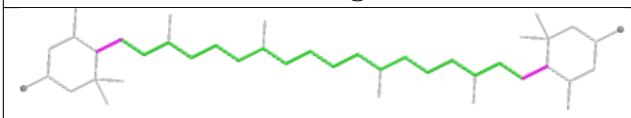
Rings

Ligand LUT 9 624

Bond lengths



Bond angles



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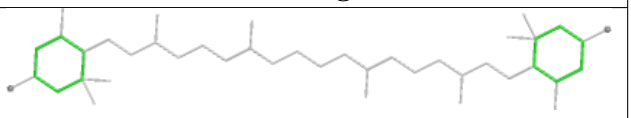
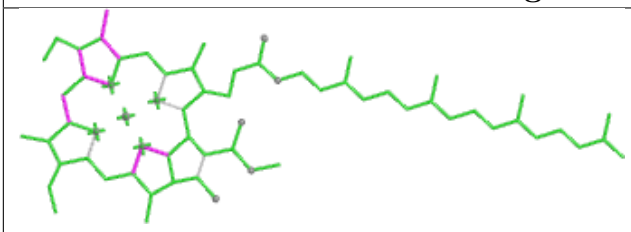
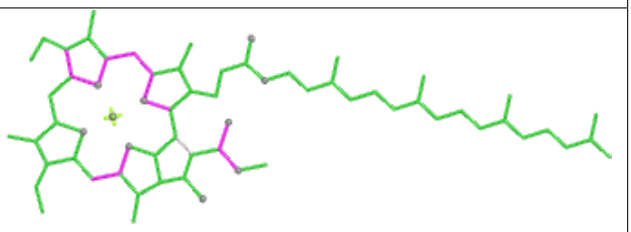
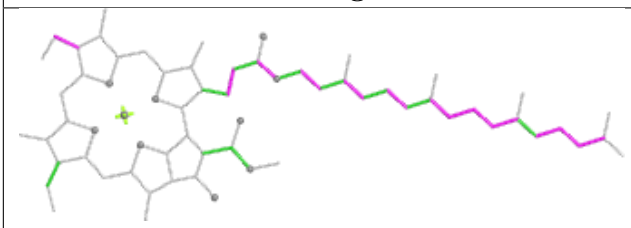
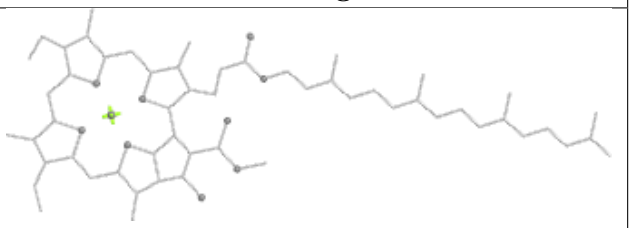


Rings

Ligand CLA B 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

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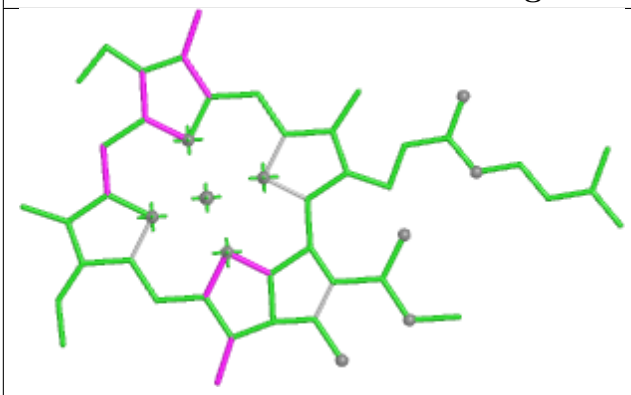
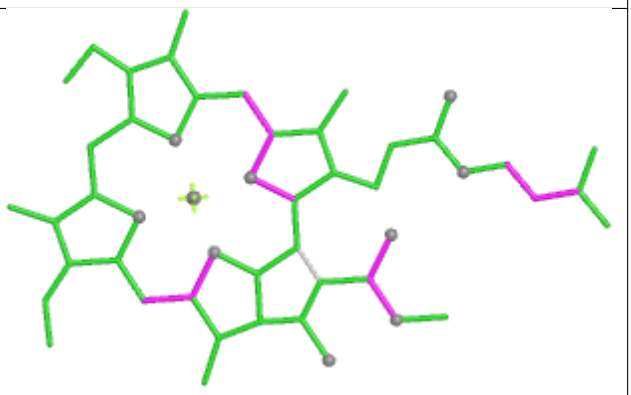
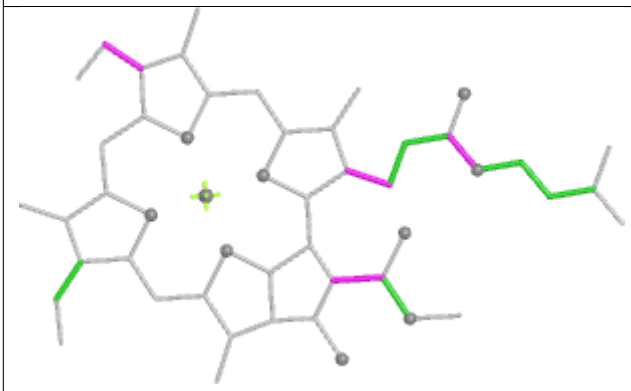
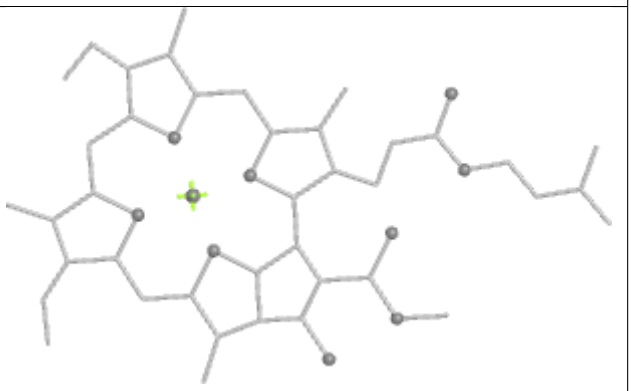
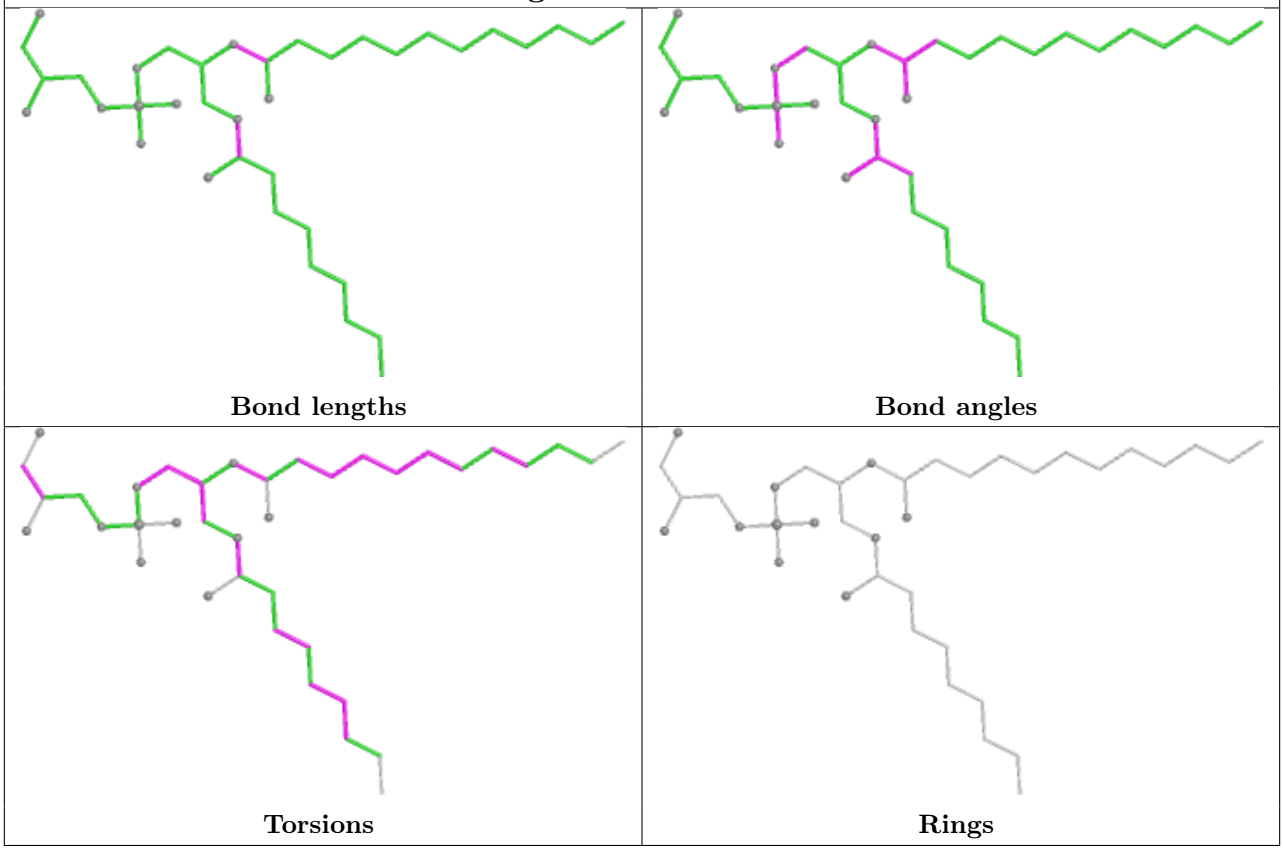
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 4 630



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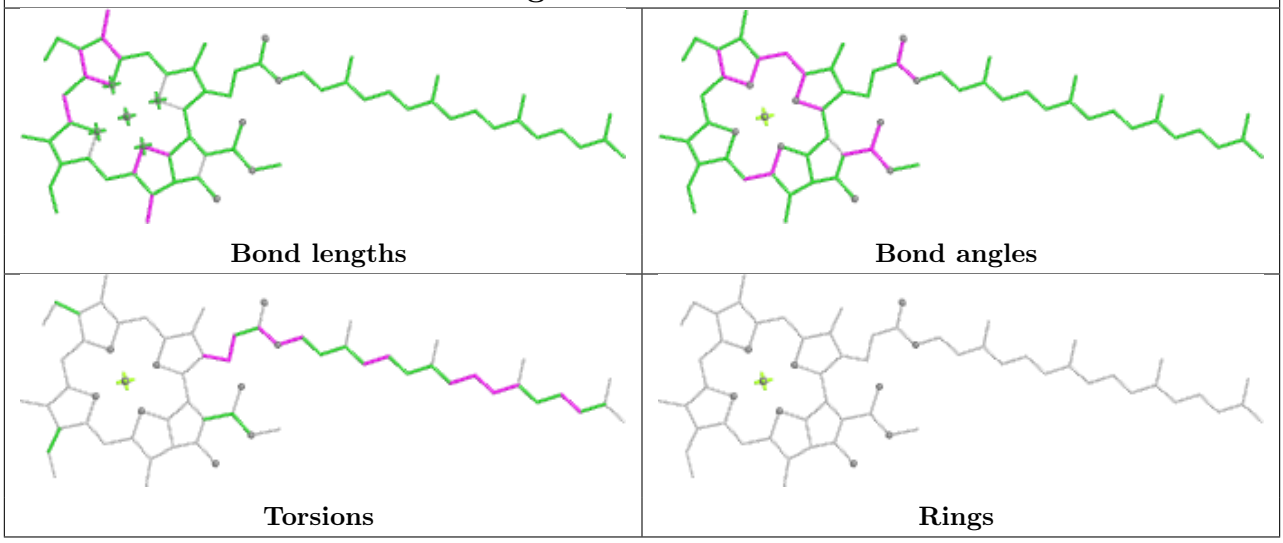
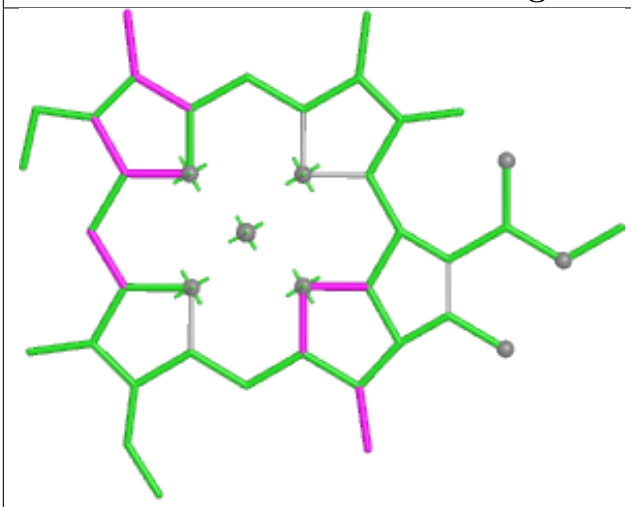
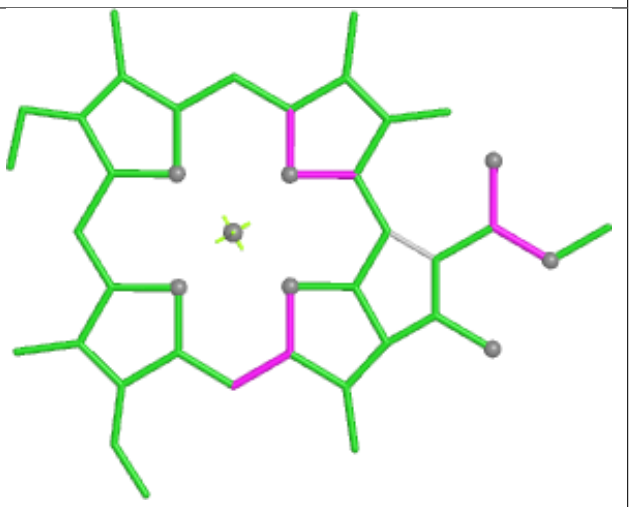


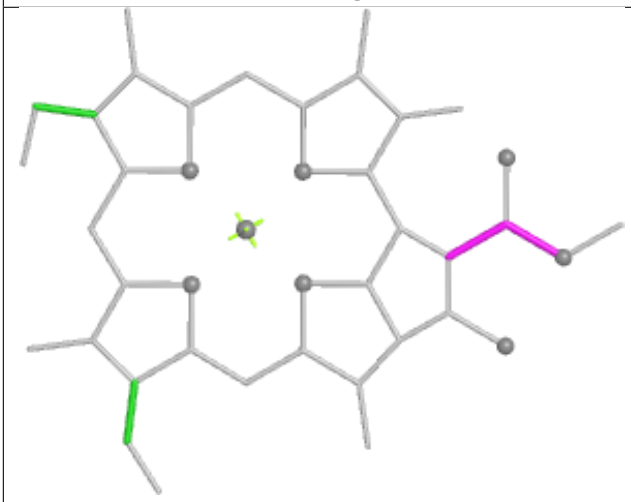
Ligand CLA 5 604



Bond lengths



Bond angles



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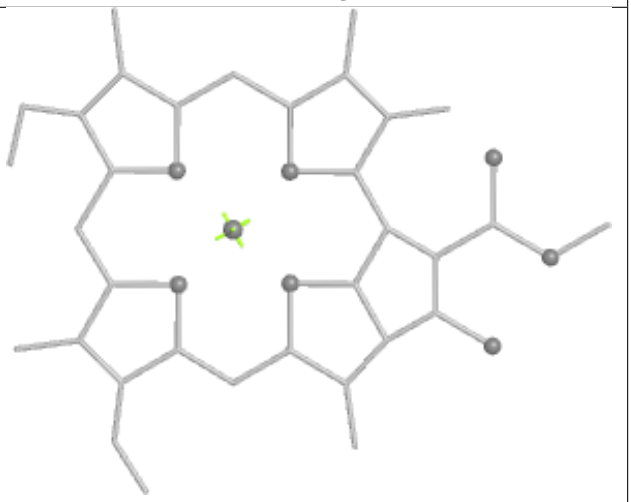
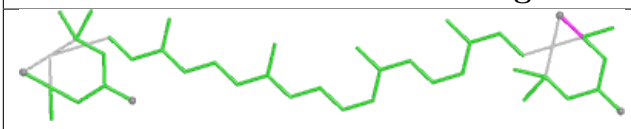


Rings

Ligand XAT V 2622



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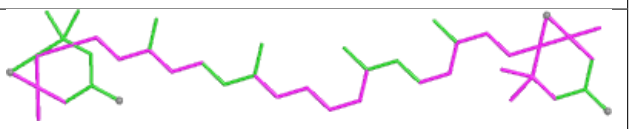

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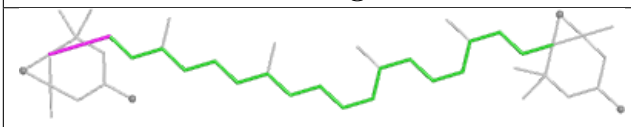

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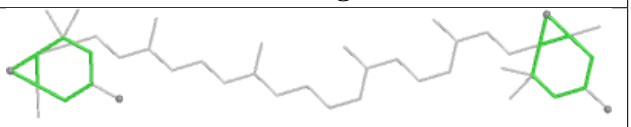
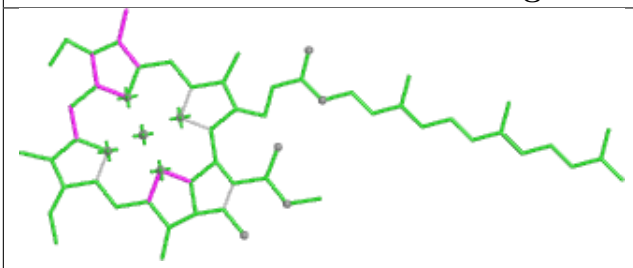


Rings

Ligand CLA A 808



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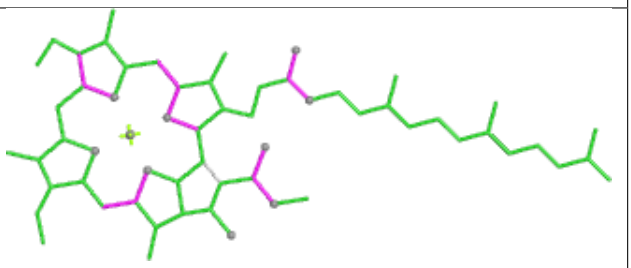

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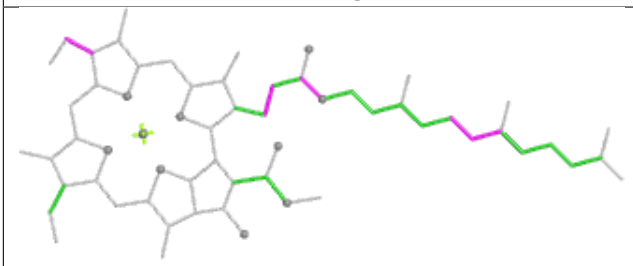

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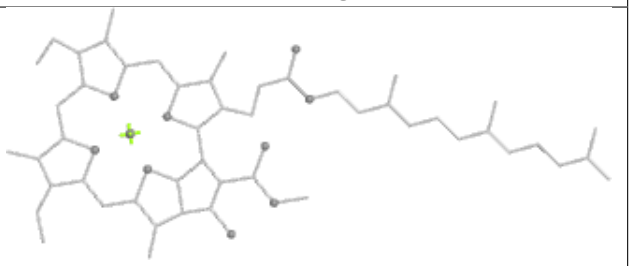
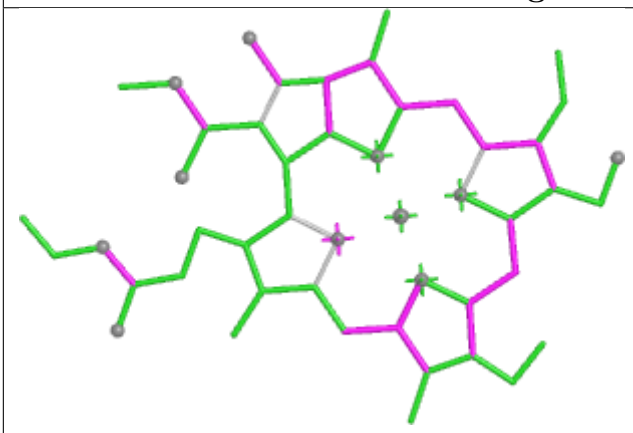


Rings

Ligand CHL 6 608



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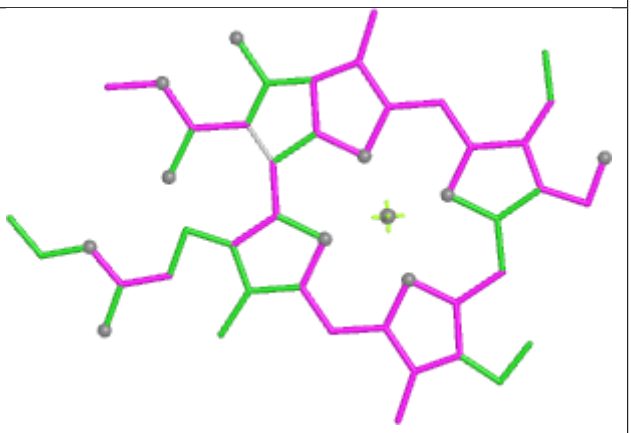

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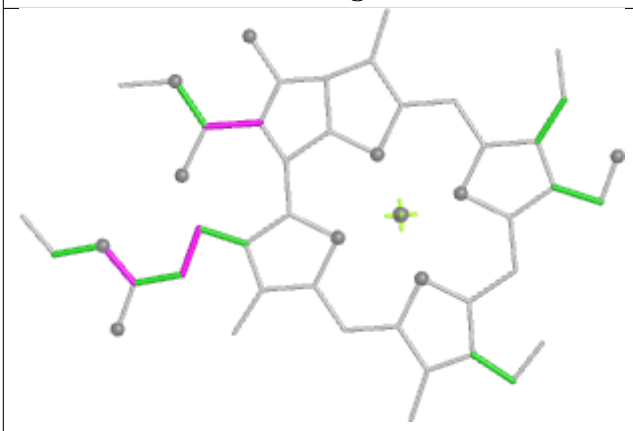
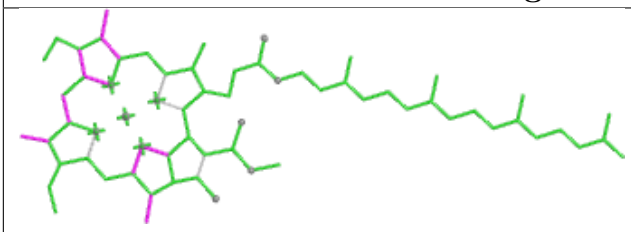
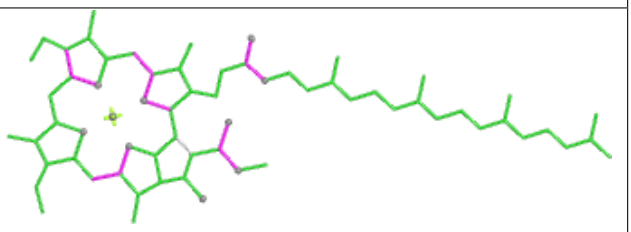
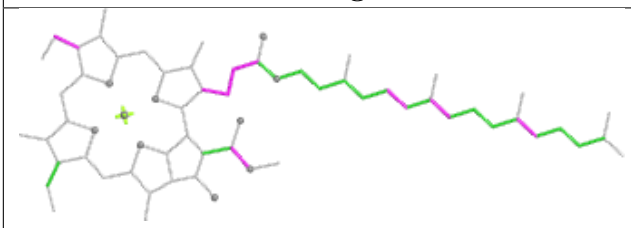
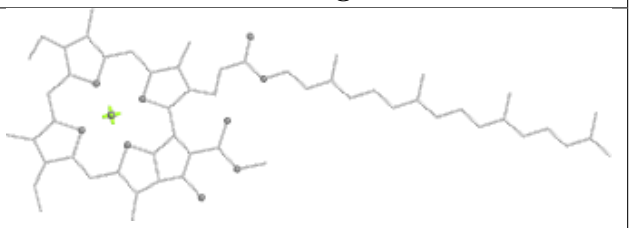
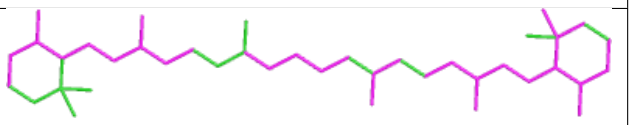
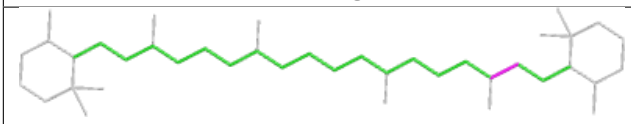
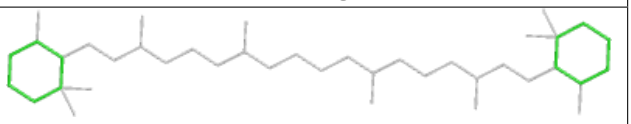


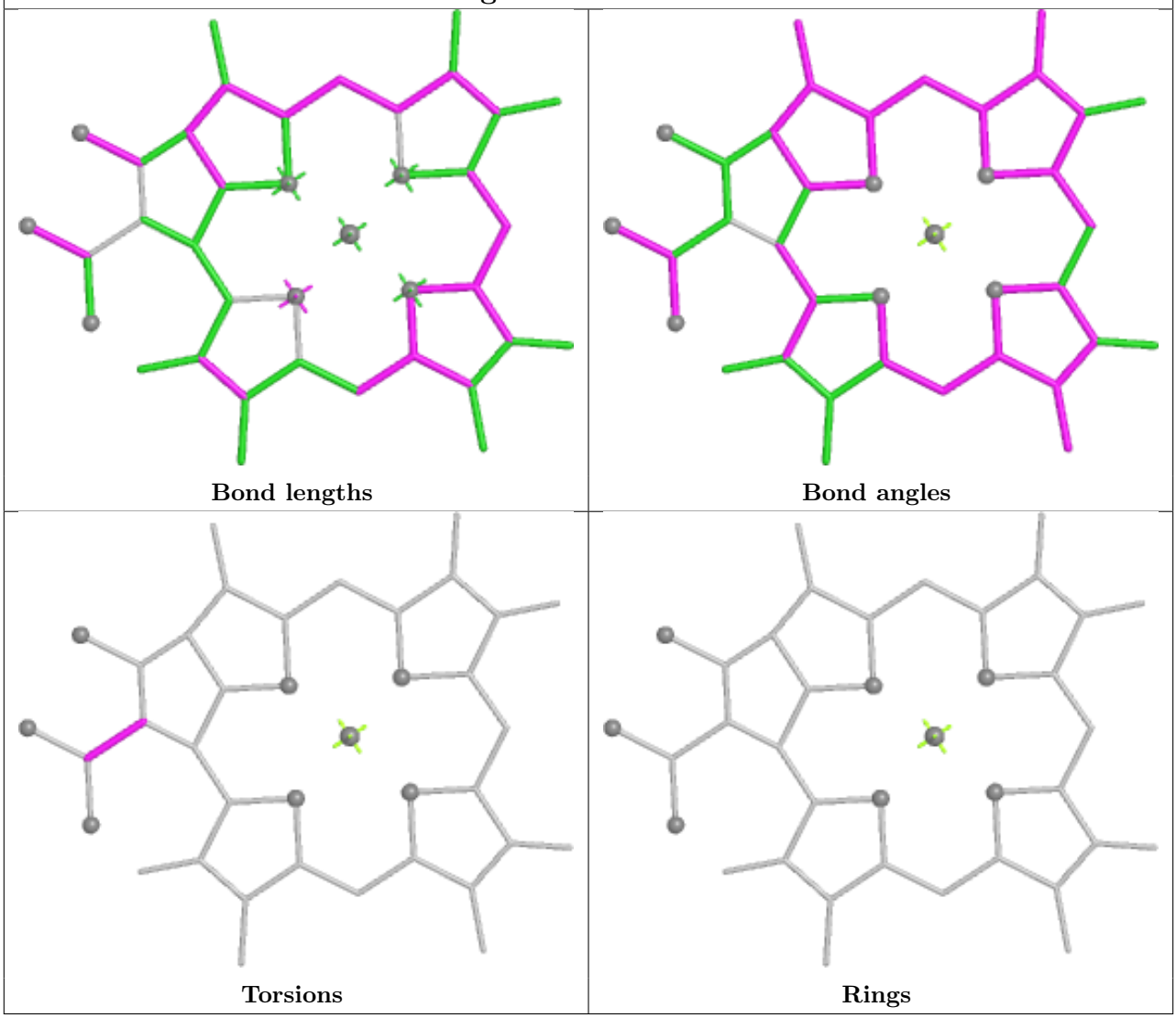
Torsions

Rings

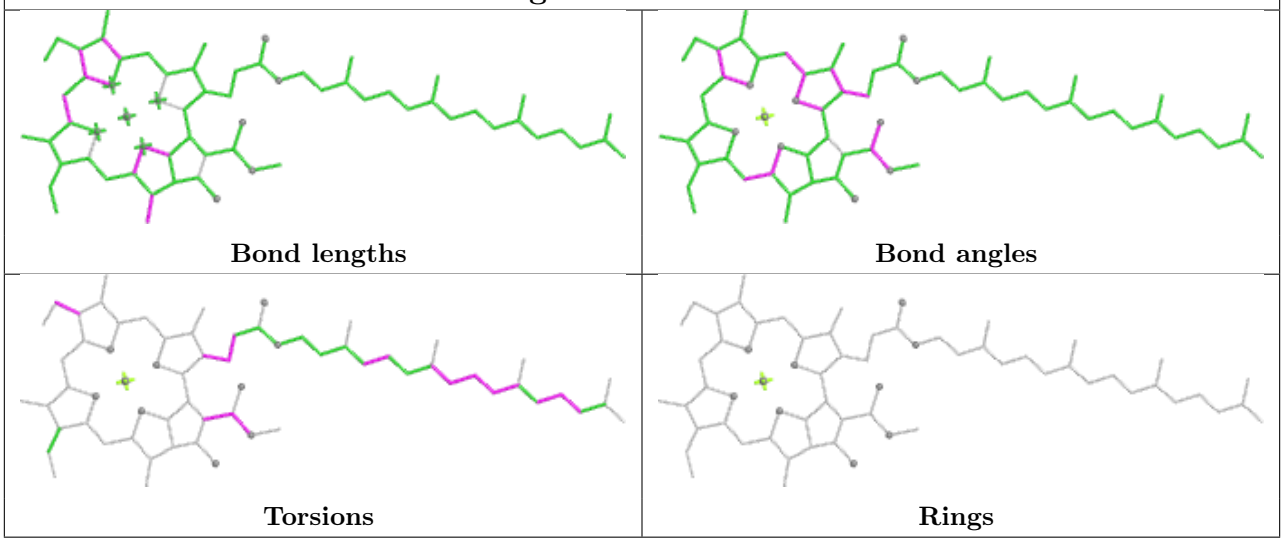
Ligand CLA B 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 847	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL V 606



Ligand CLA 9 611



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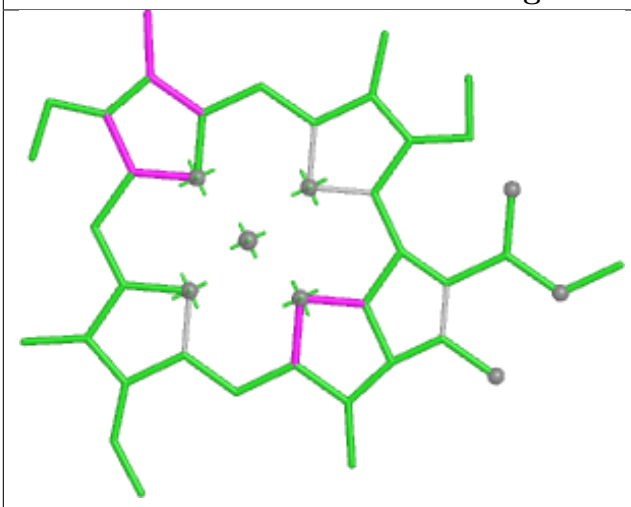

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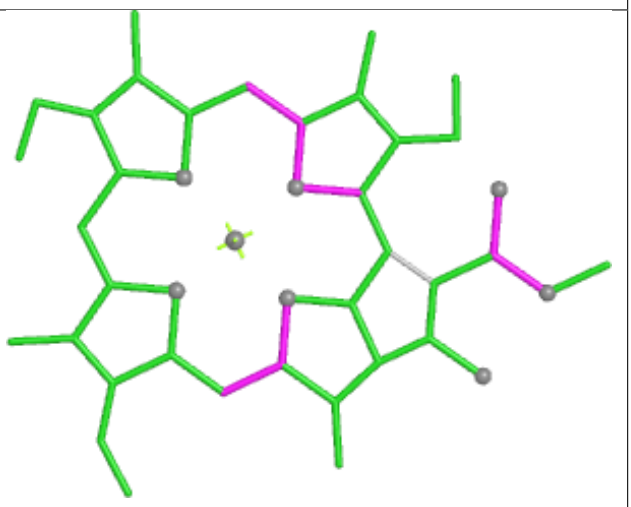
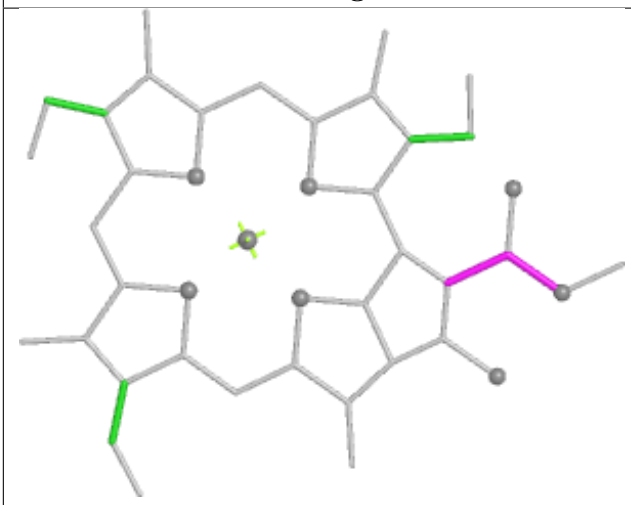


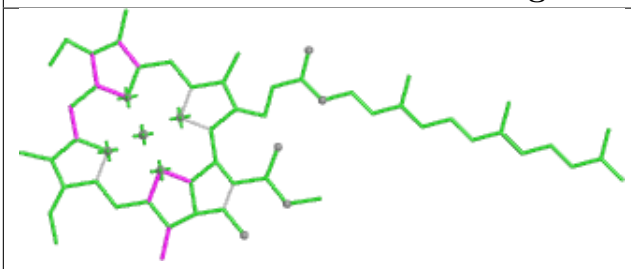
Bond angles



Torsions

Rings

Ligand CLA 5 602



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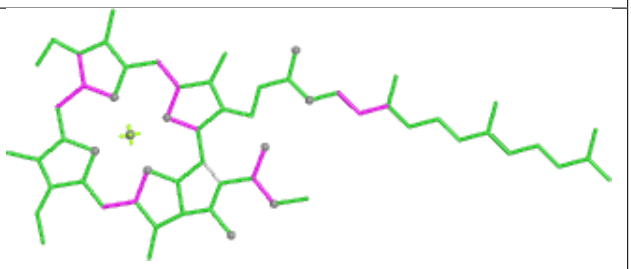
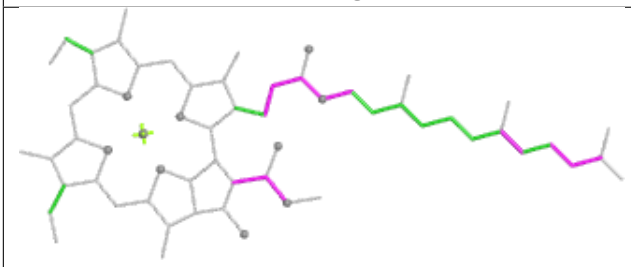


Bond angles



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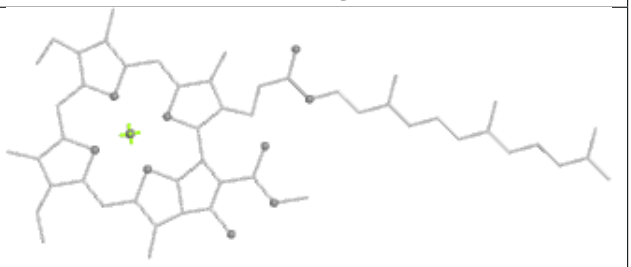
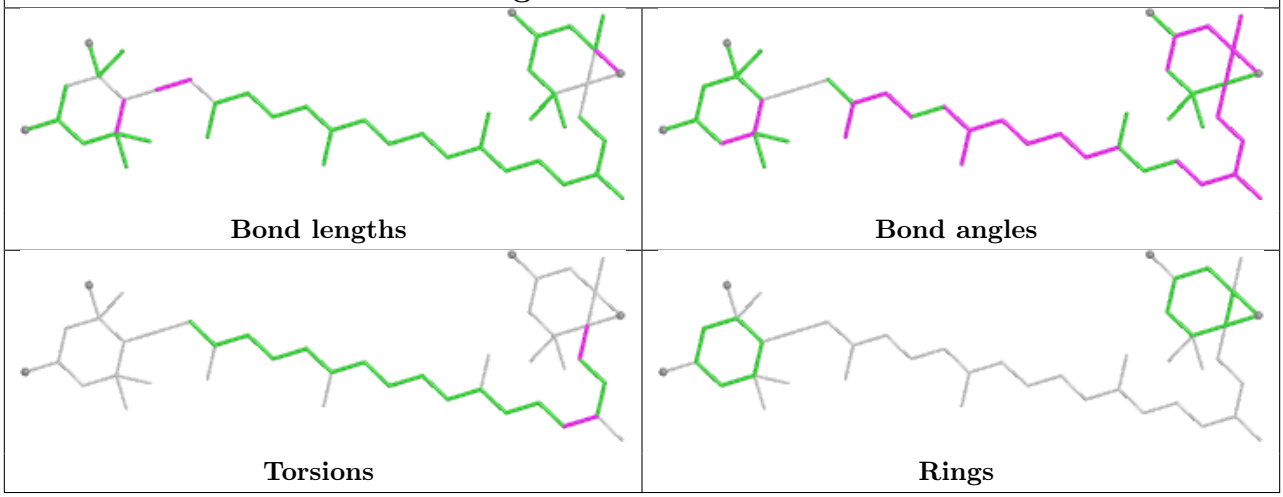
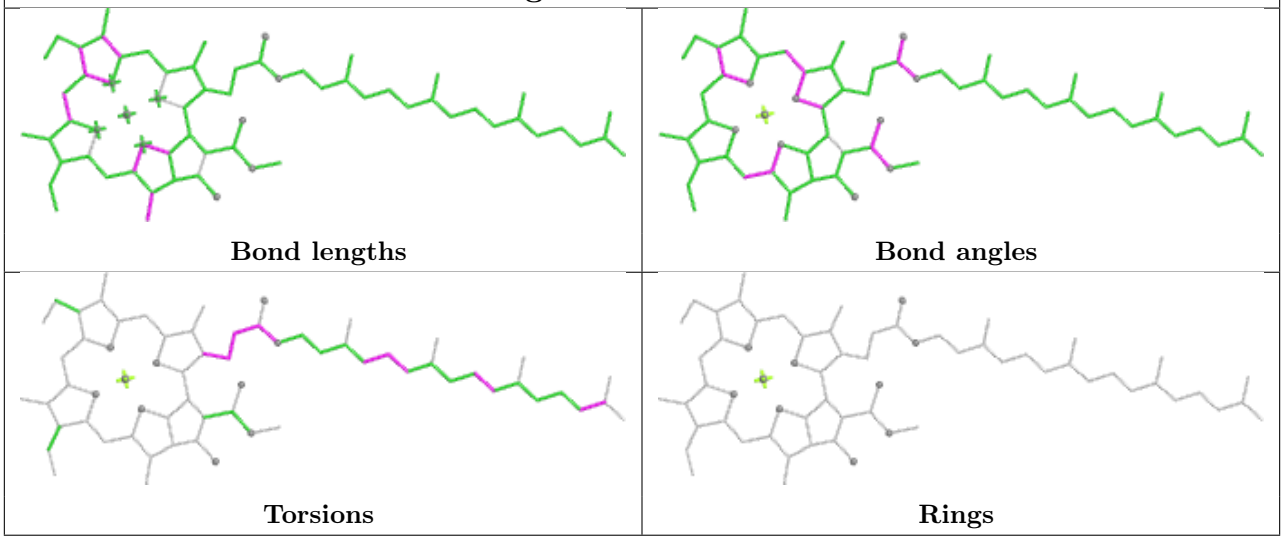


Rings

Ligand NEX U 2623



Ligand CLA B 825



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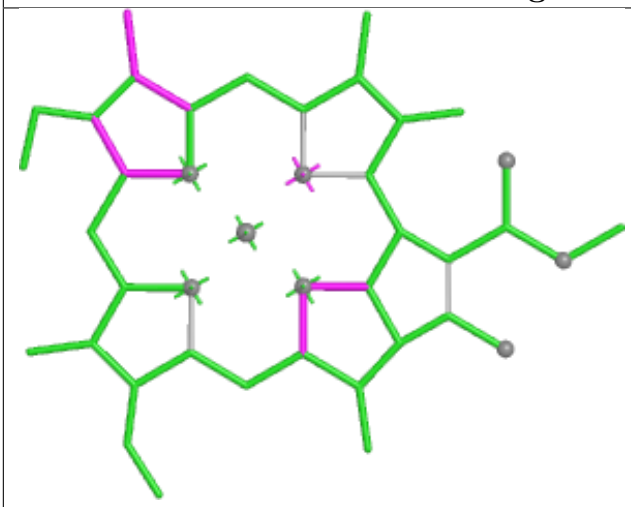

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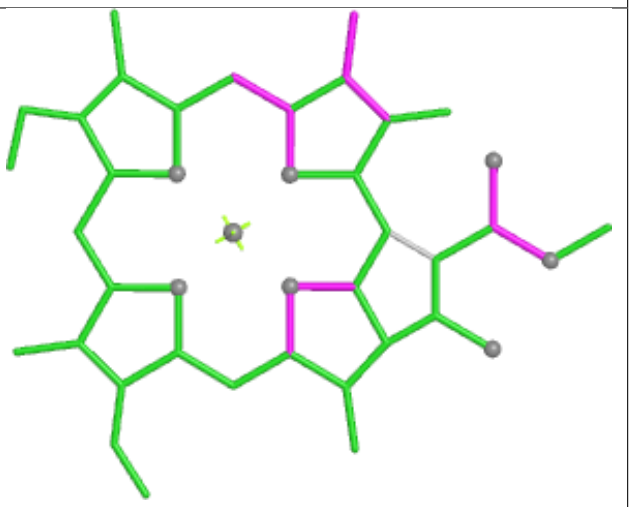
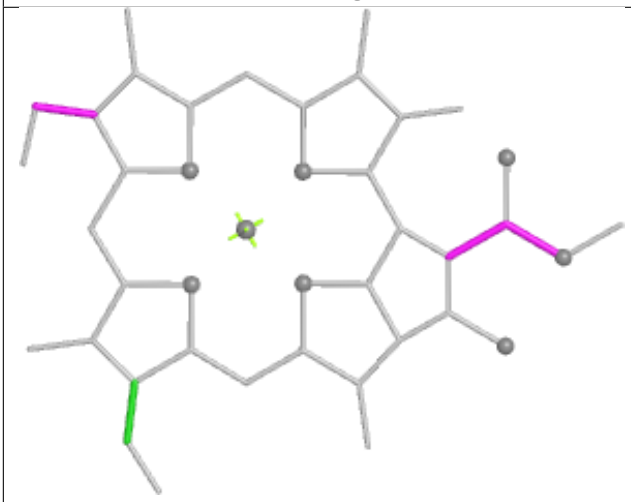


Bond angles



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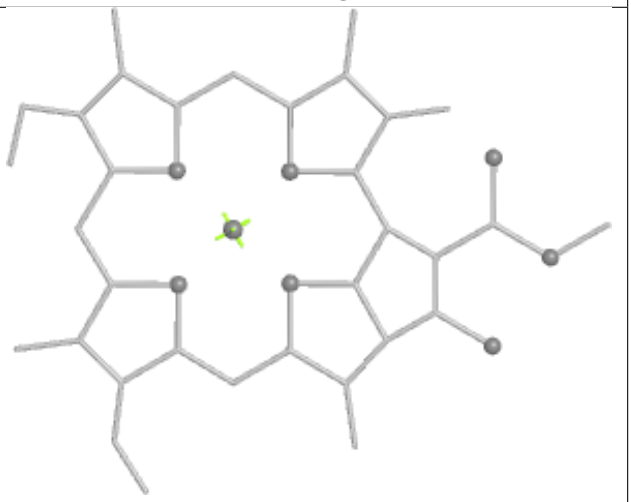
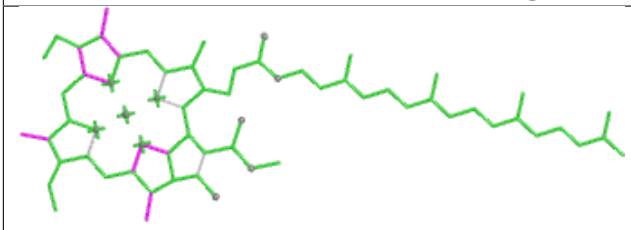
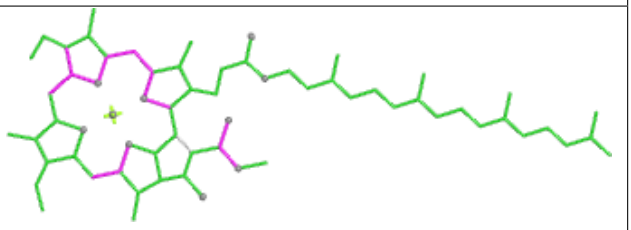


Rings

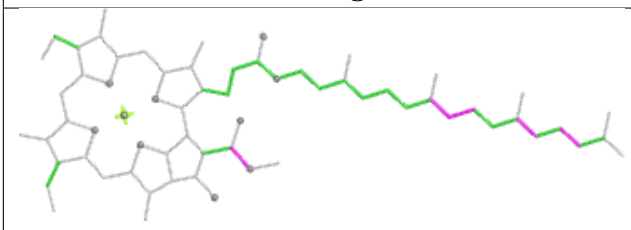
Ligand CLA A 802



Bond lengths



Bond angles



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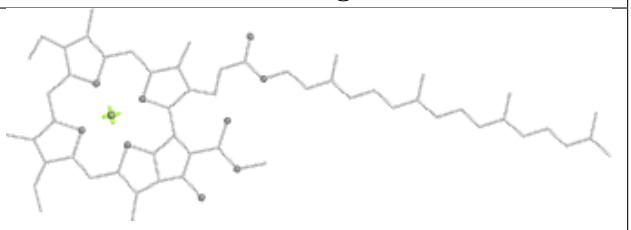
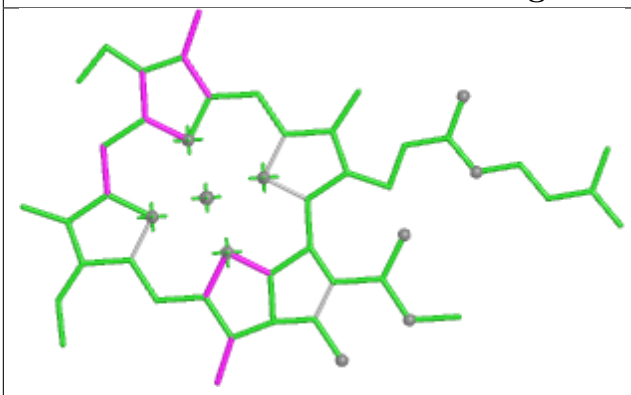
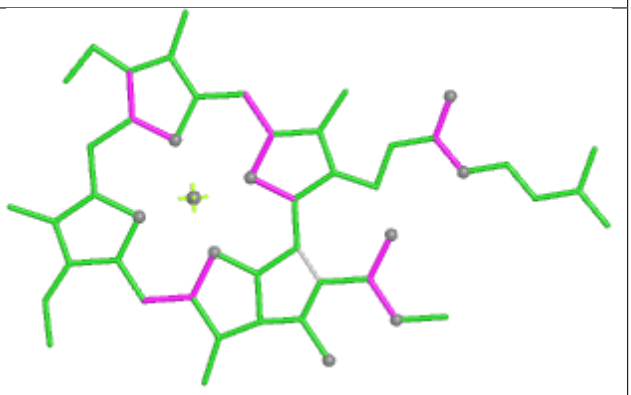
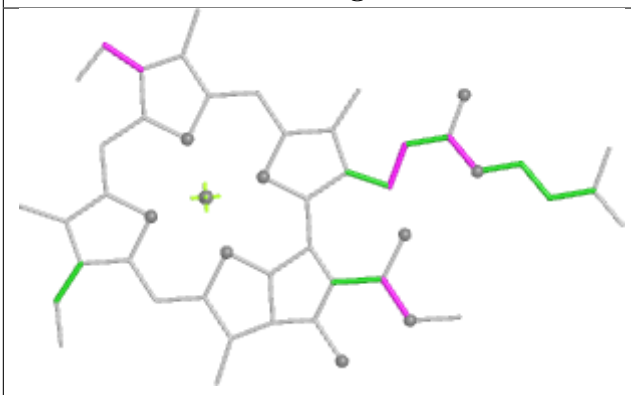
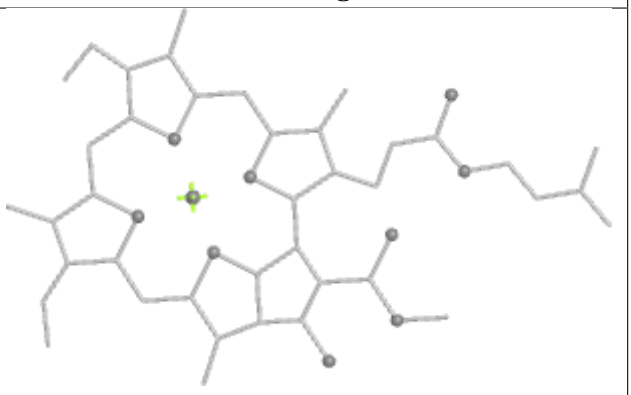
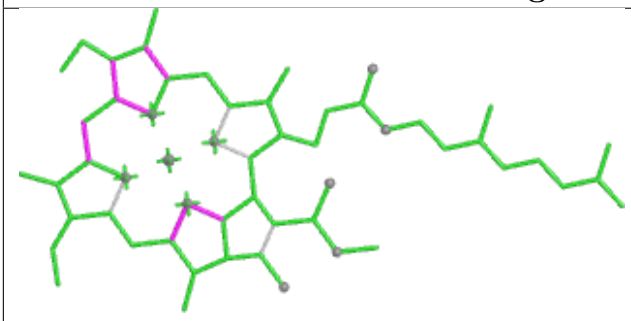
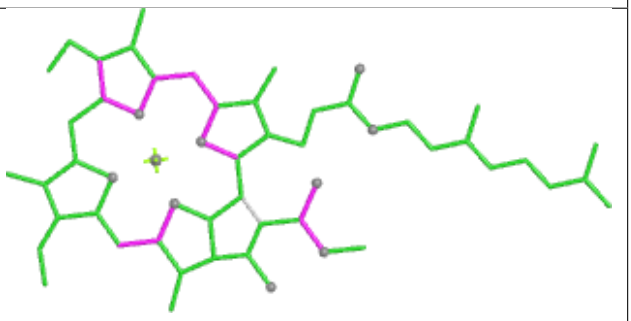
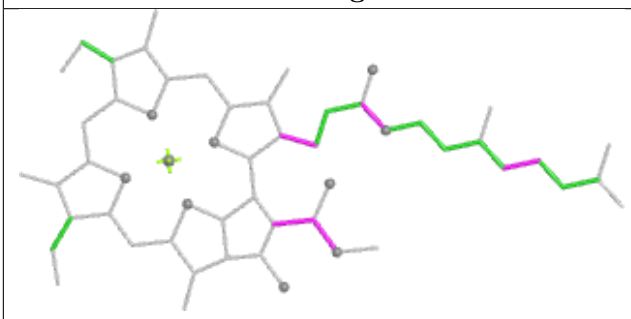
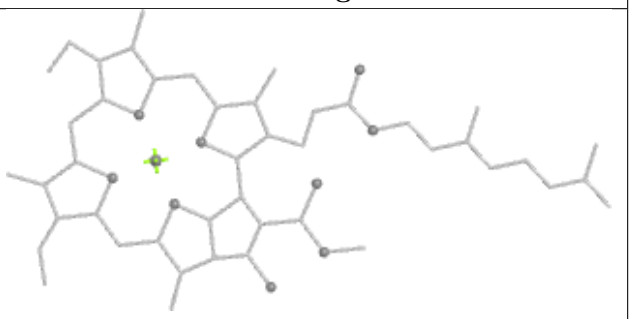
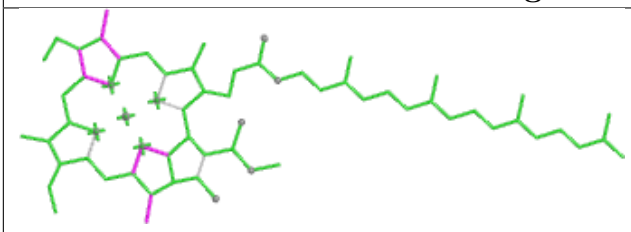


Rings

Ligand CLA J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 840



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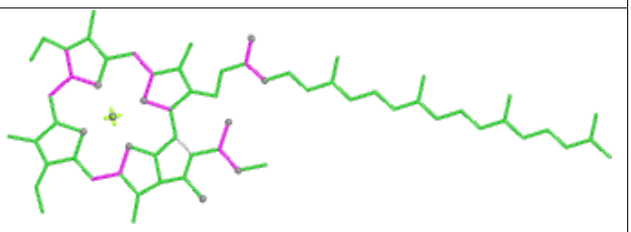
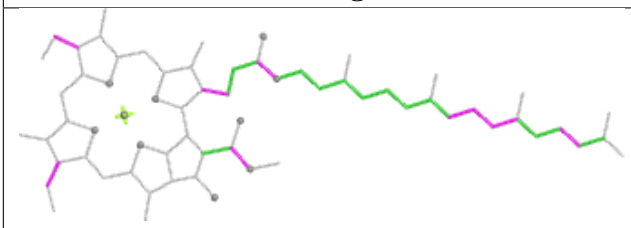


Bond angles



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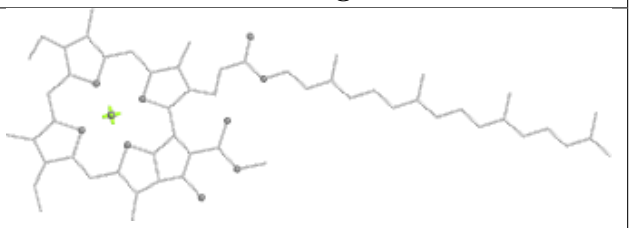
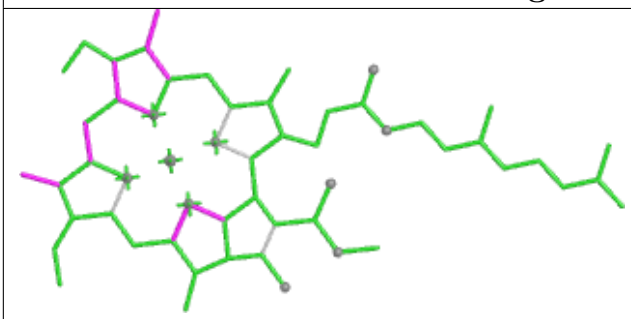


Rings

Ligand CLA 8 609



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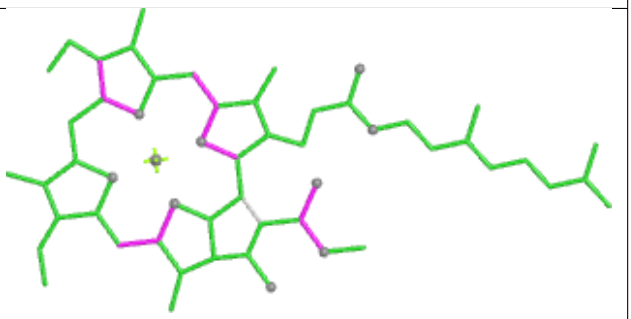

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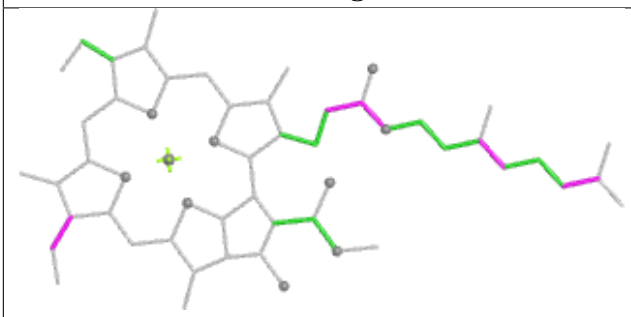

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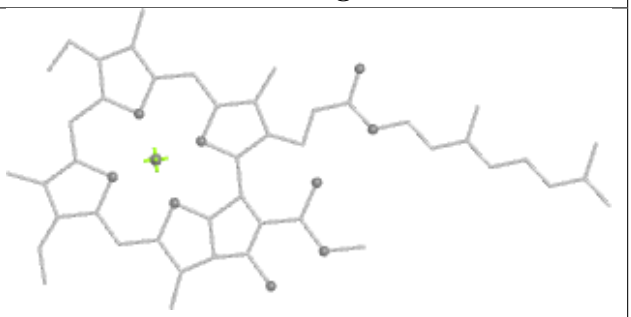
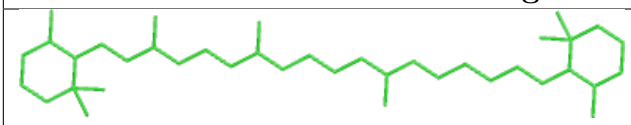


Rings

Ligand BCR A 856



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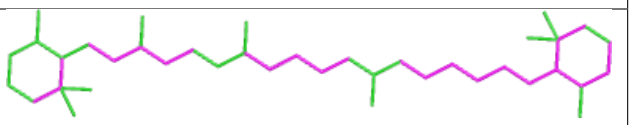

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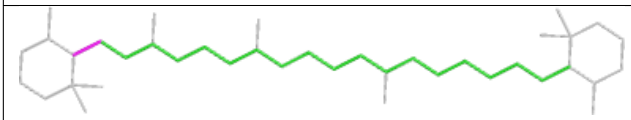

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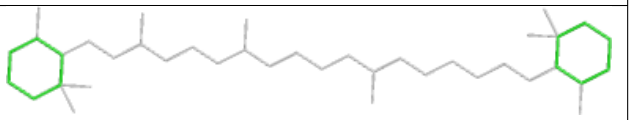
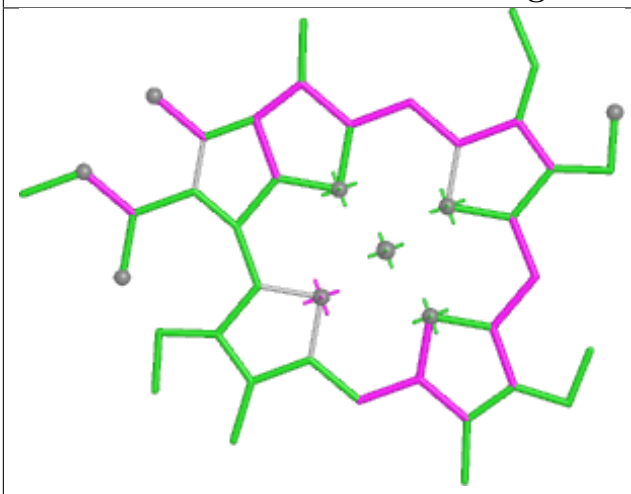


Rings

Ligand CHL 8 618



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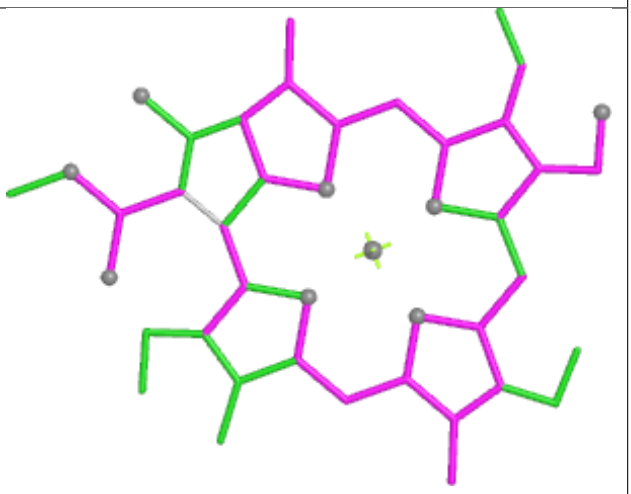

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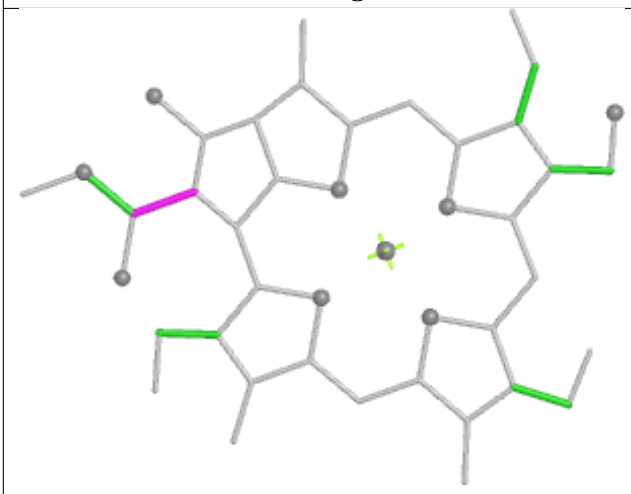
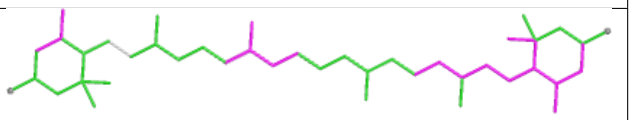


Torsions

Rings

Ligand LUT 7 618

Bond lengths



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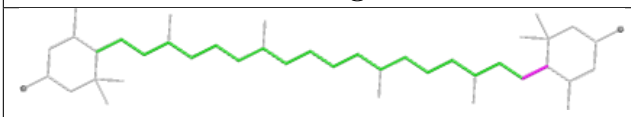

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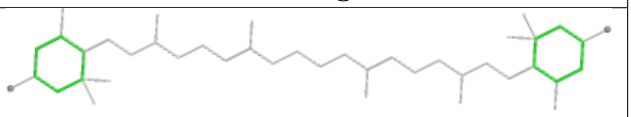
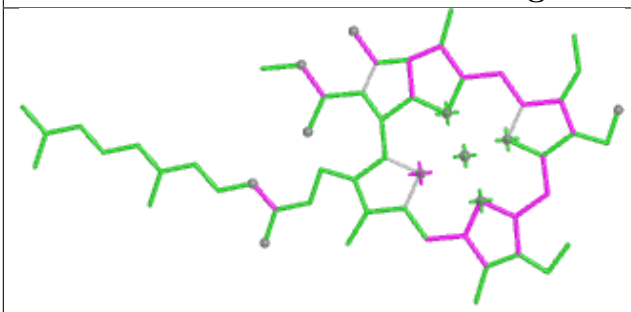
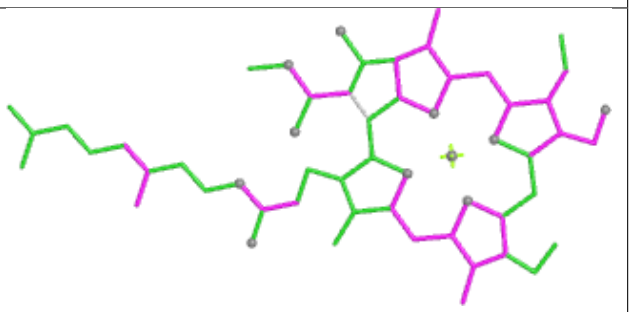
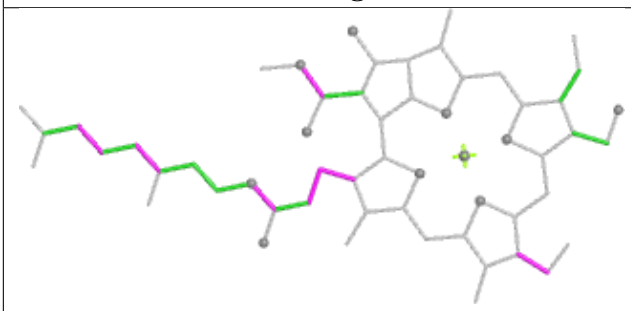
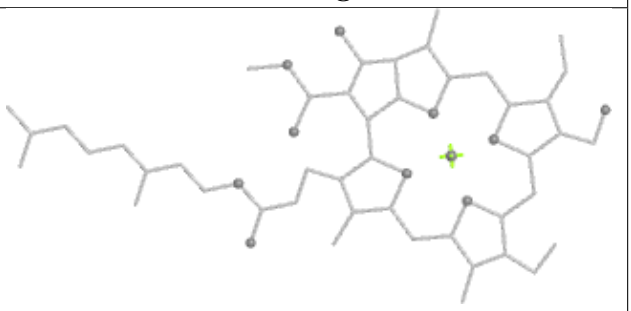
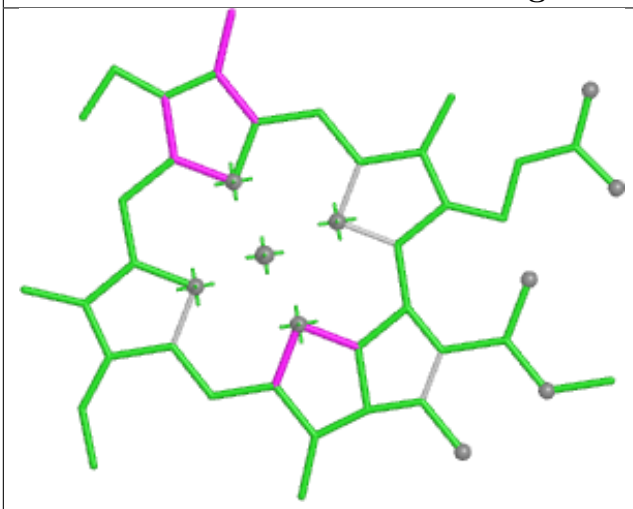


Rings

Ligand CHL 3 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 612



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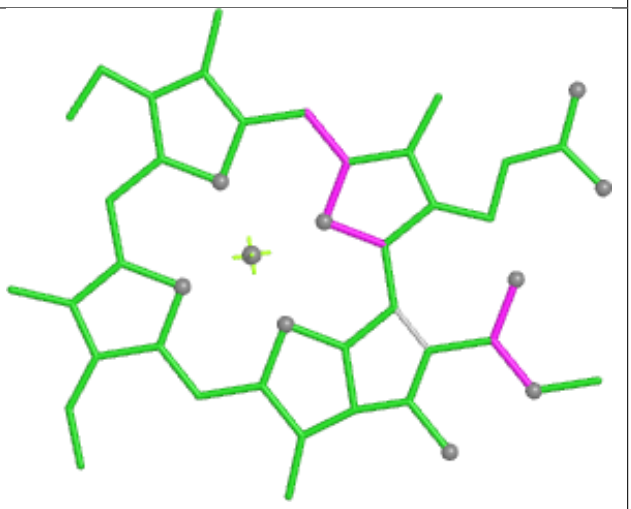
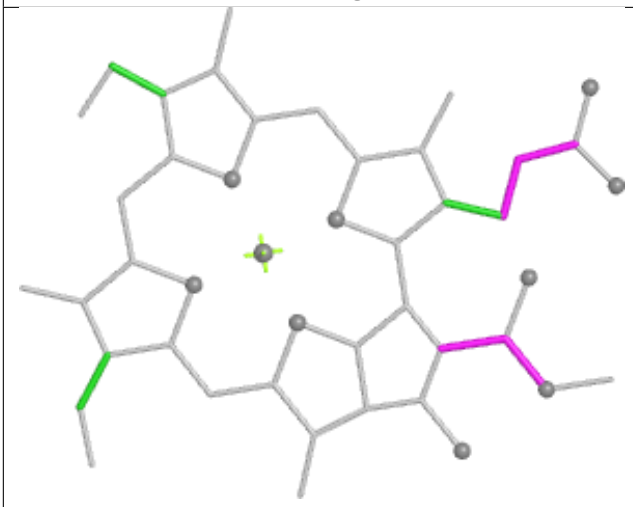


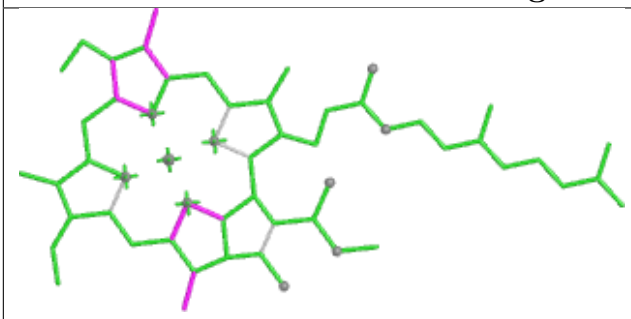
Bond angles



Torsions

Rings

Ligand CLA 7 613



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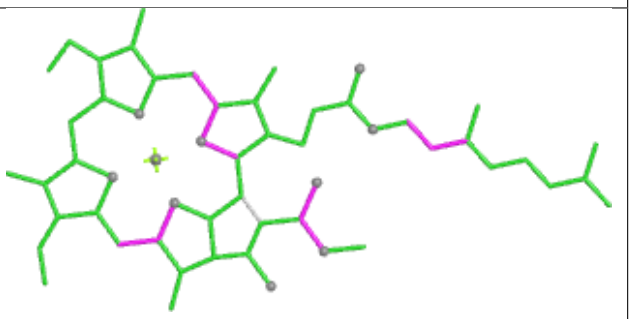

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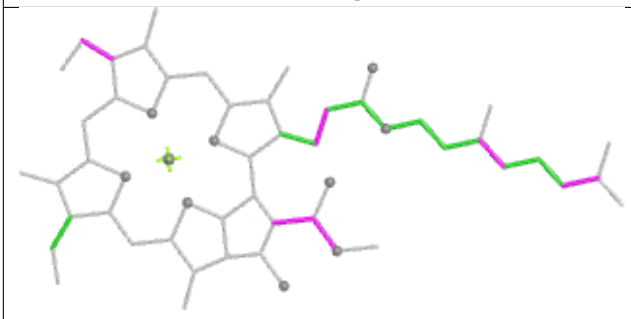

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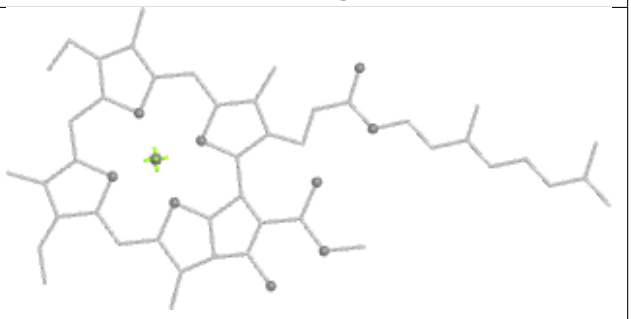
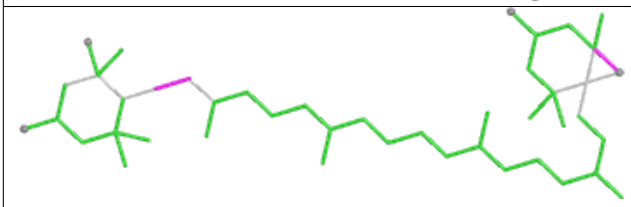


Rings

Ligand NEX 9 623



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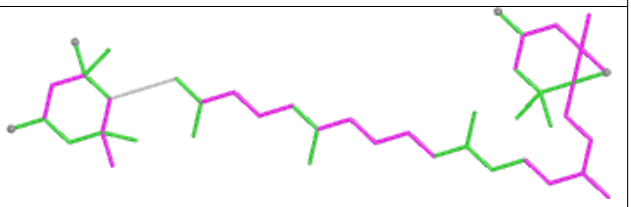

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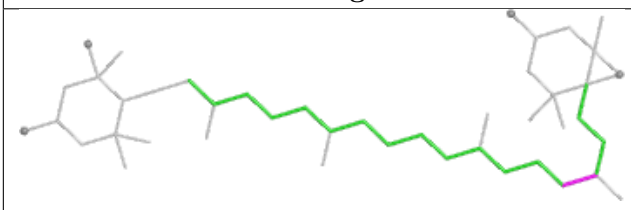

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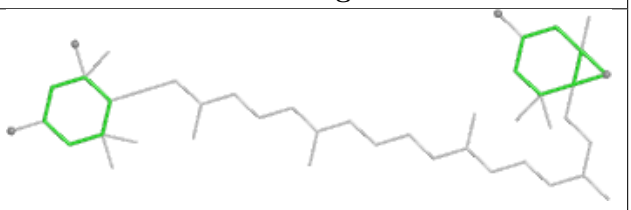
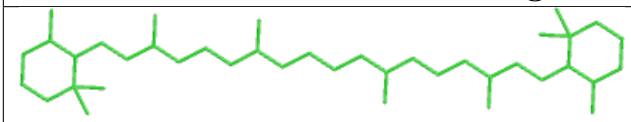


Rings

Ligand BCR 6 621



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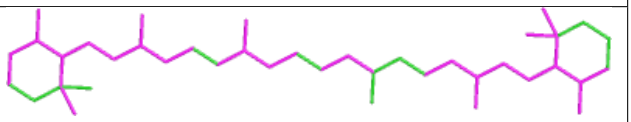
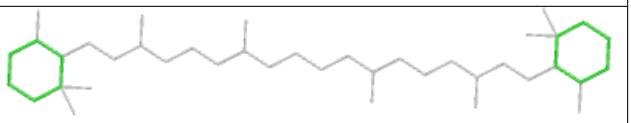


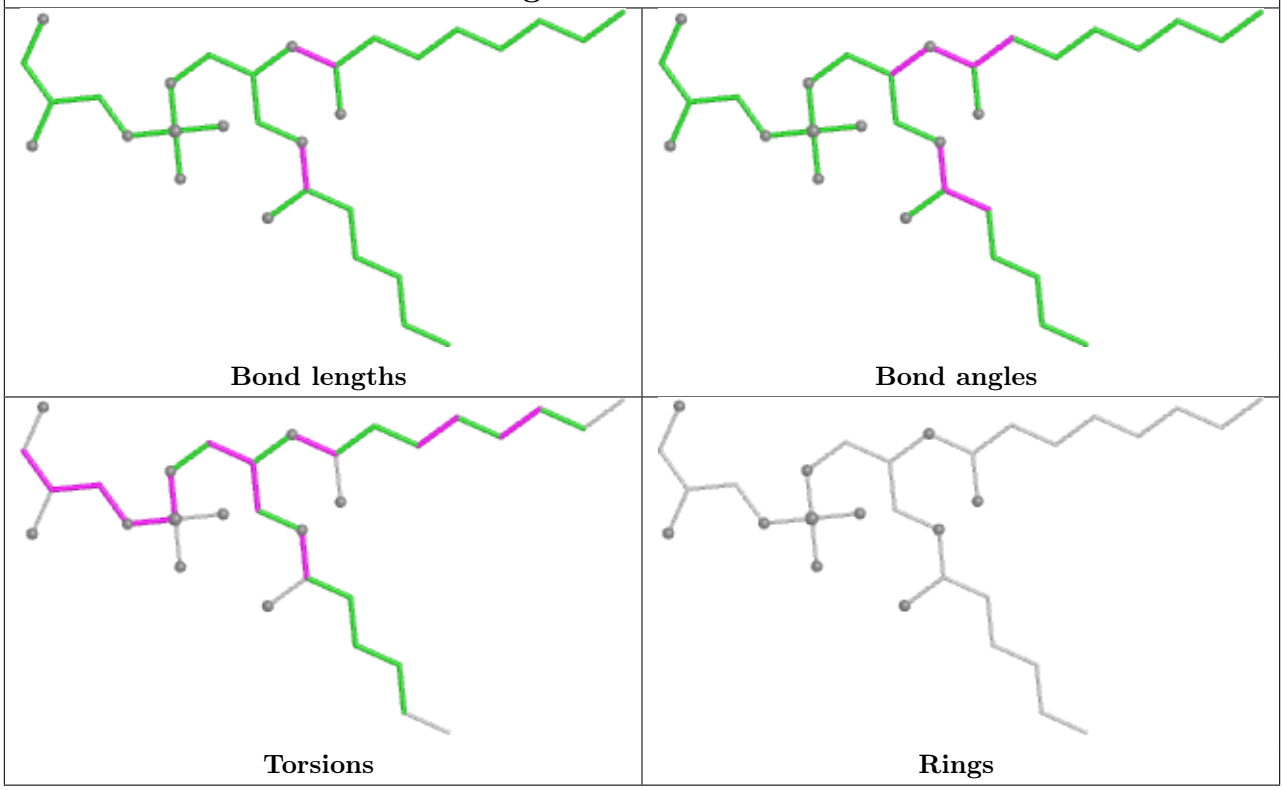
Bond angles

Torsions

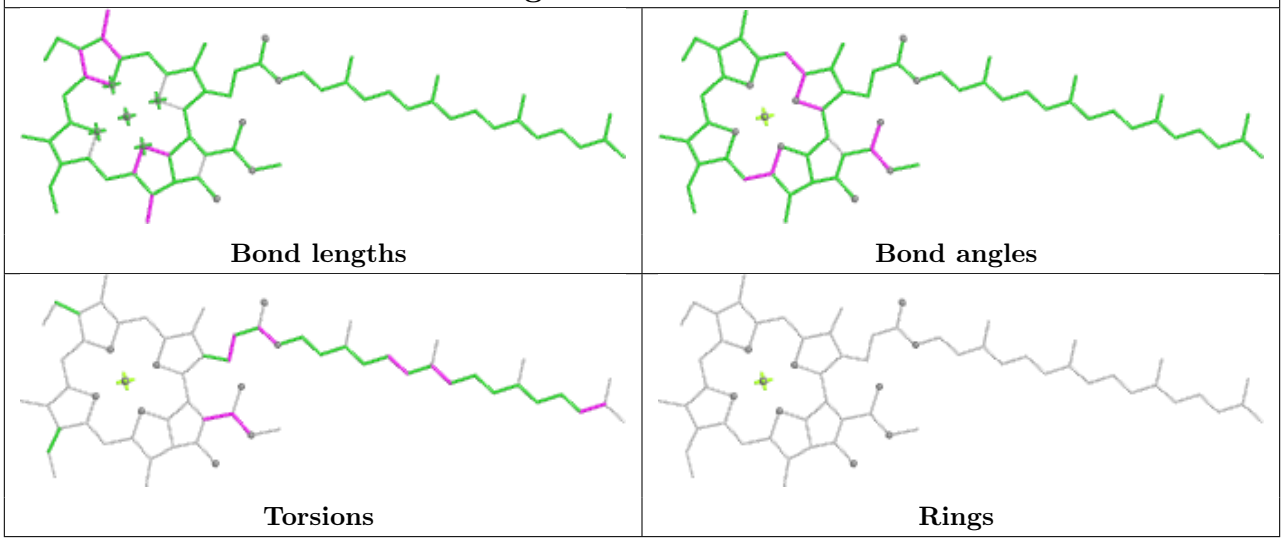


Rings

Ligand LHG A 847



Ligand CLA A 845



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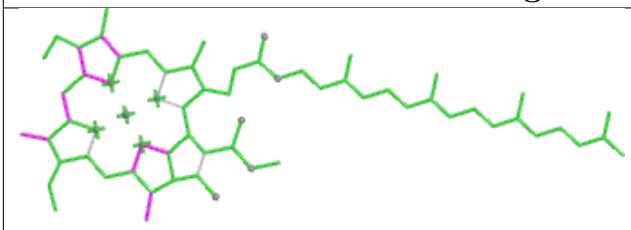
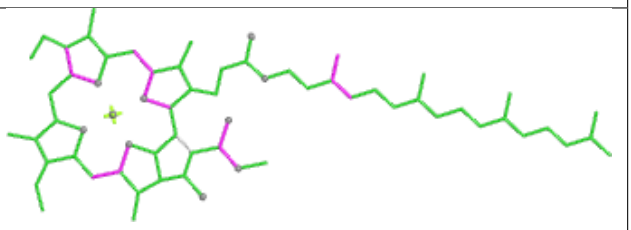
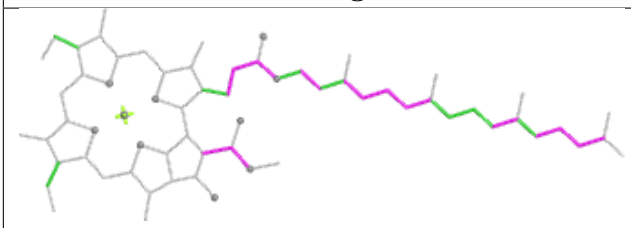
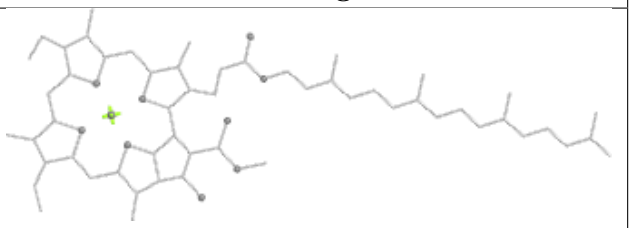
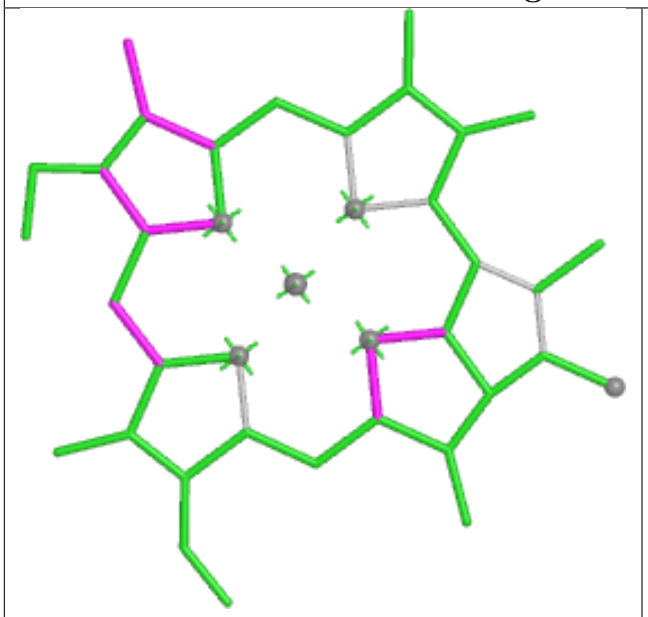
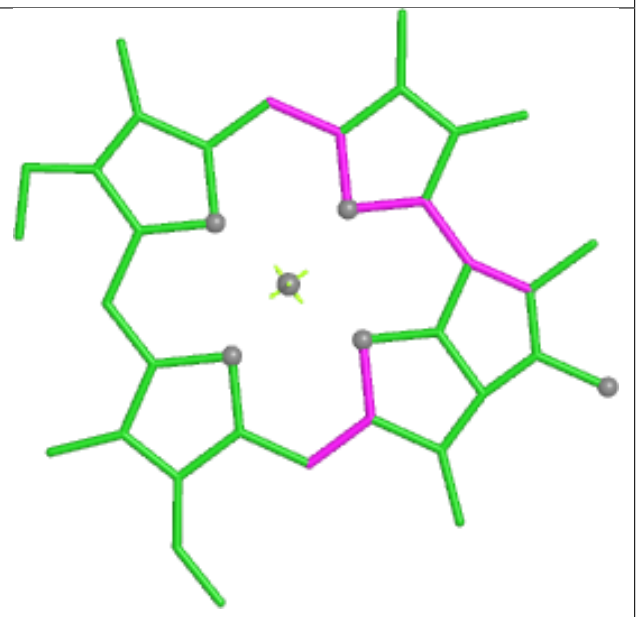
 Bond lengths	 Bond angles
 Torsions	 Rings

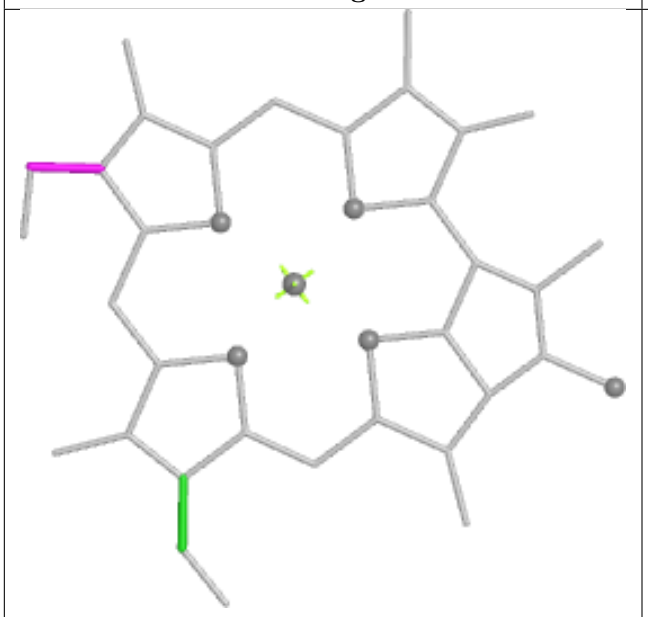
Ligand CLA H 201



Bond lengths



Bond angles



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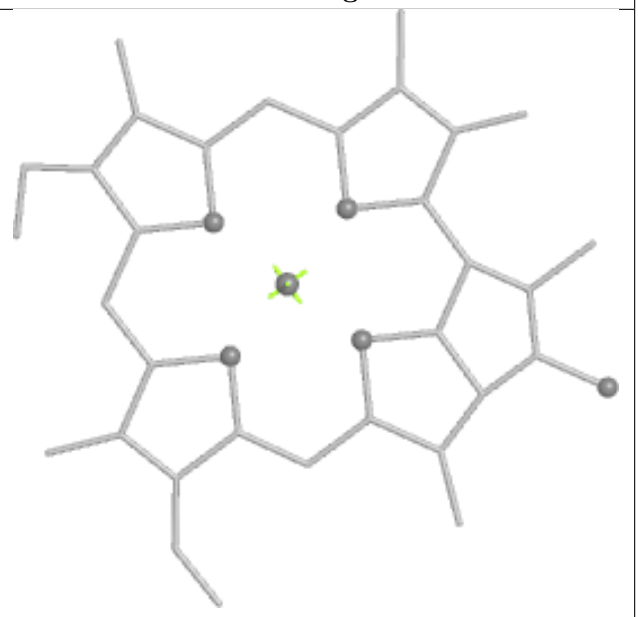
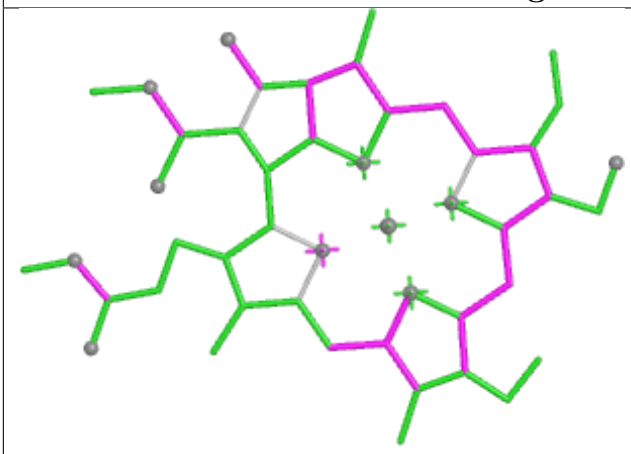


Rings

Ligand CHL 6 607



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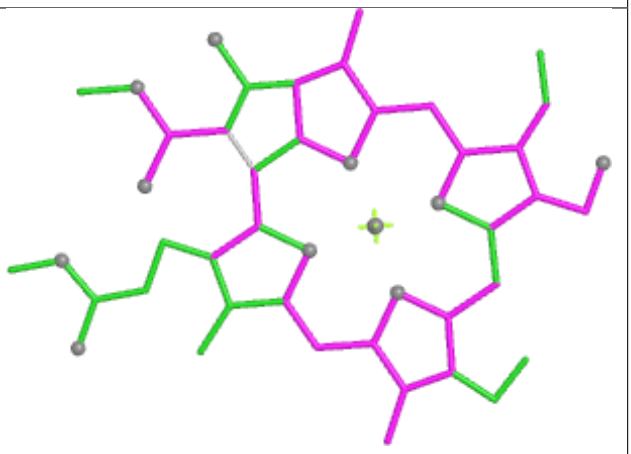
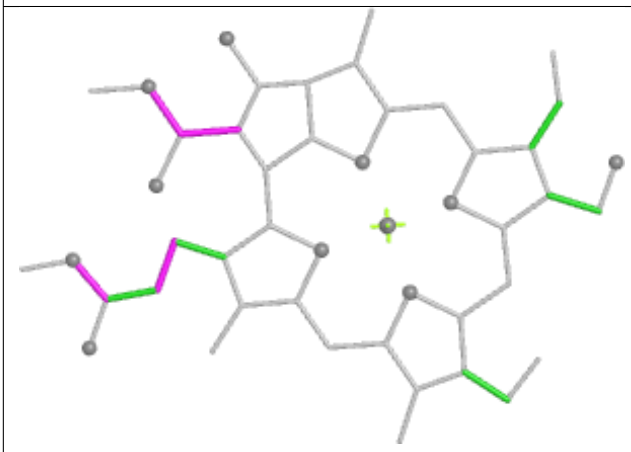


Bond angles



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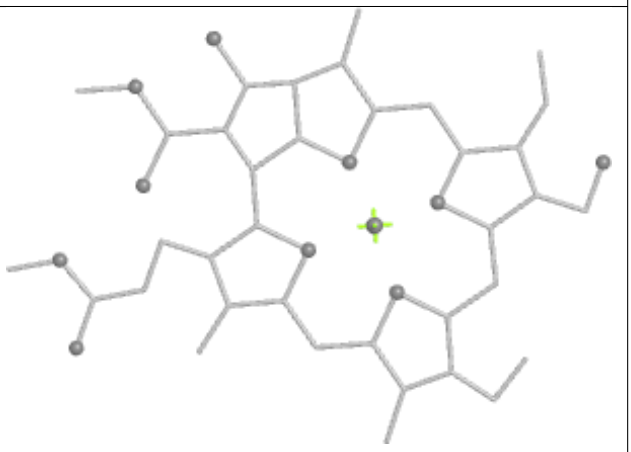
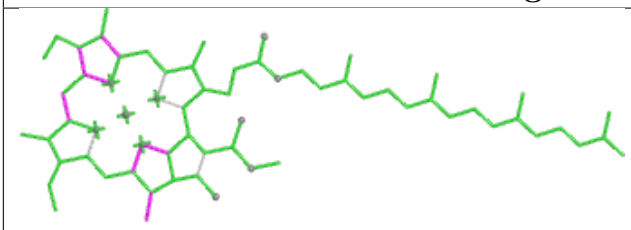


Rings

Ligand CLA B 814



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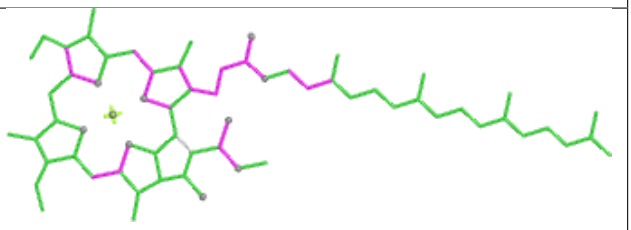
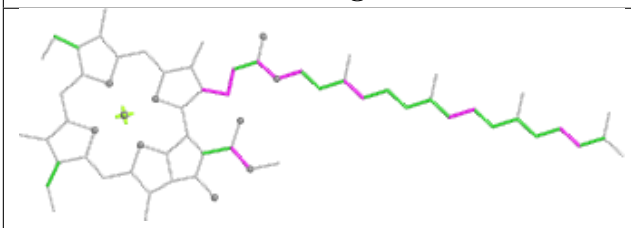


Bond angles



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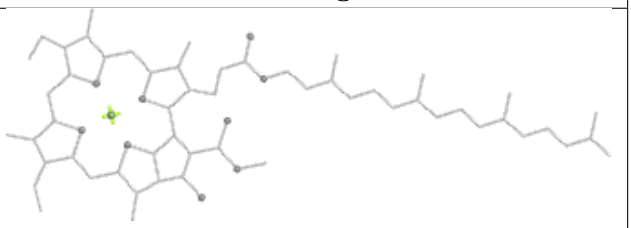
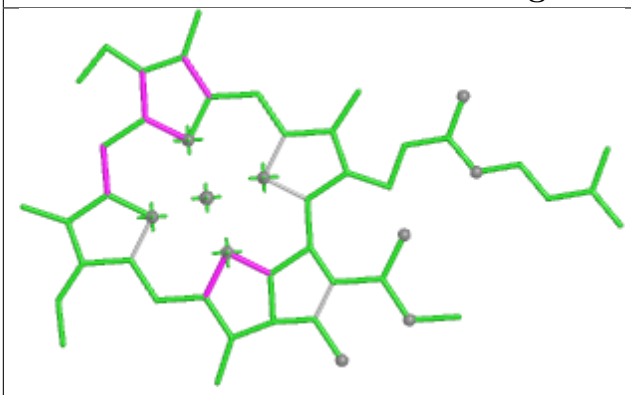
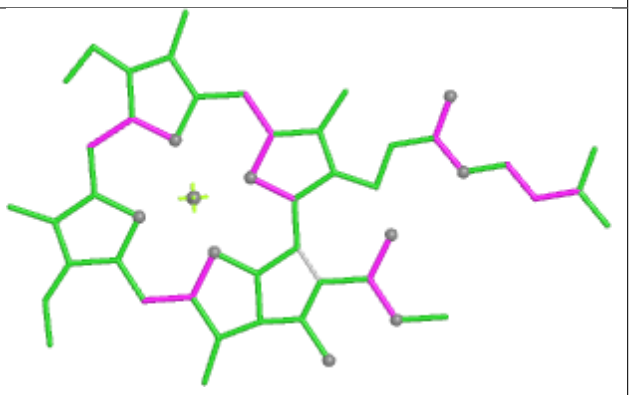


Rings

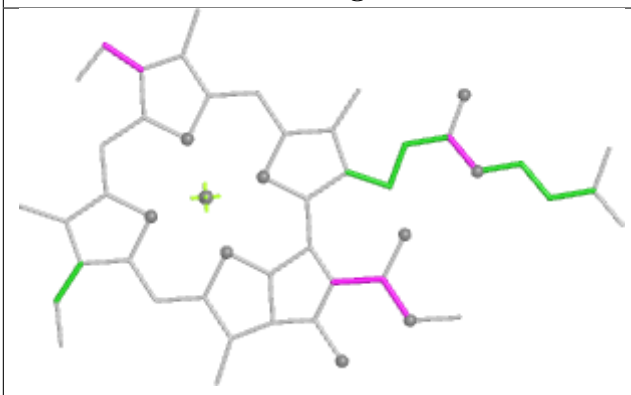
Ligand CLA 8 604



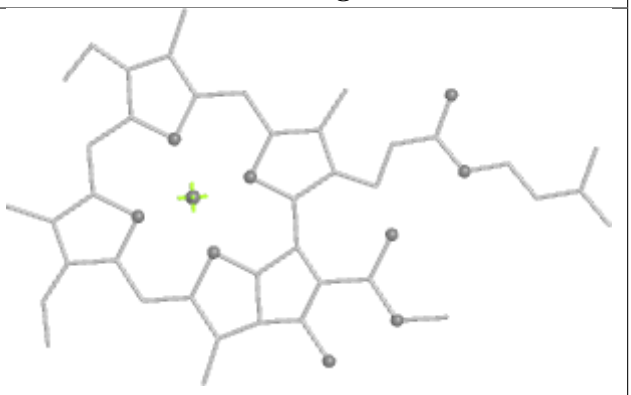
Bond lengths



Bond angles



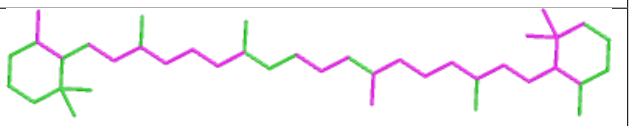
Torsions



Rings

Ligand BCR 4 621

Bond lengths



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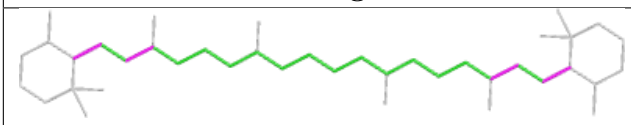

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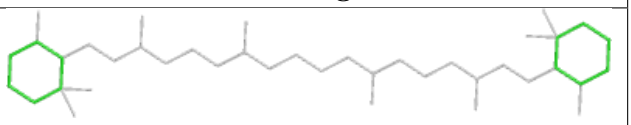

Rings

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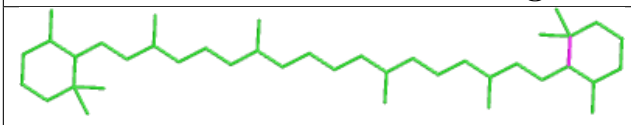

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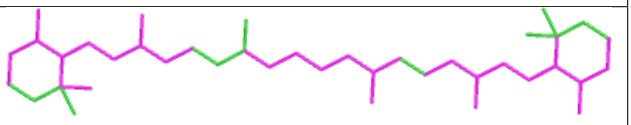
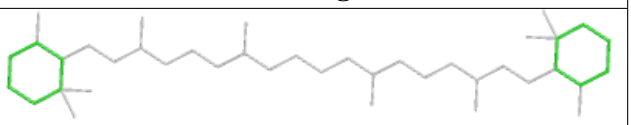
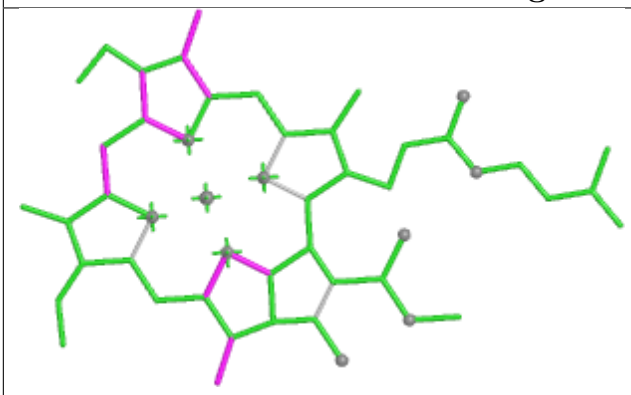
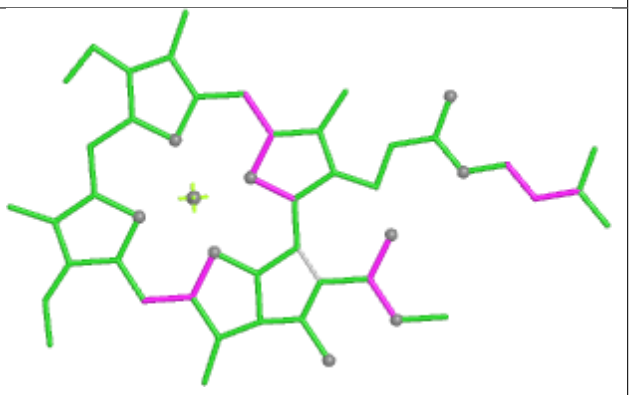
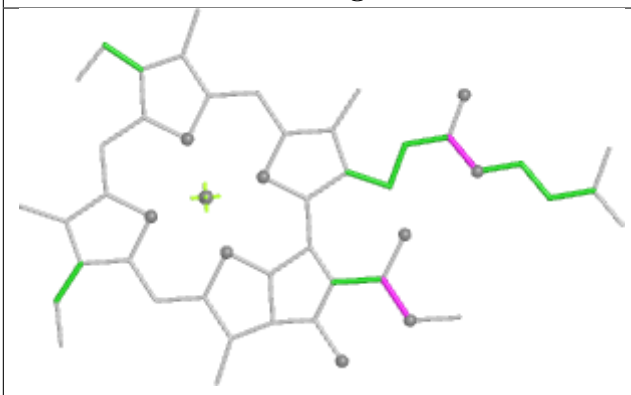
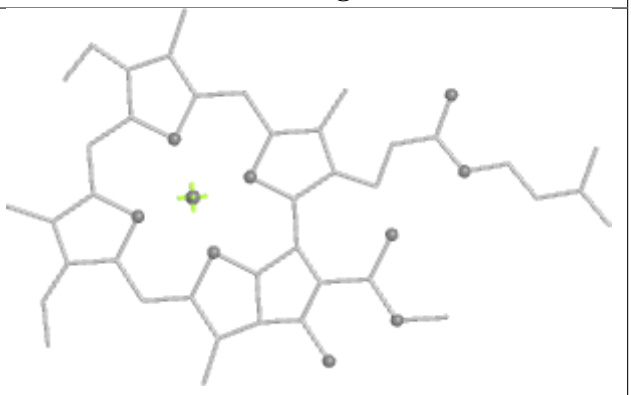


Bond angles

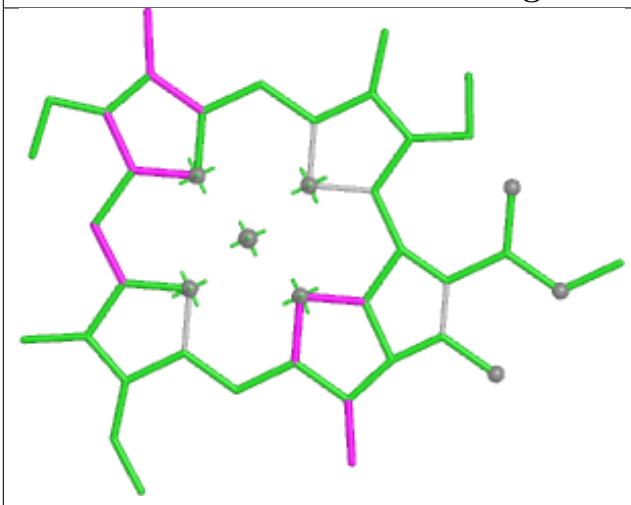
Torsions



Rings

Ligand CLA 6 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 206



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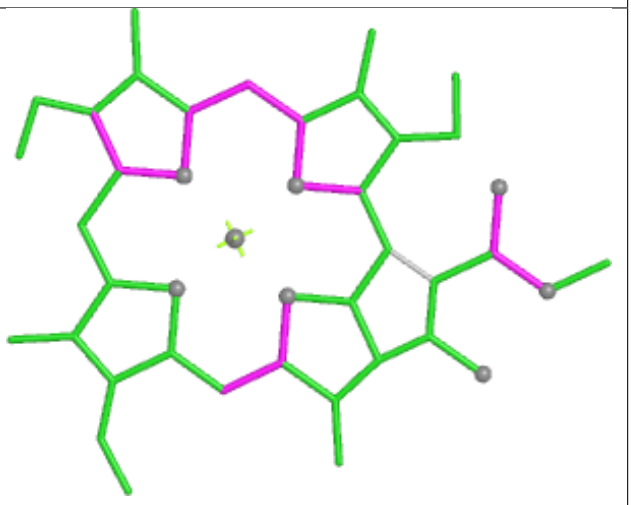
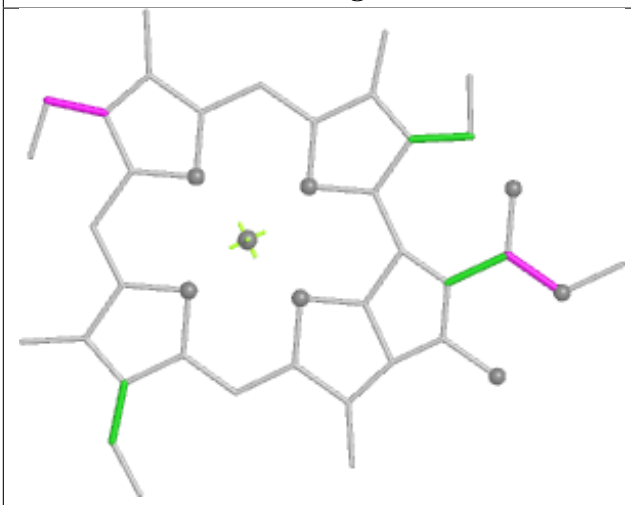


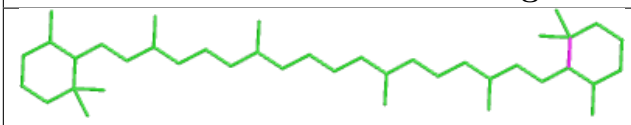
Bond angles



Torsions

Rings

Ligand BCR K 205



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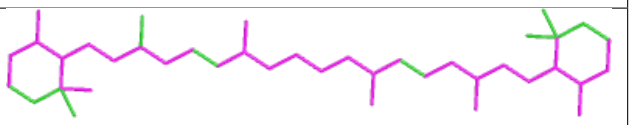

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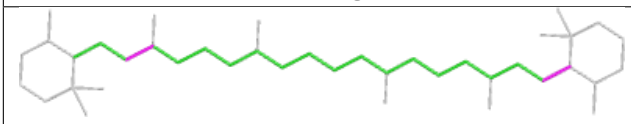

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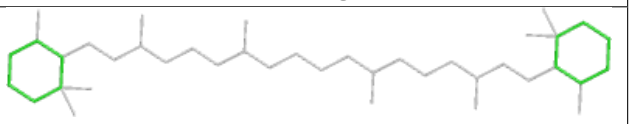
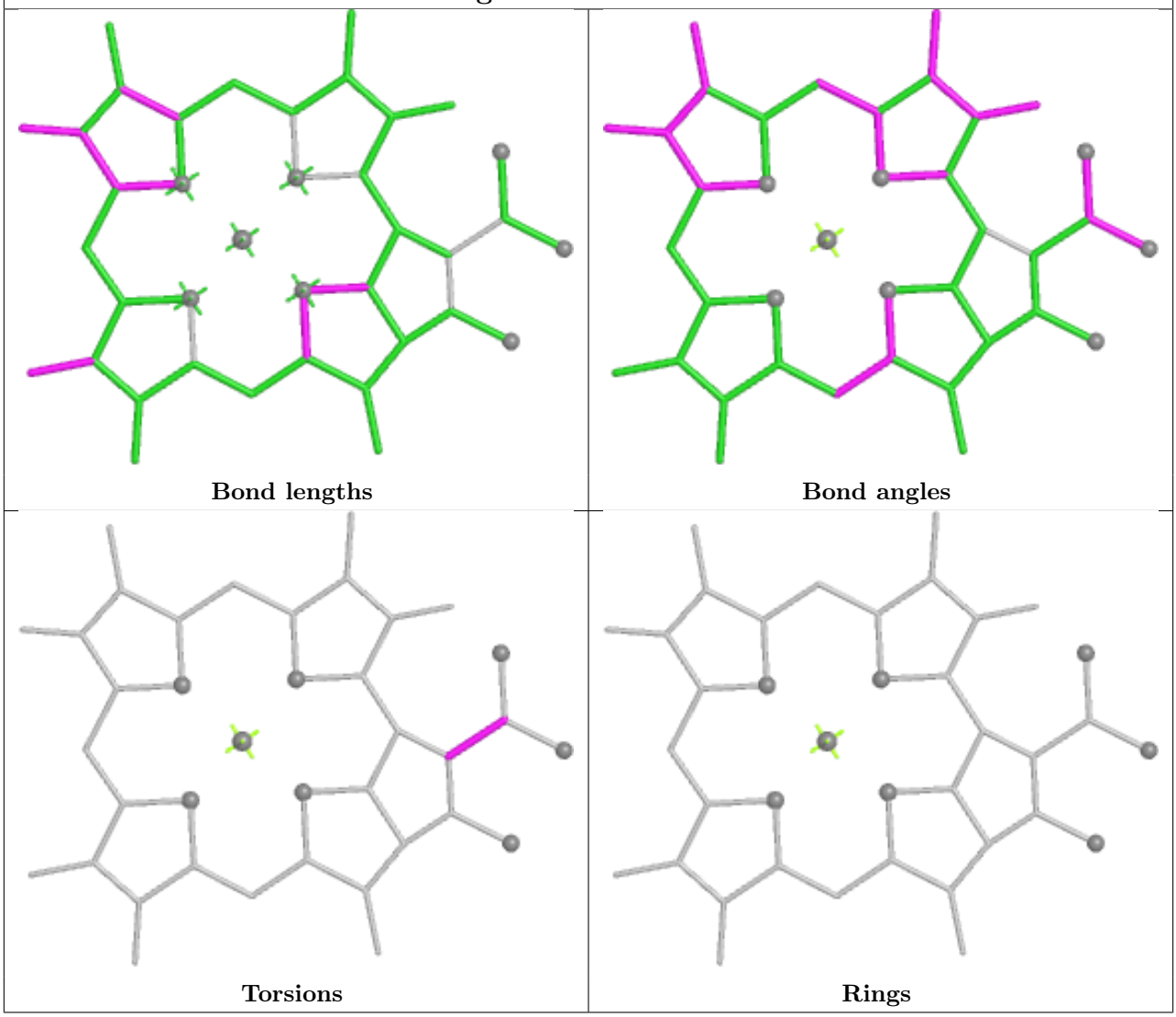
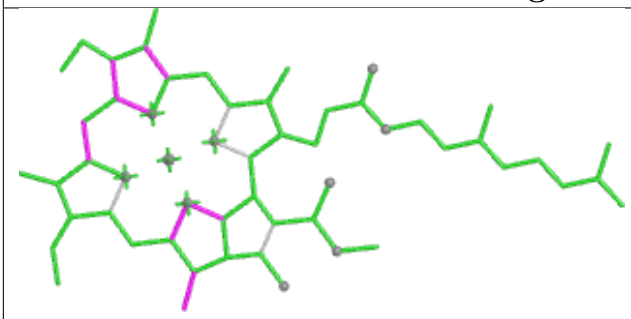
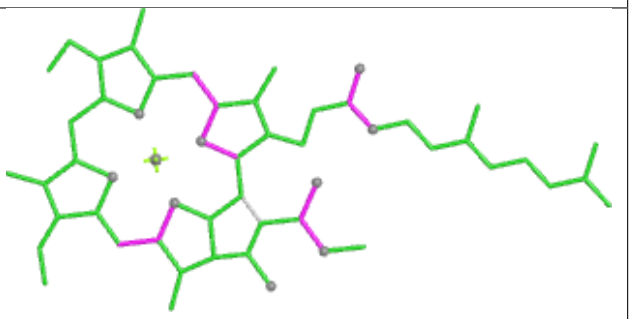
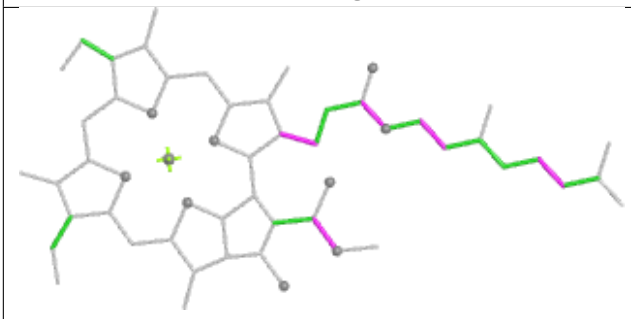
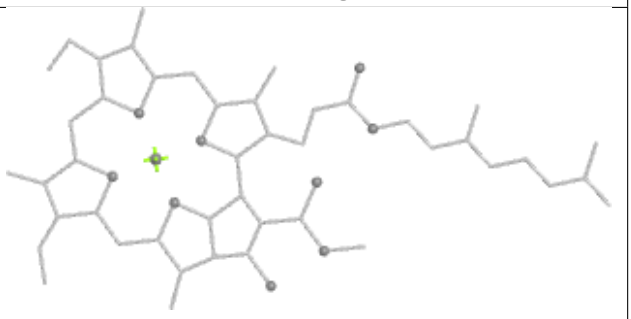


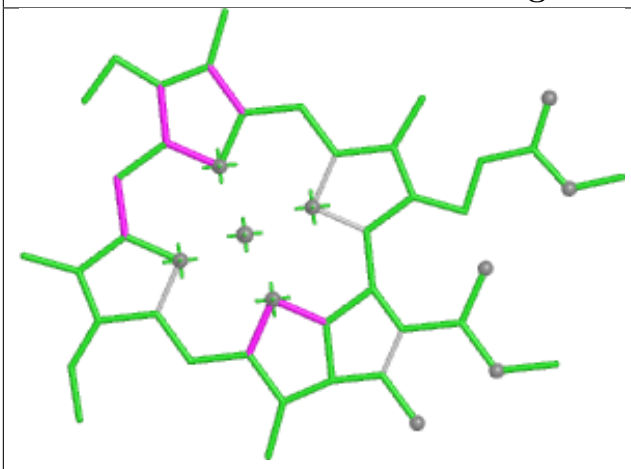
Rings

Ligand CLA W 612

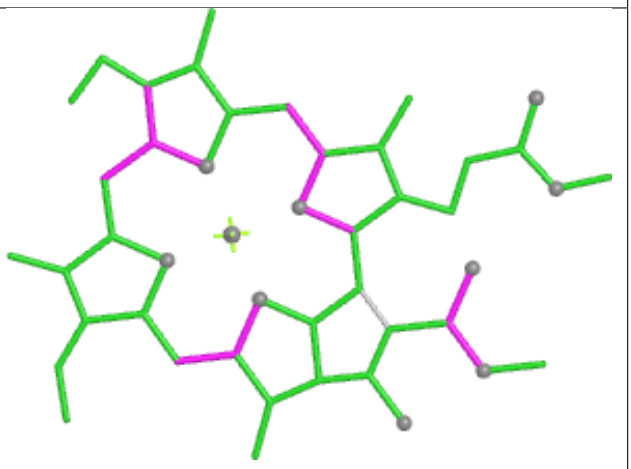


Ligand CLA 4 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

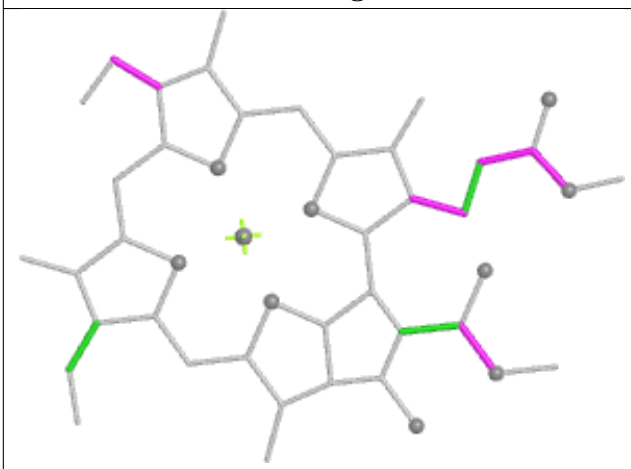
Ligand CLA 7 606



Bond lengths



Bond angles



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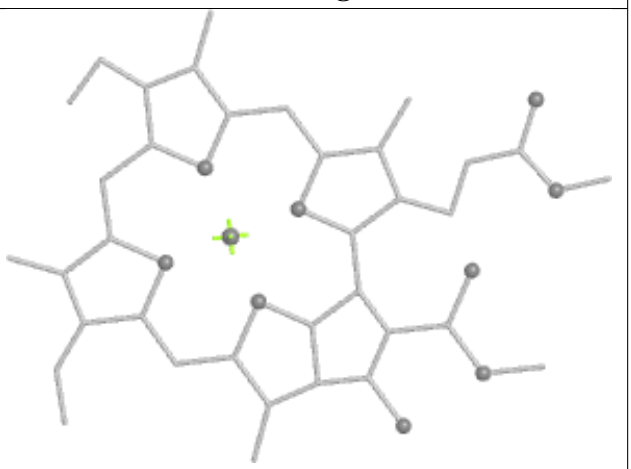
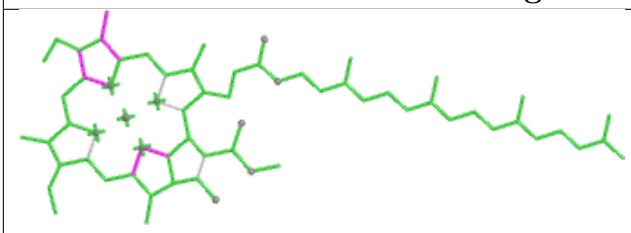


Rings

Ligand CLA B 804



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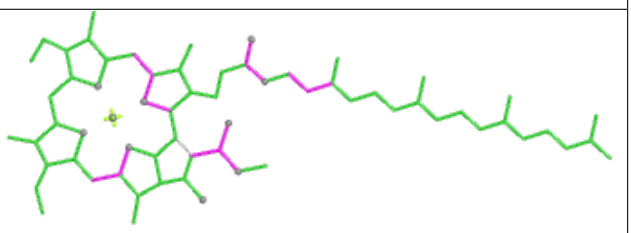
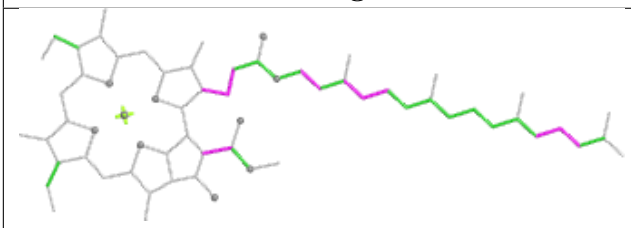


Bond angles



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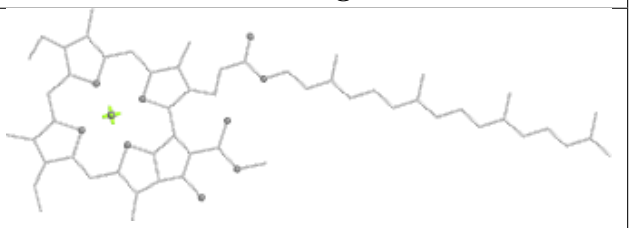
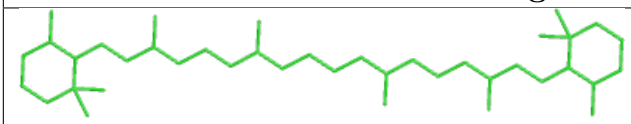


Rings

Ligand BCR I 101



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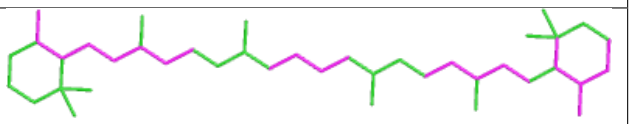
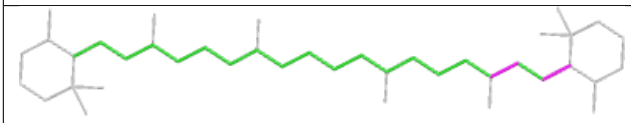


Bond angles



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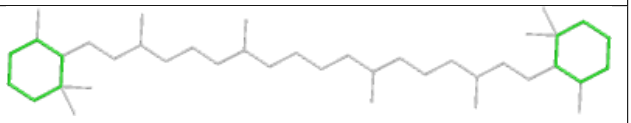
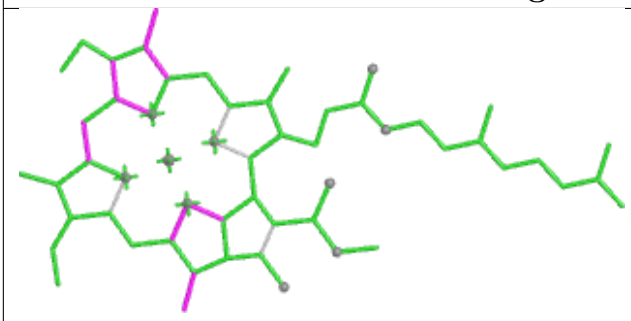
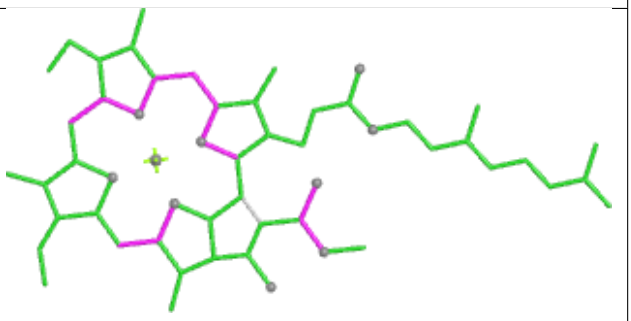


Rings

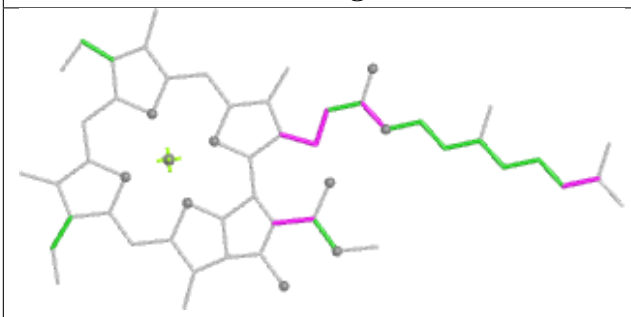
Ligand CLA 8 603



Bond lengths



Bond angles



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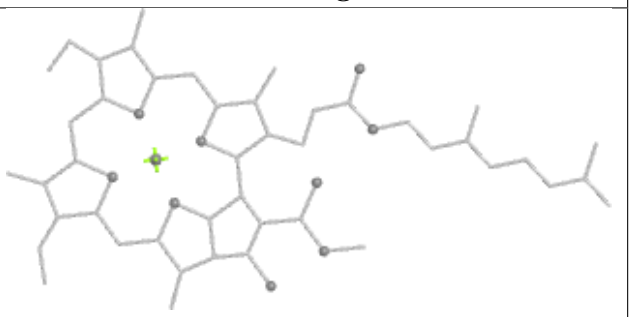
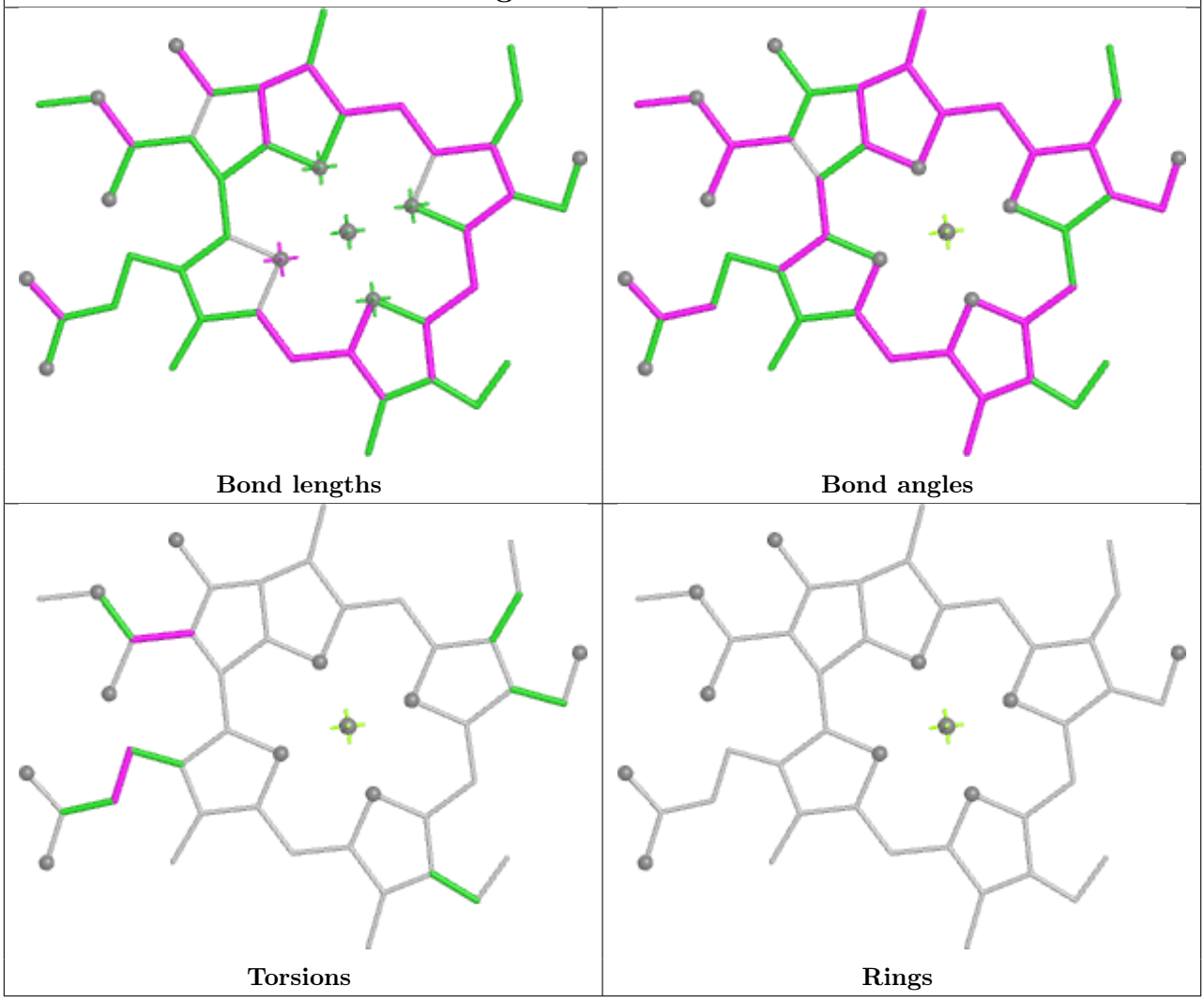
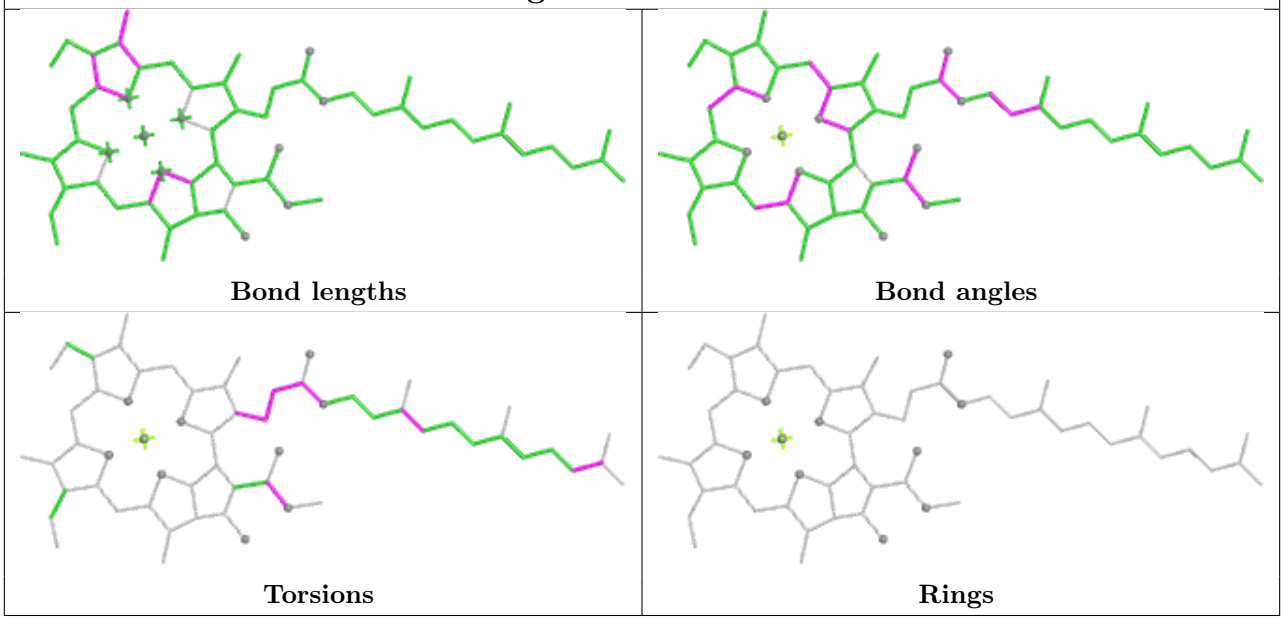


Rings

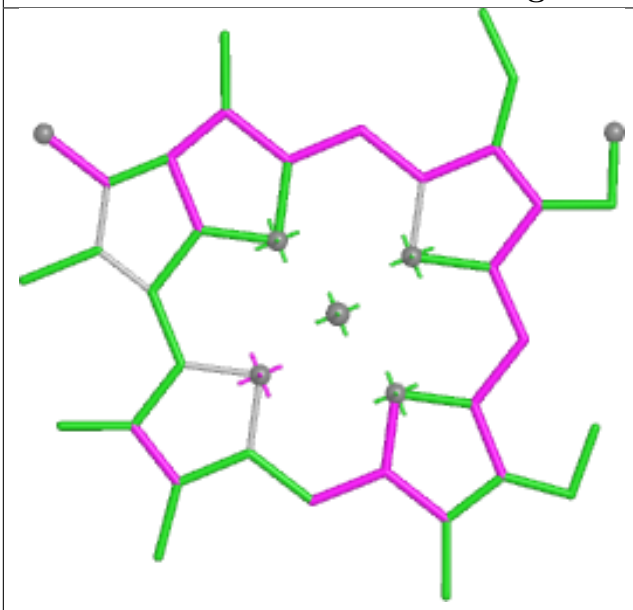
Ligand CHL 4 606



Ligand CLA L 304

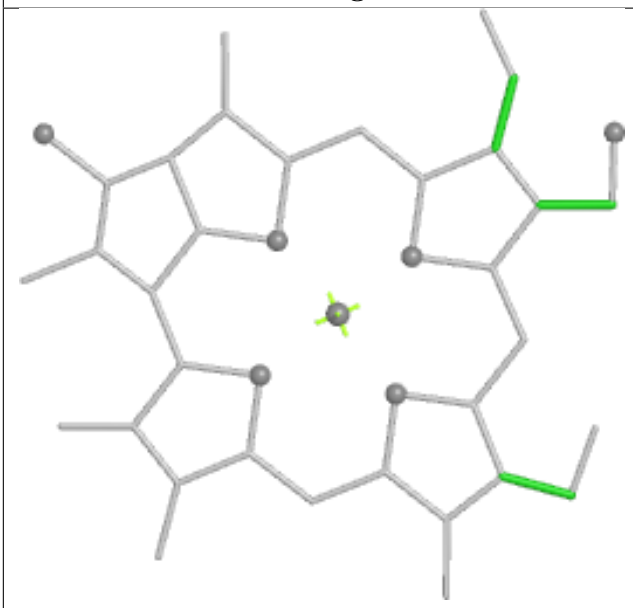


Ligand CHL 5 607



Bond lengths

Bond angles



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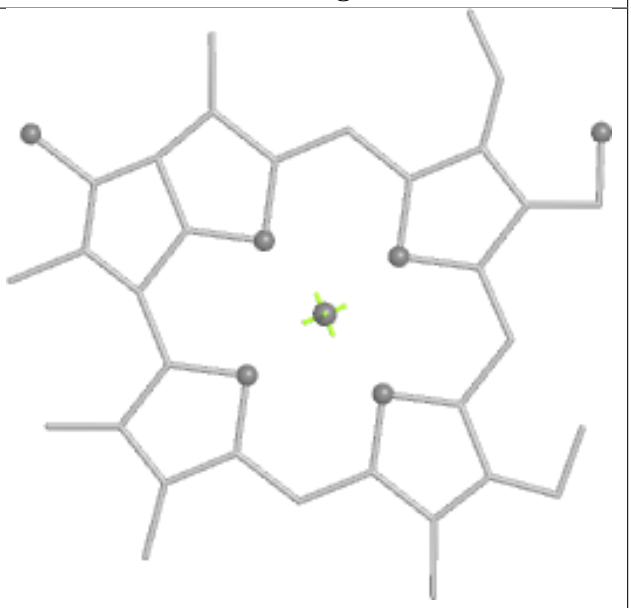
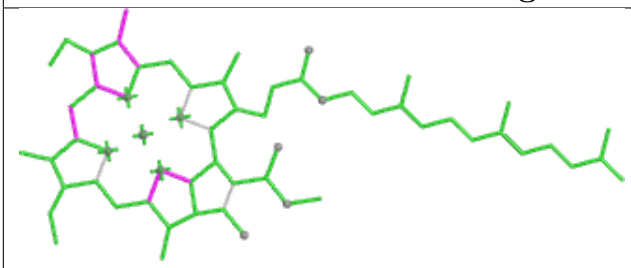
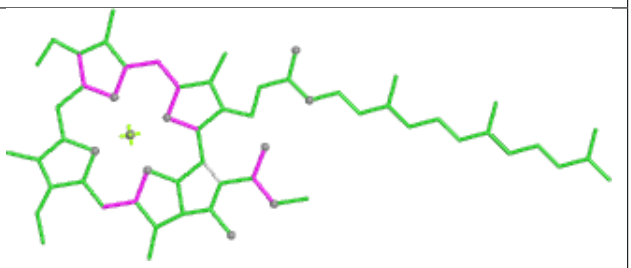
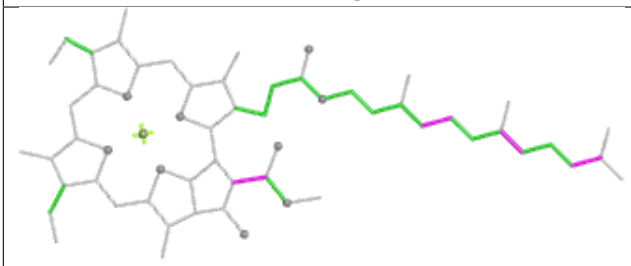
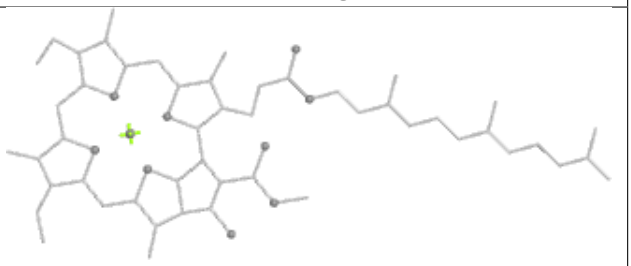
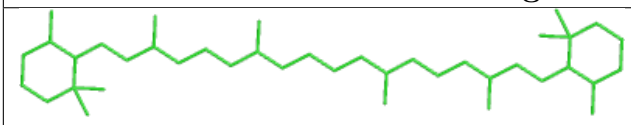
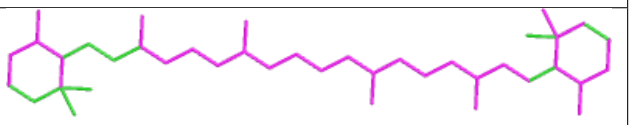
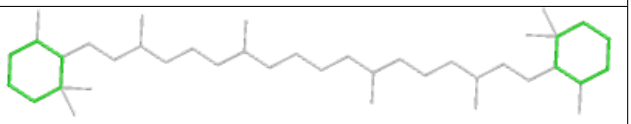
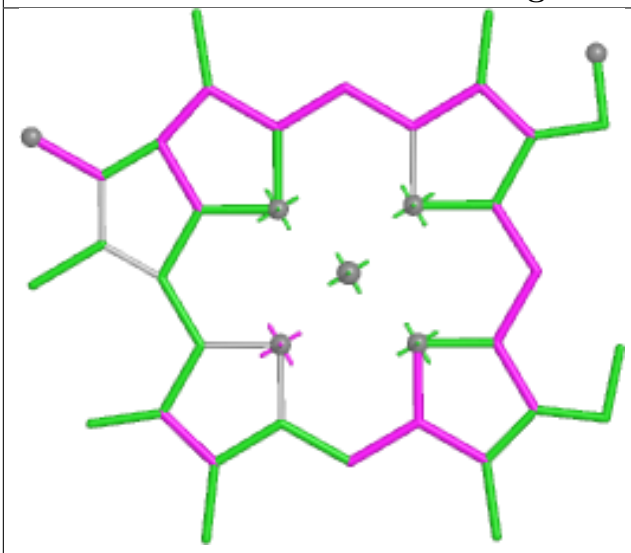


Rings

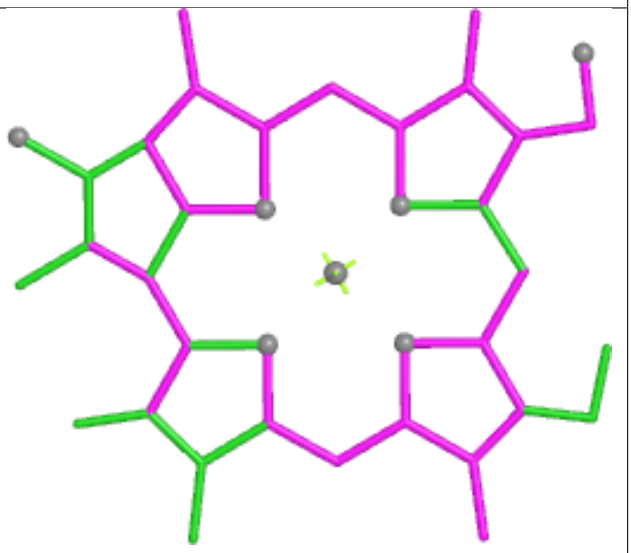
Ligand CLA W 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 845	
 Bond lengths	 Bond angles
Torsions	 Rings

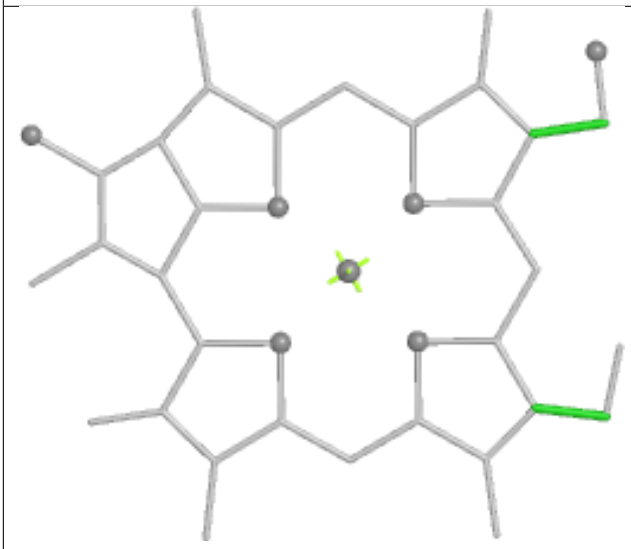
Ligand CHL 9 605



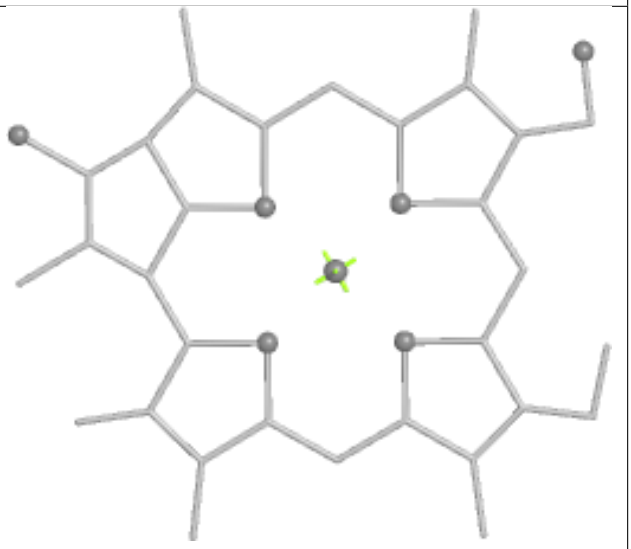
Bond lengths



Bond angles

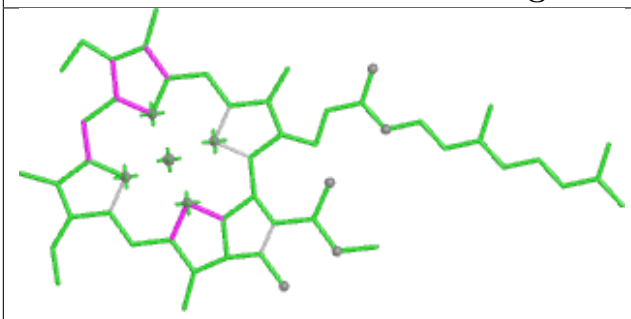


Torsions

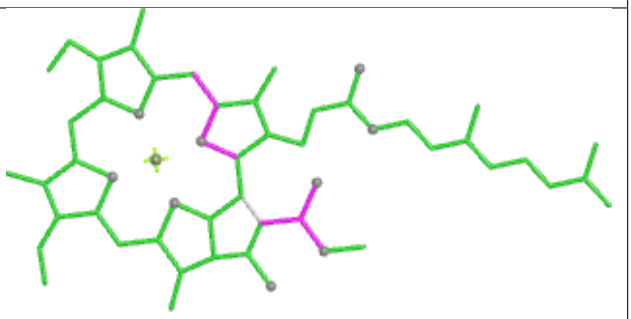


Rings

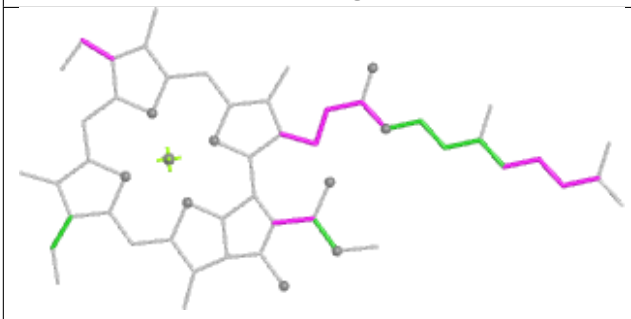
Ligand CLA 3 611



Bond lengths



Bond angles



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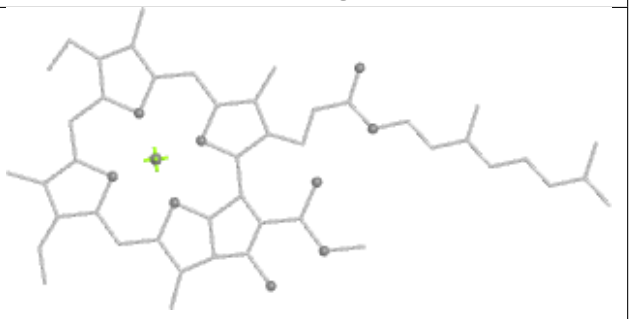
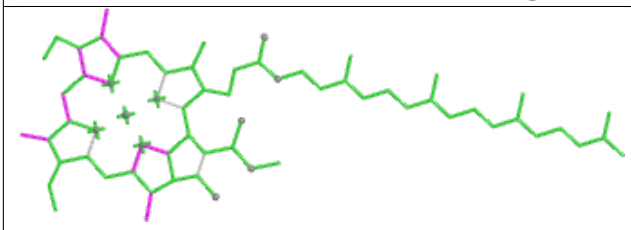


Rings

Ligand CLA A 812



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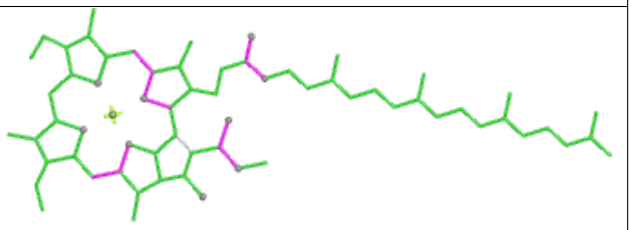

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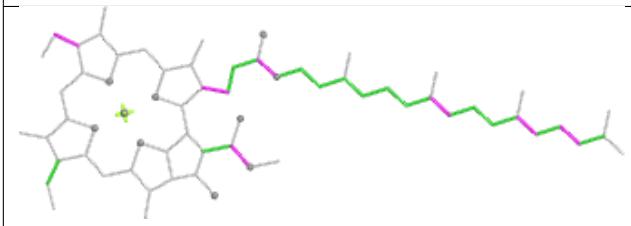

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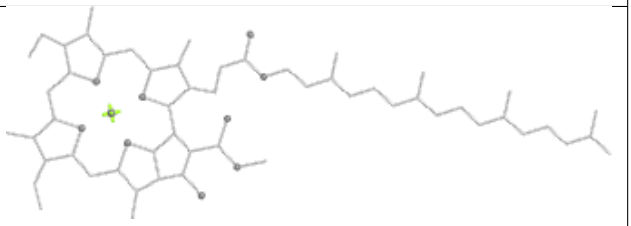

Rings

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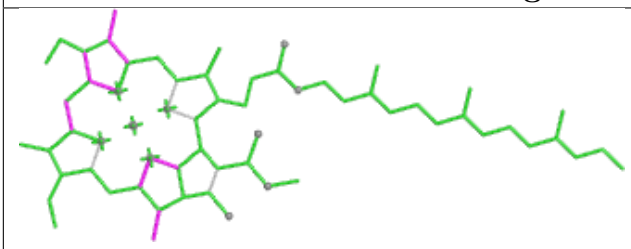
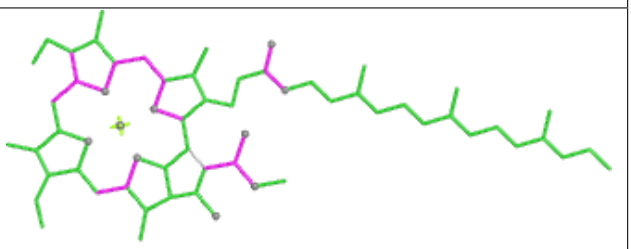
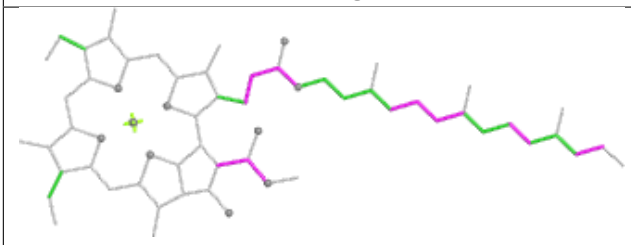
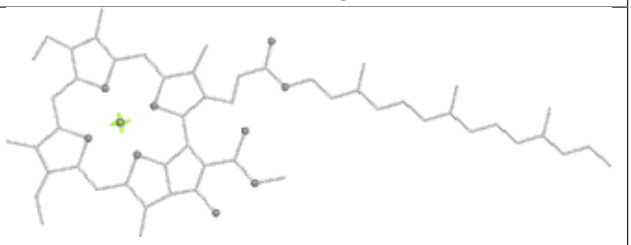
 Bond lengths	 Bond angles
 Torsions	 Rings

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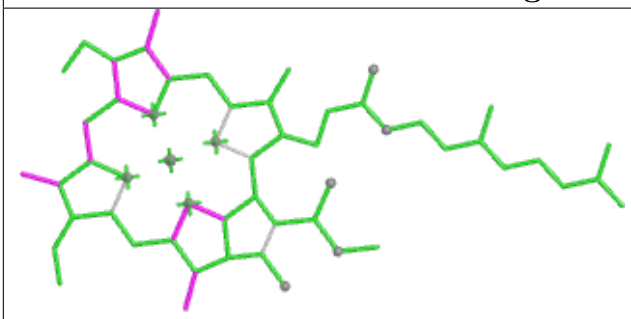
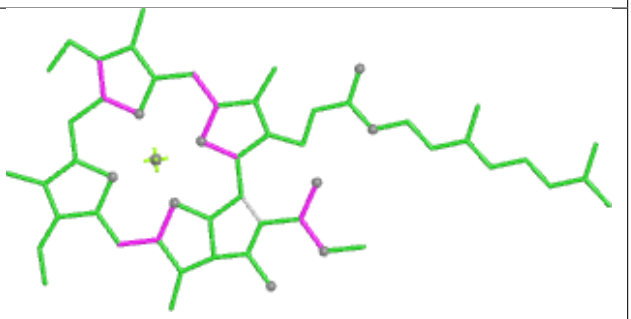
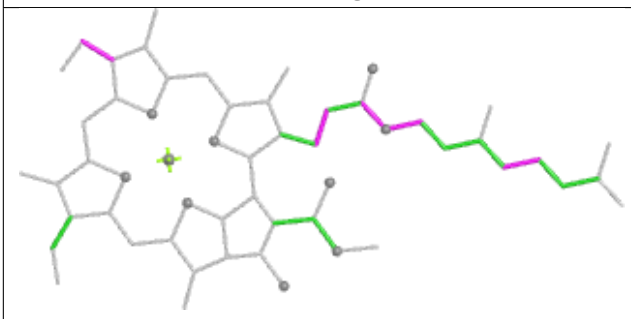
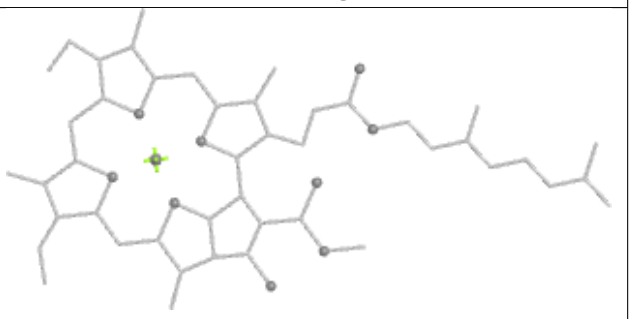
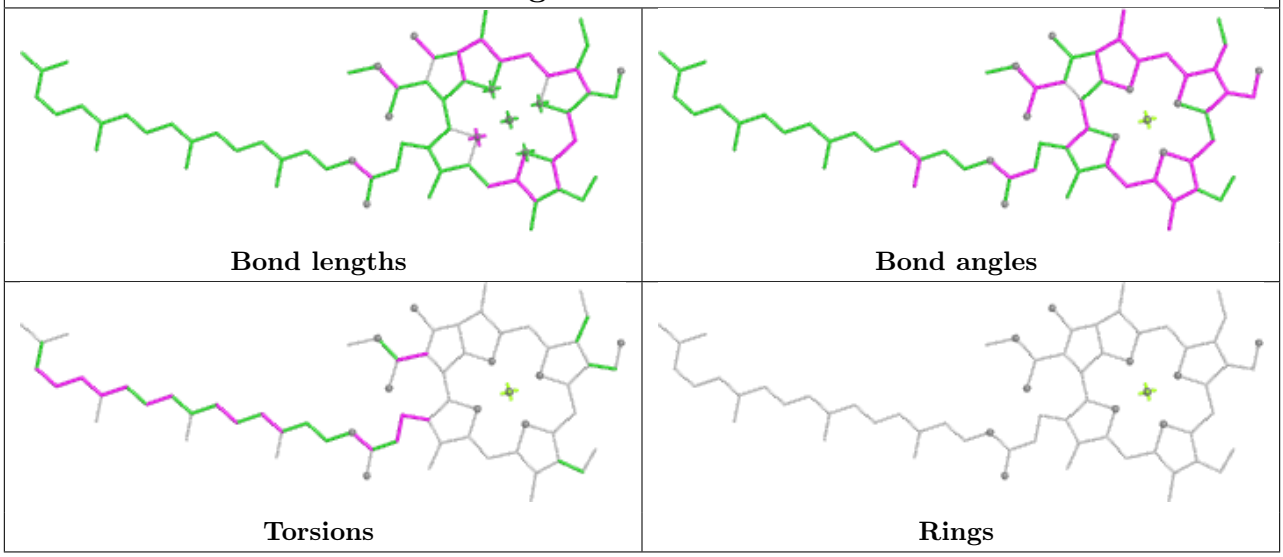
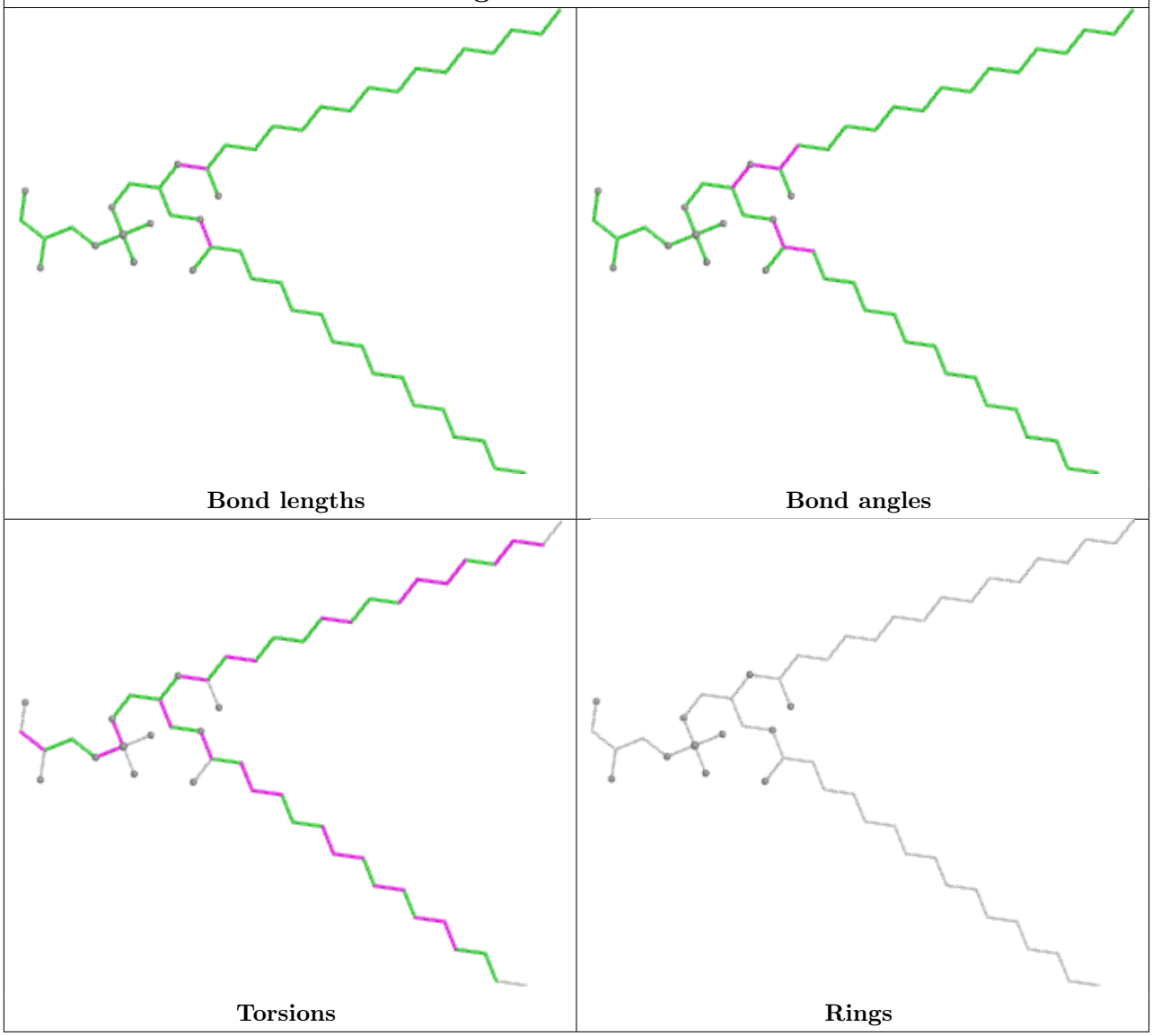
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 601



Ligand LHG 1 630



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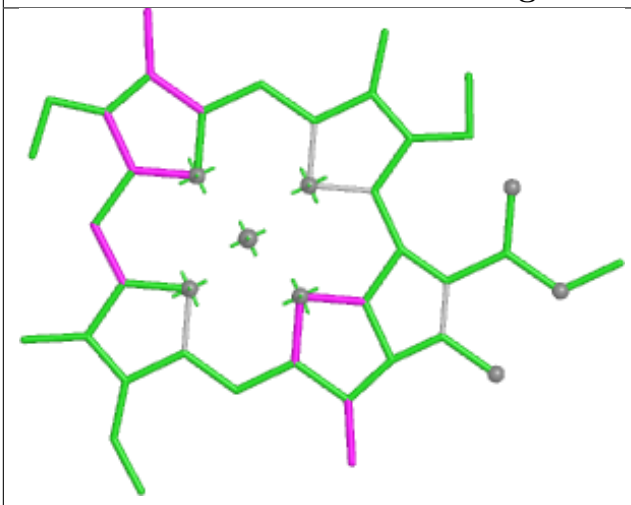
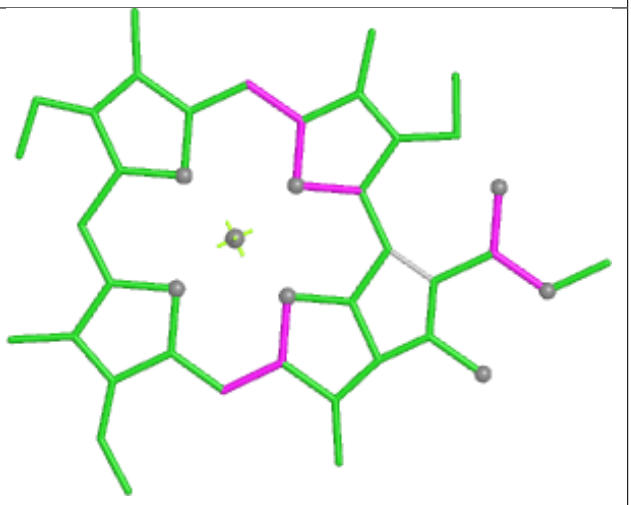
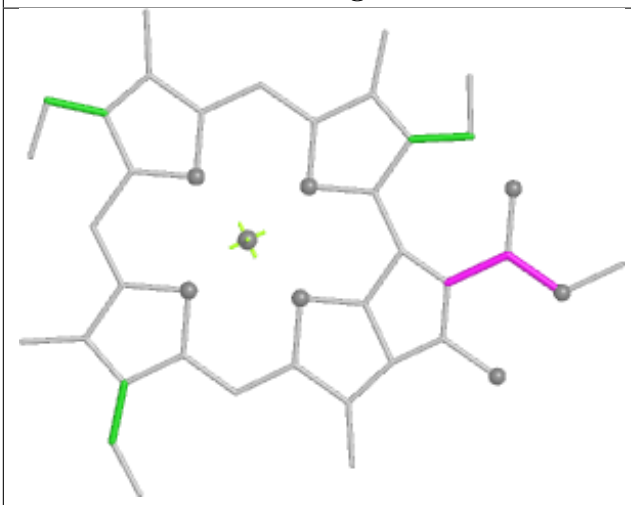


Bond lengths



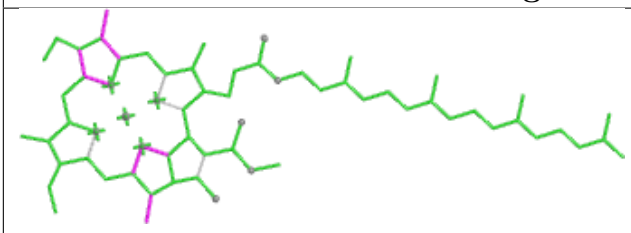
Bond angles



Torsions

Rings

Ligand CLA K 204



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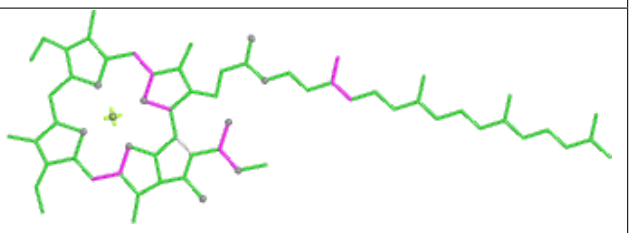

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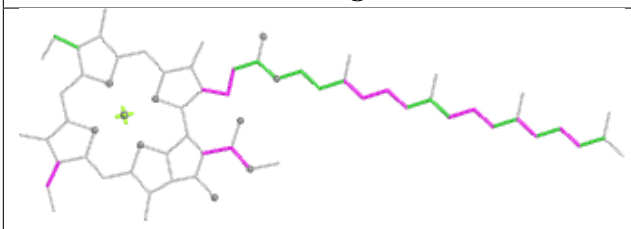

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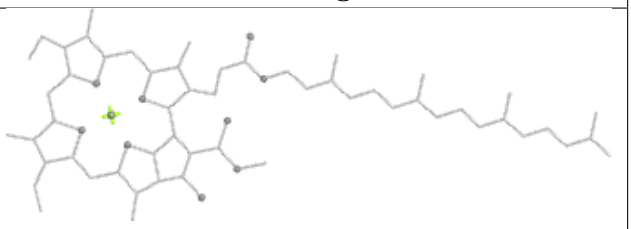
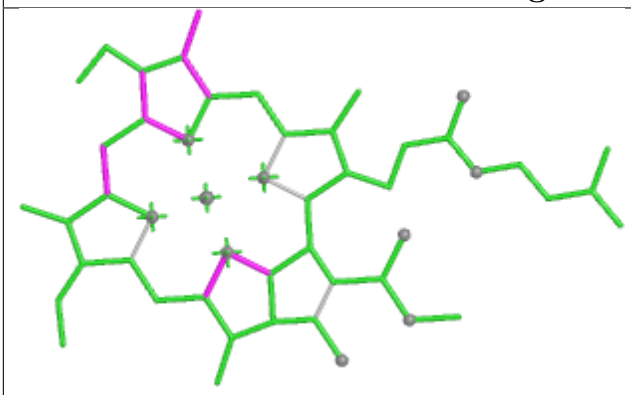
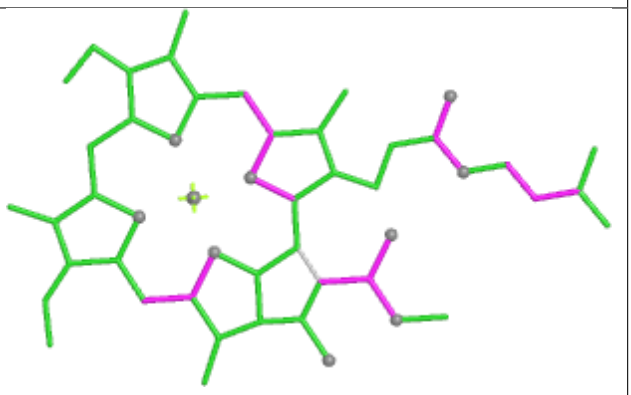
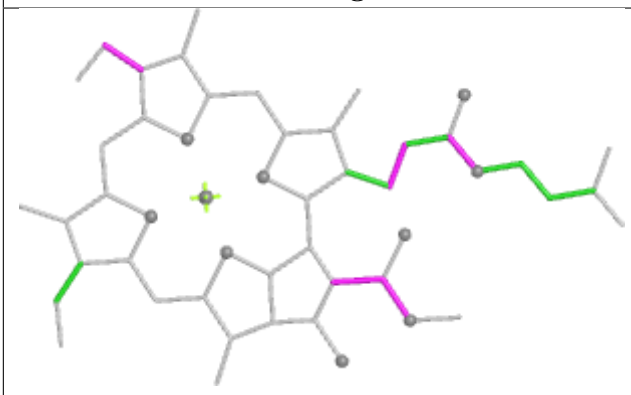
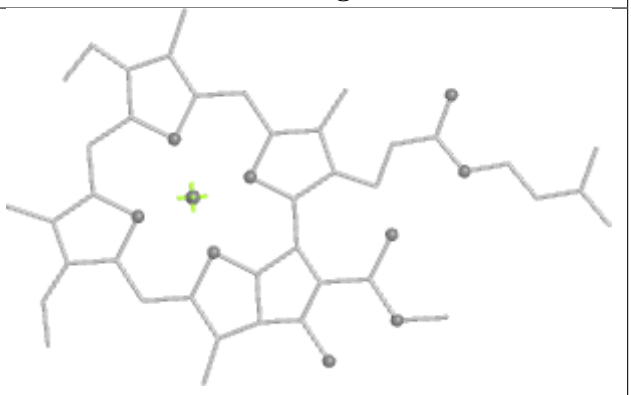


Rings

Ligand CLA 4 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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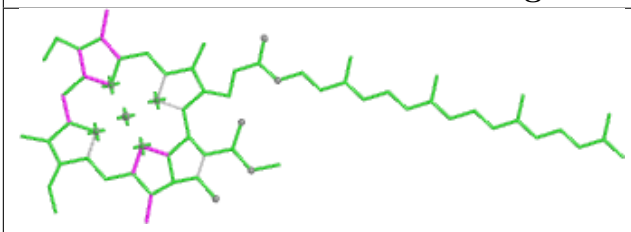
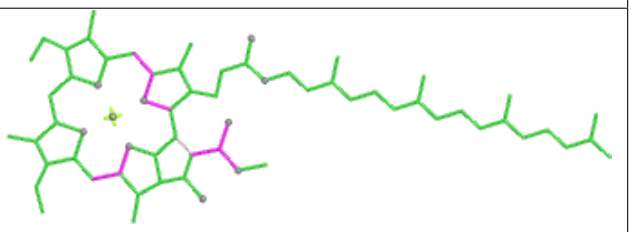
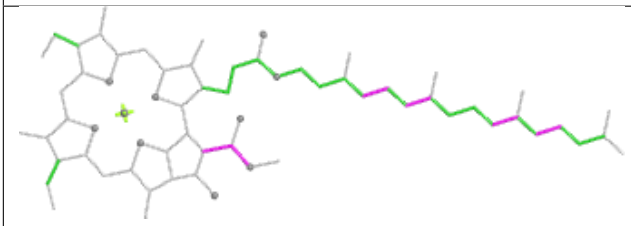
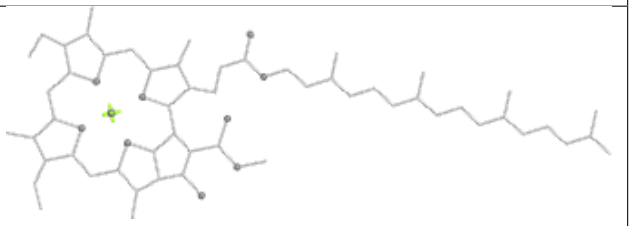
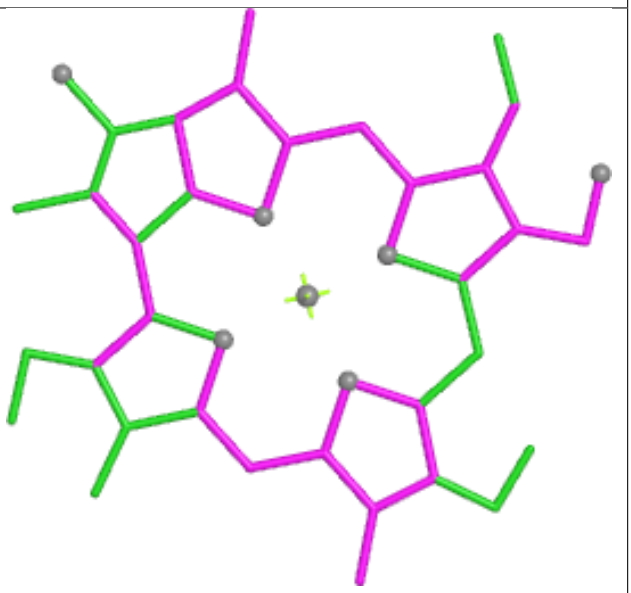
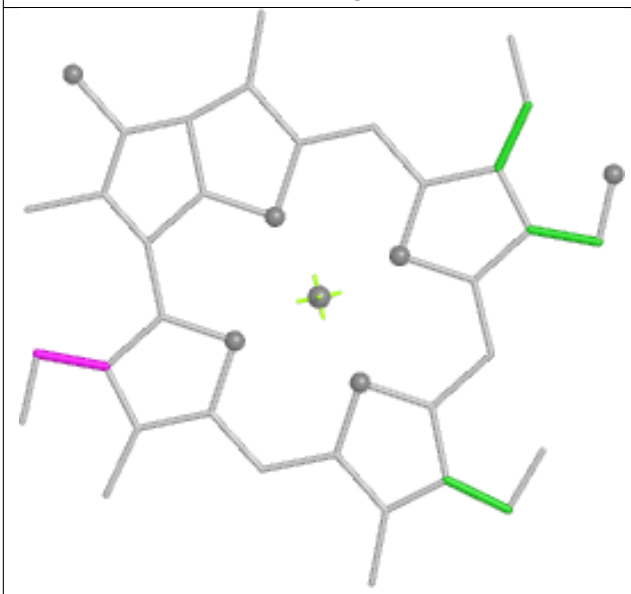
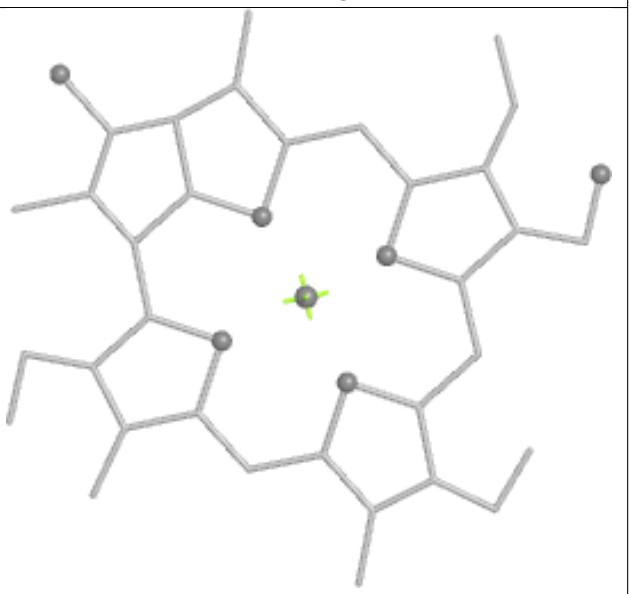
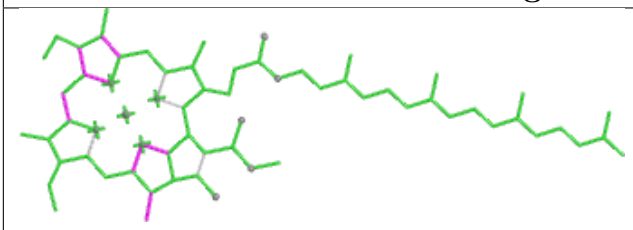
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL W 609	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 815



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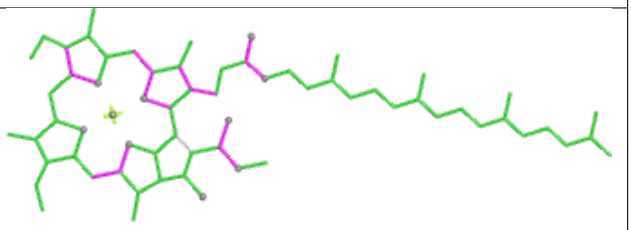
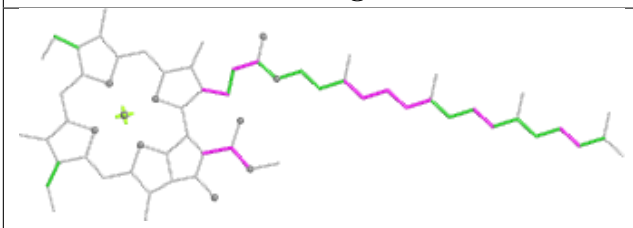


Bond angles



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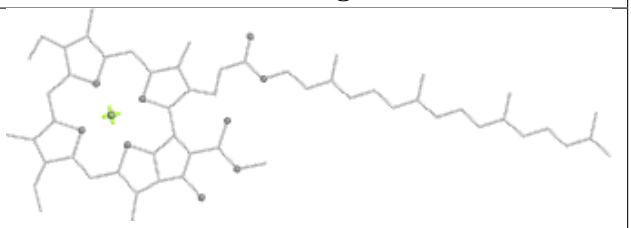
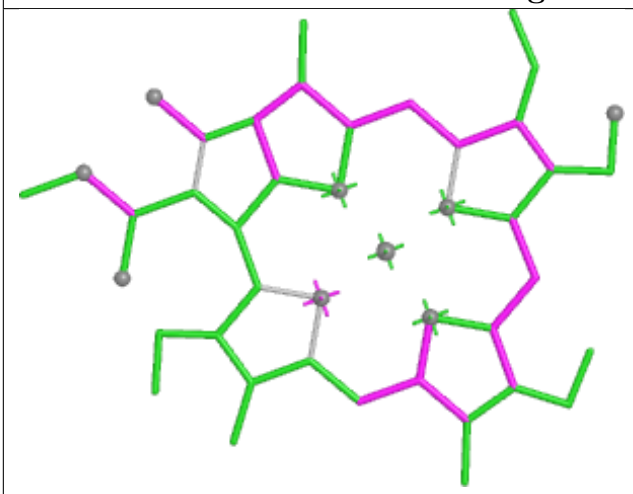


Rings

Ligand CHL 2 618



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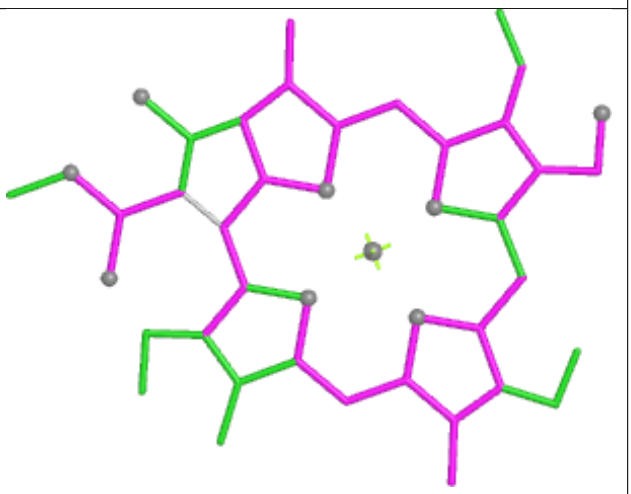
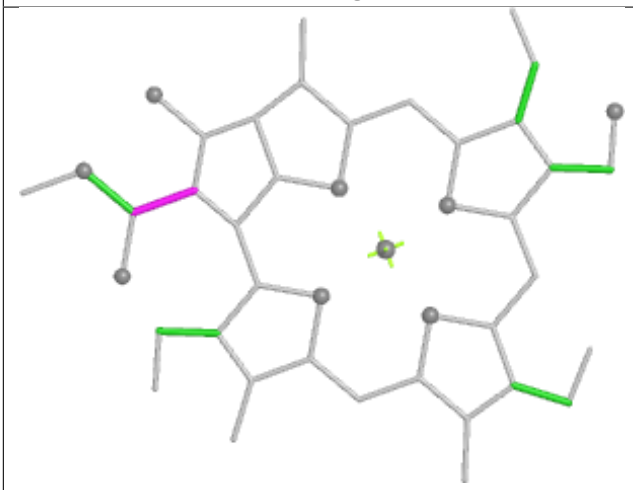


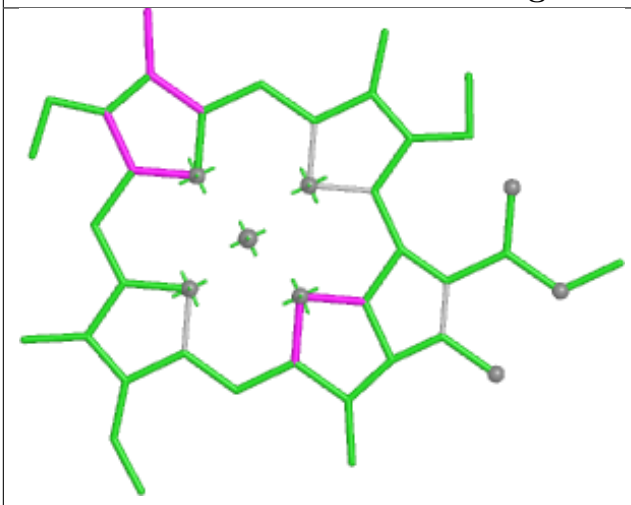
Bond angles



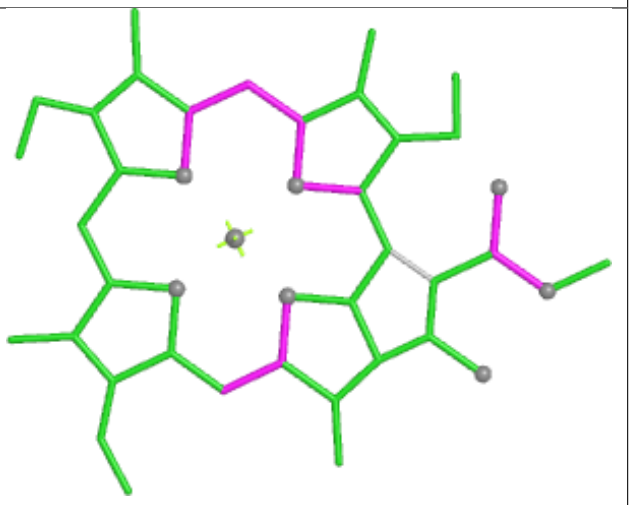
Torsions

Rings

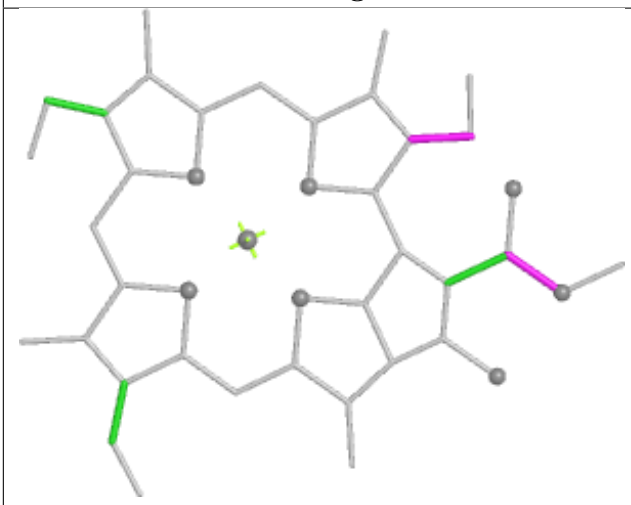
Ligand CLA 9 603



Bond lengths

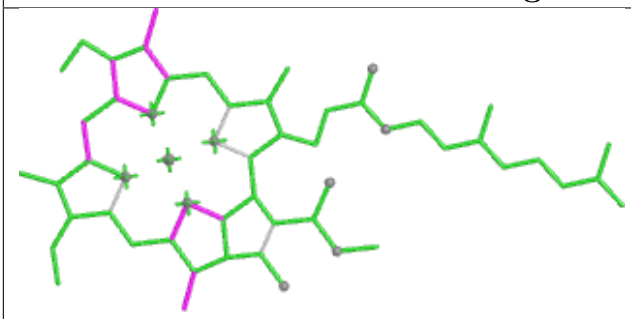
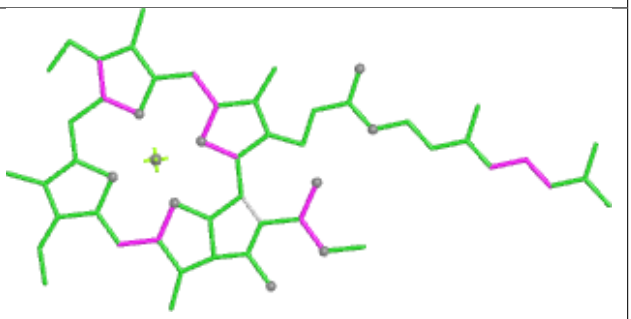
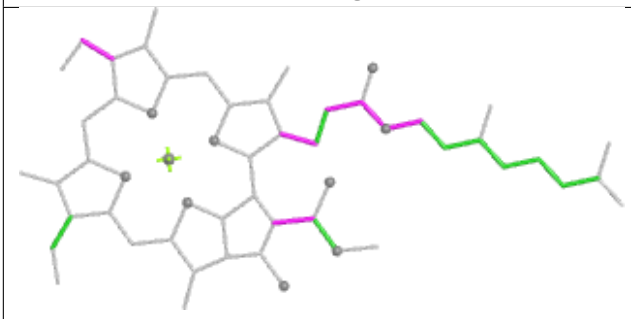
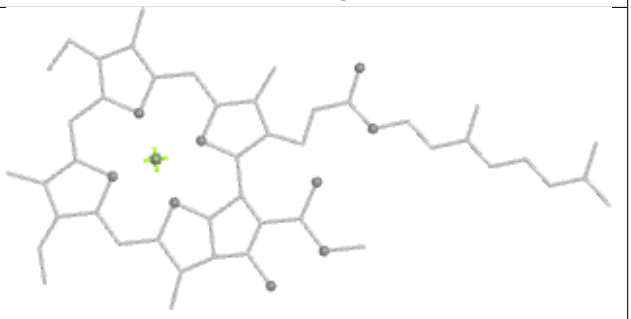


Bond angles



Torsions

Rings

Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

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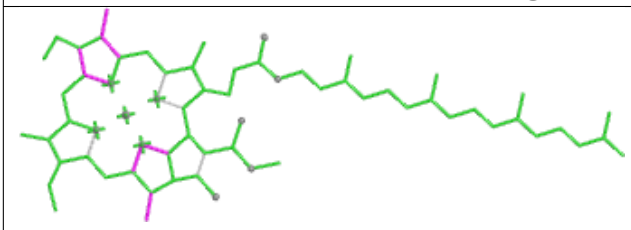
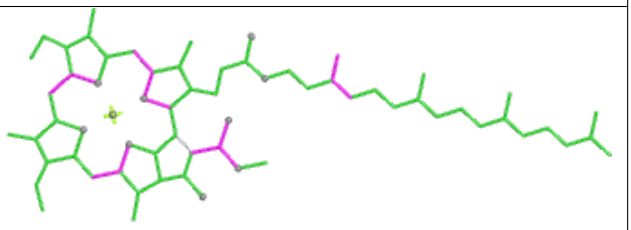
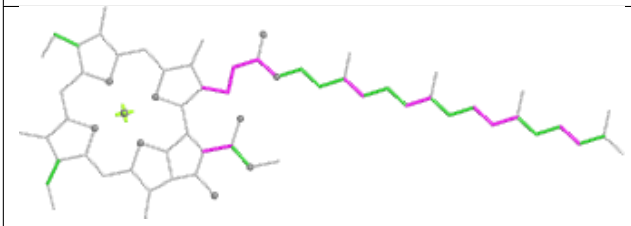
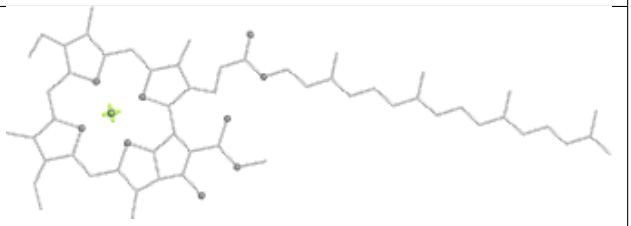
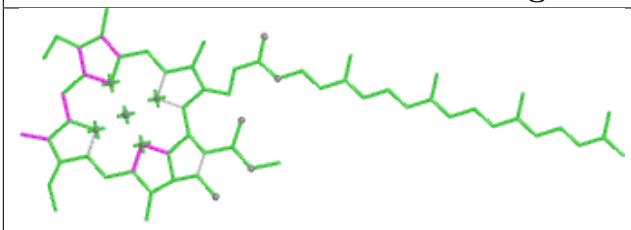
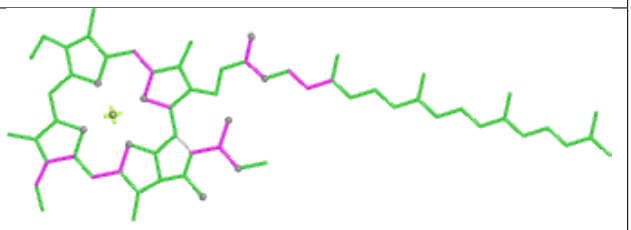
 Bond lengths	 Bond angles
 Torsions	 Rings

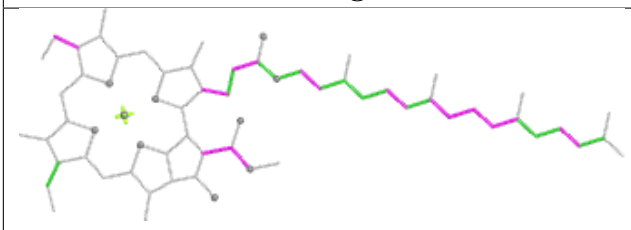
Ligand CLA 1 611



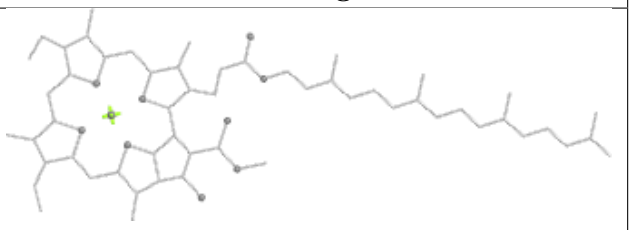
Bond lengths



Bond angles

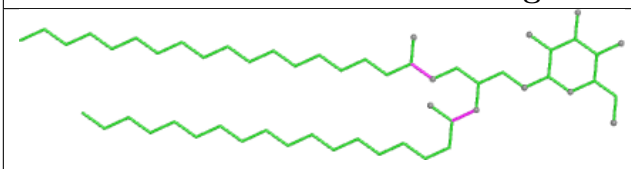


Torsions



Rings

Ligand LMG J 103



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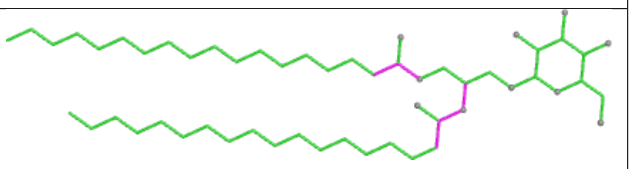

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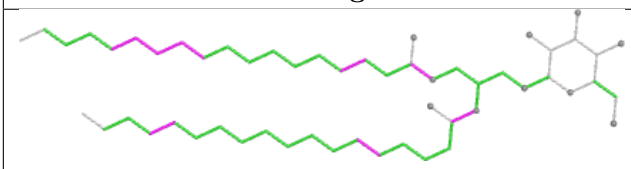

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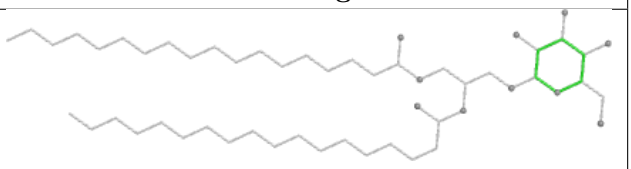
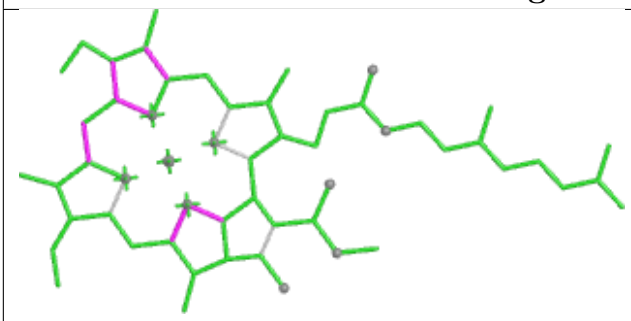


Rings

Ligand CLA 5 610



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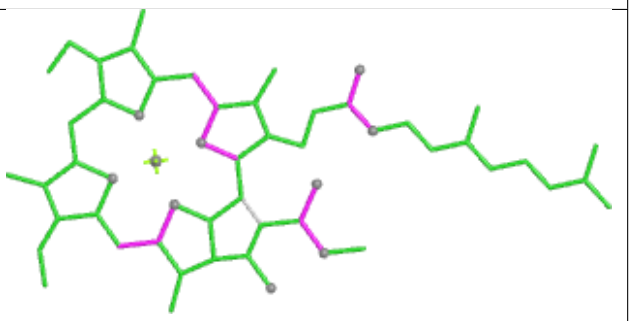

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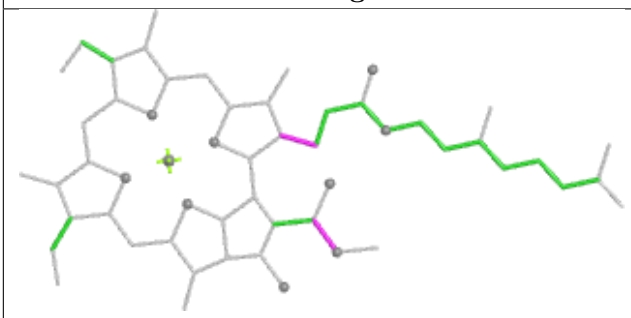

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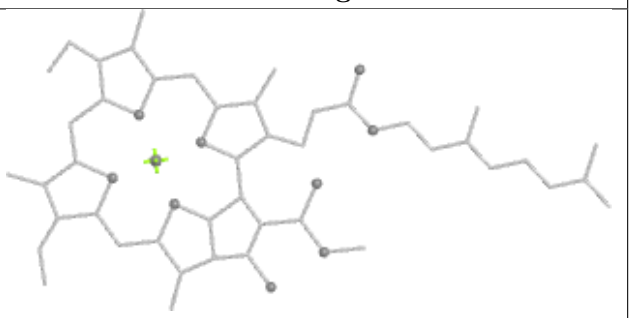
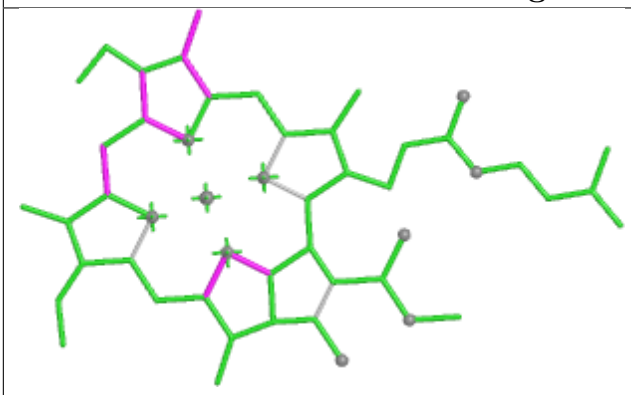


Rings

Ligand CLA 1 604



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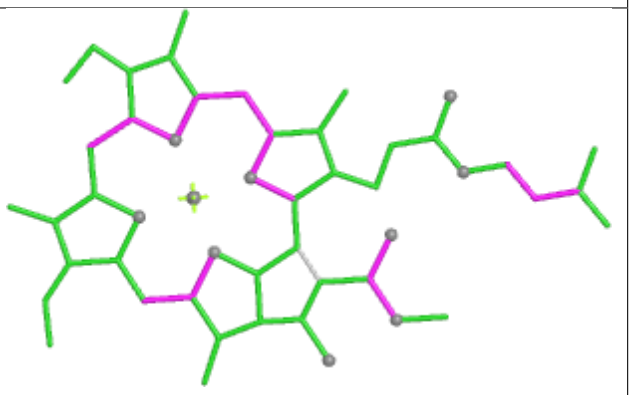

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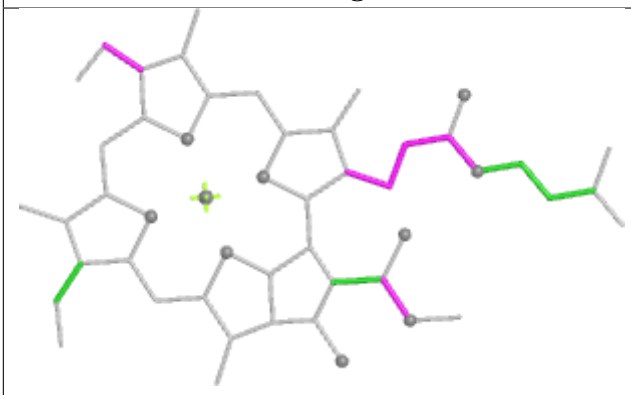

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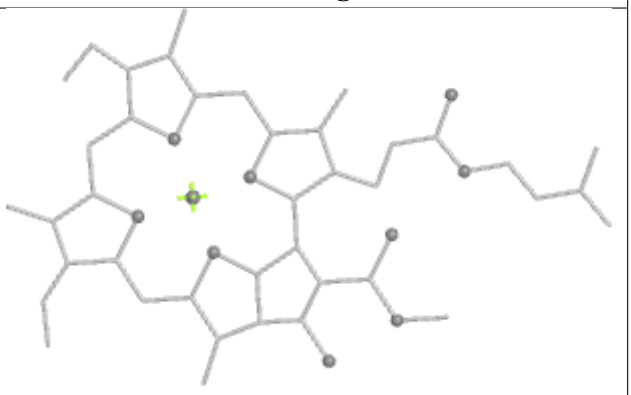
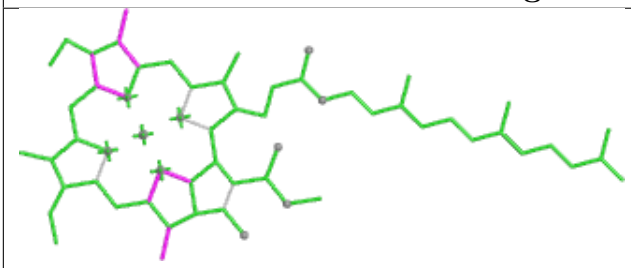


Rings

Ligand CLA A 839



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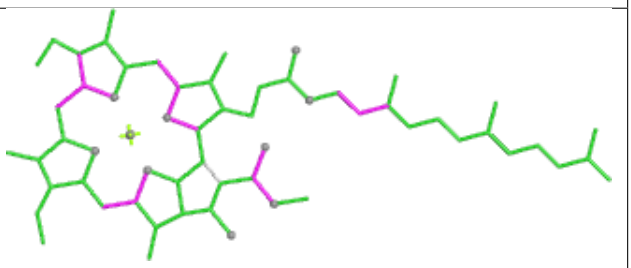
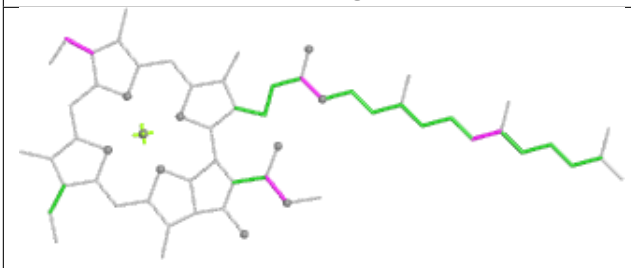


Bond angles



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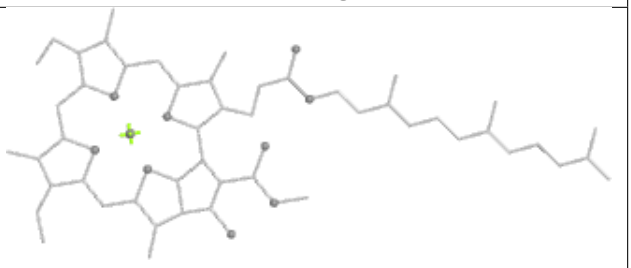
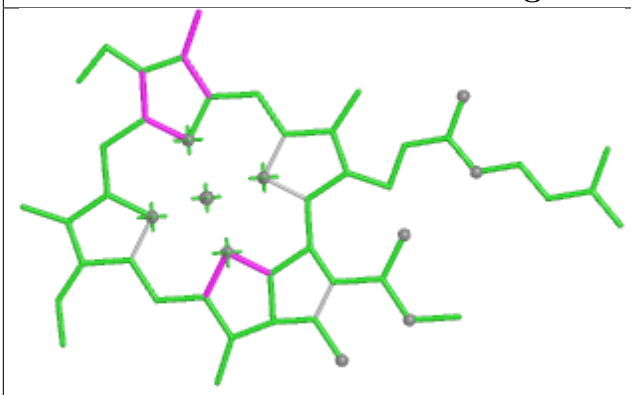
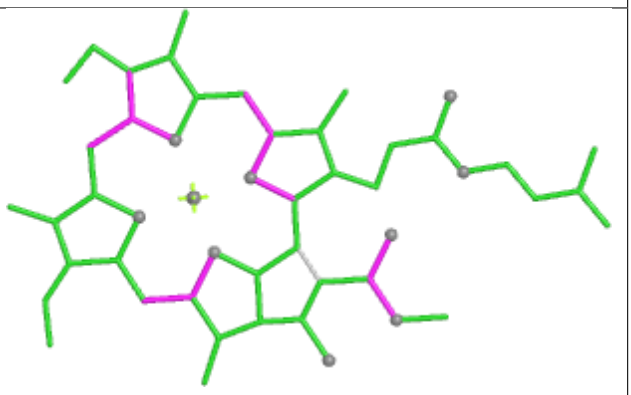
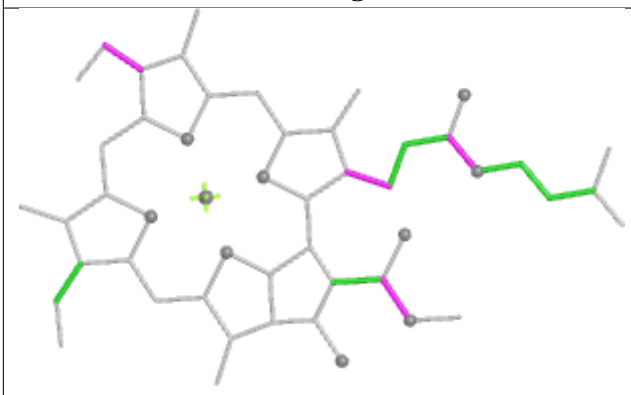
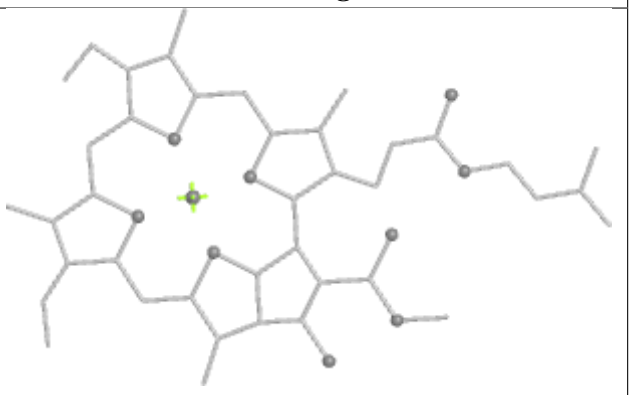
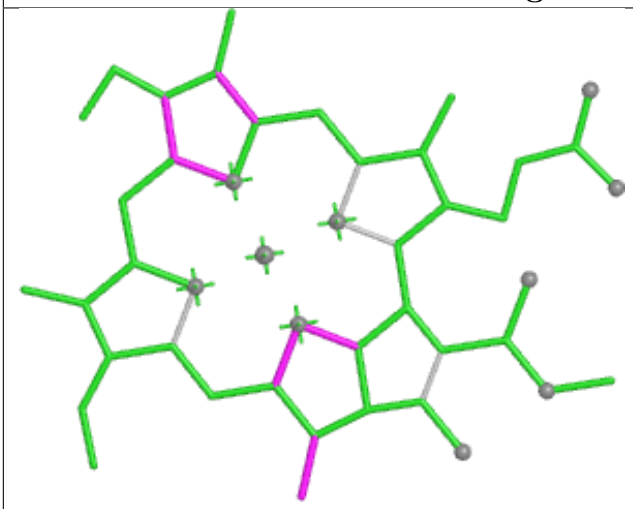


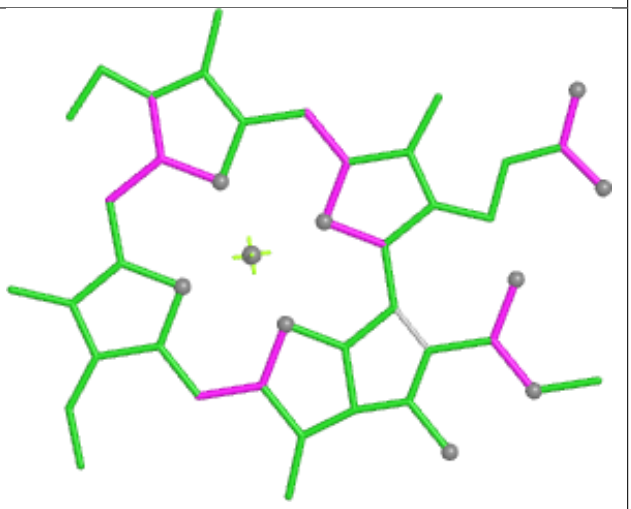
Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

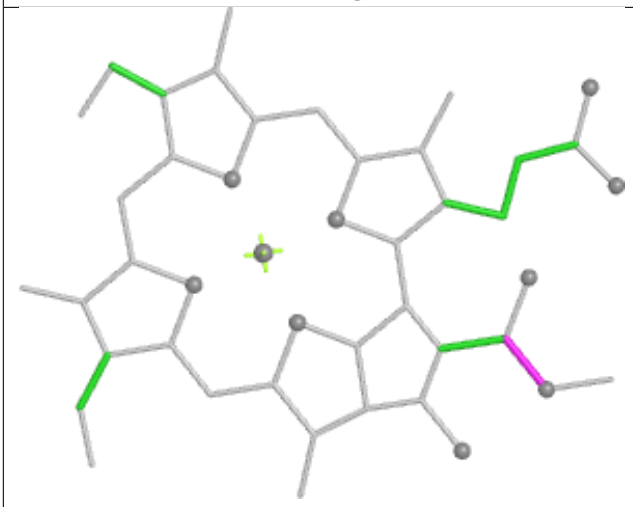
Ligand CLA F 303



Bond lengths



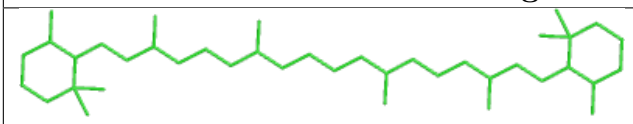
Bond angles



Torsions

Rings

Ligand BCR K 202



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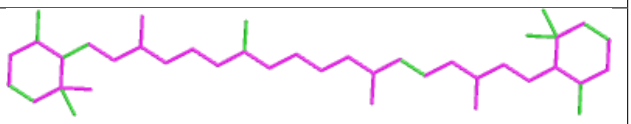

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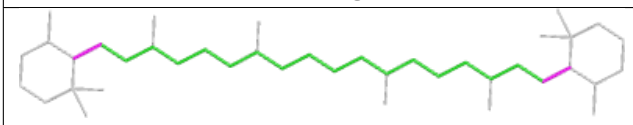

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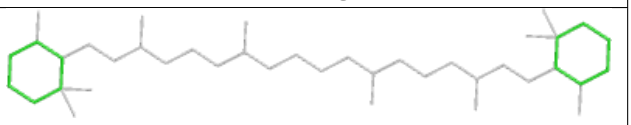
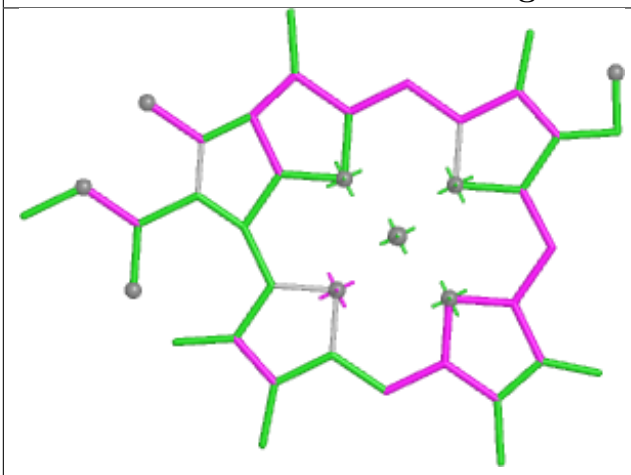


Rings

Ligand CHL W 607



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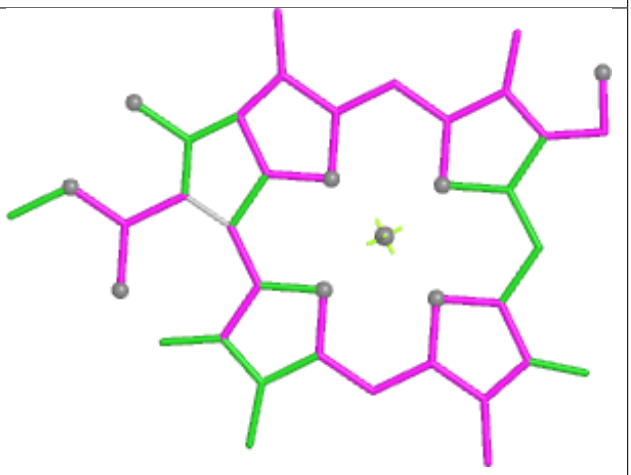

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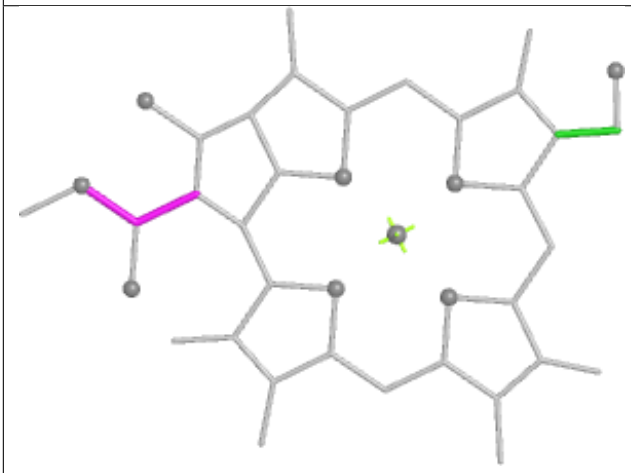

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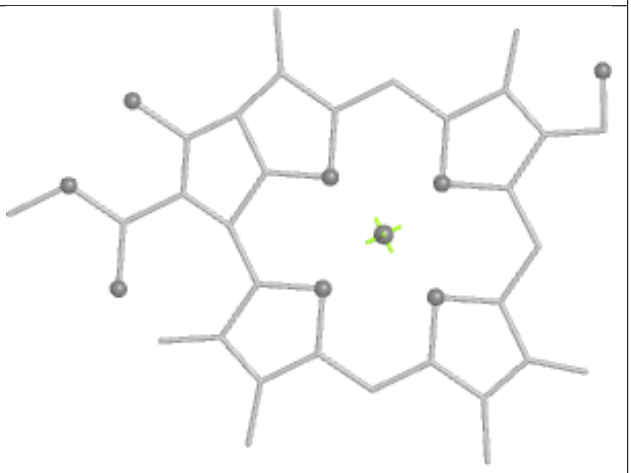
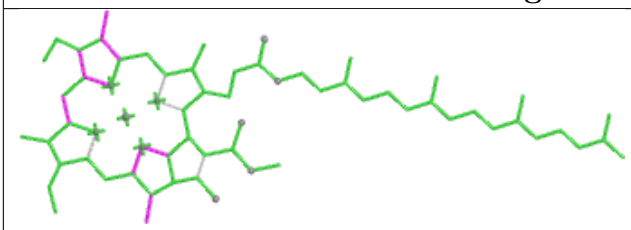
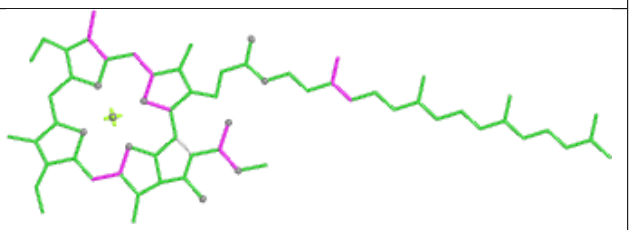


Rings

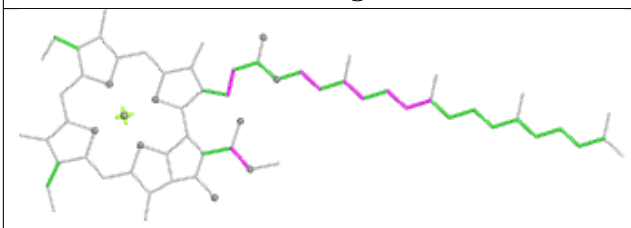
Ligand CLA B 824



Bond lengths



Bond angles



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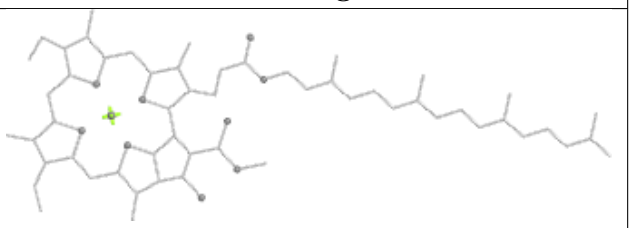
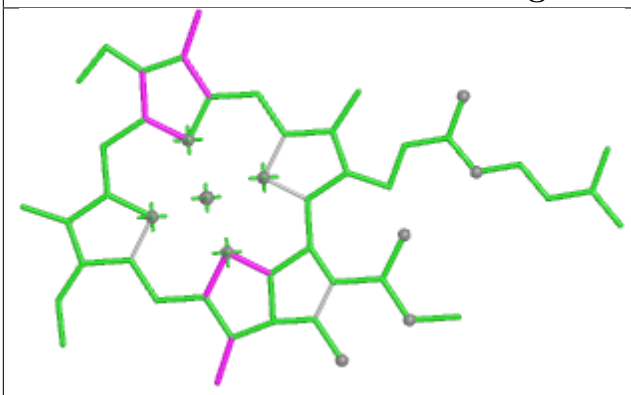


Rings

Ligand CLA 5 613



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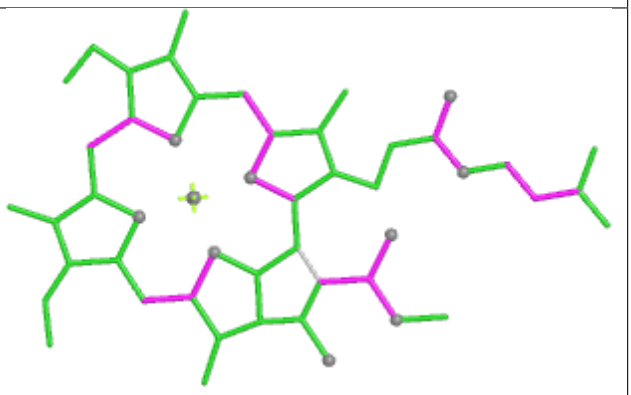
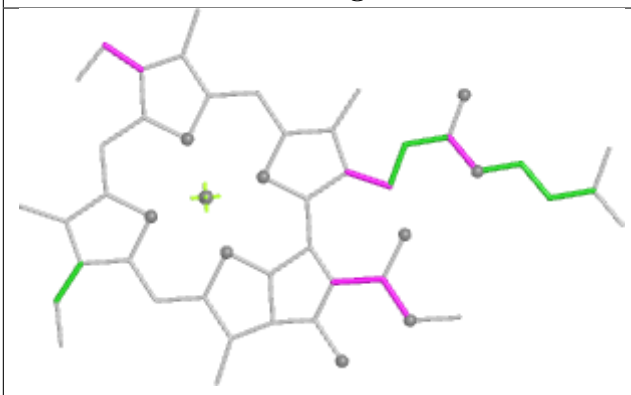


Bond angles



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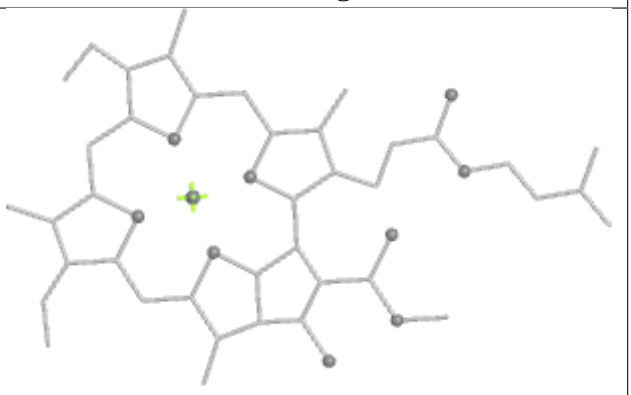
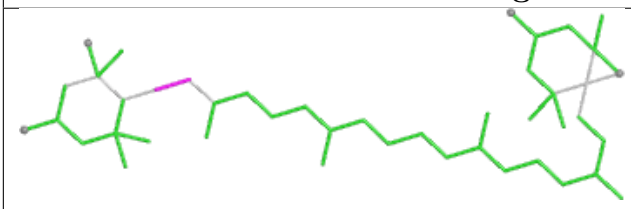


Rings

Ligand NEX V 2623



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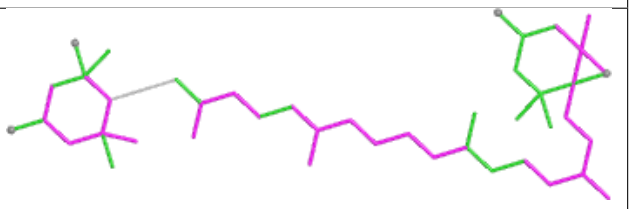

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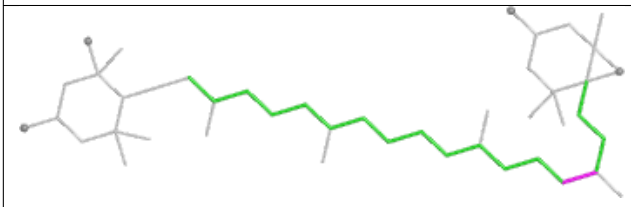

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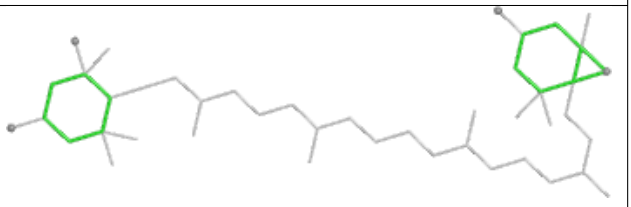
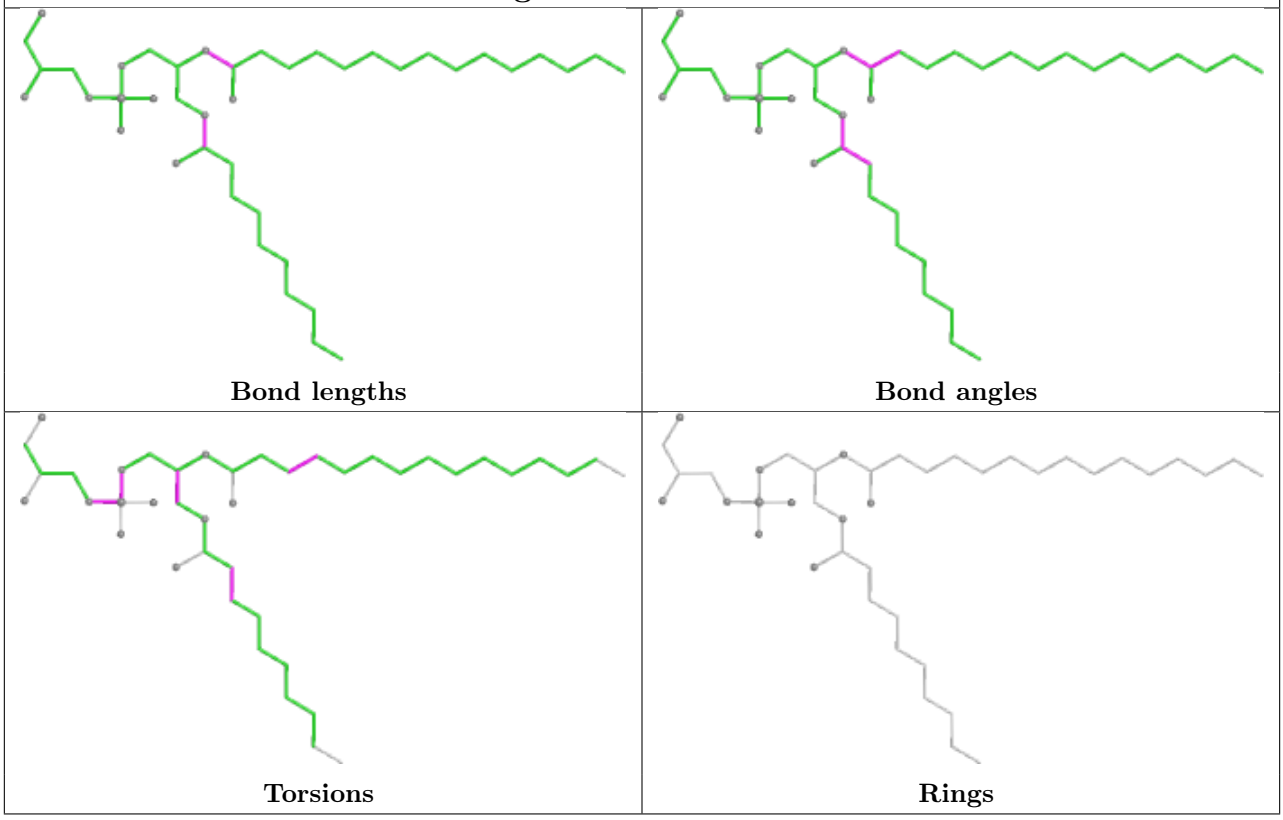
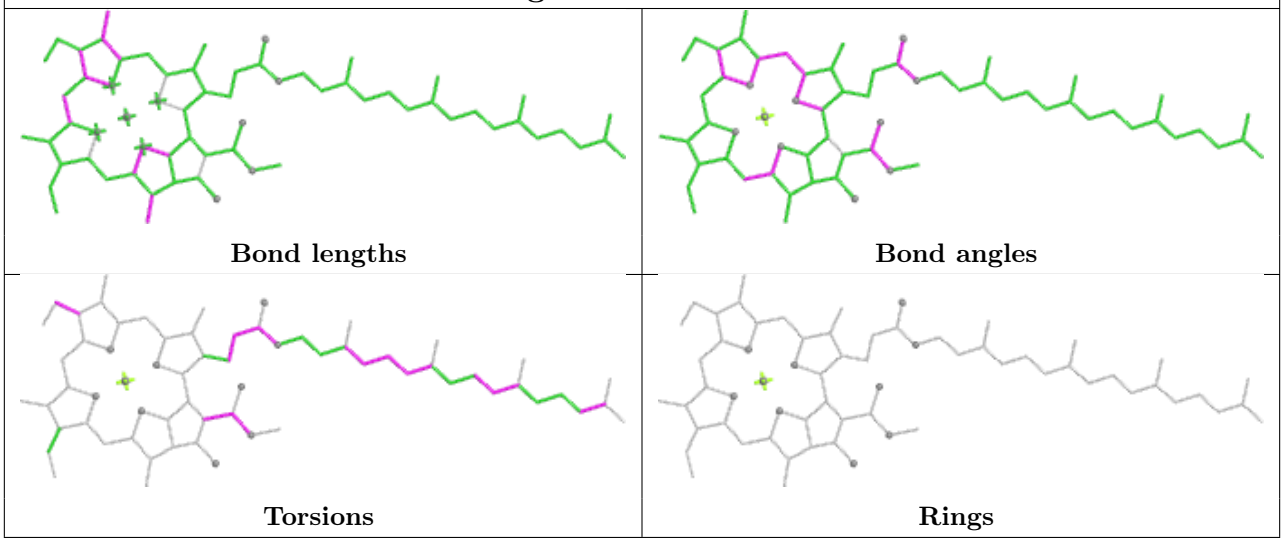


Rings

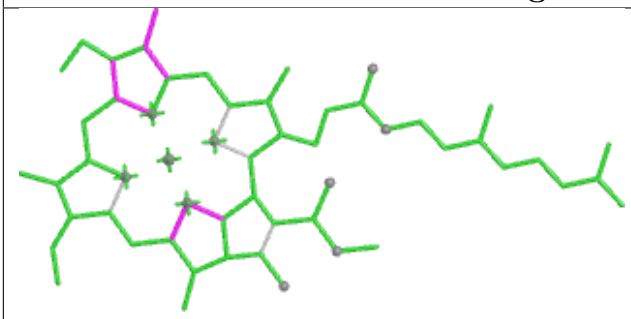
Ligand LHG V 2630



Ligand CLA L 302



Ligand CLA 8 613



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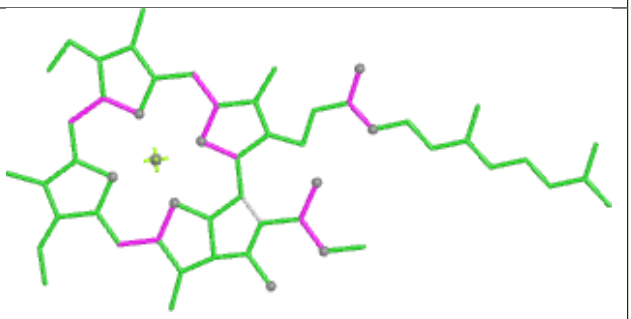

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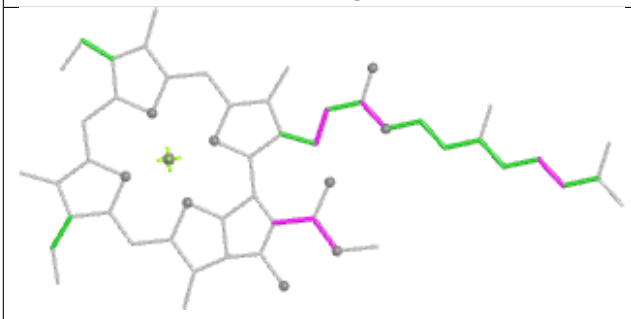

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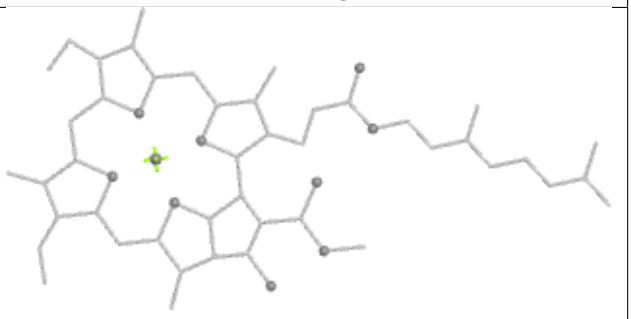
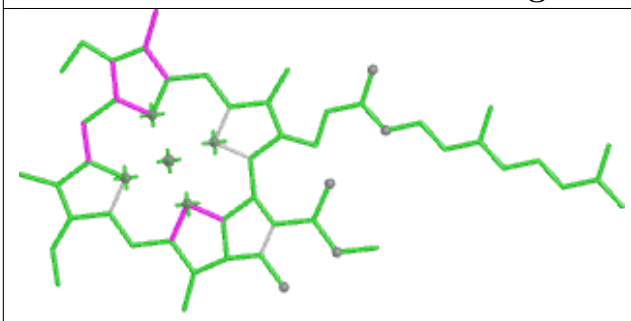


Rings

Ligand CLA 8 610



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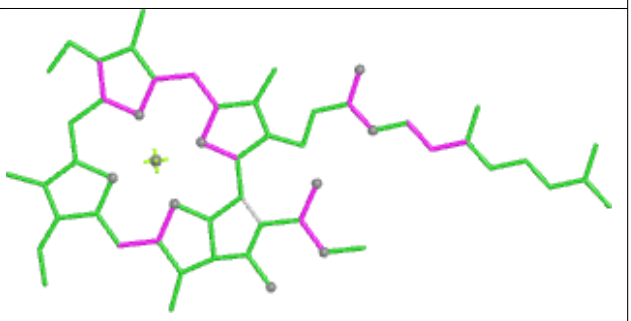
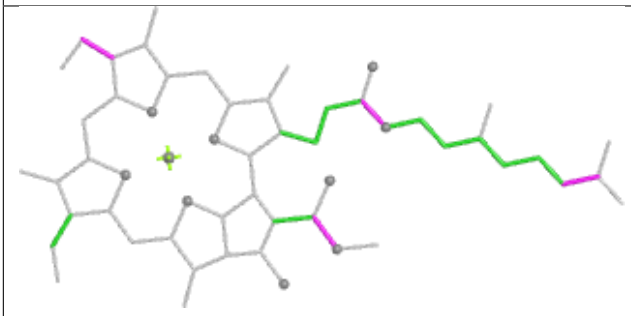


Bond angles



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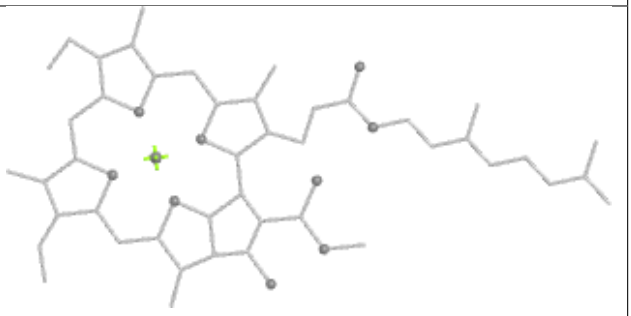
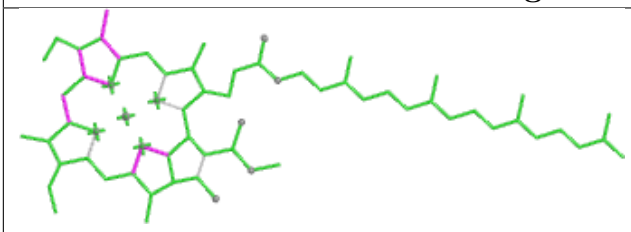


Rings

Ligand CLA B 806



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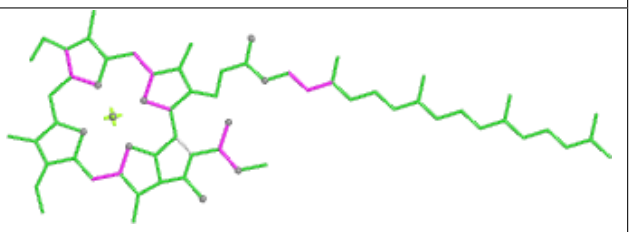
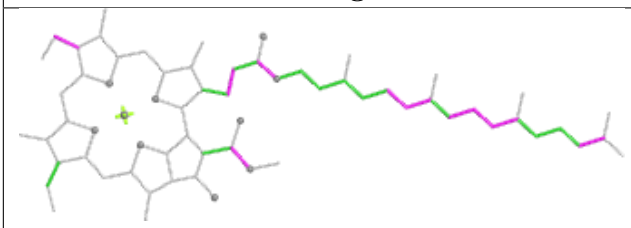
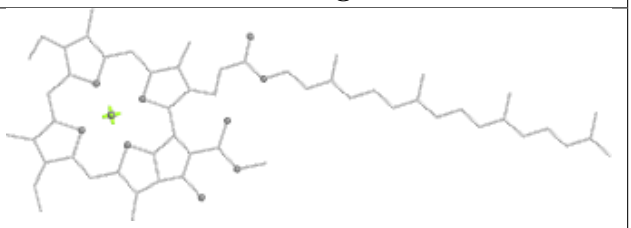


Bond angles

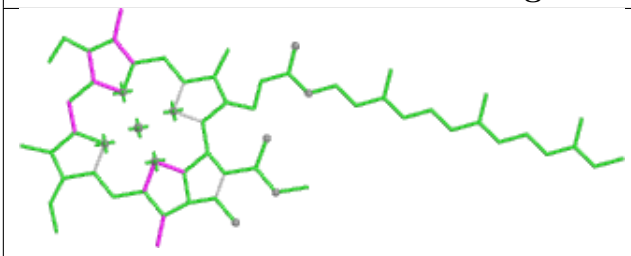


Torsions



Rings

Ligand CLA B 811



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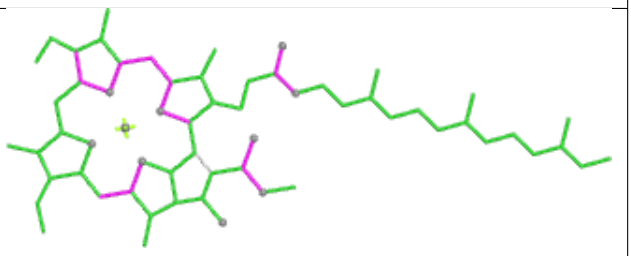

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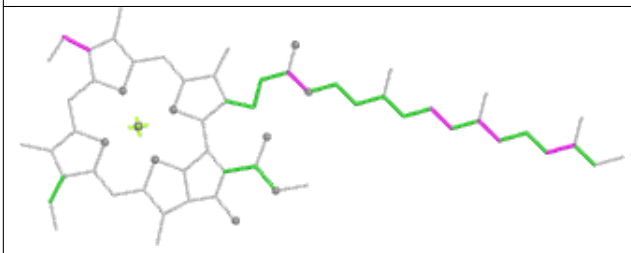

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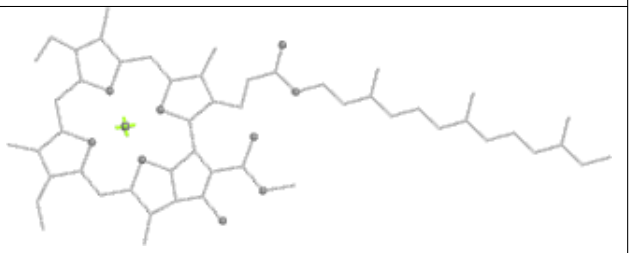
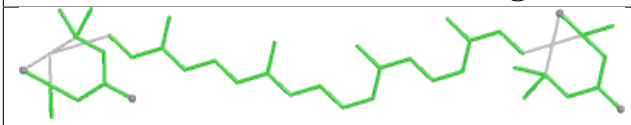


Rings

Ligand XAT W 2622



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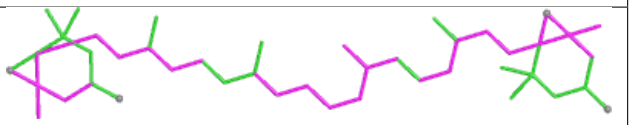

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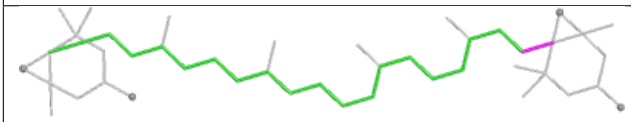

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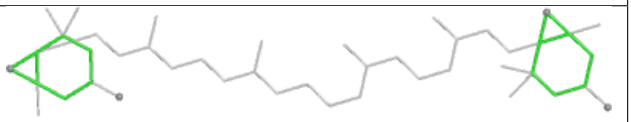
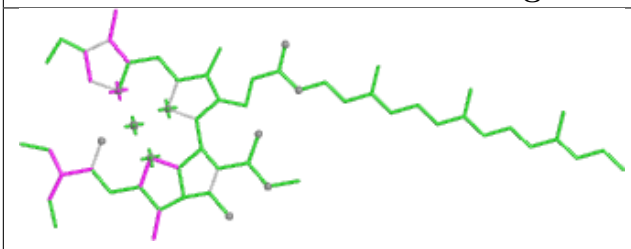


Rings

Ligand CLA A 836



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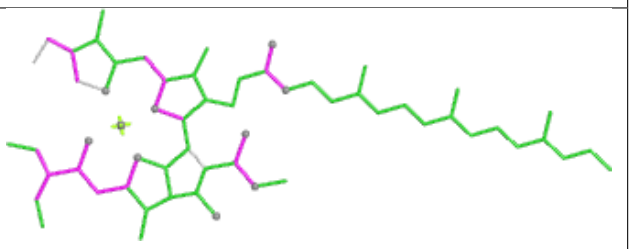

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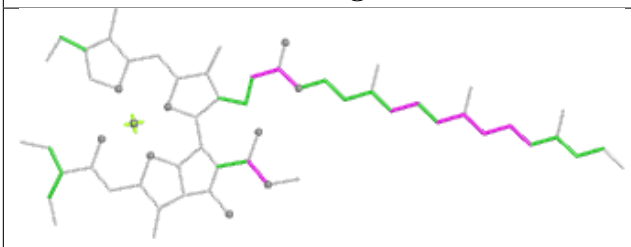

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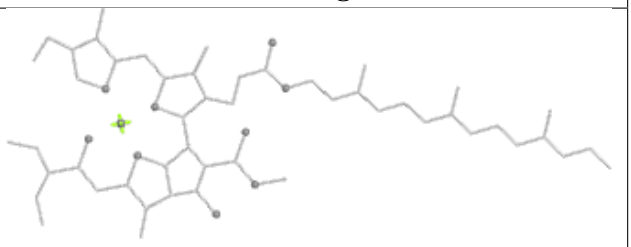
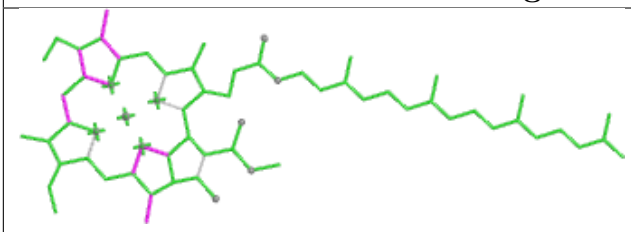


Rings

Ligand CLA A 841



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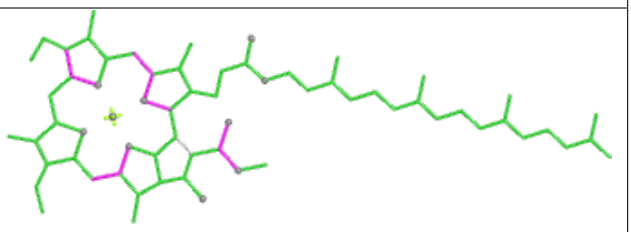

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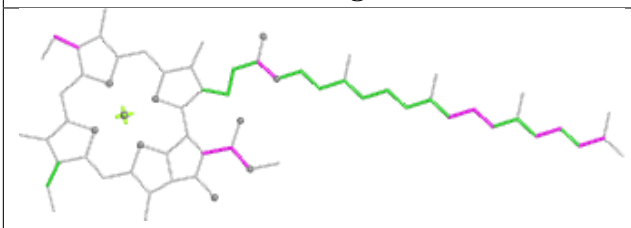

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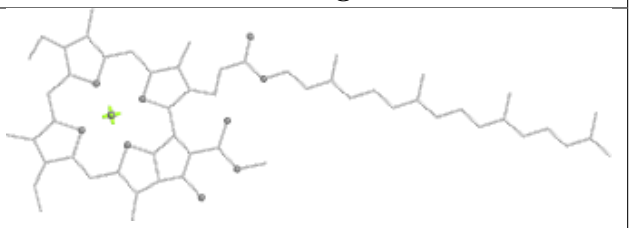
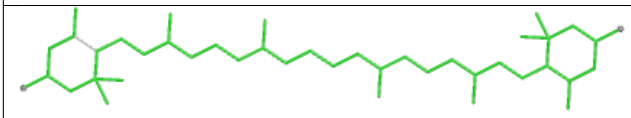


Rings

Ligand LUT U 2621



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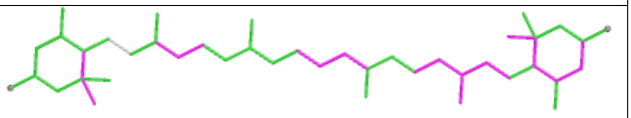

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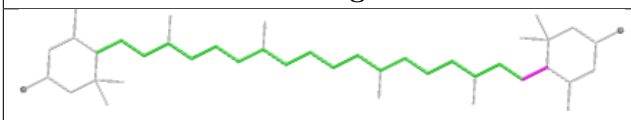

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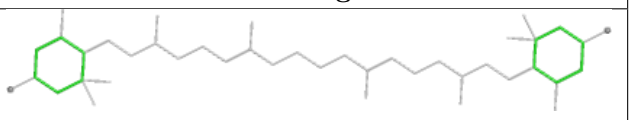
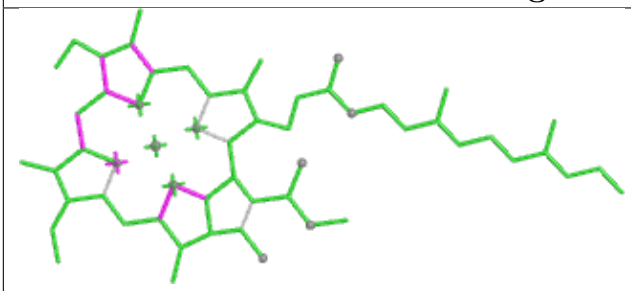


Rings

Ligand CLA 7 609



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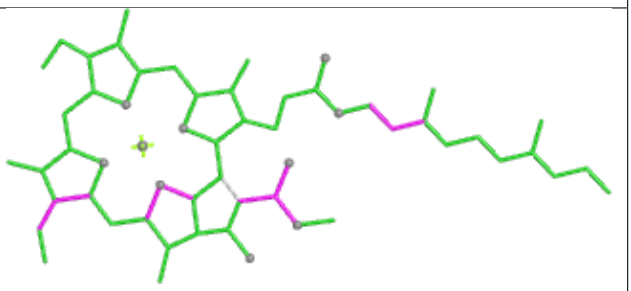
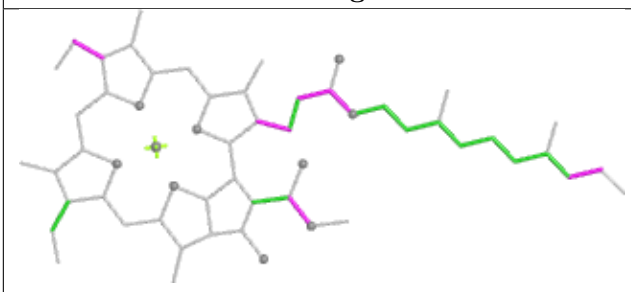


Bond angles



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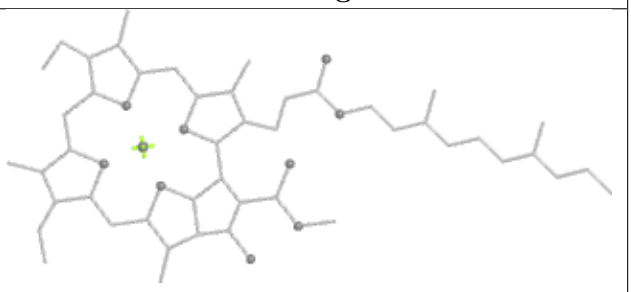
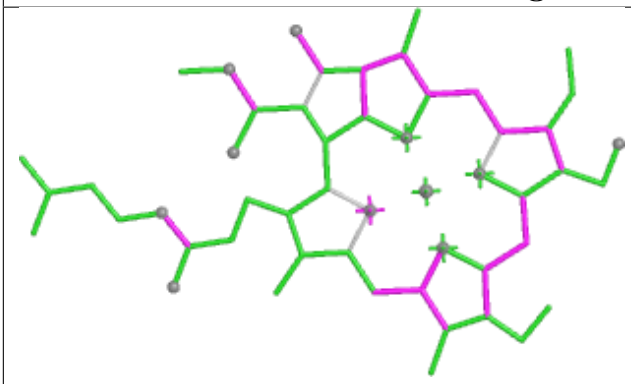


Rings

Ligand CHL 8 608



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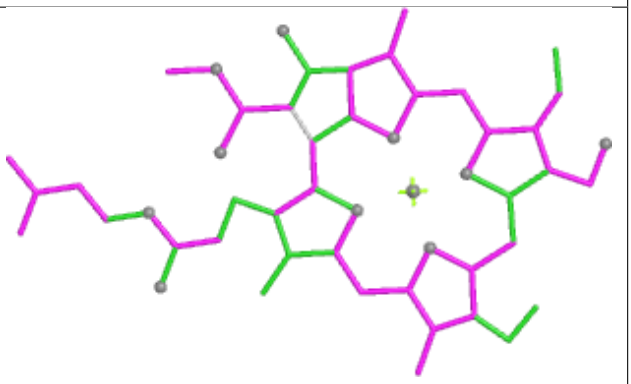

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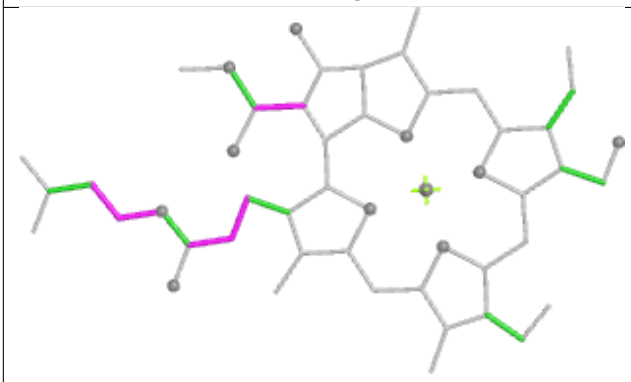

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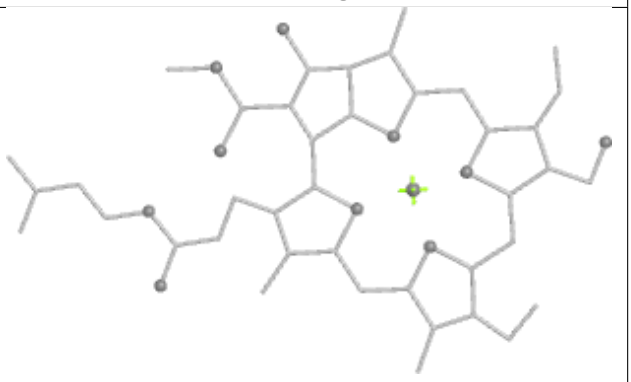
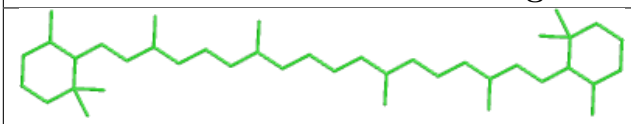


Rings

Ligand BCR 2 621



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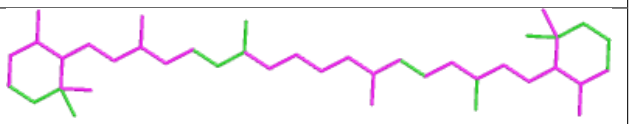

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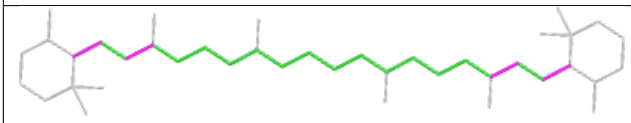

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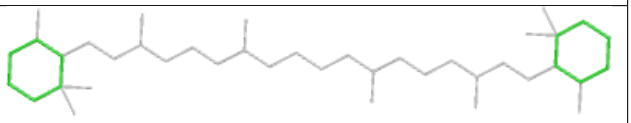
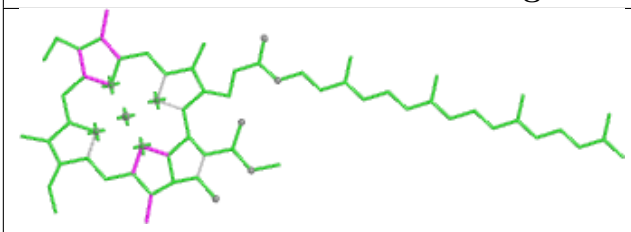


Rings

Ligand CLA U 603



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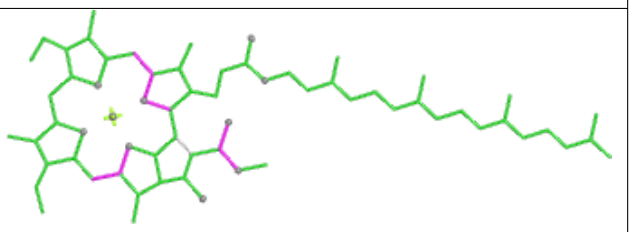

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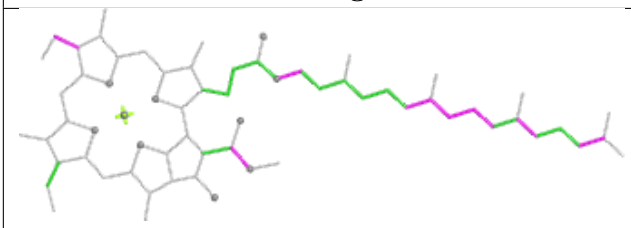

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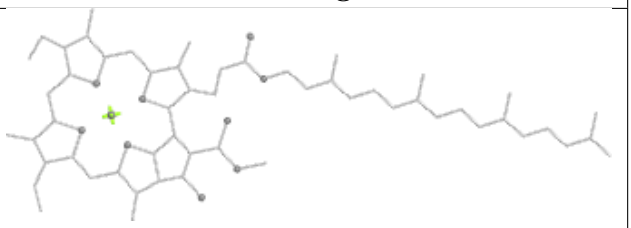
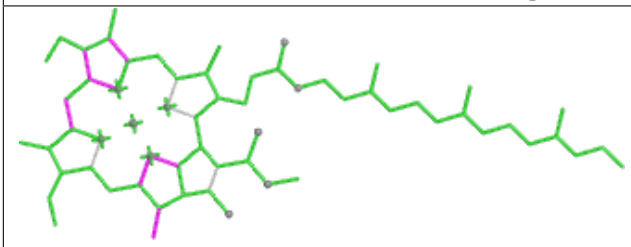


Rings

Ligand CLA A 819



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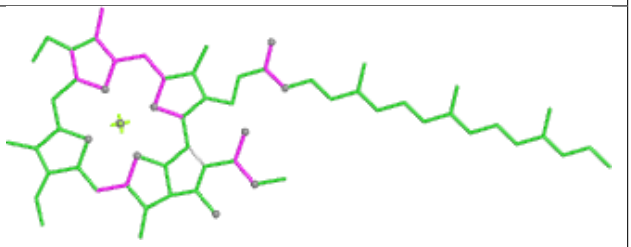

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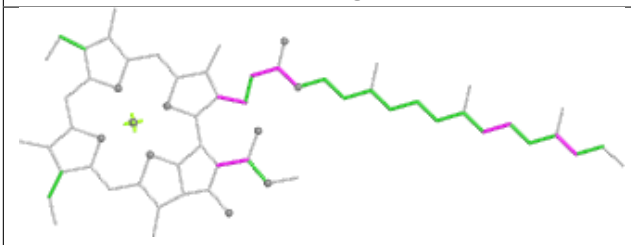

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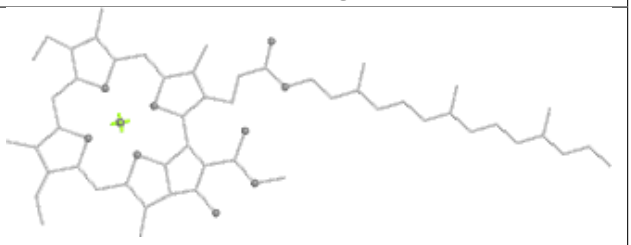
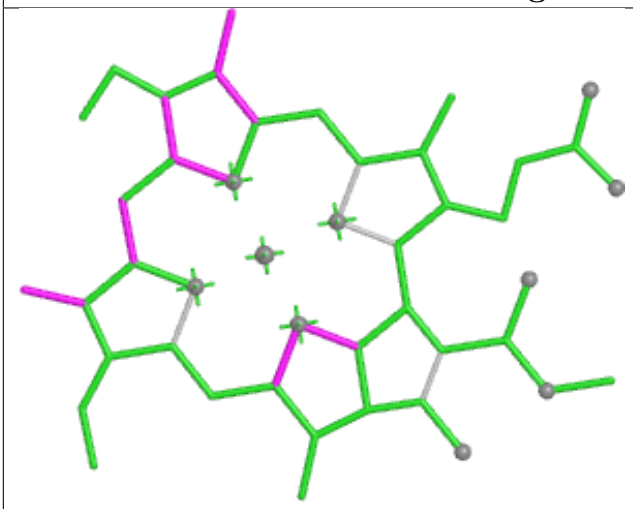


Rings

Ligand CLA 5 606



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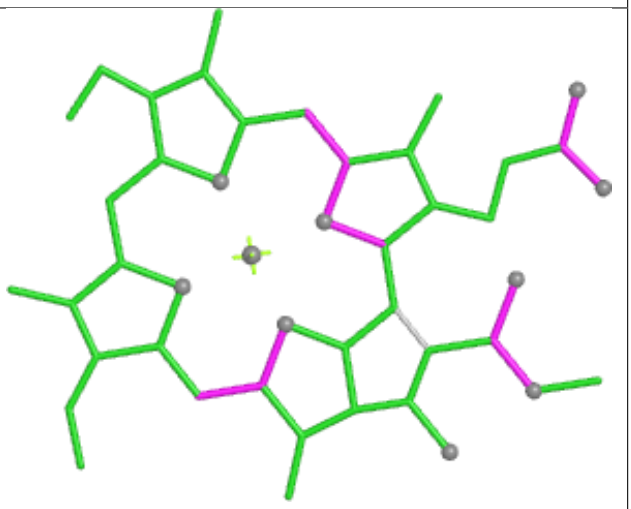

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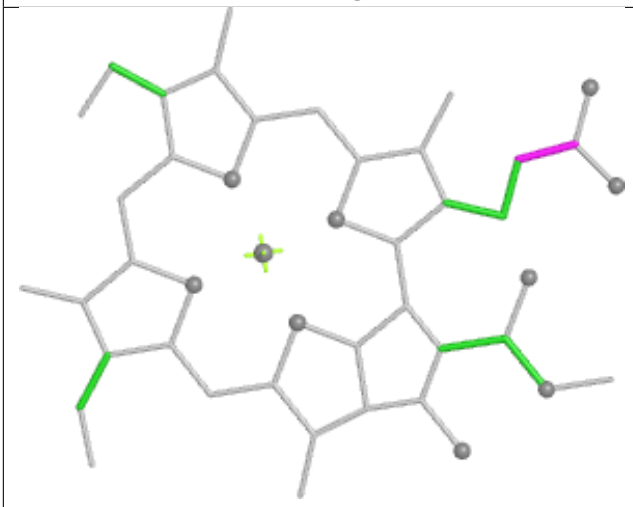
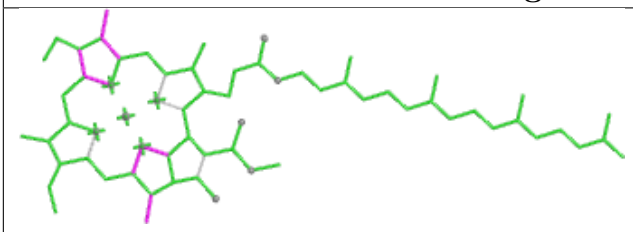


Torsions

Rings

Ligand CLA B 841



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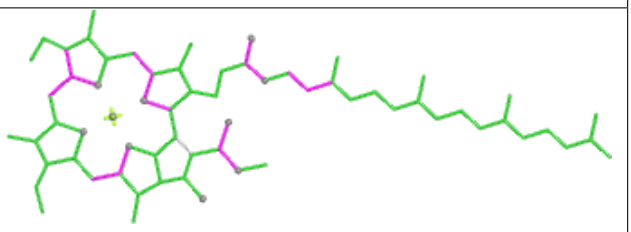

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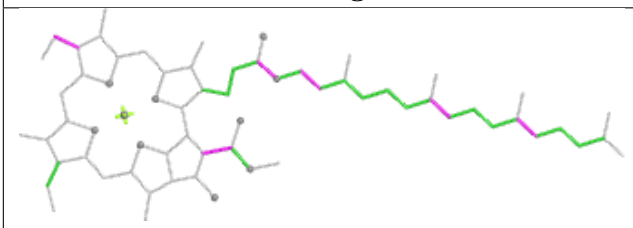

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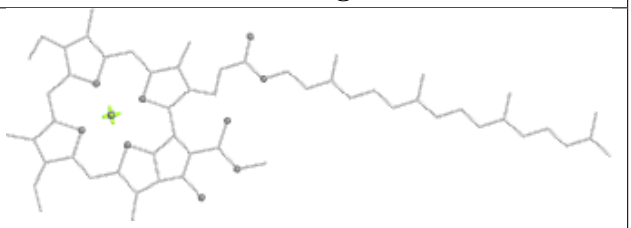
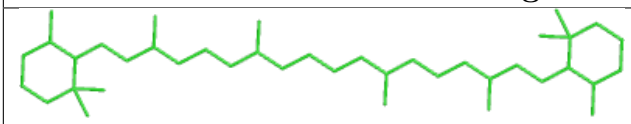
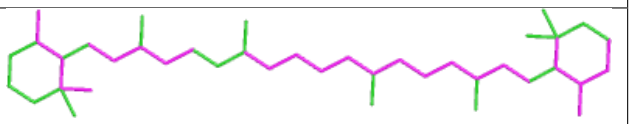
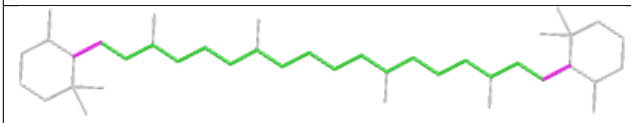
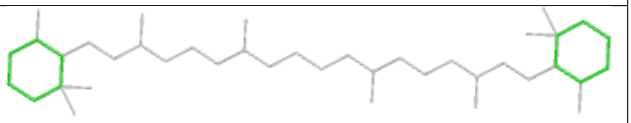
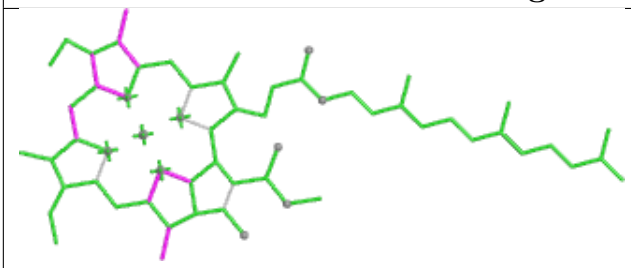
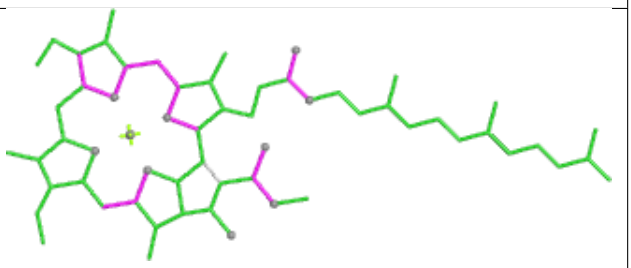
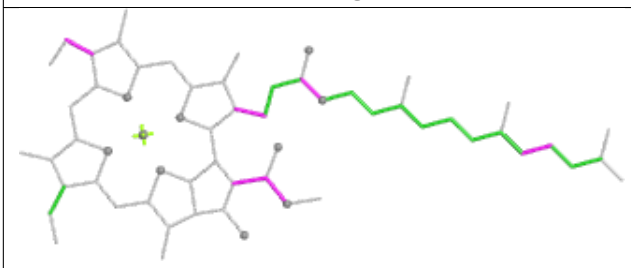
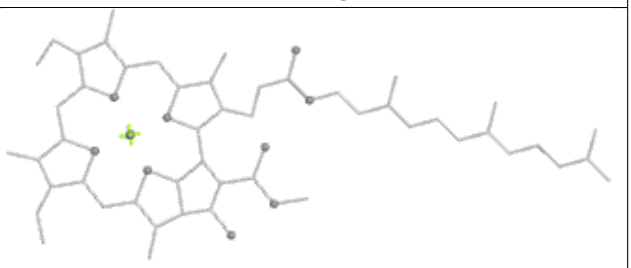
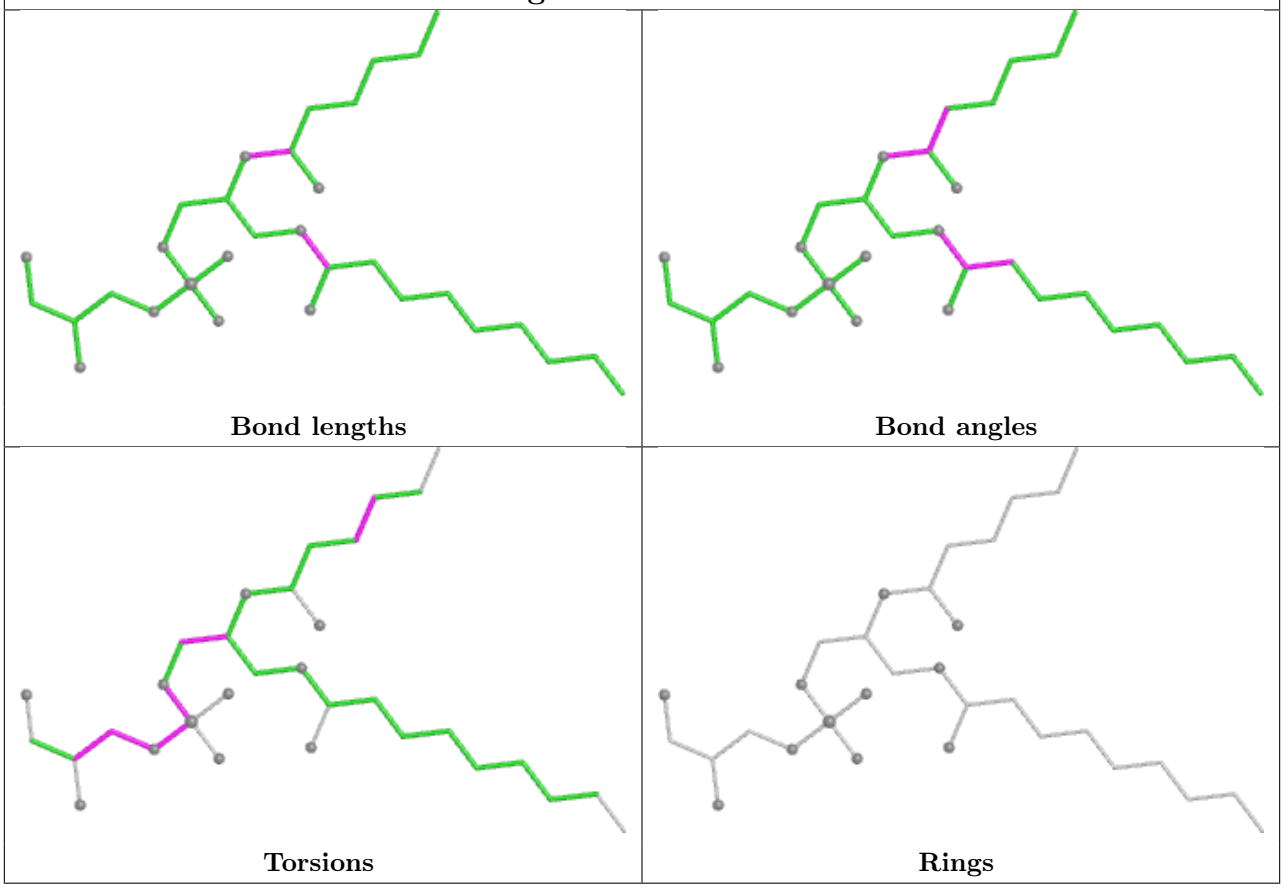


Rings

Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 2 630



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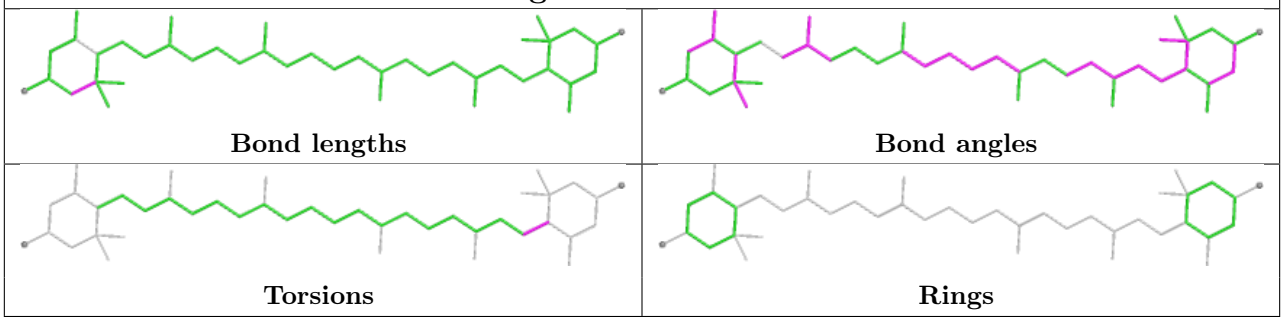

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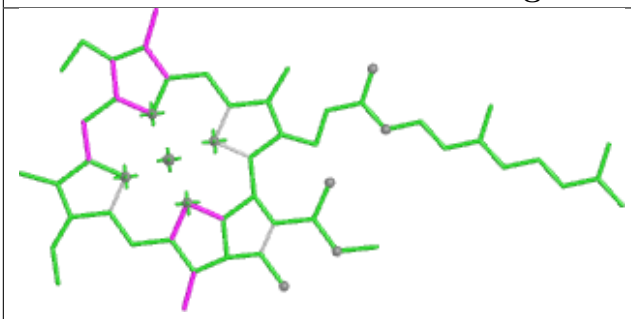
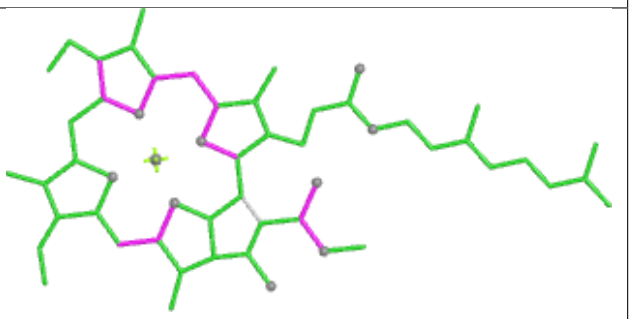
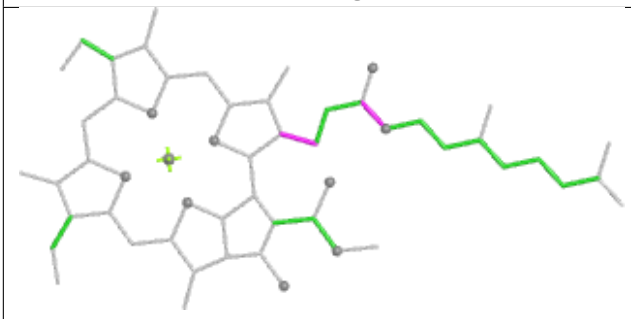
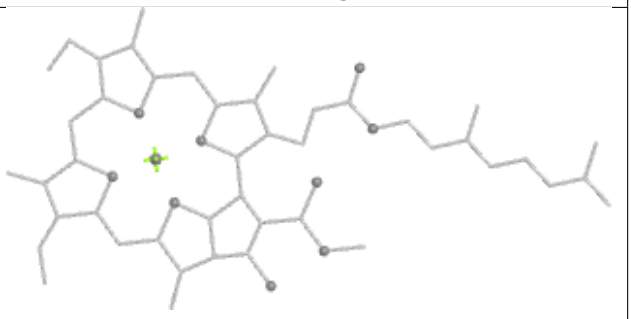
 Bond lengths	 Bond angles
 Torsions	 Rings

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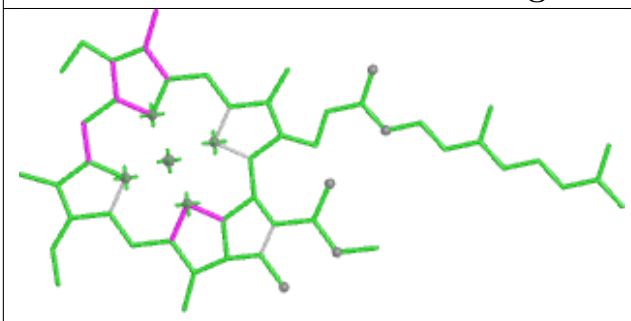
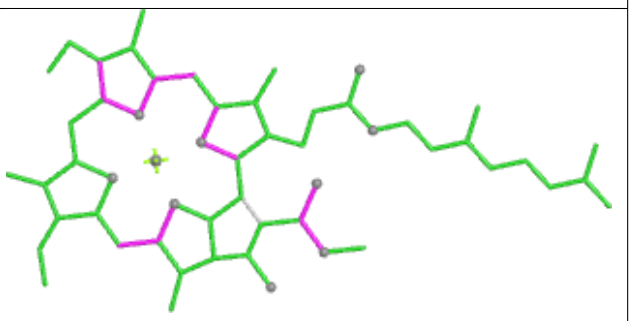
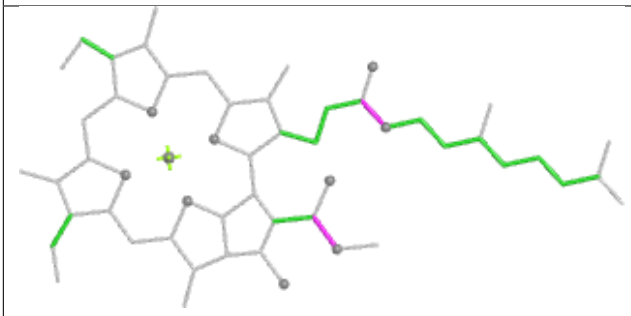
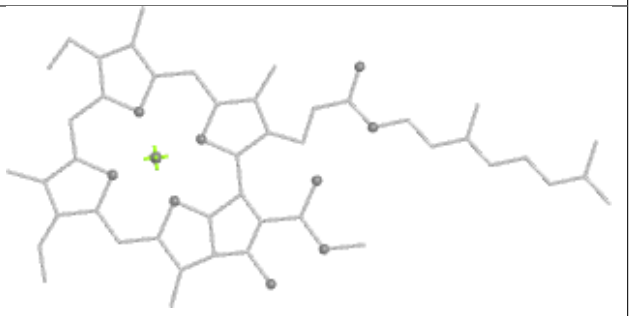
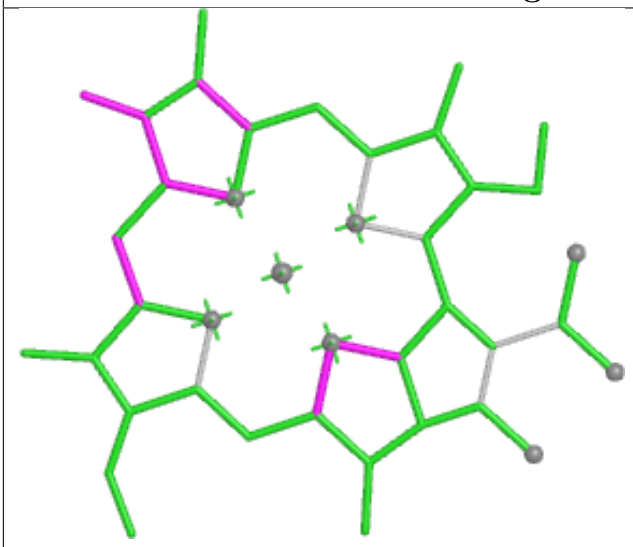
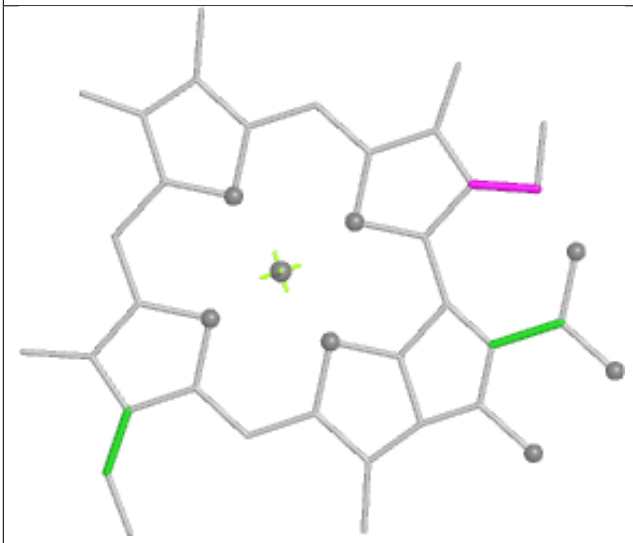
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 611



Bond lengths

Bond angles



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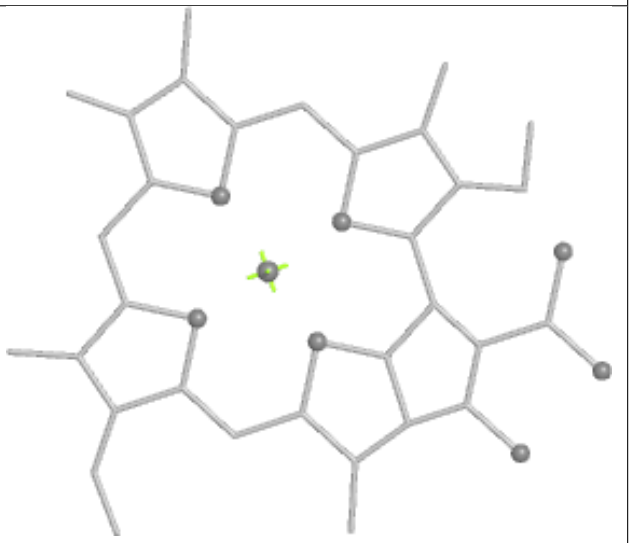
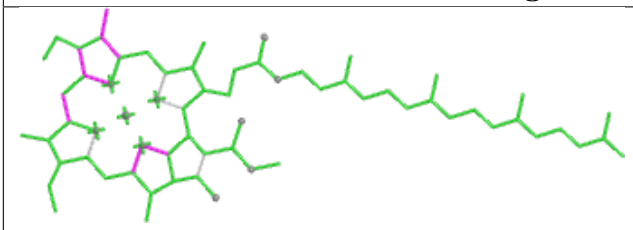


Rings

Ligand CLA A 827



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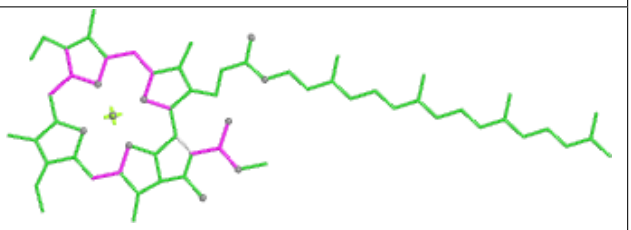
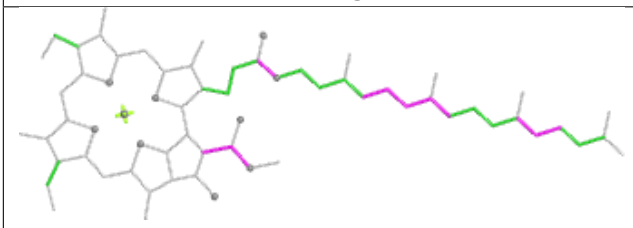


Bond angles



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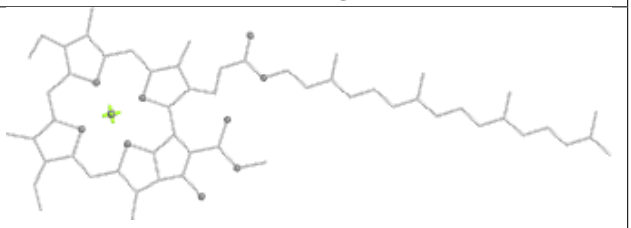

Rings

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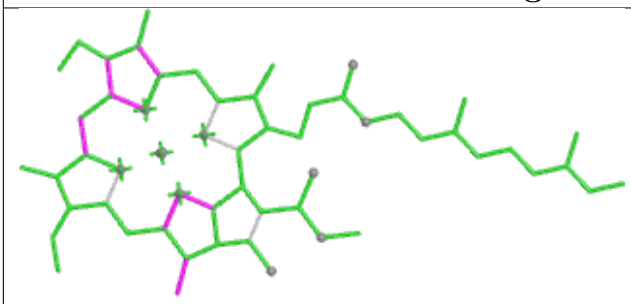
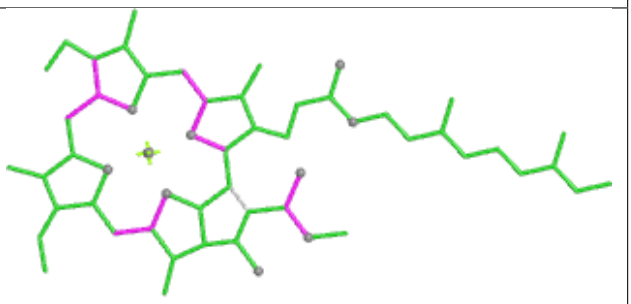
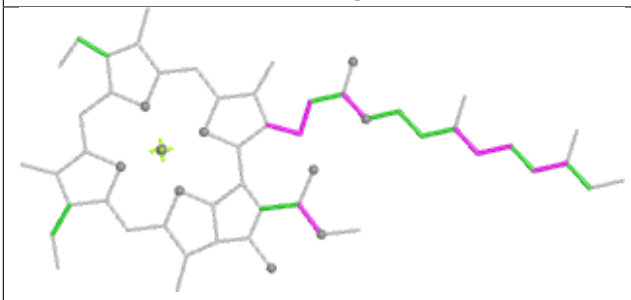
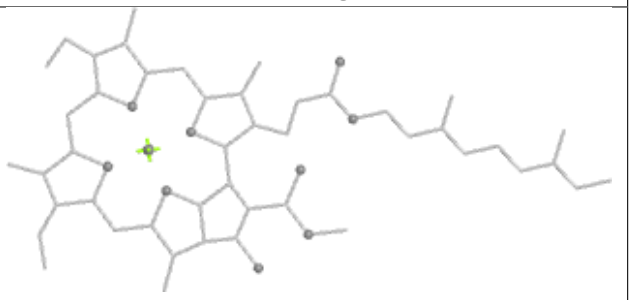
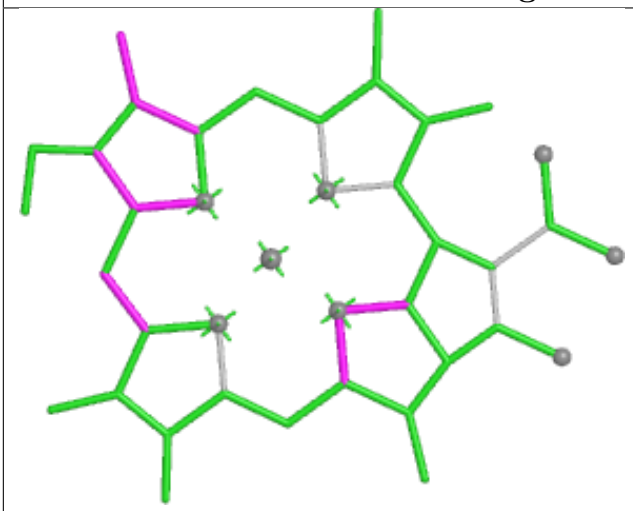
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 603



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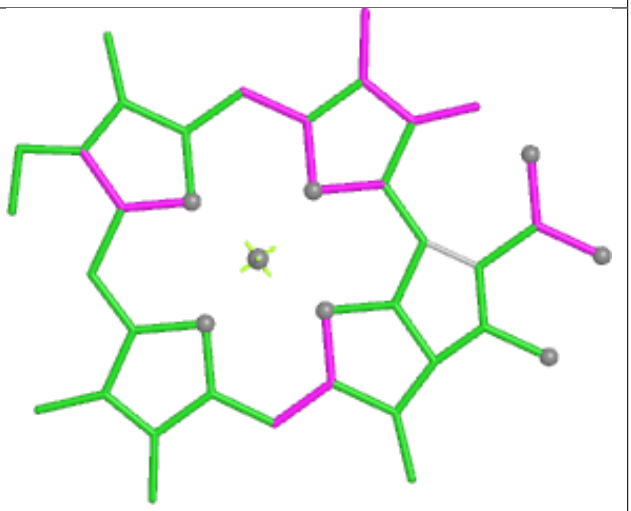
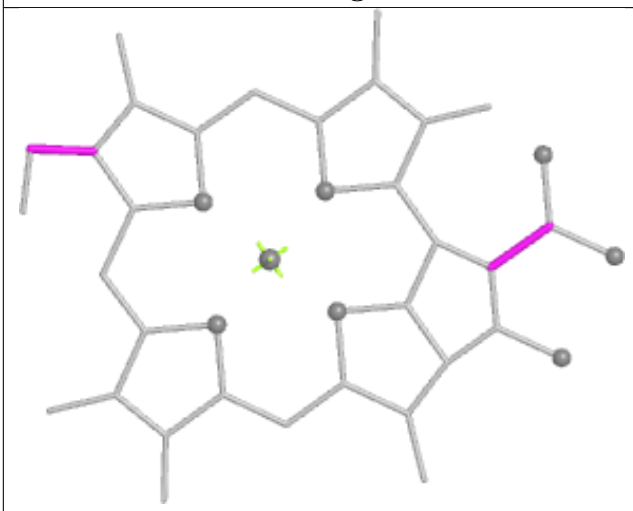


Bond angles



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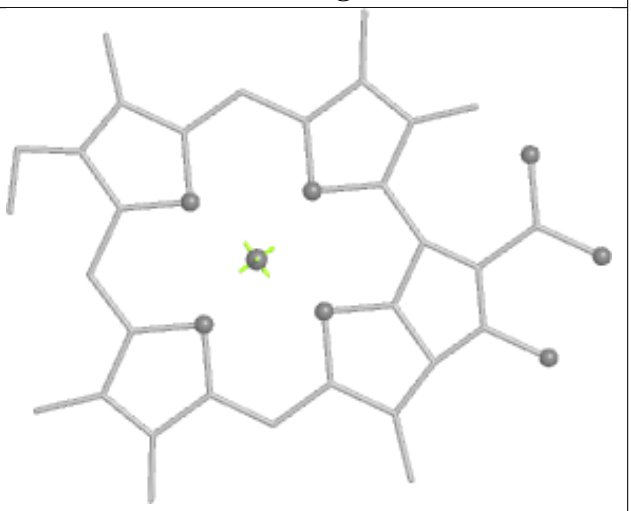
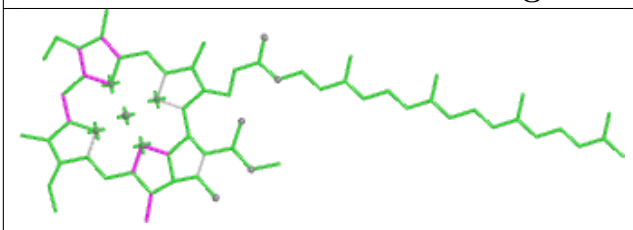


Rings

Ligand CLA U 613



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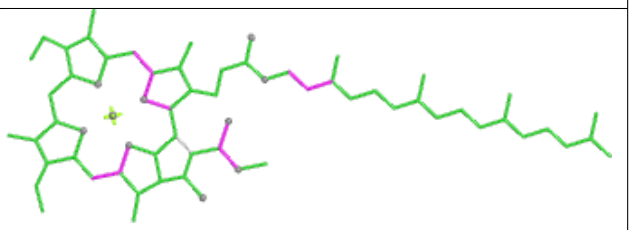
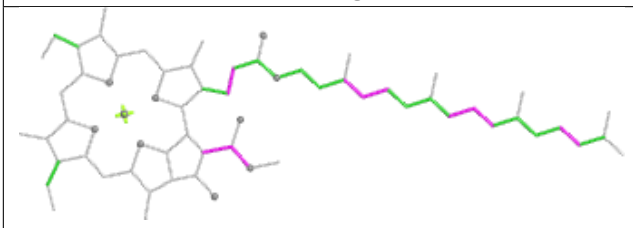


Bond angles



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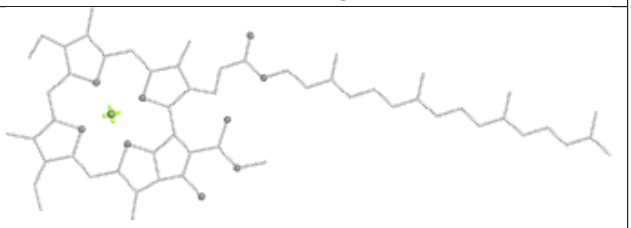
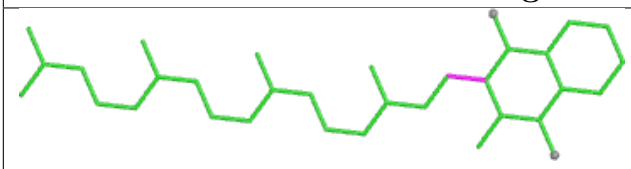


Rings

Ligand PQN B 842



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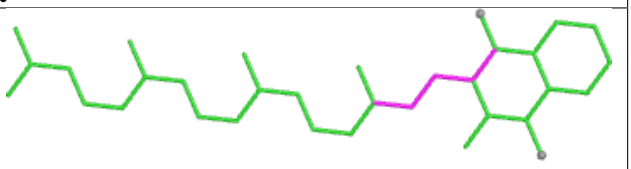

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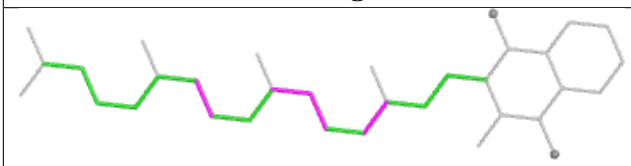

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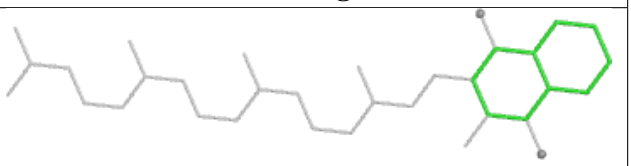
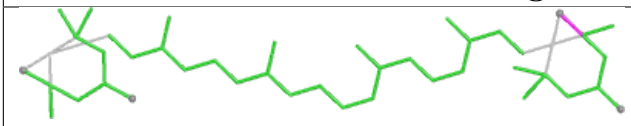


Rings

Ligand XAT 4 620



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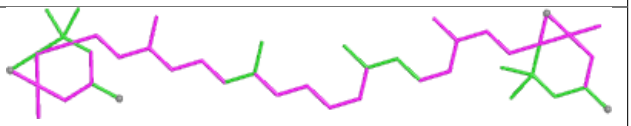

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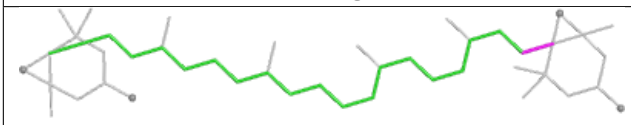

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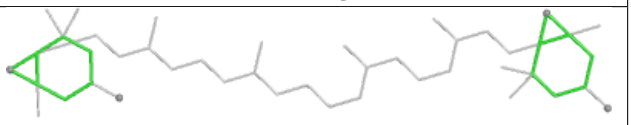

Rings

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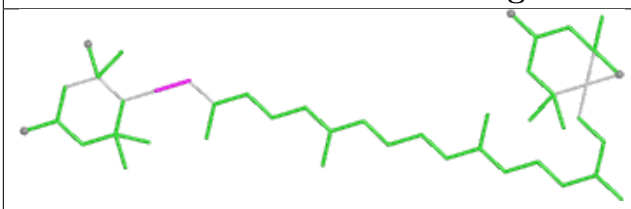

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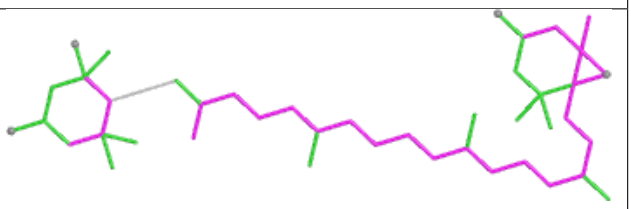

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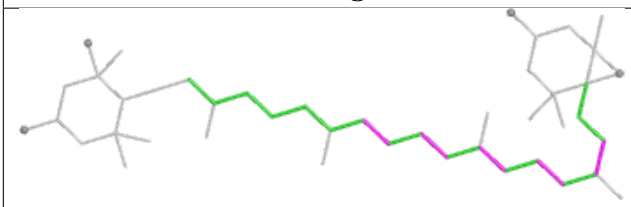

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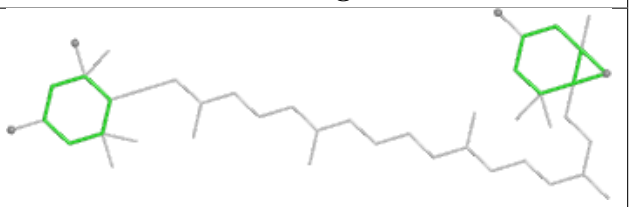
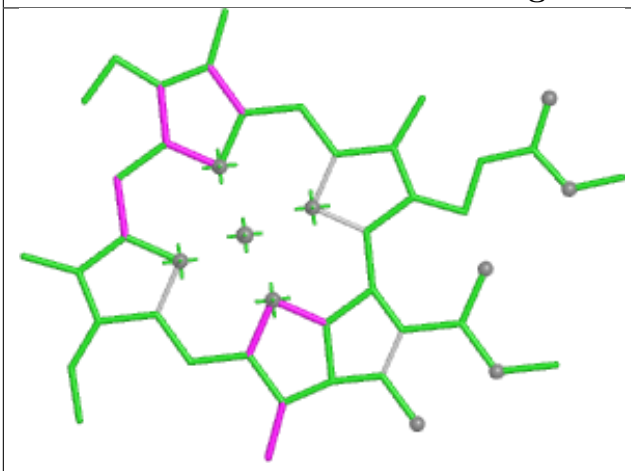
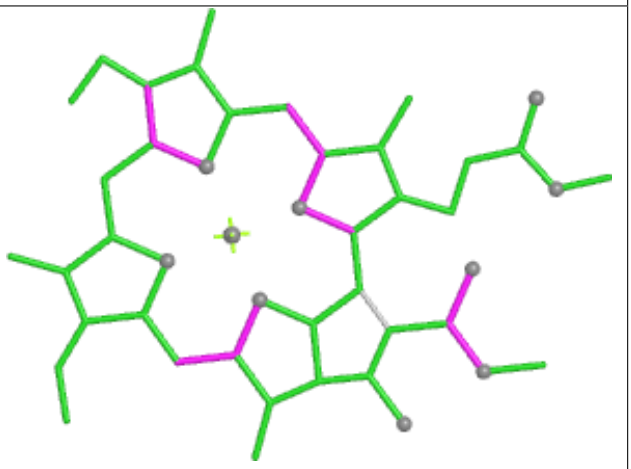
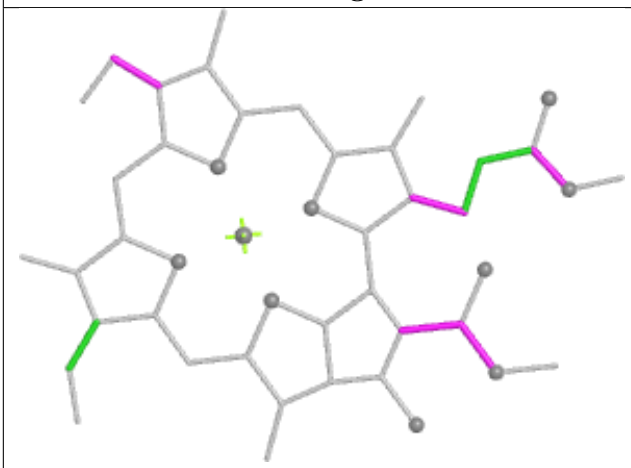
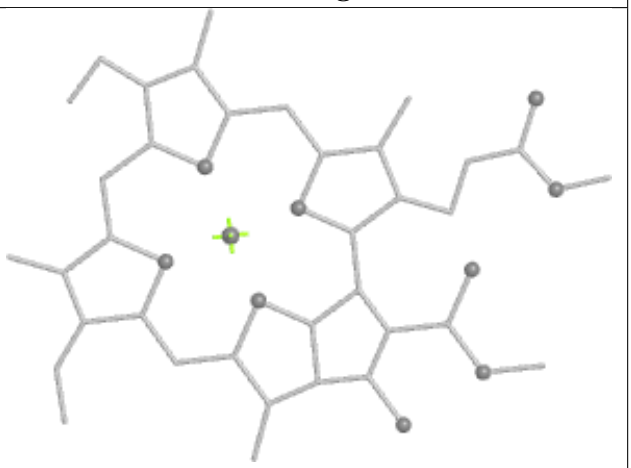
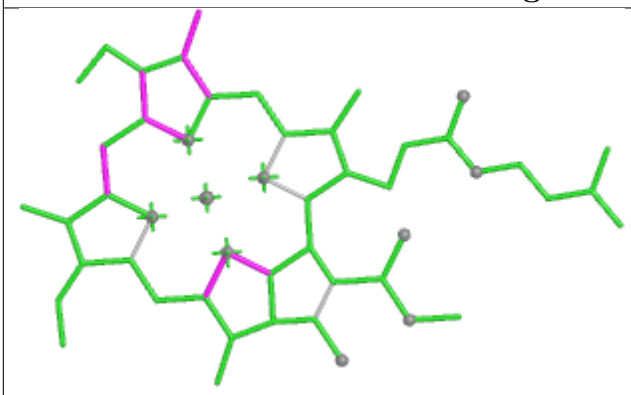


Rings

Ligand CLA 4 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 203



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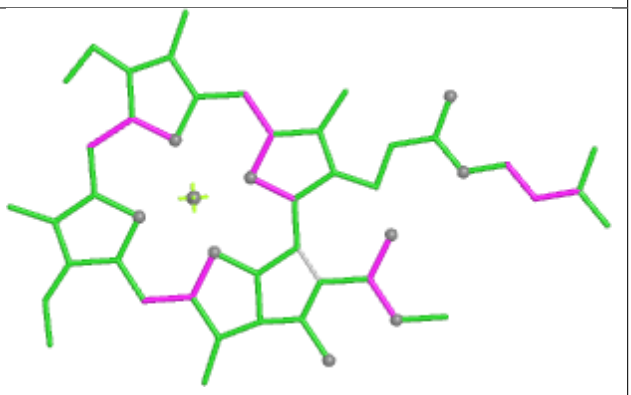
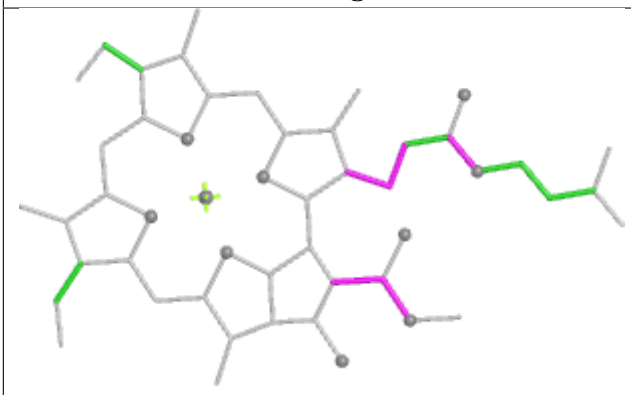


Bond angles



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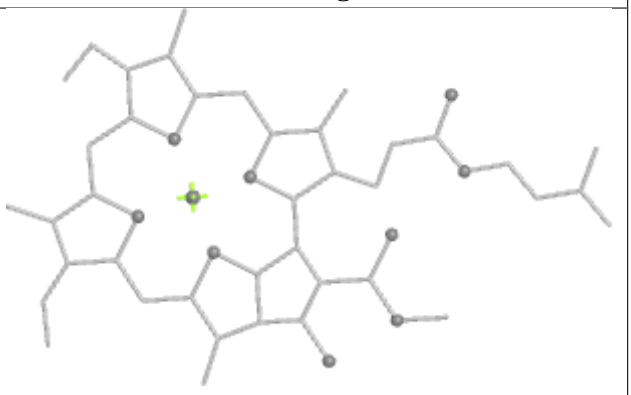
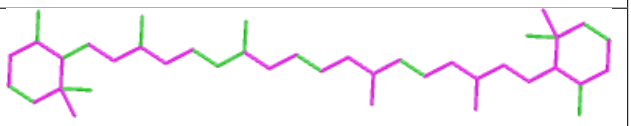


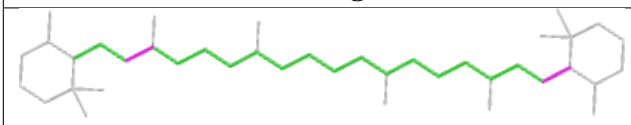
Rings

Ligand BCR 3 620

Bond lengths



Bond angles



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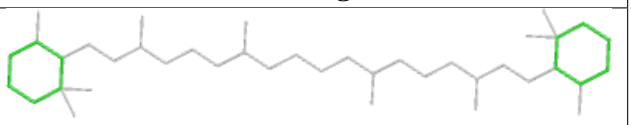
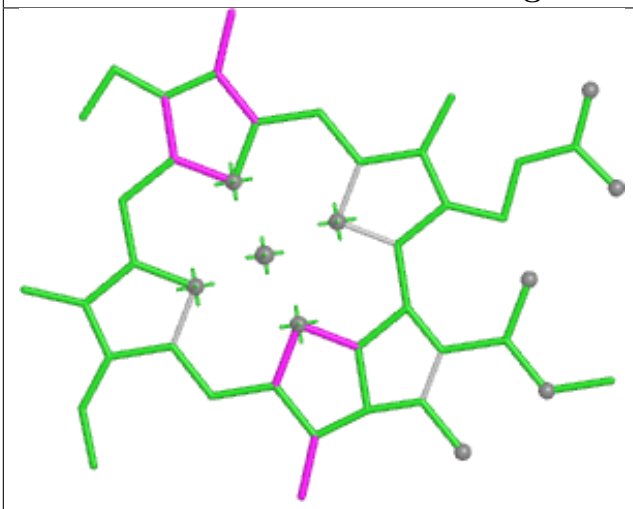


Rings

Ligand CLA A 816



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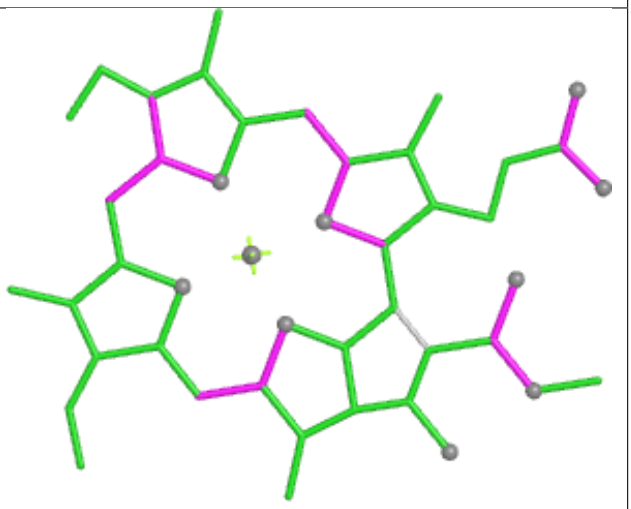
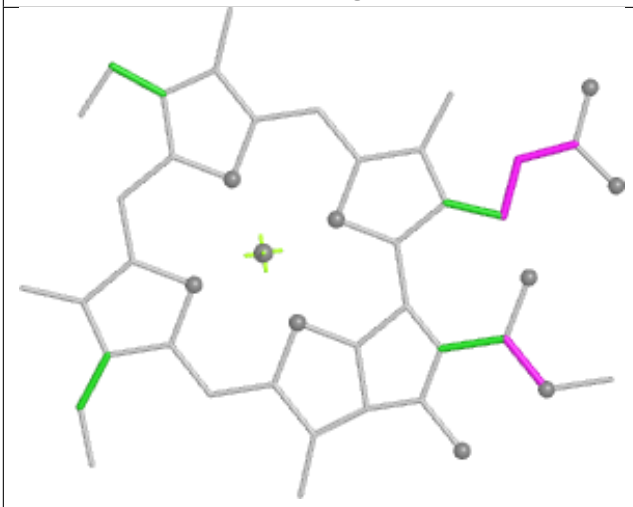


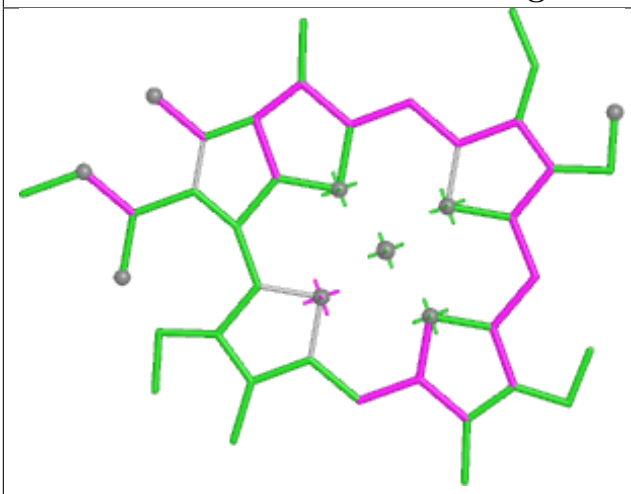
Bond angles



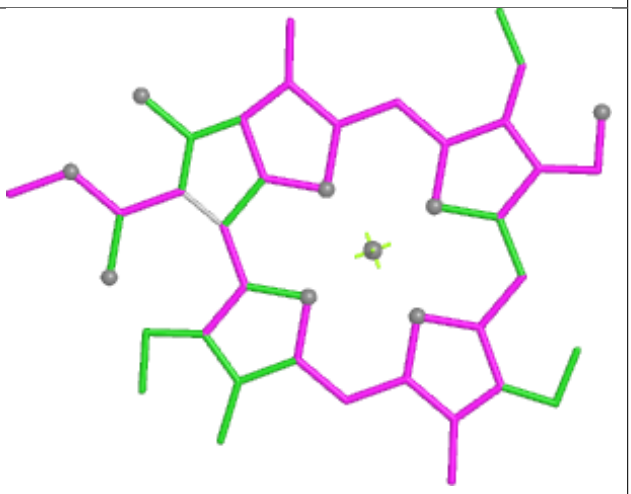
Torsions

Rings

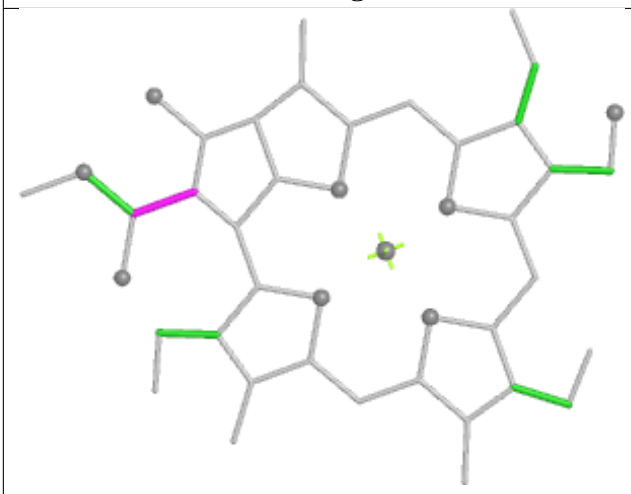
Ligand CHL 9 608



Bond lengths



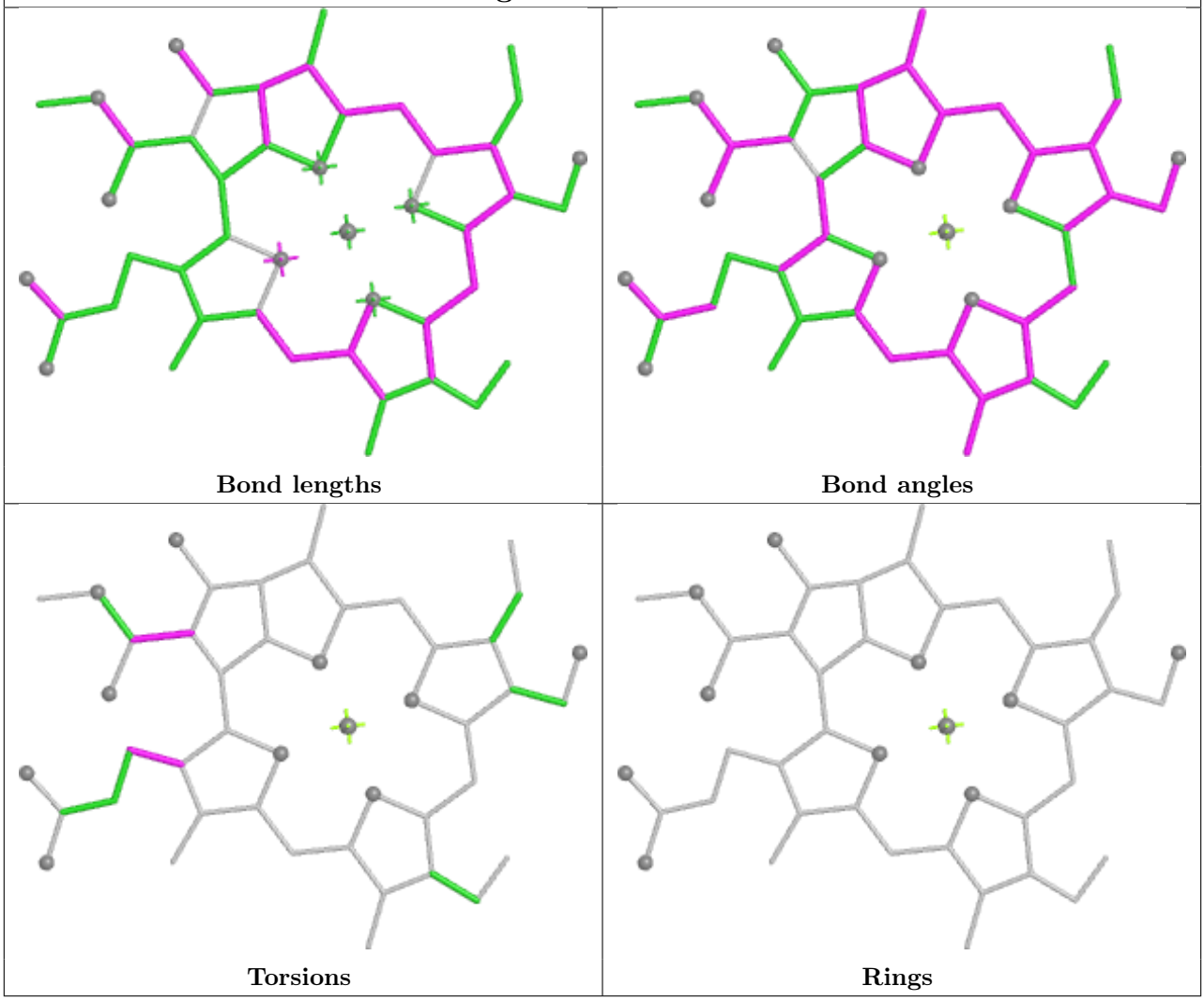
Bond angles



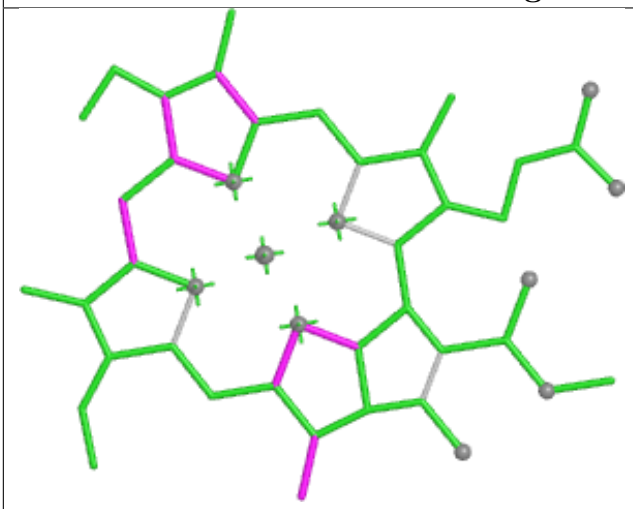
Torsions

Rings

Ligand CHL 8 606



Ligand CLA B 823



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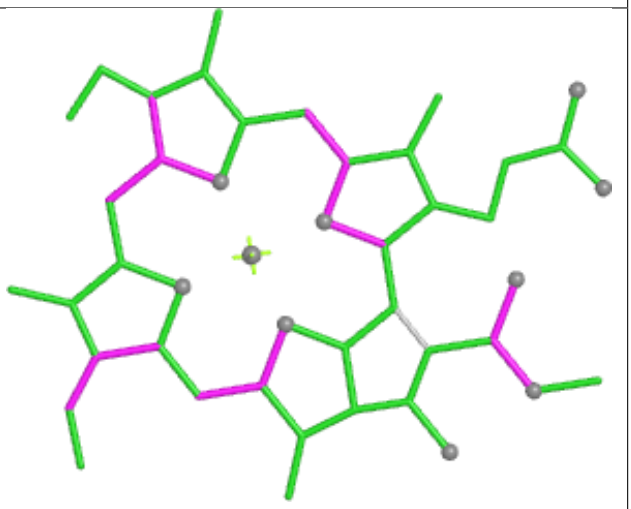

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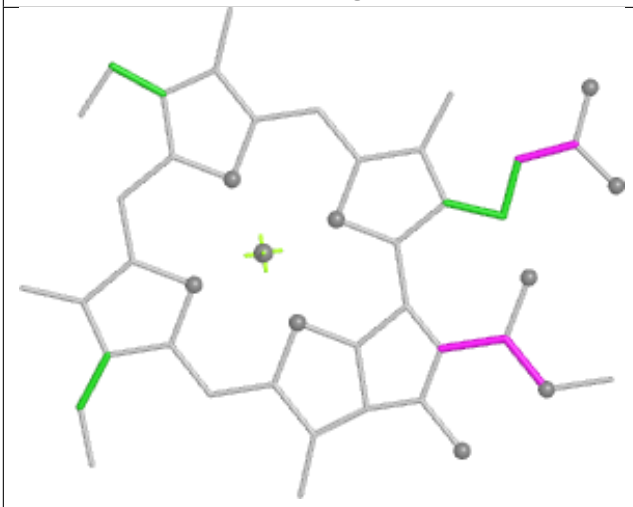
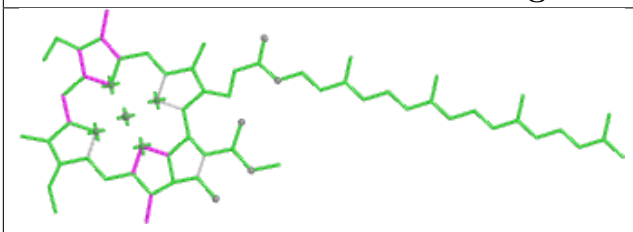


Torsions

Rings

Ligand CLA 4 603



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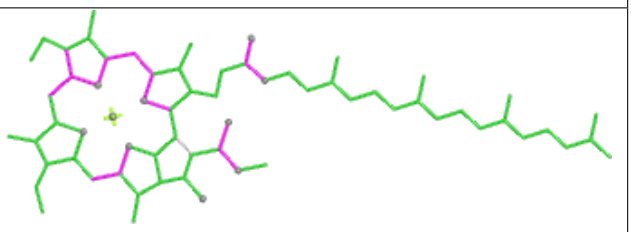
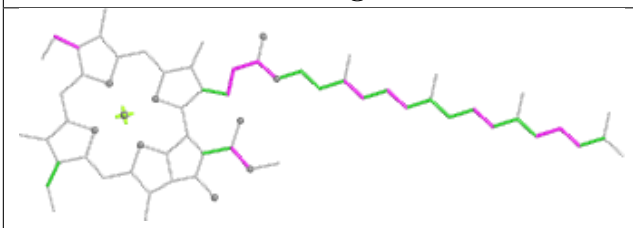


Bond angles



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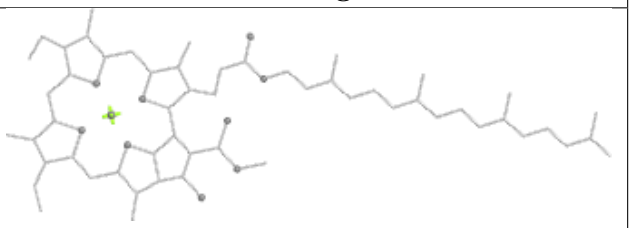
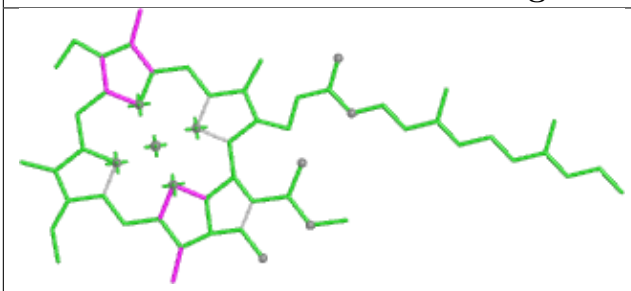


Rings

Ligand CLA 2 613



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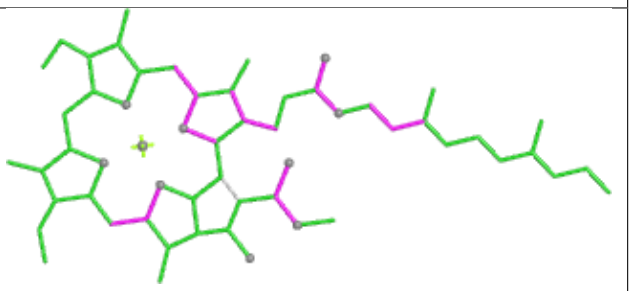
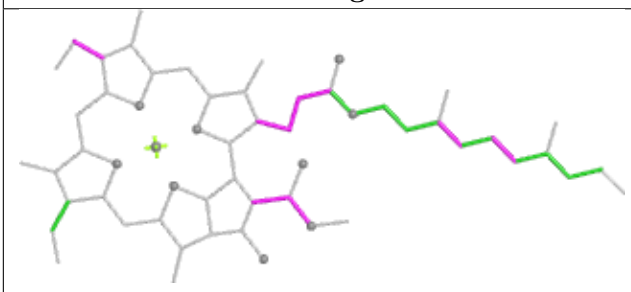


Bond angles



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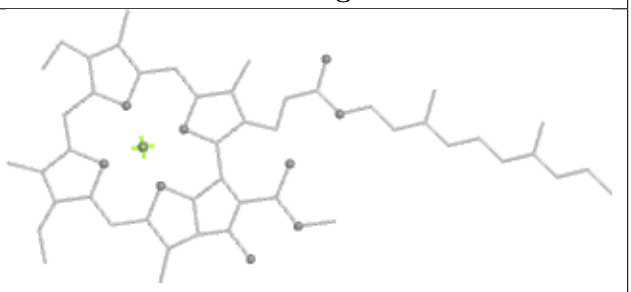
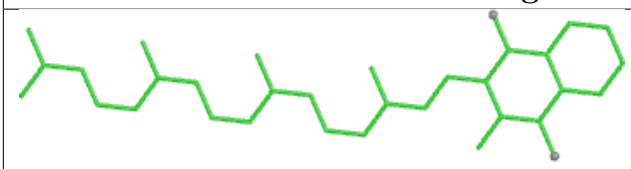


Rings

Ligand PQN A 844



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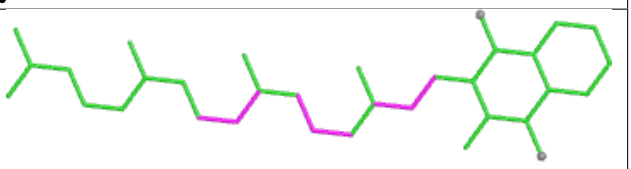
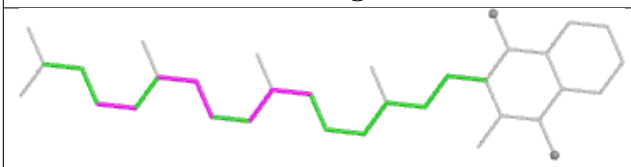


Bond angles



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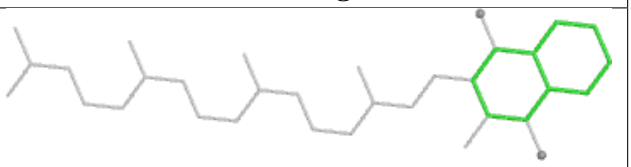
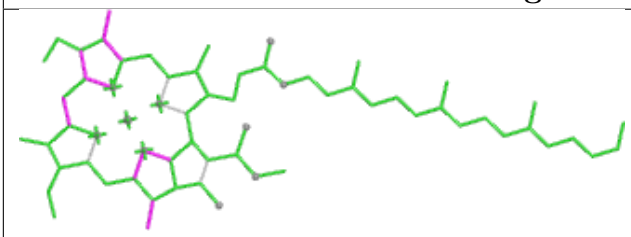


Rings

Ligand CLA B 818



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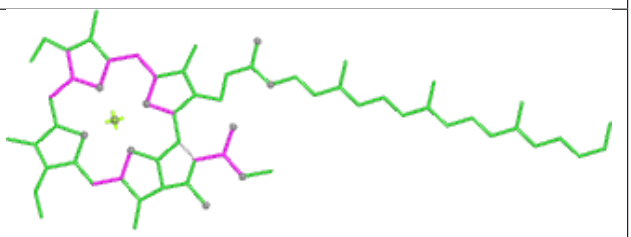
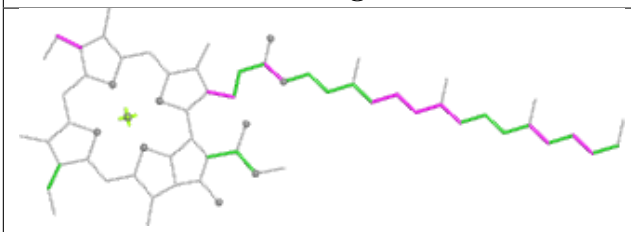


Bond angles



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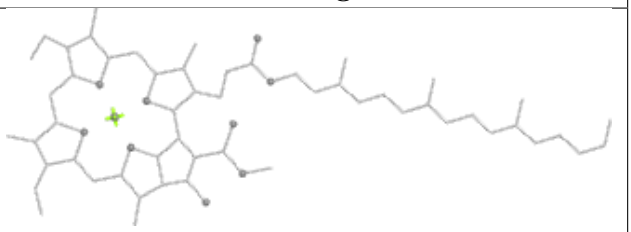
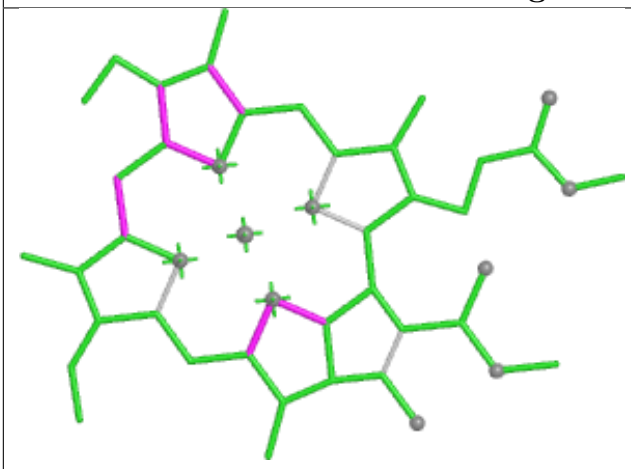


Rings

Ligand CLA 8 612



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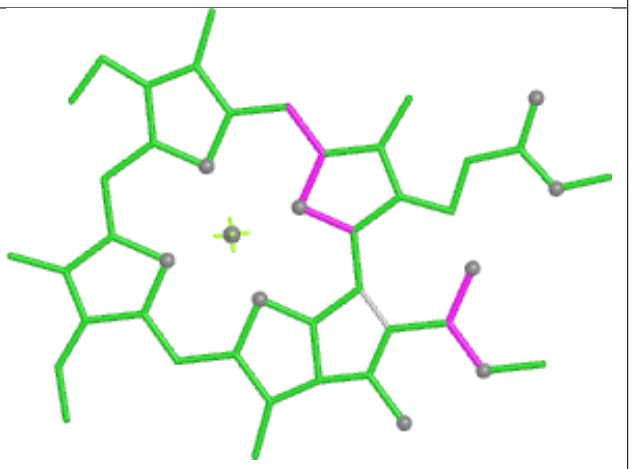
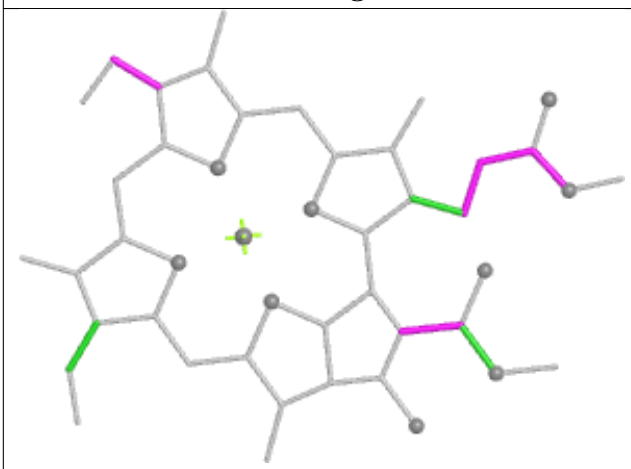


Bond angles



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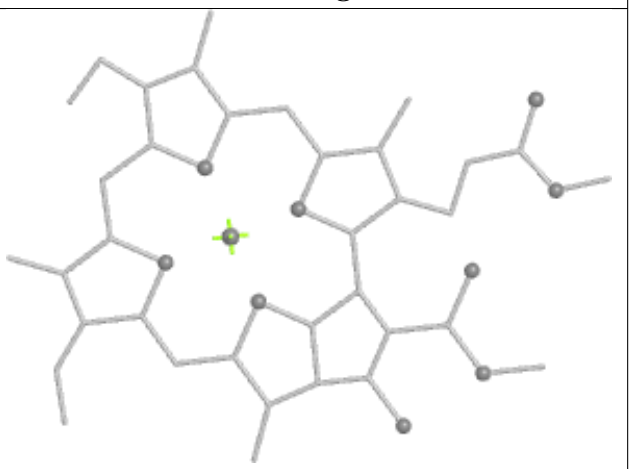
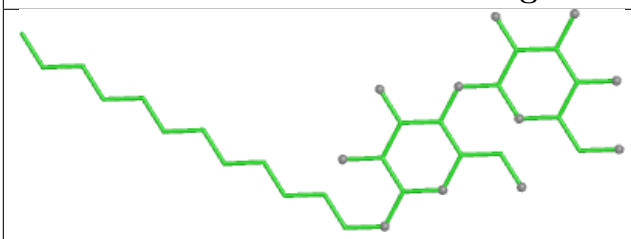


Rings

Ligand LMT G 206



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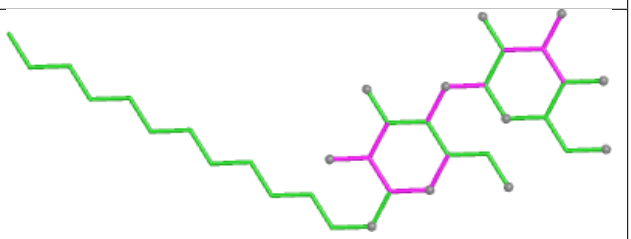
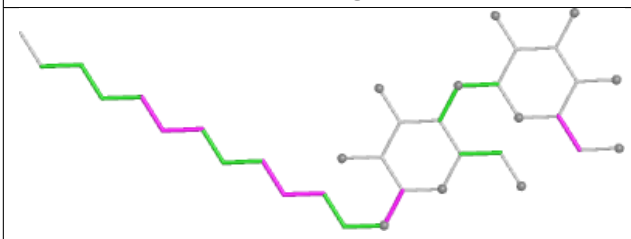


Bond angles



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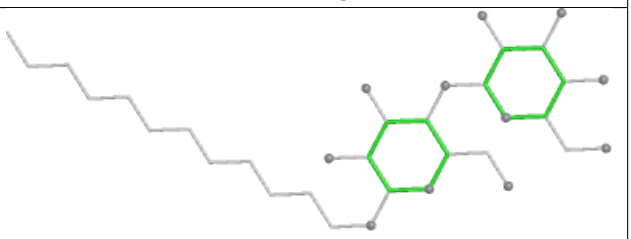
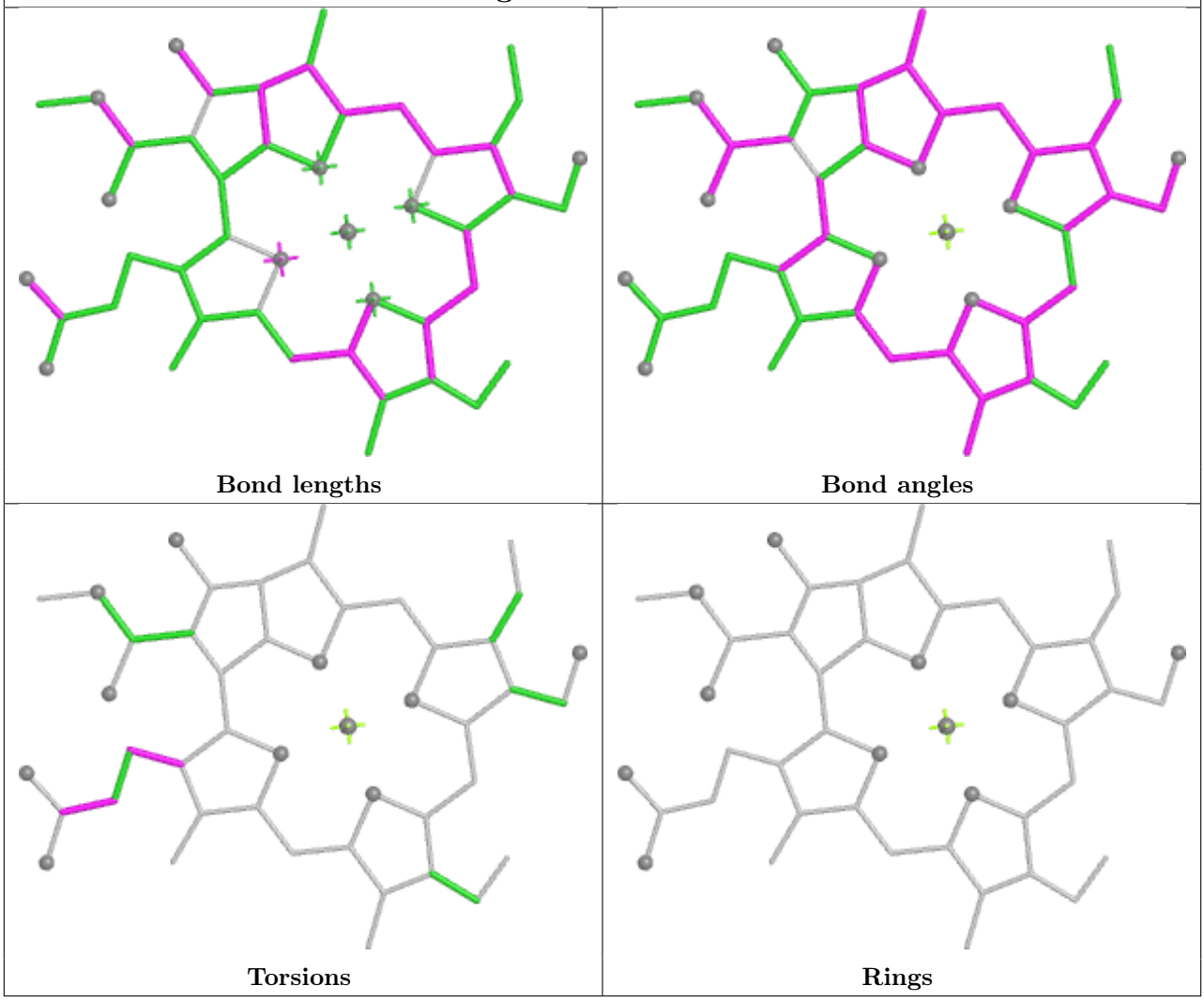


Rings

Ligand CHL 6 606



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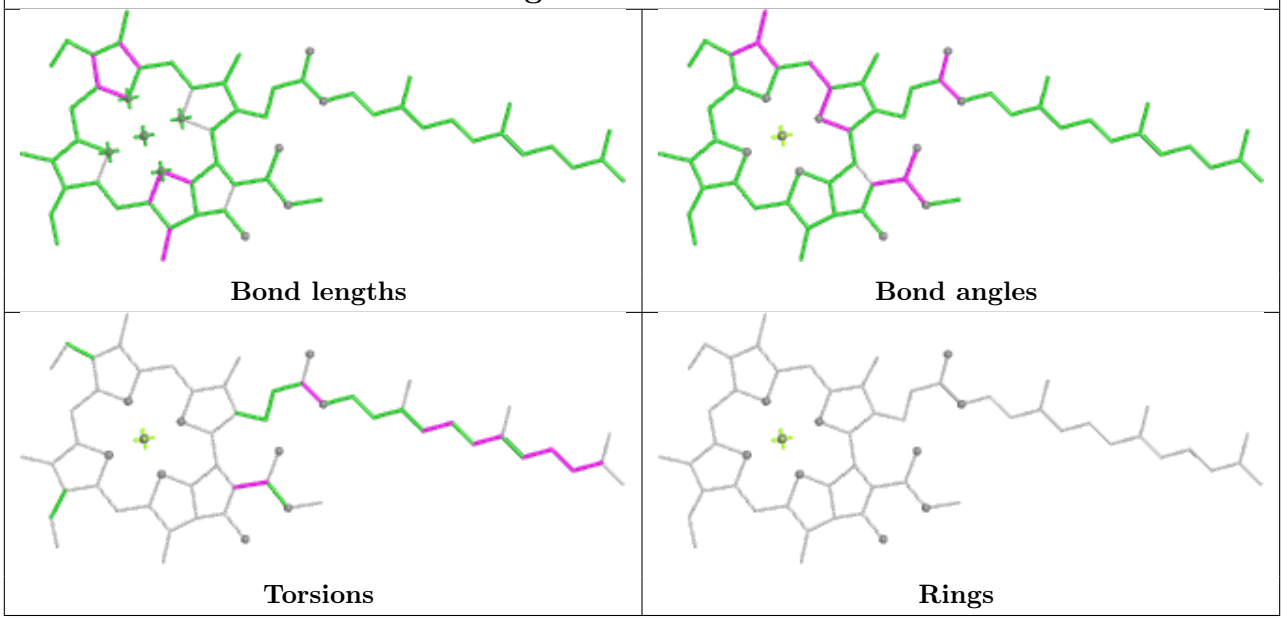
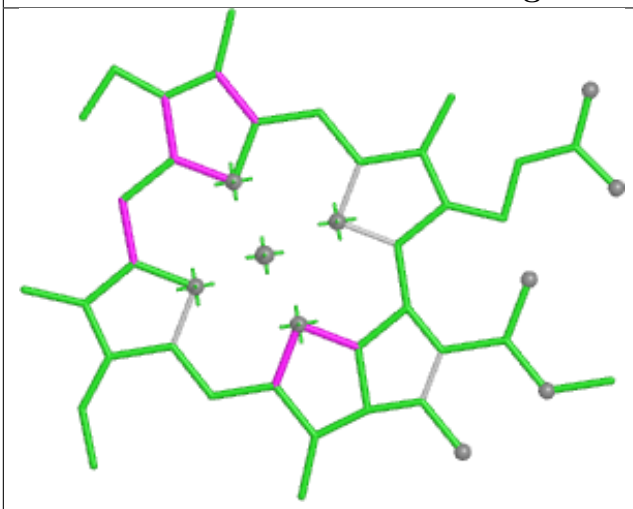


Ligand CLA U 611



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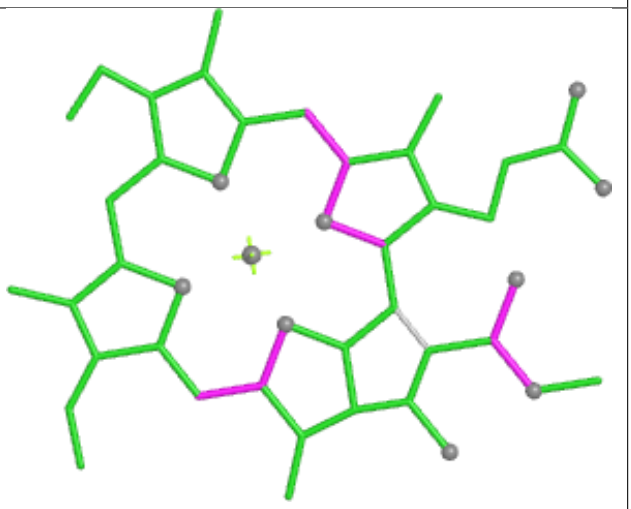
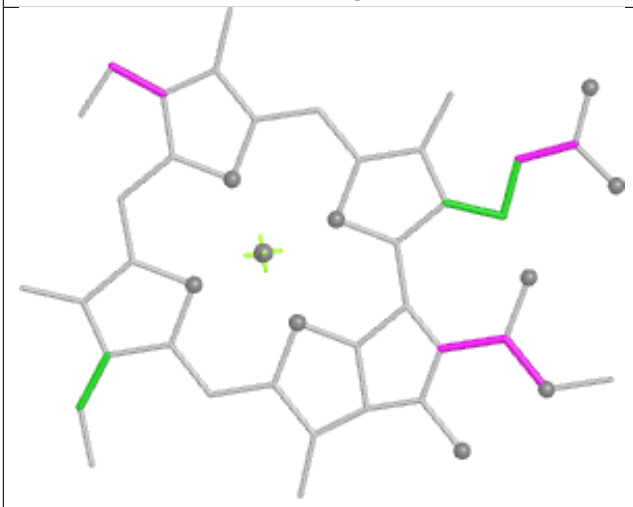


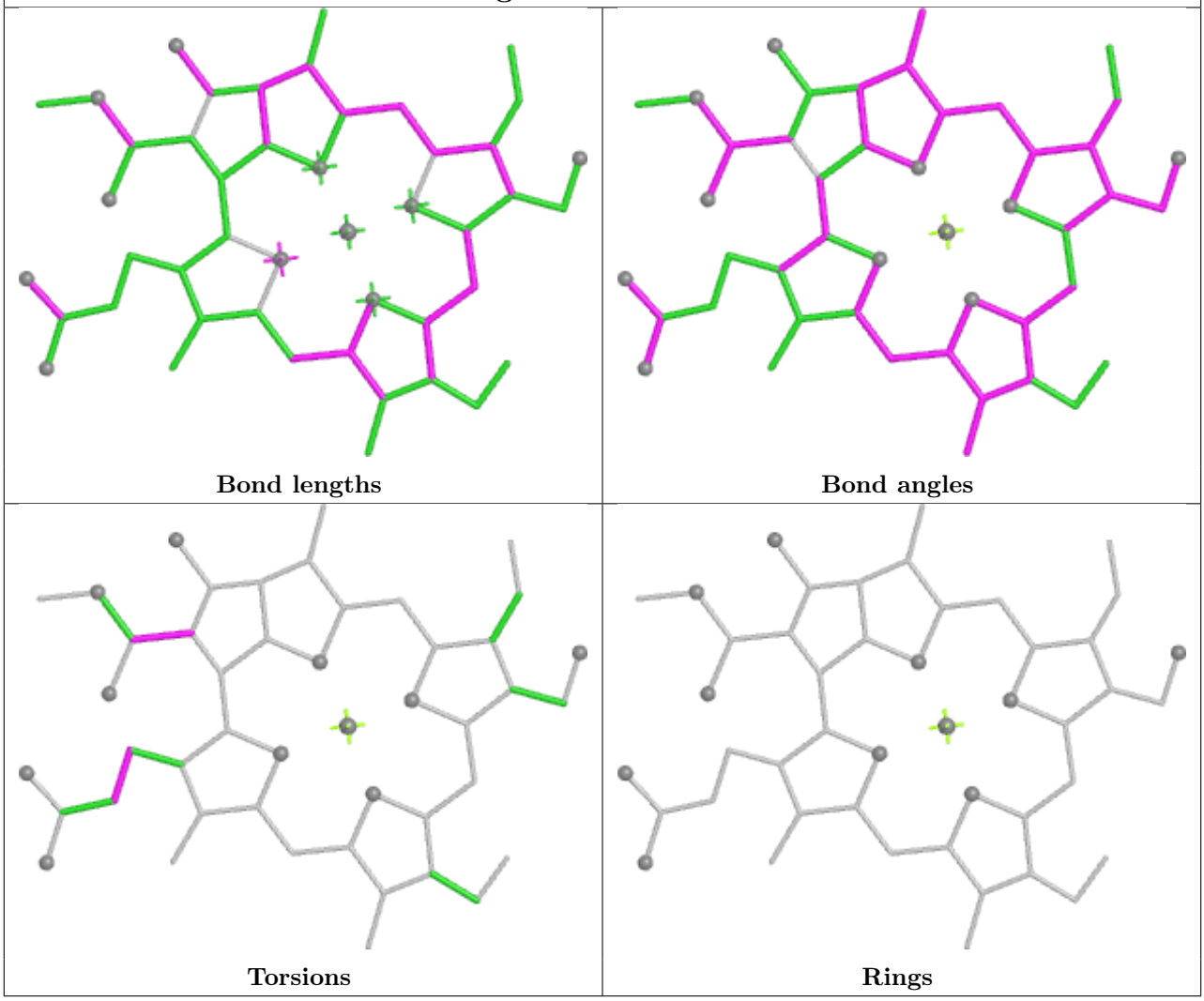
Bond angles



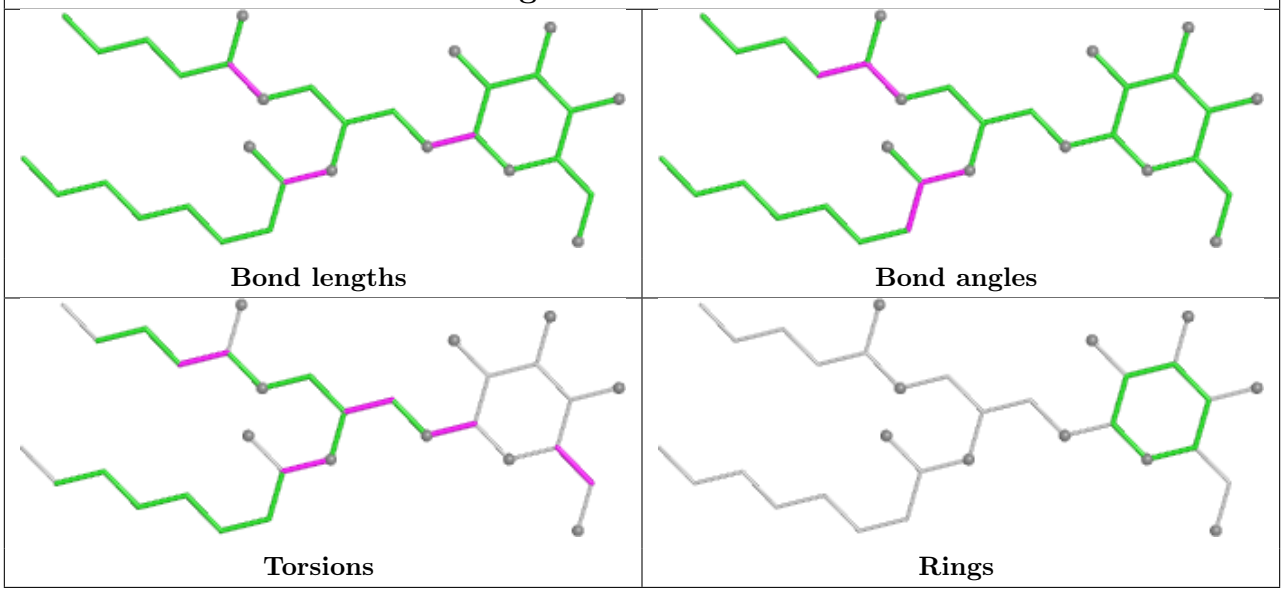
Torsions

Rings

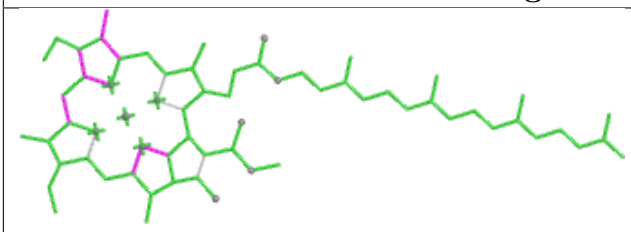
Ligand CHL 2 601



Ligand LMG G 202



Ligand CLA B 832



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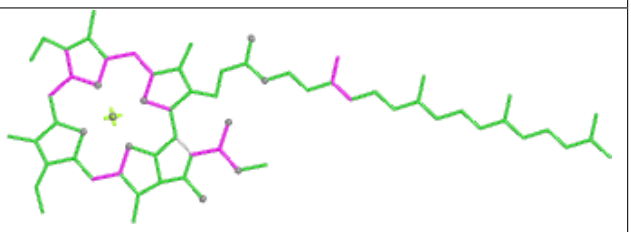
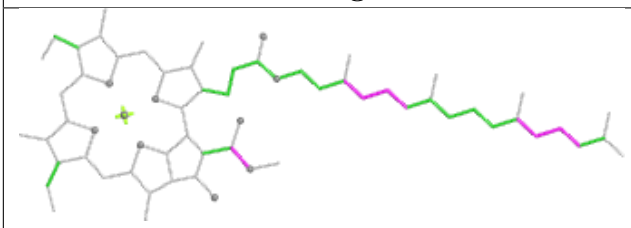
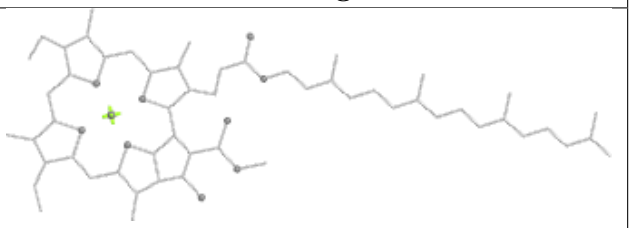


Bond angles

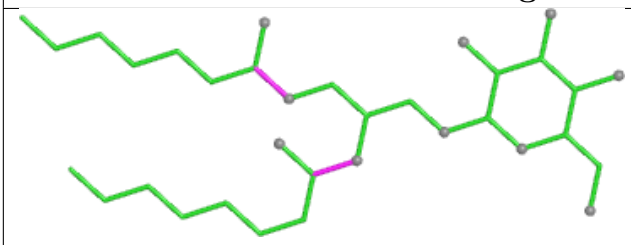


Torsions



Rings

Ligand LMG A 860



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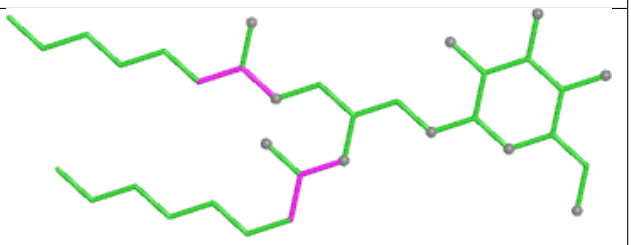
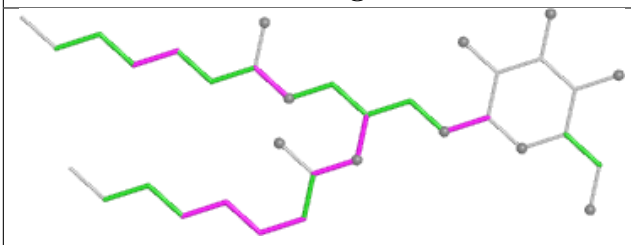


Bond angles



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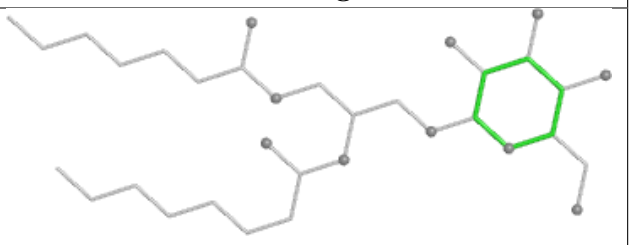
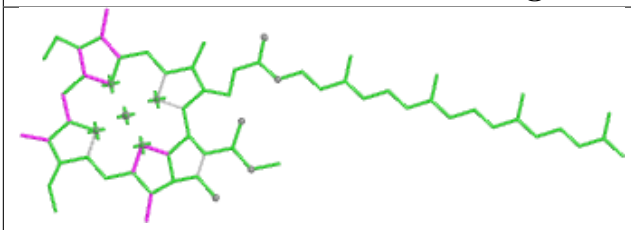


Rings

Ligand CLA F 301



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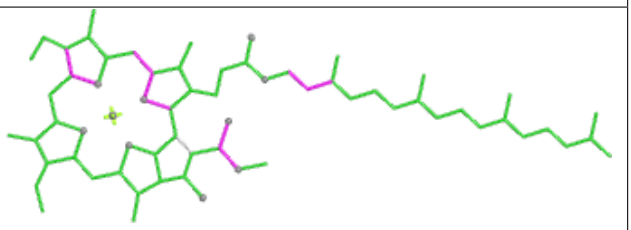
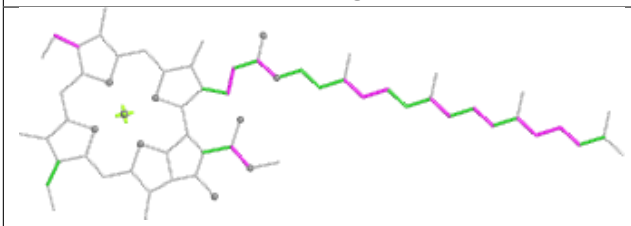


Bond angles



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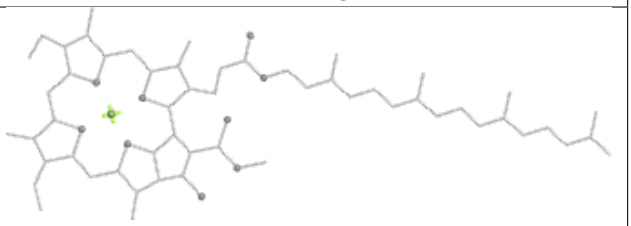
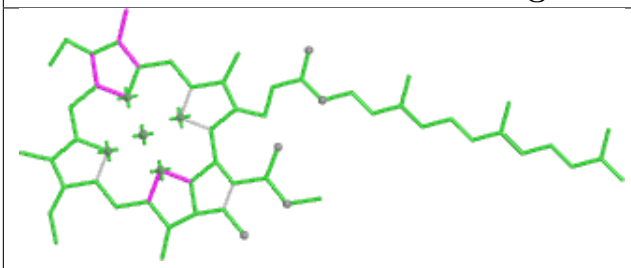


Rings

Ligand CLA 8 602



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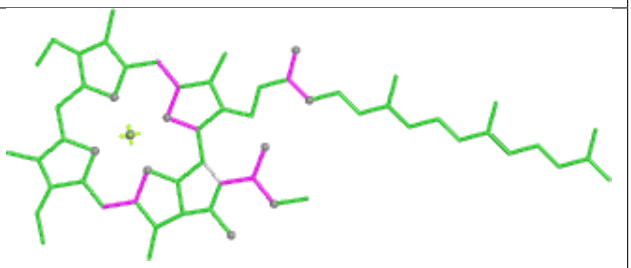
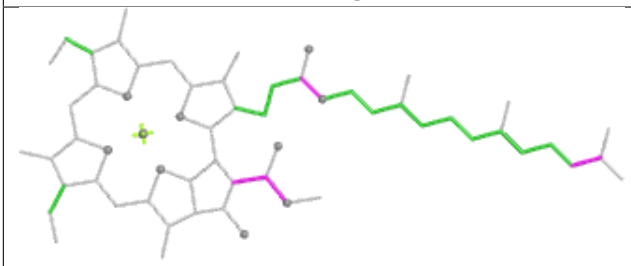


Bond angles



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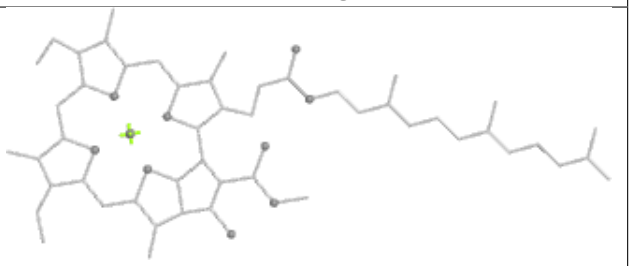
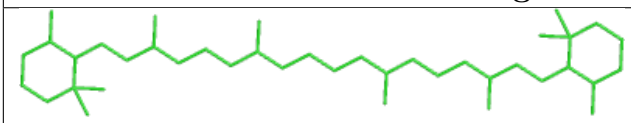
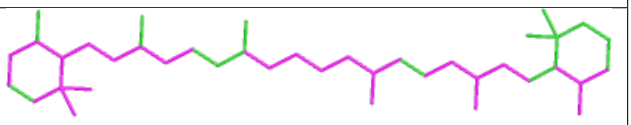


Rings

Ligand BCR O 2004

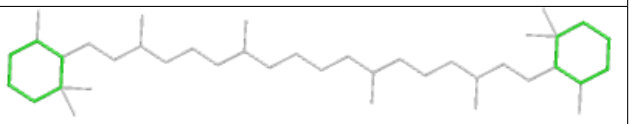


Bond lengths



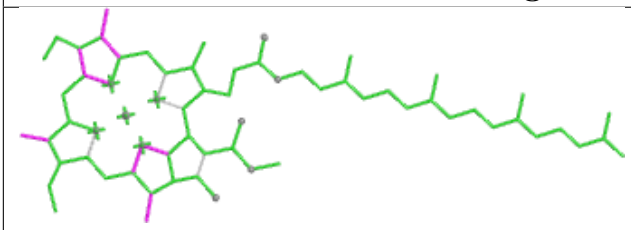
Bond angles

Torsions

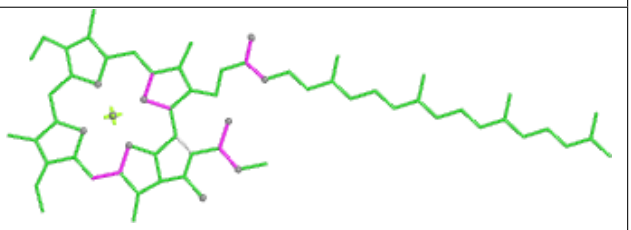


Rings

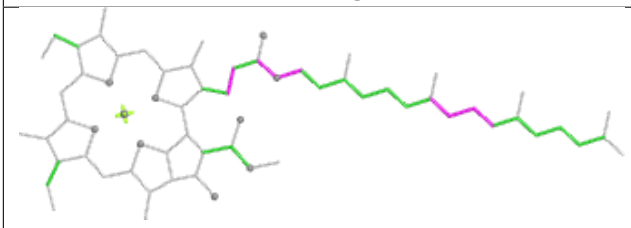
Ligand CLA A 803



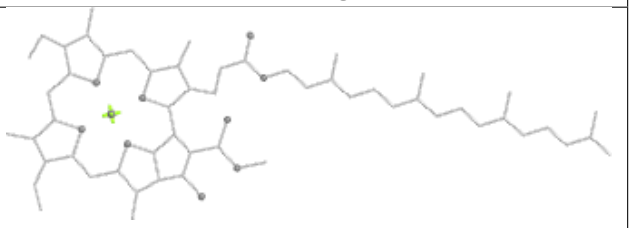
Bond lengths



Bond angles

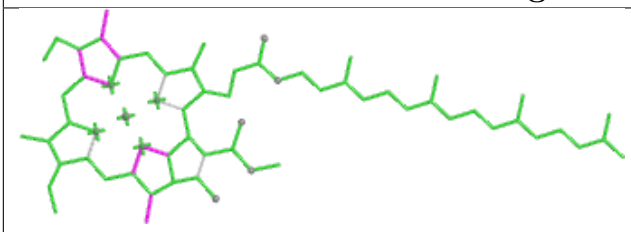


Torsions



Rings

Ligand CLA 3 612



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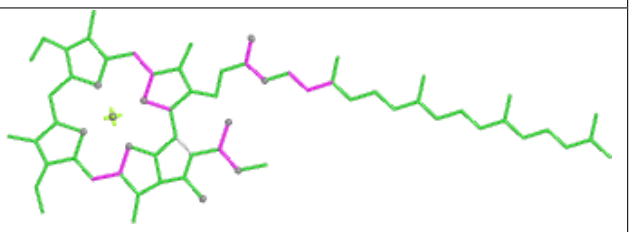

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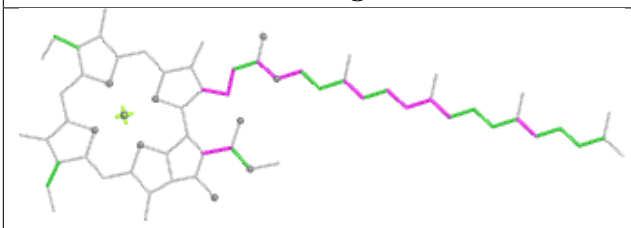

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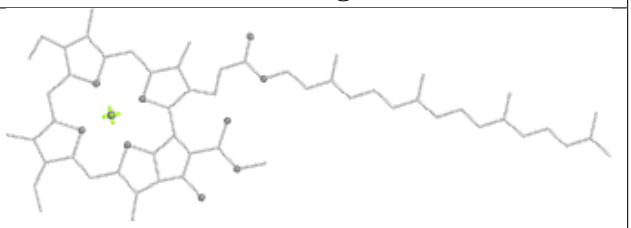
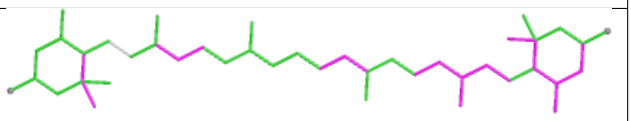


Rings

Ligand LUT V 2621

Bond lengths



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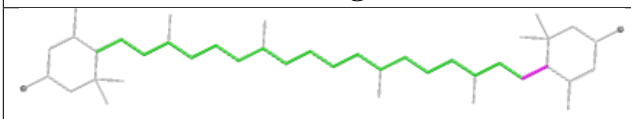

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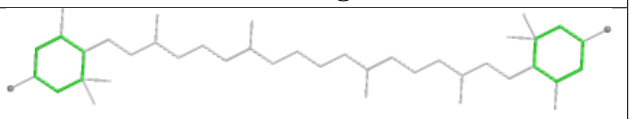
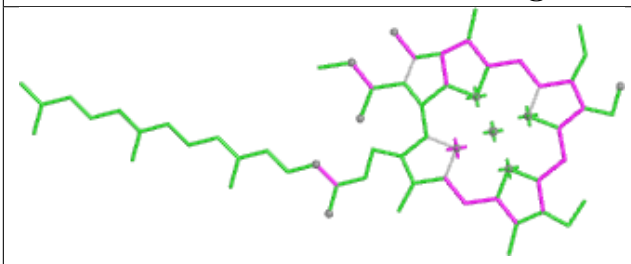


Rings

Ligand CHL 2 602



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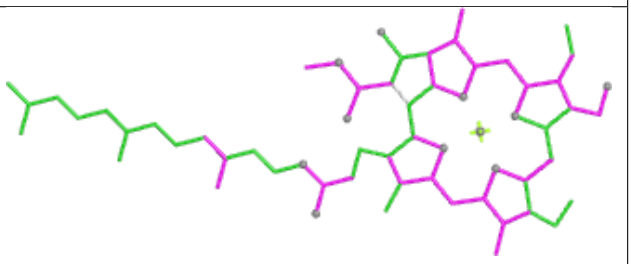

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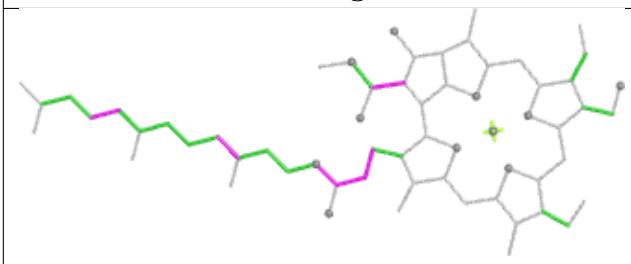

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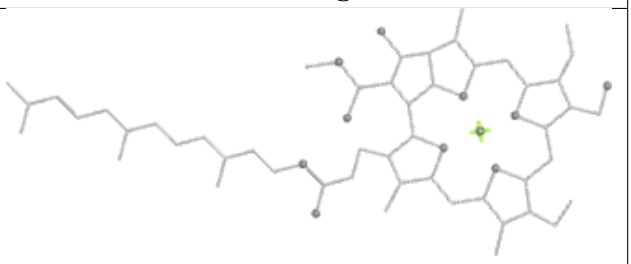
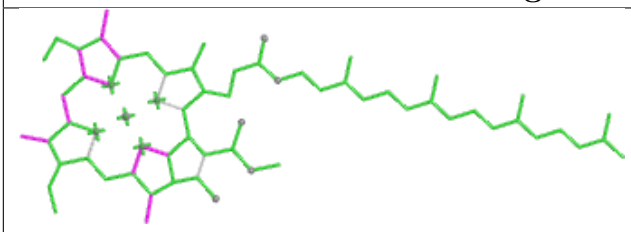


Rings

Ligand CLA B 803



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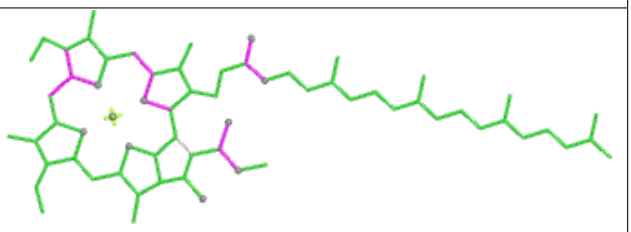

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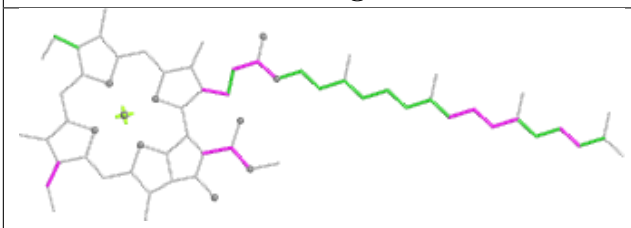

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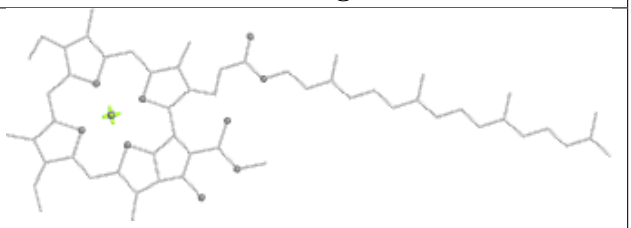
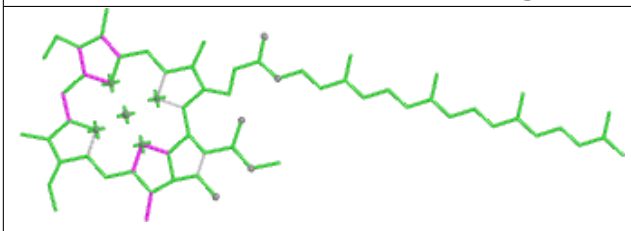


Rings

Ligand CLA W 610



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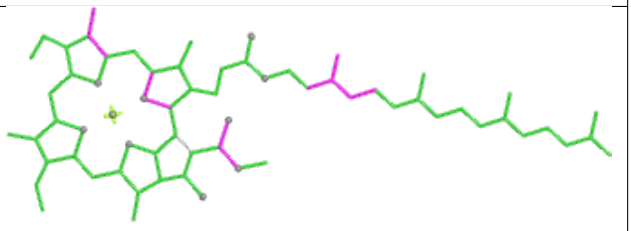

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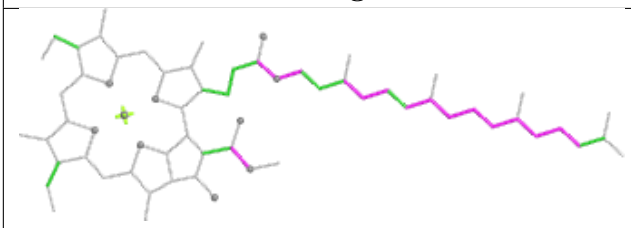

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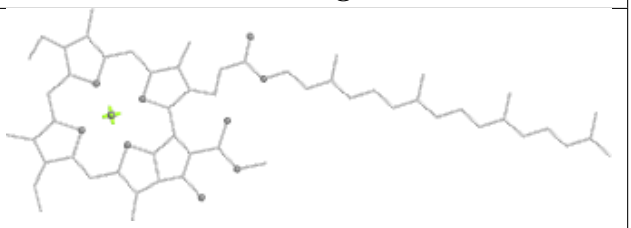
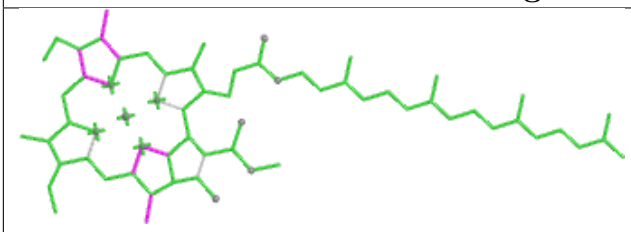


Rings

Ligand CLA A 801



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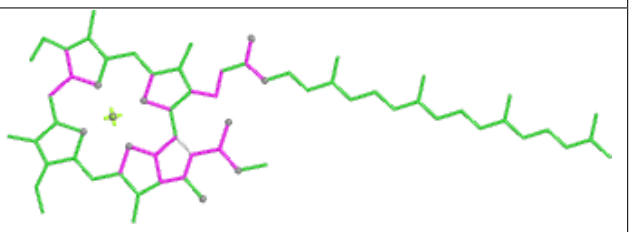

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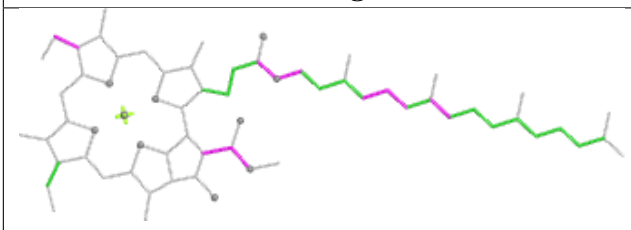

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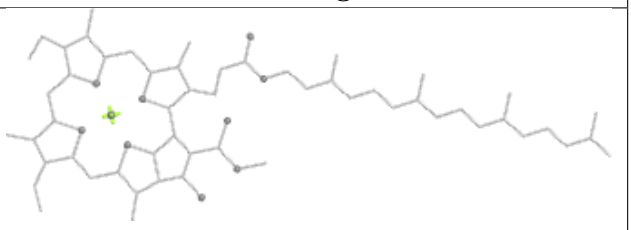
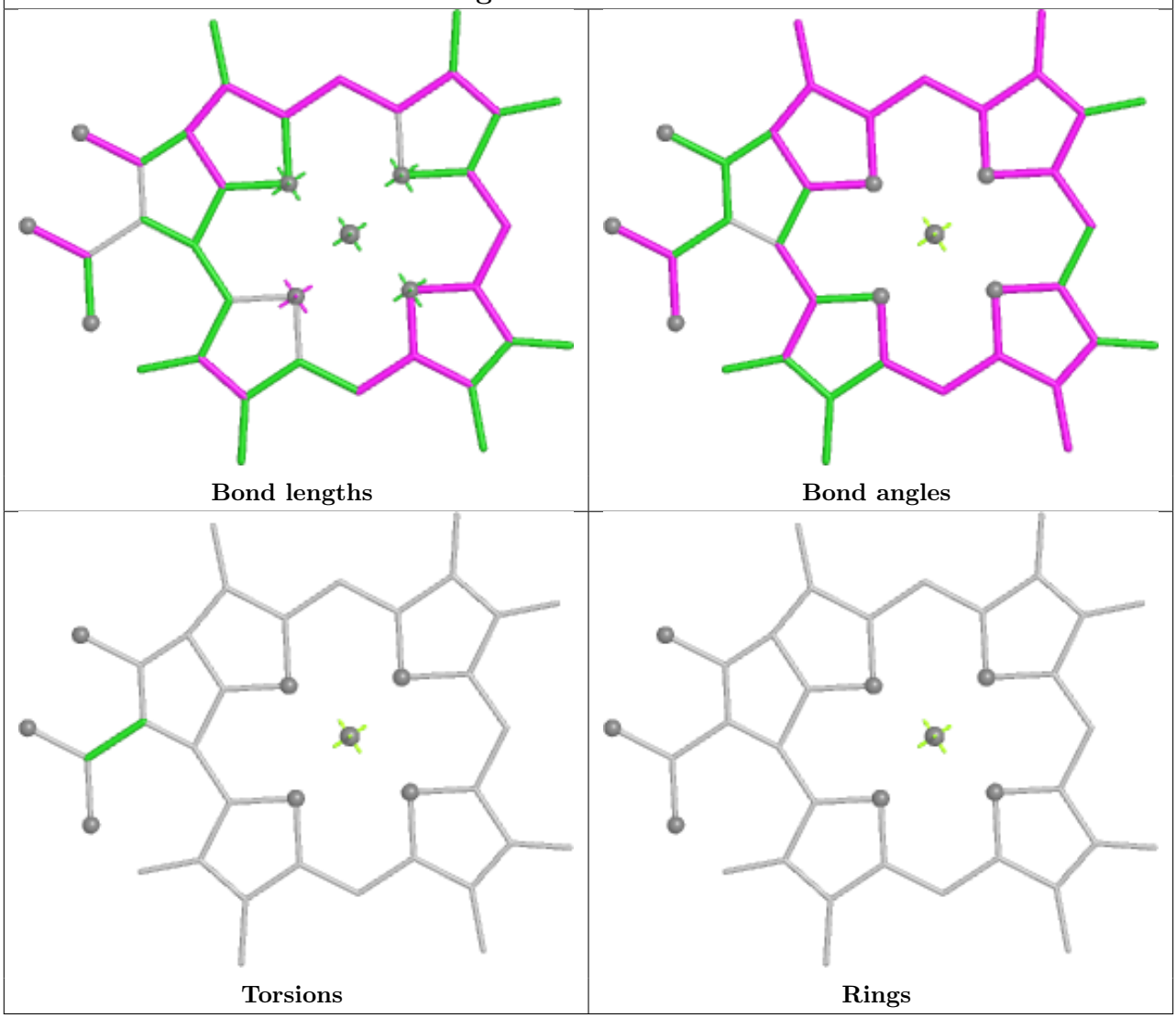
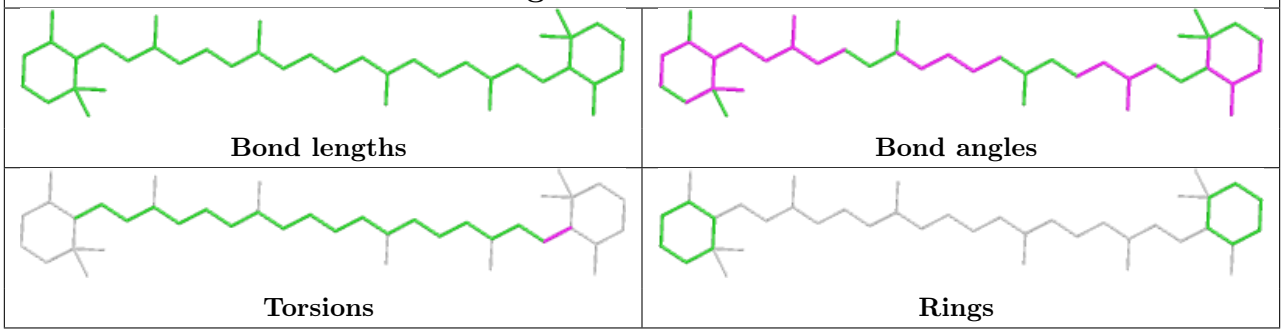


Rings

Ligand CHL W 606



Ligand BCR J 102



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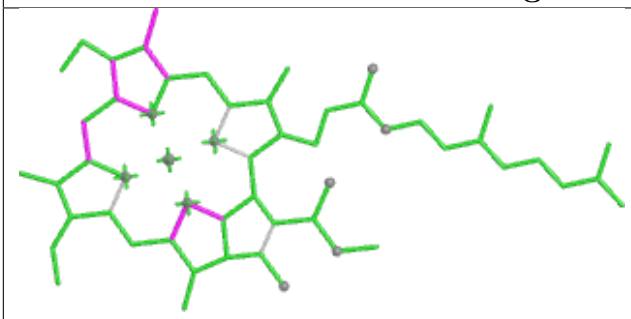

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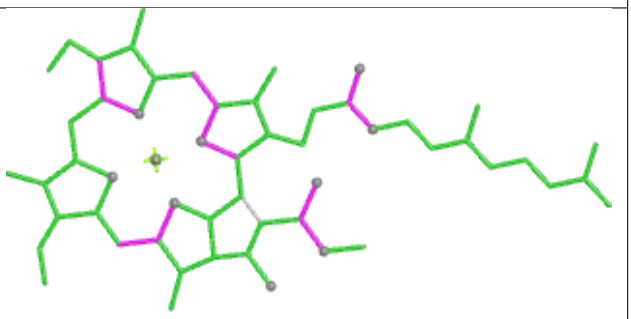
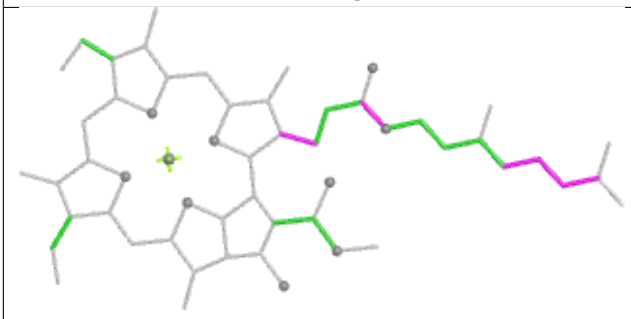


Bond angles



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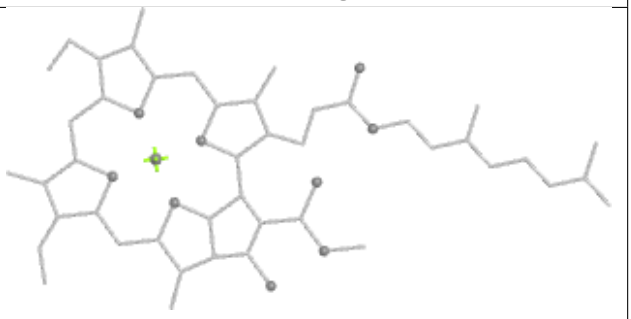
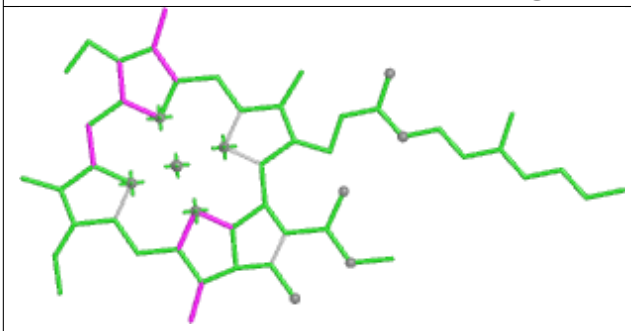


Rings

Ligand CLA 3 615



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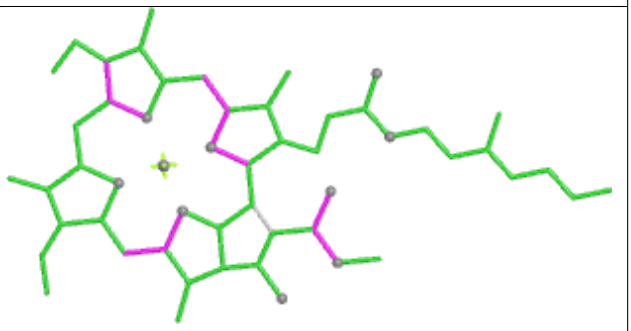
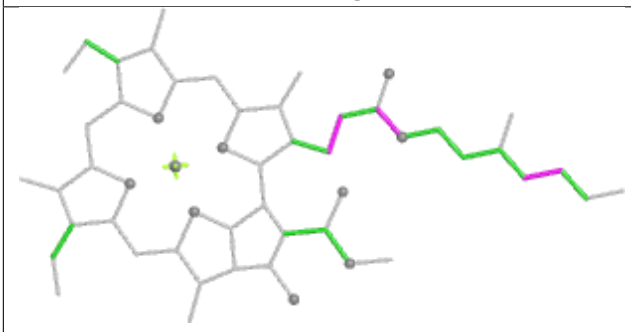


Bond angles



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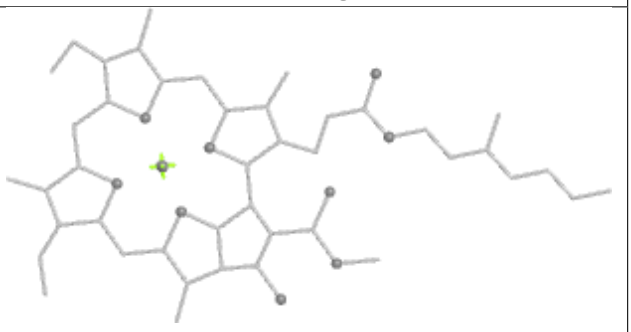
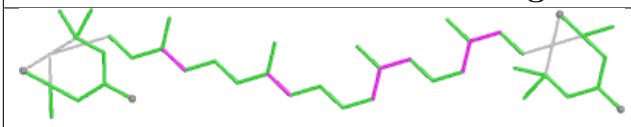
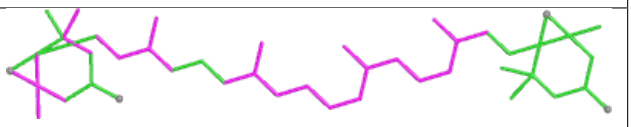
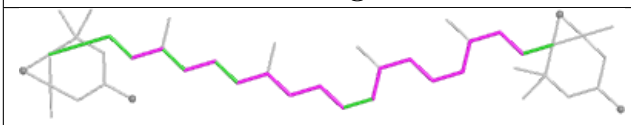
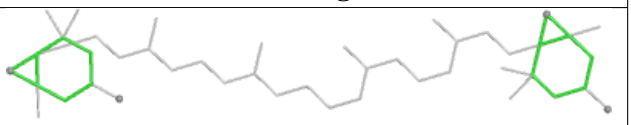
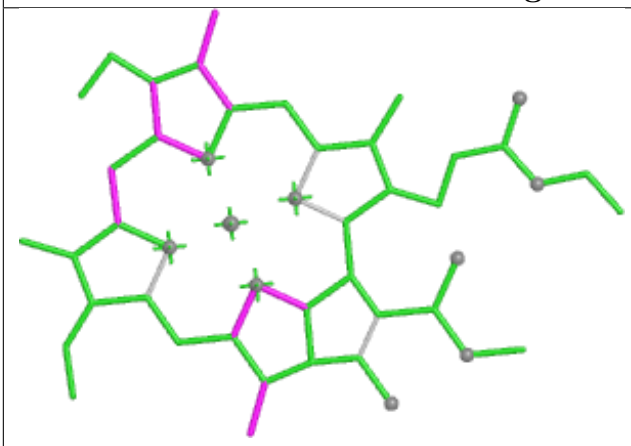
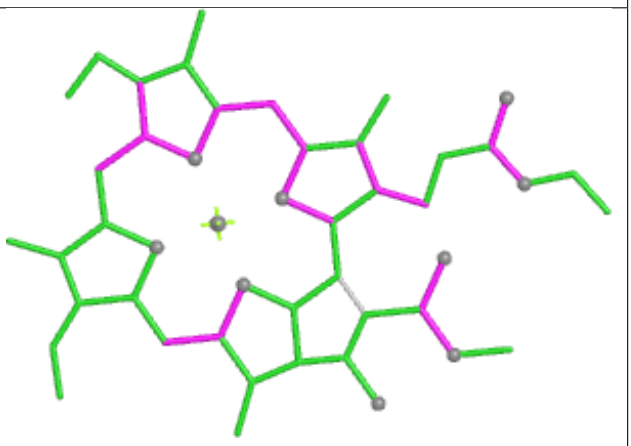
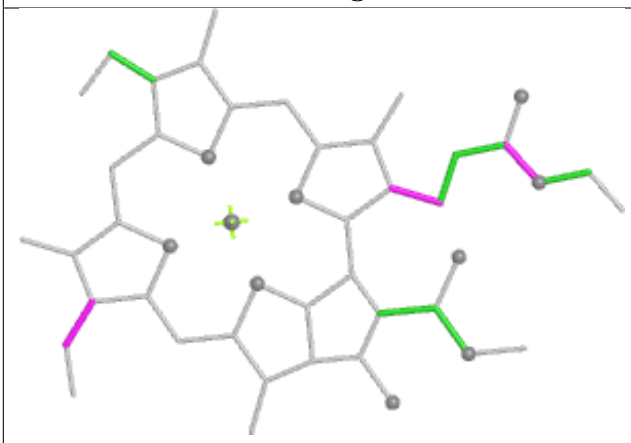
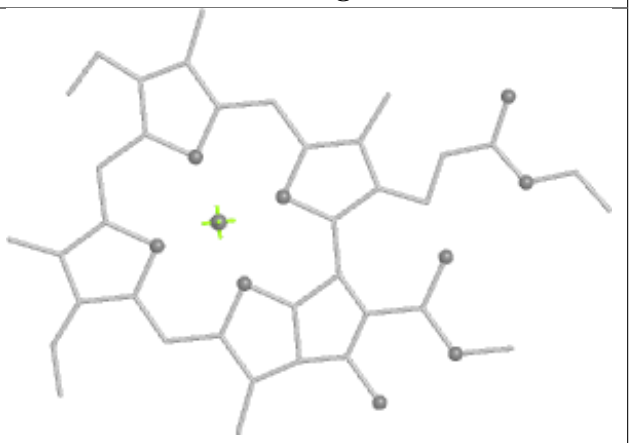
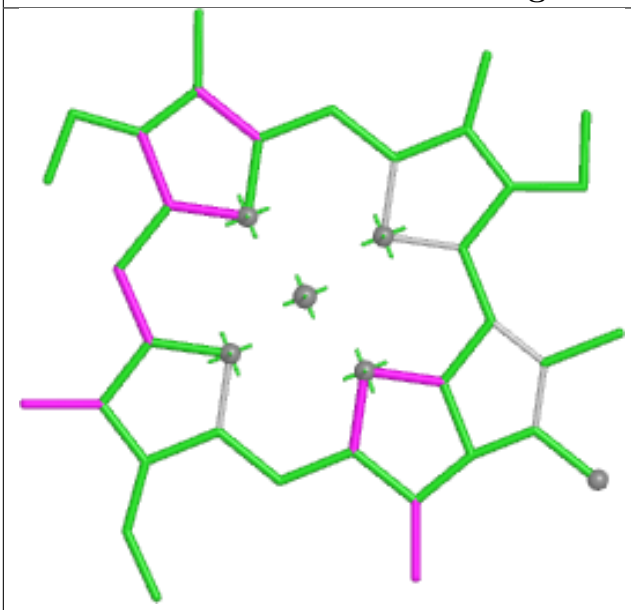


Rings

Ligand XAT 8 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 612



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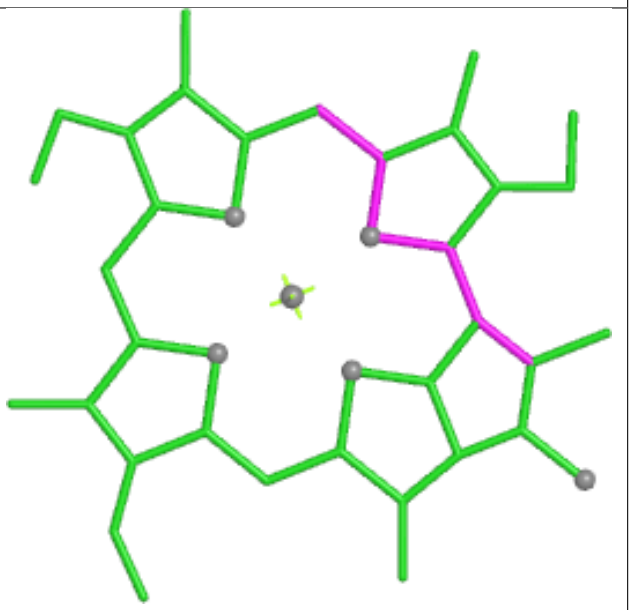
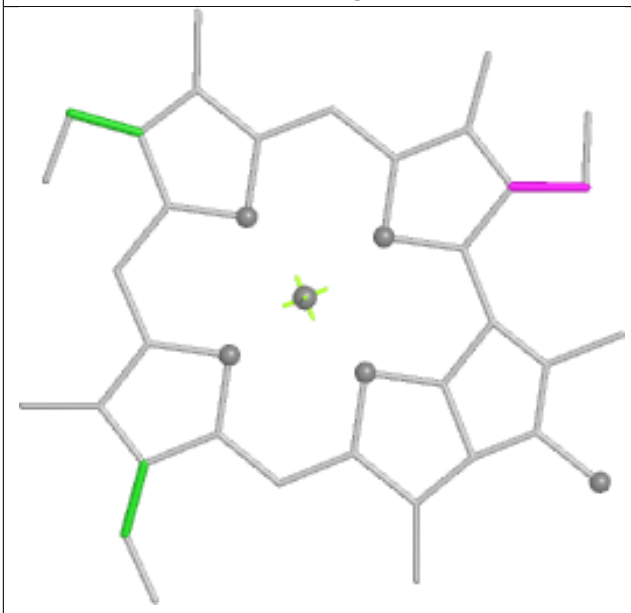


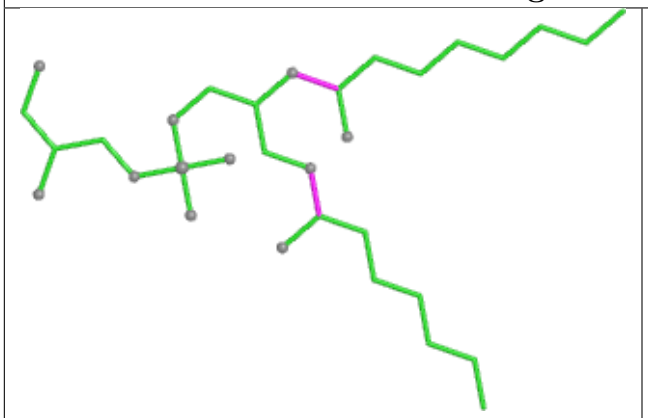
Bond angles



Torsions

Rings

Ligand LHG 3 630



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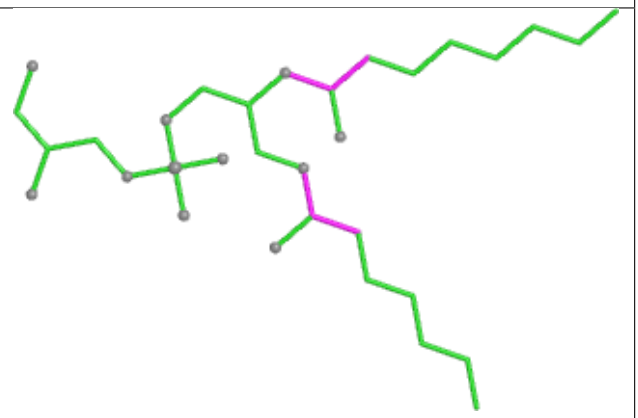
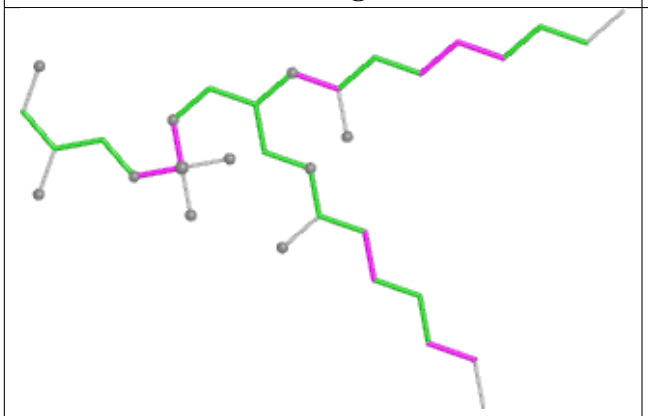


Bond angles



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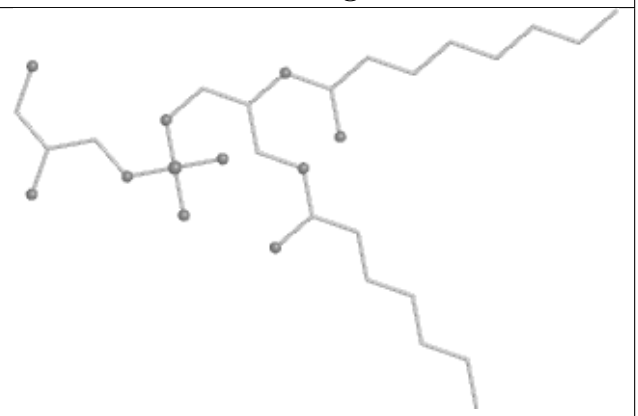
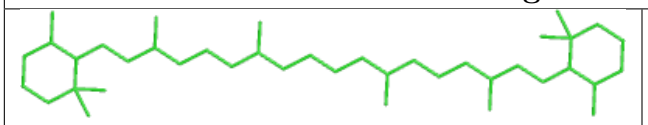


Rings

Ligand BCR A 852



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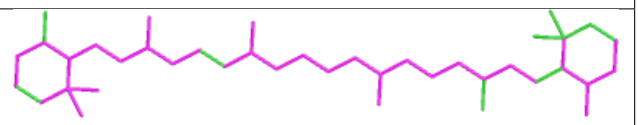
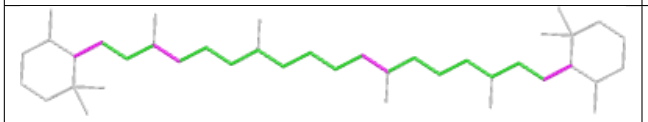


Bond angles



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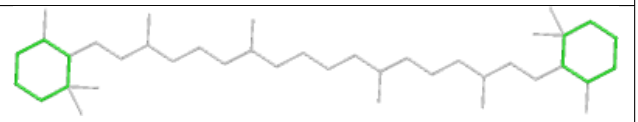

Rings

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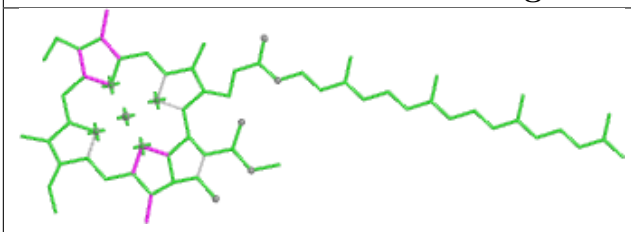
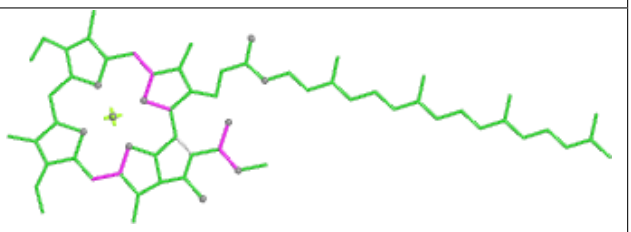
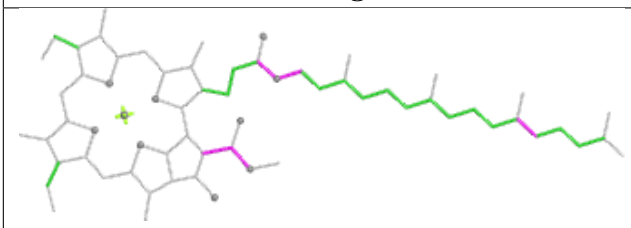
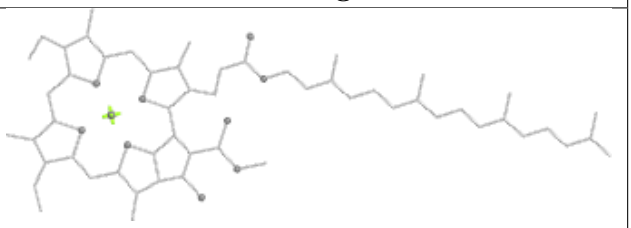
 Bond lengths	 Bond angles
 Torsions	 Rings

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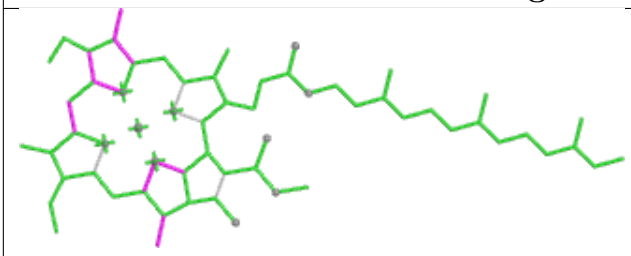
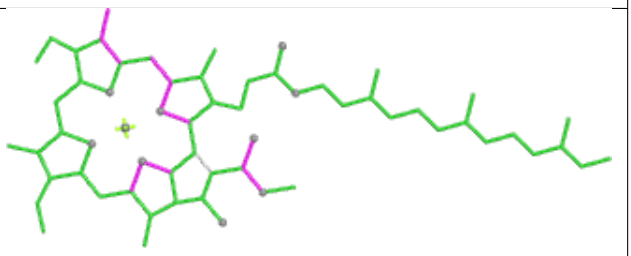
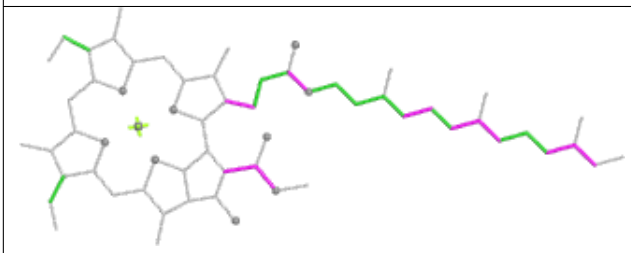
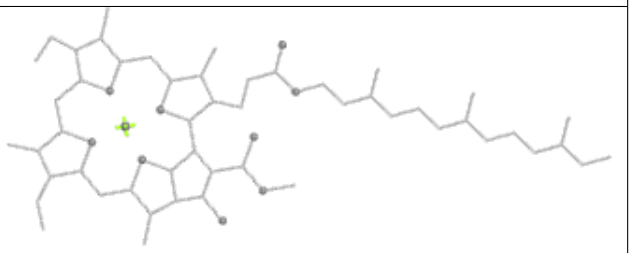
 Bond lengths	 Bond angles
 Torsions	 Rings

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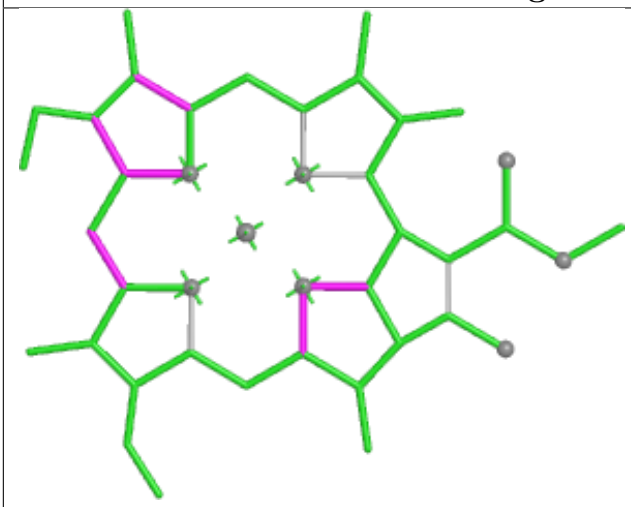

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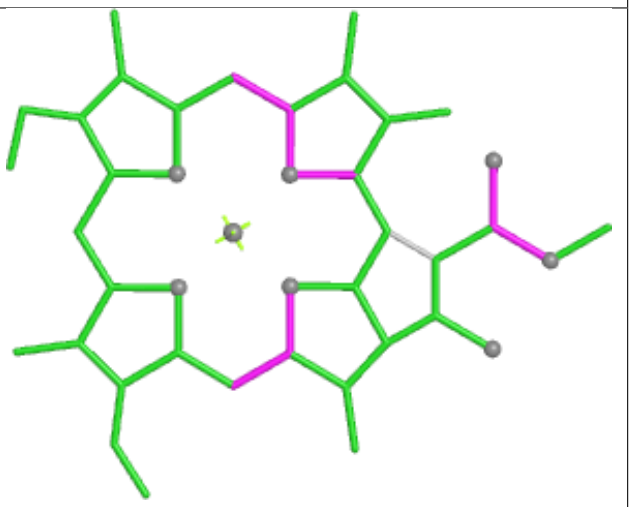

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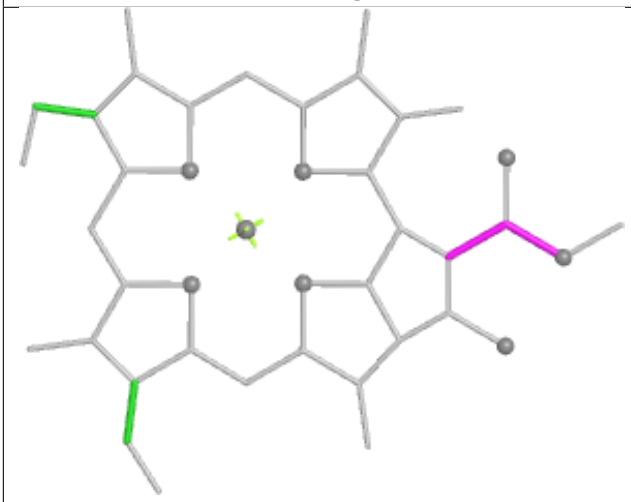

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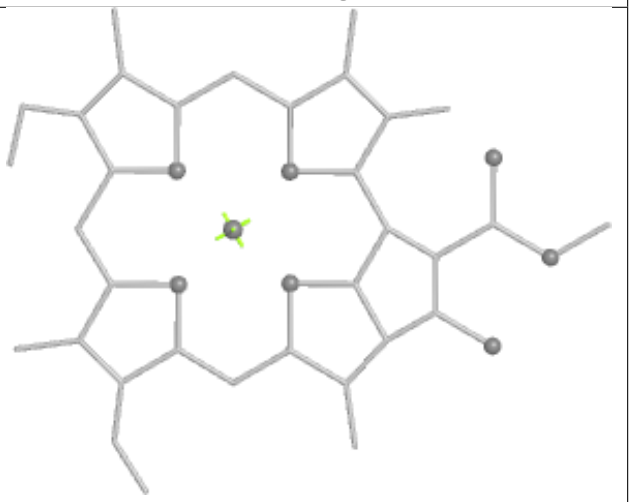

Rings

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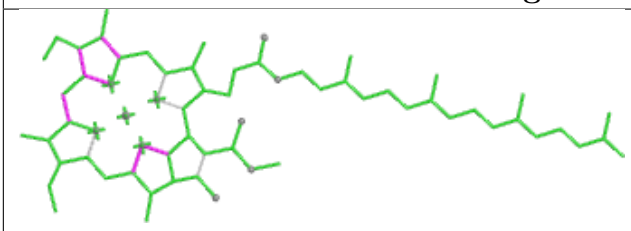

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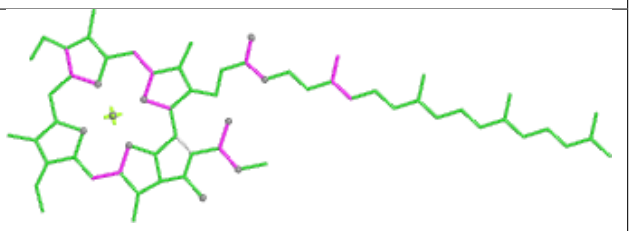

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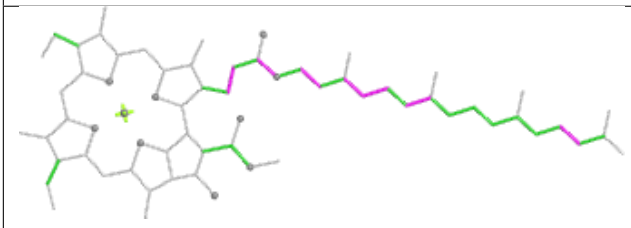

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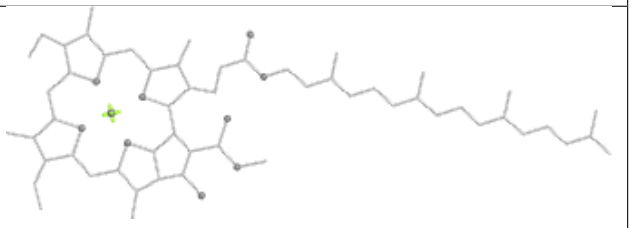

Rings

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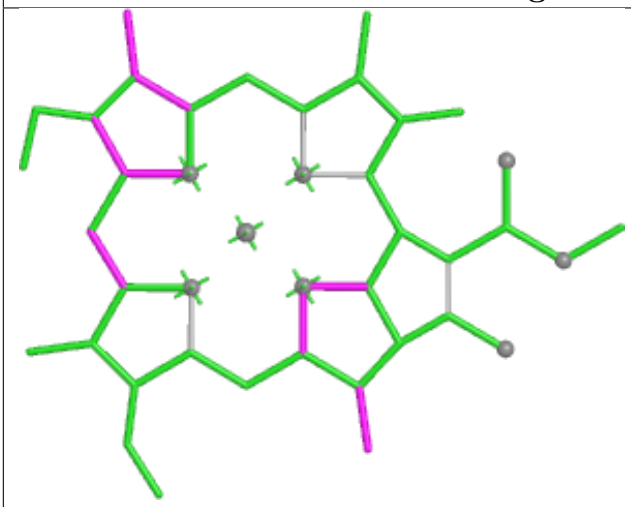

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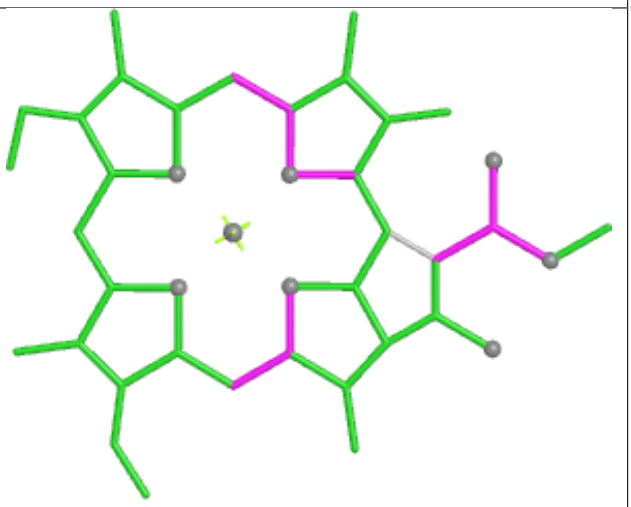

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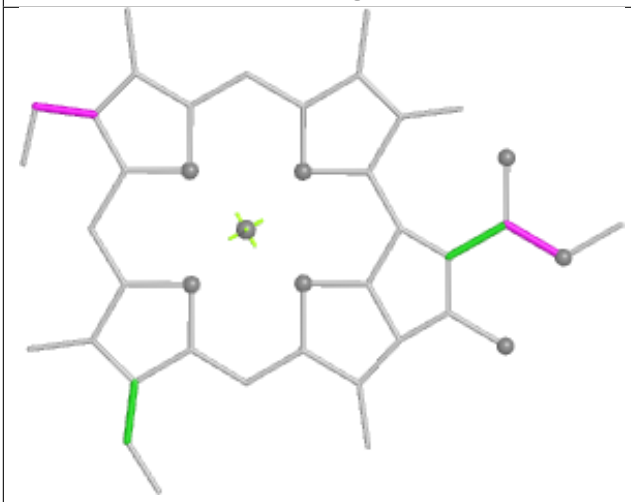

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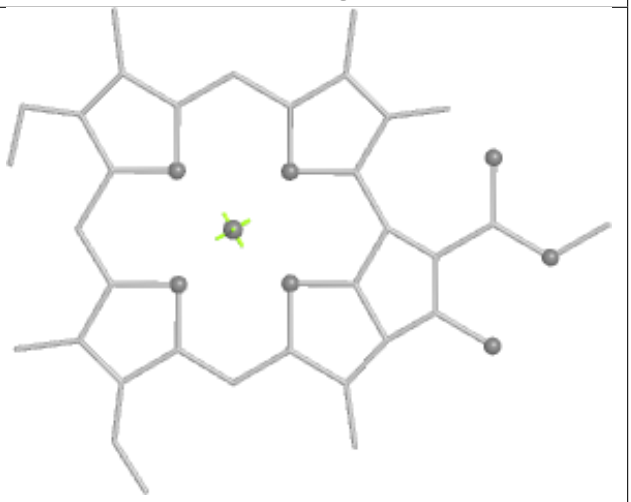

Rings

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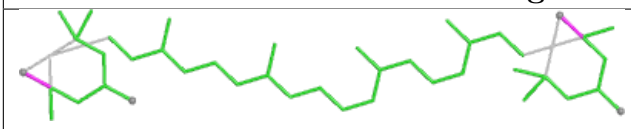

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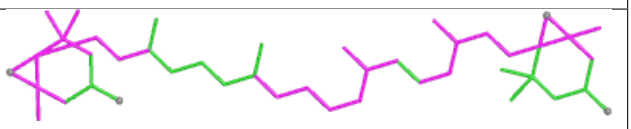

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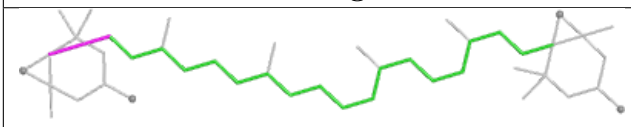

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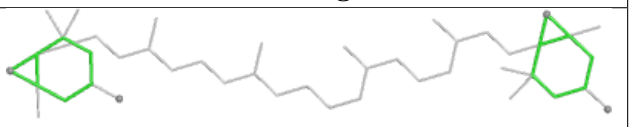

Rings

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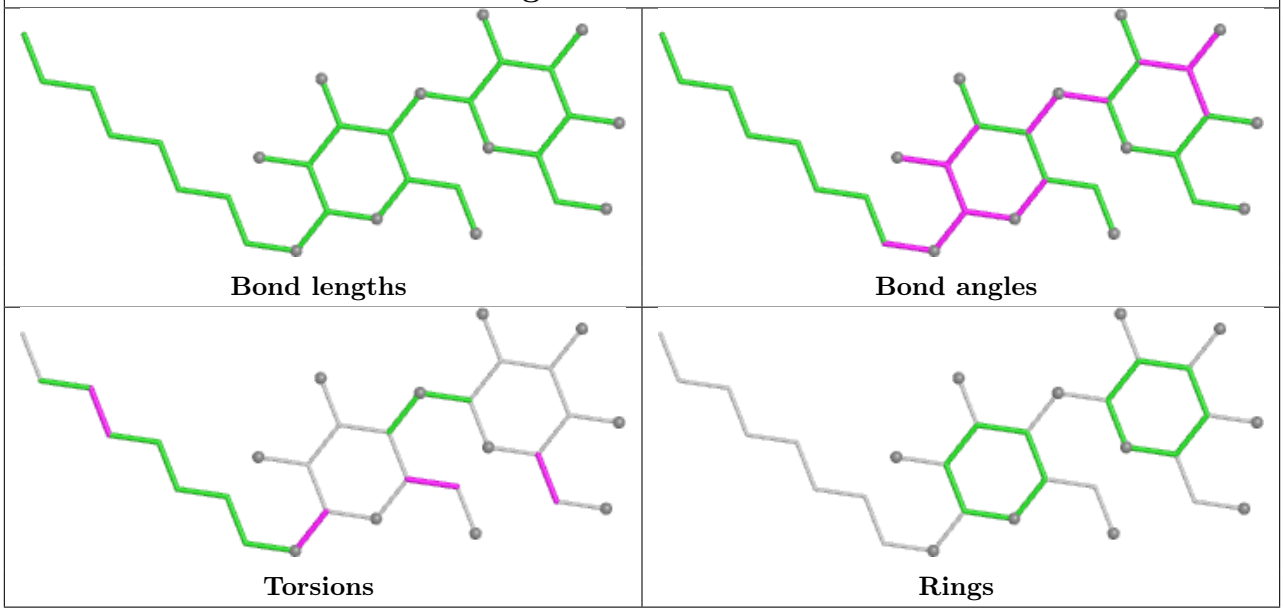

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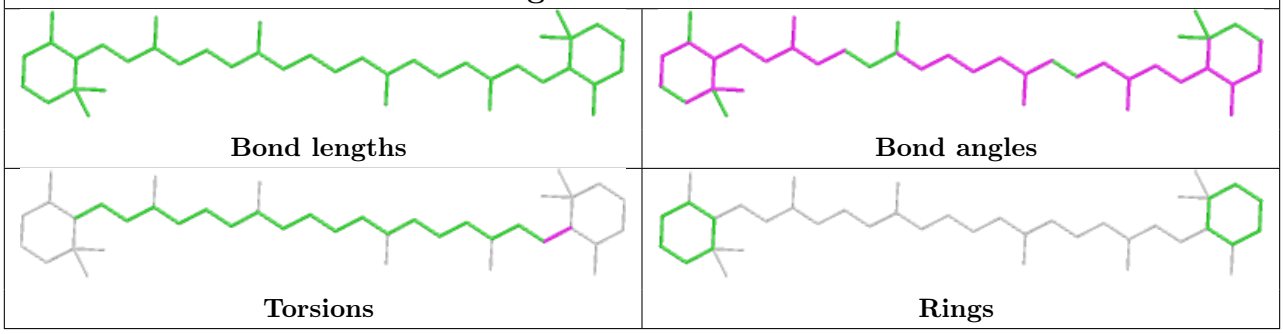

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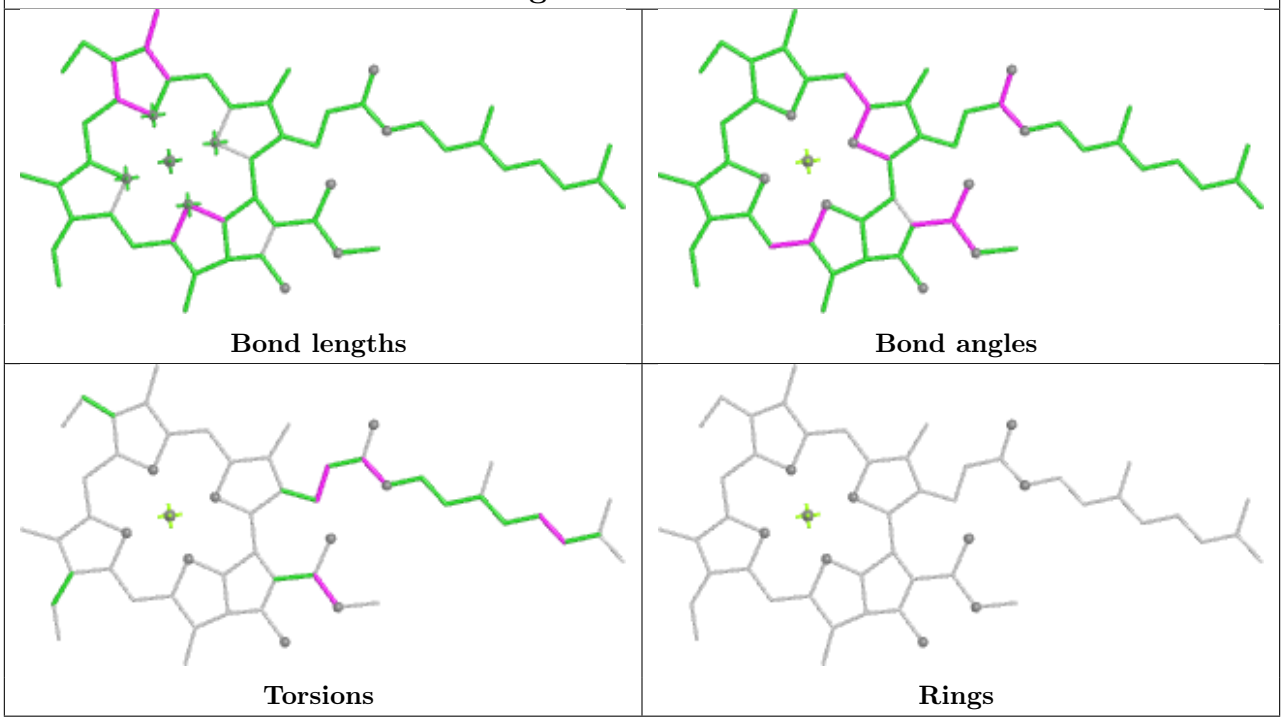

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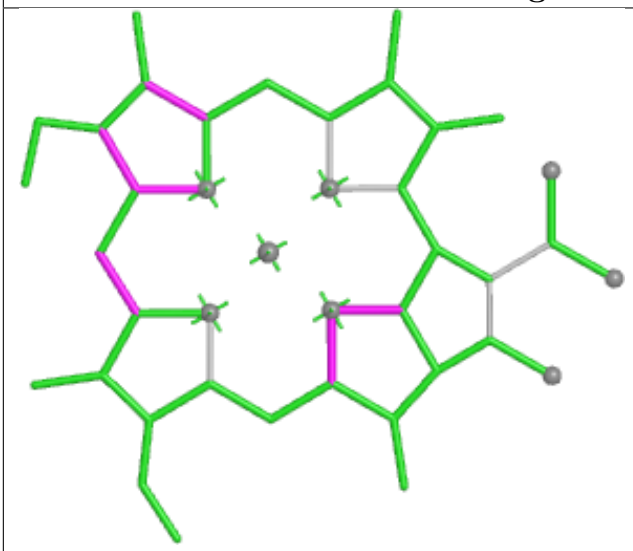

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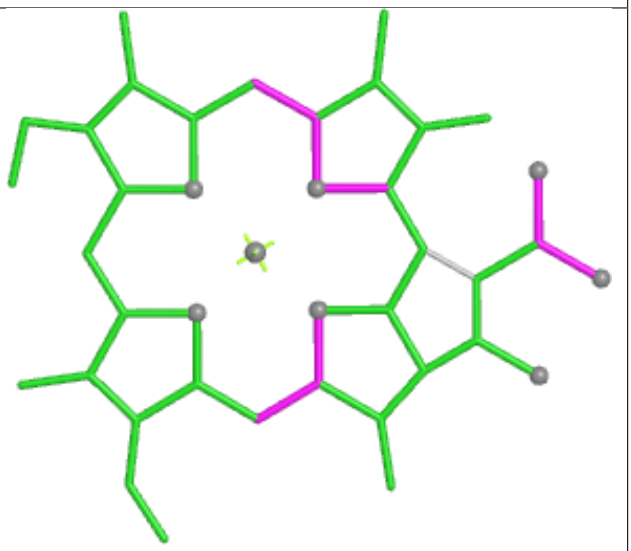
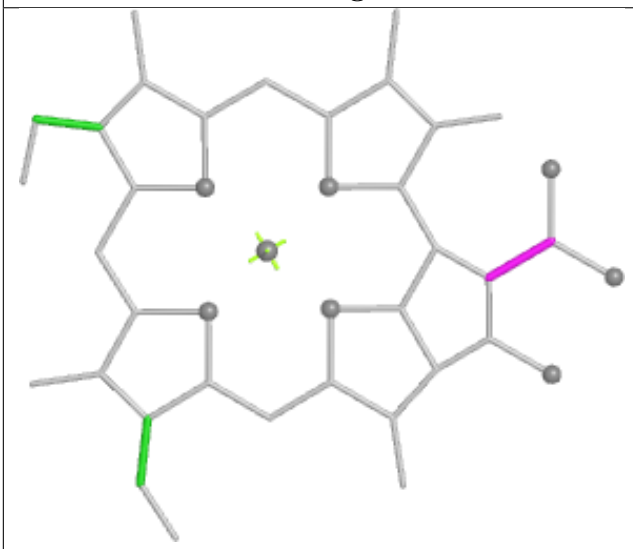


Bond angles



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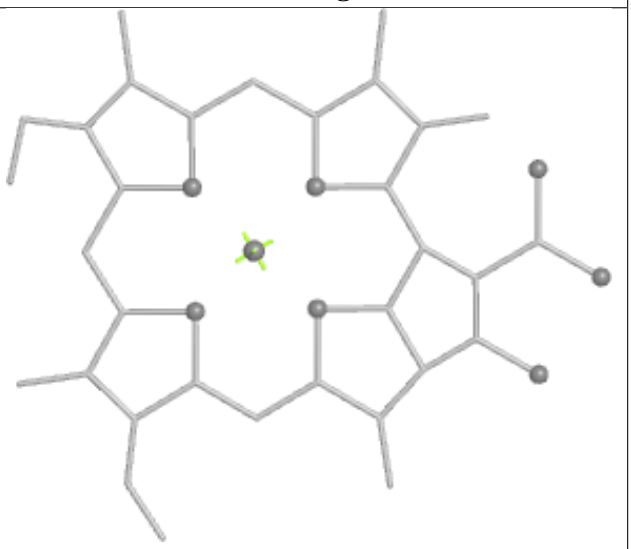
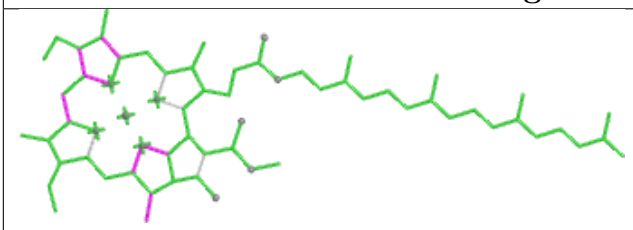


Rings

Ligand CLA A 830



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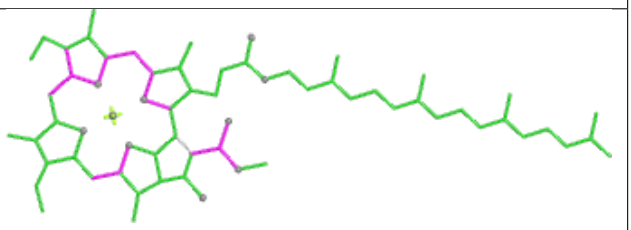

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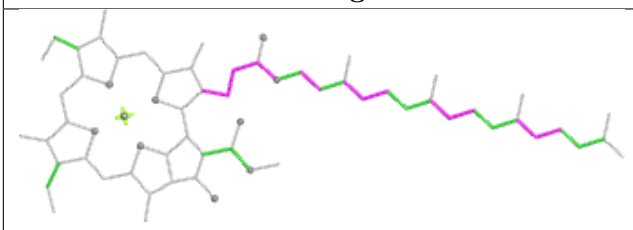

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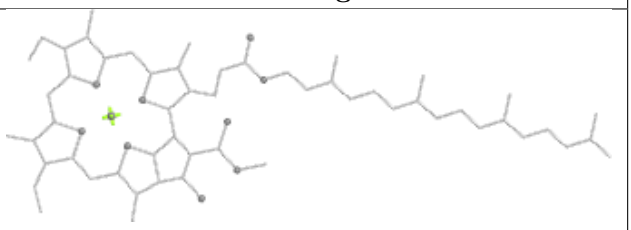
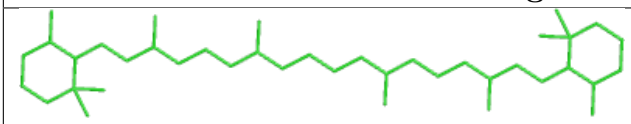


Rings

Ligand BCR 1 619



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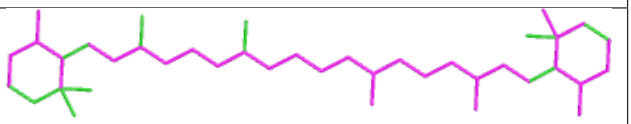

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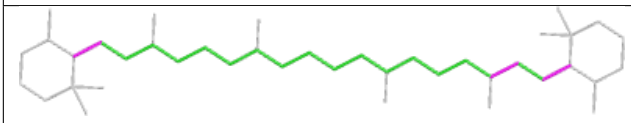

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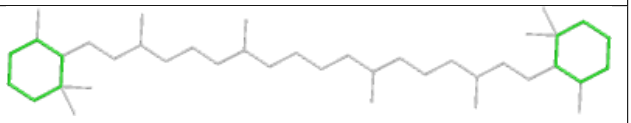
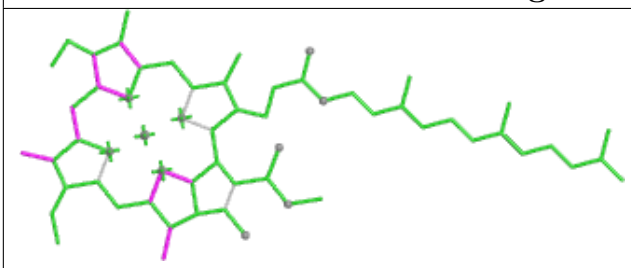


Rings

Ligand CLA 9 602



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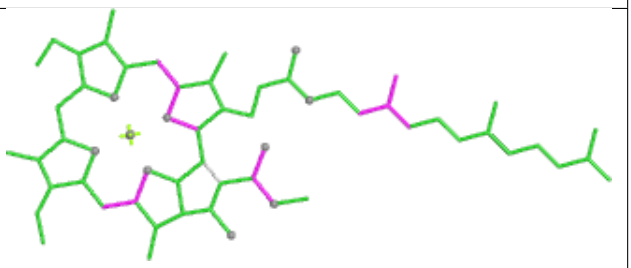

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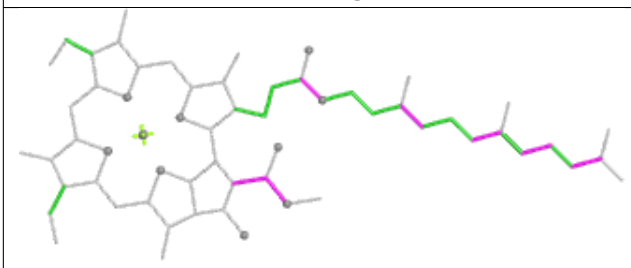

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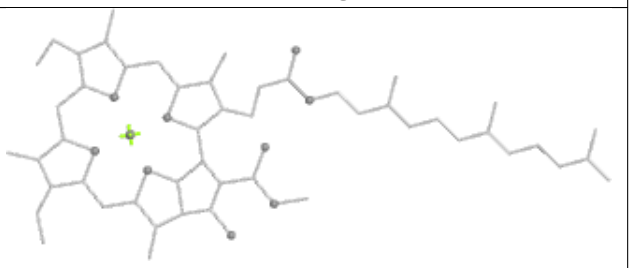

Rings

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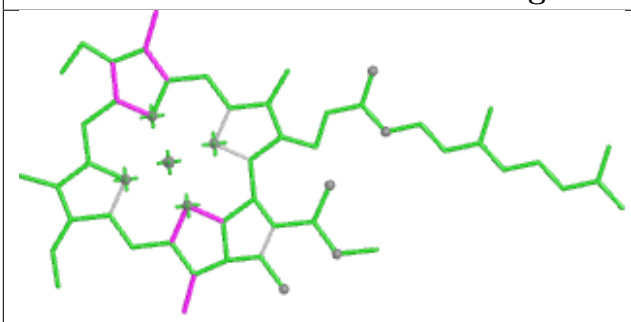

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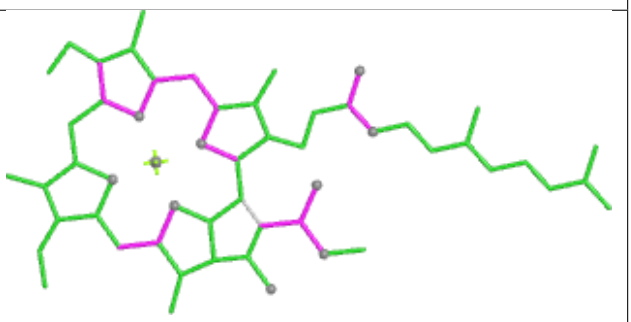

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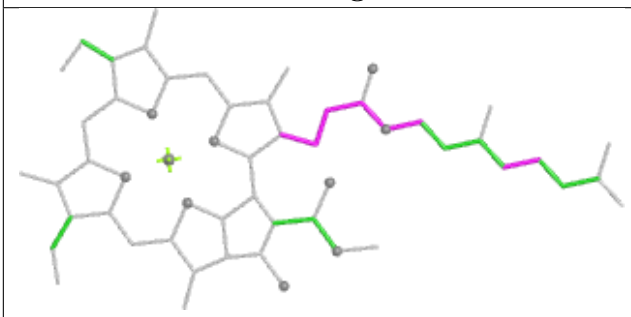

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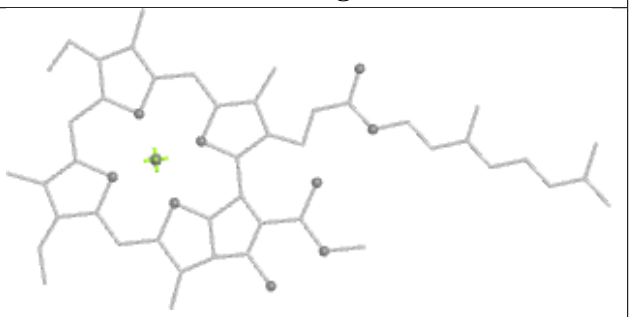
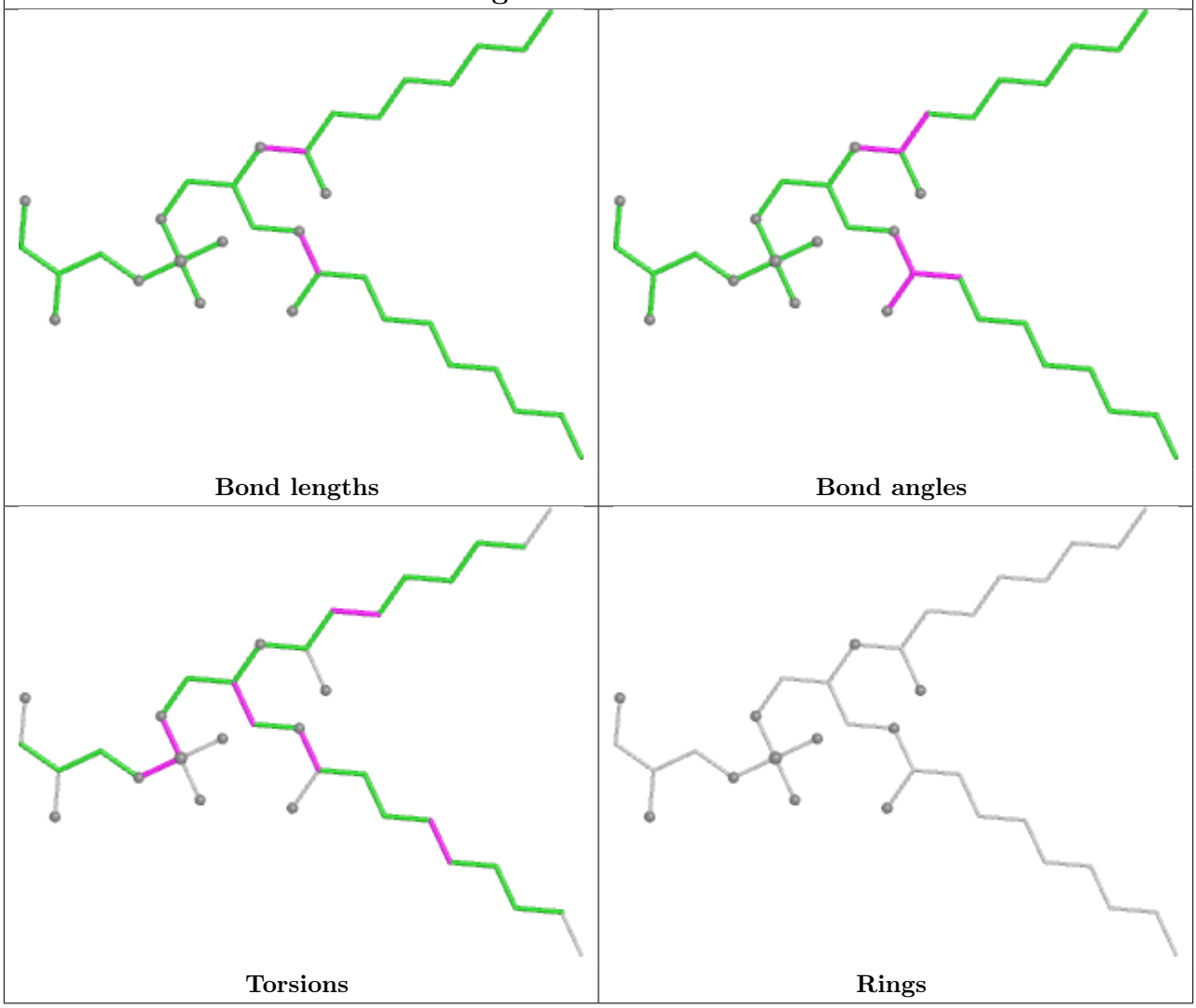


Rings

Ligand LHG 7 630



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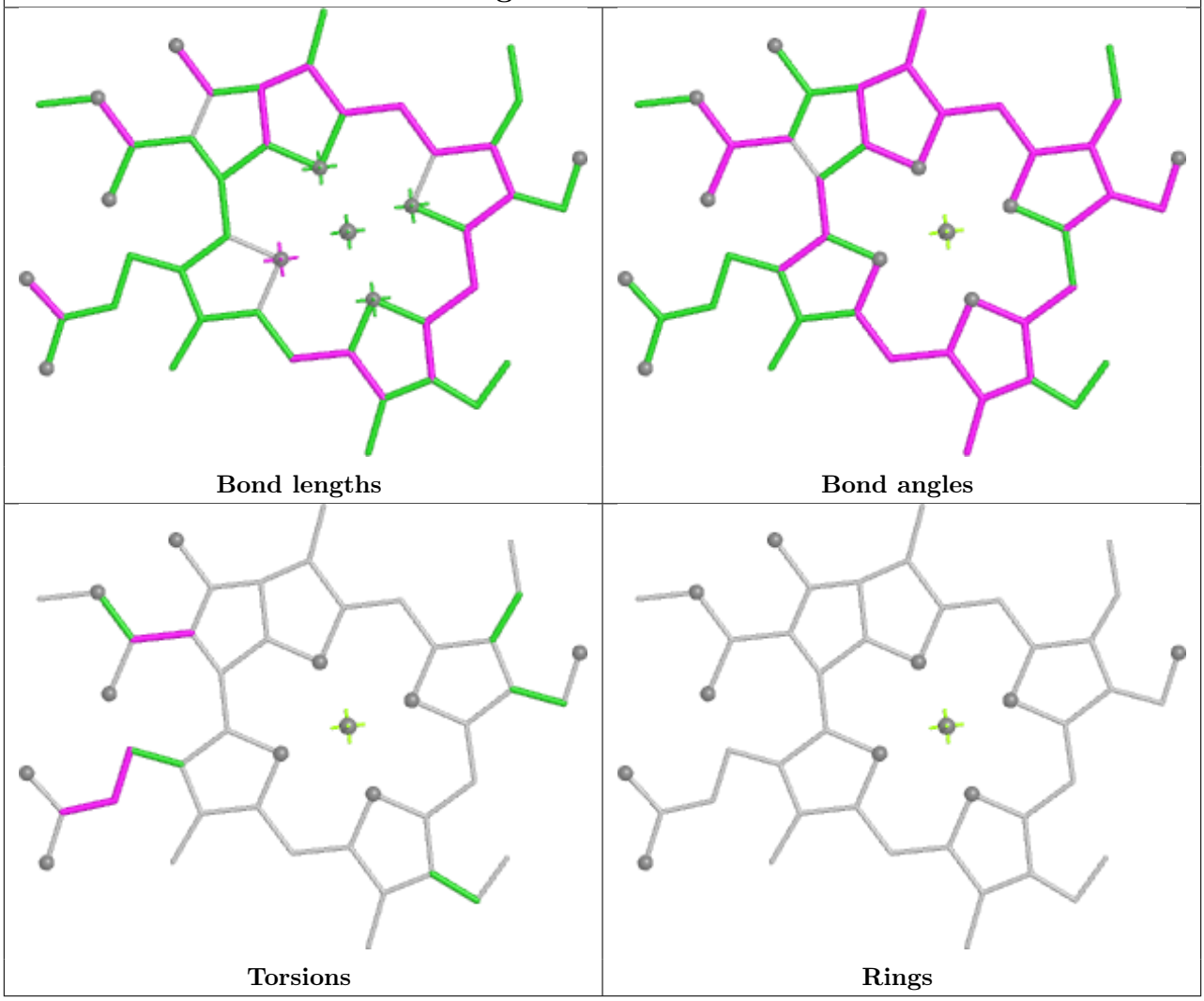

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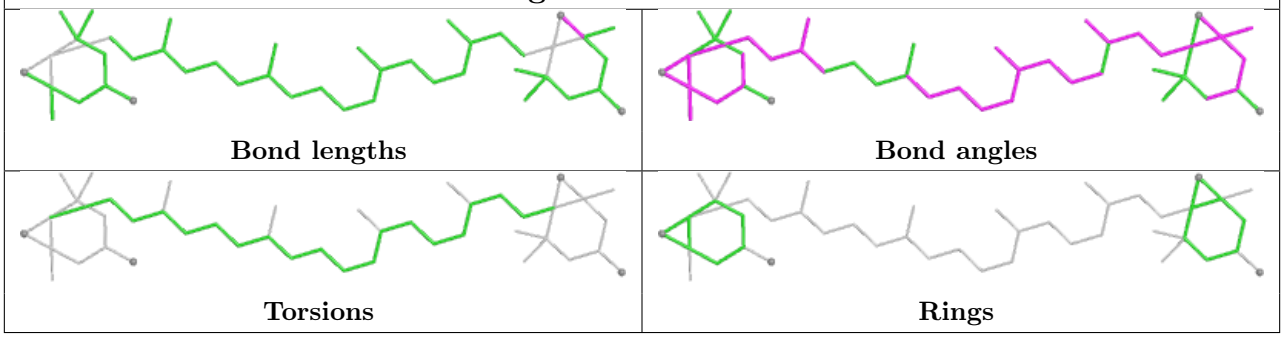

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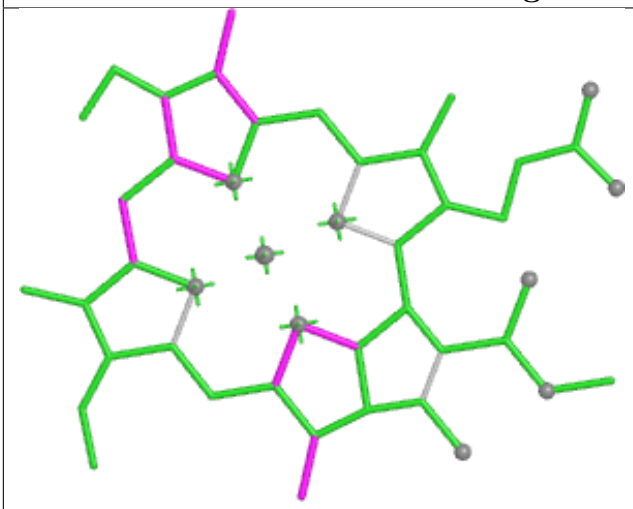

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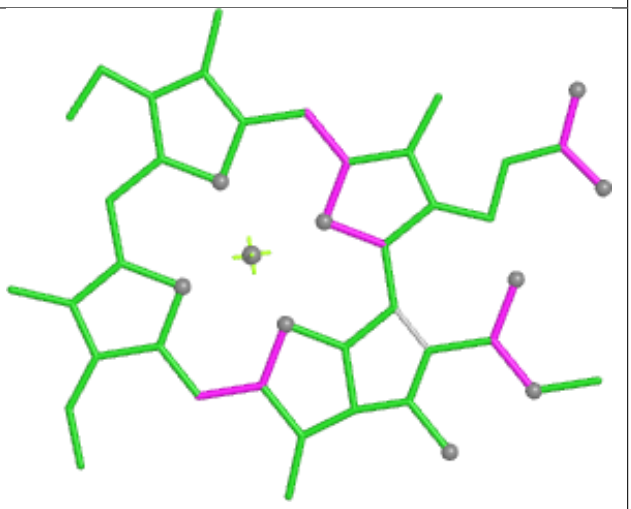

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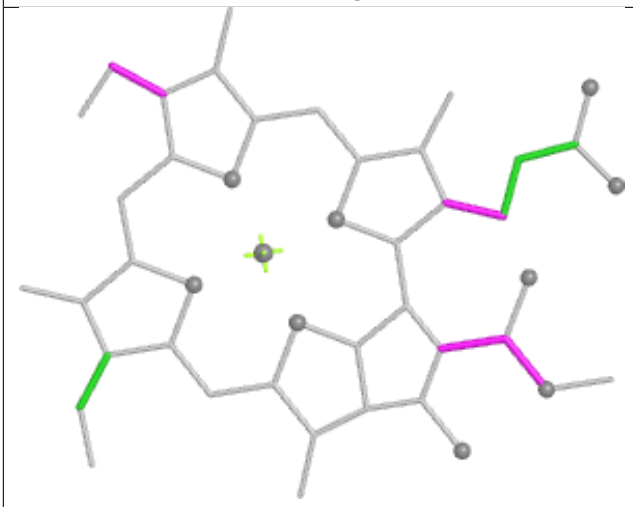
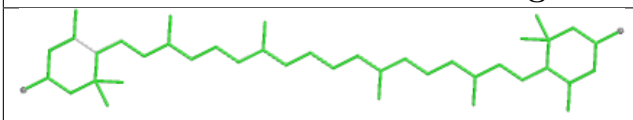


Torsions

Rings

Ligand LUT 1 617



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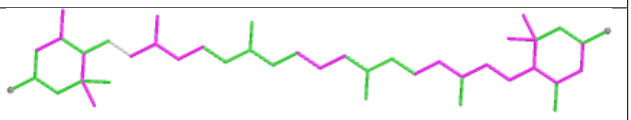

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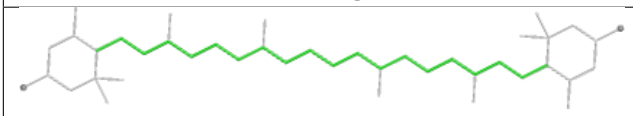
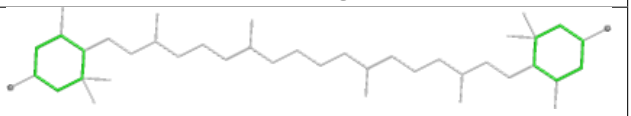
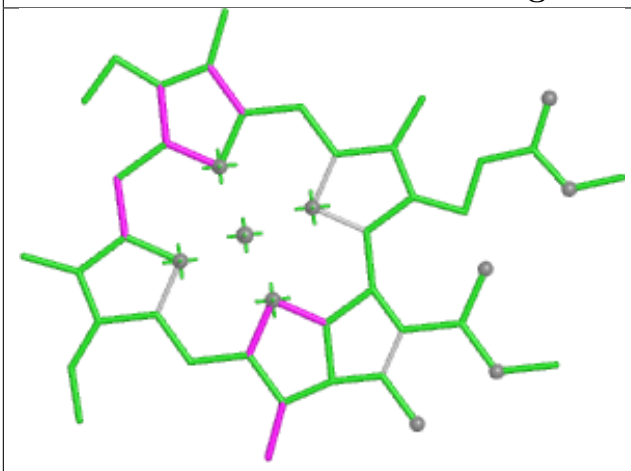
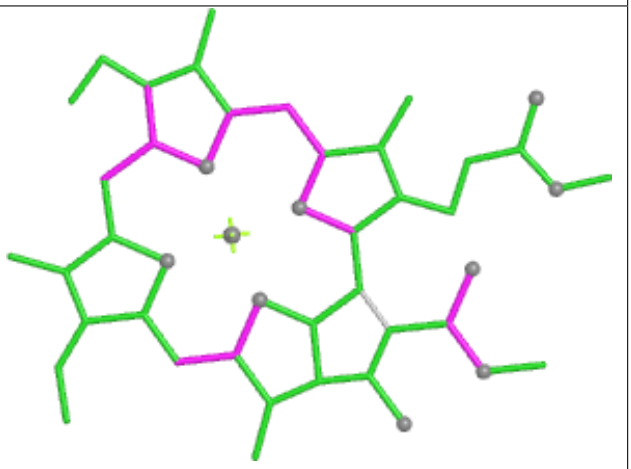
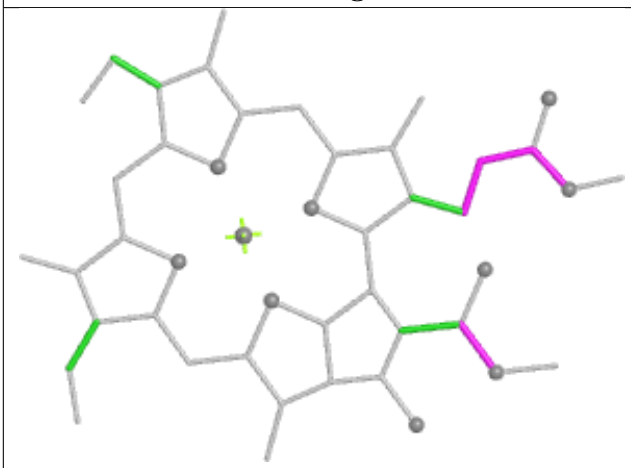
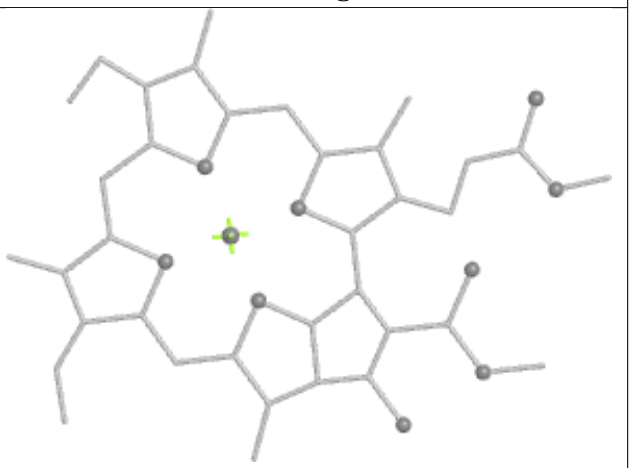


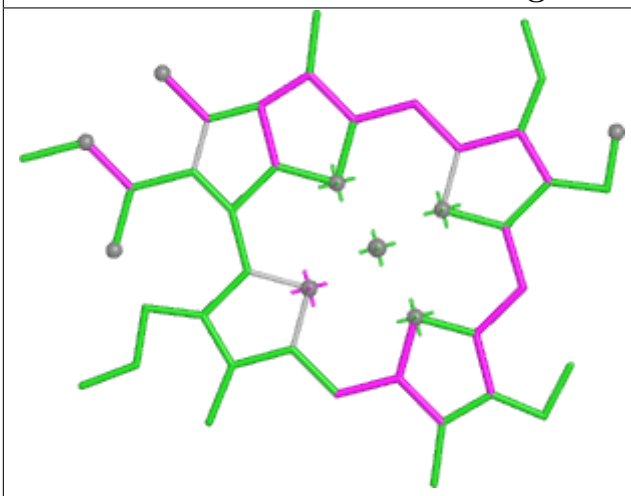
Torsions



Rings

Ligand CLA 6 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 9 606



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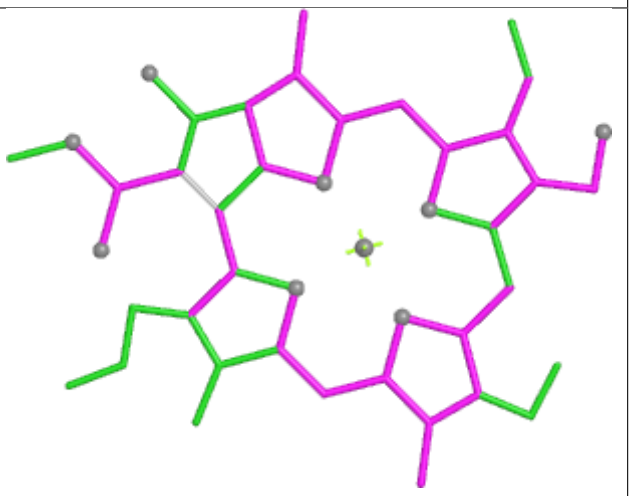

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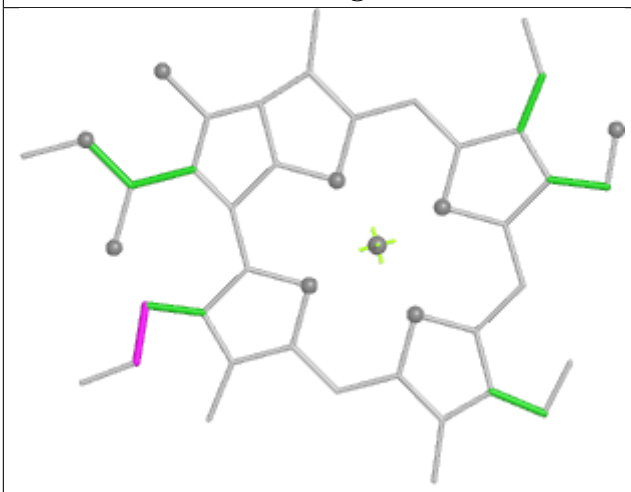

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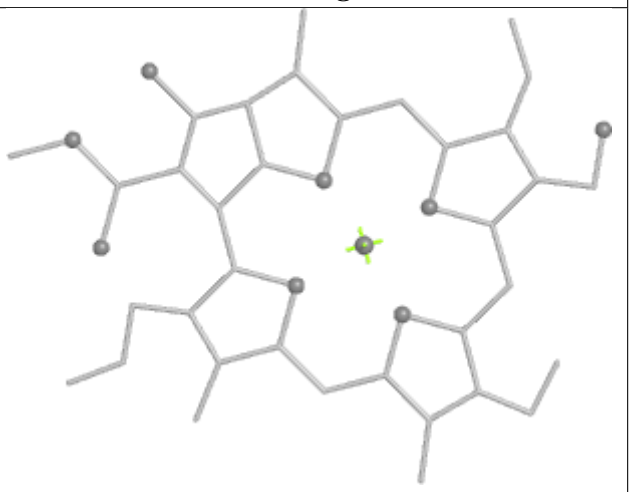

Rings

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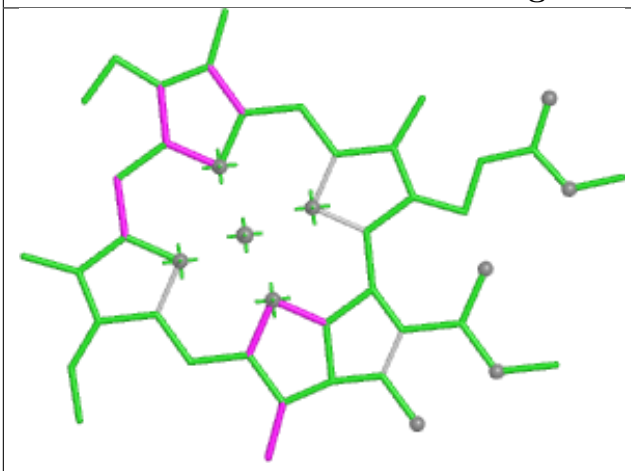
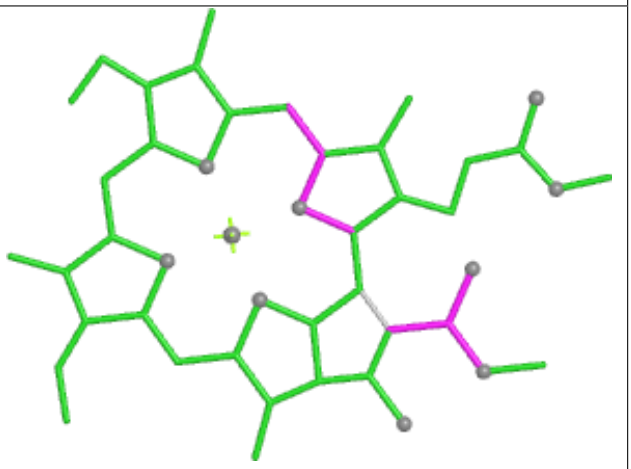
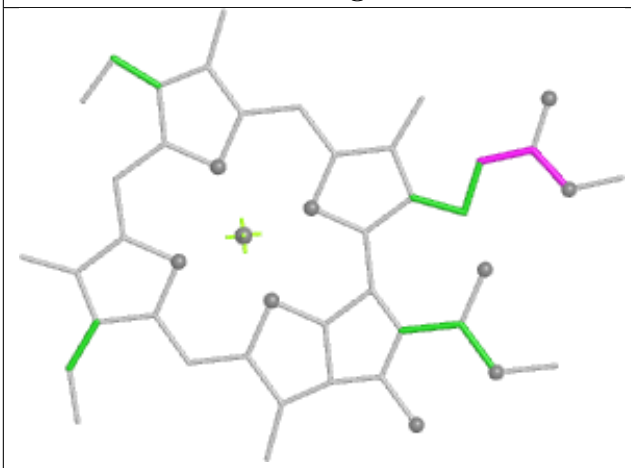
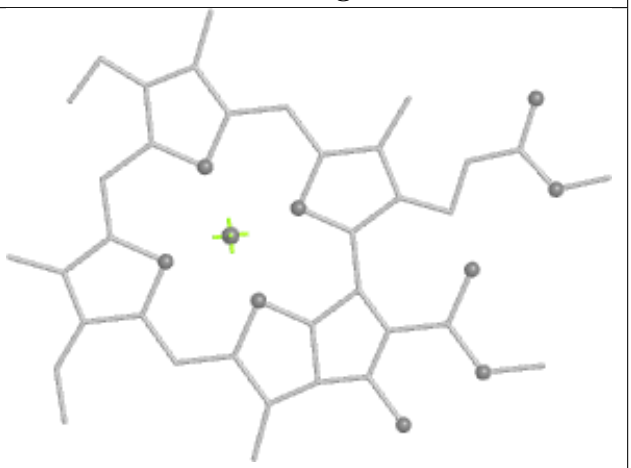
 Bond lengths	 Bond angles
 Torsions	 Rings

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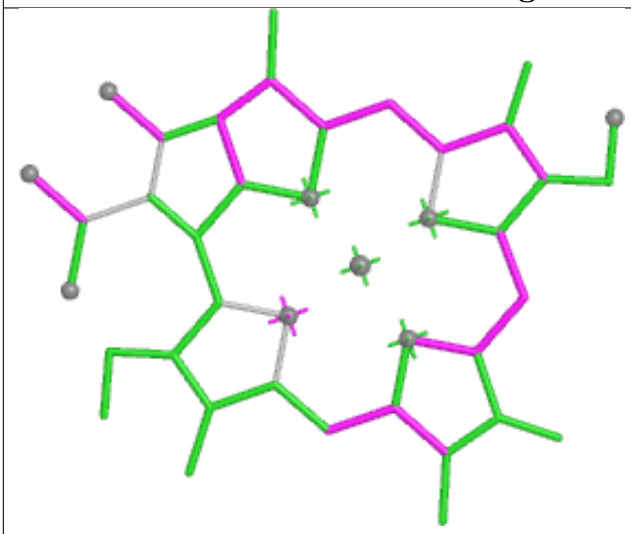

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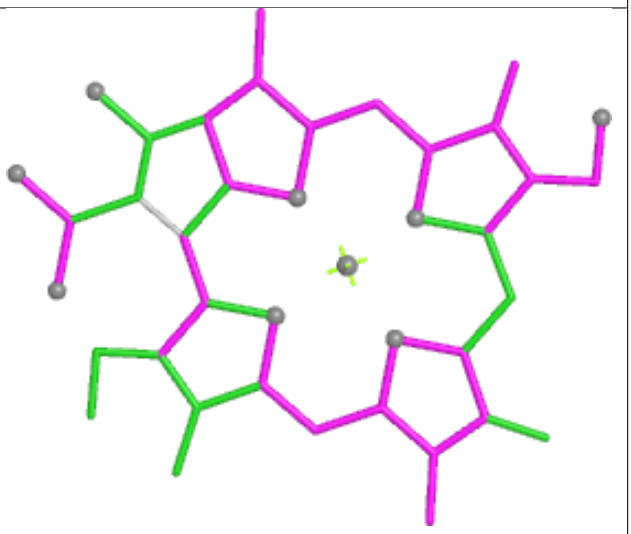

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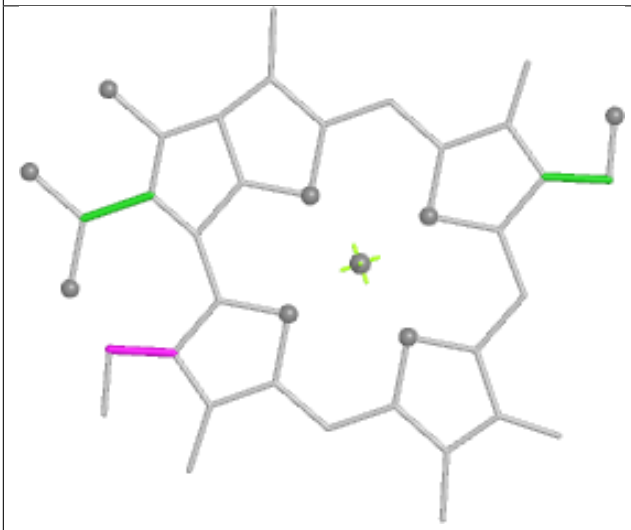

Torsions

Rings

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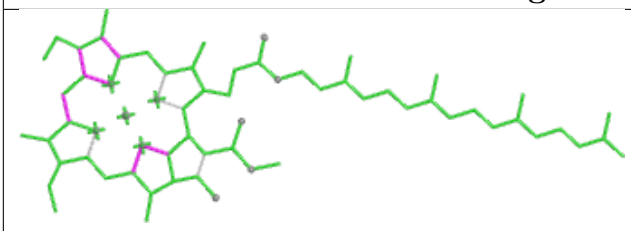

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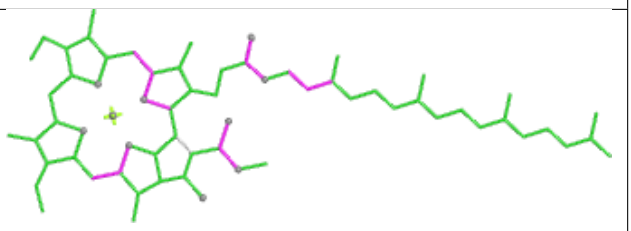

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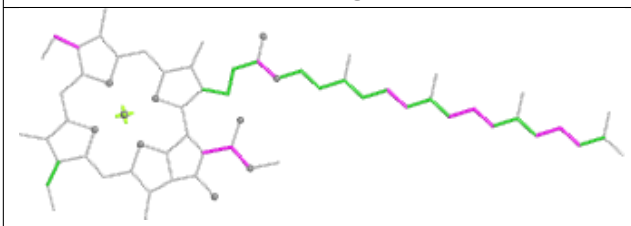

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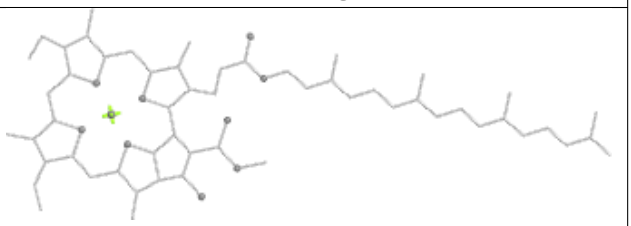

Rings

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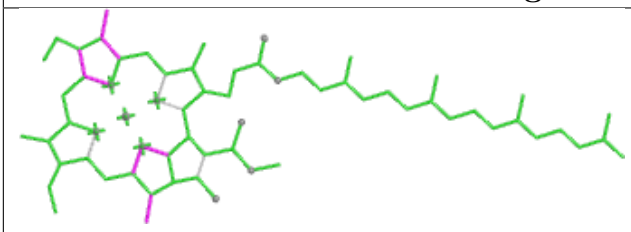

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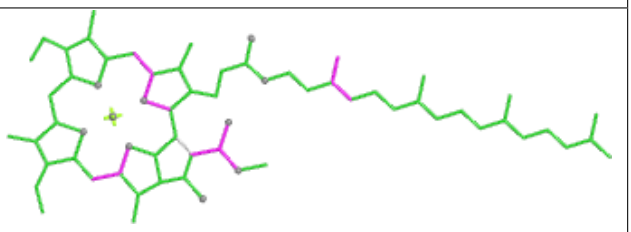

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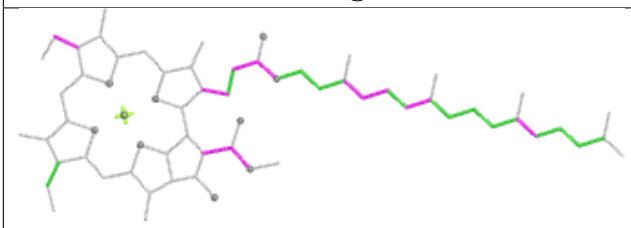

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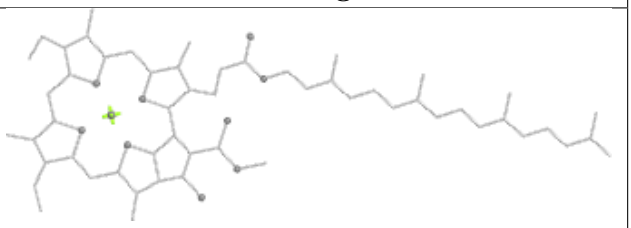
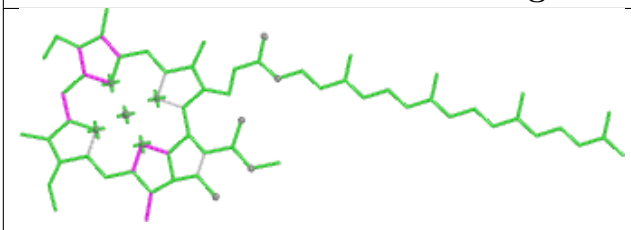


Rings

Ligand CLA 3 602



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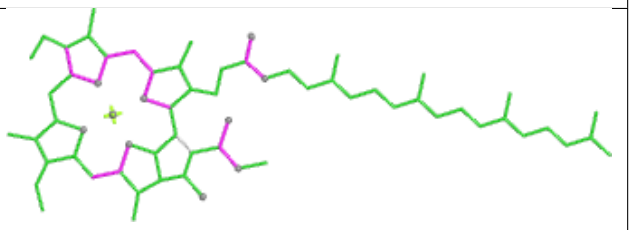

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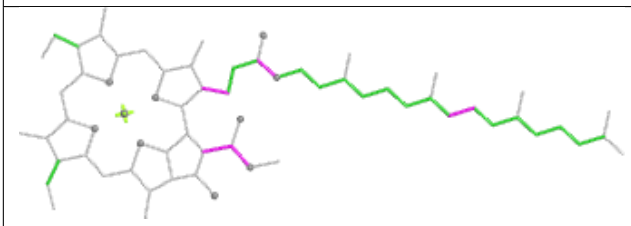

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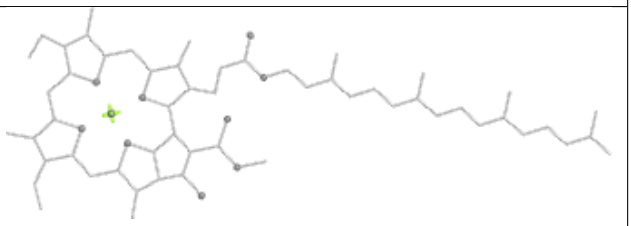

Rings

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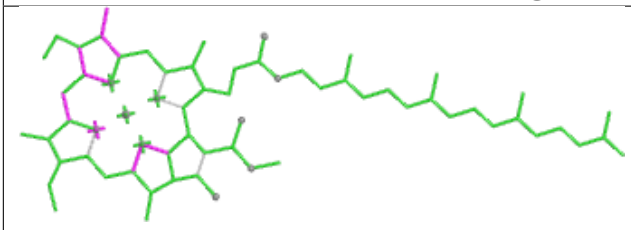

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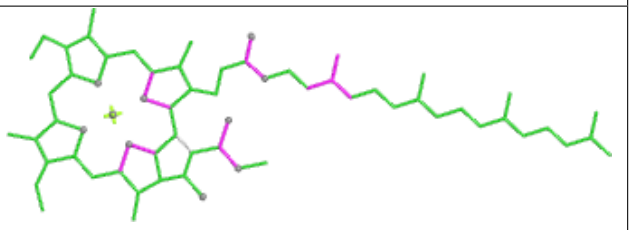

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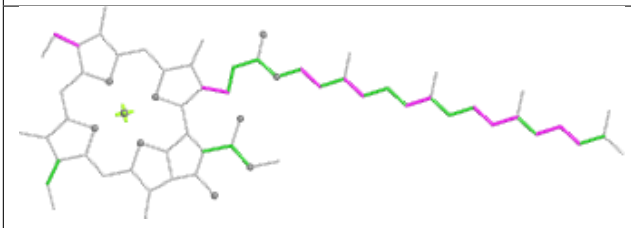

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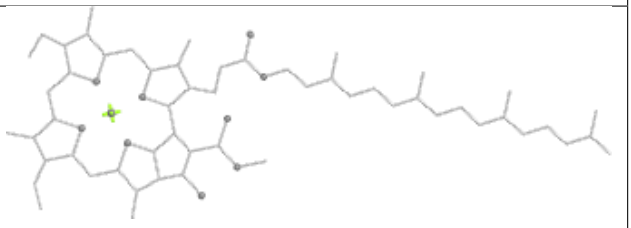
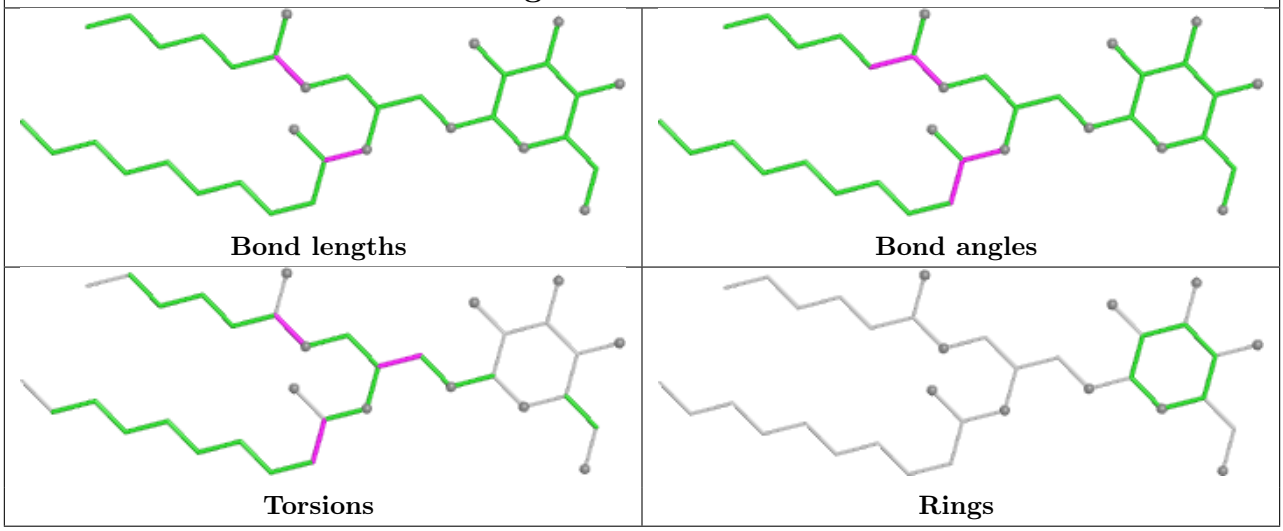


Rings

Ligand LMG J 104



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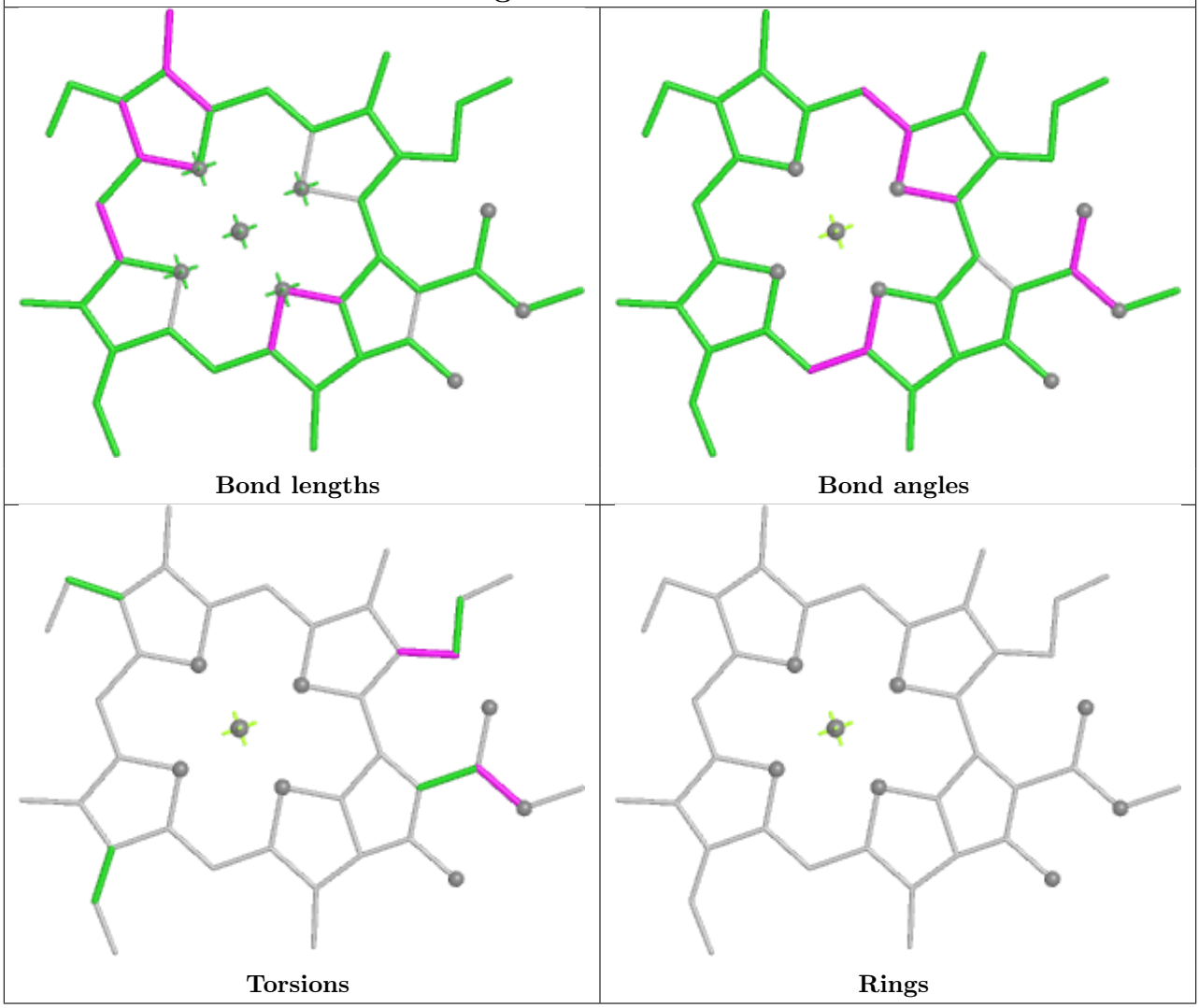

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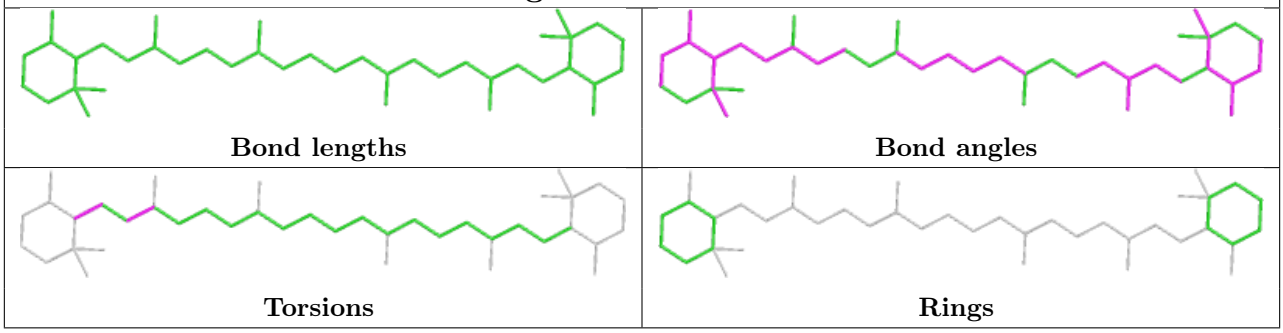

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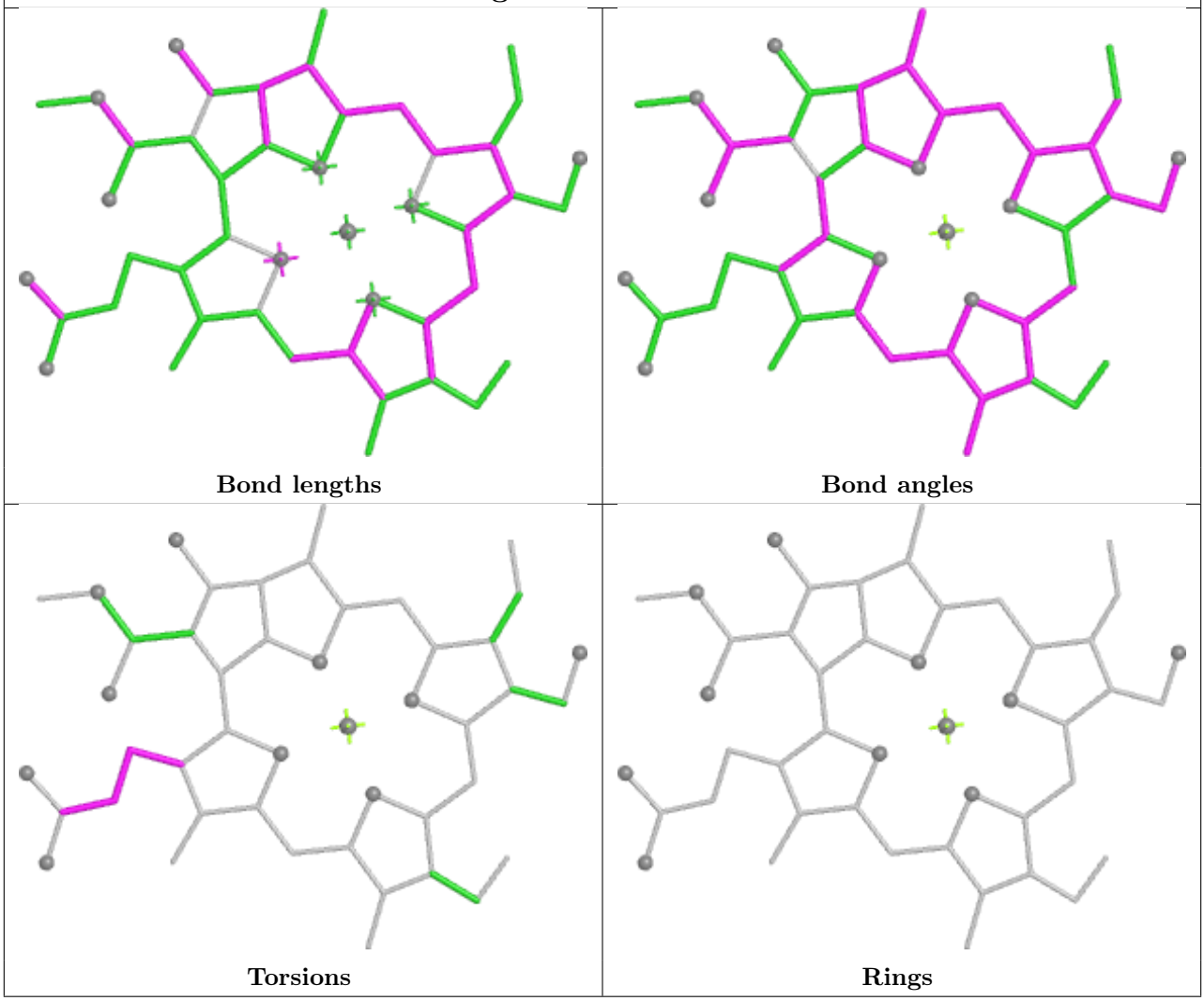

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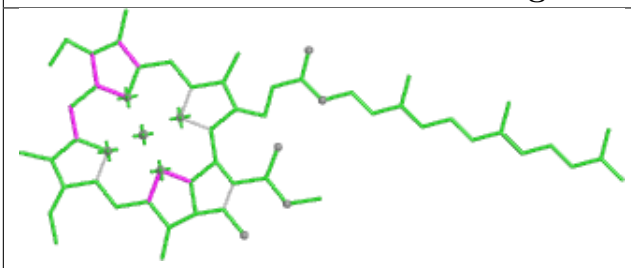
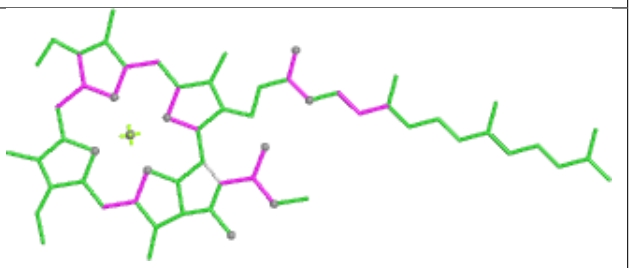
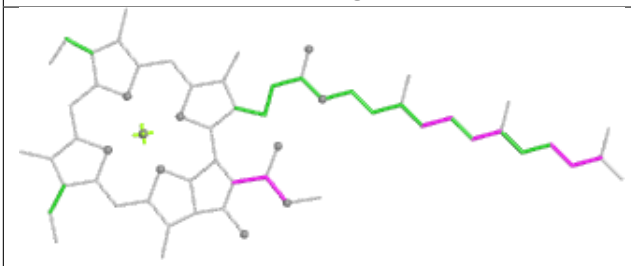
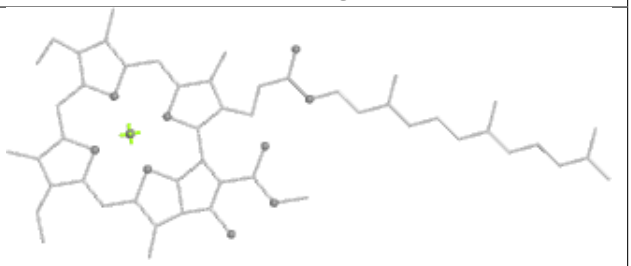
 Bond lengths	 Bond angles
 Torsions	 Rings

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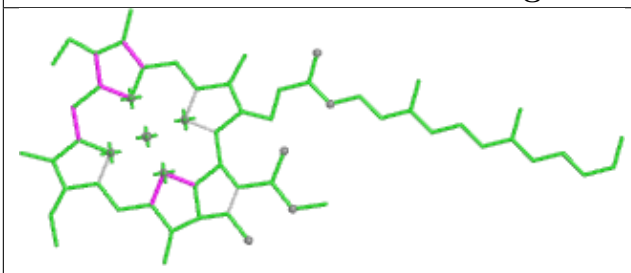
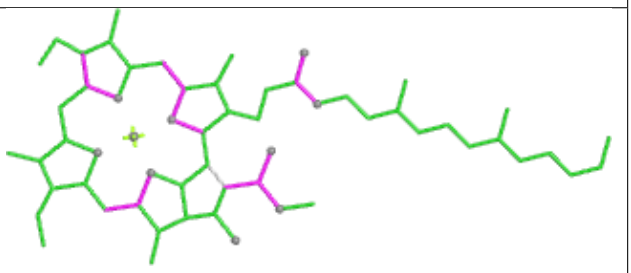
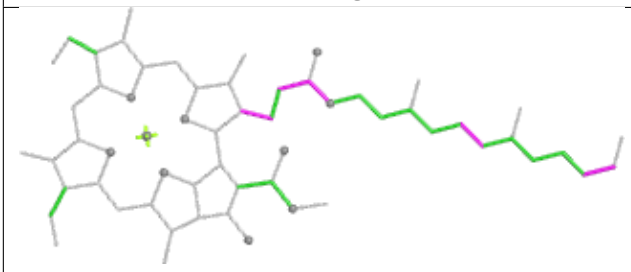
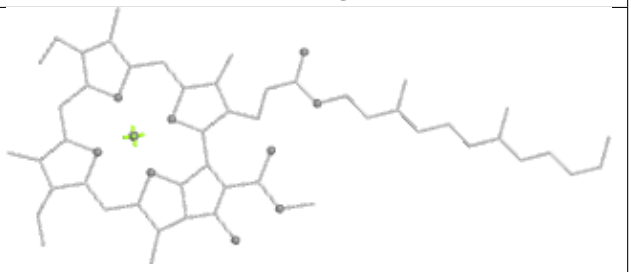
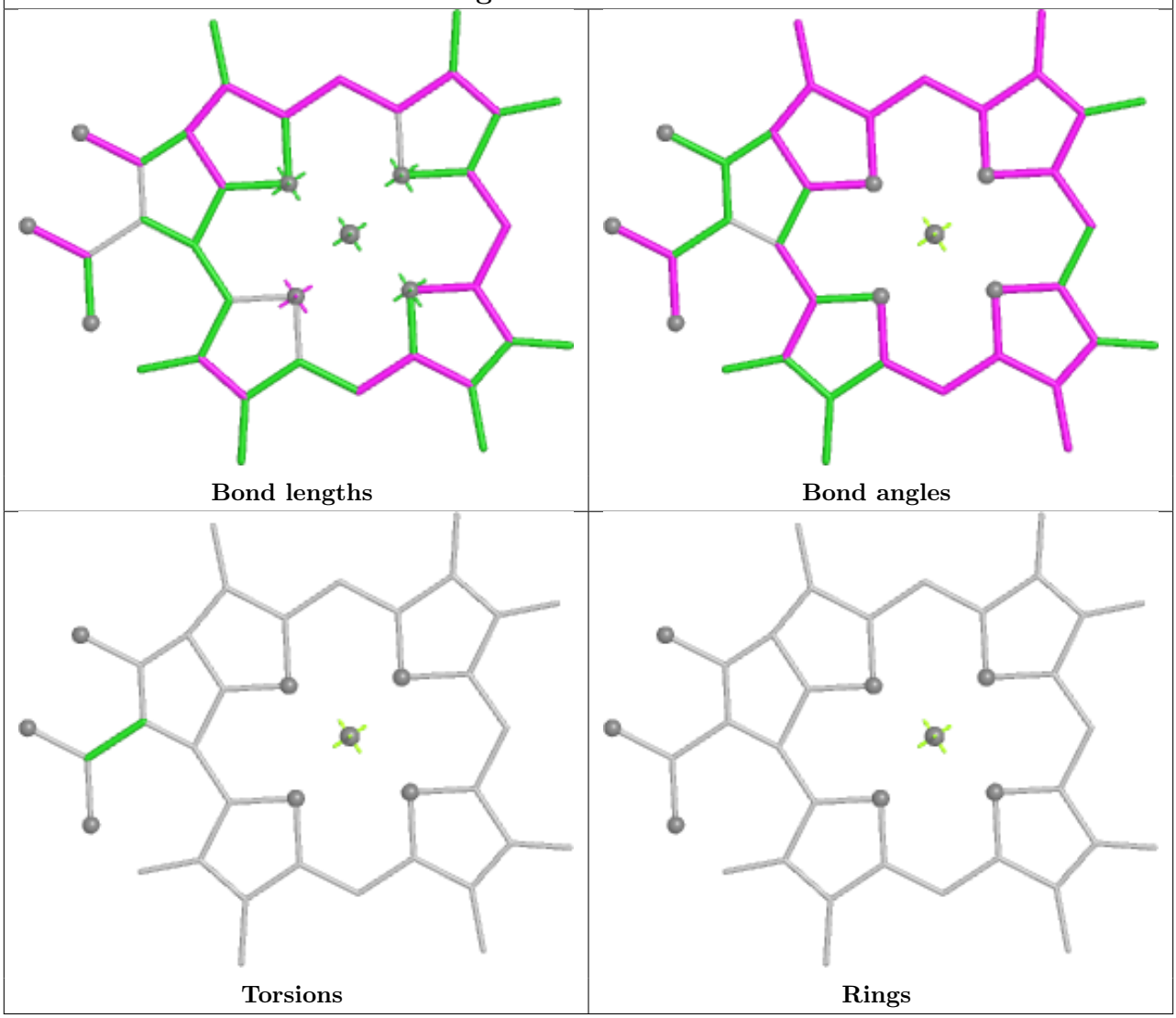
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL W 605



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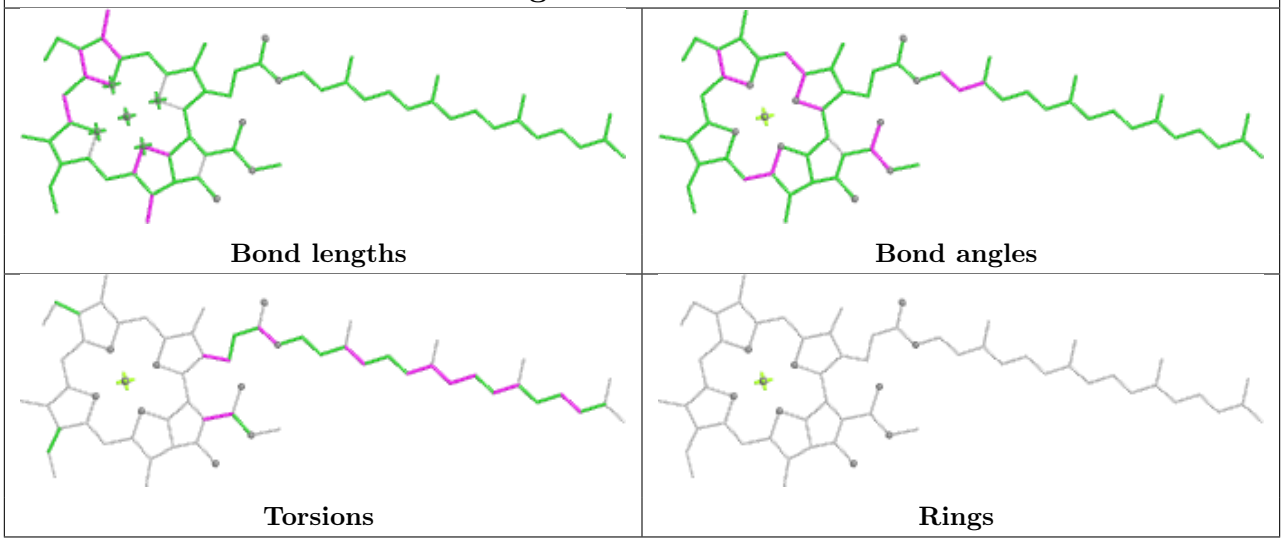

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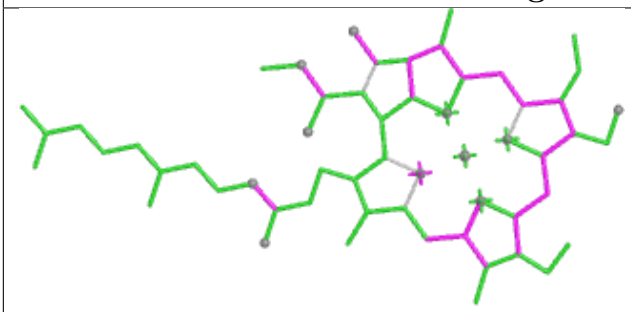

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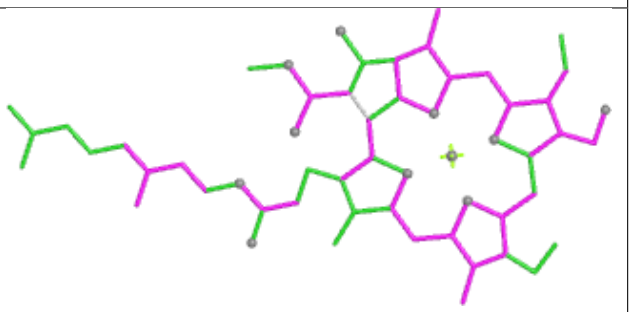

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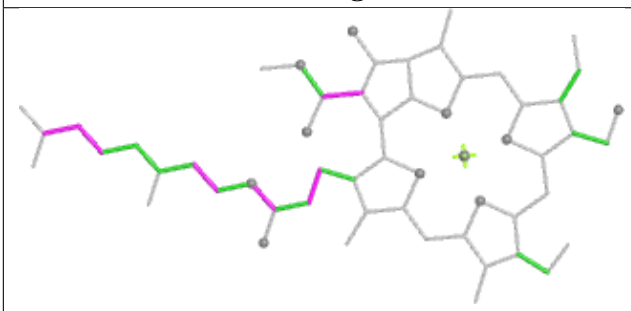

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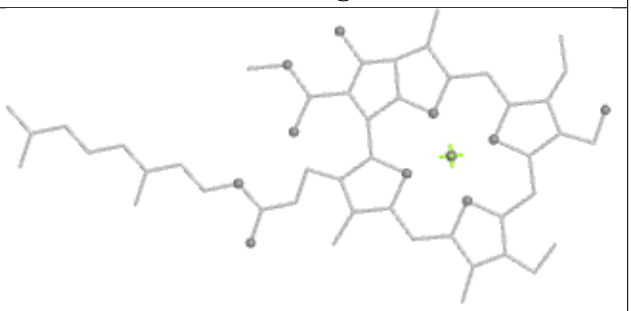
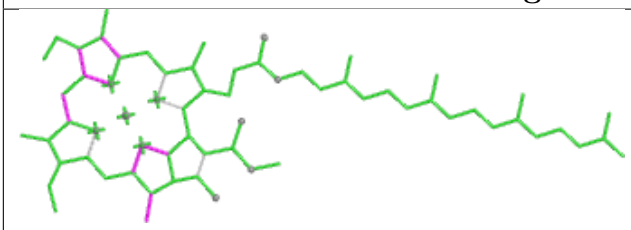


Rings

Ligand CLA A 806



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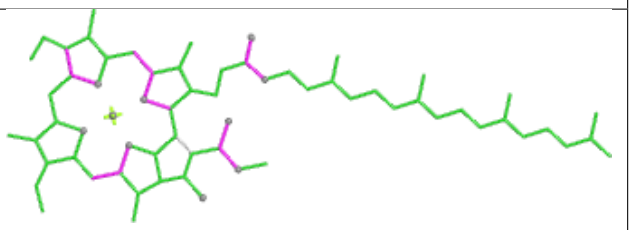

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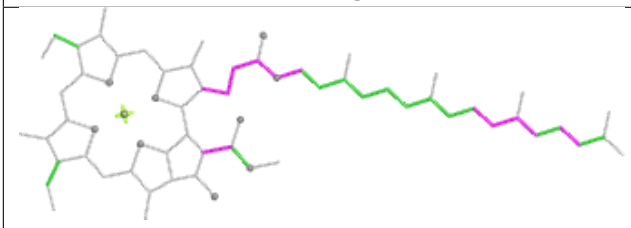

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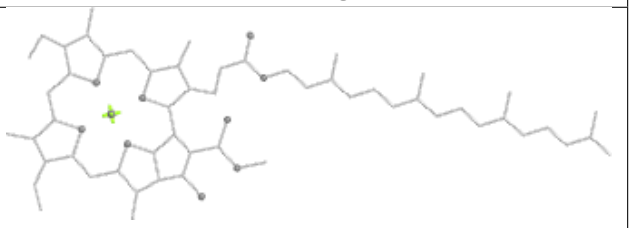
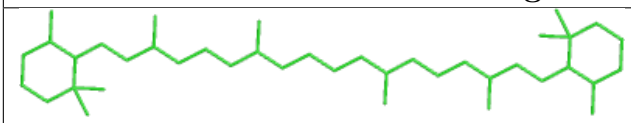


Rings

Ligand BCR F 305



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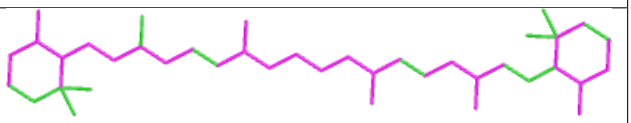
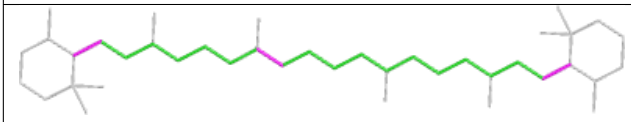


Bond angles



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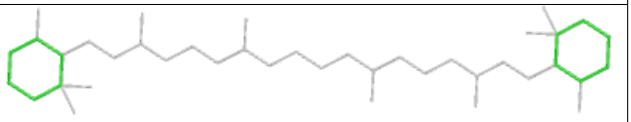
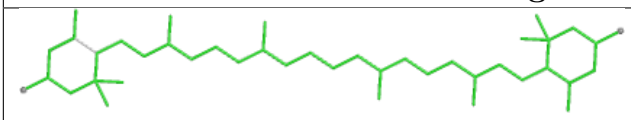
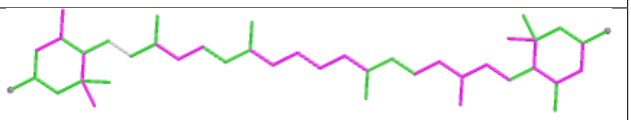


Rings

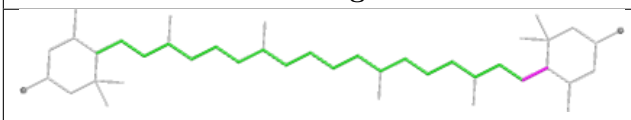
Ligand LUT 9 621



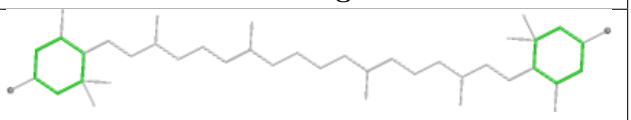
Bond lengths



Bond angles

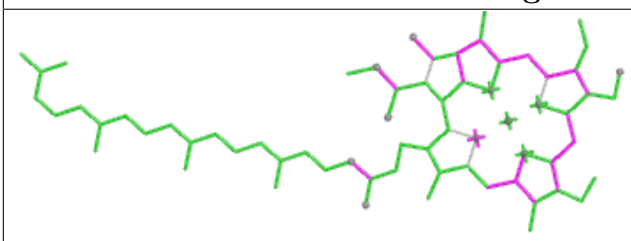


Torsions



Rings

Ligand CHL U 607



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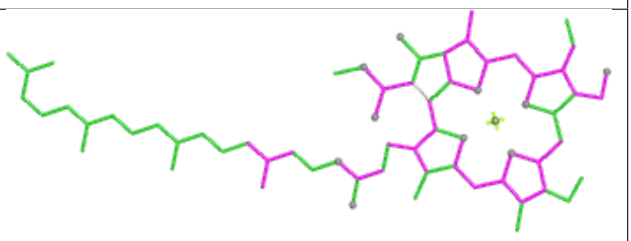
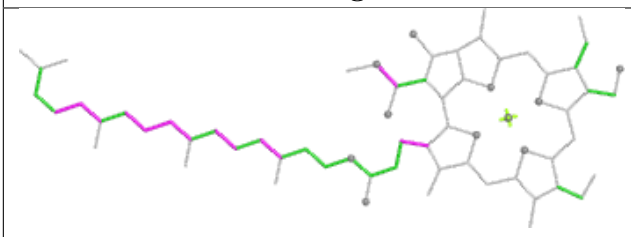


Bond angles



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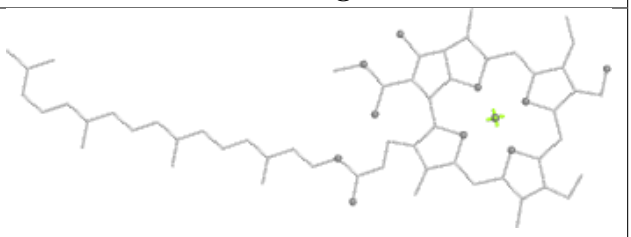
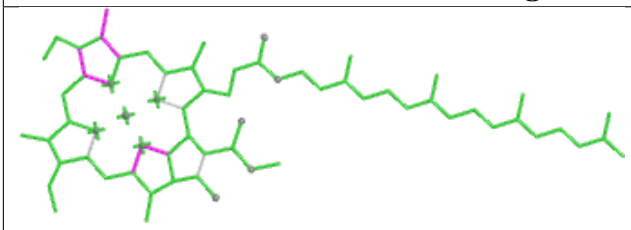


Rings

Ligand CLA A 831



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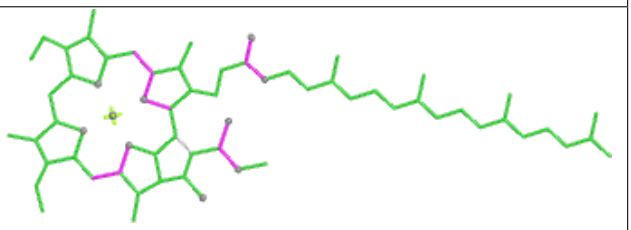

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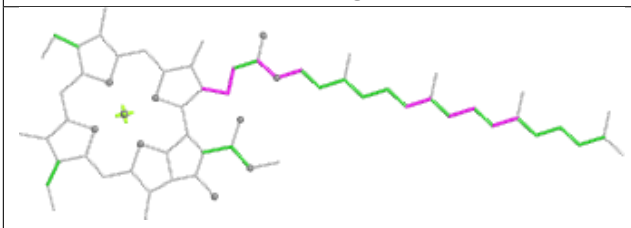

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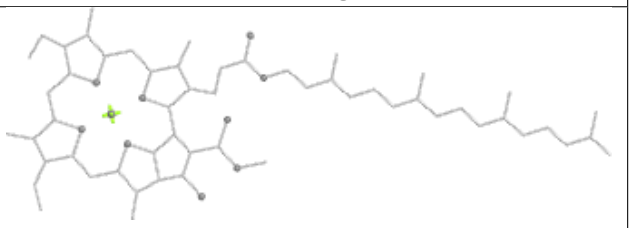
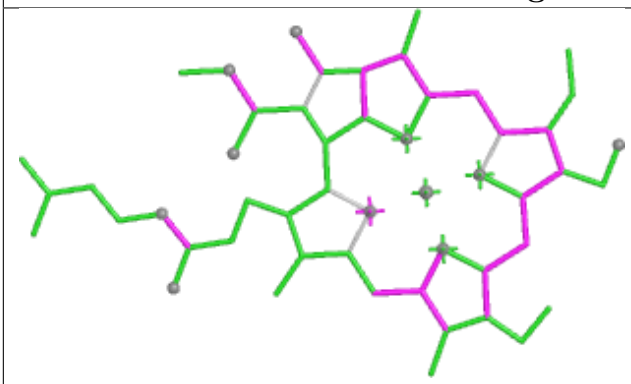
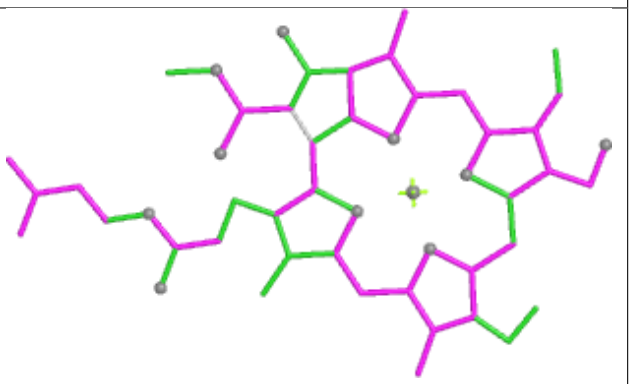
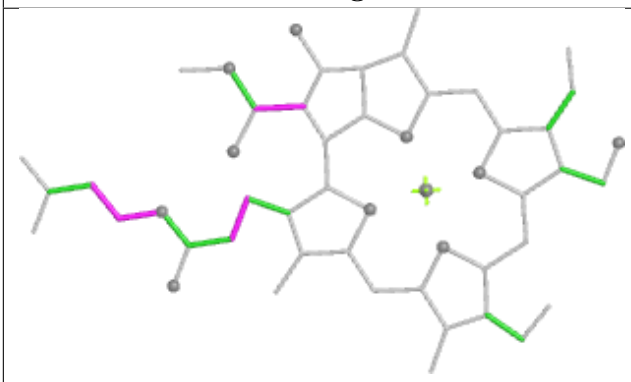
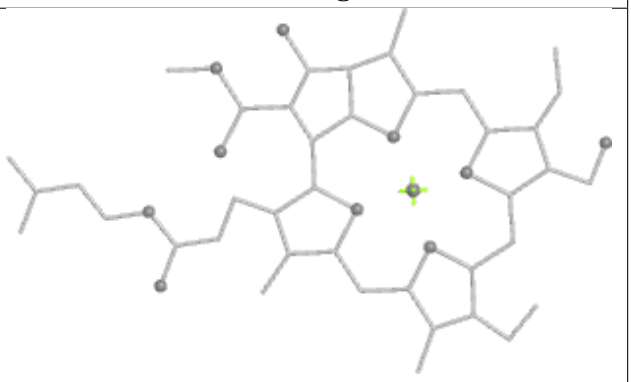
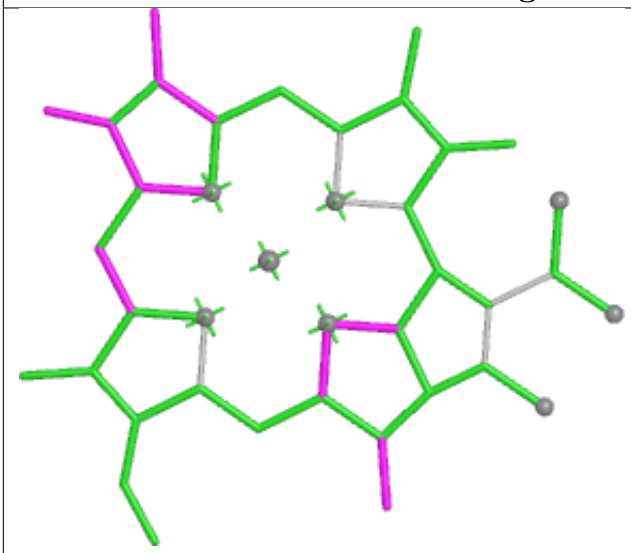


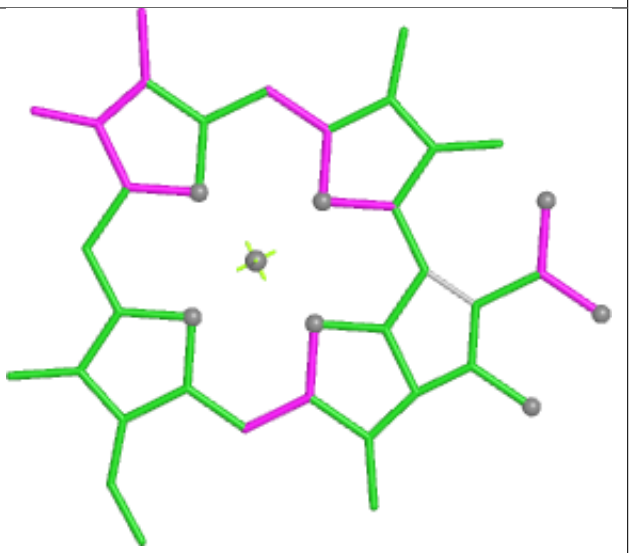
Rings

Ligand CHL 5 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

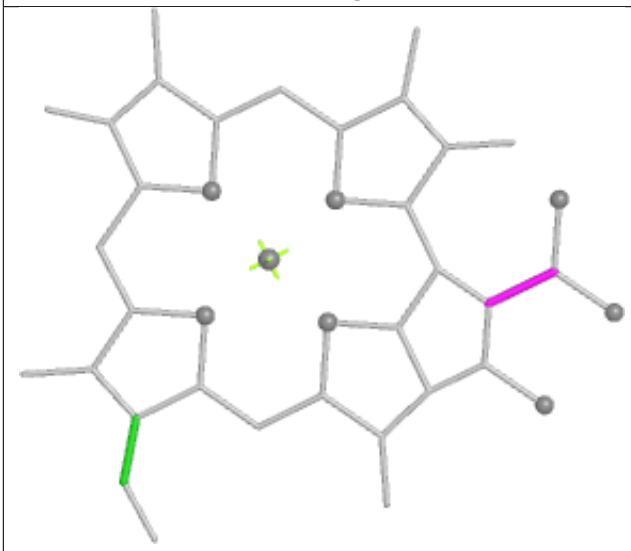
Ligand CLA W 614



Bond lengths



Bond angles



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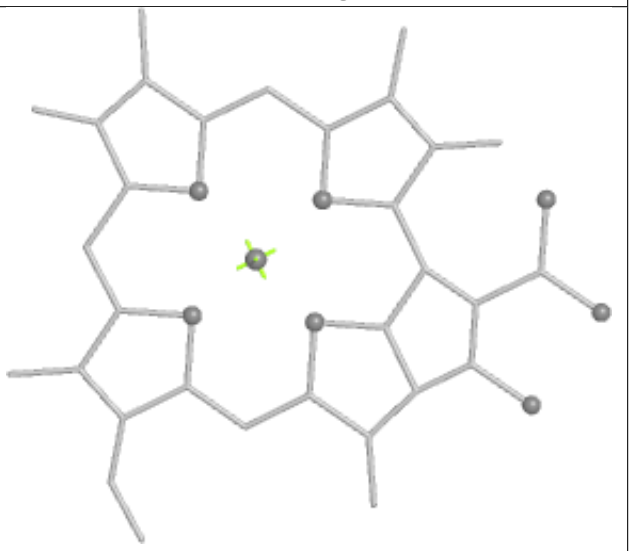
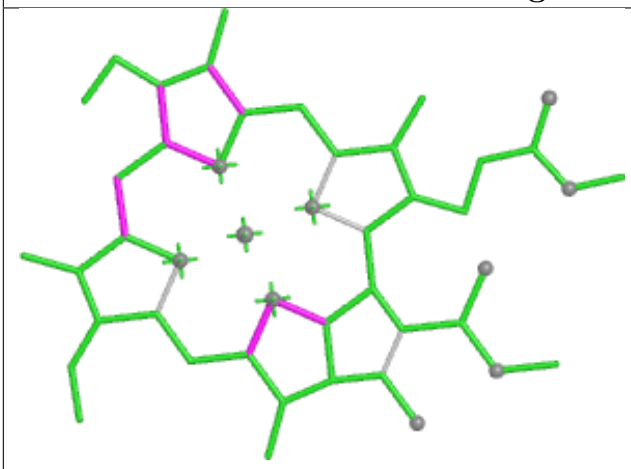


Rings

Ligand CLA 7 617



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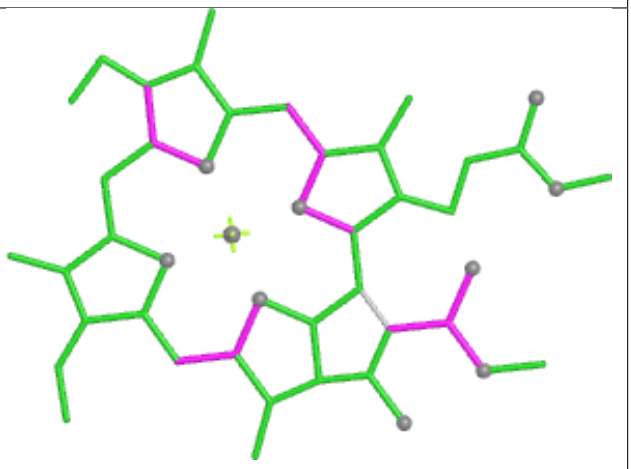
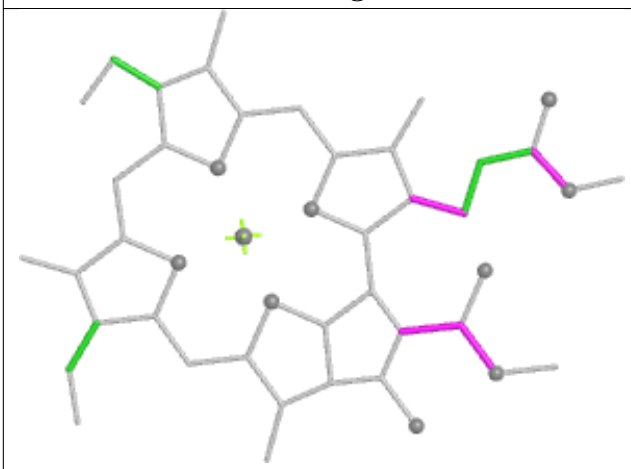


Bond angles



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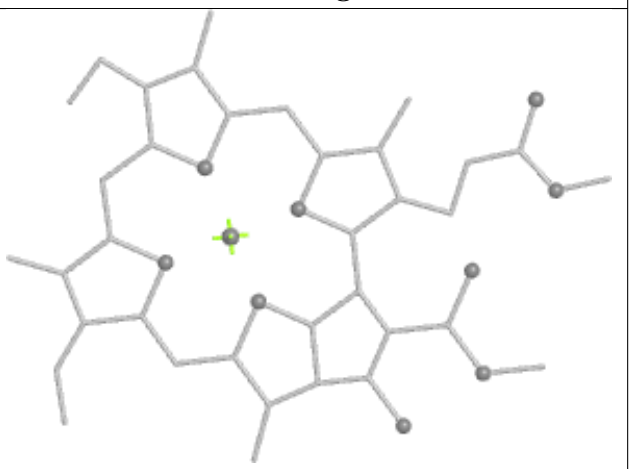
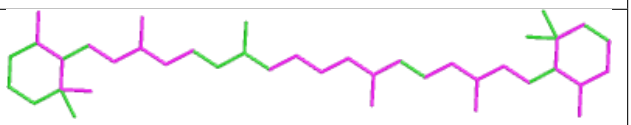


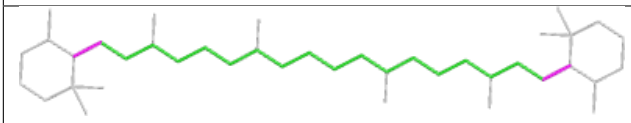
Rings

Ligand BCR B 801

Bond lengths



Bond angles



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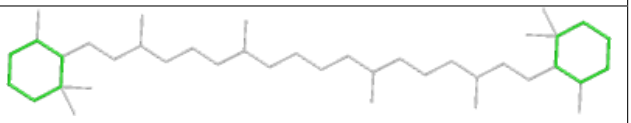
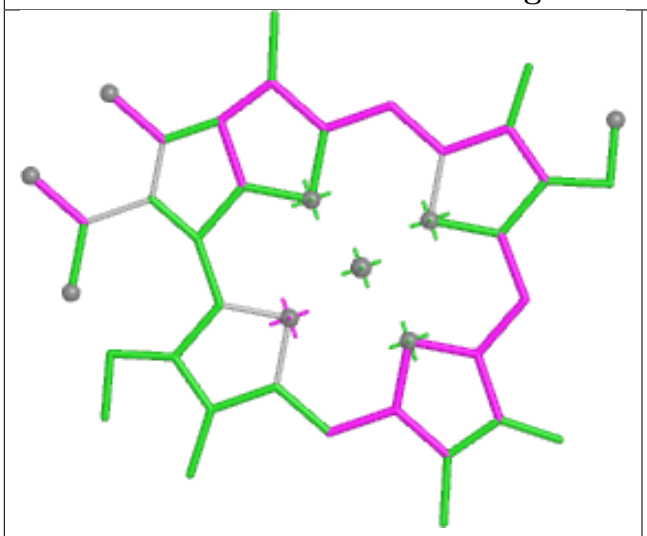


Rings

Ligand CHL U 608



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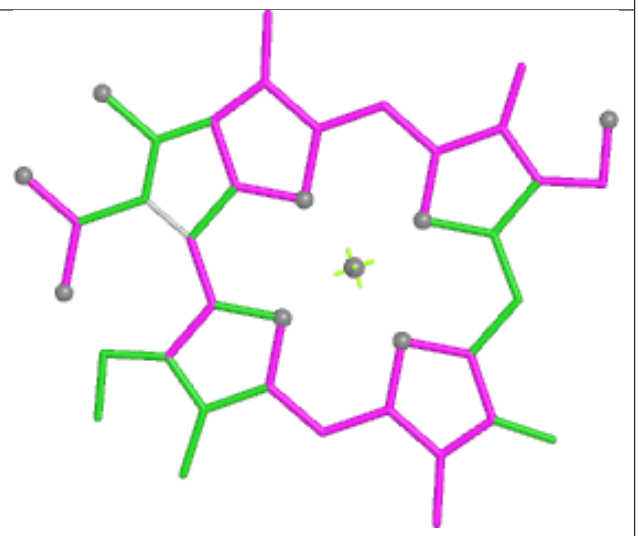

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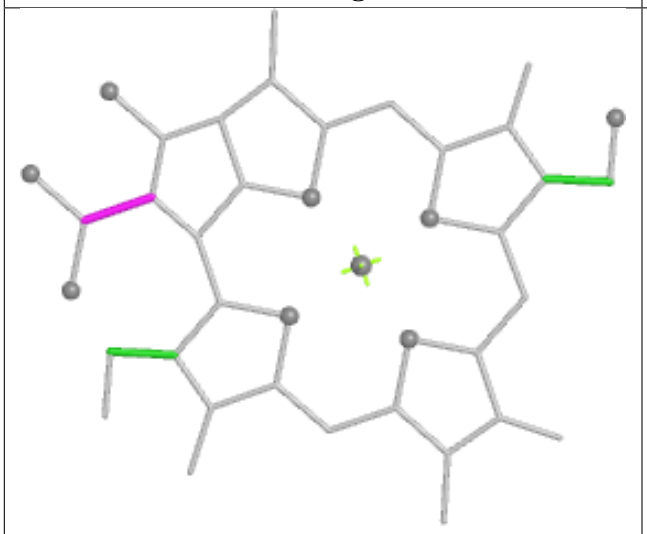
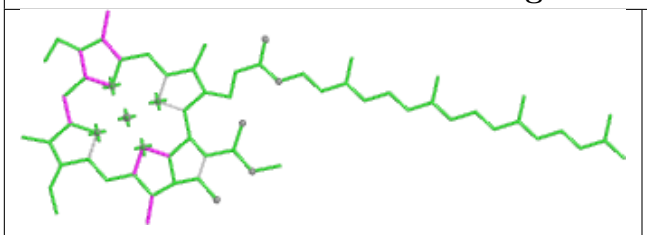


Torsions

Rings

Ligand CLA B 807



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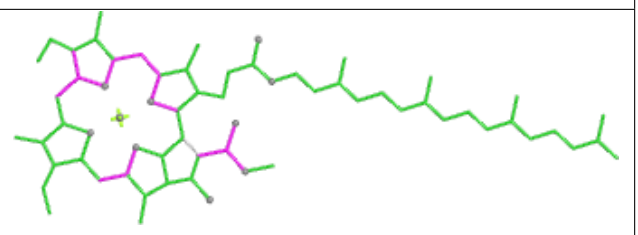
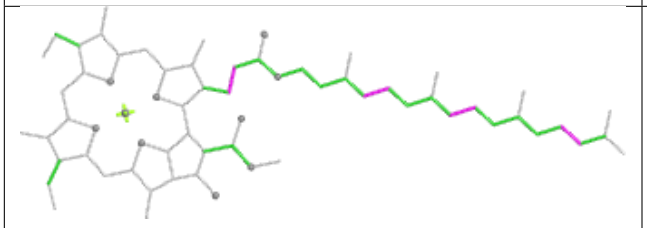
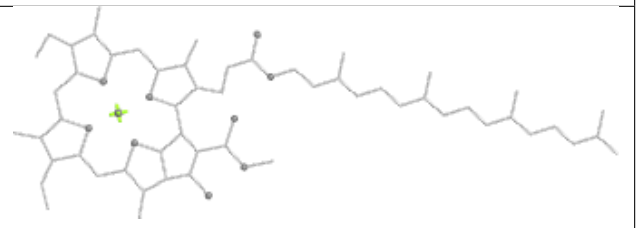


Bond angles

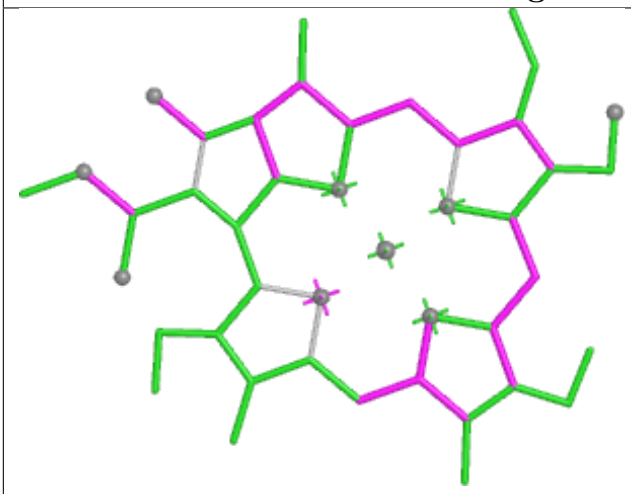


Torsions

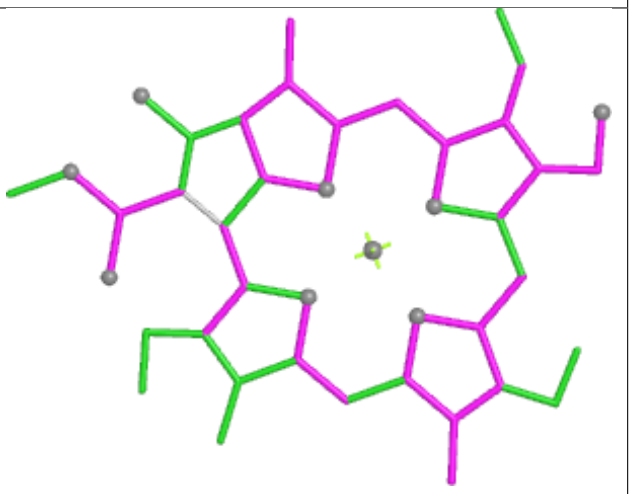


Rings

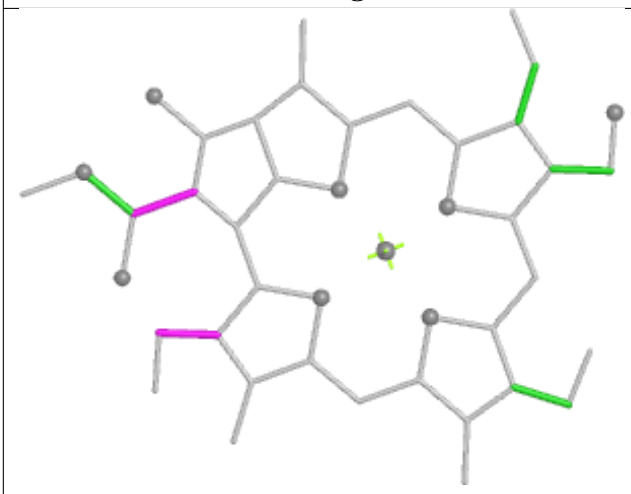
Ligand CHL 9 607



Bond lengths



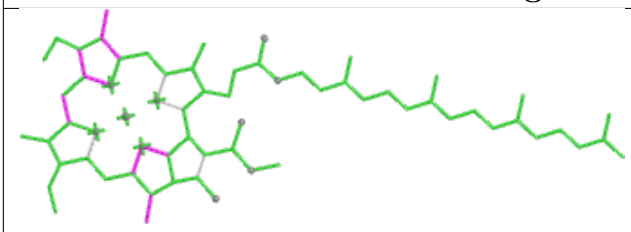
Bond angles



Torsions

Rings

Ligand CLA B 826



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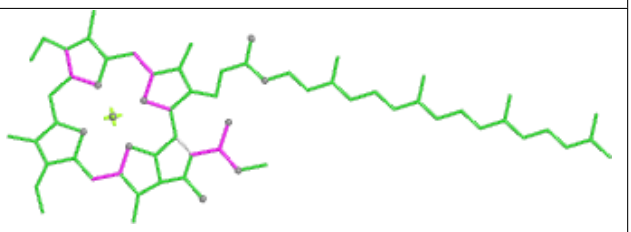
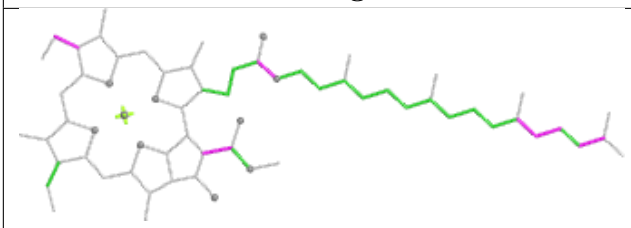


Bond angles



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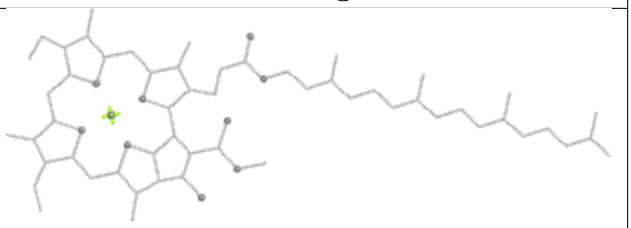
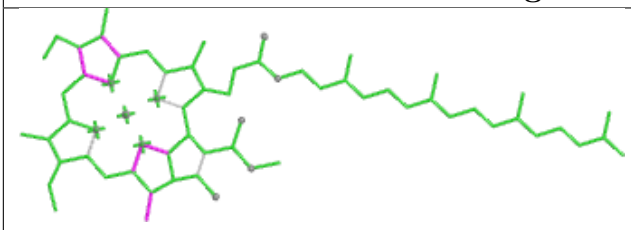
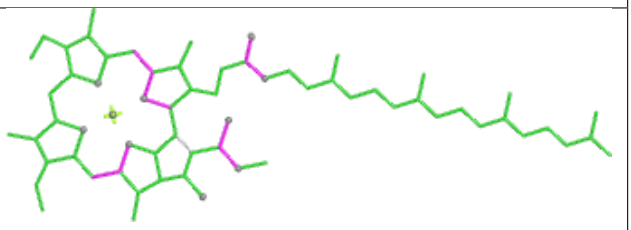
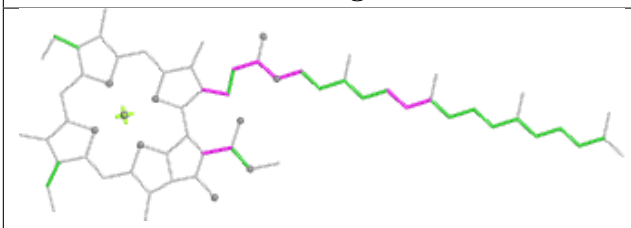
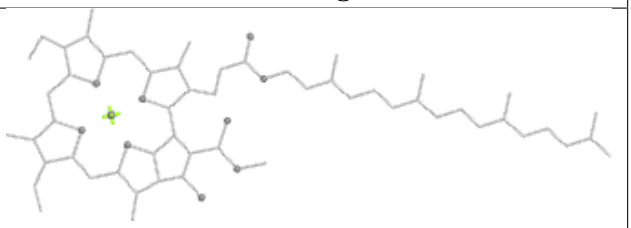
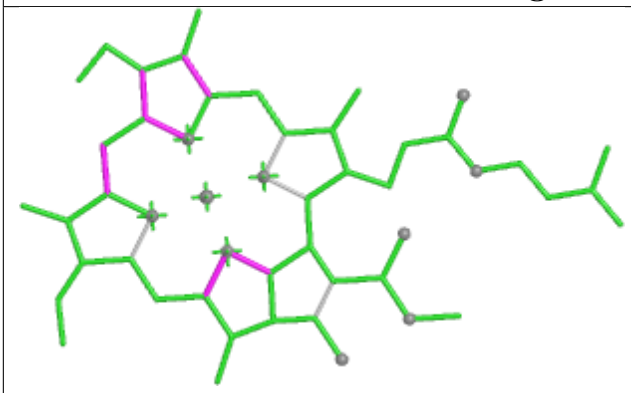
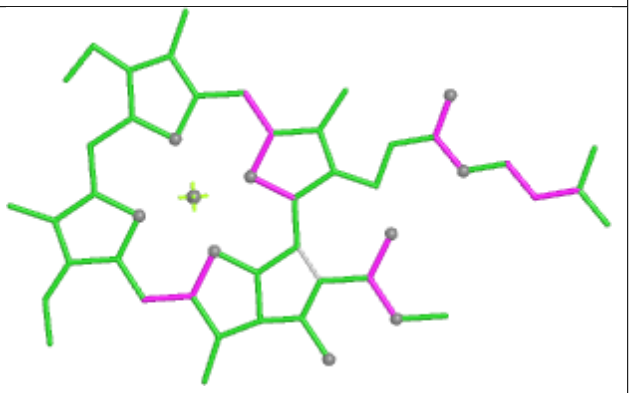
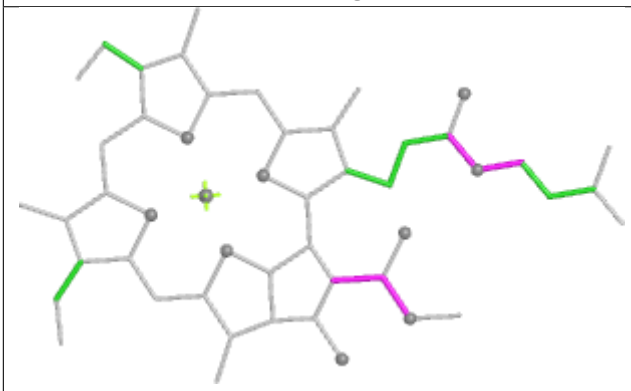
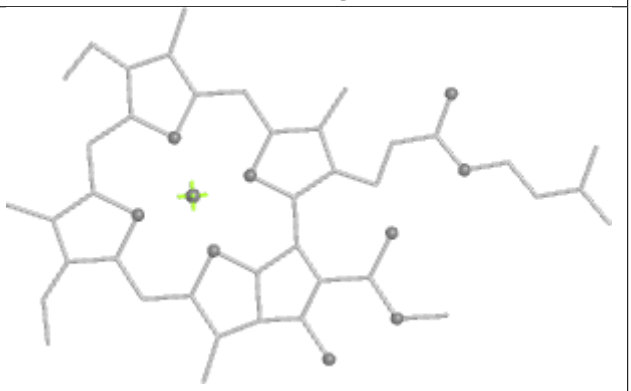
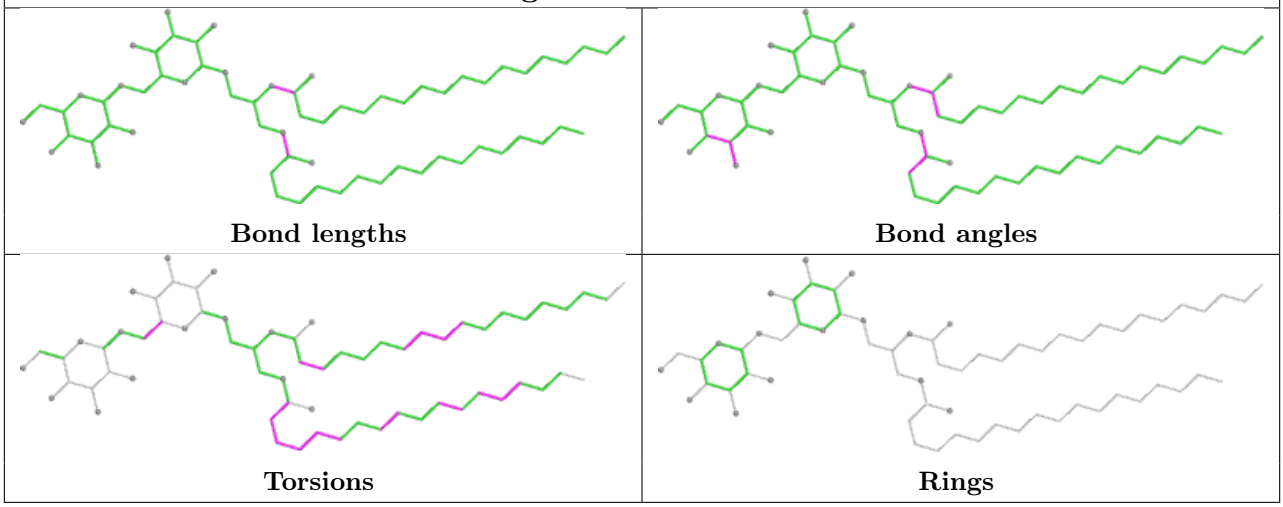


Rings

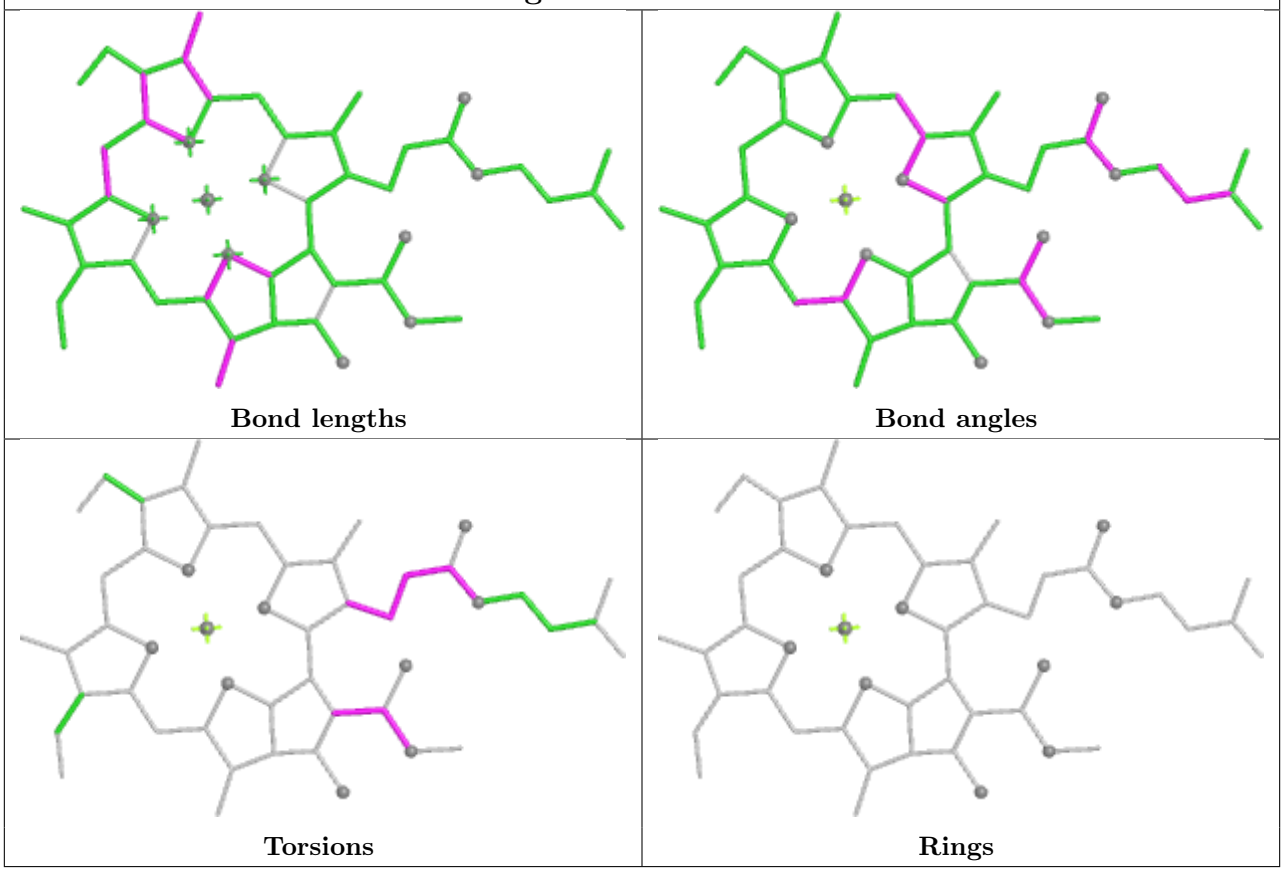
Ligand CLA B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

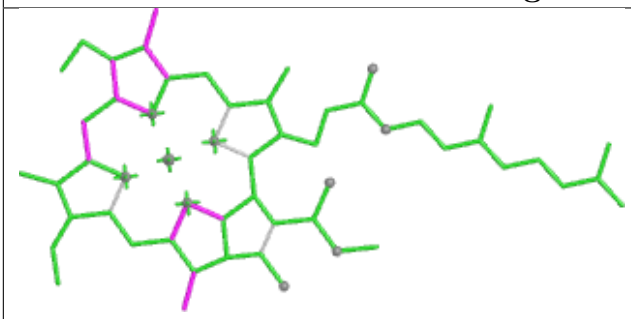
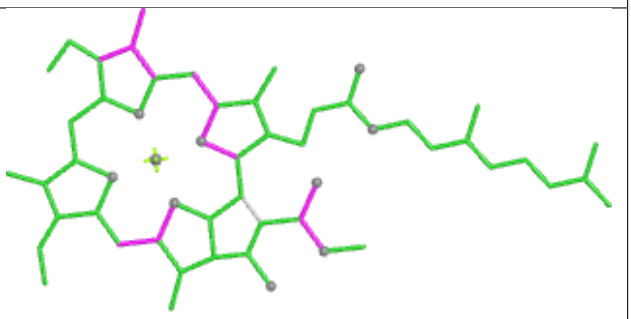
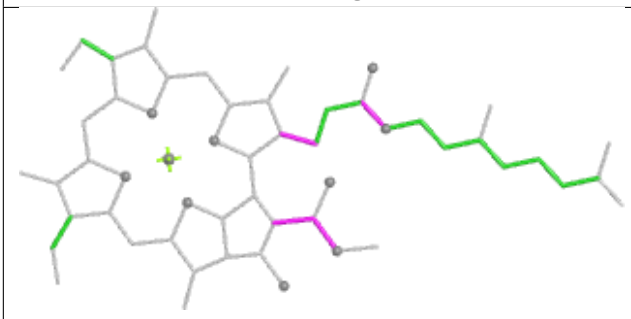
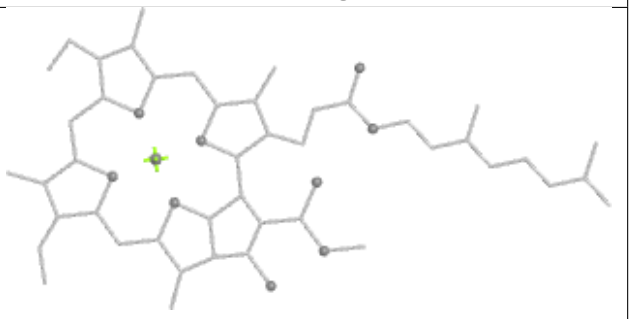
Ligand CLA 7 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD B 850

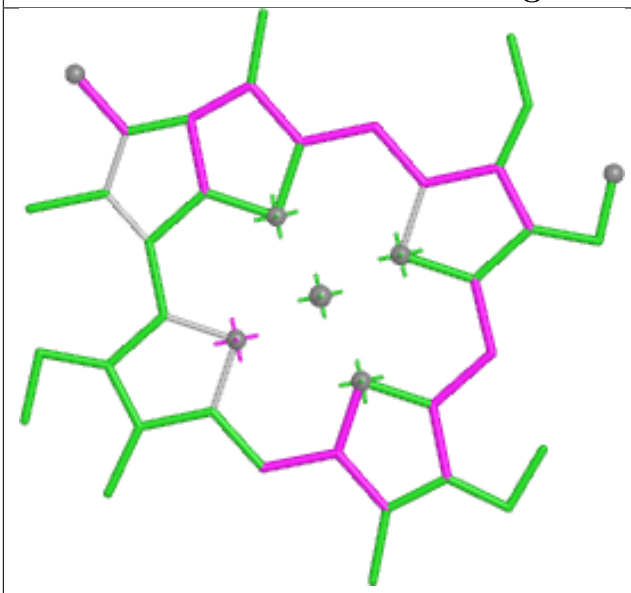


Ligand CLA V 604

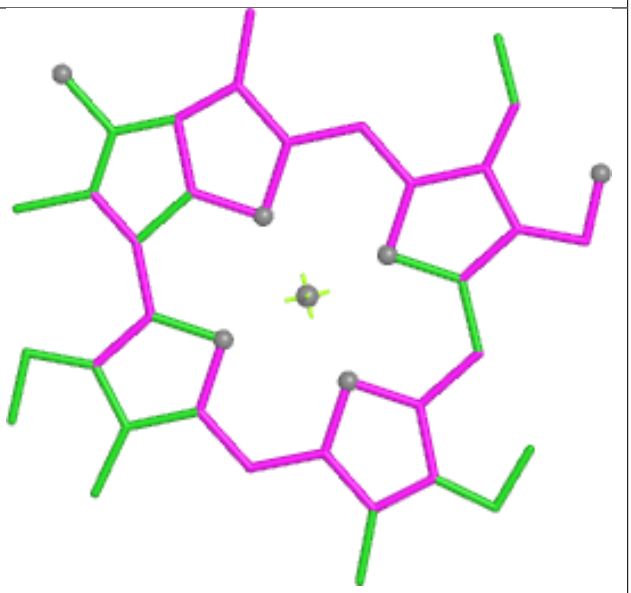


Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

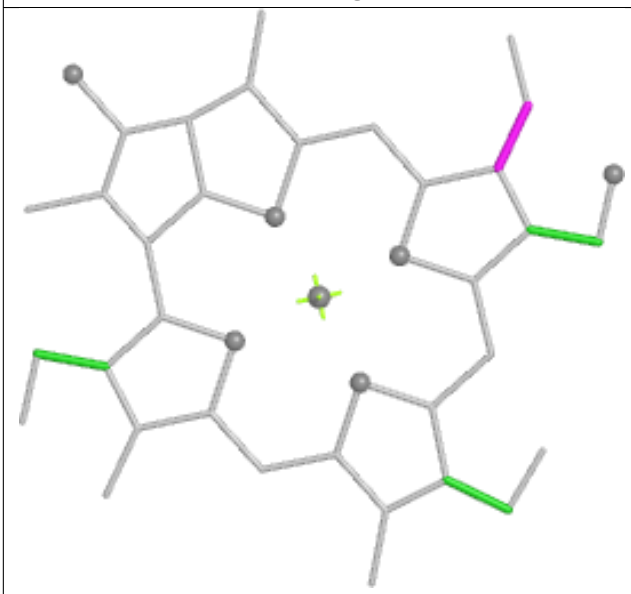
Ligand CHL V 609



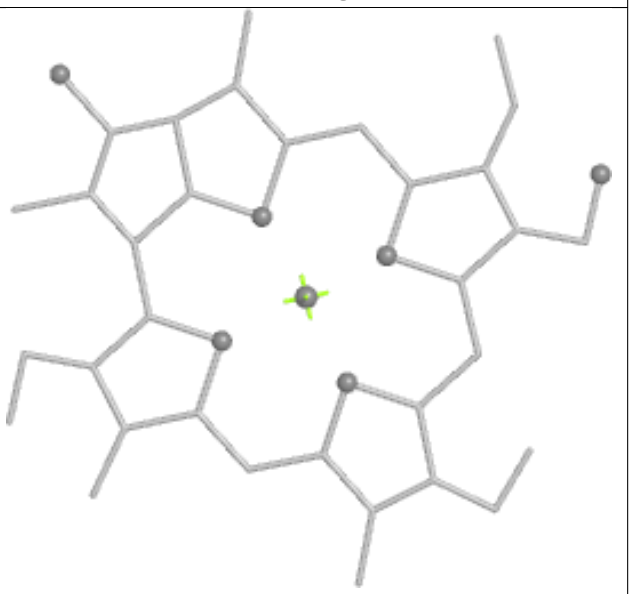
Bond lengths



Bond angles

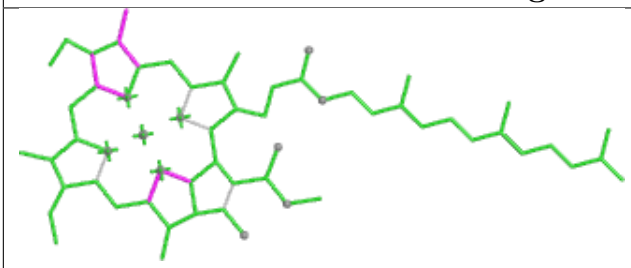


Torsions

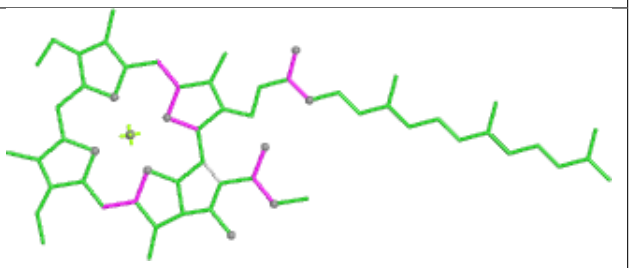


Rings

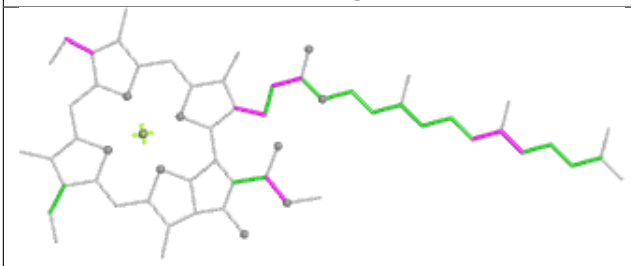
Ligand CLA 6 610



Bond lengths



Bond angles



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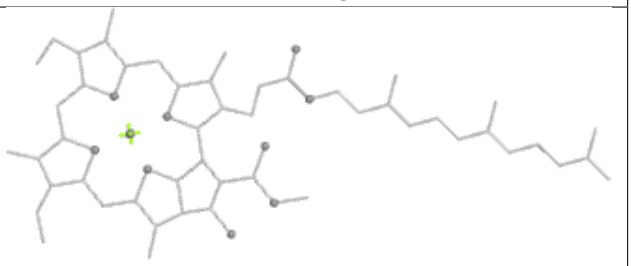
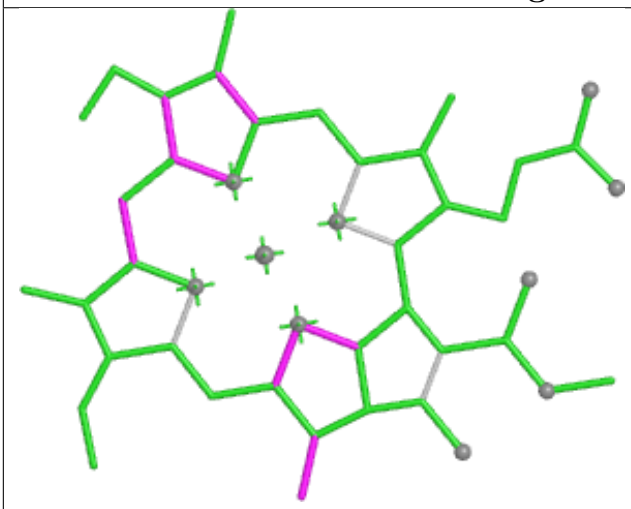


Rings

Ligand CLA 4 609



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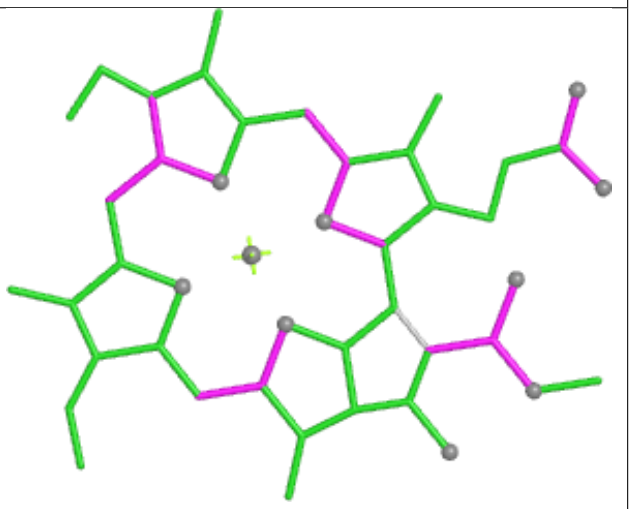

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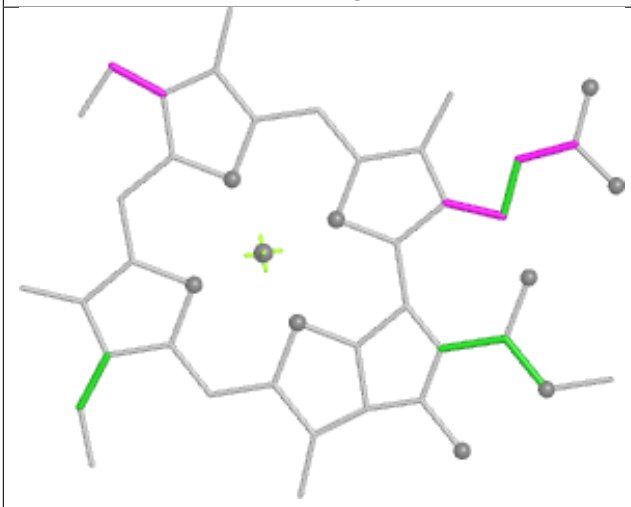
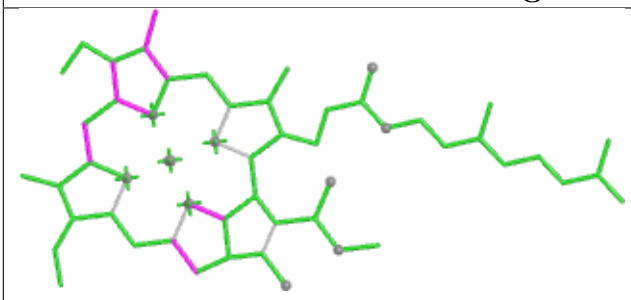
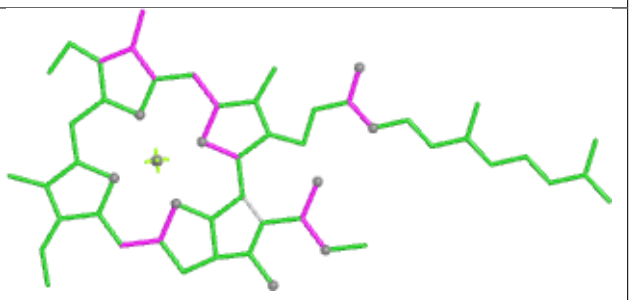
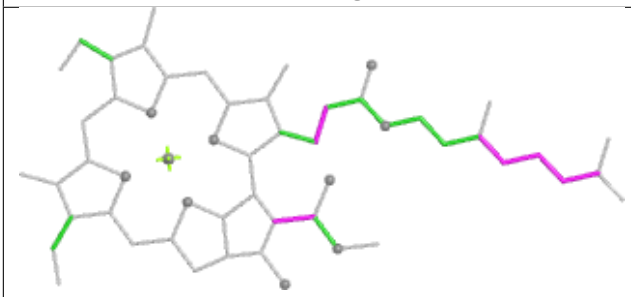
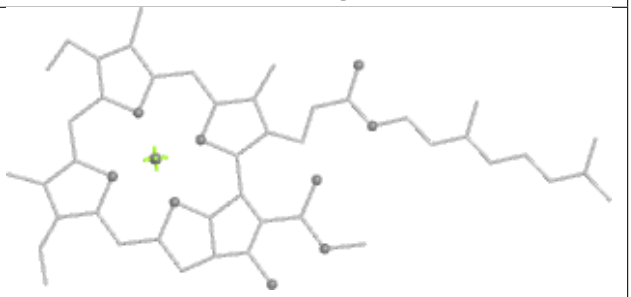
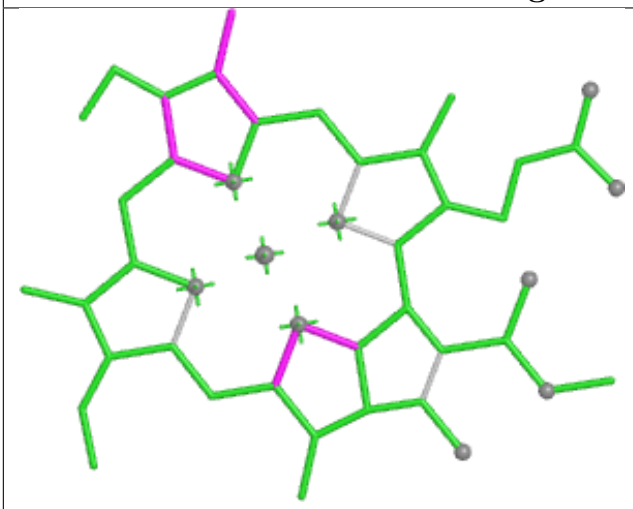


Torsions

Rings

Ligand CLA A 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 612



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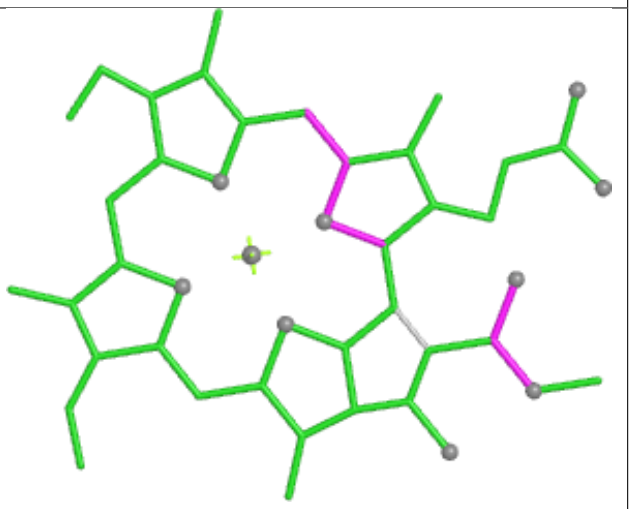
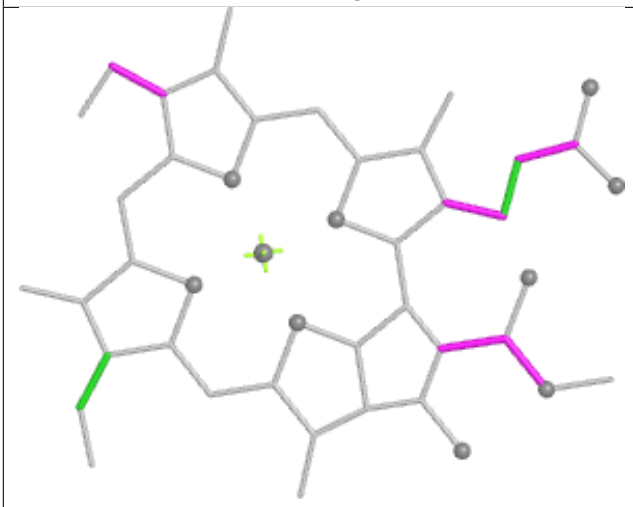


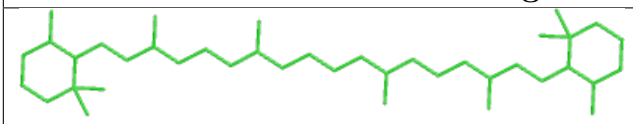
Bond angles



Torsions

Rings

Ligand BCR A 849



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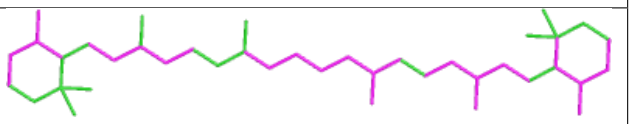

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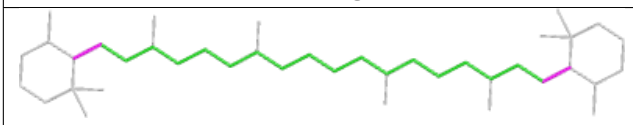

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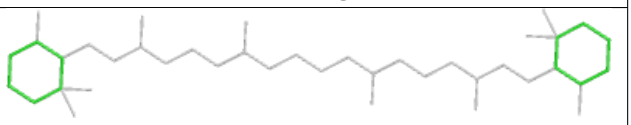
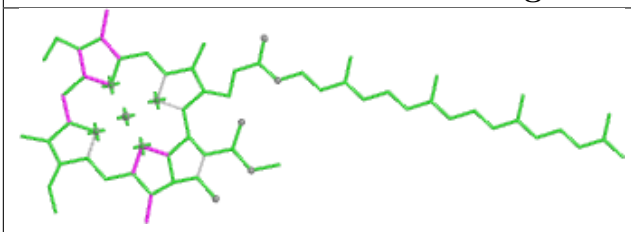


Rings

Ligand CLA B 809



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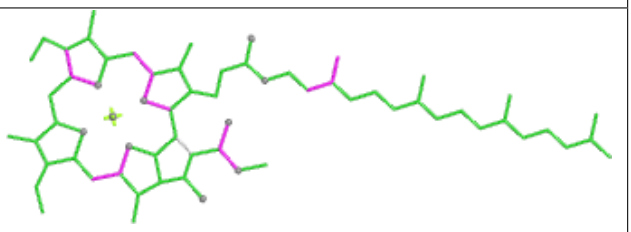

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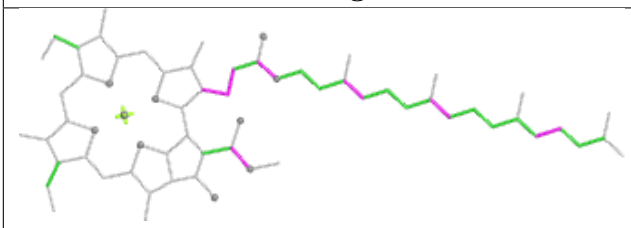

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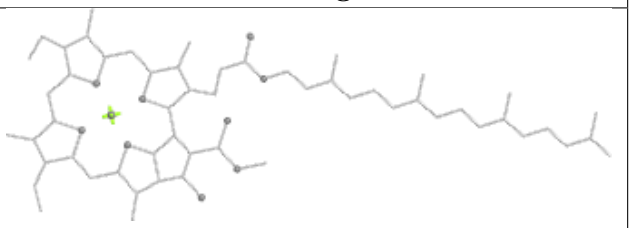

Rings

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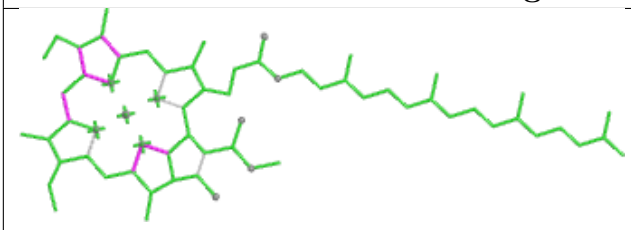

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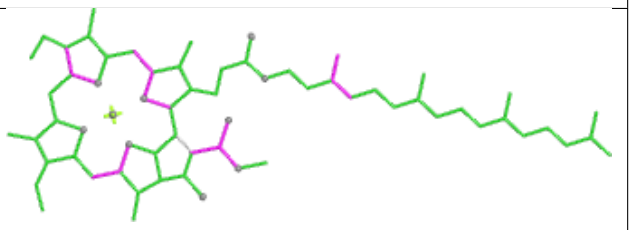
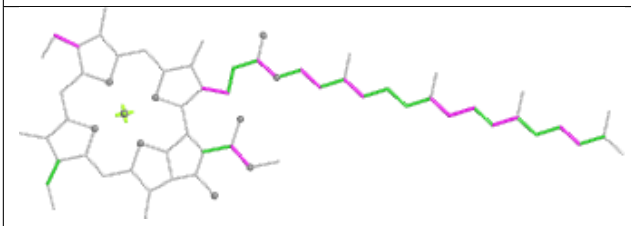


Bond angles



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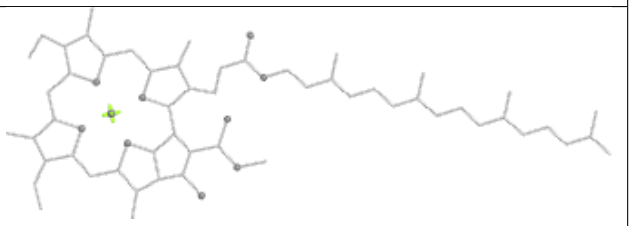
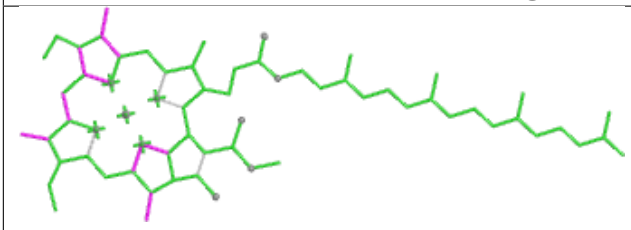


Rings

Ligand CLA A 828



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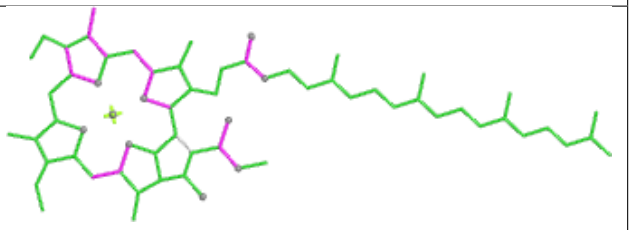

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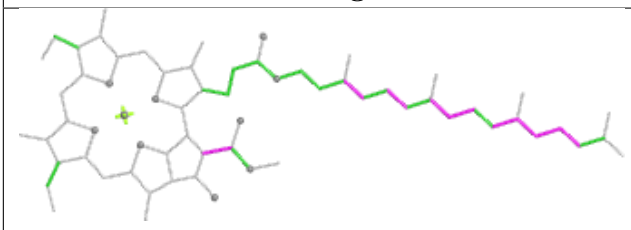

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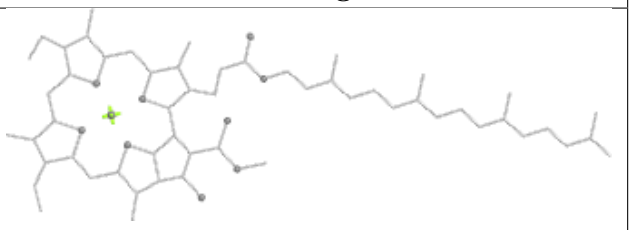
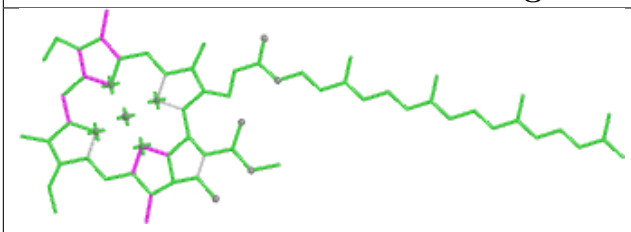
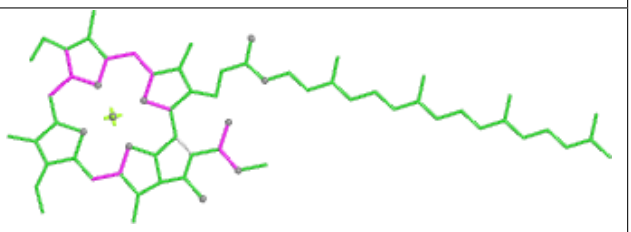
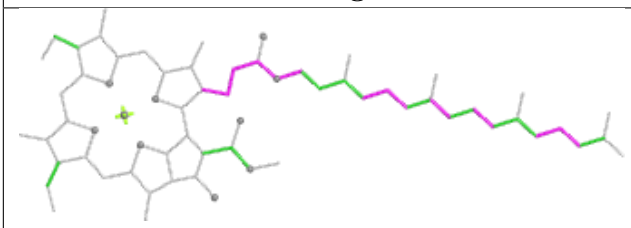
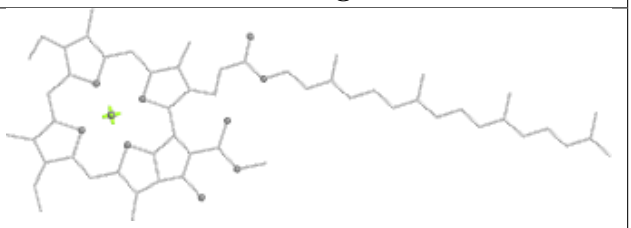


Rings

Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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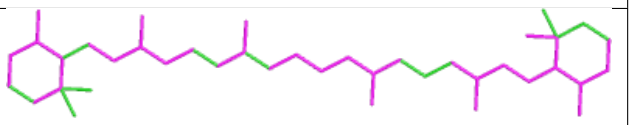
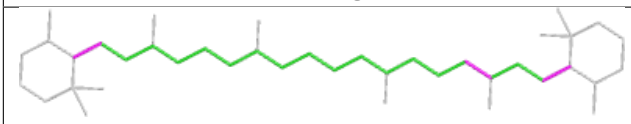
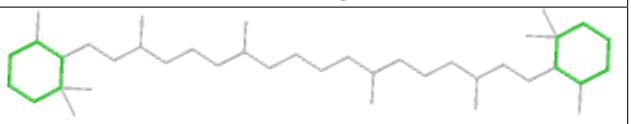
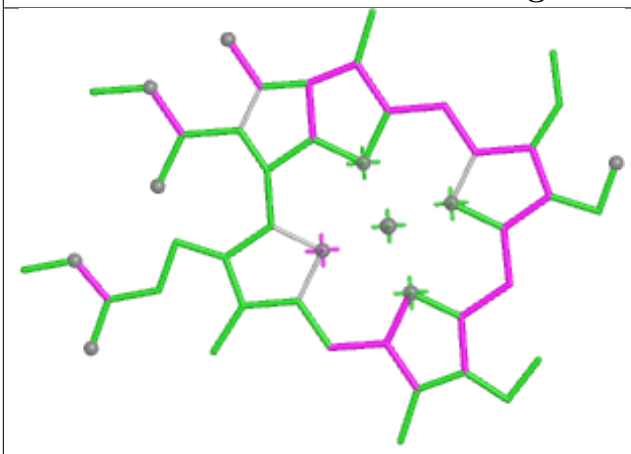
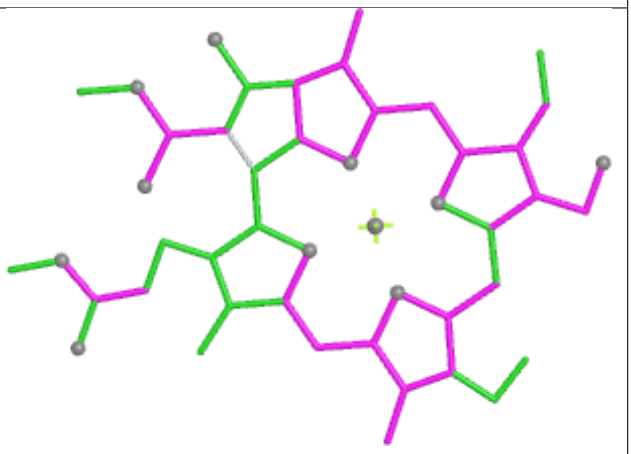
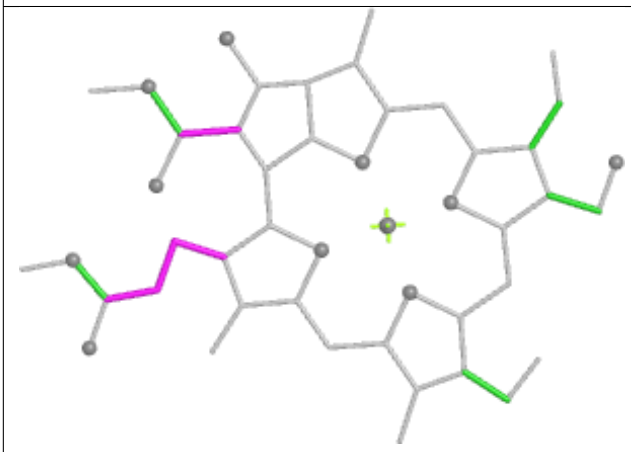
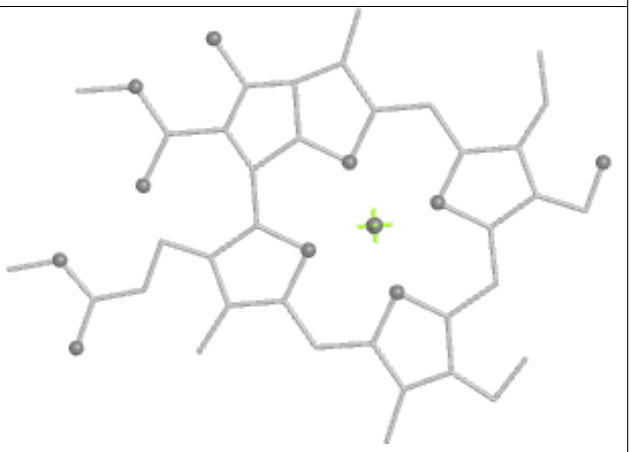
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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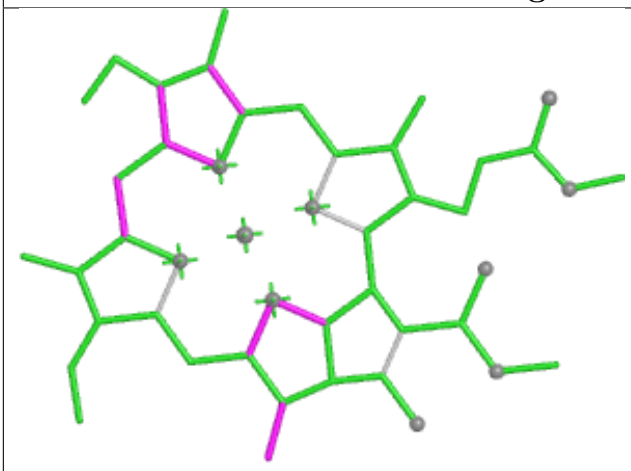
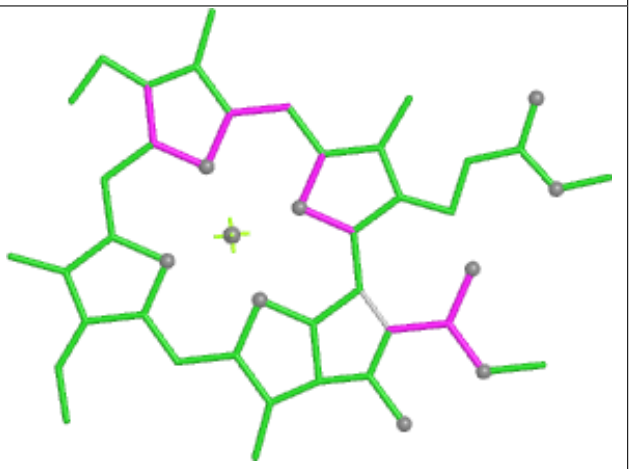
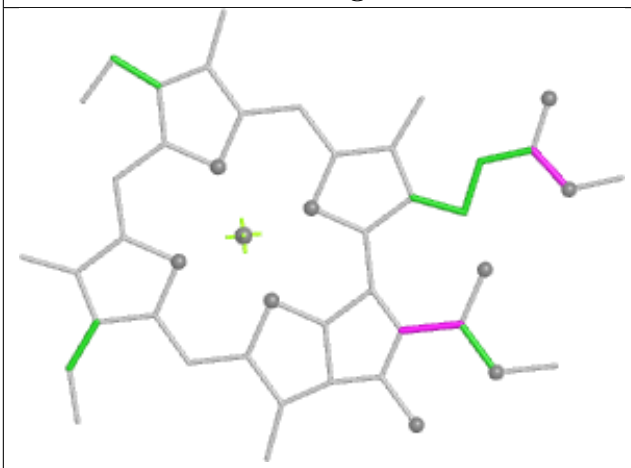
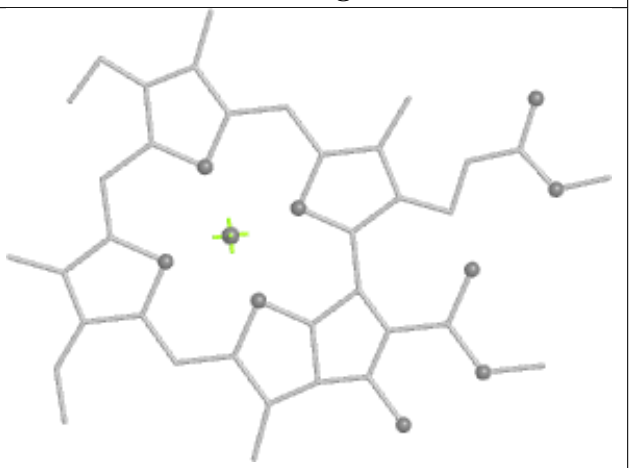
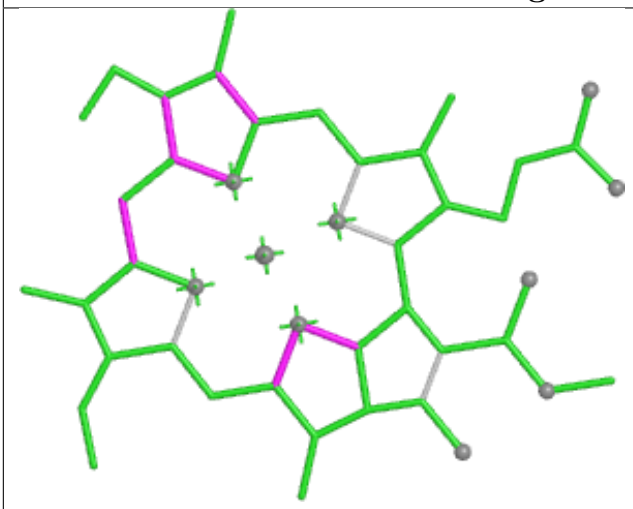
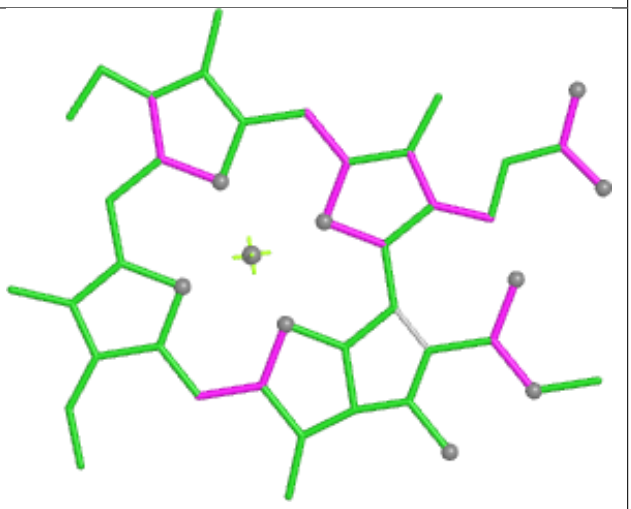
 Bond lengths	 Bond angles
 Torsions	 Rings

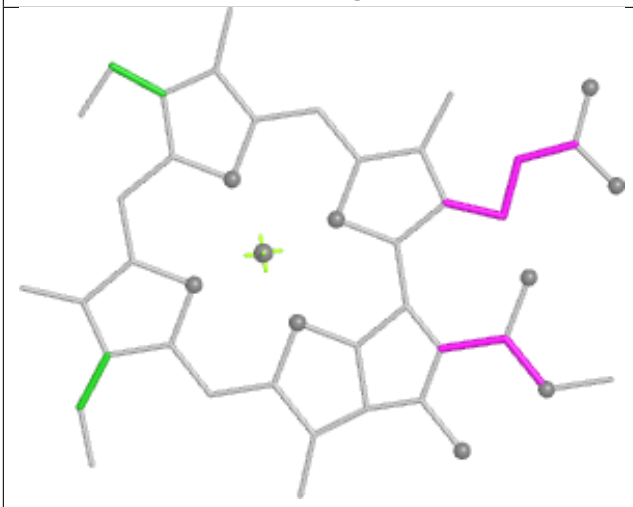
Ligand CLA 8 614



Bond lengths



Bond angles



Torsions

Rings

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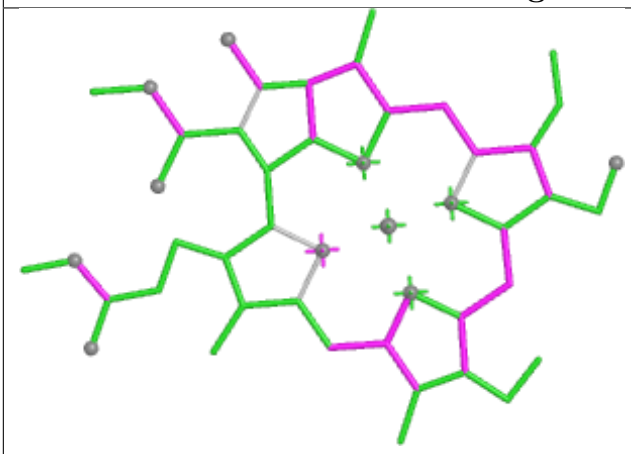
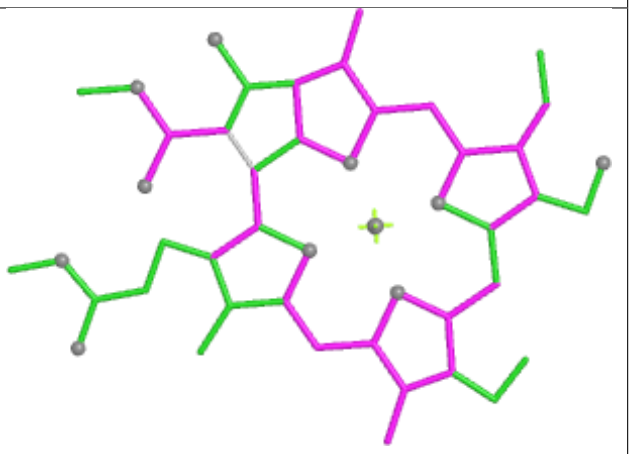
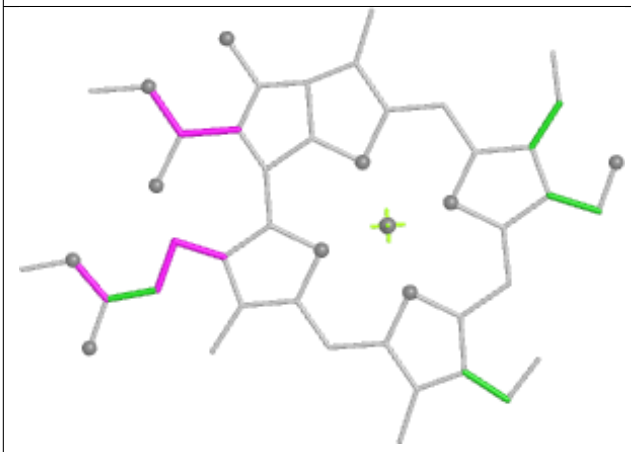
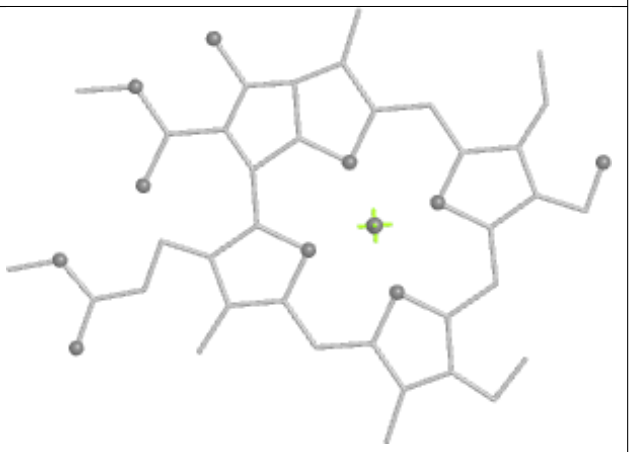
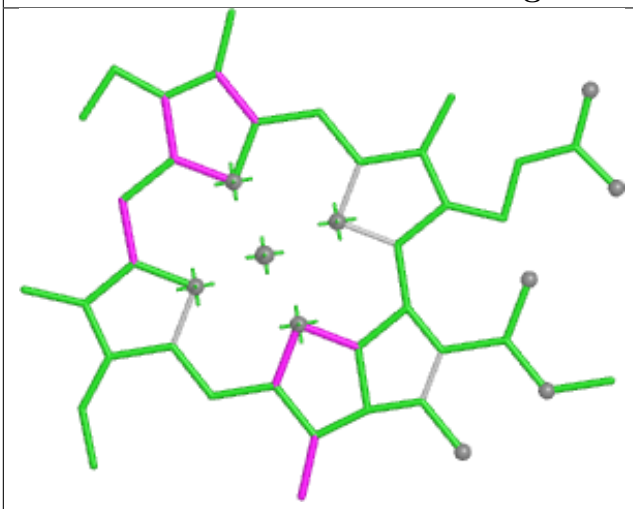
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 614



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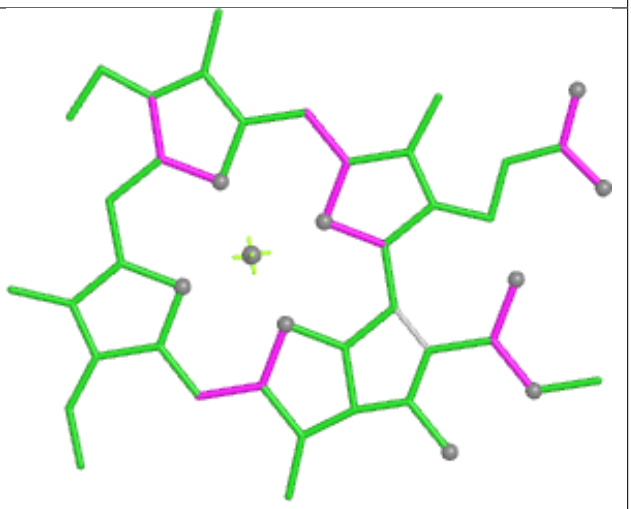

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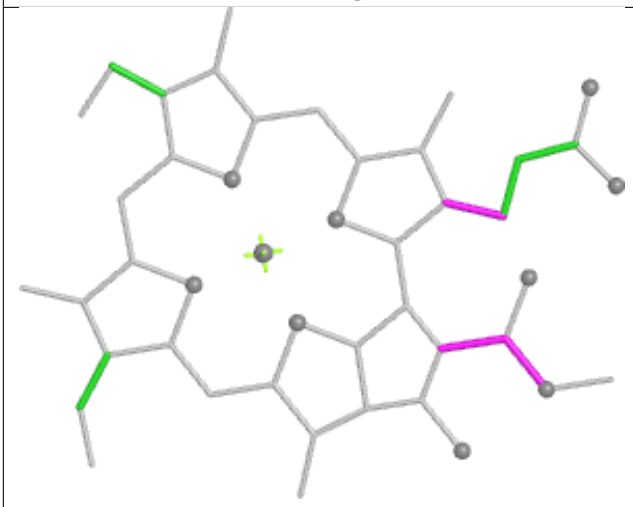
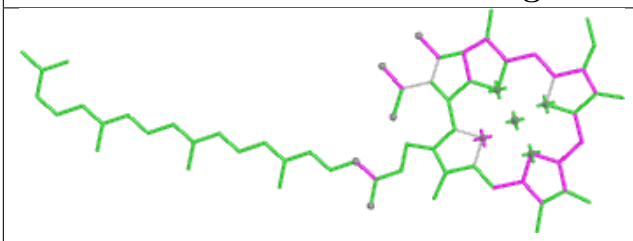


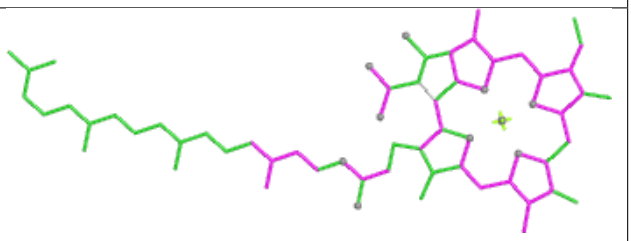
Torsions

Rings

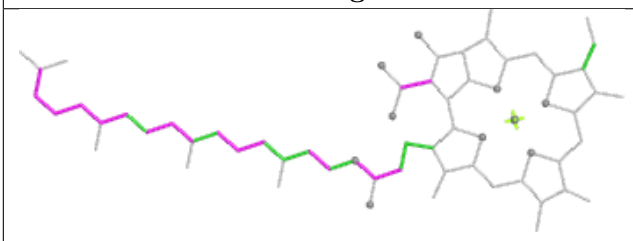
Ligand CHL U 601



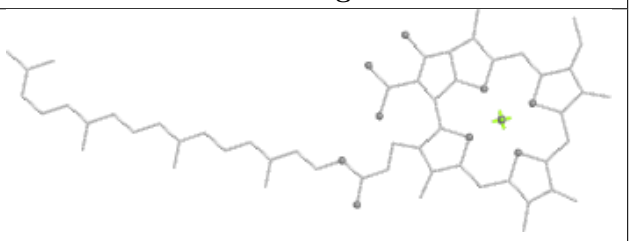
Bond lengths



Bond angles



Torsions



Rings

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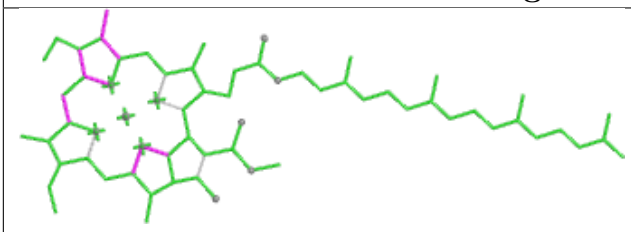
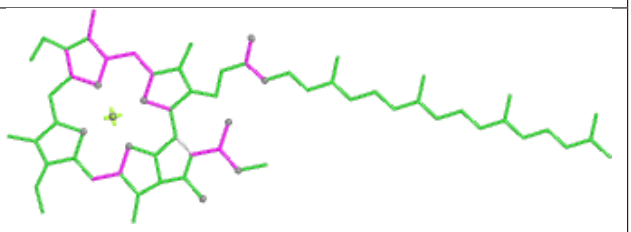
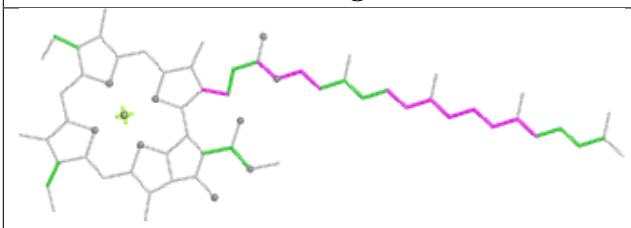
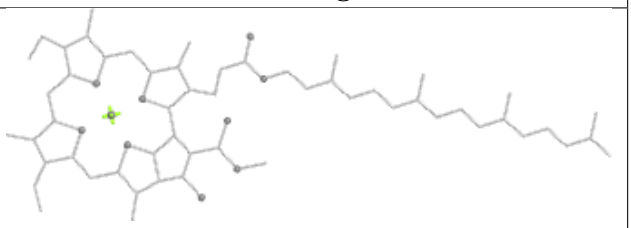
 Bond lengths	 Bond angles
 Torsions	 Rings

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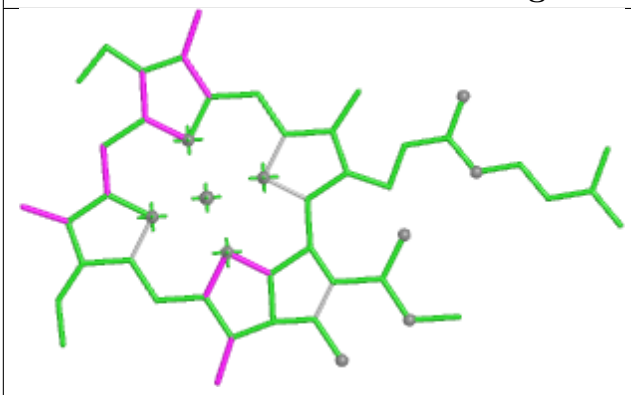
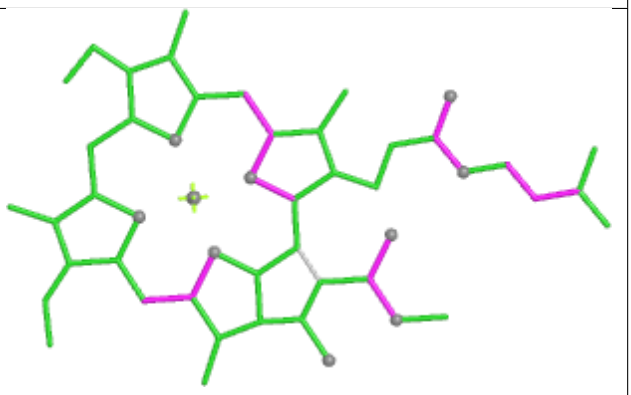
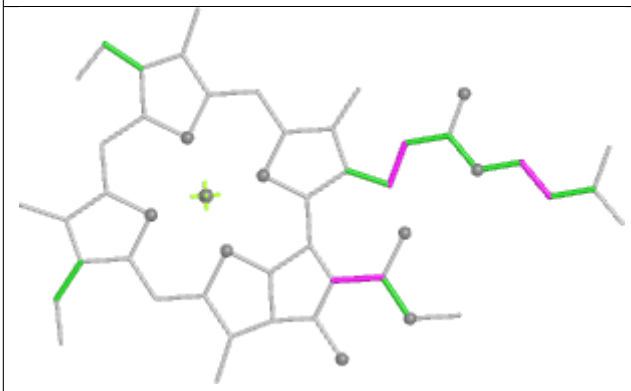
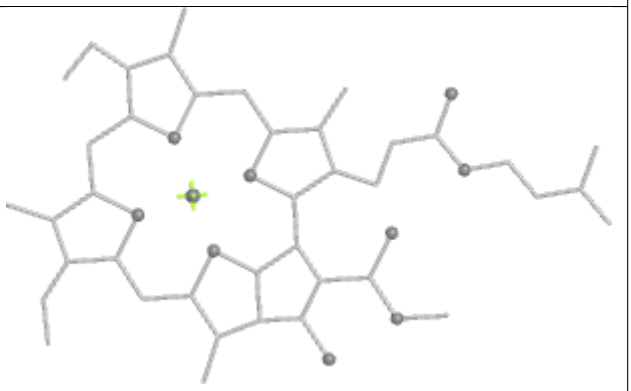
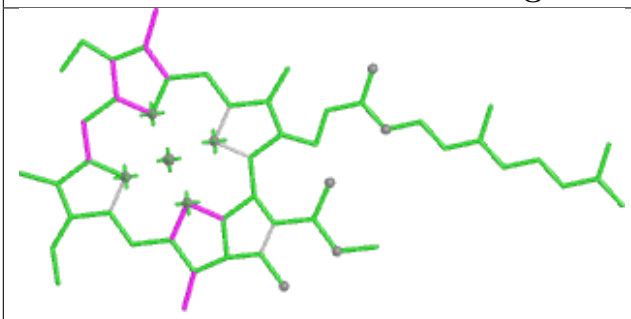
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 820



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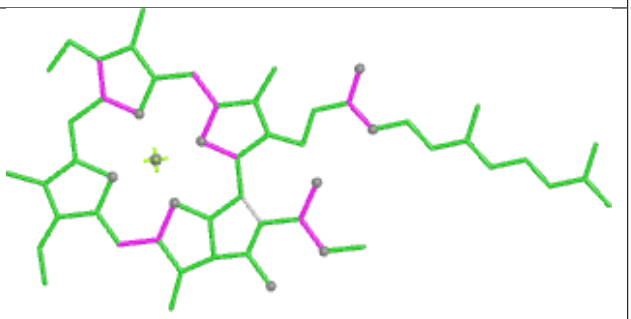
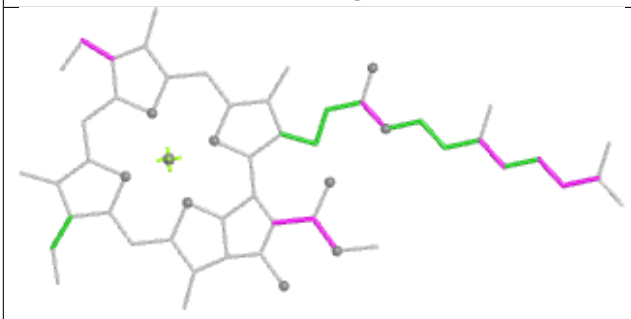


Bond angles



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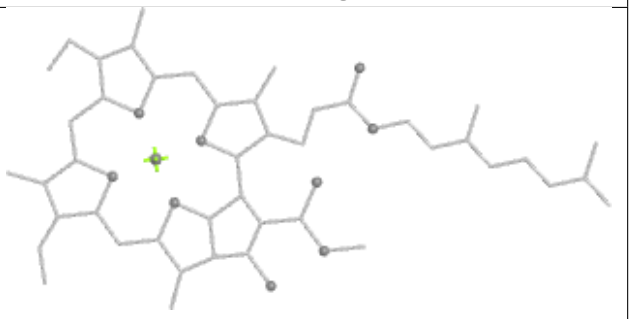
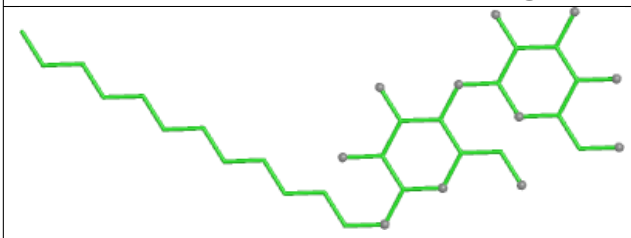


Rings

Ligand LMT A 857



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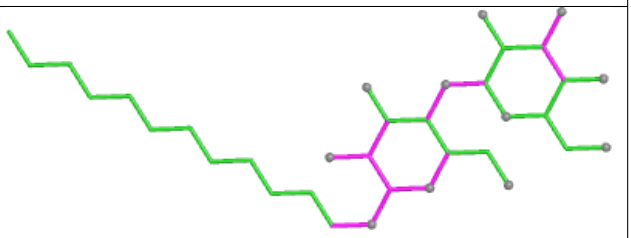
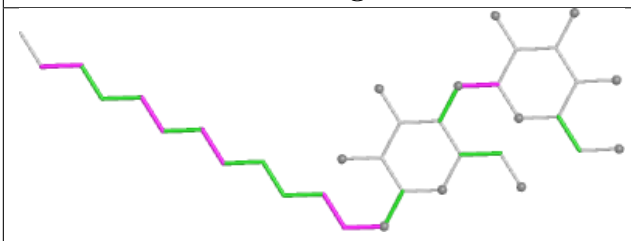


Bond angles



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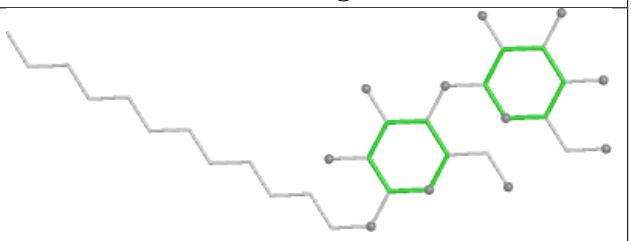
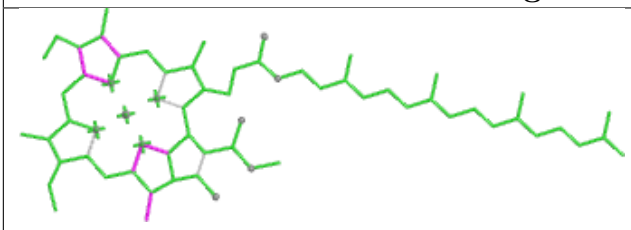
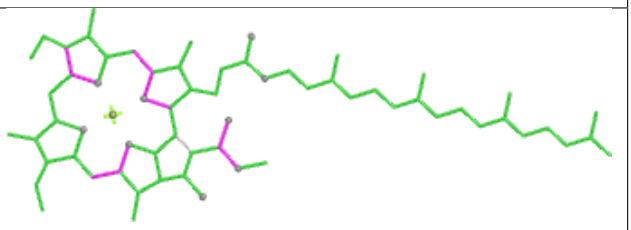
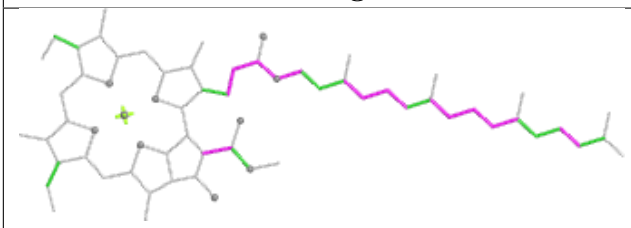
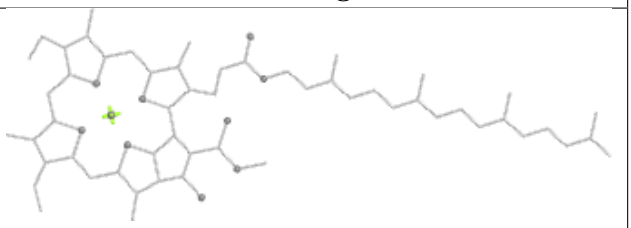


Rings

Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

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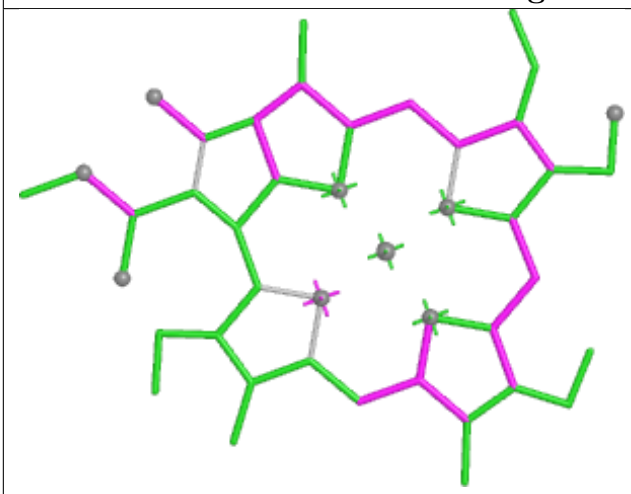
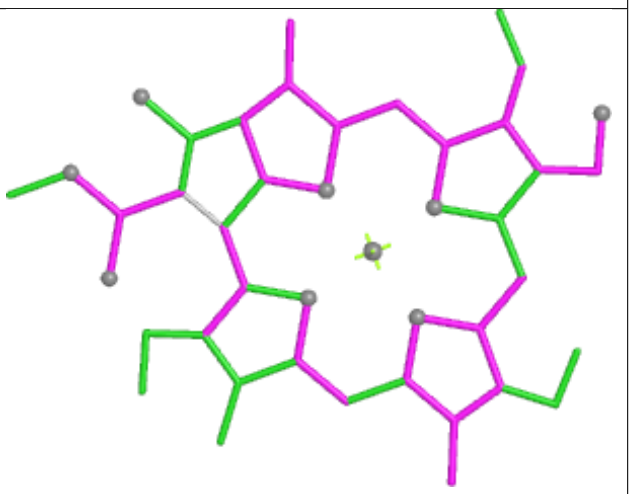
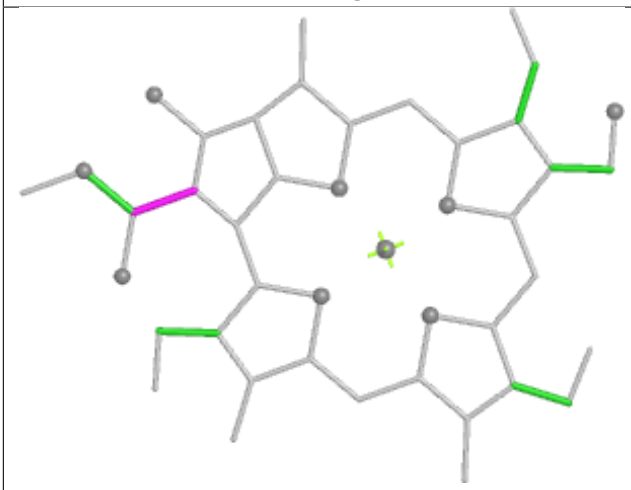
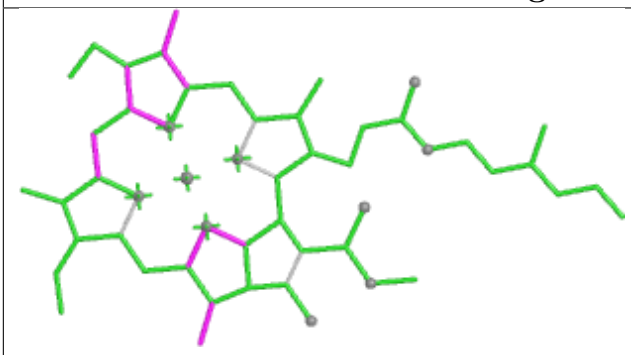
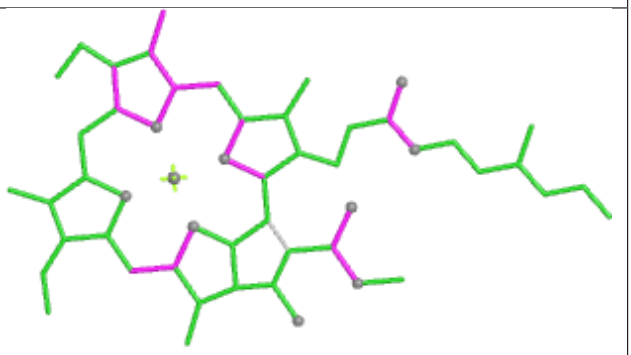
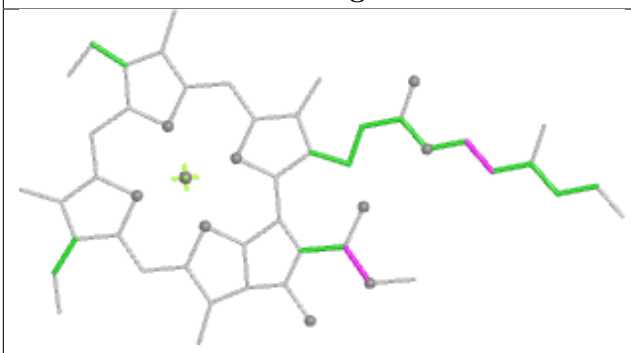
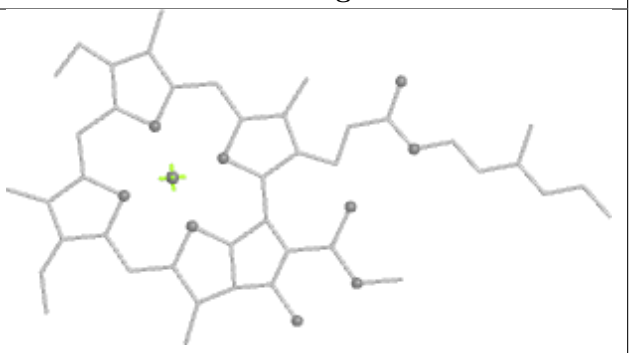
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 9 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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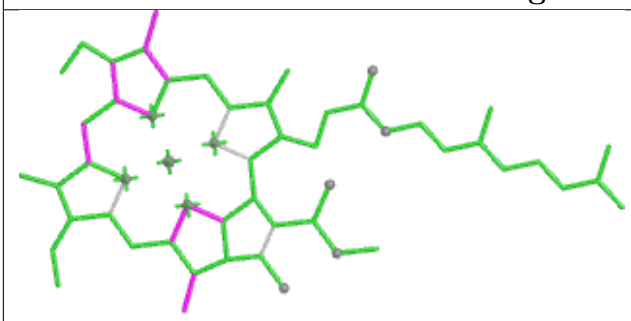
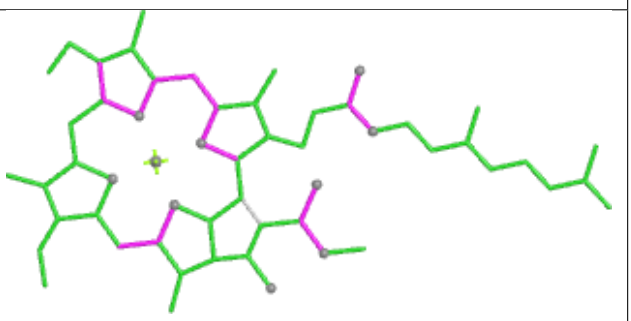
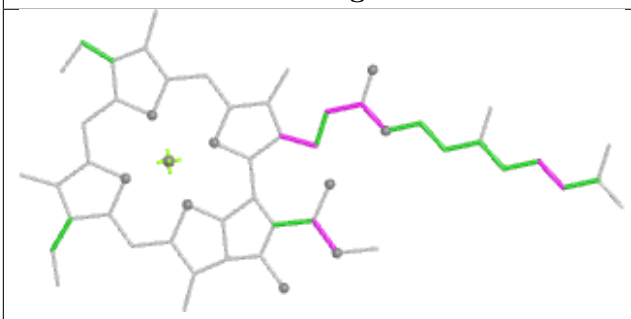
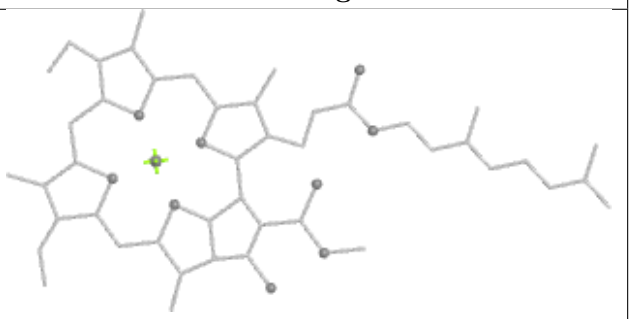
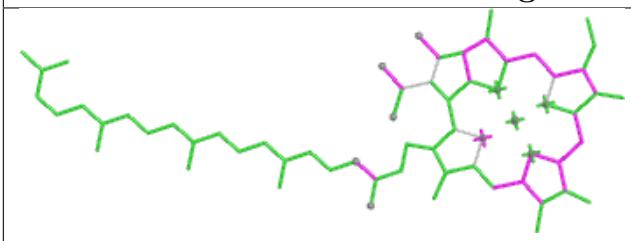
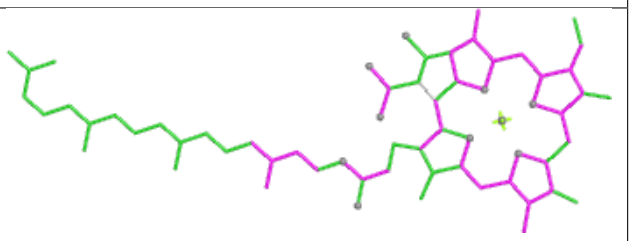
 Bond lengths	 Bond angles
 Torsions	 Rings

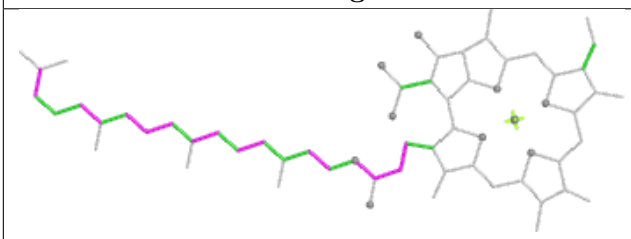
Ligand CHL W 601



Bond lengths



Bond angles



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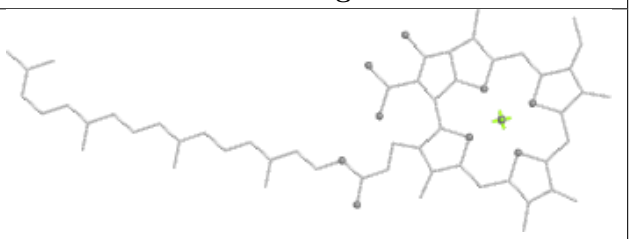
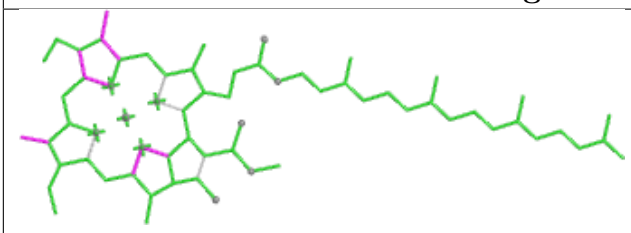


Rings

Ligand CLA U 612



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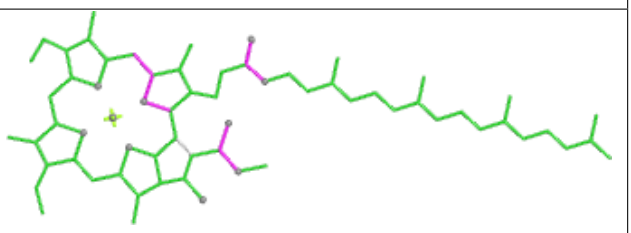

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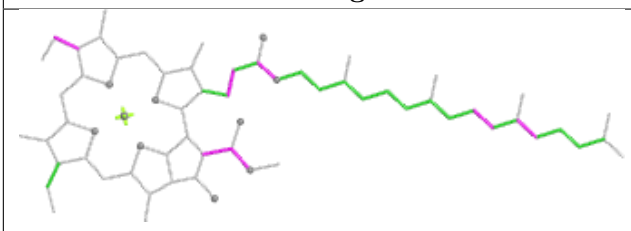

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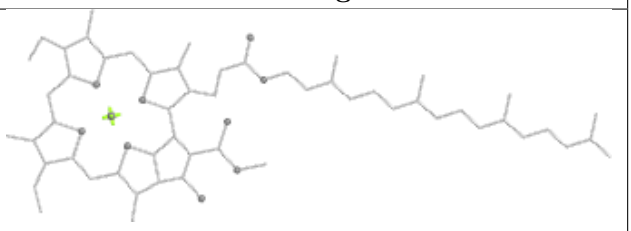
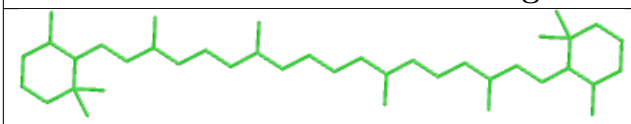


Rings

Ligand BCR A 848



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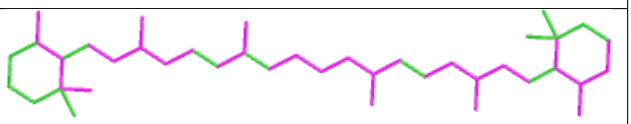

Bond angles

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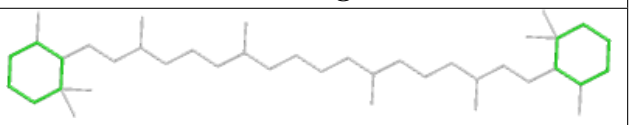
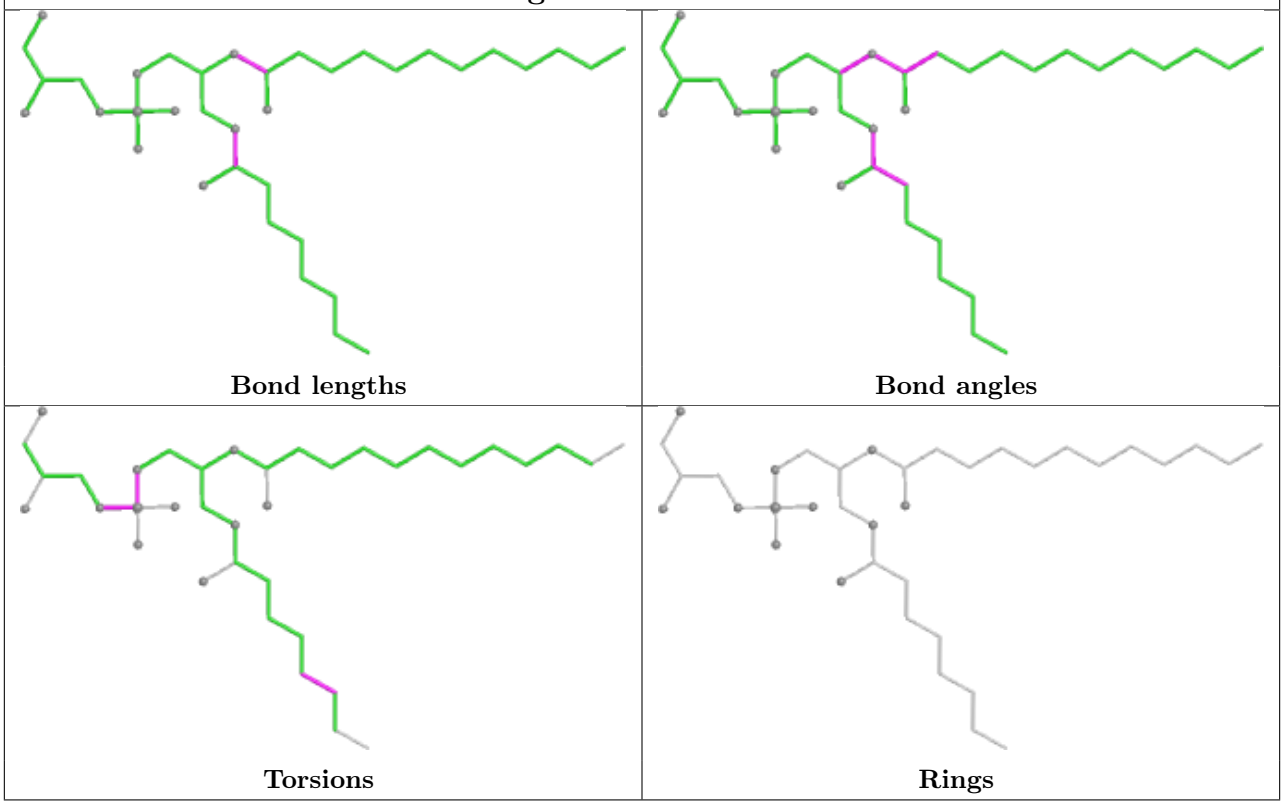
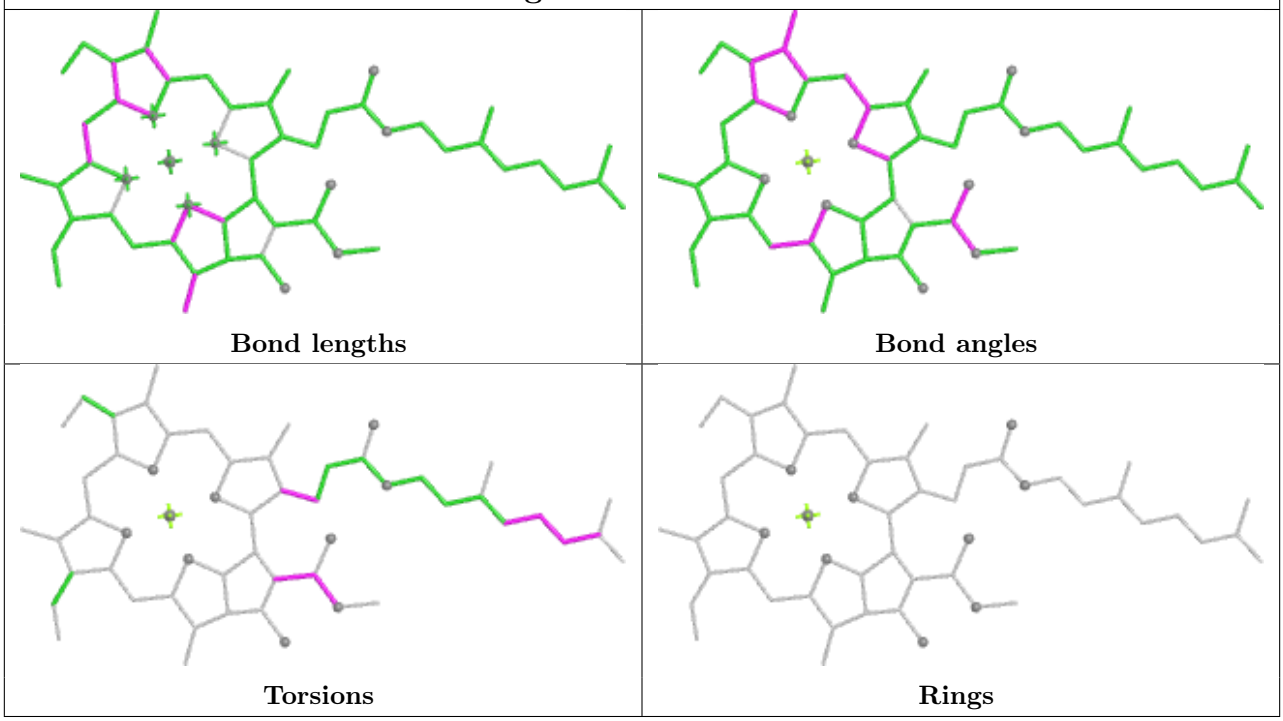


Rings

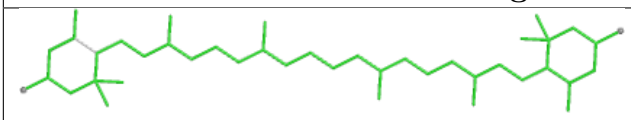
Ligand LHG 5 630



Ligand CLA A 838



Ligand LUT W 2620



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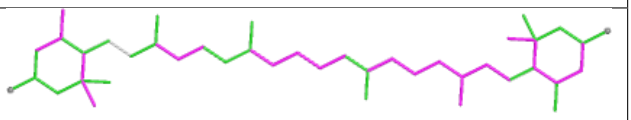
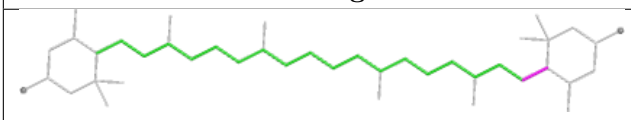


Bond angles



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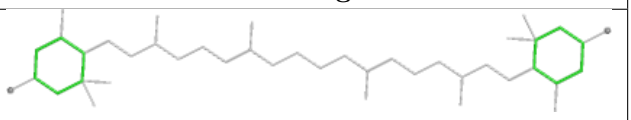
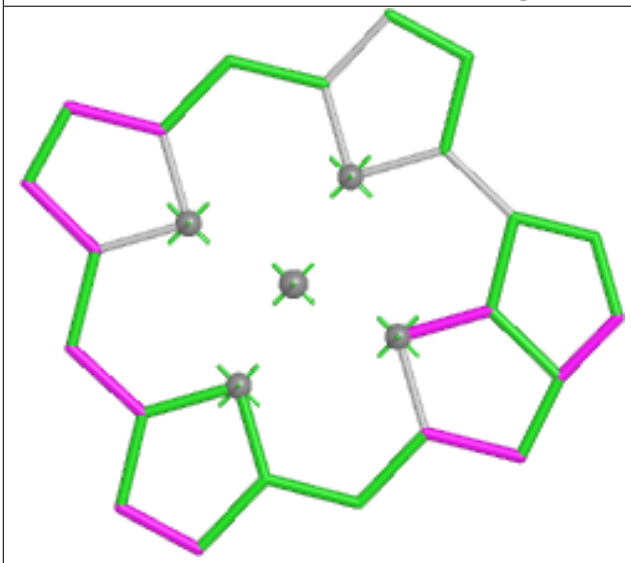


Rings

Ligand CLA O 2003



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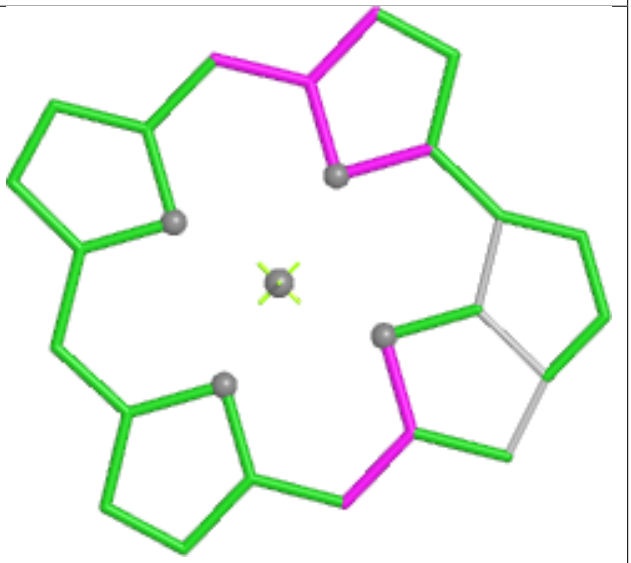
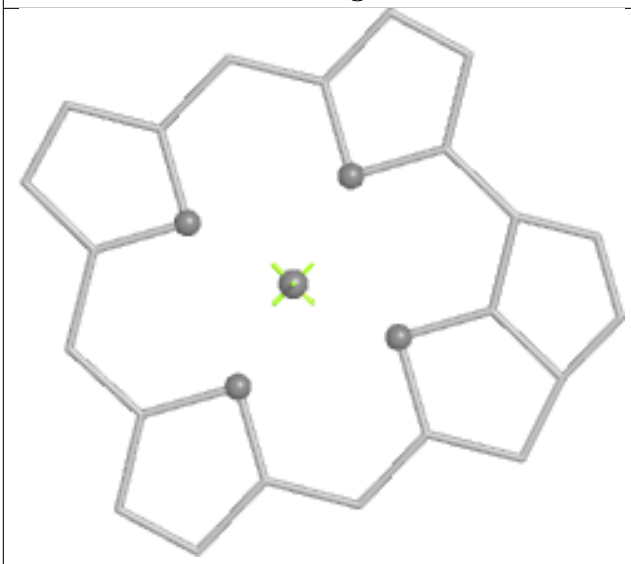


Bond angles



Torsions

Rings

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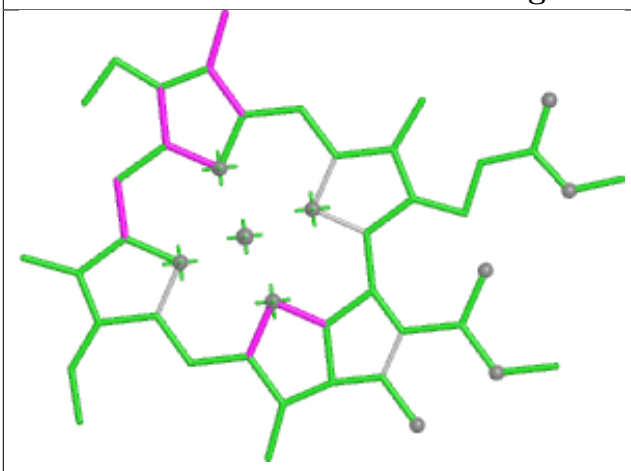

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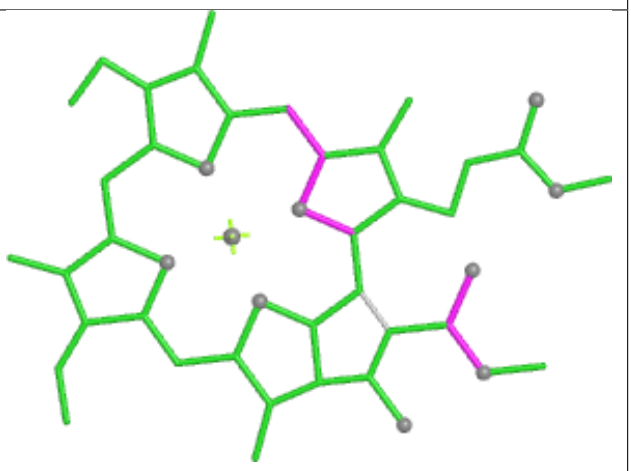
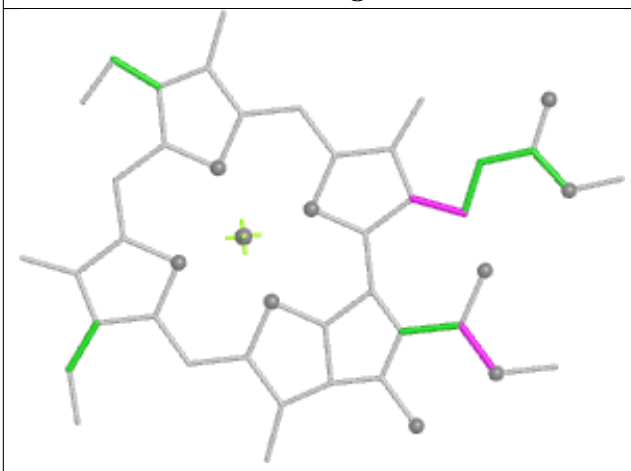
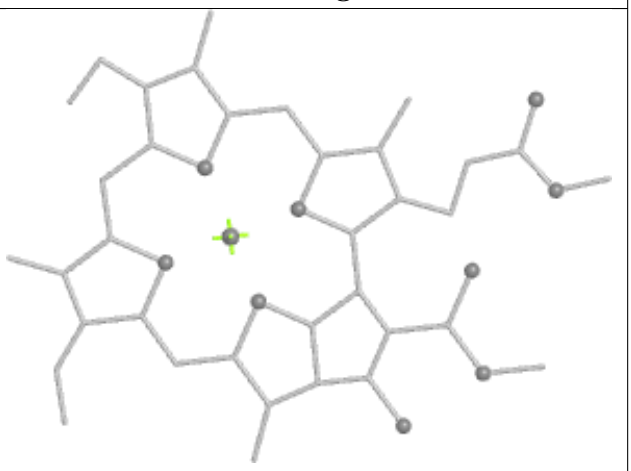


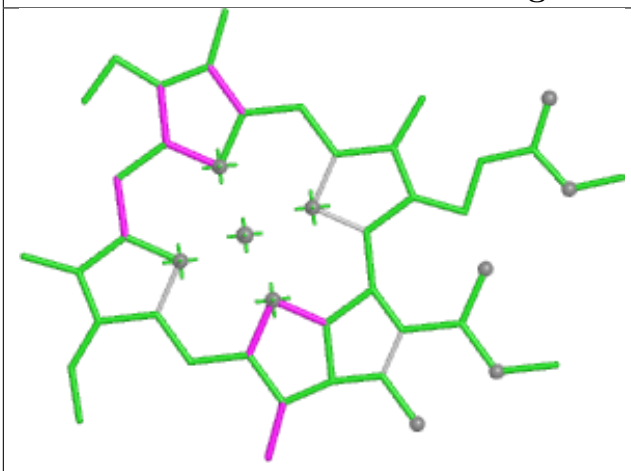
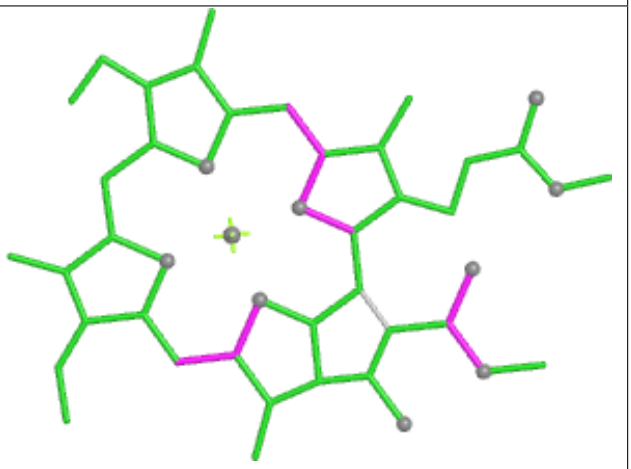
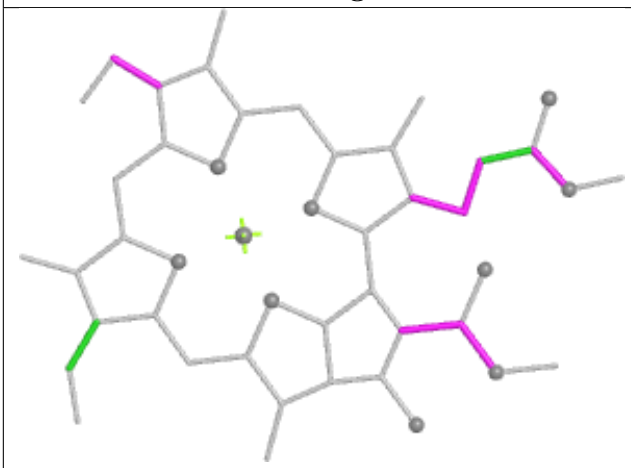
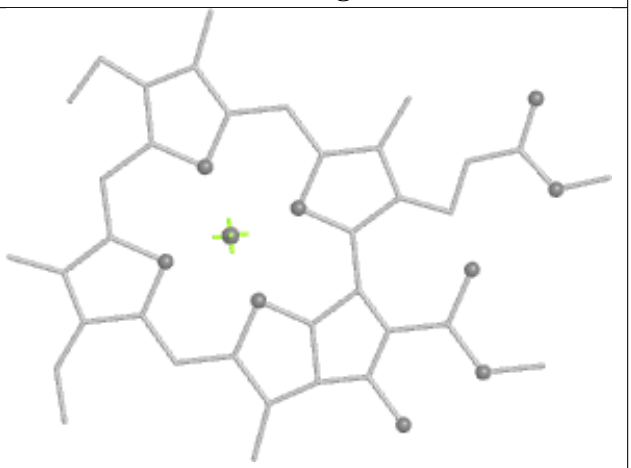
Bond angles



Torsions



Rings

Ligand CLA 3 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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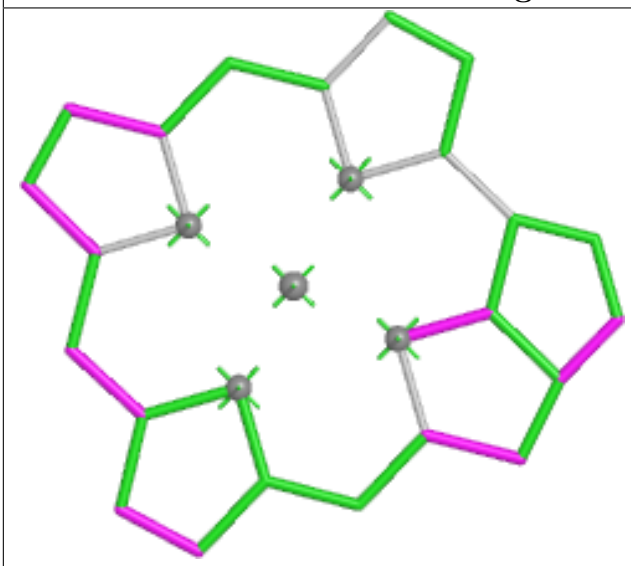

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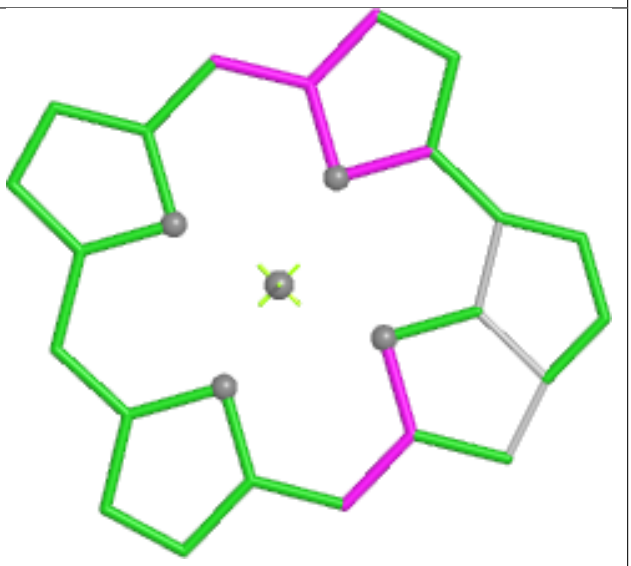

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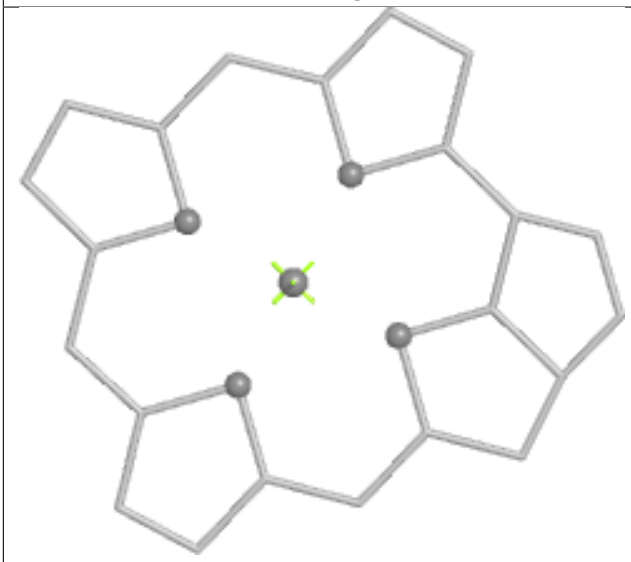

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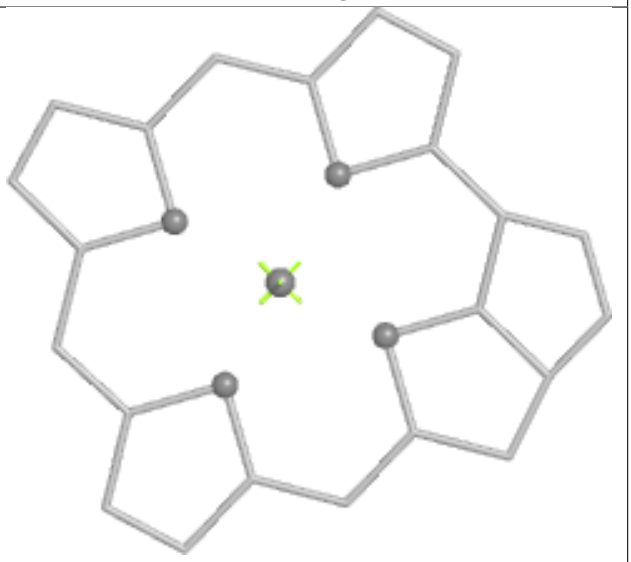

Rings

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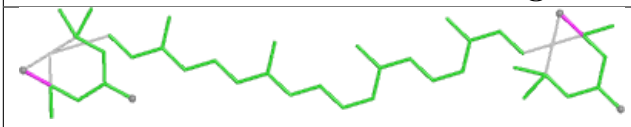

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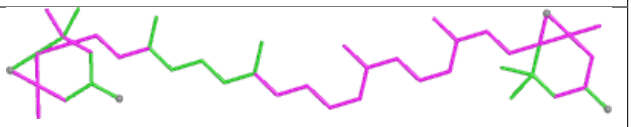

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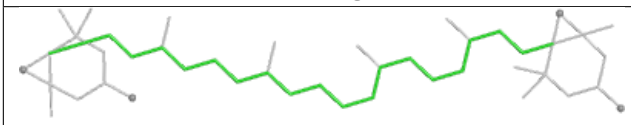

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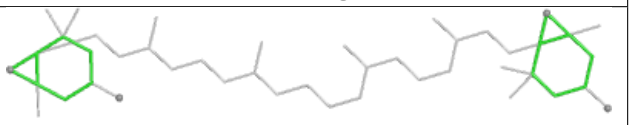

Rings

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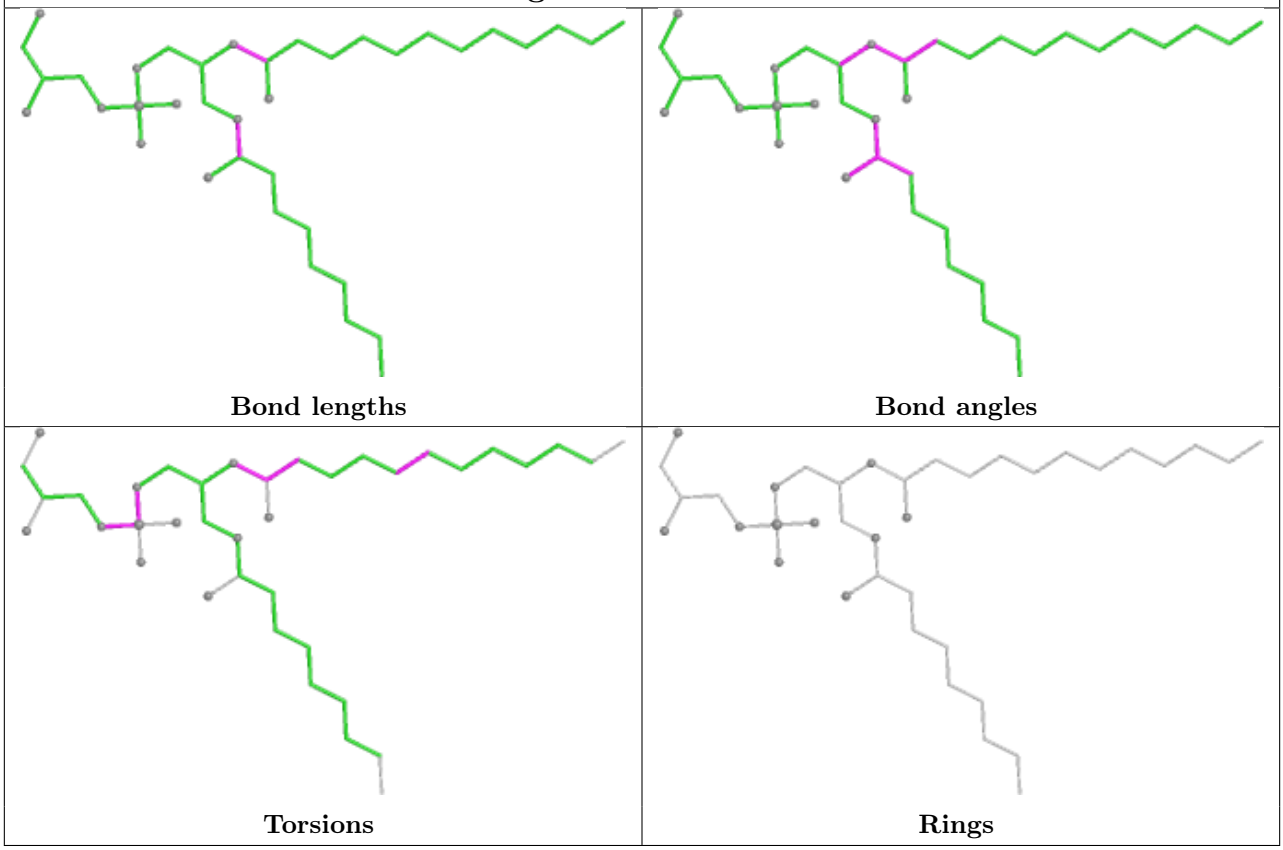

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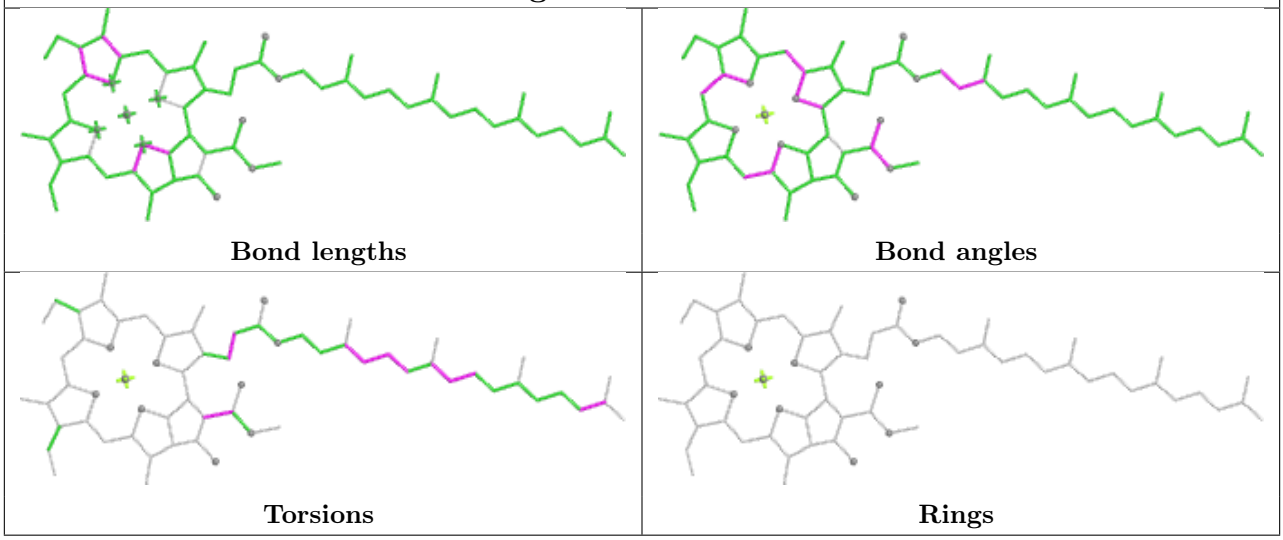

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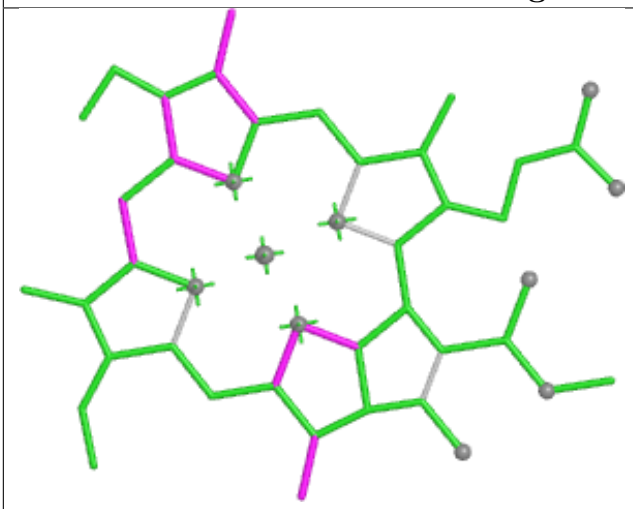

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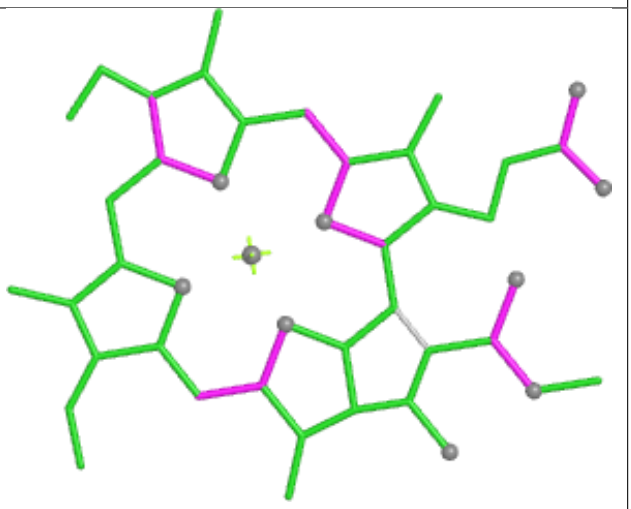

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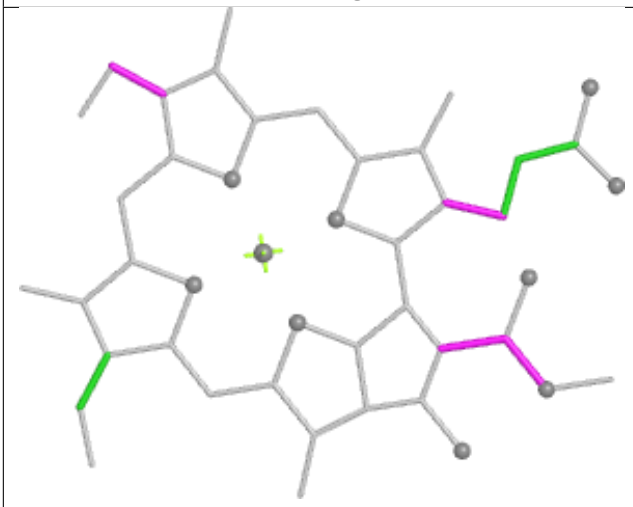

Torsions

Rings

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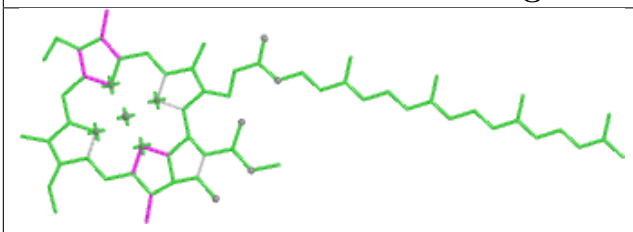

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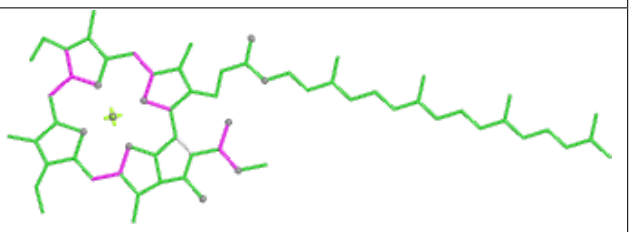

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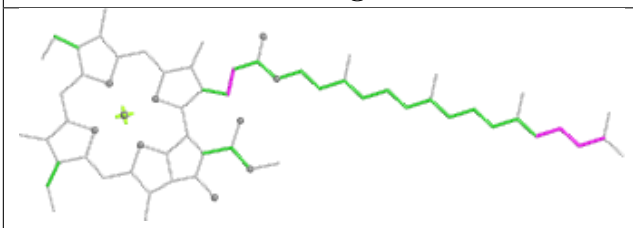

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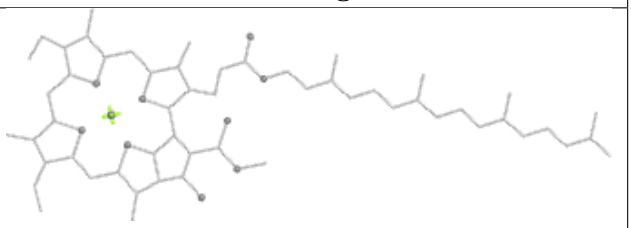

Rings

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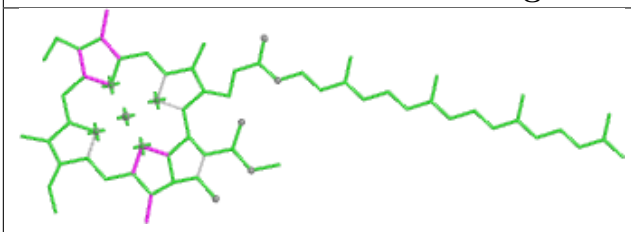

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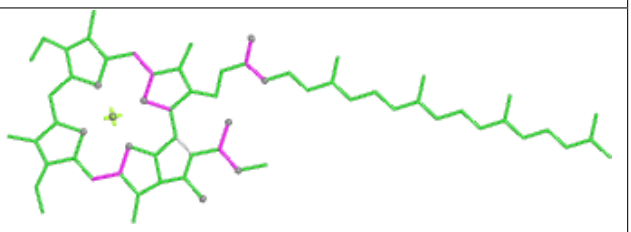

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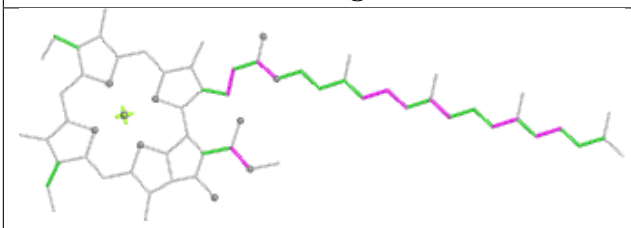

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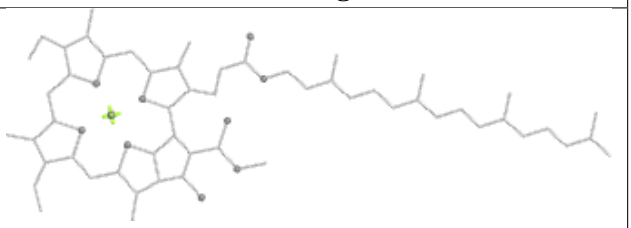

Rings

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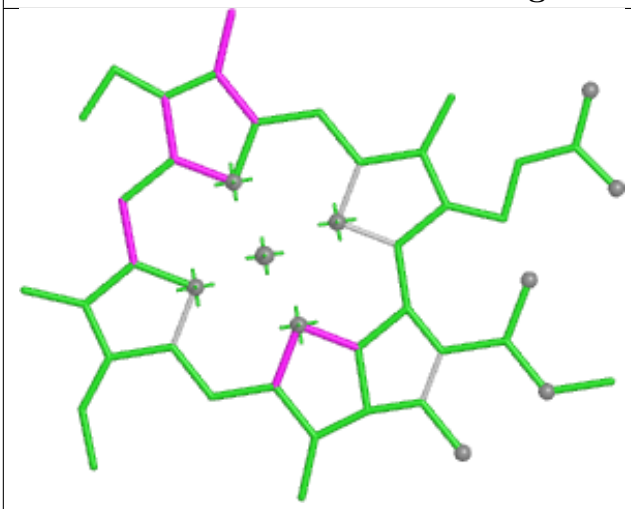

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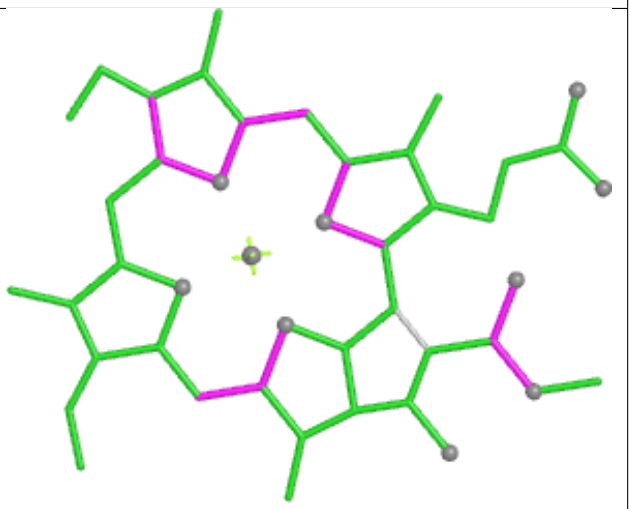

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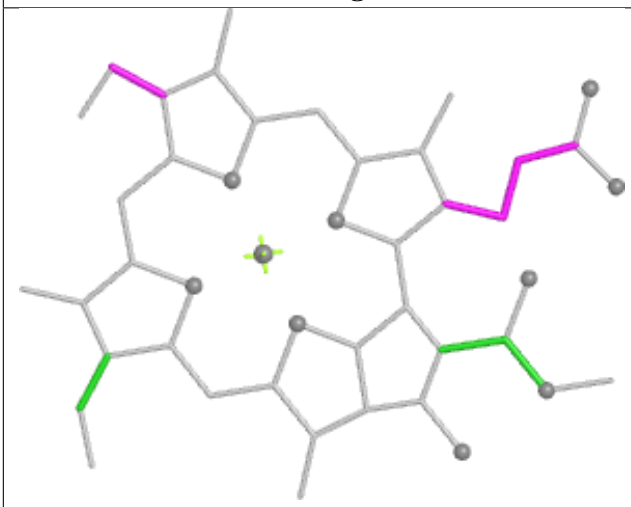

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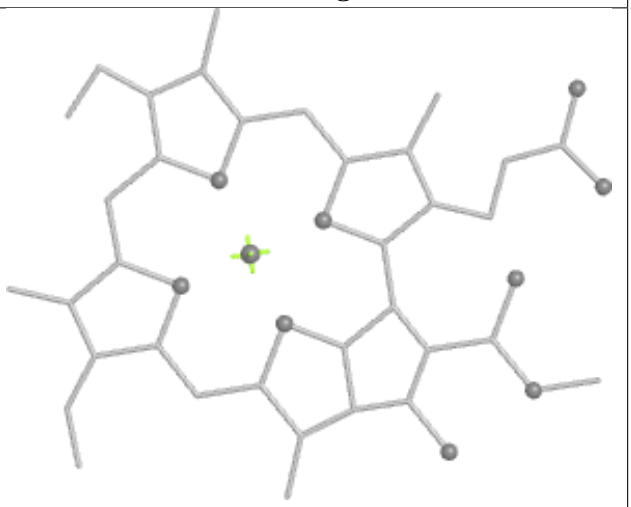
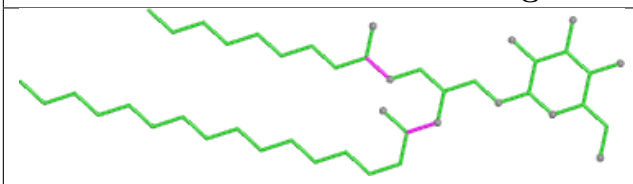


Rings

Ligand LMG L 307



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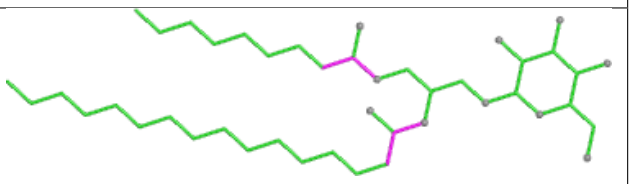

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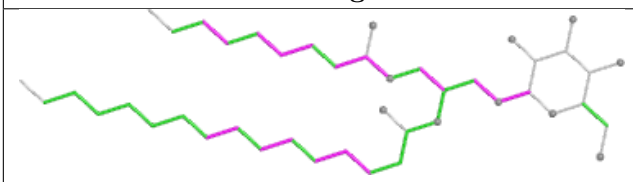

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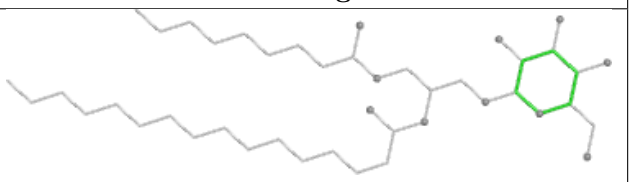
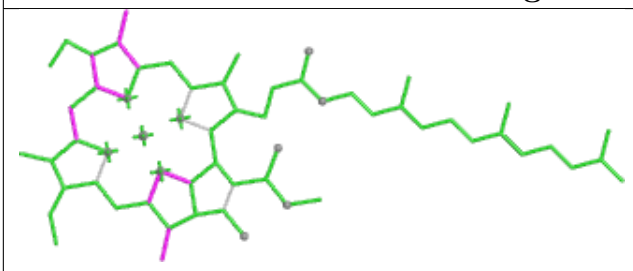


Rings

Ligand CLA A 854



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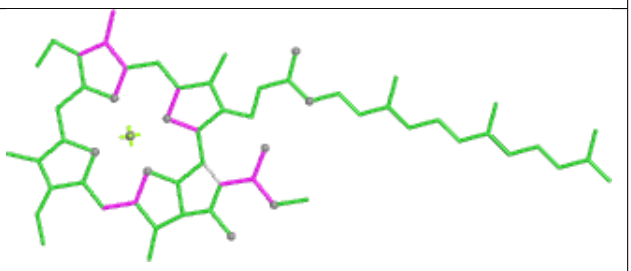

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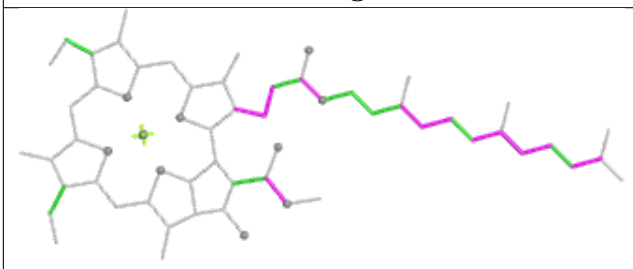

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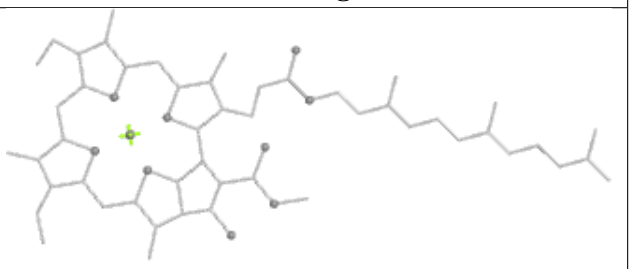

Rings

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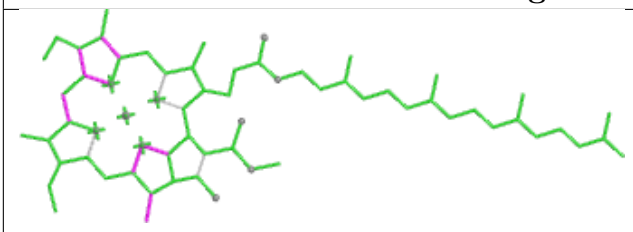

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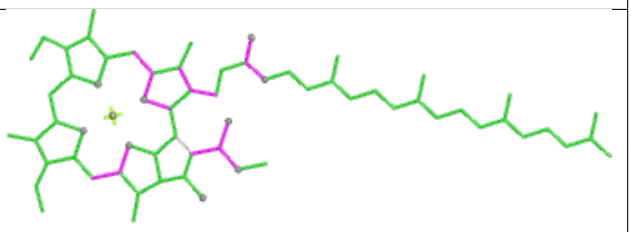

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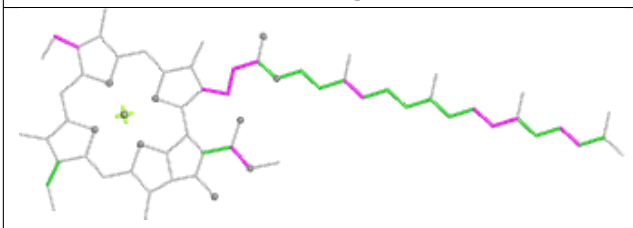

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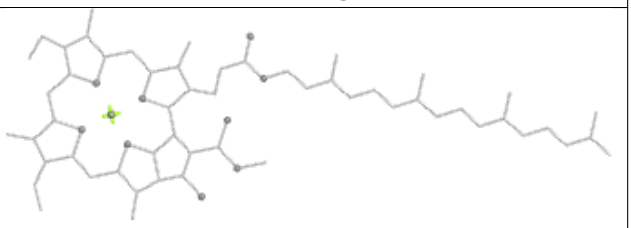
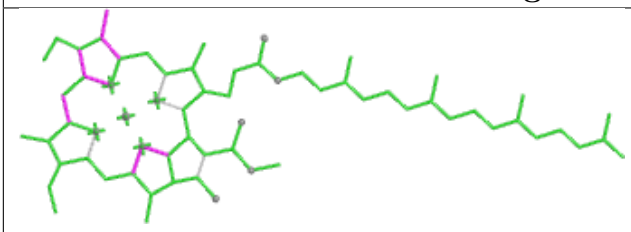


Rings

Ligand CLA A 817



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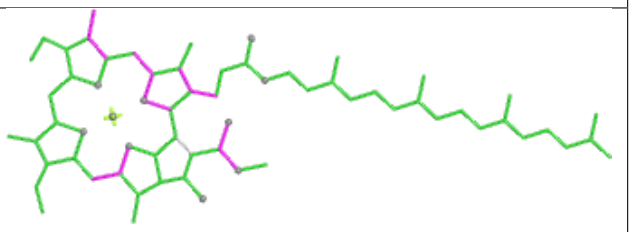

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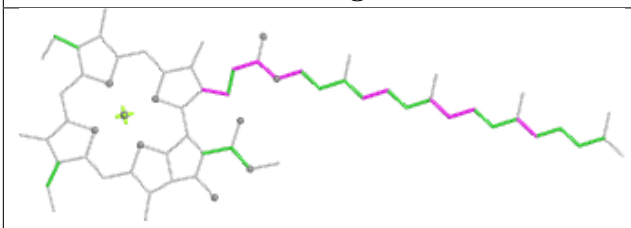

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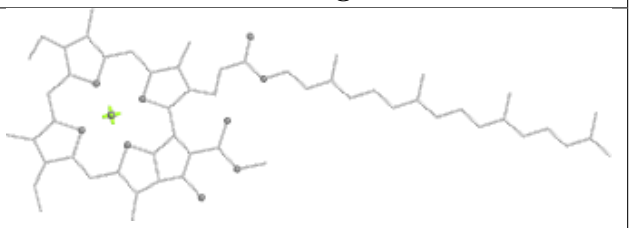
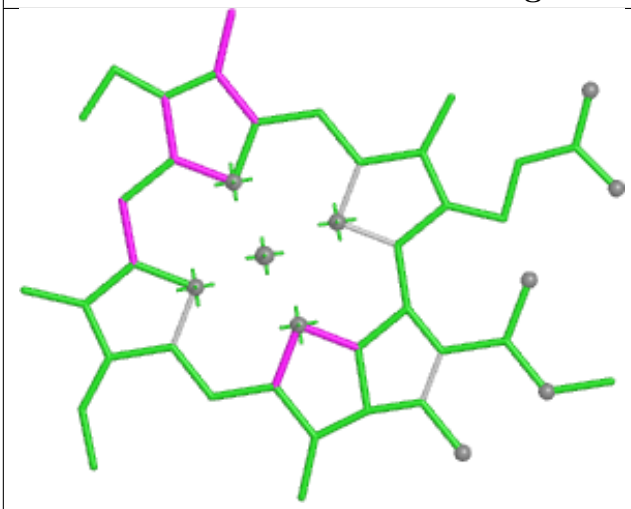


Rings

Ligand CLA B 830



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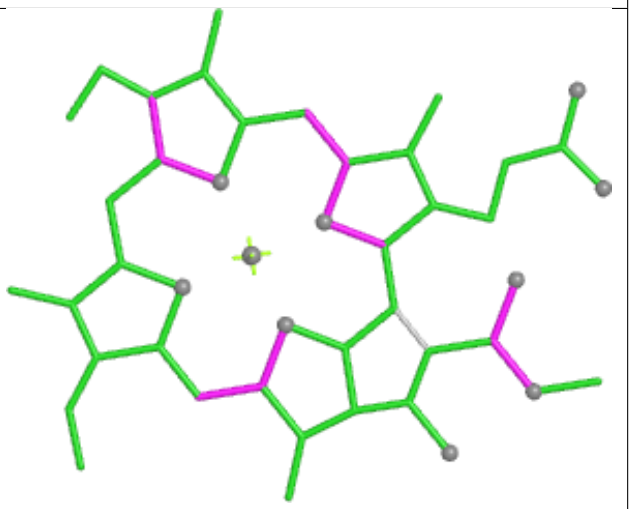

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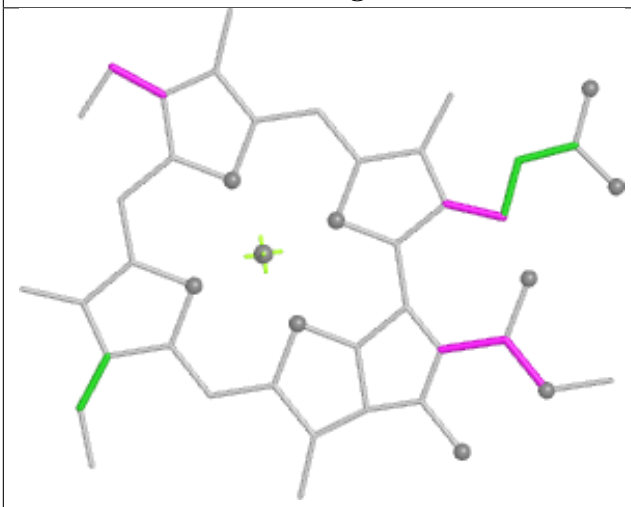

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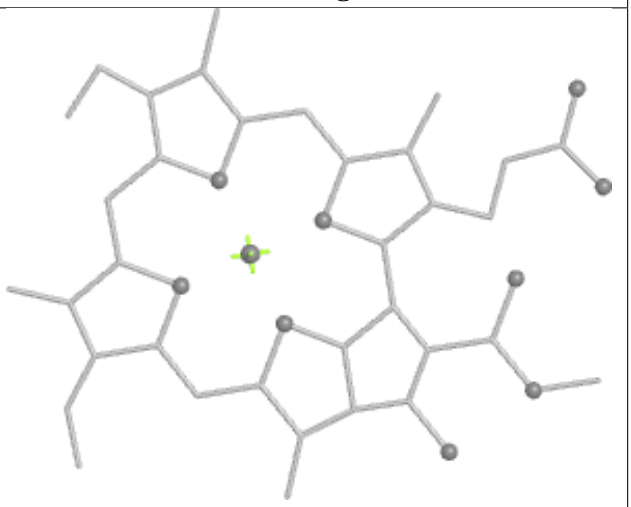
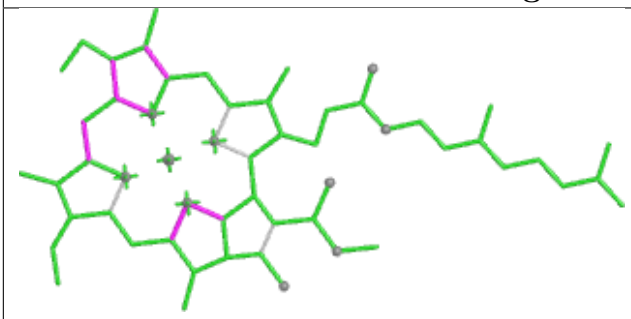


Rings

Ligand CLA K 203



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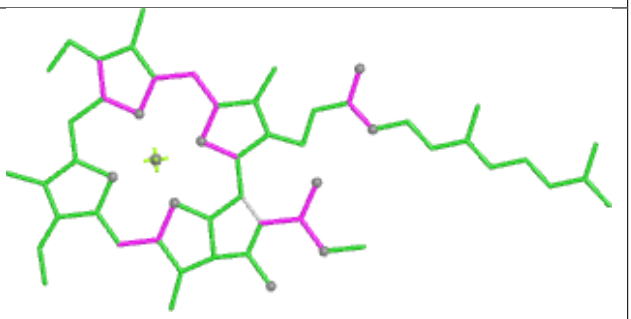
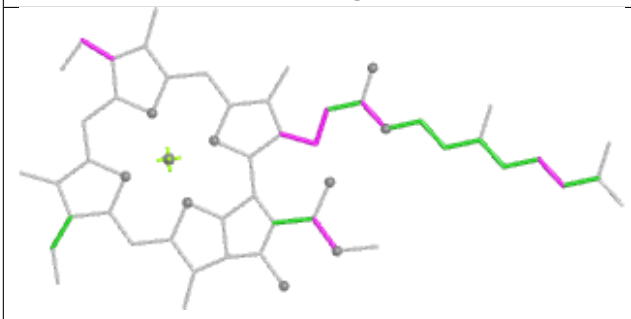


Bond angles



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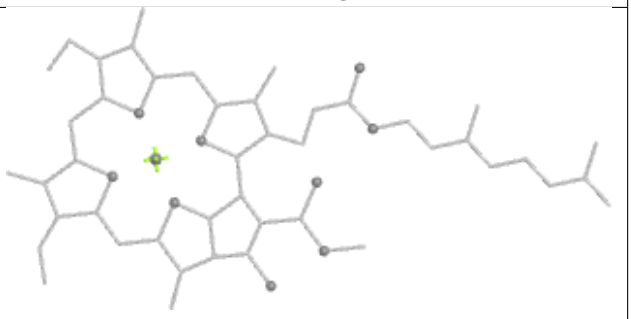
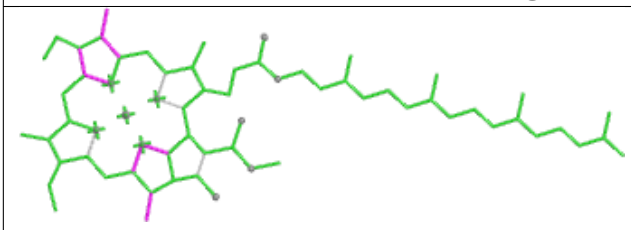


Rings

Ligand CLA A 835



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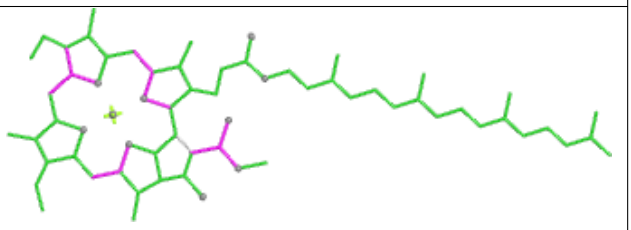
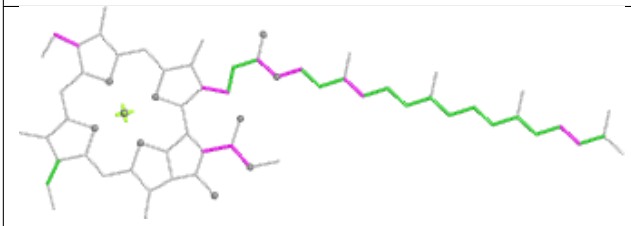
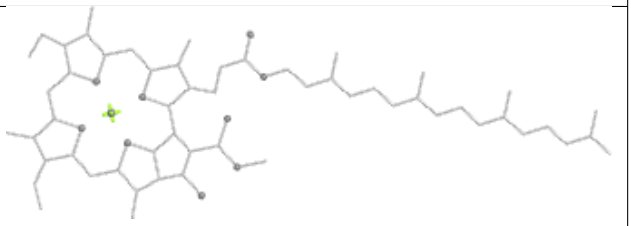


Bond angles

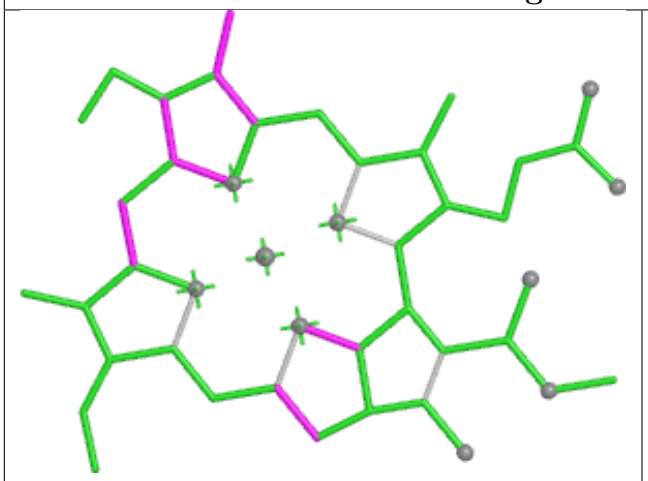


Torsions

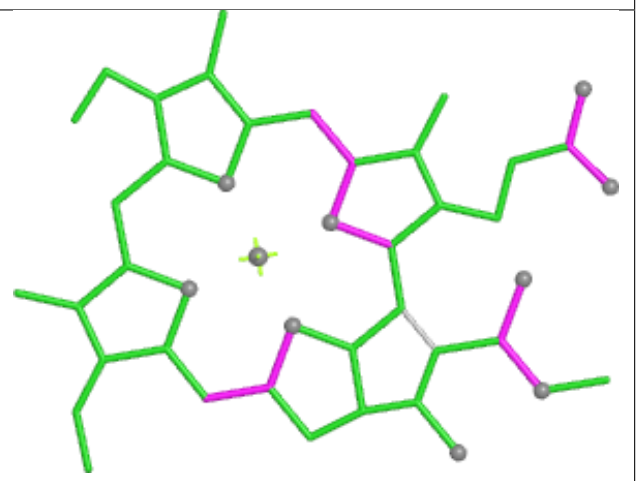


Rings

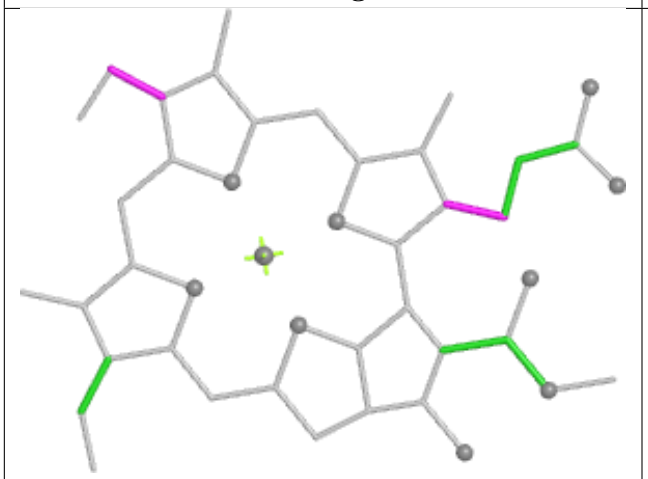
Ligand CLA B 812



Bond lengths



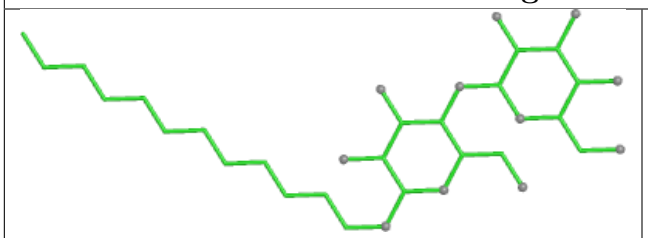
Bond angles



Torsions

Rings

Ligand LMT K 208



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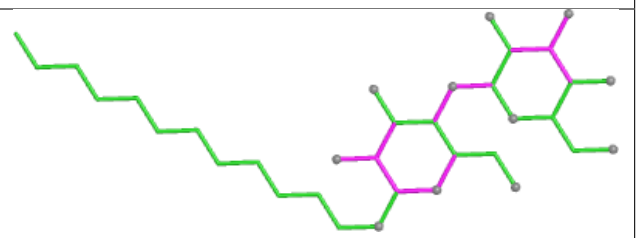
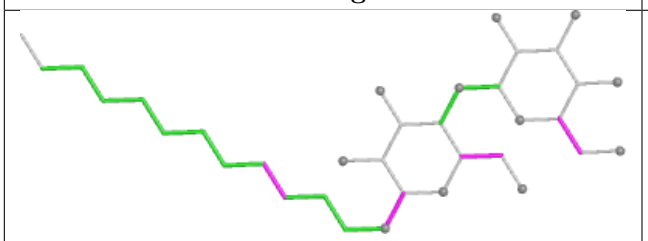


Bond angles



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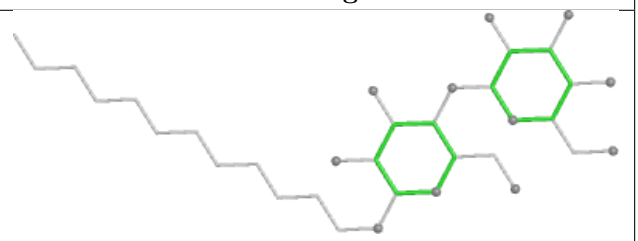
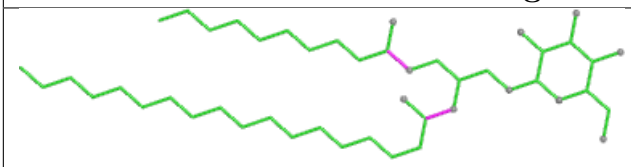
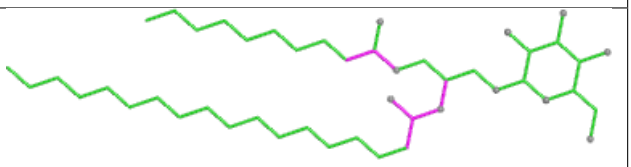
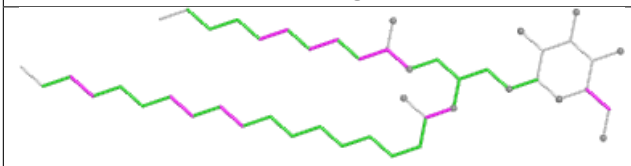
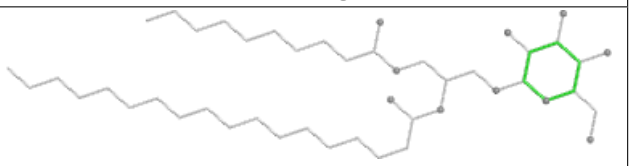


Rings

Ligand LMG 2 631	
 Bond lengths	 Bond angles
 Torsions	 Rings

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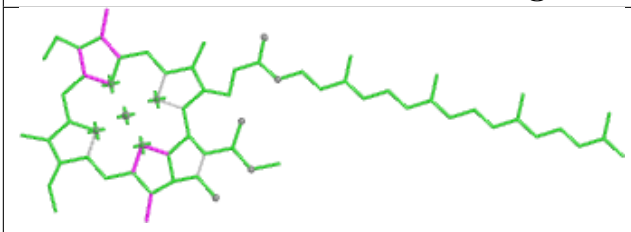
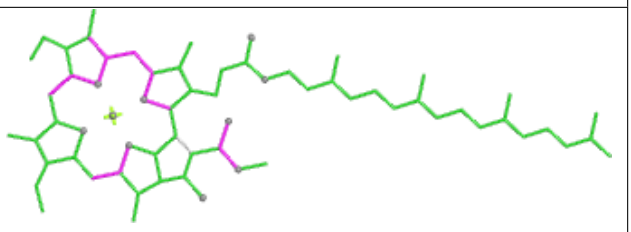
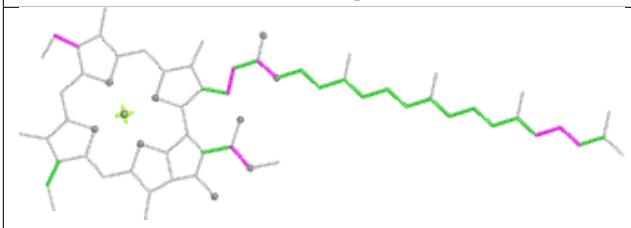
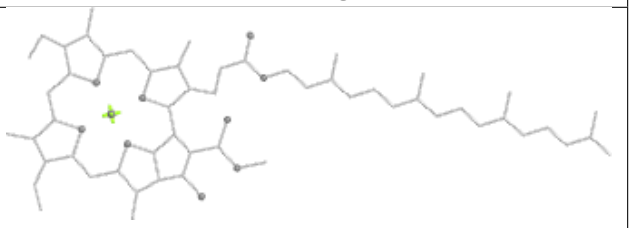
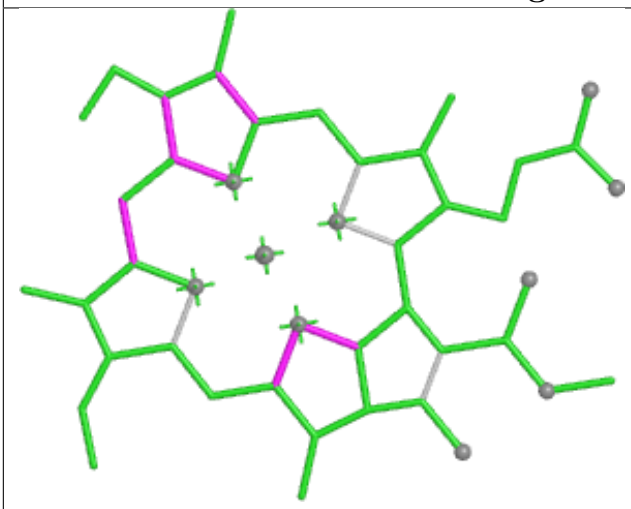
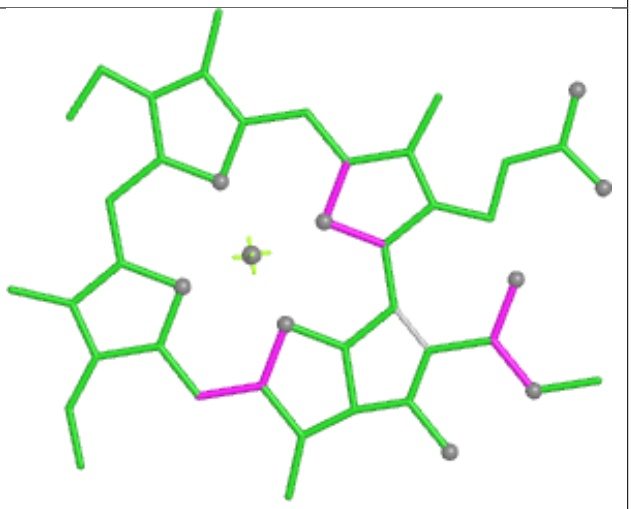
 Bond lengths	 Bond angles
 Torsions	 Rings

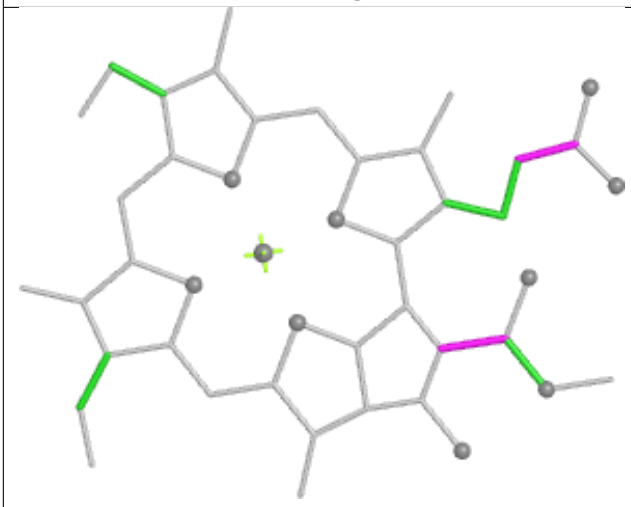
Ligand CLA 7 607



Bond lengths



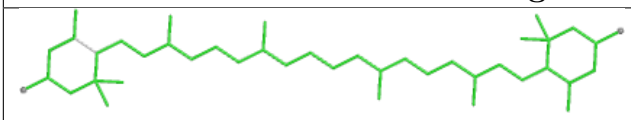
Bond angles



Torsions

Rings

Ligand LUT 9 620



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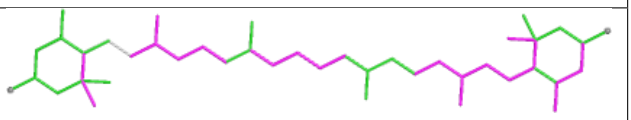
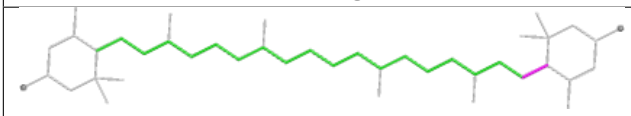


Bond angles



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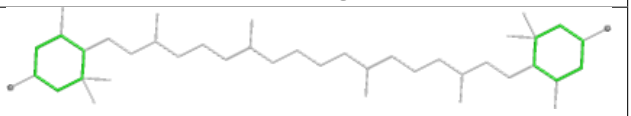
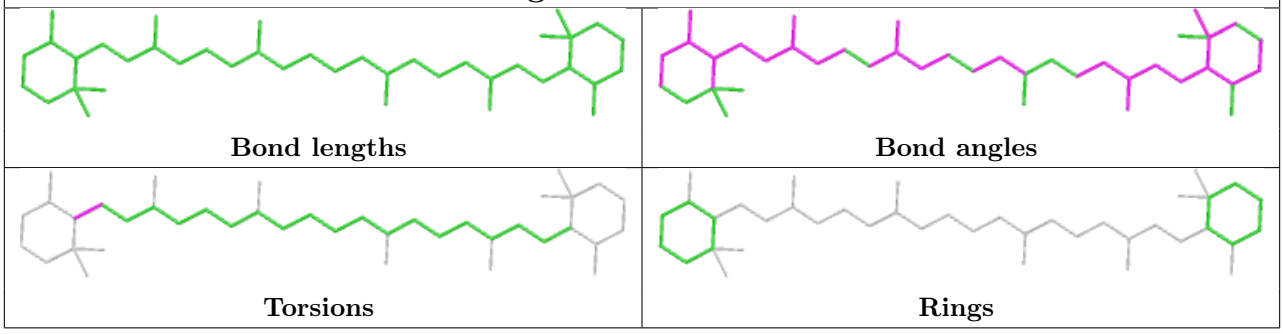
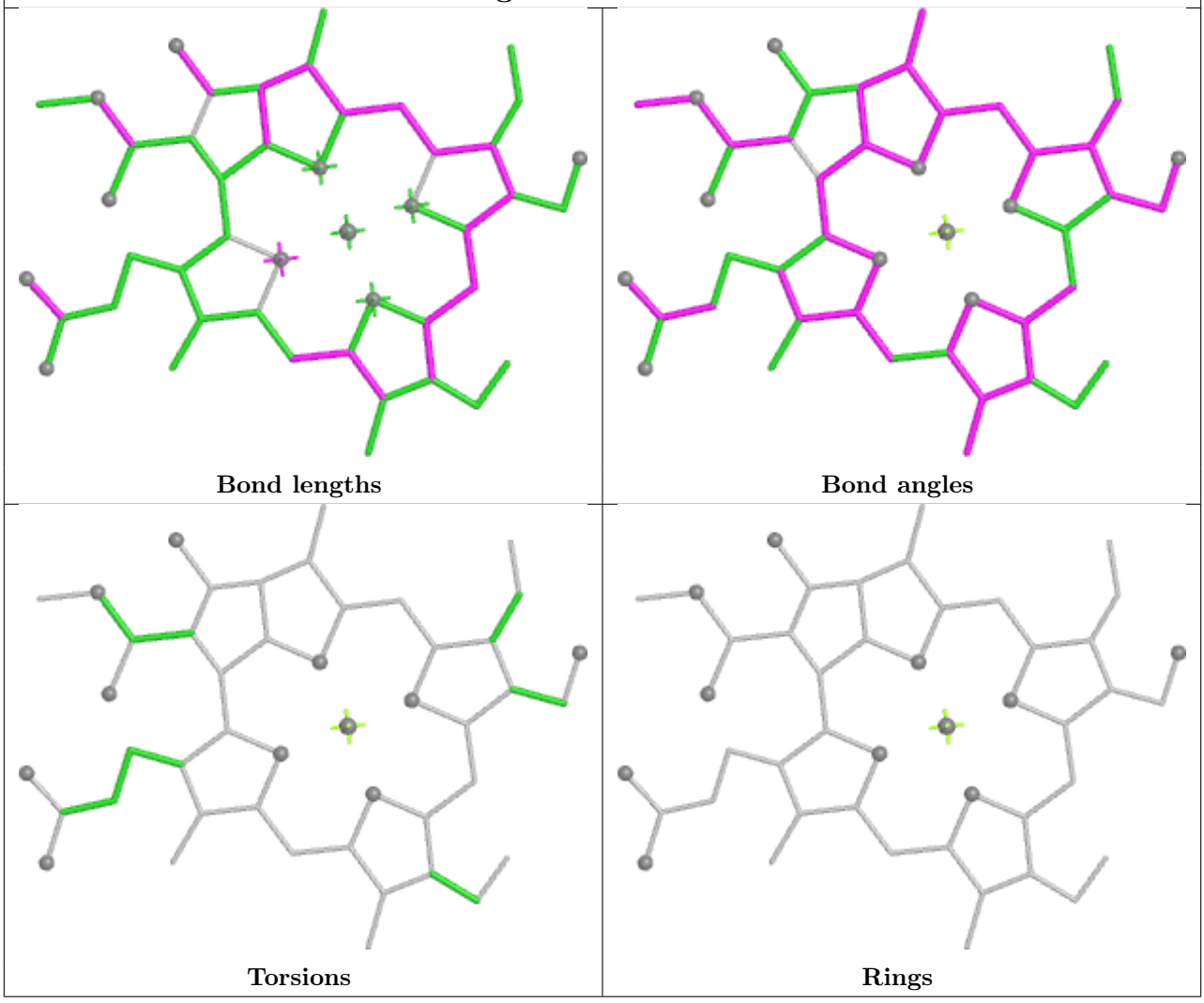


Rings

Ligand BCR 7 620



Ligand CHL 2 608



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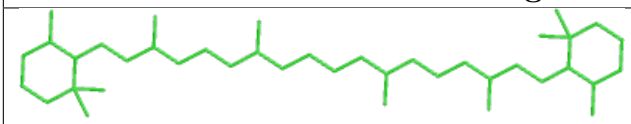

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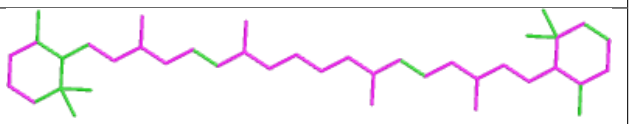
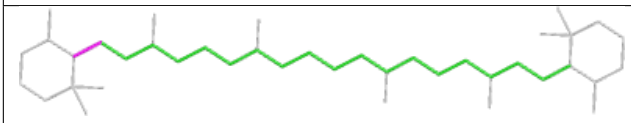


Bond angles



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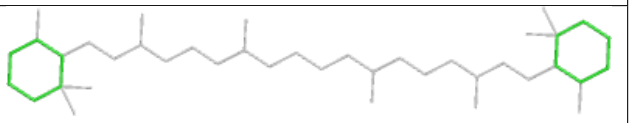
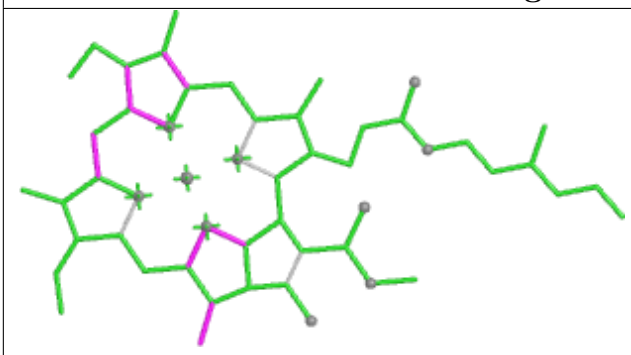


Rings

Ligand CLA B 836



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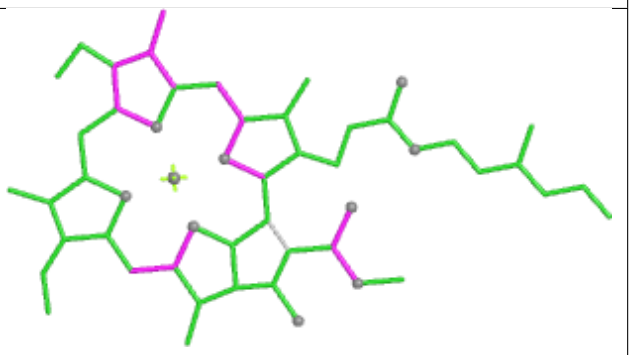
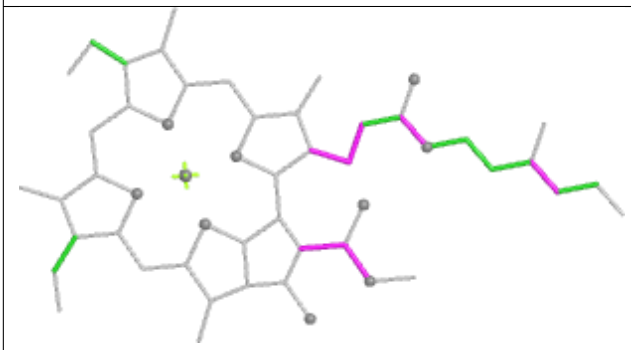


Bond angles



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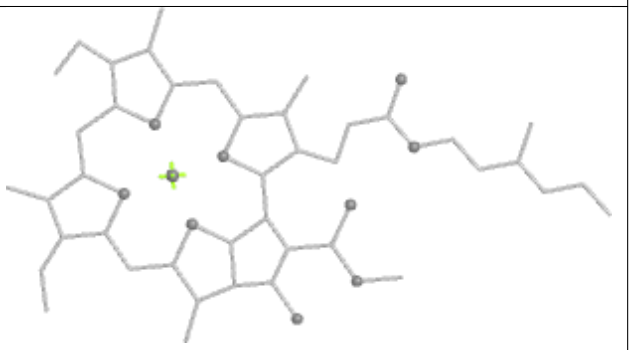
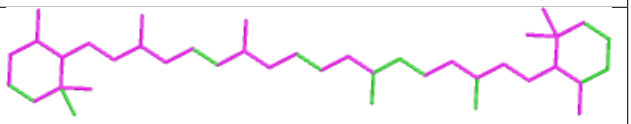


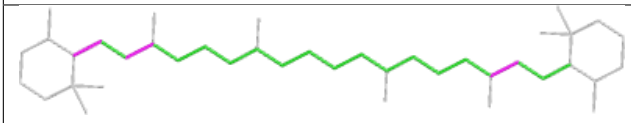
Rings

Ligand BCR B 1609

Bond lengths



Bond angles



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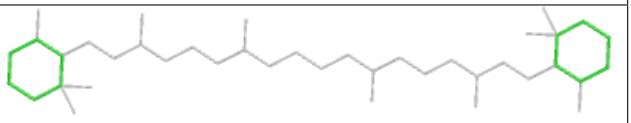
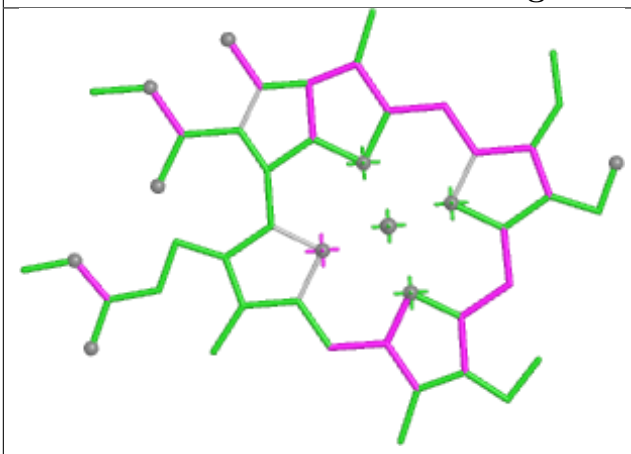


Rings

Ligand CHL 2 607



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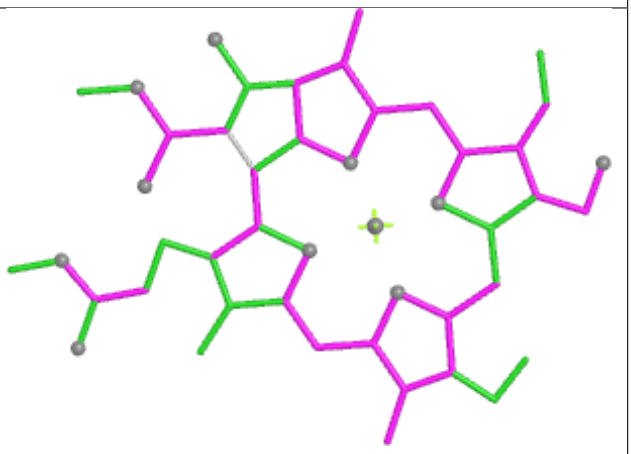
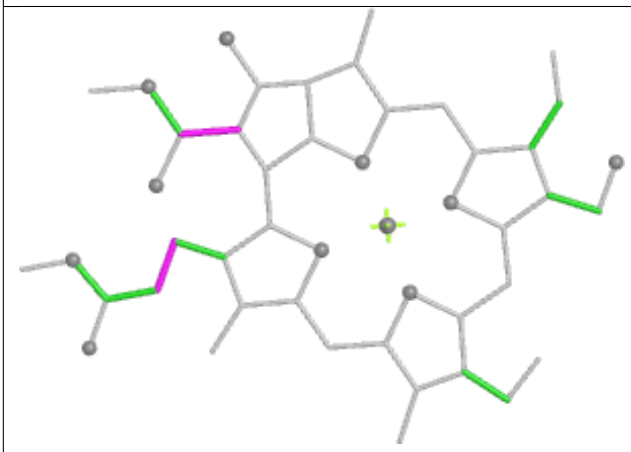
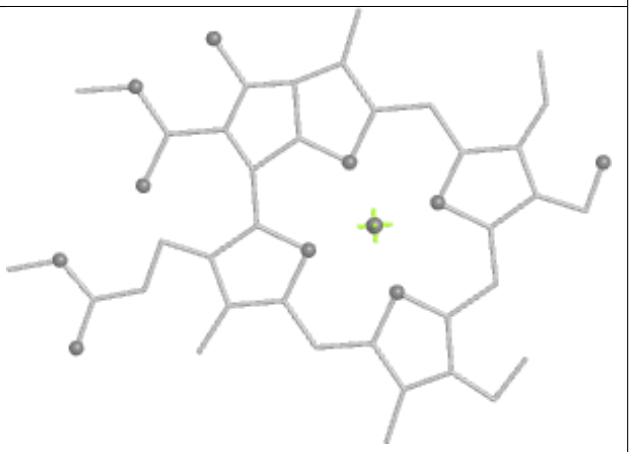


Bond angles

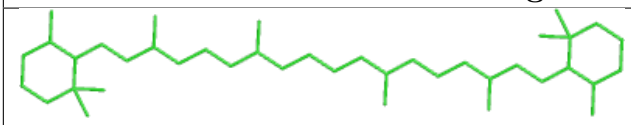


Torsions

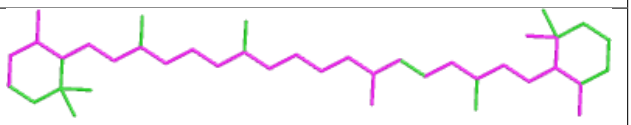


Rings

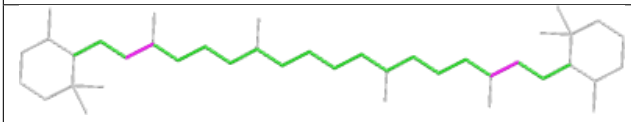
Ligand BCR 8 621



Bond lengths



Bond angles



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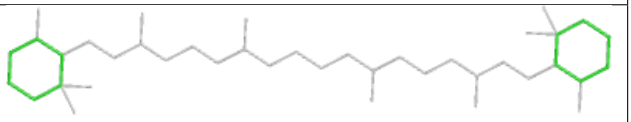
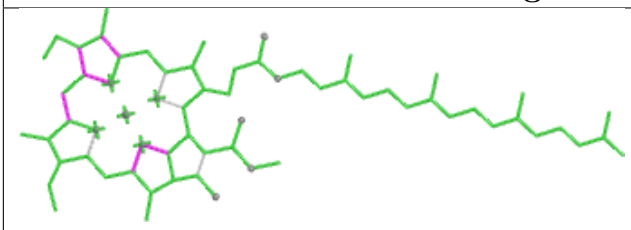
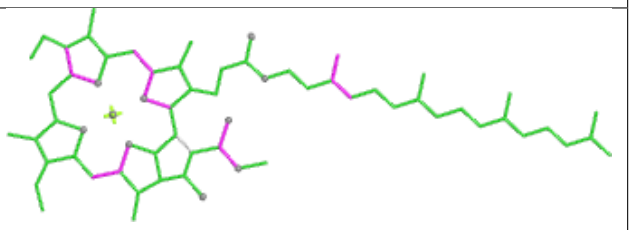
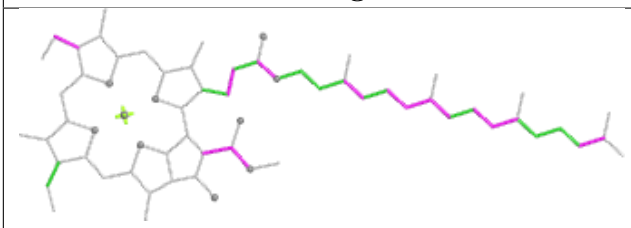
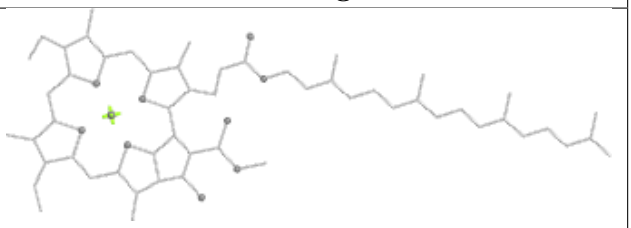
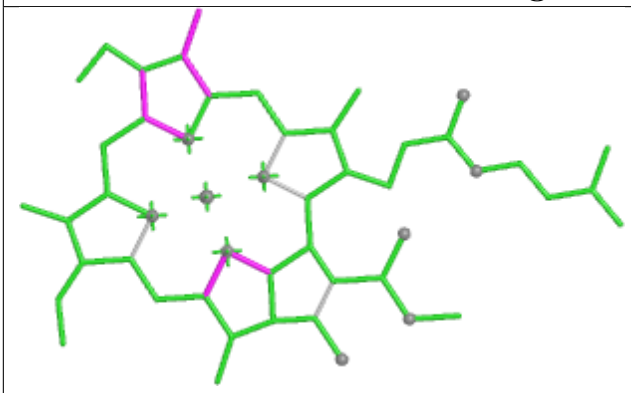
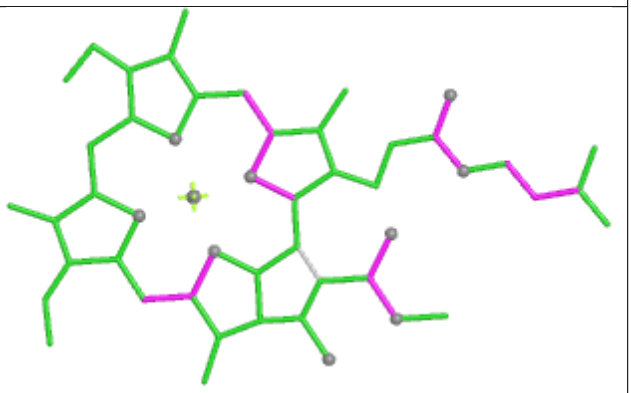
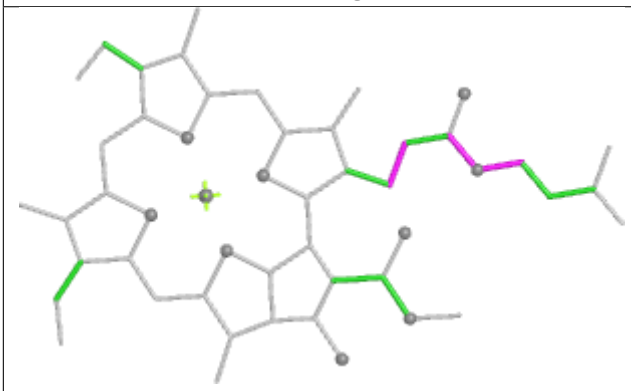
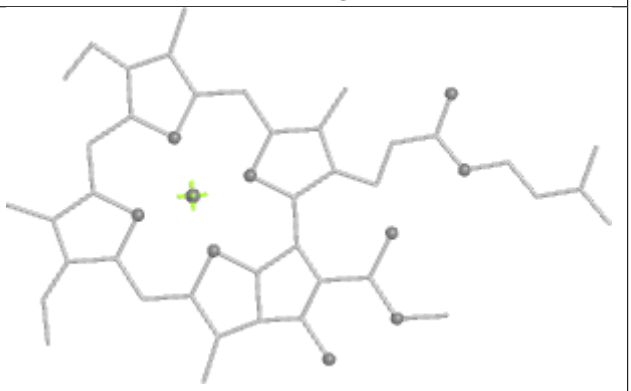
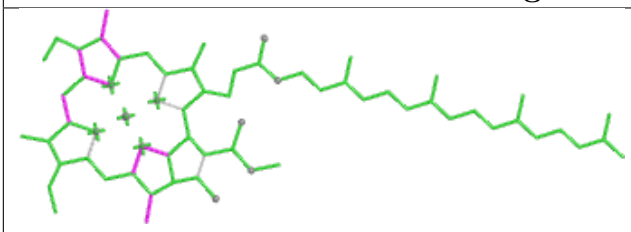
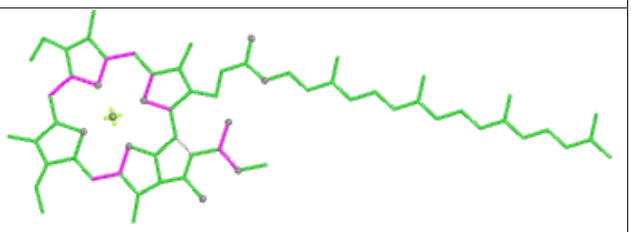
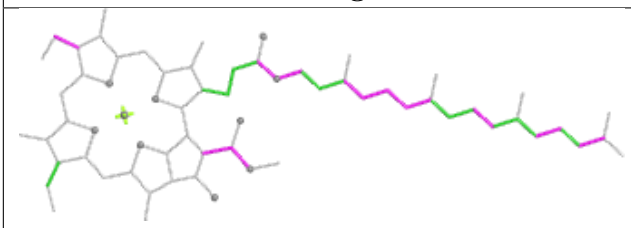
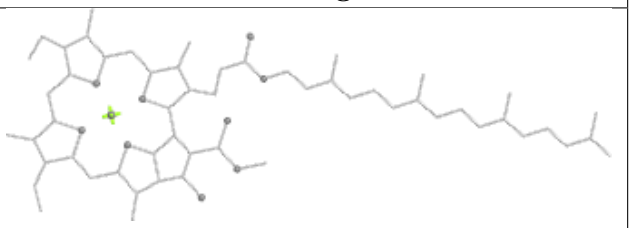
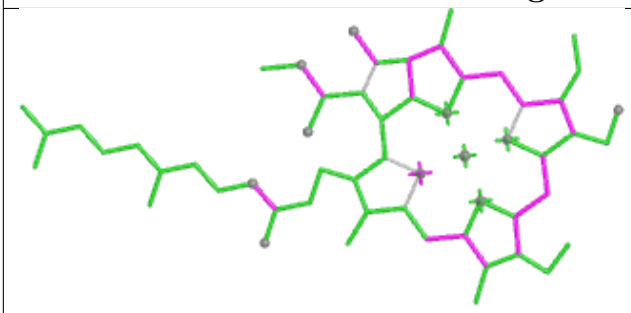
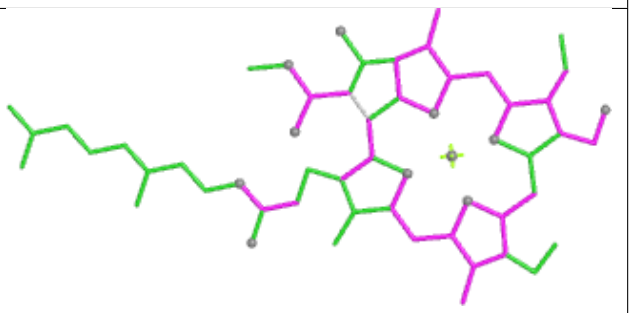
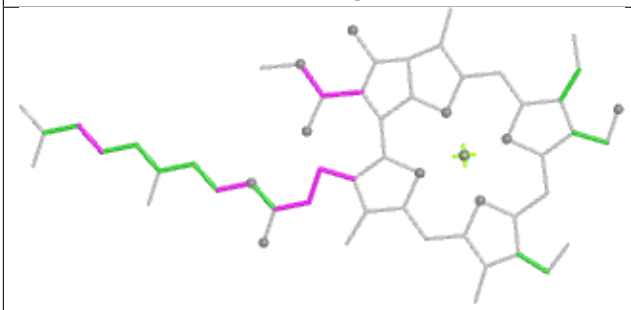
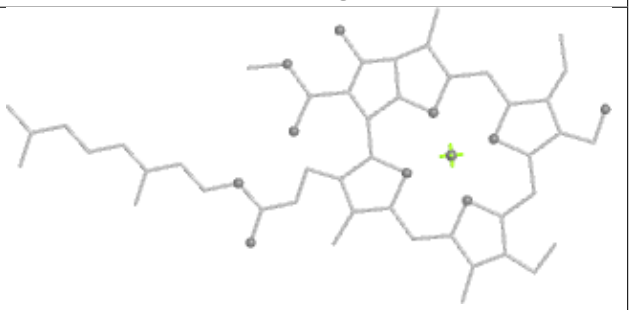


Rings

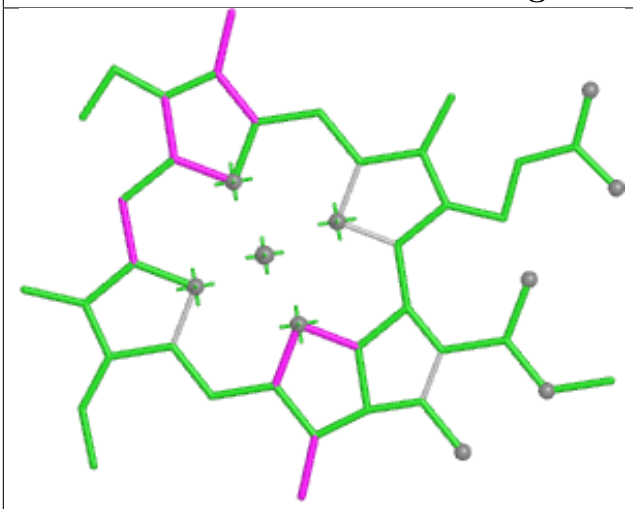
Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

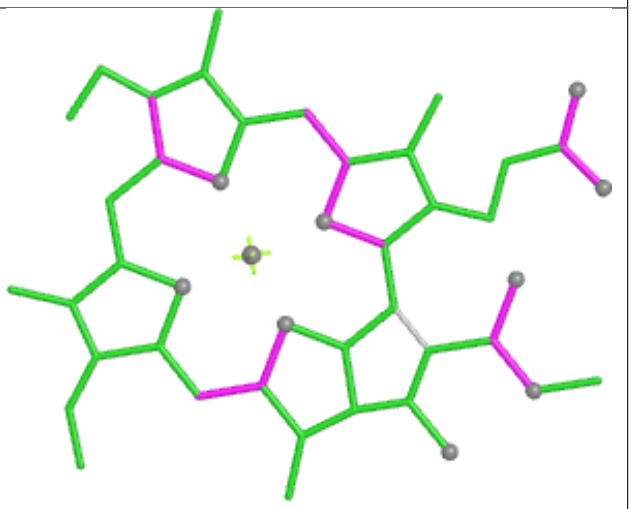
Ligand CLA A 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

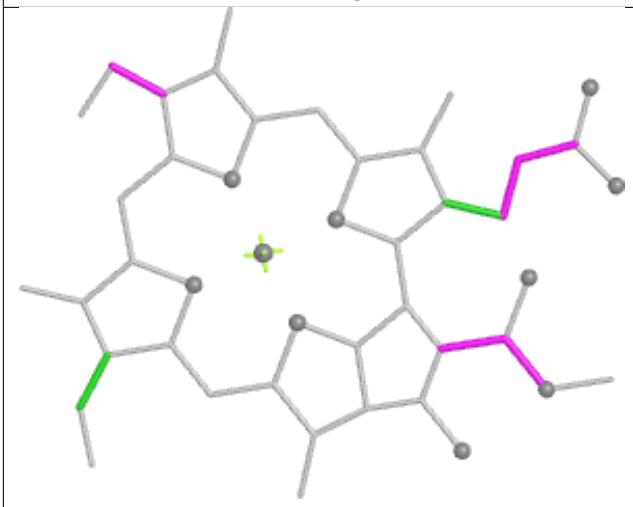
Ligand CLA 3 614



Bond lengths



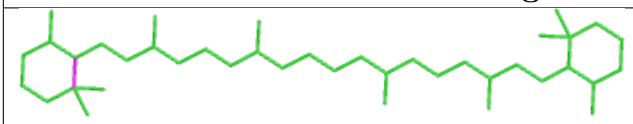
Bond angles



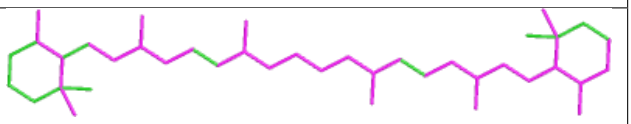
Torsions

Rings

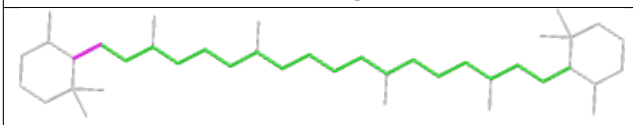
Ligand BCR A 851



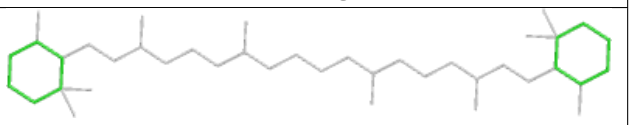
Bond lengths



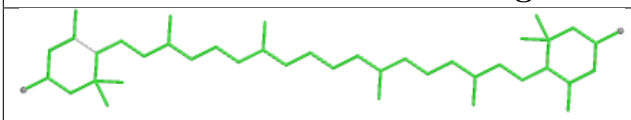
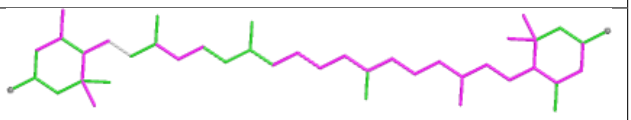
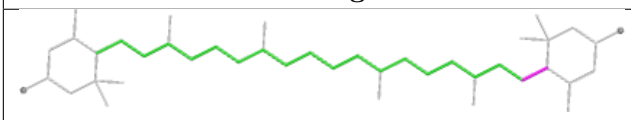
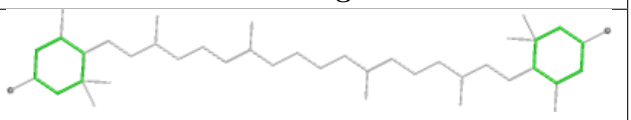
Bond angles



Torsions



Rings

Ligand LUT V 2620	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

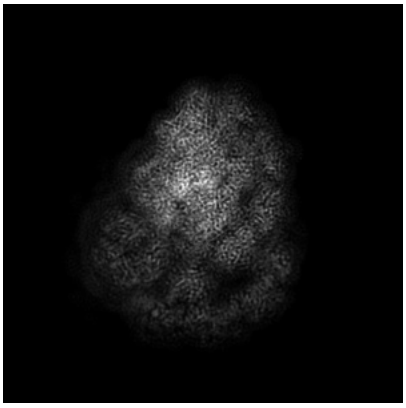
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35018. These allow visual inspection of the internal detail of the map and identification of artifacts.

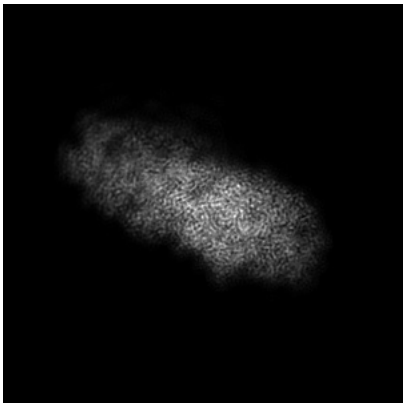
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

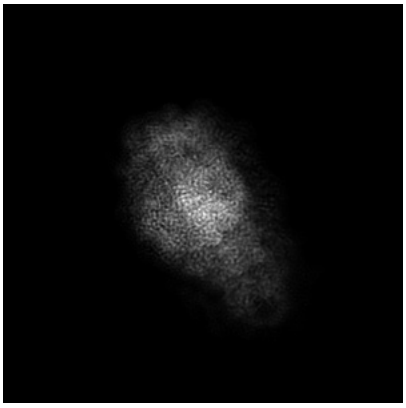
6.1.1 Primary map



X



Y

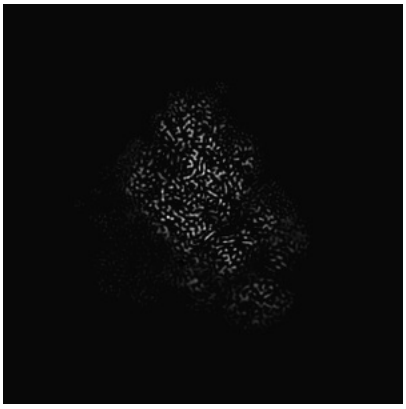


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 160

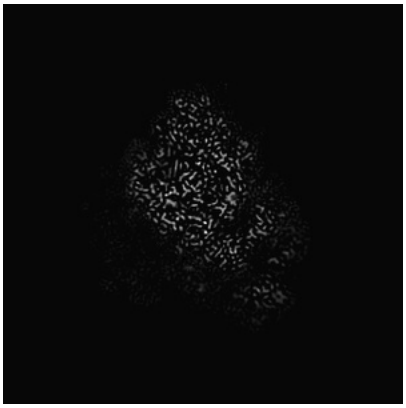
Y Index: 160

Z Index: 160

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: 158

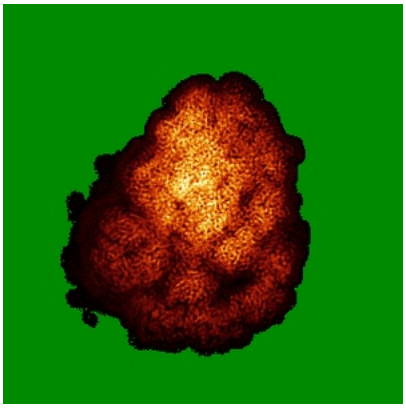
Y Index: 151

Z Index: 175

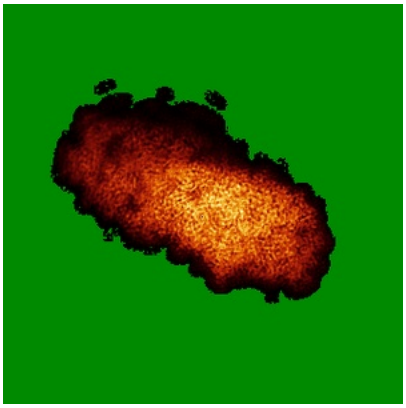
The images above show the largest variance slices of the map in three orthogonal directions.

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

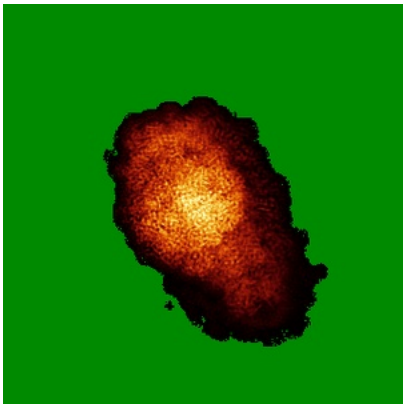
6.4.1 Primary map



X



Y

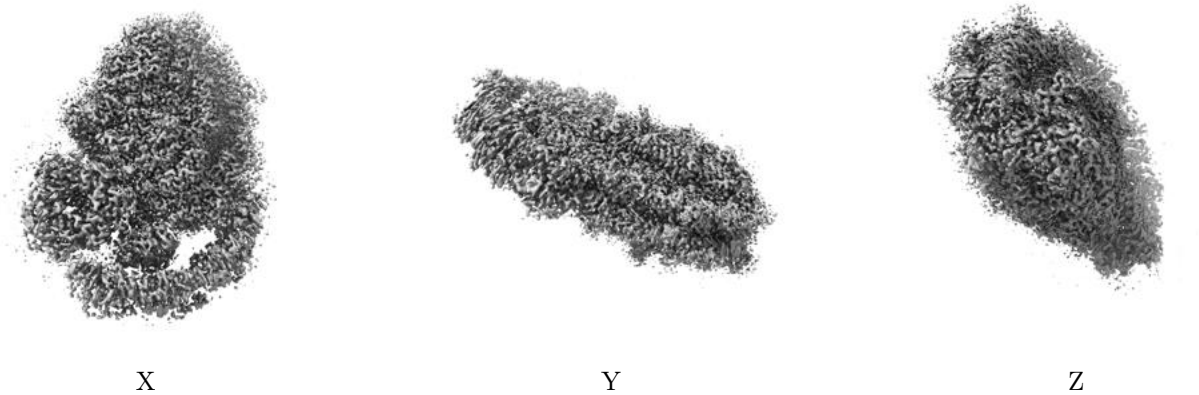


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

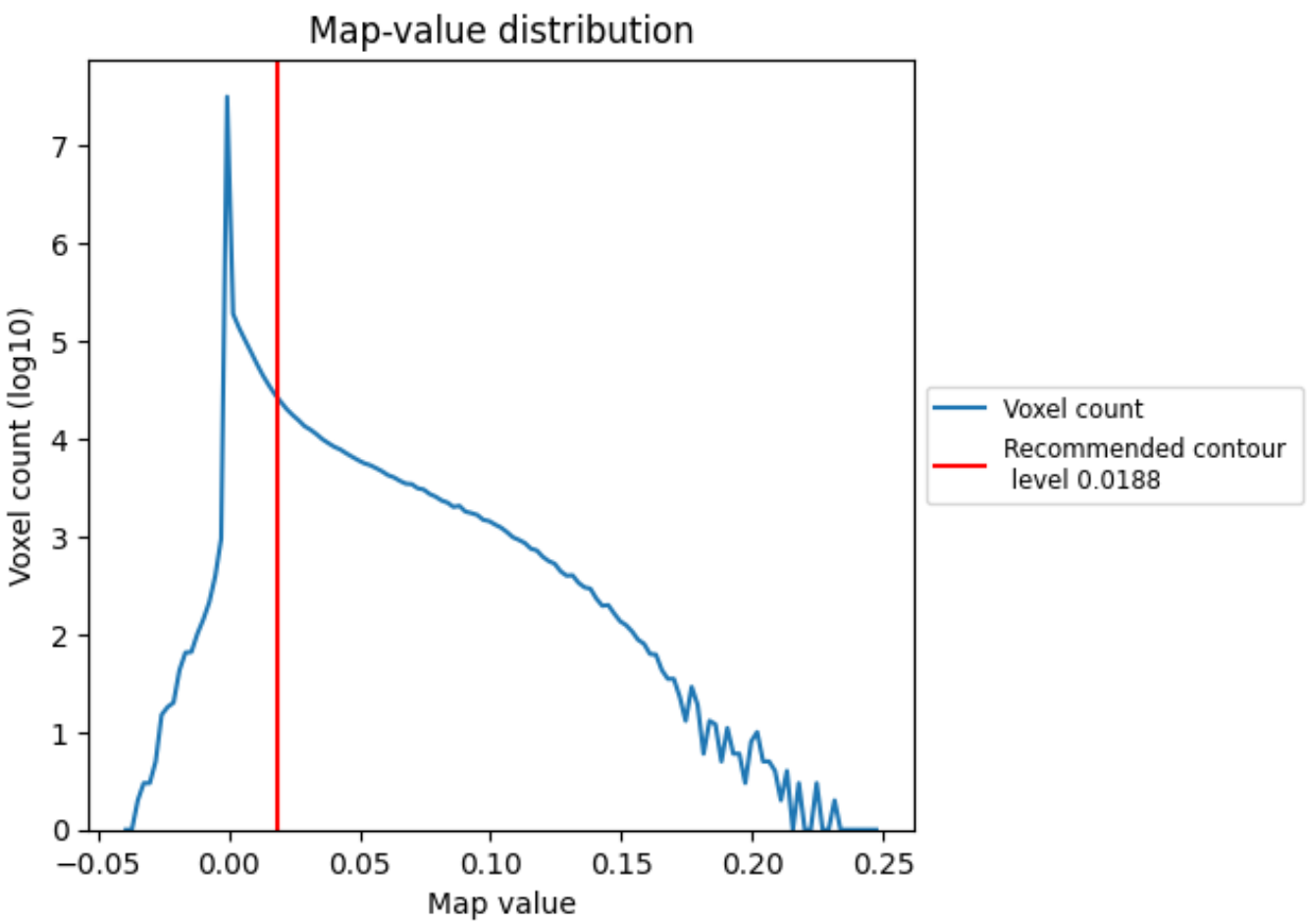
6.6 Mask visualisation (i)

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

7 Map analysis (i)

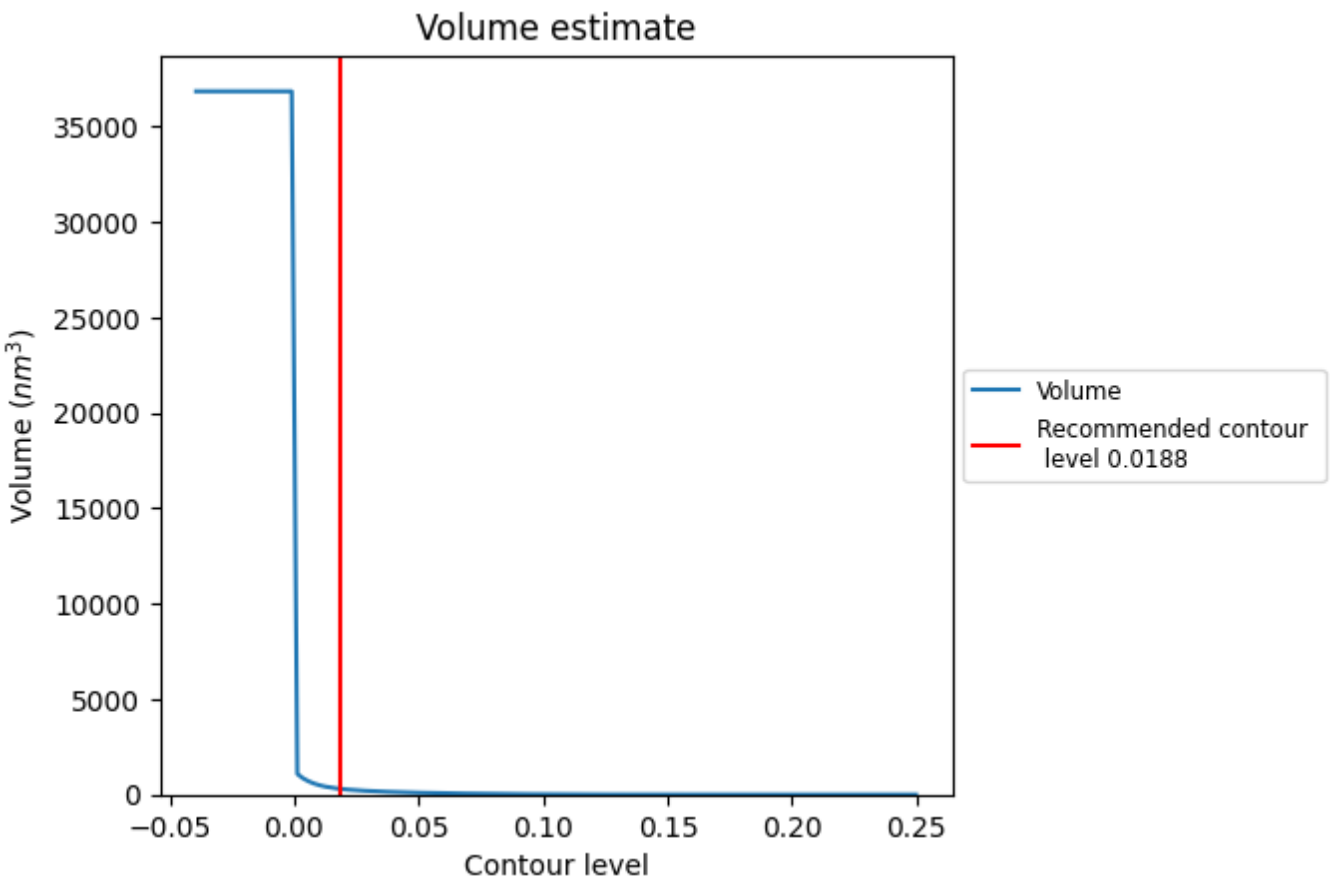
This section contains the results of statistical analysis of the map.

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.

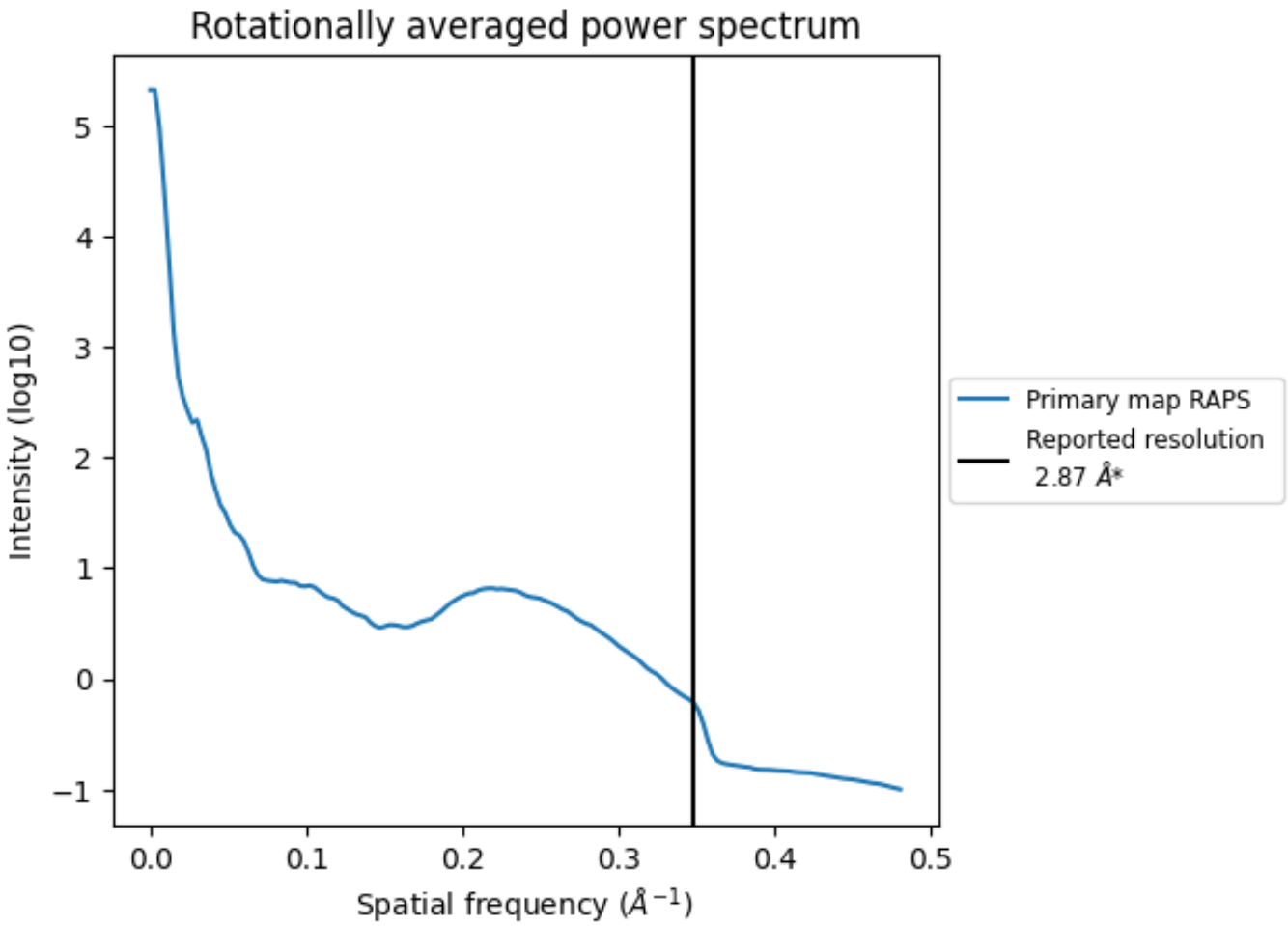
7.2 Volume estimate (i)



The volume at the recommended contour level is 296 nm^3; this corresponds to an approximate mass of 267 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 0.348 Å^{-1}

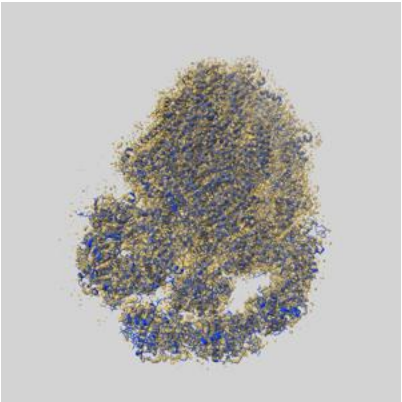
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

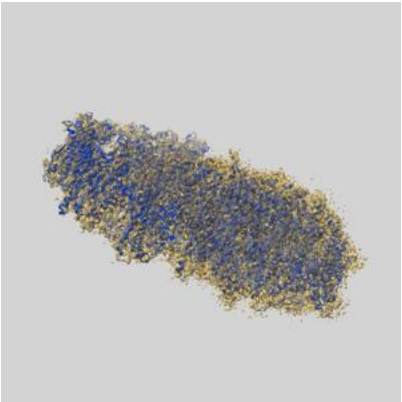
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35018 and PDB model 8HTU. Per-residue inclusion information can be found in section 3 on page 31.

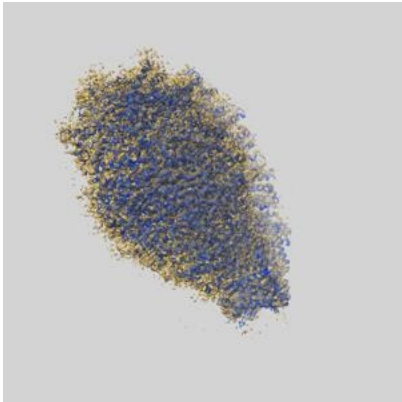
9.1 Map-model overlay (i)



X



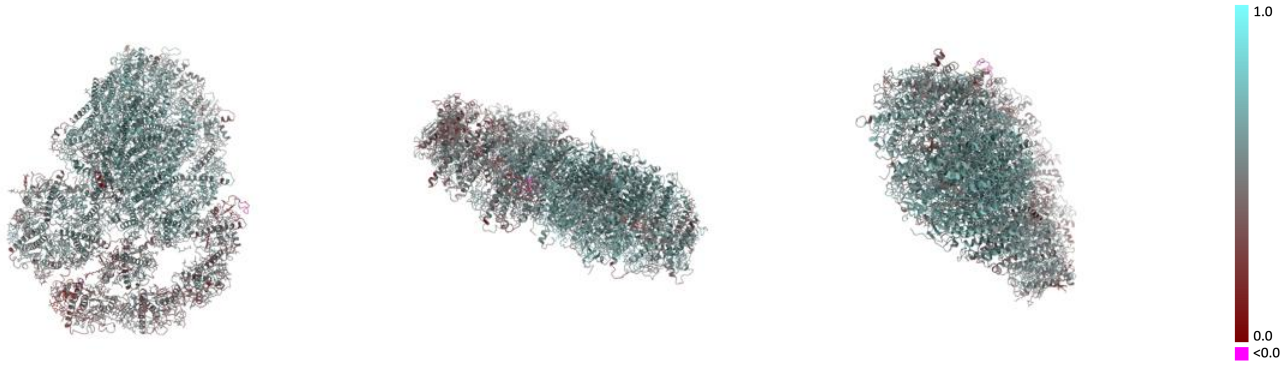
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0188 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.

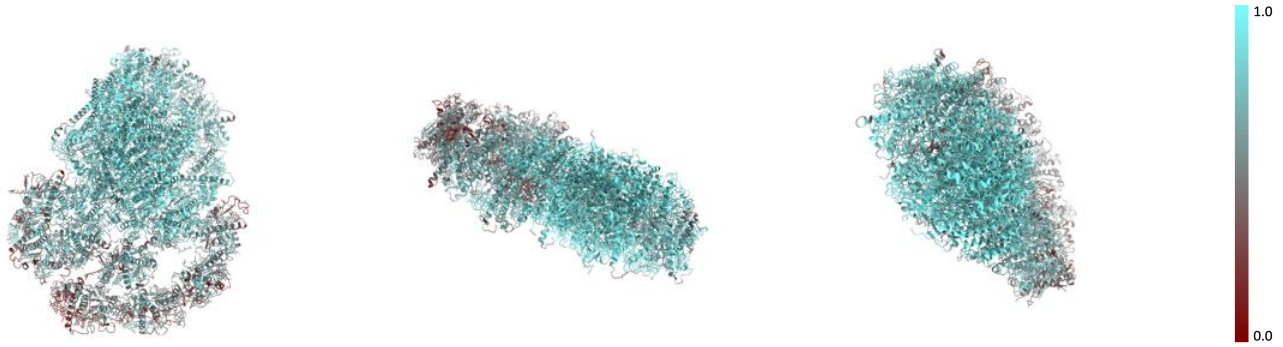
9.2 Q-score mapped to coordinate model (i)



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.

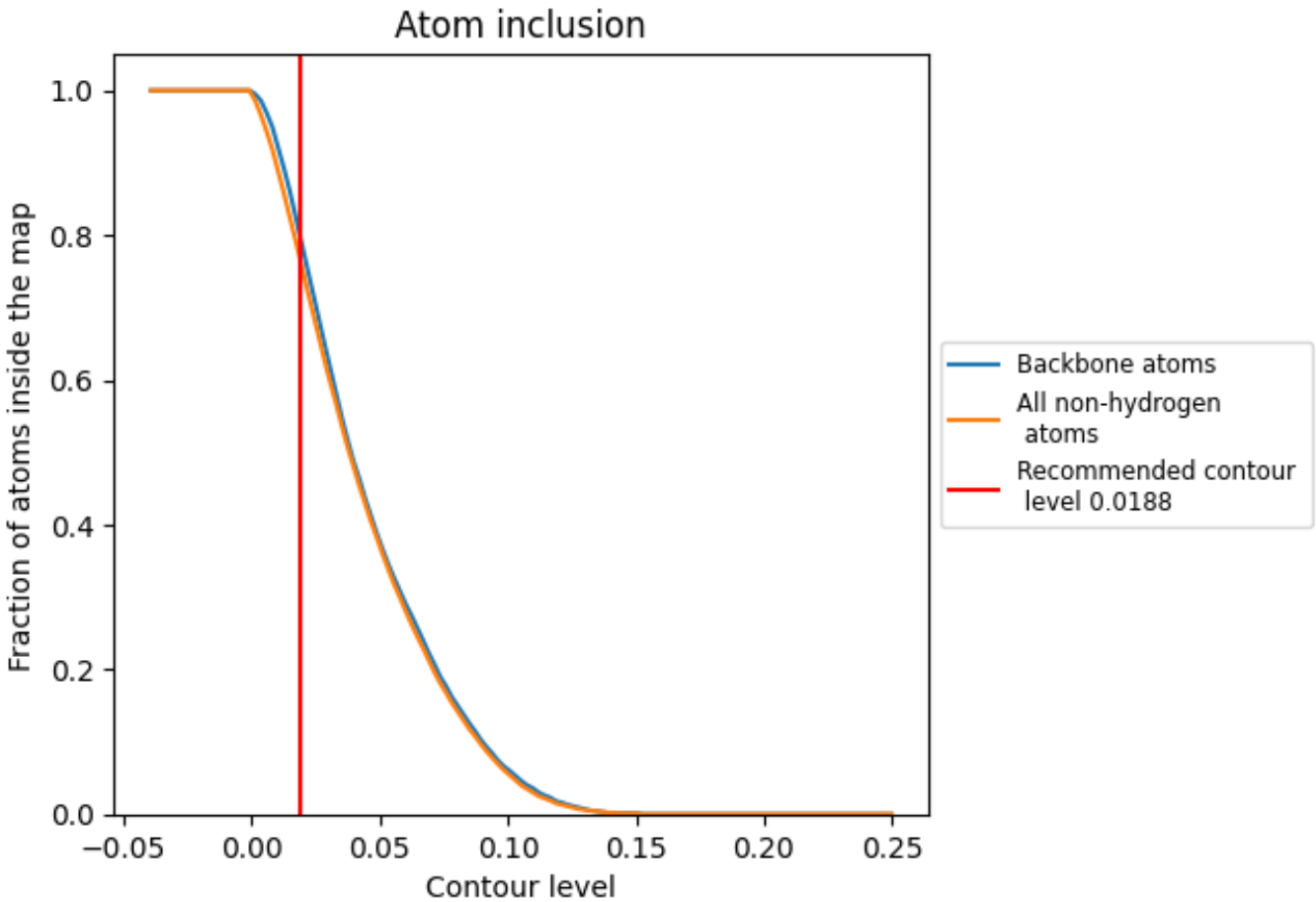
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0188).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.5500
1	0.7560	0.5390
2	0.8540	0.5860
3	0.8550	0.5880
4	0.7930	0.5400
5	0.5530	0.4110
6	0.5150	0.4410
7	0.4180	0.3830
8	0.5530	0.4610
9	0.6210	0.4420
A	0.9310	0.6320
B	0.9210	0.6270
C	0.9460	0.6200
D	0.8850	0.5910
E	0.8660	0.6050
F	0.8630	0.5990
G	0.7240	0.5410
H	0.7350	0.5080
I	0.9010	0.5910
J	0.8490	0.5860
K	0.8640	0.5880
L	0.8690	0.5870
M	0.7750	0.5580
O	0.7840	0.4770
U	0.6840	0.5290
V	0.5640	0.4930
W	0.6720	0.5220