Full wwPDB EM Validation Report (i)

Oct 15, 2024 – 06:53 AM JST

PDB ID	:	7WFE
EMDB ID	:	EMD-32463
Title	:	Right PSI in the cyclic electron transfer supercomplex NDH-PSI from Arabidopsis
Authors	:	Pan, X.W.; Li, M.
Deposited on	:	2021-12-26
Resolution	:	3.25 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 (1)) were used in the production of this report:

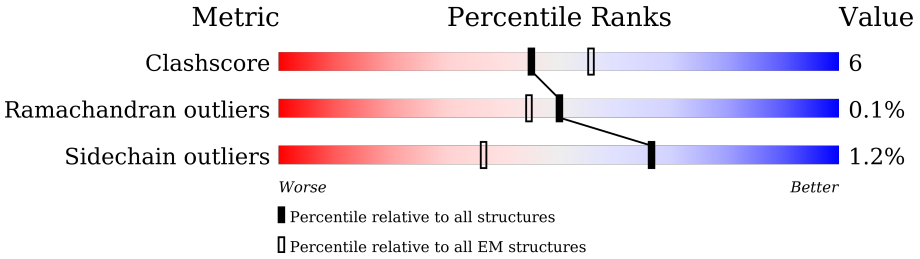
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	BA	750	87% 12% •
2	BB	734	85% 15%
3	BC	81	81% 17% •
4	BD	204	59% 10% 30%
5	BE	143	41% 7% 52%
6	BF	221	63% 7% 30%
7	BG	160	51% 8% 41%
8	BH	145	61% 5% 34%

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Mol	Chain	Length	Quality of chain
9	BI	37	84% 5% 11%
10	BJ	44	84% 14%
11	BK	130	45% 5% 51%
12	BL	219	65% 7% 27%
13	B1	241	7% 59% 13% 29%
14	B2	257	73% 8% 19%
15	B3	273	73% 8% 19%
16	B5	256	69% 11% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B1	304	X	-	-	-
17	CLA	B1	305	X	-	-	-
17	CLA	B1	306	X	-	-	-
17	CLA	B1	307	X	-	-	-
17	CLA	B1	310	X	-	-	-
17	CLA	B1	311	X	-	-	-
17	CLA	B1	312	X	-	-	-
17	CLA	B1	313	X	-	-	-
17	CLA	B1	314	X	-	-	-
17	CLA	B1	315	X	-	-	-
17	CLA	B2	301	X	-	-	-
17	CLA	B2	302	X	-	-	-
17	CLA	B2	303	X	-	-	-
17	CLA	B2	307	X	-	-	-
17	CLA	B2	308	X	-	-	-
17	CLA	B2	309	X	-	-	-
17	CLA	B2	310	X	-	-	-
17	CLA	B2	311	X	-	-	-
17	CLA	B2	312	X	-	-	-
17	CLA	B3	602	X	-	-	-
17	CLA	B3	603	X	-	-	-
17	CLA	B3	604	X	-	-	-
17	CLA	B3	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B3	606	X	-	-	-
17	CLA	B3	608	X	-	-	-
17	CLA	B3	609	X	-	-	-
17	CLA	B3	610	X	-	-	-
17	CLA	B3	611	X	-	-	-
17	CLA	B3	612	X	-	-	-
17	CLA	B3	613	X	-	-	-
17	CLA	B3	614	X	-	-	-
17	CLA	B3	615	X	-	-	-
17	CLA	B5	601	X	-	-	-
17	CLA	B5	603	X	-	-	-
17	CLA	B5	604	X	-	-	-
17	CLA	B5	608	X	-	-	-
17	CLA	B5	609	X	-	-	-
17	CLA	B5	611	X	-	-	-
17	CLA	B5	612	X	-	-	-
17	CLA	B5	613	X	-	-	-
17	CLA	BA	801	X	-	-	-
17	CLA	BA	802	X	-	-	-
17	CLA	BA	803	X	-	-	-
17	CLA	BA	805	X	-	-	-
17	CLA	BA	806	X	-	-	-
17	CLA	BA	807	X	-	-	-
17	CLA	BA	808	X	-	-	-
17	CLA	BA	810	X	-	-	-
17	CLA	BA	811	X	-	-	-
17	CLA	BA	812	X	-	-	-
17	CLA	BA	813	X	-	-	-
17	CLA	BA	814	X	-	-	-
17	CLA	BA	816	X	-	-	-
17	CLA	BA	819	X	-	-	-
17	CLA	BA	820	X	-	-	-
17	CLA	BA	822	X	-	-	-
17	CLA	BA	823	X	-	-	-
17	CLA	BA	824	X	-	-	-
17	CLA	BA	825	X	-	-	-
17	CLA	BA	827	X	-	-	-
17	CLA	BA	828	X	-	-	-
17	CLA	BA	829	X	-	-	-
17	CLA	BA	830	X	-	-	-
17	CLA	BA	831	X	-	-	-
17	CLA	BA	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	BA	835	X	-	-	-
17	CLA	BA	837	X	-	-	-
17	CLA	BA	838	X	-	-	-
17	CLA	BA	840	X	-	-	-
17	CLA	BA	841	X	-	-	-
17	CLA	BA	842	X	-	-	-
17	CLA	BA	844	X	-	-	-
17	CLA	BB	801	X	-	-	-
17	CLA	BB	802	X	-	-	-
17	CLA	BB	804	X	-	-	-
17	CLA	BB	805	X	-	-	-
17	CLA	BB	806	X	-	-	-
17	CLA	BB	807	X	-	-	-
17	CLA	BB	808	X	-	-	-
17	CLA	BB	810	X	-	-	-
17	CLA	BB	811	X	-	-	-
17	CLA	BB	812	X	-	-	-
17	CLA	BB	813	X	-	-	-
17	CLA	BB	814	X	-	-	-
17	CLA	BB	815	X	-	-	-
17	CLA	BB	816	X	-	-	-
17	CLA	BB	817	X	-	-	-
17	CLA	BB	818	X	-	-	-
17	CLA	BB	819	X	-	-	-
17	CLA	BB	820	X	-	-	-
17	CLA	BB	821	X	-	-	-
17	CLA	BB	822	X	-	-	-
17	CLA	BB	823	X	-	-	-
17	CLA	BB	825	X	-	-	-
17	CLA	BB	826	X	-	-	-
17	CLA	BB	828	X	-	-	-
17	CLA	BB	829	X	-	-	-
17	CLA	BB	830	X	-	-	-
17	CLA	BB	831	X	-	-	-
17	CLA	BB	832	X	-	-	-
17	CLA	BB	835	X	-	-	-
17	CLA	BB	837	X	-	-	-
17	CLA	BB	838	X	-	-	-
17	CLA	BB	841	X	-	-	-
17	CLA	BB	842	X	-	-	-
17	CLA	BB	843	X	-	-	-
17	CLA	BF	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	BF	302	X	-	-	-
17	CLA	BF	303	X	-	-	-
17	CLA	BG	201	X	-	-	-
17	CLA	BG	202	X	-	-	-
17	CLA	BH	201	X	-	-	-
17	CLA	BJ	102	X	-	-	-
17	CLA	BK	201	X	-	-	-
17	CLA	BK	202	X	-	-	-
17	CLA	BK	203	X	-	-	-
17	CLA	BL	304	X	-	-	-
25	CHL	B1	303	X	-	-	-
25	CHL	B1	308	X	-	-	-
25	CHL	B2	304	X	-	-	-
25	CHL	B2	305	X	-	-	-
25	CHL	B2	306	X	-	-	-
25	CHL	B2	313	X	-	-	-
25	CHL	B3	601	X	-	-	-
25	CHL	B3	607	X	-	-	-
25	CHL	B5	605	X	-	-	-
25	CHL	B5	606	X	-	-	-
25	CHL	B5	607	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 35123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	742	5841	3828	992	1003	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	733	5854	3842	998	1000	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BC	80	615	381	107	116	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BD	143	1127	723	195	205	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	BE	69	546	352	97	97	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BF	154	1220	797	209	211	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	BG	94	733	474	121	138	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	BH	95	730	476	119	135	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BI	33	257	175	41	40	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BJ	43	344	233	52	58	1	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BK	64	445	285	73	84	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BL	159	1184	781	190	211	2	0	0

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B1	172	1339	873	221	240	5	0	0

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B2	208	1607	1051	261	291	4	0	0

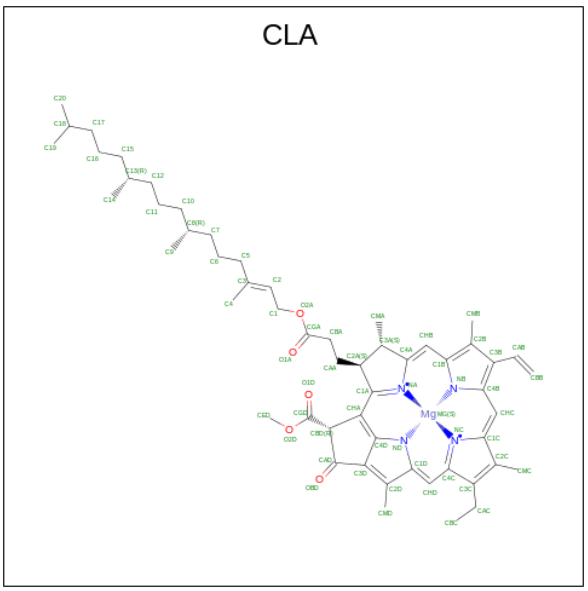
- Molecule 15 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	B3	221	1696	1111	276	304	5	0	0

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	B5	206	1603	1047	263	287	6	0	0

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	BA	1	52	42	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	50	40	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	50	40	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	54	44	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	45	35	1	4	5	0
17	BA	1	42	34	1	4	3	0
17	BA	1	45	35	1	4	5	0
17	BA	1	60	50	1	4	5	0
17	BA	1	56	46	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	45	35	1	4	5	0
17	BA	1	65	55	1	4	5	0
17	BA	1	42	34	1	4	3	0
17	BA	1	41	33	1	4	3	0
17	BA	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	54	45	1	4	4	0
			Total	C	Mg	N	O	
17	BA	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BA	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	BB	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	BB	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
17	BB	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	BB	1	45	35	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	62	52	1	4	5	0
17	BB	1	62	52	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	56	46	1	4	5	0
17	BB	1	43	35	1	4	3	0
17	BB	1	43	35	1	4	3	0
17	BB	1	65	55	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	60	50	1	4	5	0
17	BB	1	42	34	1	4	3	0
17	BB	1	50	40	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	47	37	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BB	1	65	55	1	4	5	0
17	BF	1	55	46	1	4	4	0
17	BF	1	42	34	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	BF	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	BG	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	BG	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	BH	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	BJ	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	BK	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
17	BK	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	BK	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
17	BL	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	BL	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	BL	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	B1	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
17	B1	1	54	45	1	4	4	0
			Total	C	Mg	N	O	
17	B1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B1	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
17	B1	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
17	B1	1	39	31	1	4	3	0
			Total	C	Mg	N	O	
17	B1	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
17	B1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
17	B1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B1	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B1	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
17	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
17	B2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
17	B2	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B2	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	B3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
17	B3	1	42	32	1	4	5	0
			Total	C	Mg	N	O	
17	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B3	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	B3	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
17	B3	1	40	32	1	4	3	0

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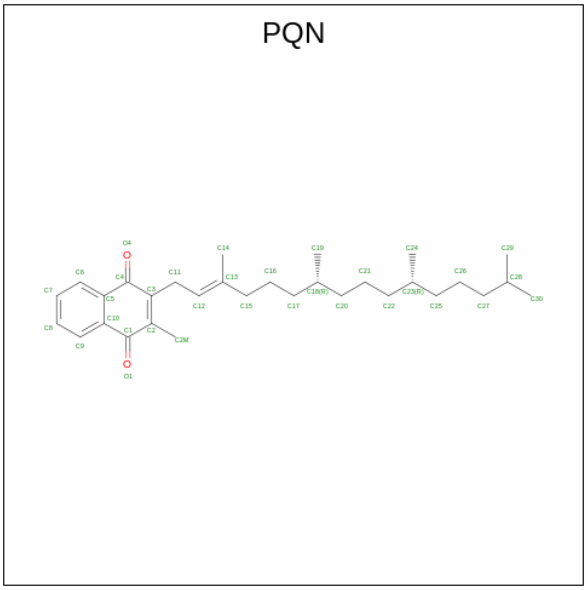
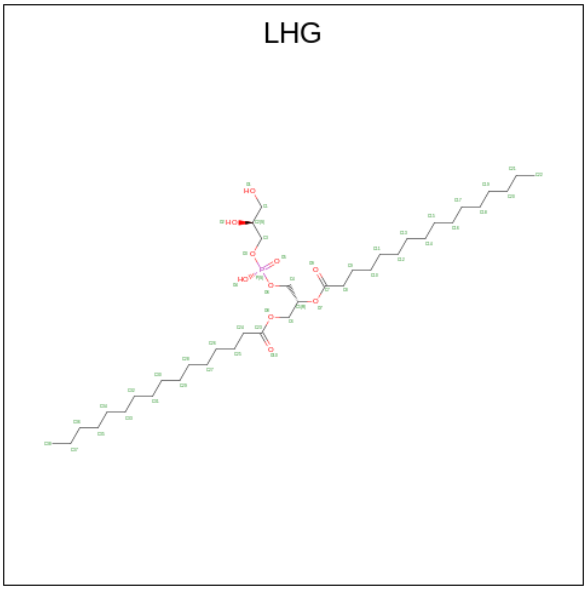
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B3	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
17	B3	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
17	B5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B5	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
17	B5	1	45	35	1	4	5	0

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



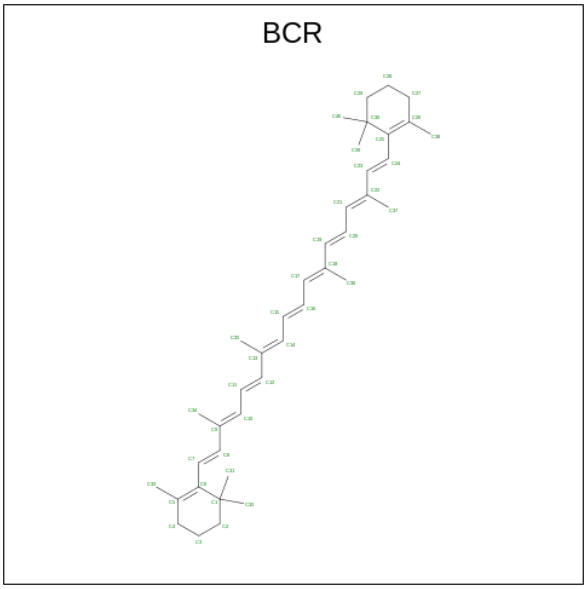
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	BA	1	33	31	2	0
			Total	C	O	
18	BB	1	33	31	2	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	BA	1	49	38	10	1	0
			Total	C	O	P	
19	BA	1	27	16	10	1	0
			Total	C	O	P	
19	BF	1	45	34	10	1	0
			Total	C	O	P	
19	B1	1	38	27	10	1	0
			Total	C	O	P	
19	B1	1	36	25	10	1	0
			Total	C	O	P	
19	B1	1	42	31	10	1	0
			Total	C	O	P	
19	B2	1	35	24	10	1	0
			Total	C	O	P	
19	B3	1	23	12	10	1	0
			Total	C	O	P	
19	B5	1	30	19	10	1	0

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BA	1	40	40	0
			Total	C	
20	BB	1	40	40	0
			Total	C	
20	BB	1	40	40	0
			Total	C	
20	BB	1	40	40	0
			Total	C	
20	BB	1	40	40	0
			Total	C	
20	BB	1	40	40	0

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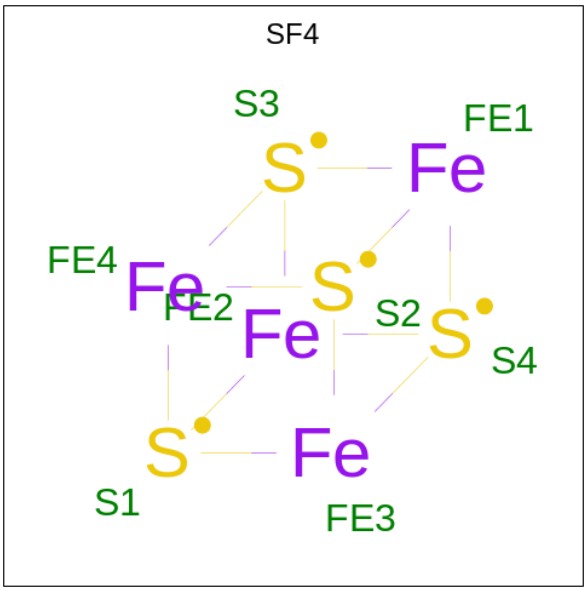
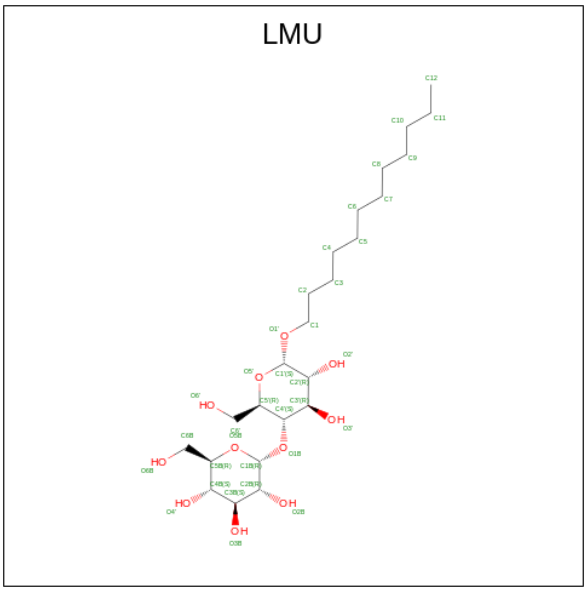
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
20	BB	1	40	40	0
20	BF	1	40	40	0
20	BG	1	40	40	0
20	BH	1	40	40	0
20	BI	1	40	40	0
20	BJ	1	40	40	0
20	BJ	1	40	40	0
20	BK	1	40	40	0
20	BL	1	40	40	0
20	BL	1	40	40	0
20	B2	1	40	40	0
20	B3	1	40	40	0
20	B5	1	40	40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



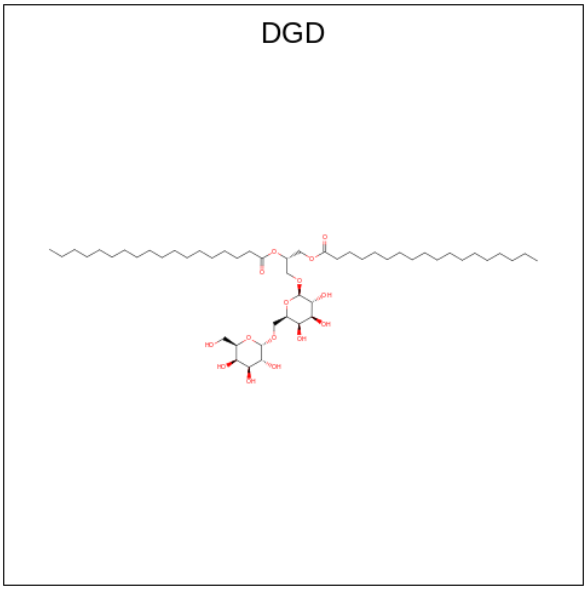
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
21	BA	1	8	4	4	0
21	BC	1	8	4	4	0
21	BC	1	8	4	4	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



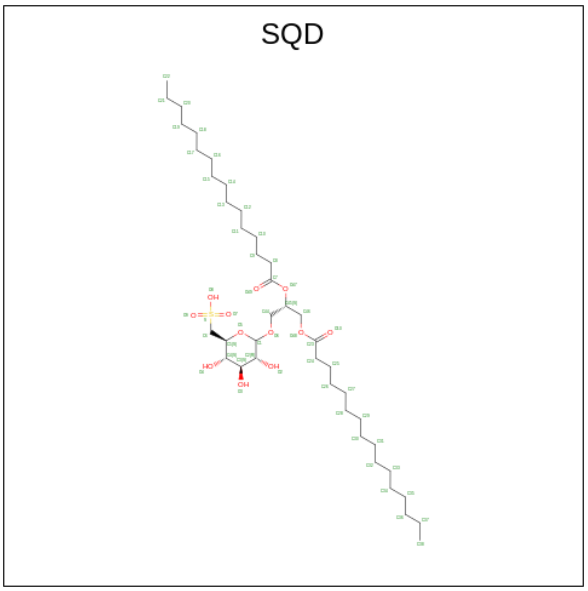
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	BA	1	34	23	11	0
			Total	C	O	
22	BA	1	33	22	11	0
			Total	C	O	
22	BB	1	35	24	11	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



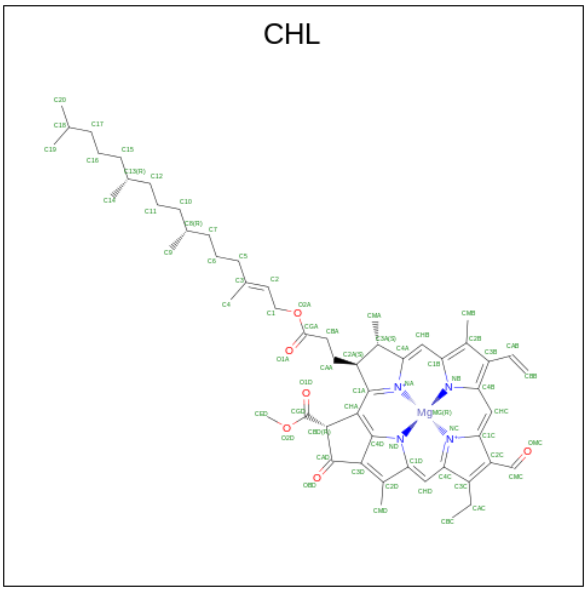
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	BB	1	66	51	15	0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
24	BJ	1	47	34	12	1	0

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B1	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
25	B1	1	41	32	1	4	4	0

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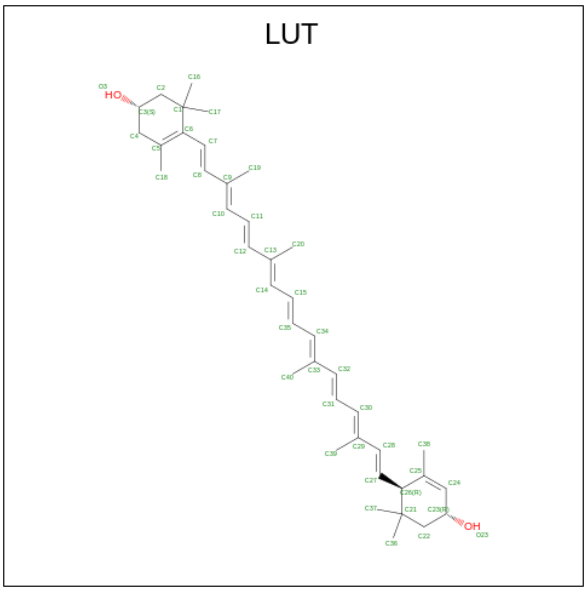
Mol	Chain	Residues	Atoms					AltConf
25	B2	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	B2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	B2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	B2	1	Total 43	C 34	Mg 1	N 4	O 4	0
25	B3	1	Total 53	C 42	Mg 1	N 4	O 6	0
25	B3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B5	1	Total 41	C 32	Mg 1	N 4	O 4	0
25	B5	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	B5	1	Total 45	C 34	Mg 1	N 4	O 6	0

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	B1	1	Total 42	C 40	O 2	0

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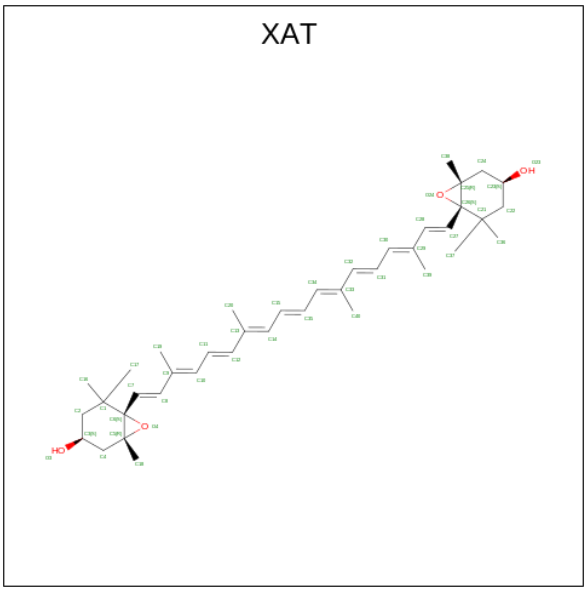
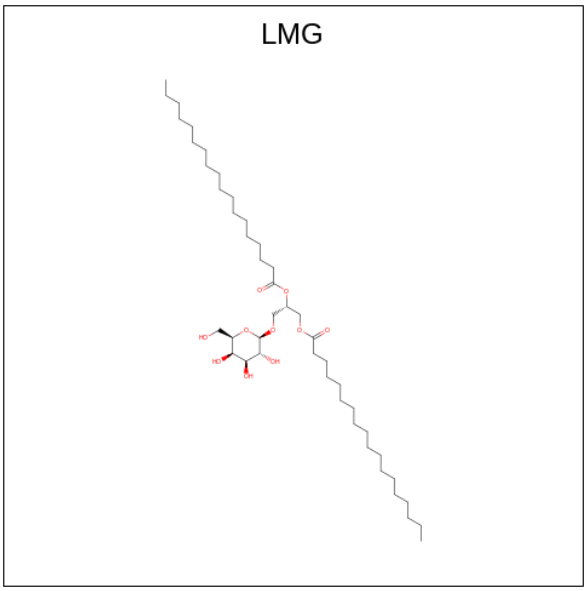
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	B2	1	42	40	2	0
26	B3	1	42	40	2	0
26	B5	1	42	40	2	0

- Molecule 27 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B1	1	44	40	4	0
27	B2	1	44	40	4	0
27	B3	1	44	40	4	0
27	B5	1	44	40	4	0

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



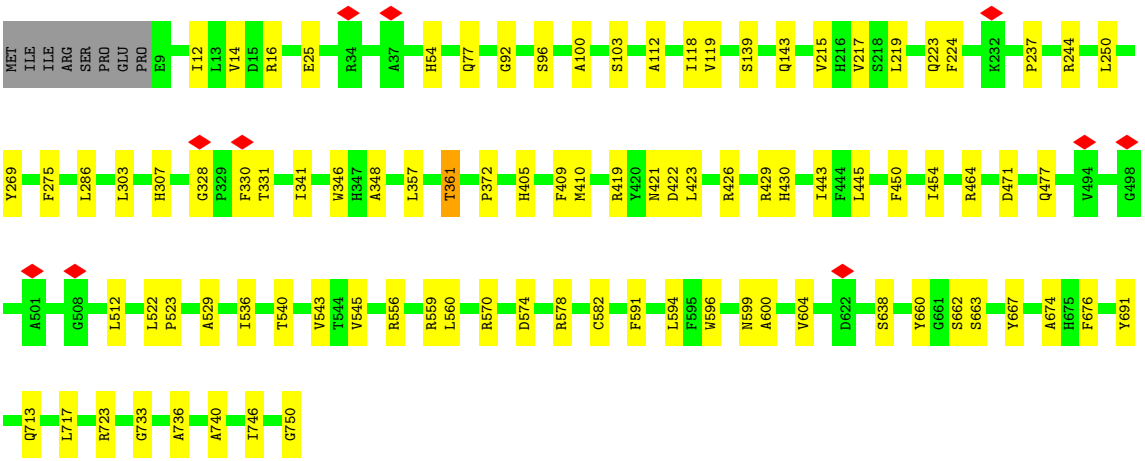
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B5	1	33	23	10	0

3 Residue-property plots (i)

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

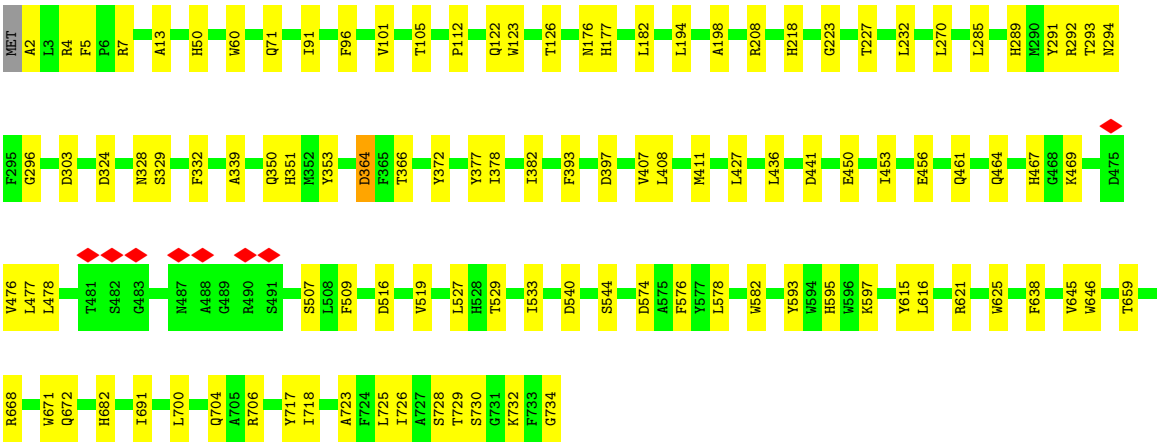
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain BA:



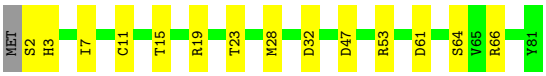
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain BB:



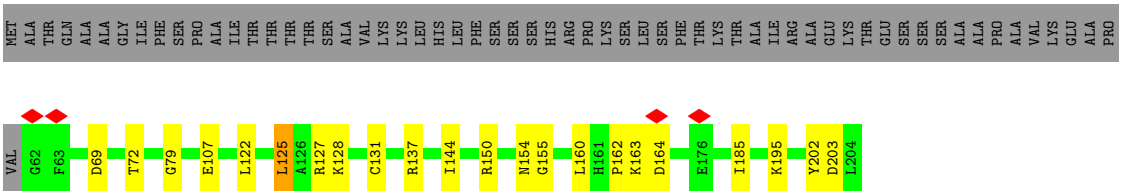
• Molecule 3: Photosystem I iron-sulfur center

Chain BC: 81% 17%



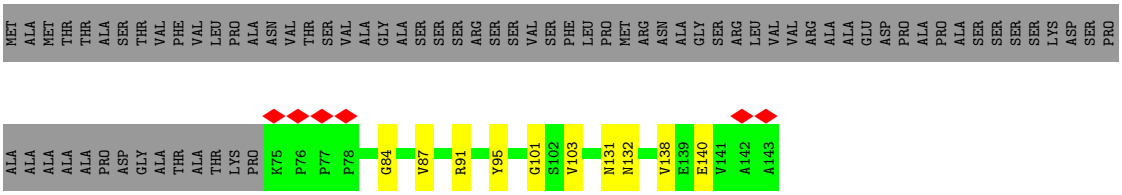
• Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD: 59% 10% 30%



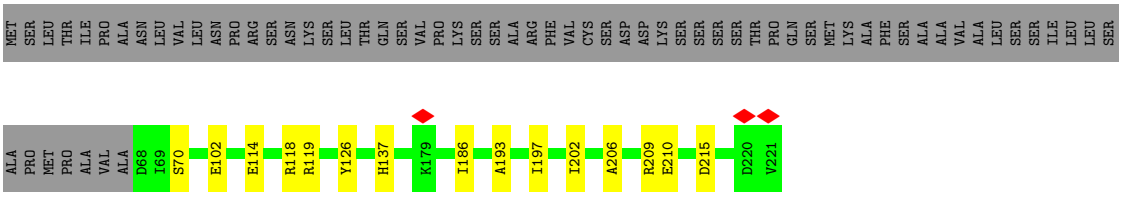
• Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain BE: 41% 7% 52%



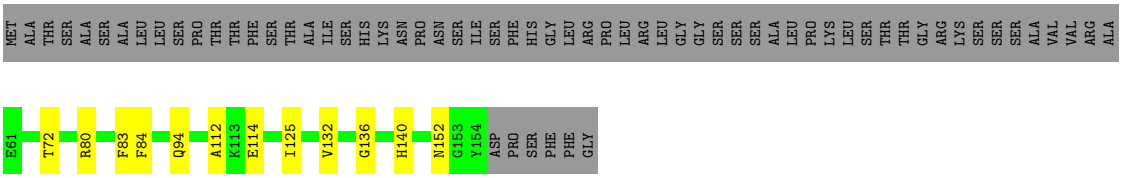
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain BF: 63% 7% 30%



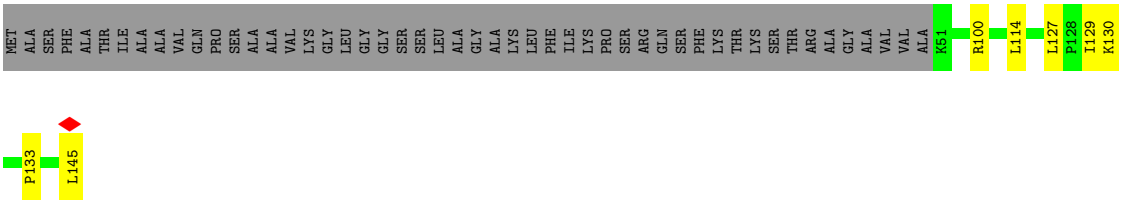
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain BG: 51% 8% 41%



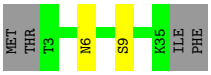
• Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

Chain BH: 61% 5% 34%



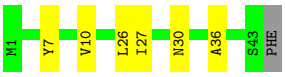
• Molecule 9: Photosystem I reaction center subunit VIII

Chain BI: 84% 5% 11%



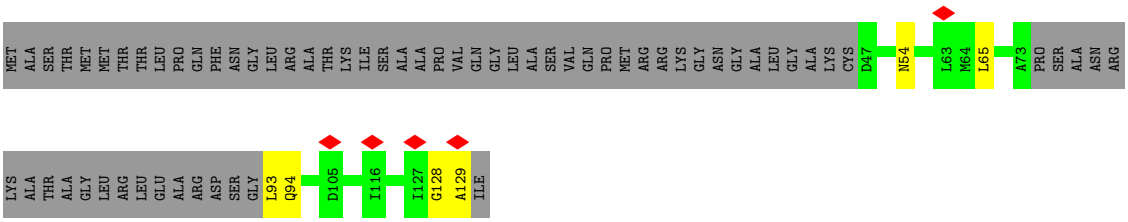
• Molecule 10: Photosystem I reaction center subunit IX

Chain BJ: 84% 14%



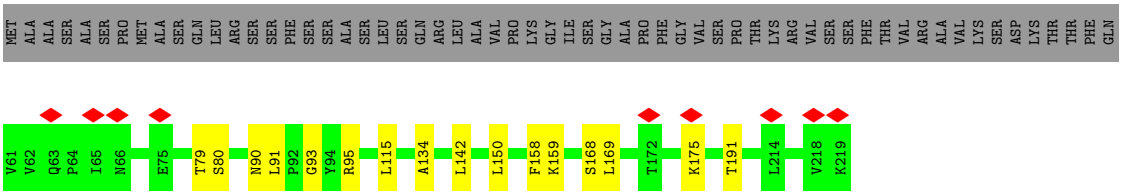
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain BK: 45% 5% 51%



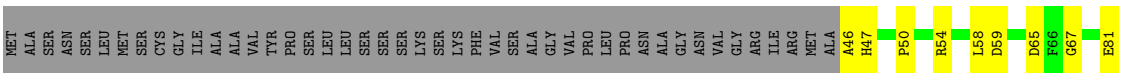
• Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

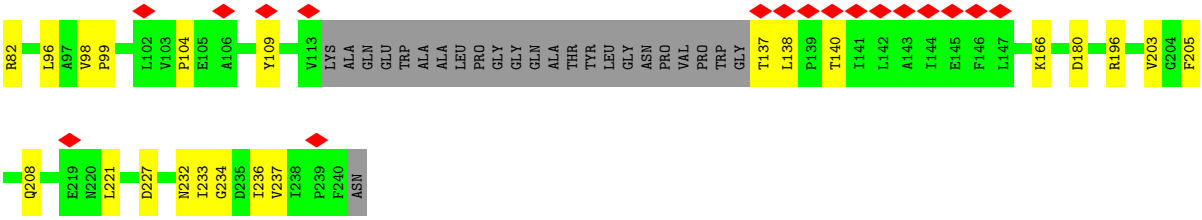
Chain BL: 65% 7% 27%



• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

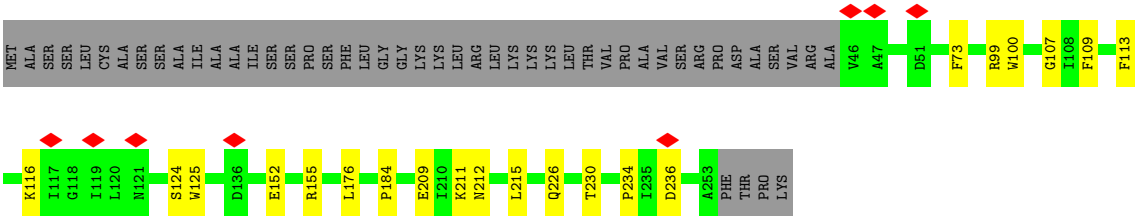
Chain B1: 7% 59% 13% 29%





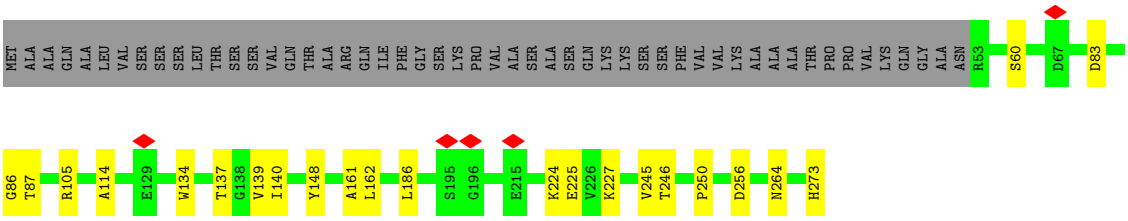
• Molecule 14: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain B2:



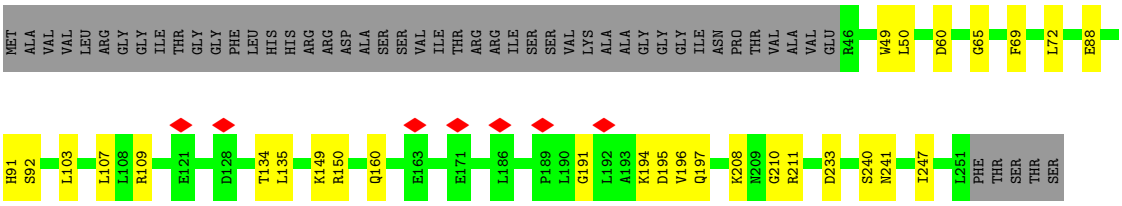
• Molecule 15: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain B3:



• Molecule 16: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic

Chain B5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	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 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	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: SQD, SF4, LMU, LHG, CLA, CHL, DGD, LMG, BCR, XAT, LUT, PQN

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	BA	0.36	0/6039	0.54	0/8239
2	BB	0.37	0/6065	0.54	1/8281 (0.0%)
3	BC	0.34	0/628	0.56	0/852
4	BD	0.35	0/1156	0.61	0/1563
5	BE	0.30	0/559	0.50	0/760
6	BF	0.31	0/1250	0.55	0/1687
7	BG	0.29	0/750	0.47	0/1016
8	BH	0.29	0/751	0.50	0/1018
9	BI	0.31	0/264	0.49	0/359
10	BJ	0.33	0/354	0.67	0/482
11	BK	0.30	0/449	0.57	0/607
12	BL	0.31	0/1218	0.52	0/1663
13	B1	0.30	0/1381	0.51	0/1879
14	B2	0.29	0/1663	0.53	0/2277
15	B3	0.30	0/1749	0.51	0/2378
16	B5	0.30	0/1650	0.54	0/2244
All	All	0.34	0/25926	0.54	1/35305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BB	427	LEU	CA-CB-CG	5.01	126.82	115.30

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	BA	5841	0	5690	93	0
2	BB	5854	0	5637	93	0
3	BC	615	0	593	19	0
4	BD	1127	0	1134	13	0
5	BE	546	0	555	13	0
6	BF	1220	0	1252	12	0
7	BG	733	0	718	11	0
8	BH	730	0	720	12	0
9	BI	257	0	274	1	0
10	BJ	344	0	356	5	0
11	BK	445	0	453	5	0
12	BL	1184	0	1179	13	0
13	B1	1339	0	1316	30	0
14	B2	1607	0	1555	14	0
15	B3	1696	0	1663	18	0
16	B5	1603	0	1585	19	0
17	B1	519	0	402	3	0
17	B2	442	0	366	5	0
17	B3	578	0	422	1	0
17	B5	476	0	368	6	0
17	BA	2446	0	2387	46	0
17	BB	2423	0	2407	57	0
17	BF	138	0	110	3	0
17	BG	87	0	64	3	0
17	BH	60	0	59	0	0
17	BJ	42	0	31	0	0
17	BK	127	0	88	1	0
17	BL	148	0	125	1	0
18	BA	33	0	46	3	0
18	BB	33	0	46	3	0
19	B1	116	0	145	0	0
19	B2	35	0	40	1	0
19	B3	23	0	16	1	0
19	B5	30	0	30	0	0
19	BA	76	0	98	2	0
19	BF	45	0	63	1	0
20	B2	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B3	40	0	56	5	0
20	B5	40	0	56	0	0
20	BA	280	0	392	15	0
20	BB	240	0	336	14	0
20	BF	40	0	56	1	0
20	BG	40	0	56	3	0
20	BH	40	0	55	1	0
20	BI	40	0	56	1	0
20	BJ	80	0	112	4	0
20	BK	40	0	56	2	0
20	BL	80	0	112	4	0
21	BA	8	0	0	1	0
21	BC	16	0	0	0	0
22	BA	67	0	80	0	0
22	BB	35	0	46	0	0
23	BB	66	0	96	1	0
24	BJ	47	0	61	3	0
25	B1	91	0	58	1	0
25	B2	174	0	113	4	0
25	B3	98	0	71	5	0
25	B5	126	0	67	1	0
26	B1	42	0	56	2	0
26	B2	42	0	56	1	0
26	B3	42	0	56	2	0
26	B5	42	0	56	1	0
27	B1	44	0	56	7	0
27	B2	44	0	56	3	0
27	B3	44	0	56	1	0
27	B5	44	0	56	1	0
28	B5	33	0	36	0	0
All	All	35123	0	34468	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (422) 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)
13:B1:203:VAL:HG21	27:B1:317:XAT:C40	1.73	1.19
8:BH:127:LEU:HD13	8:BH:129:ILE:HG22	1.28	1.13
13:B1:203:VAL:CG2	27:B1:317:XAT:C40	2.27	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:169:LEU:HD21	12:BL:175:LYS:HD2	1.32	1.09
13:B1:58:LEU:HD11	13:B1:67:GLY:HA2	1.16	1.07
13:B1:203:VAL:HG21	27:B1:317:XAT:H403	1.35	1.05
2:BB:91:ILE:HG22	17:BB:811:CLA:OBD	1.58	1.04
1:BA:224:PHE:CE1	1:BA:250:LEU:HD11	1.94	1.02
2:BB:467:HIS:HA	2:BB:478:LEU:HD12	1.02	1.02
12:BL:169:LEU:CD2	12:BL:175:LYS:HD2	1.89	1.01
13:B1:203:VAL:CG2	27:B1:317:XAT:H401	1.91	1.00
2:BB:467:HIS:HA	2:BB:478:LEU:CD1	1.92	1.00
13:B1:58:LEU:CD1	13:B1:67:GLY:HA2	1.91	0.99
2:BB:467:HIS:CA	2:BB:478:LEU:HD12	1.92	0.98
5:BE:87:VAL:HG21	5:BE:138:VAL:CG1	1.94	0.97
1:BA:341:ILE:CG2	1:BA:409:PHE:CE1	2.56	0.89
1:BA:341:ILE:HD11	1:BA:419:ARG:O	1.74	0.87
1:BA:341:ILE:HG21	1:BA:409:PHE:CZ	2.10	0.86
12:BL:169:LEU:HD21	12:BL:175:LYS:CD	2.06	0.86
3:BC:23:THR:HG21	3:BC:47:ASP:O	1.77	0.85
13:B1:203:VAL:HG23	27:B1:317:XAT:H401	1.59	0.85
1:BA:341:ILE:HG23	1:BA:409:PHE:HE1	1.42	0.84
8:BH:127:LEU:HD13	8:BH:129:ILE:CG2	2.08	0.83
2:BB:366:THR:HG23	2:BB:729:THR:CG2	2.07	0.83
1:BA:341:ILE:HG23	1:BA:409:PHE:CE1	2.15	0.81
1:BA:341:ILE:HG21	1:BA:409:PHE:HZ	1.46	0.81
8:BH:127:LEU:HD12	8:BH:127:LEU:O	1.79	0.81
3:BC:11:CYS:SG	3:BC:64:SER:HB3	2.20	0.80
1:BA:341:ILE:CG2	1:BA:409:PHE:CZ	2.64	0.79
5:BE:87:VAL:CG2	5:BE:138:VAL:CG1	2.61	0.78
6:BF:114:GLU:HB3	6:BF:118:ARG:HH21	1.49	0.77
13:B1:58:LEU:HD13	13:B1:65:ASP:OD1	1.86	0.75
8:BH:127:LEU:HD11	8:BH:130:LYS:HB2	1.68	0.75
13:B1:58:LEU:HD12	13:B1:58:LEU:O	1.85	0.75
1:BA:522:LEU:HD12	1:BA:523:PRO:O	1.87	0.74
3:BC:23:THR:HG22	3:BC:23:THR:O	1.88	0.74
4:BD:107:GLU:O	4:BD:137:ARG:NH1	2.22	0.72
3:BC:61:ASP:N	5:BE:131:ASN:OD1	2.23	0.71
1:BA:594:LEU:HD21	17:BA:830:CLA:HBC1	1.70	0.71
8:BH:127:LEU:CD1	8:BH:129:ILE:HG22	2.13	0.71
2:BB:91:ILE:CG1	2:BB:112:PRO:HB2	2.21	0.70
2:BB:303:ASP:OD2	7:BG:94:GLN:HA	1.90	0.70
25:B1:303:CHL:OBD	16:B5:149:LYS:NZ	2.23	0.70
13:B1:82:ARG:NH1	17:B1:305:CLA:O1D	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B1:203:VAL:CG2	27:B1:317:XAT:H403	2.08	0.69
13:B1:232:ASN:ND2	16:B5:134:THR:OG1	2.25	0.69
5:BE:87:VAL:HG21	5:BE:138:VAL:HG12	1.73	0.69
2:BB:294:ASN:ND2	7:BG:112:ALA:O	2.25	0.69
1:BA:713:GLN:NE2	5:BE:95:TYR:OH	2.26	0.68
2:BB:364:ASP:HB2	8:BH:145:LEU:HD11	1.75	0.68
14:B2:152:GLU:OE1	14:B2:155:ARG:NH2	2.27	0.68
1:BA:330:PHE:O	1:BA:426:ARG:NH2	2.26	0.67
15:B3:245:VAL:HG23	15:B3:246:THR:HG23	1.77	0.67
11:BK:54:ASN:ND2	17:BK:203:CLA:OBD	2.28	0.67
2:BB:450:GLU:OE2	6:BF:119:ARG:NE	2.28	0.66
2:BB:294:ASN:CG	7:BG:112:ALA:O	2.34	0.66
2:BB:436:LEU:HD22	2:BB:453:ILE:HG21	1.76	0.66
6:BF:193:ALA:O	6:BF:197:ILE:N	2.28	0.66
2:BB:350:GLN:NE2	2:BB:372:TYR:OH	2.28	0.66
4:BD:72:THR:OG1	4:BD:122:LEU:HB2	1.96	0.65
2:BB:464:GLN:NE2	17:BB:838:CLA:OBD	2.29	0.65
2:BB:71:GLN:NE2	17:BB:809:CLA:O1D	2.30	0.65
8:BH:100:ARG:NH2	12:BL:159:LYS:O	2.30	0.65
3:BC:11:CYS:SG	3:BC:64:SER:CB	2.84	0.65
1:BA:331:THR:O	1:BA:331:THR:HG22	1.95	0.64
3:BC:47:ASP:OD2	4:BD:128:LYS:NZ	2.28	0.64
20:BA:851:BCR:H401	17:BB:834:CLA:HMB3	1.78	0.64
1:BA:348:ALA:HB1	20:BA:849:BCR:H393	1.78	0.64
12:BL:115:LEU:HD22	12:BL:142:LEU:HD23	1.78	0.64
2:BB:351:HIS:ND1	17:BB:819:CLA:OBD	2.31	0.64
3:BC:7:ILE:HG23	3:BC:11:CYS:SG	2.37	0.64
5:BE:87:VAL:CG2	5:BE:138:VAL:HG13	2.27	0.64
2:BB:366:THR:OG1	2:BB:729:THR:HG23	1.98	0.63
2:BB:294:ASN:HD21	7:BG:112:ALA:HA	1.62	0.63
1:BA:12:ILE:HD11	17:BA:812:CLA:O1A	1.99	0.63
2:BB:91:ILE:HG22	17:BB:811:CLA:CAD	2.28	0.63
2:BB:91:ILE:HG13	2:BB:112:PRO:HB2	1.79	0.62
5:BE:131:ASN:ND2	5:BE:132:ASN:O	2.33	0.62
4:BD:125:LEU:HD11	4:BD:131:CYS:HB3	1.82	0.62
15:B3:186:LEU:HD22	20:B3:618:BCR:H342	1.82	0.62
12:BL:90:ASN:O	12:BL:95:ARG:NH1	2.32	0.61
1:BA:676:PHE:CG	20:BA:851:BCR:H363	2.35	0.61
17:BB:818:CLA:O1A	7:BG:152:ASN:ND2	2.32	0.61
16:B5:88:GLU:OE2	16:B5:211:ARG:NH1	2.33	0.61
1:BA:582:CYS:N	2:BB:668:ARG:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B2:211:LYS:NZ	19:B2:317:LHG:O5	2.31	0.60
2:BB:91:ILE:CG2	17:BB:811:CLA:OBD	2.42	0.60
16:B5:92:SER:HB2	16:B5:210:GLY:HA3	1.83	0.60
2:BB:126:THR:HG22	2:BB:270:LEU:HD21	1.83	0.60
2:BB:366:THR:HG23	2:BB:729:THR:HG21	1.83	0.60
2:BB:456:GLU:OE1	6:BF:137:HIS:ND1	2.35	0.60
13:B1:59:ASP:OD1	13:B1:59:ASP:N	2.35	0.60
13:B1:81:GLU:OE2	13:B1:166:LYS:NZ	2.34	0.60
5:BE:87:VAL:CG2	5:BE:138:VAL:HG12	2.32	0.59
1:BA:331:THR:HG21	19:BA:846:LHG:O2	2.03	0.59
3:BC:47:ASP:OD1	4:BD:150:ARG:NH2	2.36	0.59
1:BA:223:GLN:HG2	1:BA:250:LEU:HD13	1.85	0.58
1:BA:717:LEU:N	18:BA:843:PQN:O4	2.35	0.58
17:BB:805:CLA:HBC2	17:BB:805:CLA:HHD	1.84	0.58
2:BB:292:ARG:NH1	2:BB:296:GLY:O	2.36	0.58
1:BA:429:ARG:NH1	4:BD:79:GLY:O	2.37	0.58
20:BB:803:BCR:H353	17:BB:834:CLA:CGA	2.34	0.58
2:BB:339:ALA:HB2	20:BB:849:BCR:H372	1.85	0.57
20:BB:803:BCR:HC31	24:BJ:104:SQD:H92	1.86	0.57
1:BA:92:GLY:HA2	1:BA:96:SER:OG	2.04	0.57
14:B2:184:PRO:HB3	25:B2:306:CHL:HBC2	1.84	0.57
1:BA:559:ARG:O	4:BD:127:ARG:NH1	2.37	0.57
20:BA:855:BCR:H312	17:BB:810:CLA:HMC2	1.86	0.57
3:BC:61:ASP:OD2	5:BE:91:ARG:NE	2.38	0.57
2:BB:397:ASP:OD1	4:BD:195:LYS:NZ	2.31	0.57
1:BA:331:THR:CG2	1:BA:423:LEU:CD2	2.83	0.57
2:BB:2:ALA:O	2:BB:7:ARG:NH2	2.37	0.57
2:BB:366:THR:HA	2:BB:729:THR:HG21	1.87	0.57
20:BL:305:BCR:H23C	20:BL:305:BCR:H392	1.87	0.56
16:B5:208:LYS:NZ	17:B5:610:CLA:O1D	2.36	0.56
15:B3:224:LYS:NZ	17:B3:611:CLA:O2D	2.38	0.56
3:BC:15:THR:O	3:BC:19:ARG:NH2	2.38	0.56
3:BC:23:THR:CG2	3:BC:47:ASP:O	2.51	0.56
17:B2:302:CLA:HBC3	27:B2:315:XAT:H203	1.87	0.56
15:B3:161:ALA:HA	25:B3:601:CHL:H2	1.86	0.56
1:BA:676:PHE:CD2	20:BA:851:BCR:H363	2.40	0.56
20:BA:851:BCR:C40	17:BB:834:CLA:HMB3	2.36	0.56
13:B1:104:PRO:O	13:B1:109:TYR:N	2.36	0.56
17:B2:311:CLA:CHB	17:B2:312:CLA:HMD3	2.36	0.56
17:BA:801:CLA:HMB3	17:BB:802:CLA:OBD	2.05	0.56
2:BB:574:ASP:OD1	2:BB:706:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:536:ILE:HG23	17:BA:801:CLA:H193	1.88	0.55
13:B1:46:ALA:O	13:B1:54:ARG:NH2	2.39	0.55
1:BA:224:PHE:CZ	1:BA:250:LEU:HD11	2.40	0.55
8:BH:127:LEU:HD12	8:BH:130:LYS:H	1.70	0.55
3:BC:23:THR:HG22	3:BC:47:ASP:HB3	1.88	0.55
13:B1:137:THR:OG1	13:B1:138:LEU:N	2.39	0.55
15:B3:137:THR:OG1	15:B3:148:TYR:OH	2.20	0.55
15:B3:105:ARG:NH1	25:B3:607:CHL:OBD	2.38	0.54
17:BB:802:CLA:HMB1	17:BB:802:CLA:HBB1	1.90	0.54
1:BA:118:ILE:HD12	10:BJ:27:ILE:HG23	1.87	0.54
16:B5:65:GLY:O	16:B5:211:ARG:NH2	2.40	0.54
3:BC:66:ARG:HD2	4:BD:185:ILE:HD11	1.89	0.54
1:BA:92:GLY:O	1:BA:96:SER:HB2	2.08	0.54
2:BB:615:TYR:OH	2:BB:621:ARG:NH2	2.41	0.54
20:BB:803:BCR:H381	17:BF:301:CLA:HMC2	1.90	0.54
2:BB:182:LEU:HD13	17:BB:815:CLA:HHB	1.90	0.54
2:BB:461:GLN:OE1	6:BF:70:SER:OG	2.21	0.54
14:B2:73:PHE:N	17:B2:301:CLA:OBD	2.41	0.54
15:B3:256:ASP:O	15:B3:264:ASN:ND2	2.41	0.54
10:BJ:36:ALA:CB	24:BJ:104:SQD:H441	2.38	0.54
12:BL:150:LEU:HB3	12:BL:191:THR:HG22	1.90	0.53
9:BI:6:ASN:O	9:BI:9:SER:OG	2.26	0.53
1:BA:464:ARG:NH2	17:BA:834:CLA:O1D	2.41	0.53
16:B5:135:LEU:HD11	25:B5:605:CHL:HMD3	1.91	0.53
17:BB:828:CLA:H142	20:BB:848:BCR:C21	2.38	0.53
15:B3:139:VAL:HG13	15:B3:140:ILE:HG13	1.91	0.53
1:BA:348:ALA:HB1	20:BA:849:BCR:C39	2.38	0.53
17:BA:832:CLA:CBB	20:BL:301:BCR:H342	2.38	0.53
17:BA:804:CLA:HMA2	17:BA:811:CLA:HMD2	1.91	0.53
17:BB:806:CLA:HMC3	17:BB:808:CLA:OBD	2.09	0.53
17:BB:823:CLA:CAD	20:BB:845:BCR:H312	2.39	0.53
1:BA:143:GLN:OE1	1:BA:143:GLN:N	2.42	0.52
1:BA:599:ASN:OD1	17:BA:801:CLA:H43	2.09	0.52
2:BB:122:GLN:OE1	2:BB:122:GLN:N	2.41	0.52
1:BA:54:HIS:ND1	17:BA:806:CLA:O1A	2.39	0.52
1:BA:223:GLN:CG	1:BA:250:LEU:HD13	2.40	0.52
2:BB:700:LEU:HD22	2:BB:704:GLN:NE2	2.25	0.52
6:BF:102:GLU:OE2	6:BF:102:GLU:N	2.42	0.52
1:BA:341:ILE:CG2	1:BA:409:PHE:HE1	2.04	0.51
1:BA:570:ARG:NH1	17:BA:830:CLA:O2D	2.43	0.51
20:BA:851:BCR:H362	17:BB:802:CLA:C4	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:60:TRP:NE1	17:BB:829:CLA:OBD	2.43	0.51
20:BB:847:BCR:H383	20:BB:847:BCR:H23C	1.92	0.51
16:B5:72:LEU:HD22	27:B5:615:XAT:H372	1.92	0.51
1:BA:341:ILE:HG22	1:BA:341:ILE:O	2.09	0.51
16:B5:69:PHE:N	17:B5:602:CLA:OBD	2.38	0.51
1:BA:16:ARG:NH1	15:B3:86:GLY:O	2.43	0.51
5:BE:87:VAL:HG22	5:BE:138:VAL:HG13	1.91	0.51
6:BF:209:ARG:NH1	19:BF:305:LHG:O4	2.43	0.51
13:B1:98:VAL:HG13	13:B1:99:PRO:HD3	1.93	0.51
17:BB:801:CLA:HMB1	17:BB:801:CLA:HBB1	1.93	0.51
12:BL:169:LEU:HD23	12:BL:175:LYS:HA	1.93	0.51
1:BA:331:THR:HG22	1:BA:423:LEU:CD2	2.40	0.51
1:BA:691:TYR:OH	2:BB:533:ILE:HA	2.11	0.51
1:BA:118:ILE:HG23	1:BA:119:VAL:HG22	1.93	0.51
2:BB:303:ASP:OD1	2:BB:303:ASP:O	2.29	0.51
13:B1:98:VAL:HG23	13:B1:205:PHE:CZ	2.46	0.51
16:B5:191:GLY:O	16:B5:194:LYS:NZ	2.41	0.51
5:BE:140:GLU:OE1	5:BE:140:GLU:N	2.44	0.50
26:B3:616:LUT:H381	26:B3:616:LUT:H28	1.92	0.50
1:BA:471:ASP:OD1	1:BA:477:GLN:NE2	2.45	0.50
12:BL:79:THR:OG1	12:BL:80:SER:N	2.45	0.50
11:BK:128:GLY:O	11:BK:129:ALA:C	2.50	0.50
1:BA:331:THR:HG22	1:BA:423:LEU:HD21	1.93	0.50
1:BA:341:ILE:HG12	1:BA:419:ARG:HB3	1.92	0.50
17:BA:801:CLA:H18	17:BA:802:CLA:C1B	2.42	0.50
2:BB:726:ILE:O	2:BB:730:SER:OG	2.22	0.50
14:B2:109:PHE:O	14:B2:113:PHE:N	2.45	0.50
17:BG:201:CLA:CMC	20:BG:203:BCR:H332	2.42	0.50
1:BA:674:ALA:HB1	1:BA:733:GLY:O	2.12	0.49
2:BB:718:ILE:HG21	23:BB:850:DGD:HBG3	1.93	0.49
17:BA:840:CLA:HED3	17:BA:840:CLA:H2A	1.94	0.49
16:B5:103:LEU:O	16:B5:107:LEU:HD23	2.13	0.49
2:BB:366:THR:HG23	2:BB:729:THR:HG23	1.91	0.49
17:BA:842:CLA:H92	20:BL:305:BCR:H392	1.93	0.49
2:BB:208:ARG:NH1	17:BB:816:CLA:O1D	2.46	0.49
15:B3:105:ARG:NH2	15:B3:225:GLU:OE2	2.45	0.49
2:BB:519:VAL:HG23	17:BB:804:CLA:H141	1.94	0.48
6:BF:210:GLU:O	6:BF:215:ASP:N	2.45	0.48
14:B2:124:SER:OG	14:B2:125:TRP:N	2.46	0.48
1:BA:331:THR:O	1:BA:331:THR:CG2	2.62	0.48
20:BB:803:BCR:H23C	20:BB:803:BCR:H382	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:560:LEU:HD11	1:BA:578:ARG:HB3	1.95	0.48
2:BB:469:LYS:NZ	2:BB:509:PHE:O	2.41	0.48
20:BH:202:BCR:H382	20:BH:202:BCR:H371	1.96	0.48
14:B2:234:PRO:O	26:B2:314:LUT:O3	2.31	0.48
3:BC:32:ASP:OD1	3:BC:32:ASP:N	2.47	0.48
16:B5:109:ARG:NH2	16:B5:233:ASP:OD2	2.46	0.48
1:BA:331:THR:CG2	1:BA:423:LEU:HD21	2.44	0.48
2:BB:50:HIS:ND1	17:BB:815:CLA:OBD	2.44	0.48
13:B1:58:LEU:CD1	13:B1:67:GLY:CA	2.80	0.48
2:BB:378:ILE:HG22	2:BB:382:ILE:HD12	1.96	0.48
2:BB:285:LEU:O	2:BB:289:HIS:ND1	2.47	0.47
17:BB:835:CLA:O1A	10:BJ:30:ASN:ND2	2.47	0.47
13:B1:221:LEU:HD22	26:B1:316:LUT:H163	1.95	0.47
15:B3:162:LEU:HB3	20:B3:618:BCR:H363	1.95	0.47
17:BA:801:CLA:HAA1	17:BB:804:CLA:HMB1	1.95	0.47
17:BA:808:CLA:H92	19:BA:845:LHG:H222	1.95	0.47
20:BB:845:BCR:H383	20:BB:845:BCR:H23C	1.96	0.47
2:BB:218:HIS:NE2	2:BB:232:LEU:O	2.48	0.47
2:BB:578:LEU:HD22	17:BB:801:CLA:CBC	2.45	0.47
17:BB:824:CLA:OBD	7:BG:94:GLN:NE2	2.47	0.47
2:BB:182:LEU:HD13	17:BB:815:CLA:CHB	2.44	0.47
17:BA:801:CLA:H111	17:BA:802:CLA:CMA	2.45	0.47
17:BA:801:CLA:HBC1	2:BB:625:TRP:CD1	2.50	0.47
17:BA:819:CLA:CGA	17:BA:829:CLA:HMD1	2.45	0.47
17:BA:829:CLA:C2	20:BA:848:BCR:H342	2.45	0.47
17:BA:832:CLA:HBB1	17:BA:832:CLA:HMB1	1.97	0.47
2:BB:527:LEU:HD12	17:BB:840:CLA:HED1	1.96	0.47
2:BB:616:LEU:HD22	17:BB:802:CLA:HMA2	1.97	0.47
17:BB:815:CLA:HHD	17:BB:815:CLA:HBC2	1.97	0.47
1:BA:25:GLU:N	1:BA:25:GLU:OE1	2.48	0.47
20:BA:851:BCR:H382	20:BA:851:BCR:H23C	1.97	0.47
17:B2:309:CLA:CAB	20:B3:618:BCR:H311	2.45	0.47
15:B3:245:VAL:O	15:B3:273:HIS:N	2.44	0.47
25:B3:601:CHL:HMD2	20:B3:618:BCR:HC21	1.97	0.47
1:BA:574:ASP:OD2	1:BA:578:ARG:NH2	2.44	0.47
2:BB:177:HIS:CG	17:BB:815:CLA:HMC2	2.50	0.47
17:BB:825:CLA:HMB3	17:BB:843:CLA:O1D	2.15	0.47
7:BG:80:ARG:HE	7:BG:125:ILE:HG22	1.80	0.47
14:B2:176:LEU:HD12	25:B2:306:CHL:HBC3	1.97	0.47
1:BA:100:ALA:O	1:BA:103:SER:OG	2.30	0.46
1:BA:286:LEU:N	1:BA:372:PRO:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:328:GLY:HA3	1:BA:331:THR:HB	1.97	0.46
15:B3:227:LYS:NZ	19:B3:619:LHG:O5	2.33	0.46
1:BA:445:LEU:HD11	17:BA:838:CLA:HMB1	1.98	0.46
1:BA:450:PHE:CZ	1:BA:454:ILE:HD11	2.50	0.46
17:BA:801:CLA:HMB3	17:BB:802:CLA:CAD	2.45	0.46
2:BB:105:THR:HG21	8:BH:133:PRO:HG3	1.96	0.46
17:BB:830:CLA:H202	20:BB:846:BCR:H352	1.97	0.46
1:BA:96:SER:OG	1:BA:112:ALA:HA	2.15	0.46
17:BA:801:CLA:HBC1	2:BB:625:TRP:HD1	1.81	0.46
2:BB:324:ASP:O	2:BB:328:ASN:ND2	2.45	0.46
2:BB:377:TYR:HH	2:BB:717:TYR:HE1	1.61	0.46
13:B1:196:ARG:NH2	17:B1:304:CLA:O2D	2.48	0.46
13:B1:227:ASP:N	13:B1:227:ASP:OD1	2.49	0.46
14:B2:107:GLY:HA3	27:B2:315:XAT:H182	1.95	0.46
2:BB:408:LEU:O	2:BB:411:MET:HB3	2.15	0.46
15:B3:114:ALA:HB1	15:B3:134:TRP:HB3	1.98	0.46
1:BA:662:SER:OG	1:BA:663:SER:N	2.49	0.46
17:BB:828:CLA:H142	20:BB:848:BCR:C22	2.46	0.46
4:BD:154:ASN:OD1	4:BD:155:GLY:N	2.49	0.46
25:B2:306:CHL:HMB3	20:B2:316:BCR:H362	1.97	0.46
15:B3:250:PRO:O	26:B3:616:LUT:O3	2.34	0.46
17:BB:807:CLA:HBB1	17:BB:807:CLA:HMB1	1.98	0.46
13:B1:203:VAL:HG21	27:B1:317:XAT:H402	1.85	0.46
1:BA:303:LEU:O	1:BA:307:HIS:ND1	2.43	0.45
1:BA:746:ILE:O	1:BA:750:GLY:HA2	2.15	0.45
2:BB:540:ASP:N	2:BB:540:ASP:OD1	2.48	0.45
7:BG:72:THR:HG23	7:BG:136:GLY:HA2	1.98	0.45
2:BB:519:VAL:HG21	2:BB:593:TYR:HB2	1.99	0.45
1:BA:512:LEU:HD12	1:BA:522:LEU:CD2	2.46	0.45
14:B2:226:GLN:O	14:B2:230:THR:N	2.44	0.45
2:BB:182:LEU:HG	17:BB:815:CLA:H43	1.98	0.45
1:BA:599:ASN:HD21	17:BA:801:CLA:H191	1.80	0.45
1:BA:14:VAL:HG21	17:BA:810:CLA:HED3	1.99	0.45
17:BA:808:CLA:H93	20:BJ:103:BCR:H343	1.98	0.45
17:BF:302:CLA:HMB3	10:BJ:26:LEU:HD21	1.98	0.45
1:BA:215:VAL:HA	1:BA:219:LEU:HD12	1.99	0.45
2:BB:366:THR:CG2	2:BB:729:THR:CG2	2.89	0.45
1:BA:600:ALA:O	1:BA:604:VAL:HG23	2.17	0.45
20:BJ:101:BCR:H392	20:BJ:101:BCR:H23C	1.98	0.45
11:BK:65:LEU:HD11	20:BK:204:BCR:C36	2.47	0.45
1:BA:341:ILE:CG2	1:BA:341:ILE:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:421:ASN:OD1	1:BA:422:ASP:N	2.50	0.44
2:BB:516:ASP:OD2	2:BB:597:LYS:NZ	2.49	0.44
12:BL:93:GLY:N	17:BL:303:CLA:OBD	2.51	0.44
13:B1:50:PRO:O	16:B5:160:GLN:NE2	2.50	0.44
1:BA:410:MET:O	1:BA:556:ARG:NH2	2.46	0.44
1:BA:674:ALA:HB2	1:BA:736:ALA:HB3	1.98	0.44
2:BB:91:ILE:HG12	2:BB:112:PRO:HB2	1.99	0.44
1:BA:346:TRP:HE3	17:BA:805:CLA:HMD2	1.82	0.44
1:BA:529:ALA:HB1	1:BA:638:SER:OG	2.17	0.44
2:BB:646:TRP:O	2:BB:723:ALA:HB1	2.16	0.44
1:BA:118:ILE:HG12	1:BA:119:VAL:HG13	1.99	0.44
1:BA:717:LEU:CD2	18:BA:843:PQN:H143	2.48	0.44
17:BB:828:CLA:HMA3	20:BB:849:BCR:HC41	1.99	0.44
17:B2:301:CLA:HBC2	25:B3:601:CHL:HBB2	1.99	0.44
16:B5:247:ILE:N	17:B5:612:CLA:O1A	2.49	0.44
2:BB:529:THR:HG21	2:BB:582:TRP:CE2	2.52	0.44
2:BB:578:LEU:HD22	17:BB:801:CLA:HBC1	1.99	0.44
4:BD:69:ASP:N	4:BD:69:ASP:OD1	2.51	0.44
11:BK:94:GLN:NE2	15:B3:60:SER:OG	2.50	0.44
1:BA:139:SER:OG	17:BA:808:CLA:OBD	2.29	0.44
2:BB:700:LEU:HD21	18:BB:844:PQN:H152	1.99	0.44
3:BC:2:SER:OG	3:BC:3:HIS:N	2.48	0.44
1:BA:674:ALA:CB	1:BA:736:ALA:HB3	2.48	0.44
17:B5:611:CLA:HMB2	26:B5:614:LUT:C34	2.48	0.44
1:BA:540:THR:HB	1:BA:600:ALA:HB2	1.99	0.43
20:BF:304:BCR:H383	20:BF:304:BCR:H23C	1.99	0.43
16:B5:240:SER:OG	16:B5:241:ASN:ND2	2.51	0.43
13:B1:208:GLN:HE22	26:B1:316:LUT:H42	1.83	0.43
17:BB:823:CLA:HMB1	17:BB:823:CLA:HBB1	2.00	0.43
12:BL:168:SER:O	12:BL:168:SER:OG	2.33	0.43
15:B3:83:ASP:O	15:B3:87:THR:HG21	2.17	0.43
2:BB:725:LEU:O	2:BB:729:THR:HG22	2.18	0.43
4:BD:160:LEU:HD23	4:BD:163:LYS:HE2	2.00	0.43
17:BG:201:CLA:HMC1	20:BG:203:BCR:H332	1.99	0.43
11:BK:65:LEU:HD11	20:BK:204:BCR:H362	1.99	0.43
17:BA:827:CLA:HBB1	17:BA:827:CLA:HMB1	2.01	0.43
2:BB:293:THR:HG22	2:BB:294:ASN:H	1.83	0.43
2:BB:728:SER:O	2:BB:732:LYS:HG2	2.19	0.43
17:BB:840:CLA:HBB1	17:BB:840:CLA:HMB1	2.01	0.43
17:BA:803:CLA:CMD	6:BF:186:ILE:HG23	2.49	0.43
14:B2:100:TRP:CE2	25:B2:306:CHL:HED2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BA:801:CLA:HBD	17:BA:801:CLA:HED3	1.69	0.43
2:BB:329:SER:HG	2:BB:393:PHE:HD1	1.66	0.43
17:BB:802:CLA:HMB3	17:BB:804:CLA:H191	2.01	0.43
2:BB:101:VAL:O	2:BB:105:THR:HG23	2.19	0.43
4:BD:125:LEU:HD12	4:BD:125:LEU:H	1.84	0.43
14:B2:99:ARG:NH2	14:B2:209:GLU:OE2	2.49	0.43
5:BE:87:VAL:O	5:BE:101:GLY:N	2.52	0.42
16:B5:195:ASP:OD1	16:B5:196:VAL:N	2.52	0.42
17:BA:801:CLA:HMB1	17:BB:804:CLA:HAA1	2.01	0.42
17:BA:841:CLA:H41	18:BA:843:PQN:H191	2.00	0.42
2:BB:4:ARG:NH2	2:BB:13:ALA:O	2.52	0.42
17:BB:841:CLA:HAB	18:BB:844:PQN:H141	2.00	0.42
13:B1:233:ILE:HD12	17:B1:314:CLA:H43	2.01	0.42
17:BA:803:CLA:HMD3	6:BF:186:ILE:HG23	2.02	0.42
7:BG:84:PHE:CD2	7:BG:125:ILE:HG12	2.53	0.42
14:B2:116:LYS:NZ	14:B2:236:ASP:OD2	2.52	0.42
16:B5:247:ILE:HD12	17:B5:612:CLA:HMD2	2.01	0.42
1:BA:217:VAL:HG13	1:BA:237:PRO:HB3	2.01	0.42
2:BB:441:ASP:OD1	2:BB:616:LEU:N	2.52	0.42
2:BB:671:TRP:CH2	18:BB:844:PQN:H2M3	2.55	0.42
7:BG:132:VAL:HG21	17:BG:202:CLA:HMA1	2.01	0.42
3:BC:23:THR:CG2	3:BC:47:ASP:HB3	2.49	0.42
6:BF:126:TYR:OH	24:BJ:104:SQD:H4	2.19	0.42
1:BA:443:ILE:HD11	20:BA:855:BCR:H402	2.02	0.42
2:BB:123:TRP:CZ2	17:BB:815:CLA:H191	2.55	0.42
2:BB:476:VAL:HG22	2:BB:477:LEU:HG	2.00	0.42
17:BB:815:CLA:H41	17:BB:820:CLA:CBC	2.50	0.42
8:BH:127:LEU:CD1	8:BH:130:LYS:H	2.33	0.42
1:BA:536:ILE:HD12	17:BA:801:CLA:H172	2.01	0.42
17:BA:808:CLA:H91	17:BA:811:CLA:H193	2.02	0.42
17:BA:828:CLA:HBB1	17:BA:828:CLA:HMB1	2.02	0.42
2:BB:292:ARG:NH2	7:BG:114:GLU:OE1	2.52	0.42
17:BB:801:CLA:O1D	20:BB:803:BCR:H401	2.19	0.42
1:BA:405:HIS:CE1	17:BA:830:CLA:NA	2.87	0.42
1:BA:522:LEU:HB2	1:BA:523:PRO:HD2	2.02	0.42
1:BA:543:VAL:HG11	1:BA:596:TRP:CE2	2.55	0.42
1:BA:545:VAL:HG11	17:BA:839:CLA:HMB3	2.01	0.42
1:BA:560:LEU:HD13	2:BB:672:GLN:HG2	2.01	0.42
2:BB:194:LEU:HA	2:BB:198:ALA:HB3	2.02	0.42
2:BB:507:SER:O	2:BB:507:SER:OG	2.33	0.42
20:BA:855:BCR:H391	17:BB:805:CLA:O1D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BL:301:BCR:HC8	20:BL:301:BCR:H311	2.02	0.42
20:BA:856:BCR:H382	20:BA:856:BCR:H23C	2.01	0.41
1:BA:357:LEU:O	1:BA:361:THR:OG1	2.36	0.41
1:BA:574:ASP:OD2	3:BC:53:ARG:NH2	2.53	0.41
1:BA:667:TYR:O	1:BA:740:ALA:HB1	2.21	0.41
3:BC:23:THR:O	3:BC:23:THR:CG2	2.59	0.41
5:BE:84:GLY:N	5:BE:103:VAL:O	2.47	0.41
8:BH:127:LEU:CD1	8:BH:129:ILE:CG2	2.88	0.41
6:BF:202:ILE:HD13	6:BF:206:ALA:HB2	2.02	0.41
20:BJ:101:BCR:H11C	20:BJ:101:BCR:H341	1.94	0.41
13:B1:233:ILE:O	13:B1:236:ILE:HG22	2.20	0.41
17:BA:801:CLA:HAA2	17:BA:801:CLA:HED2	2.02	0.41
2:BB:645:VAL:HG21	17:BB:810:CLA:HAC1	2.02	0.41
17:BB:812:CLA:H142	8:BH:114:LEU:HD23	2.02	0.41
16:B5:60:ASP:OD1	16:B5:60:ASP:N	2.53	0.41
1:BA:346:TRP:CE3	17:BA:805:CLA:HMD2	2.55	0.41
2:BB:176:ASN:ND2	2:BB:291:TYR:O	2.50	0.41
20:BJ:103:BCR:H382	20:BJ:103:BCR:H23C	2.01	0.41
2:BB:366:THR:CG2	2:BB:729:THR:HG23	2.49	0.41
17:BB:821:CLA:HMB2	17:BB:826:CLA:HMA3	2.01	0.41
14:B2:212:ASN:O	14:B2:215:LEU:HD23	2.21	0.41
1:BA:426:ARG:O	1:BA:430:HIS:ND1	2.48	0.41
1:BA:599:ASN:OD1	17:BA:801:CLA:H201	2.20	0.41
2:BB:595:HIS:HE1	2:BB:728:SER:OG	2.04	0.41
17:BB:827:CLA:HMA1	20:BB:849:BCR:H14C	2.02	0.41
10:BJ:7:TYR:O	10:BJ:10:VAL:HG12	2.21	0.41
27:B2:315:XAT:C28	27:B2:315:XAT:H381	2.51	0.41
17:BA:801:CLA:H2	17:BA:802:CLA:O1D	2.21	0.41
17:BA:832:CLA:HAA1	12:BL:79:THR:HG22	2.03	0.41
2:BB:659:THR:H	2:BB:659:THR:HG1	1.65	0.41
17:BB:812:CLA:H42	12:BL:134:ALA:HB1	2.02	0.41
3:BC:15:THR:HG22	3:BC:28:MET:HG3	2.03	0.41
20:BG:203:BCR:H20C	20:BG:203:BCR:H361	1.36	0.41
13:B1:234:GLY:HA2	13:B1:237:VAL:HG22	2.02	0.41
17:BA:840:CLA:H91	17:BF:302:CLA:HBC3	2.03	0.41
20:BA:847:BCR:H311	20:BA:847:BCR:C8	2.51	0.41
13:B1:98:VAL:HG23	13:B1:205:PHE:HZ	1.84	0.41
20:B2:316:BCR:H331	20:B2:316:BCR:HC8	2.03	0.41
2:BB:682:HIS:NE2	2:BB:691:ILE:O	2.47	0.40
1:BA:723:ARG:NH2	21:BA:852:SF4:S1	2.95	0.40
2:BB:732:LYS:HG3	2:BB:734:GLY:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B5:150:ARG:NH2	17:B5:608:CLA:O1D	2.50	0.40
1:BA:77:GLN:HB2	17:BA:805:CLA:HMB2	2.02	0.40
2:BB:646:TRP:CZ2	2:BB:726:ILE:HG21	2.56	0.40
20:BA:851:BCR:H362	17:BB:802:CLA:H42	2.03	0.40
2:BB:223:GLY:O	2:BB:227:THR:OG1	2.20	0.40
17:BB:812:CLA:HMC3	20:BI:101:BCR:C18	2.50	0.40
25:B3:607:CHL:HMB3	20:B3:618:BCR:C17	2.52	0.40
1:BA:512:LEU:HD12	1:BA:522:LEU:HD22	2.04	0.40
15:B3:134:TRP:HB2	27:B3:617:XAT:H173	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	BA	740/750 (99%)	692 (94%)	48 (6%)	0	100	100
2	BB	731/734 (100%)	695 (95%)	36 (5%)	0	100	100
3	BC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	BD	141/204 (69%)	121 (86%)	18 (13%)	2 (1%)	9	34
5	BE	67/143 (47%)	61 (91%)	6 (9%)	0	100	100
6	BF	152/221 (69%)	149 (98%)	3 (2%)	0	100	100
7	BG	92/160 (58%)	85 (92%)	7 (8%)	0	100	100
8	BH	93/145 (64%)	86 (92%)	7 (8%)	0	100	100
9	BI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
10	BJ	41/44 (93%)	38 (93%)	3 (7%)	0	100	100
11	BK	60/130 (46%)	54 (90%)	6 (10%)	0	100	100
12	BL	157/219 (72%)	149 (95%)	8 (5%)	0	100	100
13	B1	168/241 (70%)	160 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	B2	206/257 (80%)	191 (93%)	15 (7%)	0	100	100
15	B3	219/273 (80%)	206 (94%)	13 (6%)	0	100	100
16	B5	204/256 (80%)	188 (92%)	15 (7%)	1 (0%)	25	56
All	All	3180/3895 (82%)	2978 (94%)	199 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	164	ASP
16	B5	49	TRP
4	BD	162	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	601/610 (98%)	595 (99%)	6 (1%)	73	82
2	BB	597/600 (100%)	588 (98%)	9 (2%)	60	75
3	BC	70/71 (99%)	70 (100%)	0	100	100
4	BD	121/170 (71%)	117 (97%)	4 (3%)	33	58
5	BE	58/114 (51%)	58 (100%)	0	100	100
6	BF	126/185 (68%)	126 (100%)	0	100	100
7	BG	79/133 (59%)	77 (98%)	2 (2%)	42	65
8	BH	77/113 (68%)	77 (100%)	0	100	100
9	BI	29/33 (88%)	29 (100%)	0	100	100
10	BJ	38/39 (97%)	38 (100%)	0	100	100
11	BK	46/95 (48%)	45 (98%)	1 (2%)	47	68
12	BL	120/174 (69%)	118 (98%)	2 (2%)	56	73
13	B1	138/190 (73%)	134 (97%)	4 (3%)	37	61
14	B2	165/205 (80%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	B3	170/211 (81%)	170 (100%)	0	100	100
16	B5	167/205 (82%)	164 (98%)	3 (2%)	54	72
All	All	2602/3148 (83%)	2571 (99%)	31 (1%)	66	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	244	ARG
1	BA	269	TYR
1	BA	275	PHE
1	BA	361	THR
1	BA	591	PHE
1	BA	660	TYR
2	BB	5	PHE
2	BB	96	PHE
2	BB	332	PHE
2	BB	353	TYR
2	BB	364	ASP
2	BB	407	VAL
2	BB	544	SER
2	BB	576	PHE
2	BB	638	PHE
4	BD	125	LEU
4	BD	144	ILE
4	BD	202	TYR
4	BD	203	ASP
7	BG	83	PHE
7	BG	140	HIS
11	BK	93	LEU
12	BL	91	LEU
12	BL	158	PHE
13	B1	47	HIS
13	B1	96	LEU
13	B1	140	THR
13	B1	180	ASP
16	B5	50	LEU
16	B5	91	HIS
16	B5	197	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	214	GLN
1	BA	713	GLN
2	BB	350	GLN
2	BB	595	HIS
4	BD	200	GLN
8	BH	86	GLN
11	BK	94	GLN
13	B1	208	GLN
15	B3	242	GLN
15	B3	253	ASN
16	B5	241	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

205 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	$\#\|Z\| > 2$
17	CLA	BA	832	-	56,64,73	1.59	8 (14%)	65,102,113	1.31	8 (12%)
17	CLA	B1	310	13	38,47,73	1.99	7 (18%)	47,82,113	1.54	10 (21%)
19	LHG	B2	317	17	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	B5	610	19	42,50,73	1.86	7 (16%)	48,85,113	1.47	7 (14%)
17	CLA	B1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.51	6 (11%)
17	CLA	BB	837	-	42,50,73	1.86	5 (11%)	48,85,113	1.45	7 (14%)
17	CLA	B3	602	15	60,68,73	1.58	9 (15%)	70,107,113	1.22	8 (11%)
17	CLA	BB	813	-	54,62,73	1.66	8 (14%)	67,100,113	1.50	11 (16%)
17	CLA	BB	831	-	56,64,73	1.63	9 (16%)	65,102,113	1.38	6 (9%)
25	CHL	B2	306	-	46,54,74	2.33	17 (36%)	49,90,114	2.82	20 (40%)
17	CLA	BB	820	-	60,68,73	1.51	7 (11%)	70,107,113	1.62	11 (15%)
17	CLA	BF	301	-	55,63,73	1.58	7 (12%)	62,100,113	1.37	7 (11%)
17	CLA	BB	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.30	7 (9%)
17	CLA	BB	814	-	43,51,73	1.78	6 (13%)	49,86,113	1.48	8 (16%)
21	SF4	BA	852	2,1	0,12,12	-	-	-		
17	CLA	BF	303	-	41,49,73	1.86	6 (14%)	47,84,113	1.47	8 (17%)
17	CLA	BJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
17	CLA	B3	606	-	41,49,73	1.89	7 (17%)	51,84,113	1.73	11 (21%)
17	CLA	BA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	9 (11%)
17	CLA	BB	823	-	47,55,73	1.72	6 (12%)	54,91,113	1.32	8 (14%)
17	CLA	BA	838	-	55,62,73	1.69	8 (14%)	59,99,113	1.45	11 (18%)
17	CLA	BB	815	-	65,73,73	1.47	9 (13%)	76,113,113	1.49	11 (14%)
17	CLA	BB	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.26	8 (10%)
17	CLA	B1	311	13	59,67,73	1.59	6 (10%)	69,106,113	1.22	8 (11%)
17	CLA	B3	603	15	55,63,73	1.61	7 (12%)	64,101,113	1.34	8 (12%)
17	CLA	BA	817	-	60,68,73	1.52	6 (10%)	70,107,113	1.37	11 (15%)
26	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
25	CHL	B2	304	-	42,50,74	2.37	16 (38%)	45,85,114	2.84	18 (40%)
20	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
17	CLA	BB	822	-	41,49,73	1.83	8 (19%)	47,84,113	1.56	7 (14%)
17	CLA	BA	831	-	47,55,73	1.79	8 (17%)	54,91,113	1.49	10 (18%)
17	CLA	B1	306	-	41,49,73	1.86	5 (12%)	47,84,113	1.45	7 (14%)
17	CLA	B2	307	14	45,53,73	1.80	7 (15%)	52,89,113	1.39	8 (15%)
17	CLA	BB	826	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	7 (9%)
17	CLA	BB	828	-	62,70,73	1.51	7 (11%)	72,109,113	1.48	11 (15%)
17	CLA	BB	838	-	50,58,73	1.67	7 (14%)	58,95,113	1.50	9 (15%)
26	LUT	B2	314	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
17	CLA	B3	609	15	41,49,73	1.85	8 (19%)	47,84,113	1.45	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
18	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
17	CLA	BB	843	19	65,73,73	1.52	9 (13%)	76,113,113	1.27	7 (9%)
24	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
17	CLA	BA	842	-	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
20	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
21	SF4	BC	101	3	0,12,12	-	-	-		
17	CLA	BA	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.23	8 (10%)
17	CLA	BA	815	-	42,50,73	1.79	8 (19%)	48,85,113	1.51	6 (12%)
17	CLA	BK	202	-	45,53,73	1.81	6 (13%)	52,89,113	1.47	7 (13%)
17	CLA	BA	822	-	42,50,73	1.83	6 (14%)	48,85,113	1.56	7 (14%)
17	CLA	B2	310	14	44,52,73	1.85	7 (15%)	51,88,113	1.42	7 (13%)
27	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)
17	CLA	B3	612	-	53,62,73	1.69	7 (13%)	61,100,113	1.25	6 (9%)
20	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
17	CLA	BA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	11 (14%)
17	CLA	BB	807	-	65,73,73	1.49	7 (10%)	76,113,113	1.33	10 (13%)
19	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
20	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)
17	CLA	BB	808	2	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
17	CLA	BB	817	-	41,50,73	1.80	7 (17%)	46,85,113	1.48	7 (15%)
17	CLA	B2	303	-	43,51,73	1.84	6 (13%)	48,86,113	1.43	7 (14%)
19	LHG	B1	318	17	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
21	SF4	BC	102	3	0,12,12	-	-	-		
26	LUT	B3	616	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
17	CLA	BA	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.23	7 (9%)
17	CLA	BG	201	-	42,50,73	1.85	7 (16%)	48,85,113	1.28	7 (14%)
25	CHL	B1	303	13	49,58,74	2.23	17 (34%)	52,95,114	2.63	22 (42%)
17	CLA	B5	608	16	44,52,73	1.86	9 (20%)	51,88,113	1.44	7 (13%)
17	CLA	BA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	8 (15%)
17	CLA	B3	613	-	39,48,73	1.93	6 (15%)	44,83,113	1.40	7 (15%)
17	CLA	BB	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.32	7 (9%)
17	CLA	BB	819	-	59,67,73	1.57	9 (15%)	68,105,113	1.40	9 (13%)
17	CLA	BL	304	-	43,51,73	1.78	6 (13%)	49,86,113	1.47	7 (14%)
25	CHL	B3	607	-	45,53,74	2.28	16 (35%)	52,89,114	2.69	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	BA	836	1	45,53,73	1.81	6 (13%)	52,89,113	1.53	8 (15%)
27	XAT	B3	617	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
17	CLA	B3	610	19	39,48,73	1.93	5 (12%)	44,83,113	1.40	7 (15%)
19	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
17	CLA	B5	601	16	46,54,73	1.75	8 (17%)	53,90,113	1.37	7 (13%)
17	CLA	BB	804	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	8 (10%)
17	CLA	B5	612	16	57,65,73	1.62	8 (14%)	66,103,113	1.28	7 (10%)
25	CHL	B1	308	-	40,49,74	2.55	18 (45%)	41,84,114	2.79	17 (41%)
20	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
17	CLA	BA	807	-	50,58,73	1.70	7 (14%)	58,95,113	1.34	7 (12%)
17	CLA	BA	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	8 (10%)
17	CLA	B3	614	-	37,44,73	1.95	9 (24%)	42,77,113	1.35	7 (16%)
17	CLA	BA	809	1	50,58,73	1.73	8 (16%)	58,95,113	1.44	10 (17%)
20	BCR	B2	316	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
20	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
17	CLA	BL	302	12	45,53,73	1.85	8 (17%)	52,89,113	1.60	11 (21%)
17	CLA	B5	611	16	40,49,73	1.87	8 (20%)	45,84,113	1.47	7 (15%)
19	LHG	B3	619	17	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
17	CLA	B2	301	14	65,73,73	1.51	9 (13%)	76,113,113	1.26	10 (13%)
25	CHL	B2	313	14	43,51,74	2.35	15 (34%)	45,86,114	2.87	19 (42%)
17	CLA	BA	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	10 (13%)
17	CLA	BA	829	-	65,73,73	1.49	9 (13%)	76,113,113	1.31	9 (11%)
20	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
19	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
20	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
17	CLA	BA	825	-	65,73,73	1.47	7 (10%)	76,113,113	1.31	6 (7%)
17	CLA	B5	613	-	45,53,73	1.80	7 (15%)	52,89,113	1.37	7 (13%)
25	CHL	B2	305	-	43,51,74	2.40	16 (37%)	45,86,114	2.78	17 (37%)
20	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
27	XAT	B2	315	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
20	BCR	BH	202	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
17	CLA	BA	837	-	51,59,73	1.63	8 (15%)	59,96,113	1.47	7 (11%)
17	CLA	B5	604	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
20	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
17	CLA	BB	827	-	62,70,73	1.52	8 (12%)	72,109,113	1.27	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	BA	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.43	6 (11%)
17	CLA	BB	811	2	65,73,73	1.48	10 (15%)	76,113,113	1.37	9 (11%)
17	CLA	BA	824	-	55,63,73	1.63	9 (16%)	64,101,113	1.39	8 (12%)
17	CLA	B1	309	-	43,52,73	1.85	7 (16%)	49,88,113	1.44	7 (14%)
17	CLA	B3	611	15	43,51,73	1.82	5 (11%)	49,86,113	1.44	8 (16%)
17	CLA	BB	818	-	55,63,73	1.61	8 (14%)	64,101,113	1.33	8 (12%)
17	CLA	BB	821	-	55,63,73	1.64	8 (14%)	64,101,113	1.14	5 (7%)
17	CLA	B1	305	-	54,62,73	1.64	8 (14%)	62,99,113	1.53	10 (16%)
17	CLA	B3	615	-	39,48,73	1.87	6 (15%)	44,83,113	1.46	7 (15%)
25	CHL	B5	605	-	40,49,74	2.42	17 (42%)	42,84,114	2.80	18 (42%)
17	CLA	BA	826	-	53,61,73	1.62	7 (13%)	61,98,113	1.40	10 (16%)
17	CLA	BA	819	-	65,73,73	1.48	9 (13%)	76,113,113	1.34	9 (11%)
17	CLA	B5	602	16	60,68,73	1.62	9 (15%)	70,107,113	1.29	6 (8%)
27	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
17	CLA	BB	825	-	45,53,73	1.79	8 (17%)	52,89,113	1.37	6 (11%)
17	CLA	BA	802	-	65,73,73	1.54	9 (13%)	76,113,113	1.38	6 (7%)
17	CLA	BA	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.28	8 (10%)
17	CLA	BB	834	-	65,73,73	1.51	10 (15%)	76,113,113	1.31	8 (10%)
20	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
17	CLA	BA	804	-	52,60,73	1.66	7 (13%)	60,97,113	1.56	11 (18%)
17	CLA	BA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	6 (7%)
28	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
20	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
17	CLA	BA	840	-	65,73,73	1.44	8 (12%)	76,113,113	1.33	8 (10%)
17	CLA	BA	818	-	56,64,73	1.64	8 (14%)	65,102,113	1.32	8 (12%)
17	CLA	BB	810	-	65,73,73	1.50	8 (12%)	76,113,113	1.33	12 (15%)
17	CLA	BB	833	-	43,51,73	1.80	7 (16%)	49,86,113	1.65	8 (16%)
17	CLA	BF	302	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
17	CLA	B2	311	14	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
23	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
17	CLA	BB	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	6 (7%)
17	CLA	BK	201	11	37,44,73	2.00	7 (18%)	46,77,113	1.73	9 (19%)
17	CLA	BB	802	-	65,73,73	1.55	9 (13%)	76,113,113	1.42	8 (10%)
18	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
22	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
17	CLA	BB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.47	13 (17%)
17	CLA	BB	809	-	52,60,73	1.69	8 (15%)	60,97,113	1.33	7 (11%)
20	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
17	CLA	B3	608	15	45,53,73	1.79	6 (13%)	52,89,113	1.50	8 (15%)
20	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
19	LHG	B5	618	17	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
17	CLA	BB	816	-	64,72,73	1.51	9 (14%)	75,112,113	1.35	8 (10%)
17	CLA	BA	841	-	65,73,73	1.47	8 (12%)	76,113,113	1.55	11 (14%)
17	CLA	BA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	8 (10%)
17	CLA	BA	810	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	7 (9%)
17	CLA	BB	805	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	12 (15%)
17	CLA	B2	308	14	55,63,73	1.66	8 (14%)	64,101,113	1.34	10 (15%)
20	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
17	CLA	BH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.29	8 (11%)
17	CLA	BA	803	-	65,73,73	1.41	7 (10%)	76,113,113	1.37	10 (13%)
22	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)
17	CLA	B1	314	-	60,68,73	1.60	7 (11%)	70,107,113	1.24	10 (14%)
26	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
17	CLA	BA	820	-	45,53,73	1.73	7 (15%)	52,89,113	1.50	6 (11%)
17	CLA	BB	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	10 (13%)
17	CLA	BG	202	7	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
20	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)
17	CLA	B5	609	16	54,62,73	1.67	9 (16%)	62,99,113	1.26	8 (12%)
20	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
17	CLA	BA	816	-	45,53,73	1.81	7 (15%)	52,89,113	1.45	8 (15%)
17	CLA	BA	823	-	41,49,73	1.86	6 (14%)	47,84,113	1.49	9 (19%)
17	CLA	BB	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
17	CLA	BA	839	-	51,59,73	1.69	8 (15%)	59,96,113	1.41	8 (13%)
17	CLA	BL	303	-	60,68,73	1.58	8 (13%)	70,107,113	1.37	10 (14%)
20	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
17	CLA	BB	806	-	41,49,73	1.80	7 (17%)	47,84,113	1.58	9 (19%)
20	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
17	CLA	B1	307	-	39,48,73	1.94	5 (12%)	45,82,113	1.55	7 (15%)
19	LHG	BA	846	17	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	B3	605	-	40,49,73	1.91	7 (17%)	45,84,113	1.44	7 (15%)
25	CHL	B5	606	-	40,48,74	2.31	13 (32%)	50,83,114	2.83	21 (42%)
25	CHL	B3	601	14	53,61,74	2.21	16 (30%)	57,98,114	2.76	25 (43%)
17	CLA	BB	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.43	8 (14%)
17	CLA	BA	821	-	65,73,73	1.50	9 (13%)	76,113,113	1.39	10 (13%)
17	CLA	B1	315	-	37,46,73	2.00	7 (18%)	46,81,113	1.61	9 (19%)
20	BCR	B3	618	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
17	CLA	BK	203	-	46,54,73	1.73	6 (13%)	53,90,113	1.54	6 (11%)
17	CLA	BB	832	-	43,51,73	1.83	8 (18%)	49,86,113	1.30	6 (12%)
17	CLA	BA	806	1	65,73,73	1.50	8 (12%)	76,113,113	1.33	7 (9%)
17	CLA	B3	604	-	41,50,73	1.94	7 (17%)	51,86,113	1.55	9 (17%)
19	LHG	B1	301	17	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
17	CLA	BA	844	19	41,49,73	1.90	5 (12%)	47,84,113	1.43	8 (17%)
17	CLA	BA	830	-	65,73,73	1.53	9 (13%)	76,113,113	1.23	8 (10%)
17	CLA	BB	836	-	60,68,73	1.56	8 (13%)	70,107,113	1.38	7 (10%)
17	CLA	B1	304	13	61,69,73	1.52	7 (11%)	71,108,113	1.39	8 (11%)
25	CHL	B5	607	-	45,53,74	2.37	17 (37%)	49,89,114	2.81	19 (38%)
17	CLA	BB	835	-	65,73,73	1.53	9 (13%)	76,113,113	1.14	5 (6%)
17	CLA	B1	312	19	37,46,73	1.97	7 (18%)	46,81,113	1.60	9 (19%)
20	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
17	CLA	BA	812	-	54,62,73	1.59	9 (16%)	62,99,113	1.46	8 (12%)
17	CLA	B5	603	-	44,52,73	1.87	7 (15%)	55,88,113	1.58	8 (14%)
17	CLA	B2	309	19	38,45,73	2.95	10 (26%)	41,76,113	1.64	10 (24%)
22	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
17	CLA	B2	302	-	43,52,73	1.85	7 (16%)	49,88,113	1.58	8 (16%)
17	CLA	B2	312	-	43,51,73	1.81	6 (13%)	49,86,113	1.44	8 (16%)
17	CLA	BB	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	10 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	BA	832	-	-	7/27/105/115	-
17	CLA	B1	310	13	1/1/10/20	3/6/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	B2	317	17	-	22/39/39/53	-
17	CLA	B5	610	19	-	4/10/88/115	-
17	CLA	B1	313	13	1/1/11/20	5/13/91/115	-
17	CLA	BB	837	-	1/1/10/20	4/10/88/115	-
17	CLA	B3	602	15	1/1/14/20	5/31/109/115	-
17	CLA	BB	813	-	1/1/13/20	4/25/101/115	-
17	CLA	BB	831	-	1/1/13/20	8/27/105/115	-
25	CHL	B2	306	-	3/3/16/26	4/15/113/137	-
17	CLA	BB	820	-	1/1/14/20	12/31/109/115	-
17	CLA	BF	301	-	1/1/12/20	8/24/102/115	-
17	CLA	BB	842	-	1/1/15/20	9/37/115/115	-
17	CLA	BB	814	-	1/1/10/20	1/11/89/115	-
21	SF4	BA	852	2,1	-	-	0/6/5/5
17	CLA	BF	303	-	1/1/10/20	2/8/86/115	-
17	CLA	BJ	102	10	1/1/10/20	4/10/88/115	-
17	CLA	B3	606	-	1/1/10/20	2/10/86/115	-
17	CLA	BA	805	-	1/1/15/20	22/37/115/115	-
17	CLA	BB	823	-	1/1/11/20	4/16/94/115	-
17	CLA	BA	838	-	1/1/12/20	11/25/99/115	-
17	CLA	BB	815	-	1/1/15/20	20/37/115/115	-
17	CLA	BB	830	-	1/1/15/20	11/37/115/115	-
17	CLA	B1	311	13	1/1/14/20	3/29/107/115	-
17	CLA	B3	603	15	1/1/13/20	6/25/103/115	-
17	CLA	BA	817	-	-	9/31/109/115	-
26	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
25	CHL	B2	304	-	3/3/15/26	3/10/108/137	-
20	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
17	CLA	BB	822	-	1/1/10/20	2/8/86/115	-
17	CLA	BA	831	-	1/1/11/20	7/16/94/115	-
17	CLA	B1	306	-	1/1/10/20	3/8/86/115	-
17	CLA	B2	307	14	1/1/11/20	3/13/91/115	-
17	CLA	BB	826	-	1/1/15/20	10/37/115/115	-
17	CLA	BB	828	-	1/1/14/20	9/34/112/115	-
17	CLA	BB	838	-	1/1/12/20	5/19/97/115	-
26	LUT	B2	314	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B3	609	15	1/1/10/20	3/8/86/115	-
20	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
18	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
17	CLA	BB	843	19	1/1/15/20	11/37/115/115	-
24	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
17	CLA	BA	842	-	1/1/15/20	13/37/115/115	-
20	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
21	SF4	BC	101	3	-	-	0/6/5/5
17	CLA	BA	808	1	1/1/15/20	10/37/115/115	-
17	CLA	BA	815	-	-	4/10/88/115	-
17	CLA	BK	202	-	1/1/11/20	6/13/91/115	-
17	CLA	BA	822	-	1/1/10/20	8/10/88/115	-
17	CLA	B2	310	14	1/1/11/20	7/11/89/115	-
27	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
17	CLA	B3	612	-	1/1/13/20	7/23/101/115	-
20	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
17	CLA	BA	828	-	1/1/15/20	14/37/115/115	-
17	CLA	BB	807	-	1/1/15/20	13/37/115/115	-
19	LHG	BF	305	-	-	18/49/49/53	-
20	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
17	CLA	BB	808	2	1/1/15/20	10/37/115/115	-
17	CLA	BB	817	-	1/1/10/20	4/9/87/115	-
17	CLA	B2	303	-	1/1/10/20	4/9/88/115	-
19	LHG	B1	318	17	-	12/46/46/53	-
21	SF4	BC	102	3	-	-	0/6/5/5
26	LUT	B3	616	-	-	4/29/67/67	0/2/2/2
17	CLA	BA	827	-	1/1/15/20	14/37/115/115	-
17	CLA	BG	201	-	1/1/10/20	7/10/88/115	-
25	CHL	B1	303	13	3/3/17/26	3/19/117/137	-
17	CLA	B5	608	16	1/1/11/20	4/11/89/115	-
17	CLA	BA	814	-	1/1/11/20	6/13/91/115	-
17	CLA	B3	613	-	1/1/10/20	0/6/84/115	-
17	CLA	BB	829	-	1/1/15/20	17/37/115/115	-
17	CLA	BB	819	-	1/1/13/20	12/30/108/115	-
17	CLA	BL	304	-	1/1/10/20	5/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	B3	607	-	3/3/16/26	5/13/111/137	-
17	CLA	BA	836	1	-	6/13/91/115	-
27	XAT	B3	617	-	-	0/31/93/93	0/4/4/4
17	CLA	B3	610	19	1/1/10/20	0/6/84/115	-
19	LHG	BA	845	-	-	29/53/53/53	-
17	CLA	B5	601	16	1/1/11/20	8/15/93/115	-
17	CLA	BB	804	-	1/1/15/20	15/37/115/115	-
17	CLA	B5	612	16	1/1/13/20	8/28/106/115	-
25	CHL	B1	308	-	3/3/15/26	0/8/106/137	-
20	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
17	CLA	BA	807	-	1/1/12/20	4/19/97/115	-
17	CLA	BA	813	-	1/1/15/20	17/37/115/115	-
17	CLA	B3	614	-	1/1/8/20	0/0/74/115	-
17	CLA	BA	809	1	-	9/19/97/115	-
20	BCR	B2	316	-	-	0/29/63/63	0/2/2/2
20	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
17	CLA	BL	302	12	-	4/13/91/115	-
17	CLA	B5	611	16	1/1/10/20	4/8/86/115	-
19	LHG	B3	619	17	-	11/26/26/53	-
17	CLA	B2	301	14	1/1/15/20	9/37/115/115	-
25	CHL	B2	313	14	3/3/15/26	0/12/110/137	-
17	CLA	BA	834	-	-	11/37/115/115	-
17	CLA	BA	829	-	1/1/15/20	11/37/115/115	-
20	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
19	LHG	B1	302	-	-	14/40/40/53	-
20	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
17	CLA	BA	825	-	1/1/15/20	15/37/115/115	-
17	CLA	B5	613	-	1/1/11/20	5/13/91/115	-
25	CHL	B2	305	-	3/3/15/26	2/12/110/137	-
20	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
27	XAT	B2	315	-	-	0/31/93/93	0/4/4/4
20	BCR	BH	202	-	-	15/29/63/63	0/2/2/2
17	CLA	BA	837	-	1/1/12/20	3/21/99/115	-
17	CLA	B5	604	-	1/1/11/20	3/11/87/115	-
20	BCR	BA	850	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	BB	827	-	-	8/34/112/115	-
17	CLA	BA	835	-	1/1/11/20	6/13/91/115	-
17	CLA	BB	811	2	1/1/15/20	15/37/115/115	-
17	CLA	BA	824	-	1/1/13/20	8/25/103/115	-
17	CLA	B1	309	-	-	2/11/89/115	-
17	CLA	B3	611	15	1/1/10/20	2/11/89/115	-
17	CLA	BB	818	-	1/1/13/20	8/25/103/115	-
17	CLA	BB	821	-	1/1/13/20	6/25/103/115	-
17	CLA	B1	305	-	1/1/12/20	6/23/101/115	-
17	CLA	B3	615	-	1/1/10/20	0/6/84/115	-
25	CHL	B5	605	-	3/3/15/26	2/8/106/137	-
17	CLA	BA	826	-	-	6/23/101/115	-
17	CLA	BA	819	-	1/1/15/20	13/37/115/115	-
17	CLA	B5	602	16	-	9/31/109/115	-
27	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
17	CLA	BB	825	-	1/1/11/20	6/13/91/115	-
17	CLA	BA	802	-	1/1/15/20	4/37/115/115	-
17	CLA	BA	811	-	1/1/15/20	14/37/115/115	-
17	CLA	BB	834	-	-	9/37/115/115	-
20	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
17	CLA	BA	804	-	-	5/22/100/115	-
17	CLA	BA	801	-	1/1/15/20	9/37/115/115	-
28	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
20	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
17	CLA	BA	840	-	1/1/15/20	13/37/115/115	-
17	CLA	BA	818	-	-	6/27/105/115	-
17	CLA	BB	810	-	1/1/15/20	15/37/115/115	-
17	CLA	BB	833	-	-	4/11/89/115	-
17	CLA	BF	302	-	1/1/10/20	3/10/88/115	-
17	CLA	B2	311	14	1/1/15/20	13/37/115/115	-
23	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
17	CLA	BB	839	-	-	8/37/115/115	-
17	CLA	BK	201	11	1/1/8/20	0/2/74/115	-
17	CLA	BB	802	-	1/1/15/20	16/37/115/115	-
18	PQN	BB	844	-	-	9/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
20	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
17	CLA	BB	801	-	1/1/15/20	17/37/115/115	-
17	CLA	BB	809	-	-	5/22/100/115	-
20	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
17	CLA	B3	608	15	1/1/11/20	3/13/91/115	-
20	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
19	LHG	B5	618	17	-	13/34/34/53	-
17	CLA	BB	816	-	1/1/15/20	15/35/113/115	-
17	CLA	BA	841	-	1/1/15/20	15/37/115/115	-
17	CLA	BA	833	-	1/1/15/20	15/37/115/115	-
17	CLA	BA	810	-	1/1/15/20	12/37/115/115	-
17	CLA	BB	805	-	1/1/15/20	14/37/115/115	-
17	CLA	B2	308	14	1/1/13/20	6/25/103/115	-
20	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
17	CLA	BH	201	-	1/1/14/20	11/31/109/115	-
17	CLA	BA	803	-	1/1/15/20	18/37/115/115	-
22	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
17	CLA	B1	314	-	1/1/14/20	9/31/109/115	-
26	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
17	CLA	BA	820	-	1/1/11/20	4/13/91/115	-
17	CLA	BB	824	-	-	18/37/115/115	-
17	CLA	BG	202	7	1/1/11/20	6/13/91/115	-
20	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
17	CLA	B5	609	16	1/1/12/20	3/24/102/115	-
20	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
17	CLA	BA	816	-	1/1/11/20	2/13/91/115	-
17	CLA	BA	823	-	1/1/10/20	4/8/86/115	-
17	CLA	BB	841	-	1/1/15/20	7/37/115/115	-
17	CLA	BA	839	-	-	6/21/99/115	-
17	CLA	BL	303	-	-	7/31/109/115	-
20	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
17	CLA	BB	806	-	1/1/10/20	2/8/86/115	-
20	BCR	BB	849	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B1	307	-	1/1/9/20	4/8/82/115	-
19	LHG	BA	846	17	-	7/30/30/53	-
17	CLA	B3	605	-	1/1/10/20	4/8/86/115	-
25	CHL	B5	606	-	3/3/15/26	2/8/104/137	-
25	CHL	B3	601	14	3/3/17/26	11/24/122/137	-
17	CLA	BB	840	-	-	4/16/94/115	-
17	CLA	BA	821	-	-	12/37/115/115	-
17	CLA	B1	315	-	1/1/10/20	0/4/80/115	-
20	BCR	B3	618	-	-	6/29/63/63	0/2/2/2
17	CLA	BK	203	-	1/1/11/20	5/15/93/115	-
17	CLA	BB	832	-	1/1/10/20	4/11/89/115	-
17	CLA	BA	806	1	1/1/15/20	18/37/115/115	-
17	CLA	B3	604	-	1/1/11/20	2/9/85/115	-
19	LHG	B1	301	17	-	7/42/42/53	-
17	CLA	BA	844	19	1/1/10/20	4/8/86/115	-
17	CLA	BA	830	-	1/1/15/20	13/37/115/115	-
17	CLA	B1	304	13	1/1/14/20	7/33/111/115	-
17	CLA	BB	836	-	-	11/31/109/115	-
25	CHL	B5	607	-	3/3/16/26	5/13/111/137	-
17	CLA	BB	835	-	1/1/15/20	16/37/115/115	-
17	CLA	B1	312	19	1/1/10/20	0/4/80/115	-
20	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
17	CLA	BA	812	-	1/1/12/20	5/24/102/115	-
17	CLA	B5	603	-	1/1/11/20	4/13/89/115	-
17	CLA	B2	309	19	1/1/7/20	1/10/70/115	-
22	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
17	CLA	B2	302	-	1/1/11/20	4/11/89/115	-
17	CLA	B2	312	-	1/1/10/20	1/11/89/115	-
17	CLA	BB	812	-	1/1/15/20	13/37/115/115	-

All (1330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B2	309	CLA	C1A-NA	12.72	1.40	1.29
18	BB	844	PQN	C12-C13	9.75	1.56	1.33
18	BA	843	PQN	C12-C13	9.52	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	844	CLA	C4B-NB	8.02	1.42	1.35
17	B3	612	CLA	C4B-NB	7.87	1.42	1.35
17	B2	310	CLA	C4B-NB	7.83	1.42	1.35
17	BG	201	CLA	C4B-NB	7.80	1.42	1.35
17	B1	311	CLA	C4B-NB	7.78	1.42	1.35
17	BF	302	CLA	C4B-NB	7.75	1.42	1.35
17	BH	201	CLA	C4B-NB	7.74	1.42	1.35
17	B2	303	CLA	C4B-NB	7.73	1.42	1.35
17	B5	610	CLA	C4B-NB	7.71	1.42	1.35
17	B3	610	CLA	C4B-NB	7.71	1.42	1.35
17	BA	822	CLA	C4B-NB	7.71	1.42	1.35
18	BA	843	PQN	O4-C4	7.70	1.39	1.23
17	B2	308	CLA	C4B-NB	7.69	1.42	1.35
17	BK	201	CLA	C4B-NB	7.68	1.42	1.35
17	B1	306	CLA	C4B-NB	7.66	1.42	1.35
17	B3	605	CLA	C4B-NB	7.65	1.42	1.35
17	B5	604	CLA	C4B-NB	7.65	1.42	1.35
17	B3	613	CLA	C4B-NB	7.65	1.42	1.35
17	B1	314	CLA	C4B-NB	7.63	1.42	1.35
17	B3	611	CLA	C4B-NB	7.63	1.42	1.35
17	B2	309	CLA	C4B-NB	7.62	1.42	1.35
17	B1	310	CLA	C4B-NB	7.62	1.42	1.35
17	BA	838	CLA	C4B-NB	7.62	1.42	1.35
17	B3	604	CLA	C4B-NB	7.62	1.42	1.35
17	B2	302	CLA	C4B-NB	7.62	1.42	1.35
17	BK	202	CLA	C4B-NB	7.61	1.42	1.35
17	BA	836	CLA	C4B-NB	7.61	1.42	1.35
17	B5	602	CLA	C4B-NB	7.61	1.42	1.35
18	BA	843	PQN	O1-C1	7.60	1.39	1.23
18	BB	844	PQN	O4-C4	7.59	1.39	1.23
18	BB	844	PQN	O1-C1	7.58	1.39	1.23
17	BB	835	CLA	C4B-NB	7.58	1.42	1.35
17	BB	810	CLA	C4B-NB	7.57	1.42	1.35
17	B2	311	CLA	C4B-NB	7.57	1.42	1.35
17	BL	304	CLA	C4B-NB	7.56	1.41	1.35
17	B1	307	CLA	C4B-NB	7.56	1.41	1.35
17	BL	302	CLA	C4B-NB	7.55	1.41	1.35
17	B5	612	CLA	C4B-NB	7.55	1.41	1.35
17	B1	309	CLA	C4B-NB	7.55	1.41	1.35
17	B5	609	CLA	C4B-NB	7.55	1.41	1.35
17	B1	315	CLA	C4B-NB	7.54	1.41	1.35
17	BB	843	CLA	C4B-NB	7.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	809	CLA	C4B-NB	7.53	1.41	1.35
17	BB	802	CLA	C4B-NB	7.53	1.41	1.35
17	BA	823	CLA	C4B-NB	7.52	1.41	1.35
17	BB	837	CLA	C4B-NB	7.51	1.41	1.35
17	BB	833	CLA	C4B-NB	7.51	1.41	1.35
17	B3	606	CLA	C4B-NB	7.51	1.41	1.35
17	B1	305	CLA	C4B-NB	7.50	1.41	1.35
17	B2	312	CLA	C4B-NB	7.50	1.41	1.35
17	BF	303	CLA	C4B-NB	7.50	1.41	1.35
17	BJ	102	CLA	C4B-NB	7.49	1.41	1.35
17	B5	608	CLA	C4B-NB	7.48	1.41	1.35
17	BG	202	CLA	C4B-NB	7.47	1.41	1.35
17	B3	602	CLA	C4B-NB	7.47	1.41	1.35
17	BB	839	CLA	C4B-NB	7.45	1.41	1.35
17	B5	603	CLA	C4B-NB	7.45	1.41	1.35
17	B5	613	CLA	C4B-NB	7.44	1.41	1.35
17	BA	827	CLA	C4B-NB	7.42	1.41	1.35
17	BB	831	CLA	C4B-NB	7.41	1.41	1.35
17	B3	615	CLA	C4B-NB	7.41	1.41	1.35
17	BA	811	CLA	C4B-NB	7.40	1.41	1.35
17	BA	831	CLA	C4B-NB	7.40	1.41	1.35
17	BB	823	CLA	C4B-NB	7.39	1.41	1.35
17	BA	802	CLA	C4B-NB	7.39	1.41	1.35
17	BA	801	CLA	C4B-NB	7.39	1.41	1.35
17	BB	836	CLA	C4B-NB	7.39	1.41	1.35
17	BK	203	CLA	C4B-NB	7.39	1.41	1.35
17	BB	813	CLA	C4B-NB	7.38	1.41	1.35
17	BA	833	CLA	C4B-NB	7.38	1.41	1.35
17	BA	806	CLA	C4B-NB	7.38	1.41	1.35
17	BB	838	CLA	C4B-NB	7.37	1.41	1.35
17	BA	807	CLA	C4B-NB	7.37	1.41	1.35
17	BB	824	CLA	C4B-NB	7.37	1.41	1.35
17	BA	814	CLA	C4B-NB	7.36	1.41	1.35
17	BB	822	CLA	C4B-NB	7.36	1.41	1.35
17	BA	842	CLA	C4B-NB	7.35	1.41	1.35
17	BA	830	CLA	C4B-NB	7.34	1.41	1.35
17	BA	804	CLA	C4B-NB	7.34	1.41	1.35
17	B1	313	CLA	C4B-NB	7.34	1.41	1.35
17	BA	835	CLA	C4B-NB	7.33	1.41	1.35
17	BA	828	CLA	C4B-NB	7.33	1.41	1.35
17	BF	301	CLA	C4B-NB	7.32	1.41	1.35
17	B1	312	CLA	C4B-NB	7.31	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B5	611	CLA	C4B-NB	7.30	1.41	1.35
17	BA	816	CLA	C4B-NB	7.30	1.41	1.35
17	B3	603	CLA	C4B-NB	7.30	1.41	1.35
17	BB	807	CLA	C4B-NB	7.30	1.41	1.35
17	B2	307	CLA	C4B-NB	7.29	1.41	1.35
17	BA	817	CLA	C4B-NB	7.29	1.41	1.35
17	B3	609	CLA	C4B-NB	7.28	1.41	1.35
17	BB	828	CLA	C4B-NB	7.28	1.41	1.35
17	B3	608	CLA	C4B-NB	7.28	1.41	1.35
17	BA	818	CLA	C4B-NB	7.27	1.41	1.35
17	BA	810	CLA	C4B-NB	7.27	1.41	1.35
17	BA	824	CLA	C4B-NB	7.26	1.41	1.35
17	BB	826	CLA	C4B-NB	7.26	1.41	1.35
17	B2	301	CLA	C4B-NB	7.24	1.41	1.35
17	B3	614	CLA	C4B-NB	7.23	1.41	1.35
17	BB	812	CLA	C4B-NB	7.21	1.41	1.35
17	BB	840	CLA	C4B-NB	7.21	1.41	1.35
17	BB	816	CLA	C4B-NB	7.20	1.41	1.35
17	BB	827	CLA	C4B-NB	7.20	1.41	1.35
17	BB	842	CLA	C4B-NB	7.18	1.41	1.35
18	BA	843	PQN	C9-C10	7.17	1.51	1.39
17	BA	825	CLA	C4B-NB	7.15	1.41	1.35
17	BL	303	CLA	C4B-NB	7.15	1.41	1.35
17	BB	832	CLA	C4B-NB	7.15	1.41	1.35
17	BB	819	CLA	C4B-NB	7.14	1.41	1.35
17	BA	839	CLA	C4B-NB	7.14	1.41	1.35
17	BB	825	CLA	C4B-NB	7.14	1.41	1.35
17	BB	809	CLA	C4B-NB	7.12	1.41	1.35
17	BB	821	CLA	C4B-NB	7.12	1.41	1.35
17	B1	304	CLA	C4B-NB	7.11	1.41	1.35
17	BB	817	CLA	C4B-NB	7.10	1.41	1.35
17	BB	814	CLA	C4B-NB	7.10	1.41	1.35
17	BB	804	CLA	C4B-NB	7.08	1.41	1.35
17	BA	841	CLA	C4B-NB	7.07	1.41	1.35
18	BA	843	PQN	C6-C5	7.04	1.51	1.39
17	BB	806	CLA	C4B-NB	7.04	1.41	1.35
17	BB	818	CLA	C4B-NB	7.03	1.41	1.35
17	BB	834	CLA	C4B-NB	7.03	1.41	1.35
17	BA	826	CLA	C4B-NB	7.02	1.41	1.35
17	BA	832	CLA	C4B-NB	7.02	1.41	1.35
18	BB	844	PQN	C10-C5	-7.00	1.29	1.40
17	BB	841	CLA	C4B-NB	7.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B5	601	CLA	C4B-NB	6.98	1.41	1.35
17	BA	813	CLA	C4B-NB	6.97	1.41	1.35
17	BA	821	CLA	C4B-NB	6.95	1.41	1.35
17	BA	815	CLA	C4B-NB	6.91	1.41	1.35
17	BB	820	CLA	C4B-NB	6.90	1.41	1.35
17	BA	819	CLA	C4B-NB	6.90	1.41	1.35
17	BA	834	CLA	C4B-NB	6.89	1.41	1.35
17	BB	829	CLA	C4B-NB	6.89	1.41	1.35
17	BB	801	CLA	C4B-NB	6.88	1.41	1.35
17	BB	830	CLA	C4B-NB	6.88	1.41	1.35
17	BA	808	CLA	C4B-NB	6.87	1.41	1.35
17	BA	820	CLA	C4B-NB	6.87	1.41	1.35
17	BB	811	CLA	C4B-NB	6.87	1.41	1.35
17	BA	837	CLA	C4B-NB	6.86	1.41	1.35
17	BA	805	CLA	C4B-NB	6.84	1.41	1.35
18	BB	844	PQN	C9-C10	6.80	1.50	1.39
17	BB	808	CLA	C4B-NB	6.78	1.41	1.35
18	BA	843	PQN	C10-C5	-6.69	1.29	1.40
17	BA	803	CLA	C4B-NB	6.64	1.41	1.35
17	BA	812	CLA	C4B-NB	6.61	1.41	1.35
17	BB	815	CLA	C4B-NB	6.60	1.41	1.35
17	BA	829	CLA	C4B-NB	6.55	1.41	1.35
18	BB	844	PQN	C6-C5	6.45	1.50	1.39
17	BA	840	CLA	C4B-NB	6.43	1.40	1.35
17	BB	805	CLA	C4B-NB	6.36	1.40	1.35
25	B3	601	CHL	C3B-C2B	5.83	1.48	1.40
25	B2	313	CHL	C3B-C2B	5.66	1.48	1.40
25	B5	607	CHL	C3B-C2B	5.58	1.48	1.40
25	B1	303	CHL	C3B-C2B	5.52	1.48	1.40
25	B1	308	CHL	C3B-C2B	5.51	1.48	1.40
25	B5	605	CHL	C3B-C2B	5.44	1.47	1.40
25	B2	306	CHL	C3B-C2B	5.42	1.47	1.40
25	B5	606	CHL	C3C-C2C	5.38	1.47	1.36
25	B1	308	CHL	C2C-C3C	5.26	1.48	1.36
25	B2	305	CHL	C3B-C2B	5.23	1.47	1.40
25	B5	606	CHL	O2D-CGD	5.22	1.45	1.33
25	B2	305	CHL	O2D-CGD	5.21	1.45	1.33
25	B2	304	CHL	O2D-CGD	5.21	1.45	1.33
25	B2	304	CHL	C3B-C2B	5.21	1.47	1.40
25	B2	313	CHL	O2D-CGD	5.15	1.45	1.33
25	B5	605	CHL	C2C-C3C	5.04	1.47	1.37
24	BJ	104	SQD	O8-S	5.00	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	308	CHL	CHC-C1C	5.00	1.47	1.35
25	B2	304	CHL	C2C-C3C	4.99	1.47	1.37
25	B3	601	CHL	C2C-C3C	4.99	1.47	1.36
25	B5	607	CHL	O2D-CGD	4.99	1.45	1.33
25	B3	601	CHL	O2D-CGD	4.99	1.45	1.33
25	B2	305	CHL	C2C-C3C	4.98	1.47	1.36
25	B3	607	CHL	O2D-CGD	4.97	1.45	1.33
25	B2	306	CHL	O2D-CGD	4.96	1.45	1.33
19	B3	619	LHG	O7-C7	4.94	1.46	1.35
25	B2	305	CHL	CHC-C1C	4.93	1.47	1.35
25	B5	607	CHL	CHC-C1C	4.92	1.47	1.35
25	B2	313	CHL	C2C-C3C	4.89	1.47	1.36
25	B5	607	CHL	C2C-C3C	4.88	1.47	1.37
25	B2	306	CHL	CHC-C1C	4.84	1.47	1.35
25	B5	605	CHL	CHC-C1C	4.83	1.47	1.35
25	B2	306	CHL	C2C-C3C	4.80	1.47	1.36
25	B3	601	CHL	CHC-C1C	4.79	1.47	1.35
25	B1	303	CHL	C2C-C3C	4.77	1.47	1.36
25	B5	606	CHL	CHC-C1C	4.75	1.47	1.35
25	B2	304	CHL	CHC-C1C	4.74	1.47	1.35
25	B1	303	CHL	CHC-C1C	4.73	1.47	1.35
25	B2	313	CHL	CHC-C1C	4.71	1.47	1.35
25	B1	308	CHL	O2D-CGD	4.67	1.45	1.30
25	B3	607	CHL	C3C-C2C	4.65	1.46	1.36
25	B5	605	CHL	O2D-CGD	4.64	1.45	1.30
25	B1	303	CHL	O2D-CGD	4.60	1.45	1.30
25	B3	607	CHL	C3B-C2B	4.57	1.46	1.40
25	B3	607	CHL	O2A-CGA	4.51	1.45	1.30
25	B5	607	CHL	O2A-CGA	4.51	1.45	1.30
25	B2	305	CHL	CHD-C1D	4.50	1.47	1.38
25	B2	306	CHL	O2A-CGA	4.46	1.45	1.30
25	B2	304	CHL	CHD-C1D	4.45	1.47	1.38
25	B5	606	CHL	CHD-C1D	4.40	1.46	1.38
25	B5	605	CHL	CHD-C1D	4.40	1.46	1.38
25	B1	308	CHL	CHD-C1D	4.39	1.46	1.38
25	B3	607	CHL	CHD-C1D	4.38	1.46	1.38
25	B3	607	CHL	CHC-C1C	4.36	1.46	1.35
19	B1	301	LHG	O7-C7	4.34	1.46	1.34
17	B2	309	CLA	CHB-C4A	4.32	1.38	1.34
28	B5	617	LMG	O7-C10	4.29	1.46	1.34
25	B3	601	CHL	CHD-C1D	4.27	1.46	1.38
19	B3	619	LHG	O8-C23	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	302	LHG	O7-C7	4.26	1.46	1.34
28	B5	617	LMG	O8-C28	4.25	1.45	1.33
19	B1	301	LHG	O8-C23	4.24	1.45	1.33
19	B1	318	LHG	O7-C7	4.23	1.46	1.34
19	B5	618	LHG	O8-C23	4.21	1.45	1.33
25	B1	303	CHL	O2A-CGA	4.20	1.45	1.33
19	B1	302	LHG	O8-C23	4.20	1.45	1.33
24	BJ	104	SQD	O47-C7	4.19	1.46	1.34
25	B3	601	CHL	C1D-ND	-4.17	1.32	1.37
23	BB	850	DGD	O1G-C1A	4.15	1.45	1.33
19	B1	318	LHG	O8-C23	4.13	1.45	1.33
19	BF	305	LHG	O8-C23	4.12	1.45	1.33
25	B2	313	CHL	C1D-ND	-4.10	1.32	1.37
24	BJ	104	SQD	O48-C23	4.10	1.45	1.33
19	BA	846	LHG	O7-C7	4.09	1.45	1.34
25	B3	601	CHL	O2A-CGA	4.09	1.45	1.33
19	BF	305	LHG	O7-C7	4.06	1.45	1.34
25	B2	306	CHL	C1D-ND	-4.03	1.32	1.37
25	B1	303	CHL	CHD-C1D	4.02	1.46	1.38
25	B5	607	CHL	C1D-ND	-4.02	1.32	1.37
25	B1	308	CHL	C3A-C2A	-4.01	1.50	1.54
25	B2	313	CHL	CHD-C1D	4.00	1.46	1.38
23	BB	850	DGD	O2G-C1B	3.98	1.45	1.34
19	B2	317	LHG	O8-C23	3.98	1.45	1.33
25	B2	306	CHL	CHD-C1D	3.98	1.46	1.38
19	B5	618	LHG	O7-C7	3.95	1.45	1.34
25	B2	305	CHL	CHD-C4C	3.95	1.48	1.39
17	BA	801	CLA	C1D-ND	3.95	1.42	1.37
25	B2	305	CHL	C1D-ND	-3.94	1.32	1.37
25	B1	303	CHL	C1D-ND	-3.94	1.32	1.37
25	B5	607	CHL	CHD-C1D	3.93	1.46	1.38
17	BB	837	CLA	C1D-ND	3.92	1.42	1.37
25	B1	308	CHL	CHD-C4C	3.92	1.48	1.39
17	BK	201	CLA	C1D-ND	3.89	1.42	1.37
26	B1	316	LUT	C10-C9	3.88	1.40	1.35
17	BL	302	CLA	C1D-ND	3.88	1.42	1.37
17	BA	844	CLA	C1D-ND	3.87	1.42	1.37
17	B1	307	CLA	C1D-ND	3.87	1.42	1.37
25	B5	605	CHL	CHD-C4C	3.85	1.48	1.39
17	B3	610	CLA	C1D-ND	3.84	1.42	1.37
25	B5	606	CHL	C1D-ND	-3.84	1.33	1.37
17	BA	836	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	317	LHG	O7-C7	3.83	1.45	1.34
25	B2	304	CHL	CHD-C4C	3.82	1.48	1.39
17	B1	309	CLA	C1D-ND	3.82	1.42	1.37
25	B3	607	CHL	C1D-ND	-3.82	1.33	1.37
19	BA	845	LHG	O8-C23	3.82	1.44	1.33
25	B5	605	CHL	C1D-ND	-3.82	1.33	1.37
25	B3	601	CHL	CHD-C4C	3.79	1.47	1.39
17	BB	842	CLA	C1D-ND	3.79	1.42	1.37
17	BG	202	CLA	C1D-ND	3.79	1.42	1.37
17	B3	611	CLA	C1D-ND	3.79	1.42	1.37
25	B2	313	CHL	CHD-C4C	3.78	1.47	1.39
17	B3	613	CLA	C1D-ND	3.78	1.42	1.37
17	BL	303	CLA	C1D-ND	3.78	1.42	1.37
25	B5	606	CHL	CHD-C4C	3.77	1.47	1.39
17	BK	202	CLA	C1D-ND	3.77	1.42	1.37
17	B5	601	CLA	C1D-ND	3.76	1.42	1.37
26	B1	316	LUT	C34-C33	3.76	1.40	1.35
25	B1	308	CHL	C1D-ND	-3.76	1.33	1.37
17	BB	818	CLA	C1D-ND	3.76	1.42	1.37
17	B1	313	CLA	C1D-ND	3.75	1.42	1.37
25	B2	304	CHL	C1D-ND	-3.75	1.33	1.37
17	BA	815	CLA	C1D-ND	3.74	1.42	1.37
17	B3	614	CLA	C1D-ND	3.74	1.42	1.37
17	B1	306	CLA	C1D-ND	3.74	1.42	1.37
17	BJ	102	CLA	C1D-ND	3.73	1.42	1.37
17	B2	310	CLA	C1D-ND	3.73	1.42	1.37
25	B5	607	CHL	CHD-C4C	3.73	1.47	1.39
25	B2	313	CHL	OBD-CAD	3.73	1.28	1.22
25	B2	305	CHL	OBD-CAD	3.73	1.28	1.22
17	B2	308	CLA	C1D-ND	3.72	1.42	1.37
17	BA	832	CLA	C1D-ND	3.72	1.42	1.37
25	B1	308	CHL	OBD-CAD	3.71	1.28	1.22
17	B3	606	CLA	C1D-ND	3.71	1.42	1.37
17	B5	604	CLA	C1D-ND	3.69	1.42	1.37
17	B1	312	CLA	C1D-ND	3.69	1.42	1.37
17	B1	305	CLA	C1D-ND	3.69	1.42	1.37
18	BB	844	PQN	C11-C12	3.68	1.56	1.50
17	BB	836	CLA	C1D-ND	3.68	1.42	1.37
17	BB	820	CLA	C1D-ND	3.67	1.42	1.37
17	B5	613	CLA	C1D-ND	3.67	1.42	1.37
17	BF	303	CLA	C1D-ND	3.67	1.42	1.37
17	BA	812	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B1	316	LUT	C14-C13	3.66	1.40	1.35
25	B5	606	CHL	OBD-CAD	3.66	1.28	1.22
17	B5	603	CLA	C1D-ND	3.66	1.42	1.37
17	BB	809	CLA	C1D-ND	3.66	1.42	1.37
17	BA	816	CLA	C1D-ND	3.66	1.42	1.37
17	BA	823	CLA	C1D-ND	3.65	1.42	1.37
17	BB	828	CLA	C1D-ND	3.65	1.42	1.37
25	B1	303	CHL	OBD-CAD	3.65	1.28	1.22
17	B5	611	CLA	C1D-ND	3.65	1.42	1.37
17	BB	833	CLA	C1D-ND	3.64	1.42	1.37
25	B5	606	CHL	C3D-C2D	3.64	1.49	1.39
17	B3	604	CLA	C1D-ND	3.64	1.42	1.37
17	BA	813	CLA	C1D-ND	3.64	1.42	1.37
19	BA	845	LHG	O7-C7	3.64	1.44	1.34
17	BA	835	CLA	C1D-ND	3.64	1.42	1.37
17	B1	310	CLA	C1D-ND	3.63	1.42	1.37
25	B2	306	CHL	CHD-C4C	3.63	1.47	1.39
17	B2	309	CLA	C1D-ND	3.63	1.42	1.37
17	B5	610	CLA	C1D-ND	3.63	1.42	1.37
17	BB	843	CLA	C1D-ND	3.62	1.42	1.37
17	BA	807	CLA	C1D-ND	3.62	1.42	1.37
17	B5	612	CLA	C1D-ND	3.62	1.42	1.37
17	BA	810	CLA	C1D-ND	3.61	1.42	1.37
25	B1	308	CHL	C3D-C2D	3.60	1.49	1.39
17	BA	802	CLA	C4D-ND	-3.60	1.32	1.37
17	B2	311	CLA	C1D-ND	3.60	1.42	1.37
17	B1	310	CLA	CAB-C3B	-3.60	1.44	1.51
17	BA	824	CLA	C1D-ND	3.60	1.42	1.37
17	BA	818	CLA	C1D-ND	3.59	1.42	1.37
17	BA	839	CLA	C1D-ND	3.59	1.42	1.37
17	BA	820	CLA	C1D-ND	3.59	1.42	1.37
17	BH	201	CLA	C1D-ND	3.59	1.42	1.37
17	B5	603	CLA	CAB-C3B	-3.58	1.44	1.51
17	BA	822	CLA	C1D-ND	3.58	1.42	1.37
17	B3	608	CLA	C1D-ND	3.58	1.42	1.37
25	B3	607	CHL	CHD-C4C	3.58	1.47	1.39
17	BA	834	CLA	C1D-ND	3.58	1.42	1.37
17	B2	303	CLA	C1D-ND	3.58	1.42	1.37
17	BF	302	CLA	C1D-ND	3.57	1.42	1.37
17	B5	604	CLA	CAB-C3B	-3.57	1.44	1.51
17	BB	813	CLA	C1D-ND	3.57	1.42	1.37
17	BA	817	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	821	CLA	C1D-ND	3.55	1.42	1.37
17	B1	311	CLA	C1D-ND	3.55	1.42	1.37
17	B3	604	CLA	CAB-C3B	-3.55	1.44	1.51
17	B2	312	CLA	C1D-ND	3.55	1.42	1.37
17	BK	203	CLA	C1D-ND	3.55	1.42	1.37
17	B5	608	CLA	C1D-ND	3.55	1.42	1.37
17	B3	603	CLA	C1D-ND	3.54	1.42	1.37
25	B2	304	CHL	OBD-CAD	3.54	1.28	1.22
17	BA	840	CLA	C1D-ND	3.54	1.42	1.37
17	B2	302	CLA	C1D-ND	3.54	1.42	1.37
17	B3	612	CLA	C1D-ND	3.54	1.42	1.37
17	BA	814	CLA	C1D-ND	3.53	1.42	1.37
17	BA	837	CLA	C1D-ND	3.53	1.42	1.37
17	B5	609	CLA	C1D-ND	3.53	1.42	1.37
17	B3	605	CLA	C1D-ND	3.53	1.42	1.37
18	BA	843	PQN	C11-C12	3.52	1.55	1.50
17	BB	813	CLA	CAB-C3B	-3.52	1.44	1.51
17	BK	201	CLA	CAB-C3B	-3.52	1.44	1.51
25	B1	303	CHL	CHD-C4C	3.52	1.47	1.39
17	BB	808	CLA	C1D-ND	3.52	1.42	1.37
25	B3	601	CHL	C3D-C2D	3.51	1.48	1.39
17	B5	602	CLA	C4D-ND	-3.51	1.32	1.37
17	B1	312	CLA	CAB-C3B	-3.51	1.44	1.51
17	B3	606	CLA	CAB-C3B	-3.51	1.44	1.51
17	B1	314	CLA	C1D-ND	3.51	1.42	1.37
17	BA	805	CLA	C1D-ND	3.51	1.42	1.37
17	B1	315	CLA	CAB-C3B	-3.51	1.44	1.51
26	B1	316	LUT	C30-C29	3.50	1.40	1.35
17	B3	609	CLA	C1D-ND	3.50	1.42	1.37
17	BB	834	CLA	C1D-ND	3.50	1.42	1.37
25	B5	605	CHL	OBD-CAD	3.49	1.28	1.22
25	B3	607	CHL	OBD-CAD	3.49	1.28	1.22
17	B2	309	CLA	CAB-C3B	-3.48	1.44	1.51
17	BB	807	CLA	C1D-ND	3.48	1.42	1.37
17	B3	602	CLA	C1D-ND	3.47	1.42	1.37
17	BA	831	CLA	C1D-ND	3.47	1.42	1.37
17	BA	841	CLA	C4D-ND	-3.46	1.32	1.37
17	B2	307	CLA	C1D-ND	3.46	1.42	1.37
25	B2	305	CHL	C3D-C2D	3.46	1.48	1.39
17	BA	830	CLA	C4D-ND	-3.46	1.32	1.37
25	B5	605	CHL	C3D-C2D	3.46	1.48	1.39
17	B1	315	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	817	CLA	C1D-ND	3.44	1.42	1.37
17	BA	808	CLA	C4D-ND	-3.44	1.33	1.37
25	B2	304	CHL	C3D-C2D	3.44	1.48	1.39
17	BB	802	CLA	C4D-ND	-3.44	1.33	1.37
17	BA	827	CLA	C1D-ND	3.44	1.42	1.37
17	BB	811	CLA	C1D-ND	3.44	1.42	1.37
17	BB	807	CLA	C4D-ND	-3.44	1.33	1.37
17	BB	821	CLA	C4D-ND	-3.42	1.33	1.37
17	BA	809	CLA	C1D-ND	3.42	1.42	1.37
17	BG	201	CLA	C1D-ND	3.42	1.42	1.37
17	BB	821	CLA	C1D-ND	3.41	1.42	1.37
25	B2	306	CHL	OBD-CAD	3.41	1.28	1.22
17	BA	828	CLA	C1D-ND	3.41	1.42	1.37
22	BA	853	LMU	O5B-C1B	3.41	1.50	1.41
17	BA	811	CLA	C1D-ND	3.41	1.42	1.37
17	BB	819	CLA	C1D-ND	3.40	1.42	1.37
17	BA	804	CLA	C1D-ND	3.40	1.42	1.37
17	BB	827	CLA	C1D-ND	3.40	1.42	1.37
17	BA	808	CLA	C1D-ND	3.40	1.42	1.37
17	B3	615	CLA	C1D-ND	3.39	1.42	1.37
17	BL	304	CLA	C1D-ND	3.39	1.41	1.37
17	BA	841	CLA	C1D-ND	3.39	1.41	1.37
17	BA	832	CLA	C4D-ND	-3.38	1.33	1.37
17	BA	819	CLA	C1D-ND	3.38	1.41	1.37
17	BA	838	CLA	C4D-ND	-3.38	1.33	1.37
17	BA	826	CLA	C4D-ND	-3.37	1.33	1.37
17	BB	827	CLA	C4D-ND	-3.37	1.33	1.37
17	BB	829	CLA	C1D-ND	3.37	1.41	1.37
17	BA	830	CLA	C1D-ND	3.37	1.41	1.37
25	B2	313	CHL	C3D-C2D	3.36	1.48	1.39
17	BA	806	CLA	C1D-ND	3.36	1.41	1.37
17	BA	821	CLA	C4D-ND	-3.36	1.33	1.37
17	BB	812	CLA	C1D-ND	3.36	1.41	1.37
17	BB	822	CLA	C1D-ND	3.36	1.41	1.37
17	BB	816	CLA	C1D-ND	3.36	1.41	1.37
17	BA	842	CLA	C1D-ND	3.35	1.41	1.37
17	BF	301	CLA	C1D-ND	3.35	1.41	1.37
17	BA	825	CLA	C1D-ND	3.34	1.41	1.37
25	B1	303	CHL	C3D-C2D	3.34	1.48	1.39
17	BA	833	CLA	C1D-ND	3.34	1.41	1.37
17	BA	807	CLA	C4D-ND	-3.34	1.33	1.37
17	BB	806	CLA	C1D-ND	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	840	CLA	C1D-ND	3.34	1.41	1.37
22	BA	854	LMU	O5B-C1B	3.33	1.50	1.41
17	BA	804	CLA	C4D-ND	-3.33	1.33	1.37
17	BA	838	CLA	C1D-ND	3.33	1.41	1.37
17	BB	802	CLA	C1D-ND	3.32	1.41	1.37
17	BB	825	CLA	C4D-ND	-3.32	1.33	1.37
17	B2	301	CLA	C4D-ND	-3.32	1.33	1.37
17	BL	303	CLA	C4D-ND	-3.32	1.33	1.37
17	B5	602	CLA	C1D-ND	3.32	1.41	1.37
17	BA	802	CLA	C1D-ND	3.31	1.41	1.37
17	BA	840	CLA	C4D-ND	-3.31	1.33	1.37
17	BB	824	CLA	C1D-ND	3.31	1.41	1.37
17	B1	307	CLA	CHC-C1C	3.31	1.43	1.35
17	BB	811	CLA	C4D-ND	-3.30	1.33	1.37
22	BA	854	LMU	O5'-C1'	3.30	1.50	1.41
17	BA	830	CLA	CMB-C2B	-3.30	1.44	1.51
17	BA	826	CLA	C1D-ND	3.30	1.41	1.37
17	BB	814	CLA	C1D-ND	3.29	1.41	1.37
17	BB	830	CLA	C1D-ND	3.29	1.41	1.37
17	BB	812	CLA	C4D-ND	-3.29	1.33	1.37
17	BB	826	CLA	C4D-ND	-3.29	1.33	1.37
17	BA	819	CLA	C4D-ND	-3.28	1.33	1.37
17	BB	804	CLA	C1D-ND	3.28	1.41	1.37
17	BB	823	CLA	C4D-ND	-3.28	1.33	1.37
17	BB	831	CLA	C4D-ND	-3.28	1.33	1.37
17	BB	824	CLA	C4D-ND	-3.28	1.33	1.37
17	BB	830	CLA	C4D-ND	-3.27	1.33	1.37
17	BA	805	CLA	C4D-ND	-3.27	1.33	1.37
17	B2	308	CLA	CHC-C1C	3.27	1.43	1.35
17	B1	304	CLA	C4D-ND	-3.27	1.33	1.37
17	BB	843	CLA	CHC-C1C	3.27	1.43	1.35
17	BB	832	CLA	C4D-ND	-3.26	1.33	1.37
17	B3	602	CLA	C4D-ND	-3.26	1.33	1.37
22	BA	853	LMU	O5'-C1'	3.26	1.50	1.41
17	BA	813	CLA	C4D-ND	-3.26	1.33	1.37
17	BA	812	CLA	C4D-ND	-3.26	1.33	1.37
17	BB	820	CLA	C4D-ND	-3.26	1.33	1.37
17	BB	841	CLA	C4D-ND	-3.26	1.33	1.37
25	B3	607	CHL	C3D-C2D	3.25	1.48	1.39
25	B5	607	CHL	C3D-C2D	3.25	1.48	1.39
17	BB	825	CLA	C1D-ND	3.25	1.41	1.37
17	BB	839	CLA	C4D-ND	-3.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	851	LMU	O5B-C1B	3.24	1.50	1.41
17	BB	808	CLA	C4D-ND	-3.24	1.33	1.37
17	B2	301	CLA	C1D-ND	3.24	1.41	1.37
17	B5	603	CLA	C4D-ND	-3.23	1.33	1.37
17	BF	302	CLA	C4D-ND	-3.23	1.33	1.37
22	BB	851	LMU	O5'-C1'	3.23	1.50	1.41
17	BB	834	CLA	C4D-ND	-3.23	1.33	1.37
17	BA	814	CLA	C4D-ND	-3.22	1.33	1.37
17	BB	816	CLA	C4D-ND	-3.22	1.33	1.37
17	B5	601	CLA	C4D-ND	-3.22	1.33	1.37
17	BB	838	CLA	C1D-ND	3.22	1.41	1.37
17	BB	809	CLA	C4D-ND	-3.20	1.33	1.37
17	BB	832	CLA	C1D-ND	3.19	1.41	1.37
17	BB	823	CLA	C1D-ND	3.19	1.41	1.37
17	BB	815	CLA	C1D-ND	3.19	1.41	1.37
17	BB	831	CLA	CMB-C2B	-3.19	1.45	1.51
17	BA	806	CLA	CHC-C1C	3.19	1.43	1.35
25	B5	607	CHL	OBD-CAD	3.19	1.28	1.22
17	BG	201	CLA	CHC-C1C	3.19	1.43	1.35
17	B5	602	CLA	CHC-C1C	3.17	1.43	1.35
17	B2	307	CLA	C4D-ND	-3.17	1.33	1.37
17	BA	818	CLA	C4D-ND	-3.17	1.33	1.37
17	BB	815	CLA	C4D-ND	-3.17	1.33	1.37
17	BB	819	CLA	C4D-ND	-3.16	1.33	1.37
17	BB	814	CLA	C4D-ND	-3.16	1.33	1.37
17	BA	824	CLA	C4D-ND	-3.16	1.33	1.37
25	B2	306	CHL	C3D-C2D	3.16	1.47	1.39
17	BA	829	CLA	C1D-ND	3.16	1.41	1.37
17	B5	609	CLA	CHC-C1C	3.15	1.43	1.35
17	BB	805	CLA	C4D-ND	-3.14	1.33	1.37
17	B3	609	CLA	C4D-ND	-3.14	1.33	1.37
17	BB	831	CLA	C1D-ND	3.14	1.41	1.37
17	BA	822	CLA	C4D-ND	-3.12	1.33	1.37
17	BA	809	CLA	CHC-C1C	3.12	1.43	1.35
17	B2	309	CLA	C4D-ND	-3.12	1.33	1.37
17	BA	811	CLA	C4D-ND	-3.12	1.33	1.37
17	BB	804	CLA	C4D-ND	-3.12	1.33	1.37
17	BB	806	CLA	C4D-ND	-3.12	1.33	1.37
17	BB	833	CLA	C4D-ND	-3.12	1.33	1.37
17	BB	805	CLA	CHC-C1C	3.11	1.42	1.35
17	BB	829	CLA	C4D-ND	-3.11	1.33	1.37
17	BA	833	CLA	CMB-C2B	-3.11	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B1	310	CLA	C4D-ND	-3.10	1.33	1.37
17	BA	829	CLA	CMD-C2D	-3.09	1.44	1.50
17	B5	609	CLA	C4D-ND	-3.09	1.33	1.37
17	BB	810	CLA	C4D-ND	-3.09	1.33	1.37
17	B1	311	CLA	CHC-C1C	3.09	1.42	1.35
17	BB	835	CLA	C1D-ND	3.09	1.41	1.37
17	BB	841	CLA	C1D-ND	3.09	1.41	1.37
17	BB	836	CLA	C4D-ND	-3.09	1.33	1.37
17	B5	612	CLA	C4D-ND	-3.09	1.33	1.37
17	B1	312	CLA	C4D-ND	-3.09	1.33	1.37
17	BA	803	CLA	C4D-ND	-3.08	1.33	1.37
17	BB	816	CLA	CHC-C1C	3.08	1.42	1.35
17	BA	834	CLA	C4D-ND	-3.08	1.33	1.37
17	BB	801	CLA	CMD-C2D	-3.08	1.44	1.50
17	BA	816	CLA	C4D-ND	-3.08	1.33	1.37
17	BB	807	CLA	CHC-C1C	3.07	1.42	1.35
17	B3	603	CLA	C4D-ND	-3.07	1.33	1.37
17	BA	839	CLA	C4D-ND	-3.07	1.33	1.37
17	BA	810	CLA	C4D-ND	-3.07	1.33	1.37
17	B3	608	CLA	C4D-ND	-3.06	1.33	1.37
17	BK	201	CLA	CHC-C1C	3.06	1.42	1.35
17	B5	613	CLA	CHC-C1C	3.06	1.42	1.35
17	B3	614	CLA	C4D-ND	-3.06	1.33	1.37
17	B5	608	CLA	C4D-ND	-3.06	1.33	1.37
17	BA	829	CLA	CHC-C1C	3.06	1.42	1.35
17	B3	604	CLA	CHC-C1C	3.06	1.42	1.35
17	BF	303	CLA	C4D-ND	-3.06	1.33	1.37
17	B5	604	CLA	CHC-C1C	3.06	1.42	1.35
17	BA	835	CLA	C4D-ND	-3.06	1.33	1.37
17	B5	610	CLA	C4D-ND	-3.06	1.33	1.37
17	BK	203	CLA	C4D-ND	-3.06	1.33	1.37
17	B1	314	CLA	C4D-ND	-3.06	1.33	1.37
17	BA	825	CLA	C4D-ND	-3.05	1.33	1.37
17	BA	827	CLA	C4D-ND	-3.05	1.33	1.37
17	BB	840	CLA	C4D-ND	-3.05	1.33	1.37
17	BK	202	CLA	CHC-C1C	3.05	1.42	1.35
17	B5	608	CLA	CHC-C1C	3.05	1.42	1.35
17	BB	826	CLA	CHC-C1C	3.05	1.42	1.35
17	BB	835	CLA	C4D-ND	-3.05	1.33	1.37
17	BB	821	CLA	CHC-C1C	3.05	1.42	1.35
17	B2	303	CLA	CHC-C1C	3.05	1.42	1.35
17	BB	839	CLA	C1D-ND	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	838	CLA	CAD-C3D	-3.04	1.45	1.50
17	B2	302	CLA	C4D-ND	-3.04	1.33	1.37
17	B5	613	CLA	C4D-ND	-3.04	1.33	1.37
17	B5	604	CLA	C4D-ND	-3.04	1.33	1.37
17	B3	615	CLA	CHC-C1C	3.04	1.42	1.35
17	BA	844	CLA	CHC-C1C	3.04	1.42	1.35
17	BA	829	CLA	C4D-ND	-3.04	1.33	1.37
17	BB	818	CLA	C4D-ND	-3.04	1.33	1.37
25	B3	601	CHL	OBD-CAD	3.03	1.27	1.22
17	B3	615	CLA	C4D-ND	-3.03	1.33	1.37
17	BB	842	CLA	C4D-ND	-3.03	1.33	1.37
17	B3	613	CLA	CHC-C1C	3.03	1.42	1.35
17	BA	831	CLA	C4D-ND	-3.03	1.33	1.37
17	BA	833	CLA	C4D-ND	-3.03	1.33	1.37
17	BJ	102	CLA	C4D-ND	-3.03	1.33	1.37
17	BB	817	CLA	C4D-ND	-3.02	1.33	1.37
17	BA	842	CLA	C4D-ND	-3.02	1.33	1.37
17	B3	602	CLA	CHC-C1C	3.02	1.42	1.35
17	BB	829	CLA	CHC-C1C	3.02	1.42	1.35
17	B1	309	CLA	CHC-C1C	3.01	1.42	1.35
17	BA	831	CLA	CHC-C1C	3.01	1.42	1.35
17	BB	815	CLA	CHC-C1C	3.01	1.42	1.35
17	BB	830	CLA	CMB-C2B	-3.01	1.45	1.51
17	B1	315	CLA	CHC-C1C	3.01	1.42	1.35
17	BA	820	CLA	C4D-ND	-3.01	1.33	1.37
17	B1	311	CLA	C4D-ND	-3.01	1.33	1.37
17	BA	814	CLA	CHC-C1C	3.01	1.42	1.35
17	BB	828	CLA	C4D-ND	-3.01	1.33	1.37
17	B3	606	CLA	CHC-C1C	3.01	1.42	1.35
17	BA	827	CLA	CHC-C1C	3.01	1.42	1.35
17	B2	311	CLA	C4D-ND	-3.00	1.33	1.37
17	B3	612	CLA	CHC-C1C	3.00	1.42	1.35
17	B3	605	CLA	C4D-ND	-3.00	1.33	1.37
17	B1	304	CLA	C1D-ND	3.00	1.41	1.37
17	B2	312	CLA	C4D-ND	-3.00	1.33	1.37
17	B2	303	CLA	C4D-ND	-3.00	1.33	1.37
17	BG	201	CLA	C4D-ND	-2.99	1.33	1.37
17	BJ	102	CLA	CHC-C1C	2.99	1.42	1.35
17	BB	843	CLA	C4D-ND	-2.99	1.33	1.37
17	BA	837	CLA	C4D-ND	-2.99	1.33	1.37
17	B1	306	CLA	C4D-ND	-2.99	1.33	1.37
17	B3	610	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	810	CLA	CHC-C1C	2.98	1.42	1.35
17	BL	302	CLA	CHC-C1C	2.98	1.42	1.35
17	B2	311	CLA	CMB-C2B	-2.98	1.45	1.51
17	BB	802	CLA	CHC-C1C	2.97	1.42	1.35
17	BB	832	CLA	CMB-C2B	-2.97	1.45	1.51
17	BA	822	CLA	CHC-C1C	2.97	1.42	1.35
17	B2	310	CLA	CHC-C1C	2.97	1.42	1.35
17	BB	819	CLA	CHC-C1C	2.97	1.42	1.35
20	BI	101	BCR	C30-C25	-2.97	1.49	1.53
17	B2	311	CLA	CHC-C1C	2.97	1.42	1.35
17	BF	301	CLA	C4D-ND	-2.97	1.33	1.37
17	B5	603	CLA	CHC-C1C	2.97	1.42	1.35
17	BK	203	CLA	CHC-C1C	2.97	1.42	1.35
17	BA	817	CLA	C4D-ND	-2.97	1.33	1.37
17	BF	303	CLA	CHC-C1C	2.97	1.42	1.35
17	BL	303	CLA	CHC-C1C	2.96	1.42	1.35
17	B2	307	CLA	CHC-C1C	2.96	1.42	1.35
17	B3	606	CLA	C4D-ND	-2.96	1.33	1.37
17	B3	609	CLA	CHC-C1C	2.96	1.42	1.35
17	BA	819	CLA	CMB-C2B	-2.96	1.45	1.51
17	BB	826	CLA	C1D-ND	2.96	1.41	1.37
17	B2	312	CLA	CHC-C1C	2.96	1.42	1.35
17	BA	813	CLA	CHC-C1C	2.96	1.42	1.35
17	BB	818	CLA	CHC-C1C	2.96	1.42	1.35
17	BB	837	CLA	CHC-C1C	2.96	1.42	1.35
17	BB	839	CLA	CHC-C1C	2.95	1.42	1.35
17	B3	604	CLA	C4D-ND	-2.95	1.33	1.37
17	BA	803	CLA	C1D-ND	2.95	1.41	1.37
17	BA	807	CLA	CHC-C1C	2.95	1.42	1.35
17	BB	813	CLA	C4D-ND	-2.95	1.33	1.37
17	BA	826	CLA	CHC-C1C	2.95	1.42	1.35
17	B1	306	CLA	CHC-C1C	2.95	1.42	1.35
17	BA	806	CLA	C4D-ND	-2.95	1.33	1.37
17	BB	825	CLA	CHC-C1C	2.95	1.42	1.35
17	BB	814	CLA	CHC-C1C	2.95	1.42	1.35
17	B2	301	CLA	CHC-C1C	2.95	1.42	1.35
17	BB	828	CLA	CHC-C1C	2.95	1.42	1.35
17	BB	822	CLA	C4D-ND	-2.95	1.33	1.37
17	BK	202	CLA	C4D-ND	-2.95	1.33	1.37
17	B5	610	CLA	CHC-C1C	2.94	1.42	1.35
17	BA	809	CLA	C4D-ND	-2.94	1.33	1.37
17	BB	827	CLA	CHC-C1C	2.94	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B2	308	CLA	C4D-ND	-2.94	1.33	1.37
17	B1	314	CLA	CHC-C1C	2.94	1.42	1.35
17	B5	601	CLA	CHC-C1C	2.94	1.42	1.35
17	B2	309	CLA	CHC-C1C	2.94	1.42	1.35
17	BB	841	CLA	CHC-C1C	2.94	1.42	1.35
17	BG	202	CLA	C4D-ND	-2.94	1.33	1.37
17	BA	831	CLA	CMB-C2B	-2.94	1.45	1.51
17	BA	808	CLA	C3B-C2B	-2.94	1.36	1.40
17	BA	823	CLA	C4D-ND	-2.93	1.33	1.37
17	B1	310	CLA	CHC-C1C	2.93	1.42	1.35
17	BB	801	CLA	C4D-ND	-2.93	1.33	1.37
17	BB	838	CLA	C4D-ND	-2.93	1.33	1.37
17	BB	835	CLA	CHC-C1C	2.93	1.42	1.35
17	B1	315	CLA	C4D-ND	-2.93	1.33	1.37
17	BA	821	CLA	CHC-C1C	2.92	1.42	1.35
17	BB	813	CLA	CHC-C1C	2.92	1.42	1.35
17	BA	817	CLA	CHC-C1C	2.92	1.42	1.35
17	B1	309	CLA	C4D-ND	-2.91	1.33	1.37
17	B1	313	CLA	CHC-C1C	2.91	1.42	1.35
17	B3	611	CLA	CHC-C1C	2.91	1.42	1.35
17	BA	823	CLA	CHC-C1C	2.91	1.42	1.35
17	BA	828	CLA	C4D-ND	-2.91	1.33	1.37
17	B5	611	CLA	C4D-ND	-2.91	1.33	1.37
17	BF	302	CLA	CHC-C1C	2.91	1.42	1.35
17	BA	804	CLA	CHC-C1C	2.91	1.42	1.35
17	B1	312	CLA	CHC-C1C	2.91	1.42	1.35
25	B3	601	CHL	MG-NA	-2.91	1.99	2.06
17	B3	612	CLA	C4D-ND	-2.91	1.33	1.37
17	BA	815	CLA	C4D-ND	-2.90	1.33	1.37
17	BL	302	CLA	C3B-C2B	-2.90	1.36	1.40
17	B3	605	CLA	CHC-C1C	2.90	1.42	1.35
17	B2	310	CLA	C4D-ND	-2.90	1.33	1.37
17	BB	808	CLA	CHC-C1C	2.90	1.42	1.35
17	BL	304	CLA	CHC-C1C	2.90	1.42	1.35
26	B3	616	LUT	C26-C27	2.90	1.54	1.50
17	BA	825	CLA	CHC-C1C	2.90	1.42	1.35
17	BB	830	CLA	CHC-C1C	2.90	1.42	1.35
17	BB	812	CLA	CHC-C1C	2.90	1.42	1.35
17	BA	805	CLA	CHC-C1C	2.89	1.42	1.35
17	BH	201	CLA	CHC-C1C	2.89	1.42	1.35
17	B5	612	CLA	CHC-C1C	2.89	1.42	1.35
17	BB	837	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	811	CLA	CHC-C1C	2.89	1.42	1.35
17	BA	818	CLA	CHC-C1C	2.88	1.42	1.35
17	BL	304	CLA	C4D-ND	-2.88	1.33	1.37
17	BA	836	CLA	CHC-C1C	2.88	1.42	1.35
17	BB	832	CLA	CHC-C1C	2.88	1.42	1.35
17	BB	836	CLA	CHC-C1C	2.88	1.42	1.35
17	BB	810	CLA	C1D-ND	2.88	1.41	1.37
25	B2	305	CHL	MG-NA	-2.88	1.99	2.06
17	B3	614	CLA	CHC-C1C	2.88	1.42	1.35
17	B2	302	CLA	CHC-C1C	2.88	1.42	1.35
17	BA	835	CLA	CHC-C1C	2.87	1.42	1.35
17	BA	837	CLA	CHC-C1C	2.87	1.42	1.35
17	BB	806	CLA	CHC-C1C	2.87	1.42	1.35
17	B5	611	CLA	CHC-C1C	2.87	1.42	1.35
17	BB	835	CLA	C3B-C2B	-2.86	1.36	1.40
17	BB	809	CLA	CHC-C1C	2.86	1.42	1.35
17	BB	840	CLA	CHC-C1C	2.85	1.42	1.35
17	BA	801	CLA	C4D-ND	-2.85	1.33	1.37
17	B3	611	CLA	C4D-ND	-2.85	1.33	1.37
17	BA	842	CLA	CHC-C1C	2.85	1.42	1.35
17	B3	603	CLA	CHC-C1C	2.85	1.42	1.35
17	B1	307	CLA	C4D-ND	-2.85	1.33	1.37
17	BA	829	CLA	CMB-C2B	-2.85	1.45	1.51
17	BB	822	CLA	CHC-C1C	2.84	1.42	1.35
17	BB	802	CLA	C3B-C2B	-2.84	1.36	1.40
17	BB	811	CLA	CHC-C1C	2.84	1.42	1.35
17	B3	613	CLA	C4D-ND	-2.84	1.33	1.37
26	B1	316	LUT	C8-C9	-2.84	1.39	1.45
17	BA	824	CLA	CHC-C1C	2.84	1.42	1.35
17	BG	202	CLA	CHC-C1C	2.83	1.42	1.35
17	BA	819	CLA	CHC-C1C	2.83	1.42	1.35
17	BA	838	CLA	CHC-C1C	2.83	1.42	1.35
17	BB	834	CLA	CHC-C1C	2.83	1.42	1.35
17	BB	801	CLA	CHC-C1C	2.83	1.42	1.35
17	BB	838	CLA	CHC-C1C	2.83	1.42	1.35
17	BA	816	CLA	CHC-C1C	2.83	1.42	1.35
17	BK	201	CLA	C4D-ND	-2.83	1.33	1.37
17	BA	841	CLA	CHC-C1C	2.82	1.42	1.35
20	BG	203	BCR	C1-C6	-2.82	1.49	1.53
17	BA	808	CLA	CHC-C1C	2.82	1.42	1.35
17	B1	304	CLA	CHC-C1C	2.82	1.42	1.35
17	B3	610	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	841	CLA	CMB-C2B	-2.82	1.45	1.51
17	B1	313	CLA	C4D-ND	-2.82	1.33	1.37
17	BA	835	CLA	CMB-C2B	-2.81	1.45	1.51
17	B1	305	CLA	C4D-ND	-2.81	1.33	1.37
17	BB	817	CLA	CHC-C1C	2.81	1.42	1.35
17	BA	810	CLA	CHC-C1C	2.81	1.42	1.35
17	BF	301	CLA	CMB-C2B	-2.81	1.45	1.51
17	BA	842	CLA	CMB-C2B	-2.81	1.45	1.51
17	BB	804	CLA	CHC-C1C	2.81	1.42	1.35
17	BA	812	CLA	CHC-C1C	2.81	1.42	1.35
17	BA	844	CLA	C4D-ND	-2.80	1.33	1.37
17	BB	820	CLA	CMB-C2B	-2.80	1.45	1.51
17	BA	801	CLA	CHC-C1C	2.79	1.42	1.35
17	BH	201	CLA	C4D-ND	-2.79	1.33	1.37
17	B3	605	CLA	CMB-C2B	-2.78	1.45	1.51
25	B5	606	CHL	MG-NA	-2.78	1.99	2.06
17	BA	815	CLA	CHC-C1C	2.78	1.42	1.35
17	BA	833	CLA	CHC-C1C	2.78	1.42	1.35
17	BA	803	CLA	CHC-C1C	2.77	1.42	1.35
17	BA	831	CLA	C3B-C2B	-2.77	1.36	1.40
17	BA	829	CLA	C3B-CAB	-2.77	1.42	1.47
17	BA	818	CLA	CMB-C2B	-2.77	1.45	1.51
17	BA	803	CLA	CMD-C2D	-2.76	1.44	1.50
17	BB	833	CLA	CHC-C1C	2.76	1.42	1.35
17	BA	808	CLA	CMB-C2B	-2.76	1.45	1.51
17	B1	305	CLA	CHC-C1C	2.76	1.42	1.35
17	BB	842	CLA	C3B-C2B	-2.75	1.36	1.40
17	BL	302	CLA	C4D-ND	-2.75	1.33	1.37
17	BH	201	CLA	CMB-C2B	-2.75	1.45	1.51
17	BA	811	CLA	CMB-C2B	-2.75	1.45	1.51
17	BA	839	CLA	C3B-C2B	-2.74	1.36	1.40
17	BB	824	CLA	CHC-C1C	2.74	1.42	1.35
17	BB	801	CLA	CMB-C2B	-2.74	1.46	1.51
17	BA	832	CLA	CHC-C1C	2.73	1.42	1.35
17	B3	608	CLA	CHC-C1C	2.73	1.42	1.35
17	BL	303	CLA	CMB-C2B	-2.73	1.46	1.51
17	B5	603	CLA	CMB-C2B	-2.72	1.46	1.51
17	BA	836	CLA	CMB-C2B	-2.72	1.46	1.51
17	BB	834	CLA	C3B-C2B	-2.72	1.36	1.40
25	B1	308	CHL	MG-NA	-2.72	1.99	2.06
25	B1	308	CHL	C4B-CHC	2.71	1.48	1.41
17	BB	823	CLA	CHC-C1C	2.71	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BA	801	CLA	CMB-C2B	-2.71	1.46	1.51
17	BA	802	CLA	CMB-C2B	-2.71	1.46	1.51
17	BA	836	CLA	C4D-ND	-2.71	1.34	1.37
17	BA	834	CLA	CHC-C1C	2.71	1.41	1.35
17	BB	839	CLA	CMB-C2B	-2.70	1.46	1.51
25	B5	605	CHL	C4C-C3C	2.70	1.49	1.44
17	BA	839	CLA	CMB-C2B	-2.70	1.46	1.51
17	BA	802	CLA	CMD-C2D	-2.70	1.45	1.50
17	BB	811	CLA	CMB-C2B	-2.70	1.46	1.51
17	B1	304	CLA	CMB-C2B	-2.70	1.46	1.51
17	BA	805	CLA	CMB-C2B	-2.69	1.46	1.51
17	BA	812	CLA	CMB-C2B	-2.69	1.46	1.51
17	B2	307	CLA	CMB-C2B	-2.69	1.46	1.51
17	B1	314	CLA	CMB-C2B	-2.68	1.46	1.51
17	BB	842	CLA	CMB-C2B	-2.68	1.46	1.51
17	BA	820	CLA	CHC-C1C	2.68	1.41	1.35
18	BA	843	PQN	C5-C4	2.68	1.53	1.48
17	BB	821	CLA	CMB-C2B	-2.67	1.46	1.51
17	BB	841	CLA	CMD-C2D	-2.67	1.45	1.50
17	BB	804	CLA	CMB-C2B	-2.67	1.46	1.51
17	BB	826	CLA	CMD-C2D	-2.67	1.45	1.50
17	BA	834	CLA	CMB-C2B	-2.67	1.46	1.51
17	BB	809	CLA	C3B-C2B	-2.67	1.36	1.40
17	BB	831	CLA	CMD-C2D	-2.66	1.45	1.50
17	BA	834	CLA	C3B-C2B	-2.66	1.36	1.40
17	BA	828	CLA	CHC-C1C	2.66	1.41	1.35
17	BA	825	CLA	CMD-C2D	-2.66	1.45	1.50
17	BA	802	CLA	CHC-C1C	2.66	1.41	1.35
25	B2	305	CHL	C4C-C3C	2.66	1.49	1.45
17	BA	821	CLA	CMB-C2B	-2.66	1.46	1.51
17	BA	816	CLA	CMB-C2B	-2.66	1.46	1.51
17	BA	825	CLA	CMB-C2B	-2.65	1.46	1.51
17	B5	602	CLA	CMB-C2B	-2.65	1.46	1.51
17	BB	836	CLA	CMB-C2B	-2.65	1.46	1.51
17	BG	202	CLA	CMB-C2B	-2.65	1.46	1.51
17	BB	809	CLA	CMB-C2B	-2.65	1.46	1.51
17	BA	842	CLA	CMD-C2D	-2.64	1.45	1.50
17	B5	608	CLA	CMB-C2B	-2.64	1.46	1.51
17	B3	608	CLA	CMB-C2B	-2.64	1.46	1.51
17	BB	826	CLA	CMB-C2B	-2.64	1.46	1.51
17	BB	835	CLA	CMD-C2D	-2.64	1.45	1.50
17	BA	839	CLA	CHC-C1C	2.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	814	CLA	CMB-C2B	-2.63	1.46	1.51
17	BB	832	CLA	C3B-C2B	-2.63	1.36	1.40
17	BB	830	CLA	CMD-C2D	-2.63	1.45	1.50
17	BB	815	CLA	CMB-C2B	-2.62	1.46	1.51
17	B2	301	CLA	CMB-C2B	-2.62	1.46	1.51
17	BB	820	CLA	CHC-C1C	2.61	1.41	1.35
17	BB	808	CLA	CMB-C2B	-2.61	1.46	1.51
17	BB	819	CLA	CMB-C2B	-2.60	1.46	1.51
17	B3	602	CLA	CMB-C2B	-2.60	1.46	1.51
18	BA	843	PQN	C11-C3	2.60	1.55	1.51
17	BA	810	CLA	CMB-C2B	-2.60	1.46	1.51
17	B5	602	CLA	C3B-C2B	-2.60	1.36	1.40
17	BA	824	CLA	CMB-C2B	-2.59	1.46	1.51
17	BB	801	CLA	C1D-ND	2.59	1.41	1.37
17	BA	840	CLA	CHC-C1C	2.59	1.41	1.35
17	BA	840	CLA	CMB-C2B	-2.58	1.46	1.51
17	BA	829	CLA	C3B-C2B	-2.58	1.36	1.40
25	B1	308	CHL	C2C-C1C	2.58	1.50	1.44
17	BA	838	CLA	CMB-C2B	-2.58	1.46	1.51
17	B3	612	CLA	CMB-C2B	-2.58	1.46	1.51
17	BA	830	CLA	C3B-C2B	-2.57	1.36	1.40
17	BB	842	CLA	CHC-C1C	2.57	1.41	1.35
17	B5	612	CLA	CMB-C2B	-2.57	1.46	1.51
17	BA	814	CLA	CMB-C2B	-2.57	1.46	1.51
17	B5	609	CLA	C3B-C2B	-2.57	1.36	1.40
17	BB	805	CLA	C1D-ND	2.57	1.40	1.37
17	BB	843	CLA	CMB-C2B	-2.56	1.46	1.51
18	BB	844	PQN	C2-C1	2.56	1.53	1.48
17	BA	809	CLA	CMB-C2B	-2.56	1.46	1.51
17	BB	838	CLA	CMB-C2B	-2.56	1.46	1.51
17	B5	611	CLA	CMB-C2B	-2.56	1.46	1.51
17	BB	802	CLA	CMB-C2B	-2.56	1.46	1.51
17	BL	303	CLA	C3B-C2B	-2.55	1.36	1.40
25	B5	607	CHL	MG-NA	-2.55	2.00	2.06
17	BA	821	CLA	C3B-C2B	-2.55	1.36	1.40
25	B1	308	CHL	C4C-C3C	2.55	1.49	1.45
17	BF	302	CLA	CMB-C2B	-2.55	1.46	1.51
17	B5	604	CLA	CMB-C2B	-2.54	1.46	1.51
17	BA	804	CLA	CMB-C2B	-2.54	1.46	1.51
17	BB	815	CLA	C3B-C2B	-2.54	1.36	1.40
17	BA	820	CLA	CMB-C2B	-2.54	1.46	1.51
26	B1	316	LUT	C32-C33	-2.54	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	822	CLA	CMB-C2B	-2.54	1.46	1.51
25	B2	306	CHL	MG-NA	-2.54	2.00	2.06
17	B3	609	CLA	CMB-C2B	-2.54	1.46	1.51
17	BB	813	CLA	CMB-C2B	-2.53	1.46	1.51
17	BB	816	CLA	CMB-C2B	-2.53	1.46	1.51
17	BB	801	CLA	C3B-C2B	-2.53	1.36	1.40
17	B2	310	CLA	CMB-C2B	-2.53	1.46	1.51
17	B2	312	CLA	CMB-C2B	-2.53	1.46	1.51
17	B1	305	CLA	CMB-C2B	-2.53	1.46	1.51
25	B3	607	CHL	MG-NA	-2.52	2.00	2.06
17	B2	302	CLA	CMB-C2B	-2.52	1.46	1.51
20	BA	851	BCR	C1-C6	-2.52	1.50	1.53
18	BA	843	PQN	C10-C1	2.52	1.53	1.48
25	B5	607	CHL	C2C-C1C	2.52	1.49	1.44
17	B2	303	CLA	CMB-C2B	-2.52	1.46	1.51
26	B1	316	LUT	C28-C29	-2.52	1.40	1.45
17	B5	610	CLA	CMB-C2B	-2.51	1.46	1.51
17	BB	821	CLA	C3B-C2B	-2.51	1.36	1.40
17	B5	608	CLA	C3B-C2B	-2.51	1.36	1.40
25	B2	313	CHL	MG-NA	-2.51	2.00	2.06
17	B1	304	CLA	CMD-C2D	-2.51	1.45	1.50
17	B5	609	CLA	CMB-C2B	-2.51	1.46	1.51
17	BA	830	CLA	CHC-C1C	2.50	1.41	1.35
17	BB	819	CLA	C3B-C2B	-2.50	1.36	1.40
17	BB	824	CLA	CMB-C2B	-2.50	1.46	1.51
17	BB	837	CLA	CMB-C2B	-2.50	1.46	1.51
17	BF	301	CLA	CHC-C1C	2.49	1.41	1.35
17	BB	825	CLA	CMB-C2B	-2.49	1.46	1.51
17	B2	309	CLA	CMB-C2B	-2.49	1.46	1.51
25	B5	605	CHL	MG-NA	-2.49	2.00	2.06
17	BA	831	CLA	C3B-CAB	-2.49	1.42	1.47
17	BB	828	CLA	CMB-C2B	-2.49	1.46	1.51
17	B3	603	CLA	CMB-C2B	-2.49	1.46	1.51
17	BB	835	CLA	CMB-C2B	-2.49	1.46	1.51
25	B2	304	CHL	MG-NA	-2.49	2.00	2.06
25	B1	303	CHL	C2C-C1C	2.49	1.49	1.44
25	B2	304	CHL	C4C-C3C	2.49	1.49	1.44
17	BB	810	CLA	CMD-C2D	-2.49	1.45	1.50
17	BA	808	CLA	C3B-CAB	-2.49	1.42	1.47
17	B2	308	CLA	CMB-C2B	-2.49	1.46	1.51
17	B1	310	CLA	CMB-C2B	-2.48	1.46	1.51
17	BA	818	CLA	C3B-C2B	-2.48	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	812	CLA	CMB-C2B	-2.48	1.46	1.51
17	BB	810	CLA	CMB-C2B	-2.48	1.46	1.51
25	B5	607	CHL	C4B-CHC	2.48	1.47	1.41
19	BA	846	LHG	O8-C23	2.48	1.45	1.33
17	BB	841	CLA	CMB-C2B	-2.48	1.46	1.51
18	BB	844	PQN	C11-C3	2.48	1.55	1.51
17	B1	313	CLA	CMB-C2B	-2.48	1.46	1.51
25	B1	308	CHL	C4D-CHA	2.48	1.47	1.38
17	BB	833	CLA	CMB-C2B	-2.48	1.46	1.51
25	B5	606	CHL	C4C-C3C	2.47	1.49	1.44
17	BA	807	CLA	CMB-C2B	-2.47	1.46	1.51
17	BB	806	CLA	CMB-C2B	-2.47	1.46	1.51
17	B1	315	CLA	CMD-C2D	-2.47	1.45	1.50
20	BF	304	BCR	C1-C6	-2.47	1.50	1.53
17	BB	825	CLA	CMD-C2D	-2.47	1.45	1.50
17	BA	837	CLA	CMB-C2B	-2.47	1.46	1.51
17	BA	806	CLA	CMD-C2D	-2.46	1.45	1.50
17	BJ	102	CLA	CMB-C2B	-2.46	1.46	1.51
25	B2	306	CHL	C4B-CHC	2.46	1.47	1.41
25	B2	305	CHL	C4B-CHC	2.46	1.47	1.41
17	B3	614	CLA	CMB-C2B	-2.46	1.46	1.51
17	B1	315	CLA	CMB-C2B	-2.46	1.46	1.51
17	BA	826	CLA	CMB-C2B	-2.46	1.46	1.51
17	B1	309	CLA	CMB-C2B	-2.45	1.46	1.51
17	B5	613	CLA	CMB-C2B	-2.45	1.46	1.51
17	BB	827	CLA	CMD-C2D	-2.45	1.45	1.50
17	BA	810	CLA	C3B-C2B	-2.45	1.37	1.40
17	B5	601	CLA	CMB-C2B	-2.45	1.46	1.51
25	B2	305	CHL	C4D-CHA	2.44	1.47	1.38
17	BB	810	CLA	CMC-C2C	-2.44	1.45	1.50
25	B3	601	CHL	C4D-CHA	2.43	1.47	1.38
17	BB	807	CLA	CMB-C2B	-2.43	1.46	1.51
17	BB	834	CLA	CMC-C2C	-2.43	1.45	1.50
17	B2	301	CLA	C3B-C2B	-2.43	1.37	1.40
25	B2	306	CHL	C2C-C1C	2.43	1.49	1.44
17	B3	606	CLA	CMB-C2B	-2.43	1.46	1.51
17	BB	830	CLA	C3B-C2B	-2.43	1.37	1.40
25	B2	306	CHL	C4C-C3C	2.43	1.49	1.45
17	BF	303	CLA	CMB-C2B	-2.43	1.46	1.51
25	B5	606	CHL	C4D-CHA	2.43	1.47	1.38
17	BB	805	CLA	CMB-C2B	-2.42	1.46	1.51
17	BB	841	CLA	C3B-CAB	-2.42	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	838	CLA	CMD-C2D	-2.42	1.45	1.50
17	BB	805	CLA	CMC-C2C	-2.42	1.45	1.50
17	BA	802	CLA	C3B-C2B	-2.42	1.37	1.40
17	BA	834	CLA	C3B-CAB	-2.42	1.43	1.47
17	B1	314	CLA	C3B-C2B	-2.41	1.37	1.40
17	BA	812	CLA	CMC-C2C	-2.41	1.45	1.50
17	BA	803	CLA	CMB-C2B	-2.41	1.46	1.51
25	B2	304	CHL	C2C-C1C	2.41	1.49	1.44
17	BL	302	CLA	CMB-C2B	-2.41	1.46	1.51
17	B3	613	CLA	CMB-C2B	-2.41	1.46	1.51
17	BB	840	CLA	CMB-C2B	-2.41	1.46	1.51
17	BB	834	CLA	CMD-C2D	-2.40	1.45	1.50
17	BA	823	CLA	CMB-C2B	-2.40	1.46	1.51
17	BB	819	CLA	C3B-CAB	-2.40	1.43	1.47
17	BB	815	CLA	C3B-CAB	-2.40	1.43	1.47
17	BA	827	CLA	CMD-C2D	-2.39	1.45	1.50
17	BA	828	CLA	CMD-C2D	-2.39	1.45	1.50
17	BA	809	CLA	CMD-C2D	-2.39	1.45	1.50
17	BA	818	CLA	CMD-C2D	-2.39	1.45	1.50
17	BA	806	CLA	CMB-C2B	-2.39	1.46	1.51
17	BA	838	CLA	C3B-C2B	-2.39	1.37	1.40
17	B2	308	CLA	C3B-C2B	-2.39	1.37	1.40
25	B1	303	CHL	C4C-C3C	2.39	1.49	1.45
17	BA	806	CLA	C3B-C2B	-2.38	1.37	1.40
17	BB	802	CLA	CMD-C2D	-2.38	1.45	1.50
17	BB	832	CLA	CMD-C2D	-2.38	1.45	1.50
17	B3	610	CLA	CMB-C2B	-2.38	1.46	1.51
18	BA	843	PQN	C2-C1	2.38	1.53	1.48
17	BA	841	CLA	CMC-C2C	-2.38	1.45	1.50
17	BB	840	CLA	CMD-C2D	-2.38	1.45	1.50
17	BA	832	CLA	CMB-C2B	-2.38	1.46	1.51
17	BA	820	CLA	CMD-C2D	-2.37	1.45	1.50
17	BK	202	CLA	CMB-C2B	-2.37	1.46	1.51
17	BB	831	CLA	C3B-C2B	-2.37	1.37	1.40
17	BB	818	CLA	CMB-C2B	-2.37	1.46	1.51
17	BB	823	CLA	CMB-C2B	-2.37	1.46	1.51
17	BA	806	CLA	CMC-C2C	-2.37	1.45	1.50
17	BA	833	CLA	C3B-C2B	-2.37	1.37	1.40
25	B2	313	CHL	C4B-CHC	2.37	1.47	1.41
17	BA	814	CLA	CMC-C2C	-2.37	1.45	1.50
17	BL	304	CLA	CMB-C2B	-2.36	1.46	1.51
17	BA	844	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	810	CLA	C3B-C2B	-2.36	1.37	1.40
25	B2	304	CHL	C4D-CHA	2.36	1.46	1.38
17	BB	834	CLA	CMB-C2B	-2.36	1.46	1.51
25	B3	607	CHL	C4C-C3C	2.36	1.49	1.45
17	BB	805	CLA	CMD-C2D	-2.36	1.45	1.50
25	B3	607	CHL	C4D-CHA	2.36	1.46	1.38
17	B1	307	CLA	CMB-C2B	-2.36	1.46	1.51
17	BB	801	CLA	MG-ND	-2.36	2.01	2.05
17	BB	831	CLA	CHC-C1C	2.36	1.41	1.35
17	BB	808	CLA	C3B-C2B	-2.36	1.37	1.40
17	BA	816	CLA	C3B-C2B	-2.35	1.37	1.40
17	BA	809	CLA	C3B-C2B	-2.35	1.37	1.40
17	BB	839	CLA	CMD-C2D	-2.35	1.45	1.50
17	B3	604	CLA	CMB-C2B	-2.35	1.46	1.51
17	BA	813	CLA	CMB-C2B	-2.35	1.46	1.51
17	B5	612	CLA	C3B-C2B	-2.35	1.37	1.40
17	B1	312	CLA	CMB-C2B	-2.35	1.46	1.51
17	B3	608	CLA	CMD-C2D	-2.35	1.45	1.50
17	BB	825	CLA	C3B-C2B	-2.34	1.37	1.40
17	BA	811	CLA	CMD-C2D	-2.34	1.45	1.50
17	BA	840	CLA	CMD-C2D	-2.34	1.45	1.50
27	B3	617	XAT	O24-C25	-2.34	1.42	1.46
26	B1	316	LUT	C12-C13	-2.34	1.40	1.45
17	BA	802	CLA	CMC-C2C	-2.34	1.45	1.50
17	BB	817	CLA	CMB-C2B	-2.34	1.46	1.51
17	BB	814	CLA	CMD-C2D	-2.34	1.45	1.50
17	B5	608	CLA	CMD-C2D	-2.34	1.45	1.50
17	BA	815	CLA	CMB-C2B	-2.33	1.46	1.51
17	B3	605	CLA	C3B-C2B	-2.33	1.37	1.40
17	B1	306	CLA	CMB-C2B	-2.33	1.46	1.51
17	BK	201	CLA	CMB-C2B	-2.33	1.46	1.51
25	B1	303	CHL	C4D-CHA	2.33	1.46	1.38
25	B2	313	CHL	C4C-C3C	2.33	1.49	1.45
17	BB	822	CLA	CMD-C2D	-2.33	1.45	1.50
17	BA	840	CLA	C3B-C2B	-2.33	1.37	1.40
17	BA	821	CLA	C3B-CAB	-2.33	1.43	1.47
17	B3	615	CLA	CMB-C2B	-2.32	1.46	1.51
17	B3	612	CLA	C3B-C2B	-2.32	1.37	1.40
17	BB	816	CLA	C3B-CAB	-2.32	1.43	1.47
17	B2	301	CLA	C3B-CAB	-2.32	1.43	1.47
17	BB	802	CLA	CMC-C2C	-2.32	1.45	1.50
17	BB	804	CLA	C3B-C2B	-2.32	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	809	CLA	C3B-CAB	-2.32	1.43	1.47
17	BB	807	CLA	CMC-C2C	-2.32	1.45	1.50
17	B5	601	CLA	C3B-CAB	-2.32	1.43	1.47
25	B1	303	CHL	MG-NA	-2.32	2.00	2.06
17	B3	611	CLA	CMB-C2B	-2.31	1.46	1.51
17	BB	843	CLA	C3B-C2B	-2.31	1.37	1.40
17	B3	615	CLA	CMD-C2D	-2.31	1.45	1.50
17	BB	829	CLA	CMB-C2B	-2.31	1.46	1.51
17	BB	807	CLA	CMD-C2D	-2.31	1.45	1.50
25	B5	605	CHL	C4D-CHA	2.31	1.46	1.38
25	B1	303	CHL	C4B-CHC	2.31	1.47	1.41
17	BF	301	CLA	CMD-C2D	-2.30	1.45	1.50
17	BA	805	CLA	CMD-C2D	-2.30	1.45	1.50
17	B5	608	CLA	C3B-CAB	-2.30	1.43	1.47
17	BB	830	CLA	C3B-CAB	-2.30	1.43	1.47
17	B1	311	CLA	CMB-C2B	-2.30	1.46	1.51
20	BG	203	BCR	C30-C25	-2.30	1.50	1.53
25	B2	305	CHL	C2C-C1C	2.30	1.49	1.44
20	BA	847	BCR	C8-C9	2.30	1.50	1.45
25	B5	607	CHL	C4D-CHA	2.29	1.46	1.38
17	BB	806	CLA	CMD-C2D	-2.29	1.45	1.50
17	BB	816	CLA	CMD-C2D	-2.29	1.45	1.50
17	BB	831	CLA	C4B-CHC	-2.29	1.34	1.41
17	BB	805	CLA	C3B-CAB	-2.29	1.43	1.47
17	B1	305	CLA	C3B-C2B	-2.29	1.37	1.40
17	BB	804	CLA	CMC-C2C	-2.29	1.45	1.50
17	B2	311	CLA	C3B-C2B	-2.28	1.37	1.40
17	BA	818	CLA	C3B-CAB	-2.28	1.43	1.47
17	BA	805	CLA	C3B-C2B	-2.28	1.37	1.40
17	BA	809	CLA	C3B-CAB	-2.28	1.43	1.47
17	BB	832	CLA	C3B-CAB	-2.28	1.43	1.47
17	BB	811	CLA	CMC-C2C	-2.28	1.46	1.50
17	BA	804	CLA	CMD-C2D	-2.28	1.46	1.50
17	BA	822	CLA	CMB-C2B	-2.28	1.46	1.51
25	B1	308	CHL	C1B-CHB	2.28	1.47	1.41
17	BH	201	CLA	C3B-C2B	-2.28	1.37	1.40
17	BA	837	CLA	CMD-C2D	-2.28	1.46	1.50
17	BB	819	CLA	CMD-C2D	-2.27	1.46	1.50
27	B2	315	XAT	O24-C25	-2.27	1.43	1.46
17	BG	201	CLA	CMB-C2B	-2.27	1.46	1.51
17	BB	824	CLA	CMD-C2D	-2.27	1.46	1.50
17	B2	307	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B5	602	CLA	CMD-C2D	-2.26	1.46	1.50
24	BJ	104	SQD	C6-S	-2.25	1.69	1.77
17	BB	804	CLA	CMD-C2D	-2.25	1.46	1.50
17	BA	831	CLA	CMD-C2D	-2.25	1.46	1.50
17	B5	612	CLA	CMC-C2C	-2.25	1.46	1.50
17	BB	828	CLA	CMD-C2D	-2.25	1.46	1.50
17	B5	602	CLA	C3B-CAB	-2.25	1.43	1.47
25	B2	306	CHL	C4D-CHA	2.25	1.46	1.38
17	BA	841	CLA	CMD-C2D	-2.25	1.46	1.50
17	B3	609	CLA	C3B-C2B	-2.24	1.37	1.40
18	BA	843	PQN	C3-C4	2.24	1.52	1.47
17	BB	818	CLA	C3B-CAB	-2.24	1.43	1.47
17	BB	842	CLA	CMD-C2D	-2.24	1.46	1.50
17	B5	603	CLA	CMD-C2D	-2.24	1.46	1.50
17	BA	829	CLA	MG-ND	-2.24	2.01	2.05
17	BA	817	CLA	CMB-C2B	-2.24	1.47	1.51
17	BA	834	CLA	CMD-C2D	-2.23	1.46	1.50
17	BA	830	CLA	CMC-C2C	-2.23	1.46	1.50
17	BA	828	CLA	CMB-C2B	-2.23	1.47	1.51
25	B5	605	CHL	C4B-CHC	2.23	1.47	1.41
17	B3	602	CLA	CMC-C2C	-2.23	1.46	1.50
17	BA	833	CLA	CMD-C2D	-2.23	1.46	1.50
25	B2	313	CHL	C4D-CHA	2.23	1.46	1.38
17	BB	834	CLA	C3B-CAB	-2.23	1.43	1.47
25	B2	304	CHL	C4B-CHC	2.23	1.47	1.41
17	BA	819	CLA	CMC-C2C	-2.23	1.46	1.50
20	BH	202	BCR	C1-C6	-2.23	1.50	1.53
17	BB	808	CLA	CMD-C2D	-2.23	1.46	1.50
17	BA	830	CLA	CMD-C2D	-2.22	1.46	1.50
17	BA	819	CLA	C3B-C2B	-2.22	1.37	1.40
25	B5	607	CHL	C1B-CHB	2.22	1.47	1.41
17	BB	823	CLA	CMD-C2D	-2.22	1.46	1.50
17	B3	602	CLA	C3B-C2B	-2.22	1.37	1.40
17	BA	827	CLA	CMB-C2B	-2.22	1.47	1.51
17	B5	611	CLA	C3B-C2B	-2.22	1.37	1.40
17	BB	827	CLA	CMB-C2B	-2.21	1.47	1.51
17	BA	802	CLA	C3B-CAB	-2.21	1.43	1.47
17	BB	842	CLA	CMC-C2C	-2.21	1.46	1.50
17	B3	612	CLA	CMD-C2D	-2.21	1.46	1.50
25	B1	308	CHL	CMC-C2C	2.21	1.49	1.45
17	BA	839	CLA	CMD-C2D	-2.21	1.46	1.50
17	B2	309	CLA	C1A-CHA	-2.21	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B3	609	CLA	CMD-C2D	-2.21	1.46	1.50
17	B5	613	CLA	CMD-C2D	-2.21	1.46	1.50
20	BB	849	BCR	C19-C18	2.21	1.50	1.45
17	BA	826	CLA	CMD-C2D	-2.21	1.46	1.50
17	BA	824	CLA	CMC-C2C	-2.21	1.46	1.50
17	BB	805	CLA	MG-ND	-2.20	2.01	2.05
17	B2	301	CLA	CMD-C2D	-2.20	1.46	1.50
17	BA	821	CLA	CMC-C2C	-2.20	1.46	1.50
25	B2	313	CHL	C1B-CHB	2.20	1.47	1.41
27	B1	317	XAT	O24-C25	-2.20	1.43	1.46
17	B5	609	CLA	CMD-C2D	-2.20	1.46	1.50
17	BB	817	CLA	CMD-C2D	-2.20	1.46	1.50
17	BA	815	CLA	C3B-CAB	-2.20	1.43	1.47
17	BA	828	CLA	CMC-C2C	-2.19	1.46	1.50
17	BB	805	CLA	C3B-C2B	-2.19	1.37	1.40
17	BA	812	CLA	CMD-C2D	-2.19	1.46	1.50
17	B3	603	CLA	C3B-C2B	-2.19	1.37	1.40
25	B2	313	CHL	C2C-C1C	2.19	1.49	1.44
25	B5	607	CHL	C3D-C4D	-2.19	1.39	1.44
17	BB	839	CLA	CMC-C2C	-2.19	1.46	1.50
25	B3	601	CHL	C1B-CHB	2.18	1.47	1.41
27	B5	615	XAT	O24-C25	-2.18	1.43	1.46
17	BA	808	CLA	CMD-C2D	-2.18	1.46	1.50
17	BK	203	CLA	CMB-C2B	-2.18	1.47	1.51
17	BA	814	CLA	CMD-C2D	-2.18	1.46	1.50
26	B5	614	LUT	C22-C21	-2.18	1.52	1.54
17	BL	303	CLA	CMD-C2D	-2.18	1.46	1.50
17	B5	610	CLA	CMD-C2D	-2.18	1.46	1.50
17	BB	835	CLA	C3B-CAB	-2.17	1.43	1.47
17	BB	813	CLA	CMC-C2C	-2.17	1.46	1.50
17	BF	302	CLA	CMD-C2D	-2.17	1.46	1.50
25	B3	607	CHL	C4B-CHC	2.17	1.47	1.41
17	BA	838	CLA	CMD-C2D	-2.17	1.46	1.50
17	BA	811	CLA	C3B-C2B	-2.17	1.37	1.40
17	BG	202	CLA	C3B-C2B	-2.17	1.37	1.40
17	BB	811	CLA	C3B-C2B	-2.17	1.37	1.40
17	BA	819	CLA	CMD-C2D	-2.17	1.46	1.50
17	BA	814	CLA	C3B-C2B	-2.17	1.37	1.40
17	BB	843	CLA	CMD-C2D	-2.17	1.46	1.50
17	BA	840	CLA	C3B-CAB	-2.16	1.43	1.47
17	BB	816	CLA	C3B-C2B	-2.16	1.37	1.40
17	BB	812	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B2	307	CLA	C3B-C2B	-2.16	1.37	1.40
17	BA	813	CLA	CMC-C2C	-2.16	1.46	1.50
17	BF	302	CLA	CMC-C2C	-2.16	1.46	1.50
17	BA	814	CLA	C3B-CAB	-2.16	1.43	1.47
17	B2	302	CLA	CMD-C2D	-2.16	1.46	1.50
17	B1	309	CLA	CMD-C2D	-2.16	1.46	1.50
17	BB	811	CLA	C3B-CAB	-2.16	1.43	1.47
25	B5	607	CHL	C4C-C3C	2.16	1.48	1.44
17	BA	821	CLA	CMD-C2D	-2.16	1.46	1.50
17	BB	820	CLA	C4B-CHC	-2.16	1.35	1.41
25	B2	304	CHL	CMC-C2C	2.15	1.49	1.45
17	BH	201	CLA	CMD-C2D	-2.15	1.46	1.50
17	BA	803	CLA	CMC-C2C	-2.15	1.46	1.50
17	BL	304	CLA	CMD-C2D	-2.15	1.46	1.50
17	BA	810	CLA	C3B-CAB	-2.15	1.43	1.47
17	B3	614	CLA	CBD-CAD	2.15	1.56	1.51
17	BA	824	CLA	C3B-C2B	-2.15	1.37	1.40
17	BG	201	CLA	C3B-C2B	-2.15	1.37	1.40
25	B5	606	CHL	C1B-CHB	2.15	1.47	1.41
17	BB	829	CLA	CMD-C2D	-2.15	1.46	1.50
17	BB	808	CLA	C3B-CAB	-2.15	1.43	1.47
17	BA	812	CLA	C4B-CHC	-2.15	1.35	1.41
17	BB	821	CLA	CMD-C2D	-2.15	1.46	1.50
17	BB	843	CLA	C3B-CAB	-2.14	1.43	1.47
17	BA	807	CLA	CMC-C2C	-2.14	1.46	1.50
17	BA	813	CLA	CMD-C2D	-2.14	1.46	1.50
25	B5	605	CHL	C1B-CHB	2.14	1.46	1.41
17	BB	811	CLA	CMD-C2D	-2.14	1.46	1.50
18	BB	844	PQN	C10-C1	2.14	1.52	1.48
17	BA	811	CLA	CMC-C2C	-2.14	1.46	1.50
17	BB	825	CLA	C3B-CAB	-2.14	1.43	1.47
17	BA	807	CLA	CMD-C2D	-2.14	1.46	1.50
17	BA	839	CLA	C4B-CHC	-2.14	1.35	1.41
17	BA	830	CLA	C4B-CHC	-2.14	1.35	1.41
17	B3	614	CLA	C3B-C2B	-2.14	1.37	1.40
17	BA	835	CLA	C3B-CAB	-2.14	1.43	1.47
17	BB	822	CLA	CMC-C2C	-2.13	1.46	1.50
17	BB	815	CLA	CMD-C2D	-2.13	1.46	1.50
17	BL	302	CLA	CMD-C2D	-2.13	1.46	1.50
17	BB	821	CLA	C3B-CAB	-2.13	1.43	1.47
17	BB	836	CLA	CMD-C2D	-2.13	1.46	1.50
17	B5	609	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BB	818	CLA	CMD-C2D	-2.13	1.46	1.50
20	BB	847	BCR	C8-C9	2.13	1.50	1.45
17	BB	813	CLA	CMD-C2D	-2.13	1.46	1.50
17	BA	834	CLA	CMC-C2C	-2.13	1.46	1.50
17	B1	314	CLA	CMD-C2D	-2.13	1.46	1.50
17	BB	836	CLA	C3B-C2B	-2.13	1.37	1.40
17	BB	840	CLA	C3B-C2B	-2.13	1.37	1.40
25	B5	605	CHL	C2C-C1C	2.12	1.49	1.44
17	BB	818	CLA	C3B-C2B	-2.12	1.37	1.40
25	B2	305	CHL	CMC-C2C	2.12	1.49	1.45
17	BA	836	CLA	C3B-C2B	-2.12	1.37	1.40
17	BB	816	CLA	CMC-C2C	-2.12	1.46	1.50
17	BB	826	CLA	C3B-CAB	-2.12	1.43	1.47
17	B1	310	CLA	CMD-C2D	-2.12	1.46	1.50
17	BA	805	CLA	CMC-C2C	-2.12	1.46	1.50
17	BA	823	CLA	CMD-C2D	-2.12	1.46	1.50
17	BB	833	CLA	CMC-C2C	-2.12	1.46	1.50
17	BA	822	CLA	CMD-C2D	-2.12	1.46	1.50
17	BA	801	CLA	CMD-C2D	-2.12	1.46	1.50
17	BB	808	CLA	CMC-C2C	-2.12	1.46	1.50
17	BB	839	CLA	C3B-C2B	-2.12	1.37	1.40
17	BB	826	CLA	C3B-C2B	-2.12	1.37	1.40
17	BB	830	CLA	MG-ND	-2.12	2.01	2.05
17	BB	826	CLA	MG-ND	-2.11	2.01	2.05
17	BB	809	CLA	CMD-C2D	-2.11	1.46	1.50
17	BL	303	CLA	C3B-CAB	-2.11	1.43	1.47
17	B5	602	CLA	CMC-C2C	-2.11	1.46	1.50
17	BB	829	CLA	C3B-C2B	-2.11	1.37	1.40
17	B5	612	CLA	CMD-C2D	-2.11	1.46	1.50
17	BA	801	CLA	C3B-C2B	-2.11	1.37	1.40
25	B2	306	CHL	C3D-C4D	-2.11	1.39	1.44
17	BG	201	CLA	CMD-C2D	-2.11	1.46	1.50
17	BA	815	CLA	C3B-C2B	-2.10	1.37	1.40
17	BA	804	CLA	CMC-C2C	-2.10	1.46	1.50
17	B5	601	CLA	C3B-C2B	-2.10	1.37	1.40
25	B3	601	CHL	C4B-CHC	2.10	1.46	1.41
17	BA	826	CLA	C3B-CAB	-2.10	1.43	1.47
17	B3	603	CLA	CMD-C2D	-2.10	1.46	1.50
17	B3	614	CLA	C3B-CAB	-2.10	1.43	1.47
17	B1	305	CLA	C4B-CHC	-2.10	1.35	1.41
17	BK	203	CLA	CMD-C2D	-2.10	1.46	1.50
17	BA	835	CLA	C3B-C2B	-2.10	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B5	610	CLA	C3B-C2B	-2.10	1.37	1.40
17	BB	835	CLA	CMC-C2C	-2.09	1.46	1.50
17	B2	303	CLA	CMD-C2D	-2.09	1.46	1.50
17	BB	812	CLA	C3B-C2B	-2.09	1.37	1.40
25	B3	607	CHL	C1C-NC	-2.09	1.34	1.37
17	BA	816	CLA	C3B-CAB	-2.09	1.43	1.47
17	B2	302	CLA	C3B-C2B	-2.09	1.37	1.40
24	BJ	104	SQD	O6-C1	2.09	1.43	1.40
20	BL	301	BCR	C8-C9	2.09	1.50	1.45
17	B2	301	CLA	CMC-C2C	-2.09	1.46	1.50
17	BB	831	CLA	CMC-C2C	-2.09	1.46	1.50
17	B2	308	CLA	CMD-C2D	-2.08	1.46	1.50
17	BB	820	CLA	CMD-C2D	-2.08	1.46	1.50
25	B5	605	CHL	C1D-C2D	2.08	1.49	1.45
17	BA	815	CLA	CMD-C2D	-2.08	1.46	1.50
17	BB	815	CLA	MG-ND	-2.08	2.01	2.05
17	BB	817	CLA	CMC-C2C	-2.08	1.46	1.50
25	B3	601	CHL	C4C-C3C	2.08	1.48	1.45
17	B5	609	CLA	C3B-CAB	-2.08	1.43	1.47
17	BB	829	CLA	C3B-CAB	-2.08	1.43	1.47
20	BA	856	BCR	C12-C13	2.08	1.50	1.45
17	BA	817	CLA	CMD-C2D	-2.08	1.46	1.50
17	B2	309	CLA	CMD-C2D	-2.08	1.46	1.50
17	B1	304	CLA	C3B-C2B	-2.08	1.37	1.40
25	B2	305	CHL	C1B-CHB	2.07	1.46	1.41
17	B3	605	CLA	CMD-C2D	-2.07	1.46	1.50
17	BB	824	CLA	C3B-C2B	-2.07	1.37	1.40
17	B2	311	CLA	CMD-C2D	-2.07	1.46	1.50
17	BB	838	CLA	MG-ND	-2.07	2.01	2.05
17	BB	804	CLA	C3B-CAB	-2.07	1.43	1.47
25	B2	306	CHL	C1B-CHB	2.07	1.46	1.41
17	BB	826	CLA	CMC-C2C	-2.07	1.46	1.50
17	BA	841	CLA	C3B-C2B	-2.07	1.37	1.40
17	BA	837	CLA	CMC-C2C	-2.07	1.46	1.50
17	B2	310	CLA	CMD-C2D	-2.07	1.46	1.50
17	B5	611	CLA	CMD-C2D	-2.07	1.46	1.50
17	BL	302	CLA	C3B-CAB	-2.06	1.43	1.47
17	B1	305	CLA	CMD-C2D	-2.06	1.46	1.50
17	BB	833	CLA	CMD-C2D	-2.06	1.46	1.50
17	B3	604	CLA	CMD-C2D	-2.06	1.46	1.50
27	B1	317	XAT	O4-C5	-2.06	1.43	1.46
17	BA	810	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B3	609	CLA	C3B-CAB	-2.06	1.43	1.47
17	BA	832	CLA	CMD-C2D	-2.06	1.46	1.50
17	BB	811	CLA	MG-ND	-2.06	2.01	2.05
17	BB	802	CLA	MG-ND	-2.06	2.01	2.05
17	B3	602	CLA	CMD-C2D	-2.06	1.46	1.50
17	BB	842	CLA	C4B-CHC	-2.05	1.35	1.41
17	B1	312	CLA	CMD-C2D	-2.05	1.46	1.50
17	B2	312	CLA	CMD-C2D	-2.05	1.46	1.50
17	BK	201	CLA	CBD-CAD	2.05	1.56	1.51
17	BB	806	CLA	CMC-C2C	-2.05	1.46	1.50
17	B5	601	CLA	CMD-C2D	-2.05	1.46	1.50
17	B3	602	CLA	C3B-CAB	-2.05	1.43	1.47
17	BA	824	CLA	CMD-C2D	-2.05	1.46	1.50
17	BB	801	CLA	CMC-C2C	-2.05	1.46	1.50
17	BB	836	CLA	C3B-CAB	-2.05	1.43	1.47
17	B3	606	CLA	CMD-C2D	-2.05	1.46	1.50
25	B1	308	CHL	C1D-C2D	2.05	1.49	1.45
17	B3	614	CLA	CMD-C2D	-2.05	1.46	1.50
17	BB	824	CLA	CMC-C2C	-2.04	1.46	1.50
25	B5	606	CHL	C4B-CHC	2.04	1.46	1.41
17	BB	827	CLA	C3B-C2B	-2.04	1.37	1.40
17	BA	832	CLA	C3B-CAB	-2.04	1.43	1.47
17	BA	824	CLA	C3B-CAB	-2.04	1.43	1.47
17	B5	613	CLA	C3B-C2B	-2.04	1.37	1.40
17	BB	828	CLA	CMC-C2C	-2.04	1.46	1.50
17	BB	841	CLA	CMC-C2C	-2.04	1.46	1.50
25	B1	303	CHL	C1B-CHB	2.03	1.46	1.41
17	BB	822	CLA	C3B-C2B	-2.03	1.37	1.40
17	B5	611	CLA	CMC-C2C	-2.03	1.46	1.50
17	BF	301	CLA	C4B-CHC	-2.03	1.35	1.41
27	B5	615	XAT	O4-C5	-2.03	1.43	1.46
17	BA	819	CLA	C4B-CHC	-2.03	1.35	1.41
25	B2	304	CHL	C1D-C2D	2.03	1.49	1.45
25	B3	601	CHL	C3D-C4D	-2.03	1.39	1.44
17	B1	313	CLA	CMD-C2D	-2.03	1.46	1.50
17	BA	812	CLA	C3B-C2B	-2.03	1.37	1.40
17	BK	202	CLA	C3B-C2B	-2.02	1.37	1.40
20	BB	845	BCR	C8-C9	2.02	1.50	1.45
17	BF	302	CLA	C3B-C2B	-2.02	1.37	1.40
20	BB	846	BCR	C8-C9	2.02	1.50	1.45
17	BB	841	CLA	C3B-C2B	-2.02	1.37	1.40
20	B2	316	BCR	C8-C9	2.02	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B1	313	CLA	C3B-C2B	-2.02	1.37	1.40
25	B3	607	CHL	C3D-C4D	-2.02	1.39	1.44
25	B1	303	CHL	CMC-C2C	2.02	1.49	1.45
17	BB	827	CLA	CMC-C2C	-2.02	1.46	1.50
17	BA	842	CLA	C3B-C2B	-2.02	1.37	1.40
20	BK	204	BCR	C8-C9	2.02	1.50	1.45
17	B1	311	CLA	CMD-C2D	-2.02	1.46	1.50
17	B5	604	CLA	CMD-C2D	-2.02	1.46	1.50
25	B5	605	CHL	CMC-C2C	2.02	1.49	1.45
20	BI	101	BCR	C1-C6	-2.02	1.51	1.53
17	B2	310	CLA	C3B-C2B	-2.02	1.37	1.40
17	B2	308	CLA	C3B-CAB	-2.02	1.43	1.47
17	B3	613	CLA	CMD-C2D	-2.01	1.46	1.50
17	BB	834	CLA	C4B-CHC	-2.01	1.35	1.41
17	BB	819	CLA	CMC-C2C	-2.01	1.46	1.50
17	BA	820	CLA	CMC-C2C	-2.01	1.46	1.50
17	BA	825	CLA	MG-ND	-2.01	2.01	2.05
17	BA	832	CLA	CMC-C2C	-2.01	1.46	1.50
17	BB	843	CLA	CMC-C2C	-2.00	1.46	1.50
17	B5	608	CLA	CMC-C2C	-2.00	1.46	1.50
17	BB	829	CLA	CMC-C2C	-2.00	1.46	1.50
17	BF	303	CLA	C3B-C2B	-2.00	1.37	1.40
17	BA	810	CLA	CMC-C2C	-2.00	1.46	1.50
17	B1	309	CLA	C3B-C2B	-2.00	1.37	1.40
17	BA	837	CLA	MG-ND	-2.00	2.01	2.05

All (2027) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BH	202	BCR	C37-C22-C21	-32.50	77.40	122.92
20	BH	202	BCR	C35-C13-C14	-31.52	78.78	122.92
20	BH	202	BCR	C34-C9-C10	-29.92	81.01	122.92
20	BG	203	BCR	C35-C13-C14	-29.72	81.29	122.92
20	BH	202	BCR	C37-C22-C23	-27.87	74.16	118.08
20	BH	202	BCR	C34-C9-C8	-26.08	76.99	118.08
20	BG	203	BCR	C12-C13-C14	25.53	158.12	118.94
20	BG	203	BCR	C35-C13-C12	-25.33	78.17	118.08
20	BH	202	BCR	C8-C9-C10	25.31	157.78	118.94
20	BH	202	BCR	C35-C13-C12	-25.07	78.58	118.08
20	BH	202	BCR	C12-C13-C14	24.99	157.29	118.94
20	BH	202	BCR	C23-C22-C21	21.15	151.40	118.94
24	BJ	104	SQD	O9-S-C6	-20.25	82.88	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B3	618	BCR	C40-C30-C25	-12.49	90.04	110.30
24	BJ	104	SQD	O8-S-O9	-12.10	81.70	111.27
20	B3	618	BCR	C39-C30-C25	10.57	127.44	110.30
27	B5	615	XAT	O4-C5-C4	9.81	120.75	113.38
20	BJ	103	BCR	C28-C27-C26	-9.80	96.58	114.08
24	BJ	104	SQD	O8-S-C6	9.79	121.34	105.74
20	BG	203	BCR	C7-C8-C9	-9.32	112.15	126.23
20	BA	850	BCR	C28-C27-C26	-9.27	97.53	114.08
24	BJ	104	SQD	O7-S-C6	9.11	117.77	106.94
20	B2	316	BCR	C33-C5-C6	9.10	134.74	124.53
24	BJ	104	SQD	O9-S-O7	-8.81	83.46	113.95
20	BG	203	BCR	C20-C21-C22	-8.57	115.08	127.31
27	B2	315	XAT	O4-C5-C4	7.96	119.36	113.38
20	B3	618	BCR	C30-C25-C26	-7.95	111.41	122.61
27	B1	317	XAT	O4-C5-C4	7.82	119.25	113.38
20	BH	202	BCR	C20-C21-C22	7.77	138.41	127.31
20	BH	202	BCR	C19-C18-C17	7.67	130.72	118.94
20	B3	618	BCR	C24-C23-C22	-7.65	114.67	126.23
25	B2	305	CHL	C4D-CHA-C1A	-7.47	112.16	121.25
20	BB	845	BCR	C3-C4-C5	-7.34	100.96	114.08
25	B2	313	CHL	C4D-CHA-C1A	-7.34	112.31	121.25
25	B2	306	CHL	C4D-CHA-C1A	-7.33	112.33	121.25
25	B5	607	CHL	C4D-CHA-C1A	-7.30	112.37	121.25
25	B1	308	CHL	C4D-CHA-C1A	-7.21	112.47	121.25
20	BH	202	BCR	C20-C19-C18	-7.12	106.43	126.42
25	B1	303	CHL	C4D-CHA-C1A	-7.12	112.59	121.25
25	B5	605	CHL	C4D-CHA-C1A	-7.07	112.65	121.25
25	B5	606	CHL	C4D-CHA-C1A	-7.02	112.70	121.25
20	B3	618	BCR	C3-C4-C5	-6.94	101.69	114.08
25	B2	304	CHL	C4D-CHA-C1A	-6.91	112.83	121.25
17	BB	842	CLA	C4A-NA-C1A	6.80	109.77	106.71
25	B3	607	CHL	C4D-CHA-C1A	-6.80	112.97	121.25
24	BJ	104	SQD	O47-C7-C8	6.78	126.11	111.50
17	BB	828	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	BA	843	PQN	C11-C12-C13	-6.63	115.76	126.79
20	BB	847	BCR	C37-C22-C21	-6.53	113.77	122.92
27	B3	617	XAT	O24-C25-C38	6.52	122.86	115.06
17	BA	813	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	B3	601	CHL	C4D-CHA-C1A	-6.37	113.50	121.25
20	BA	849	BCR	C28-C27-C26	-6.33	102.77	114.08
20	BL	301	BCR	C8-C7-C6	-6.31	109.48	127.20
17	BB	805	CLA	C4A-NA-C1A	6.30	109.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BL	301	BCR	C34-C9-C10	-6.30	114.10	122.92
27	B5	615	XAT	O24-C25-C24	6.26	118.09	113.38
17	B1	305	CLA	C4A-NA-C1A	6.25	109.51	106.71
20	B5	616	BCR	C28-C27-C26	-6.24	102.93	114.08
27	B3	617	XAT	O4-C5-C4	6.19	118.03	113.38
27	B1	317	XAT	O24-C25-C24	6.15	118.00	113.38
17	BB	812	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	B3	601	CHL	C1B-CHB-C4A	-6.12	118.01	130.12
27	B3	617	XAT	O4-C5-C18	6.10	122.36	115.06
17	BA	840	CLA	C4A-NA-C1A	6.05	109.43	106.71
17	BA	820	CLA	C4A-NA-C1A	6.03	109.42	106.71
26	B2	314	LUT	C3-C4-C5	-6.01	99.88	111.85
17	BG	202	CLA	C4A-NA-C1A	5.99	109.40	106.71
20	BA	856	BCR	C28-C27-C26	-5.98	103.39	114.08
17	B3	606	CLA	C4A-NA-C1A	5.96	109.39	106.71
20	B2	316	BCR	C28-C27-C26	-5.95	103.46	114.08
17	BB	822	CLA	C4A-NA-C1A	5.94	109.38	106.71
17	BK	203	CLA	C4A-NA-C1A	5.89	109.35	106.71
20	BA	855	BCR	C3-C4-C5	-5.87	103.60	114.08
17	BA	806	CLA	C4A-NA-C1A	5.84	109.33	106.71
17	BB	820	CLA	C4A-NA-C1A	5.83	109.33	106.71
20	BI	101	BCR	C38-C26-C25	-5.82	117.99	124.53
25	B3	601	CHL	C1D-ND-C4D	5.82	110.47	106.33
25	B3	601	CHL	O2D-CGD-CBD	5.80	121.58	111.27
20	BG	203	BCR	C8-C9-C10	5.79	127.83	118.94
17	BB	815	CLA	CAC-C3C-C4C	5.79	132.32	124.81
20	BA	856	BCR	C3-C4-C5	-5.77	103.78	114.08
20	B5	616	BCR	C1-C6-C5	-5.76	114.50	122.61
20	BA	848	BCR	C3-C4-C5	-5.73	103.84	114.08
17	BA	812	CLA	C4A-NA-C1A	5.73	109.28	106.71
17	BB	833	CLA	C4A-NA-C1A	5.73	109.28	106.71
18	BB	844	PQN	C15-C13-C12	-5.70	109.59	121.12
20	BG	203	BCR	C33-C5-C6	-5.69	118.14	124.53
20	BA	847	BCR	C38-C26-C25	-5.68	118.15	124.53
17	BB	808	CLA	C4A-NA-C1A	5.67	109.26	106.71
17	B5	603	CLA	C4A-NA-C1A	5.67	109.25	106.71
20	B3	618	BCR	C33-C5-C6	-5.66	118.17	124.53
20	BH	202	BCR	C21-C20-C19	5.65	140.85	123.22
20	BB	848	BCR	C28-C27-C26	-5.64	104.00	114.08
17	BA	822	CLA	C4A-NA-C1A	5.64	109.24	106.71
20	BG	203	BCR	C24-C23-C22	-5.63	117.73	126.23
25	B2	313	CHL	O2D-CGD-CBD	5.61	121.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BF	302	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	B2	306	CHL	C2C-C3C-C4C	-5.58	102.51	106.49
17	BL	302	CLA	C4A-NA-C1A	5.57	109.21	106.71
17	BA	837	CLA	C4A-NA-C1A	5.55	109.20	106.71
17	BB	802	CLA	C4A-NA-C1A	5.53	109.19	106.71
17	BB	811	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	B5	607	CHL	C4A-NA-C1A	-5.52	104.22	106.71
17	BB	840	CLA	C4A-NA-C1A	5.52	109.19	106.71
20	BH	202	BCR	C36-C18-C17	-5.49	115.23	122.92
20	BA	855	BCR	C32-C1-C6	-5.49	101.40	110.30
25	B5	607	CHL	CHD-C4C-C3C	-5.48	116.42	124.98
17	B2	302	CLA	C4A-NA-C1A	5.47	109.17	106.71
17	BA	814	CLA	C4A-NA-C1A	5.46	109.16	106.71
25	B2	306	CHL	CHB-C4A-NA	5.45	132.05	124.51
17	BA	833	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	B5	605	CHL	C2C-C3C-C4C	-5.39	102.49	106.49
25	B1	303	CHL	CHD-C4C-C3C	-5.39	116.92	124.84
20	BL	301	BCR	C31-C1-C6	5.39	119.04	110.30
25	B5	607	CHL	OBD-CAD-C3D	-5.36	115.62	128.52
25	B2	305	CHL	CHB-C4A-NA	5.36	131.92	124.51
17	BK	201	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	B2	304	CHL	CHB-C4A-NA	5.34	131.89	124.51
17	BA	805	CLA	C4A-NA-C1A	5.33	109.10	106.71
17	BA	809	CLA	C4A-NA-C1A	5.33	109.10	106.71
17	BB	843	CLA	C4A-NA-C1A	5.33	109.10	106.71
25	B3	607	CHL	CHB-C4A-NA	5.32	131.86	124.51
20	B3	618	BCR	C40-C30-C39	-5.31	92.22	108.53
17	BB	826	CLA	C4A-NA-C1A	5.31	109.09	106.71
17	BA	841	CLA	C4-C3-C5	5.31	124.21	115.27
20	BL	301	BCR	C28-C27-C26	-5.31	104.60	114.08
25	B5	606	CHL	CHB-C4A-NA	5.31	131.85	124.51
25	B5	605	CHL	CHB-C4A-NA	5.30	131.84	124.51
17	BB	836	CLA	C4A-NA-C1A	5.29	109.08	106.71
20	B3	618	BCR	C1-C6-C5	-5.29	115.17	122.61
17	BA	839	CLA	C4A-NA-C1A	5.28	109.08	106.71
20	BB	849	BCR	C23-C24-C25	-5.26	112.42	127.20
25	B5	606	CHL	C4C-C3C-C2C	-5.26	102.25	107.07
17	BA	819	CLA	C4A-NA-C1A	5.25	109.06	106.71
25	B2	304	CHL	O2D-CGD-CBD	5.25	120.59	111.27
25	B3	601	CHL	OBD-CAD-C3D	-5.25	115.90	128.52
17	BB	804	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	B2	313	CHL	CHB-C4A-NA	5.24	131.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B2	306	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
17	BA	824	CLA	C4A-NA-C1A	5.24	109.06	106.71
17	BB	838	CLA	C4A-NA-C1A	5.24	109.06	106.71
17	BA	815	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	B5	606	CHL	C1B-CHB-C4A	-5.23	119.77	130.12
17	BB	813	CLA	C4A-NA-C1A	5.22	109.06	106.71
25	B1	303	CHL	C2C-C3C-C4C	-5.22	102.77	106.49
25	B1	308	CHL	C1B-CHB-C4A	-5.22	119.78	130.12
17	BA	817	CLA	C4A-NA-C1A	5.22	109.05	106.71
17	BA	836	CLA	C4A-NA-C1A	5.22	109.05	106.71
26	B3	616	LUT	C17-C1-C6	-5.21	101.85	110.30
25	B2	305	CHL	C1B-CHB-C4A	-5.20	119.81	130.12
25	B1	308	CHL	C2C-C3C-C4C	-5.17	102.80	106.49
17	BF	301	CLA	C4A-NA-C1A	5.17	109.03	106.71
20	BG	203	BCR	C15-C16-C17	-5.17	112.89	123.47
20	BG	203	BCR	C15-C14-C13	-5.17	119.94	127.31
27	B3	617	XAT	C18-C5-C6	-5.14	113.65	122.26
25	B1	303	CHL	CHB-C4A-NA	5.13	131.61	124.51
20	BB	845	BCR	C30-C25-C26	-5.13	115.39	122.61
17	BA	841	CLA	C4A-NA-C1A	5.13	109.01	106.71
17	BA	827	CLA	C4A-NA-C1A	5.12	109.01	106.71
17	B5	612	CLA	C4A-NA-C1A	5.11	109.00	106.71
25	B2	313	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
25	B3	607	CHL	CHD-C4C-C3C	-5.09	117.35	124.84
25	B1	308	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
20	BB	803	BCR	C28-C27-C26	-5.09	104.98	114.08
17	BA	834	CLA	C4A-NA-C1A	5.09	108.99	106.71
17	BB	839	CLA	C4A-NA-C1A	5.09	108.99	106.71
25	B5	607	CHL	C2C-C3C-C4C	-5.08	102.71	106.49
20	BB	846	BCR	C34-C9-C10	-5.08	115.80	122.92
25	B2	306	CHL	C2A-C1A-CHA	-5.08	114.97	123.86
17	BA	842	CLA	C4A-NA-C1A	5.08	108.99	106.71
20	BB	848	BCR	C3-C4-C5	-5.08	105.00	114.08
25	B3	601	CHL	CHD-C4C-C3C	-5.08	117.37	124.84
20	B3	618	BCR	C27-C26-C25	-5.08	115.36	122.73
17	B1	304	CLA	C4A-NA-C1A	5.07	108.98	106.71
17	B1	313	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	B5	605	CHL	C2A-C1A-CHA	-5.05	115.03	123.86
17	BB	834	CLA	C4A-NA-C1A	5.05	108.97	106.71
17	B5	611	CLA	C4A-NA-C1A	5.04	108.97	106.71
17	B3	605	CLA	C4A-NA-C1A	5.03	108.97	106.71
20	BB	846	BCR	C30-C25-C26	-5.02	115.55	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BA	804	CLA	C4A-NA-C1A	5.01	108.96	106.71
17	BA	828	CLA	C4A-NA-C1A	5.00	108.96	106.71
20	BF	304	BCR	C28-C27-C26	-5.00	105.14	114.08
20	BL	305	BCR	C28-C27-C26	-4.98	105.18	114.08
17	BA	825	CLA	C4A-NA-C1A	4.96	108.94	106.71
25	B2	304	CHL	CHD-C4C-C3C	-4.96	117.23	124.98
17	B1	309	CLA	C4A-NA-C1A	4.96	108.94	106.71
25	B1	308	CHL	CHB-C4A-NA	4.96	131.37	124.51
25	B5	606	CHL	C1B-C2B-C3B	-4.95	102.31	106.92
25	B2	313	CHL	C2A-C1A-CHA	-4.95	115.21	123.86
25	B2	306	CHL	OBD-CAD-C3D	-4.95	116.62	128.52
25	B3	607	CHL	C1B-CHB-C4A	-4.94	120.33	130.12
17	BB	837	CLA	C4A-NA-C1A	4.93	108.92	106.71
20	B5	616	BCR	C3-C4-C5	-4.92	105.30	114.08
20	BK	204	BCR	C3-C4-C5	-4.90	105.33	114.08
17	BB	831	CLA	C4A-NA-C1A	4.90	108.91	106.71
25	B1	303	CHL	C2A-C1A-CHA	-4.90	115.30	123.86
20	BA	851	BCR	C37-C22-C23	4.90	125.79	118.08
17	BJ	102	CLA	C4A-NA-C1A	4.89	108.91	106.71
25	B2	304	CHL	C1B-CHB-C4A	-4.89	120.43	130.12
17	BA	811	CLA	C4A-NA-C1A	4.89	108.90	106.71
17	BA	802	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
17	BA	808	CLA	C4A-NA-C1A	4.87	108.90	106.71
17	BF	303	CLA	C4A-NA-C1A	4.86	108.89	106.71
17	BB	823	CLA	C4A-NA-C1A	4.86	108.89	106.71
17	B3	612	CLA	C4A-NA-C1A	4.85	108.89	106.71
20	BG	203	BCR	C20-C19-C18	-4.85	112.80	126.42
19	B3	619	LHG	O7-C7-C8	4.85	120.01	111.09
17	BB	829	CLA	C4A-NA-C1A	4.84	108.88	106.71
25	B1	303	CHL	OBD-CAD-C3D	-4.84	116.88	128.52
25	B5	607	CHL	C2A-C1A-CHA	-4.83	115.41	123.86
20	BA	848	BCR	C36-C18-C19	4.83	125.69	118.08
25	B5	606	CHL	CHD-C4C-C3C	-4.83	117.44	124.98
20	BH	202	BCR	C15-C14-C13	-4.83	120.42	127.31
17	BB	806	CLA	C4A-NA-C1A	4.82	108.87	106.71
25	B1	308	CHL	OBD-CAD-C3D	-4.80	116.98	128.52
25	B5	605	CHL	C1B-CHB-C4A	-4.79	120.63	130.12
25	B2	306	CHL	C1B-CHB-C4A	-4.79	120.64	130.12
25	B5	607	CHL	CHB-C4A-NA	4.77	131.11	124.51
17	BA	834	CLA	C4-C3-C5	4.77	123.29	115.27
25	B2	305	CHL	OBD-CAD-C3D	-4.76	117.06	128.52
25	B3	607	CHL	OBD-CAD-C3D	-4.76	117.06	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BB	847	BCR	C34-C9-C10	-4.75	116.26	122.92
24	BJ	104	SQD	C45-O47-C7	-4.75	106.10	117.79
20	BG	203	BCR	C19-C18-C17	4.74	126.21	118.94
17	BB	817	CLA	C4A-NA-C1A	4.74	108.83	106.71
25	B5	606	CHL	C1D-ND-C4D	4.73	109.70	106.33
17	BB	820	CLA	C4-C3-C5	4.72	123.21	115.27
25	B2	304	CHL	C2A-C1A-CHA	-4.71	115.62	123.86
25	B2	305	CHL	C1D-ND-C4D	4.70	109.67	106.33
20	BB	846	BCR	C27-C26-C25	-4.70	115.91	122.73
20	BA	855	BCR	C37-C22-C23	4.70	125.48	118.08
17	B3	603	CLA	C4A-NA-C1A	4.69	108.82	106.71
25	B2	313	CHL	OBD-CAD-C3D	-4.69	117.23	128.52
18	BA	843	PQN	C15-C13-C12	-4.69	111.63	121.12
25	B5	606	CHL	OBD-CAD-C3D	-4.69	117.23	128.52
25	B2	313	CHL	C2C-C3C-C4C	-4.69	103.15	106.49
25	B3	601	CHL	C2C-C3C-C4C	-4.68	103.16	106.49
25	B2	313	CHL	C1B-CHB-C4A	-4.67	120.87	130.12
17	BA	821	CLA	C4A-NA-C1A	4.66	108.80	106.71
17	B3	611	CLA	C4A-NA-C1A	4.65	108.80	106.71
25	B2	305	CHL	C2C-C3C-C4C	-4.65	103.18	106.49
25	B2	304	CHL	OBD-CAD-C3D	-4.64	117.35	128.52
20	BJ	103	BCR	C36-C18-C19	4.63	125.37	118.08
17	BB	814	CLA	C4A-NA-C1A	4.61	108.78	106.71
17	B5	601	CLA	C4A-NA-C1A	4.60	108.78	106.71
20	BB	848	BCR	C38-C26-C25	-4.60	119.36	124.53
26	B2	314	LUT	C39-C29-C28	4.60	125.32	118.08
25	B5	607	CHL	C1B-CHB-C4A	-4.58	121.04	130.12
25	B5	605	CHL	CHD-C4C-C3C	-4.58	117.83	124.98
17	BA	818	CLA	C4A-NA-C1A	4.57	108.76	106.71
20	BG	203	BCR	C31-C1-C6	-4.57	102.88	110.30
25	B5	606	CHL	O2D-CGD-CBD	4.56	119.37	111.27
20	BB	848	BCR	C37-C22-C23	4.55	125.25	118.08
17	BA	838	CLA	C4A-NA-C1A	4.55	108.75	106.71
20	BB	845	BCR	C36-C18-C19	4.55	125.24	118.08
27	B2	315	XAT	O24-C25-C24	4.54	116.79	113.38
25	B2	304	CHL	C4A-NA-C1A	-4.53	104.67	106.71
25	B1	303	CHL	C1B-CHB-C4A	-4.51	121.19	130.12
20	BK	204	BCR	C36-C18-C19	4.50	125.17	118.08
17	BB	807	CLA	C4A-NA-C1A	4.49	108.73	106.71
20	BG	203	BCR	C34-C9-C10	-4.49	116.63	122.92
20	BJ	101	BCR	C8-C7-C6	-4.48	114.61	127.20
25	B3	607	CHL	C1D-ND-C4D	4.48	109.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B5	607	CHL	O2D-CGD-CBD	4.48	119.23	111.27
17	BB	818	CLA	C4A-NA-C1A	4.48	108.72	106.71
20	B5	616	BCR	C37-C22-C23	4.48	125.13	118.08
17	B2	311	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
17	B2	310	CLA	C4A-NA-C1A	4.47	108.72	106.71
17	BL	304	CLA	C4A-NA-C1A	4.47	108.72	106.71
25	B2	306	CHL	O2D-CGD-CBD	4.47	119.21	111.27
25	B2	304	CHL	C2C-C3C-C4C	-4.47	103.17	106.49
17	BK	202	CLA	C4A-NA-C1A	4.46	108.71	106.71
25	B3	601	CHL	C1D-CHD-C4C	-4.46	116.43	126.06
25	B5	605	CHL	C4A-NA-C1A	-4.46	104.70	106.71
17	BB	809	CLA	C4A-NA-C1A	4.45	108.71	106.71
17	BB	811	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
25	B3	607	CHL	C2A-C1A-CHA	-4.44	116.09	123.86
17	BB	833	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
17	BH	201	CLA	C4A-NA-C1A	4.42	108.69	106.71
20	BF	304	BCR	C35-C13-C14	-4.41	116.74	122.92
17	B3	602	CLA	C4A-NA-C1A	4.41	108.69	106.71
20	BL	305	BCR	C27-C26-C25	-4.41	116.33	122.73
25	B5	605	CHL	OBD-CAD-C3D	-4.41	117.92	128.52
17	BA	832	CLA	C4A-NA-C1A	4.40	108.69	106.71
20	BL	305	BCR	C37-C22-C23	4.40	125.01	118.08
20	BL	305	BCR	C40-C30-C25	-4.39	103.18	110.30
17	B3	610	CLA	C4A-NA-C1A	4.39	108.68	106.71
25	B2	305	CHL	CAC-C3C-C4C	4.38	130.49	124.81
17	BA	802	CLA	CMB-C2B-C3B	4.37	132.86	124.68
20	BB	846	BCR	C37-C22-C23	4.37	124.96	118.08
17	BB	801	CLA	C4A-NA-C1A	4.37	108.67	106.71
20	BL	305	BCR	C31-C1-C6	4.37	117.38	110.30
20	BH	202	BCR	C15-C16-C17	-4.36	114.55	123.47
20	BB	849	BCR	C36-C18-C19	4.35	124.93	118.08
17	BA	803	CLA	C4A-NA-C1A	4.35	108.66	106.71
20	BA	856	BCR	C36-C18-C19	4.35	124.92	118.08
25	B2	305	CHL	CHD-C4C-C3C	-4.34	118.46	124.84
17	B5	604	CLA	C4A-NA-C1A	4.33	108.65	106.71
17	B1	312	CLA	C4A-NA-C1A	4.32	108.65	106.71
20	BB	803	BCR	C35-C13-C12	4.32	124.88	118.08
17	B1	306	CLA	C4A-NA-C1A	4.31	108.64	106.71
17	B2	311	CLA	C4A-NA-C1A	4.31	108.64	106.71
25	B1	308	CHL	C1D-ND-C4D	4.31	109.40	106.33
17	B3	614	CLA	C4A-NA-C1A	4.30	108.64	106.71
20	BA	856	BCR	C27-C26-C25	-4.29	116.50	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BA	850	BCR	C37-C22-C23	4.29	124.83	118.08
26	B3	616	LUT	C3-C4-C5	-4.28	103.33	111.85
25	B3	607	CHL	O2D-CGD-CBD	4.27	118.86	111.27
17	BA	841	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
17	B3	608	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
17	BB	810	CLA	C4A-NA-C1A	4.25	108.62	106.71
20	BG	203	BCR	C36-C18-C17	-4.25	116.97	122.92
17	B2	303	CLA	C4A-NA-C1A	4.24	108.61	106.71
27	B2	315	XAT	C6-C7-C8	-4.22	117.06	125.99
27	B1	317	XAT	C18-C5-C6	-4.21	115.20	122.26
20	BB	845	BCR	C27-C26-C25	-4.21	116.62	122.73
20	BB	846	BCR	C36-C18-C19	4.20	124.70	118.08
20	BL	305	BCR	C36-C18-C19	4.20	124.69	118.08
20	B5	616	BCR	C30-C25-C26	-4.20	116.70	122.61
26	B5	614	LUT	C39-C29-C28	4.19	124.67	118.08
17	BA	830	CLA	C4A-NA-C1A	4.18	108.58	106.71
25	B5	607	CHL	C1D-CHD-C4C	-4.15	117.10	126.06
17	BB	830	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
17	BA	838	CLA	C4-C3-C5	4.14	122.24	115.27
20	BA	851	BCR	C34-C9-C10	-4.14	117.13	122.92
17	BK	203	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
17	B3	609	CLA	C4A-NA-C1A	4.13	108.56	106.71
25	B2	306	CHL	C4A-NA-C1A	-4.13	104.85	106.71
25	B2	304	CHL	C1D-ND-C4D	4.13	109.27	106.33
20	BB	845	BCR	C28-C27-C26	-4.13	106.70	114.08
25	B3	601	CHL	CHB-C4A-NA	4.13	130.22	124.51
17	BA	816	CLA	C4A-NA-C1A	4.13	108.56	106.71
17	BA	807	CLA	C4A-NA-C1A	4.12	108.56	106.71
17	BB	824	CLA	C4A-NA-C1A	4.12	108.56	106.71
17	BB	805	CLA	CHB-C4A-NA	4.11	130.20	124.51
27	B2	315	XAT	O4-C5-C18	4.11	119.98	115.06
17	B2	303	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
17	BA	822	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
25	B2	306	CHL	CAC-C3C-C4C	4.10	130.13	124.81
17	BB	841	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
25	B5	606	CHL	C1D-CHD-C4C	-4.09	117.23	126.06
17	B3	615	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
25	B5	606	CHL	C2A-C1A-CHA	-4.09	116.71	123.86
20	BB	803	BCR	C36-C18-C19	4.09	124.52	118.08
17	BA	812	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
20	BA	849	BCR	C1-C6-C5	-4.09	116.86	122.61
17	BF	301	CLA	CMB-C2B-C1B	-4.09	122.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BA	810	CLA	C4A-NA-C1A	4.08	108.54	106.71
17	BB	825	CLA	C4A-NA-C1A	4.08	108.54	106.71
20	BB	848	BCR	C36-C18-C19	4.08	124.51	118.08
20	BI	101	BCR	C33-C5-C6	-4.08	119.95	124.53
20	BI	101	BCR	C36-C18-C19	4.08	124.50	118.08
25	B3	607	CHL	CMC-C2C-C1C	4.07	131.24	125.04
17	BB	828	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
17	BA	802	CLA	C4A-NA-C1A	4.06	108.53	106.71
17	BB	816	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
17	BA	804	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
27	B1	317	XAT	O24-C25-C38	4.04	119.90	115.06
17	B1	315	CLA	CAB-C3B-C4B	-4.04	122.25	128.46
20	BL	305	BCR	C30-C25-C26	-4.04	116.92	122.61
20	BA	851	BCR	C33-C5-C6	-4.04	119.99	124.53
19	BF	305	LHG	O7-C7-C8	4.04	120.20	111.50
20	BA	856	BCR	C37-C22-C23	4.03	124.43	118.08
17	BK	201	CLA	CAB-C3B-C4B	-4.03	122.27	128.46
20	BK	204	BCR	C1-C6-C5	-4.03	116.94	122.61
17	BB	832	CLA	C4A-NA-C1A	4.02	108.52	106.71
20	BA	851	BCR	C1-C6-C5	-4.02	116.95	122.61
27	B3	617	XAT	C38-C25-C26	-4.01	115.53	122.26
25	B2	313	CHL	C4A-NA-C1A	-4.01	104.91	106.71
25	B2	305	CHL	C1D-CHD-C4C	-4.00	117.42	126.06
25	B1	308	CHL	C1D-CHD-C4C	-4.00	117.43	126.06
17	B1	311	CLA	C4A-NA-C1A	4.00	108.50	106.71
27	B2	315	XAT	O24-C25-C38	4.00	119.84	115.06
20	B3	618	BCR	C40-C30-C29	-3.99	92.93	108.91
17	BA	823	CLA	C4A-NA-C1A	3.99	108.50	106.71
25	B3	607	CHL	C1D-CHD-C4C	-3.99	117.46	126.06
20	BG	203	BCR	C33-C5-C4	3.99	121.27	113.62
25	B1	303	CHL	C1D-CHD-C4C	-3.98	117.47	126.06
20	BL	301	BCR	C3-C4-C5	-3.98	106.97	114.08
20	BL	301	BCR	C36-C18-C19	3.97	124.34	118.08
17	B3	606	CLA	CAB-C3B-C4B	-3.97	122.36	128.46
17	B5	610	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
17	BA	826	CLA	C4A-NA-C1A	3.97	108.49	106.71
25	B3	607	CHL	CHC-C1C-NC	3.97	130.22	124.20
17	BA	835	CLA	C4A-NA-C1A	3.96	108.49	106.71
27	B3	617	XAT	C39-C29-C28	3.95	124.30	118.08
27	B1	317	XAT	C20-C13-C12	3.95	124.30	118.08
27	B3	617	XAT	C19-C9-C8	3.95	124.30	118.08
17	BA	828	CLA	CMB-C2B-C1B	-3.95	122.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BB	841	CLA	CMB-C2B-C3B	3.95	132.06	124.68
28	B5	617	LMG	O7-C10-C11	3.94	120.00	111.50
17	BA	844	CLA	C4A-NA-C1A	3.94	108.48	106.71
25	B3	607	CHL	C4A-NA-C1A	-3.94	104.94	106.71
25	B2	306	CHL	C1D-CHD-C4C	-3.93	117.58	126.06
17	B1	310	CLA	C4A-NA-C1A	3.93	108.47	106.71
17	B2	312	CLA	C4A-NA-C1A	3.93	108.47	106.71
17	B1	307	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
17	BB	841	CLA	C4A-NA-C1A	3.92	108.47	106.71
27	B1	317	XAT	C39-C29-C28	3.91	124.24	118.08
17	BA	826	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
17	B3	604	CLA	CAB-C3B-C4B	-3.91	122.46	128.46
17	BB	806	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
25	B2	305	CHL	O2D-CGD-CBD	3.89	118.19	111.27
17	B1	312	CLA	CAB-C3B-C4B	-3.89	122.48	128.46
17	BA	829	CLA	C4A-NA-C1A	3.89	108.45	106.71
17	BA	831	CLA	C4A-NA-C1A	3.88	108.45	106.71
17	BA	802	CLA	C1B-CHB-C4A	-3.88	122.43	130.12
17	BB	838	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
17	B2	312	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
17	B3	608	CLA	C4A-NA-C1A	3.88	108.45	106.71
25	B2	305	CHL	C2A-C1A-CHA	-3.88	117.08	123.86
20	B2	316	BCR	C30-C25-C26	-3.88	117.15	122.61
25	B3	601	CHL	C6-C5-C3	-3.88	108.28	114.62
27	B5	615	XAT	C39-C29-C28	3.87	124.18	118.08
26	B1	316	LUT	C19-C9-C10	-3.87	117.50	122.92
25	B1	303	CHL	C1D-ND-C4D	3.87	109.08	106.33
17	BB	811	CLA	CMB-C2B-C3B	3.87	131.91	124.68
19	B1	318	LHG	O7-C7-C8	3.87	119.83	111.50
25	B3	601	CHL	CHD-C4C-NC	3.86	130.29	124.20
20	BK	204	BCR	C30-C25-C26	-3.86	117.18	122.61
17	BB	815	CLA	C4A-NA-C1A	3.85	108.44	106.71
20	BK	204	BCR	C37-C22-C23	3.85	124.14	118.08
26	B2	314	LUT	C40-C33-C32	3.85	124.14	118.08
20	BK	204	BCR	C38-C26-C27	3.85	121.00	113.62
17	BB	814	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	B5	607	CHL	CHD-C4C-NC	3.84	130.26	124.20
17	B5	603	CLA	CAB-C3B-C4B	-3.84	122.56	128.46
25	B3	601	CHL	C1-C2-C3	-3.84	119.41	126.04
18	BB	844	PQN	C11-C12-C13	-3.83	120.41	126.79
26	B1	316	LUT	C15-C35-C34	3.83	131.33	123.47
17	B1	313	CLA	CMB-C2B-C1B	-3.83	122.57	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B5	618	LHG	O7-C7-C8	3.83	119.76	111.50
17	B3	604	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	B1	308	CHL	C2A-C1A-CHA	-3.82	117.18	123.85
20	BB	849	BCR	C3-C4-C5	-3.82	107.25	114.08
23	BB	850	DGD	O2G-C1B-C2B	3.82	119.73	111.50
20	BB	845	BCR	C38-C26-C27	3.82	120.95	113.62
17	B3	606	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
27	B3	617	XAT	C6-C7-C8	-3.82	117.92	125.99
17	BB	819	CLA	C4A-NA-C1A	3.81	108.42	106.71
25	B2	304	CHL	C1D-CHD-C4C	-3.81	117.83	126.06
26	B1	316	LUT	C39-C29-C30	-3.81	117.58	122.92
25	B2	313	CHL	C1D-CHD-C4C	-3.81	117.85	126.06
20	B2	316	BCR	C23-C24-C25	-3.81	116.51	127.20
17	BL	304	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
17	B3	604	CLA	C4A-NA-C1A	3.80	108.42	106.71
26	B3	616	LUT	C21-C26-C27	-3.80	107.90	112.70
17	BB	820	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
17	B2	307	CLA	C4A-NA-C1A	3.79	108.41	106.71
26	B3	616	LUT	C38-C25-C24	-3.79	115.44	123.56
17	BB	802	CLA	C4-C3-C5	3.79	121.65	115.27
17	BA	837	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	B5	606	CHL	CHC-C1C-NC	3.78	129.94	124.20
20	BL	301	BCR	C30-C25-C26	-3.78	117.29	122.61
20	BG	203	BCR	C38-C26-C25	-3.78	120.28	124.53
17	BB	813	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
27	B5	615	XAT	O24-C25-C38	3.78	119.58	115.06
20	BB	849	BCR	C33-C5-C6	-3.76	120.30	124.53
17	B1	315	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
17	B2	301	CLA	C4A-NA-C1A	3.76	108.40	106.71
17	B3	613	CLA	C4A-NA-C1A	3.76	108.40	106.71
17	B5	610	CLA	C4A-NA-C1A	3.75	108.39	106.71
25	B5	605	CHL	C1D-ND-C4D	3.75	109.00	106.33
20	BJ	103	BCR	C32-C1-C6	-3.75	104.22	110.30
17	BK	201	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
17	BL	303	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	B3	616	LUT	C39-C29-C28	3.73	123.95	118.08
20	BI	101	BCR	C31-C1-C6	-3.72	104.26	110.30
20	B2	316	BCR	C40-C30-C25	-3.72	104.26	110.30
17	BA	842	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
20	BA	849	BCR	C36-C18-C19	3.72	123.94	118.08
17	BA	825	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
17	B1	310	CLA	CAB-C3B-C4B	-3.72	122.75	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BA	851	BCR	C23-C22-C21	-3.72	113.24	118.94
26	B5	614	LUT	C1-C6-C5	-3.72	117.38	122.61
20	BG	203	BCR	C37-C22-C21	-3.72	117.72	122.92
27	B2	315	XAT	C20-C13-C12	3.71	123.93	118.08
17	BL	303	CLA	C4A-NA-C1A	3.71	108.37	106.71
17	B5	604	CLA	CAB-C3B-C4B	-3.71	122.77	128.46
20	B5	616	BCR	C33-C5-C6	-3.70	120.37	124.53
26	B5	614	LUT	C36-C21-C26	3.70	115.16	109.55
20	BA	848	BCR	C34-C9-C8	3.70	123.91	118.08
17	B2	302	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
17	BA	807	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
20	BB	803	BCR	C30-C25-C26	-3.70	117.41	122.61
17	BB	816	CLA	CMB-C2B-C3B	3.69	131.59	124.68
17	B5	613	CLA	C4A-NA-C1A	3.69	108.37	106.71
17	B2	309	CLA	CAB-C3B-C4B	-3.69	122.79	128.46
17	BB	826	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
20	BK	204	BCR	C30-C25-C24	3.69	126.22	115.78
20	BL	305	BCR	C32-C1-C6	-3.69	104.32	110.30
25	B5	607	CHL	C1D-ND-C4D	3.68	108.95	106.33
17	B5	604	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
20	B2	316	BCR	C32-C1-C6	-3.68	104.33	110.30
17	BK	203	CLA	CMB-C2B-C3B	3.68	131.56	124.68
20	BL	301	BCR	C38-C26-C25	-3.68	120.40	124.53
17	BB	836	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
20	BA	848	BCR	C30-C25-C26	-3.67	117.45	122.61
20	BA	850	BCR	C30-C25-C26	-3.66	117.45	122.61
20	BA	849	BCR	C38-C26-C25	-3.66	120.42	124.53
17	BA	829	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
17	BA	821	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	BA	831	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	B2	309	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	BA	836	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
17	B1	315	CLA	C4A-NA-C1A	3.64	108.34	106.71
25	B5	605	CHL	C1D-CHD-C4C	-3.63	118.22	126.06
25	B2	313	CHL	CHD-C4C-NC	3.63	129.93	124.20
17	BA	803	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
17	B5	602	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
20	BA	848	BCR	C38-C26-C27	3.62	120.58	113.62
17	BB	833	CLA	CMB-C2B-C3B	3.62	131.45	124.68
25	B2	306	CHL	C1D-ND-C4D	3.62	108.91	106.33
17	BA	828	CLA	CMB-C2B-C3B	3.62	131.44	124.68
20	B3	618	BCR	C37-C22-C23	3.61	123.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B2	316	BCR	C36-C18-C19	3.61	123.76	118.08
17	B5	602	CLA	C4A-NA-C1A	3.60	108.33	106.71
20	BG	203	BCR	C10-C11-C12	-3.60	111.97	123.22
20	BL	305	BCR	C30-C25-C24	3.60	125.96	115.78
20	BB	803	BCR	C37-C22-C23	3.60	123.75	118.08
20	BA	851	BCR	C33-C5-C4	3.60	120.53	113.62
20	BB	846	BCR	C8-C7-C6	-3.59	117.12	127.20
20	BB	845	BCR	C1-C6-C5	-3.59	117.56	122.61
27	B3	617	XAT	C35-C15-C14	-3.58	116.14	123.47
17	BB	813	CLA	CAB-C3B-C4B	-3.58	122.96	128.46
17	BB	821	CLA	C4A-NA-C1A	3.57	108.31	106.71
17	B3	615	CLA	C4A-NA-C1A	3.57	108.31	106.71
20	BI	101	BCR	C39-C30-C25	-3.57	104.50	110.30
27	B1	317	XAT	C6-C7-C8	-3.56	118.46	125.99
17	BB	824	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
20	BB	846	BCR	C3-C4-C5	-3.56	107.73	114.08
20	BH	202	BCR	C33-C5-C6	-3.55	120.55	124.53
25	B2	304	CHL	C1C-C2C-C3C	-3.54	104.30	107.11
17	BA	826	CLA	CMB-C2B-C3B	3.54	131.31	124.68
17	BB	835	CLA	C4A-NA-C1A	3.54	108.30	106.71
17	BB	815	CLA	CAC-C3C-C2C	-3.54	121.47	127.53
17	B1	304	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
17	BJ	102	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
25	B3	601	CHL	CMB-C2B-C3B	3.54	131.29	124.68
17	B3	608	CLA	CMB-C2B-C3B	3.53	131.29	124.68
17	BB	817	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
20	BB	847	BCR	C8-C9-C10	3.53	124.35	118.94
25	B2	304	CHL	CHD-C4C-NC	3.53	129.76	124.20
17	BB	801	CLA	O2D-CGD-O1D	-3.53	116.95	123.84
17	BA	841	CLA	CMB-C2B-C3B	3.52	131.27	124.68
25	B2	313	CHL	CAC-C3C-C4C	3.52	129.38	124.81
27	B5	615	XAT	C6-C7-C8	-3.52	118.55	125.99
19	BF	305	LHG	C5-O7-C7	-3.52	109.12	117.79
17	B3	615	CLA	CMB-C2B-C3B	3.52	131.26	124.68
17	BA	837	CLA	CMB-C2B-C3B	3.52	131.26	124.68
17	BA	822	CLA	CMB-C2B-C3B	3.52	131.26	124.68
20	BJ	101	BCR	C3-C4-C5	-3.52	107.80	114.08
17	BB	843	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
17	BA	811	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
17	B2	309	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
25	B1	308	CHL	CHD-C4C-NC	3.50	129.72	124.20
25	B3	607	CHL	CHD-C4C-NC	3.50	129.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BJ	103	BCR	C39-C30-C25	-3.50	104.62	110.30
17	B5	608	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
17	BA	835	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
20	BI	101	BCR	C38-C26-C27	3.49	120.33	113.62
25	B1	303	CHL	CHD-C4C-NC	3.49	129.71	124.20
20	BJ	103	BCR	C8-C9-C10	-3.49	113.58	118.94
20	BA	850	BCR	C36-C18-C19	3.49	123.57	118.08
19	B1	301	LHG	O7-C7-C8	3.49	119.02	111.50
17	BA	844	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
25	B5	605	CHL	CHC-C1C-NC	3.48	129.49	124.20
17	B1	307	CLA	C4A-NA-C1A	3.48	108.27	106.71
17	B2	310	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
17	BA	829	CLA	CMB-C2B-C3B	3.48	131.19	124.68
20	BA	847	BCR	C30-C25-C26	-3.48	117.72	122.61
20	BA	856	BCR	C30-C25-C26	-3.48	117.72	122.61
20	BA	855	BCR	C24-C23-C22	-3.47	120.98	126.23
18	BB	844	PQN	C11-C3-C4	-3.47	114.78	118.50
17	BA	814	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	BA	803	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
26	B3	616	LUT	C40-C33-C32	3.47	123.54	118.08
27	B2	315	XAT	C36-C21-C22	-3.47	102.96	108.98
17	B1	312	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
17	BB	805	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	B3	601	CHL	C2A-C1A-CHA	-3.46	117.80	123.86
25	B2	306	CHL	CHD-C4C-NC	3.46	129.66	124.20
17	B5	608	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
25	B5	606	CHL	CMC-C2C-C1C	3.46	130.31	125.04
17	BB	801	CLA	CHB-C4A-NA	3.46	129.29	124.51
25	B5	606	CHL	CHD-C4C-NC	3.46	129.65	124.20
17	BA	821	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
17	BB	834	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
17	BA	834	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
20	BI	101	BCR	C30-C25-C26	-3.45	117.75	122.61
17	BK	201	CLA	CAA-C2A-C3A	-3.45	108.05	116.10
20	BA	855	BCR	C34-C9-C8	3.45	123.51	118.08
20	BA	856	BCR	C37-C22-C21	-3.44	118.10	122.92
17	BB	828	CLA	CMB-C2B-C3B	3.43	131.10	124.68
17	BB	839	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	B3	607	CHL	CHC-C1C-C2C	-3.43	117.23	126.72
20	BB	847	BCR	C36-C18-C19	3.43	123.48	118.08
25	B1	303	CHL	C4A-NA-C1A	-3.43	105.17	106.71
17	B1	307	CLA	CMB-C2B-C3B	3.42	131.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B1	317	XAT	C40-C33-C32	3.42	123.47	118.08
17	B2	311	CLA	CMB-C2B-C3B	3.42	131.07	124.68
17	BA	812	CLA	CMB-C2B-C3B	3.42	131.07	124.68
20	BB	848	BCR	C39-C30-C25	-3.41	104.77	110.30
27	B2	315	XAT	C39-C29-C28	3.41	123.44	118.08
17	BA	803	CLA	CMB-C2B-C3B	3.41	131.05	124.68
20	BA	851	BCR	C8-C9-C10	3.40	124.16	118.94
17	BA	804	CLA	CMB-C2B-C3B	3.40	131.04	124.68
17	B3	611	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
27	B1	317	XAT	O4-C5-C18	3.40	119.13	115.06
17	B2	308	CLA	C4A-NA-C1A	3.40	108.23	106.71
17	B2	307	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
17	B1	305	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
17	BB	812	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
20	BF	304	BCR	C30-C25-C26	-3.39	117.84	122.61
25	B3	607	CHL	CAC-C3C-C4C	3.39	129.20	124.81
20	BI	101	BCR	C37-C22-C23	3.38	123.40	118.08
20	B2	316	BCR	C33-C5-C4	-3.37	107.14	113.62
26	B3	616	LUT	C19-C9-C8	3.37	123.39	118.08
27	B2	315	XAT	C40-C33-C32	3.37	123.39	118.08
17	BB	807	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
20	BA	855	BCR	C16-C15-C14	-3.37	116.58	123.47
27	B5	615	XAT	C18-C5-C6	-3.36	116.63	122.26
17	BA	817	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
20	BA	856	BCR	C38-C26-C25	3.36	128.30	124.53
20	BH	202	BCR	C38-C26-C25	-3.36	120.76	124.53
27	B5	615	XAT	C36-C21-C22	-3.36	103.15	108.98
17	B5	608	CLA	C4A-NA-C1A	3.36	108.22	106.71
17	BA	819	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
17	B5	610	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
17	BG	201	CLA	C4A-NA-C1A	3.35	108.21	106.71
18	BB	844	PQN	C14-C13-C12	-3.34	115.10	123.68
19	B1	302	LHG	O7-C7-C8	3.34	118.70	111.50
17	BB	819	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
24	BJ	104	SQD	O47-C7-O49	-3.34	115.64	123.70
19	BA	846	LHG	O7-C7-C8	3.33	118.69	111.50
17	BB	831	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	B1	309	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
18	BA	843	PQN	C16-C15-C13	-3.33	104.73	113.45
20	BB	846	BCR	C38-C26-C27	3.32	120.00	113.62
17	B5	609	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
20	BJ	101	BCR	C34-C9-C8	3.32	123.31	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B1	317	XAT	C38-C25-C26	-3.32	116.70	122.26
17	B5	603	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
20	BG	203	BCR	C11-C10-C9	3.31	132.04	127.31
17	B2	308	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
20	BA	847	BCR	C38-C26-C27	3.31	119.97	113.62
17	BA	823	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
17	B5	610	CLA	CMB-C2B-C3B	3.31	130.87	124.68
17	BB	830	CLA	CMB-C2B-C3B	3.30	130.86	124.68
17	BA	839	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	B3	601	CHL	CHC-C1C-NC	3.30	129.21	124.20
17	B1	304	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
17	BB	806	CLA	CMB-C2B-C3B	3.30	130.85	124.68
20	BG	203	BCR	C16-C17-C18	3.29	132.01	127.31
17	BA	836	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	BB	847	BCR	C33-C5-C6	-3.29	120.83	124.53
20	BI	101	BCR	C16-C15-C14	-3.29	116.74	123.47
17	B2	303	CLA	CMB-C2B-C3B	3.29	130.83	124.68
20	B5	616	BCR	C33-C5-C4	3.28	119.92	113.62
20	BK	204	BCR	C27-C26-C25	-3.28	117.97	122.73
20	BJ	101	BCR	C32-C1-C6	-3.28	104.98	110.30
17	BG	202	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
17	BB	814	CLA	CMB-C2B-C3B	3.28	130.81	124.68
20	BA	856	BCR	C29-C30-C25	3.27	115.52	110.48
17	B2	308	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
17	BA	821	CLA	CMB-C2B-C3B	3.27	130.80	124.68
20	B3	618	BCR	C33-C5-C4	3.26	119.89	113.62
17	B3	610	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
20	B2	316	BCR	C4-C5-C6	-3.26	117.99	122.73
17	BL	303	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
25	B2	305	CHL	CHD-C4C-NC	3.26	129.34	124.20
17	BA	818	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
17	BB	840	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
20	BL	305	BCR	C3-C4-C5	-3.25	108.27	114.08
17	BA	841	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
17	BB	826	CLA	CMB-C2B-C3B	3.25	130.76	124.68
20	BA	848	BCR	C27-C26-C25	-3.25	118.01	122.73
17	BA	840	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
20	BK	204	BCR	C36-C18-C17	-3.25	118.37	122.92
17	B2	312	CLA	CMB-C2B-C3B	3.25	130.76	124.68
17	B5	613	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
17	BA	828	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	BB	816	CLA	C1B-CHB-C4A	-3.24	123.69	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B1	303	CHL	CAC-C3C-C4C	3.24	129.02	124.81
17	BB	829	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	BK	202	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
17	BA	833	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
17	B1	311	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
20	B3	618	BCR	C28-C29-C30	-3.23	103.05	114.60
20	BB	803	BCR	C16-C15-C14	-3.23	116.86	123.47
17	BB	810	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
17	BA	830	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
17	B1	313	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	B2	305	CHL	CHC-C1C-NC	3.22	129.09	124.20
17	BB	816	CLA	C4A-NA-C1A	3.22	108.15	106.71
17	BB	812	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
17	BA	818	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
20	BG	203	BCR	C38-C26-C27	3.21	119.79	113.62
17	BB	824	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
20	BF	304	BCR	C31-C1-C6	-3.20	105.11	110.30
26	B5	614	LUT	C21-C26-C27	-3.20	108.66	112.70
17	BA	804	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
17	BB	820	CLA	CMB-C2B-C3B	3.19	130.65	124.68
17	BB	841	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
17	B1	314	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
25	B2	313	CHL	C1D-ND-C4D	3.19	108.60	106.33
17	B1	310	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
17	BB	829	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
17	BG	201	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
17	B3	604	CLA	CMB-C2B-C3B	3.18	130.92	124.69
17	BL	304	CLA	CMB-C2B-C3B	3.18	130.63	124.68
17	B5	601	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
17	BB	819	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
17	B2	302	CLA	CMB-C2B-C3B	3.18	130.62	124.68
17	BB	819	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
24	BJ	104	SQD	C3-C4-C5	3.17	115.90	110.24
17	BL	303	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	BA	849	BCR	C36-C18-C17	-3.17	118.48	122.92
20	BK	204	BCR	C38-C26-C25	-3.17	120.97	124.53
17	B3	606	CLA	CMB-C2B-C3B	3.17	130.89	124.69
17	BK	201	CLA	CMB-C2B-C3B	3.16	130.88	124.69
17	B3	606	CLA	CAB-C3B-C2B	3.16	130.88	124.69
17	B2	312	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	B5	616	BCR	C23-C22-C21	-3.16	114.09	118.94
17	BB	827	CLA	C1B-CHB-C4A	-3.16	123.86	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BA	832	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
20	BF	304	BCR	C37-C22-C23	3.15	123.05	118.08
17	BA	834	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
20	BB	803	BCR	C29-C30-C25	3.15	115.33	110.48
17	BB	830	CLA	C4A-NA-C1A	3.15	108.12	106.71
17	B3	613	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
17	BK	201	CLA	CAB-C3B-C2B	3.15	130.86	124.69
20	BJ	103	BCR	C1-C6-C5	-3.15	118.18	122.61
20	BF	304	BCR	C16-C15-C14	-3.15	117.02	123.47
20	BA	855	BCR	C8-C9-C10	-3.15	114.11	118.94
17	B2	307	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
25	B2	306	CHL	CHC-C1C-NC	3.15	128.98	124.20
26	B1	316	LUT	C20-C13-C14	-3.15	118.52	122.92
17	BB	817	CLA	CMB-C2B-C3B	3.14	130.56	124.68
17	BB	814	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
17	BK	202	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	B1	308	CHL	C4A-NA-C1A	-3.14	105.30	106.71
17	B3	606	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
17	BB	836	CLA	CMB-C2B-C3B	3.14	130.55	124.68
17	BB	809	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
27	B1	317	XAT	C35-C15-C14	-3.13	117.06	123.47
17	BB	838	CLA	CMB-C2B-C3B	3.13	130.54	124.68
17	BA	808	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
20	BL	301	BCR	C34-C9-C8	3.13	123.00	118.08
27	B1	317	XAT	C26-C27-C28	-3.13	119.38	125.99
17	BB	825	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
17	BL	304	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
17	BB	827	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
20	BI	101	BCR	C28-C27-C26	-3.12	108.50	114.08
17	B5	612	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
17	BF	301	CLA	CMB-C2B-C3B	3.12	130.52	124.68
20	BA	847	BCR	C37-C22-C23	3.12	123.00	118.08
17	BB	828	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
17	BB	819	CLA	CMB-C2B-C3B	3.12	130.52	124.68
20	BF	304	BCR	C7-C8-C9	-3.12	121.52	126.23
17	BB	810	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
17	BF	303	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
26	B1	316	LUT	C40-C33-C34	-3.12	118.55	122.92
20	BB	848	BCR	C29-C30-C25	3.12	115.28	110.48
25	B5	605	CHL	CHD-C4C-NC	3.11	129.11	124.20
17	BB	802	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
17	BL	303	CLA	CMB-C2B-C3B	3.11	130.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BA	850	BCR	C19-C18-C17	-3.11	114.17	118.94
17	B2	301	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
20	BL	301	BCR	C37-C22-C23	3.11	122.97	118.08
17	B3	605	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
17	B3	609	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
20	BA	855	BCR	C39-C30-C25	-3.10	105.26	110.30
25	B5	607	CHL	CHA-C4D-ND	3.10	138.99	132.50
17	BB	802	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
20	BA	850	BCR	C27-C26-C25	-3.10	118.23	122.73
17	BB	829	CLA	CMB-C2B-C3B	3.10	130.47	124.68
17	BA	829	CLA	C2D-C1D-ND	-3.10	107.82	110.10
17	BB	830	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
17	BA	810	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
20	B5	616	BCR	C23-C24-C25	-3.09	118.52	127.20
17	BA	807	CLA	CMB-C2B-C3B	3.09	130.46	124.68
17	BB	824	CLA	CMB-C2B-C3B	3.09	130.45	124.68
23	BB	850	DGD	O1G-C1A-C2A	3.08	121.58	111.91
20	BB	849	BCR	C15-C16-C17	-3.08	117.16	123.47
17	BA	828	CLA	O2D-CGD-CBD	3.08	116.74	111.27
17	BB	824	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	BB	818	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	BB	827	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
17	BF	302	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
26	B3	616	LUT	C15-C35-C34	-3.08	117.17	123.47
17	BB	827	CLA	C4A-NA-C1A	3.07	108.09	106.71
17	BA	817	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
20	BB	849	BCR	C38-C26-C25	-3.07	121.08	124.53
17	BB	829	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
17	BA	806	CLA	CHB-C4A-NA	3.06	128.75	124.51
25	B5	606	CHL	CHC-C1C-C2C	-3.06	118.25	126.72
20	BB	849	BCR	C28-C27-C26	-3.06	108.61	114.08
17	BA	821	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
17	B1	315	CLA	CAB-C3B-C2B	3.06	130.69	124.69
17	B3	608	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
17	BB	805	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
20	BB	803	BCR	C12-C13-C14	-3.06	114.24	118.94
17	B1	315	CLA	CMB-C2B-C3B	3.06	130.68	124.69
17	B5	608	CLA	CMB-C2B-C3B	3.06	130.40	124.68
17	BA	841	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
17	BA	824	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
17	BA	844	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
26	B2	314	LUT	C17-C1-C6	-3.05	105.35	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BH	201	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
17	B5	603	CLA	CAB-C3B-C2B	3.05	130.66	124.69
17	BA	814	CLA	CMB-C2B-C3B	3.04	130.38	124.68
17	BA	820	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	B2	312	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
17	BA	835	CLA	CMB-C2B-C3B	3.04	130.37	124.68
17	B1	314	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	B2	306	CHL	CHA-C4D-ND	3.04	138.86	132.50
17	BB	833	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
17	B3	613	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
17	BB	829	CLA	CHB-C4A-NA	3.04	128.71	124.51
17	B5	602	CLA	CMB-C2B-C3B	3.04	130.36	124.68
17	B2	309	CLA	C1A-CHA-C4D	-3.04	121.47	125.72
17	BA	809	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
17	B3	602	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
17	BL	302	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
17	BA	806	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
20	BJ	103	BCR	C19-C18-C17	-3.03	114.28	118.94
25	B3	601	CHL	C4-C3-C5	3.03	120.37	115.27
17	BA	820	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
17	B5	613	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
17	BA	842	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	BH	201	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	BB	813	CLA	CMB-C2B-C3B	3.03	130.62	124.69
17	BB	836	CLA	CHD-C1D-ND	-3.03	121.67	124.45
17	BA	819	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
20	BI	101	BCR	C1-C6-C5	-3.03	118.35	122.61
17	B5	609	CLA	C4A-NA-C1A	3.03	108.07	106.71
17	B1	306	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
17	BA	831	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
17	BA	835	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
17	B5	601	CLA	CMB-C2B-C3B	3.01	130.32	124.68
17	B1	310	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
17	BA	811	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
17	BB	836	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
17	BB	822	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	B2	313	CHL	C1C-C2C-C3C	-3.01	104.72	107.11
26	B2	314	LUT	C28-C29-C30	-3.01	114.32	118.94
17	BB	813	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
17	BA	822	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
17	BJ	102	CLA	CMB-C2B-C3B	3.01	130.30	124.68
20	BF	304	BCR	C1-C6-C5	-3.00	118.38	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B3	609	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
20	BA	855	BCR	C4-C5-C6	-3.00	118.37	122.73
17	BB	818	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
17	BA	825	CLA	CMB-C2B-C3B	3.00	130.29	124.68
17	BB	824	CLA	CHD-C1D-ND	-3.00	121.70	124.45
17	BA	833	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
27	B5	615	XAT	C40-C33-C32	3.00	122.80	118.08
25	B3	607	CHL	CHA-C4D-ND	3.00	138.77	132.50
17	BA	815	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	B1	303	CHL	CHA-C4D-ND	2.99	138.76	132.50
20	B2	316	BCR	C38-C26-C25	-2.99	121.17	124.53
20	B5	616	BCR	C12-C13-C14	-2.99	114.36	118.94
17	BA	831	CLA	CMB-C2B-C3B	2.99	130.26	124.68
17	BA	839	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
17	B5	604	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
19	BA	845	LHG	O7-C7-C8	2.98	117.93	111.50
17	BA	834	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
20	BB	847	BCR	C37-C22-C23	2.98	122.77	118.08
17	BB	820	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
17	BB	843	CLA	CMB-C2B-C3B	2.98	130.25	124.68
17	BA	815	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
20	BA	848	BCR	C8-C9-C10	-2.97	114.38	118.94
17	BB	809	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
20	BA	848	BCR	C38-C26-C25	-2.97	121.19	124.53
17	BA	817	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	BB	841	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	B3	604	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
20	BB	803	BCR	C40-C30-C25	-2.97	105.48	110.30
25	B1	303	CHL	CHC-C1C-NC	2.97	128.71	124.20
17	BA	844	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	BA	826	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
17	BB	827	CLA	CMB-C2B-C3B	2.96	130.22	124.68
17	B2	301	CLA	CAC-C3C-C4C	2.96	128.65	124.81
17	BB	801	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
17	B5	601	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
19	B1	301	LHG	O8-C23-C24	2.96	121.19	111.91
17	BF	302	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
17	BB	810	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
17	B5	602	CLA	CHD-C1D-ND	-2.96	121.74	124.45
17	B1	312	CLA	CAB-C3B-C2B	2.96	130.48	124.69
17	BB	836	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
17	B5	610	CLA	O2D-CGD-O1D	-2.95	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	850	DGD	C2G-O2G-C1B	-2.95	110.52	117.79
17	BA	810	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
17	BB	808	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
17	BA	816	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
25	B2	304	CHL	CHA-C4D-ND	2.95	138.67	132.50
20	B2	316	BCR	C37-C22-C23	2.95	122.72	118.08
26	B5	614	LUT	C8-C9-C10	-2.95	114.42	118.94
20	BB	848	BCR	C15-C16-C17	-2.95	117.44	123.47
17	BA	801	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
20	B3	618	BCR	C15-C16-C17	-2.94	117.44	123.47
20	BA	856	BCR	C15-C16-C17	-2.94	117.44	123.47
27	B3	617	XAT	C36-C21-C22	-2.94	103.87	108.98
17	B1	305	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
20	BB	846	BCR	C37-C22-C21	-2.94	118.81	122.92
17	B2	310	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	BA	832	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	B5	614	LUT	C35-C15-C14	-2.94	117.46	123.47
17	BK	202	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
17	BB	821	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
17	BA	806	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	B2	313	CHL	CHC-C1C-NC	2.93	128.65	124.20
17	B2	301	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	B2	305	CHL	CHA-C4D-ND	2.93	138.63	132.50
17	BK	202	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	B2	308	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	B3	604	CLA	CAB-C3B-C2B	2.93	130.42	124.69
17	BA	817	CLA	CHD-C1D-ND	-2.93	121.77	124.45
17	B1	307	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
17	BA	825	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	BA	849	BCR	C3-C4-C5	-2.92	108.86	114.08
25	B3	601	CHL	CHA-C4D-ND	2.92	138.61	132.50
17	BA	807	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	B5	607	CHL	CHC-C1C-NC	2.92	128.63	124.20
17	BB	837	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
17	BB	807	CLA	CHD-C1D-ND	-2.92	121.78	124.45
26	B3	616	LUT	C8-C9-C10	-2.91	114.47	118.94
17	BB	815	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
26	B3	616	LUT	C37-C21-C22	-2.91	103.92	109.44
17	B3	611	CLA	CMB-C2B-C3B	2.91	130.13	124.68
25	B2	304	CHL	CHC-C1C-NC	2.91	128.62	124.20
20	BK	204	BCR	C28-C27-C26	-2.91	108.88	114.08
17	BJ	102	CLA	O2D-CGD-O1D	-2.91	118.15	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BA	849	BCR	C37-C22-C23	2.91	122.66	118.08
20	BB	848	BCR	C23-C22-C21	-2.90	114.49	118.94
17	BA	811	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
17	B2	308	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	B5	605	CHL	CHA-C4D-ND	2.90	138.56	132.50
17	B2	309	CLA	CMB-C2B-C3B	2.90	130.37	124.69
20	BB	847	BCR	C23-C22-C21	2.90	123.39	118.94
17	BA	812	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
17	B1	311	CLA	CHB-C4A-NA	2.90	128.52	124.51
17	BA	824	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	BA	816	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
17	B1	312	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
17	BA	828	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
17	B2	309	CLA	O2D-CGD-CBD	2.90	116.41	111.27
17	BA	818	CLA	CMB-C2B-C3B	2.90	130.09	124.68
17	BB	806	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
17	BB	833	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	BB	804	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
17	BB	804	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	BB	801	CLA	C2D-C1D-ND	-2.89	107.97	110.10
17	B3	602	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
27	B1	317	XAT	C12-C13-C14	-2.89	114.50	118.94
17	BB	838	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
17	B1	314	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
17	BB	813	CLA	CAB-C3B-C2B	2.89	130.35	124.69
17	BA	836	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
17	B2	311	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
17	BA	823	CLA	CMB-C2B-C3B	2.89	130.08	124.68
17	B5	604	CLA	CMB-C2B-C3B	2.89	130.34	124.69
17	BA	831	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
20	B2	316	BCR	C38-C26-C27	2.88	119.16	113.62
17	BB	834	CLA	CHB-C4A-NA	2.88	128.50	124.51
17	B5	604	CLA	CAB-C3B-C2B	2.88	130.34	124.69
17	BA	827	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	BA	848	BCR	C36-C18-C17	-2.88	118.89	122.92
20	B3	618	BCR	C23-C22-C21	-2.88	114.52	118.94
17	BA	805	CLA	CHD-C1D-ND	-2.88	121.81	124.45
20	BA	851	BCR	C31-C1-C6	-2.88	105.63	110.30
17	BA	803	CLA	O2D-CGD-CBD	2.88	116.38	111.27
17	B2	309	CLA	CAB-C3B-C2B	2.88	130.32	124.69
17	BB	806	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
17	B1	315	CLA	C1B-CHB-C4A	-2.88	124.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BB	834	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
17	BB	840	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
17	BA	813	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
20	BJ	103	BCR	C7-C8-C9	-2.87	121.89	126.23
27	B3	617	XAT	C12-C13-C14	-2.87	114.53	118.94
17	BB	812	CLA	CMB-C2B-C3B	2.87	130.05	124.68
17	BA	829	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	BB	801	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
20	BJ	103	BCR	C16-C15-C14	-2.87	117.59	123.47
17	B3	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	BA	849	BCR	C16-C15-C14	-2.87	117.59	123.47
17	B1	306	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	BA	807	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	BJ	103	BCR	C15-C16-C17	-2.87	117.60	123.47
17	BA	814	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
17	BA	819	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
17	BA	815	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
17	B5	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	BA	850	BCR	C23-C22-C21	-2.86	114.55	118.94
17	B1	309	CLA	CMB-C2B-C3B	2.86	130.04	124.68
17	BB	801	CLA	CAA-C2A-C1A	-2.86	102.59	111.97
17	B1	312	CLA	CMB-C2B-C3B	2.86	130.29	124.69
17	BB	805	CLA	CMC-C2C-C1C	-2.86	120.68	125.04
17	BB	842	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	BB	834	CLA	C6-C5-C3	2.86	120.95	113.45
20	BL	305	BCR	C1-C6-C5	-2.86	118.59	122.61
17	BB	820	CLA	C6-C5-C3	2.86	120.95	113.45
17	BH	201	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
17	BA	827	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
25	B3	601	CHL	O1D-CGD-CBD	-2.85	118.65	124.48
17	B5	608	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	BA	842	CLA	CMB-C2B-C3B	2.85	130.01	124.68
26	B2	314	LUT	C1-C6-C5	-2.85	118.60	122.61
27	B2	315	XAT	C38-C25-C26	-2.85	117.49	122.26
17	BB	820	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
20	BB	848	BCR	C30-C25-C26	-2.84	118.61	122.61
17	B1	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	B2	316	BCR	C31-C1-C6	2.84	114.91	110.30
25	B1	303	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
25	B3	601	CHL	O2A-CGA-CBA	2.84	120.82	111.91
17	B5	604	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	B5	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B2	302	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
20	BA	849	BCR	C33-C5-C4	2.84	119.07	113.62
17	BB	832	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
17	BB	826	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	B3	603	CLA	CMB-C2B-C1B	-2.84	124.11	128.46
25	B1	308	CHL	CHC-C1C-NC	2.84	128.50	124.20
17	BL	302	CLA	CHB-C4A-NA	2.83	128.43	124.51
17	BA	835	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	BB	837	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	BB	821	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
17	BB	807	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
17	BA	830	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
20	BJ	103	BCR	C30-C25-C26	-2.83	118.63	122.61
20	BF	304	BCR	C33-C5-C6	-2.83	121.36	124.53
17	BA	816	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	BA	838	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
17	B5	613	CLA	CHD-C1D-ND	-2.82	121.86	124.45
17	B1	309	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
26	B5	614	LUT	C40-C33-C32	2.82	122.52	118.08
17	BB	826	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	BA	811	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	B5	605	CHL	CAC-C3C-C4C	2.82	129.33	125.04
17	B1	311	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	BG	202	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	BK	204	BCR	C4-C5-C6	-2.82	118.64	122.73
20	B2	316	BCR	C34-C9-C8	2.82	122.51	118.08
20	BG	203	BCR	C23-C22-C21	2.81	123.26	118.94
17	B3	614	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
20	BL	301	BCR	C36-C18-C17	-2.81	118.98	122.92
17	BB	814	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
17	BB	817	CLA	O2D-CGD-O1D	-2.81	117.70	124.09
17	BA	824	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
17	BB	809	CLA	O2D-CGD-CBD	2.81	116.26	111.27
17	BB	837	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
17	BA	838	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	BB	812	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
20	B5	616	BCR	C36-C18-C19	2.80	122.49	118.08
17	B3	612	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
17	B5	612	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	B1	308	CHL	CHA-C4D-ND	2.80	138.35	132.50
17	BA	836	CLA	CMB-C2B-C3B	2.80	129.91	124.68
17	B2	311	CLA	O2D-CGD-O1D	-2.80	118.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B3	616	LUT	C32-C33-C34	-2.79	114.66	118.94
17	BA	815	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	B2	313	CHL	CHA-C4D-ND	2.79	138.34	132.50
17	BA	844	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	BA	802	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
20	BB	846	BCR	C8-C9-C10	2.79	123.22	118.94
20	BL	301	BCR	C38-C26-C27	2.79	118.97	113.62
17	B2	303	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	B2	314	LUT	C15-C35-C34	-2.79	117.76	123.47
17	B5	609	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
20	BJ	101	BCR	C37-C22-C23	2.79	122.47	118.08
17	BB	805	CLA	CAC-C3C-C4C	2.79	128.43	124.81
17	BA	804	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
17	BA	821	CLA	CHD-C1D-ND	-2.78	121.89	124.45
17	BB	819	CLA	CHB-C4A-NA	2.78	128.36	124.51
20	BB	846	BCR	C28-C27-C26	-2.78	109.11	114.08
17	BB	839	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
20	BK	204	BCR	C37-C22-C21	-2.78	119.02	122.92
17	BB	809	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
20	B5	616	BCR	C8-C9-C10	-2.78	114.67	118.94
17	BA	823	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	B5	606	CHL	CHA-C4D-ND	2.78	138.32	132.50
20	BJ	103	BCR	C31-C1-C6	2.78	114.81	110.30
17	B2	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	B5	616	BCR	C16-C15-C14	-2.78	117.78	123.47
20	BB	847	BCR	C1-C6-C5	-2.77	118.71	122.61
17	B3	612	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
25	B3	601	CHL	C1C-C2C-C3C	-2.77	104.92	107.11
17	BB	819	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
17	BA	817	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
20	B3	618	BCR	C20-C21-C22	-2.77	123.36	127.31
17	BA	801	CLA	C4A-NA-C1A	2.76	107.95	106.71
17	B5	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	B3	618	BCR	C36-C18-C19	2.76	122.43	118.08
27	B3	617	XAT	C26-C27-C28	-2.76	120.15	125.99
25	B1	308	CHL	C1C-C2C-C3C	-2.76	104.92	107.11
20	BK	204	BCR	C34-C9-C8	2.76	122.43	118.08
17	BA	819	CLA	CMB-C2B-C3B	2.76	129.84	124.68
17	B5	613	CLA	CMB-C2B-C3B	2.76	129.84	124.68
17	B1	310	CLA	CAB-C3B-C2B	2.76	130.09	124.69
25	B3	607	CHL	C4C-C3C-C2C	-2.75	102.88	106.90
17	BF	303	CLA	CMB-C2B-C3B	2.75	129.83	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B5	618	LHG	C5-O7-C7	-2.75	111.02	117.79
19	B3	619	LHG	O8-C23-C24	2.75	120.54	111.91
17	BA	813	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	B3	607	CHL	C2C-C1C-NC	2.75	112.55	109.97
20	B2	316	BCR	C36-C18-C17	-2.75	119.07	122.92
17	BA	818	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	BA	820	CLA	CMB-C2B-C3B	2.75	129.81	124.68
17	B3	610	CLA	CMB-C2B-C3B	2.75	129.81	124.68
17	BB	822	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
17	BB	839	CLA	CMB-C2B-C3B	2.74	129.81	124.68
26	B5	614	LUT	C28-C29-C30	-2.74	114.73	118.94
27	B1	317	XAT	C36-C21-C22	-2.74	104.22	108.98
17	BA	833	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
17	BB	822	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	B2	305	CHL	C4A-NA-C1A	-2.74	105.47	106.71
17	BA	809	CLA	CMB-C2B-C3B	2.74	129.81	124.68
17	BA	834	CLA	CMB-C2B-C3B	2.74	129.81	124.68
26	B2	314	LUT	C8-C7-C6	-2.74	119.51	127.20
17	BB	822	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
17	B1	305	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	BB	827	CLA	CHD-C1D-ND	-2.73	121.94	124.45
17	BA	836	CLA	O2D-CGD-CBD	2.73	116.12	111.27
17	BA	830	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
20	BI	101	BCR	C32-C1-C6	2.73	114.72	110.30
17	BB	817	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
17	B1	310	CLA	CMA-C3A-C2A	-2.72	109.74	116.10
17	BA	842	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
17	BB	818	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
20	BF	304	BCR	C34-C9-C8	2.72	122.36	118.08
17	B1	313	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
17	BG	202	CLA	CMB-C2B-C3B	2.72	129.76	124.68
17	B3	613	CLA	CMB-C2B-C3B	2.71	129.76	124.68
17	BA	801	CLA	C1D-ND-C4D	-2.71	104.41	106.33
17	B5	611	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	BF	303	CLA	CAA-C2A-C3A	-2.71	109.77	116.10
20	BB	848	BCR	C19-C18-C17	-2.71	114.78	118.94
17	BA	824	CLA	CHB-C4A-NA	2.71	128.26	124.51
27	B2	315	XAT	C26-C27-C28	-2.71	120.26	125.99
17	B3	611	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	BB	826	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
20	BA	856	BCR	C36-C18-C17	-2.71	119.13	122.92
18	BA	843	PQN	C21-C22-C23	-2.71	107.17	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BA	823	CLA	CHD-C1D-ND	-2.71	121.97	124.45
17	BA	805	CLA	CMC-C2C-C1C	-2.71	120.92	125.04
17	BA	840	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
26	B1	316	LUT	C32-C33-C34	2.70	123.09	118.94
20	BA	848	BCR	C12-C13-C14	-2.70	114.80	118.94
17	BB	824	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	BI	101	BCR	C24-C23-C22	-2.70	122.15	126.23
20	BA	855	BCR	C36-C18-C19	2.70	122.33	118.08
20	BA	855	BCR	C12-C13-C14	-2.70	114.80	118.94
20	BH	202	BCR	C7-C8-C9	-2.70	122.16	126.23
17	BB	820	CLA	CHD-C1D-ND	-2.70	121.97	124.45
20	BA	850	BCR	C16-C15-C14	-2.70	117.94	123.47
27	B5	615	XAT	C39-C29-C30	-2.70	119.14	122.92
17	BA	803	CLA	CAC-C3C-C4C	2.70	128.31	124.81
17	BB	816	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
20	BJ	103	BCR	C3-C4-C5	-2.70	109.26	114.08
17	B5	602	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
17	BA	805	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
17	BL	302	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
20	BL	305	BCR	C38-C26-C27	2.69	118.78	113.62
17	B3	606	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
17	B1	304	CLA	CAC-C3C-C4C	2.69	128.30	124.81
17	B1	304	CLA	CMB-C2B-C3B	2.69	129.71	124.68
17	B2	308	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	B5	615	XAT	C38-C25-C26	-2.69	117.76	122.26
17	BB	820	CLA	C5-C3-C2	-2.68	115.69	121.12
17	BA	805	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
17	BK	203	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	B3	610	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	BF	303	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	BB	840	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
17	BA	828	CLA	C11-C10-C8	2.68	124.58	115.92
17	BK	201	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
20	BB	849	BCR	C8-C7-C6	-2.68	119.68	127.20
17	B5	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
17	BB	818	CLA	CMB-C2B-C3B	2.68	129.69	124.68
17	BB	838	CLA	CHB-C4A-NA	2.68	128.21	124.51
17	BA	822	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
17	BB	828	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	BF	301	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
20	BL	301	BCR	C2-C1-C6	-2.67	106.37	110.48
20	B2	316	BCR	C1-C6-C5	-2.67	118.85	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BB	802	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
17	BA	801	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
20	B3	618	BCR	C1-C6-C7	2.67	123.33	115.78
20	BF	304	BCR	C38-C26-C25	-2.67	121.53	124.53
26	B2	314	LUT	C8-C9-C10	-2.67	114.85	118.94
20	BB	848	BCR	C38-C26-C27	2.67	118.74	113.62
26	B5	614	LUT	C3-C4-C5	-2.67	106.54	111.85
17	BA	829	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
20	BH	202	BCR	C33-C5-C4	2.66	118.73	113.62
17	BL	303	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
17	B1	307	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	BF	304	BCR	C12-C13-C14	2.66	123.03	118.94
20	BA	855	BCR	C29-C28-C27	-2.66	105.43	111.38
17	BA	839	CLA	O2D-CGD-CBD	2.66	116.00	111.27
17	B1	309	CLA	O2D-CGD-O1D	-2.66	118.05	124.09
20	BJ	103	BCR	C12-C13-C14	-2.66	114.86	118.94
26	B2	314	LUT	C32-C33-C34	-2.66	114.86	118.94
17	B3	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	B3	616	LUT	C7-C8-C9	-2.66	122.22	126.23
19	B2	317	LHG	O7-C7-C8	2.66	117.23	111.50
18	BB	844	PQN	O4-C4-C5	-2.66	117.26	121.56
17	BA	840	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	BI	101	BCR	C12-C13-C14	-2.65	114.87	118.94
17	BA	840	CLA	CMB-C2B-C3B	2.65	129.64	124.68
20	BB	848	BCR	C40-C30-C25	-2.65	106.00	110.30
25	B2	305	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
26	B3	616	LUT	C12-C13-C14	-2.65	114.87	118.94
17	BA	806	CLA	CMB-C2B-C3B	2.65	129.63	124.68
17	B3	609	CLA	CMB-C2B-C3B	2.65	129.63	124.68
17	BA	821	CLA	C4-C3-C5	2.65	119.73	115.27
17	BB	815	CLA	CBC-CAC-C3C	2.65	119.73	112.43
20	BA	849	BCR	C24-C23-C22	-2.65	122.23	126.23
20	BA	855	BCR	C37-C22-C21	-2.64	119.22	122.92
17	BA	823	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	BA	820	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
20	B5	616	BCR	C38-C26-C27	2.64	118.69	113.62
17	BL	303	CLA	O2D-CGD-CBD	2.64	115.97	111.27
27	B5	615	XAT	C8-C9-C10	-2.64	114.89	118.94
20	B3	618	BCR	C19-C18-C17	-2.64	114.89	118.94
25	B5	607	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
20	BA	851	BCR	C36-C18-C17	-2.64	119.22	122.92
17	BA	840	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B5	618	LHG	O8-C23-C24	2.64	120.19	111.91
17	B3	615	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	BA	831	CLA	CHD-C1D-ND	-2.64	122.03	124.45
17	BJ	102	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	BB	813	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	B2	310	CLA	CMB-C2B-C3B	2.64	129.61	124.68
20	BA	847	BCR	C1-C6-C5	-2.64	118.90	122.61
17	BL	304	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
17	B1	310	CLA	CMB-C2B-C3B	2.64	129.85	124.69
17	B5	609	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
17	BB	823	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	B2	303	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
17	BB	843	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
17	B2	301	CLA	CMB-C2B-C3B	2.63	129.60	124.68
17	BA	801	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
20	BJ	103	BCR	C27-C26-C25	-2.63	118.91	122.73
17	BB	808	CLA	CMB-C2B-C3B	2.63	129.60	124.68
20	BB	847	BCR	C32-C1-C6	-2.63	106.03	110.30
20	BB	845	BCR	C16-C15-C14	-2.63	118.09	123.47
17	B1	306	CLA	CMB-C2B-C3B	2.63	129.59	124.68
17	B1	313	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	BA	851	BCR	C3-C4-C5	-2.62	109.39	114.08
17	B1	305	CLA	C5-C3-C2	2.62	126.43	121.12
17	B3	611	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
17	B1	311	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
17	BA	826	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
17	BB	816	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	BA	808	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
27	B3	617	XAT	C8-C9-C10	-2.62	114.92	118.94
17	BA	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	BB	811	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	B5	611	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
17	B2	307	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	BB	809	CLA	CMB-C2B-C3B	2.62	129.57	124.68
17	B1	315	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
17	BA	808	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	BF	303	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	BF	302	CLA	CHB-C4A-NA	2.61	128.13	124.51
17	B5	601	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
17	BA	832	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
17	BA	805	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
17	BA	804	CLA	CHD-C1D-ND	-2.61	122.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BB	831	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
20	BB	803	BCR	C3-C4-C5	-2.61	109.42	114.08
17	BA	837	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
28	B5	617	LMG	O8-C28-C29	2.61	120.08	111.91
19	B2	317	LHG	O8-C23-C24	2.60	120.08	111.91
17	BB	825	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
17	BB	838	CLA	C1-C2-C3	-2.60	122.54	126.75
17	BB	808	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	B1	306	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
17	B5	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
17	B5	612	CLA	CMB-C2B-C3B	2.59	129.53	124.68
17	B3	615	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
17	BB	801	CLA	O1D-CGD-CBD	2.59	129.79	124.48
17	BF	302	CLA	CAA-C2A-C3A	-2.59	107.78	114.26
20	BK	204	BCR	C1-C6-C7	2.59	123.11	115.78
17	BA	813	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
20	B3	618	BCR	C38-C26-C27	2.59	118.59	113.62
17	BL	302	CLA	O2A-CGA-O1A	-2.59	116.85	123.30
20	BA	848	BCR	C15-C16-C17	-2.59	118.18	123.47
17	BA	838	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
17	B1	310	CLA	O2D-CGD-O1D	-2.58	118.22	124.09
17	BA	824	CLA	CBA-CAA-C2A	2.58	121.49	113.86
20	BA	851	BCR	C39-C30-C25	-2.58	106.11	110.30
17	B2	312	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
17	B5	603	CLA	CMB-C2B-C3B	2.58	129.74	124.69
17	B3	602	CLA	CMB-C2B-C3B	2.58	129.50	124.68
17	BB	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	BB	808	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
20	BA	855	BCR	C24-C25-C26	2.58	127.70	121.46
17	BA	812	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
20	BL	305	BCR	C15-C16-C17	-2.58	118.20	123.47
17	BB	810	CLA	CMB-C2B-C3B	2.58	129.50	124.68
17	BA	824	CLA	CMB-C2B-C3B	2.58	129.50	124.68
17	BB	807	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	B2	309	CLA	C3A-C4A-CHB	-2.57	117.46	124.50
20	BL	301	BCR	C8-C9-C10	2.57	122.89	118.94
17	BB	811	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	B1	316	LUT	C35-C15-C14	2.57	128.74	123.47
17	BA	809	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	B5	611	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
17	BA	828	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
25	B5	605	CHL	C1C-C2C-C3C	-2.57	105.08	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BA	834	CLA	CHD-C1D-ND	-2.56	122.10	124.45
20	BA	849	BCR	C4-C5-C6	-2.56	119.01	122.73
17	BA	814	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	BA	812	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	BB	839	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
27	B5	615	XAT	C26-C27-C28	-2.56	120.58	125.99
17	BG	201	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	BB	808	CLA	CHD-C1D-ND	-2.56	122.10	124.45
20	BH	202	BCR	C36-C18-C19	-2.55	114.05	118.08
25	B5	606	CHL	CAC-C3C-C4C	2.55	128.93	125.04
17	BB	831	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
17	BA	808	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
26	B2	314	LUT	C19-C9-C8	2.55	122.10	118.08
17	B1	312	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
17	B2	302	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
27	B3	617	XAT	C24-C23-C22	-2.55	105.85	110.77
17	BB	817	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	B2	316	BCR	C7-C6-C5	2.55	127.63	121.46
17	B1	313	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
20	BJ	101	BCR	C36-C18-C19	2.54	122.08	118.08
17	BB	813	CLA	CHB-C4A-NA	2.54	128.03	124.51
17	B1	304	CLA	O1D-CGD-CBD	2.54	129.68	124.48
17	B3	605	CLA	CHD-C1D-ND	-2.54	122.12	124.45
17	BA	808	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
17	B5	611	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
20	BB	849	BCR	C36-C18-C17	-2.54	119.37	122.92
17	B3	613	CLA	O2D-CGD-O1D	-2.54	118.33	124.09
17	BB	842	CLA	CAC-C3C-C4C	2.54	128.10	124.81
17	BA	813	CLA	CMB-C2B-C3B	2.54	129.43	124.68
19	BA	845	LHG	O8-C23-C24	2.53	119.86	111.91
17	BA	807	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
17	BL	302	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
17	BA	837	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	BK	203	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	B2	313	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
17	B2	311	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	BA	848	BCR	C35-C13-C12	2.53	122.06	118.08
17	BA	832	CLA	CMB-C2B-C3B	2.53	129.41	124.68
20	BB	845	BCR	C15-C16-C17	-2.53	118.30	123.47
20	BA	855	BCR	C2-C3-C4	-2.53	105.73	111.38
17	B5	609	CLA	CHD-C1D-ND	-2.52	122.13	124.45
17	BL	302	CLA	O1A-CGA-CBA	2.52	131.19	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B1	304	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
17	B1	311	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	B5	607	CHL	C3C-C4C-NC	2.52	113.33	110.57
17	B3	605	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
17	BB	843	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
17	BA	813	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
17	BB	810	CLA	CBA-CAA-C2A	2.52	121.30	113.86
17	BB	805	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	B5	604	CLA	CHD-C1D-ND	-2.52	122.14	124.45
17	B3	612	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
17	BA	816	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	BA	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	BA	843	PQN	C14-C13-C12	-2.51	117.23	123.68
17	BA	841	CLA	C5-C3-C2	-2.51	116.03	121.12
17	BB	812	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	BB	805	CLA	CMD-C2D-C3D	2.51	133.40	127.61
17	B5	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	BA	844	CLA	CHD-C1D-ND	-2.51	122.14	124.45
17	B1	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	BL	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	BB	848	BCR	C23-C24-C25	-2.51	120.15	127.20
17	BB	801	CLA	C1-O2A-CGA	2.51	123.03	116.44
17	BA	816	CLA	CAC-C3C-C4C	2.51	128.06	124.81
17	B5	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B3	610	CLA	O2D-CGD-O1D	-2.51	118.40	124.09
17	BA	839	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	BA	810	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
17	BB	839	CLA	CHD-C1D-ND	-2.50	122.15	124.45
17	BA	809	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
19	B1	302	LHG	O8-C23-C24	2.50	119.76	111.91
17	B1	315	CLA	CMA-C3A-C2A	-2.50	110.26	116.10
17	BA	813	CLA	C4-C3-C5	2.50	119.48	115.27
20	BJ	103	BCR	C7-C6-C5	2.50	127.52	121.46
25	B1	303	CHL	C3C-C4C-NC	2.50	113.37	110.57
20	BB	846	BCR	C36-C18-C17	-2.50	119.42	122.92
17	BA	836	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	BA	855	BCR	C30-C25-C26	-2.50	119.09	122.61
17	BA	831	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	BJ	101	BCR	C30-C25-C26	-2.50	119.10	122.61
17	B3	604	CLA	O2D-CGD-O1D	-2.50	118.42	124.09
17	BA	817	CLA	CHB-C4A-NA	2.50	127.96	124.51
20	B2	316	BCR	C16-C15-C14	-2.50	118.36	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BB	834	CLA	C4-C3-C5	-2.49	111.08	115.27
17	BA	819	CLA	CHD-C1D-ND	-2.49	122.16	124.45
17	BA	832	CLA	CHB-C4A-NA	2.49	127.96	124.51
17	BB	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
17	BB	833	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	BA	812	CLA	CHD-C1D-ND	-2.49	122.17	124.45
20	BK	204	BCR	C16-C15-C14	-2.49	118.38	123.47
17	B1	311	CLA	CMB-C2B-C3B	2.49	129.34	124.68
20	BA	855	BCR	C8-C7-C6	-2.49	120.21	127.20
17	BA	838	CLA	C4-C3-C2	-2.49	117.30	123.68
17	BK	203	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	B3	603	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
17	BK	202	CLA	CHD-C1D-ND	-2.48	122.17	124.45
17	BB	812	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
17	BB	832	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
17	BB	832	CLA	CHD-C1D-ND	-2.48	122.17	124.45
17	B3	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	BA	849	BCR	C31-C1-C6	-2.48	106.28	110.30
19	BA	845	LHG	C5-O7-C7	-2.48	111.69	117.79
20	BF	304	BCR	C33-C5-C4	2.48	118.38	113.62
26	B1	316	LUT	C12-C13-C14	2.48	122.74	118.94
17	BA	827	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	B3	609	CLA	CMA-C3A-C2A	-2.48	110.31	116.10
17	BB	837	CLA	CMB-C2B-C3B	2.47	129.31	124.68
17	BB	834	CLA	CHD-C1D-ND	-2.47	122.18	124.45
17	B5	603	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
20	B5	616	BCR	C15-C16-C17	-2.47	118.41	123.47
17	BA	814	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	BB	845	BCR	C36-C18-C17	-2.47	119.46	122.92
20	B5	616	BCR	C1-C6-C7	2.47	122.77	115.78
17	BB	807	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	B1	316	LUT	C39-C29-C28	2.47	121.97	118.08
17	B3	612	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	BA	851	BCR	C38-C26-C25	-2.47	121.76	124.53
17	B5	608	CLA	CHD-C1D-ND	-2.47	122.19	124.45
17	BA	840	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
17	B2	311	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
17	B3	604	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	BB	832	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
17	BB	809	CLA	CHD-C1D-ND	-2.46	122.19	124.45
17	B1	314	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	BA	812	CLA	O2D-CGD-O1D	-2.46	119.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BL	304	CLA	O2D-CGD-CBD	2.46	115.64	111.27
27	B3	617	XAT	C4-C3-C2	-2.46	106.02	110.77
17	B5	609	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	BA	837	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	BB	816	CLA	CHD-C1D-ND	-2.46	122.20	124.45
17	BB	806	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	BG	201	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	B3	609	CLA	CHB-C4A-NA	2.45	127.91	124.51
17	BB	804	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
17	BB	840	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	BB	805	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
20	BB	846	BCR	C12-C13-C14	-2.45	115.18	118.94
20	B2	316	BCR	C29-C30-C25	2.45	114.25	110.48
17	B2	302	CLA	CHD-C1D-ND	-2.45	122.20	124.45
20	BA	847	BCR	C28-C27-C26	-2.45	109.70	114.08
24	BJ	104	SQD	O48-C23-C24	2.45	119.59	111.91
20	BA	855	BCR	C19-C18-C17	-2.45	115.19	118.94
17	B3	602	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	BJ	102	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	BA	811	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	BB	835	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
17	BA	808	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	BB	806	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	BA	826	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	BF	302	CLA	CHD-C1D-ND	-2.44	122.21	124.45
20	BA	855	BCR	C23-C22-C21	-2.44	115.20	118.94
17	B3	603	CLA	CMB-C2B-C3B	2.44	129.24	124.68
17	BA	834	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	BA	849	BCR	C33-C5-C6	-2.44	121.79	124.53
17	BA	827	CLA	CMB-C2B-C3B	2.44	129.24	124.68
17	B5	610	CLA	CHD-C1D-ND	-2.44	122.22	124.45
17	B5	612	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
17	BB	808	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
17	BB	823	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
17	B2	307	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B1	303	CHL	O2A-CGA-O1A	-2.43	117.46	123.59
25	B5	606	CHL	C4A-NA-C1A	-2.43	105.61	106.71
17	B2	309	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
20	BB	848	BCR	C32-C1-C6	-2.43	106.36	110.30
20	B5	616	BCR	C38-C26-C25	-2.42	121.81	124.53
20	BG	203	BCR	C39-C30-C25	-2.42	106.37	110.30
25	B3	601	CHL	C3D-C2D-C1D	-2.42	102.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	BA	829	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
20	B2	316	BCR	C23-C22-C21	-2.42	115.23	118.94
27	B2	315	XAT	C8-C9-C10	-2.42	115.23	118.94
20	BL	305	BCR	C37-C22-C21	-2.42	119.54	122.92
20	BA	847	BCR	C40-C30-C25	-2.42	106.38	110.30
17	BA	804	CLA	CHB-C4A-NA	2.42	127.85	124.51
17	BA	834	CLA	O2D-CGD-CBD	2.42	115.56	111.27
17	B3	613	CLA	CHD-C1D-ND	-2.42	122.23	124.45
20	BB	846	BCR	C16-C15-C14	-2.41	118.53	123.47
17	BA	809	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	BA	816	CLA	CHD-C1D-ND	-2.41	122.24	124.45
17	BA	818	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
17	BB	833	CLA	CHD-C1D-ND	-2.41	122.24	124.45
17	BB	831	CLA	CHD-C1D-ND	-2.41	122.24	124.45
17	B1	307	CLA	CBD-CHA-C1A	2.41	131.34	128.50
20	BH	202	BCR	C23-C24-C25	-2.41	120.44	127.20
17	B3	603	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	B2	310	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	BA	824	CLA	CHD-C1D-ND	-2.40	122.25	124.45
20	BB	803	BCR	C24-C25-C26	2.40	127.28	121.46
20	BA	847	BCR	C23-C22-C21	-2.40	115.25	118.94
17	BB	818	CLA	CHD-C1D-ND	-2.40	122.25	124.45
20	BB	803	BCR	C29-C28-C27	-2.40	106.02	111.38
17	B3	608	CLA	CHD-C1D-ND	-2.40	122.25	124.45
17	B3	608	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	BH	202	BCR	C16-C17-C18	2.40	130.73	127.31
17	BB	805	CLA	C2A-C1A-CHA	2.40	128.05	123.86
17	BB	829	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
20	BI	101	BCR	C33-C5-C4	2.40	118.22	113.62
26	B5	614	LUT	C37-C21-C36	2.40	111.42	107.89
17	BB	841	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	B3	603	CLA	C5-C3-C2	2.39	125.96	121.12
17	B3	604	CLA	CHD-C1D-ND	-2.39	122.25	124.45
17	BA	837	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
17	BA	816	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	BF	301	CLA	CHB-C4A-NA	2.39	127.82	124.51
17	B1	312	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	BA	851	BCR	C4-C5-C6	-2.39	119.26	122.73
20	B5	616	BCR	C27-C26-C25	-2.39	119.26	122.73
17	BA	827	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	B1	310	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	B1	317	XAT	C39-C29-C30	-2.39	119.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B1	317	XAT	C8-C9-C10	-2.39	115.28	118.94
25	B1	308	CHL	CAC-C3C-C4C	2.39	127.91	124.81
20	B3	618	BCR	C29-C30-C25	2.39	114.15	110.48
17	B3	605	CLA	CMB-C2B-C3B	2.38	129.14	124.68
17	B1	314	CLA	CHD-C1D-ND	-2.38	122.26	124.45
20	BB	845	BCR	C19-C18-C17	-2.38	115.28	118.94
25	B2	304	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
17	B3	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	B3	616	LUT	C36-C21-C26	2.38	113.15	109.55
17	B5	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
17	BA	830	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
17	BA	832	CLA	CHD-C1D-ND	-2.38	122.27	124.45
17	BA	838	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
20	BA	851	BCR	C30-C25-C26	-2.38	119.27	122.61
20	BL	305	BCR	C19-C18-C17	-2.37	115.30	118.94
17	BB	807	CLA	CMB-C2B-C3B	2.37	129.12	124.68
20	BJ	101	BCR	C2-C1-C6	2.37	114.13	110.48
17	BA	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	B1	305	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
17	B2	311	CLA	CHD-C1D-ND	-2.37	122.28	124.45
17	BK	202	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	B3	602	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
19	B1	318	LHG	O8-C23-C24	2.37	119.33	111.91
20	BF	304	BCR	C11-C10-C9	-2.36	123.94	127.31
17	B2	308	CLA	C4-C3-C5	2.36	119.25	115.27
27	B2	315	XAT	C35-C15-C14	-2.36	118.63	123.47
17	BB	814	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	BA	820	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	BA	850	BCR	C38-C26-C27	2.36	118.15	113.62
28	B5	617	LMG	C6-C5-C4	-2.36	107.47	113.00
17	BA	828	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	BB	814	CLA	CHD-C1D-ND	-2.36	122.29	124.45
17	BA	821	CLA	CHB-C4A-NA	2.36	127.77	124.51
20	BB	845	BCR	C16-C17-C18	-2.36	123.94	127.31
17	BA	815	CLA	CHB-C4A-NA	2.36	127.77	124.51
17	BB	801	CLA	CMB-C2B-C3B	2.36	129.09	124.68
20	BB	849	BCR	C15-C14-C13	-2.36	123.95	127.31
17	B3	605	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	B5	616	BCR	C29-C30-C25	2.35	114.10	110.48
27	B1	317	XAT	C32-C33-C34	-2.35	115.33	118.94
27	B5	615	XAT	C4-C3-C2	-2.35	106.23	110.77
25	B2	306	CHL	C3C-C4C-NC	2.35	113.21	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BB	848	BCR	C2-C1-C6	2.35	114.10	110.48
17	BA	811	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	BA	818	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	BA	856	BCR	C40-C30-C25	-2.35	106.49	110.30
25	B2	305	CHL	CED-O2D-CGD	2.35	121.24	115.94
17	BB	815	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
17	B3	606	CLA	CAA-C2A-C3A	-2.34	108.40	114.26
17	BF	303	CLA	CHB-C4A-NA	2.34	127.75	124.51
27	B2	315	XAT	C32-C33-C34	-2.34	115.34	118.94
17	B1	306	CLA	CAA-C2A-C3A	-2.34	110.63	116.10
17	BL	302	CLA	CBA-CAA-C2A	2.34	120.78	113.86
17	BA	808	CLA	CMB-C2B-C3B	2.34	129.06	124.68
20	BB	803	BCR	C8-C9-C10	-2.34	115.35	118.94
20	BB	803	BCR	C19-C18-C17	-2.34	115.35	118.94
17	BB	842	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	B2	301	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	BF	302	CLA	CMB-C2B-C3B	2.34	129.05	124.68
17	BB	807	CLA	CMC-C2C-C1C	-2.34	121.48	125.04
17	BB	840	CLA	O2D-CGD-CBD	2.33	115.42	111.27
27	B3	617	XAT	C10-C11-C12	-2.33	115.93	123.22
17	B2	308	CLA	C6-C5-C3	2.33	119.58	113.45
17	BA	831	CLA	CAC-C3C-C4C	2.33	127.84	124.81
17	BB	835	CLA	CHD-C1D-ND	-2.33	122.31	124.45
17	BB	837	CLA	CHD-C1D-ND	-2.33	122.31	124.45
17	BG	201	CLA	O1D-CGD-CBD	2.33	129.26	124.48
20	BI	101	BCR	C3-C4-C5	-2.33	109.92	114.08
17	B1	305	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	B1	309	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	BB	848	BCR	C1-C6-C5	-2.33	119.33	122.61
20	BJ	103	BCR	C10-C11-C12	-2.33	115.95	123.22
20	B3	618	BCR	C24-C25-C26	2.33	127.10	121.46
17	BA	823	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	B3	617	XAT	C36-C21-C26	2.33	116.33	110.05
17	BB	806	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
17	BA	805	CLA	CHB-C4A-NA	2.32	127.73	124.51
17	BF	301	CLA	C6-C5-C3	2.32	119.55	113.45
20	BB	846	BCR	C40-C30-C25	-2.32	106.53	110.30
17	BB	830	CLA	CBA-CAA-C2A	2.32	120.72	113.86
20	BA	848	BCR	C28-C27-C26	-2.32	109.93	114.08
20	B2	316	BCR	C8-C9-C10	-2.32	115.38	118.94
17	BL	304	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	BG	202	CLA	C1B-CHB-C4A	-2.32	125.52	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B2	301	CLA	C1-C2-C3	-2.32	122.03	126.04
17	BA	804	CLA	O2D-CGD-CBD	2.32	115.39	111.27
20	BA	849	BCR	C38-C26-C27	2.32	118.07	113.62
20	BA	848	BCR	C19-C18-C17	-2.32	115.38	118.94
27	B2	315	XAT	C19-C9-C8	2.32	121.73	118.08
17	B1	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
17	BL	302	CLA	CMB-C2B-C3B	2.32	129.01	124.68
17	BA	803	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	B3	616	LUT	C28-C29-C30	-2.31	115.39	118.94
17	B3	602	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	BK	201	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	B5	616	BCR	C21-C20-C19	-2.31	116.00	123.22
20	B3	618	BCR	C39-C30-C29	2.31	118.15	108.91
17	BA	821	CLA	C7-C6-C5	-2.31	107.08	113.36
20	BB	803	BCR	C16-C17-C18	-2.31	124.01	127.31
20	BI	101	BCR	C36-C18-C17	-2.31	119.69	122.92
17	BB	801	CLA	O2A-C1-C2	-2.31	102.57	108.64
17	BB	812	CLA	O1D-CGD-CBD	2.31	129.20	124.48
20	BB	849	BCR	C37-C22-C23	2.31	121.71	118.08
26	B1	316	LUT	C19-C9-C8	2.31	121.71	118.08
17	B1	305	CLA	C4-C3-C2	-2.30	117.77	123.68
25	B2	306	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
17	BA	806	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	B3	614	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	BB	823	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
20	BA	847	BCR	C36-C18-C17	-2.30	119.70	122.92
20	B2	316	BCR	C27-C26-C25	-2.30	119.39	122.73
17	BB	838	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	BB	810	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	BA	848	BCR	C16-C15-C14	-2.30	118.77	123.47
20	BH	202	BCR	C3-C4-C5	-2.29	109.98	114.08
17	BB	828	CLA	O2D-CGD-CBD	2.29	115.34	111.27
17	BB	807	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
17	BB	834	CLA	O2D-CGD-CBD	2.29	115.34	111.27
20	BA	856	BCR	C24-C23-C22	-2.29	122.78	126.23
20	BJ	103	BCR	C34-C9-C8	2.29	121.68	118.08
27	B3	617	XAT	C16-C1-C2	-2.29	105.01	108.98
17	BB	825	CLA	CHD-C1D-ND	-2.29	122.35	124.45
17	BG	201	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
25	B1	303	CHL	O2A-CGA-CBA	2.29	119.08	111.91
17	BA	829	CLA	O2D-CGD-CBD	2.29	115.33	111.27
17	BA	826	CLA	C5-C3-C2	2.28	125.74	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BF	303	CLA	CHD-C1D-ND	-2.28	122.36	124.45
20	BA	849	BCR	C40-C30-C25	-2.28	106.60	110.30
17	BB	821	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	BB	836	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	BF	302	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
20	BA	847	BCR	C16-C15-C14	-2.28	118.80	123.47
20	BL	305	BCR	C23-C22-C21	-2.28	115.44	118.94
17	BB	830	CLA	C2D-C1D-ND	-2.28	108.42	110.10
20	BI	101	BCR	C16-C17-C18	-2.28	124.06	127.31
20	BB	845	BCR	C20-C21-C22	-2.28	124.06	127.31
17	B3	606	CLA	CHD-C1D-ND	-2.28	122.36	124.45
17	B2	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
25	B5	605	CHL	C3C-C4C-NC	2.28	113.06	110.57
17	BL	303	CLA	CBA-CAA-C2A	2.28	120.58	113.86
17	BB	823	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
20	BB	848	BCR	C21-C20-C19	-2.28	116.12	123.22
20	BJ	103	BCR	C37-C22-C23	2.27	121.66	118.08
20	B5	616	BCR	C19-C18-C17	-2.27	115.45	118.94
17	B5	613	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	B1	301	LHG	O8-C23-O10	-2.27	117.86	123.59
17	B2	303	CLA	CHD-C1D-ND	-2.27	122.37	124.45
17	BB	804	CLA	CHB-C4A-NA	2.27	127.65	124.51
20	BJ	101	BCR	C30-C25-C24	2.27	122.20	115.78
17	BA	804	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
20	BA	847	BCR	C36-C18-C19	2.27	121.65	118.08
17	BA	803	CLA	C2D-C1D-ND	-2.27	108.43	110.10
17	BB	805	CLA	CMD-C2D-C1D	-2.27	120.72	124.71
17	BA	821	CLA	O2D-CGD-CBD	2.27	115.30	111.27
17	B5	611	CLA	CAA-C2A-C3A	-2.27	108.60	114.26
17	BB	804	CLA	C5-C3-C2	-2.27	116.53	121.12
17	BB	813	CLA	C5-C3-C2	2.26	125.70	121.12
17	BA	814	CLA	CHD-C1D-ND	-2.26	122.37	124.45
17	BB	828	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
20	BB	845	BCR	C37-C22-C23	2.26	121.64	118.08
25	B1	303	CHL	O2D-CGD-O1D	-2.26	118.95	124.09
17	BB	810	CLA	O2D-CGD-CBD	2.26	115.29	111.27
17	BA	810	CLA	CMB-C2B-C3B	2.26	128.91	124.68
17	BA	803	CLA	C1-C2-C3	-2.26	122.13	126.04
26	B5	614	LUT	C12-C13-C14	-2.26	115.47	118.94
25	B2	313	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
26	B2	314	LUT	C12-C13-C14	-2.26	115.48	118.94
17	BA	826	CLA	CHB-C4A-NA	2.26	127.63	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B2	315	XAT	C18-C5-C6	-2.26	118.48	122.26
17	BL	302	CLA	C3A-C2A-C1A	2.25	104.72	101.34
20	BK	204	BCR	C20-C21-C22	-2.25	124.09	127.31
17	BB	843	CLA	CHB-C4A-NA	2.25	127.63	124.51
20	B3	618	BCR	C12-C13-C14	-2.25	115.48	118.94
17	BB	824	CLA	CBA-CAA-C2A	2.25	120.51	113.86
17	B5	604	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	BH	201	CLA	CMB-C2B-C3B	2.25	128.89	124.68
17	B2	301	CLA	CHD-C1D-ND	-2.25	122.39	124.45
17	BB	842	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	B5	606	CHL	CED-O2D-CGD	2.25	121.02	115.94
17	BL	302	CLA	CHD-C1D-ND	-2.25	122.39	124.45
17	BA	817	CLA	C5-C3-C2	2.25	125.66	121.12
17	BH	201	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	BB	802	CLA	C7-C6-C5	-2.25	107.26	113.36
20	BA	856	BCR	C29-C28-C27	-2.25	106.36	111.38
19	BF	305	LHG	O8-C23-C24	2.25	118.95	111.91
17	BB	811	CLA	CHB-C4A-NA	2.24	127.62	124.51
17	BB	832	CLA	CHB-C4A-NA	2.24	127.62	124.51
17	B2	312	CLA	CHB-C4A-NA	2.24	127.62	124.51
17	BA	805	CLA	CMC-C2C-C3C	2.24	132.20	126.12
20	BB	849	BCR	C20-C21-C22	-2.24	124.11	127.31
27	B2	315	XAT	C24-C23-C22	-2.24	106.45	110.77
17	BB	830	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	BB	849	BCR	C8-C9-C10	-2.24	115.50	118.94
17	BA	803	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	B3	614	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
17	BA	813	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	B2	304	CHL	C3C-C4C-NC	2.24	113.01	110.57
20	BJ	101	BCR	C16-C15-C14	-2.24	118.89	123.47
17	BJ	102	CLA	CHD-C1D-ND	-2.24	122.40	124.45
20	BL	305	BCR	C8-C9-C10	-2.23	115.51	118.94
17	BB	802	CLA	O2D-CGD-CBD	2.23	115.24	111.27
17	BA	828	CLA	C6-C7-C8	-2.23	108.71	115.92
17	BB	824	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
17	BB	840	CLA	CHB-C4A-NA	2.22	127.59	124.51
25	B2	306	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
17	BB	804	CLA	CMB-C2B-C3B	2.22	128.84	124.68
17	BB	828	CLA	C2A-C1A-CHA	2.22	127.75	123.86
20	BF	304	BCR	C8-C9-C10	-2.22	115.53	118.94
17	BB	822	CLA	CMB-C2B-C3B	2.22	128.83	124.68
25	B5	607	CHL	C3D-C2D-C1D	-2.22	102.81	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BB	846	BCR	C33-C5-C6	-2.22	122.04	124.53
17	BA	841	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	B2	314	LUT	C30-C31-C32	-2.21	116.31	123.22
17	BB	840	CLA	CHD-C1D-ND	-2.21	122.42	124.45
17	BB	807	CLA	CBA-CAA-C2A	2.21	120.39	113.86
27	B5	615	XAT	C40-C33-C34	-2.21	119.83	122.92
20	BA	850	BCR	C21-C20-C19	-2.21	116.32	123.22
17	BB	835	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	B2	301	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	BB	802	CLA	CHB-C4A-NA	2.21	127.56	124.51
20	BA	849	BCR	C12-C13-C14	-2.21	115.56	118.94
26	B5	614	LUT	C16-C1-C6	2.21	113.88	110.30
17	B5	611	CLA	CMB-C2B-C3B	2.21	128.81	124.68
20	BJ	101	BCR	C28-C27-C26	-2.21	110.14	114.08
27	B5	615	XAT	C24-C23-C22	-2.21	106.51	110.77
20	BL	305	BCR	C12-C13-C14	-2.20	115.56	118.94
17	BB	815	CLA	C7-C6-C5	2.20	119.34	113.36
17	BB	817	CLA	CAC-C3C-C4C	2.20	127.67	124.81
20	BG	203	BCR	C21-C20-C19	2.20	130.09	123.22
27	B3	617	XAT	C39-C29-C30	-2.20	119.84	122.92
17	BB	830	CLA	CHB-C4A-NA	2.20	127.56	124.51
17	B3	613	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	BB	815	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
17	BB	810	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	B1	304	CLA	CHB-C4A-NA	2.20	127.55	124.51
20	BF	304	BCR	C3-C4-C5	-2.20	110.16	114.08
28	B5	617	LMG	O6-C5-C4	2.19	113.68	109.69
17	BB	814	CLA	O2D-CGD-CBD	2.19	115.17	111.27
17	BA	839	CLA	C1-C2-C3	-2.19	122.25	126.04
18	BB	844	PQN	O1-C1-C10	-2.19	118.01	121.56
20	BA	848	BCR	C40-C30-C25	-2.19	106.74	110.30
17	BA	838	CLA	CHD-C1D-ND	-2.19	122.45	124.45
17	B3	614	CLA	CMB-C2B-C3B	2.18	128.77	124.68
17	BB	810	CLA	C5-C3-C2	2.18	125.54	121.12
17	BH	201	CLA	CAC-C3C-C4C	2.18	127.64	124.81
20	BG	203	BCR	C28-C27-C26	-2.18	110.18	114.08
17	BB	819	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	BB	847	BCR	C15-C16-C17	-2.18	119.01	123.47
17	BB	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	BB	838	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
17	BB	823	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	B5	616	BCR	C4-C5-C6	-2.18	119.57	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B2	302	CLA	O2A-CGA-O1A	-2.18	117.88	123.30
17	B2	303	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	BA	854	LMU	C1-O1'-C1'	2.18	117.45	113.84
17	BA	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	BA	801	CLA	CMB-C2B-C3B	2.17	128.75	124.68
17	B2	307	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	B2	306	CHL	CMD-C2D-C1D	2.17	128.54	124.71
17	BB	828	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
27	B2	315	XAT	C4-C3-C2	-2.17	106.58	110.77
17	BB	841	CLA	O2D-CGD-CBD	2.17	115.13	111.27
17	B1	312	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	BB	846	BCR	C7-C8-C9	-2.17	122.96	126.23
17	BB	837	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	B5	612	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	BB	804	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
17	B1	315	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	BB	838	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	B1	314	CLA	CAC-C3C-C4C	2.16	127.61	124.81
17	BA	842	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	BB	810	CLA	CMD-C2D-C3D	2.16	132.58	127.61
18	BB	844	PQN	C12-C11-C3	-2.16	106.22	112.05
17	B2	302	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
17	BA	811	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
17	BA	810	CLA	CAC-C3C-C4C	2.15	127.61	124.81
17	BB	835	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
17	BA	809	CLA	O1D-CGD-CBD	2.15	128.89	124.48
17	BA	823	CLA	CAA-C2A-C3A	-2.15	111.07	116.10
20	BJ	101	BCR	C2-C3-C4	-2.15	106.57	111.38
17	B3	610	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	B1	311	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
20	BA	851	BCR	C19-C18-C17	2.15	122.24	118.94
20	BA	850	BCR	C12-C13-C14	-2.15	115.64	118.94
17	BB	824	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	BA	819	CLA	CBA-CAA-C2A	2.15	120.20	113.86
20	BA	851	BCR	C12-C13-C14	-2.15	115.65	118.94
17	B3	603	CLA	CAC-C3C-C4C	2.15	127.59	124.81
17	BF	301	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	B3	607	CHL	C1C-C2C-C3C	-2.14	104.70	106.96
17	BA	844	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	B5	605	CHL	CHC-C1C-C2C	-2.14	118.34	126.11
26	B5	614	LUT	C8-C7-C6	-2.14	121.19	127.20
17	B1	314	CLA	CMC-C2C-C1C	-2.13	121.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B5	607	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
20	BA	855	BCR	C23-C24-C25	2.13	133.19	127.20
17	BA	833	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	BA	851	BCR	C21-C20-C19	-2.13	116.56	123.22
17	BA	840	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
17	B3	615	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	B3	618	BCR	C2-C1-C6	-2.13	107.20	110.48
17	B1	306	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	B5	606	CHL	C3C-C4C-NC	2.13	112.90	110.57
17	B3	612	CLA	CMB-C2B-C3B	2.13	128.66	124.68
17	BA	817	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
17	BA	829	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	BB	842	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
17	BA	817	CLA	C4-C3-C2	-2.13	118.22	123.68
17	BA	835	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	BB	849	BCR	C19-C18-C17	-2.13	115.67	118.94
20	BB	849	BCR	C37-C22-C21	-2.13	119.94	122.92
17	BA	834	CLA	C5-C3-C2	-2.13	116.82	121.12
27	B5	615	XAT	C36-C21-C26	2.13	115.78	110.05
26	B3	616	LUT	C30-C31-C32	-2.12	116.59	123.22
17	BB	842	CLA	CHD-C1D-ND	-2.12	122.50	124.45
17	B1	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
17	B5	610	CLA	CHB-C4A-NA	2.12	127.45	124.51
17	B2	308	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
20	BB	845	BCR	C12-C13-C14	-2.12	115.68	118.94
17	BB	815	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
17	BB	828	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
17	BA	841	CLA	CAC-C3C-C4C	2.12	127.56	124.81
20	BI	101	BCR	C20-C21-C22	-2.12	124.29	127.31
27	B5	615	XAT	O4-C5-C18	2.12	117.59	115.06
17	B3	610	CLA	CHD-C1D-ND	-2.12	122.51	124.45
17	BB	815	CLA	CHB-C4A-NA	2.12	127.44	124.51
20	B3	618	BCR	C8-C9-C10	-2.11	115.70	118.94
20	BA	855	BCR	C20-C21-C22	-2.11	124.29	127.31
20	BJ	103	BCR	C35-C13-C14	2.11	125.88	122.92
17	B2	310	CLA	CHB-C4A-NA	2.11	127.43	124.51
17	B1	314	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	BH	202	BCR	C1-C6-C5	-2.11	119.64	122.61
25	B3	601	CHL	CAC-C3C-C4C	2.11	127.55	124.81
17	BL	303	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	BA	831	CLA	O1D-CGD-CBD	2.11	128.80	124.48
25	B5	605	CHL	O2D-CGD-O1D	-2.11	119.30	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	BG	202	CLA	CHD-C1D-ND	-2.11	122.52	124.45
27	B2	315	XAT	C12-C13-C14	-2.11	115.71	118.94
20	BB	803	BCR	C10-C11-C12	-2.11	116.65	123.22
17	BA	807	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	B3	607	CHL	C3C-C4C-NC	2.10	112.93	110.57
25	B5	606	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
25	B1	308	CHL	O2D-CGD-O1D	-2.10	119.32	124.09
20	BA	851	BCR	C24-C23-C22	-2.10	123.06	126.23
26	B3	616	LUT	C11-C10-C9	-2.10	124.31	127.31
20	BB	845	BCR	C23-C22-C21	-2.10	115.72	118.94
17	B2	310	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	BB	801	CLA	CMD-C2D-C1D	-2.10	121.02	124.71
17	BA	805	CLA	CMB-C2B-C3B	2.10	128.60	124.68
17	BA	831	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
17	B1	314	CLA	C4A-NA-C1A	2.10	107.65	106.71
17	BA	819	CLA	O2D-CGD-CBD	2.10	114.99	111.27
17	BG	201	CLA	CMB-C2B-C3B	2.09	128.60	124.68
20	BL	305	BCR	C16-C15-C14	-2.09	119.19	123.47
17	BA	822	CLA	CHD-C1D-ND	-2.09	122.53	124.45
20	BL	305	BCR	C36-C18-C17	-2.09	119.99	122.92
17	BB	812	CLA	C2A-C1A-CHA	2.09	127.52	123.86
17	BA	826	CLA	C1-C2-C3	-2.09	122.42	126.04
17	BB	805	CLA	O2D-CGD-CBD	2.09	114.98	111.27
17	BA	841	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	BB	803	BCR	C23-C22-C21	-2.09	115.73	118.94
17	BB	815	CLA	CMB-C2B-C3B	2.09	128.59	124.68
17	BB	806	CLA	CAC-C3C-C4C	2.09	127.52	124.81
25	B5	607	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
17	BK	201	CLA	CHD-C1D-ND	-2.09	122.54	124.45
17	BA	822	CLA	CHB-C4A-NA	2.08	127.39	124.51
25	B2	304	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
17	BA	842	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
17	BB	831	CLA	CMB-C2B-C3B	2.08	128.57	124.68
17	BB	827	CLA	CHB-C4A-NA	2.08	127.39	124.51
25	B3	601	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
17	BA	838	CLA	CHB-C4A-NA	2.08	127.39	124.51
25	B1	303	CHL	C1-C2-C3	-2.08	123.39	126.75
22	BA	854	LMU	C1B-O1B-C4'	-2.08	112.82	117.96
17	BB	811	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
17	BA	832	CLA	O2D-CGD-CBD	2.08	114.96	111.27
17	BA	809	CLA	CHD-C1D-ND	-2.08	122.55	124.45
17	B3	615	CLA	CAA-C2A-C3A	-2.07	111.26	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BK	204	BCR	C40-C30-C39	2.07	114.90	108.53
20	B5	616	BCR	C10-C11-C12	-2.07	116.74	123.22
20	BF	304	BCR	C23-C22-C21	-2.07	115.76	118.94
17	B2	307	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
17	B3	614	CLA	CAA-C2A-C3A	-2.07	111.26	116.10
17	BA	838	CLA	CMB-C2B-C3B	2.07	128.56	124.68
20	BB	845	BCR	C32-C1-C6	-2.07	106.94	110.30
20	BA	849	BCR	C16-C17-C18	-2.07	124.35	127.31
27	B3	617	XAT	C32-C33-C34	-2.07	115.76	118.94
17	BB	818	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
20	BA	856	BCR	C20-C21-C22	-2.07	124.36	127.31
17	BB	816	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
17	BA	830	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	BB	847	BCR	C29-C30-C25	2.07	113.66	110.48
20	BI	101	BCR	C23-C22-C21	-2.07	115.77	118.94
17	B2	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	B5	601	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	B1	308	CHL	C3C-C4C-NC	2.06	112.89	110.57
20	BB	846	BCR	C15-C16-C17	-2.06	119.25	123.47
20	BH	202	BCR	C28-C27-C26	-2.06	110.40	114.08
26	B2	314	LUT	C35-C15-C14	-2.06	119.25	123.47
17	BA	830	CLA	CMB-C2B-C3B	2.06	128.53	124.68
20	BB	803	BCR	C36-C18-C17	-2.06	120.04	122.92
17	BA	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
17	BB	801	CLA	C3C-C4C-NC	-2.06	108.26	110.57
20	BJ	101	BCR	C19-C18-C17	-2.06	115.79	118.94
20	BA	856	BCR	C24-C25-C26	2.06	126.44	121.46
20	BA	849	BCR	C20-C21-C22	-2.06	124.38	127.31
17	BA	802	CLA	C2D-C1D-ND	-2.05	108.59	110.10
17	B3	611	CLA	C2A-C1A-CHA	2.05	127.45	123.86
25	B3	601	CHL	O2A-CGA-O1A	-2.05	118.41	123.59
17	BA	833	CLA	C4-C3-C2	-2.05	118.42	123.68
17	B3	611	CLA	CHA-C1A-NA	-2.05	121.70	126.40
20	BA	848	BCR	C37-C22-C23	2.05	121.31	118.08
20	BB	849	BCR	C34-C9-C8	2.05	121.31	118.08
17	BA	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	BB	811	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	BB	828	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	BA	855	BCR	C10-C11-C12	-2.05	116.83	123.22
20	BI	101	BCR	C19-C18-C17	-2.05	115.80	118.94
20	B2	316	BCR	C16-C17-C18	-2.05	124.39	127.31
17	BB	812	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BB	845	BCR	C31-C1-C6	2.05	113.62	110.30
17	BA	804	CLA	C5-C3-C2	2.04	125.25	121.12
17	B3	603	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
17	BA	817	CLA	O2D-CGD-CBD	2.04	114.90	111.27
17	BA	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	B3	617	XAT	C28-C29-C30	-2.04	115.81	118.94
17	B3	606	CLA	C3A-C2A-C1A	2.04	104.40	101.34
20	BA	851	BCR	C24-C25-C26	2.04	126.41	121.46
20	BJ	103	BCR	C16-C17-C18	-2.04	124.40	127.31
17	BA	828	CLA	C14-C13-C15	2.04	118.68	111.29
24	BJ	104	SQD	C4-C3-C2	2.04	114.38	110.82
26	B5	614	LUT	C7-C8-C9	-2.04	123.16	126.23
25	B1	303	CHL	C5-C3-C4	2.04	119.10	114.60
17	BB	823	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	BA	825	CLA	C6-C5-C3	2.04	118.79	113.45
17	BA	827	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	BA	814	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
20	BB	848	BCR	C2-C3-C4	-2.04	106.83	111.38
27	B2	315	XAT	O4-C5-C6	-2.04	57.27	58.96
20	BA	855	BCR	C29-C30-C25	2.04	113.61	110.48
17	BG	202	CLA	CHB-C4A-NA	2.03	127.33	124.51
17	BA	833	CLA	C5-C3-C2	2.03	125.23	121.12
20	BB	803	BCR	C2-C3-C4	-2.03	106.83	111.38
18	BB	844	PQN	C6-C5-C10	2.03	121.52	119.26
20	BA	855	BCR	C35-C13-C12	2.03	121.28	118.08
17	BH	201	CLA	CED-O2D-CGD	2.03	120.53	115.94
25	B1	303	CHL	OMC-CMC-C2C	-2.03	121.10	125.69
17	BB	813	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
17	BB	819	CLA	C6-C5-C3	2.03	118.78	113.45
17	B3	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	BJ	104	SQD	O47-C45-C44	2.03	115.75	108.40
26	B5	614	LUT	C38-C25-C24	-2.03	119.22	123.56
27	B1	317	XAT	C35-C34-C33	-2.03	124.42	127.31
20	BF	304	BCR	C20-C21-C22	-2.03	124.42	127.31
17	B2	301	CLA	O1D-CGD-CBD	2.03	128.63	124.48
17	BB	825	CLA	CHB-C4A-NA	2.03	127.31	124.51
17	BB	826	CLA	C1-O2A-CGA	2.03	121.76	116.44
17	BB	827	CLA	O1D-CGD-CBD	2.03	128.63	124.48
17	BB	810	CLA	CMD-C2D-C1D	-2.03	121.14	124.71
20	BK	204	BCR	C15-C16-C17	-2.02	119.33	123.47
17	BB	822	CLA	CMA-C3A-C2A	-2.02	111.37	116.10
17	BA	825	CLA	C5-C3-C2	2.02	125.21	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B3	601	CHL	C4D-C3D-CAD	-2.02	105.71	108.10
17	BA	844	CLA	O2D-CGD-CBD	2.02	114.86	111.27
17	BA	806	CLA	CHD-C1D-ND	-2.02	122.59	124.45
17	BB	825	CLA	CAA-C2A-C3A	2.02	118.31	112.78
17	BA	804	CLA	C6-C5-C3	2.02	117.93	114.62
17	BB	823	CLA	CMB-C2B-C3B	2.02	128.46	124.68
20	BA	856	BCR	C7-C8-C9	-2.02	123.18	126.23
17	BB	820	CLA	CAA-C2A-C3A	2.02	118.30	112.78
27	B5	615	XAT	C15-C35-C34	-2.02	119.35	123.47
17	BB	843	CLA	CHD-C1D-ND	-2.01	122.60	124.45
20	BK	204	BCR	C24-C25-C26	-2.01	116.58	121.46
17	B3	608	CLA	O1D-CGD-CBD	2.01	128.60	124.48
20	B3	618	BCR	C30-C25-C24	2.01	121.47	115.78
25	B2	306	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
17	B3	602	CLA	O1D-CGD-CBD	2.01	128.60	124.48
17	BB	821	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
20	B3	618	BCR	C28-C27-C26	-2.01	110.48	114.08
17	BA	839	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
20	BA	851	BCR	C32-C1-C6	2.01	113.56	110.30
17	B5	604	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
20	BF	304	BCR	C29-C28-C27	-2.01	106.88	111.38
25	B2	313	CHL	C3D-C2D-C1D	-2.01	103.09	105.83
17	BA	823	CLA	CMA-C3A-C2A	-2.01	111.41	116.10
20	BJ	101	BCR	C20-C21-C22	-2.01	124.44	127.31
26	B2	314	LUT	C38-C25-C24	-2.01	119.26	123.56
17	B1	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	BB	811	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	BA	809	CLA	CAA-C2A-C1A	2.01	118.56	111.97
17	BA	833	CLA	CMB-C2B-C3B	2.01	128.43	124.68
17	B2	312	CLA	O2D-CGD-CBD	2.01	114.83	111.27
20	BK	204	BCR	C16-C17-C18	-2.01	124.45	127.31
17	BA	830	CLA	O1D-CGD-CBD	2.01	128.59	124.48
23	BB	850	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
17	BB	833	CLA	CMC-C2C-C1C	-2.00	121.99	125.04
20	BB	846	BCR	C19-C18-C17	-2.00	115.87	118.94
17	B5	609	CLA	CBA-CAA-C2A	2.00	119.78	113.86
17	BA	836	CLA	CHD-C1D-ND	-2.00	122.61	124.45
17	B1	314	CLA	C2D-C1D-ND	-2.00	108.63	110.10
17	B3	605	CLA	CHB-C4A-NA	2.00	127.28	124.51
17	BA	838	CLA	O2D-CGD-CBD	2.00	114.83	111.49

All (150) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	BA	801	CLA	ND
17	BA	802	CLA	ND
17	BA	803	CLA	ND
17	BA	805	CLA	ND
17	BA	806	CLA	ND
17	BA	807	CLA	ND
17	BA	808	CLA	ND
17	BA	810	CLA	ND
17	BA	811	CLA	ND
17	BA	812	CLA	ND
17	BA	813	CLA	ND
17	BA	814	CLA	ND
17	BA	816	CLA	ND
17	BA	819	CLA	ND
17	BA	820	CLA	ND
17	BA	822	CLA	ND
17	BA	823	CLA	ND
17	BA	824	CLA	ND
17	BA	825	CLA	ND
17	BA	827	CLA	ND
17	BA	828	CLA	ND
17	BA	829	CLA	ND
17	BA	830	CLA	ND
17	BA	831	CLA	ND
17	BA	833	CLA	ND
17	BA	835	CLA	ND
17	BA	837	CLA	ND
17	BA	838	CLA	ND
17	BA	840	CLA	ND
17	BA	841	CLA	ND
17	BA	842	CLA	ND
17	BA	844	CLA	ND
17	BB	801	CLA	ND
17	BB	802	CLA	ND
17	BB	804	CLA	ND
17	BB	805	CLA	ND
17	BB	806	CLA	ND
17	BB	807	CLA	ND
17	BB	808	CLA	ND
17	BB	810	CLA	ND
17	BB	811	CLA	ND
17	BB	812	CLA	ND
17	BB	813	CLA	ND

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Mol	Chain	Res	Type	Atom
17	BB	814	CLA	ND
17	BB	815	CLA	ND
17	BB	816	CLA	ND
17	BB	817	CLA	ND
17	BB	818	CLA	ND
17	BB	819	CLA	ND
17	BB	820	CLA	ND
17	BB	821	CLA	ND
17	BB	822	CLA	ND
17	BB	823	CLA	ND
17	BB	825	CLA	ND
17	BB	826	CLA	ND
17	BB	828	CLA	ND
17	BB	829	CLA	ND
17	BB	830	CLA	ND
17	BB	831	CLA	ND
17	BB	832	CLA	ND
17	BB	835	CLA	ND
17	BB	837	CLA	ND
17	BB	838	CLA	ND
17	BB	841	CLA	ND
17	BB	842	CLA	ND
17	BB	843	CLA	ND
17	BF	301	CLA	ND
17	BF	302	CLA	ND
17	BF	303	CLA	ND
17	BG	201	CLA	ND
17	BG	202	CLA	ND
17	BH	201	CLA	ND
17	BJ	102	CLA	ND
17	BK	201	CLA	ND
17	BK	202	CLA	ND
17	BK	203	CLA	ND
17	BL	304	CLA	ND
17	B1	304	CLA	ND
17	B1	305	CLA	ND
17	B1	306	CLA	ND
17	B1	307	CLA	ND
17	B1	310	CLA	ND
17	B1	311	CLA	ND
17	B1	312	CLA	ND
17	B1	313	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B1	314	CLA	ND
17	B1	315	CLA	ND
17	B2	301	CLA	ND
17	B2	302	CLA	ND
17	B2	303	CLA	ND
17	B2	307	CLA	ND
17	B2	308	CLA	ND
17	B2	309	CLA	ND
17	B2	310	CLA	ND
17	B2	311	CLA	ND
17	B2	312	CLA	ND
17	B3	602	CLA	ND
17	B3	603	CLA	ND
17	B3	604	CLA	ND
17	B3	605	CLA	ND
17	B3	606	CLA	ND
17	B3	608	CLA	ND
17	B3	609	CLA	ND
17	B3	610	CLA	ND
17	B3	611	CLA	ND
17	B3	612	CLA	ND
17	B3	613	CLA	ND
17	B3	614	CLA	ND
17	B3	615	CLA	ND
17	B5	601	CLA	ND
17	B5	603	CLA	ND
17	B5	604	CLA	ND
17	B5	608	CLA	ND
17	B5	609	CLA	ND
17	B5	611	CLA	ND
17	B5	612	CLA	ND
17	B5	613	CLA	ND
25	B1	303	CHL	NC
25	B1	303	CHL	NA
25	B1	303	CHL	ND
25	B1	308	CHL	NC
25	B1	308	CHL	NA
25	B1	308	CHL	ND
25	B2	304	CHL	NC
25	B2	304	CHL	NA
25	B2	304	CHL	ND
25	B2	305	CHL	NC

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Mol	Chain	Res	Type	Atom
25	B2	305	CHL	NA
25	B2	305	CHL	ND
25	B2	306	CHL	NC
25	B2	306	CHL	NA
25	B2	306	CHL	ND
25	B2	313	CHL	NC
25	B2	313	CHL	NA
25	B2	313	CHL	ND
25	B3	601	CHL	NC
25	B3	601	CHL	NA
25	B3	601	CHL	ND
25	B3	607	CHL	NC
25	B3	607	CHL	NA
25	B3	607	CHL	ND
25	B5	605	CHL	NC
25	B5	605	CHL	NA
25	B5	605	CHL	ND
25	B5	606	CHL	NC
25	B5	606	CHL	NA
25	B5	606	CHL	ND
25	B5	607	CHL	NC
25	B5	607	CHL	NA
25	B5	607	CHL	ND

All (1453) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	BA	801	CLA	CBD-CGD-O2D-CED
17	BA	802	CLA	CBD-CGD-O2D-CED
17	BA	804	CLA	C1A-C2A-CAA-CBA
17	BA	804	CLA	C3A-C2A-CAA-CBA
17	BA	809	CLA	C1A-C2A-CAA-CBA
17	BA	813	CLA	CHA-CBD-CGD-O1D
17	BA	813	CLA	CHA-CBD-CGD-O2D
17	BA	814	CLA	CHA-CBD-CGD-O1D
17	BA	818	CLA	C1A-C2A-CAA-CBA
17	BA	818	CLA	C3A-C2A-CAA-CBA
17	BA	819	CLA	C3A-C2A-CAA-CBA
17	BA	819	CLA	CHA-CBD-CGD-O1D
17	BA	819	CLA	CHA-CBD-CGD-O2D
17	BA	821	CLA	CBD-CGD-O2D-CED
17	BA	822	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	BA	822	CLA	CAD-CBD-CGD-O1D
17	BA	822	CLA	CAD-CBD-CGD-O2D
17	BA	823	CLA	CHA-CBD-CGD-O1D
17	BA	823	CLA	CHA-CBD-CGD-O2D
17	BA	824	CLA	C1A-C2A-CAA-CBA
17	BA	824	CLA	C3A-C2A-CAA-CBA
17	BA	827	CLA	C6-C7-C8-C9
17	BA	828	CLA	CBD-CGD-O2D-CED
17	BA	833	CLA	CHA-CBD-CGD-O1D
17	BA	833	CLA	CHA-CBD-CGD-O2D
17	BA	833	CLA	CAD-CBD-CGD-O1D
17	BA	833	CLA	CBD-CGD-O2D-CED
17	BA	834	CLA	C4-C3-C5-C6
17	BA	835	CLA	CBD-CGD-O2D-CED
17	BA	840	CLA	CBD-CGD-O2D-CED
17	BA	841	CLA	CHA-CBD-CGD-O1D
17	BA	841	CLA	CHA-CBD-CGD-O2D
17	BA	841	CLA	C2-C3-C5-C6
17	BA	841	CLA	C4-C3-C5-C6
17	BA	844	CLA	CBD-CGD-O2D-CED
17	BB	802	CLA	CHA-CBD-CGD-O1D
17	BB	802	CLA	CHA-CBD-CGD-O2D
17	BB	802	CLA	C2-C3-C5-C6
17	BB	802	CLA	C4-C3-C5-C6
17	BB	804	CLA	CHA-CBD-CGD-O1D
17	BB	804	CLA	CHA-CBD-CGD-O2D
17	BB	804	CLA	CBD-CGD-O2D-CED
17	BB	805	CLA	C1A-C2A-CAA-CBA
17	BB	805	CLA	C3A-C2A-CAA-CBA
17	BB	805	CLA	CBD-CGD-O2D-CED
17	BB	807	CLA	C3A-C2A-CAA-CBA
17	BB	809	CLA	CHA-CBD-CGD-O1D
17	BB	809	CLA	CHA-CBD-CGD-O2D
17	BB	810	CLA	C1A-C2A-CAA-CBA
17	BB	811	CLA	CBD-CGD-O2D-CED
17	BB	812	CLA	C1A-C2A-CAA-CBA
17	BB	812	CLA	C2A-CAA-CBA-CGA
17	BB	813	CLA	CBD-CGD-O2D-CED
17	BB	815	CLA	C4C-C3C-CAC-CBC
17	BB	815	CLA	CBD-CGD-O2D-CED
17	BB	816	CLA	CHA-CBD-CGD-O1D
17	BB	816	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	BB	816	CLA	CBD-CGD-O2D-CED
17	BB	818	CLA	CBD-CGD-O2D-CED
17	BB	820	CLA	C3A-C2A-CAA-CBA
17	BB	820	CLA	C4-C3-C5-C6
17	BB	823	CLA	C1A-C2A-CAA-CBA
17	BB	825	CLA	C1A-C2A-CAA-CBA
17	BB	825	CLA	C3A-C2A-CAA-CBA
17	BB	825	CLA	CHA-CBD-CGD-O1D
17	BB	825	CLA	CHA-CBD-CGD-O2D
17	BB	830	CLA	C1A-C2A-CAA-CBA
17	BB	835	CLA	C6-C7-C8-C9
17	BB	836	CLA	CBD-CGD-O2D-CED
17	BB	837	CLA	C1A-C2A-CAA-CBA
17	BB	837	CLA	CBD-CGD-O2D-CED
17	BB	838	CLA	CBD-CGD-O2D-CED
17	BF	301	CLA	C1A-C2A-CAA-CBA
17	BF	301	CLA	C3A-C2A-CAA-CBA
17	BF	303	CLA	CBD-CGD-O2D-CED
17	BG	201	CLA	C1A-C2A-CAA-CBA
17	BG	201	CLA	C3A-C2A-CAA-CBA
17	BG	201	CLA	CBD-CGD-O2D-CED
17	BG	202	CLA	CBD-CGD-O2D-CED
17	BH	201	CLA	C1A-C2A-CAA-CBA
17	BH	201	CLA	CBD-CGD-O2D-CED
17	BH	201	CLA	O1D-CGD-O2D-CED
17	BJ	102	CLA	CHA-CBD-CGD-O1D
17	BJ	102	CLA	CHA-CBD-CGD-O2D
17	BL	303	CLA	C1A-C2A-CAA-CBA
17	B1	307	CLA	CHA-CBD-CGD-O1D
17	B1	307	CLA	CHA-CBD-CGD-O2D
17	B1	307	CLA	CBD-CGD-O2D-CED
17	B1	311	CLA	CBD-CGD-O2D-CED
17	B2	302	CLA	CHA-CBD-CGD-O2D
17	B3	603	CLA	C1A-C2A-CAA-CBA
17	B3	603	CLA	C3A-C2A-CAA-CBA
17	B3	605	CLA	C1A-C2A-CAA-CBA
17	B3	605	CLA	C3A-C2A-CAA-CBA
17	B5	601	CLA	CHA-CBD-CGD-O1D
17	B5	601	CLA	CHA-CBD-CGD-O2D
17	B5	601	CLA	CAD-CBD-CGD-O1D
17	B5	604	CLA	CBD-CGD-O2D-CED
17	B5	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B5	610	CLA	C1A-C2A-CAA-CBA
17	B5	610	CLA	C3A-C2A-CAA-CBA
17	B5	611	CLA	C1A-C2A-CAA-CBA
17	B5	612	CLA	CHA-CBD-CGD-O1D
17	B5	612	CLA	CHA-CBD-CGD-O2D
18	BB	844	PQN	C11-C12-C13-C14
18	BB	844	PQN	C19-C18-C20-C21
19	BA	845	LHG	C3-O3-P-O5
19	BA	846	LHG	C1-C2-C3-O3
19	BA	846	LHG	C3-O3-P-O4
19	BA	846	LHG	C3-O3-P-O5
19	BA	846	LHG	C3-O3-P-O6
19	BF	305	LHG	C3-O3-P-O5
19	BF	305	LHG	C4-O6-P-O5
19	BF	305	LHG	C8-C7-O7-C5
19	B1	301	LHG	O10-C23-O8-C6
19	B1	301	LHG	C24-C23-O8-C6
19	B1	302	LHG	C3-O3-P-O4
19	B1	302	LHG	C3-O3-P-O5
19	B1	302	LHG	C3-O3-P-O6
19	B1	318	LHG	C3-O3-P-O6
19	B1	318	LHG	C4-O6-P-O5
19	B2	317	LHG	O2-C2-C3-O3
19	B2	317	LHG	C3-O3-P-O4
19	B2	317	LHG	C3-O3-P-O5
19	B2	317	LHG	C3-O3-P-O6
19	B2	317	LHG	C4-O6-P-O5
19	B2	317	LHG	O7-C5-C6-O8
19	B3	619	LHG	C4-O6-P-O4
19	B5	618	LHG	C3-O3-P-O5
19	B5	618	LHG	C8-C7-O7-C5
20	BA	848	BCR	C23-C24-C25-C26
20	BA	848	BCR	C23-C24-C25-C30
20	BA	849	BCR	C1-C6-C7-C8
20	BA	849	BCR	C5-C6-C7-C8
20	BA	849	BCR	C21-C22-C23-C24
20	BA	850	BCR	C23-C24-C25-C26
20	BA	851	BCR	C5-C6-C7-C8
20	BA	851	BCR	C23-C24-C25-C26
20	BA	855	BCR	C23-C24-C25-C26
20	BA	856	BCR	C23-C24-C25-C26
20	BB	803	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	BB	803	BCR	C23-C24-C25-C30
20	BB	845	BCR	C1-C6-C7-C8
20	BB	845	BCR	C5-C6-C7-C8
20	BB	845	BCR	C23-C24-C25-C26
20	BB	846	BCR	C7-C8-C9-C10
20	BB	846	BCR	C7-C8-C9-C34
20	BB	846	BCR	C23-C24-C25-C26
20	BB	846	BCR	C23-C24-C25-C30
20	BB	849	BCR	C21-C22-C23-C24
20	BF	304	BCR	C5-C6-C7-C8
20	BH	202	BCR	C37-C22-C23-C24
20	BH	202	BCR	C23-C24-C25-C30
20	BJ	103	BCR	C5-C6-C7-C8
20	BL	301	BCR	C1-C6-C7-C8
20	BL	305	BCR	C1-C6-C7-C8
20	BL	305	BCR	C5-C6-C7-C8
20	B3	618	BCR	C37-C22-C23-C24
20	B3	618	BCR	C23-C24-C25-C26
20	B3	618	BCR	C23-C24-C25-C30
22	BA	853	LMU	C2-C1-O1'-C1'
22	BA	854	LMU	C2'-C1'-O1'-C1
22	BA	854	LMU	O5'-C1'-O1'-C1
23	BB	850	DGD	C2B-C1B-O2G-C2G
23	BB	850	DGD	O1B-C1B-O2G-C2G
24	BJ	104	SQD	C24-C23-O48-C46
24	BJ	104	SQD	C5-C6-S-O7
25	B3	601	CHL	C1C-C2C-CMC-OMC
25	B3	601	CHL	C3C-C2C-CMC-OMC
25	B3	607	CHL	CBD-CGD-O2D-CED
26	B1	316	LUT	C1-C6-C7-C8
26	B1	316	LUT	C10-C11-C12-C13
26	B1	316	LUT	C11-C12-C13-C14
26	B1	316	LUT	C11-C12-C13-C20
26	B1	316	LUT	C27-C28-C29-C30
26	B1	316	LUT	C27-C28-C29-C39
26	B3	616	LUT	C21-C26-C27-C28
26	B3	616	LUT	C25-C26-C27-C28
17	BB	815	CLA	C2C-C3C-CAC-CBC
17	BA	801	CLA	O1D-CGD-O2D-CED
17	BB	818	CLA	O1D-CGD-O2D-CED
17	BB	833	CLA	O1D-CGD-O2D-CED
17	B1	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B5	602	CLA	O1D-CGD-O2D-CED
25	B2	306	CHL	O1D-CGD-O2D-CED
17	BB	805	CLA	C2C-C3C-CAC-CBC
19	B3	619	LHG	C8-C7-O7-C5
17	BA	802	CLA	O1D-CGD-O2D-CED
17	BA	810	CLA	O1D-CGD-O2D-CED
17	BA	821	CLA	O1D-CGD-O2D-CED
17	BB	805	CLA	O1D-CGD-O2D-CED
17	BB	813	CLA	O1D-CGD-O2D-CED
17	BB	816	CLA	O1D-CGD-O2D-CED
17	BB	837	CLA	O1D-CGD-O2D-CED
17	BG	202	CLA	O1D-CGD-O2D-CED
17	B2	310	CLA	O1D-CGD-O2D-CED
17	BA	810	CLA	CBD-CGD-O2D-CED
17	BA	811	CLA	CBD-CGD-O2D-CED
17	BA	814	CLA	CBD-CGD-O2D-CED
17	BA	820	CLA	CBD-CGD-O2D-CED
17	BA	834	CLA	CBD-CGD-O2D-CED
17	BA	841	CLA	CBD-CGD-O2D-CED
17	BB	808	CLA	CBD-CGD-O2D-CED
17	BB	812	CLA	CBD-CGD-O2D-CED
17	BB	826	CLA	CBD-CGD-O2D-CED
17	BB	833	CLA	CBD-CGD-O2D-CED
17	BB	834	CLA	CBD-CGD-O2D-CED
17	BB	843	CLA	CBD-CGD-O2D-CED
17	BF	302	CLA	CBD-CGD-O2D-CED
17	BK	203	CLA	CBD-CGD-O2D-CED
17	B1	305	CLA	CBD-CGD-O2D-CED
17	B1	306	CLA	CBD-CGD-O2D-CED
17	B2	303	CLA	CBD-CGD-O2D-CED
17	B2	308	CLA	CBD-CGD-O2D-CED
17	B2	310	CLA	CBD-CGD-O2D-CED
17	B3	603	CLA	CBD-CGD-O2D-CED
17	B3	609	CLA	CBD-CGD-O2D-CED
17	B5	602	CLA	CBD-CGD-O2D-CED
17	B5	610	CLA	CBD-CGD-O2D-CED
25	B2	306	CHL	CBD-CGD-O2D-CED
25	B3	601	CHL	CBD-CGD-O2D-CED
25	B5	607	CHL	CBD-CGD-O2D-CED
17	BA	832	CLA	O1A-CGA-O2A-C1
17	B3	603	CLA	O1A-CGA-O2A-C1
19	B1	302	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	BJ	104	SQD	O10-C23-O48-C46
17	BA	814	CLA	O1D-CGD-O2D-CED
17	BA	844	CLA	O1D-CGD-O2D-CED
17	BB	804	CLA	O1D-CGD-O2D-CED
17	B1	311	CLA	O1D-CGD-O2D-CED
17	B5	604	CLA	O1D-CGD-O2D-CED
17	B5	609	CLA	O1D-CGD-O2D-CED
17	B5	610	CLA	O1D-CGD-O2D-CED
25	B5	607	CHL	O1D-CGD-O2D-CED
17	BK	203	CLA	CBA-CGA-O2A-C1
17	BA	833	CLA	O1D-CGD-O2D-CED
17	BB	826	CLA	O1D-CGD-O2D-CED
17	BB	836	CLA	O1D-CGD-O2D-CED
17	BF	303	CLA	O1D-CGD-O2D-CED
17	BG	201	CLA	O1D-CGD-O2D-CED
17	B1	307	CLA	O1D-CGD-O2D-CED
25	B3	607	CHL	O1D-CGD-O2D-CED
17	BA	832	CLA	CBA-CGA-O2A-C1
19	B1	302	LHG	C24-C23-O8-C6
17	BA	813	CLA	CBD-CGD-O2D-CED
17	BA	817	CLA	CBD-CGD-O2D-CED
17	BA	823	CLA	CBD-CGD-O2D-CED
17	BA	825	CLA	CBD-CGD-O2D-CED
17	BA	831	CLA	CBD-CGD-O2D-CED
17	BA	836	CLA	CBD-CGD-O2D-CED
17	BB	822	CLA	CBD-CGD-O2D-CED
17	BB	831	CLA	CBD-CGD-O2D-CED
17	BB	839	CLA	CBD-CGD-O2D-CED
17	BL	304	CLA	CBD-CGD-O2D-CED
17	B3	602	CLA	CBD-CGD-O2D-CED
17	B5	601	CLA	CBD-CGD-O2D-CED
17	B5	612	CLA	CBD-CGD-O2D-CED
25	B2	304	CHL	CBD-CGD-O2D-CED
17	BA	817	CLA	O1A-CGA-O2A-C1
17	BA	821	CLA	O1A-CGA-O2A-C1
17	BA	827	CLA	O1A-CGA-O2A-C1
17	BA	833	CLA	O1A-CGA-O2A-C1
17	BA	837	CLA	O1A-CGA-O2A-C1
17	BA	838	CLA	O1A-CGA-O2A-C1
17	BB	812	CLA	O1A-CGA-O2A-C1
17	BB	843	CLA	O1A-CGA-O2A-C1
17	BL	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B1	303	CHL	O1A-CGA-O2A-C1
17	BA	835	CLA	O1D-CGD-O2D-CED
17	BB	838	CLA	O1D-CGD-O2D-CED
17	BA	828	CLA	O1D-CGD-O2D-CED
17	BA	840	CLA	O1D-CGD-O2D-CED
17	BB	811	CLA	O1D-CGD-O2D-CED
17	BA	815	CLA	CBD-CGD-O2D-CED
17	B3	611	CLA	CBD-CGD-O2D-CED
25	B2	305	CHL	CBD-CGD-O2D-CED
17	BA	811	CLA	O1D-CGD-O2D-CED
17	BB	815	CLA	O1D-CGD-O2D-CED
19	BF	305	LHG	O9-C7-O7-C5
19	B5	618	LHG	O9-C7-O7-C5
17	BK	203	CLA	O1A-CGA-O2A-C1
17	BA	828	CLA	C3-C5-C6-C7
17	BA	832	CLA	C3-C5-C6-C7
17	BF	301	CLA	C3-C5-C6-C7
17	BH	201	CLA	C3-C5-C6-C7
17	B1	305	CLA	C3-C5-C6-C7
17	B1	314	CLA	C3-C5-C6-C7
17	B2	301	CLA	C3-C5-C6-C7
18	BA	843	PQN	C13-C15-C16-C17
17	BA	806	CLA	CBA-CGA-O2A-C1
17	BA	811	CLA	CBA-CGA-O2A-C1
17	BA	821	CLA	CBA-CGA-O2A-C1
17	BA	837	CLA	CBA-CGA-O2A-C1
17	B3	603	CLA	CBA-CGA-O2A-C1
17	B3	603	CLA	O1D-CGD-O2D-CED
25	B3	601	CHL	O1D-CGD-O2D-CED
17	B2	301	CLA	CBD-CGD-O2D-CED
17	BA	805	CLA	C2A-CAA-CBA-CGA
17	BA	806	CLA	C2A-CAA-CBA-CGA
17	BA	821	CLA	C2A-CAA-CBA-CGA
17	BA	827	CLA	C2A-CAA-CBA-CGA
17	BA	829	CLA	C2A-CAA-CBA-CGA
17	BA	842	CLA	C2A-CAA-CBA-CGA
17	BB	811	CLA	C2A-CAA-CBA-CGA
17	BB	841	CLA	C2A-CAA-CBA-CGA
17	BA	805	CLA	C3-C5-C6-C7
17	BB	824	CLA	C3-C5-C6-C7
17	BB	842	CLA	C3-C5-C6-C7
17	BA	810	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	BA	817	CLA	CBA-CGA-O2A-C1
17	BA	824	CLA	CBA-CGA-O2A-C1
17	BA	827	CLA	CBA-CGA-O2A-C1
17	BA	833	CLA	CBA-CGA-O2A-C1
17	BA	838	CLA	CBA-CGA-O2A-C1
17	BA	842	CLA	CBA-CGA-O2A-C1
17	BB	812	CLA	CBA-CGA-O2A-C1
17	BB	819	CLA	CBA-CGA-O2A-C1
17	BB	823	CLA	CBA-CGA-O2A-C1
17	BB	828	CLA	CBA-CGA-O2A-C1
17	BB	843	CLA	CBA-CGA-O2A-C1
17	BL	303	CLA	CBA-CGA-O2A-C1
25	B1	303	CHL	CBA-CGA-O2A-C1
19	B3	619	LHG	O9-C7-O7-C5
17	BA	841	CLA	O1D-CGD-O2D-CED
17	BB	808	CLA	O1D-CGD-O2D-CED
17	B2	303	CLA	O1D-CGD-O2D-CED
17	B2	308	CLA	O1D-CGD-O2D-CED
18	BA	843	PQN	C11-C12-C13-C14
25	B5	606	CHL	CBD-CGD-O2D-CED
17	BB	812	CLA	O1D-CGD-O2D-CED
17	BF	302	CLA	O1D-CGD-O2D-CED
17	BK	203	CLA	O1D-CGD-O2D-CED
17	B3	609	CLA	O1D-CGD-O2D-CED
17	BA	806	CLA	O1A-CGA-O2A-C1
17	BA	810	CLA	O1A-CGA-O2A-C1
17	BA	811	CLA	O1A-CGA-O2A-C1
17	BA	842	CLA	O1A-CGA-O2A-C1
17	BB	804	CLA	O1A-CGA-O2A-C1
17	BB	819	CLA	O1A-CGA-O2A-C1
17	BB	828	CLA	O1A-CGA-O2A-C1
20	BH	202	BCR	C19-C20-C21-C22
17	BA	803	CLA	CBD-CGD-O2D-CED
17	BA	807	CLA	CBD-CGD-O2D-CED
17	BA	838	CLA	CBD-CGD-O2D-CED
17	BB	821	CLA	CBD-CGD-O2D-CED
17	BB	824	CLA	CBD-CGD-O2D-CED
17	BB	829	CLA	CBD-CGD-O2D-CED
17	BB	835	CLA	CBD-CGD-O2D-CED
17	B1	304	CLA	CBD-CGD-O2D-CED
17	B1	313	CLA	CBD-CGD-O2D-CED
17	B2	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B3	606	CLA	CBD-CGD-O2D-CED
17	B5	613	CLA	CBD-CGD-O2D-CED
17	BB	834	CLA	O1D-CGD-O2D-CED
19	BF	305	LHG	O2-C2-C3-O3
17	BA	829	CLA	C3-C5-C6-C7
17	BA	833	CLA	C3-C5-C6-C7
17	BB	808	CLA	C3-C5-C6-C7
17	BB	816	CLA	C3-C5-C6-C7
17	BB	836	CLA	C3-C5-C6-C7
17	BB	841	CLA	C3-C5-C6-C7
17	B2	311	CLA	C3-C5-C6-C7
17	BA	804	CLA	CBA-CGA-O2A-C1
17	BB	804	CLA	CBA-CGA-O2A-C1
19	B3	619	LHG	O10-C23-O8-C6
17	BA	834	CLA	O1D-CGD-O2D-CED
17	B1	305	CLA	O1D-CGD-O2D-CED
17	BA	839	CLA	CBD-CGD-O2D-CED
17	BA	820	CLA	O1D-CGD-O2D-CED
17	BB	843	CLA	O1D-CGD-O2D-CED
17	BB	815	CLA	C5-C6-C7-C8
17	BA	803	CLA	C3-C5-C6-C7
17	BA	827	CLA	C3-C5-C6-C7
19	B3	619	LHG	C24-C23-O8-C6
17	BA	804	CLA	O1A-CGA-O2A-C1
17	BA	824	CLA	O1A-CGA-O2A-C1
17	BA	838	CLA	C4-C3-C5-C6
17	BA	834	CLA	C2-C3-C5-C6
17	BA	838	CLA	C2-C3-C5-C6
17	BB	820	CLA	C2-C3-C5-C6
17	BA	833	CLA	C2A-CAA-CBA-CGA
17	BA	840	CLA	C2A-CAA-CBA-CGA
17	BB	802	CLA	C2A-CAA-CBA-CGA
17	BA	819	CLA	O1A-CGA-O2A-C1
17	BB	823	CLA	O1A-CGA-O2A-C1
17	BA	819	CLA	CBA-CGA-O2A-C1
17	BA	826	CLA	CBA-CGA-O2A-C1
17	BB	802	CLA	CBA-CGA-O2A-C1
17	BB	807	CLA	CBA-CGA-O2A-C1
17	BB	839	CLA	CBA-CGA-O2A-C1
17	BF	301	CLA	CBA-CGA-O2A-C1
17	B5	612	CLA	CBA-CGA-O2A-C1
17	BA	836	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	BB	831	CLA	O1D-CGD-O2D-CED
17	BL	304	CLA	O1D-CGD-O2D-CED
17	B5	601	CLA	O1D-CGD-O2D-CED
17	BA	826	CLA	O1A-CGA-O2A-C1
17	BB	805	CLA	C4C-C3C-CAC-CBC
17	BB	839	CLA	O1D-CGD-O2D-CED
17	B3	602	CLA	O1D-CGD-O2D-CED
17	BA	823	CLA	O1D-CGD-O2D-CED
19	B2	317	LHG	C1-C2-C3-O3
17	BB	802	CLA	O1A-CGA-O2A-C1
17	BB	807	CLA	O1A-CGA-O2A-C1
17	BF	301	CLA	O1A-CGA-O2A-C1
17	BA	813	CLA	O1D-CGD-O2D-CED
17	BA	808	CLA	CBA-CGA-O2A-C1
17	BA	834	CLA	CBA-CGA-O2A-C1
17	BA	840	CLA	CBA-CGA-O2A-C1
17	BB	805	CLA	CBA-CGA-O2A-C1
17	BB	813	CLA	CBA-CGA-O2A-C1
17	BB	815	CLA	CBA-CGA-O2A-C1
17	BB	816	CLA	CBA-CGA-O2A-C1
17	BB	820	CLA	CBA-CGA-O2A-C1
17	B1	314	CLA	CBA-CGA-O2A-C1
17	B2	311	CLA	CBA-CGA-O2A-C1
19	BA	845	LHG	C24-C23-O8-C6
19	B2	317	LHG	C24-C23-O8-C6
25	B3	601	CHL	CBA-CGA-O2A-C1
17	BA	834	CLA	C5-C6-C7-C8
18	BA	843	PQN	C18-C20-C21-C22
22	BB	851	LMU	C4'-C5'-C6'-O6'
19	BA	846	LHG	O2-C2-C3-O3
19	B3	619	LHG	O2-C2-C3-O3
17	BB	830	CLA	CBA-CGA-O2A-C1
17	BB	820	CLA	O1A-CGA-O2A-C1
19	B2	317	LHG	O10-C23-O8-C6
17	BA	806	CLA	C14-C13-C15-C16
17	BA	828	CLA	C14-C13-C15-C16
17	BA	840	CLA	C11-C12-C13-C14
17	BB	801	CLA	C6-C7-C8-C9
17	BB	824	CLA	C6-C7-C8-C9
17	BB	830	CLA	C14-C13-C15-C16
17	BB	842	CLA	C6-C7-C8-C9
17	BA	831	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B2	304	CHL	O1D-CGD-O2D-CED
17	BB	842	CLA	CBD-CGD-O2D-CED
17	B5	601	CLA	C2A-CAA-CBA-CGA
20	BA	849	BCR	C37-C22-C23-C24
20	BB	849	BCR	C37-C22-C23-C24
20	BH	202	BCR	C11-C12-C13-C35
20	B3	618	BCR	C21-C22-C23-C24
17	BA	834	CLA	O1A-CGA-O2A-C1
17	BA	840	CLA	O1A-CGA-O2A-C1
17	BB	816	CLA	O1A-CGA-O2A-C1
17	B2	311	CLA	O1A-CGA-O2A-C1
17	BA	828	CLA	C13-C15-C16-C17
17	BA	808	CLA	CBD-CGD-O2D-CED
17	BB	835	CLA	CBA-CGA-O2A-C1
17	BA	811	CLA	C15-C16-C17-C18
17	BA	819	CLA	C13-C15-C16-C17
17	BA	827	CLA	C10-C11-C12-C13
17	BA	829	CLA	C10-C11-C12-C13
17	BB	808	CLA	C10-C11-C12-C13
17	BB	816	CLA	C10-C11-C12-C13
17	BB	816	CLA	C13-C15-C16-C17
17	BB	826	CLA	C8-C10-C11-C12
17	BB	826	CLA	C13-C15-C16-C17
17	B3	602	CLA	C10-C11-C12-C13
17	BA	831	CLA	C2-C1-O2A-CGA
24	BJ	104	SQD	C23-C24-C25-C26
17	BA	827	CLA	C15-C16-C17-C18
17	BA	833	CLA	C13-C15-C16-C17
17	BA	842	CLA	C5-C6-C7-C8
17	BB	804	CLA	C10-C11-C12-C13
17	BB	807	CLA	C10-C11-C12-C13
18	BB	844	PQN	C25-C26-C27-C28
17	BA	817	CLA	O1D-CGD-O2D-CED
17	BA	825	CLA	O1D-CGD-O2D-CED
19	B5	618	LHG	C23-C24-C25-C26
24	BJ	104	SQD	C7-C8-C9-C10
28	B5	617	LMG	C10-C11-C12-C13
17	BA	822	CLA	CBD-CGD-O2D-CED
17	BB	826	CLA	C10-C11-C12-C13
18	BB	844	PQN	C15-C16-C17-C18
17	B2	308	CLA	CBA-CGA-O2A-C1
28	B5	617	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
17	BB	805	CLA	C2-C1-O2A-CGA
17	BA	825	CLA	C10-C11-C12-C13
17	BA	825	CLA	C13-C15-C16-C17
17	BB	839	CLA	C15-C16-C17-C18
17	BL	303	CLA	C5-C6-C7-C8
17	B5	612	CLA	C8-C10-C11-C12
17	BB	801	CLA	C10-C11-C12-C13
18	BA	843	PQN	C23-C25-C26-C27
17	B3	611	CLA	O1D-CGD-O2D-CED
17	BA	842	CLA	C12-C13-C15-C16
17	BB	824	CLA	C11-C12-C13-C15
18	BA	843	PQN	C21-C22-C23-C25
18	BB	844	PQN	C21-C22-C23-C25
17	BB	828	CLA	C3-C5-C6-C7
17	BA	808	CLA	O1A-CGA-O2A-C1
17	BB	805	CLA	O1A-CGA-O2A-C1
17	BB	813	CLA	O1A-CGA-O2A-C1
17	BB	830	CLA	O1A-CGA-O2A-C1
25	B3	601	CHL	O1A-CGA-O2A-C1
17	BA	802	CLA	C2A-CAA-CBA-CGA
17	BA	808	CLA	C2A-CAA-CBA-CGA
25	B3	607	CHL	C2A-CAA-CBA-CGA
17	BA	815	CLA	O1D-CGD-O2D-CED
17	BB	822	CLA	O1D-CGD-O2D-CED
17	B5	612	CLA	O1D-CGD-O2D-CED
25	B2	305	CHL	O1D-CGD-O2D-CED
17	BA	830	CLA	C13-C15-C16-C17
17	BB	839	CLA	O1A-CGA-O2A-C1
17	BA	809	CLA	CBD-CGD-O2D-CED
17	BA	829	CLA	C8-C10-C11-C12
17	BA	801	CLA	C3-C5-C6-C7
17	BA	810	CLA	C5-C6-C7-C8
17	BA	840	CLA	C5-C6-C7-C8
17	BB	827	CLA	C8-C10-C11-C12
17	BB	835	CLA	C8-C10-C11-C12
17	BB	839	CLA	C5-C6-C7-C8
17	BB	827	CLA	CBA-CGA-O2A-C1
17	BB	815	CLA	O1A-CGA-O2A-C1
17	BB	835	CLA	O1A-CGA-O2A-C1
17	B1	314	CLA	O1A-CGA-O2A-C1
17	B5	612	CLA	O1A-CGA-O2A-C1
19	BA	845	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
17	BA	803	CLA	C5-C6-C7-C8
17	BA	803	CLA	C13-C15-C16-C17
17	BA	810	CLA	C13-C15-C16-C17
17	BA	819	CLA	C10-C11-C12-C13
17	BA	833	CLA	C15-C16-C17-C18
17	BB	829	CLA	C10-C11-C12-C13
17	BB	831	CLA	C5-C6-C7-C8
17	BB	843	CLA	C8-C10-C11-C12
17	BB	802	CLA	CBD-CGD-O2D-CED
17	BA	830	CLA	C10-C11-C12-C13
17	BB	828	CLA	C10-C11-C12-C13
17	BB	836	CLA	C8-C10-C11-C12
19	BF	305	LHG	C3-O3-P-O6
19	B2	317	LHG	C4-O6-P-O3
19	B3	619	LHG	C4-O6-P-O3
19	B5	618	LHG	C4-O6-P-O3
17	BB	820	CLA	C8-C10-C11-C12
17	BA	817	CLA	C2A-CAA-CBA-CGA
17	BA	841	CLA	C2A-CAA-CBA-CGA
17	B2	311	CLA	C2A-CAA-CBA-CGA
17	BA	830	CLA	CBA-CGA-O2A-C1
17	BB	818	CLA	CBA-CGA-O2A-C1
17	BB	824	CLA	CBA-CGA-O2A-C1
17	BB	842	CLA	CBA-CGA-O2A-C1
17	BA	821	CLA	C13-C15-C16-C17
17	BA	828	CLA	C15-C16-C17-C18
19	BA	845	LHG	C8-C7-O7-C5
17	BA	821	CLA	C15-C16-C17-C18
22	BA	853	LMU	O5B-C5B-C6B-O6B
26	B1	316	LUT	C11-C10-C9-C19
26	B1	316	LUT	C39-C29-C30-C31
19	BA	845	LHG	C14-C15-C16-C17
17	BB	804	CLA	C16-C17-C18-C19
17	BA	812	CLA	CBA-CGA-O2A-C1
19	B1	318	LHG	C28-C29-C30-C31
17	B2	301	CLA	O1D-CGD-O2D-CED
25	B5	606	CHL	O1D-CGD-O2D-CED
19	BA	845	LHG	O9-C7-O7-C5
24	BJ	104	SQD	C10-C11-C12-C13
24	BJ	104	SQD	C13-C14-C15-C16
19	BF	305	LHG	C27-C28-C29-C30
24	BJ	104	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	BA	803	CLA	O1D-CGD-O2D-CED
17	B2	311	CLA	O1D-CGD-O2D-CED
24	BJ	104	SQD	C2-C1-O6-C44
26	B1	316	LUT	C11-C10-C9-C8
26	B1	316	LUT	C28-C29-C30-C31
22	BB	851	LMU	C6-C7-C8-C9
17	BB	839	CLA	C8-C10-C11-C12
17	BB	818	CLA	O1A-CGA-O2A-C1
17	BA	806	CLA	C16-C17-C18-C19
17	BB	807	CLA	C16-C17-C18-C19
22	BB	851	LMU	O5'-C5'-C6'-O6'
19	BF	305	LHG	C11-C10-C9-C8
17	BA	821	CLA	C11-C12-C13-C14
17	BA	825	CLA	C11-C10-C8-C9
17	BA	829	CLA	C14-C13-C15-C16
17	B2	311	CLA	C14-C13-C15-C16
17	BA	838	CLA	O1D-CGD-O2D-CED
17	BB	824	CLA	O1D-CGD-O2D-CED
17	B1	313	CLA	O1D-CGD-O2D-CED
22	BA	853	LMU	C5-C6-C7-C8
23	BB	850	DGD	CAA-CBA-CCA-CDA
24	BJ	104	SQD	C11-C12-C13-C14
17	B2	308	CLA	O1A-CGA-O2A-C1
20	BH	202	BCR	C7-C8-C9-C34
19	B2	317	LHG	O1-C1-C2-C3
20	BH	202	BCR	C21-C22-C23-C24
19	BF	305	LHG	C30-C31-C32-C33
17	BB	829	CLA	O1D-CGD-O2D-CED
17	B5	613	CLA	O1D-CGD-O2D-CED
19	BA	845	LHG	C25-C26-C27-C28
19	B1	318	LHG	C11-C12-C13-C14
17	BB	824	CLA	O1A-CGA-O2A-C1
17	BA	813	CLA	C16-C17-C18-C19
17	BA	825	CLA	C16-C17-C18-C20
24	BJ	104	SQD	O5-C1-O6-C44
17	BA	802	CLA	C15-C16-C17-C18
17	BB	824	CLA	C8-C10-C11-C12
17	BB	841	CLA	CBD-CGD-O2D-CED
17	BJ	102	CLA	CBD-CGD-O2D-CED
17	B1	304	CLA	O1D-CGD-O2D-CED
23	BB	850	DGD	CCA-CDA-CEA-CFA
17	BB	843	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	BA	853	LMU	O5B-C1B-O1B-C4'
17	BA	830	CLA	O1A-CGA-O2A-C1
17	BB	827	CLA	O1A-CGA-O2A-C1
19	BF	305	LHG	C11-C12-C13-C14
17	BB	843	CLA	C3-C5-C6-C7
17	BB	831	CLA	CBA-CGA-O2A-C1
17	BB	821	CLA	O1D-CGD-O2D-CED
17	BA	803	CLA	C3A-C2A-CAA-CBA
17	BA	805	CLA	C3A-C2A-CAA-CBA
17	BA	809	CLA	C3A-C2A-CAA-CBA
17	BB	810	CLA	C3A-C2A-CAA-CBA
17	BB	815	CLA	C3A-C2A-CAA-CBA
17	BL	303	CLA	C3A-C2A-CAA-CBA
17	B2	310	CLA	C3A-C2A-CAA-CBA
25	B3	601	CHL	C3A-C2A-CAA-CBA
22	BB	851	LMU	C2-C1-O1'-C1'
17	BA	807	CLA	O1D-CGD-O2D-CED
17	BA	825	CLA	C16-C17-C18-C19
17	BB	835	CLA	C16-C17-C18-C20
17	BB	836	CLA	C11-C12-C13-C14
17	BB	836	CLA	C11-C12-C13-C15
17	B3	606	CLA	O1D-CGD-O2D-CED
19	BA	845	LHG	C29-C30-C31-C32
17	BA	842	CLA	C4-C3-C5-C6
18	BB	844	PQN	C14-C13-C15-C16
17	BA	842	CLA	C2-C3-C5-C6
19	B2	317	LHG	C8-C7-O7-C5
17	BB	807	CLA	C16-C17-C18-C20
17	BA	841	CLA	C2-C1-O2A-CGA
19	BA	845	LHG	C32-C33-C34-C35
17	BA	812	CLA	O1A-CGA-O2A-C1
17	BB	842	CLA	O1A-CGA-O2A-C1
17	BA	806	CLA	C16-C17-C18-C20
17	BB	804	CLA	C16-C17-C18-C20
20	BA	847	BCR	C5-C6-C7-C8
20	BA	847	BCR	C23-C24-C25-C26
20	BA	848	BCR	C5-C6-C7-C8
20	BA	850	BCR	C5-C6-C7-C8
20	BA	850	BCR	C23-C24-C25-C30
20	BA	851	BCR	C1-C6-C7-C8
20	BA	851	BCR	C23-C24-C25-C30
20	BA	855	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
20	BA	856	BCR	C1-C6-C7-C8
20	BA	856	BCR	C5-C6-C7-C8
20	BA	856	BCR	C23-C24-C25-C30
20	BB	803	BCR	C5-C6-C7-C8
20	BB	845	BCR	C23-C24-C25-C30
20	BB	847	BCR	C1-C6-C7-C8
20	BB	847	BCR	C5-C6-C7-C8
20	BB	848	BCR	C5-C6-C7-C8
20	BF	304	BCR	C1-C6-C7-C8
20	BF	304	BCR	C23-C24-C25-C26
20	BH	202	BCR	C1-C6-C7-C8
20	BH	202	BCR	C5-C6-C7-C8
20	BH	202	BCR	C23-C24-C25-C26
20	BI	101	BCR	C1-C6-C7-C8
20	BI	101	BCR	C5-C6-C7-C8
20	BI	101	BCR	C23-C24-C25-C26
20	BJ	103	BCR	C1-C6-C7-C8
20	BJ	103	BCR	C23-C24-C25-C26
20	BJ	103	BCR	C23-C24-C25-C30
20	BL	301	BCR	C5-C6-C7-C8
20	BL	301	BCR	C23-C24-C25-C26
20	B3	618	BCR	C1-C6-C7-C8
20	B3	618	BCR	C5-C6-C7-C8
20	B5	616	BCR	C1-C6-C7-C8
20	B5	616	BCR	C5-C6-C7-C8
26	B1	316	LUT	C5-C6-C7-C8
17	BB	835	CLA	O1D-CGD-O2D-CED
17	BA	805	CLA	CBA-CGA-O2A-C1
17	BB	840	CLA	CBA-CGA-O2A-C1
17	BA	833	CLA	C5-C6-C7-C8
17	BB	831	CLA	O1A-CGA-O2A-C1
17	BB	811	CLA	C13-C15-C16-C17
17	BA	801	CLA	C12-C13-C15-C16
17	BA	806	CLA	C2-C3-C5-C6
17	BA	806	CLA	C12-C13-C15-C16
17	BA	808	CLA	C11-C12-C13-C15
17	BA	810	CLA	C6-C7-C8-C10
17	BA	821	CLA	C11-C12-C13-C15
17	BA	829	CLA	C11-C10-C8-C7
17	BA	829	CLA	C12-C13-C15-C16
17	BB	815	CLA	C6-C7-C8-C10
17	BB	828	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	BB	828	CLA	C11-C12-C13-C15
17	BB	835	CLA	C11-C12-C13-C15
17	B2	311	CLA	C12-C13-C15-C16
17	BA	810	CLA	C10-C11-C12-C13
19	B2	317	LHG	O9-C7-O7-C5
28	B5	617	LMG	O9-C10-O7-C8
17	BA	828	CLA	C2A-CAA-CBA-CGA
17	B1	314	CLA	C2A-CAA-CBA-CGA
17	BA	839	CLA	O1D-CGD-O2D-CED
17	B2	301	CLA	C13-C15-C16-C17
19	B1	318	LHG	C9-C10-C11-C12
23	BB	850	DGD	CDA-CEA-CFA-CGA
17	BA	830	CLA	C5-C6-C7-C8
17	B2	311	CLA	C8-C10-C11-C12
19	BA	845	LHG	C15-C16-C17-C18
22	BB	851	LMU	O5B-C1B-O1B-C4'
17	BB	820	CLA	CBD-CGD-O2D-CED
17	BB	821	CLA	CBA-CGA-O2A-C1
17	BA	805	CLA	C16-C17-C18-C19
17	BB	834	CLA	C5-C6-C7-C8
17	B1	314	CLA	C8-C10-C11-C12
19	B1	318	LHG	C8-C7-O7-C5
28	B5	617	LMG	C11-C10-O7-C8
17	BB	808	CLA	C15-C16-C17-C18
17	BB	829	CLA	C15-C16-C17-C18
17	BA	838	CLA	C6-C7-C8-C10
17	B3	612	CLA	C6-C7-C8-C9
17	BA	806	CLA	C4-C3-C5-C6
19	BA	845	LHG	C23-C24-C25-C26
17	BA	808	CLA	C11-C12-C13-C14
17	BA	810	CLA	C6-C7-C8-C9
17	BA	813	CLA	C11-C10-C8-C9
17	BA	842	CLA	C14-C13-C15-C16
17	BB	811	CLA	C14-C13-C15-C16
17	BB	815	CLA	C6-C7-C8-C9
17	BB	824	CLA	C11-C12-C13-C14
17	BB	826	CLA	C14-C13-C15-C16
17	BB	835	CLA	C11-C12-C13-C14
17	B5	602	CLA	C11-C10-C8-C9
18	BA	843	PQN	C21-C22-C23-C24
24	BJ	104	SQD	C11-C10-C9-C8
17	BB	818	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	BB	830	CLA	C2A-CAA-CBA-CGA
17	BA	811	CLA	C13-C15-C16-C17
17	BA	805	CLA	O1A-CGA-O2A-C1
17	BA	803	CLA	C1A-C2A-CAA-CBA
17	BA	807	CLA	C1A-C2A-CAA-CBA
17	BA	810	CLA	C1A-C2A-CAA-CBA
17	BA	819	CLA	C1A-C2A-CAA-CBA
17	BA	830	CLA	C1A-C2A-CAA-CBA
17	BA	832	CLA	C1A-C2A-CAA-CBA
17	BB	807	CLA	C1A-C2A-CAA-CBA
17	BB	820	CLA	C1A-C2A-CAA-CBA
17	BB	834	CLA	C1A-C2A-CAA-CBA
17	BB	836	CLA	C1A-C2A-CAA-CBA
17	BL	304	CLA	C1A-C2A-CAA-CBA
17	B2	310	CLA	C1A-C2A-CAA-CBA
17	B2	312	CLA	C1A-C2A-CAA-CBA
17	B5	613	CLA	C1A-C2A-CAA-CBA
17	BA	805	CLA	C16-C17-C18-C20
17	BA	813	CLA	C16-C17-C18-C20
19	B1	302	LHG	C8-C7-O7-C5
19	BA	845	LHG	C10-C11-C12-C13
17	BB	801	CLA	C5-C6-C7-C8
17	BB	811	CLA	C10-C11-C12-C13
19	BA	845	LHG	C34-C35-C36-C37
17	BB	840	CLA	O1A-CGA-O2A-C1
17	BA	809	CLA	CBA-CGA-O2A-C1
19	B1	318	LHG	O9-C7-O7-C5
17	BA	811	CLA	C4-C3-C5-C6
17	BA	822	CLA	C3A-C2A-CAA-CBA
17	B5	611	CLA	C3A-C2A-CAA-CBA
17	BB	812	CLA	C5-C6-C7-C8
17	BA	801	CLA	C16-C17-C18-C19
17	B2	301	CLA	C16-C17-C18-C19
19	BA	845	LHG	C4-C5-C6-O8
19	B2	317	LHG	C4-C5-C6-O8
28	B5	617	LMG	O1-C7-C8-C9
17	BB	806	CLA	C2C-C3C-CAC-CBC
17	BA	828	CLA	C10-C11-C12-C13
28	B5	617	LMG	C31-C32-C33-C34
24	BJ	104	SQD	C15-C16-C17-C18
17	BA	806	CLA	C10-C11-C12-C13
17	BA	809	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	BB	821	CLA	O1A-CGA-O2A-C1
17	BA	808	CLA	O1D-CGD-O2D-CED
17	B1	305	CLA	C2A-CAA-CBA-CGA
17	BB	819	CLA	C4-C3-C5-C6
17	BB	836	CLA	C4-C3-C5-C6
17	BF	301	CLA	C4-C3-C5-C6
17	BB	836	CLA	C2-C3-C5-C6
17	BA	811	CLA	C16-C17-C18-C19
19	B5	618	LHG	C24-C23-O8-C6
17	BA	813	CLA	C15-C16-C17-C18
17	BB	830	CLA	C5-C6-C7-C8
24	BJ	104	SQD	C19-C20-C21-C22
17	BA	806	CLA	C5-C6-C7-C8
17	BH	201	CLA	C10-C11-C12-C13
17	BB	807	CLA	C2-C1-O2A-CGA
17	BA	822	CLA	O1D-CGD-O2D-CED
19	B2	317	LHG	C9-C10-C11-C12
17	BA	805	CLA	C8-C10-C11-C12
17	BB	842	CLA	O1D-CGD-O2D-CED
17	BA	838	CLA	C6-C7-C8-C9
17	B3	612	CLA	C6-C7-C8-C10
17	BA	809	CLA	O1D-CGD-O2D-CED
17	BB	825	CLA	CBD-CGD-O2D-CED
23	BB	850	DGD	O1G-C1G-C2G-O2G
19	BF	305	LHG	C10-C11-C12-C13
19	B1	302	LHG	O9-C7-O7-C5
17	BA	811	CLA	C2-C3-C5-C6
17	BA	813	CLA	C11-C10-C8-C7
17	BA	819	CLA	C11-C12-C13-C15
17	BA	828	CLA	C6-C7-C8-C10
17	BA	828	CLA	C12-C13-C15-C16
17	BB	802	CLA	C6-C7-C8-C10
17	BB	808	CLA	C11-C10-C8-C7
17	BB	811	CLA	C6-C7-C8-C10
17	BB	811	CLA	C11-C10-C8-C7
17	BB	824	CLA	C6-C7-C8-C10
17	BB	826	CLA	C12-C13-C15-C16
17	BB	836	CLA	C11-C10-C8-C7
17	BB	843	CLA	C6-C7-C8-C10
17	BF	301	CLA	C2-C3-C5-C6
17	BL	303	CLA	C11-C10-C8-C7
17	B5	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	BB	819	CLA	CAA-CBA-CGA-O2A
17	BA	803	CLA	C11-C10-C8-C9
17	BA	819	CLA	C6-C7-C8-C9
17	BA	819	CLA	C11-C12-C13-C14
17	BA	842	CLA	C11-C10-C8-C9
17	BB	807	CLA	C6-C7-C8-C9
17	BB	807	CLA	C11-C12-C13-C14
17	BB	811	CLA	C6-C7-C8-C9
17	BB	811	CLA	C11-C10-C8-C9
17	BB	819	CLA	C6-C7-C8-C9
17	BB	826	CLA	C6-C7-C8-C9
17	BB	828	CLA	C11-C12-C13-C14
17	BB	829	CLA	C11-C10-C8-C9
17	BB	836	CLA	C11-C10-C8-C9
17	BB	843	CLA	C6-C7-C8-C9
17	BL	303	CLA	C11-C10-C8-C9
17	B1	314	CLA	C6-C7-C8-C9
17	BB	801	CLA	CBA-CGA-O2A-C1
17	B2	301	CLA	C16-C17-C18-C20
20	BA	855	BCR	C21-C22-C23-C24
20	BI	101	BCR	C21-C22-C23-C24
17	BA	818	CLA	CBA-CGA-O2A-C1
17	BA	839	CLA	CBA-CGA-O2A-C1
17	BA	841	CLA	CBA-CGA-O2A-C1
17	B2	311	CLA	C10-C11-C12-C13
17	BA	826	CLA	C5-C6-C7-C8
17	BB	819	CLA	C11-C12-C13-C14
17	BB	833	CLA	C2A-CAA-CBA-CGA
17	BA	811	CLA	C16-C17-C18-C20
17	BB	824	CLA	C16-C17-C18-C20
17	BB	810	CLA	CBA-CGA-O2A-C1
19	B2	317	LHG	O8-C23-C24-C25
17	BB	801	CLA	O1A-CGA-O2A-C1
17	BA	825	CLA	C3A-C2A-CAA-CBA
17	BB	823	CLA	C3A-C2A-CAA-CBA
17	BB	829	CLA	C3A-C2A-CAA-CBA
17	BB	830	CLA	C3A-C2A-CAA-CBA
17	BH	201	CLA	C3A-C2A-CAA-CBA
17	BA	811	CLA	C5-C6-C7-C8
22	BA	854	LMU	C2-C1-O1'-C1'
17	BB	820	CLA	O1D-CGD-O2D-CED
17	BB	835	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	B5	602	CLA	CBA-CGA-O2A-C1
24	BJ	104	SQD	O6-C44-C45-C46
19	B5	618	LHG	O10-C23-O8-C6
19	B1	302	LHG	C10-C11-C12-C13
17	BA	830	CLA	O2A-C1-C2-C3
23	BB	850	DGD	O6E-C5E-C6E-O5E
17	BB	829	CLA	CAA-CBA-CGA-O2A
17	BA	801	CLA	C16-C17-C18-C20
17	BB	819	CLA	C2-C3-C5-C6
17	BA	805	CLA	C15-C16-C17-C18
19	B1	302	LHG	C4-O6-P-O3
17	BJ	102	CLA	O1D-CGD-O2D-CED
17	BB	818	CLA	C3-C5-C6-C7
23	BB	850	DGD	CAB-CBB-CCB-CDB
17	BB	802	CLA	O1D-CGD-O2D-CED
19	B1	318	LHG	O2-C2-C3-O3
22	BA	854	LMU	C1-C2-C3-C4
19	BA	845	LHG	O7-C5-C6-O8
28	B5	617	LMG	O7-C8-C9-O8
17	BB	834	CLA	CBA-CGA-O2A-C1
17	BA	801	CLA	CAA-CBA-CGA-O2A
17	BB	824	CLA	C16-C17-C18-C19
17	BA	819	CLA	C5-C6-C7-C8
19	BF	305	LHG	C1-C2-C3-O3
17	BB	816	CLA	C2-C1-O2A-CGA
17	BB	810	CLA	C11-C10-C8-C9
17	BB	820	CLA	C11-C10-C8-C9
17	BA	805	CLA	C10-C11-C12-C13
17	BB	812	CLA	C15-C16-C17-C18
19	B3	619	LHG	C5-C4-O6-P
17	BB	829	CLA	C2C-C3C-CAC-CBC
17	BB	819	CLA	C2A-CAA-CBA-CGA
25	B1	303	CHL	C2A-CAA-CBA-CGA
17	BB	834	CLA	C3-C5-C6-C7
20	BF	304	BCR	C23-C24-C25-C30
17	B1	314	CLA	C2C-C3C-CAC-CBC
20	BG	203	BCR	C11-C12-C13-C35
20	BH	202	BCR	C7-C8-C9-C10
17	BA	818	CLA	O1A-CGA-O2A-C1
17	BA	839	CLA	O1A-CGA-O2A-C1
19	B3	619	LHG	O6-C4-C5-C6
17	BA	803	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	BA	819	CLA	C6-C7-C8-C10
17	BA	827	CLA	C6-C7-C8-C10
17	BA	830	CLA	C12-C13-C15-C16
17	BA	840	CLA	C11-C10-C8-C7
17	BA	841	CLA	C11-C10-C8-C7
17	BA	842	CLA	C11-C10-C8-C7
17	BB	804	CLA	C6-C7-C8-C10
17	BB	807	CLA	C11-C12-C13-C15
17	BB	815	CLA	C11-C12-C13-C15
17	BB	816	CLA	C11-C10-C8-C7
17	BB	819	CLA	C6-C7-C8-C10
17	BB	820	CLA	C11-C10-C8-C7
17	BB	826	CLA	C6-C7-C8-C10
17	BB	829	CLA	C11-C10-C8-C7
17	B1	304	CLA	C11-C12-C13-C15
17	B1	314	CLA	C6-C7-C8-C10
18	BB	844	PQN	C17-C18-C20-C21
17	BA	817	CLA	CAD-CBD-CGD-O2D
17	BA	818	CLA	CAD-CBD-CGD-O2D
17	BA	833	CLA	CAD-CBD-CGD-O2D
17	BA	836	CLA	CAD-CBD-CGD-O2D
17	BB	821	CLA	CAD-CBD-CGD-O2D
17	BB	824	CLA	CAD-CBD-CGD-O2D
17	BB	832	CLA	CAD-CBD-CGD-O2D
17	BB	833	CLA	CAD-CBD-CGD-O2D
17	BB	835	CLA	CAD-CBD-CGD-O2D
17	BF	302	CLA	CAD-CBD-CGD-O2D
17	B1	306	CLA	CAD-CBD-CGD-O2D
17	B1	313	CLA	CAD-CBD-CGD-O2D
17	B2	309	CLA	CAD-CBD-CGD-O2D
17	B3	602	CLA	CAD-CBD-CGD-O2D
17	B3	608	CLA	CAD-CBD-CGD-O2D
17	B5	601	CLA	CAD-CBD-CGD-O2D
17	B5	609	CLA	CAD-CBD-CGD-O2D
17	BB	801	CLA	C13-C15-C16-C17
17	BB	801	CLA	CBD-CGD-O2D-CED
17	BB	810	CLA	O1A-CGA-O2A-C1
19	B3	619	LHG	O6-C4-C5-O7
19	BA	845	LHG	C12-C13-C14-C15
17	BB	821	CLA	C5-C6-C7-C8
17	BA	803	CLA	CHA-CBD-CGD-O1D
17	BA	803	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	BA	805	CLA	CHA-CBD-CGD-O1D
17	BA	805	CLA	CHA-CBD-CGD-O2D
17	BA	814	CLA	CHA-CBD-CGD-O2D
17	BA	815	CLA	CHA-CBD-CGD-O1D
17	BA	815	CLA	CHA-CBD-CGD-O2D
17	BA	820	CLA	CHA-CBD-CGD-O1D
17	BA	824	CLA	CHA-CBD-CGD-O1D
17	BA	824	CLA	CHA-CBD-CGD-O2D
17	BA	831	CLA	CHA-CBD-CGD-O1D
17	BA	831	CLA	CHA-CBD-CGD-O2D
17	BA	834	CLA	CHA-CBD-CGD-O1D
17	BA	834	CLA	CHA-CBD-CGD-O2D
17	BA	844	CLA	CHA-CBD-CGD-O1D
17	BA	844	CLA	CHA-CBD-CGD-O2D
17	BB	810	CLA	CHA-CBD-CGD-O1D
17	BB	810	CLA	CHA-CBD-CGD-O2D
17	BB	815	CLA	CHA-CBD-CGD-O1D
17	BB	815	CLA	CHA-CBD-CGD-O2D
17	BB	840	CLA	CHA-CBD-CGD-O1D
17	BB	840	CLA	CHA-CBD-CGD-O2D
17	BG	201	CLA	CHA-CBD-CGD-O1D
17	BG	201	CLA	CHA-CBD-CGD-O2D
17	BK	202	CLA	CHA-CBD-CGD-O1D
17	BK	202	CLA	CHA-CBD-CGD-O2D
17	BL	304	CLA	CHA-CBD-CGD-O1D
17	BL	304	CLA	CHA-CBD-CGD-O2D
17	B1	305	CLA	CHA-CBD-CGD-O1D
17	B3	602	CLA	CHA-CBD-CGD-O1D
17	BA	841	CLA	O1A-CGA-O2A-C1
17	BB	834	CLA	O1A-CGA-O2A-C1
17	B5	602	CLA	O1A-CGA-O2A-C1
23	BB	850	DGD	C9B-CAB-CBB-CCB
28	B5	617	LMG	O1-C7-C8-O7
19	B2	317	LHG	C29-C30-C31-C32
17	B3	612	CLA	C4-C3-C5-C6
17	B3	612	CLA	C2-C3-C5-C6
17	BB	841	CLA	O1D-CGD-O2D-CED
17	BB	838	CLA	CBA-CGA-O2A-C1
17	BB	801	CLA	C2A-CAA-CBA-CGA
17	BB	810	CLA	C2A-CAA-CBA-CGA
20	BI	101	BCR	C37-C22-C23-C24
26	B1	316	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
22	BA	853	LMU	C3'-C4'-O1B-C1B
17	BB	802	CLA	C3-C5-C6-C7
17	BA	811	CLA	C1A-C2A-CAA-CBA
17	BB	815	CLA	C1A-C2A-CAA-CBA
17	BB	829	CLA	C1A-C2A-CAA-CBA
17	B1	310	CLA	CHA-CBD-CGD-O2D
17	B3	604	CLA	CHA-CBD-CGD-O2D
25	B3	601	CHL	C1A-C2A-CAA-CBA
25	B5	605	CHL	CHA-CBD-CGD-O2D
17	BB	820	CLA	C5-C6-C7-C8
17	BA	825	CLA	C2-C1-O2A-CGA
17	BA	838	CLA	C2-C1-O2A-CGA
17	BA	803	CLA	CBA-CGA-O2A-C1
17	B3	612	CLA	CBA-CGA-O2A-C1
19	BA	845	LHG	C35-C36-C37-C38
17	BB	824	CLA	C5-C6-C7-C8
19	BF	305	LHG	C3-O3-P-O4
19	B1	318	LHG	C3-O3-P-O4
19	B2	317	LHG	C4-O6-P-O4
19	B5	618	LHG	C4-O6-P-O5
17	BA	803	CLA	C8-C10-C11-C12
17	BB	835	CLA	C10-C11-C12-C13
19	BF	305	LHG	C13-C14-C15-C16
17	BA	803	CLA	O1A-CGA-O2A-C1
17	BB	801	CLA	C3-C5-C6-C7
17	BB	825	CLA	O1D-CGD-O2D-CED
17	BA	805	CLA	CAD-CBD-CGD-O1D
17	BA	812	CLA	CAD-CBD-CGD-O1D
17	BA	813	CLA	CAD-CBD-CGD-O1D
17	BA	814	CLA	CAD-CBD-CGD-O1D
17	BA	824	CLA	CAD-CBD-CGD-O1D
17	BA	831	CLA	CAD-CBD-CGD-O1D
17	BA	841	CLA	CAD-CBD-CGD-O1D
17	BB	815	CLA	CAD-CBD-CGD-O1D
17	BB	827	CLA	CAD-CBD-CGD-O1D
17	BG	201	CLA	CAD-CBD-CGD-O1D
17	BK	202	CLA	CAD-CBD-CGD-O1D
17	BL	302	CLA	CAD-CBD-CGD-O1D
24	BJ	104	SQD	C5-C6-S-O9
17	B3	612	CLA	O1A-CGA-O2A-C1
17	BB	819	CLA	C3-C5-C6-C7
19	BA	845	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	BF	305	LHG	C14-C15-C16-C17
17	BA	805	CLA	C11-C12-C13-C15
17	BA	827	CLA	C11-C10-C8-C7
17	BB	801	CLA	C6-C7-C8-C10
17	BB	804	CLA	C12-C13-C15-C16
17	BB	808	CLA	C12-C13-C15-C16
17	BB	810	CLA	C6-C7-C8-C10
17	BB	830	CLA	C12-C13-C15-C16
17	B3	605	CLA	CAD-CBD-CGD-O2D
17	B3	612	CLA	C2A-CAA-CBA-CGA
22	BA	853	LMU	C5'-C4'-O1B-C1B
17	BA	818	CLA	CAA-CBA-CGA-O2A
17	B3	605	CLA	CAD-CBD-CGD-O1D
17	B5	611	CLA	CAD-CBD-CGD-O1D
17	BB	838	CLA	O1A-CGA-O2A-C1
24	BJ	104	SQD	O6-C44-C45-O47
17	BB	819	CLA	O2A-C1-C2-C3
17	BA	817	CLA	C5-C6-C7-C8
17	BB	812	CLA	C3-C5-C6-C7
19	BA	845	LHG	C31-C32-C33-C34
17	BB	841	CLA	O1A-CGA-O2A-C1
17	BB	808	CLA	C5-C6-C7-C8
17	BB	829	CLA	C4-C3-C5-C6
17	BB	841	CLA	CBA-CGA-O2A-C1
17	BA	830	CLA	C14-C13-C15-C16
17	BA	840	CLA	C11-C10-C8-C9
17	BA	841	CLA	C11-C10-C8-C9
17	BB	804	CLA	C6-C7-C8-C9
17	BB	805	CLA	C11-C12-C13-C14
17	BB	810	CLA	C6-C7-C8-C9
17	BB	815	CLA	C11-C12-C13-C14
17	BB	816	CLA	C11-C10-C8-C9
17	B1	304	CLA	C11-C12-C13-C14
17	BA	841	CLA	C16-C17-C18-C19
20	BA	855	BCR	C37-C22-C23-C24
19	BF	305	LHG	C24-C25-C26-C27
19	B1	301	LHG	C28-C29-C30-C31
20	BA	856	BCR	C21-C22-C23-C24
17	BA	829	CLA	CAA-CBA-CGA-O2A
17	BA	805	CLA	C2C-C3C-CAC-CBC
17	BB	806	CLA	C4C-C3C-CAC-CBC
17	BK	202	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	BB	805	CLA	C5-C6-C7-C8
17	BA	806	CLA	C2-C1-O2A-CGA
17	BA	829	CLA	C2-C1-O2A-CGA
17	BA	840	CLA	C3-C5-C6-C7
19	BA	845	LHG	C11-C10-C9-C8
22	BA	854	LMU	C6-C7-C8-C9
22	BA	853	LMU	C3-C4-C5-C6
19	BA	845	LHG	C3-O3-P-O6
19	BF	305	LHG	C4-O6-P-O3
19	B5	618	LHG	C3-O3-P-O6
23	BB	850	DGD	O1G-C1G-C2G-C3G
22	BA	853	LMU	C11-C10-C9-C8
17	BA	825	CLA	C11-C10-C8-C7
17	BB	810	CLA	C11-C10-C8-C7
19	BA	845	LHG	C9-C10-C11-C12
17	BB	802	CLA	C6-C7-C8-C9
17	BB	808	CLA	C14-C13-C15-C16
18	BB	844	PQN	C21-C22-C23-C24
26	B1	316	LUT	C9-C10-C11-C12
22	BB	851	LMU	C3-C4-C5-C6
17	BA	830	CLA	C16-C17-C18-C20
17	BA	840	CLA	C13-C15-C16-C17
26	B3	616	LUT	C7-C8-C9-C10
17	BA	826	CLA	CBD-CGD-O2D-CED
17	BA	821	CLA	C4-C3-C5-C6
28	B5	617	LMG	C29-C28-O8-C9
17	BA	806	CLA	CBD-CGD-O2D-CED
17	BB	811	CLA	CBA-CGA-O2A-C1
17	BB	805	CLA	C10-C11-C12-C13
17	BB	843	CLA	C10-C11-C12-C13
22	BB	851	LMU	C4B-C5B-C6B-O6B
17	BA	828	CLA	C2-C1-O2A-CGA
17	BB	818	CLA	C2-C1-O2A-CGA
17	BA	838	CLA	C2A-CAA-CBA-CGA
17	BB	834	CLA	CAA-CBA-CGA-O2A
17	BK	202	CLA	CAA-CBA-CGA-O2A
17	BB	830	CLA	C4-C3-C5-C6
19	B1	301	LHG	C11-C10-C9-C8
17	BB	832	CLA	CBD-CGD-O2D-CED
17	BA	805	CLA	C11-C12-C13-C14
17	BA	830	CLA	C11-C10-C8-C9
17	BB	802	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B2	301	CLA	C11-C10-C8-C9
17	BA	830	CLA	C16-C17-C18-C19
17	B2	301	CLA	C8-C10-C11-C12
17	BB	829	CLA	CBA-CGA-O2A-C1
19	B3	619	LHG	C1-C2-C3-O3
20	BA	851	BCR	C11-C10-C9-C34
20	BA	851	BCR	C16-C17-C18-C36
20	BB	846	BCR	C11-C10-C9-C34
20	BB	847	BCR	C11-C10-C9-C34
20	BB	847	BCR	C20-C21-C22-C37
20	BF	304	BCR	C35-C13-C14-C15
20	BG	203	BCR	C11-C10-C9-C34
20	BG	203	BCR	C35-C13-C14-C15
20	BG	203	BCR	C16-C17-C18-C36
20	BH	202	BCR	C11-C10-C9-C34
20	BH	202	BCR	C35-C13-C14-C15
20	BH	202	BCR	C16-C17-C18-C36
20	BH	202	BCR	C20-C21-C22-C37
20	BL	301	BCR	C11-C10-C9-C34
17	BB	843	CLA	C2A-CAA-CBA-CGA
22	BA	854	LMU	C3'-C4'-O1B-C1B
17	B2	311	CLA	C16-C17-C18-C20
17	BK	202	CLA	CAA-CBA-CGA-O1A
18	BA	843	PQN	C20-C21-C22-C23
23	BB	850	DGD	C9A-CAA-CBA-CCA
20	BJ	103	BCR	C7-C8-C9-C10
17	BA	806	CLA	C15-C16-C17-C18
17	BA	805	CLA	C1A-C2A-CAA-CBA
17	BA	825	CLA	C1A-C2A-CAA-CBA
17	BA	827	CLA	C1A-C2A-CAA-CBA
17	BB	832	CLA	C1A-C2A-CAA-CBA
24	BJ	104	SQD	C27-C28-C29-C30
17	BA	803	CLA	C11-C12-C13-C15
17	BA	805	CLA	C12-C13-C15-C16
17	BA	811	CLA	C12-C13-C15-C16
17	BA	840	CLA	C12-C13-C15-C16
17	BB	816	CLA	C11-C12-C13-C15
17	BB	824	CLA	C11-C10-C8-C7
17	BB	824	CLA	C12-C13-C15-C16
17	BB	842	CLA	C6-C7-C8-C10
17	BA	813	CLA	C8-C10-C11-C12
17	B5	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	B1	318	LHG	C4-O6-P-O3
17	BH	201	CLA	CBA-CGA-O2A-C1
17	BG	202	CLA	CAA-CBA-CGA-O1A
25	B5	607	CHL	CAA-CBA-CGA-O1A
17	BH	201	CLA	C11-C12-C13-C14
17	BB	827	CLA	C3-C5-C6-C7
17	BA	831	CLA	C2A-CAA-CBA-CGA
17	BB	839	CLA	C2A-CAA-CBA-CGA
17	B5	612	CLA	C2A-CAA-CBA-CGA
17	BA	813	CLA	C10-C11-C12-C13
17	BB	818	CLA	C5-C6-C7-C8
17	BF	301	CLA	C5-C6-C7-C8
17	B1	311	CLA	C5-C6-C7-C8
17	BA	824	CLA	C5-C6-C7-C8
17	BG	202	CLA	CAA-CBA-CGA-O2A
25	B5	607	CHL	CAA-CBA-CGA-O2A
28	B5	617	LMG	O10-C28-O8-C9
17	BB	831	CLA	C2-C3-C5-C6
17	B2	307	CLA	CAA-CBA-CGA-O2A
17	BB	827	CLA	C5-C6-C7-C8
17	BB	829	CLA	O1A-CGA-O2A-C1
22	BB	851	LMU	C3'-C4'-O1B-C1B
20	BA	851	BCR	C11-C10-C9-C8
20	BA	851	BCR	C16-C17-C18-C19
20	BB	846	BCR	C11-C10-C9-C8
20	BB	847	BCR	C11-C10-C9-C8
20	BB	847	BCR	C20-C21-C22-C23
20	BF	304	BCR	C12-C13-C14-C15
20	BG	203	BCR	C11-C10-C9-C8
20	BG	203	BCR	C16-C17-C18-C19
20	BH	202	BCR	C16-C17-C18-C19
20	BL	301	BCR	C11-C10-C9-C8
17	BB	812	CLA	C10-C11-C12-C13
17	BA	836	CLA	CAA-CBA-CGA-O1A
19	B2	317	LHG	O10-C23-C24-C25
17	BB	827	CLA	C13-C15-C16-C17
17	BB	811	CLA	O1A-CGA-O2A-C1
17	BH	201	CLA	O1A-CGA-O2A-C1
17	B5	613	CLA	CAA-CBA-CGA-O2A
17	BA	826	CLA	O1D-CGD-O2D-CED
17	BA	806	CLA	O1D-CGD-O2D-CED
17	BA	841	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B2	317	LHG	C26-C27-C28-C29
24	BJ	104	SQD	C17-C18-C19-C20
20	BA	847	BCR	C1-C6-C7-C8
20	BB	803	BCR	C1-C6-C7-C8
20	BB	848	BCR	C1-C6-C7-C8
20	BI	101	BCR	C23-C24-C25-C30
20	BL	301	BCR	C23-C24-C25-C30
26	B3	616	LUT	C5-C6-C7-C8
17	BB	832	CLA	O1D-CGD-O2D-CED
17	B2	307	CLA	CAA-CBA-CGA-O1A
17	BA	808	CLA	C5-C6-C7-C8
17	BA	805	CLA	C4-C3-C5-C6
17	BA	840	CLA	C4-C3-C5-C6
26	B5	614	LUT	C7-C8-C9-C10
17	BB	829	CLA	C2-C3-C5-C6
17	BA	836	CLA	CAA-CBA-CGA-O2A
17	BA	825	CLA	C8-C10-C11-C12
19	BA	845	LHG	O6-C4-C5-O7
19	B1	301	LHG	O6-C4-C5-O7
25	B2	306	CHL	CAA-CBA-CGA-O2A
17	BB	829	CLA	C2A-CAA-CBA-CGA
17	BB	810	CLA	C3-C5-C6-C7
17	B2	310	CLA	CAA-CBA-CGA-O2A
19	B1	301	LHG	O6-C4-C5-C6
19	B1	302	LHG	O6-C4-C5-C6
17	BB	816	CLA	C4-C3-C5-C6
17	BB	827	CLA	C4-C3-C5-C6
17	BB	819	CLA	CAA-CBA-CGA-O1A
17	BA	806	CLA	C11-C12-C13-C15
17	BA	813	CLA	C11-C12-C13-C15
17	BA	821	CLA	C2-C3-C5-C6
17	BB	801	CLA	C12-C13-C15-C16
17	BB	811	CLA	C12-C13-C15-C16
17	BB	830	CLA	C2-C3-C5-C6
17	BB	834	CLA	C11-C12-C13-C15
17	BB	801	CLA	C8-C10-C11-C12
17	BB	830	CLA	C13-C15-C16-C17
19	B2	317	LHG	O1-C1-C2-O2
22	BB	851	LMU	C2B-C1B-O1B-C4'
28	B5	617	LMG	C4-C5-C6-O5
17	B1	304	CLA	CBA-CGA-O2A-C1
17	BB	802	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	BA	835	CLA	CAA-CBA-CGA-O2A
17	B1	309	CLA	CAA-CBA-CGA-O2A
17	BA	832	CLA	O1D-CGD-O2D-CED
17	BA	813	CLA	C4-C3-C5-C6
17	BB	804	CLA	C4-C3-C5-C6
19	BA	845	LHG	C19-C20-C21-C22
28	B5	617	LMG	O7-C10-C11-C12
17	BA	811	CLA	C14-C13-C15-C16
17	BA	827	CLA	C11-C10-C8-C9
17	BA	828	CLA	C6-C7-C8-C9
17	BB	808	CLA	C11-C10-C8-C9
17	BB	828	CLA	C11-C10-C8-C9
17	B2	302	CLA	CAA-CBA-CGA-O1A
22	BA	853	LMU	C2B-C1B-O1B-C4'
17	BA	827	CLA	C3A-C2A-CAA-CBA
17	B5	608	CLA	C3A-C2A-CAA-CBA
17	BA	832	CLA	CBD-CGD-O2D-CED
17	BA	804	CLA	CAD-CBD-CGD-O2D
17	BA	807	CLA	CAD-CBD-CGD-O2D
17	BA	809	CLA	CAD-CBD-CGD-O2D
17	BA	826	CLA	CAD-CBD-CGD-O2D
17	BA	830	CLA	CAD-CBD-CGD-O2D
17	BA	832	CLA	CAD-CBD-CGD-O2D
17	BA	837	CLA	CAD-CBD-CGD-O2D
17	BB	814	CLA	CAD-CBD-CGD-O2D
17	BB	831	CLA	CAD-CBD-CGD-O2D
17	BB	837	CLA	CAD-CBD-CGD-O2D
17	BB	838	CLA	CAD-CBD-CGD-O2D
17	BB	841	CLA	CAD-CBD-CGD-O2D
17	BK	203	CLA	CAD-CBD-CGD-O2D
17	B1	314	CLA	CAD-CBD-CGD-O2D
17	B2	303	CLA	CAD-CBD-CGD-O2D
17	B2	307	CLA	CAD-CBD-CGD-O2D
17	B2	308	CLA	CAD-CBD-CGD-O2D
17	B3	609	CLA	CAD-CBD-CGD-O2D
25	B3	601	CHL	CAD-CBD-CGD-O2D
17	B1	313	CLA	CAA-CBA-CGA-O2A
22	BB	851	LMU	C5'-C4'-O1B-C1B
19	B2	317	LHG	C30-C31-C32-C33
17	B2	308	CLA	C4-C3-C5-C6
25	B2	306	CHL	CAA-CBA-CGA-O1A
17	BB	829	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	BA	805	CLA	C2-C3-C5-C6
17	BB	810	CLA	C2-C3-C5-C6
17	BB	815	CLA	CAA-CBA-CGA-O2A
19	B1	301	LHG	C27-C28-C29-C30
20	BA	847	BCR	C21-C22-C23-C24
20	BA	848	BCR	C11-C12-C13-C14
26	B1	316	LUT	C31-C32-C33-C34
28	B5	617	LMG	C7-C8-C9-O8
17	B2	310	CLA	CAA-CBA-CGA-O1A
17	B5	603	CLA	CAA-CBA-CGA-O2A
17	B1	304	CLA	O1A-CGA-O2A-C1
19	BA	846	LHG	O6-C4-C5-O7
19	B1	302	LHG	O6-C4-C5-O7
17	BA	833	CLA	CAA-CBA-CGA-O2A
17	BA	835	CLA	CAA-CBA-CGA-O1A
25	B3	607	CHL	CAA-CBA-CGA-O1A
25	B3	607	CHL	CAA-CBA-CGA-O2A
17	BA	803	CLA	O2A-C1-C2-C3
17	BA	839	CLA	O2A-C1-C2-C3
17	BB	801	CLA	O2A-C1-C2-C3
17	BB	802	CLA	O2A-C1-C2-C3
17	BB	805	CLA	O2A-C1-C2-C3
17	BB	835	CLA	O2A-C1-C2-C3
23	BB	850	DGD	CEA-CFA-CGA-CHA
17	BA	806	CLA	CAA-CBA-CGA-O2A
19	B5	618	LHG	O7-C7-C8-C9
17	B3	608	CLA	CAA-CBA-CGA-O2A
17	BH	201	CLA	C11-C12-C13-C15
18	BA	843	PQN	C26-C27-C28-C29
17	BA	808	CLA	CHA-CBD-CGD-O1D
17	BA	808	CLA	CHA-CBD-CGD-O2D
17	BA	810	CLA	CHA-CBD-CGD-O1D
17	BA	816	CLA	CHA-CBD-CGD-O1D
17	BA	816	CLA	CHA-CBD-CGD-O2D
17	BA	820	CLA	CHA-CBD-CGD-O2D
17	BA	822	CLA	CHA-CBD-CGD-O1D
17	BA	822	CLA	CHA-CBD-CGD-O2D
17	BA	825	CLA	CHA-CBD-CGD-O1D
17	BA	827	CLA	CHA-CBD-CGD-O1D
17	BA	835	CLA	CHA-CBD-CGD-O1D
17	BA	835	CLA	CHA-CBD-CGD-O2D
17	BA	839	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	BA	842	CLA	CHA-CBD-CGD-O1D
17	BA	842	CLA	CHA-CBD-CGD-O2D
17	BB	807	CLA	CHA-CBD-CGD-O1D
17	BB	812	CLA	CHA-CBD-CGD-O1D
17	BB	826	CLA	CHA-CBD-CGD-O1D
17	BG	202	CLA	CHA-CBD-CGD-O2D
17	B1	304	CLA	CHA-CBD-CGD-O2D
17	B1	305	CLA	CHA-CBD-CGD-O2D
17	B5	603	CLA	CHA-CBD-CGD-O1D
17	B5	603	CLA	CHA-CBD-CGD-O2D
17	B1	313	CLA	CAA-CBA-CGA-O1A
17	B3	608	CLA	CAA-CBA-CGA-O1A
17	B5	603	CLA	CAA-CBA-CGA-O1A
17	BB	831	CLA	C4-C3-C5-C6
19	BA	845	LHG	C30-C31-C32-C33
17	BA	825	CLA	CAA-CBA-CGA-O2A
17	BA	834	CLA	CAA-CBA-CGA-O2A
19	B1	302	LHG	O7-C7-C8-C9
25	B3	601	CHL	CAA-CBA-CGA-O2A
17	BB	804	CLA	C5-C6-C7-C8
17	BB	828	CLA	C5-C6-C7-C8
17	BA	812	CLA	CAA-CBA-CGA-O2A
17	BA	828	CLA	CAA-CBA-CGA-O2A
19	BA	845	LHG	O8-C23-C24-C25
19	BA	845	LHG	C17-C18-C19-C20
17	BA	817	CLA	CAA-CBA-CGA-O2A
17	BB	801	CLA	CAA-CBA-CGA-O2A
17	BA	805	CLA	C6-C7-C8-C10
17	BB	842	CLA	C11-C10-C8-C7
17	B2	311	CLA	C16-C17-C18-C19
17	B1	309	CLA	CAA-CBA-CGA-O1A
17	BA	801	CLA	C14-C13-C15-C16
17	BA	803	CLA	C11-C12-C13-C14
17	BA	805	CLA	C6-C7-C8-C9
17	BB	816	CLA	C11-C12-C13-C14
17	B2	302	CLA	CAA-CBA-CGA-O2A
17	B5	608	CLA	CAA-CBA-CGA-O2A
17	BB	811	CLA	C5-C6-C7-C8
17	BA	801	CLA	CAA-CBA-CGA-O1A
24	BJ	104	SQD	C4-C5-C6-S
22	BA	854	LMU	C5'-C4'-O1B-C1B
17	BB	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	BB	824	CLA	C2A-CAA-CBA-CGA
17	B5	602	CLA	C2A-CAA-CBA-CGA
17	BB	815	CLA	CAA-CBA-CGA-O1A
28	B5	617	LMG	O9-C10-C11-C12
19	BF	305	LHG	C32-C33-C34-C35
17	BB	815	CLA	C2-C3-C5-C6
22	BA	854	LMU	C4-C5-C6-C7
20	BF	304	BCR	C7-C8-C9-C10
17	BA	814	CLA	C1A-C2A-CAA-CBA
17	BB	817	CLA	C1A-C2A-CAA-CBA
17	BB	817	CLA	CHA-CBD-CGD-O2D
17	BL	302	CLA	C1A-C2A-CAA-CBA
17	B2	303	CLA	C1A-C2A-CAA-CBA
17	B5	608	CLA	C1A-C2A-CAA-CBA
25	B5	607	CHL	C1A-C2A-CAA-CBA
19	B1	318	LHG	C27-C28-C29-C30
17	BB	829	CLA	C13-C15-C16-C17
17	BA	833	CLA	CAA-CBA-CGA-O1A
19	B5	618	LHG	O9-C7-C8-C9
17	BA	838	CLA	CAD-CBD-CGD-O2D
17	BA	829	CLA	C5-C6-C7-C8
17	BB	835	CLA	C15-C16-C17-C18
17	BB	835	CLA	CAA-CBA-CGA-O2A
17	BA	812	CLA	CAA-CBA-CGA-O1A
25	B3	601	CHL	CAA-CBA-CGA-O1A
18	BB	844	PQN	C12-C13-C15-C16
19	B1	302	LHG	C4-O6-P-O5
17	BA	829	CLA	C16-C17-C18-C20
17	BA	806	CLA	CAA-CBA-CGA-O1A
19	BA	845	LHG	O10-C23-C24-C25
17	BB	804	CLA	CAA-CBA-CGA-O2A
20	BA	847	BCR	C23-C24-C25-C30
20	BK	204	BCR	C5-C6-C7-C8
17	BA	817	CLA	CAA-CBA-CGA-O1A
19	B1	302	LHG	O9-C7-C8-C9
19	B1	318	LHG	C23-C24-C25-C26
17	BB	815	CLA	C2A-CAA-CBA-CGA
17	BA	842	CLA	CAA-CBA-CGA-O2A
17	B2	301	CLA	CAA-CBA-CGA-O2A
17	BB	801	CLA	O1D-CGD-O2D-CED
23	BB	850	DGD	C1B-C2B-C3B-C4B
17	BA	834	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	B5	608	CLA	CAA-CBA-CGA-O1A
17	BA	803	CLA	CAD-CBD-CGD-O1D
17	BA	810	CLA	CAD-CBD-CGD-O1D
17	BA	827	CLA	CAD-CBD-CGD-O1D
17	BA	836	CLA	CAD-CBD-CGD-O1D
17	BB	807	CLA	CAD-CBD-CGD-O1D
17	BB	812	CLA	CAD-CBD-CGD-O1D
17	BG	202	CLA	CAD-CBD-CGD-O1D
17	BH	201	CLA	CAD-CBD-CGD-O1D
17	B2	311	CLA	CAD-CBD-CGD-O1D
24	BJ	104	SQD	O5-C5-C6-S
25	B2	304	CHL	CAD-CBD-CGD-O1D
17	BA	809	CLA	CAA-CBA-CGA-O2A
17	B5	601	CLA	CAA-CBA-CGA-O2A
17	BA	813	CLA	C11-C12-C13-C14
17	BB	801	CLA	C14-C13-C15-C16
17	BB	824	CLA	C14-C13-C15-C16
17	BA	825	CLA	CAA-CBA-CGA-O1A
17	BA	828	CLA	CAA-CBA-CGA-O1A
17	BA	813	CLA	CAA-CBA-CGA-O2A
17	B5	602	CLA	C10-C11-C12-C13
17	B2	310	CLA	C2A-CAA-CBA-CGA
17	BB	842	CLA	C15-C16-C17-C18
17	BB	805	CLA	C11-C10-C8-C7
17	BB	810	CLA	C11-C12-C13-C15
17	BB	812	CLA	C3A-C2A-CAA-CBA
17	BB	817	CLA	CHA-CBD-CGD-O1D
17	BB	817	CLA	CAD-CBD-CGD-O2D
17	B1	310	CLA	CHA-CBD-CGD-O1D
17	B1	310	CLA	CAD-CBD-CGD-O2D
17	B2	302	CLA	CHA-CBD-CGD-O1D
17	B3	604	CLA	CAD-CBD-CGD-O2D
17	B5	611	CLA	CAD-CBD-CGD-O2D
25	B5	605	CHL	CHA-CBD-CGD-O1D
17	BL	302	CLA	CAA-CBA-CGA-O1A
17	BB	809	CLA	CAA-CBA-CGA-O2A
19	B5	618	LHG	O8-C23-C24-C25
17	BA	813	CLA	CAA-CBA-CGA-O1A
17	BB	809	CLA	CAA-CBA-CGA-O1A
19	B5	618	LHG	O10-C23-C24-C25
17	BL	302	CLA	CAA-CBA-CGA-O2A
17	BA	821	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	BA	846	LHG	O7-C7-C8-C9
17	B5	602	CLA	C8-C10-C11-C12
17	BA	809	CLA	CAA-CBA-CGA-O1A
17	BB	801	CLA	CAA-CBA-CGA-O1A
17	BB	835	CLA	CAA-CBA-CGA-O1A
17	BB	802	CLA	C13-C15-C16-C17
17	BB	811	CLA	C15-C16-C17-C18
19	BA	845	LHG	O7-C7-C8-C9
17	BB	810	CLA	C4-C3-C5-C6
17	B5	604	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

119 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	BA	832	CLA	3	0
19	B2	317	LHG	1	0
17	B5	610	CLA	1	0
25	B2	306	CHL	4	0
17	BB	820	CLA	1	0
17	BF	301	CLA	1	0
21	BA	852	SF4	1	0
17	BA	805	CLA	3	0
17	BB	823	CLA	2	0
17	BA	838	CLA	1	0
17	BB	815	CLA	8	0
17	BB	830	CLA	1	0
26	B5	614	LUT	1	0
20	BK	204	BCR	2	0
17	BB	826	CLA	1	0
17	BB	828	CLA	3	0
17	BB	838	CLA	1	0
26	B2	314	LUT	1	0
20	BL	305	BCR	2	0
18	BA	843	PQN	3	0
17	BB	843	CLA	1	0
24	BJ	104	SQD	3	0
17	BA	842	CLA	1	0
20	BA	855	BCR	3	0
17	BA	808	CLA	4	0
27	B1	317	XAT	7	0
20	BB	845	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	BA	828	CLA	1	0
17	BB	807	CLA	1	0
19	BF	305	LHG	1	0
20	BB	846	BCR	1	0
17	BB	808	CLA	1	0
26	B3	616	LUT	2	0
17	BA	827	CLA	1	0
17	BG	201	CLA	2	0
25	B1	303	CHL	1	0
17	B5	608	CLA	1	0
17	BB	829	CLA	1	0
17	BB	819	CLA	1	0
25	B3	607	CHL	2	0
27	B3	617	XAT	1	0
19	BA	845	LHG	1	0
17	BB	804	CLA	4	0
17	B5	612	CLA	2	0
20	BA	851	BCR	7	0
20	B2	316	BCR	2	0
20	BF	304	BCR	1	0
17	B5	611	CLA	1	0
19	B3	619	LHG	1	0
17	B2	301	CLA	2	0
17	BA	834	CLA	1	0
17	BA	829	CLA	2	0
20	BA	847	BCR	1	0
20	BI	101	BCR	1	0
27	B2	315	XAT	3	0
20	BH	202	BCR	1	0
17	BB	827	CLA	1	0
17	BB	811	CLA	3	0
17	B3	611	CLA	1	0
17	BB	818	CLA	1	0
17	BB	821	CLA	1	0
17	B1	305	CLA	1	0
25	B5	605	CHL	1	0
17	BA	819	CLA	1	0
17	B5	602	CLA	1	0
27	B5	615	XAT	1	0
17	BB	825	CLA	1	0
17	BA	802	CLA	3	0
17	BA	811	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	BB	834	CLA	3	0
20	BJ	103	BCR	2	0
17	BA	804	CLA	1	0
17	BA	801	CLA	16	0
20	BB	847	BCR	1	0
17	BA	840	CLA	2	0
17	BB	810	CLA	2	0
17	BF	302	CLA	2	0
17	B2	311	CLA	1	0
23	BB	850	DGD	1	0
17	BB	802	CLA	7	0
18	BB	844	PQN	3	0
20	BA	856	BCR	1	0
17	BB	801	CLA	4	0
17	BB	809	CLA	1	0
20	BA	848	BCR	1	0
20	BL	301	BCR	2	0
17	BB	816	CLA	1	0
17	BA	841	CLA	1	0
17	BA	810	CLA	1	0
17	BB	805	CLA	2	0
20	BA	849	BCR	2	0
17	BA	803	CLA	2	0
17	B1	314	CLA	1	0
26	B1	316	LUT	2	0
17	BB	824	CLA	1	0
17	BG	202	CLA	1	0
20	BG	203	BCR	3	0
20	BB	803	BCR	5	0
17	BB	841	CLA	1	0
17	BA	839	CLA	1	0
17	BL	303	CLA	1	0
20	BJ	101	BCR	2	0
17	BB	806	CLA	1	0
20	BB	849	BCR	3	0
19	BA	846	LHG	1	0
25	B3	601	CHL	3	0
17	BB	840	CLA	2	0
20	B3	618	BCR	5	0
17	BK	203	CLA	1	0
17	BA	806	CLA	1	0
17	BA	830	CLA	3	0

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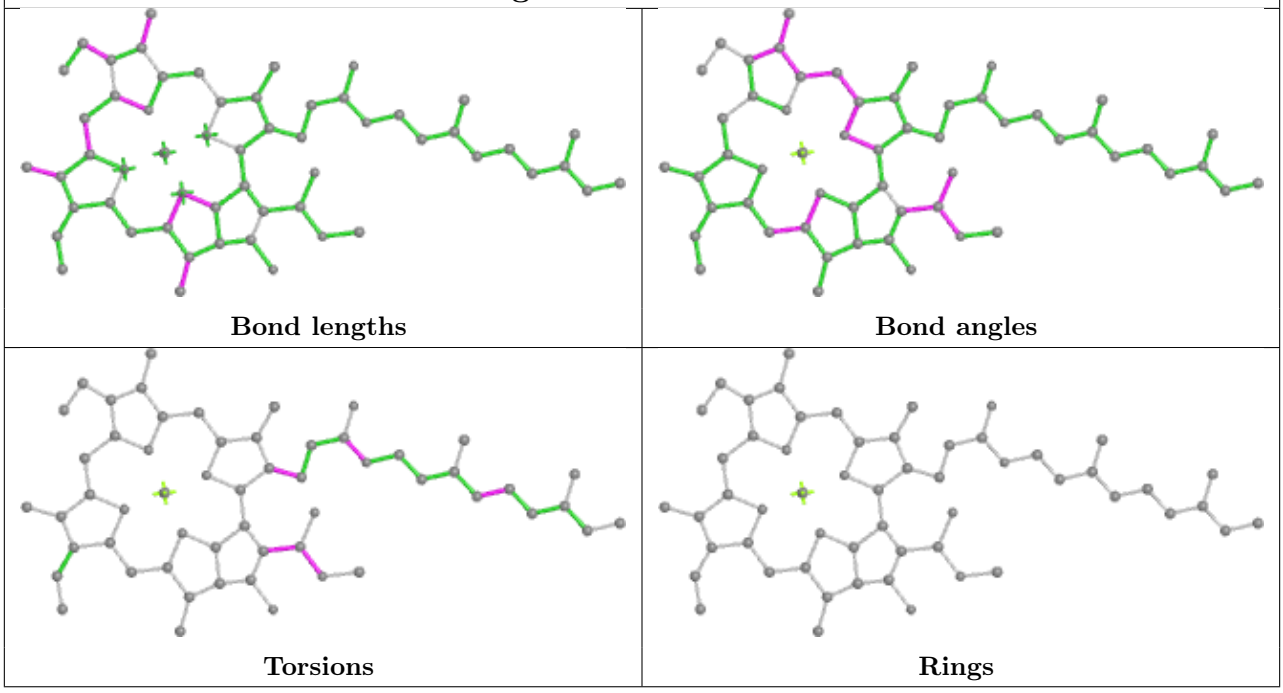
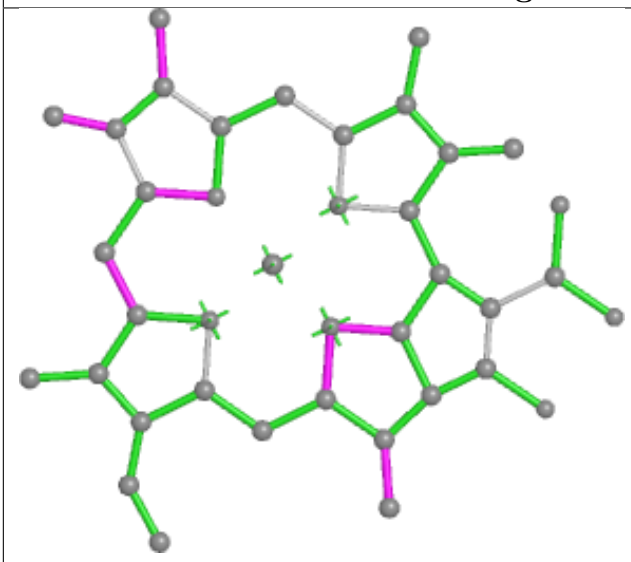
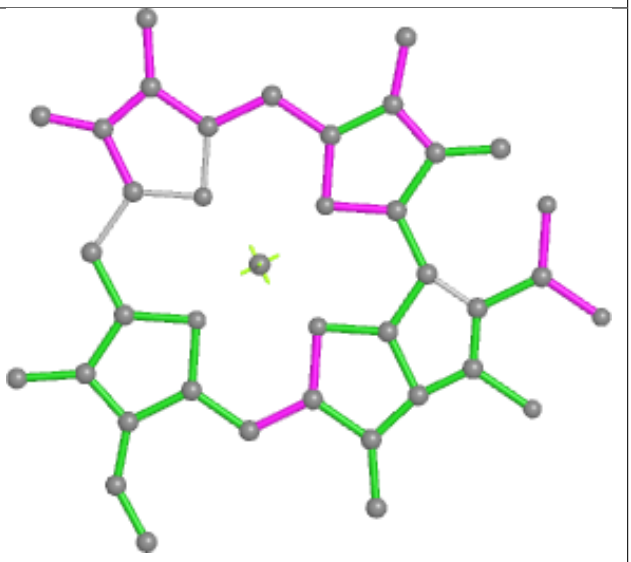
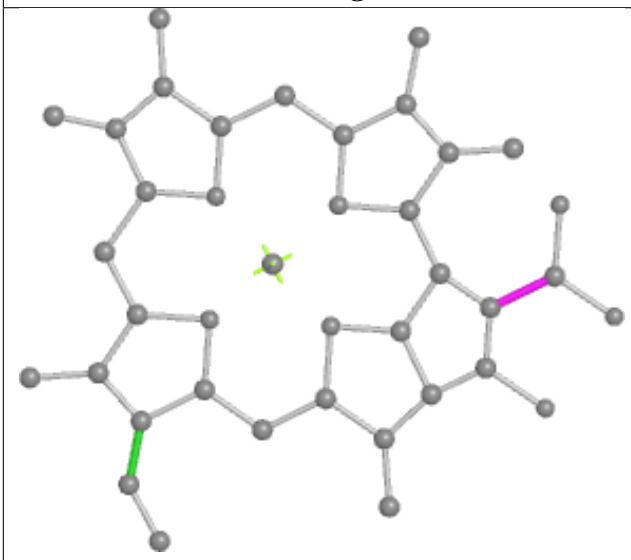
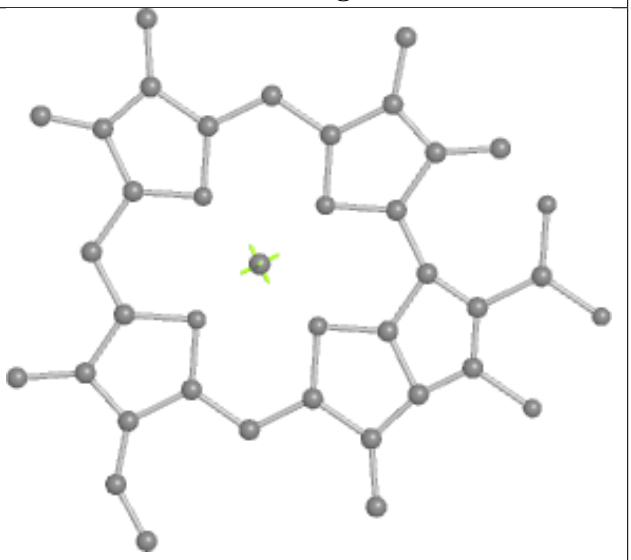
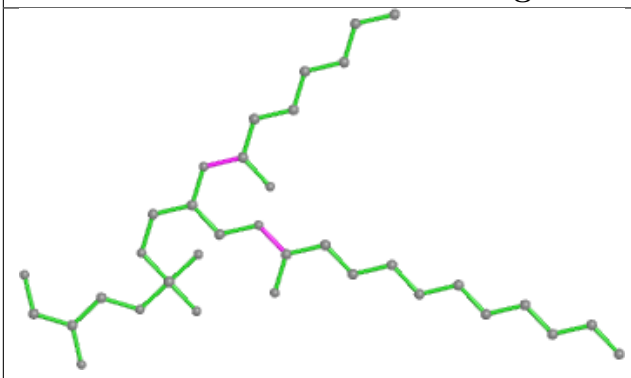
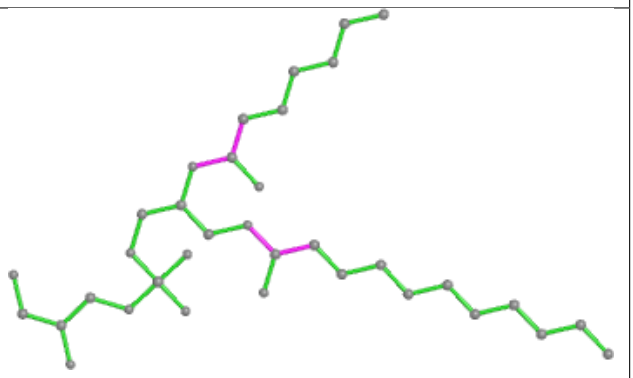
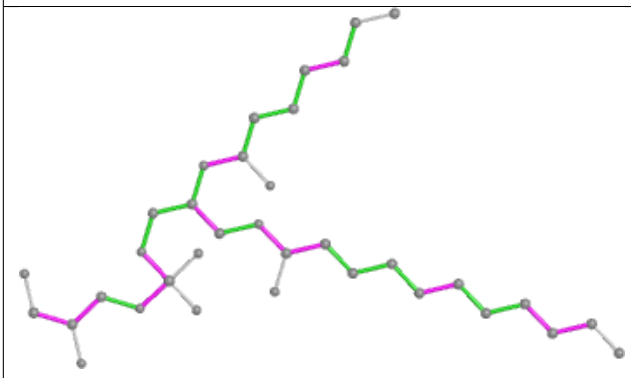
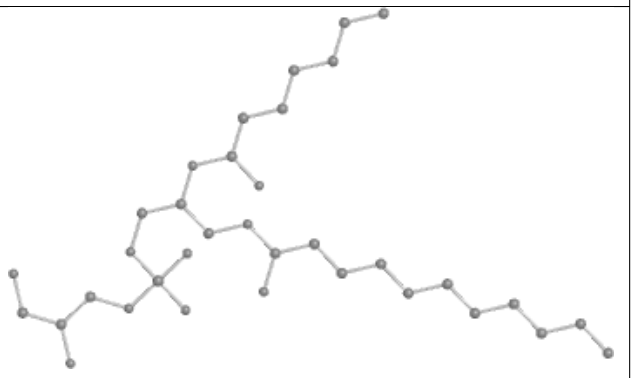
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B1	304	CLA	1	0
17	BB	835	CLA	1	0
20	BB	848	BCR	2	0
17	BA	812	CLA	1	0
17	B2	309	CLA	1	0
17	B2	302	CLA	1	0
17	B2	312	CLA	1	0
17	BB	812	CLA	3	0

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

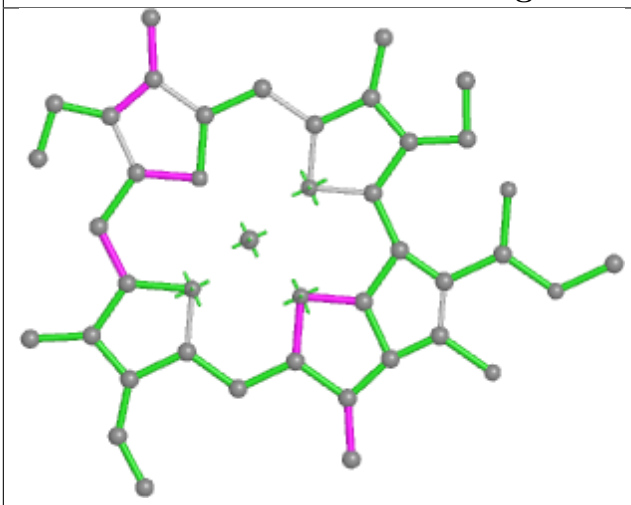
Ligand CLA BA 832



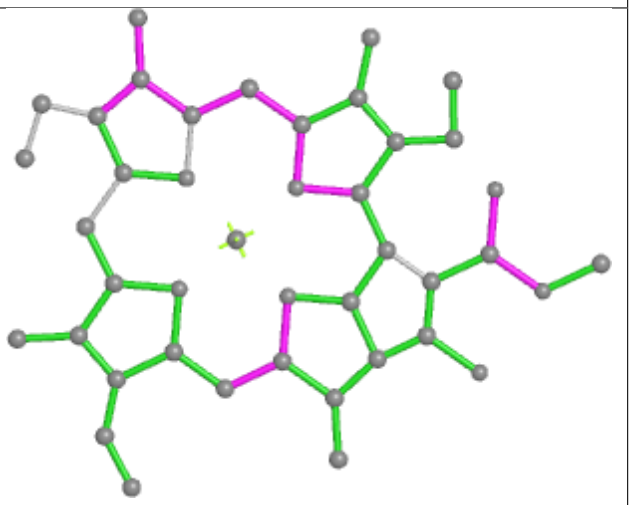
Ligand CLA B1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B2 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

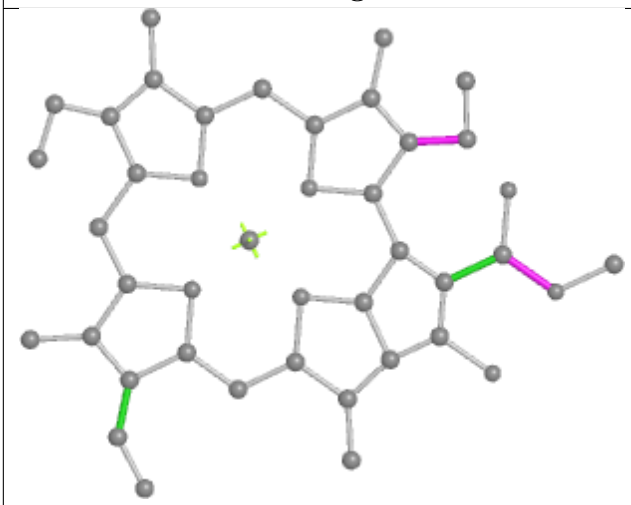
Ligand CLA B5 610



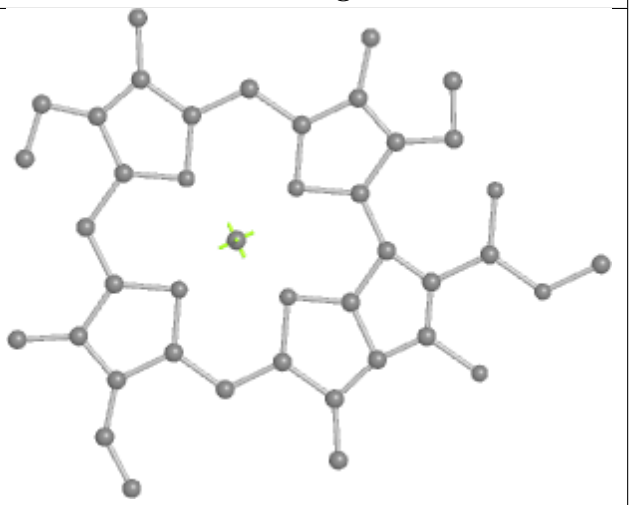
Bond lengths



Bond angles

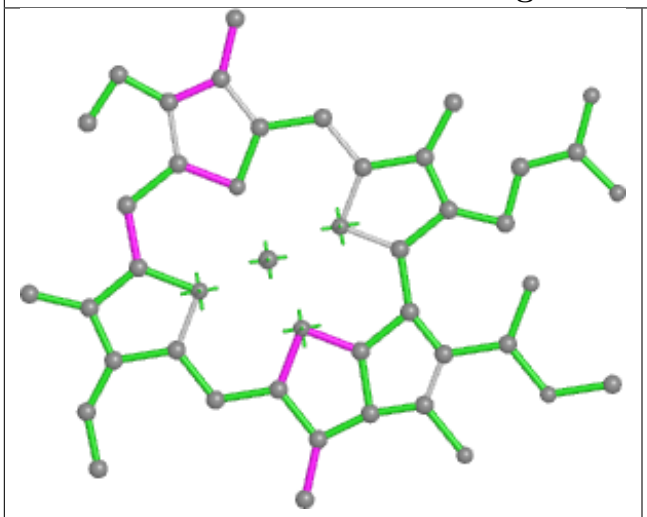


Torsions

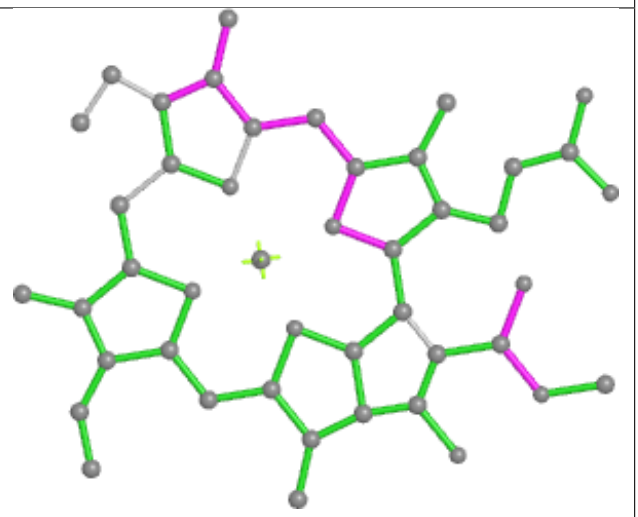


Rings

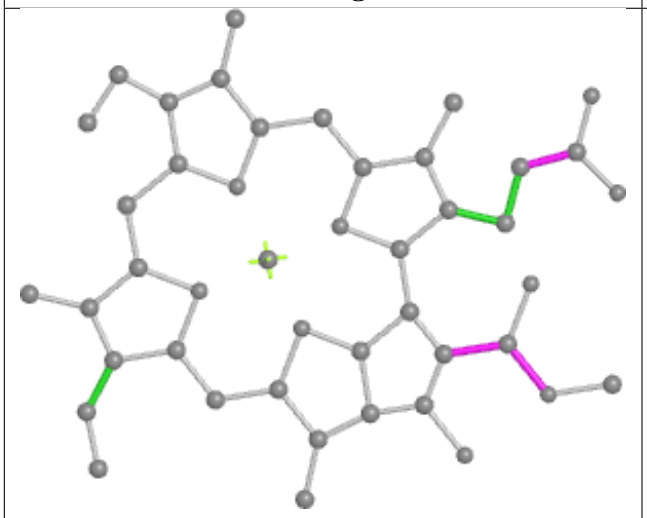
Ligand CLA B1 313



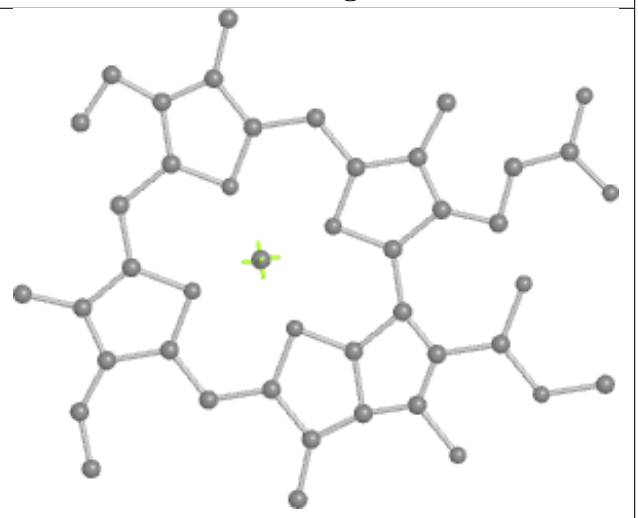
Bond lengths



Bond angles

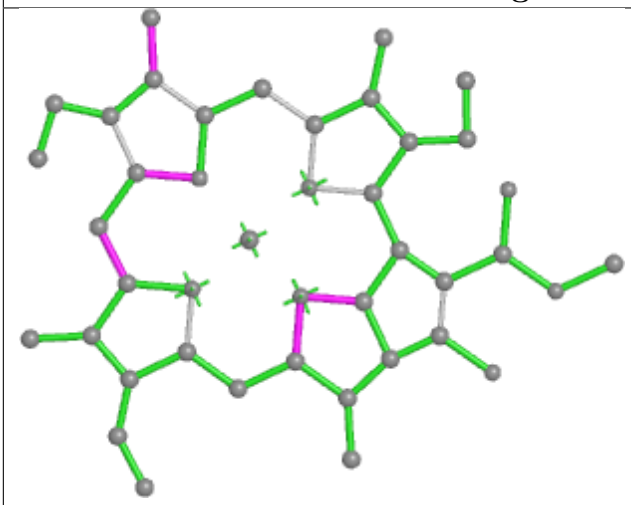


Torsions

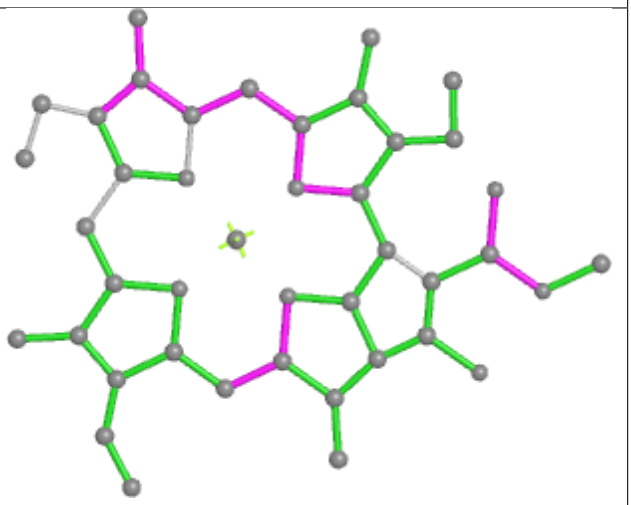


Rings

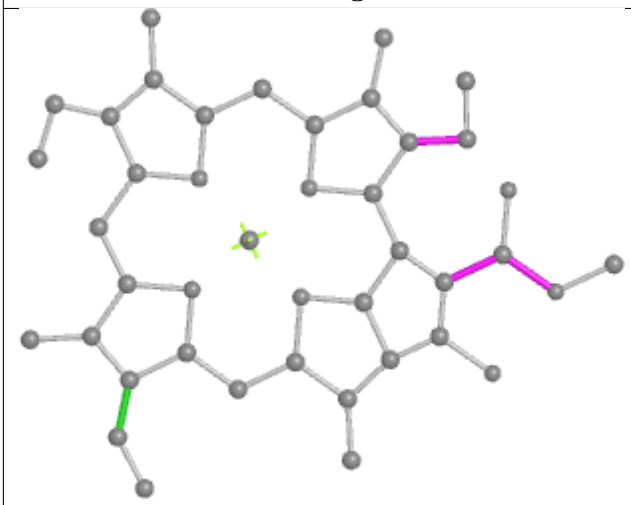
Ligand CLA BB 837



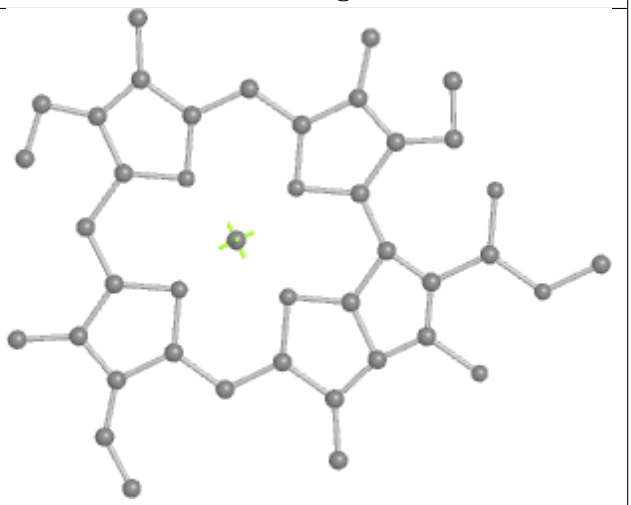
Bond lengths



Bond angles

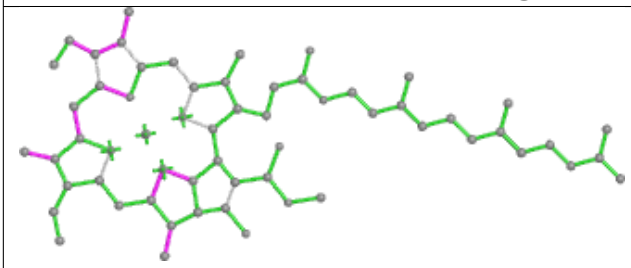


Torsions



Rings

Ligand CLA B3 602



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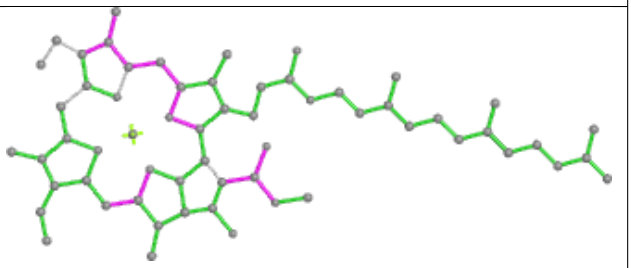
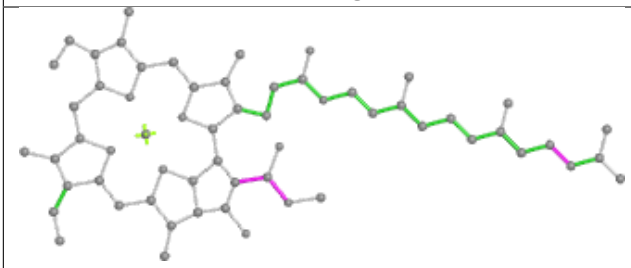


Bond angles



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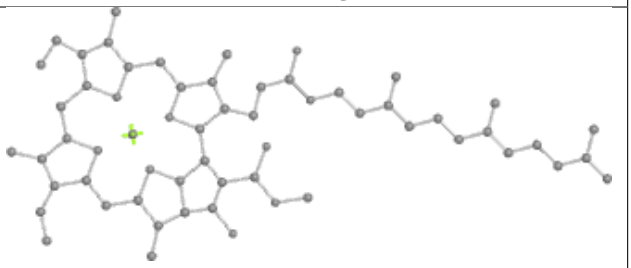
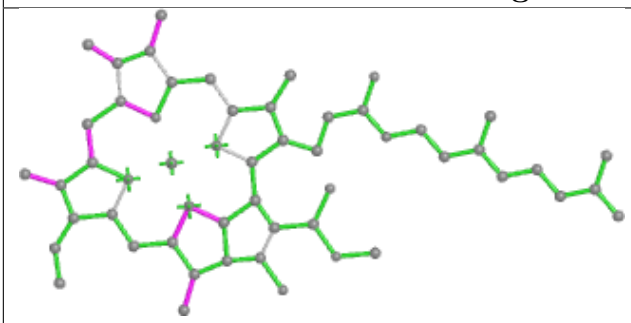
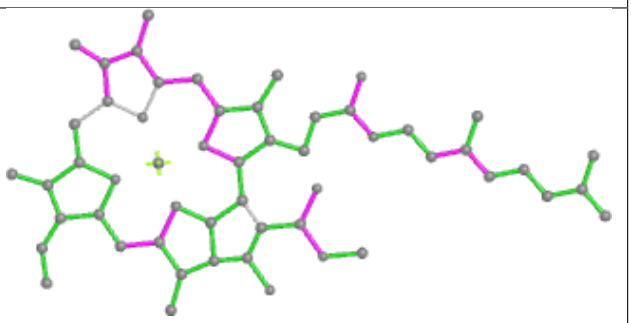
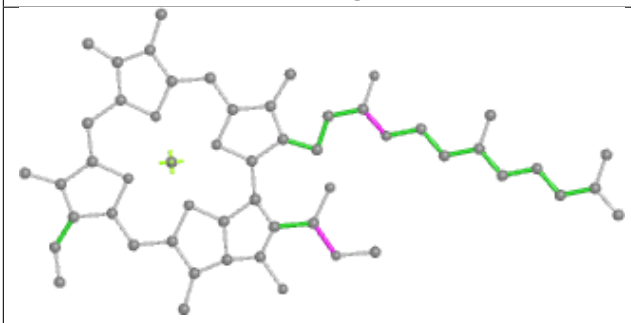
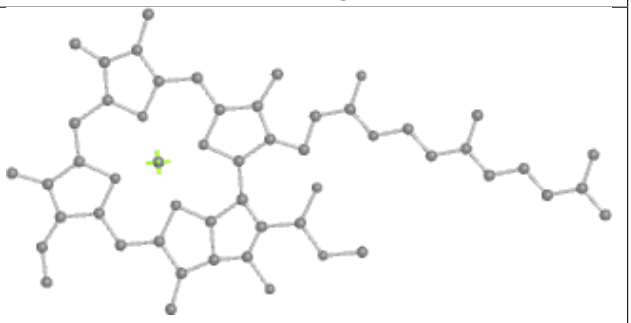


Rings

Ligand CLA BB 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

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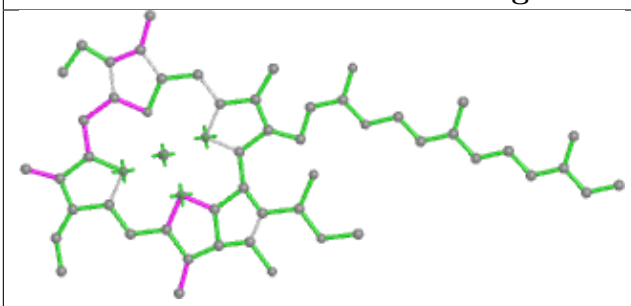
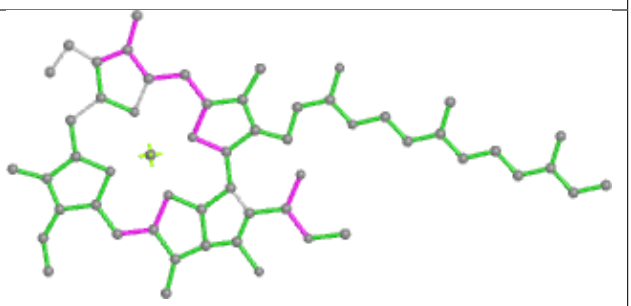
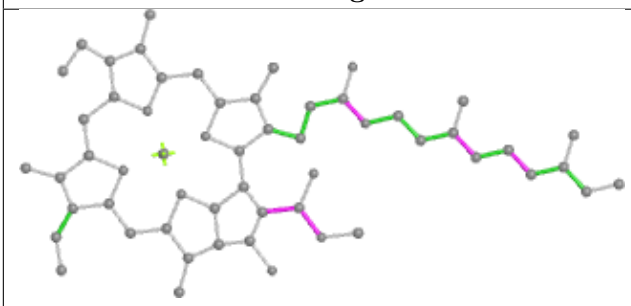
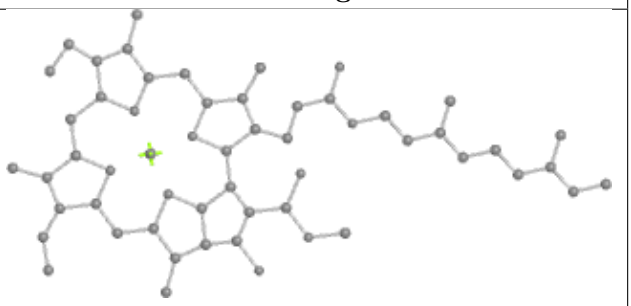
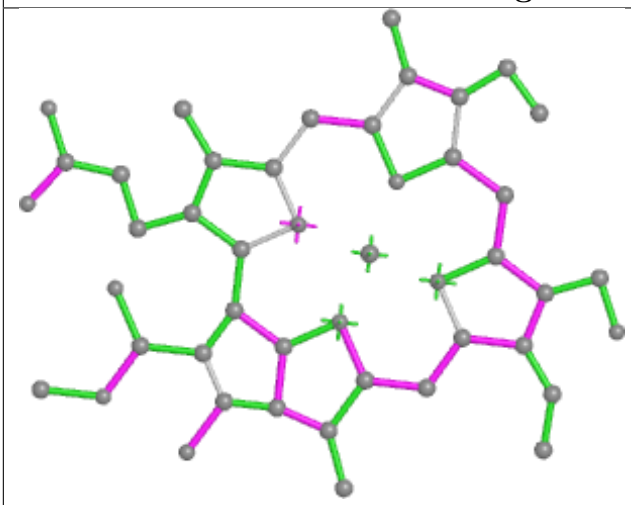
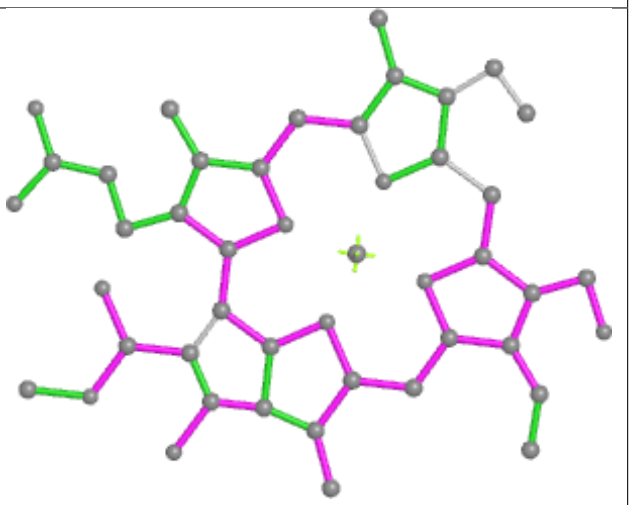
 Bond lengths	 Bond angles
 Torsions	 Rings

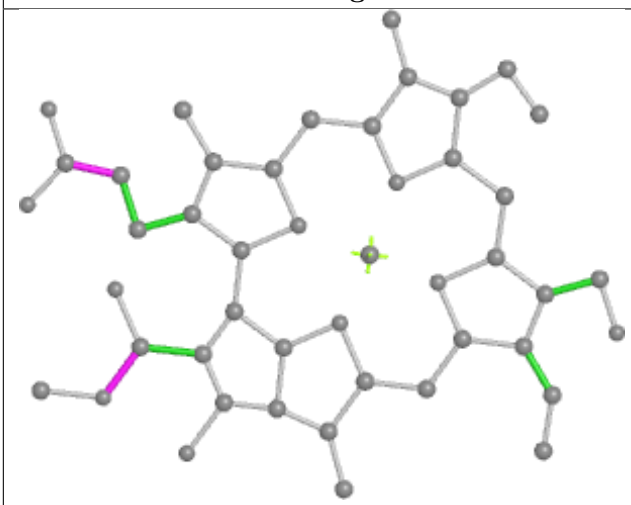
Ligand CHL B2 306



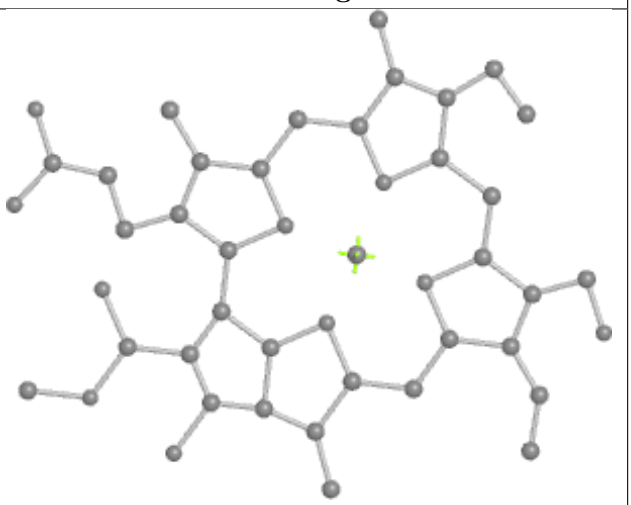
Bond lengths



Bond angles

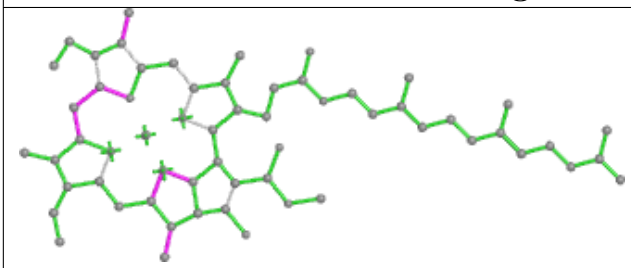


Torsions

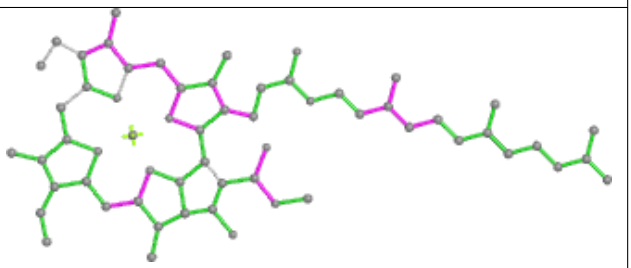


Rings

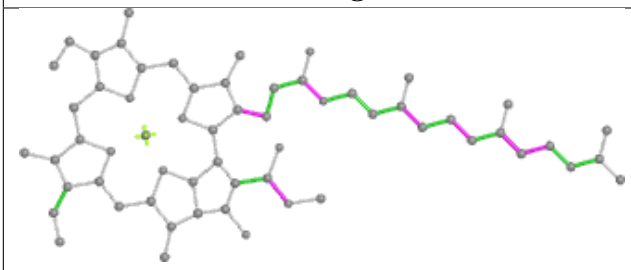
Ligand CLA BB 820



Bond lengths



Bond angles



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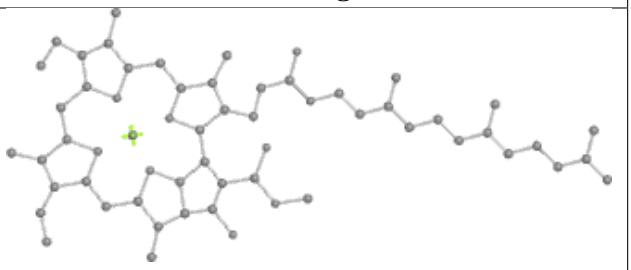
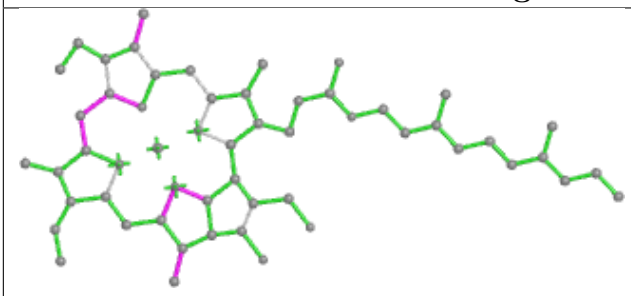
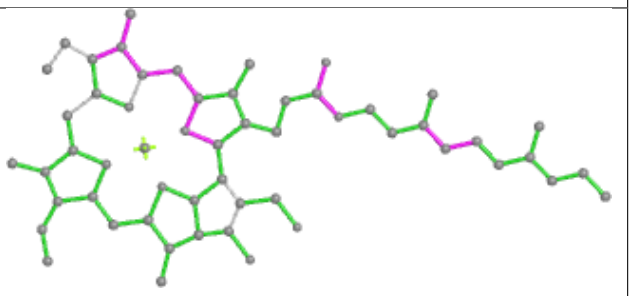
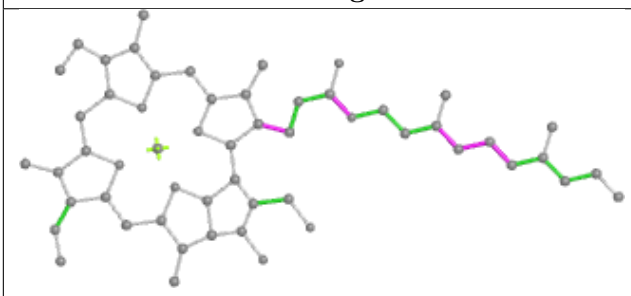
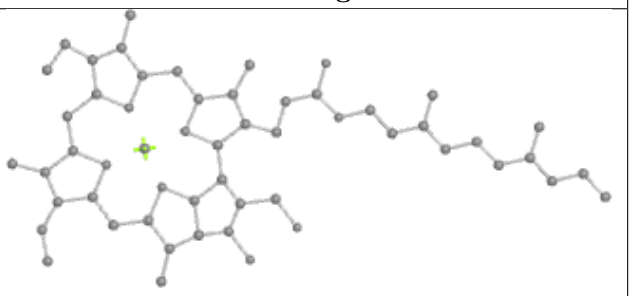
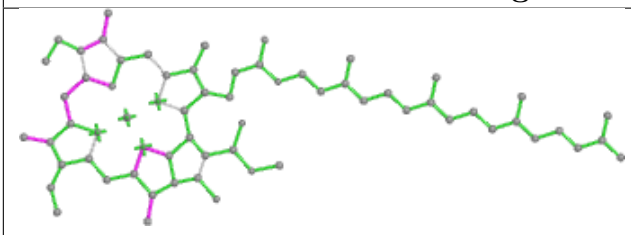
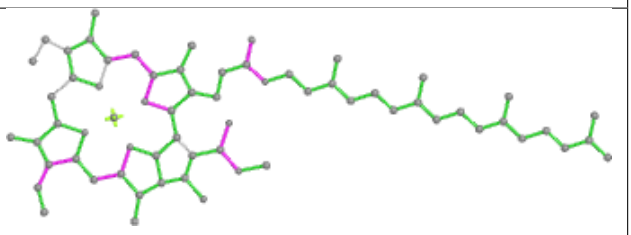
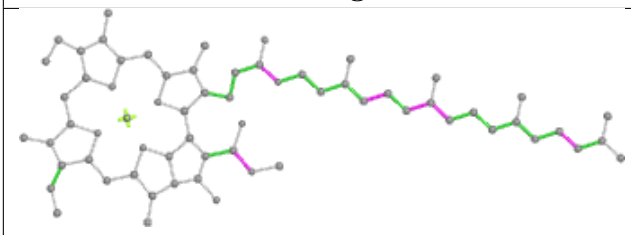
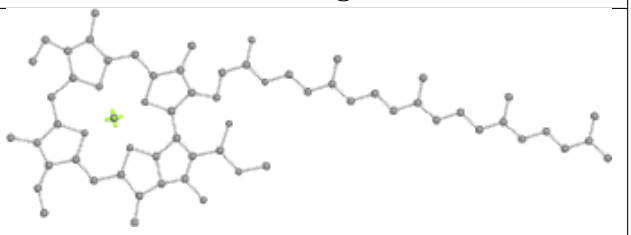
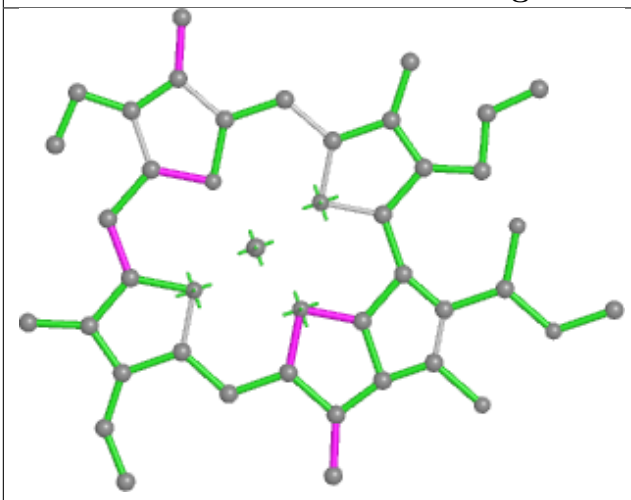


Rings

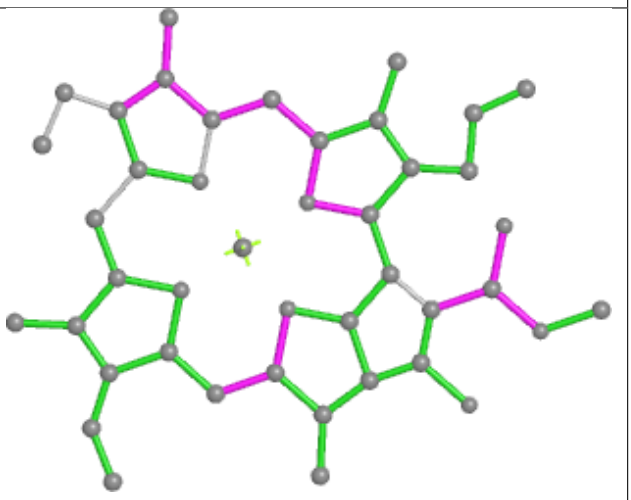
Ligand CLA BF 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

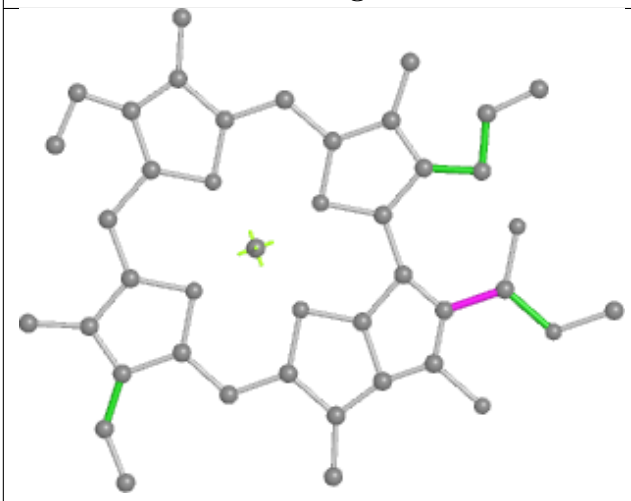
Ligand CLA BB 814



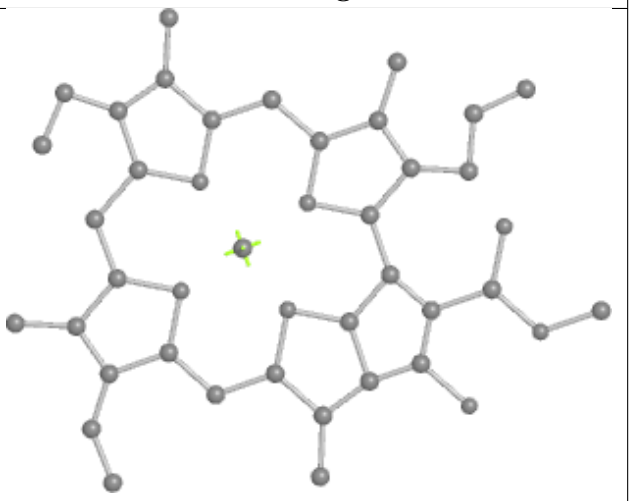
Bond lengths



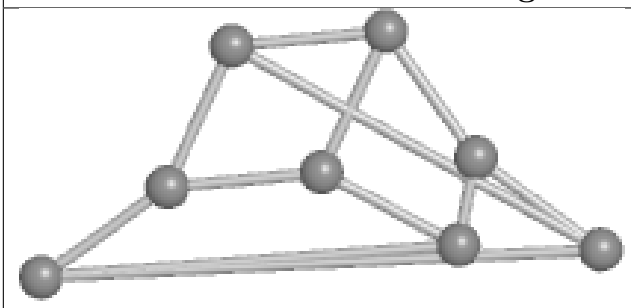
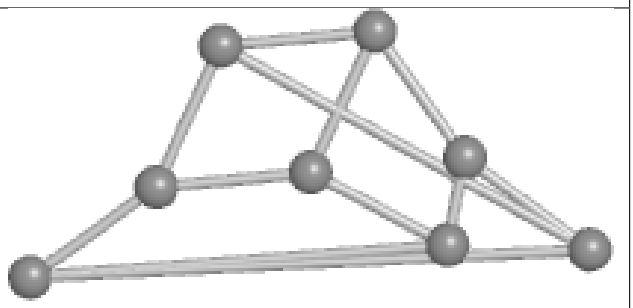
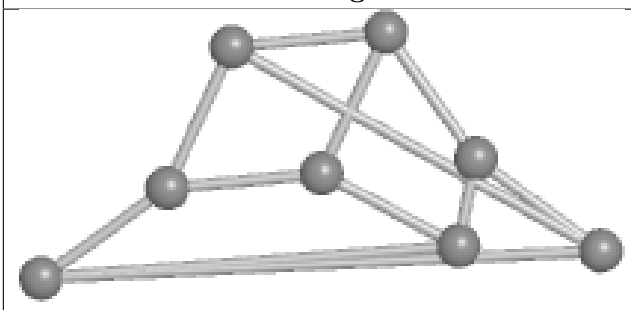
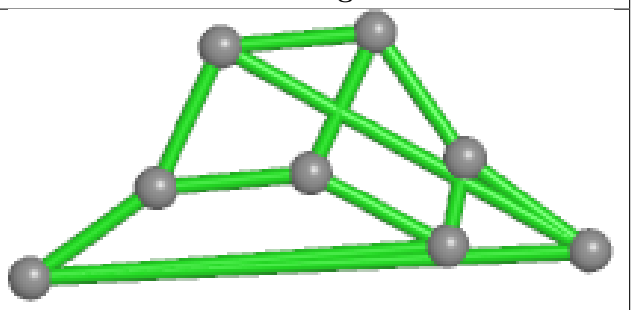
Bond angles

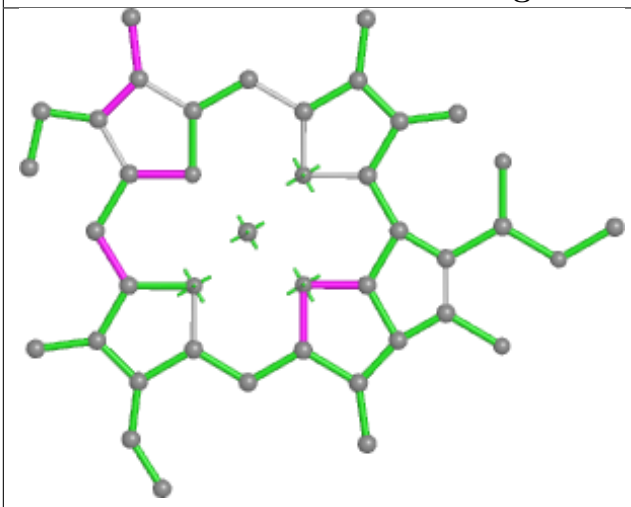
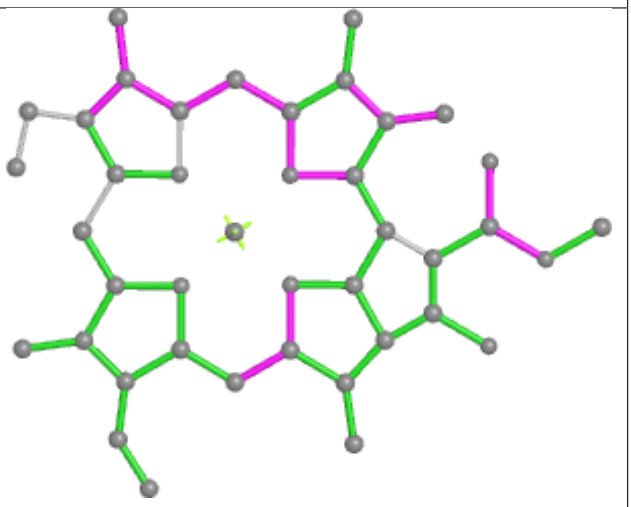
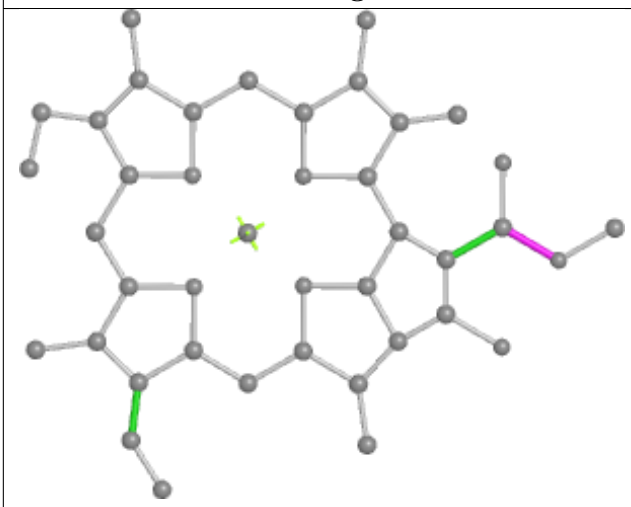
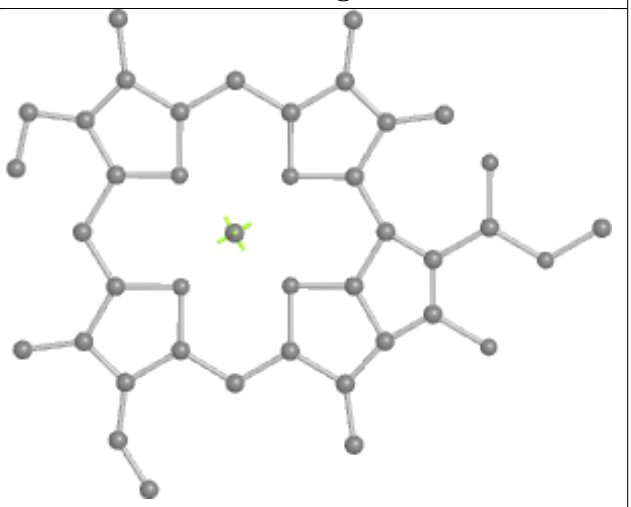


Torsions

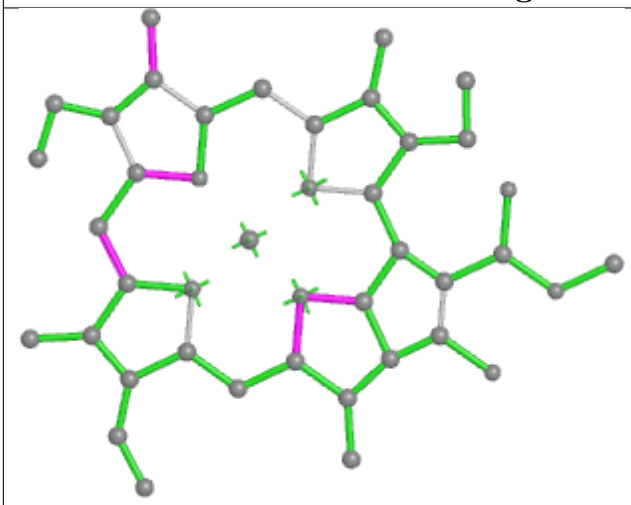


Rings

Ligand SF4 BA 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BF 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BJ 102



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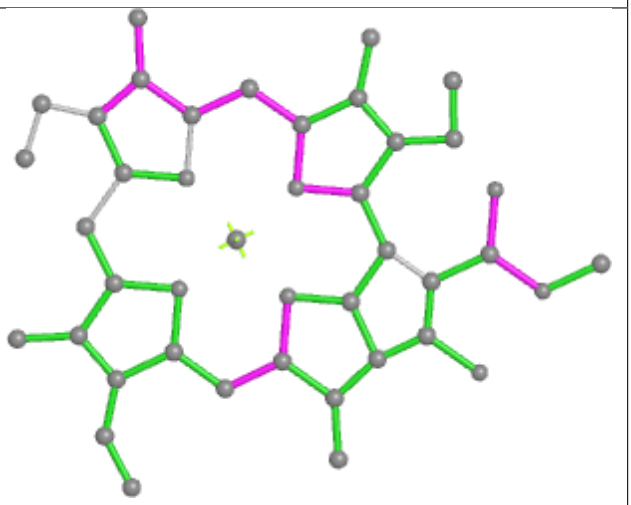

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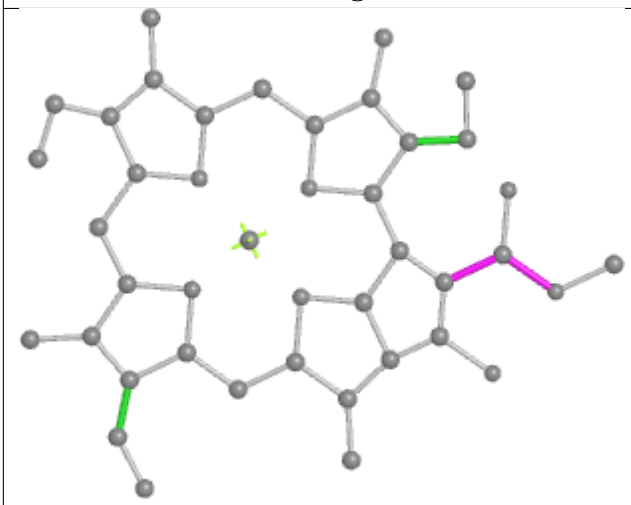

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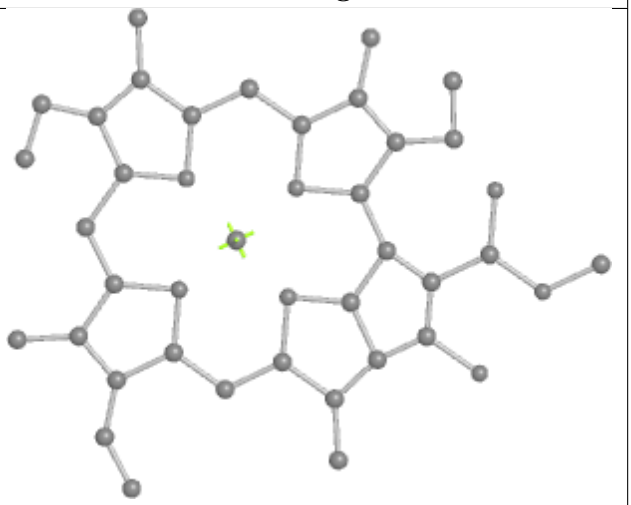
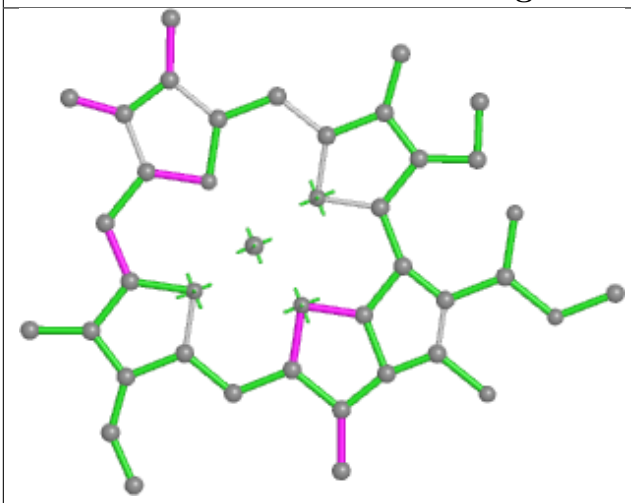


Rings

Ligand CLA B3 606



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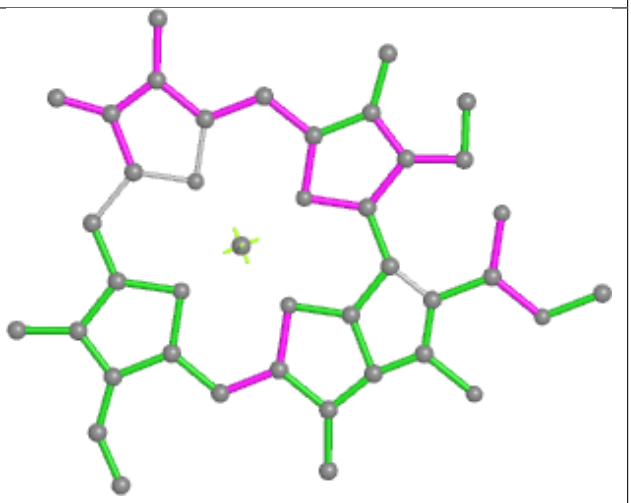

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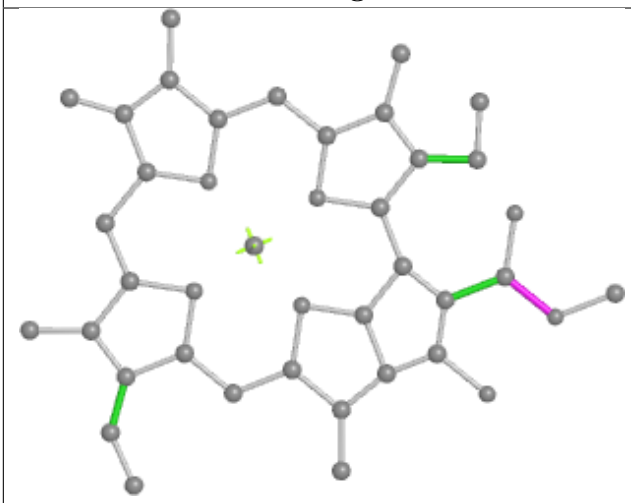

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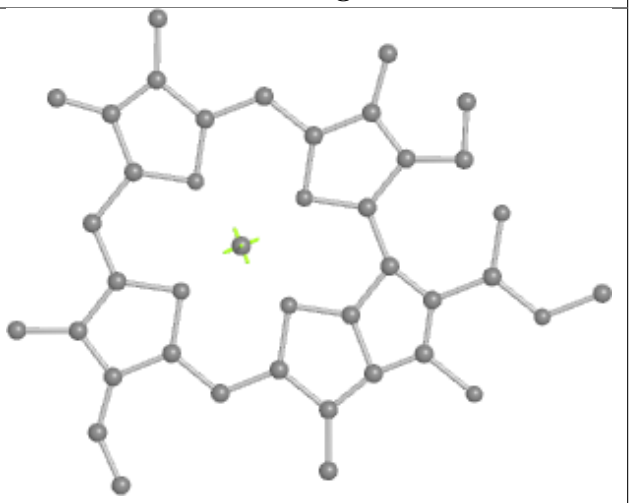
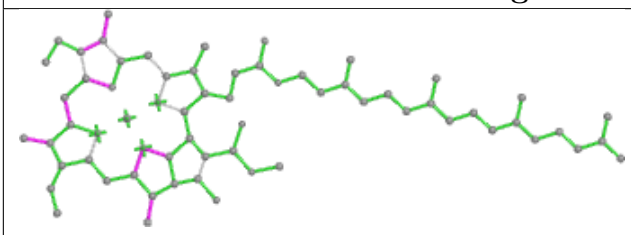


Rings

Ligand CLA BA 805



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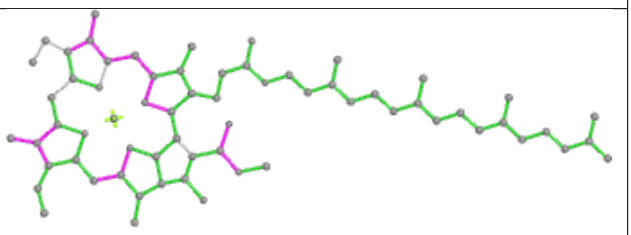

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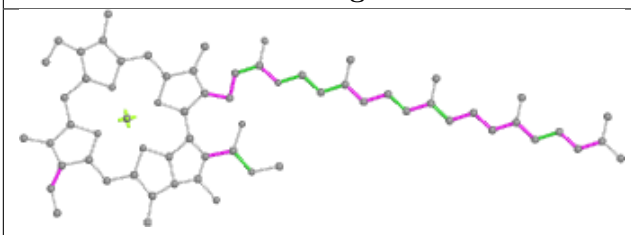

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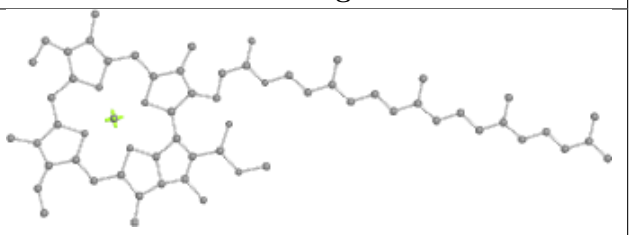
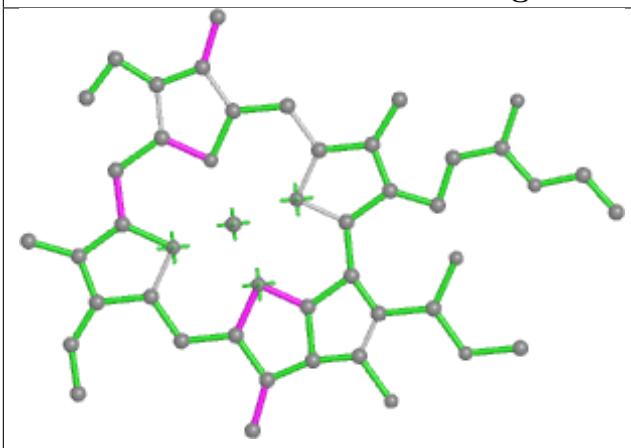


Rings

Ligand CLA BB 823



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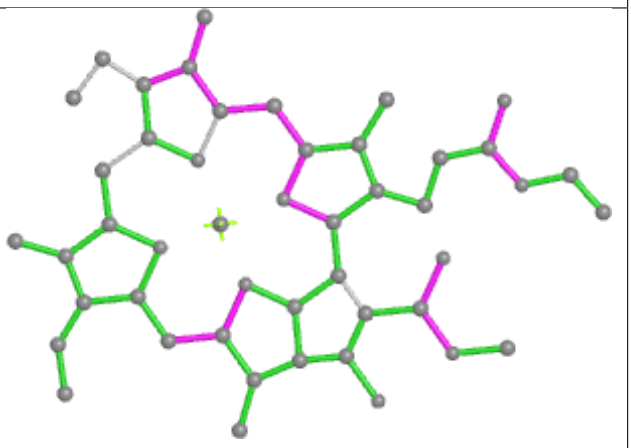

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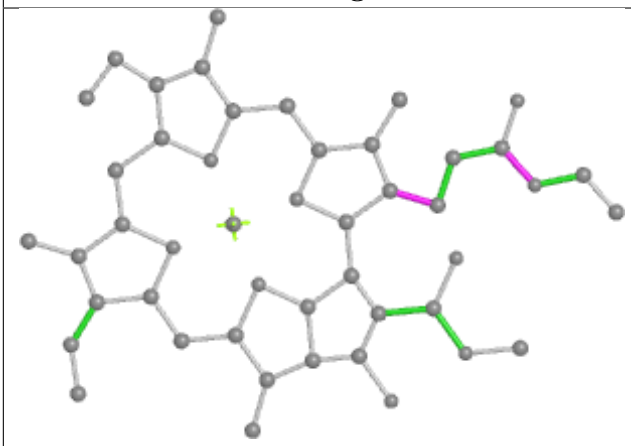

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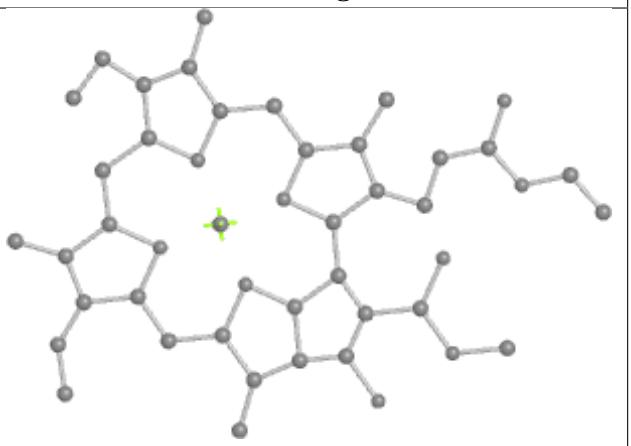

Rings

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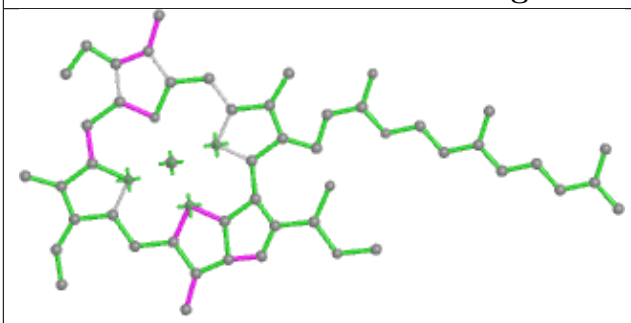

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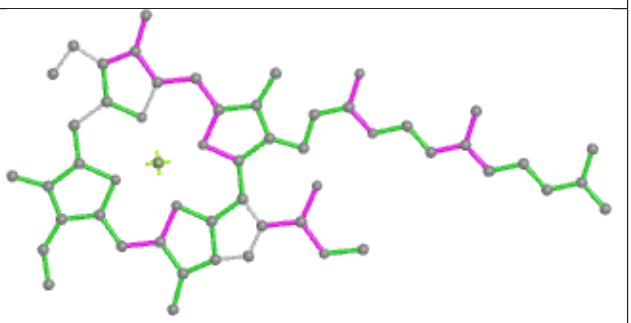

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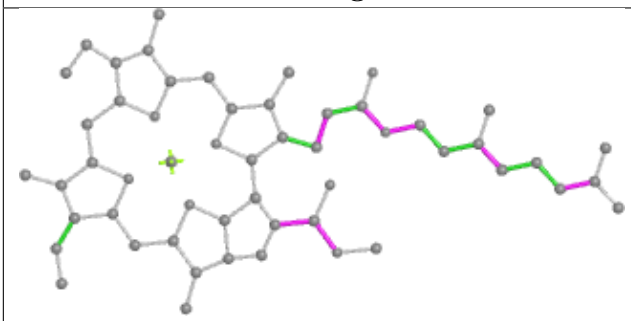

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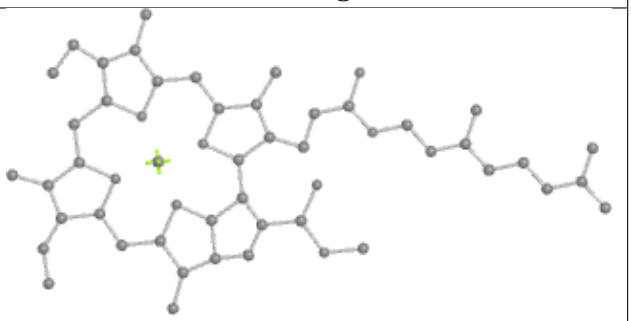

Rings

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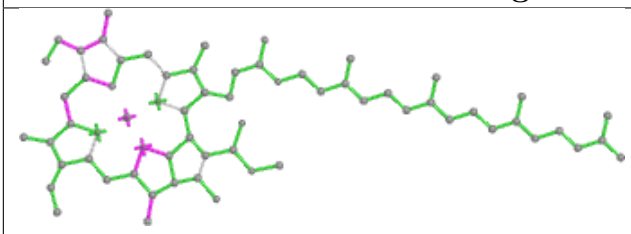
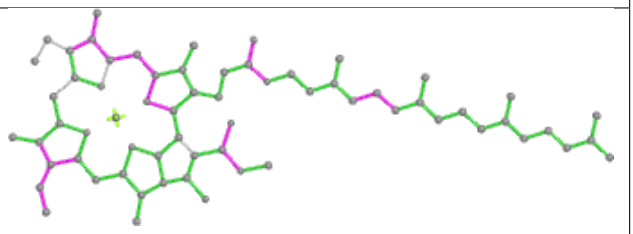
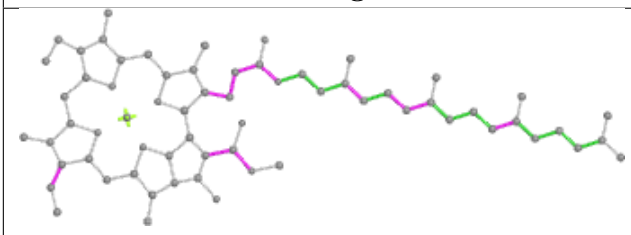
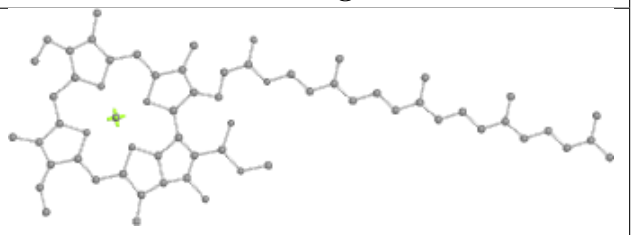
 Bond lengths	 Bond angles
 Torsions	 Rings

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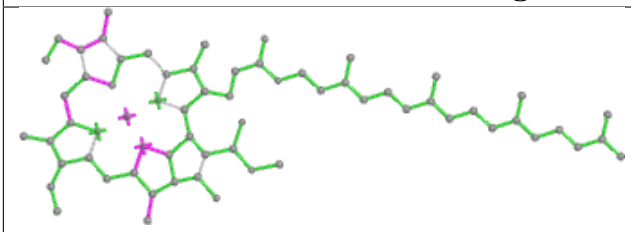
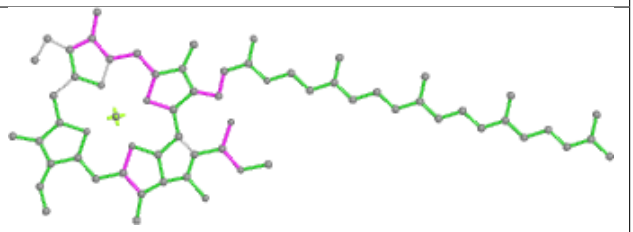
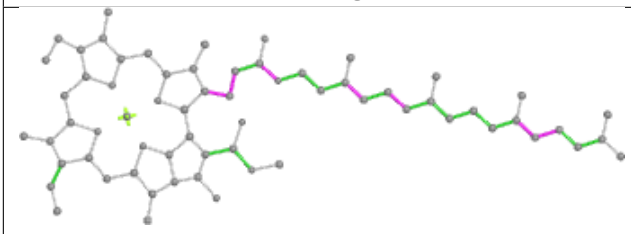
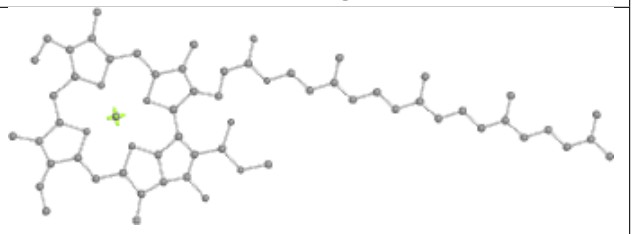
 Bond lengths	 Bond angles
 Torsions	 Rings

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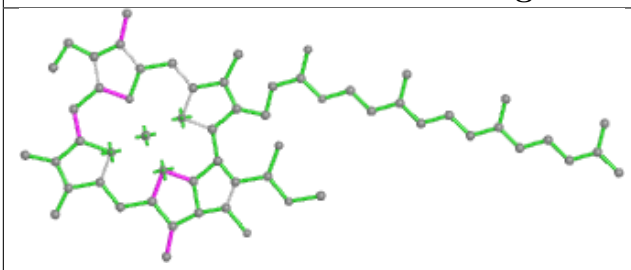
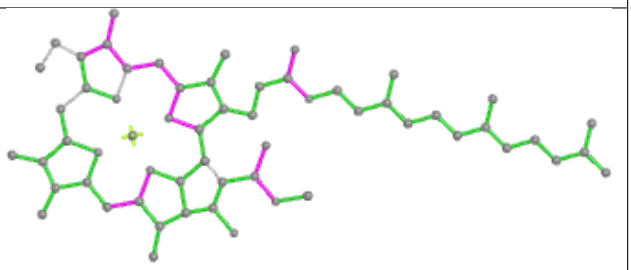
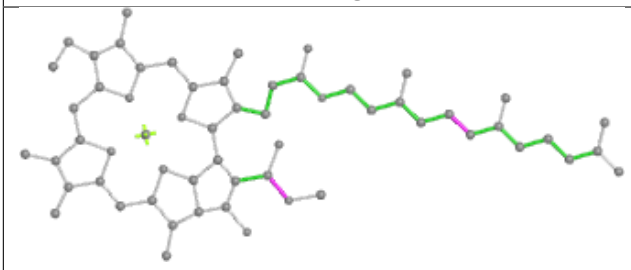
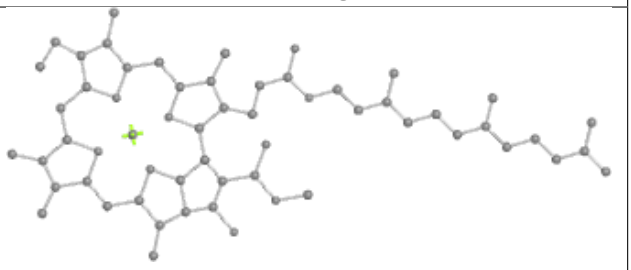
 Bond lengths	 Bond angles
 Torsions	 Rings

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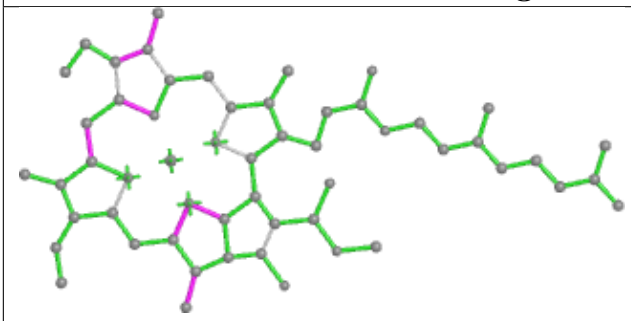
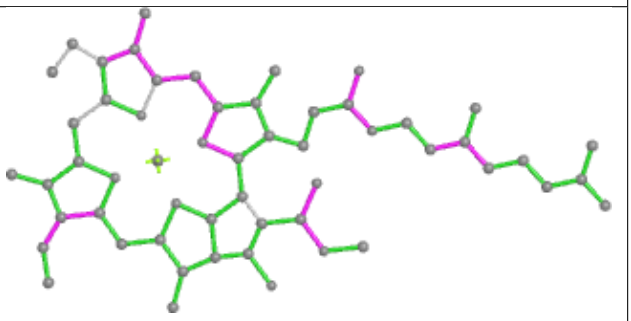
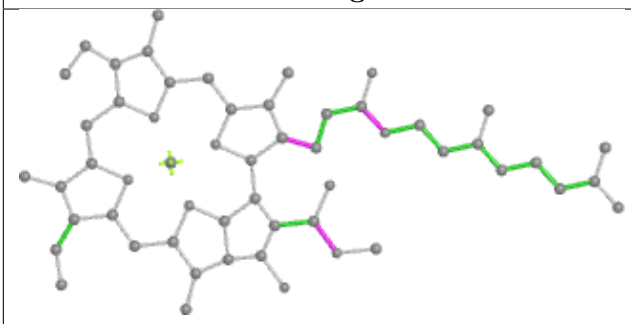
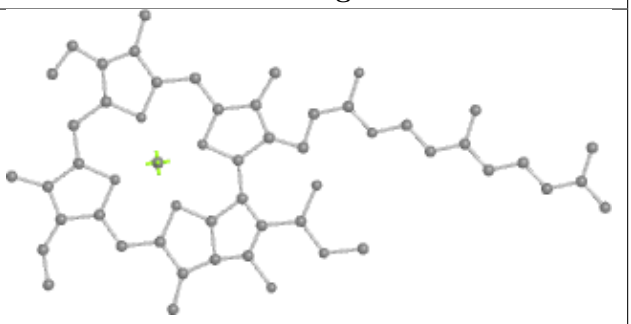
 Bond lengths	 Bond angles
 Torsions	 Rings

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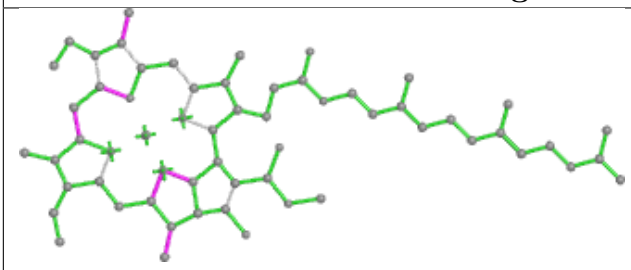
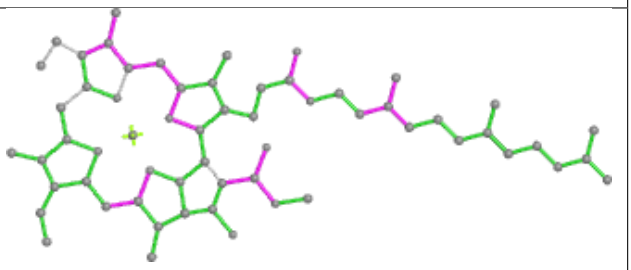
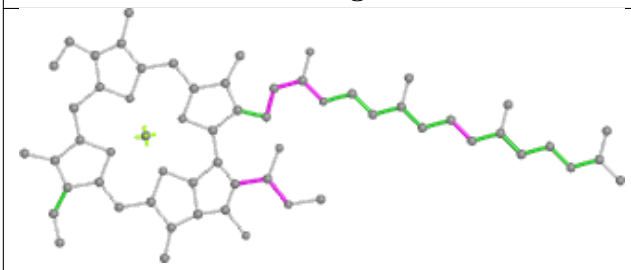
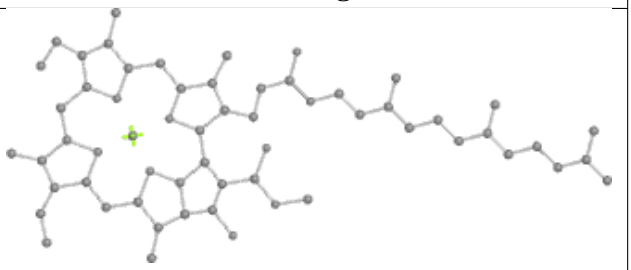
 Bond lengths	 Bond angles
 Torsions	 Rings

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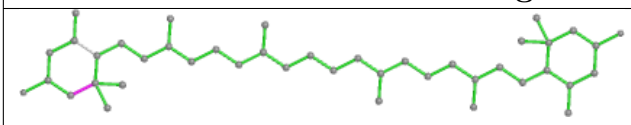
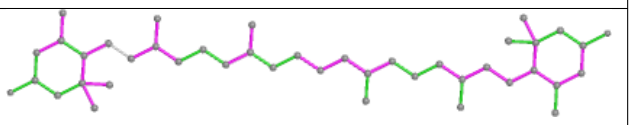
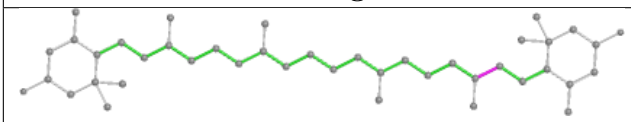
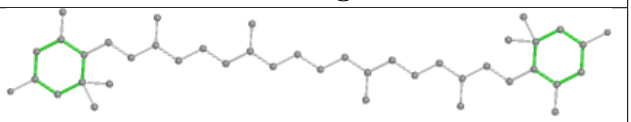
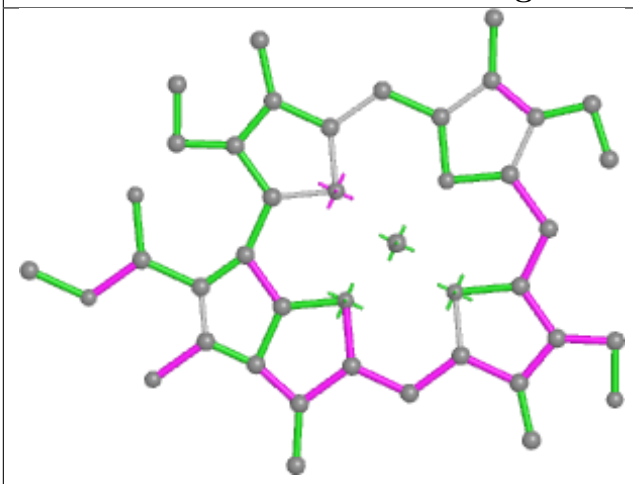
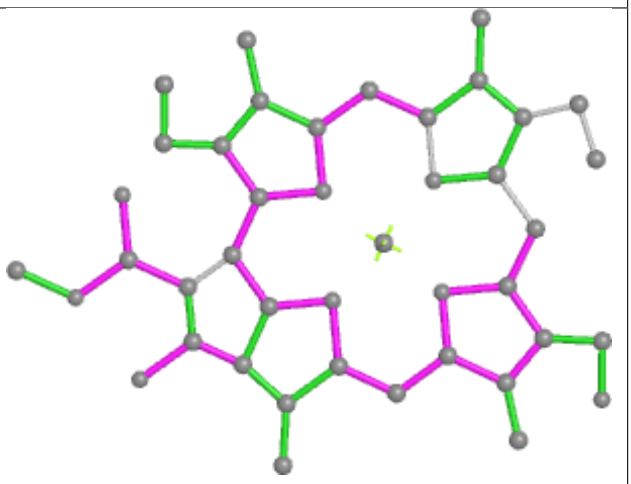
 Bond lengths	 Bond angles
 Torsions	 Rings

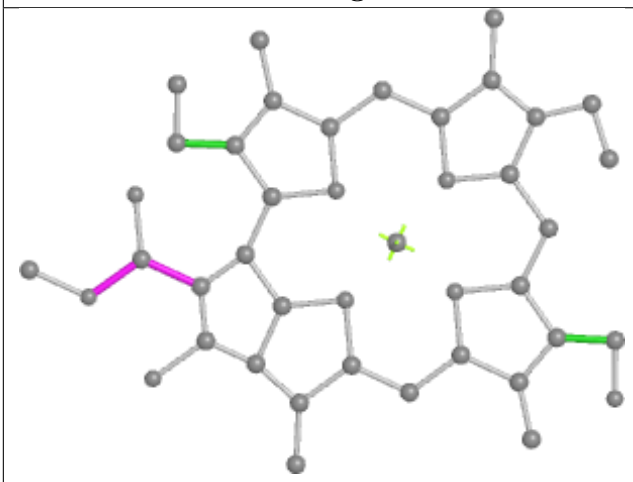
Ligand CHL B2 304



Bond lengths



Bond angles



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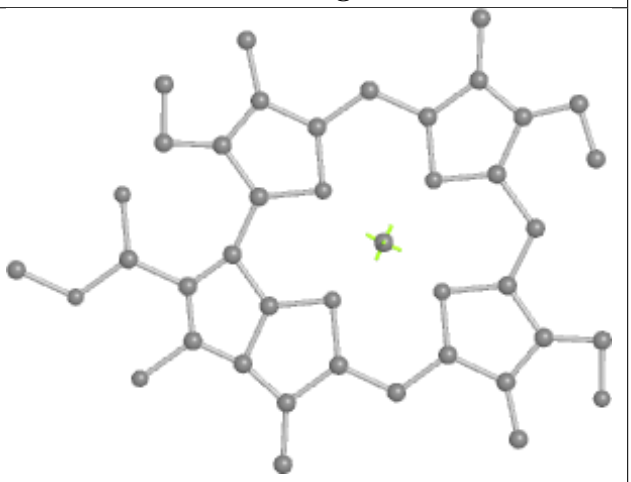
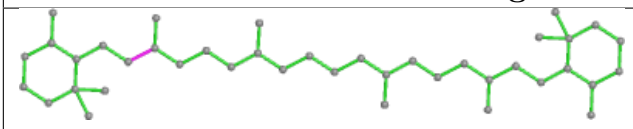
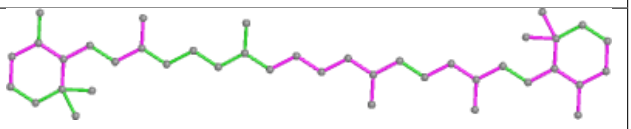


Rings

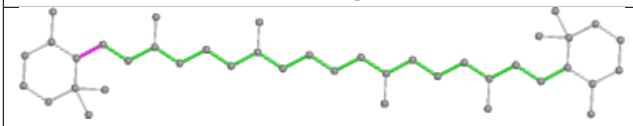
Ligand BCR BK 204



Bond lengths

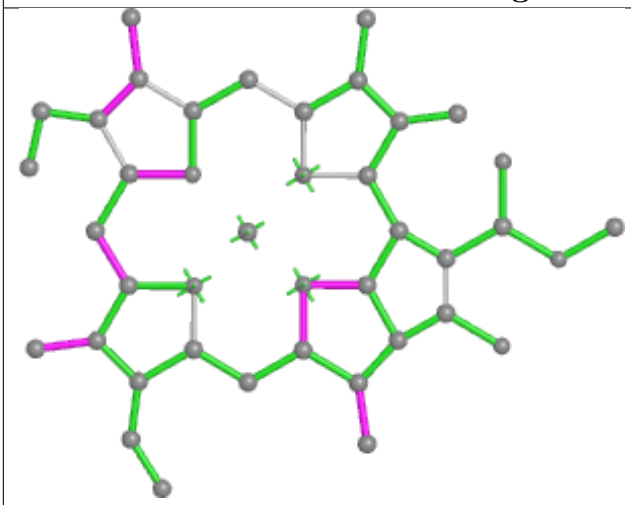
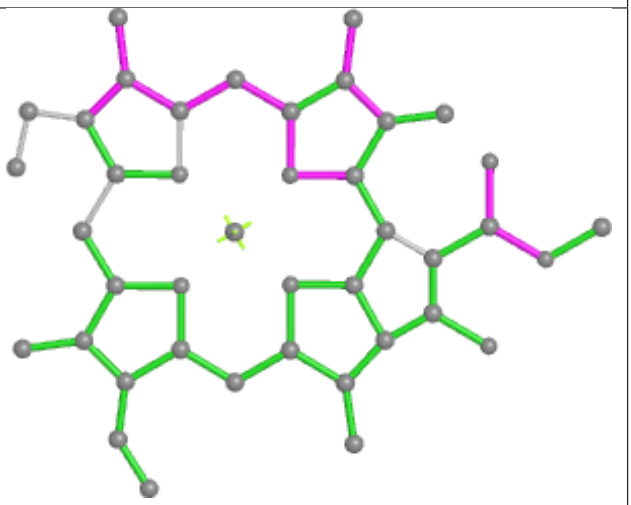
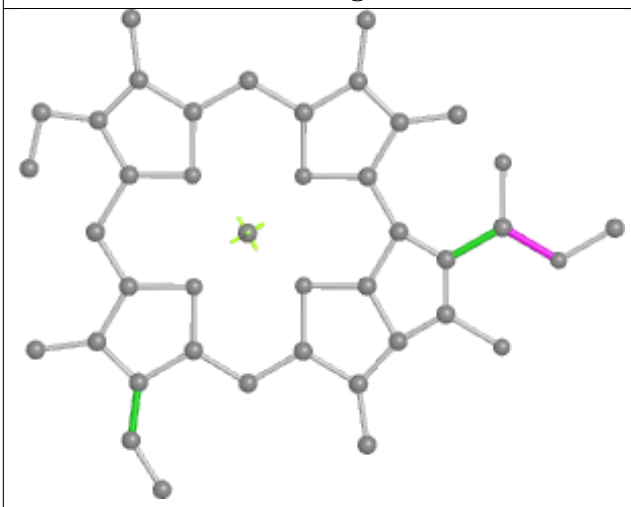
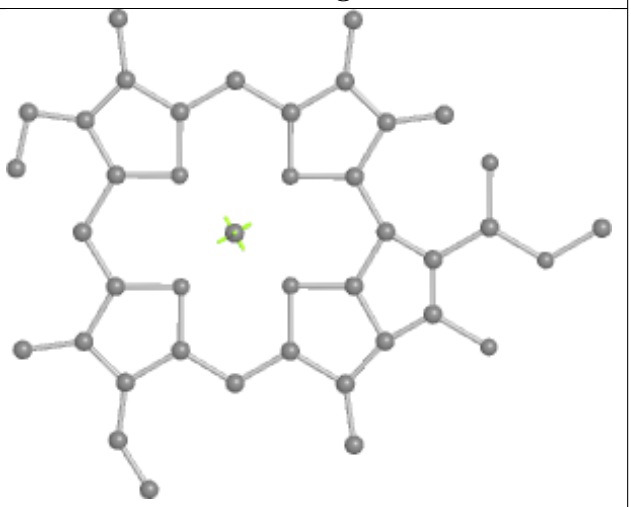


Bond angles



Torsions

Rings

Ligand CLA BB 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

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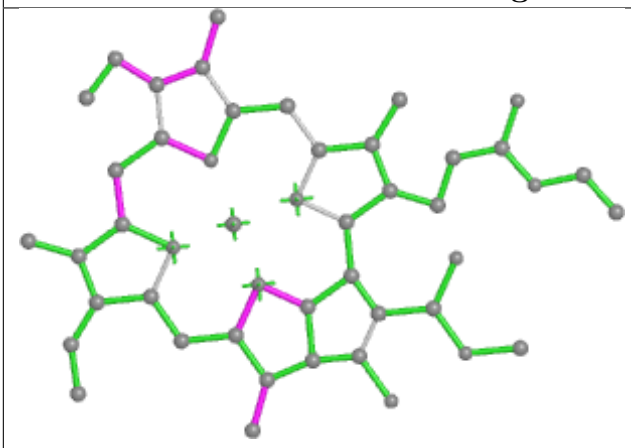
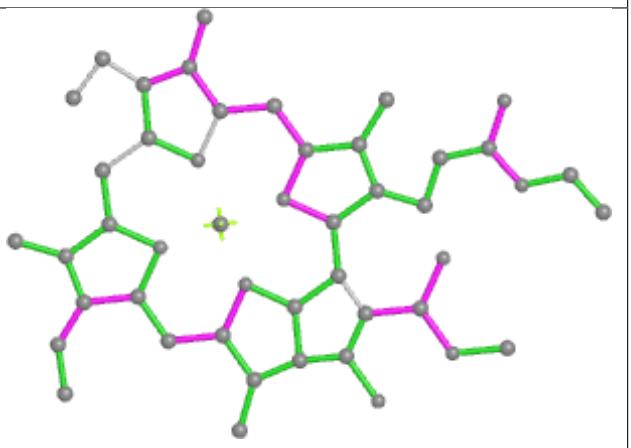
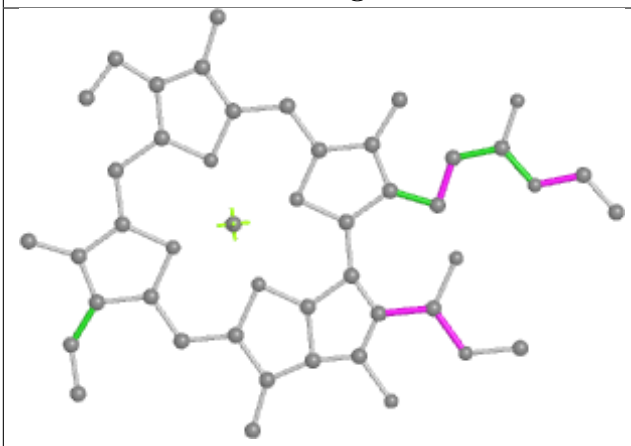
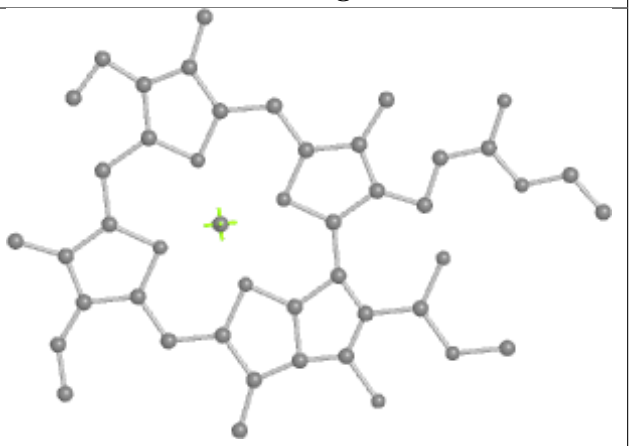
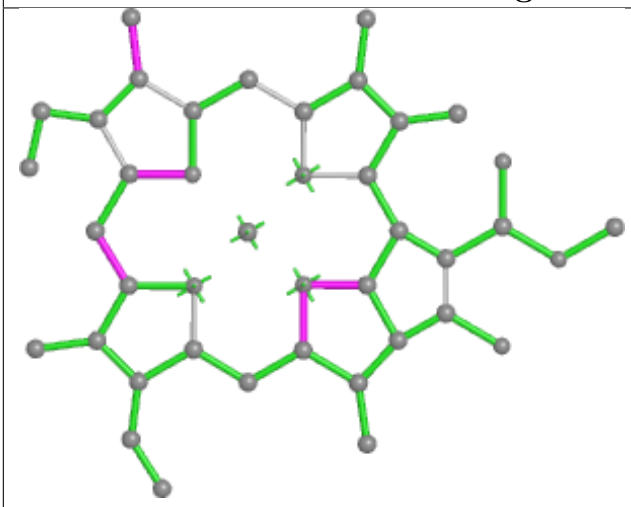
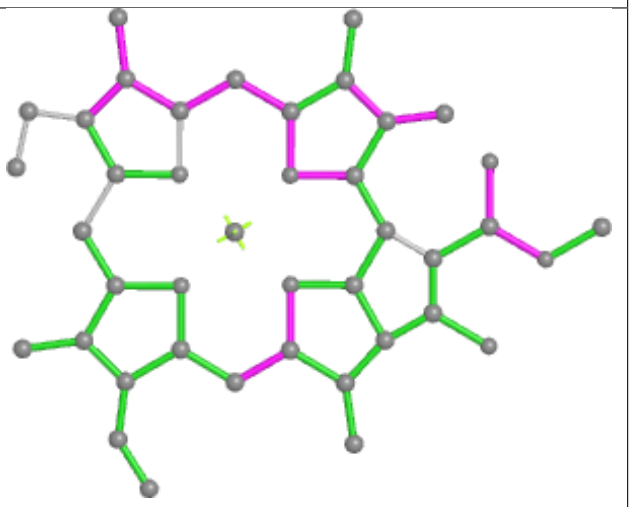
 Bond lengths	 Bond angles
 Torsions	 Rings

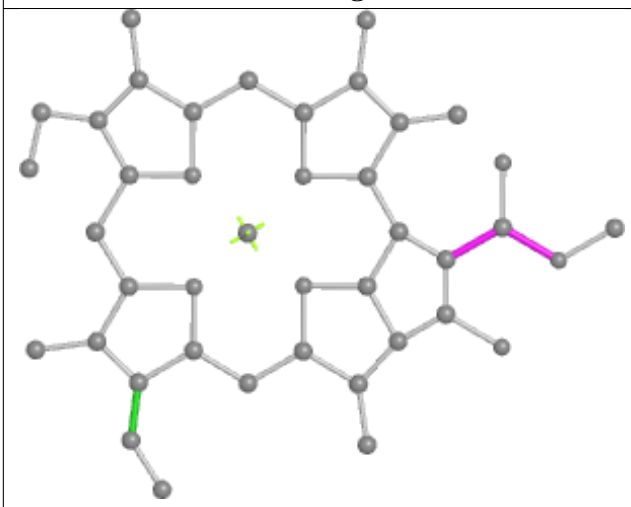
Ligand CLA B1 306



Bond lengths



Bond angles



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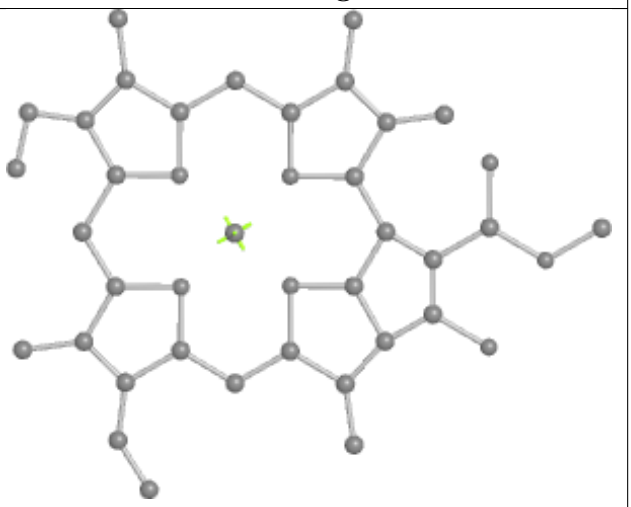
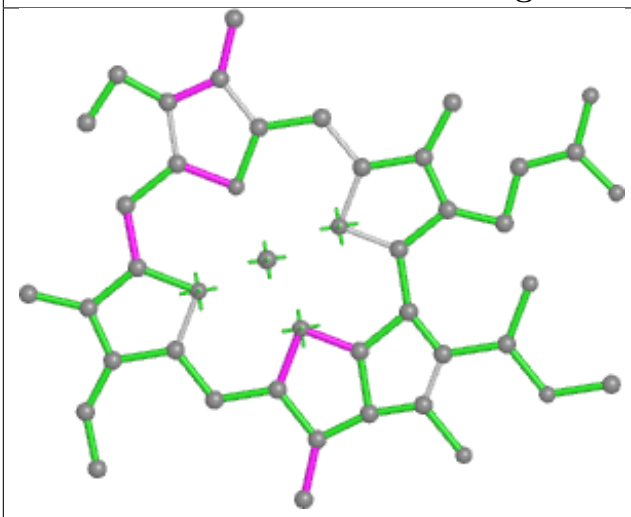


Rings

Ligand CLA B2 307



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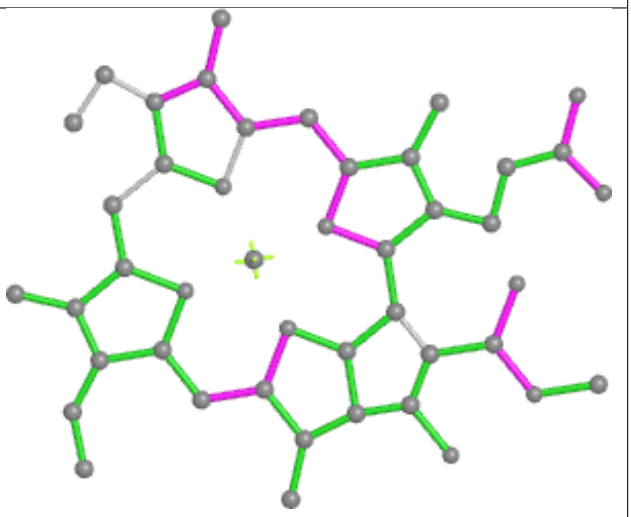
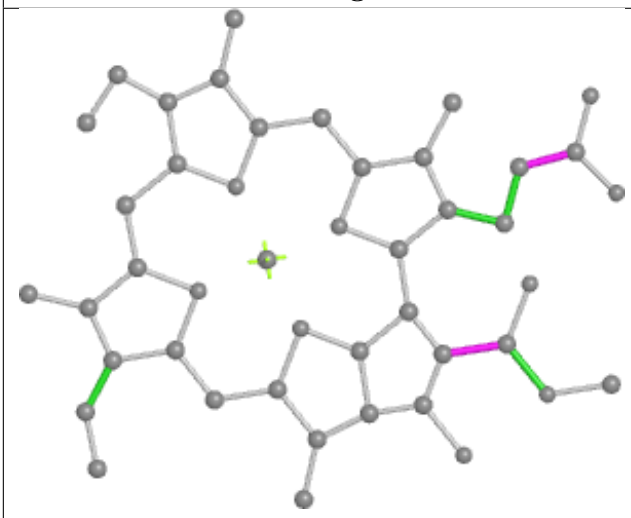


Bond angles



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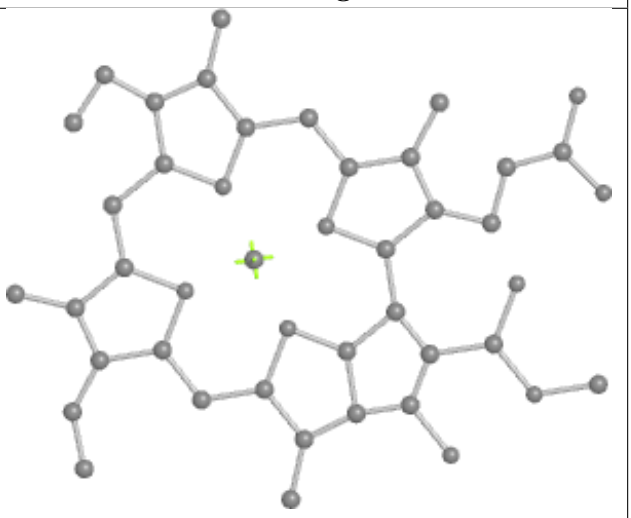
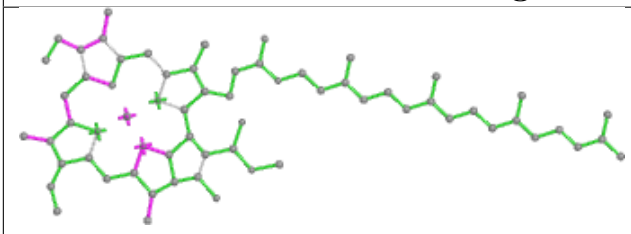


Rings

Ligand CLA BB 826



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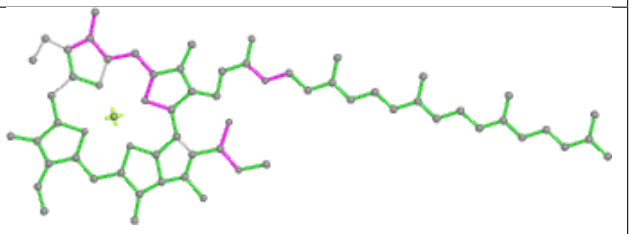
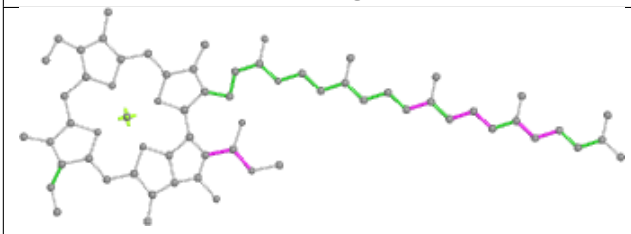


Bond angles



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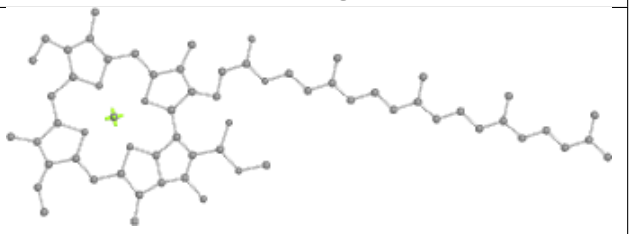
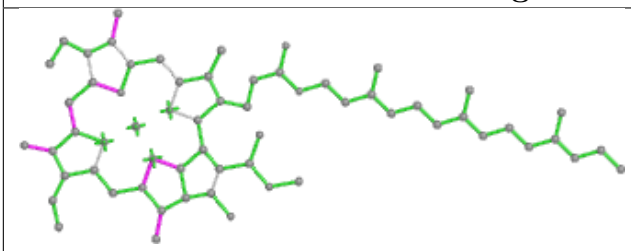
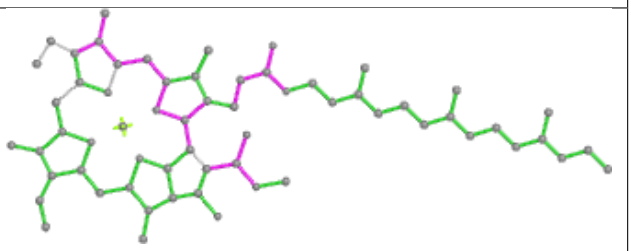
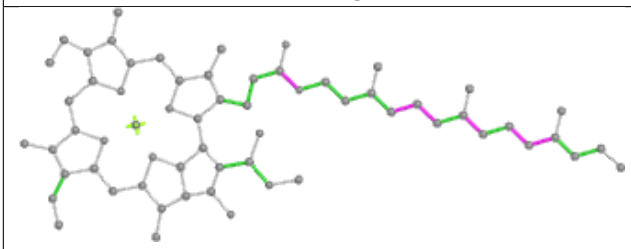
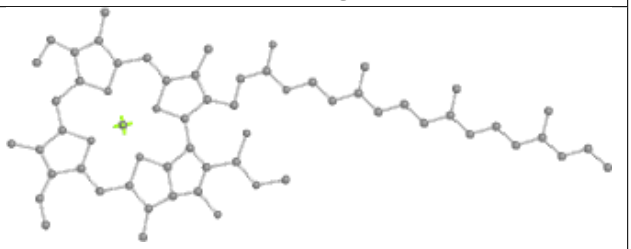


Rings

Ligand CLA BB 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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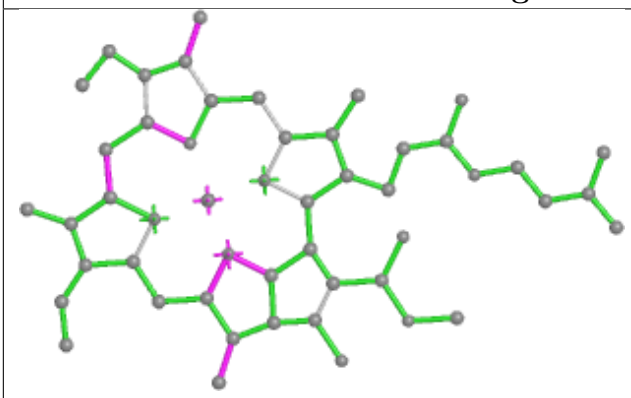
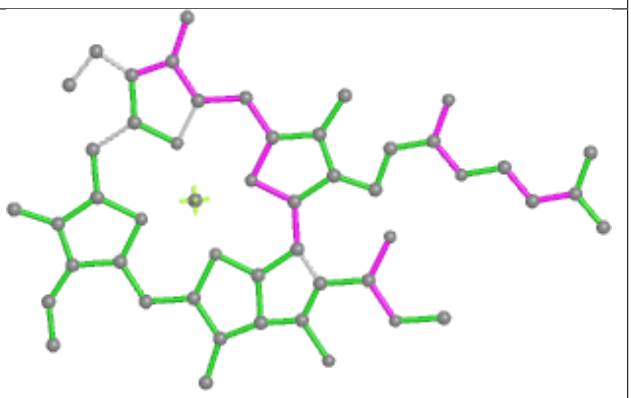
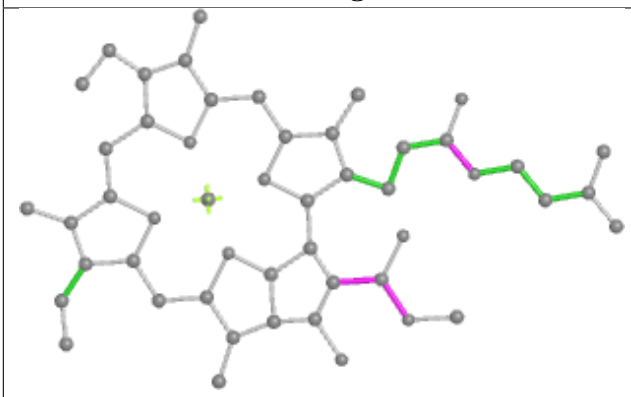
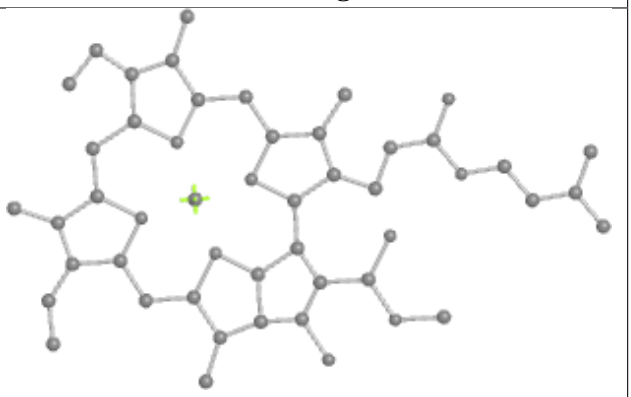
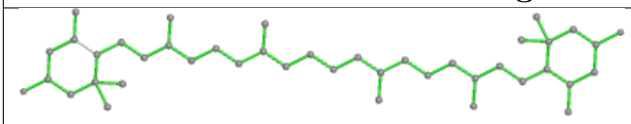
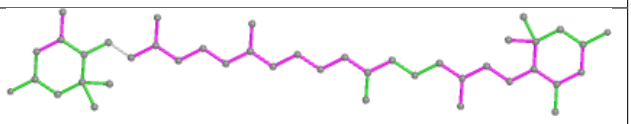
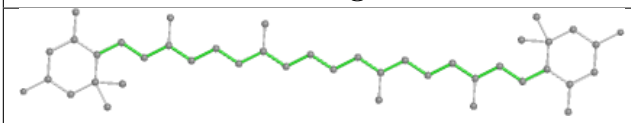
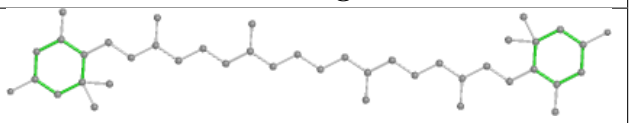
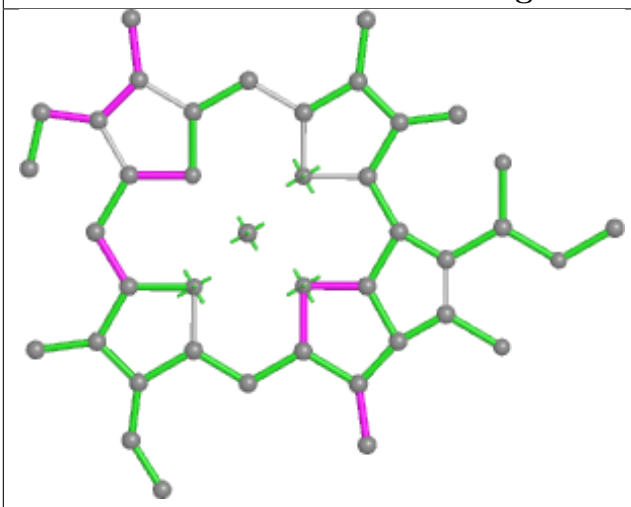
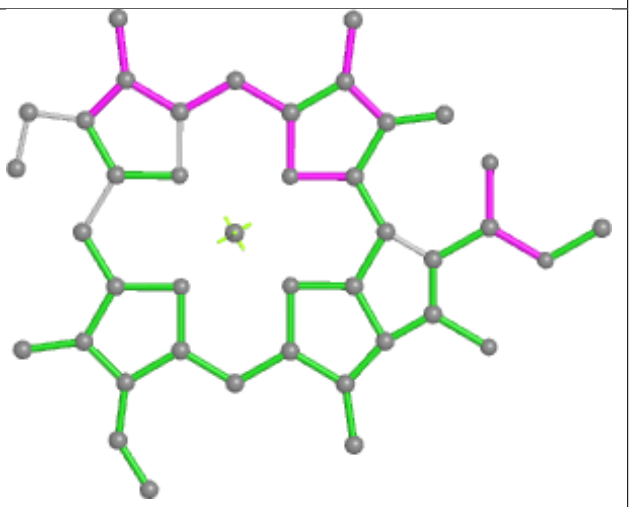
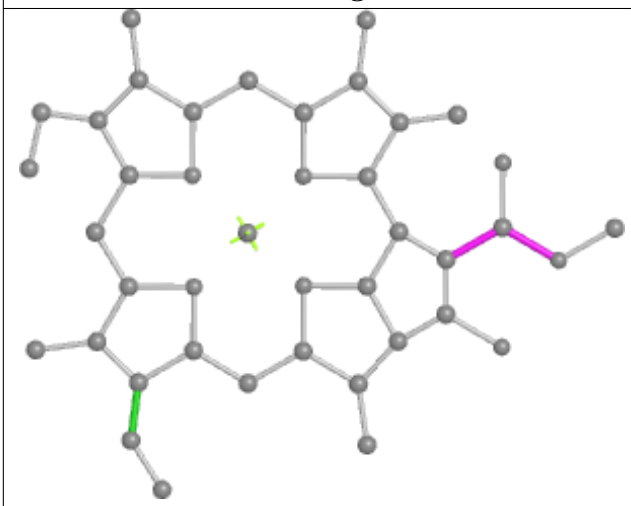
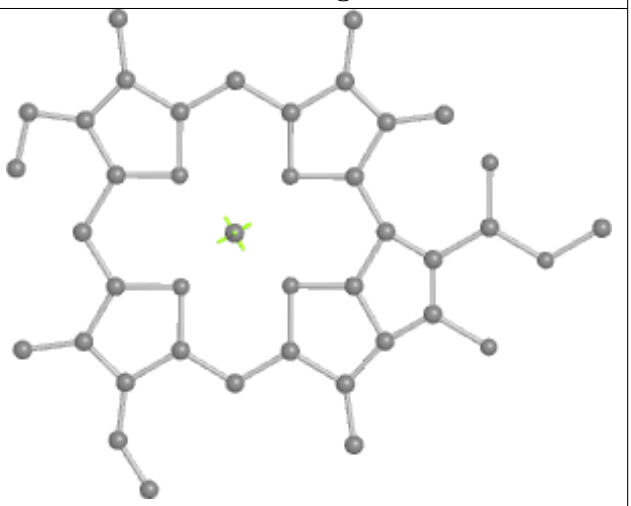
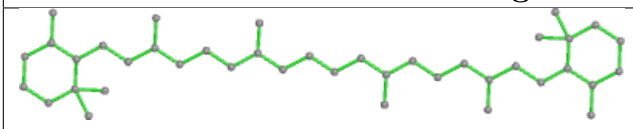
 Bond lengths	 Bond angles
 Torsions	 Rings

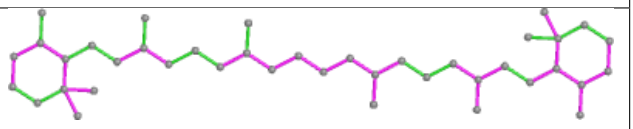
Ligand LUT B2 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

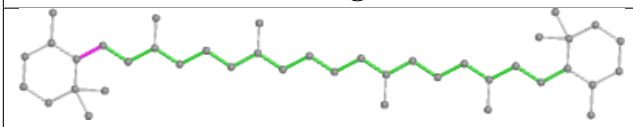
Ligand BCR BL 305



Bond lengths



Bond angles



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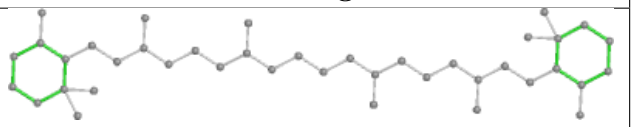
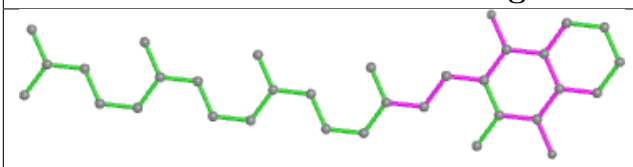
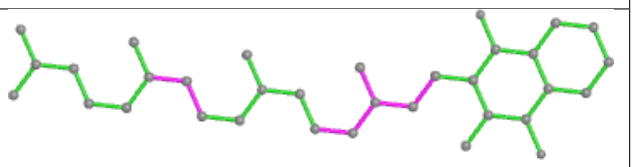


Rings

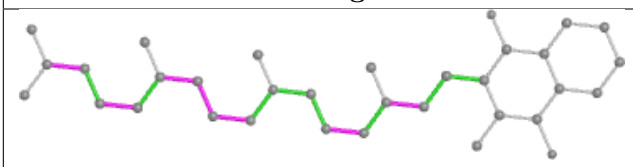
Ligand PQN BA 843



Bond lengths



Bond angles



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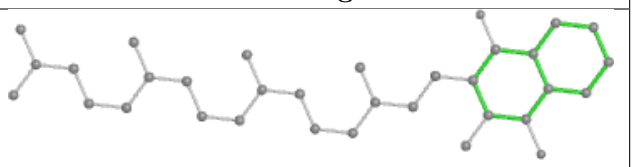
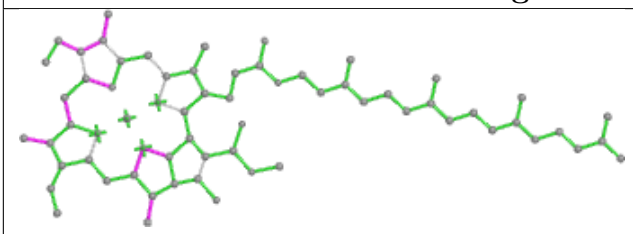
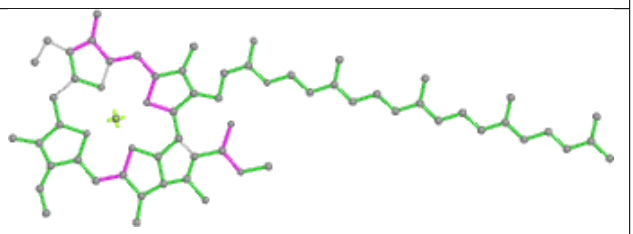


Rings

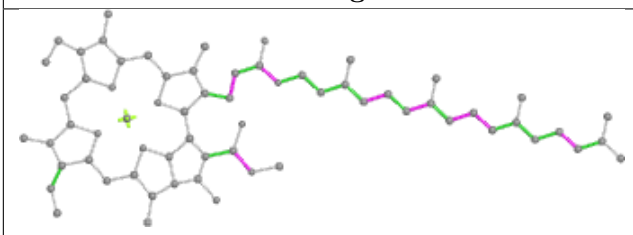
Ligand CLA BB 843



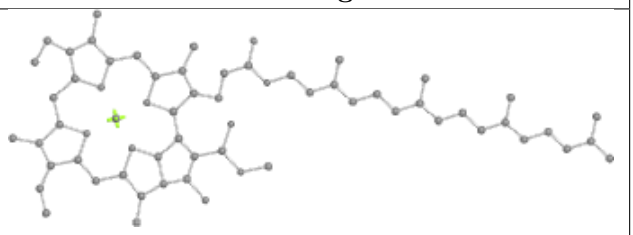
Bond lengths



Bond angles

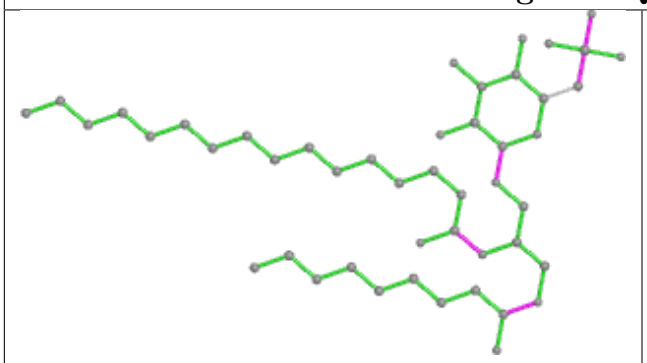


Torsions



Rings

Ligand SQD BJ 104



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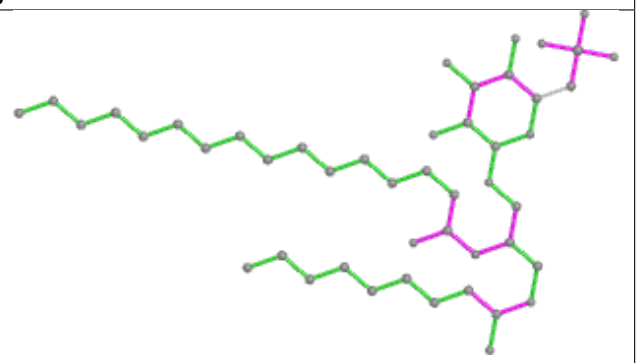
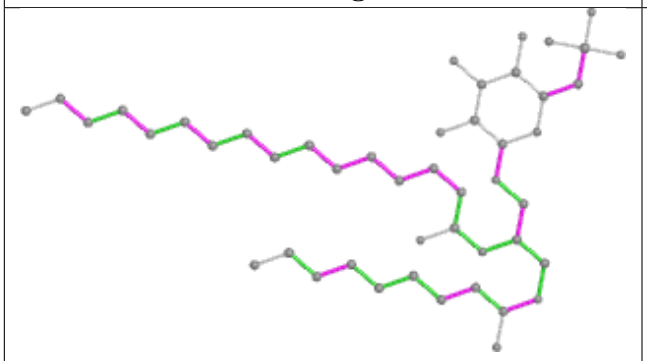


Bond angles



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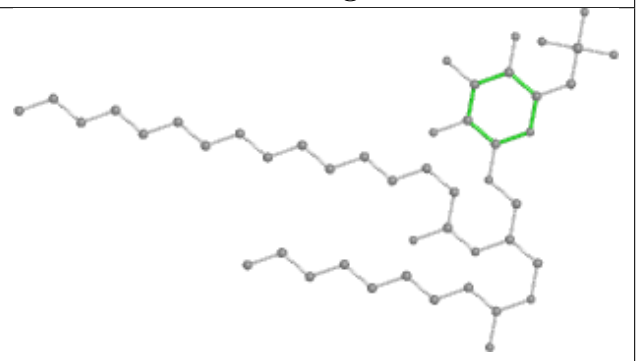
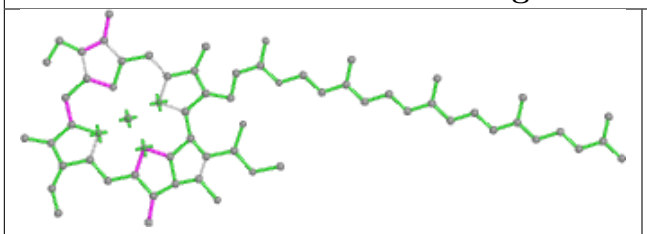
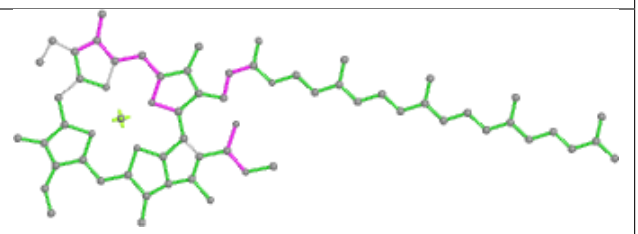


Rings

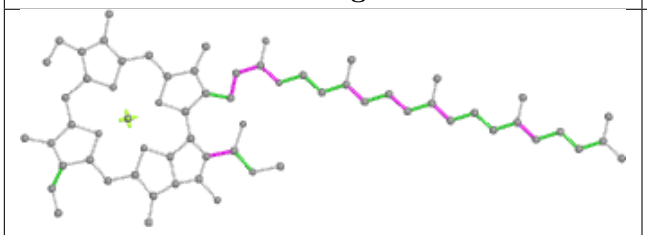
Ligand CLA BA 842



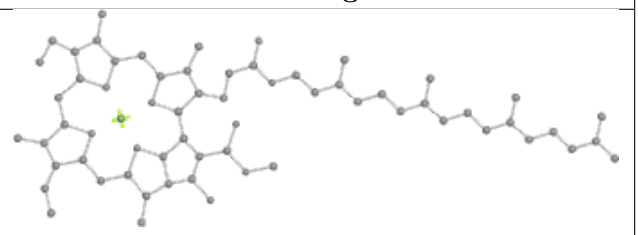
Bond lengths



Bond angles

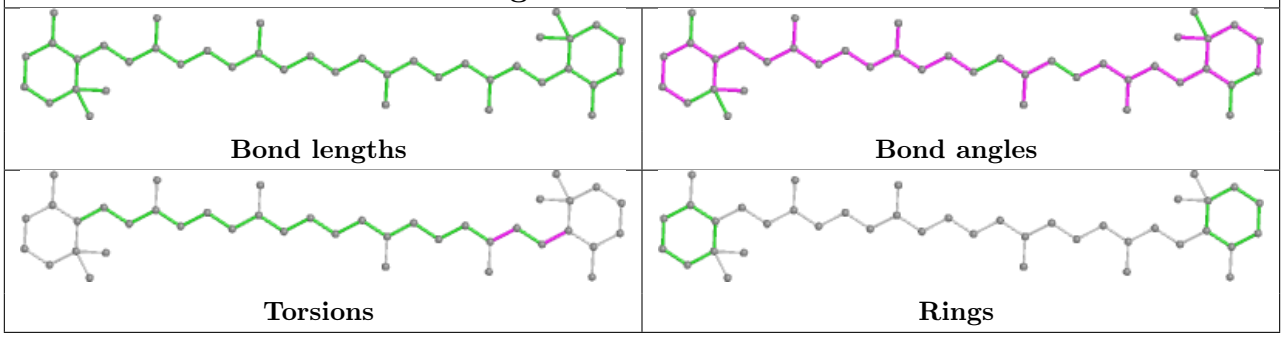


Torsions

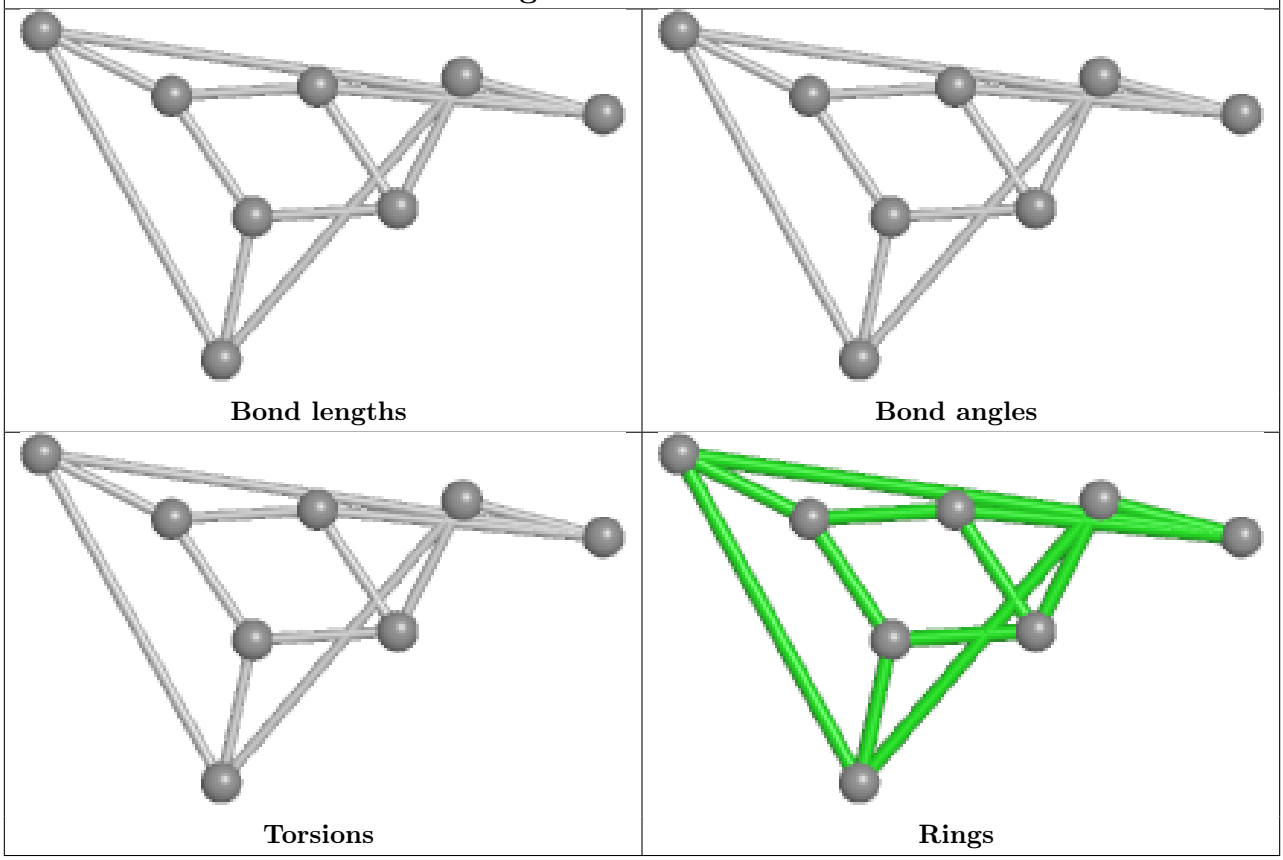


Rings

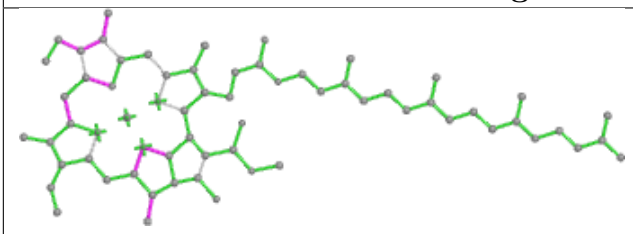
Ligand BCR BA 855



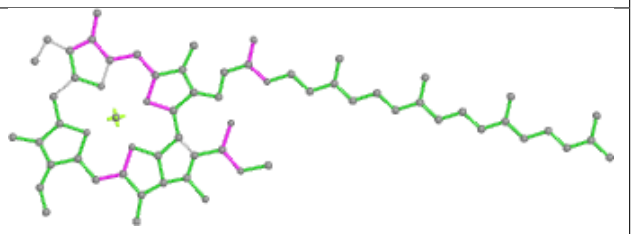
Ligand SF4 BC 101



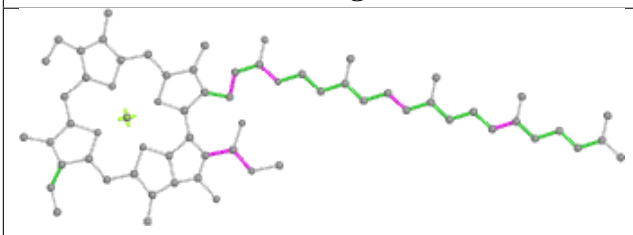
Ligand CLA BA 808



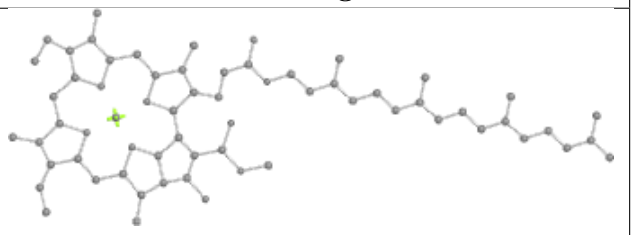
Bond lengths



Bond angles

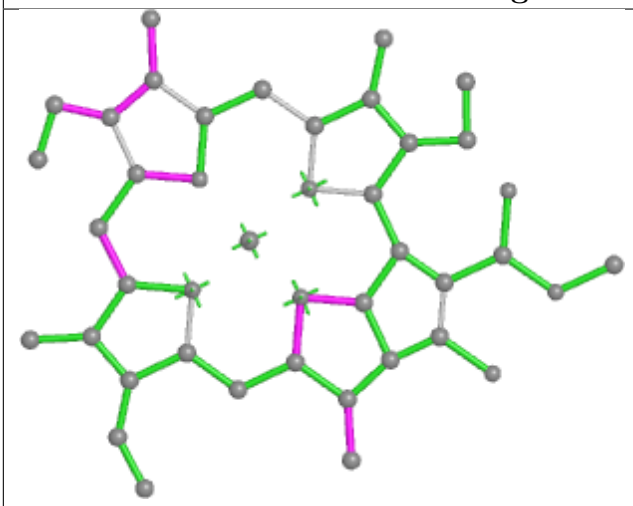


Torsions

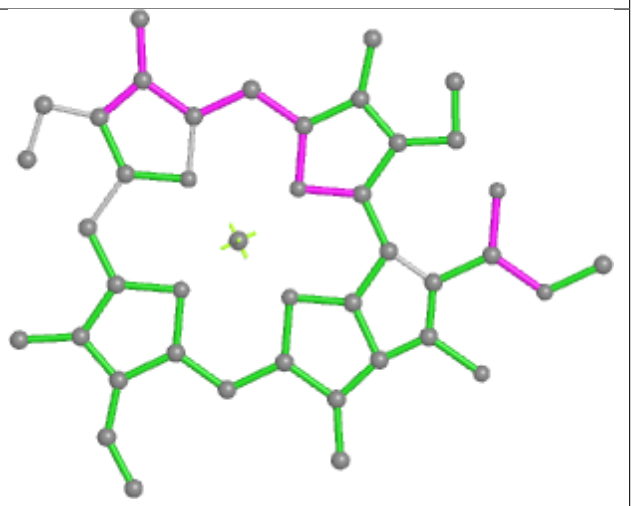


Rings

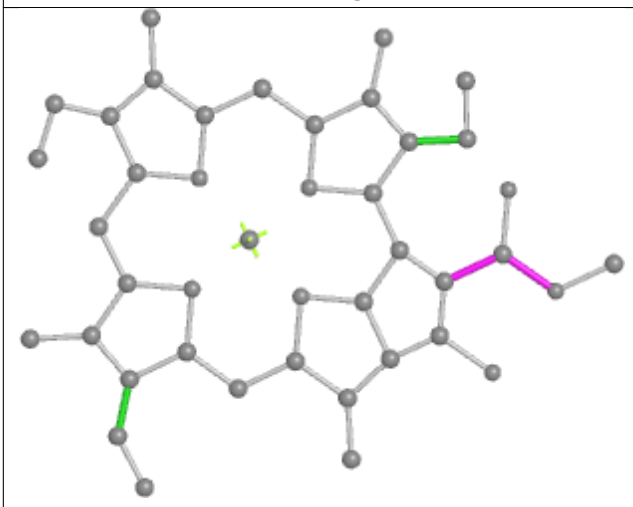
Ligand CLA BA 815



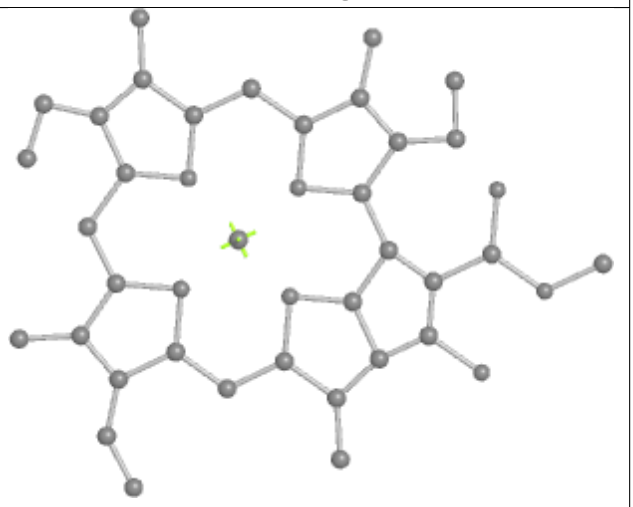
Bond lengths



Bond angles

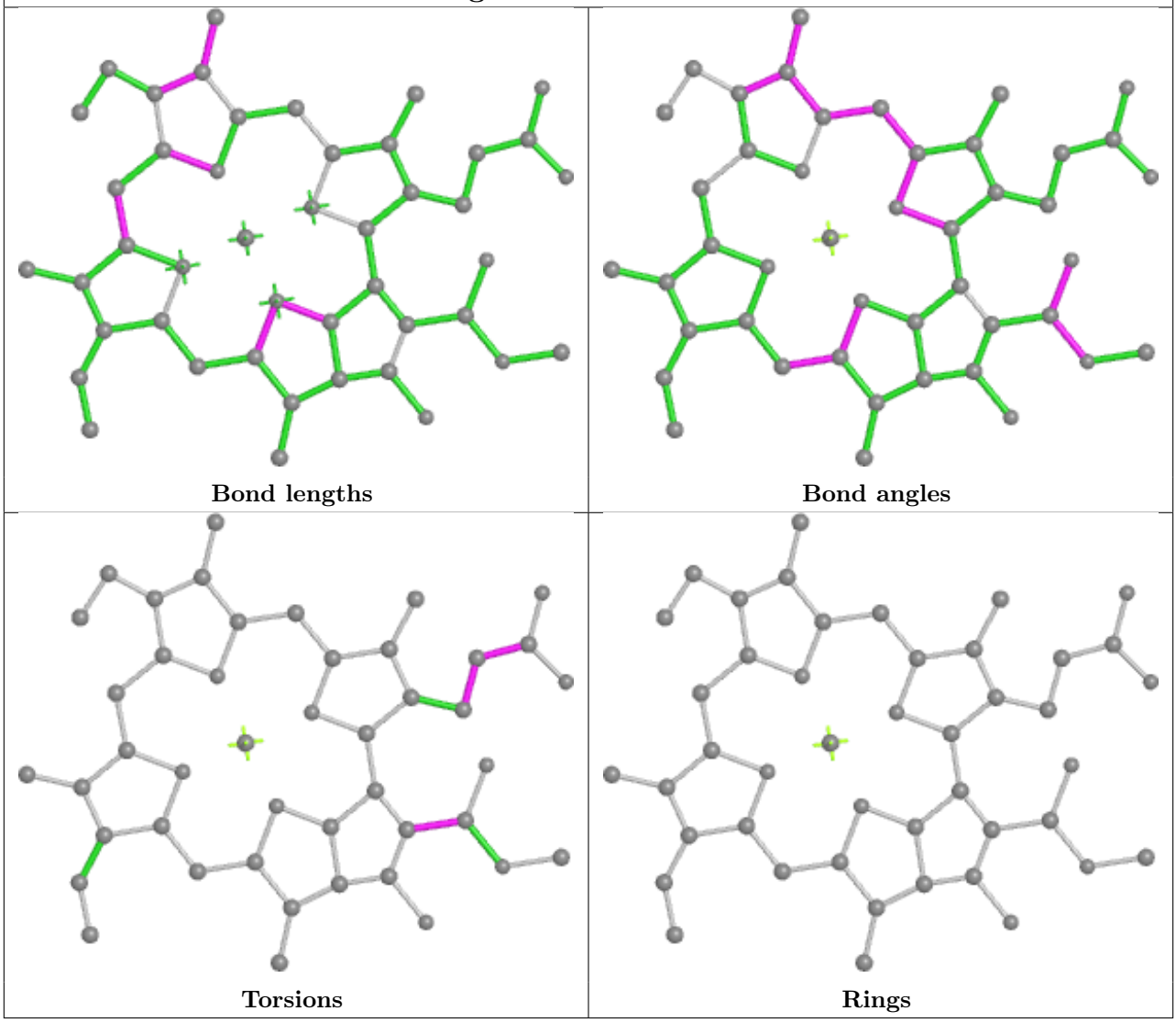


Torsions

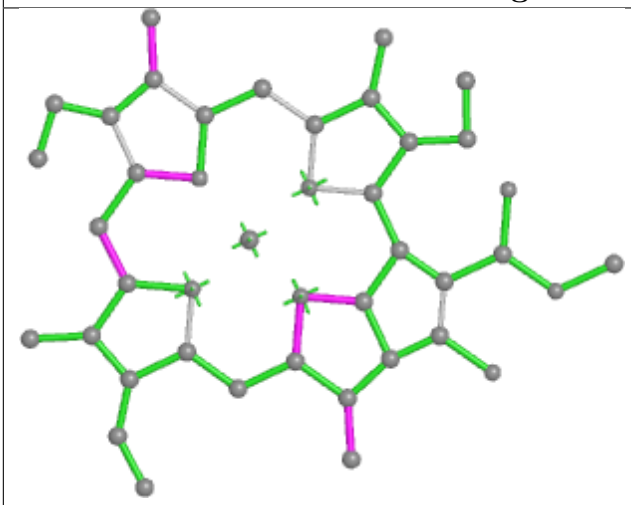


Rings

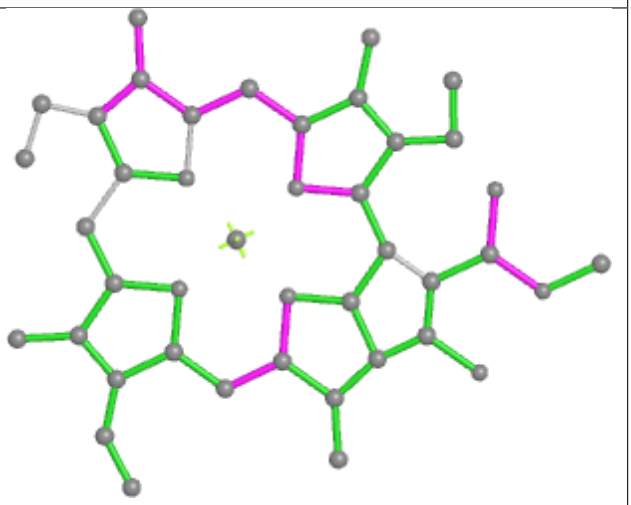
Ligand CLA BK 202



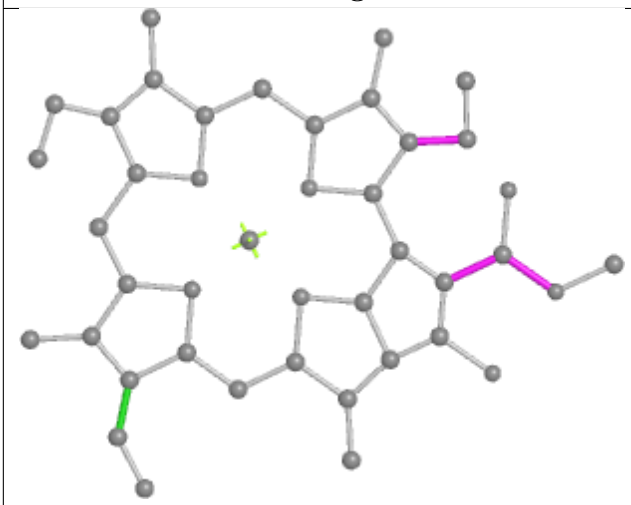
Ligand CLA BA 822



Bond lengths



Bond angles



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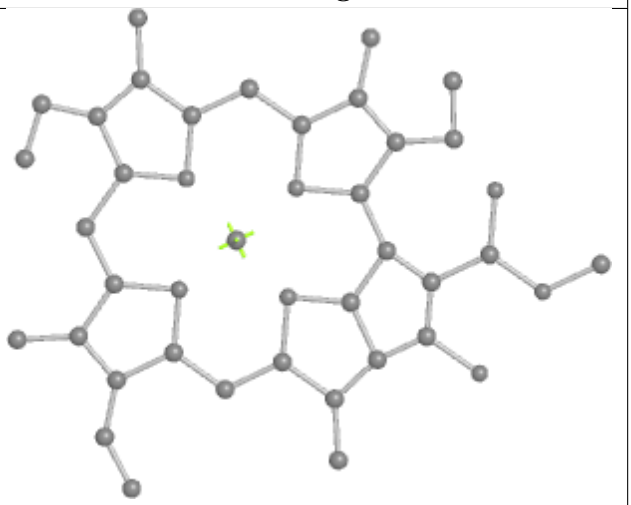
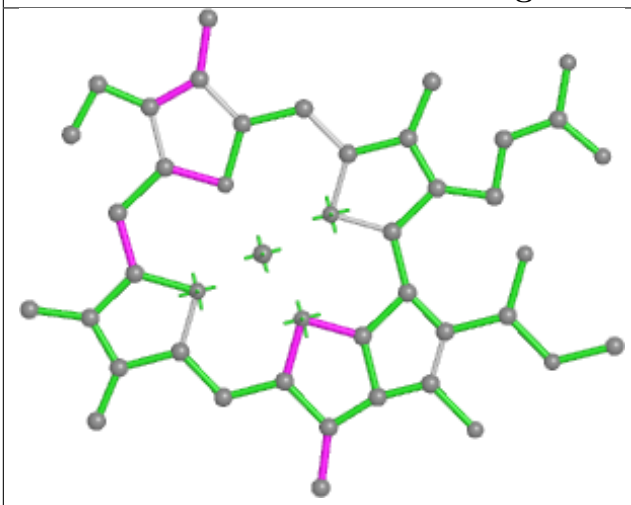
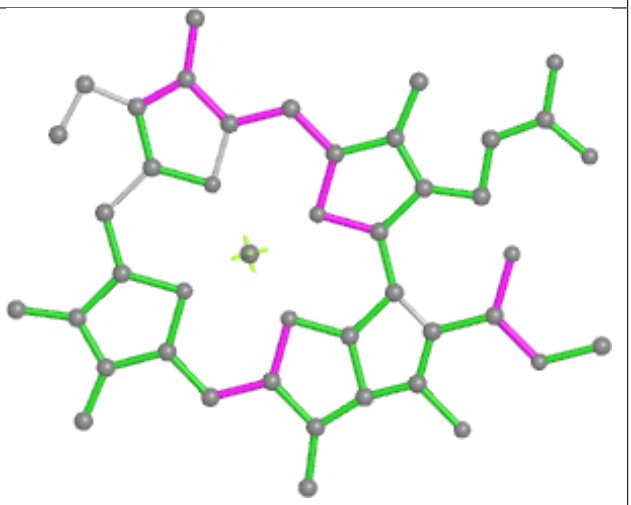


Rings

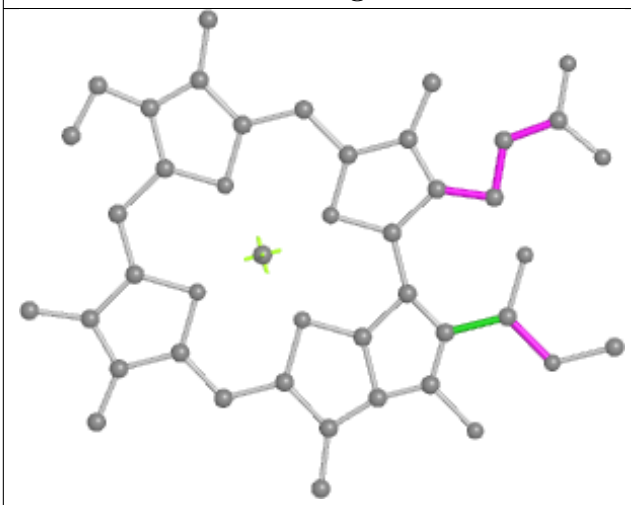
Ligand CLA B2 310



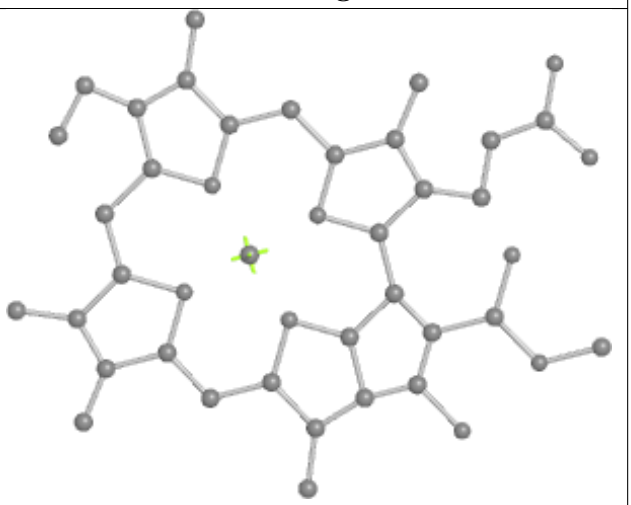
Bond lengths



Bond angles

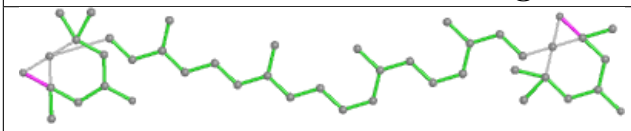


Torsions

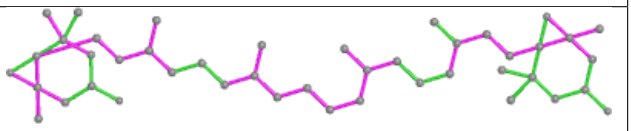


Rings

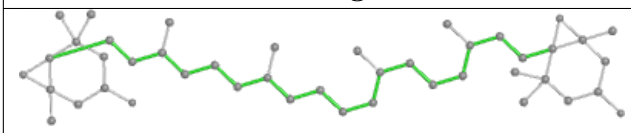
Ligand XAT B1 317



Bond lengths



Bond angles



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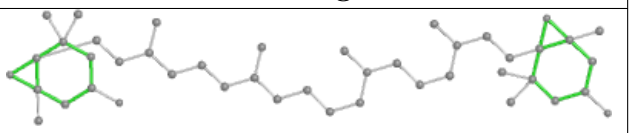
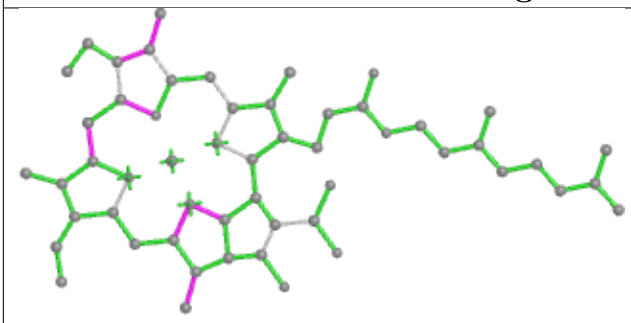
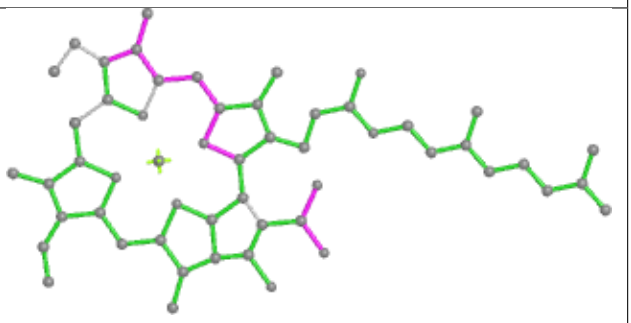


Rings

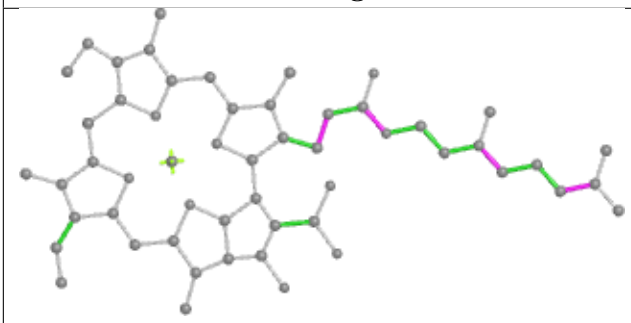
Ligand CLA B3 612



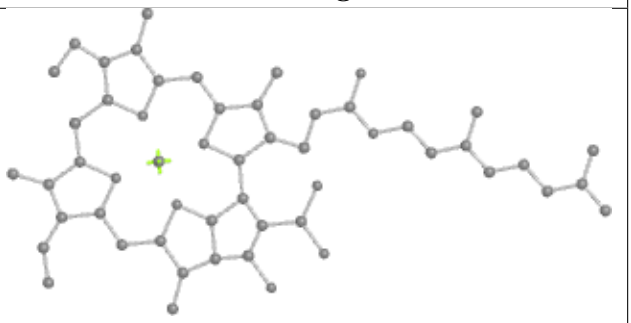
Bond lengths



Bond angles

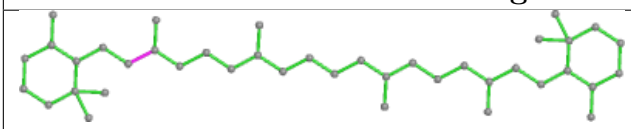


Torsions



Rings

Ligand BCR BB 845



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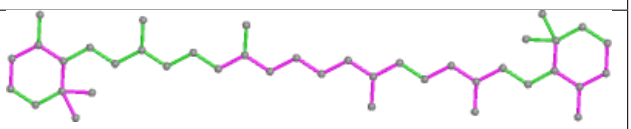
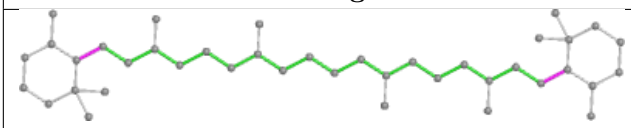


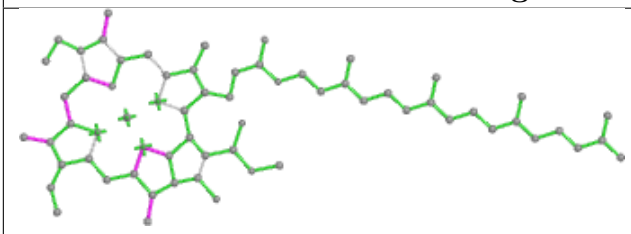
Bond angles



Torsions

Rings

Ligand CLA BA 828



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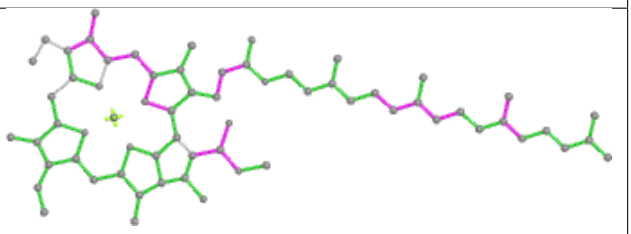
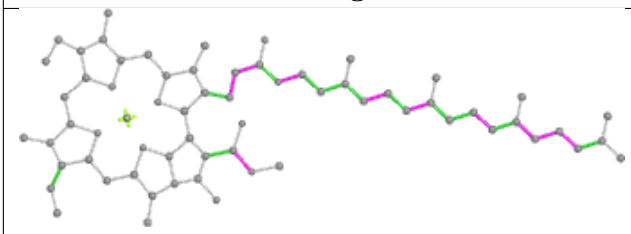
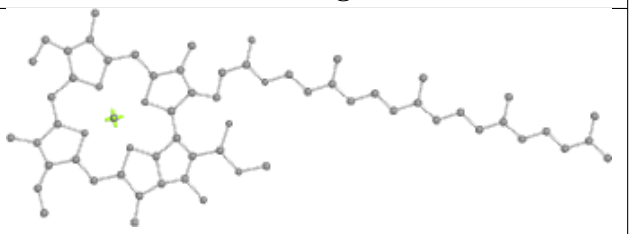


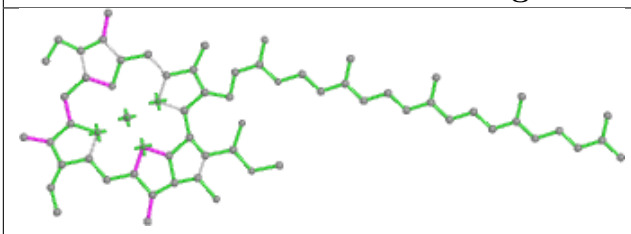
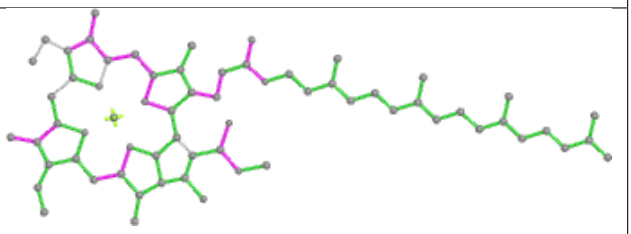
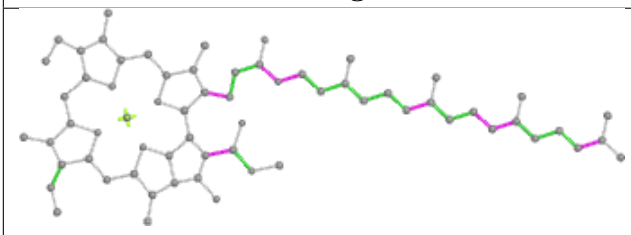
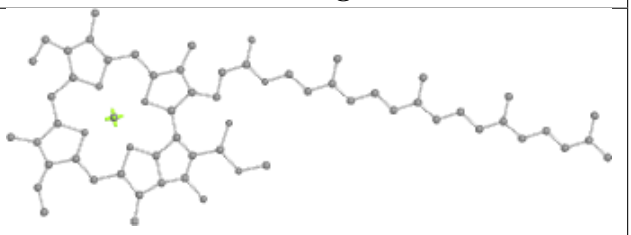
Bond angles

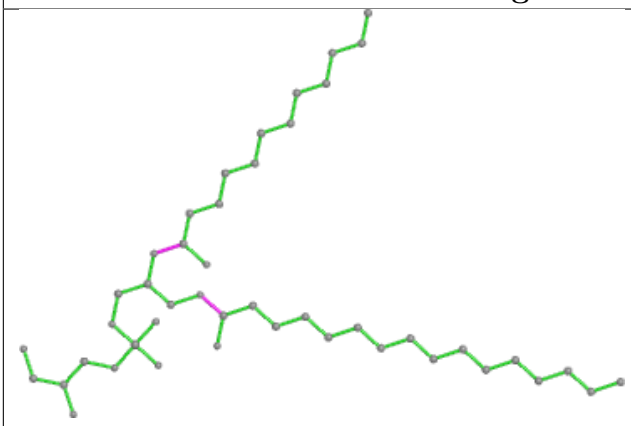
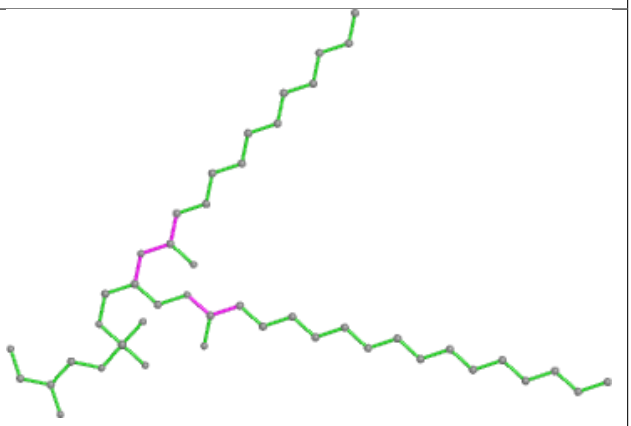
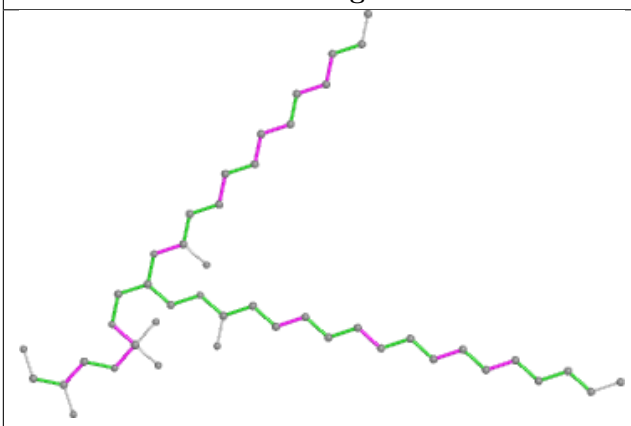
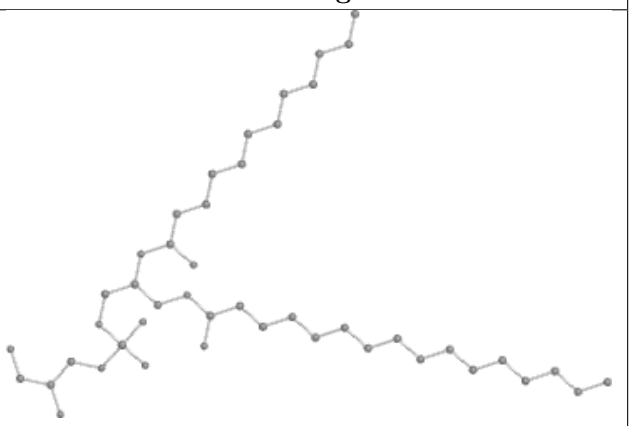


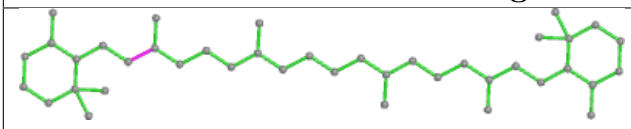
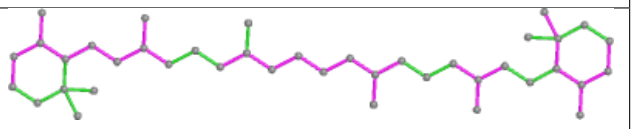
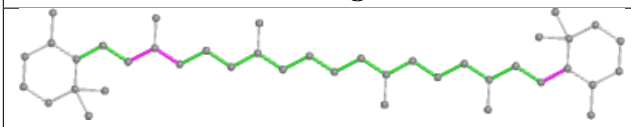
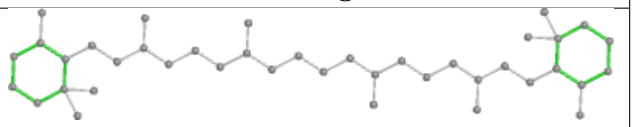
Torsions

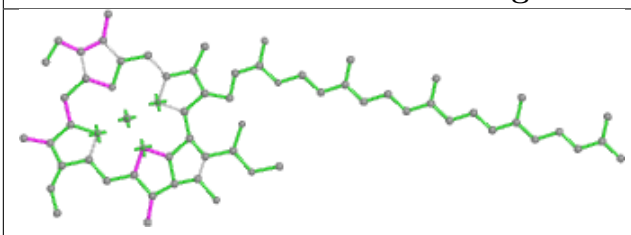
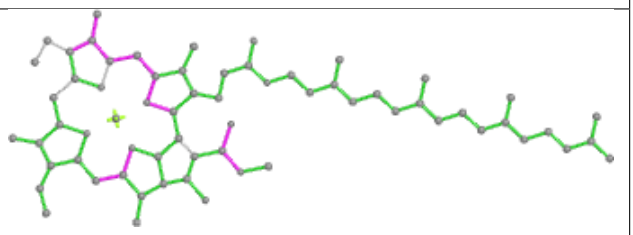
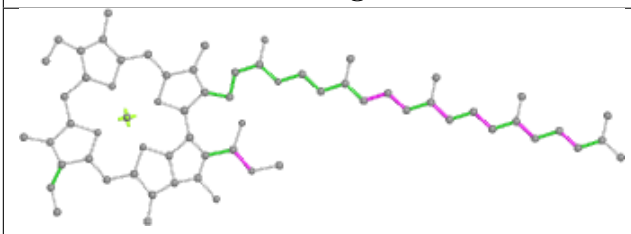
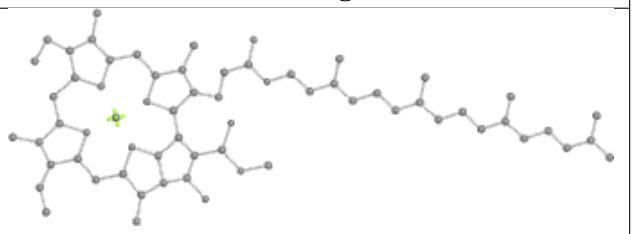


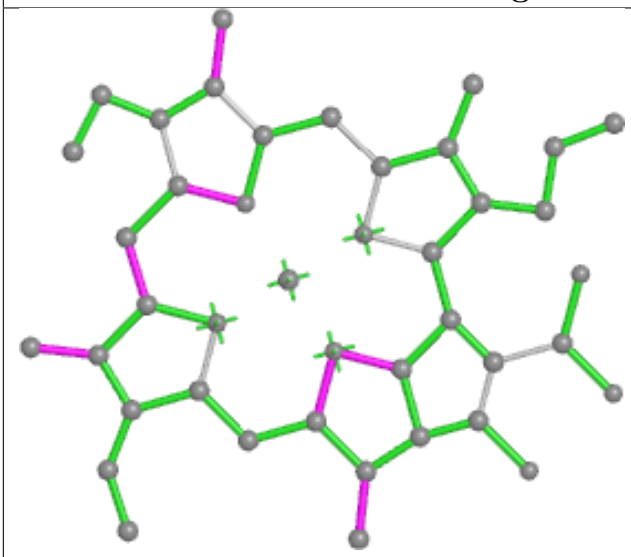
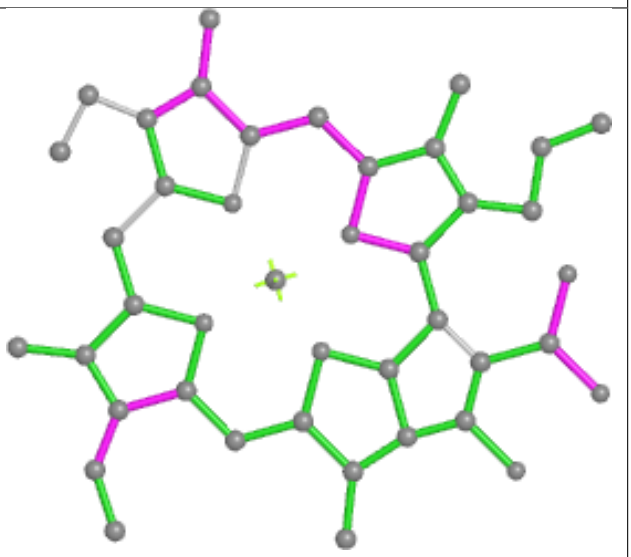
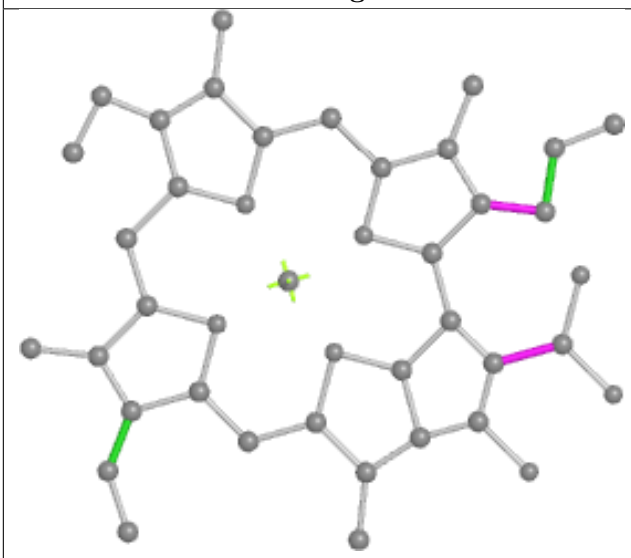
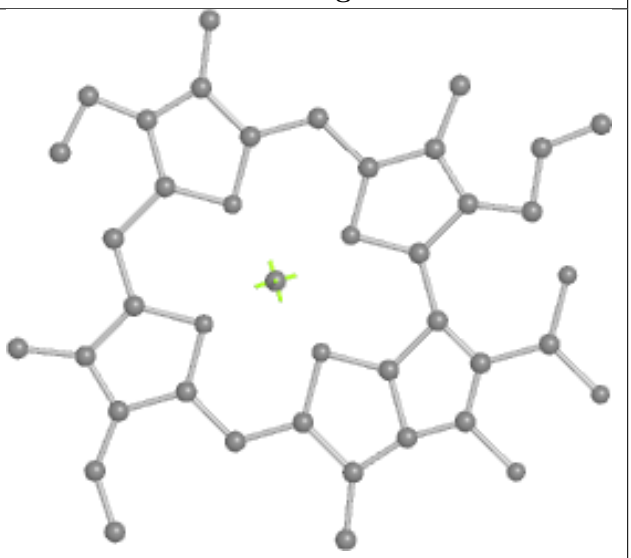
Rings

Ligand CLA BB 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

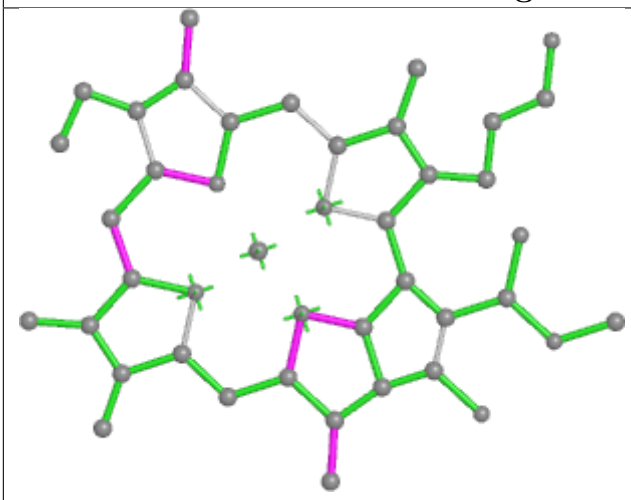
Ligand LHG BF 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR BB 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

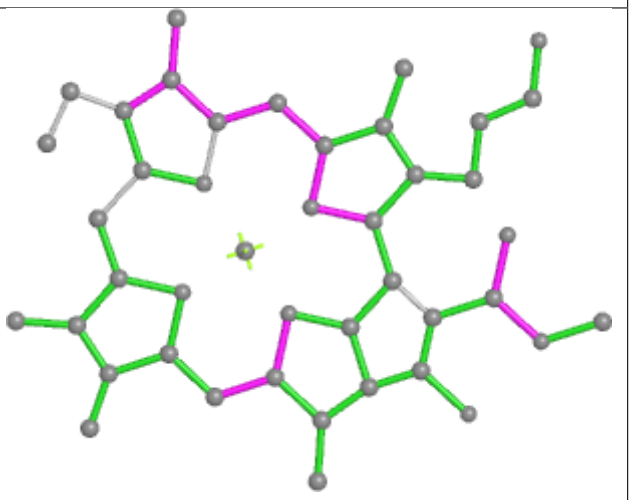
Ligand CLA BB 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

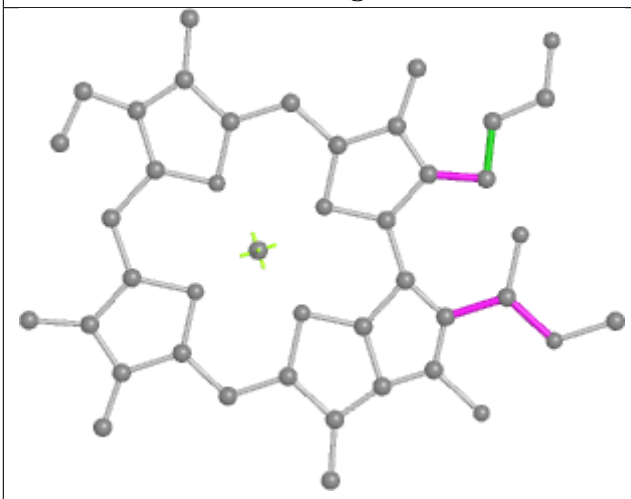
Ligand CLA B2 303



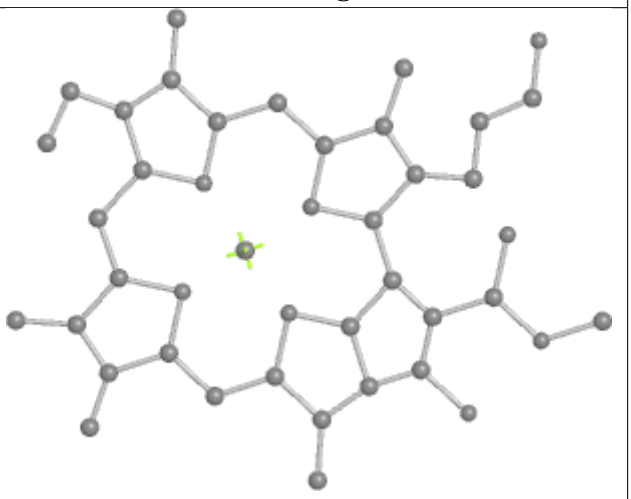
Bond lengths



Bond angles

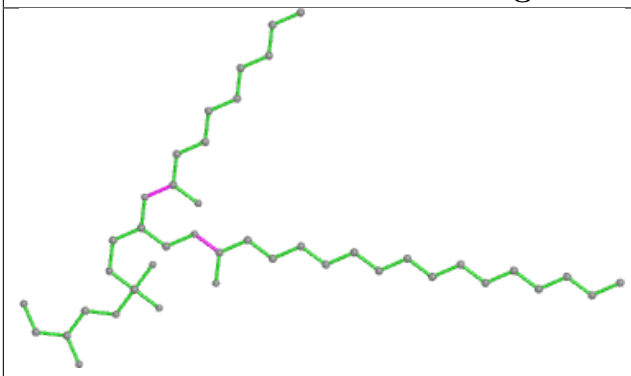


Torsions

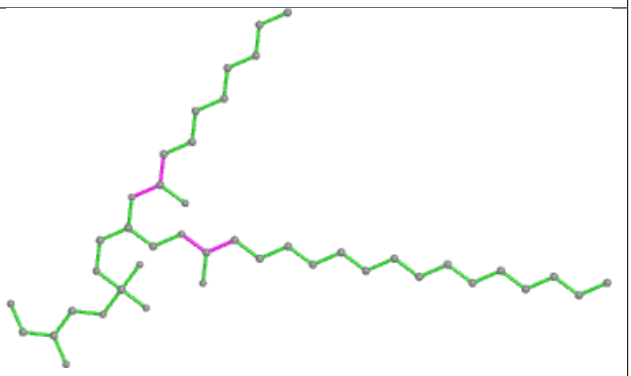


Rings

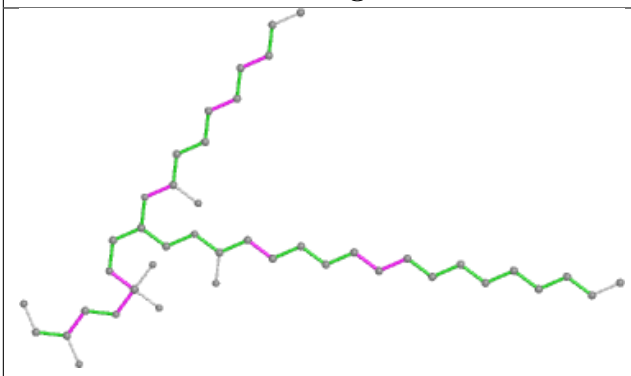
Ligand LHG B1 318



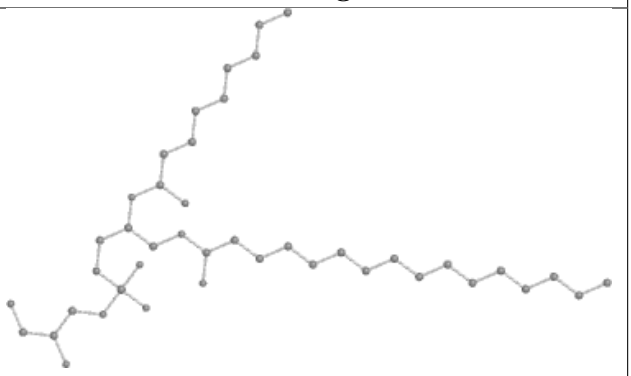
Bond lengths



Bond angles

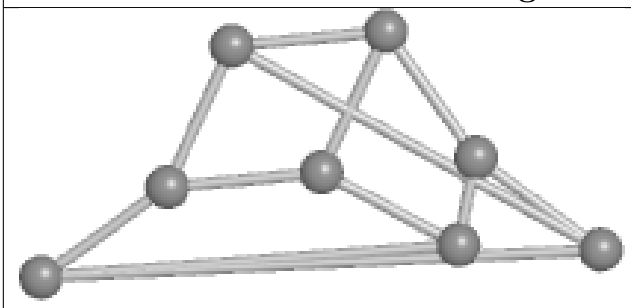


Torsions

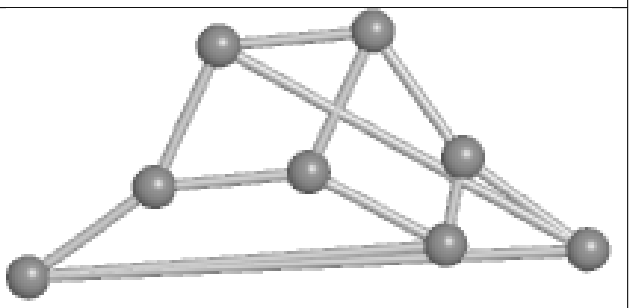


Rings

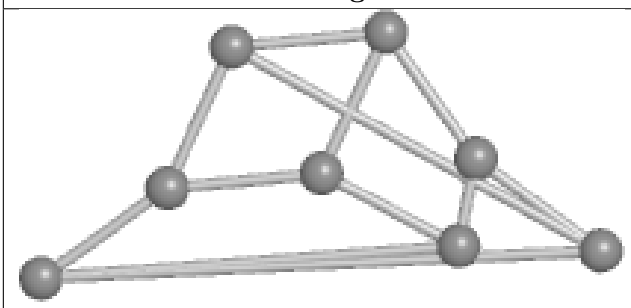
Ligand SF4 BC 102



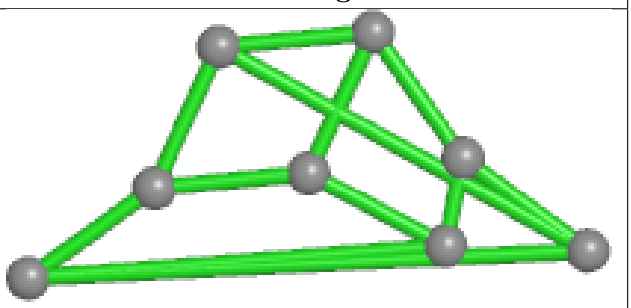
Bond lengths



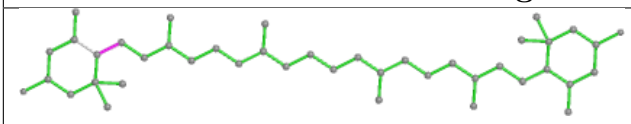
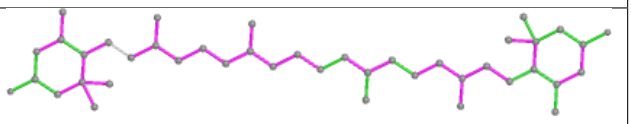
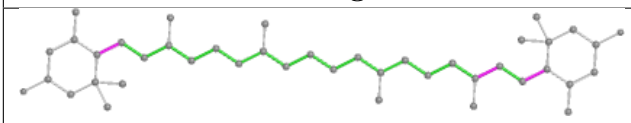
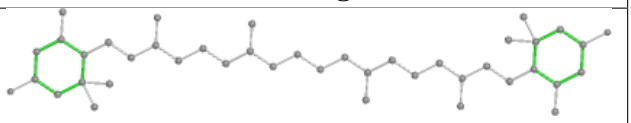
Bond angles



Torsions



Rings

Ligand LUT B3 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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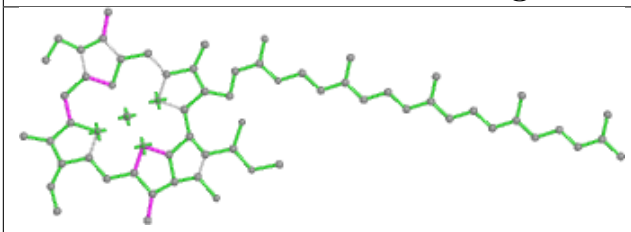
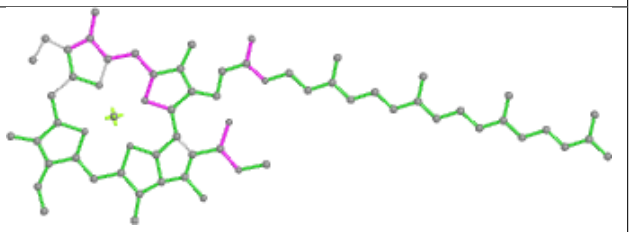
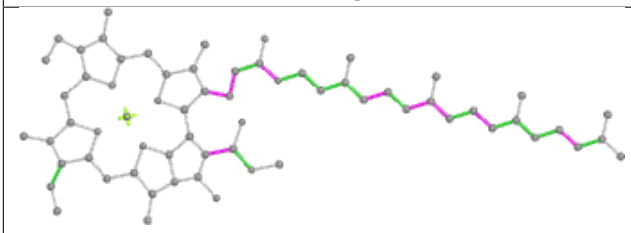
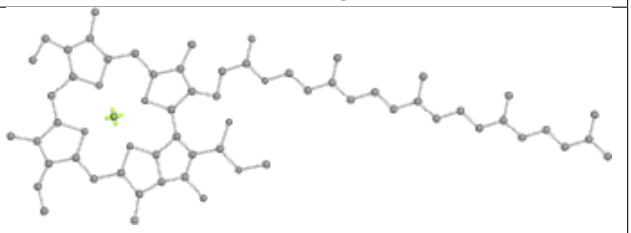
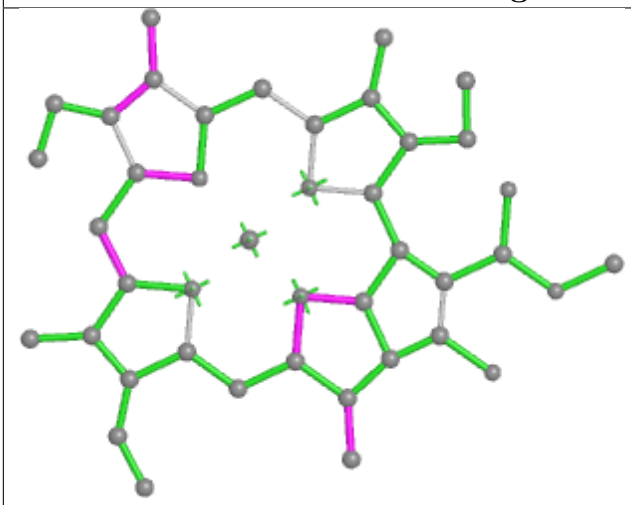
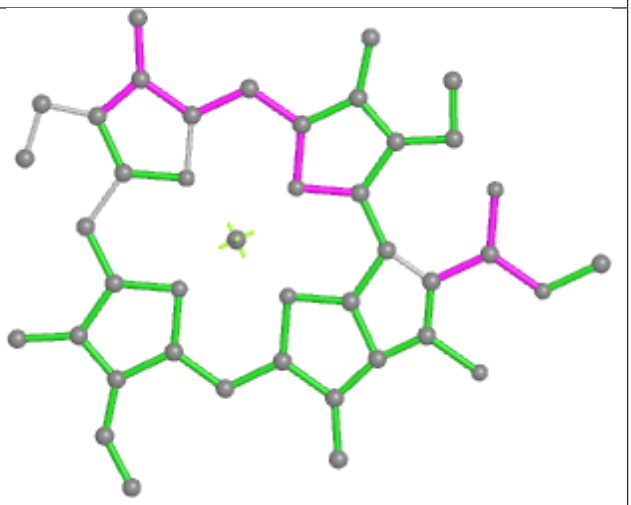
 Bond lengths	 Bond angles
 Torsions	 Rings

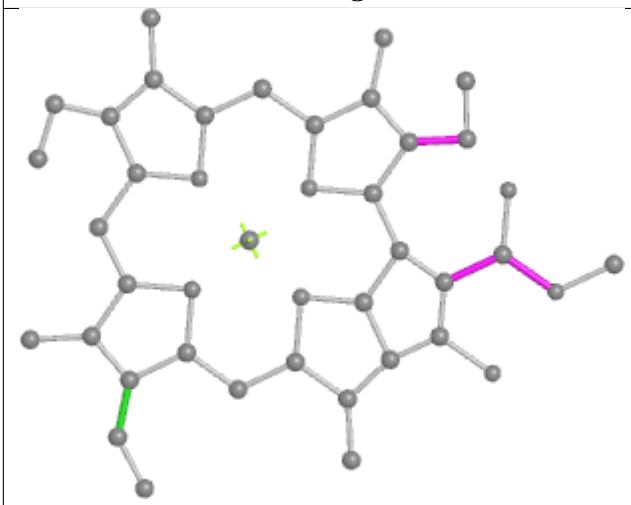
Ligand CLA BG 201



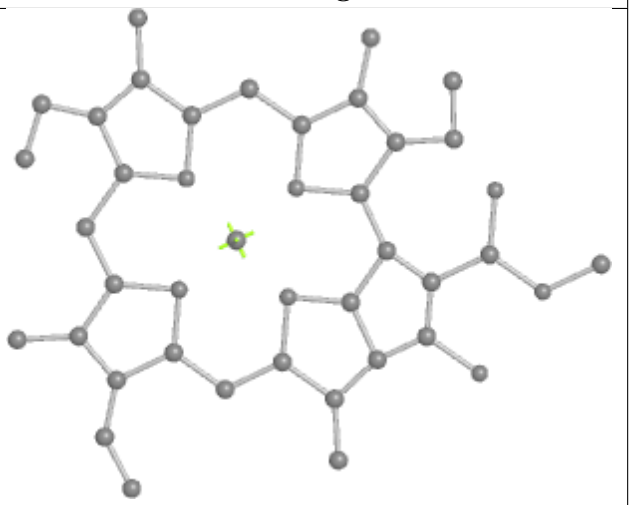
Bond lengths



Bond angles



Torsions



Rings

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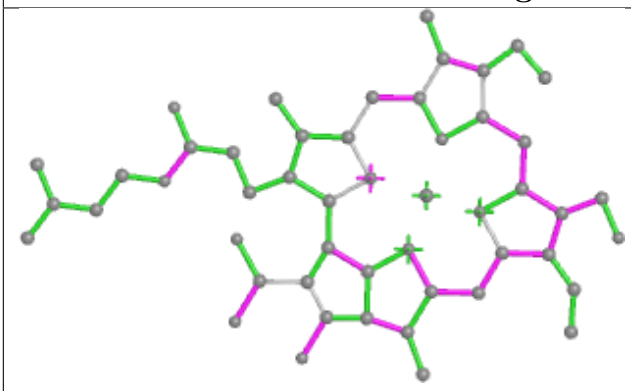
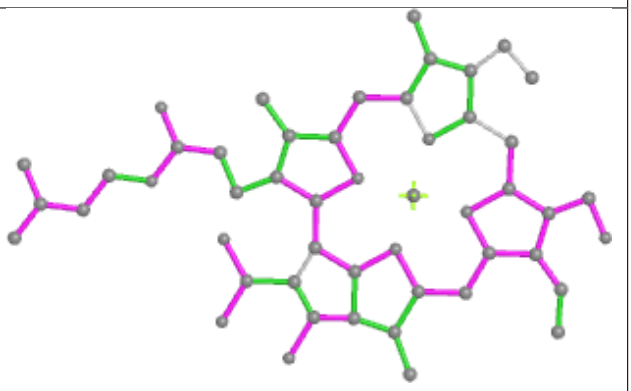
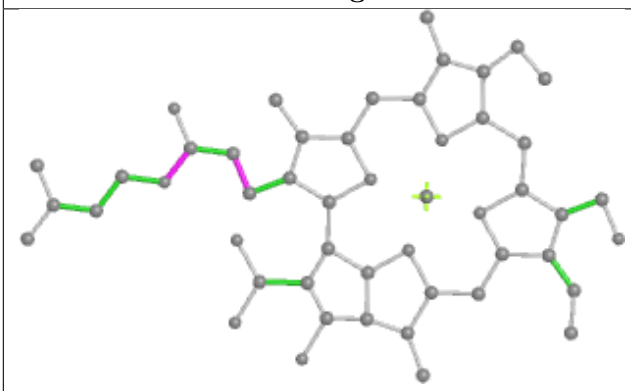
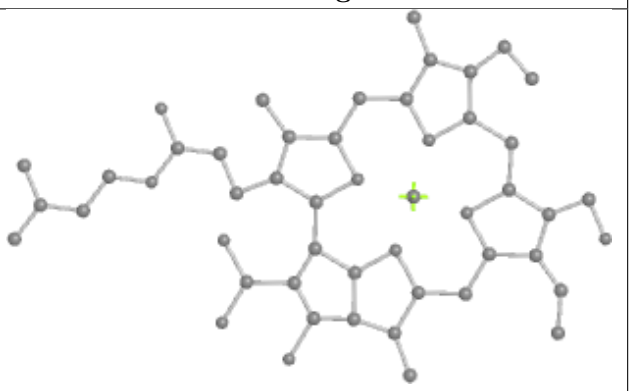
 Bond lengths	 Bond angles
 Torsions	 Rings

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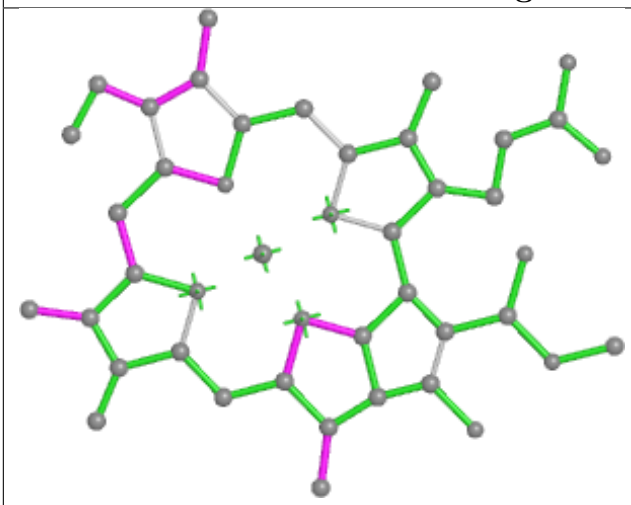
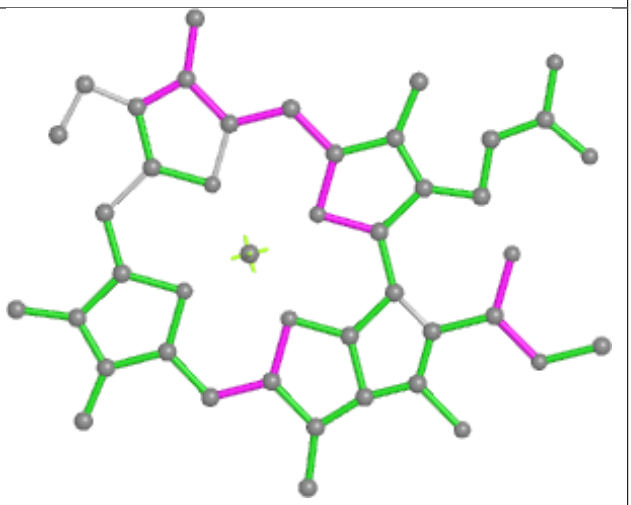
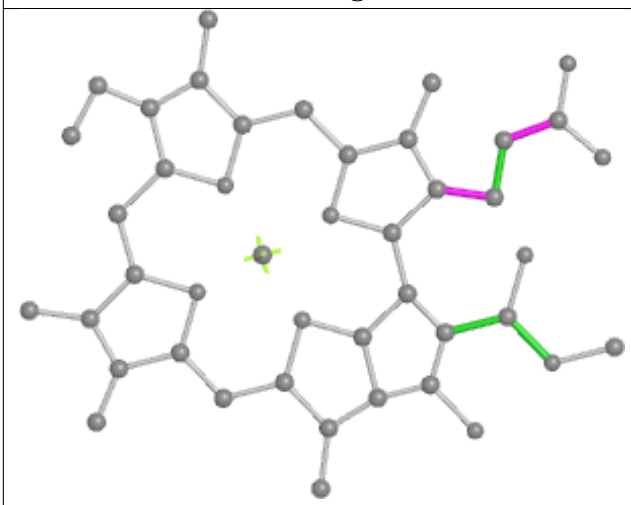
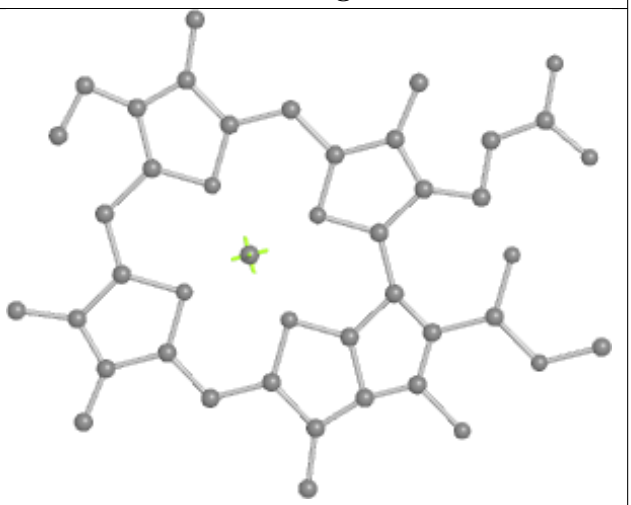
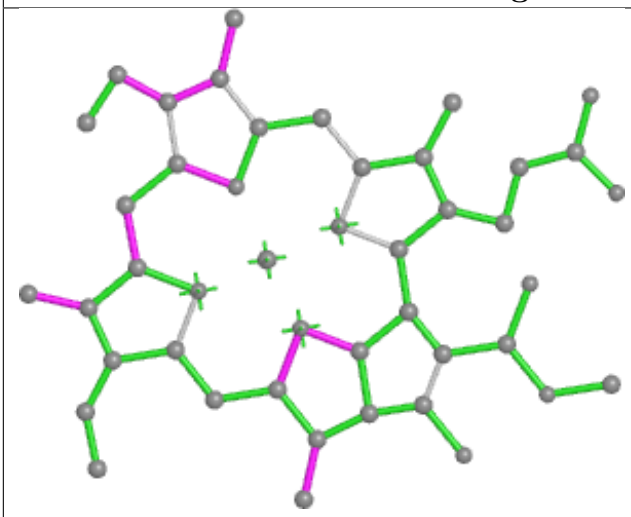
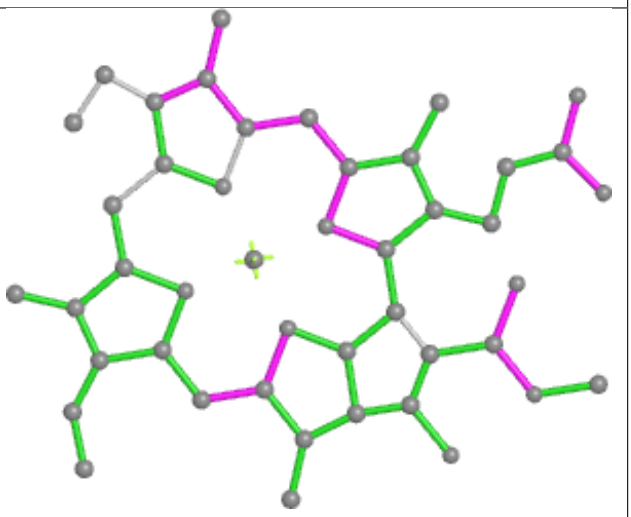
 Bond lengths	 Bond angles
 Torsions	 Rings

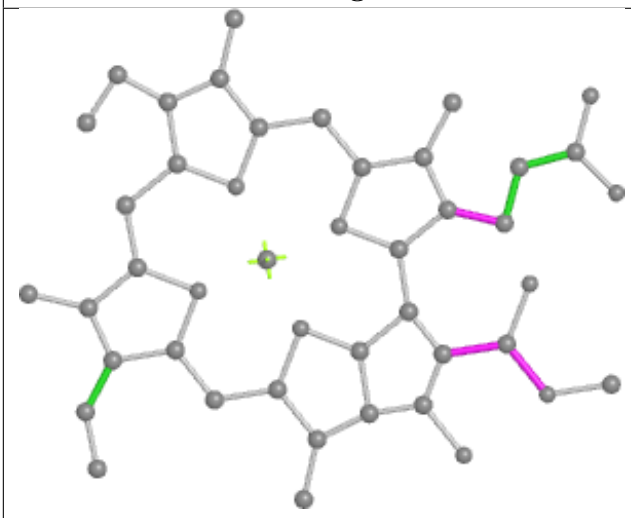
Ligand CLA BA 814



Bond lengths



Bond angles



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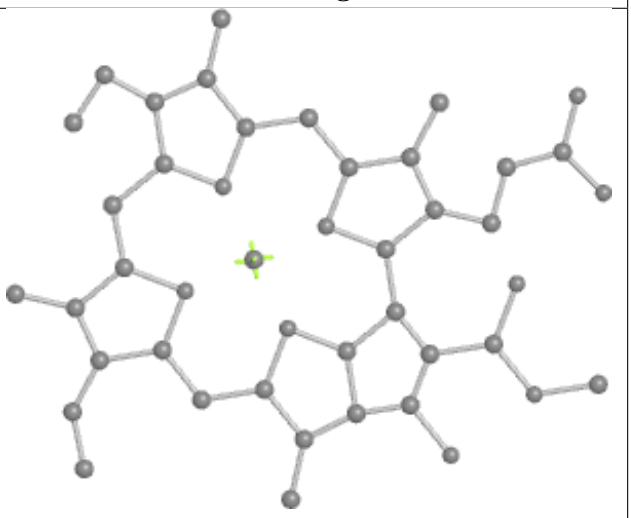
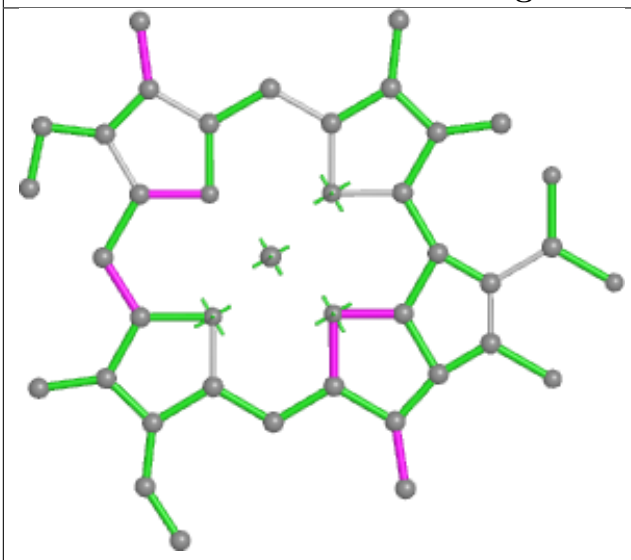


Rings

Ligand CLA B3 613



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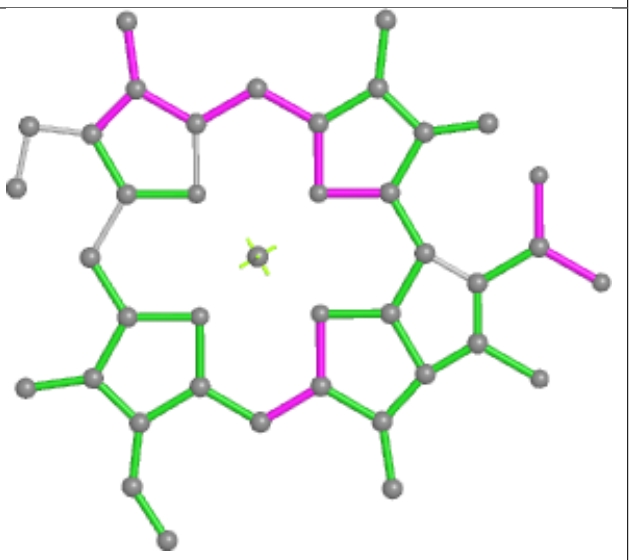
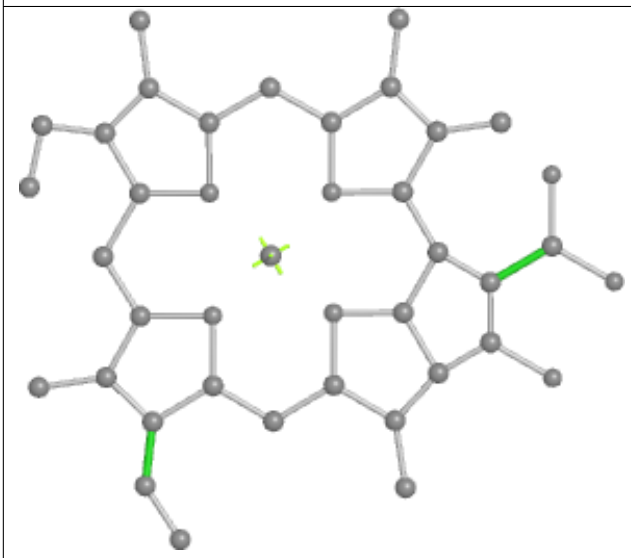


Bond angles



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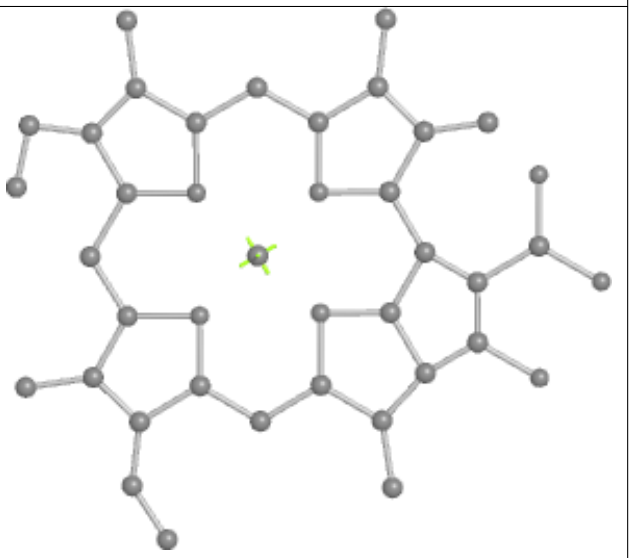

Rings

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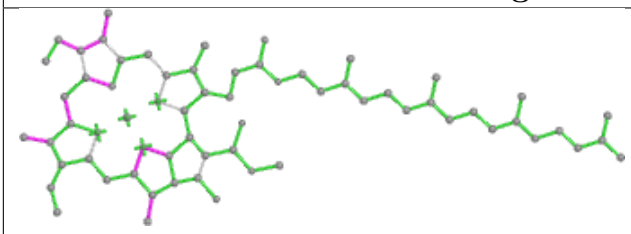
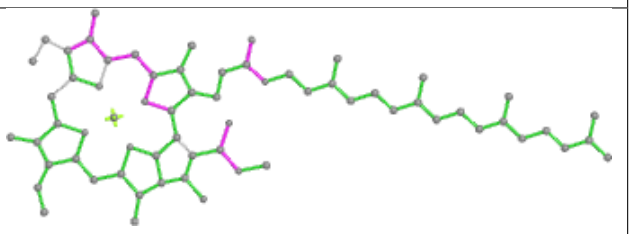
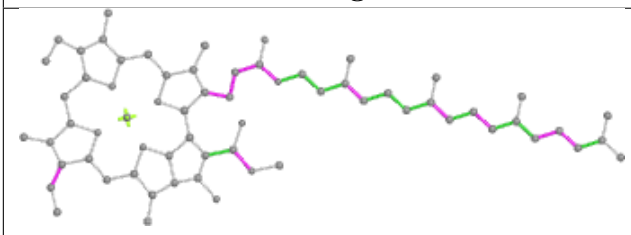
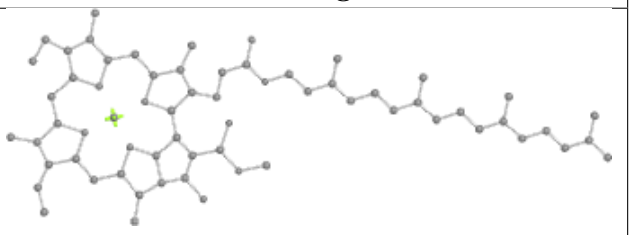
 Bond lengths	 Bond angles
 Torsions	 Rings

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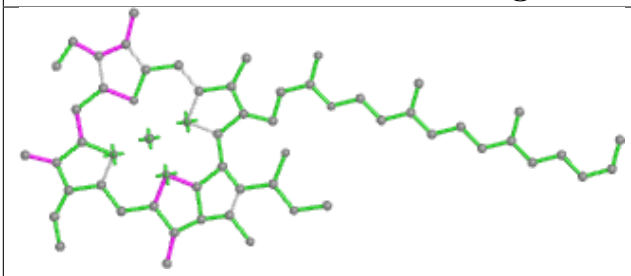
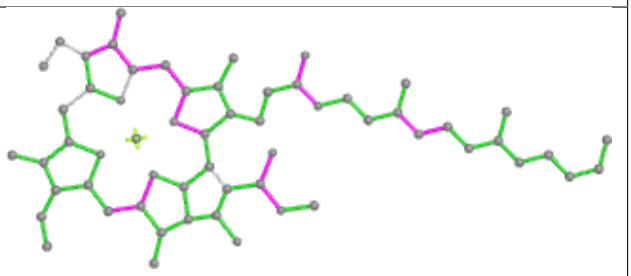
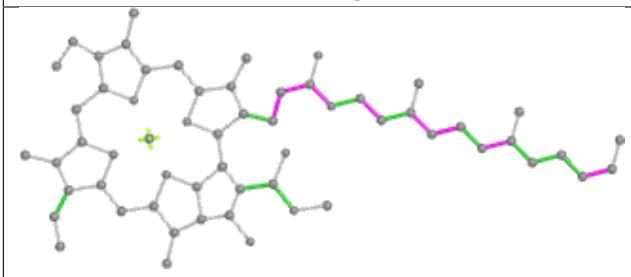
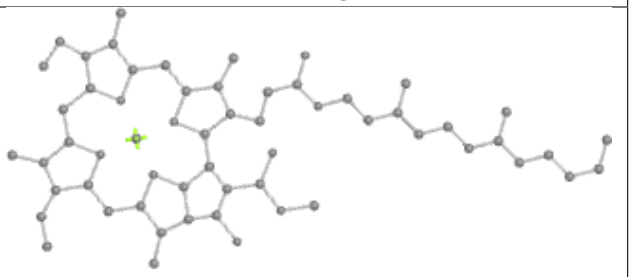
 Bond lengths	 Bond angles
 Torsions	 Rings

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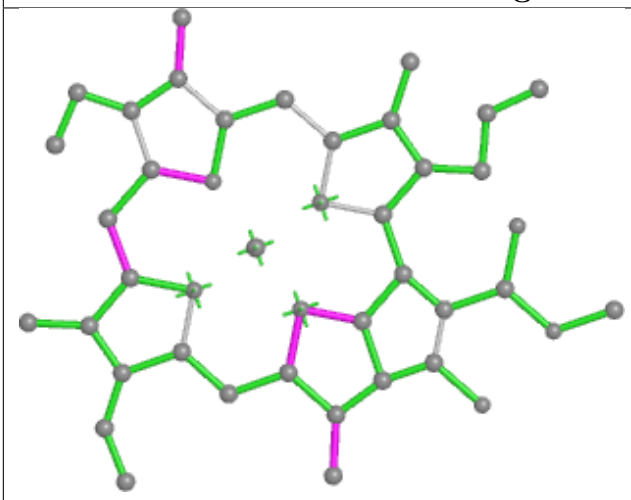
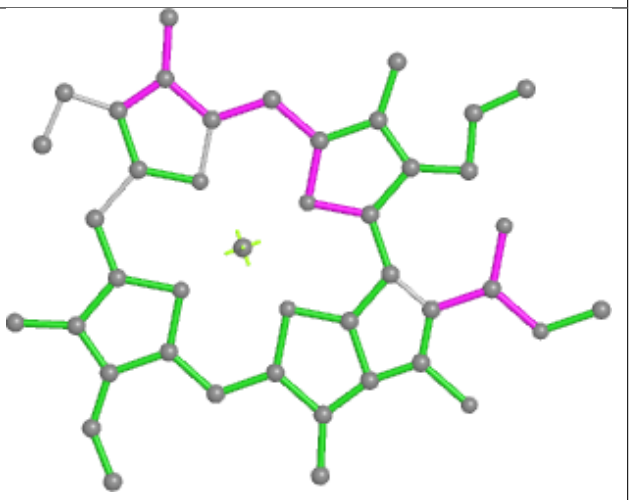
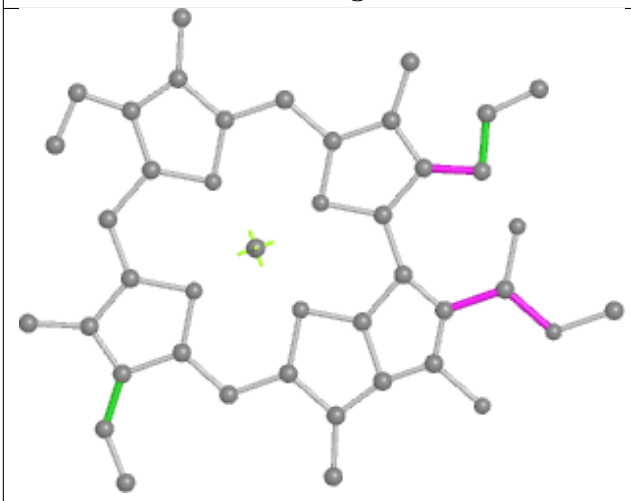
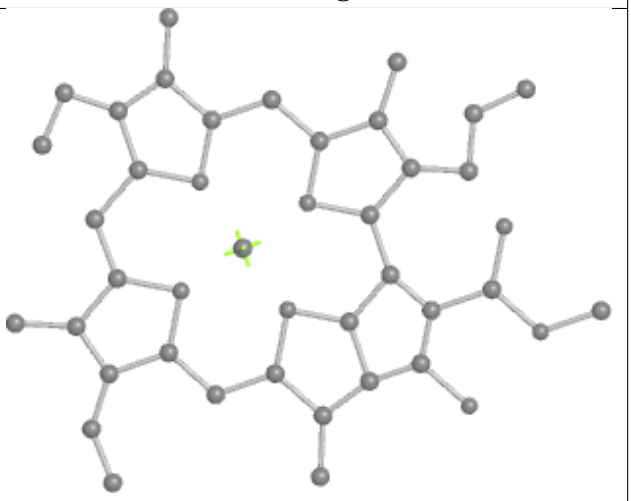
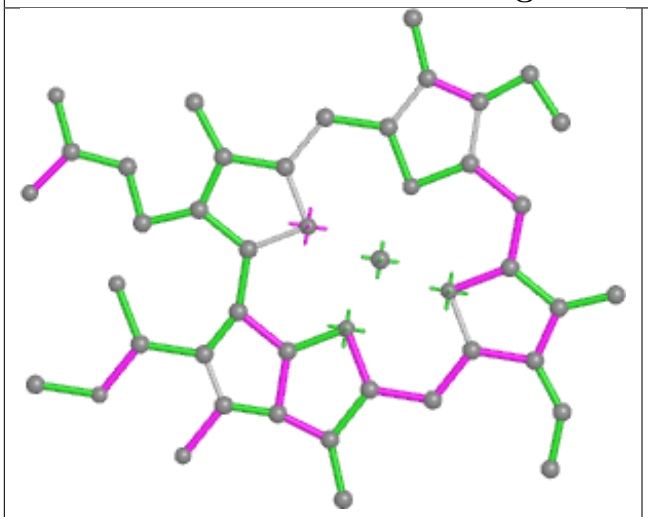
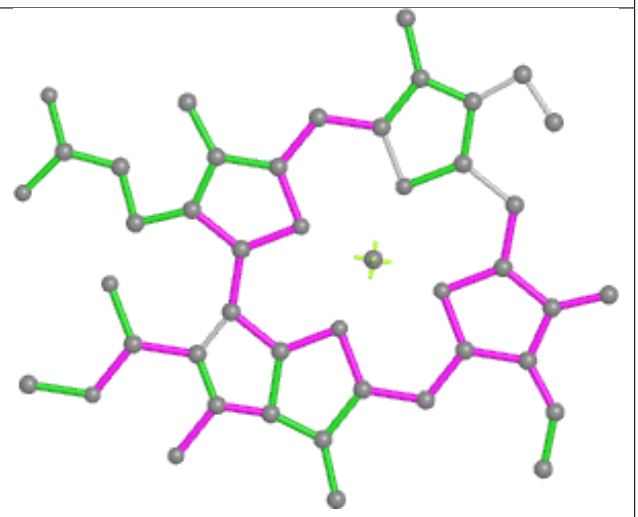
 Bond lengths	 Bond angles
 Torsions	 Rings

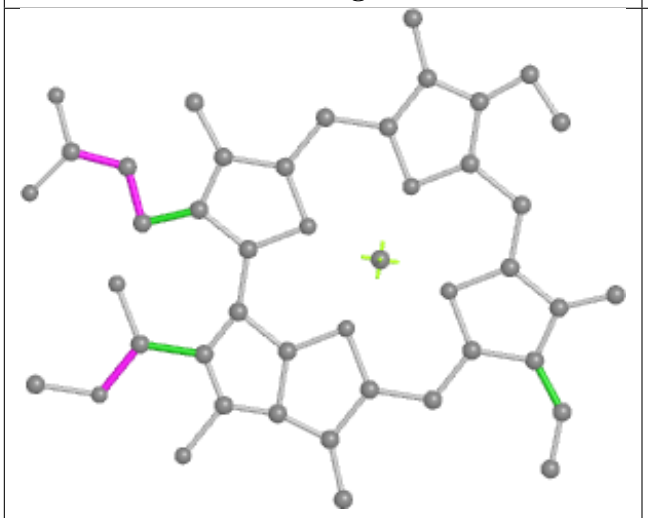
Ligand CHL B3 607



Bond lengths



Bond angles



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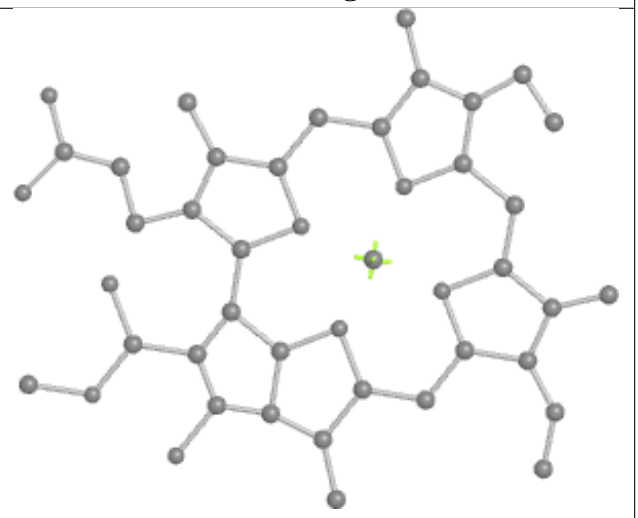
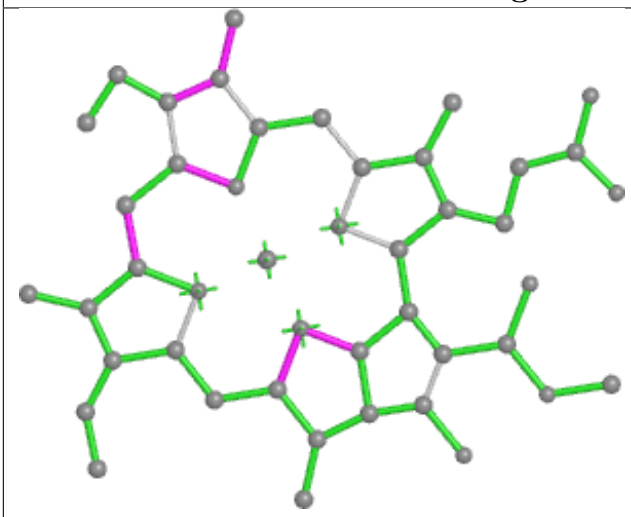
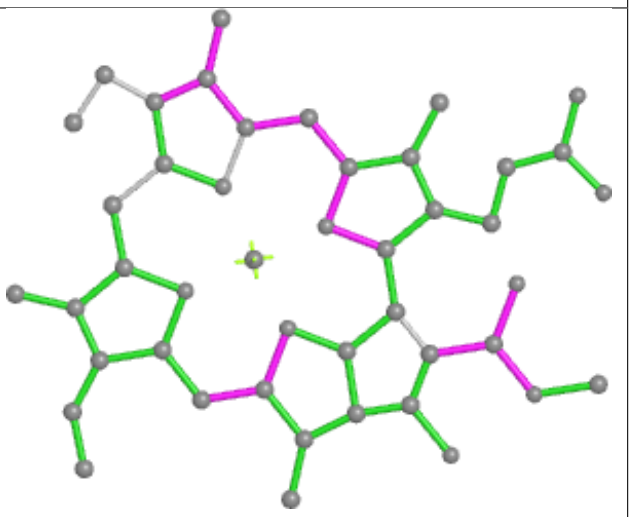


Rings

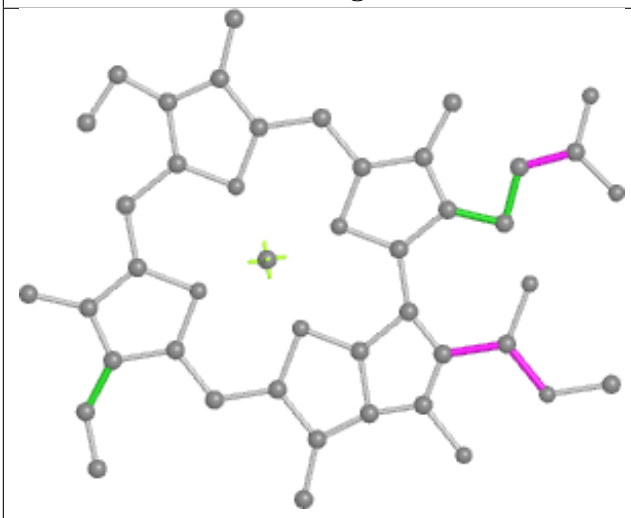
Ligand CLA BA 836



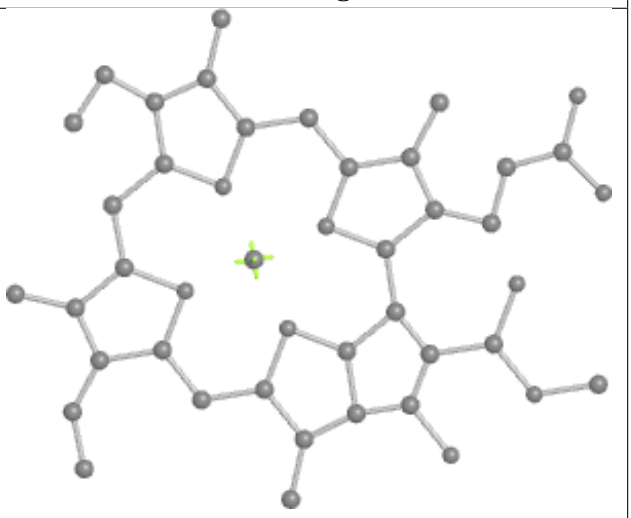
Bond lengths



Bond angles

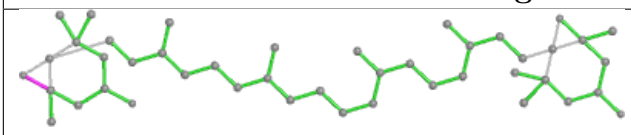


Torsions

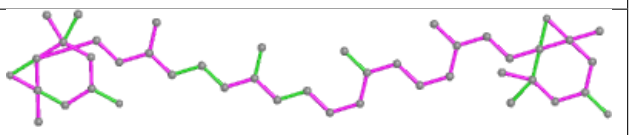


Rings

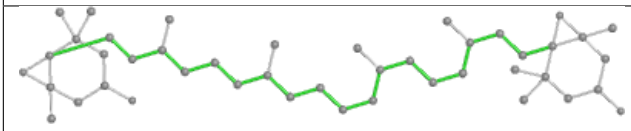
Ligand XAT B3 617



Bond lengths



Bond angles



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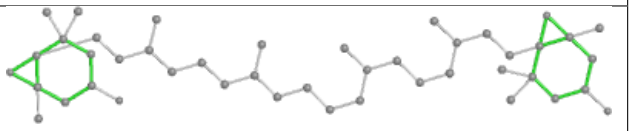
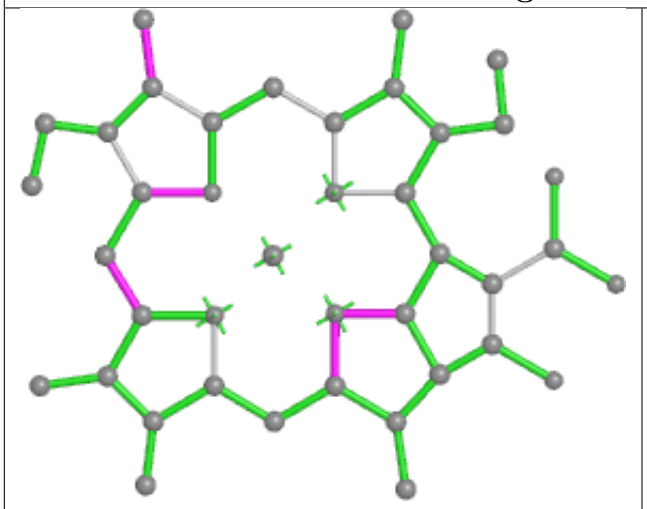
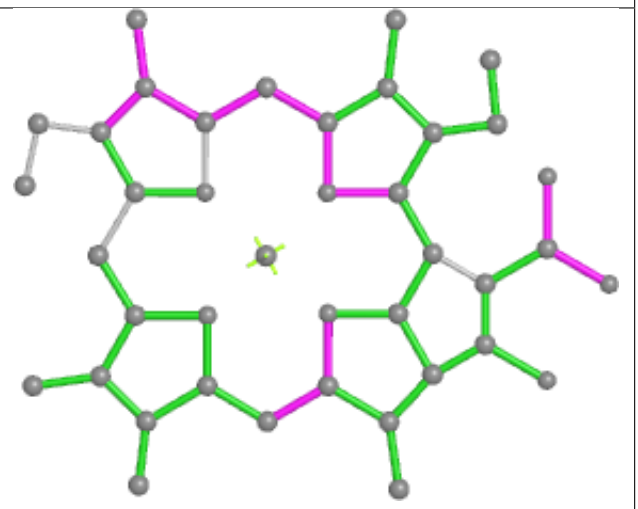


Rings

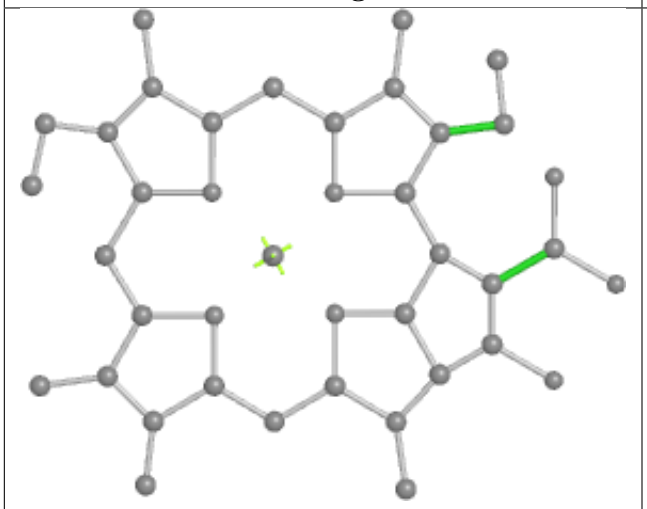
Ligand CLA B3 610



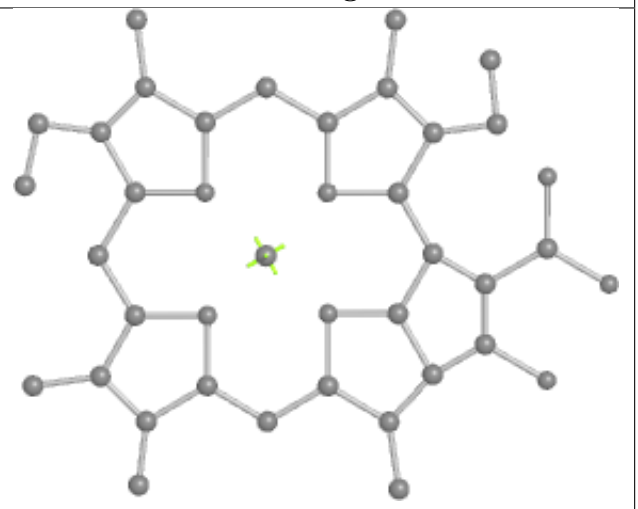
Bond lengths



Bond angles

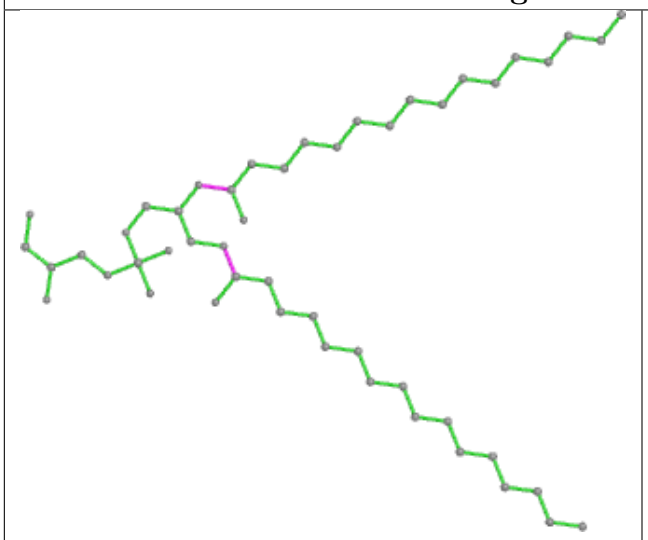


Torsions

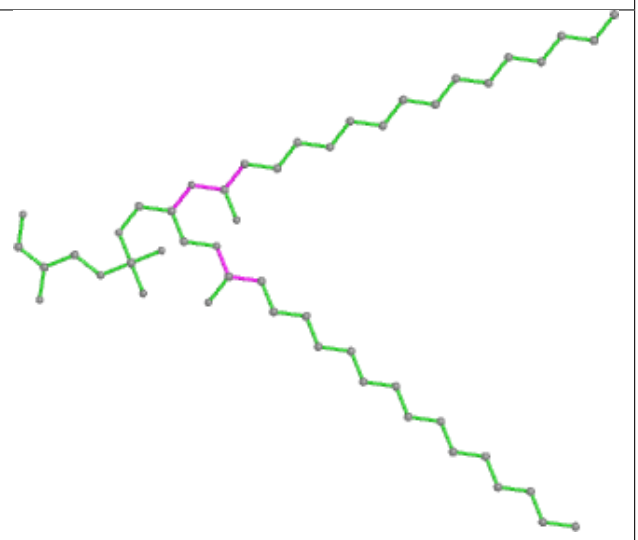


Rings

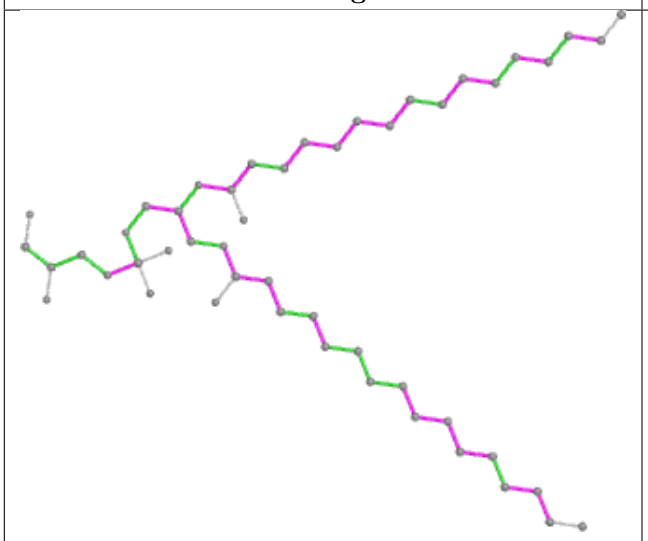
Ligand LHG BA 845



Bond lengths



Bond angles



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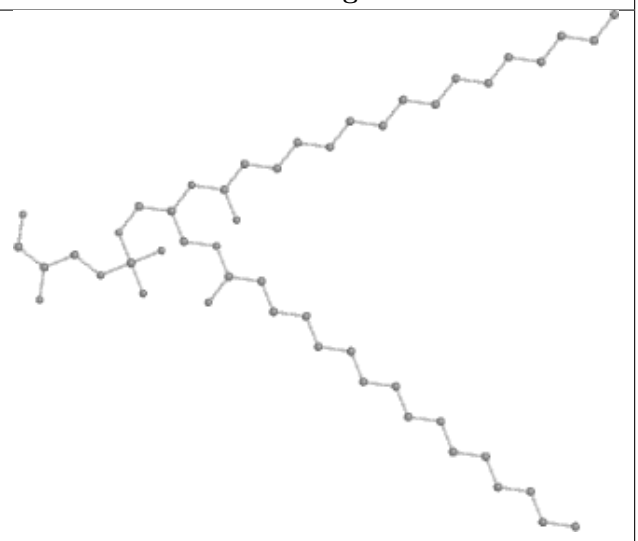
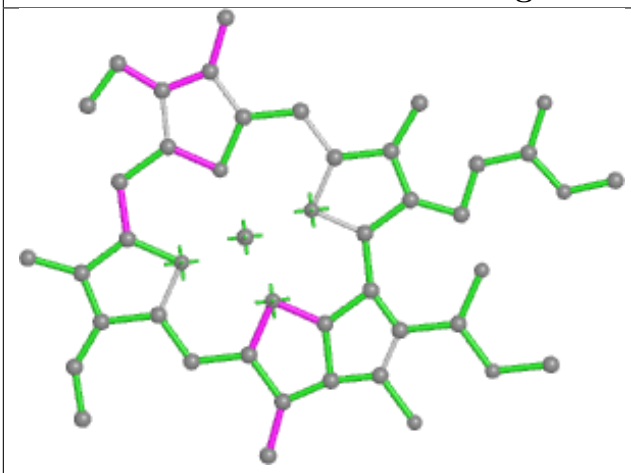
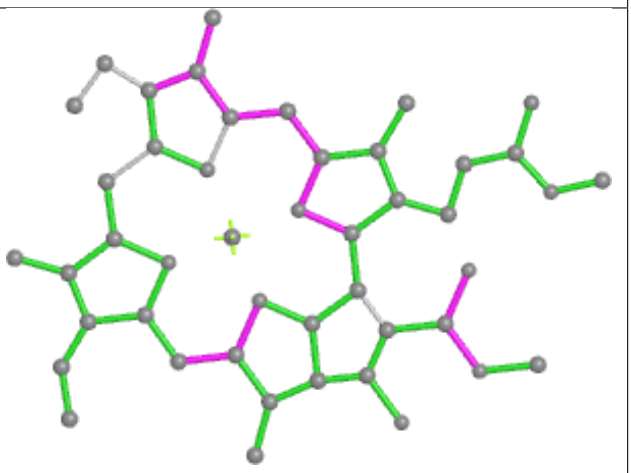


Rings

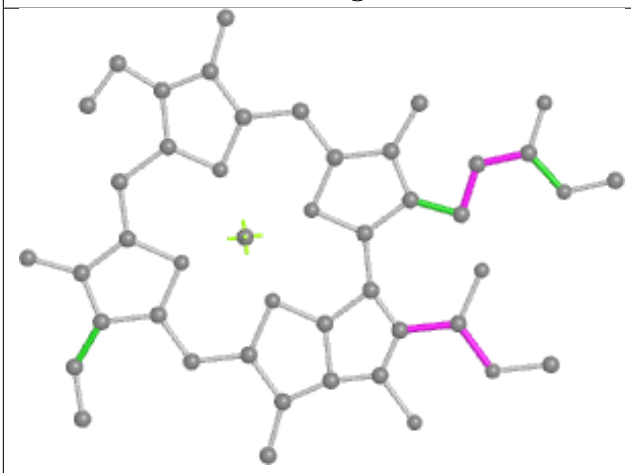
Ligand CLA B5 601



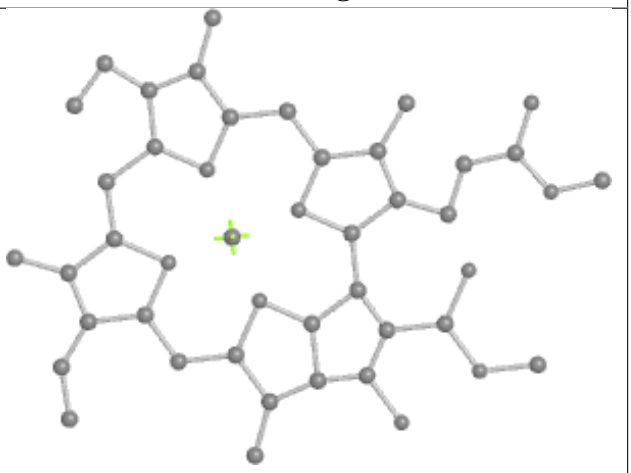
Bond lengths



Bond angles

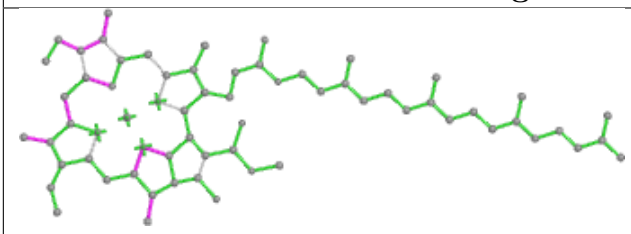


Torsions

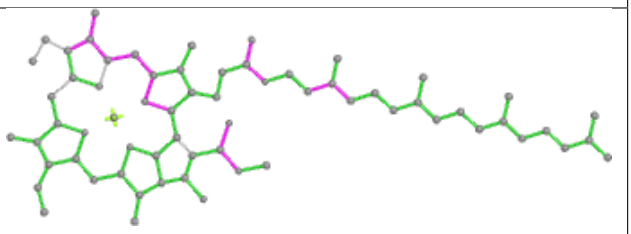


Rings

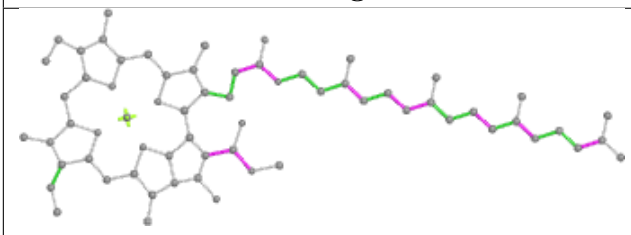
Ligand CLA BB 804



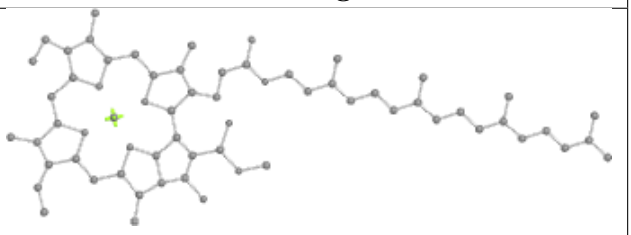
Bond lengths



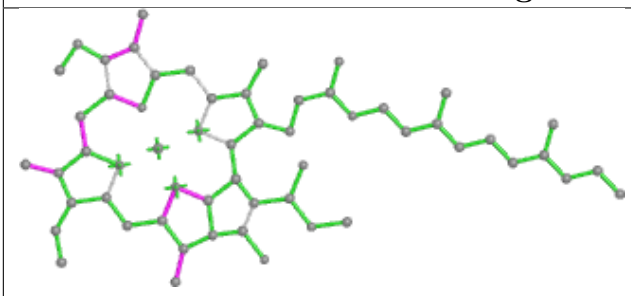
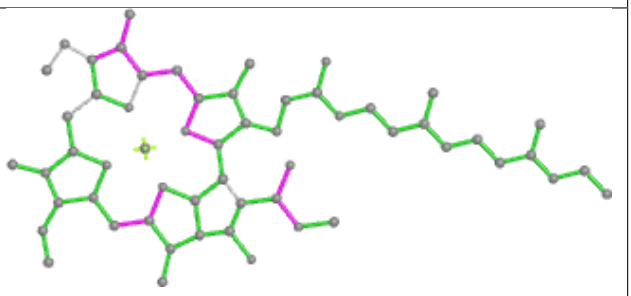
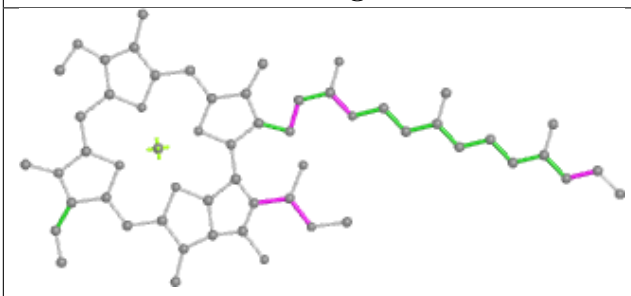
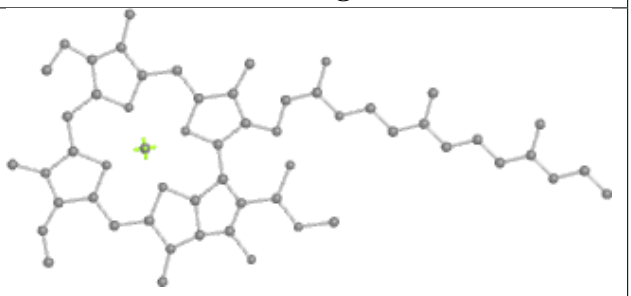
Bond angles



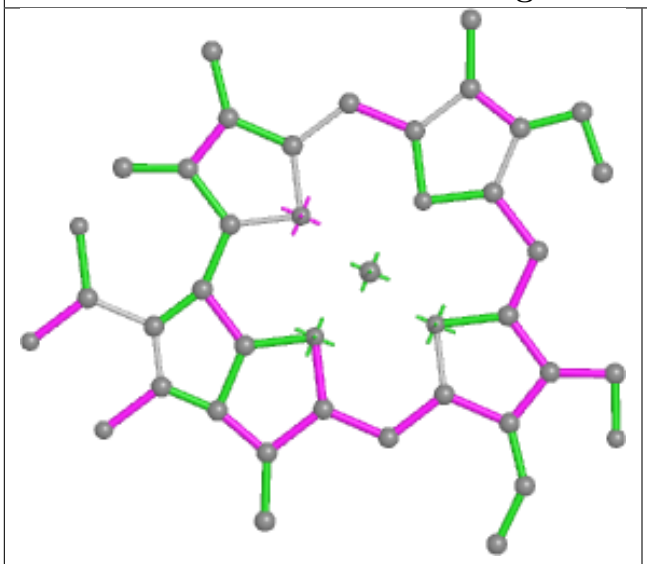
Torsions



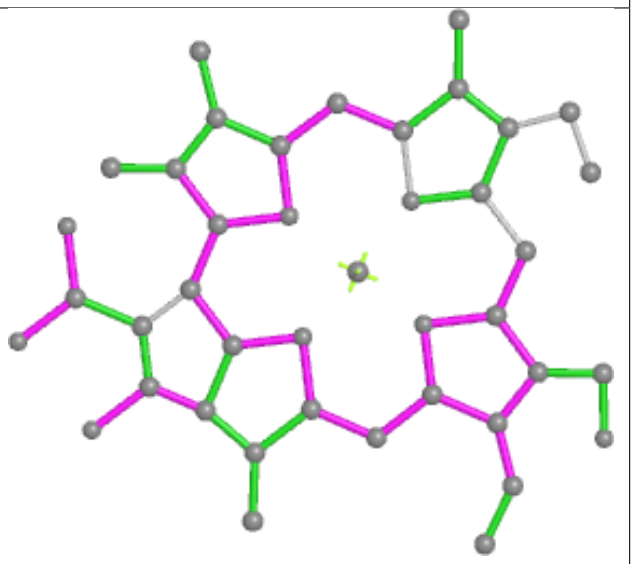
Rings

Ligand CLA B5 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

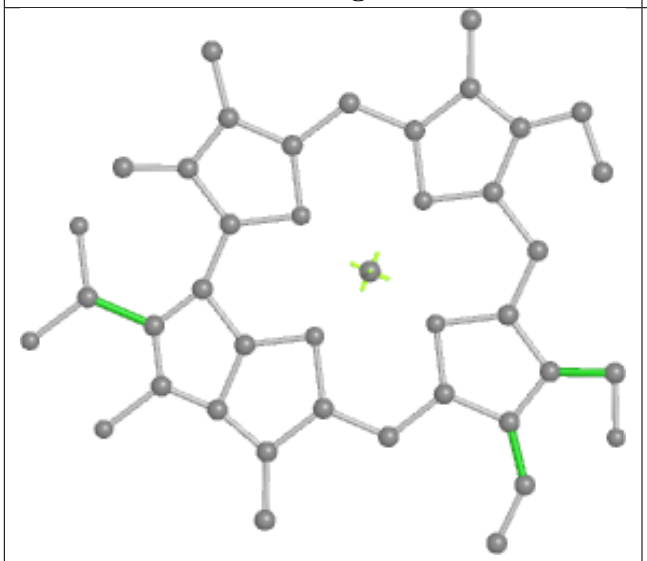
Ligand CHL B1 308



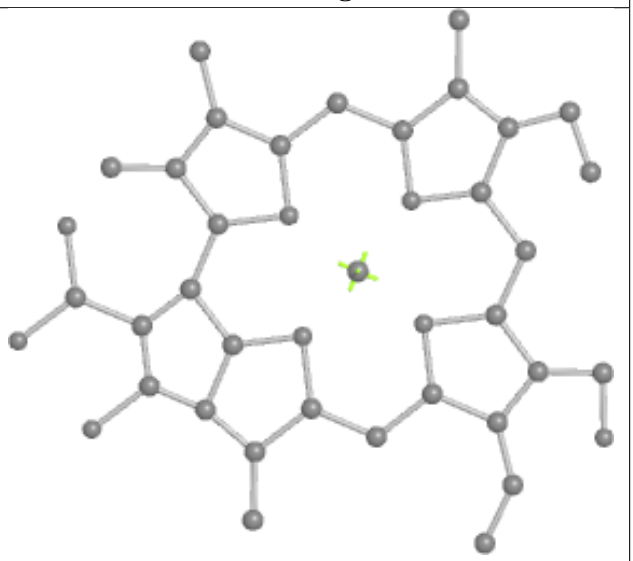
Bond lengths



Bond angles

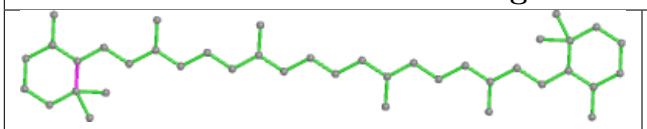


Torsions

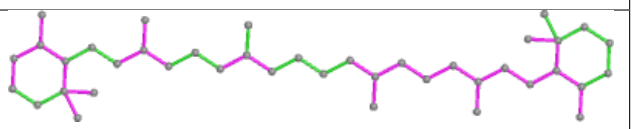


Rings

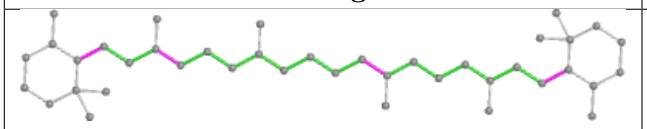
Ligand BCR BA 851



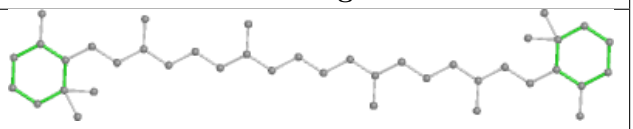
Bond lengths



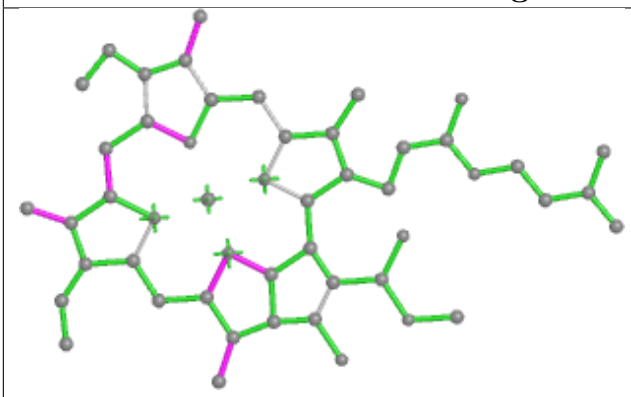
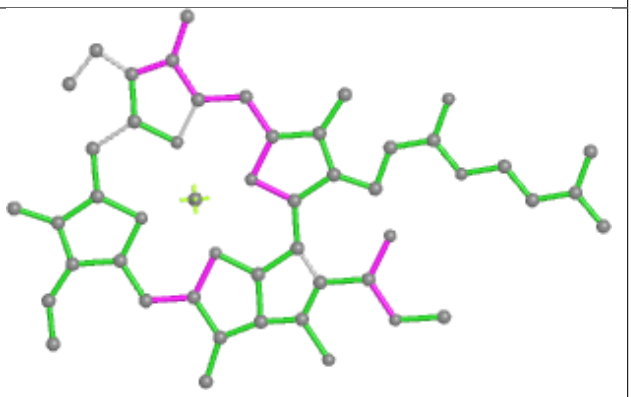
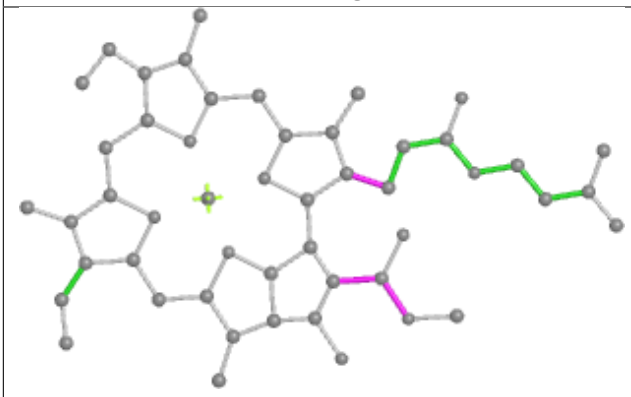
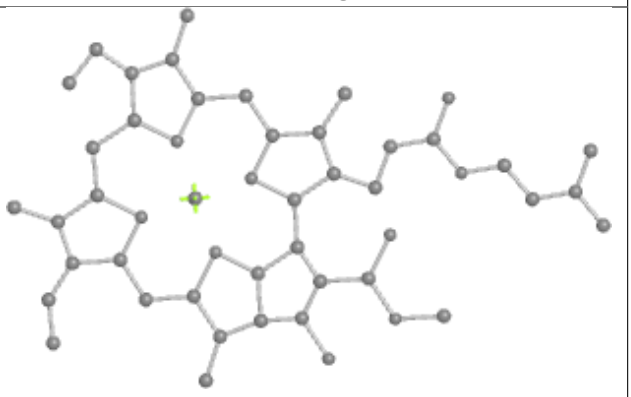
Bond angles

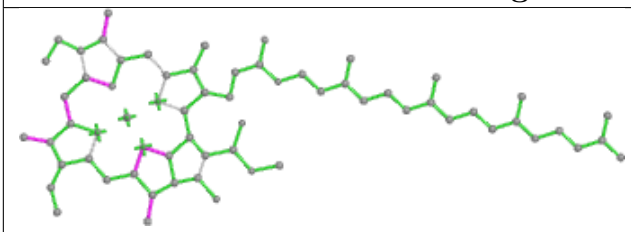
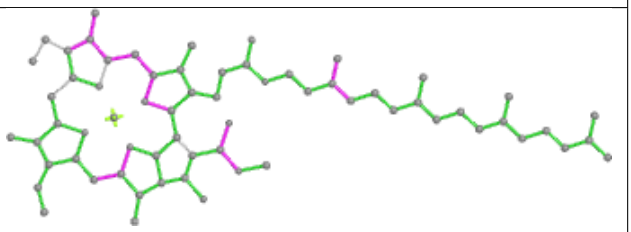
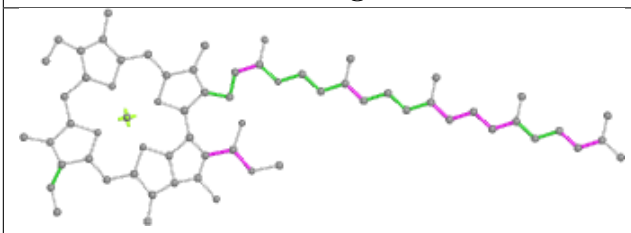
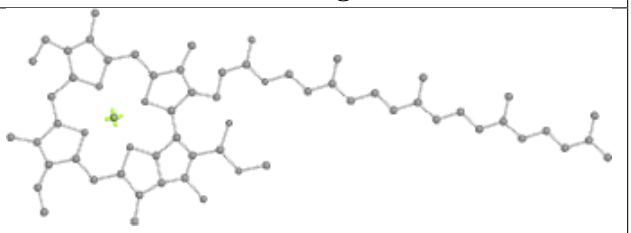


Torsions

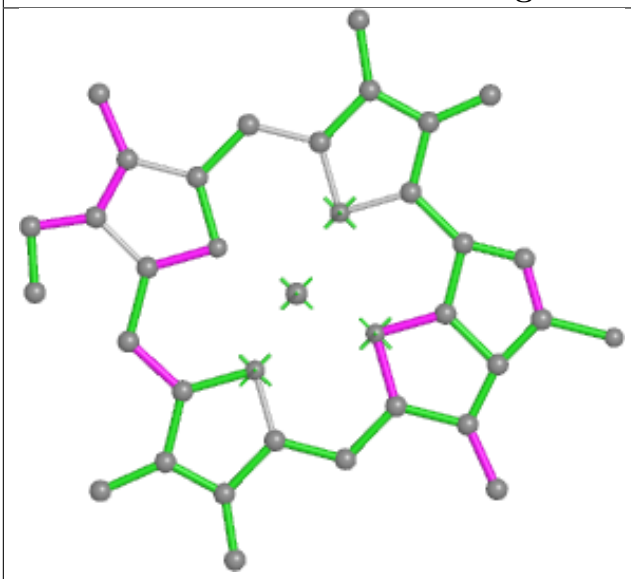


Rings

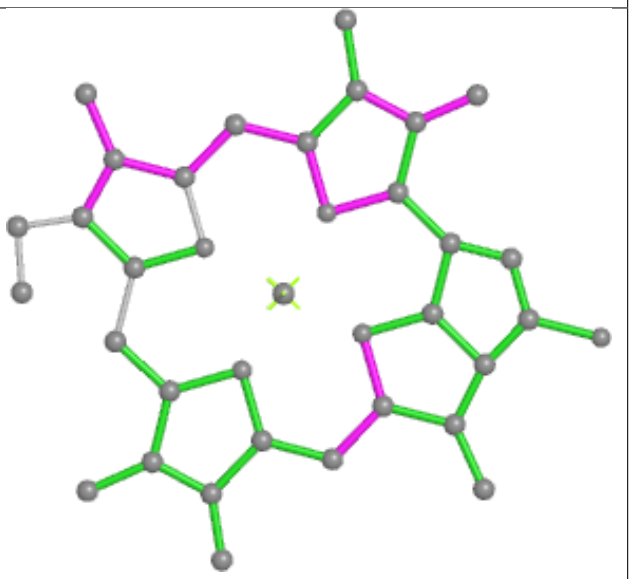
Ligand CLA BA 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BA 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

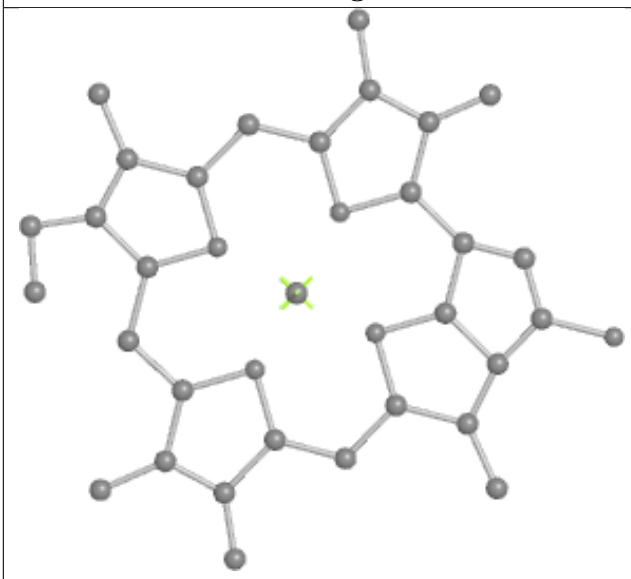
Ligand CLA B3 614



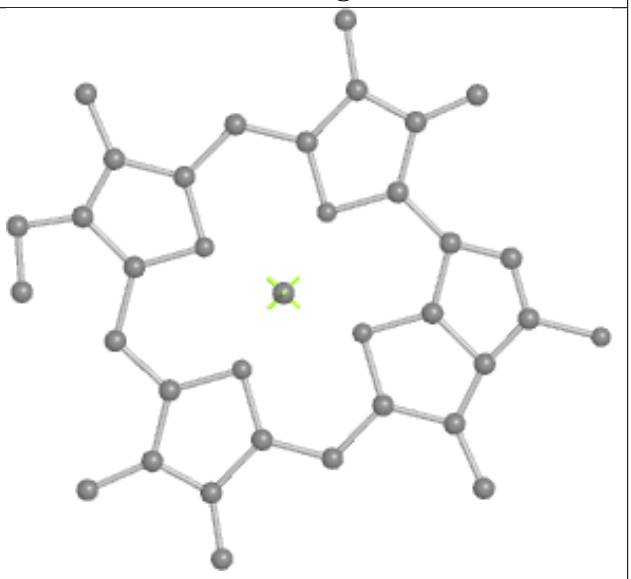
Bond lengths



Bond angles

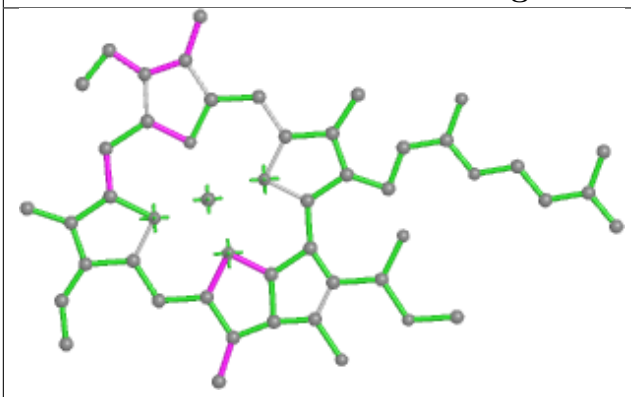


Torsions



Rings

Ligand CLA BA 809



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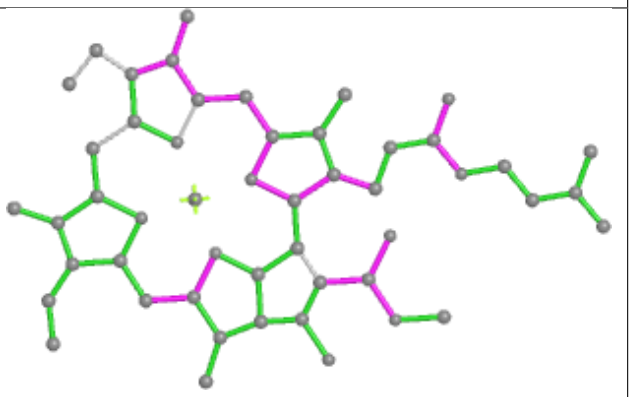
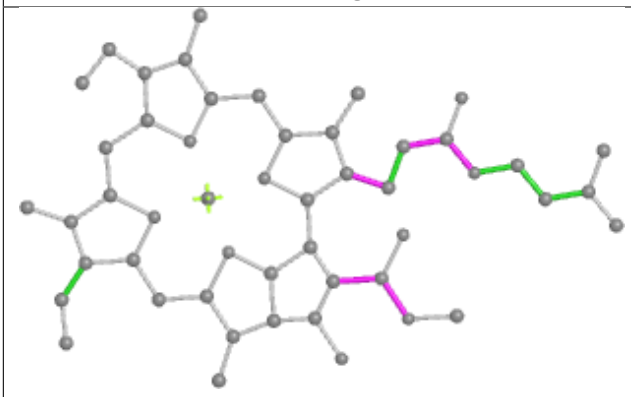


Bond angles



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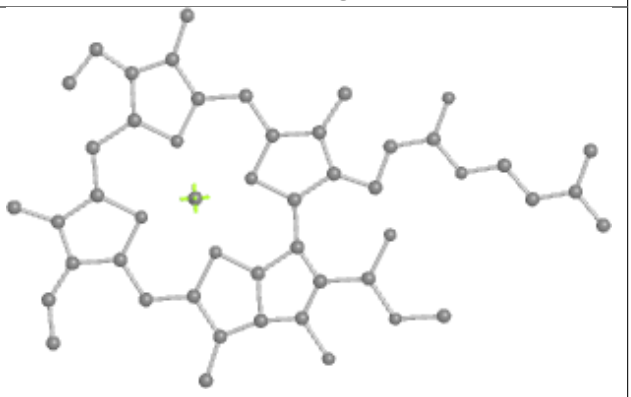
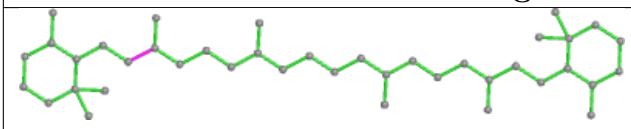
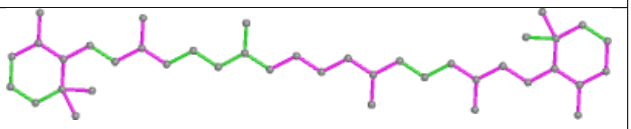


Rings

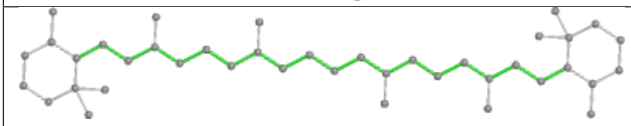
Ligand BCR B2 316



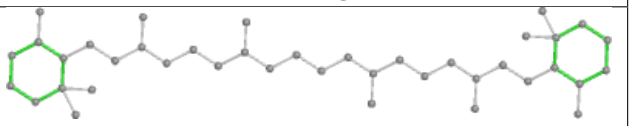
Bond lengths



Bond angles

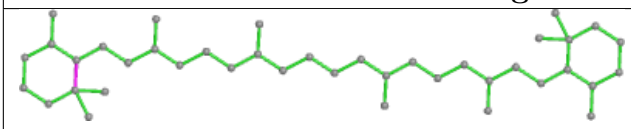


Torsions

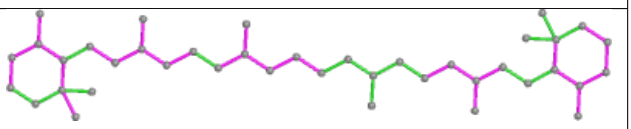


Rings

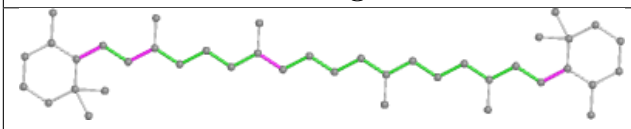
Ligand BCR BF 304



Bond lengths



Bond angles



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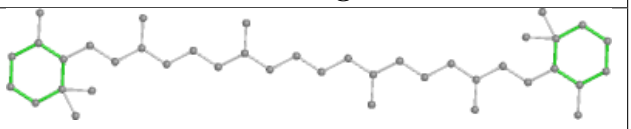
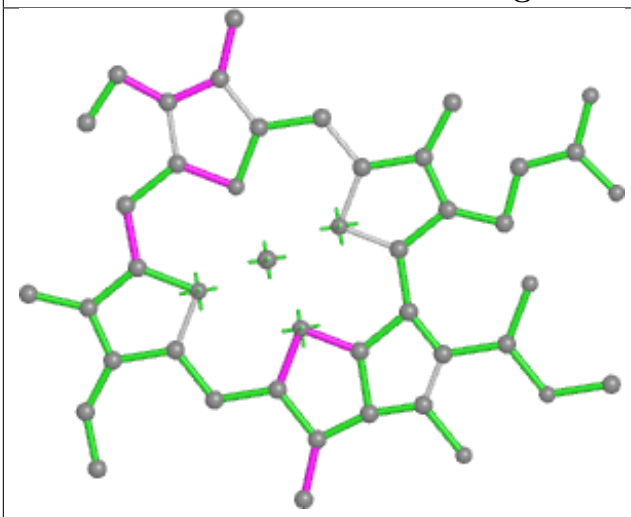
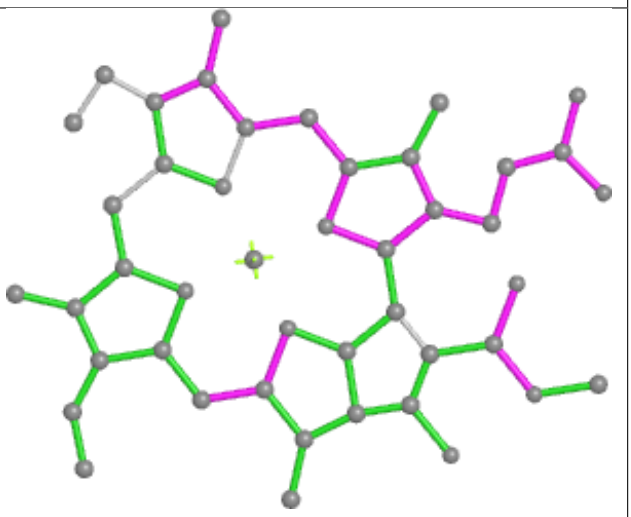


Rings

Ligand CLA BL 302



Bond lengths



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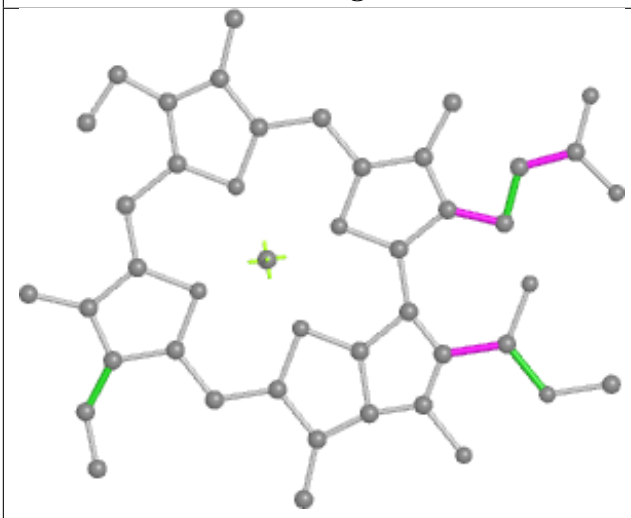

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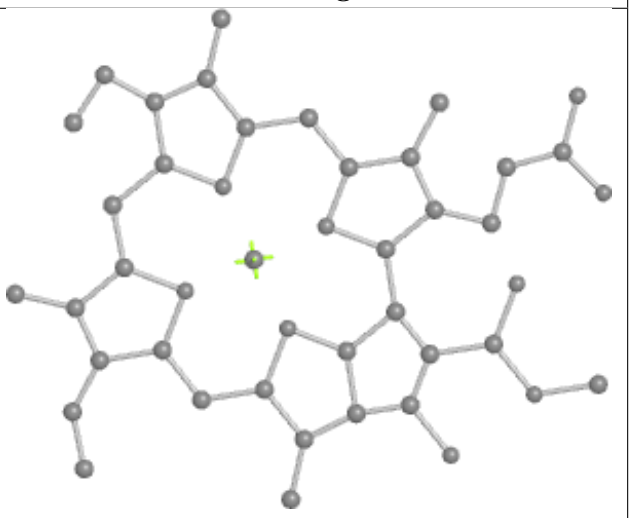
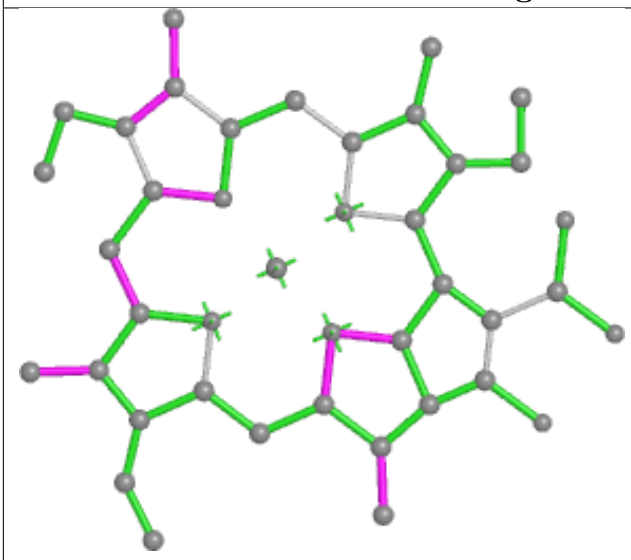
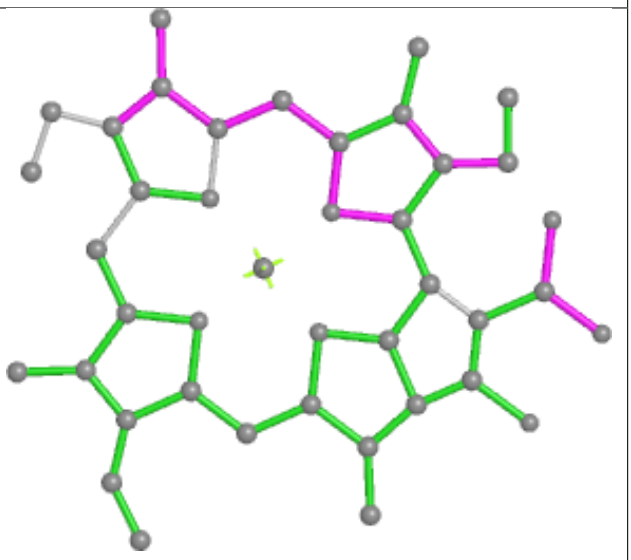
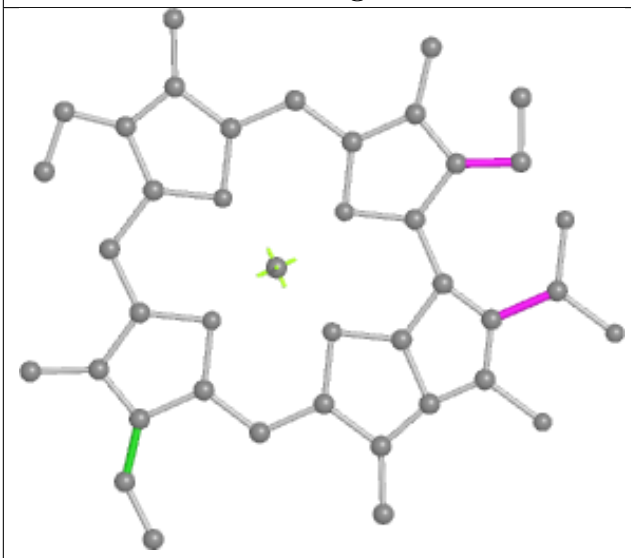
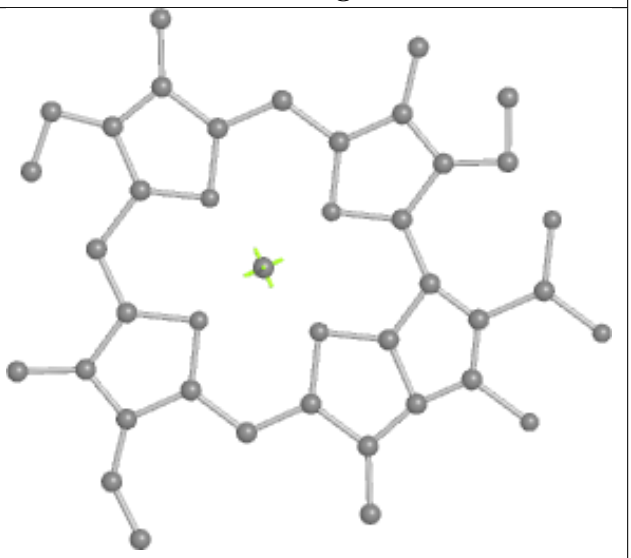
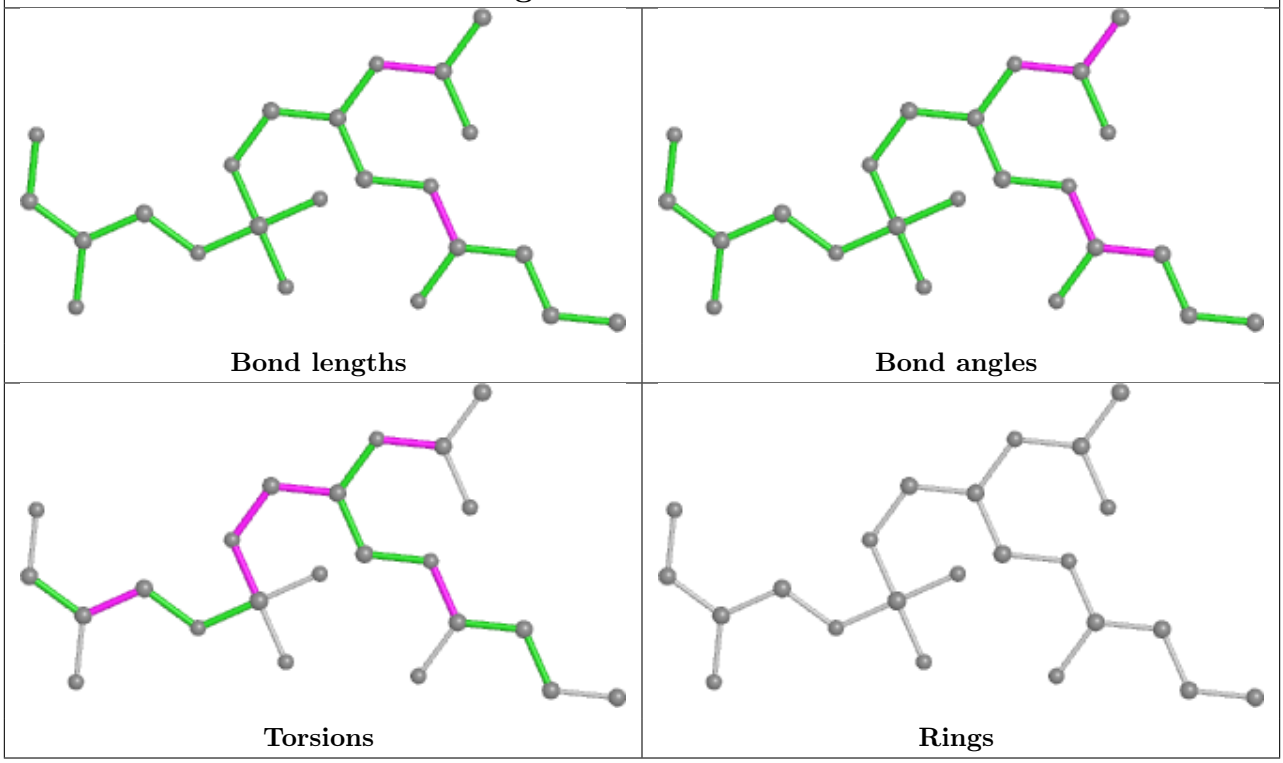


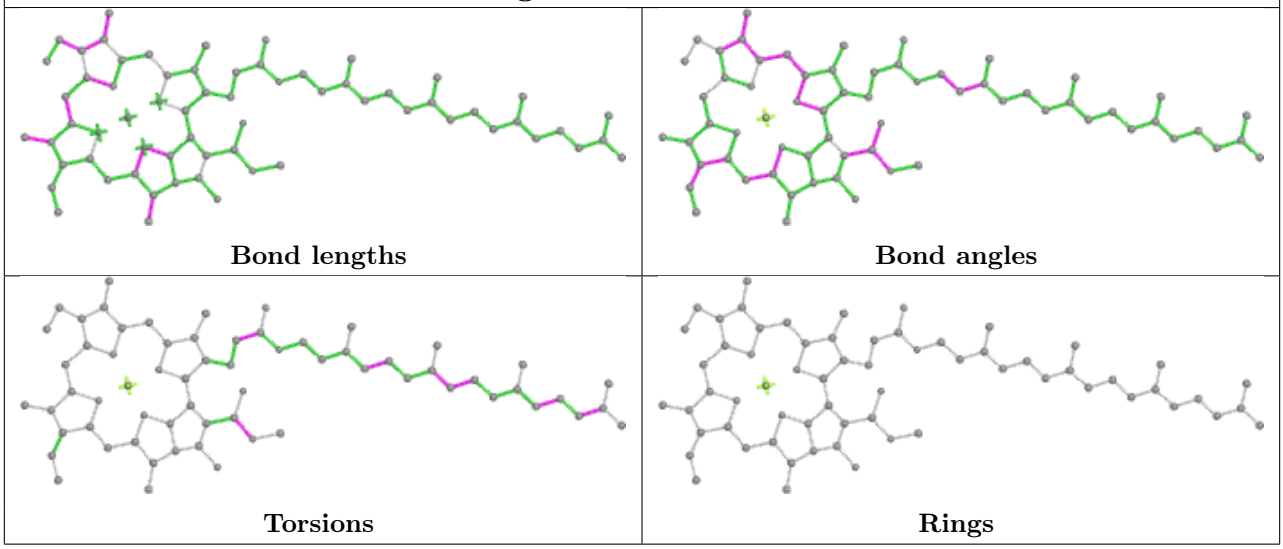
Rings

Ligand CLA B5 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

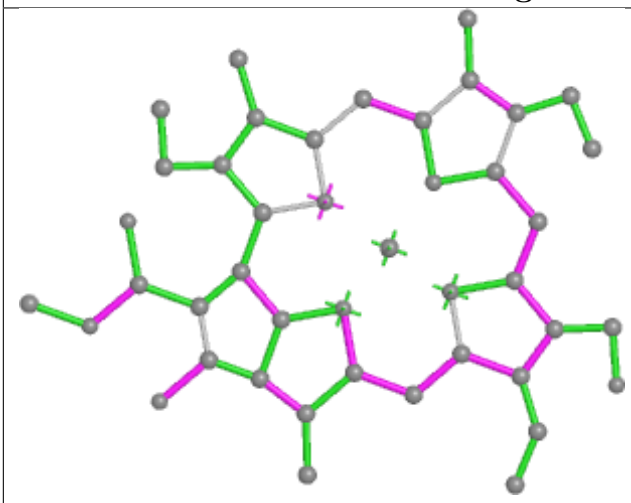
Ligand LHG B3 619



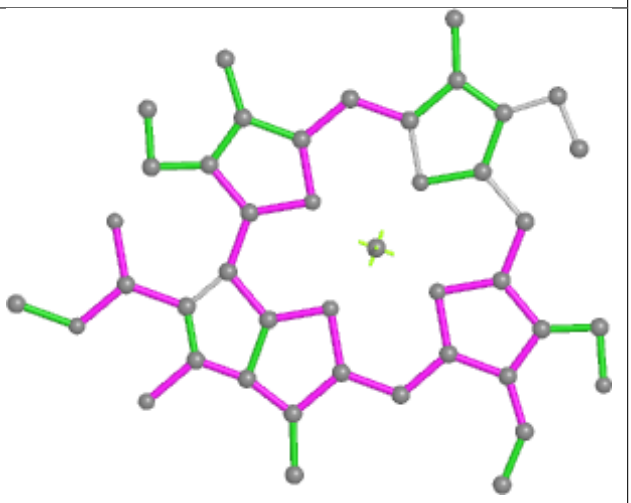
Ligand CLA B2 301



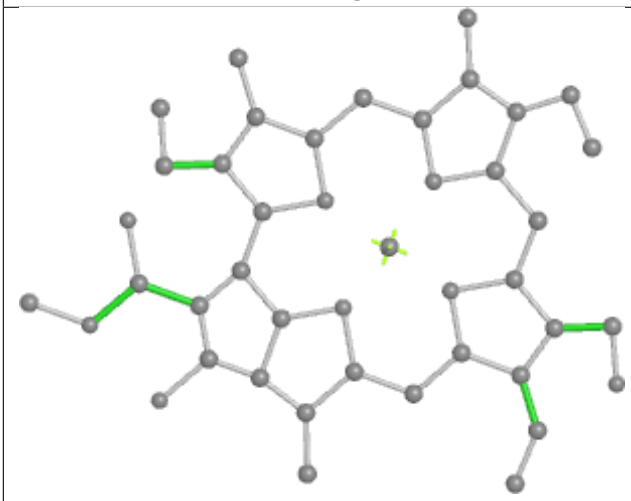
Ligand CHL B2 313



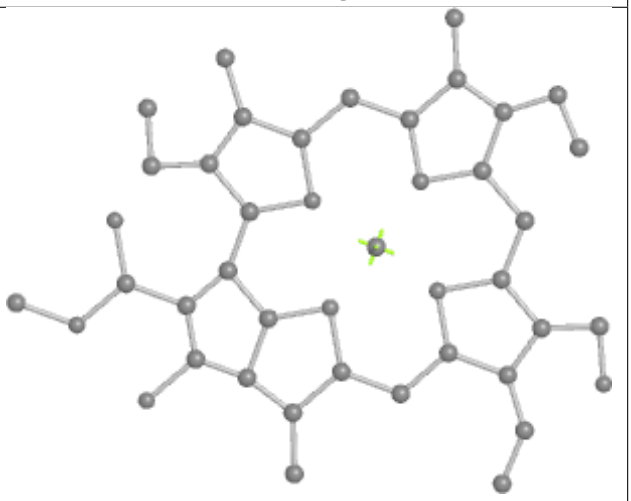
Bond lengths



Bond angles

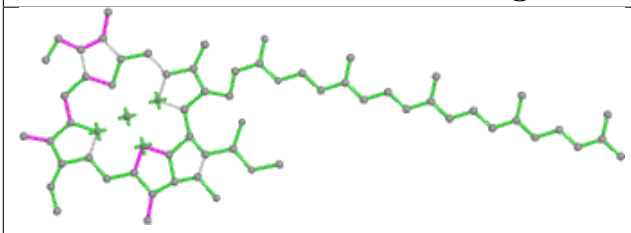


Torsions

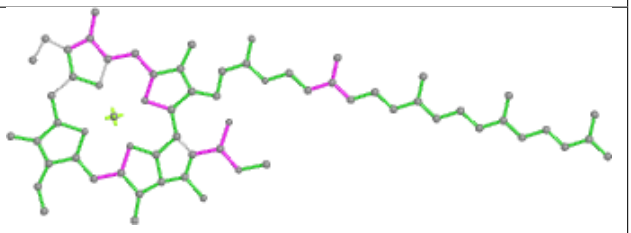


Rings

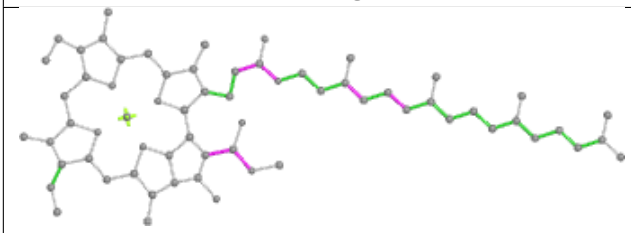
Ligand CLA BA 834



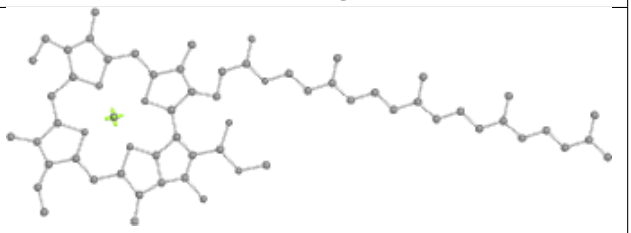
Bond lengths



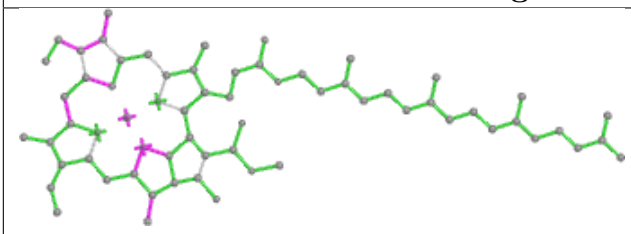
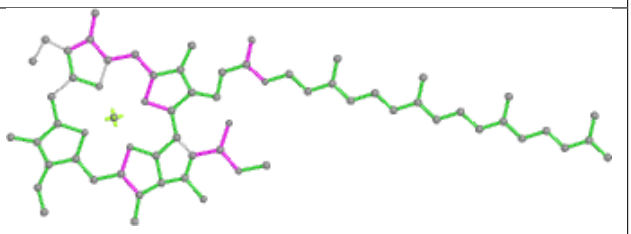
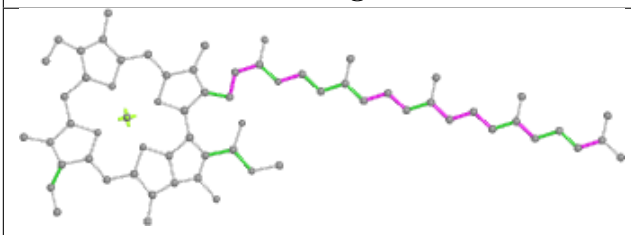
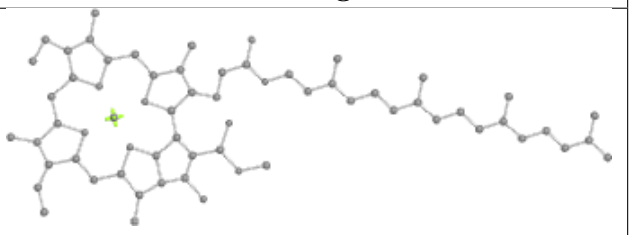
Bond angles

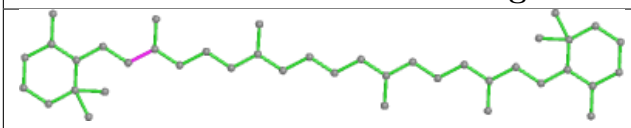
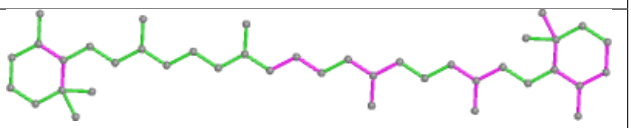
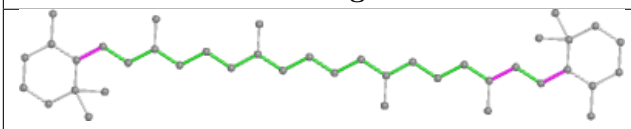


Torsions

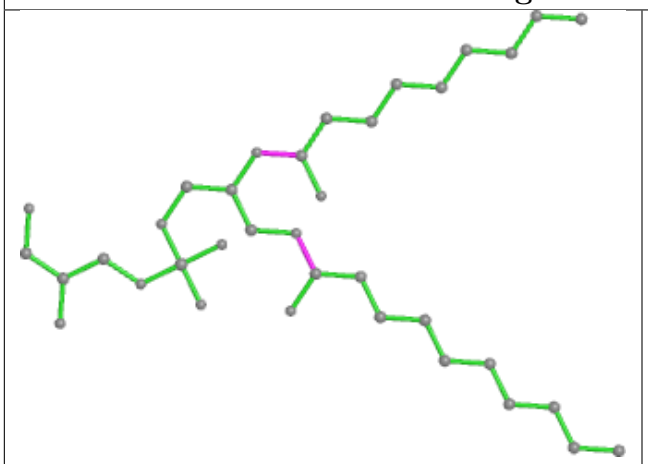


Rings

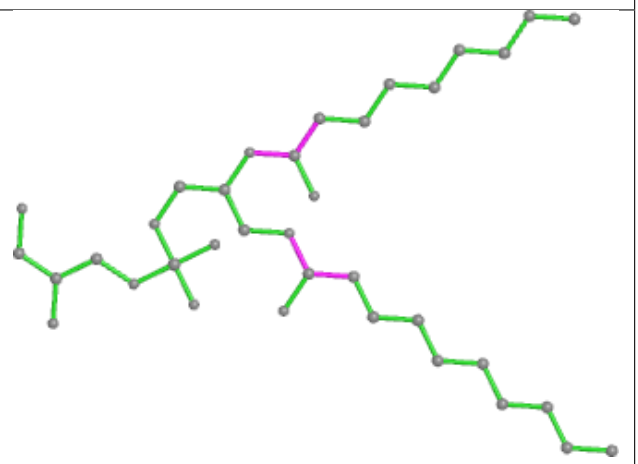
Ligand CLA BA 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR BA 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

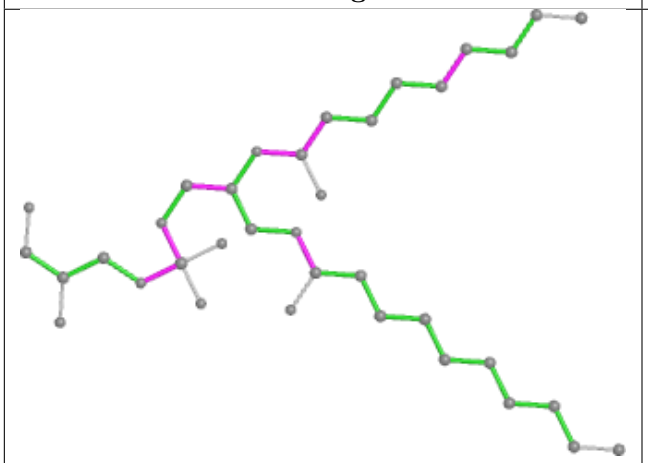
Ligand LHG B1 302



Bond lengths



Bond angles



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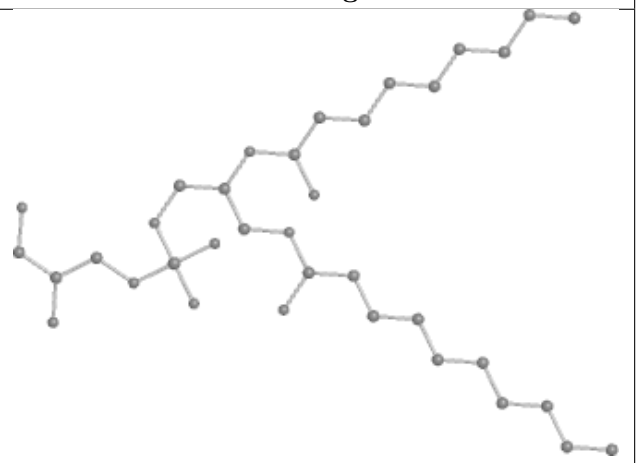
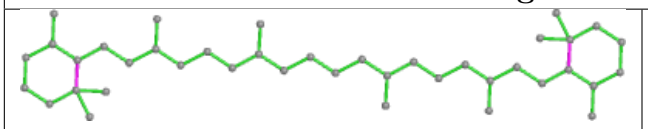


Rings

Ligand BCR BI 101



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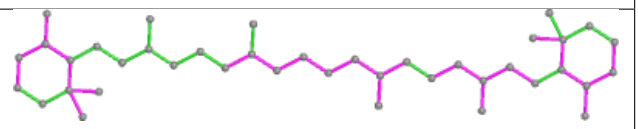
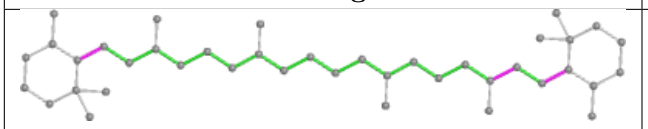


Bond angles



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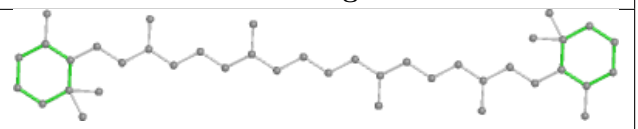
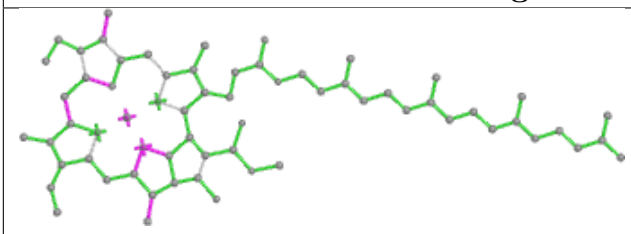
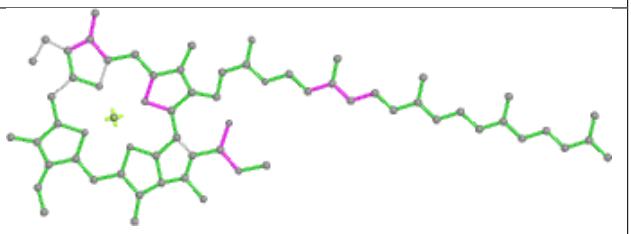


Rings

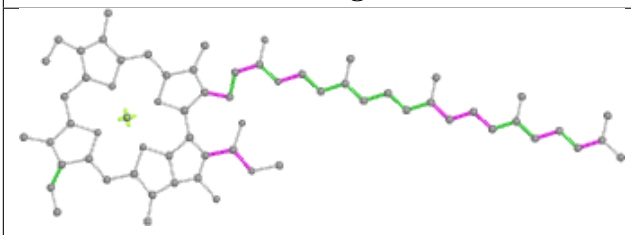
Ligand CLA BA 825



Bond lengths



Bond angles



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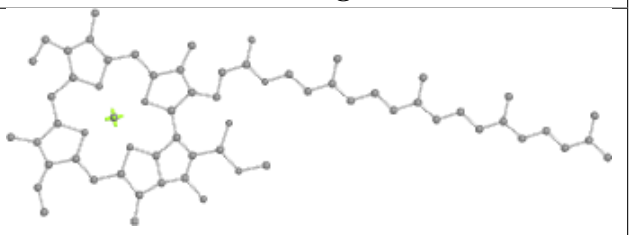
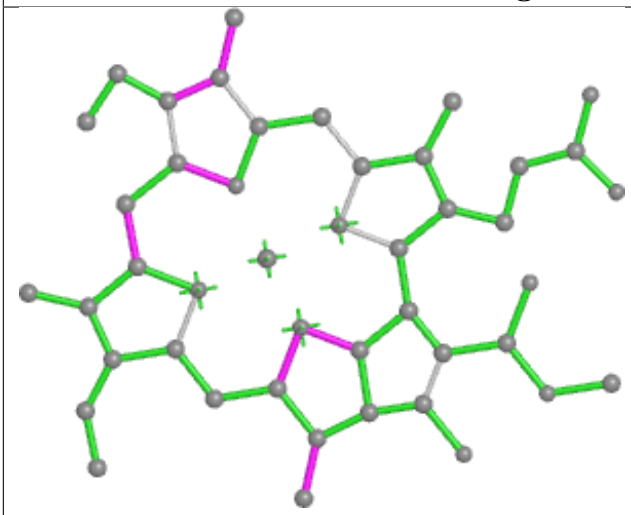


Rings

Ligand CLA B5 613



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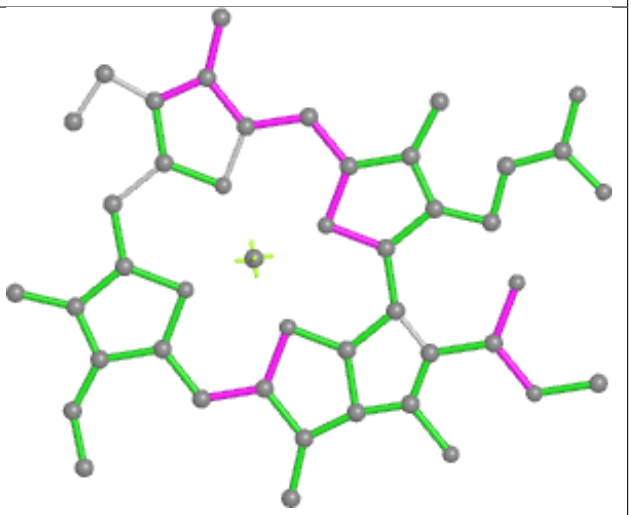

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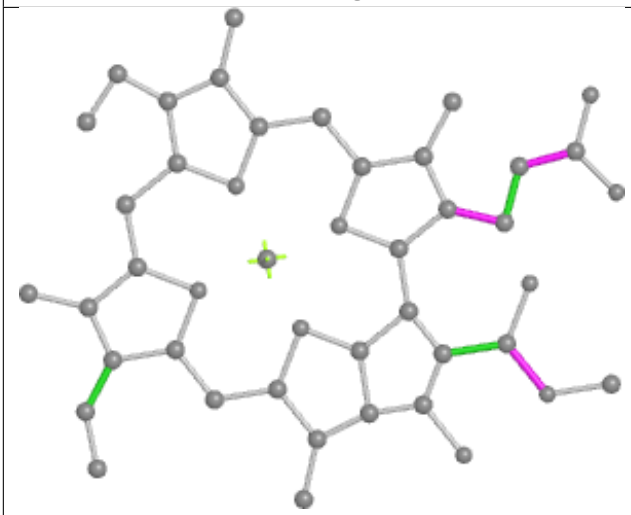

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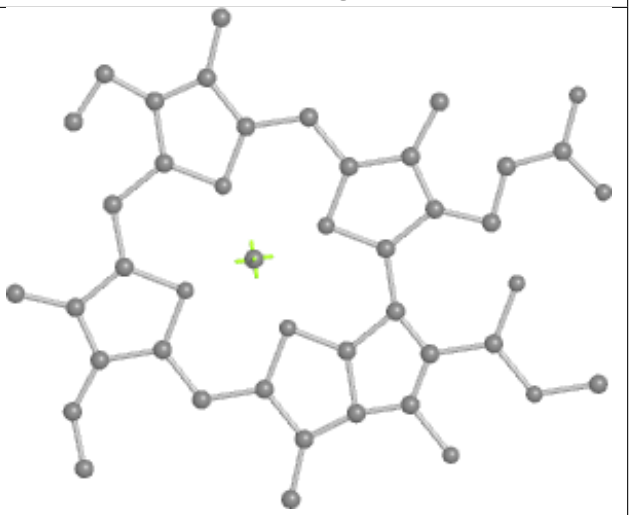
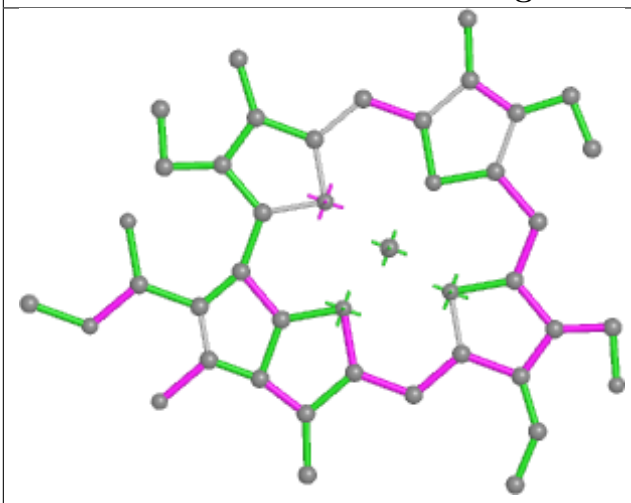


Rings

Ligand CHL B2 305



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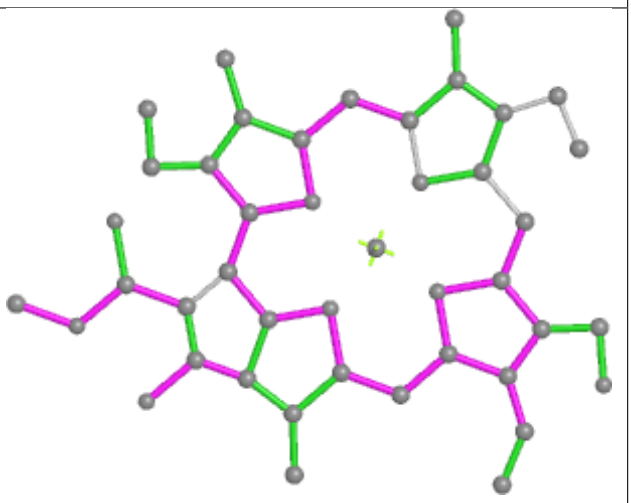
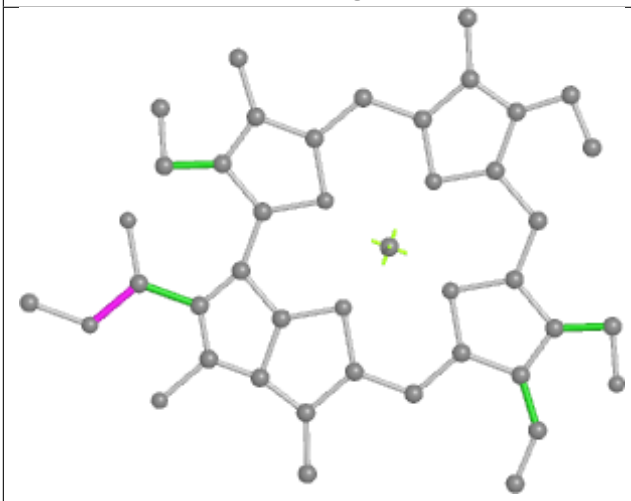


Bond angles



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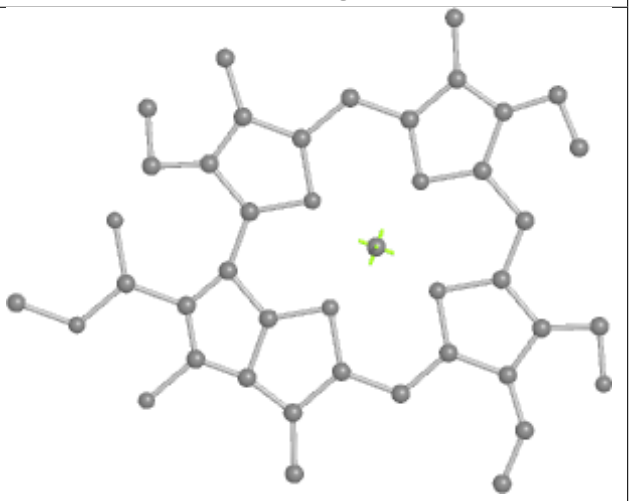
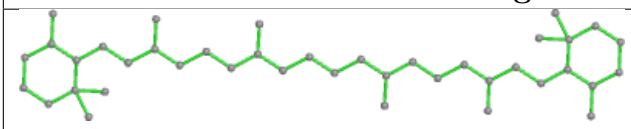


Rings

Ligand BCR B5 616



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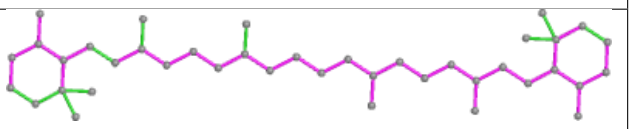

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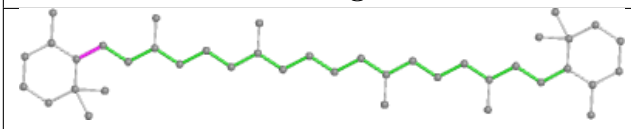
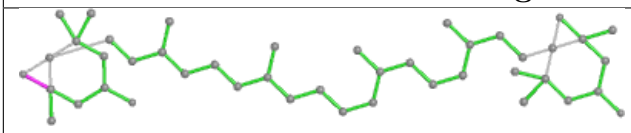


Torsions

Rings

Ligand XAT B2 315



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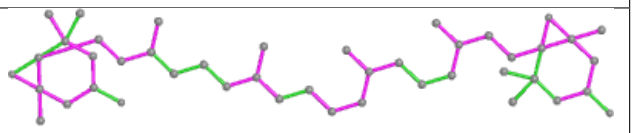
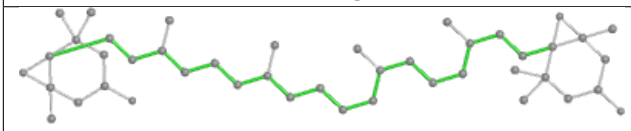
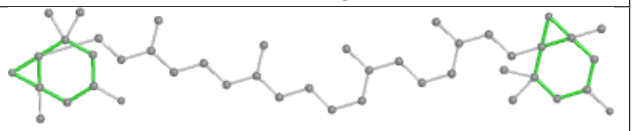


Bond angles

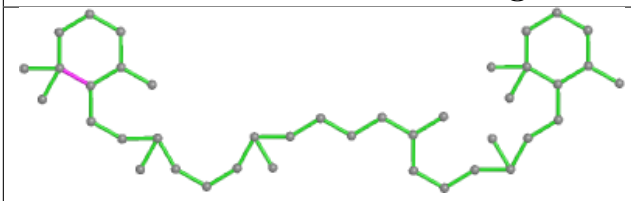


Torsions



Rings

Ligand BCR BH 202



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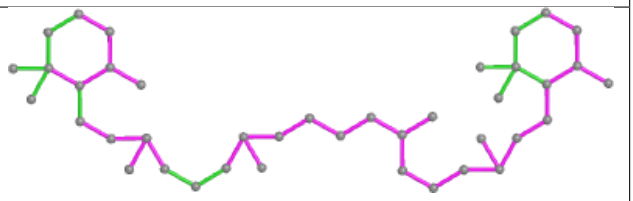
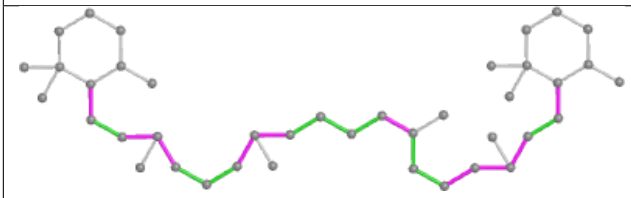


Bond angles



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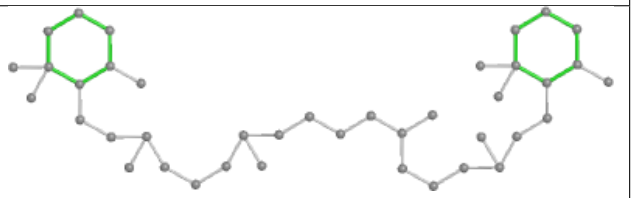
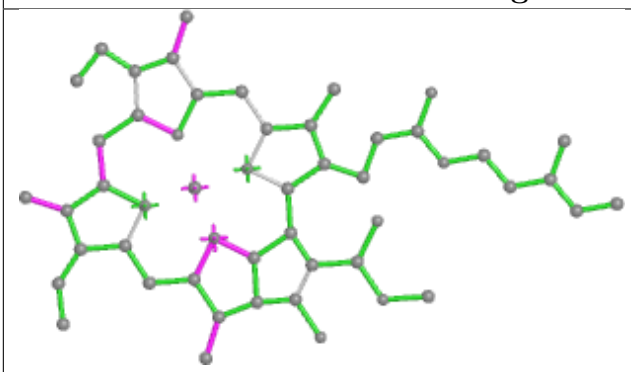


Rings

Ligand CLA BA 837



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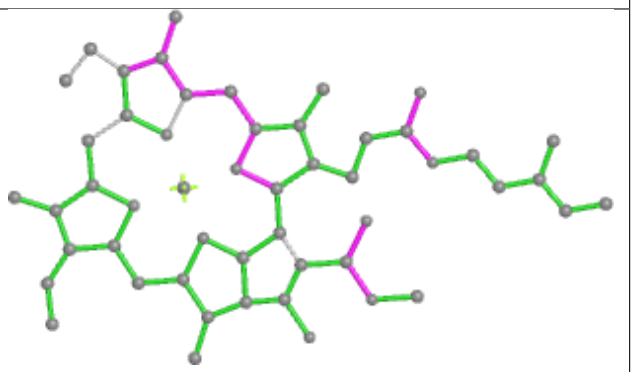
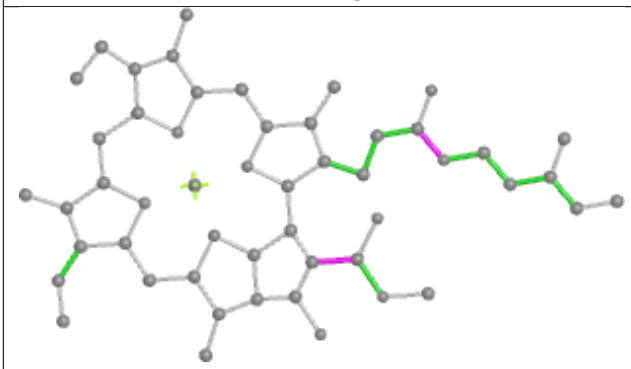


Bond angles



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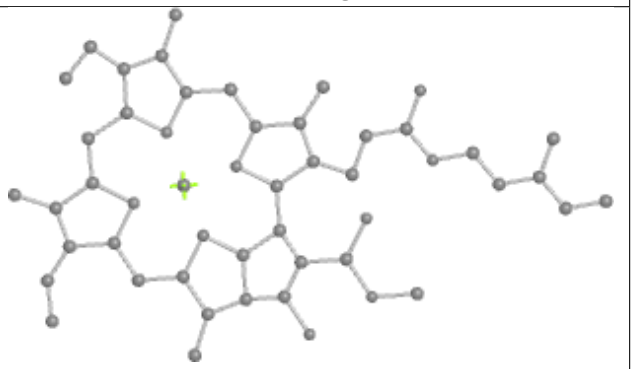
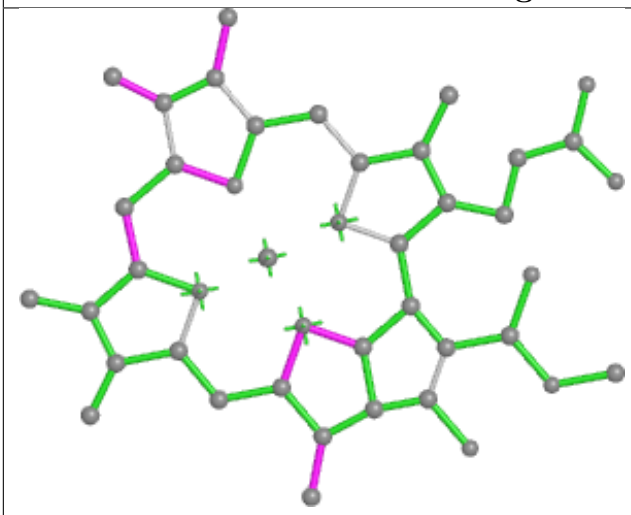


Rings

Ligand CLA B5 604



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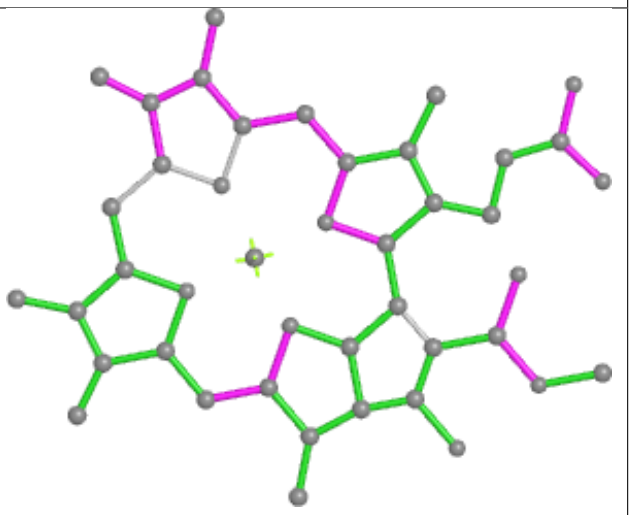
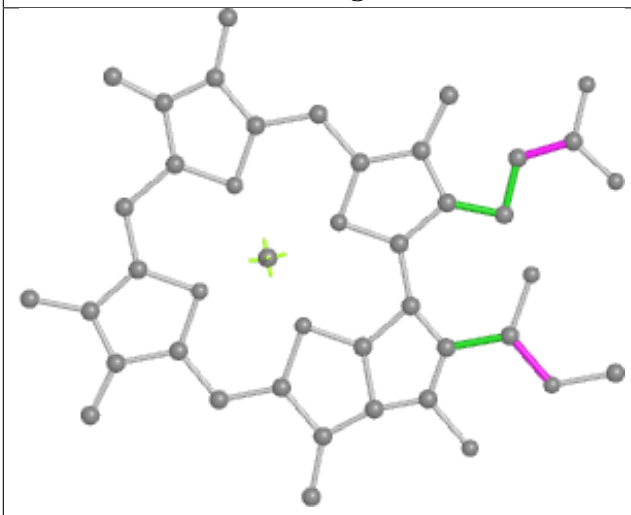


Bond angles



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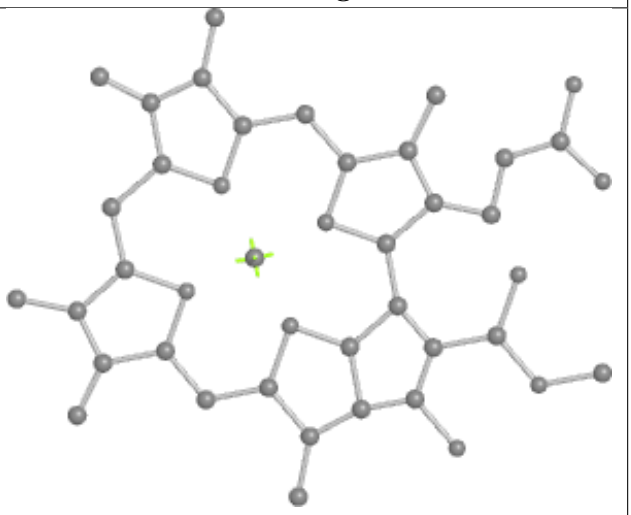
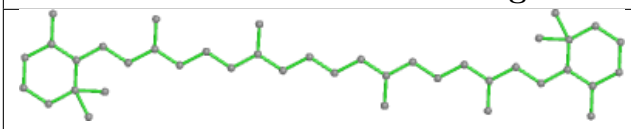
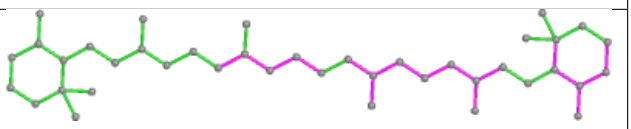


Rings

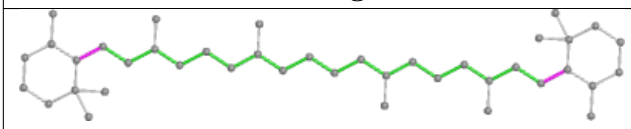
Ligand BCR BA 850



Bond lengths



Bond angles



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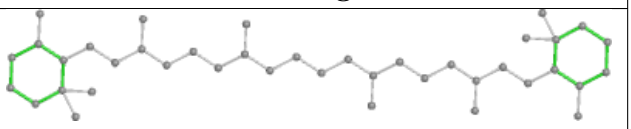
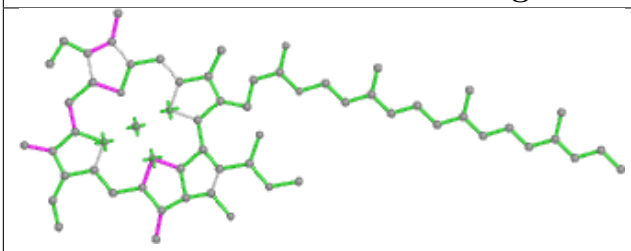
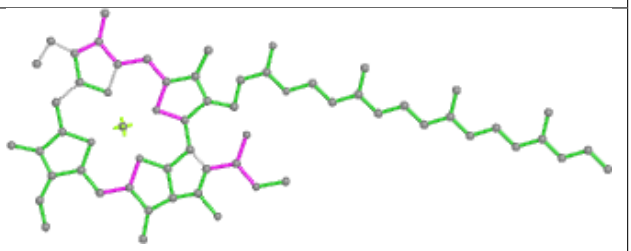
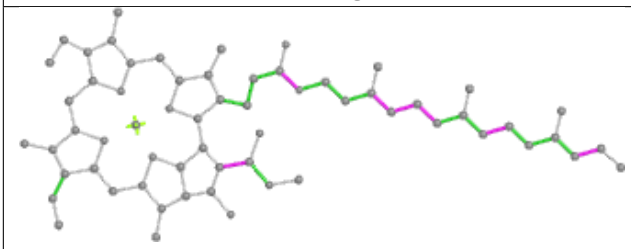
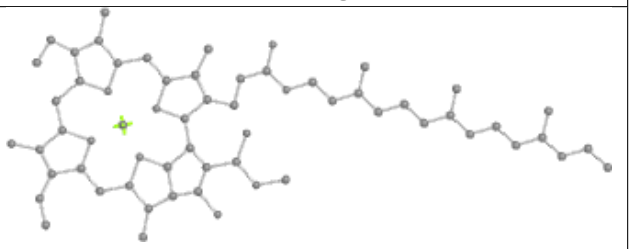


Rings

Ligand CLA BB 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

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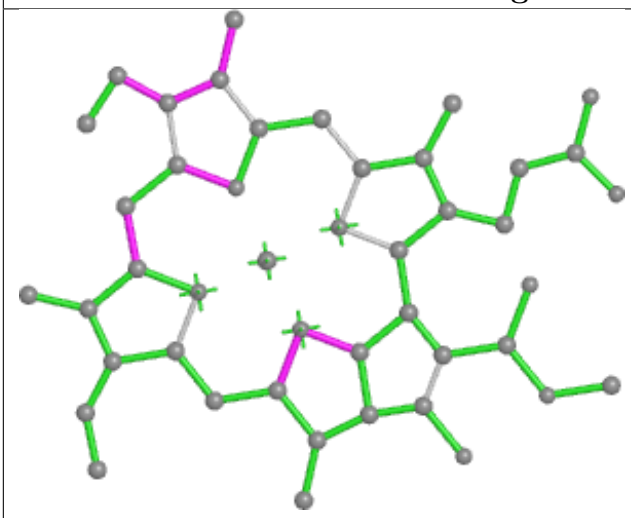
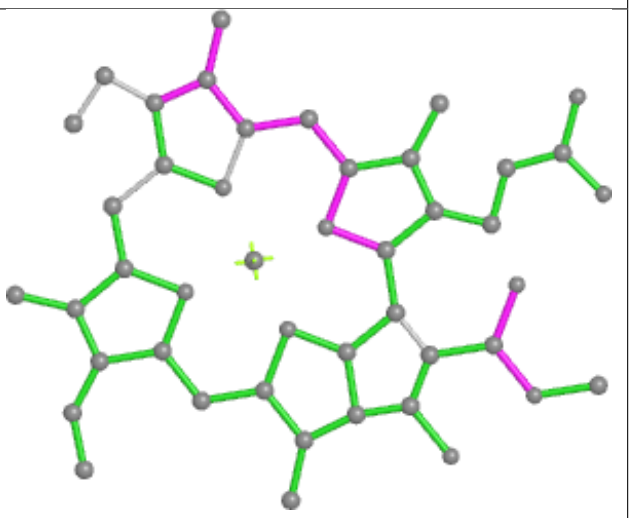
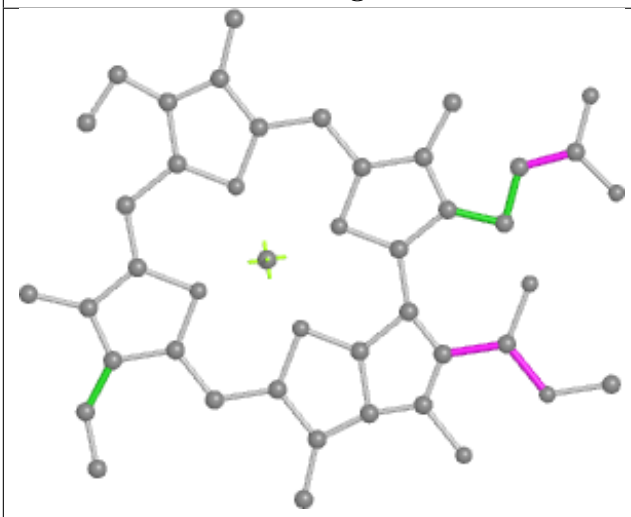
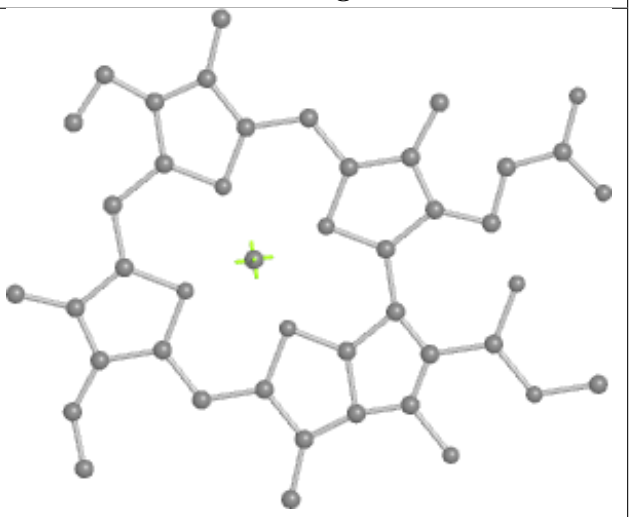
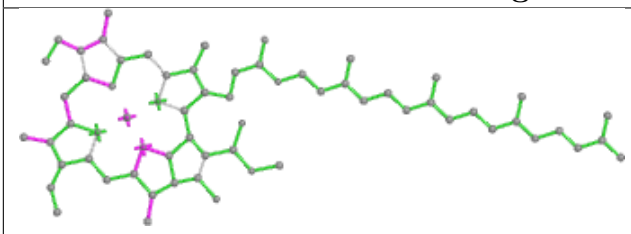
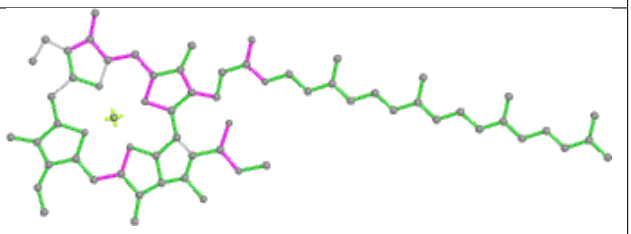
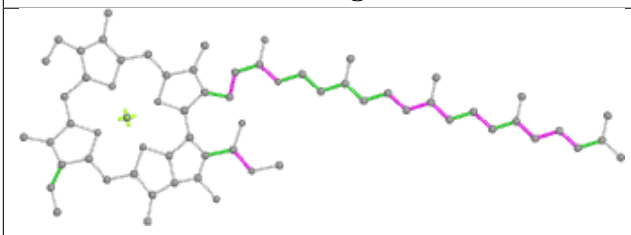
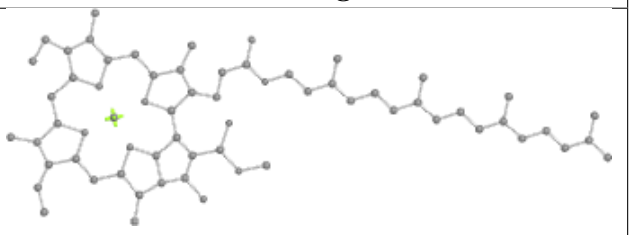
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

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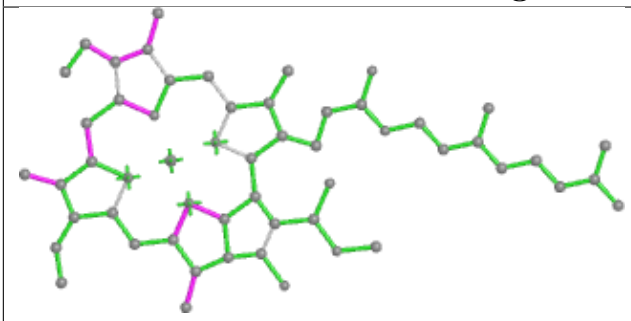
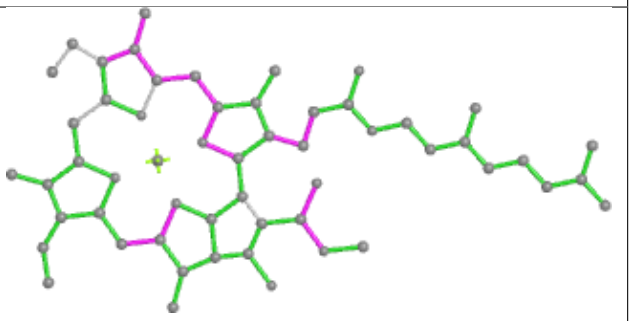
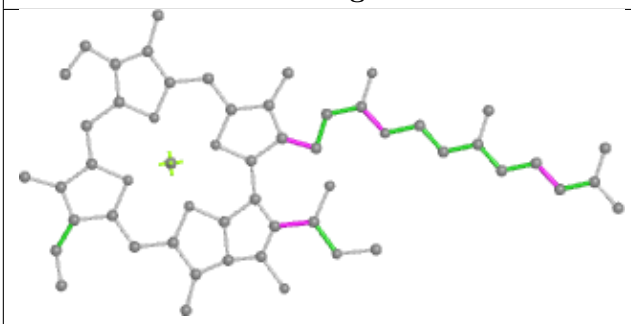
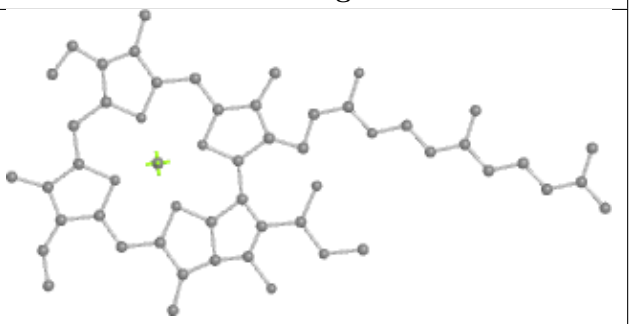
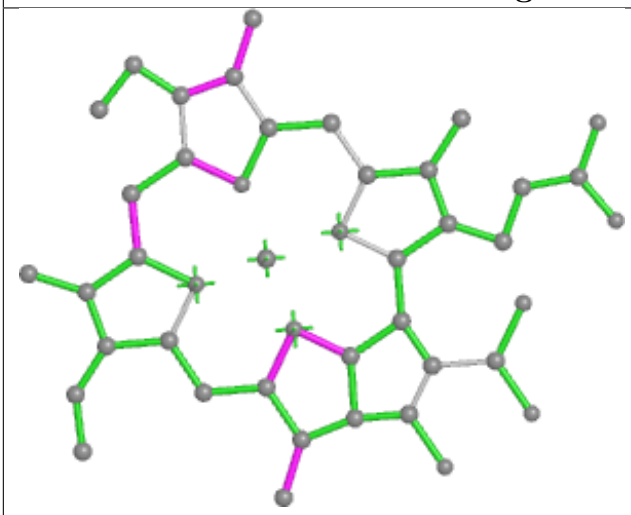
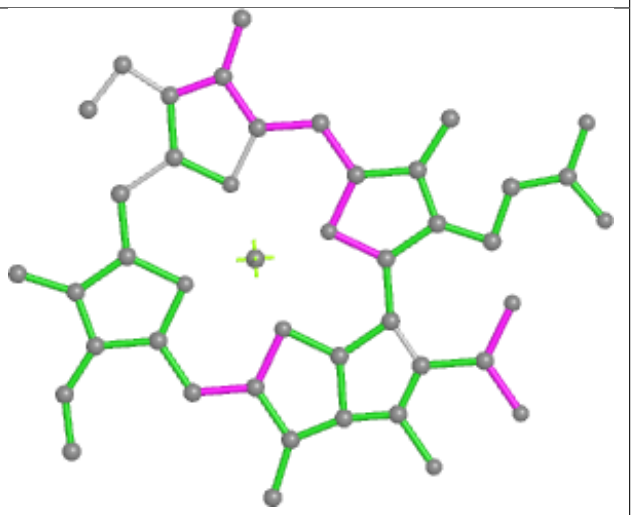
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 309	
	
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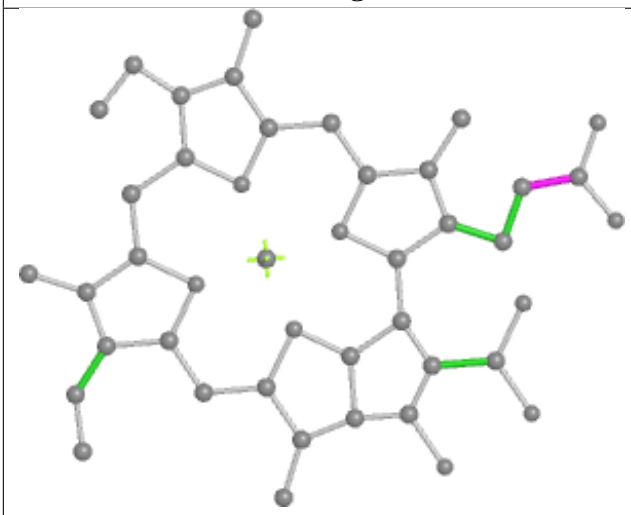
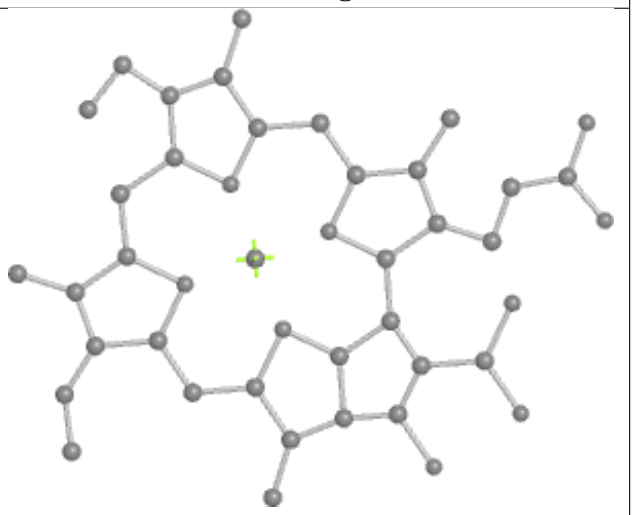
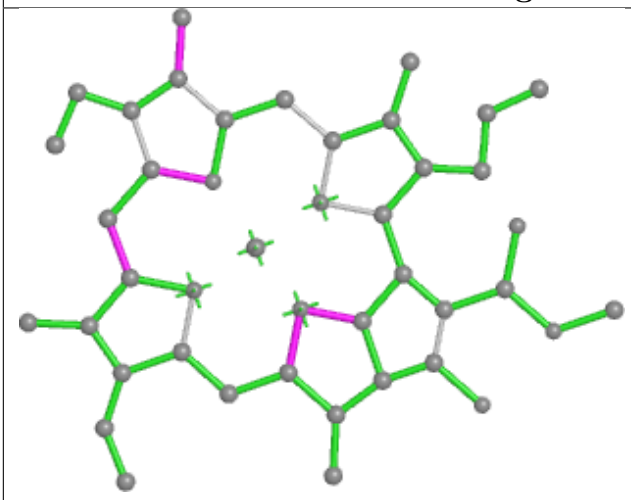
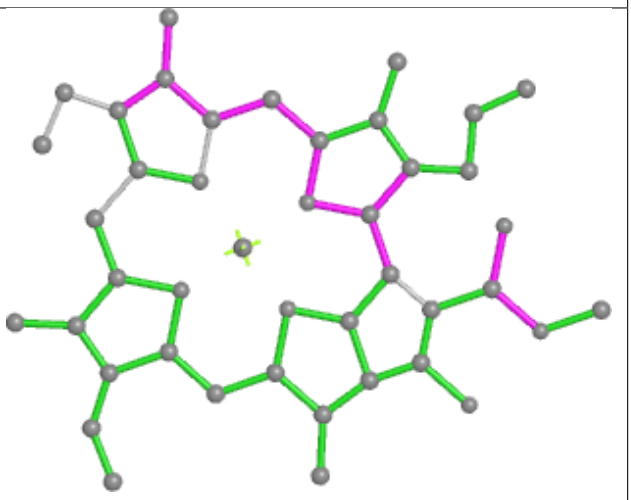
	
Torsions	**Rings**

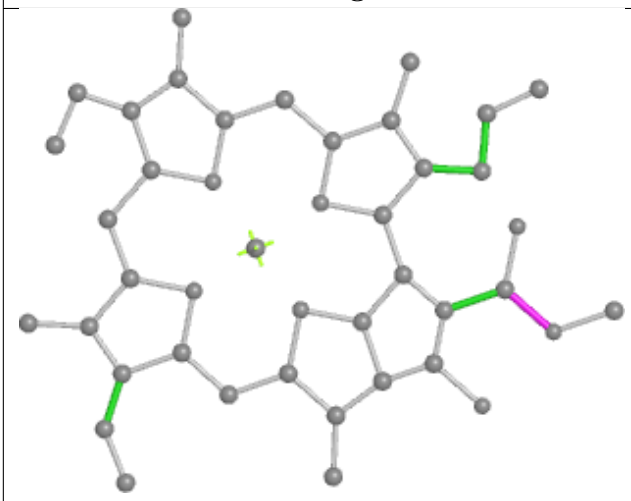
Ligand CLA B3 611



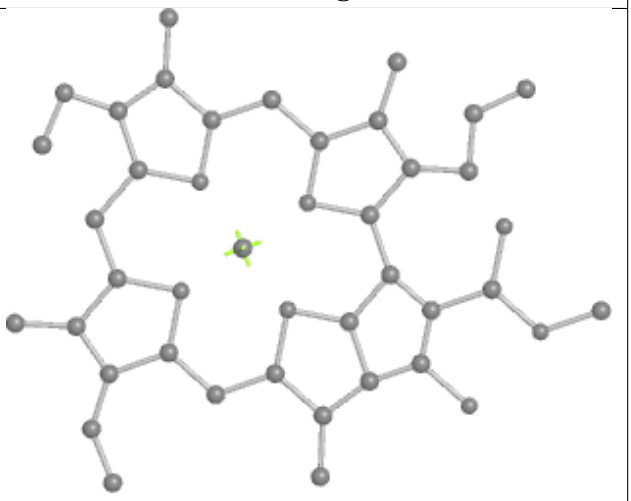
Bond lengths



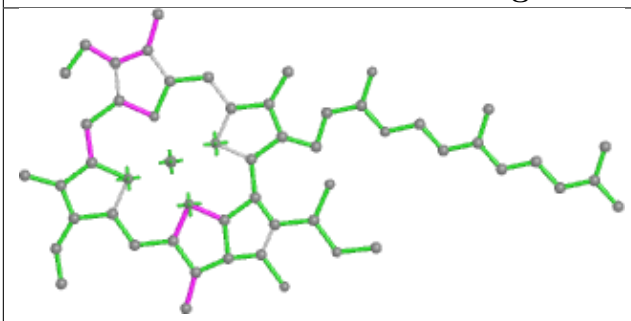
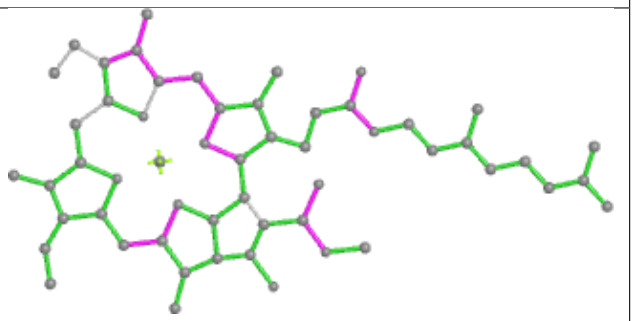
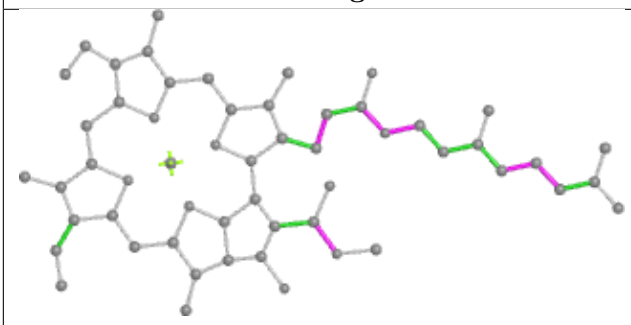
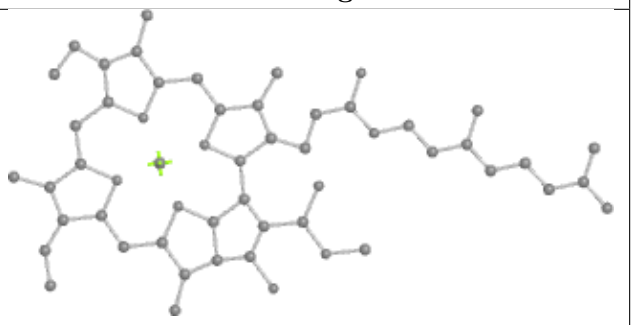
Bond angles



Torsions



Rings

Ligand CLA BB 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

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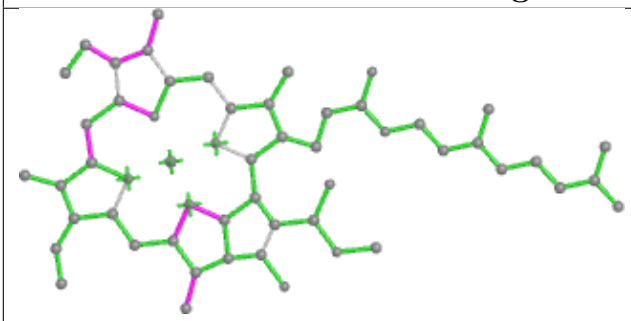
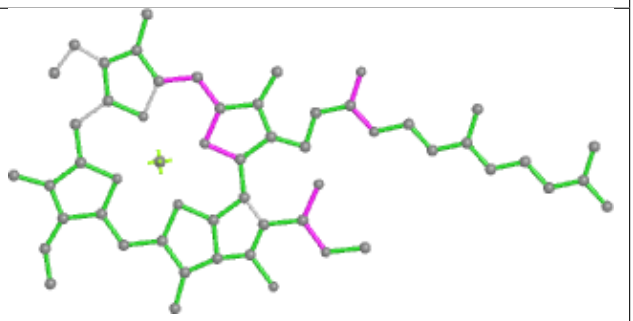
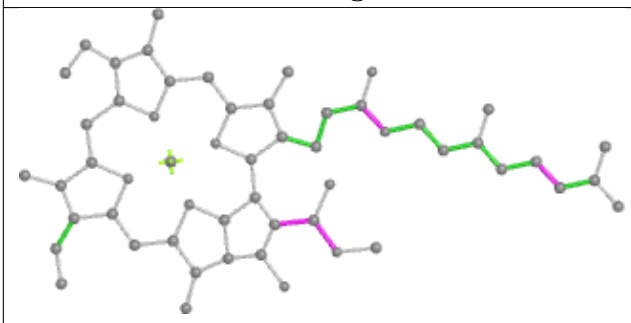
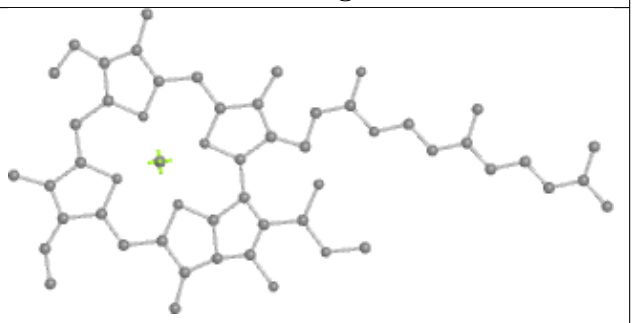
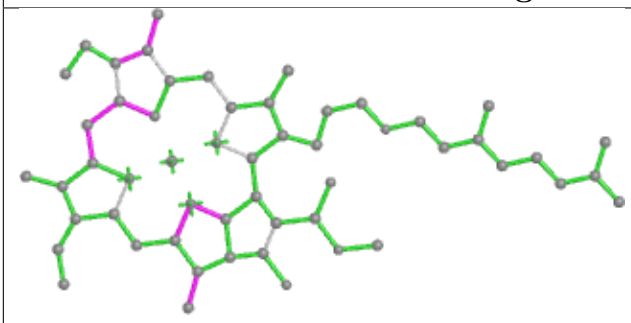
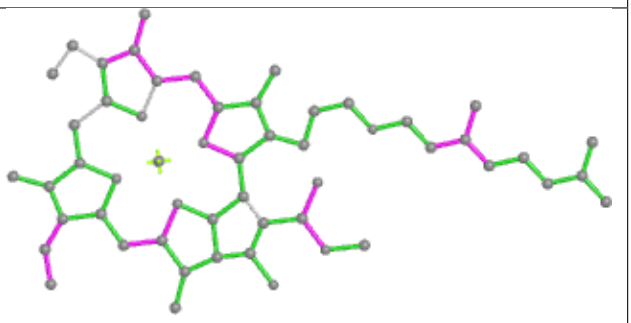
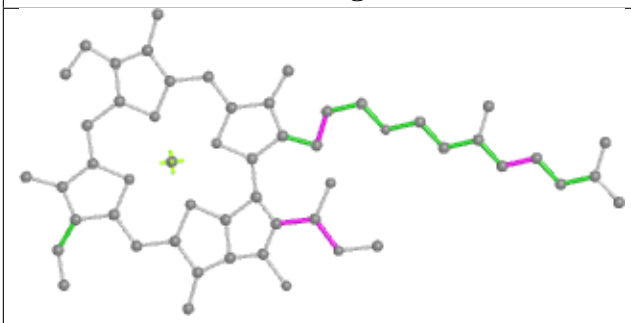
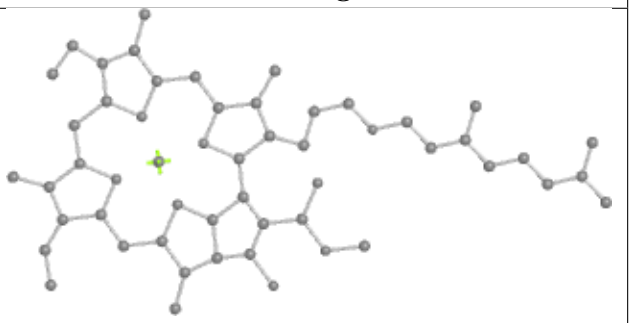
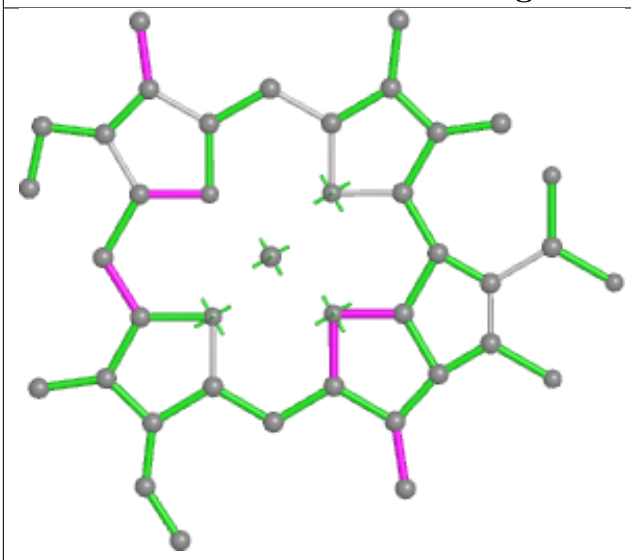
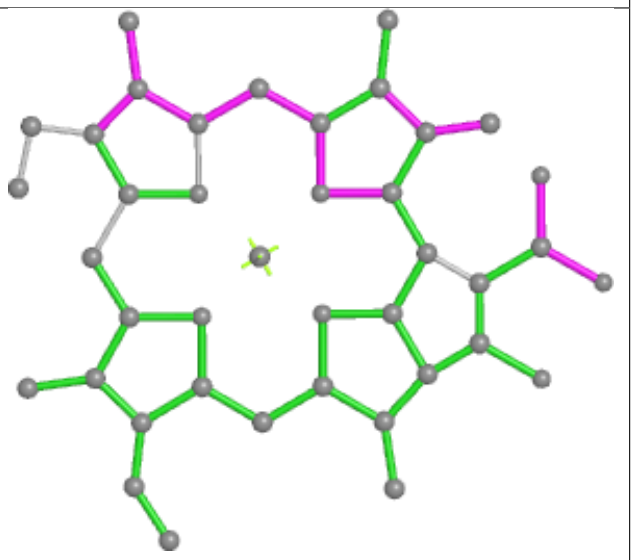
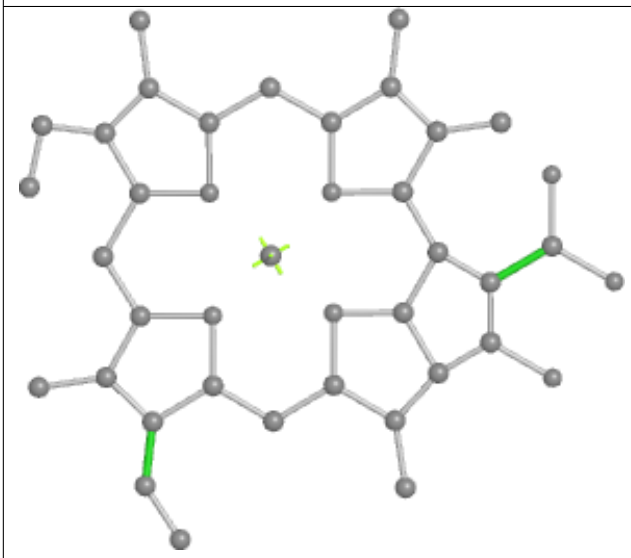
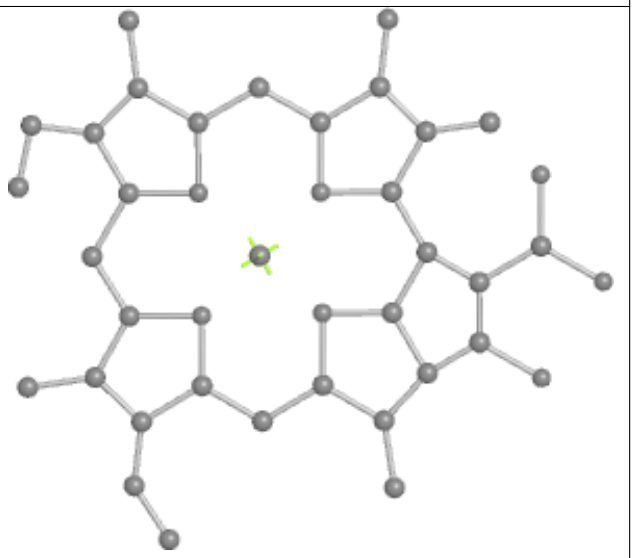
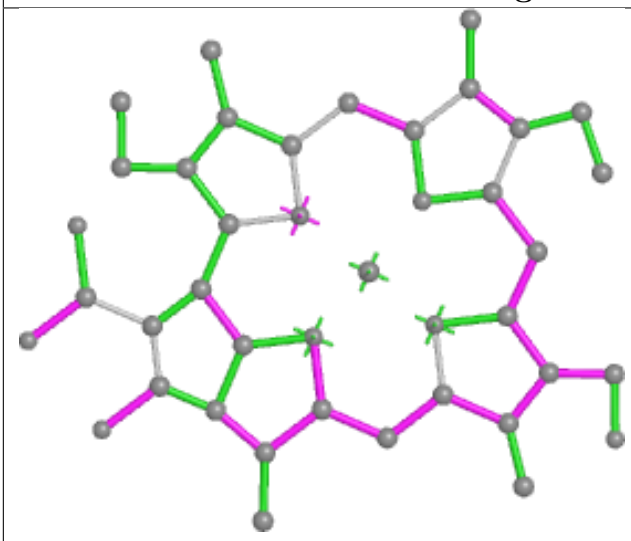
 Bond lengths	 Bond angles
 Torsions	 Rings

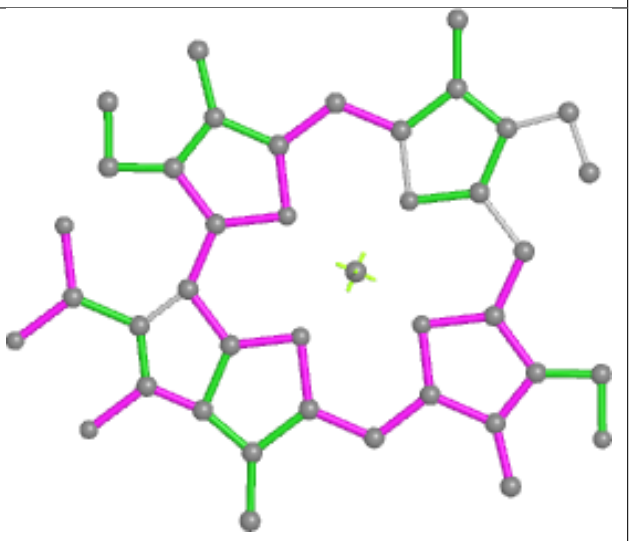
Ligand CLA B1 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

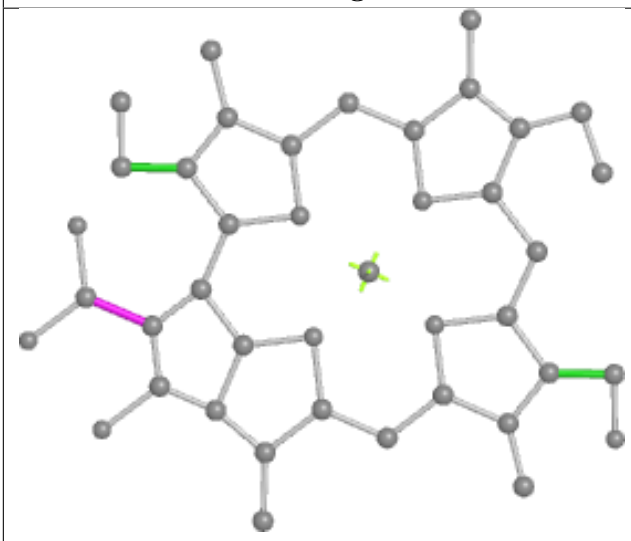
Ligand CHL B5 605



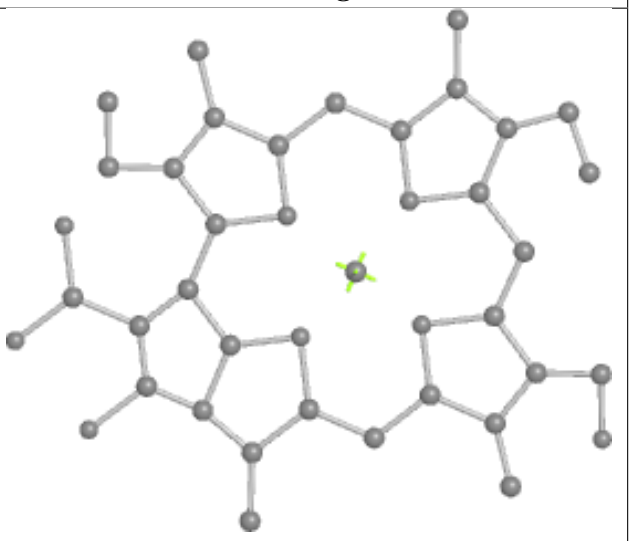
Bond lengths



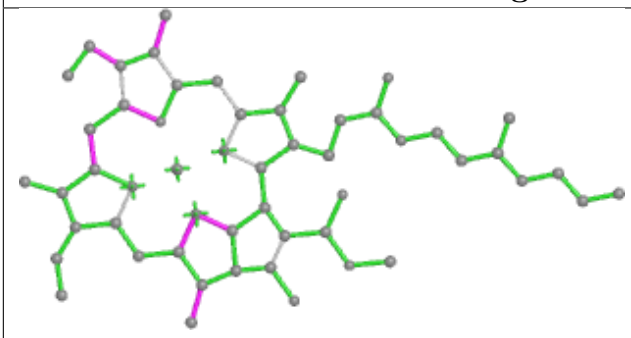
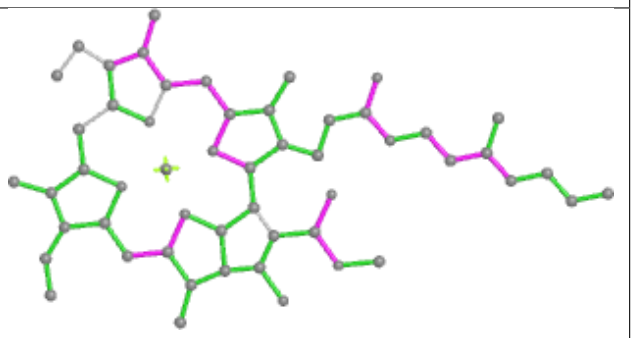
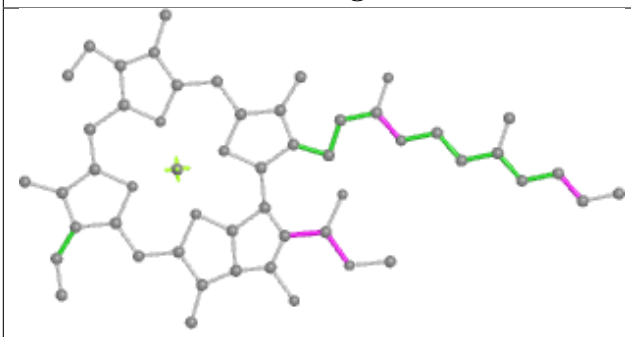
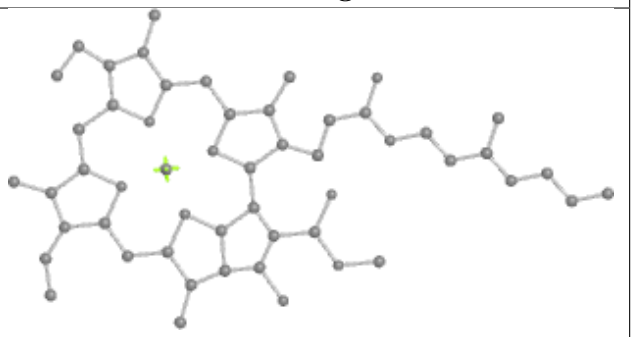
Bond angles



Torsions



Rings

Ligand CLA BA 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

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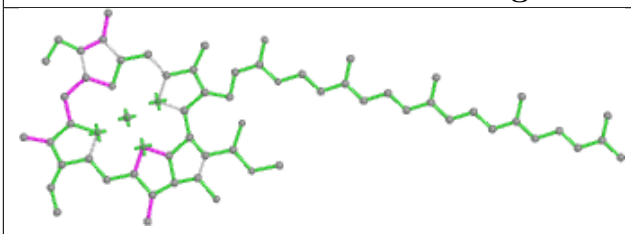
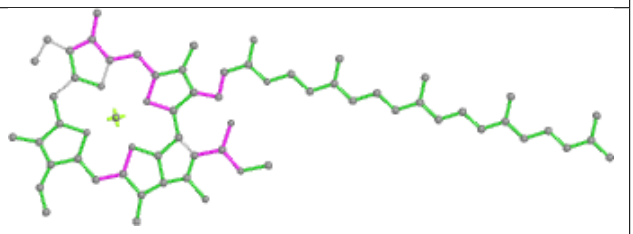
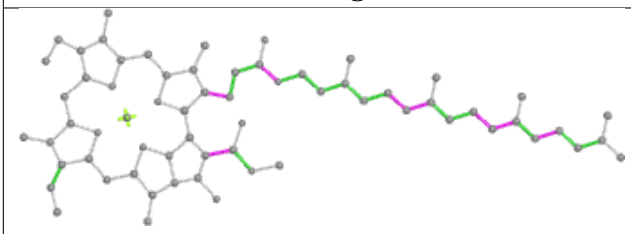
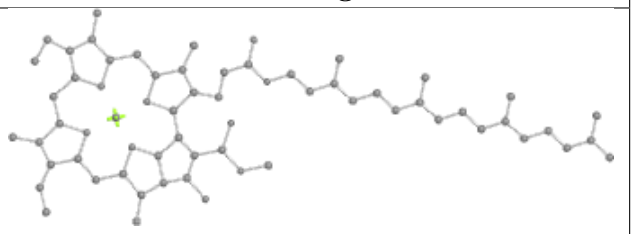
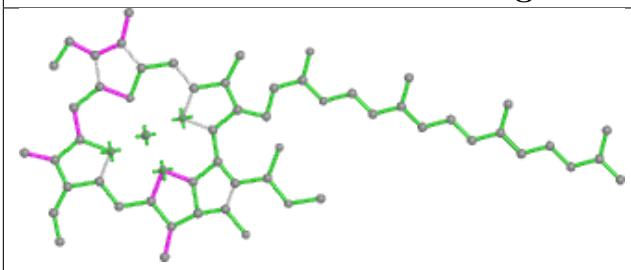
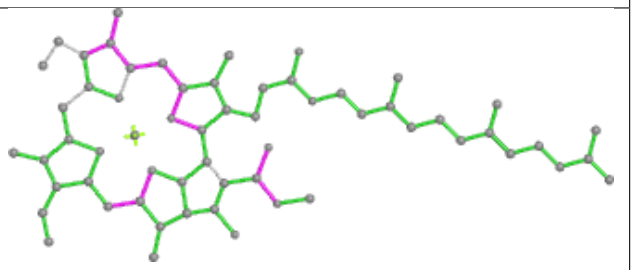
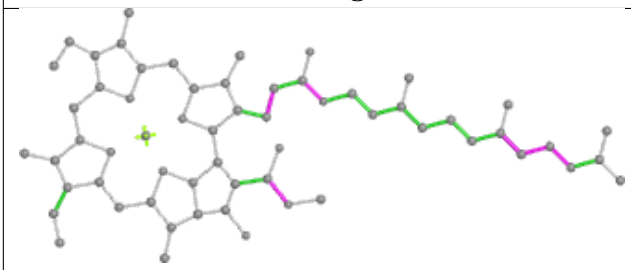
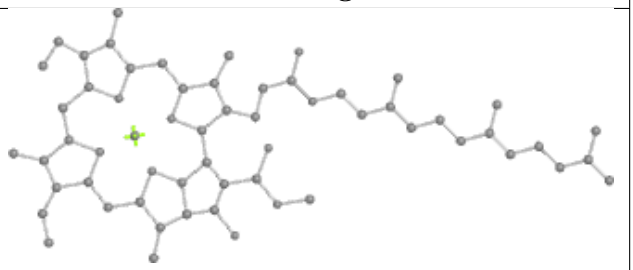
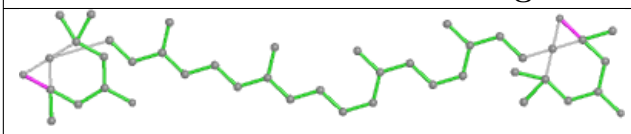
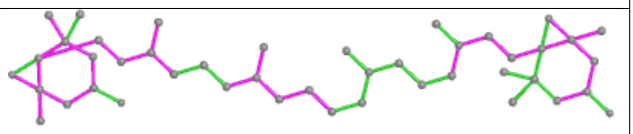
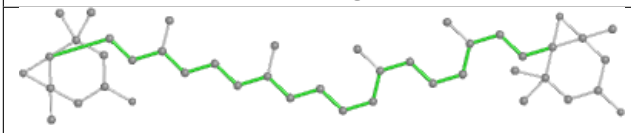
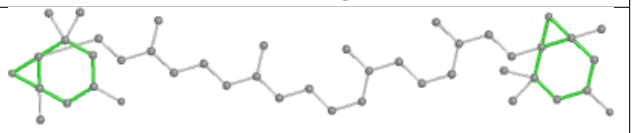
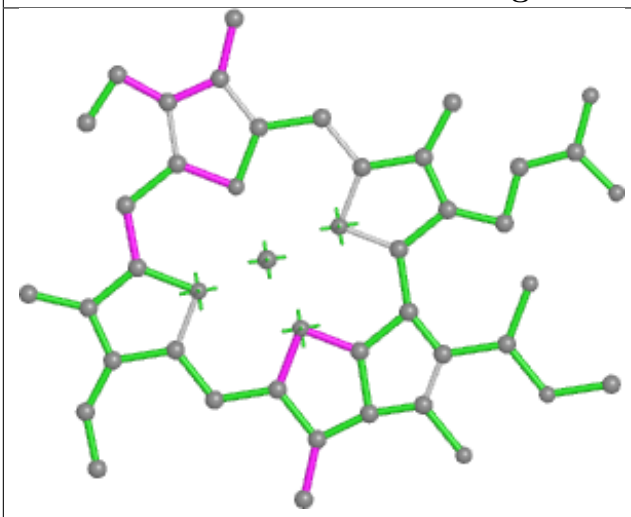
 Bond lengths	 Bond angles
 Torsions	 Rings

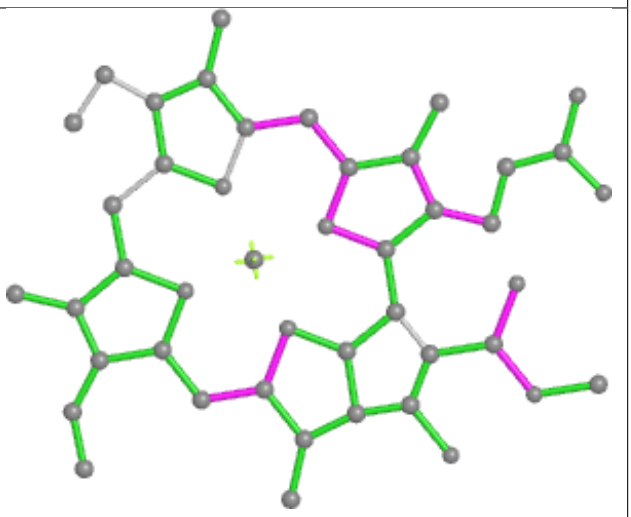
Ligand CLA B5 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT B5 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

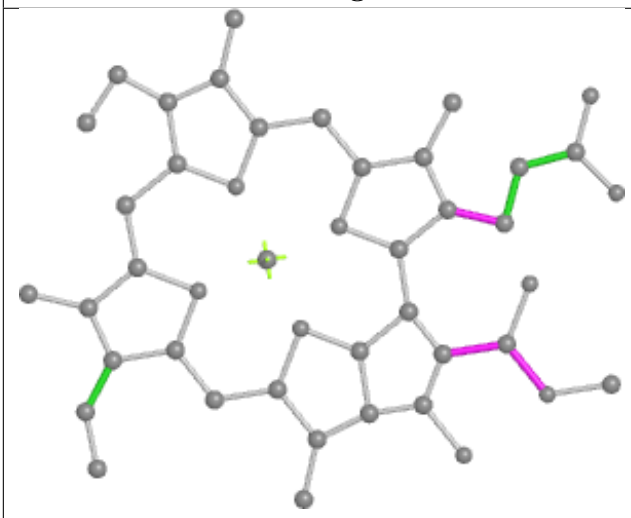
Ligand CLA BB 825



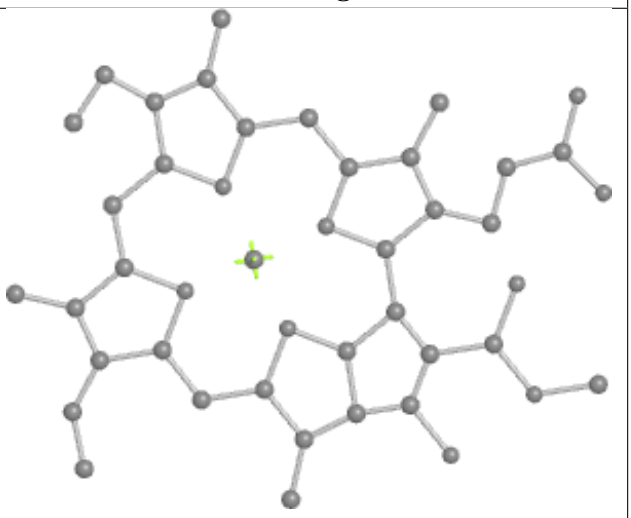
Bond lengths



Bond angles

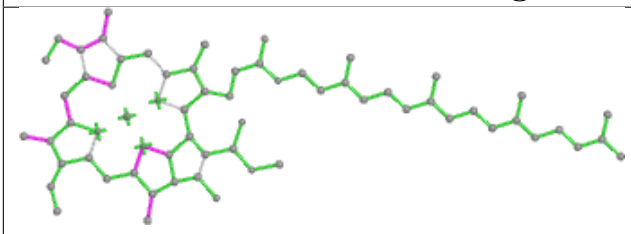


Torsions

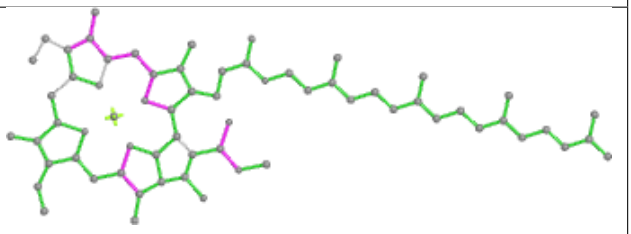


Rings

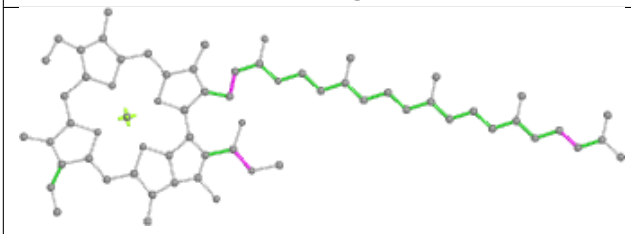
Ligand CLA BA 802



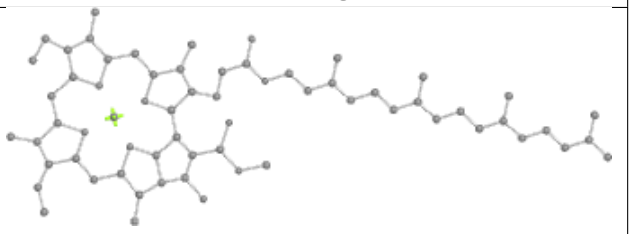
Bond lengths



Bond angles

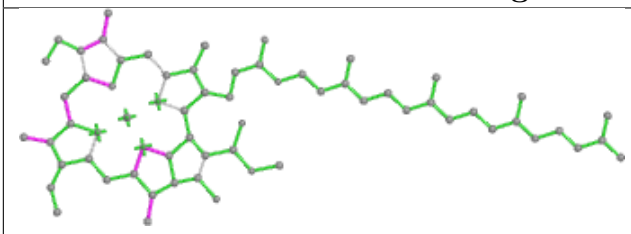


Torsions

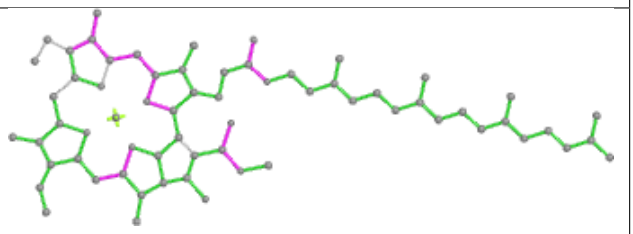


Rings

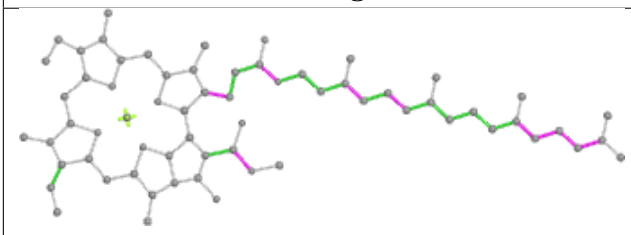
Ligand CLA BA 811



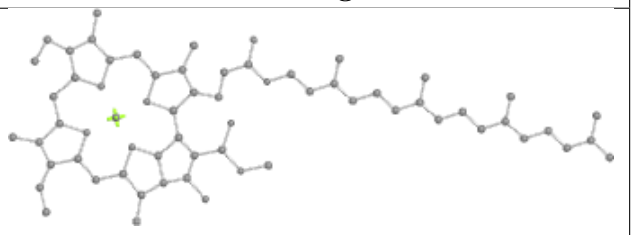
Bond lengths



Bond angles

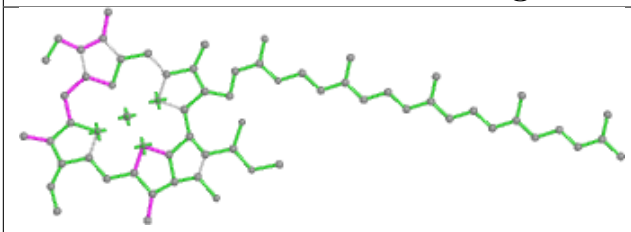


Torsions

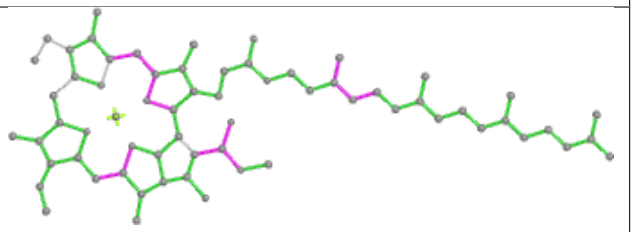


Rings

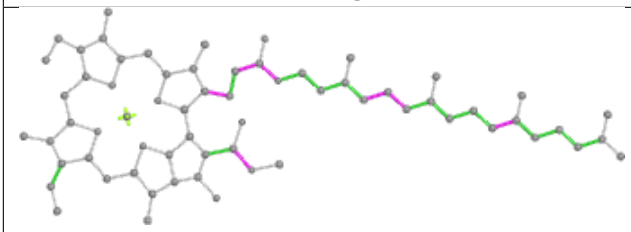
Ligand CLA BB 834



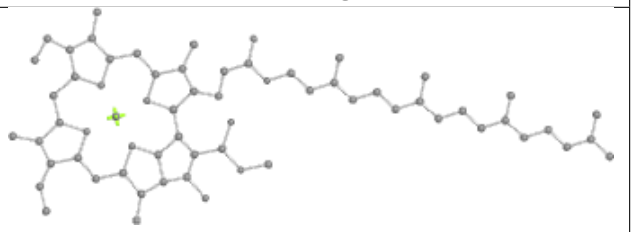
Bond lengths



Bond angles

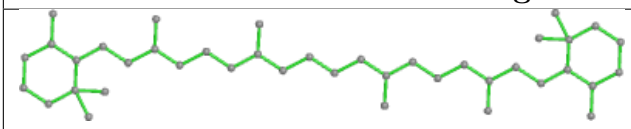


Torsions

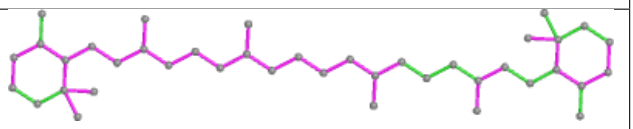


Rings

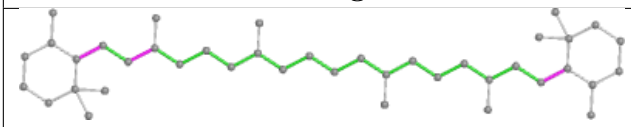
Ligand BCR BJ 103



Bond lengths

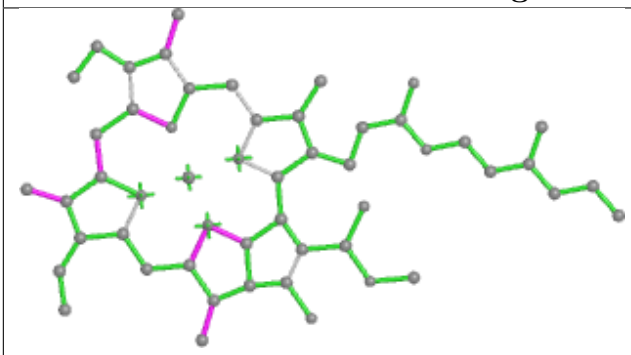
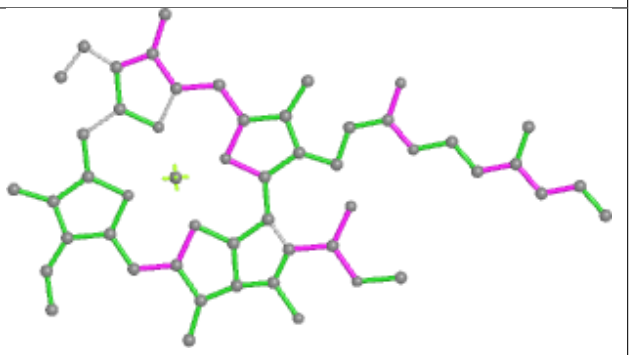
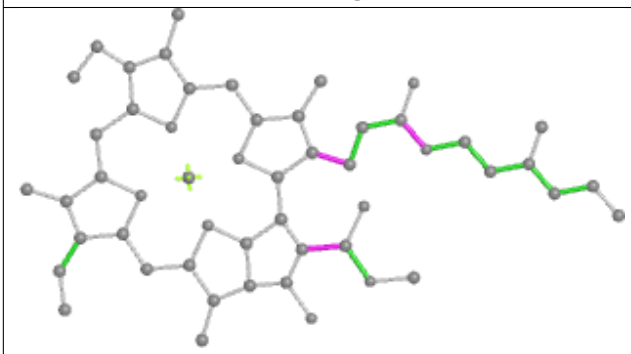
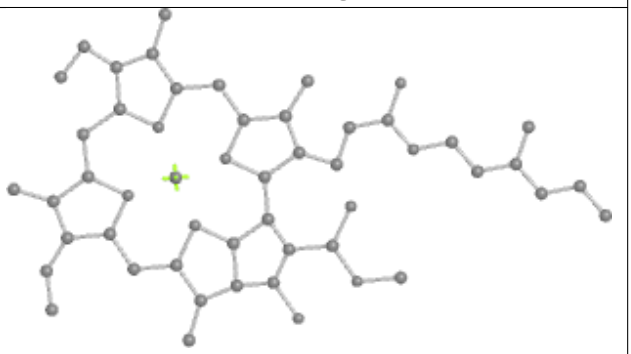


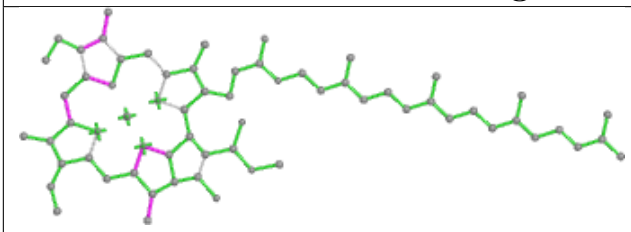
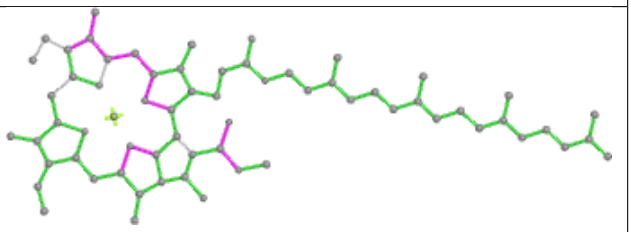
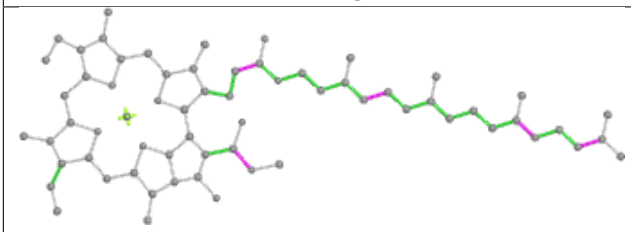
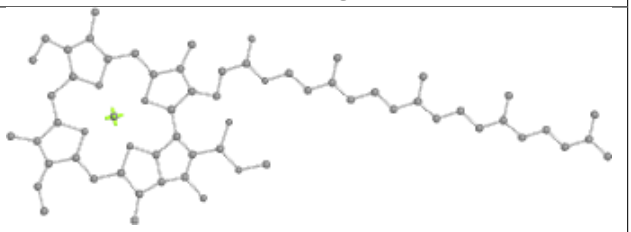
Bond angles



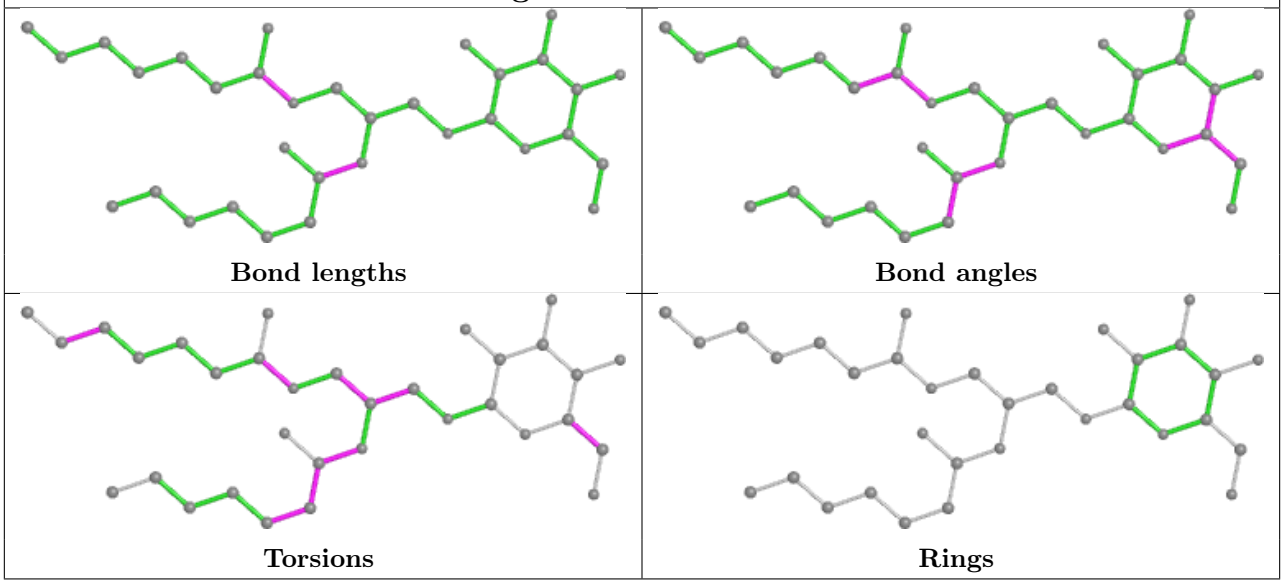
Torsions

Rings

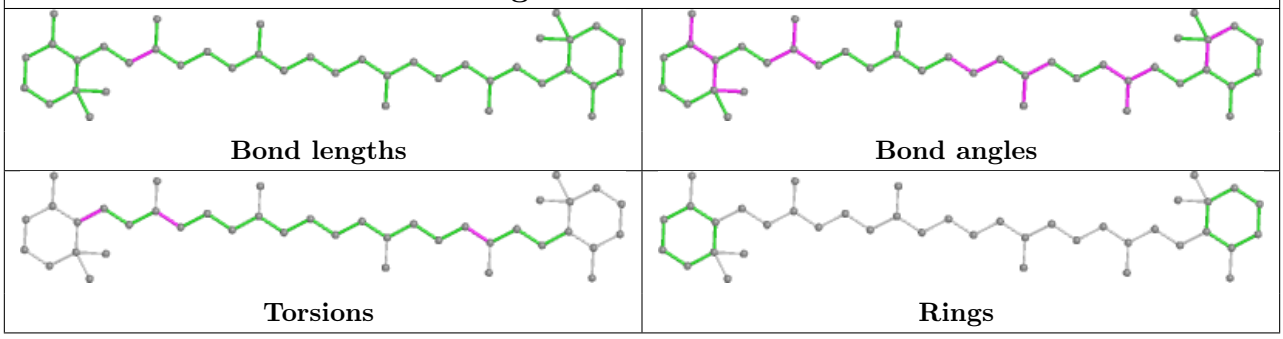
Ligand CLA BA 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BA 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

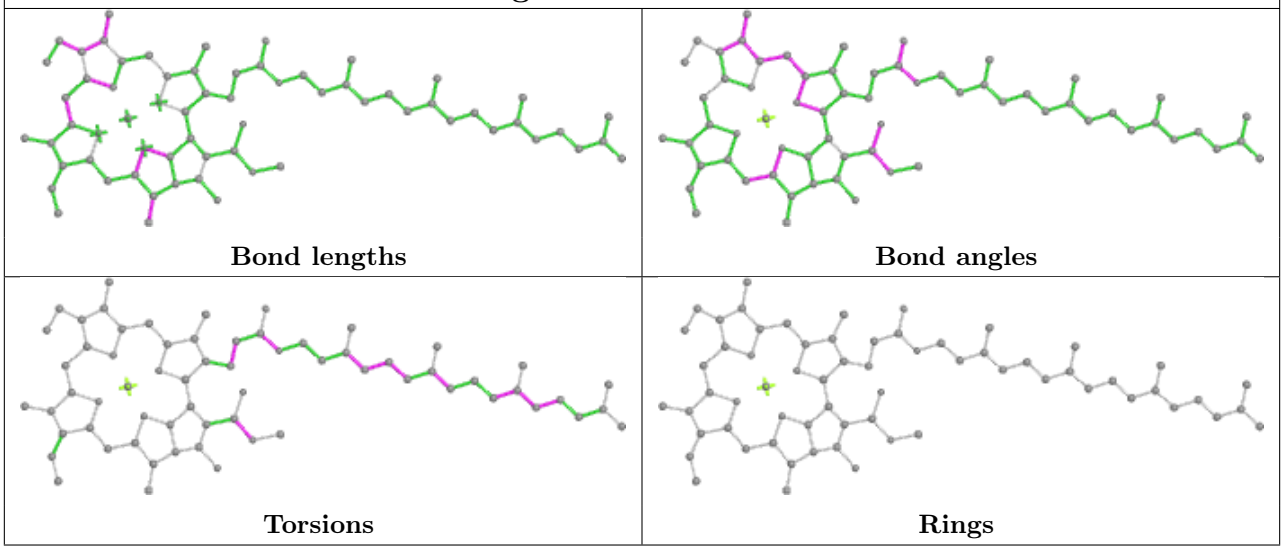
Ligand LMG B5 617



Ligand BCR BB 847



Ligand CLA BA 840



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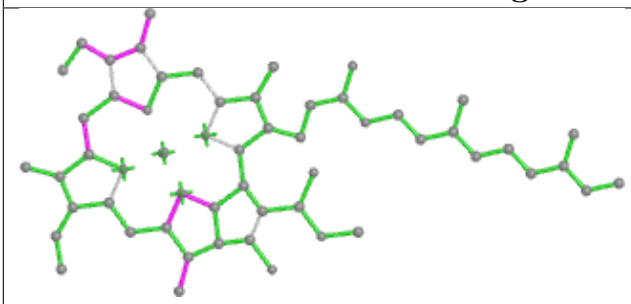
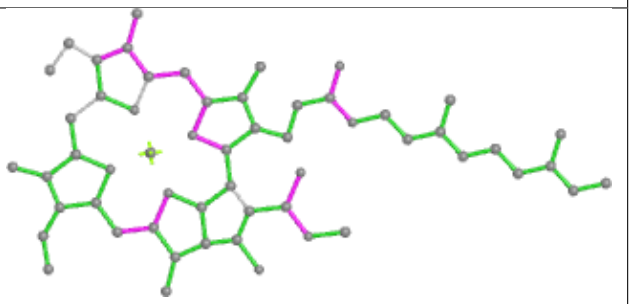
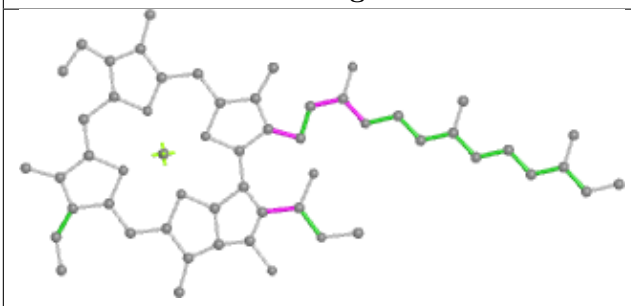
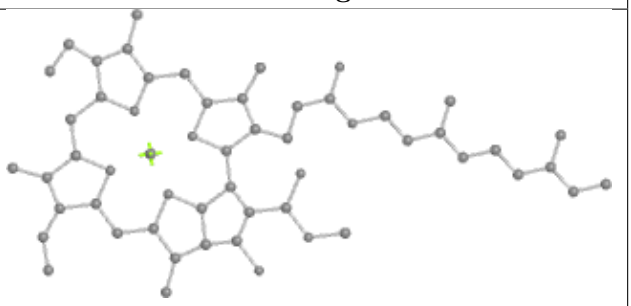
 Bond lengths	 Bond angles
 Torsions	 Rings

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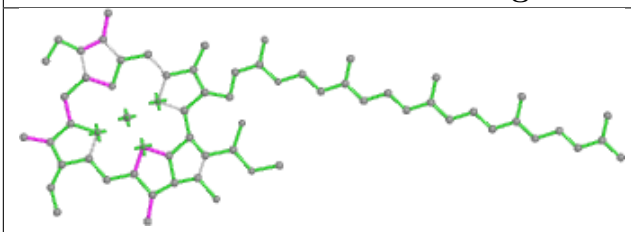
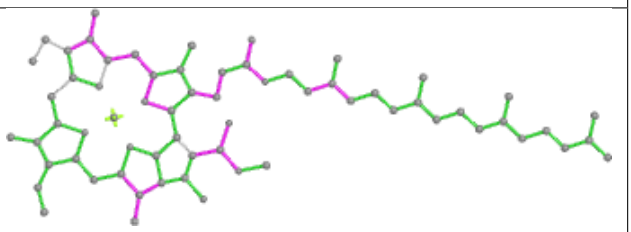
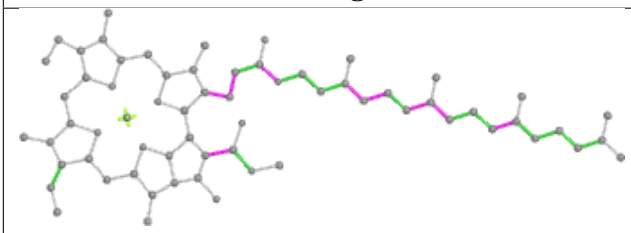
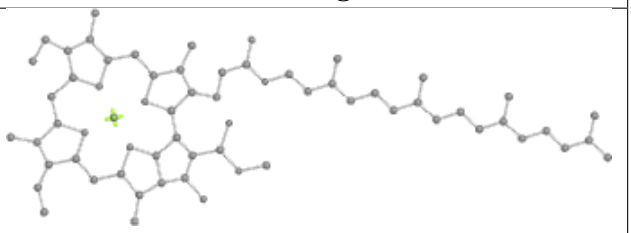
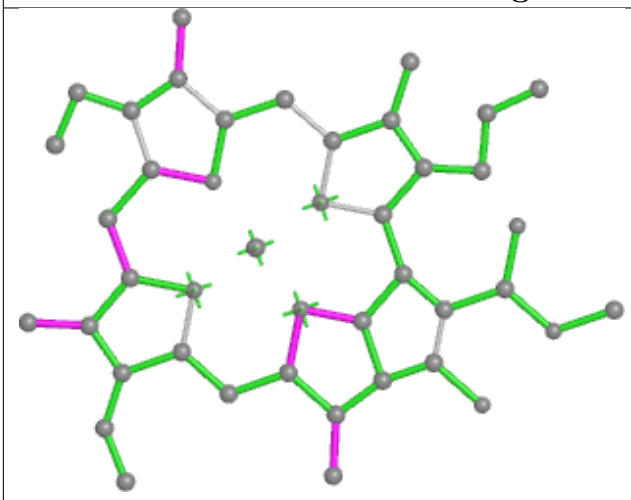
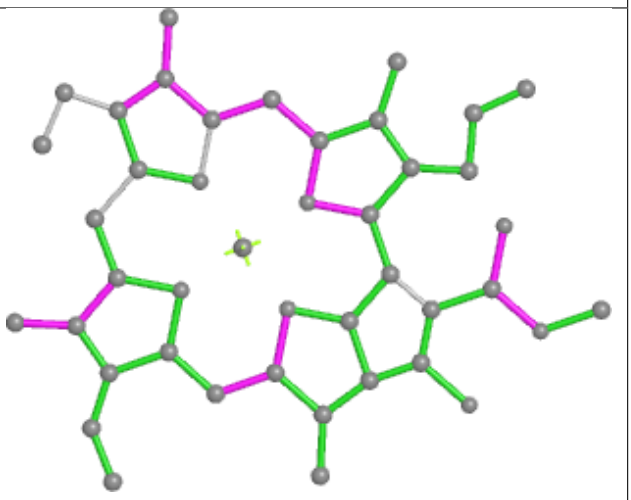
 Bond lengths	 Bond angles
 Torsions	 Rings

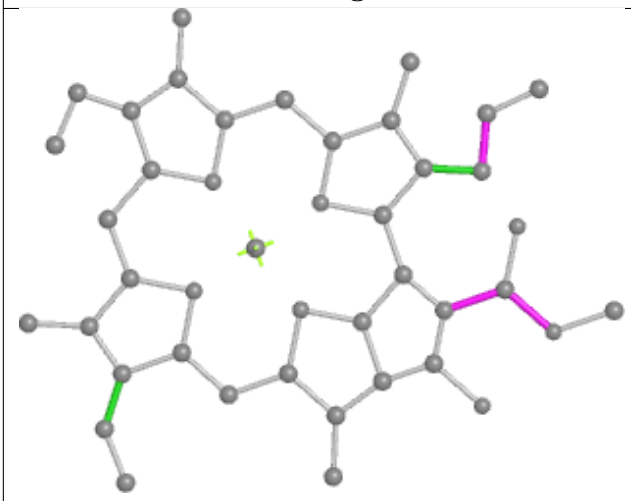
Ligand CLA BB 833



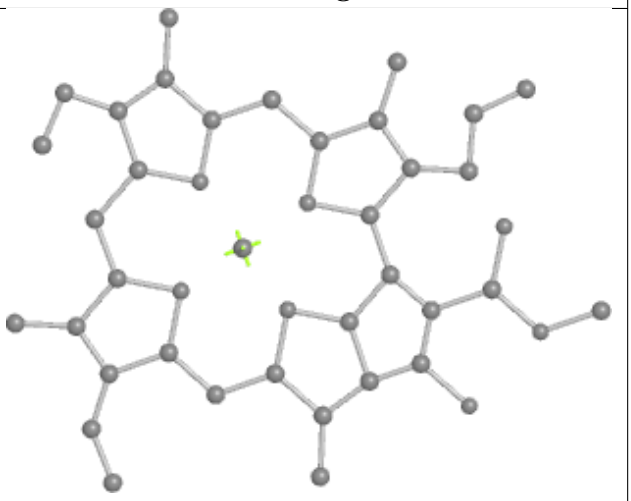
Bond lengths



Bond angles

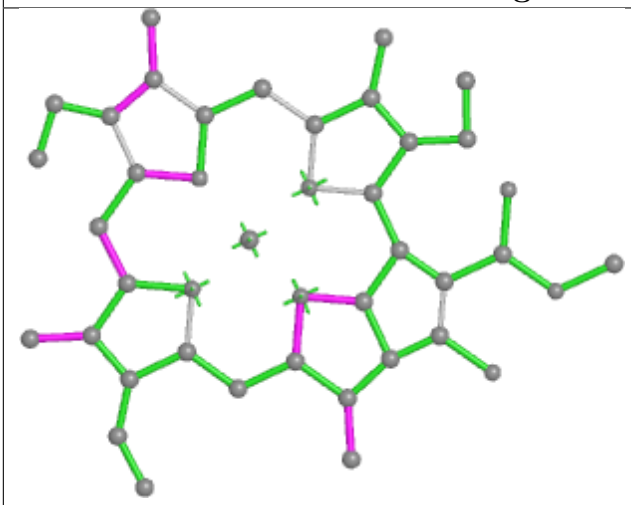


Torsions

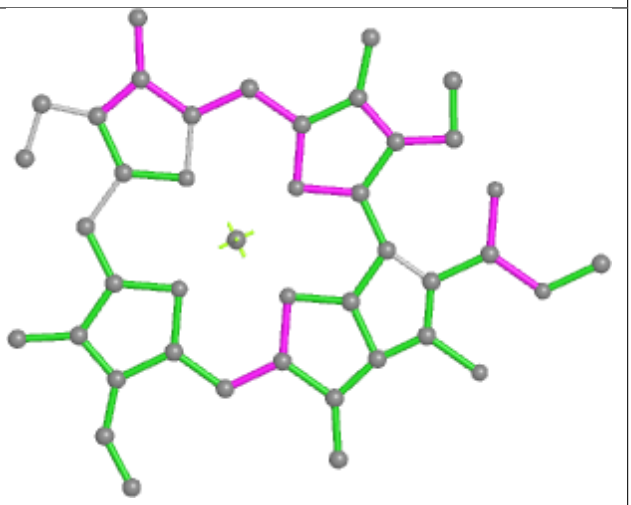


Rings

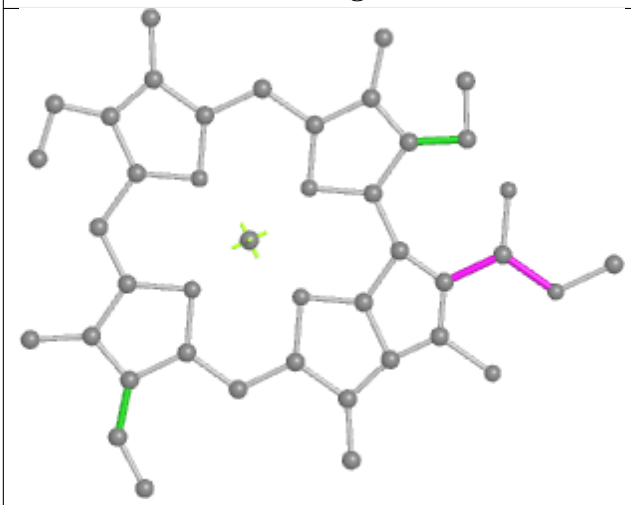
Ligand CLA BF 302



Bond lengths



Bond angles



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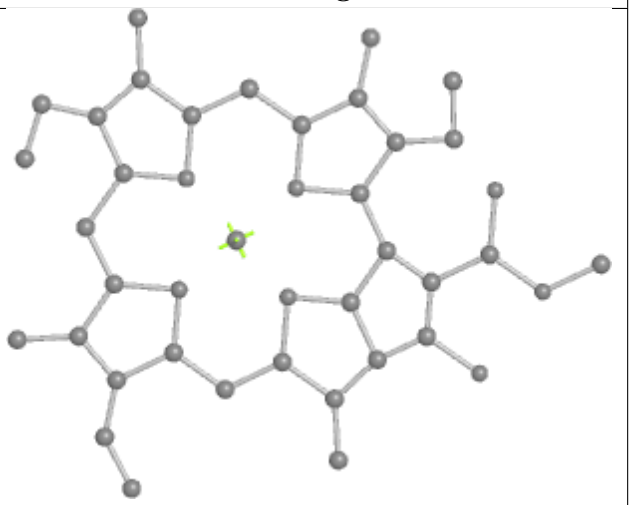
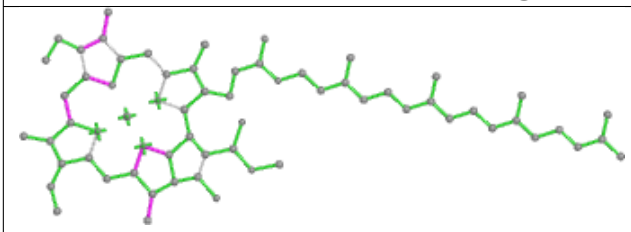
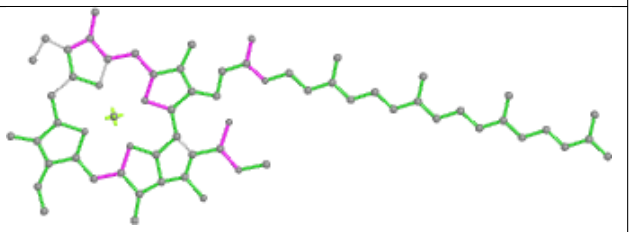


Rings

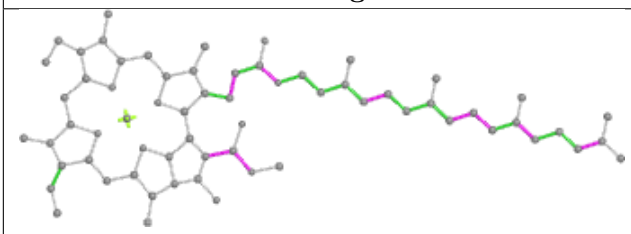
Ligand CLA B2 311



Bond lengths



Bond angles



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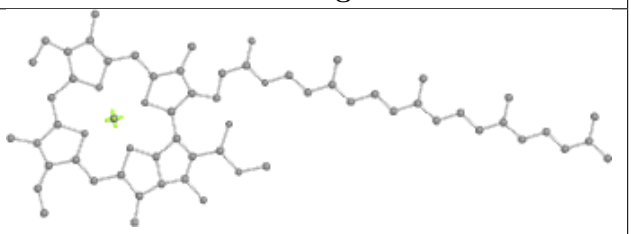
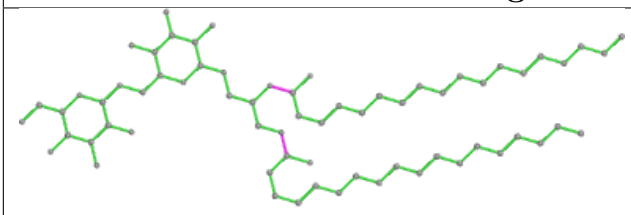
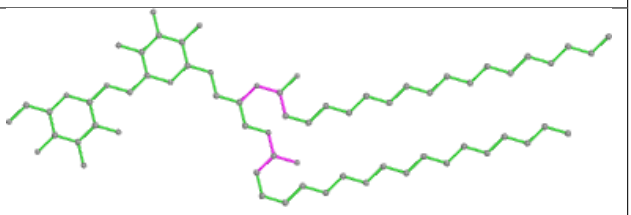
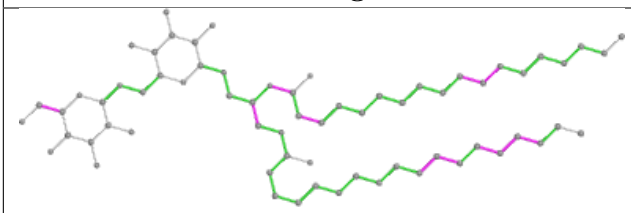
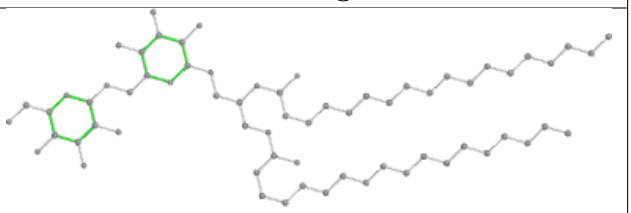
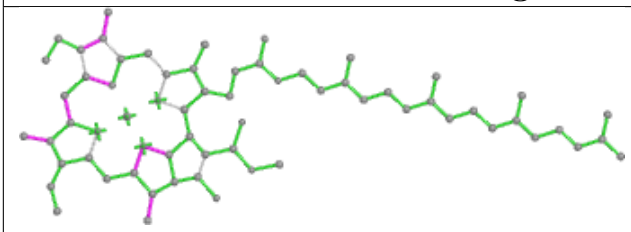
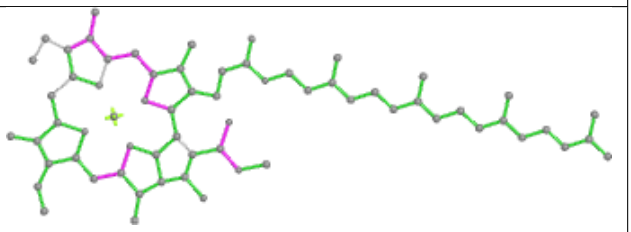
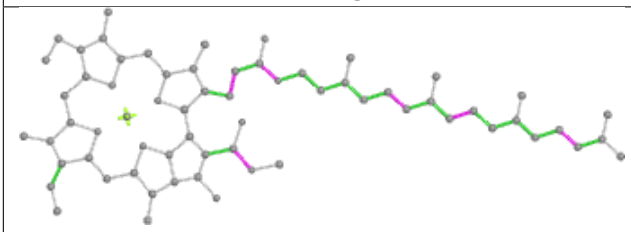
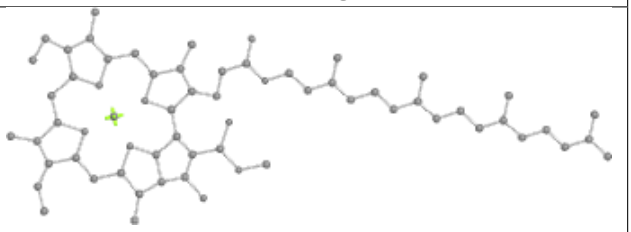
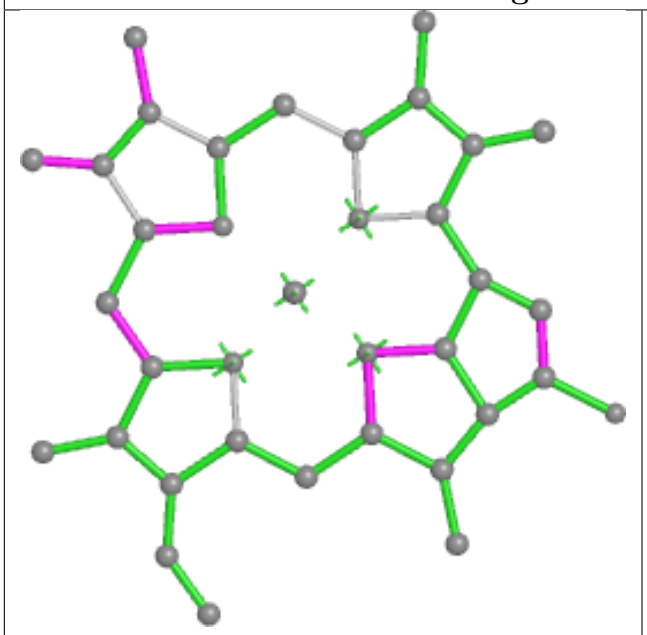


Rings

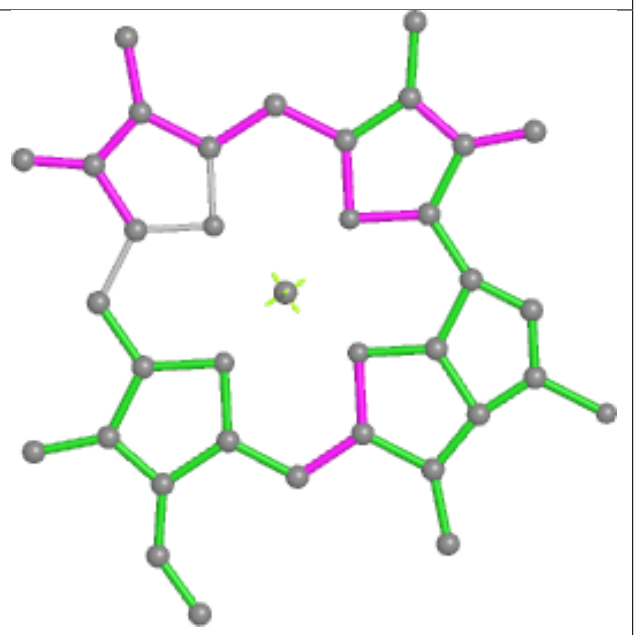
Ligand DGD BB 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

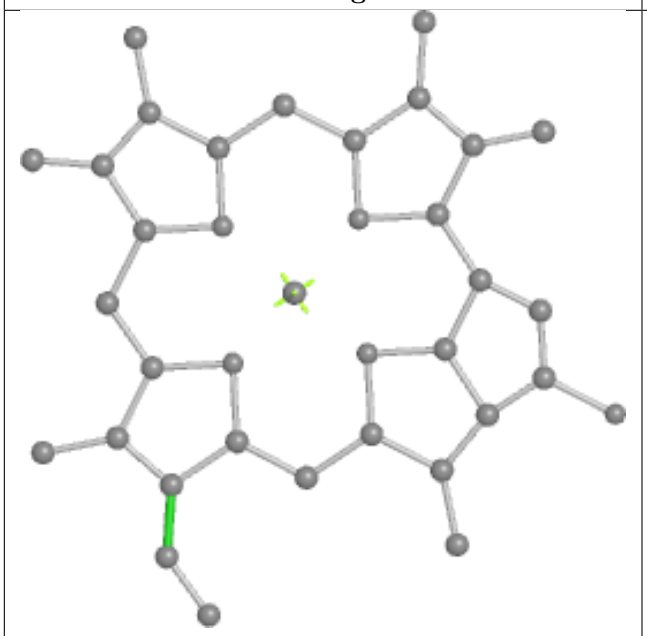
Ligand CLA BK 201



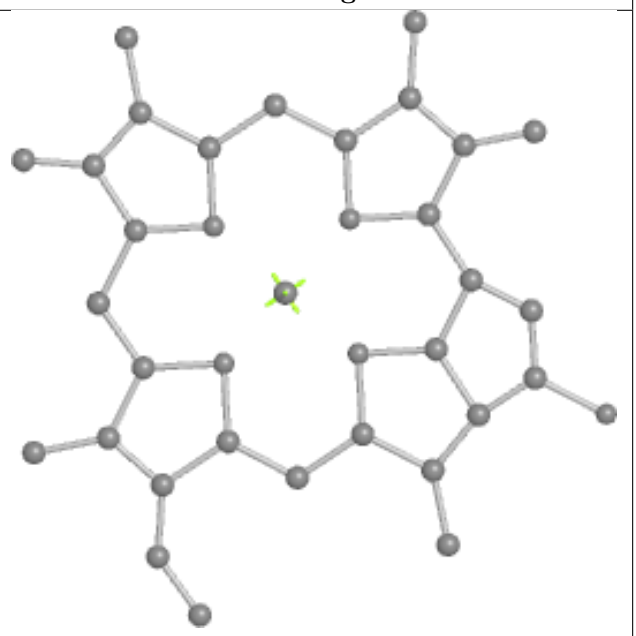
Bond lengths



Bond angles

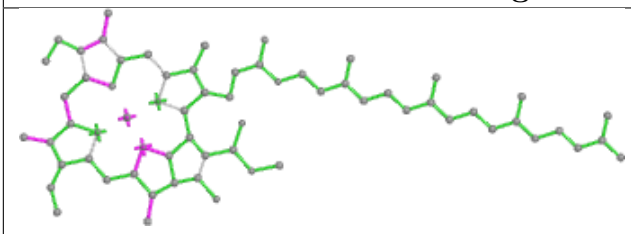


Torsions

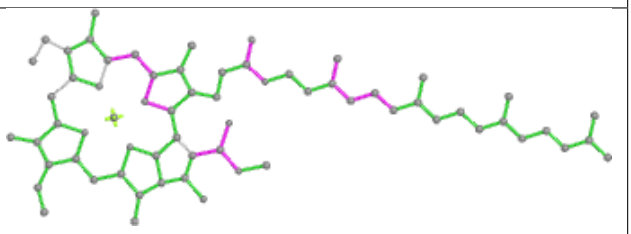


Rings

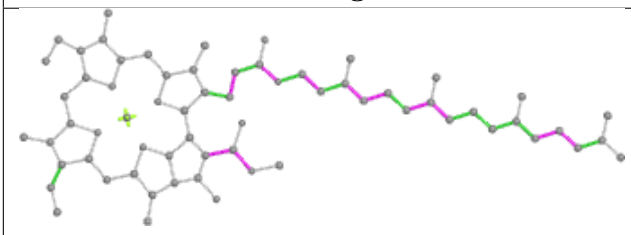
Ligand CLA BB 802



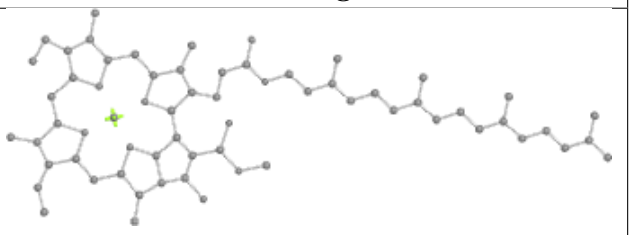
Bond lengths



Bond angles

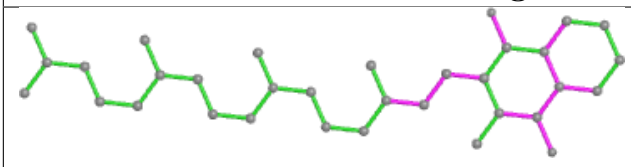


Torsions

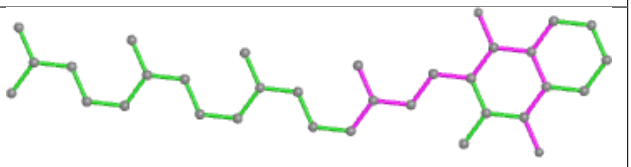


Rings

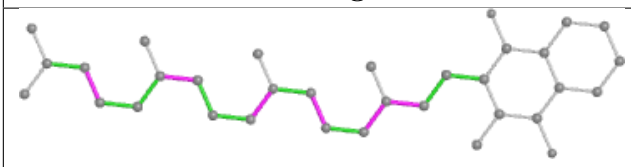
Ligand PQN BB 844



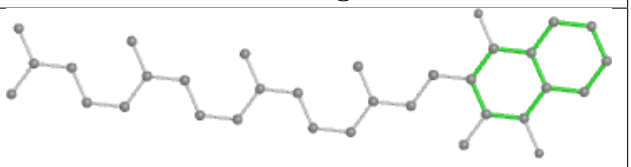
Bond lengths



Bond angles

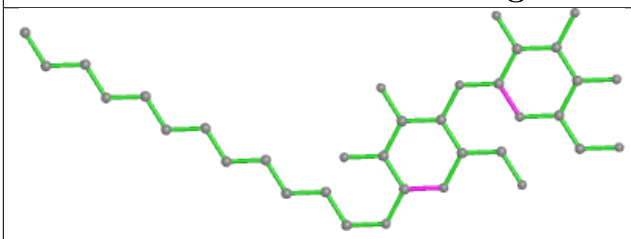


Torsions

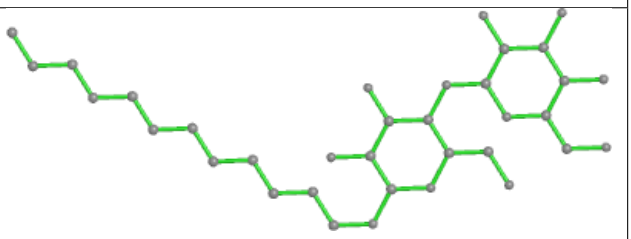


Rings

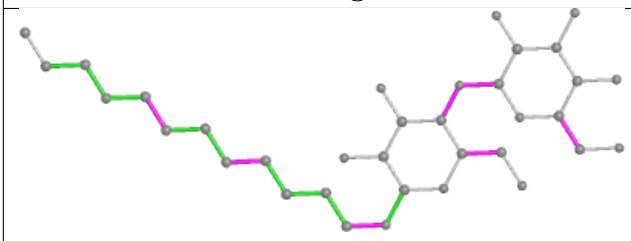
Ligand LMU BB 851



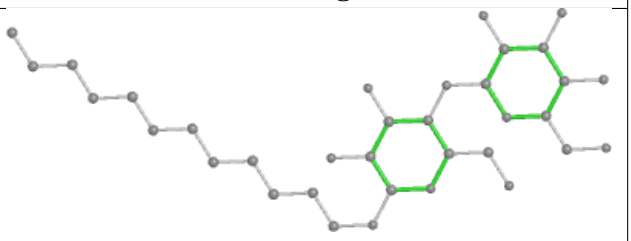
Bond lengths



Bond angles

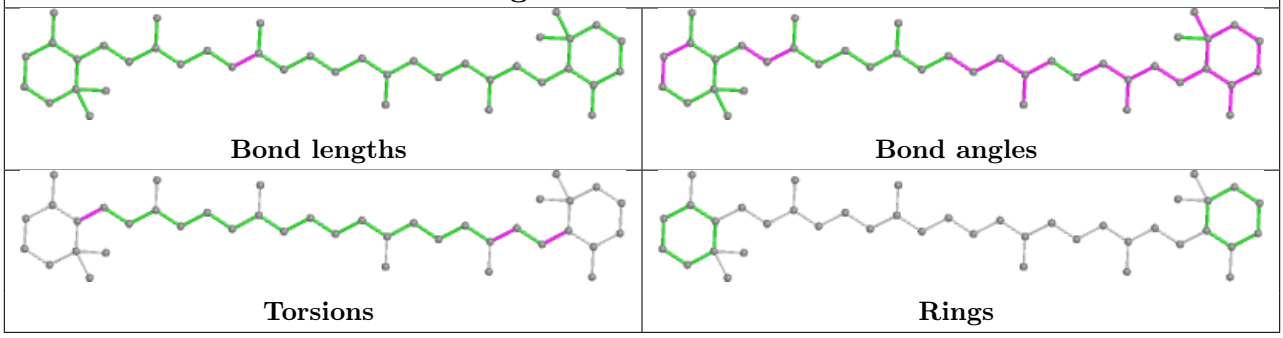


Torsions

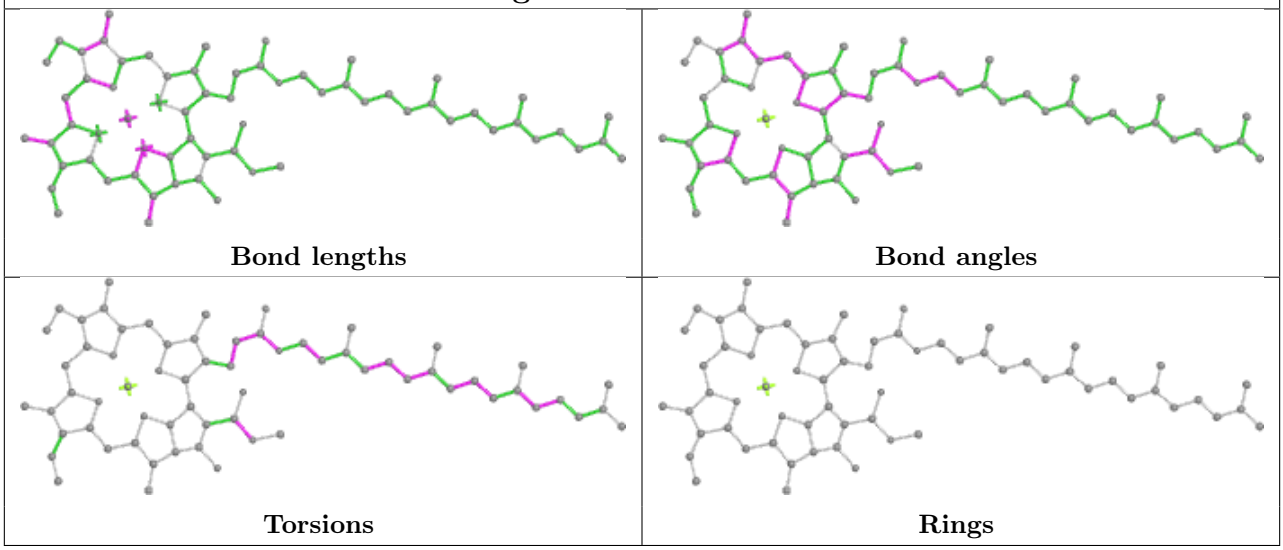


Rings

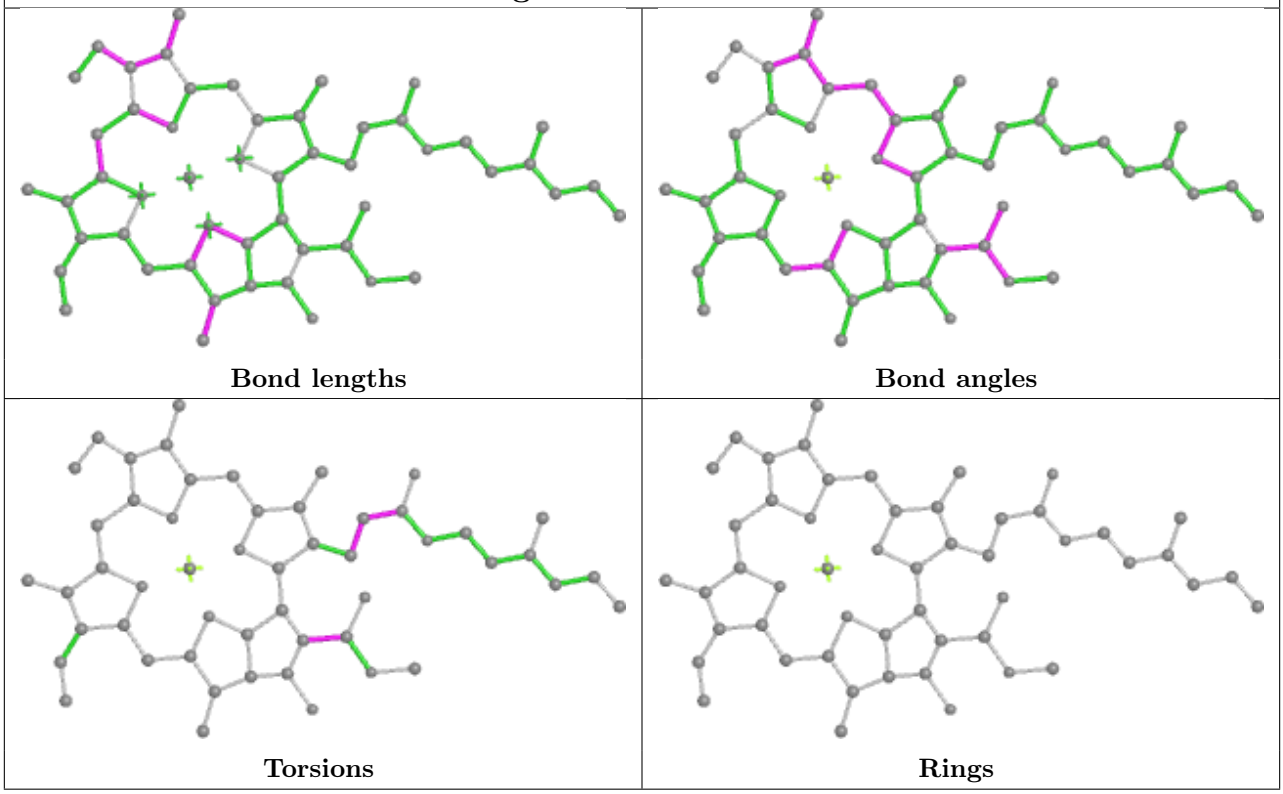
Ligand BCR BA 856



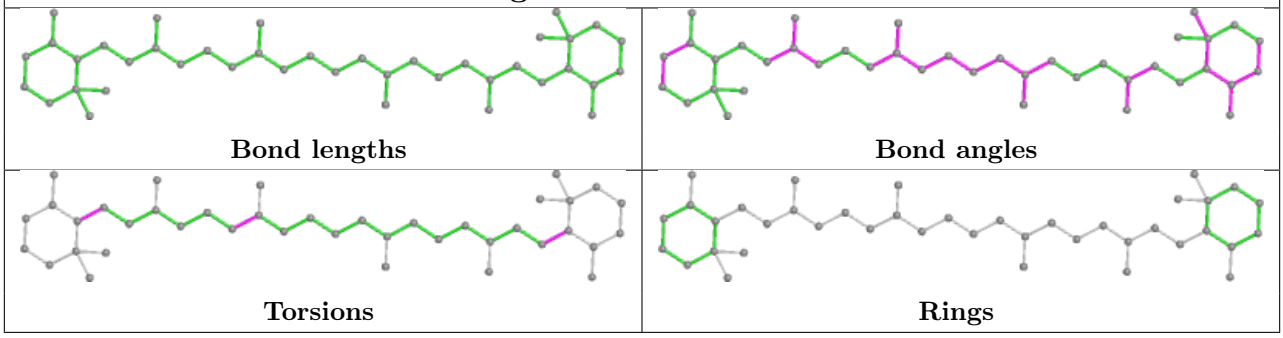
Ligand CLA BB 801



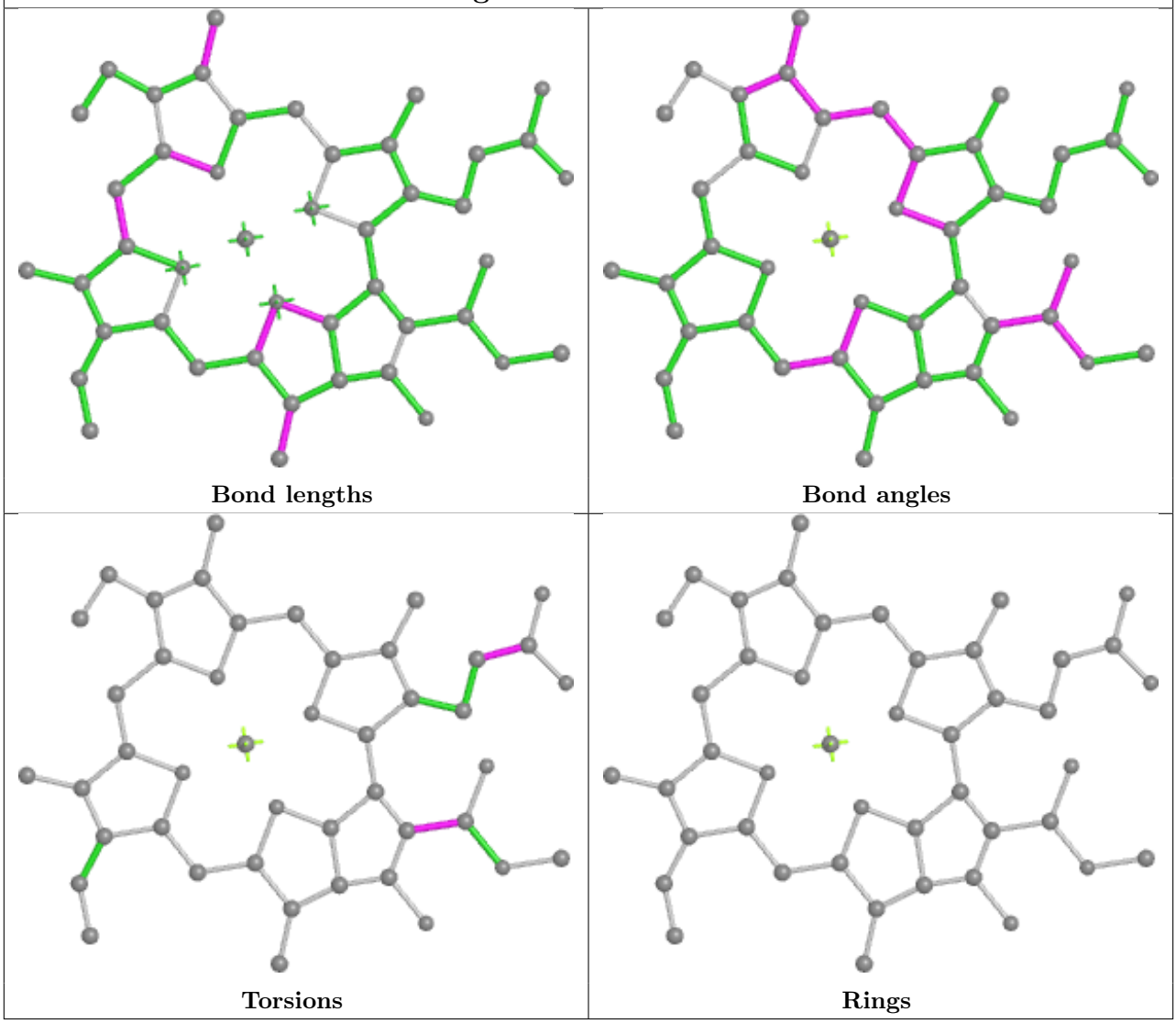
Ligand CLA BB 809



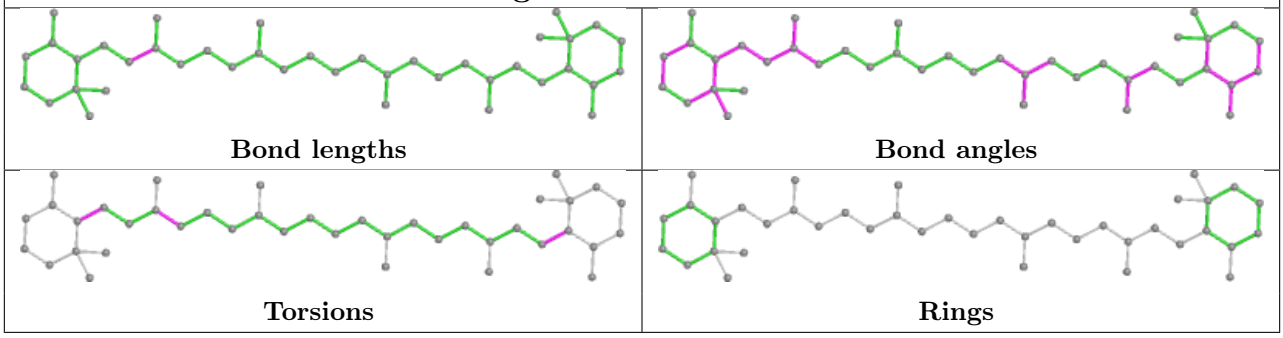
Ligand BCR BA 848



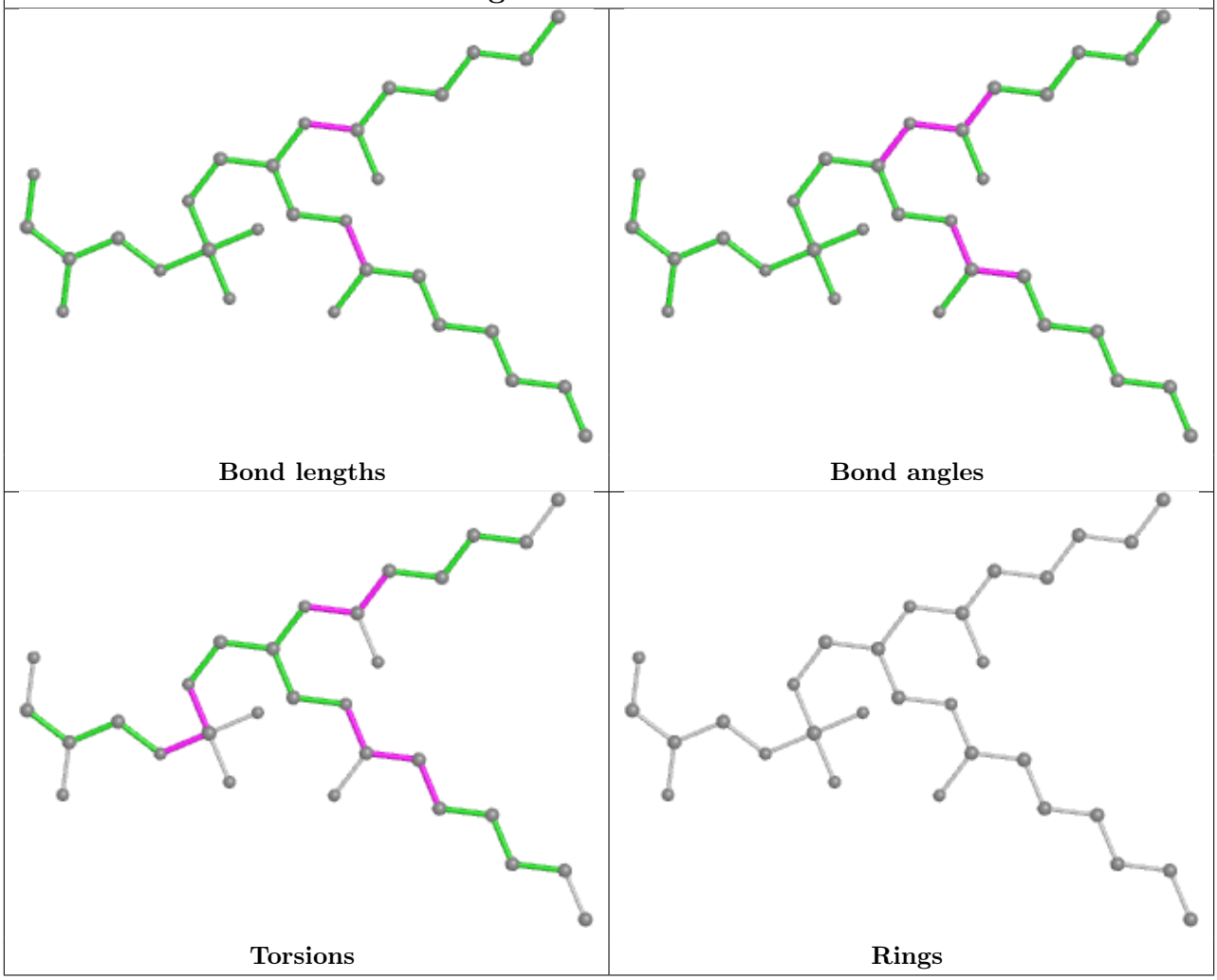
Ligand CLA B3 608



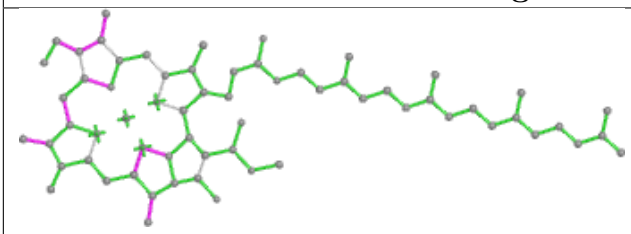
Ligand BCR BL 301



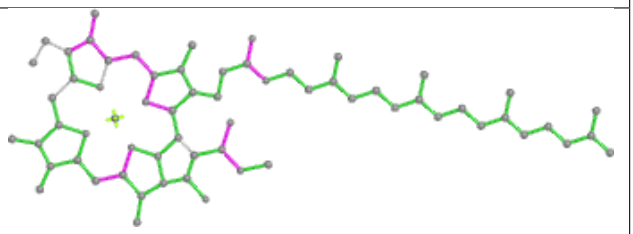
Ligand LHG B5 618



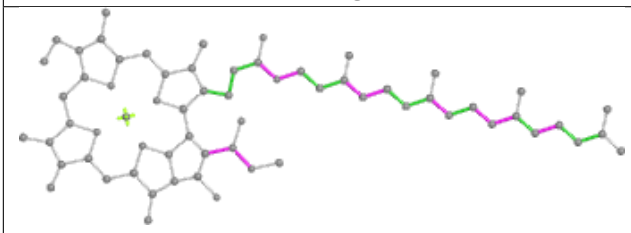
Ligand CLA BB 816



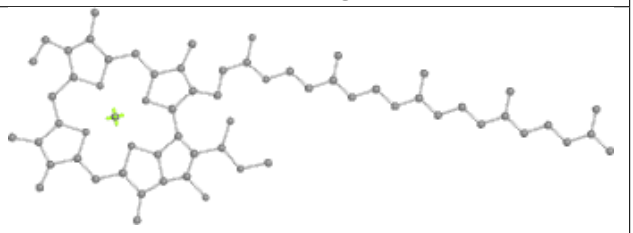
Bond lengths



Bond angles

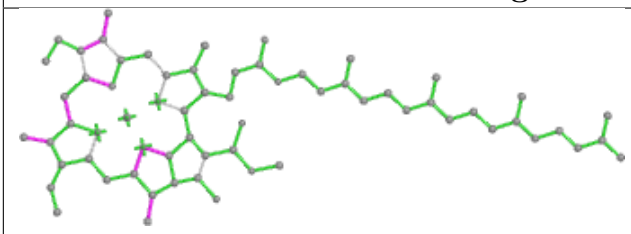


Torsions

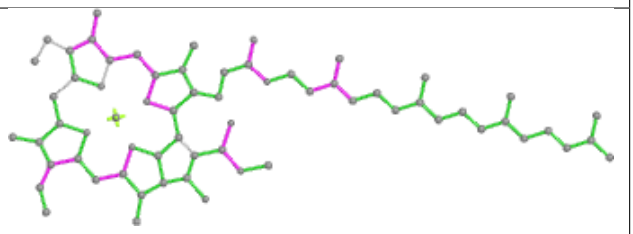


Rings

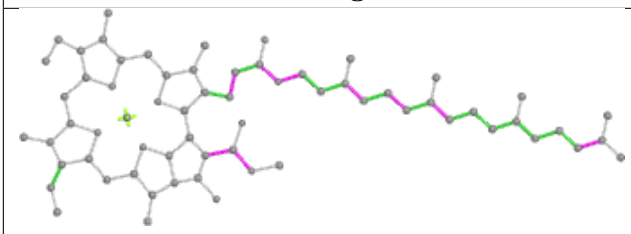
Ligand CLA BA 841



Bond lengths



Bond angles



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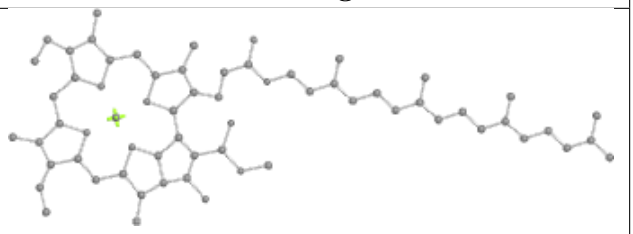
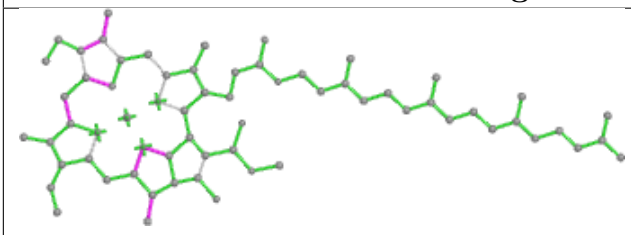
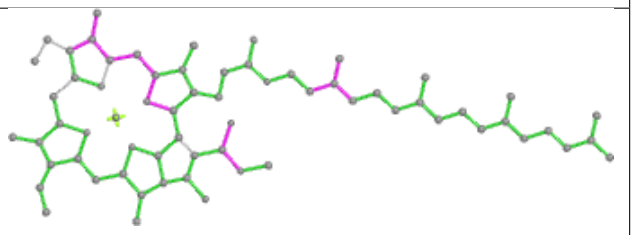


Rings

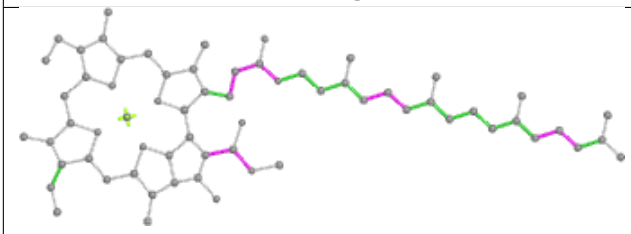
Ligand CLA BA 833



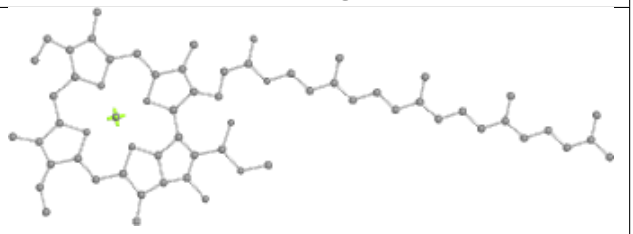
Bond lengths



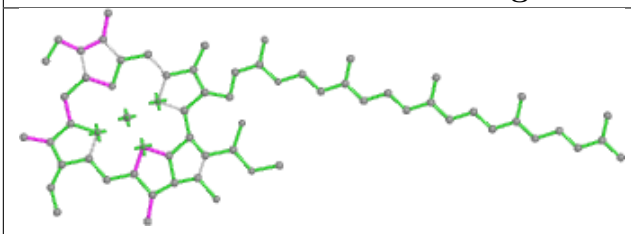
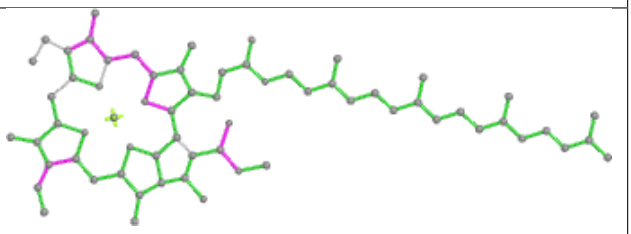
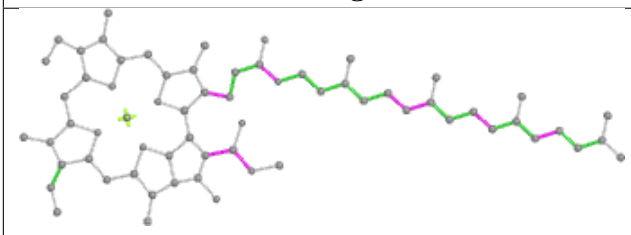
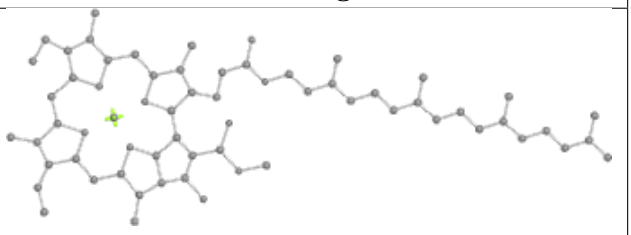
Bond angles

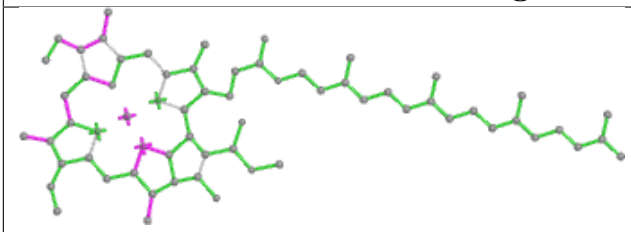
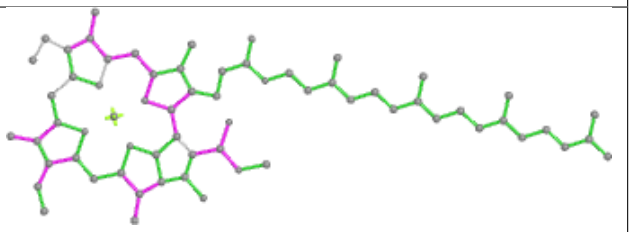
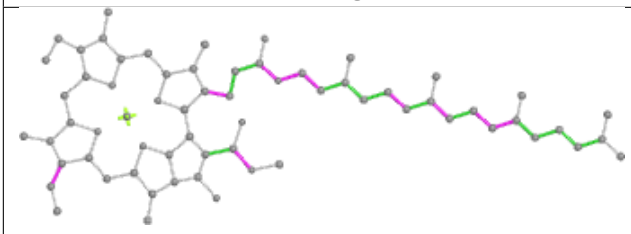
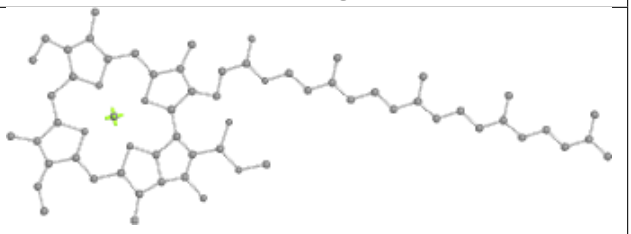


Torsions

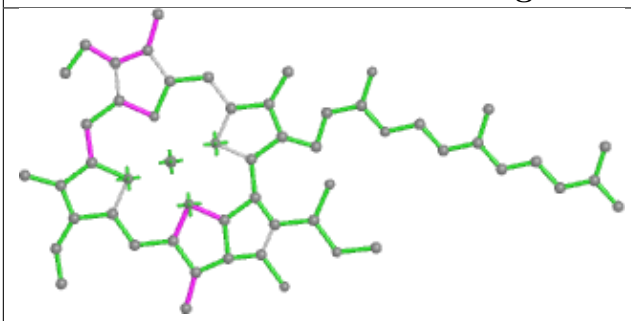


Rings

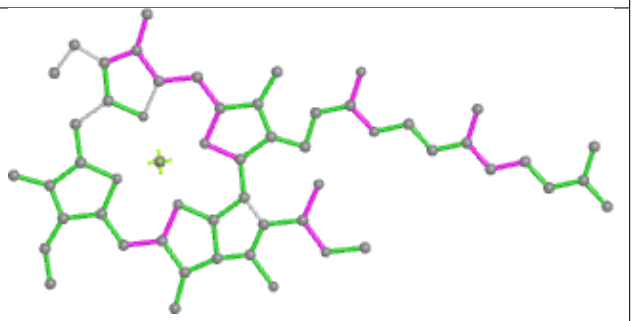
Ligand CLA BA 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BB 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

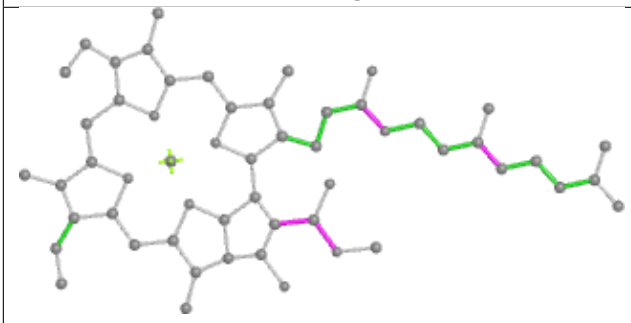
Ligand CLA B2 308



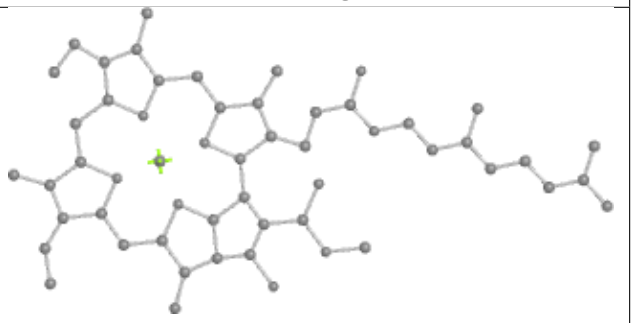
Bond lengths



Bond angles

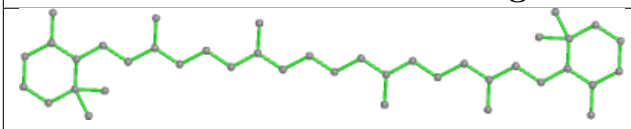


Torsions

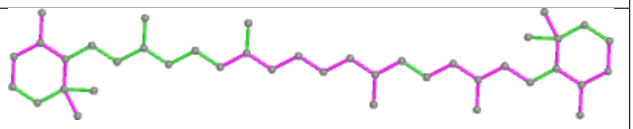


Rings

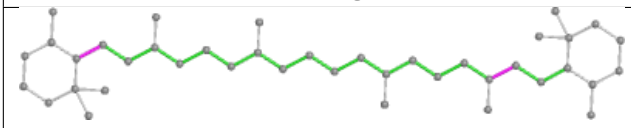
Ligand BCR BA 849



Bond lengths



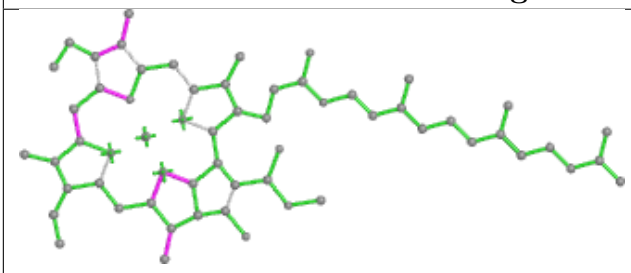
Bond angles



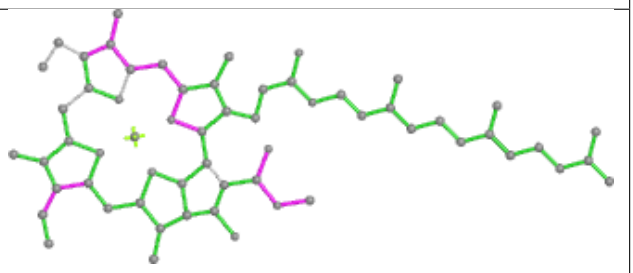
Torsions

Rings

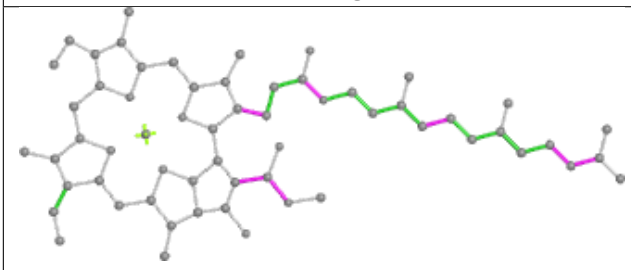
Ligand CLA BH 201



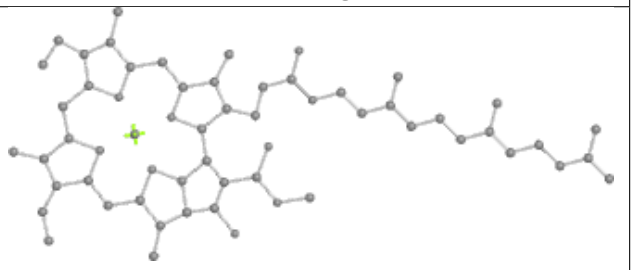
Bond lengths



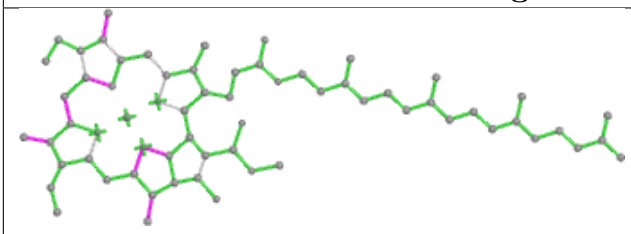
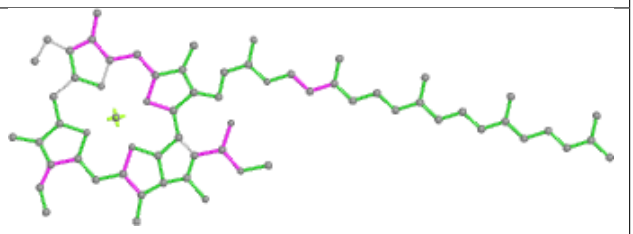
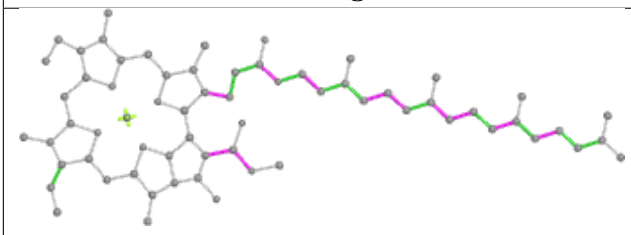
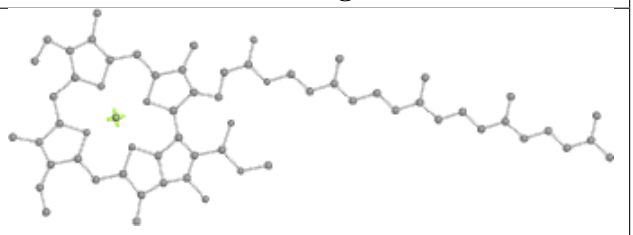
Bond angles

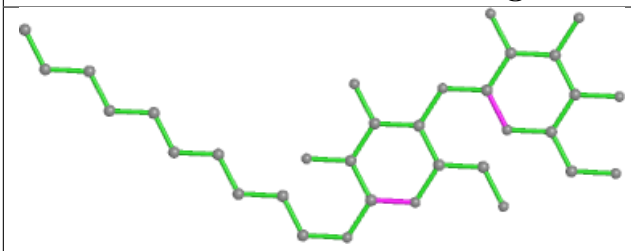
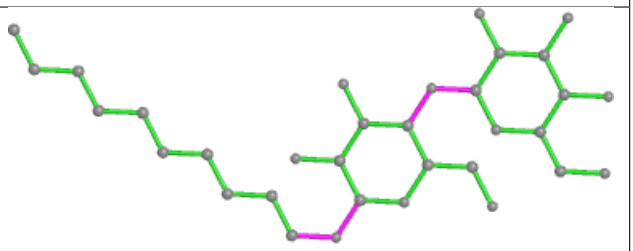
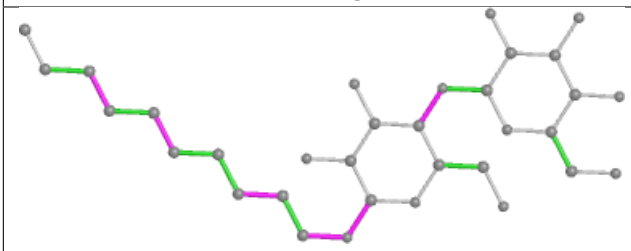
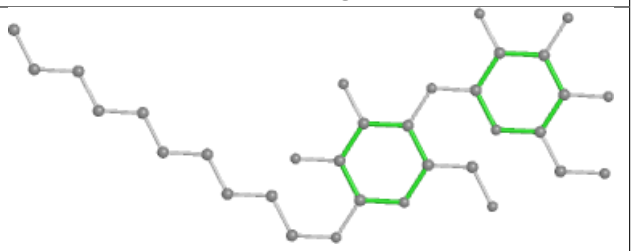


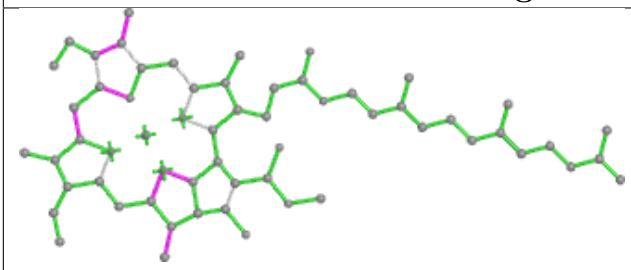
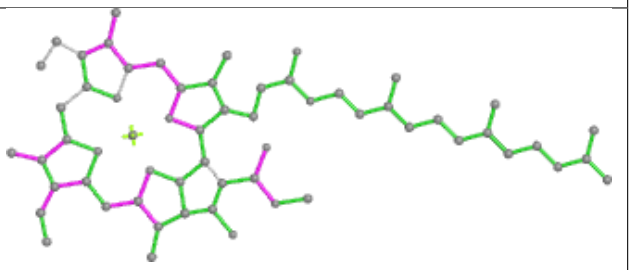
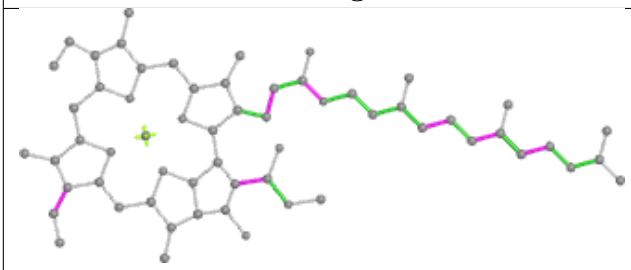
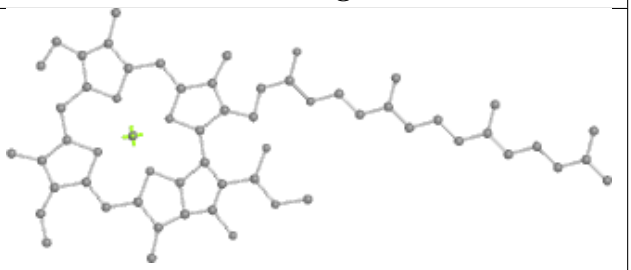
Torsions

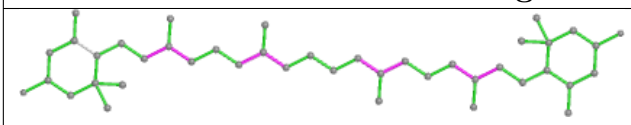
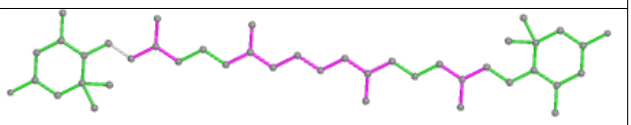
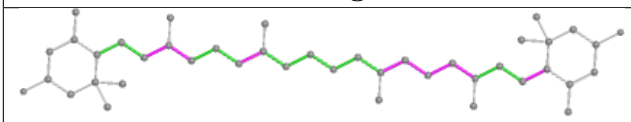
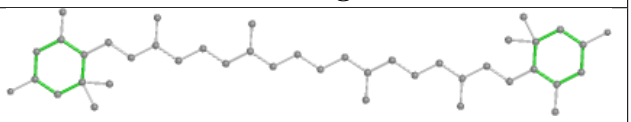


Rings

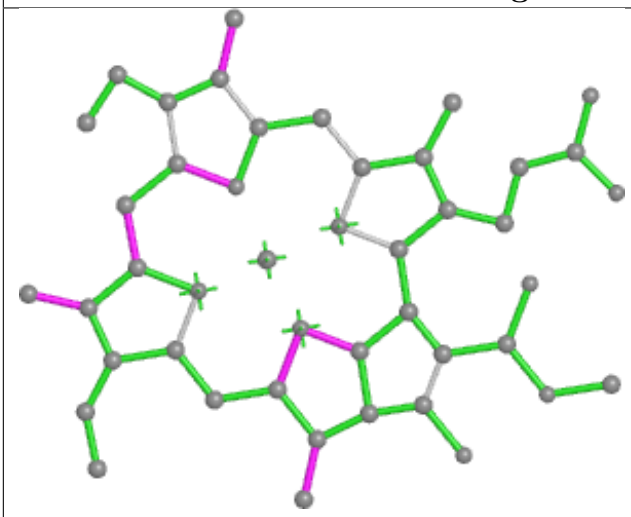
Ligand CLA BA 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU BA 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

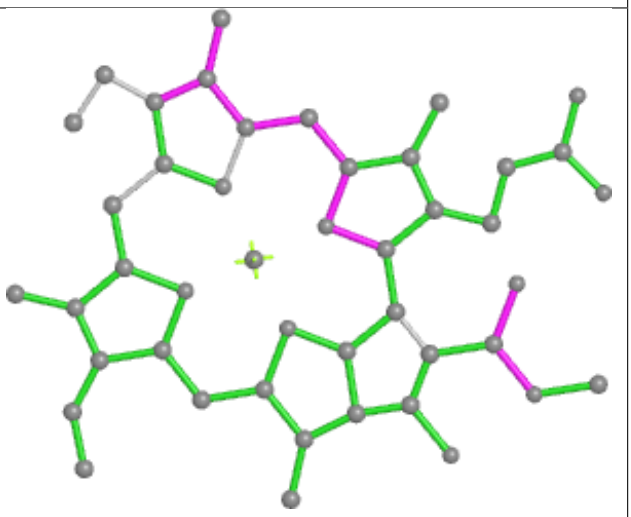
Ligand CLA B1 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT B1 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

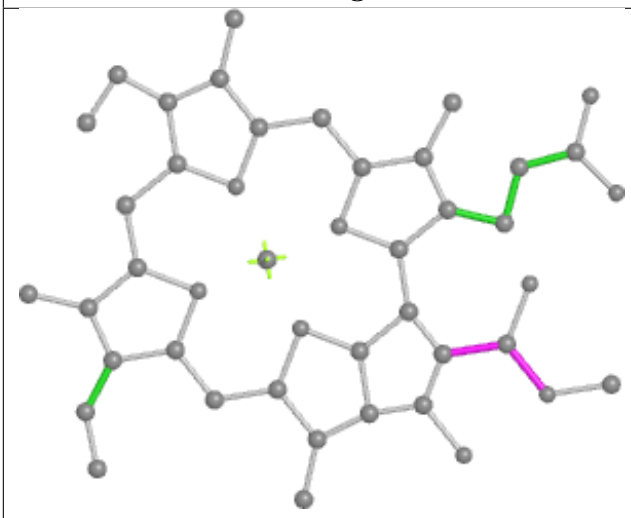
Ligand CLA BA 820



Bond lengths



Bond angles



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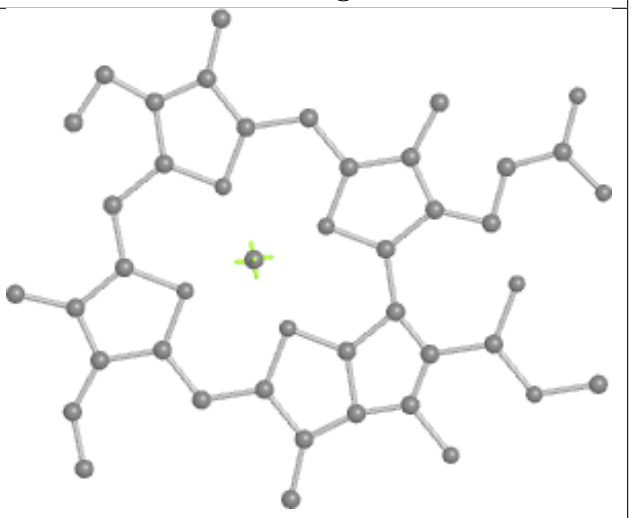
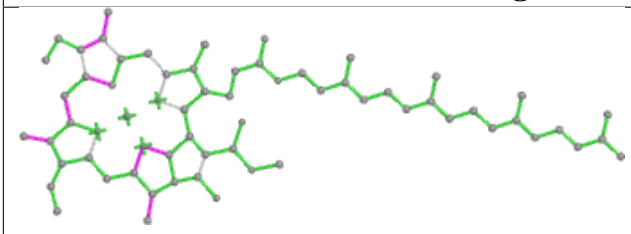


Rings

Ligand CLA BB 824



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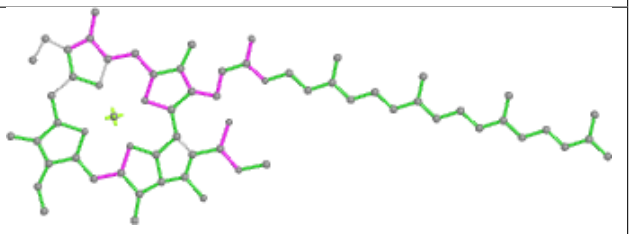
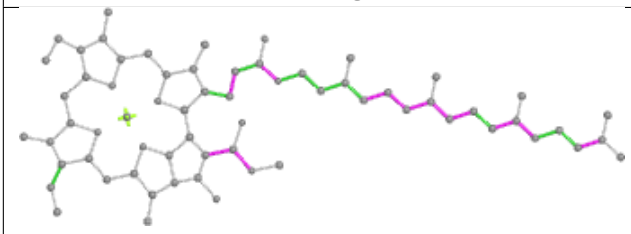


Bond angles



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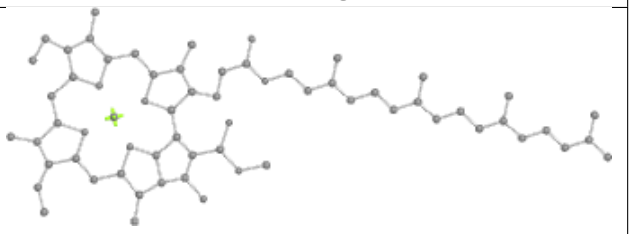
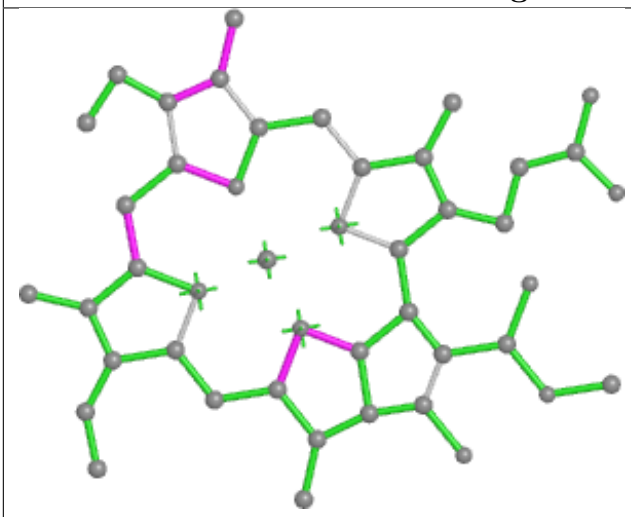


Rings

Ligand CLA BG 202



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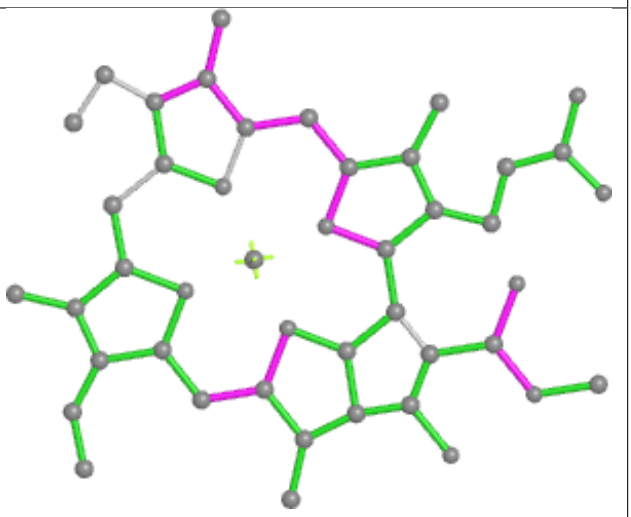
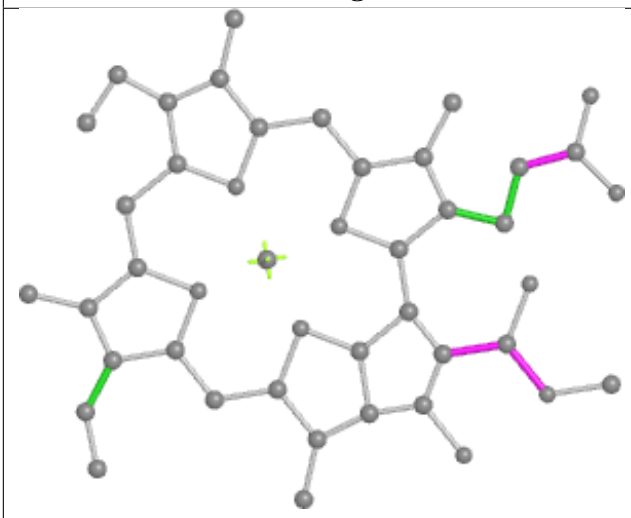


Bond angles



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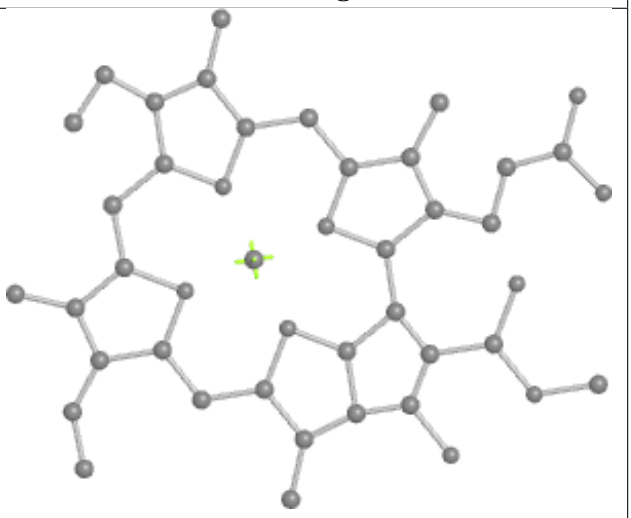
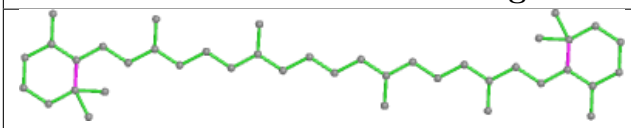
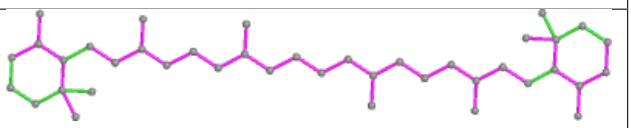


Rings

Ligand BCR BG 203



Bond lengths



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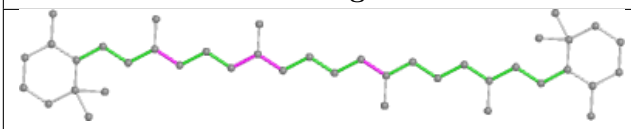
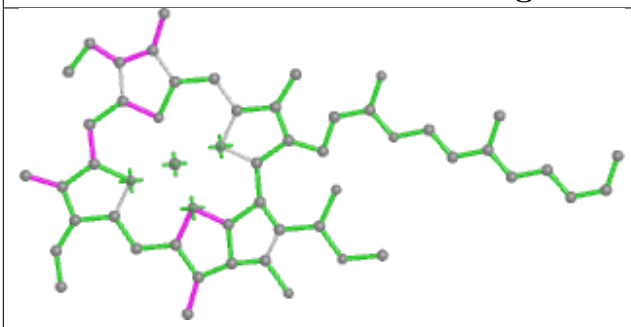
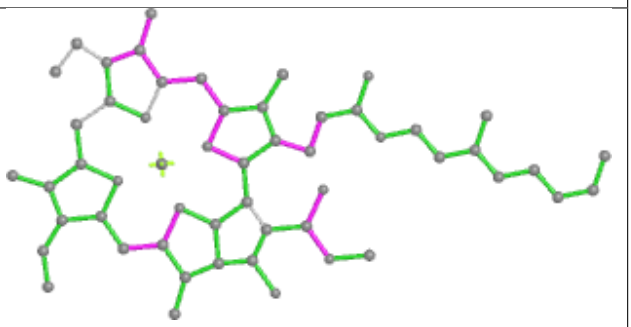
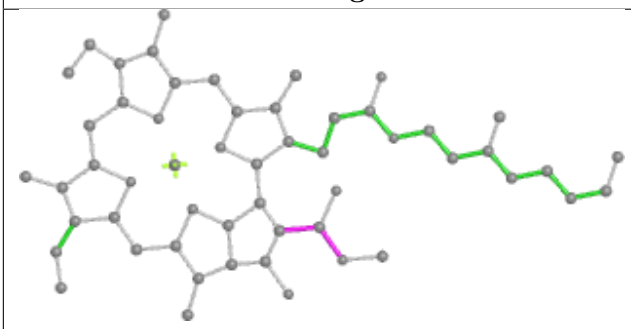
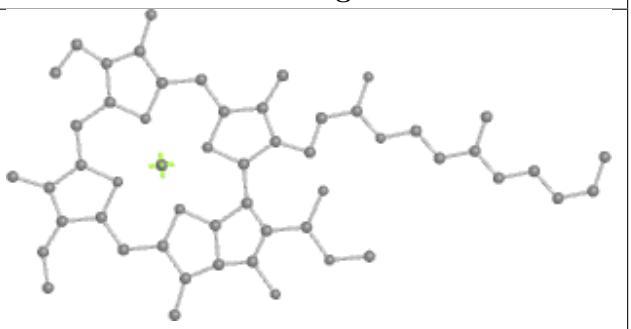


Torsions

Rings

Ligand CLA B5 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

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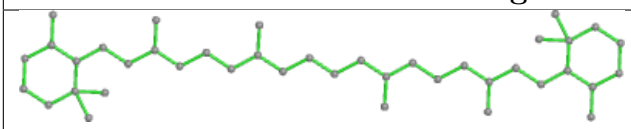
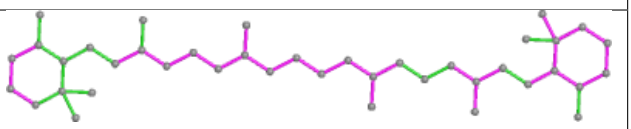
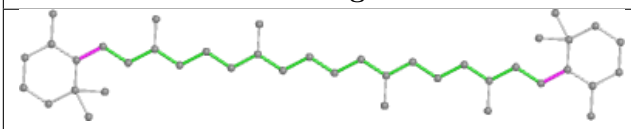
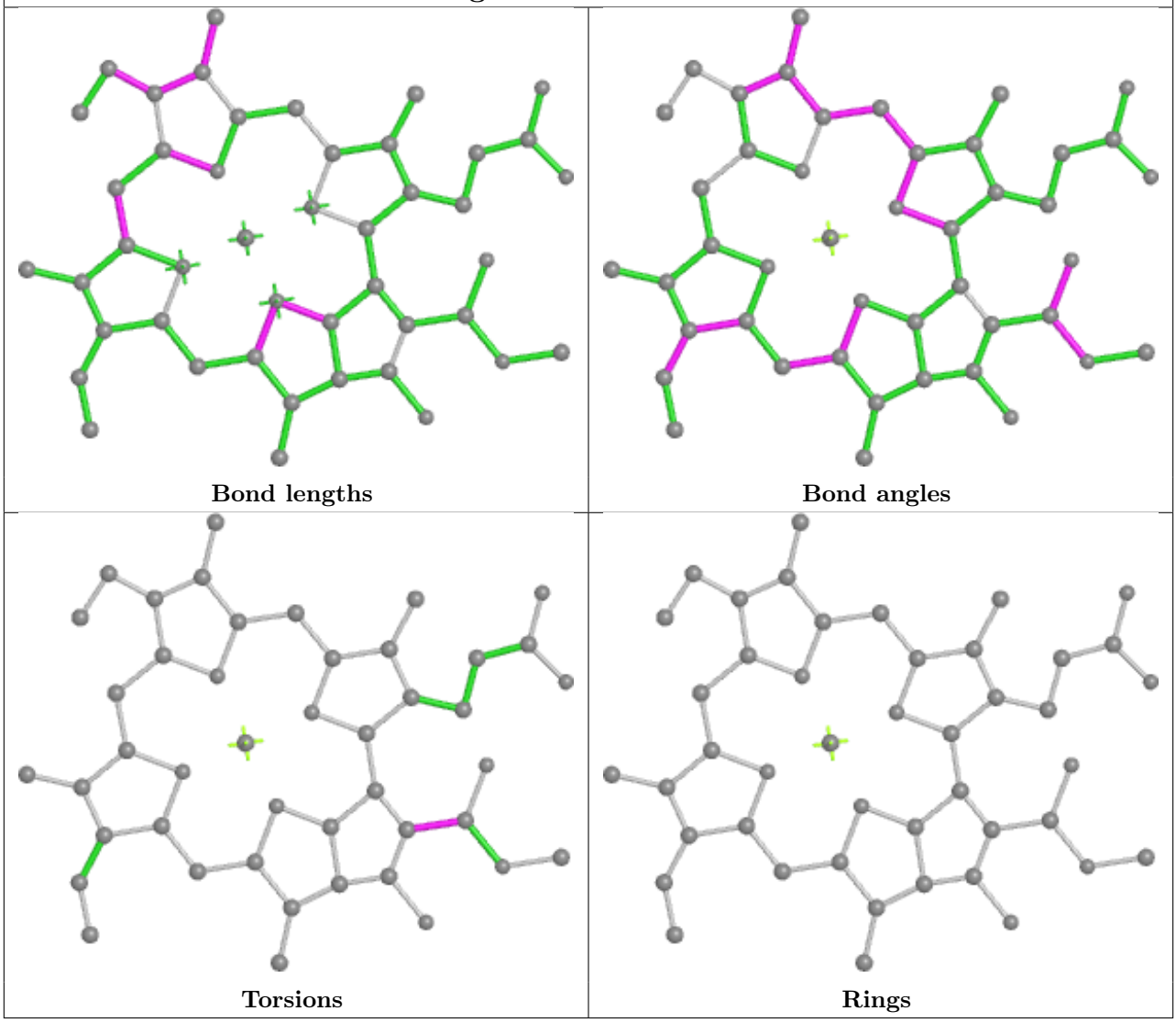
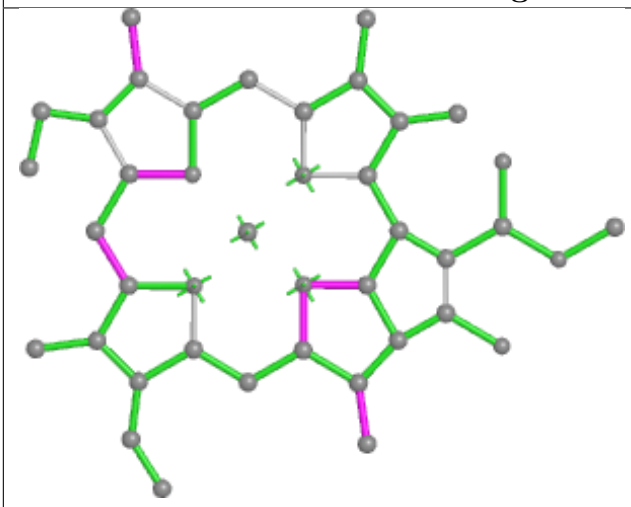
 Bond lengths	 Bond angles
 Torsions	 Rings

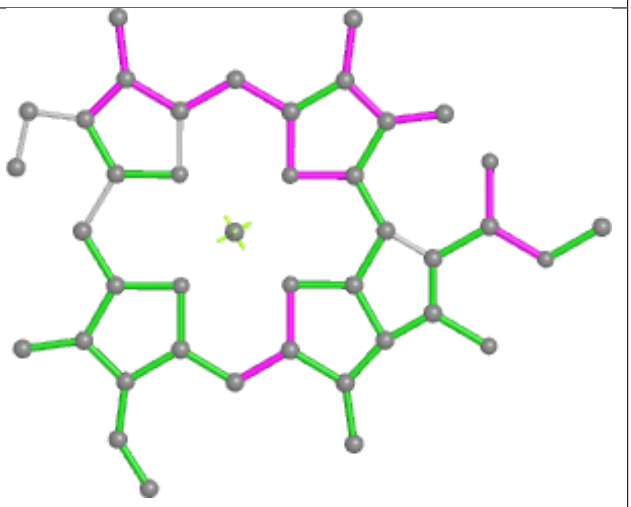
Ligand CLA BA 816



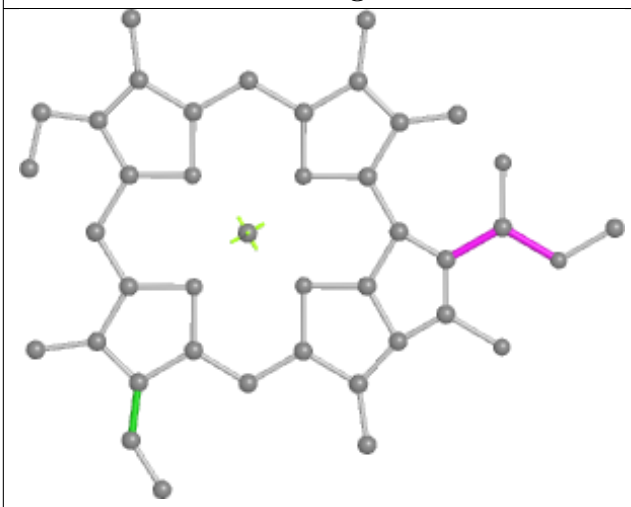
Ligand CLA BA 823



Bond lengths



Bond angles



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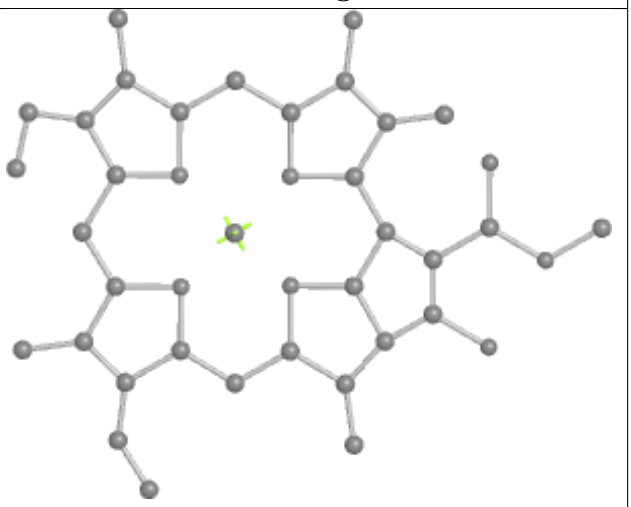
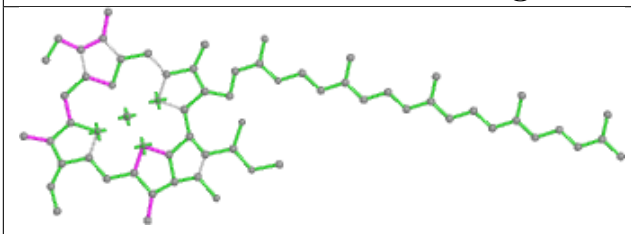


Rings

Ligand CLA BB 841



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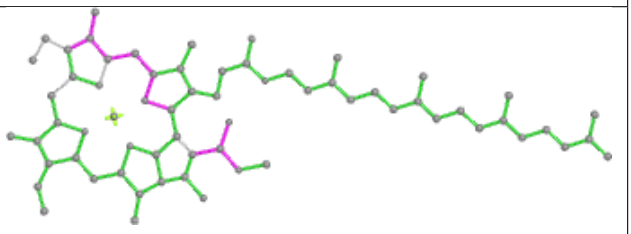
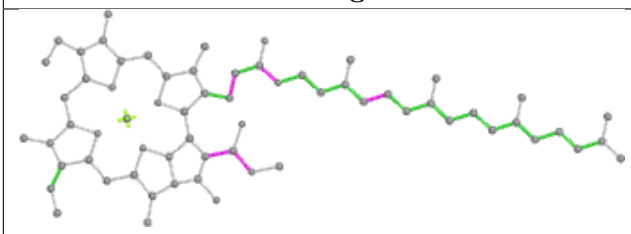


Bond angles



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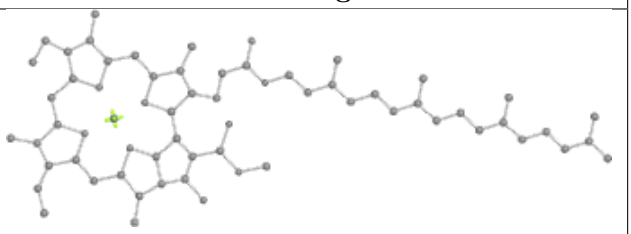
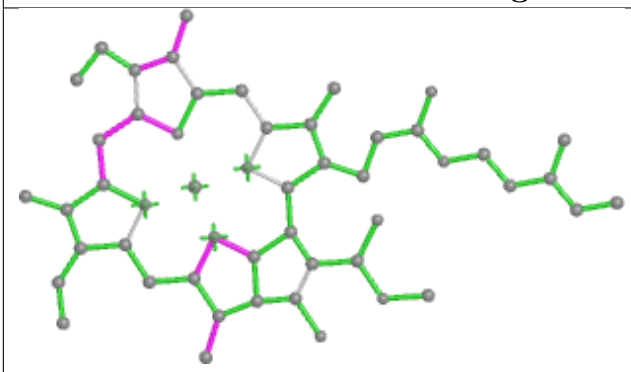
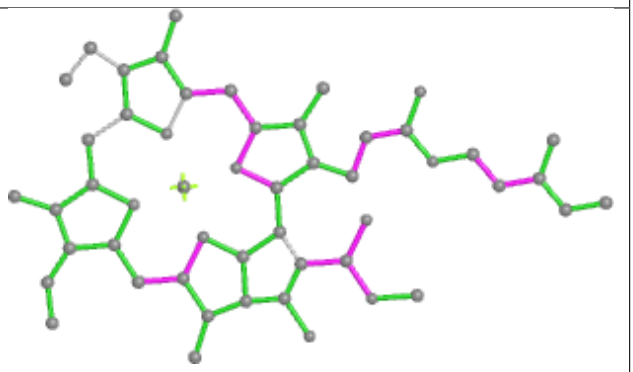
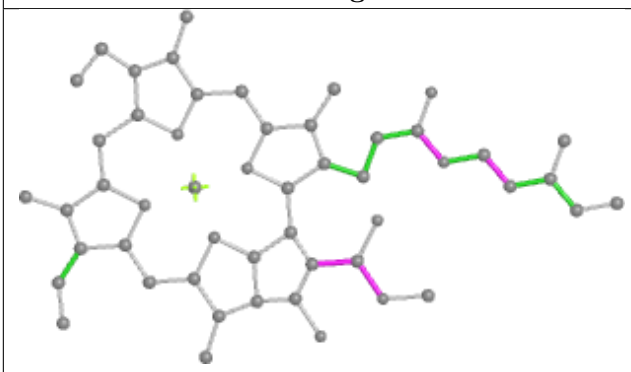
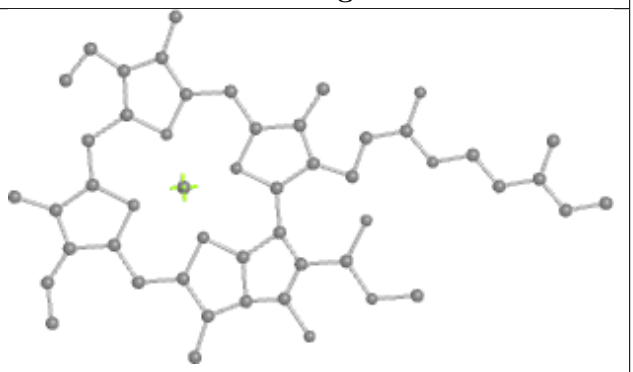
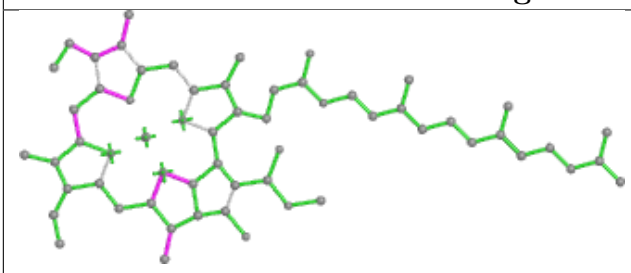
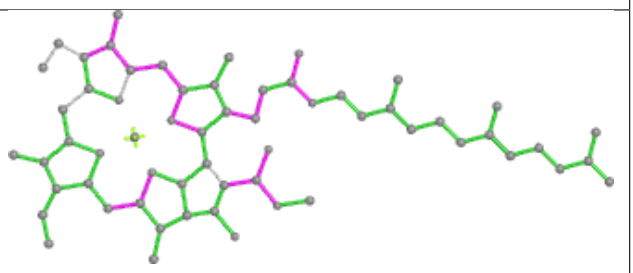
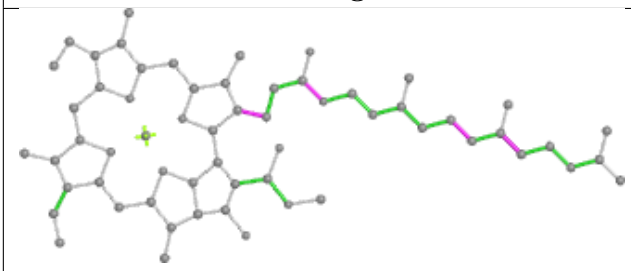
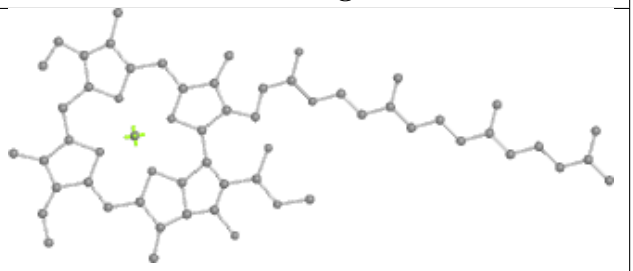
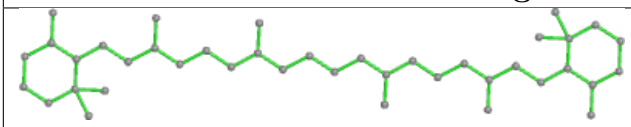


Rings

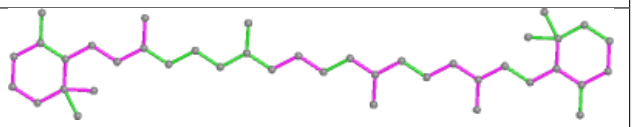
Ligand CLA BA 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BL 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

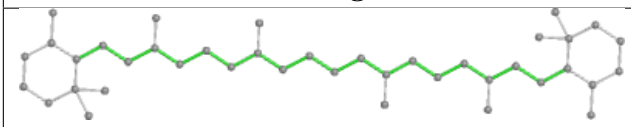
Ligand BCR BJ 101



Bond lengths



Bond angles



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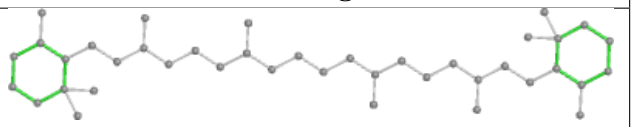
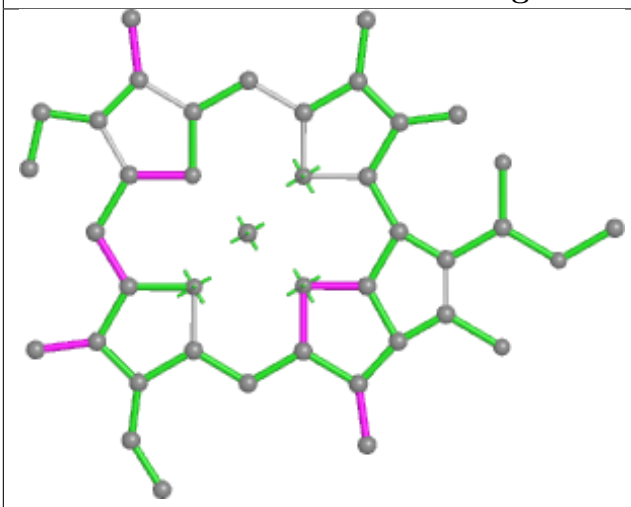
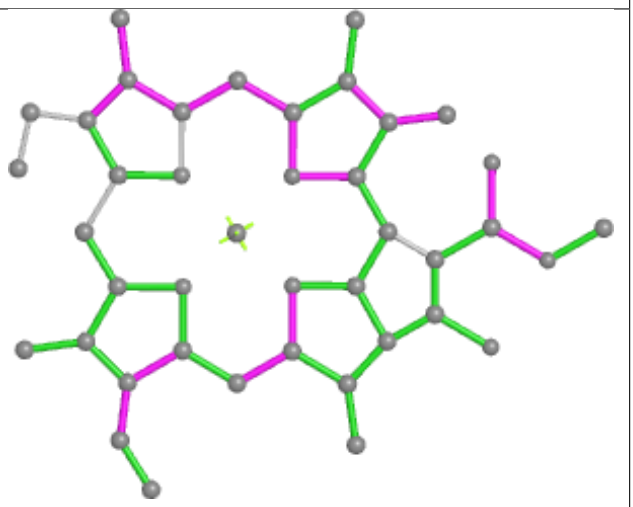


Rings

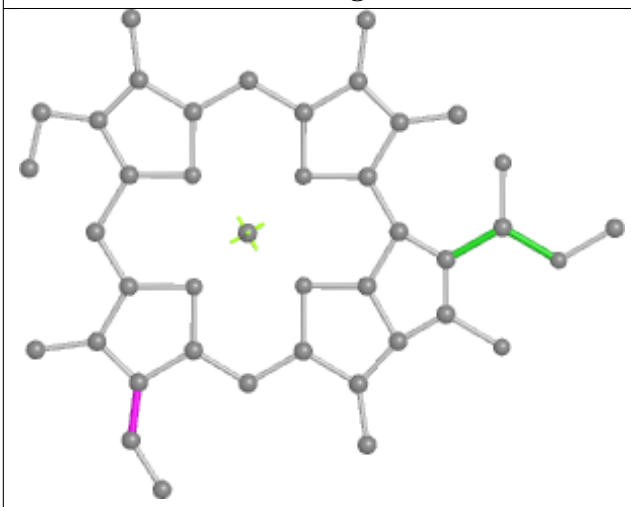
Ligand CLA BB 806



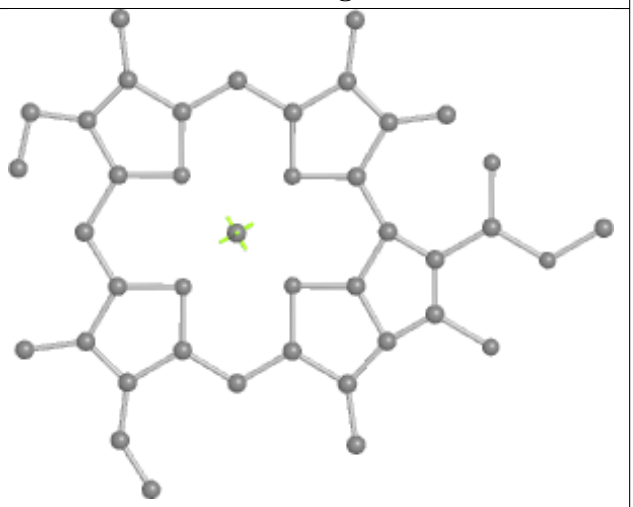
Bond lengths



Bond angles

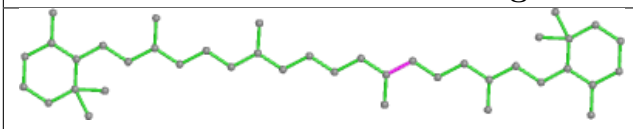


Torsions

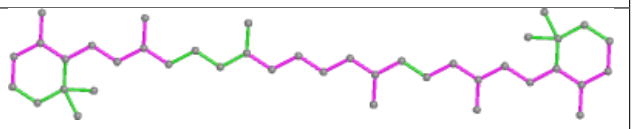


Rings

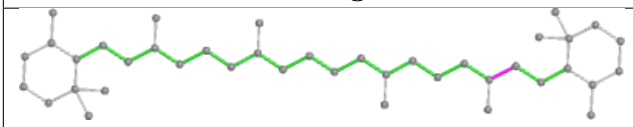
Ligand BCR BB 849



Bond lengths



Bond angles



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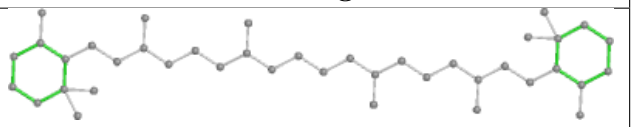
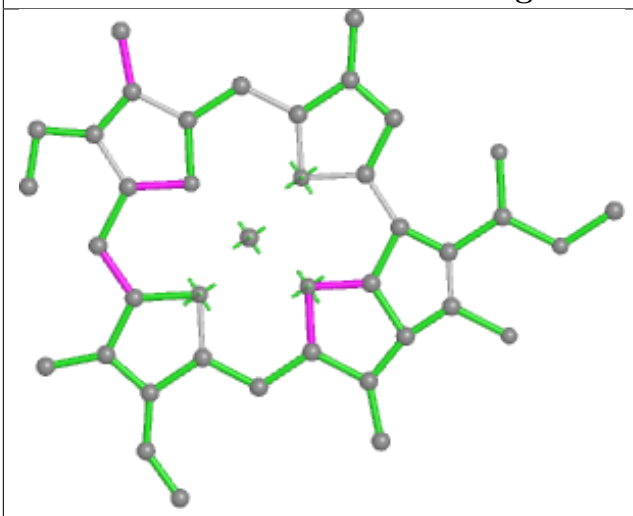
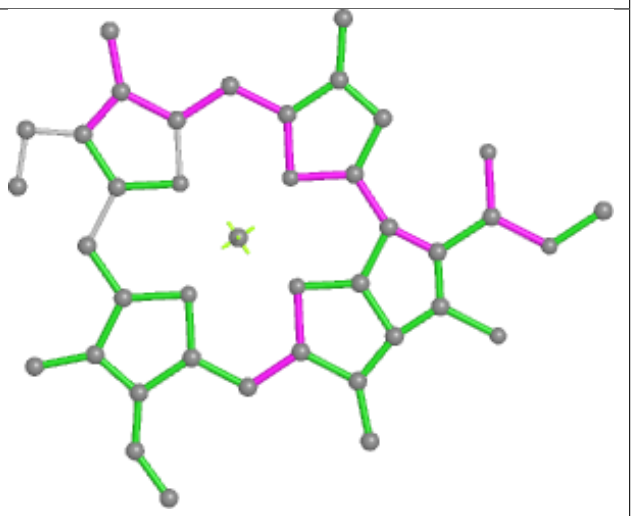


Rings

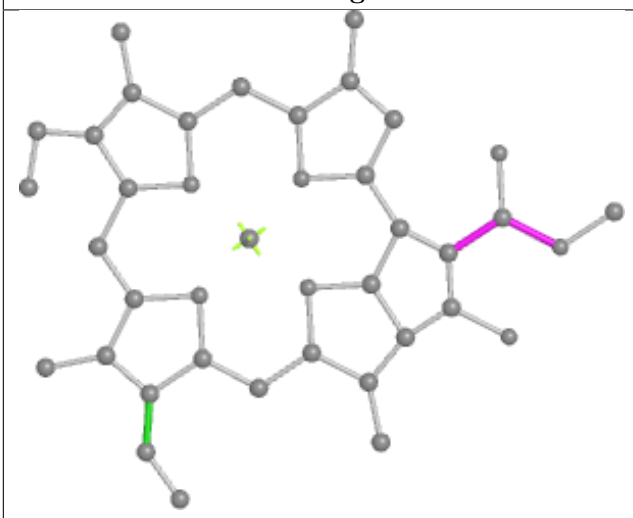
Ligand CLA B1 307



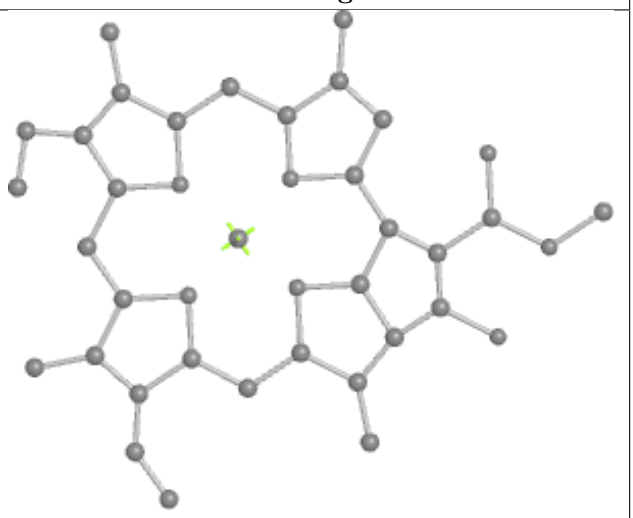
Bond lengths



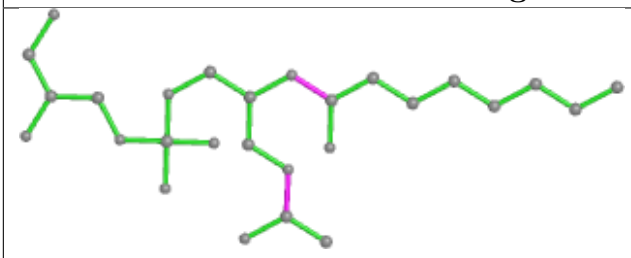
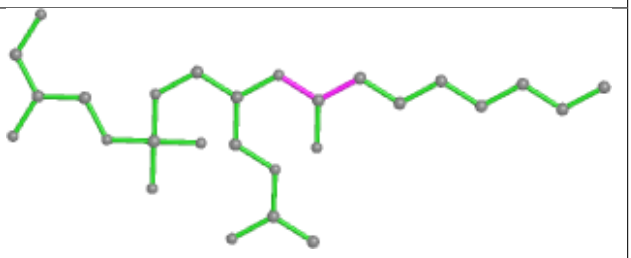
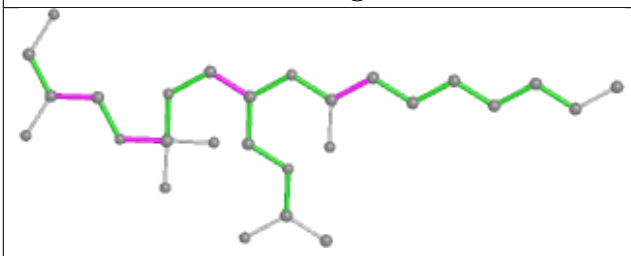
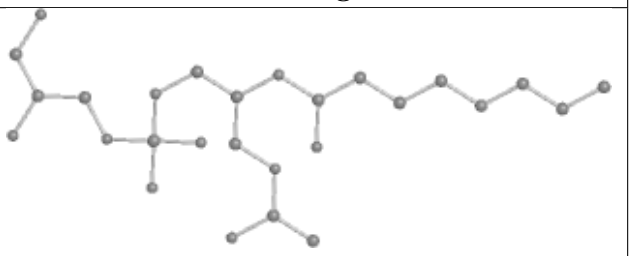
Bond angles

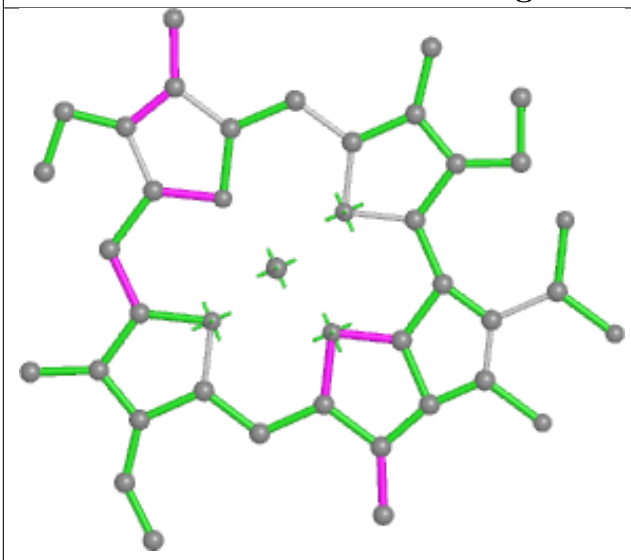
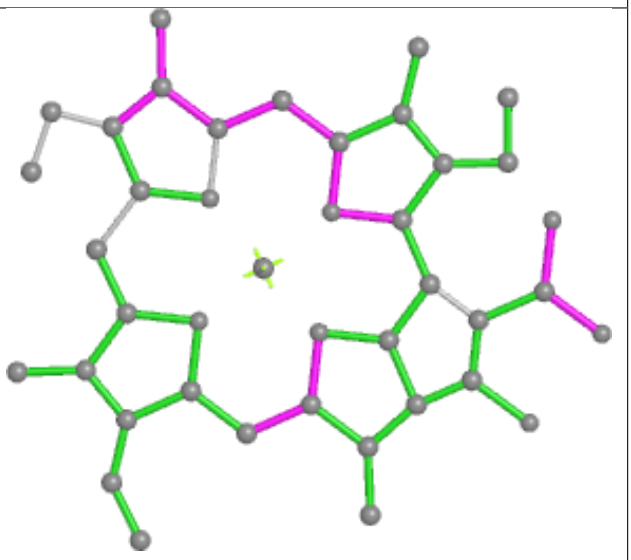
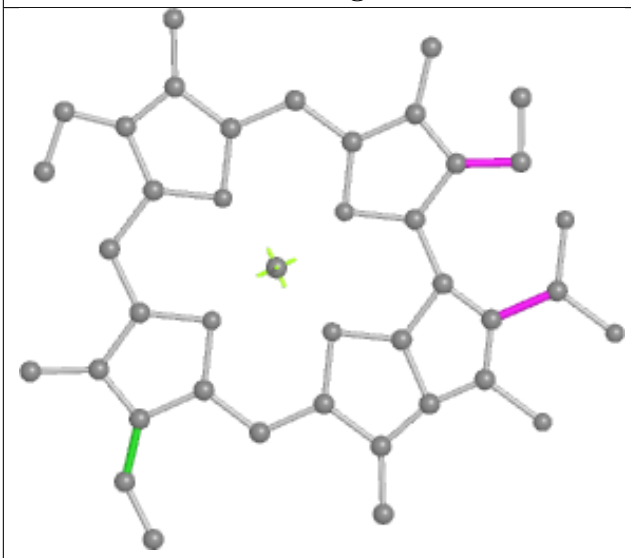
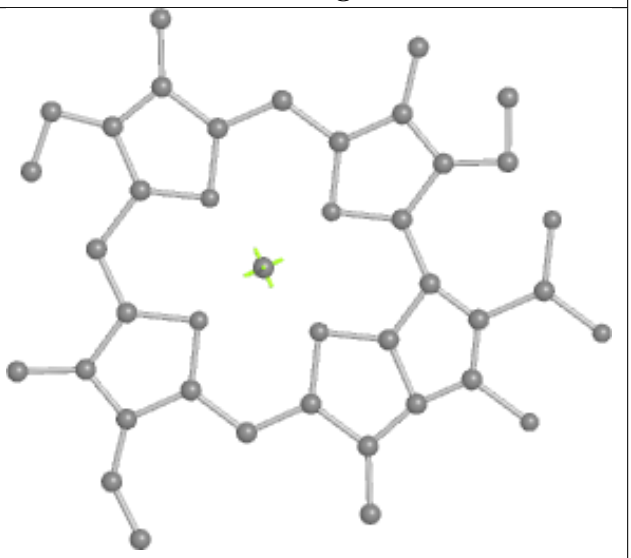


Torsions



Rings

Ligand LHG BA 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B3 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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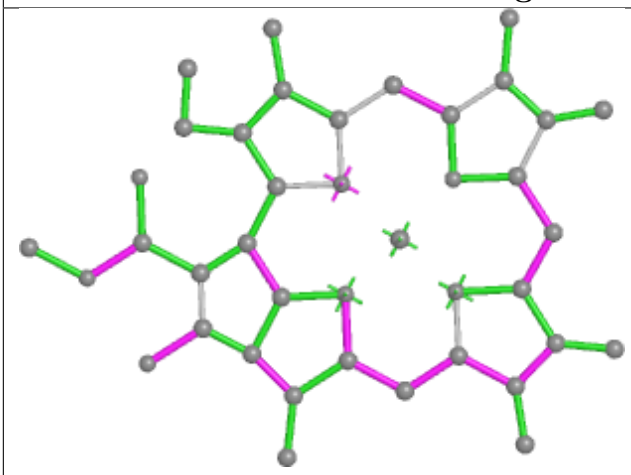
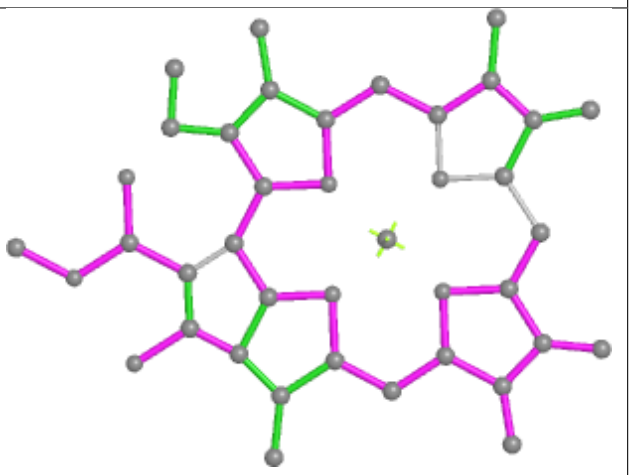
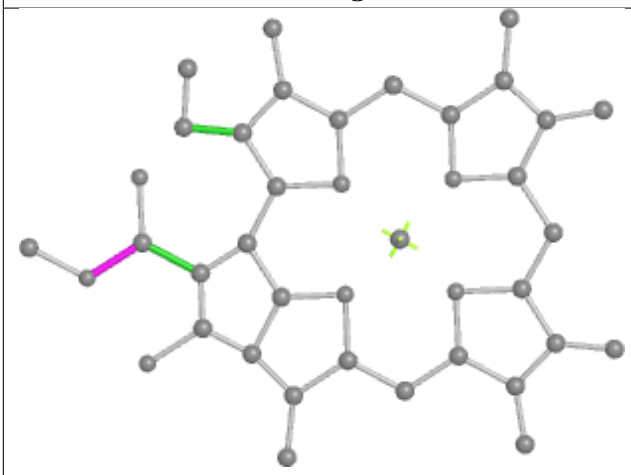
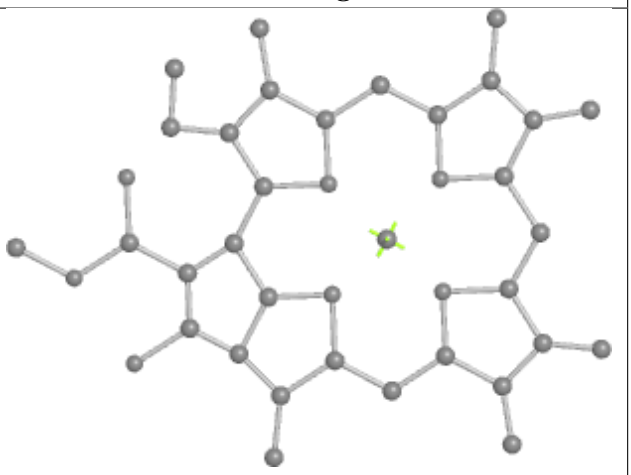
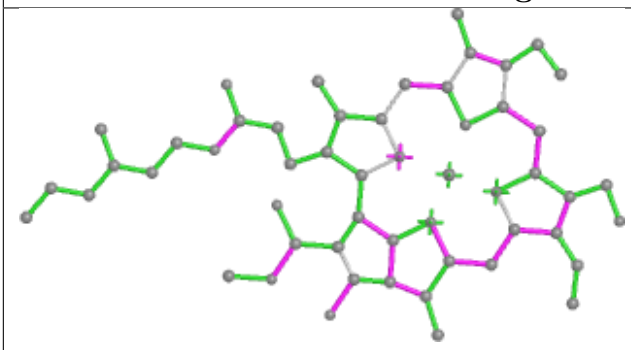
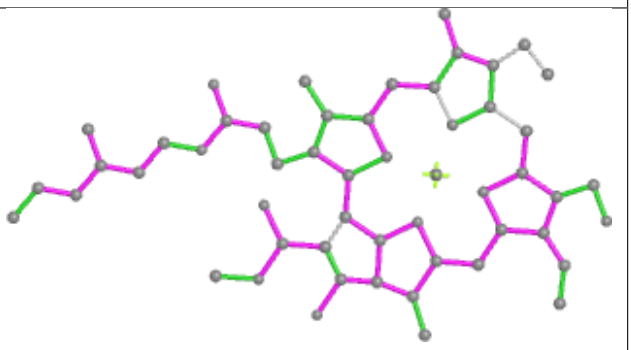
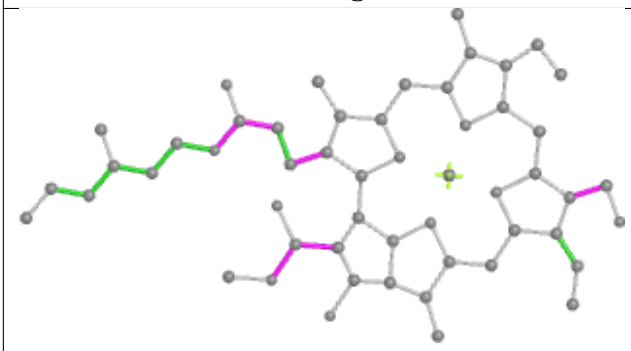
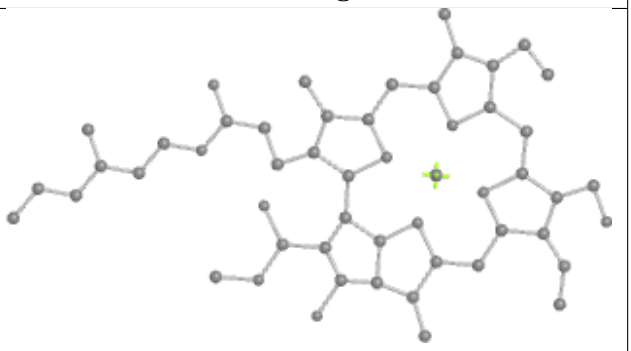
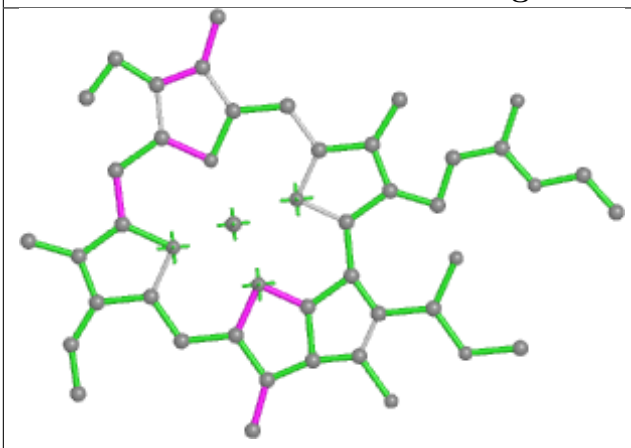
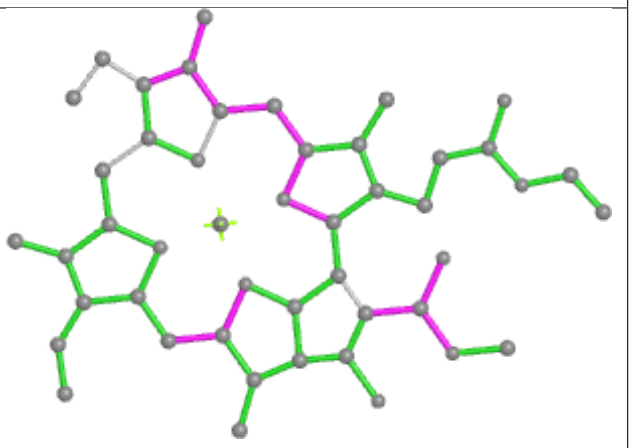
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL B3 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

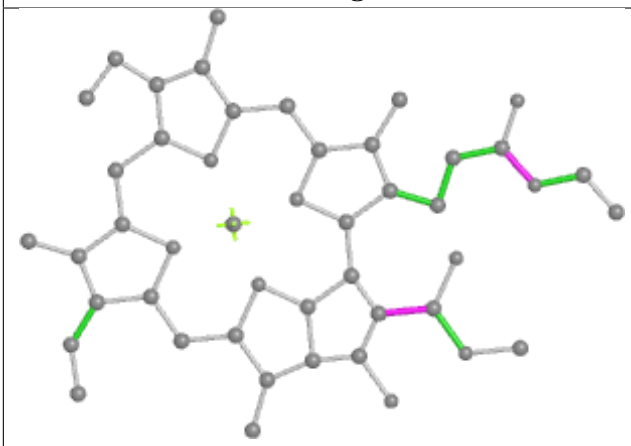
Ligand CLA BB 840



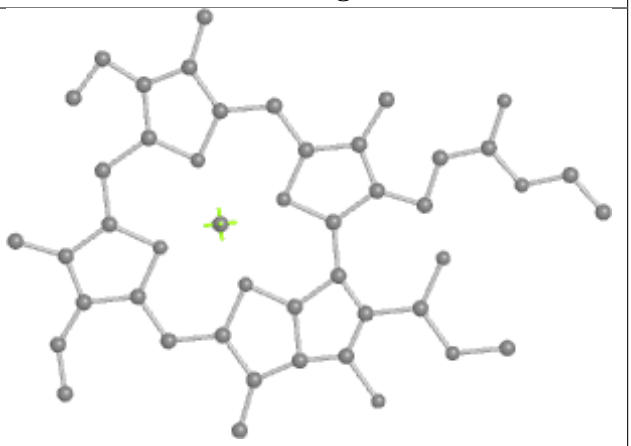
Bond lengths



Bond angles

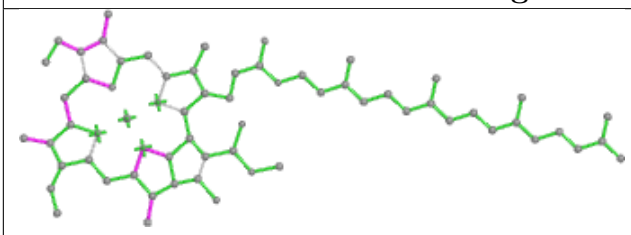


Torsions



Rings

Ligand CLA BA 821



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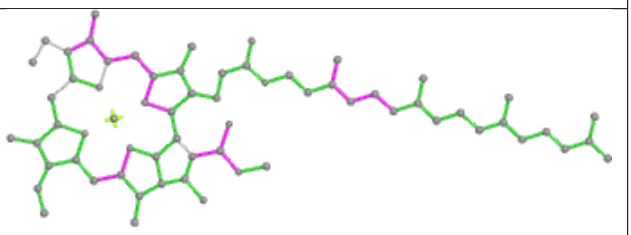

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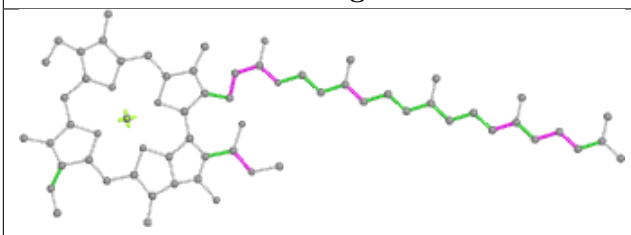

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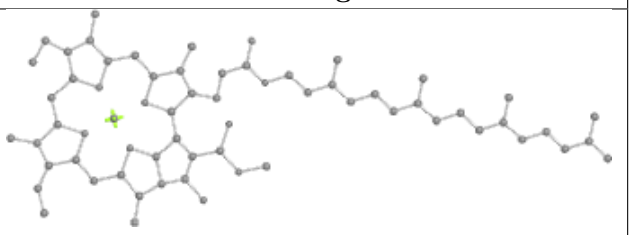
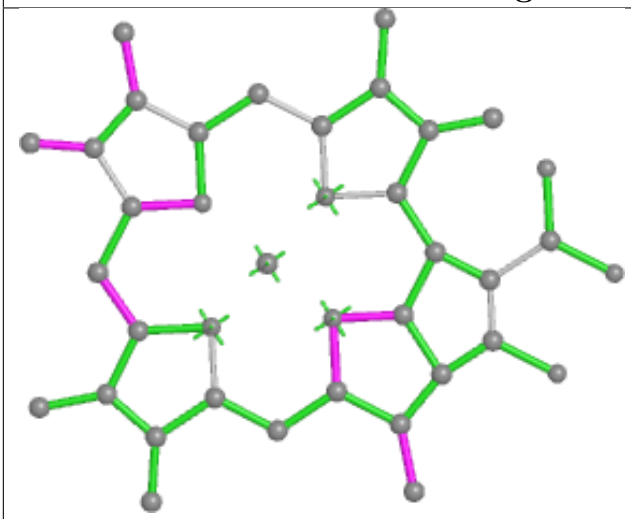


Rings

Ligand CLA B1 315



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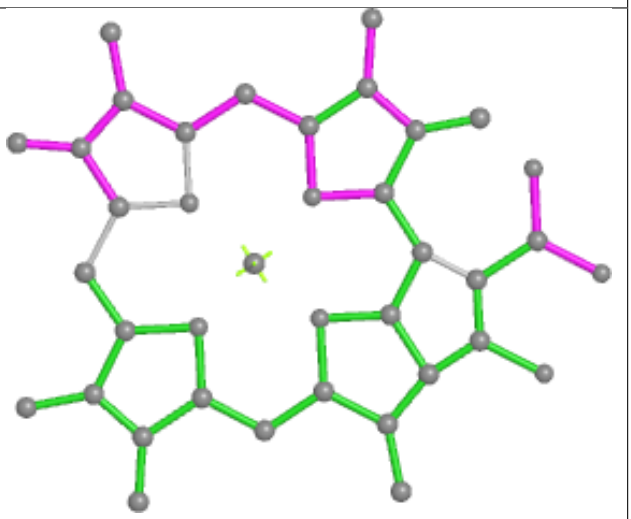
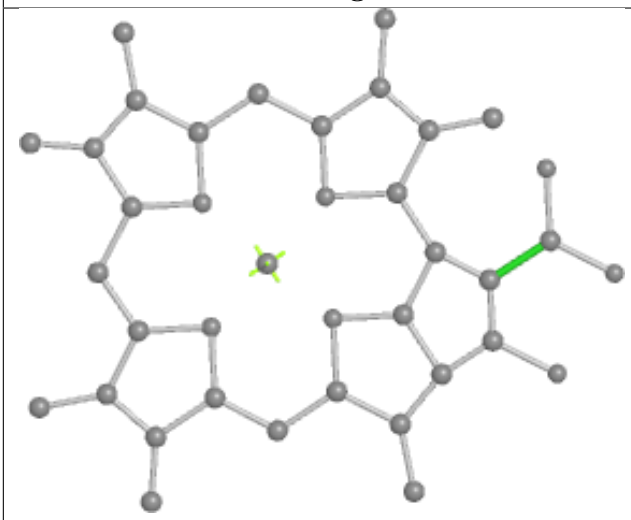


Bond angles



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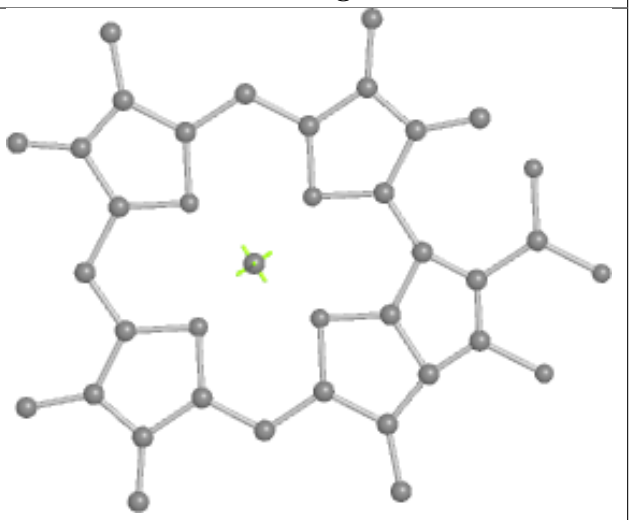
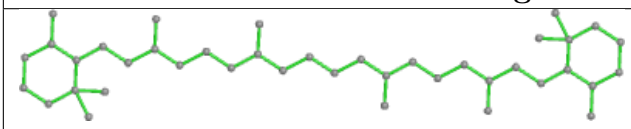


Rings

Ligand BCR B3 618



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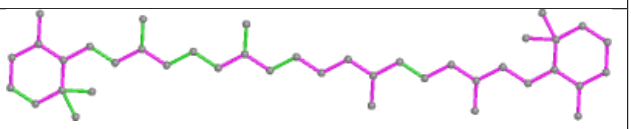
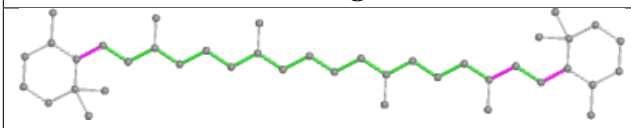
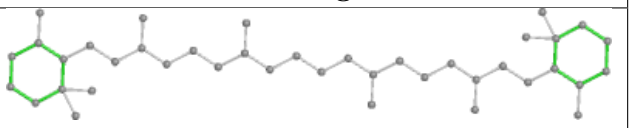


Bond angles

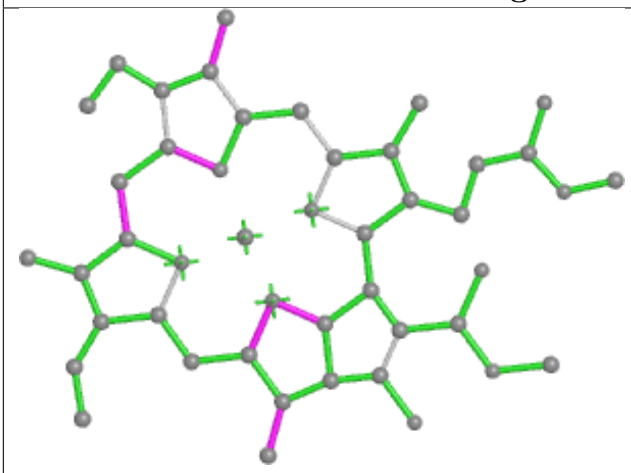


Torsions



Rings

Ligand CLA BK 203



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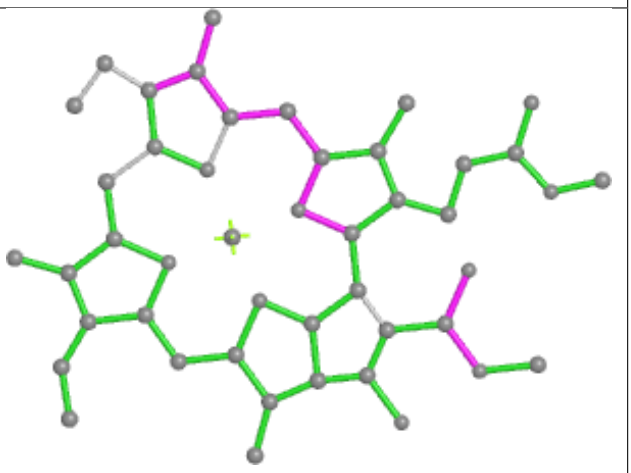

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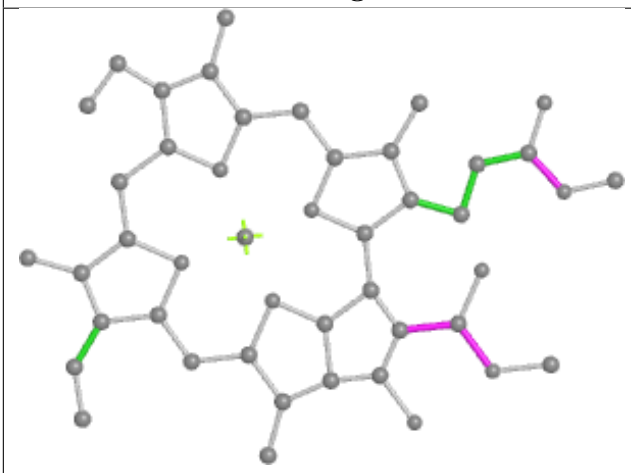

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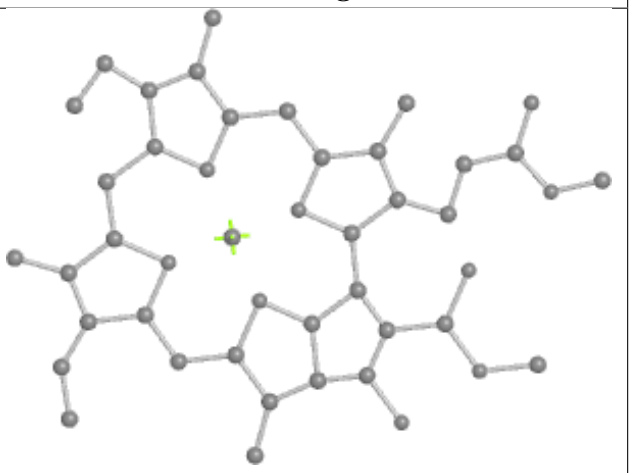
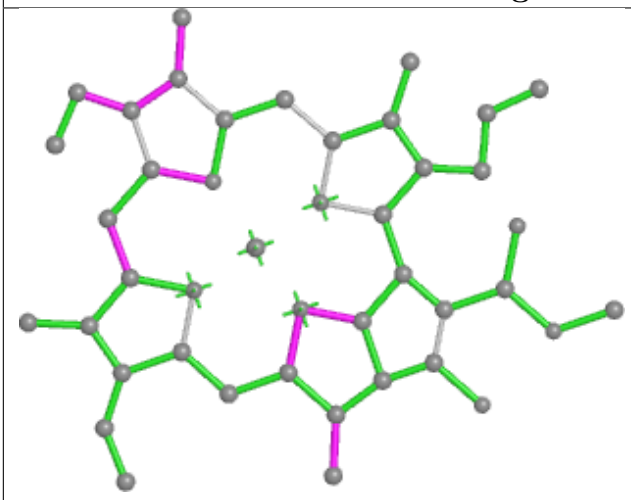


Rings

Ligand CLA BB 832



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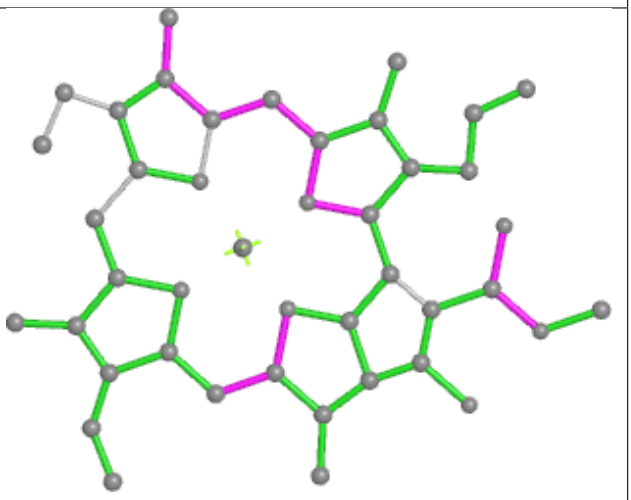
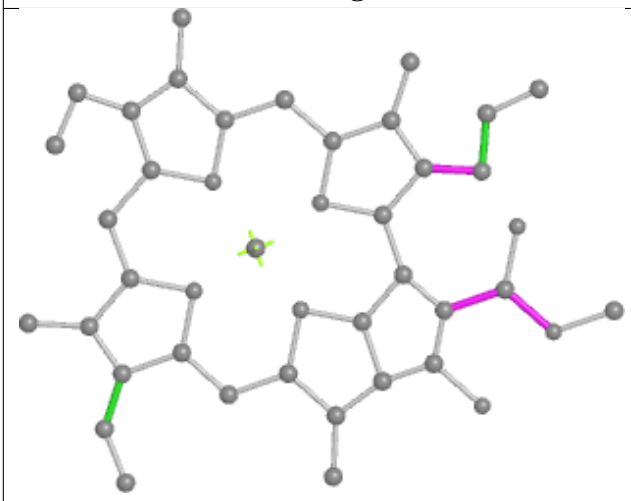


Bond angles



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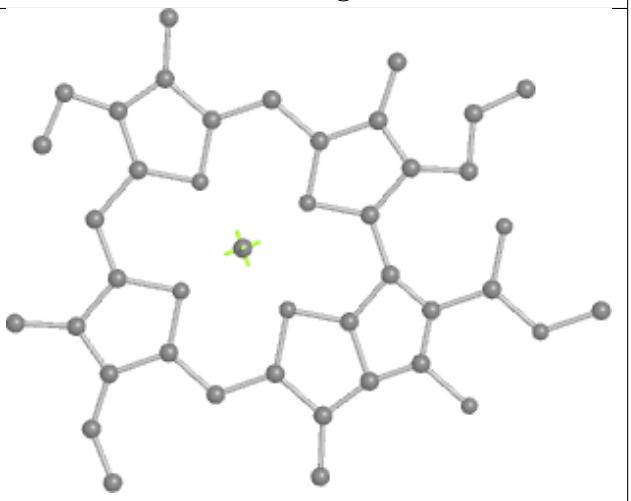
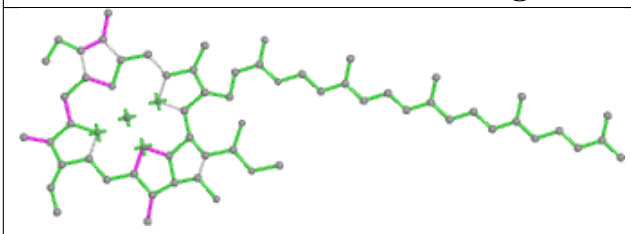
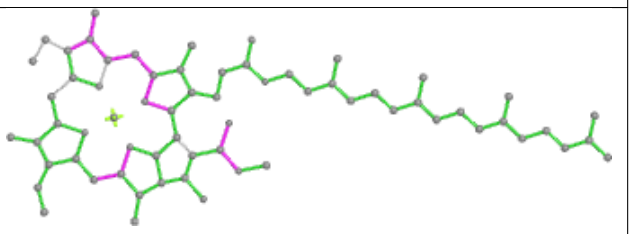


Rings

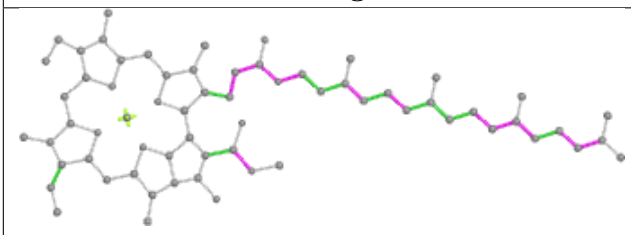
Ligand CLA BA 806



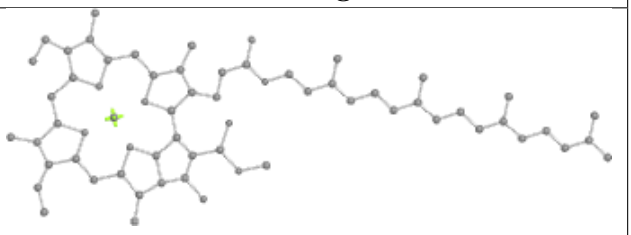
Bond lengths



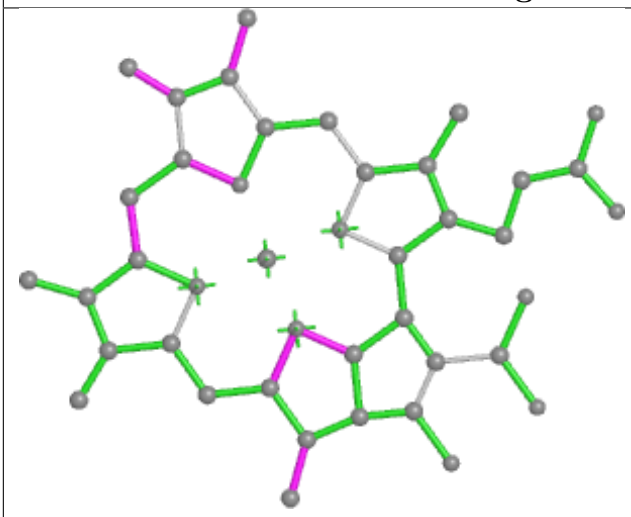
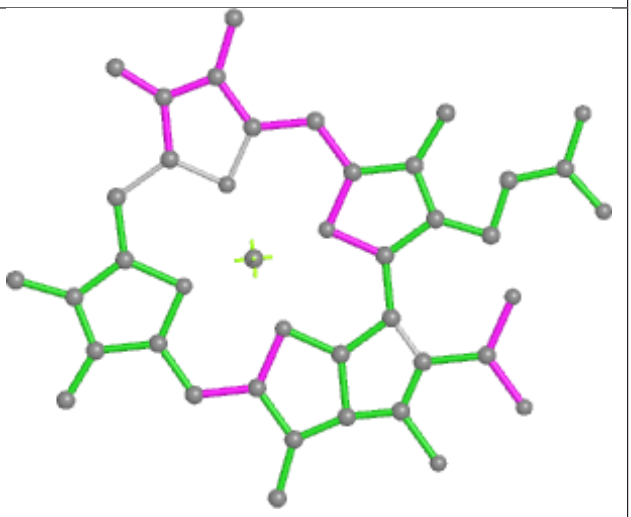
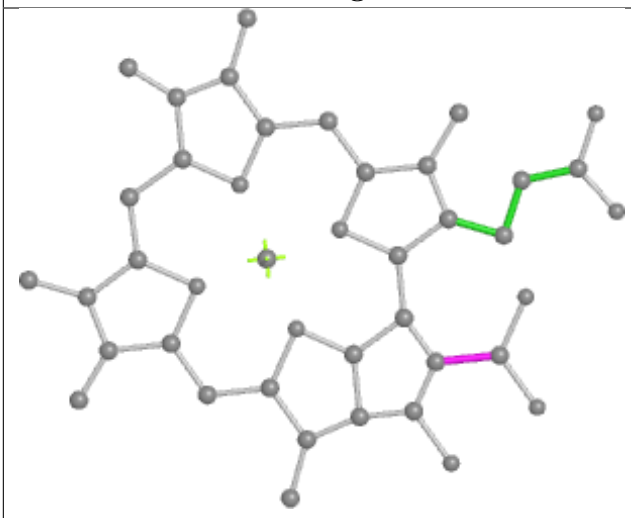
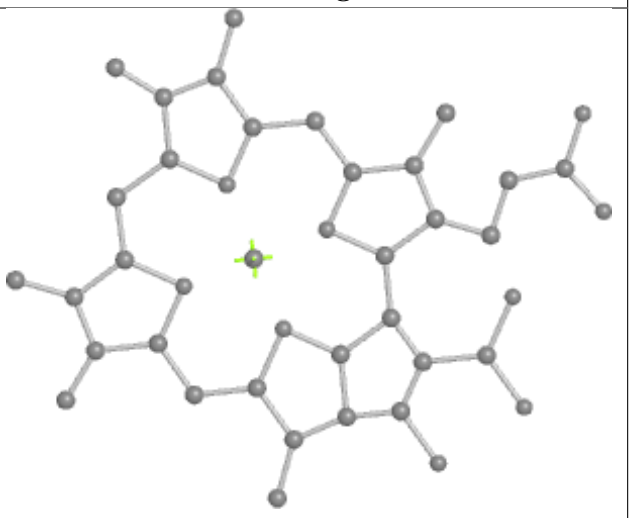
Bond angles



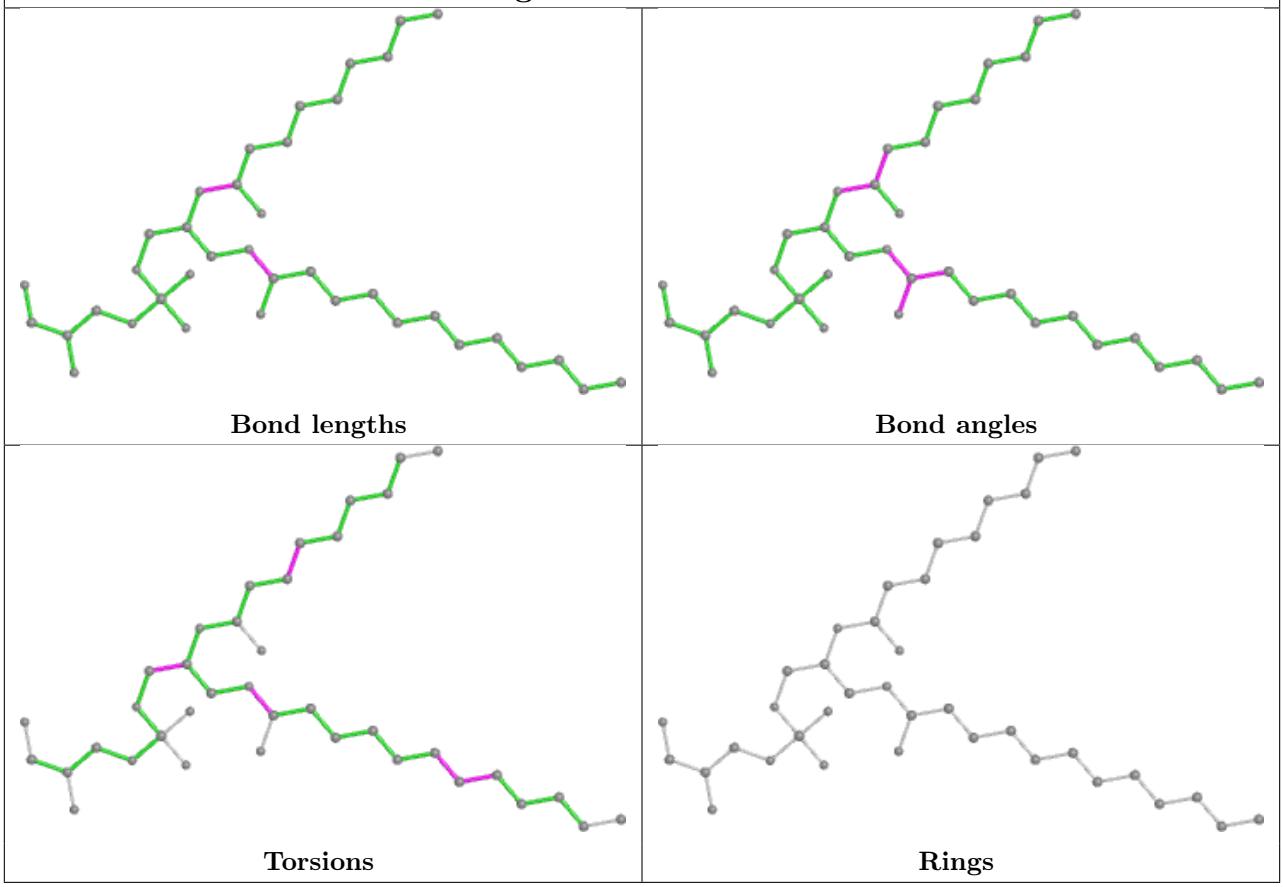
Torsions



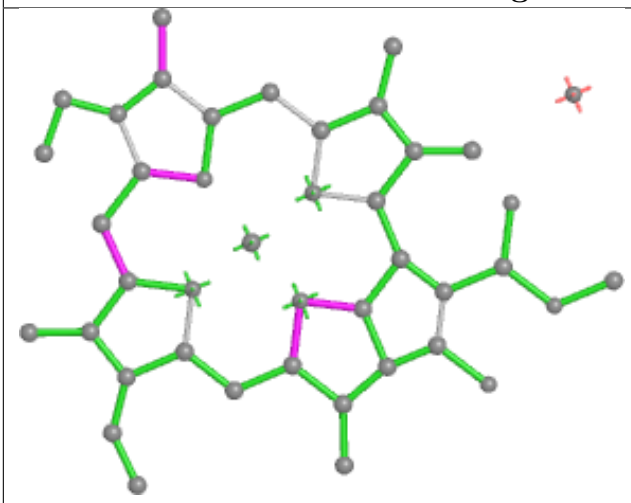
Rings

Ligand CLA B3 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

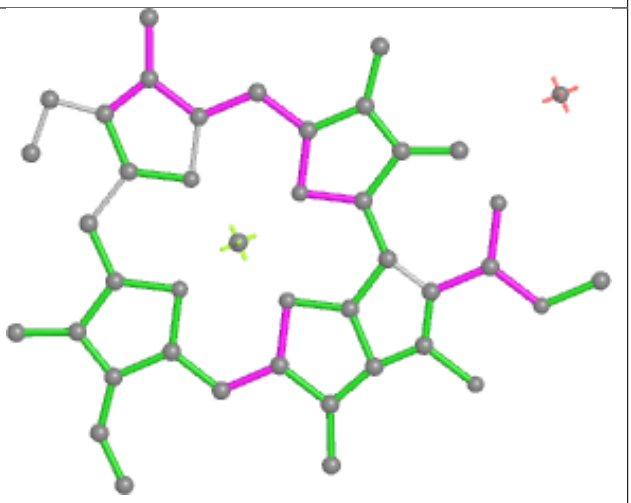
Ligand LHG B1 301



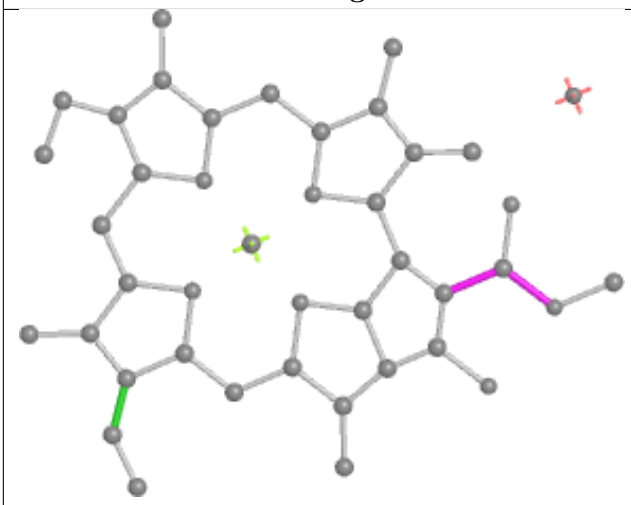
Ligand CLA BA 844



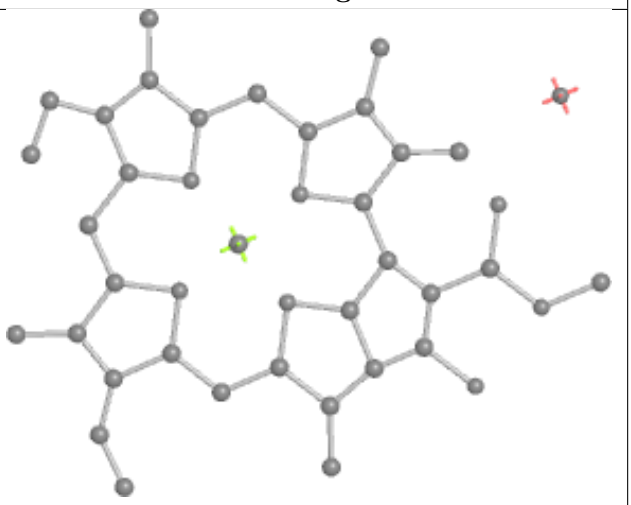
Bond lengths



Bond angles

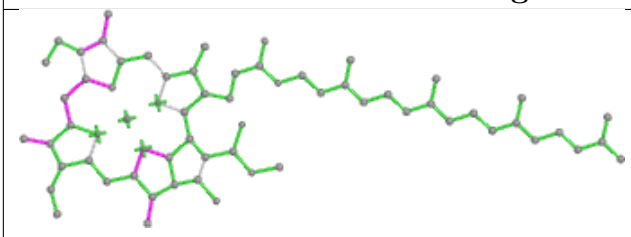


Torsions

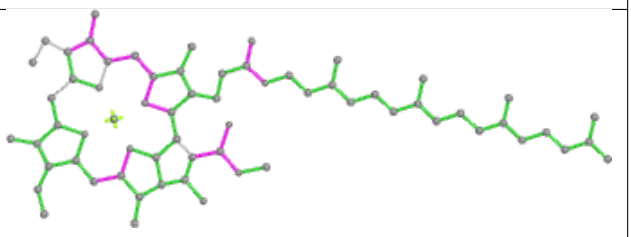


Rings

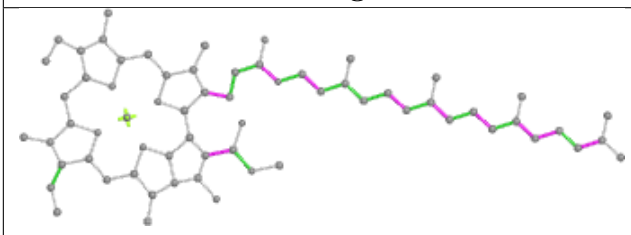
Ligand CLA BA 830



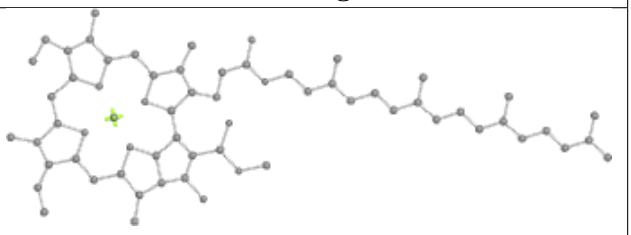
Bond lengths



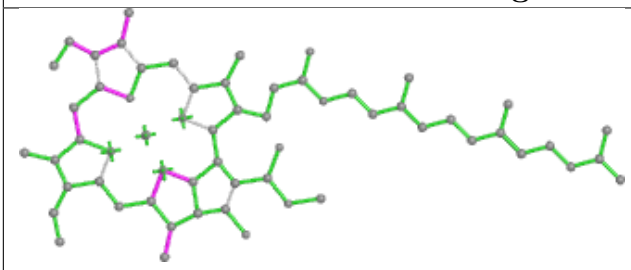
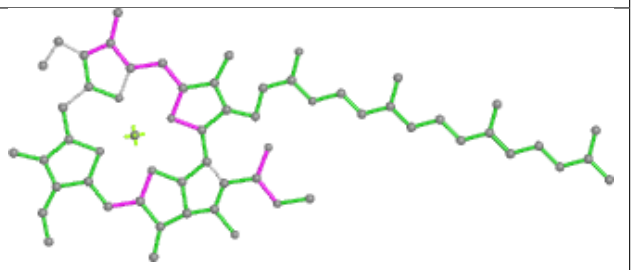
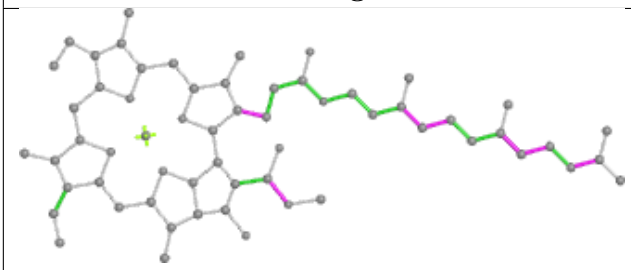
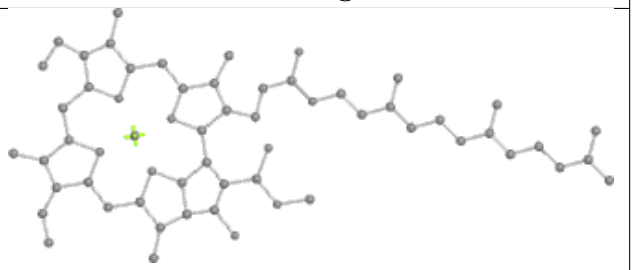
Bond angles

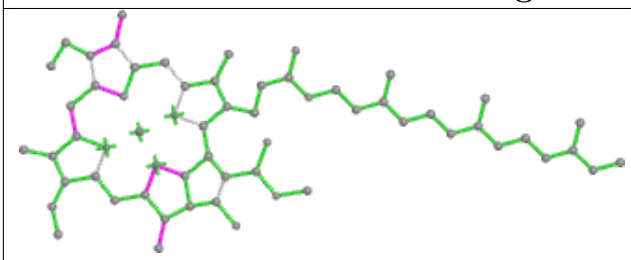
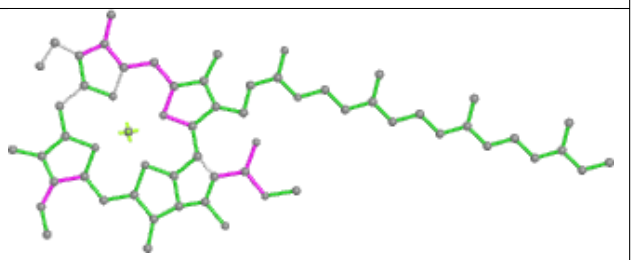
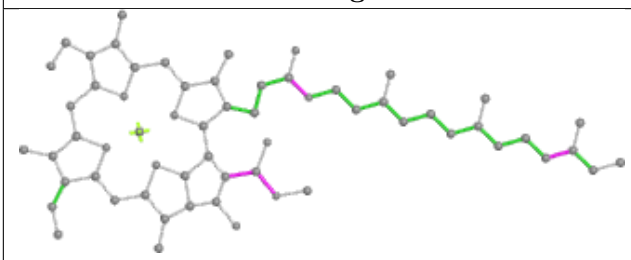
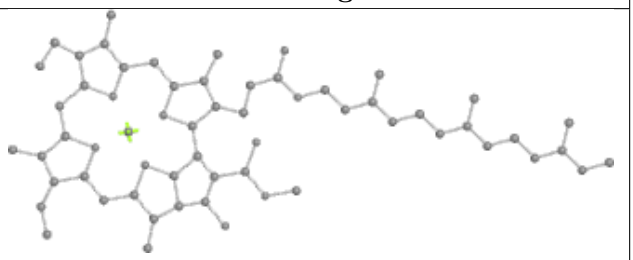


Torsions

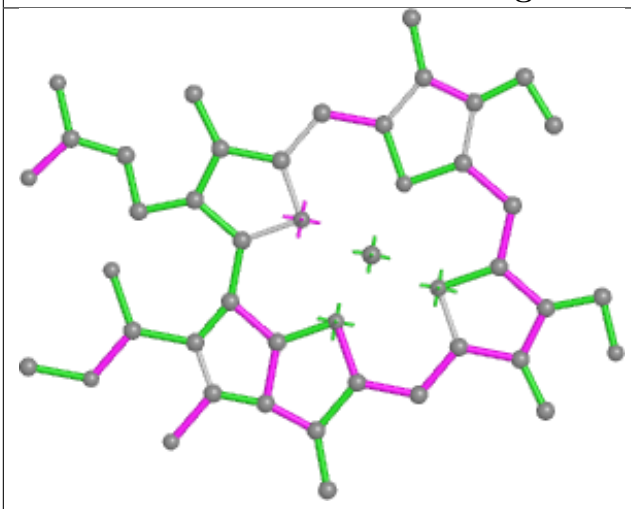


Rings

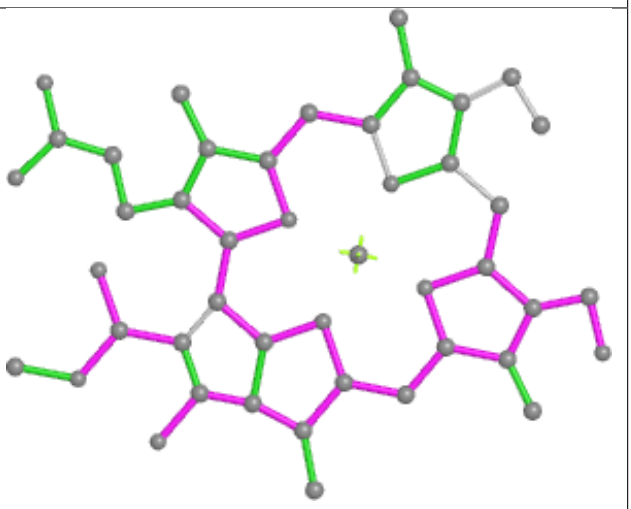
Ligand CLA BB 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

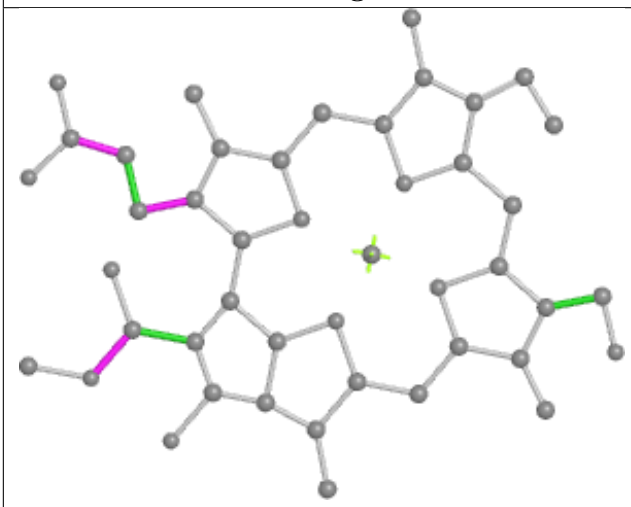
Ligand CHL B5 607



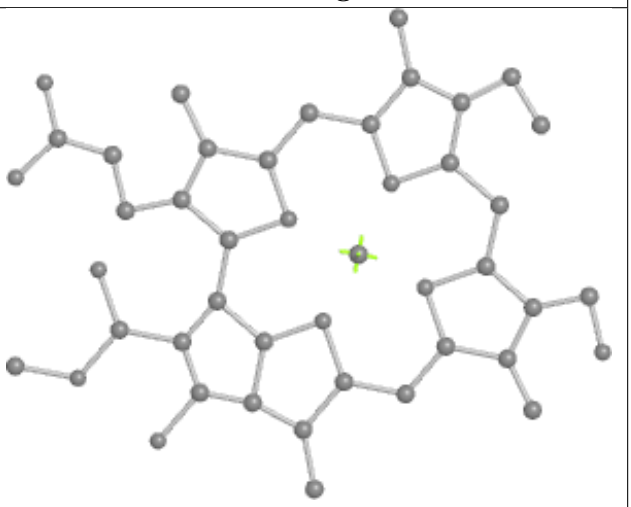
Bond lengths



Bond angles

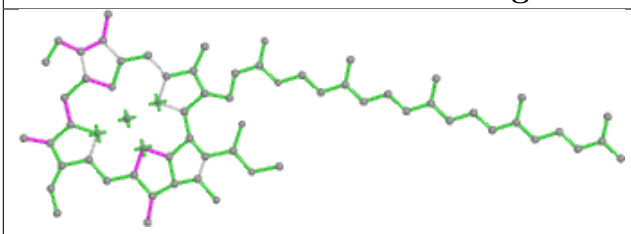


Torsions

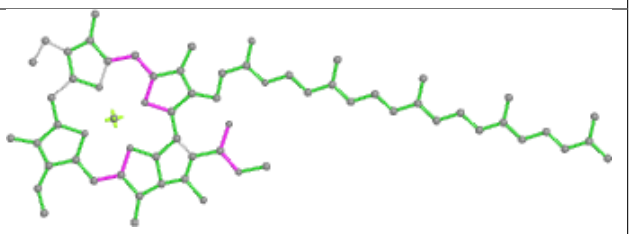


Rings

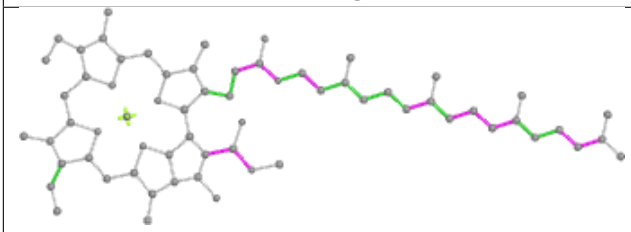
Ligand CLA BB 835



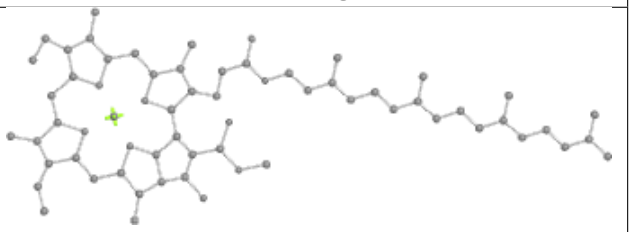
Bond lengths



Bond angles

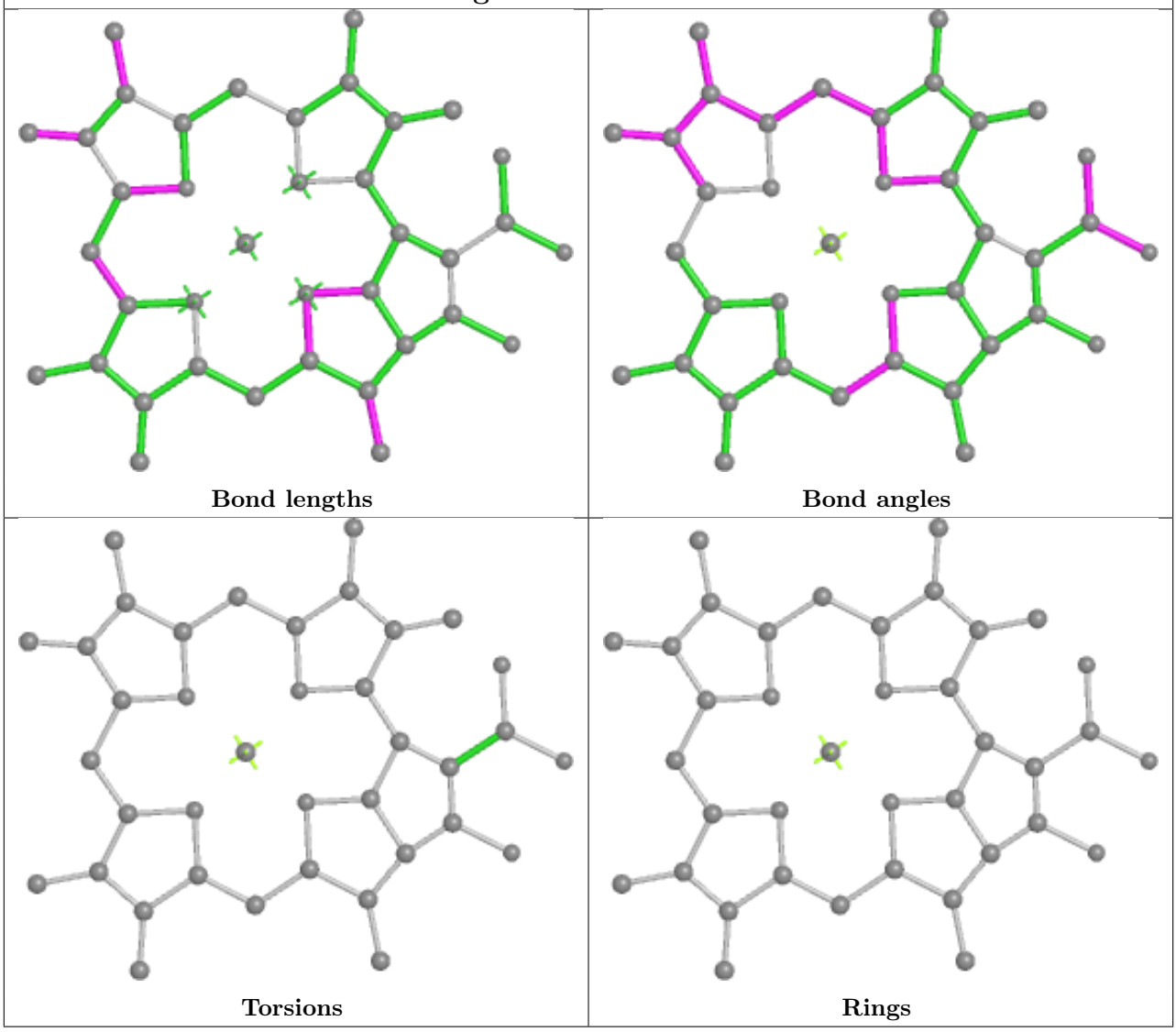


Torsions

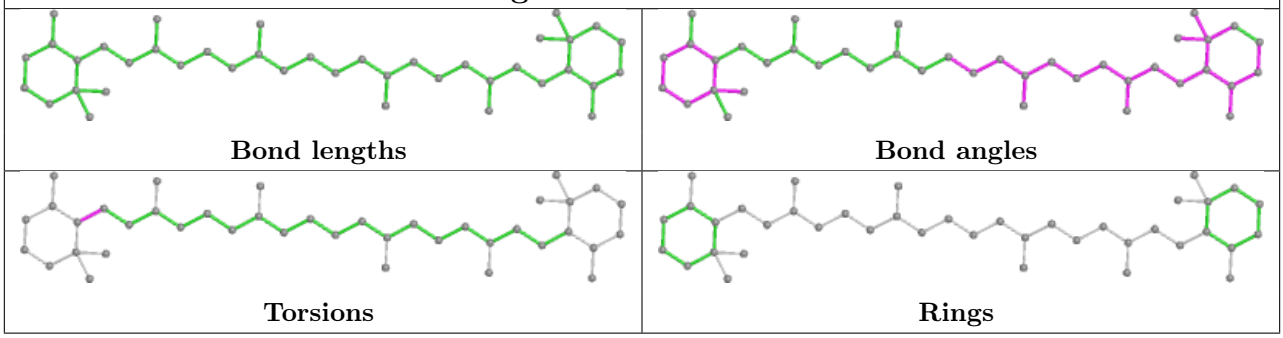


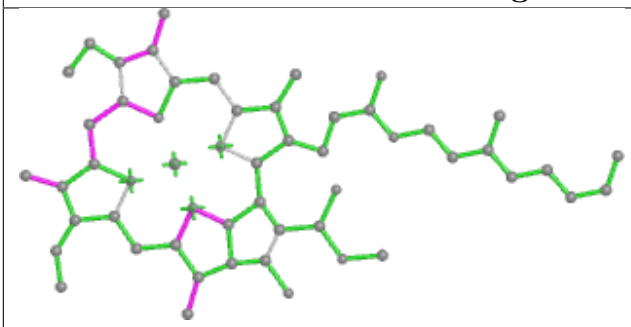
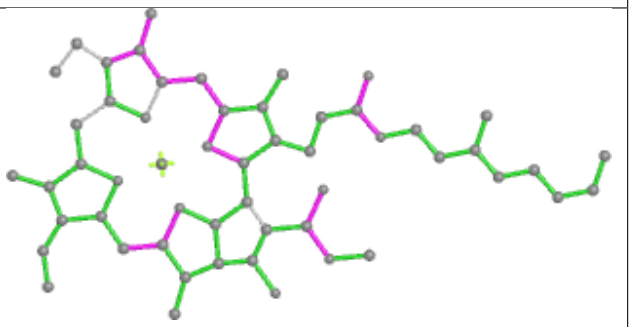
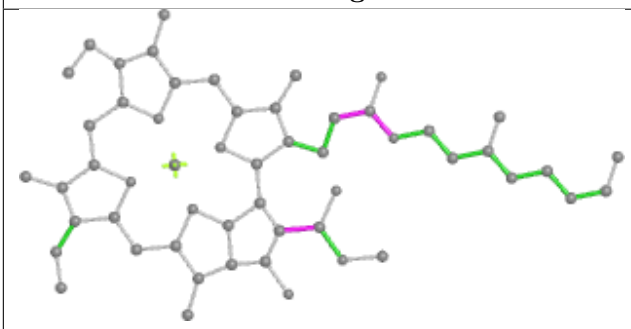
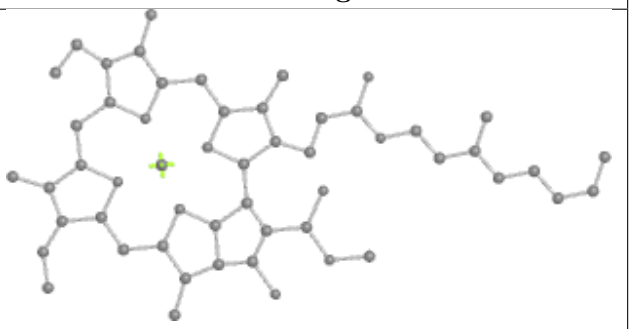
Rings

Ligand CLA B1 312

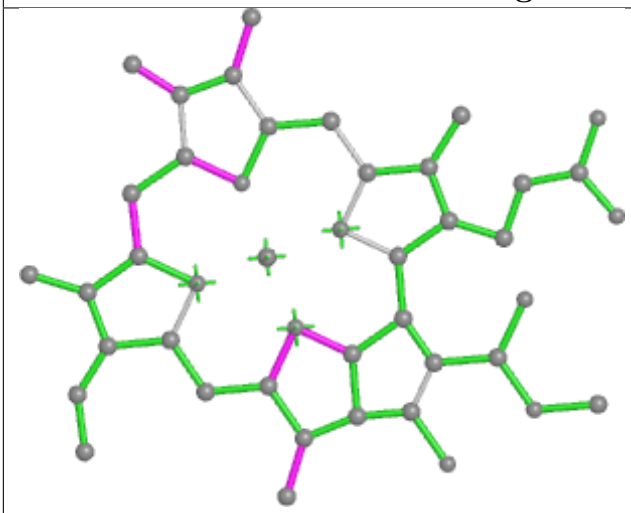


Ligand BCR BB 848

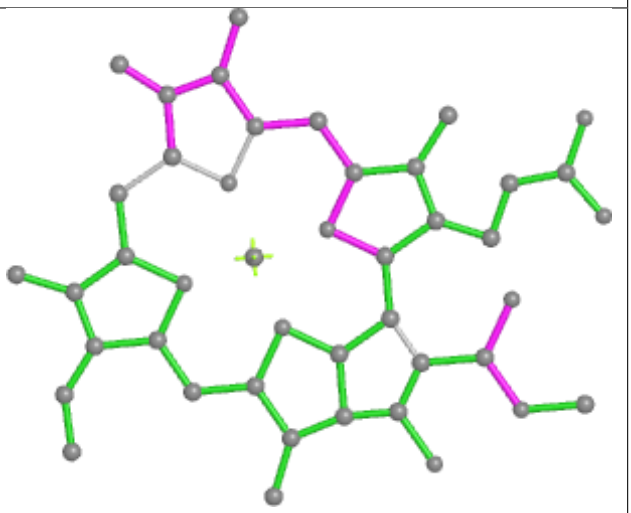


Ligand CLA BA 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

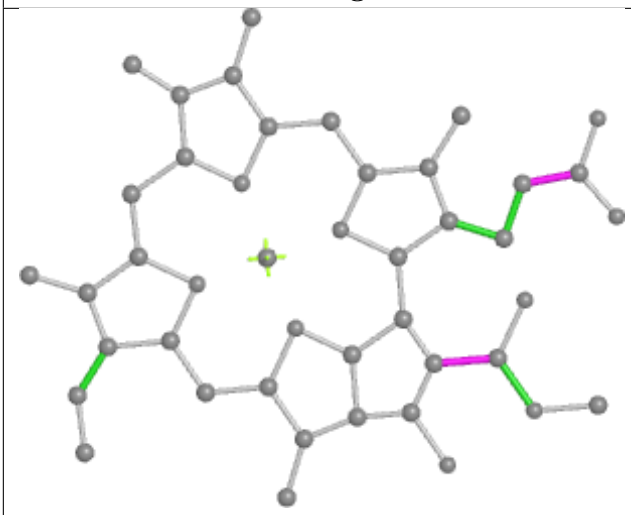
Ligand CLA B5 603



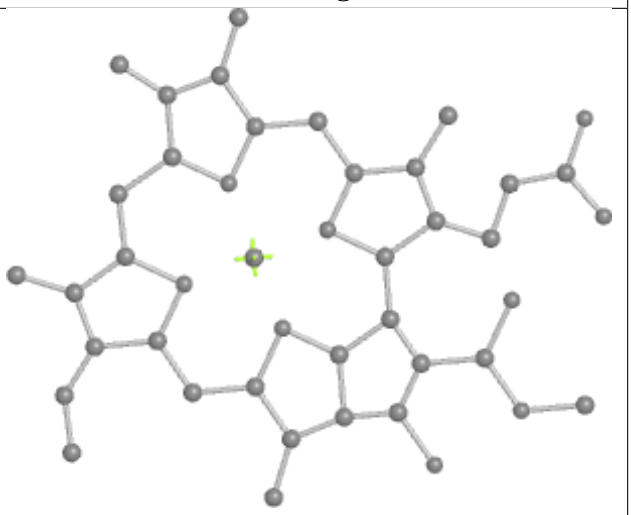
Bond lengths



Bond angles

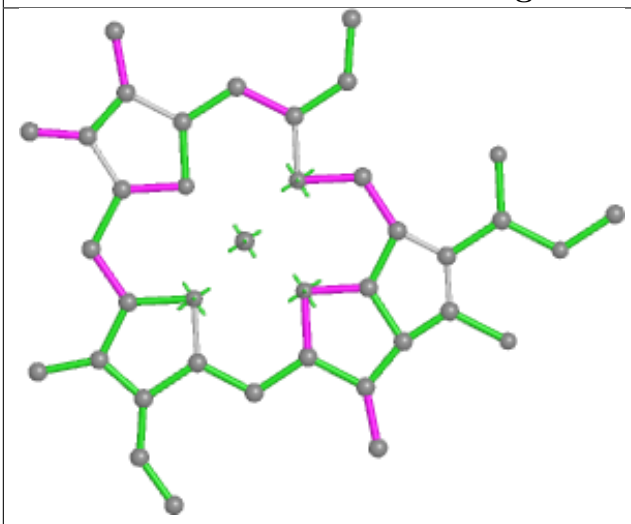


Torsions

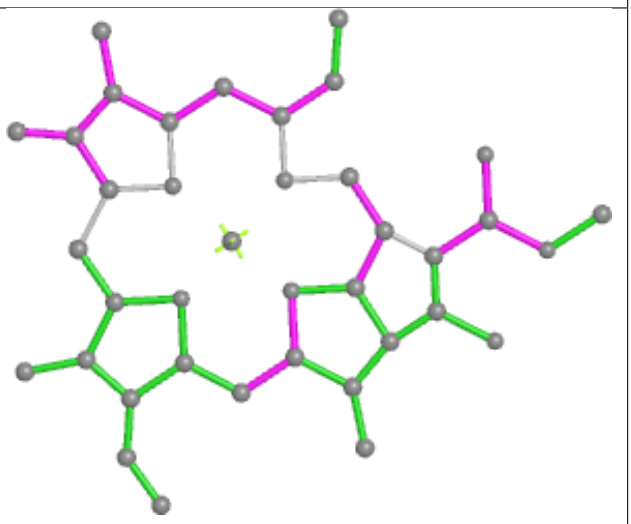


Rings

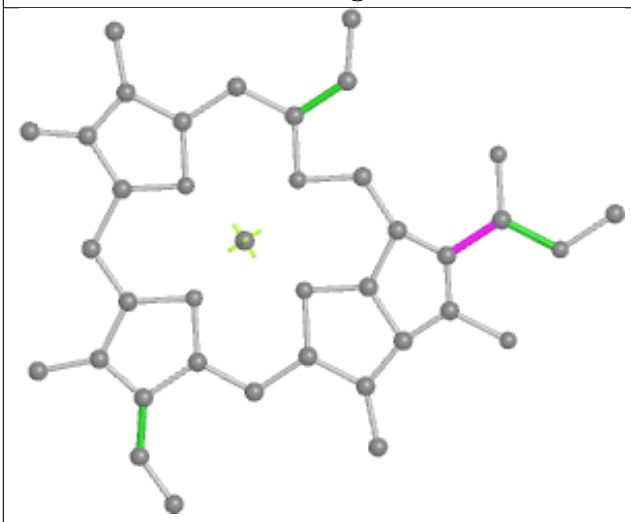
Ligand CLA B2 309



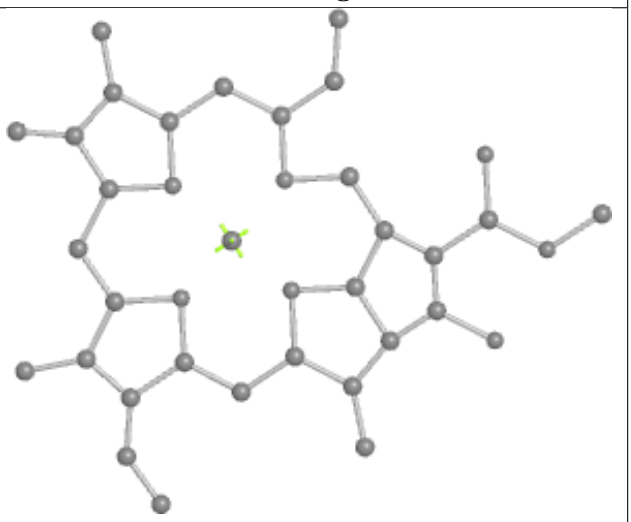
Bond lengths



Bond angles

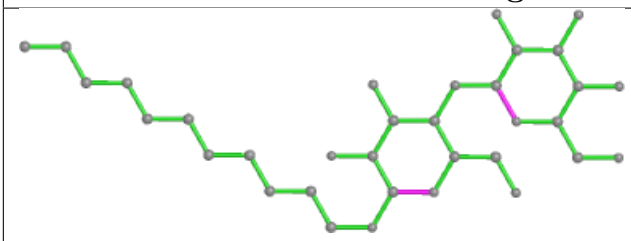


Torsions

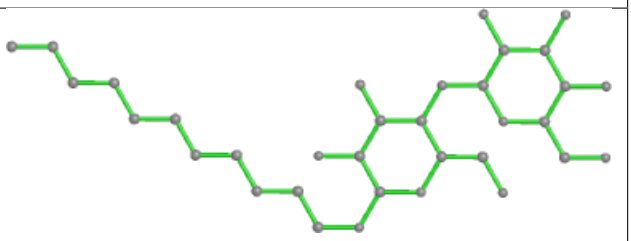


Rings

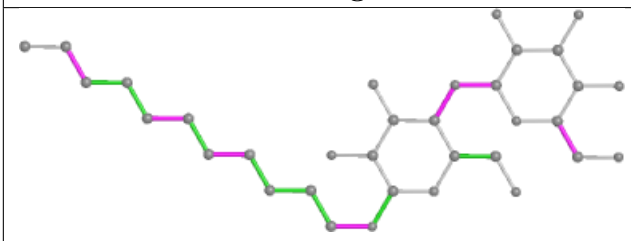
Ligand LMU BA 853



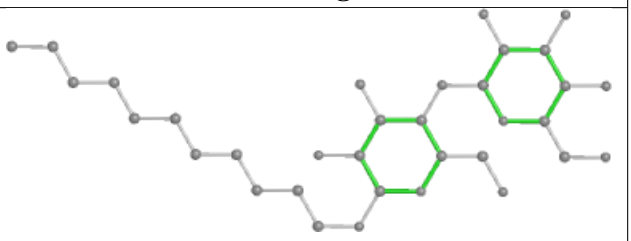
Bond lengths



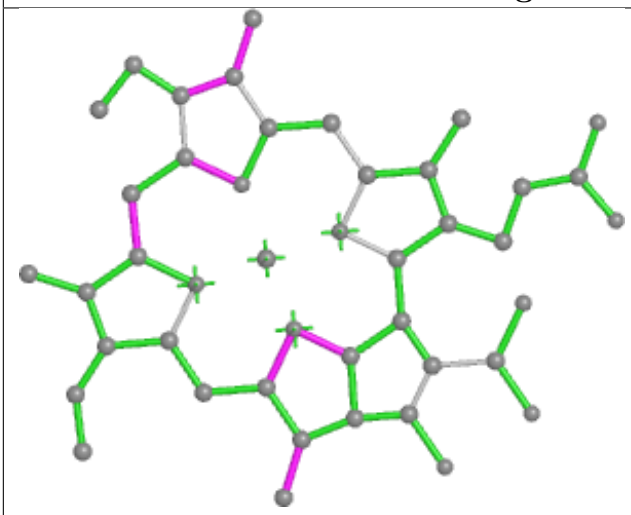
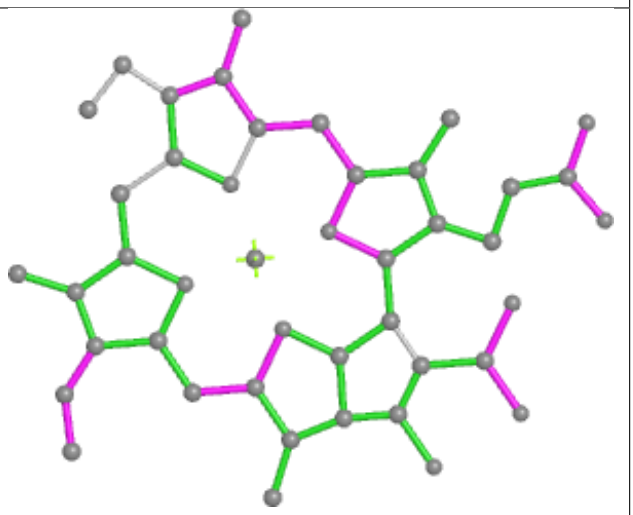
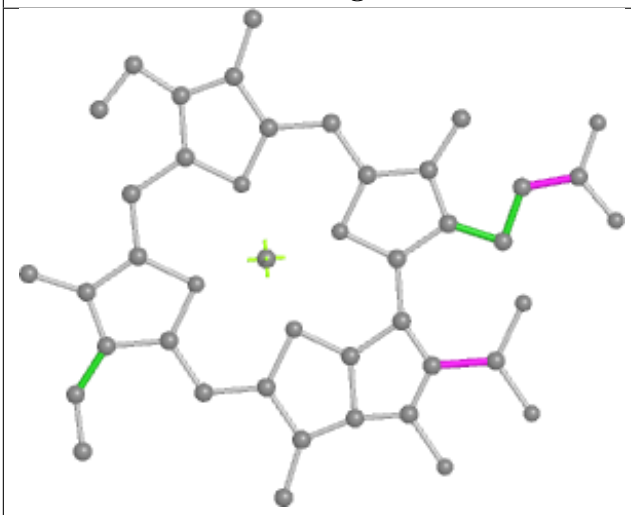
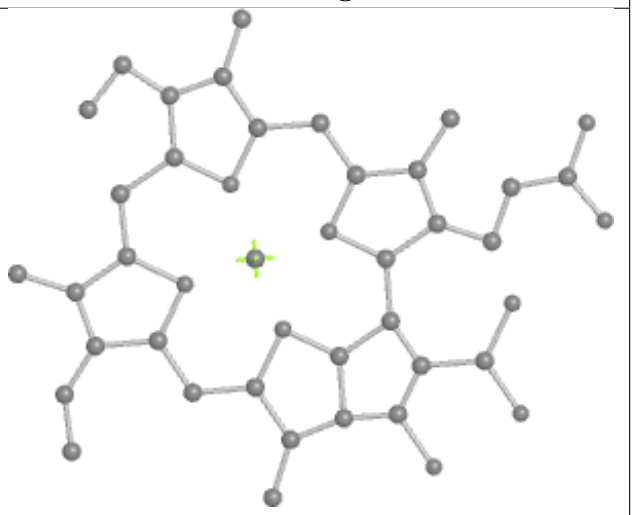
Bond angles



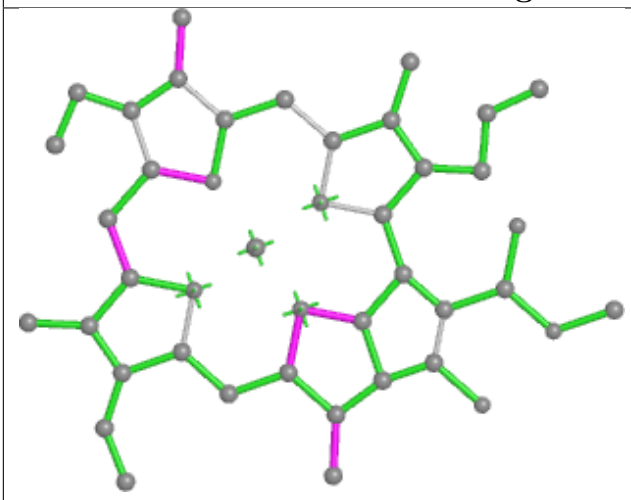
Torsions



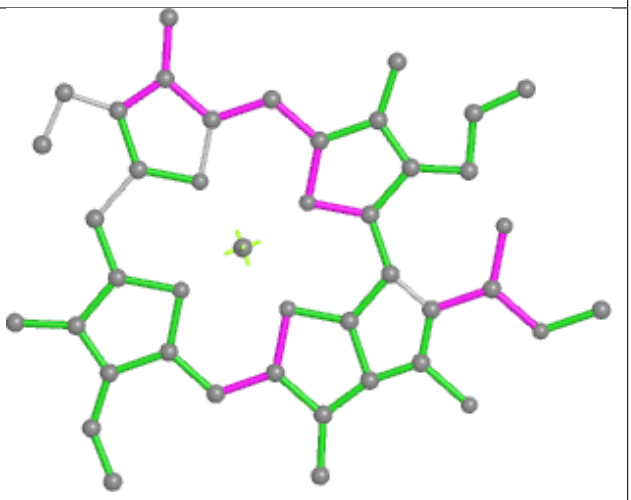
Rings

Ligand CLA B2 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

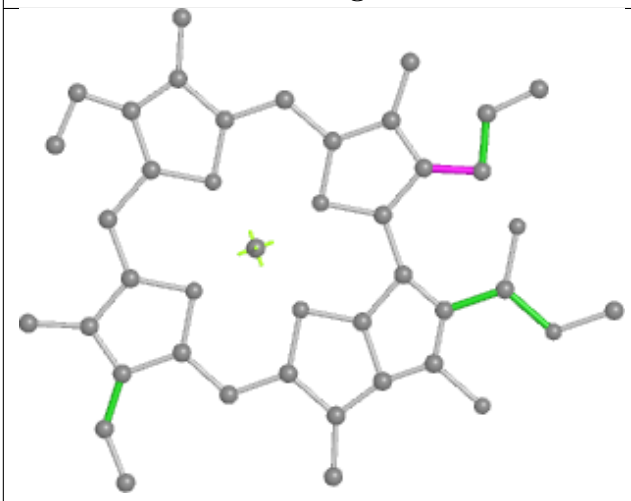
Ligand CLA B2 312



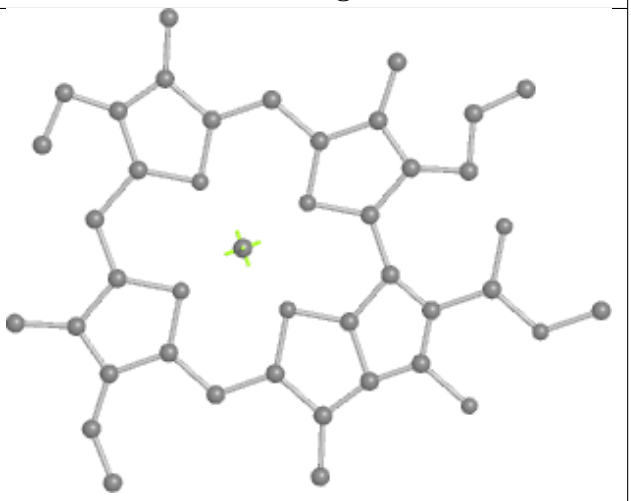
Bond lengths



Bond angles

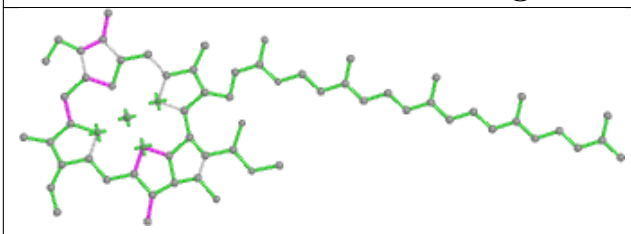


Torsions

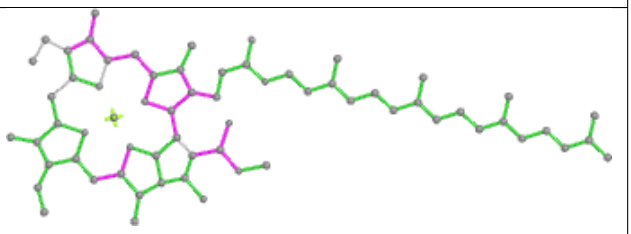


Rings

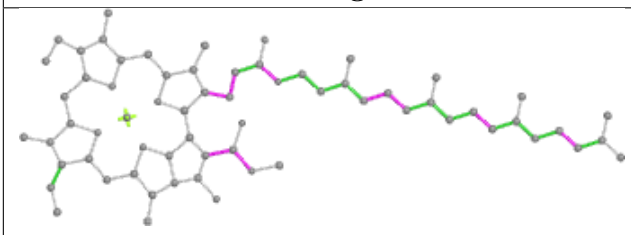
Ligand CLA BB 812



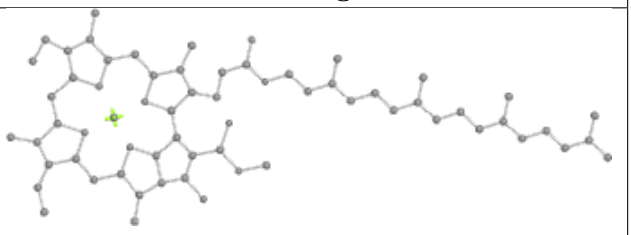
Bond lengths



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.

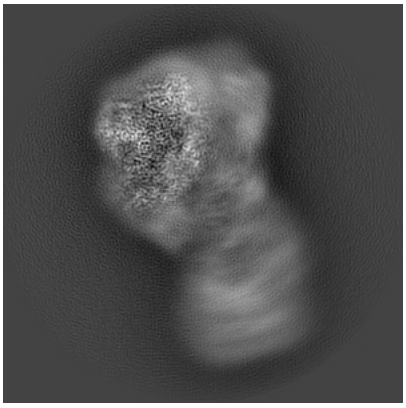
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32463. These allow visual inspection of the internal detail of the map and identification of artifacts.

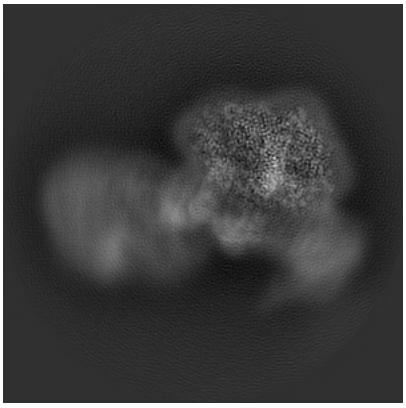
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

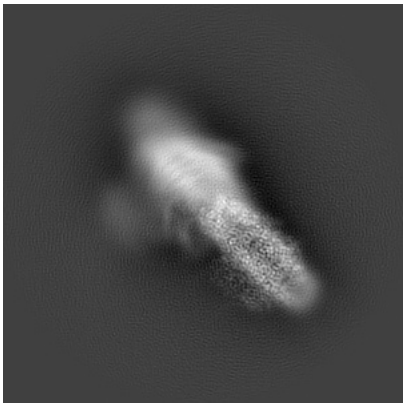
6.1.1 Primary map



X



Y

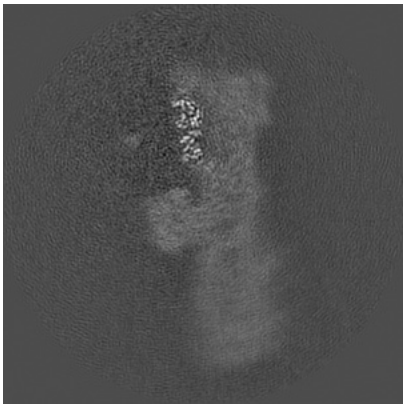


Z

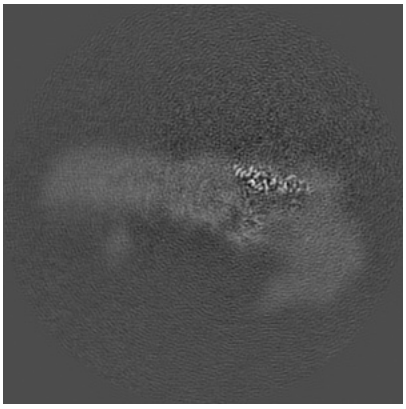
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

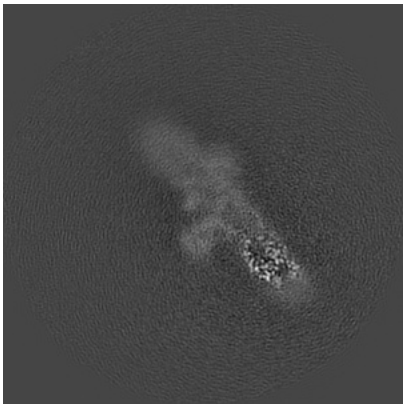
6.2.1 Primary map



X Index: 200



Y Index: 200

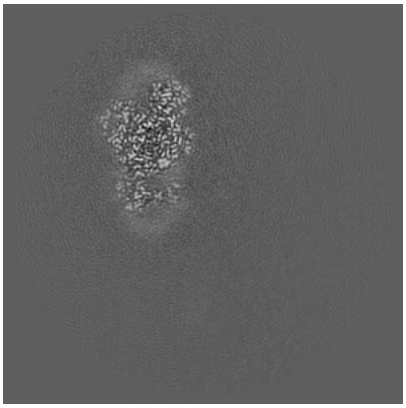


Z Index: 200

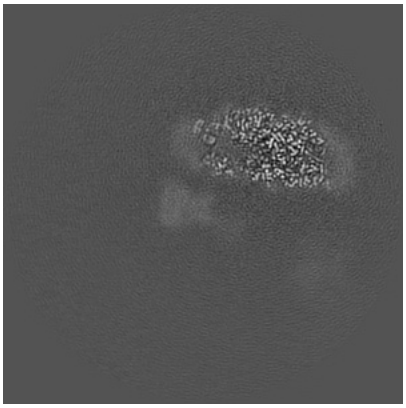
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

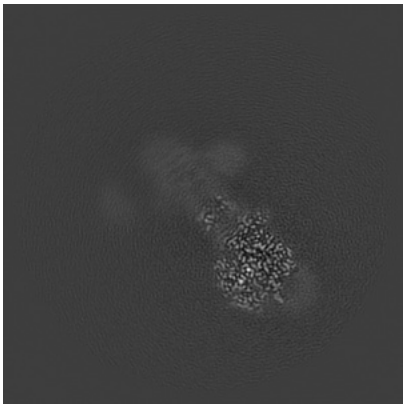
6.3.1 Primary map



X Index: 262



Y Index: 156

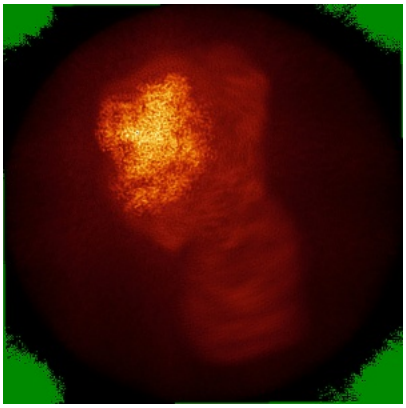


Z Index: 272

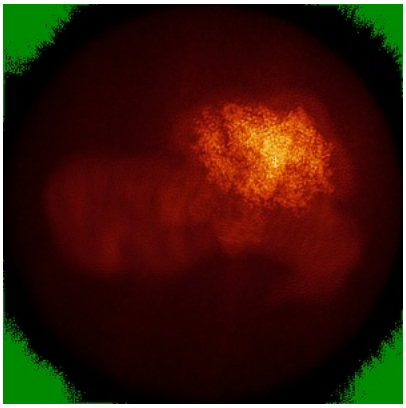
The images above show the largest variance slices of the map in three orthogonal directions.

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

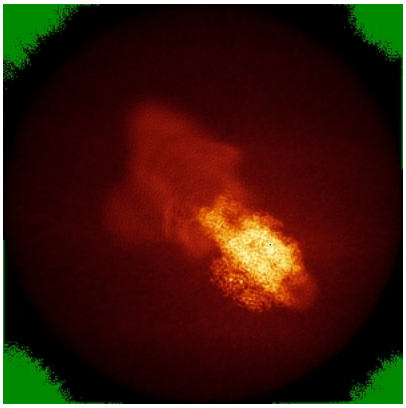
6.4.1 Primary map



X



Y

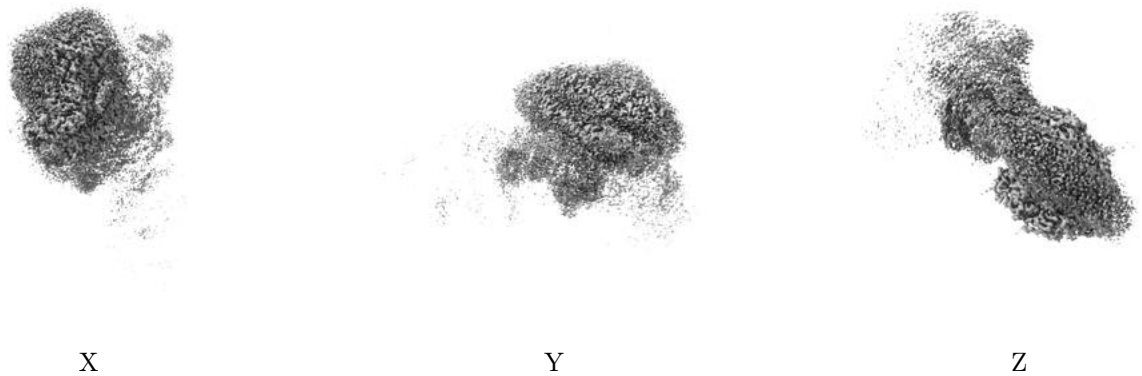


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

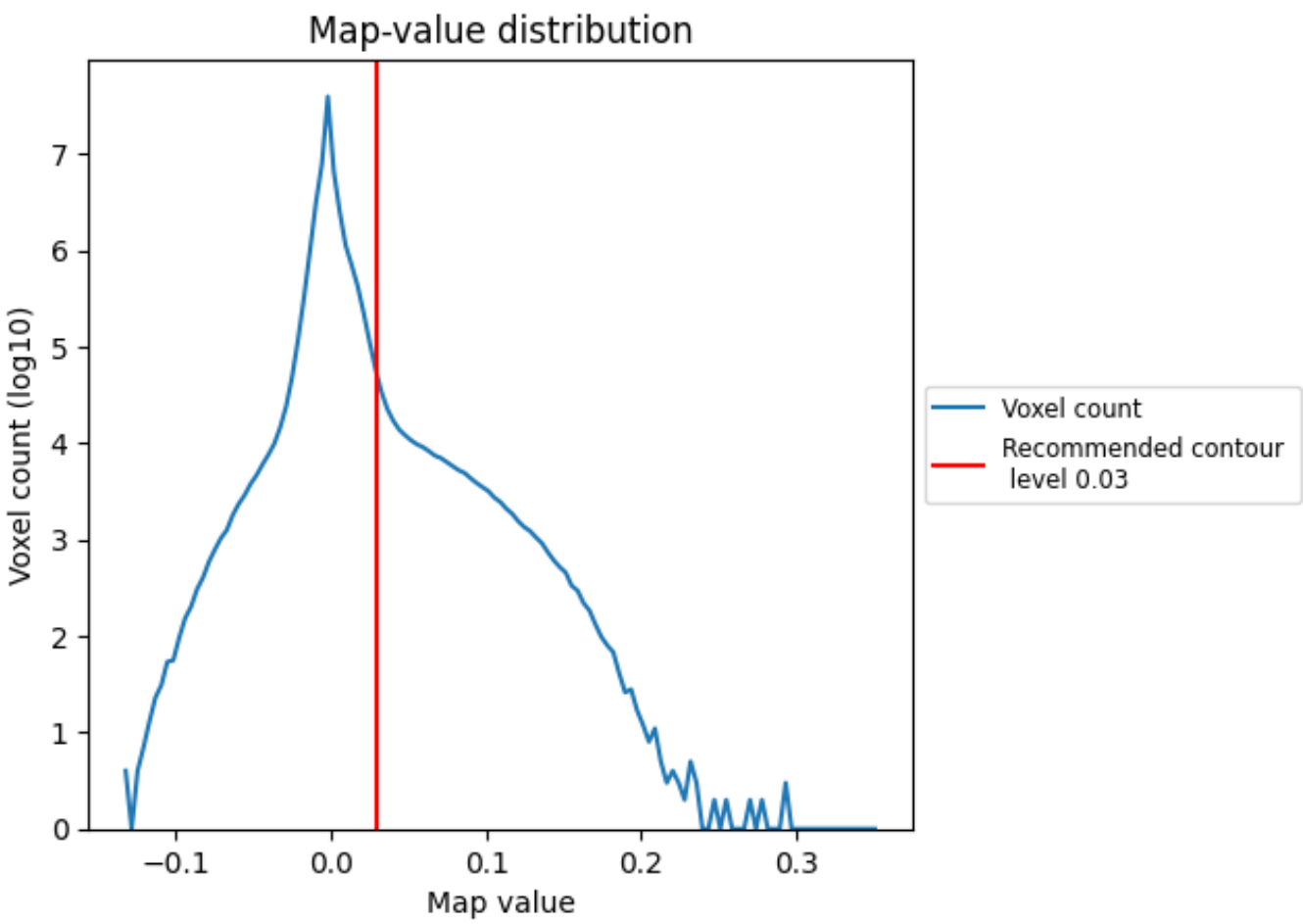
6.6 Mask visualisation (i)

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

7 Map analysis (i)

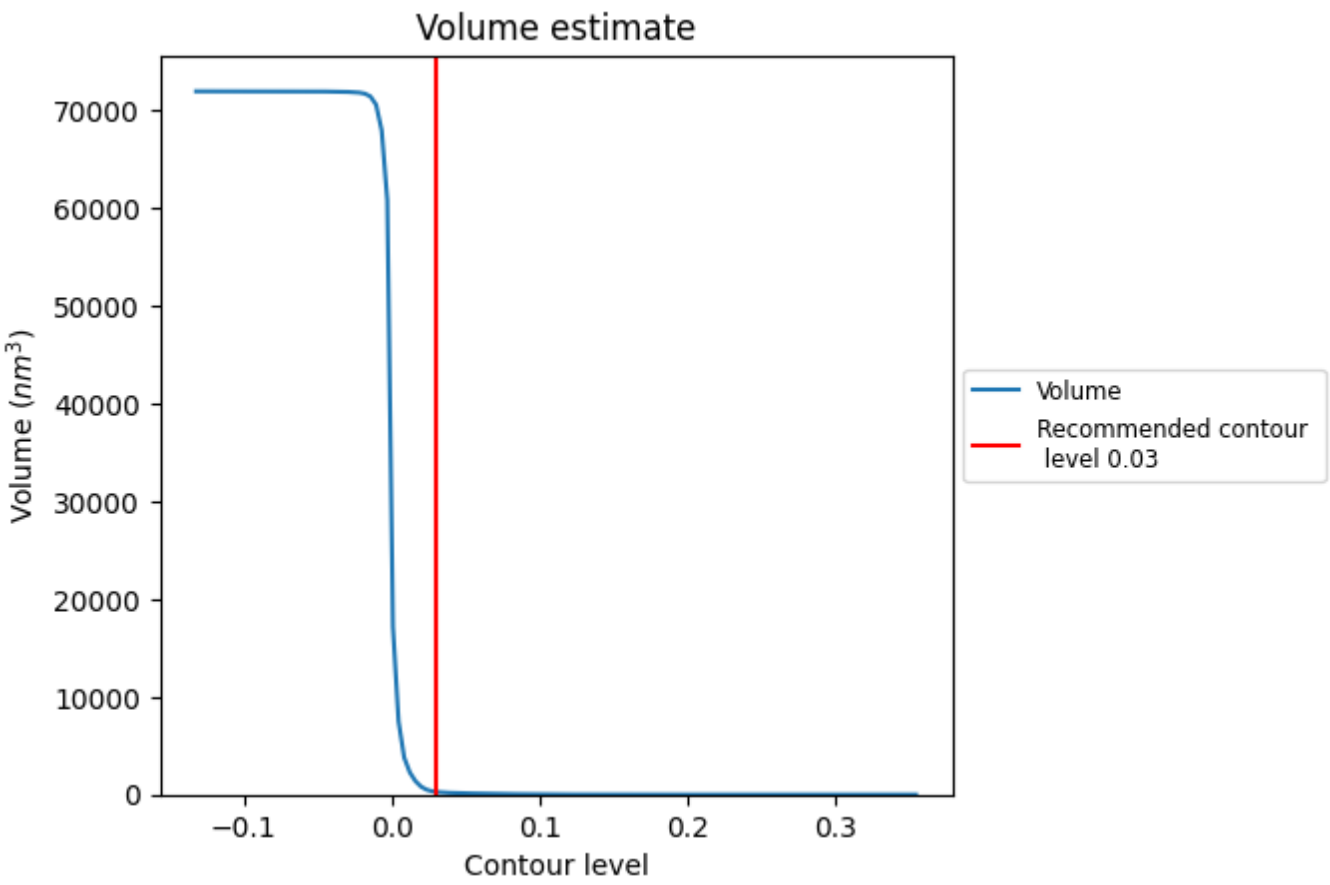
This section contains the results of statistical analysis of the map.

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.

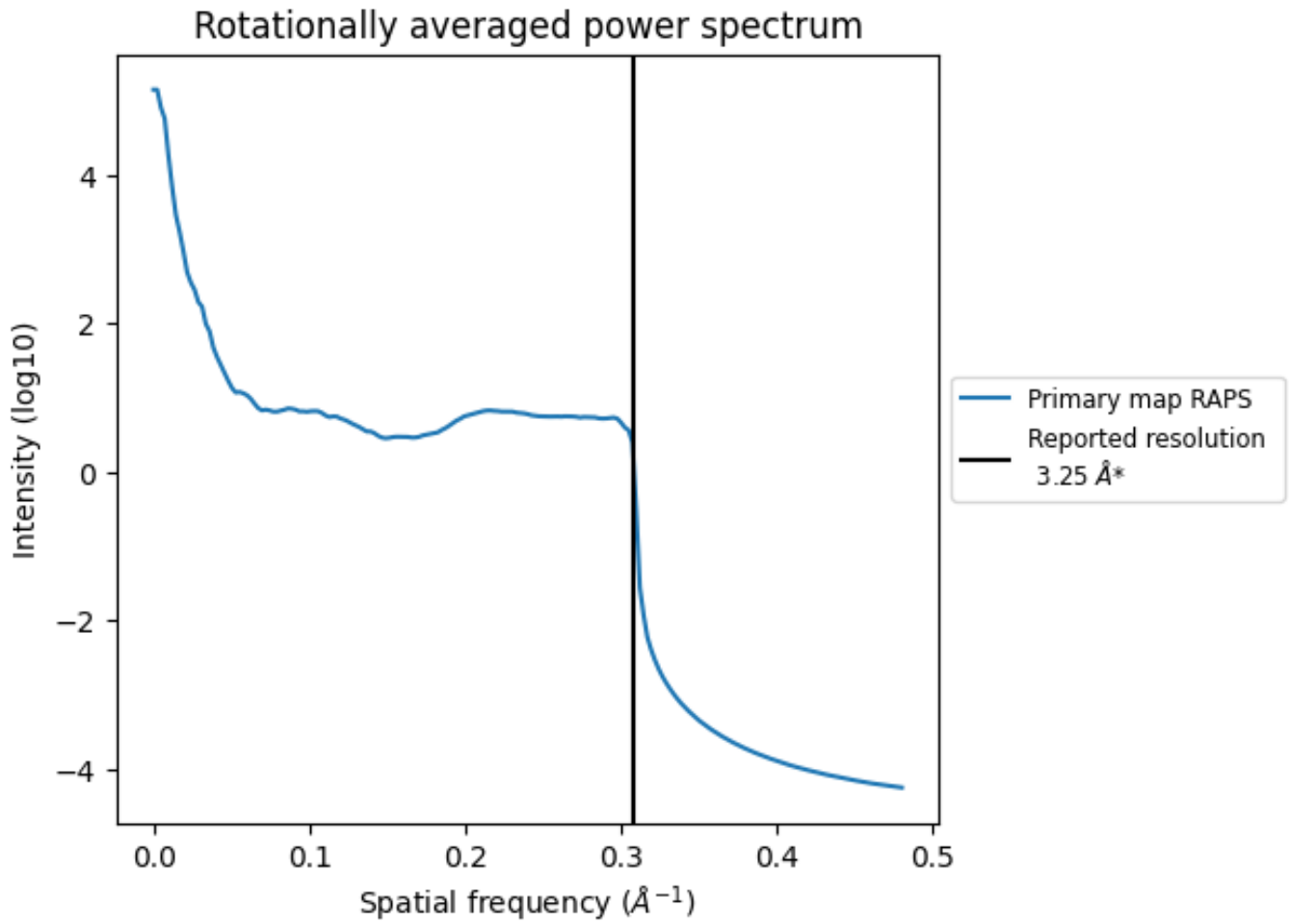
7.2 Volume estimate (i)



The volume at the recommended contour level is 281 nm^3; this corresponds to an approximate mass of 254 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 0.308 Å^{-1}

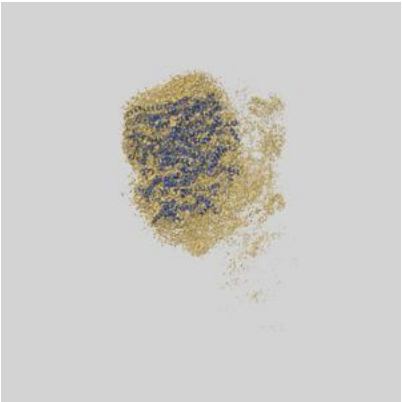
8 Fourier-Shell correlation (i)

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

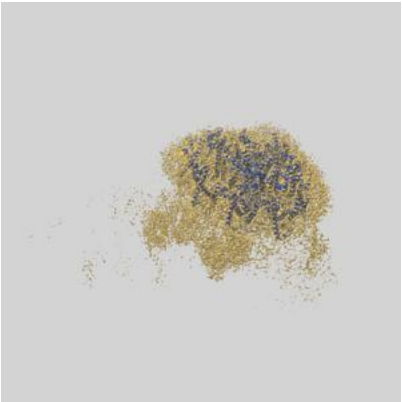
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32463 and PDB model 7WFE. Per-residue inclusion information can be found in section 3 on page 26.

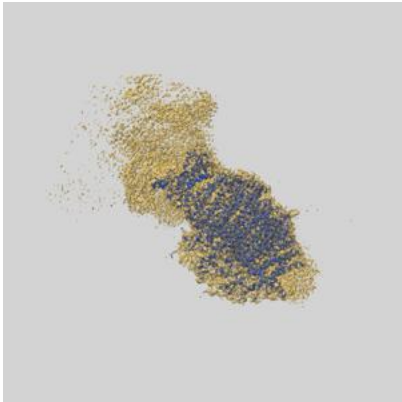
9.1 Map-model overlay (i)



X



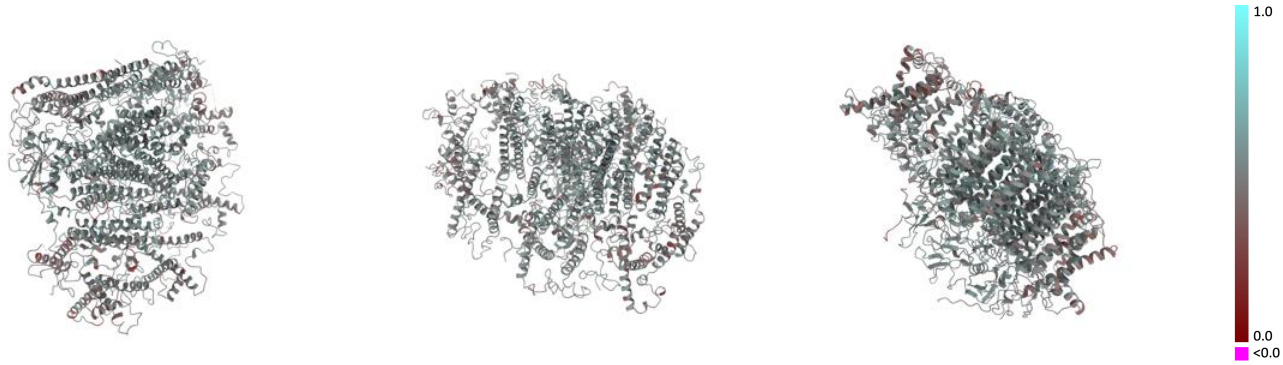
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

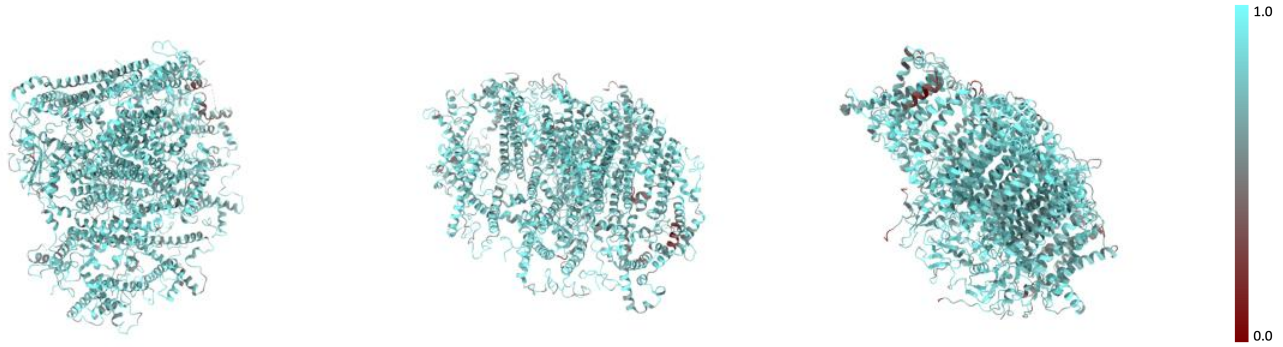
9.2 Q-score mapped to coordinate model (i)



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.

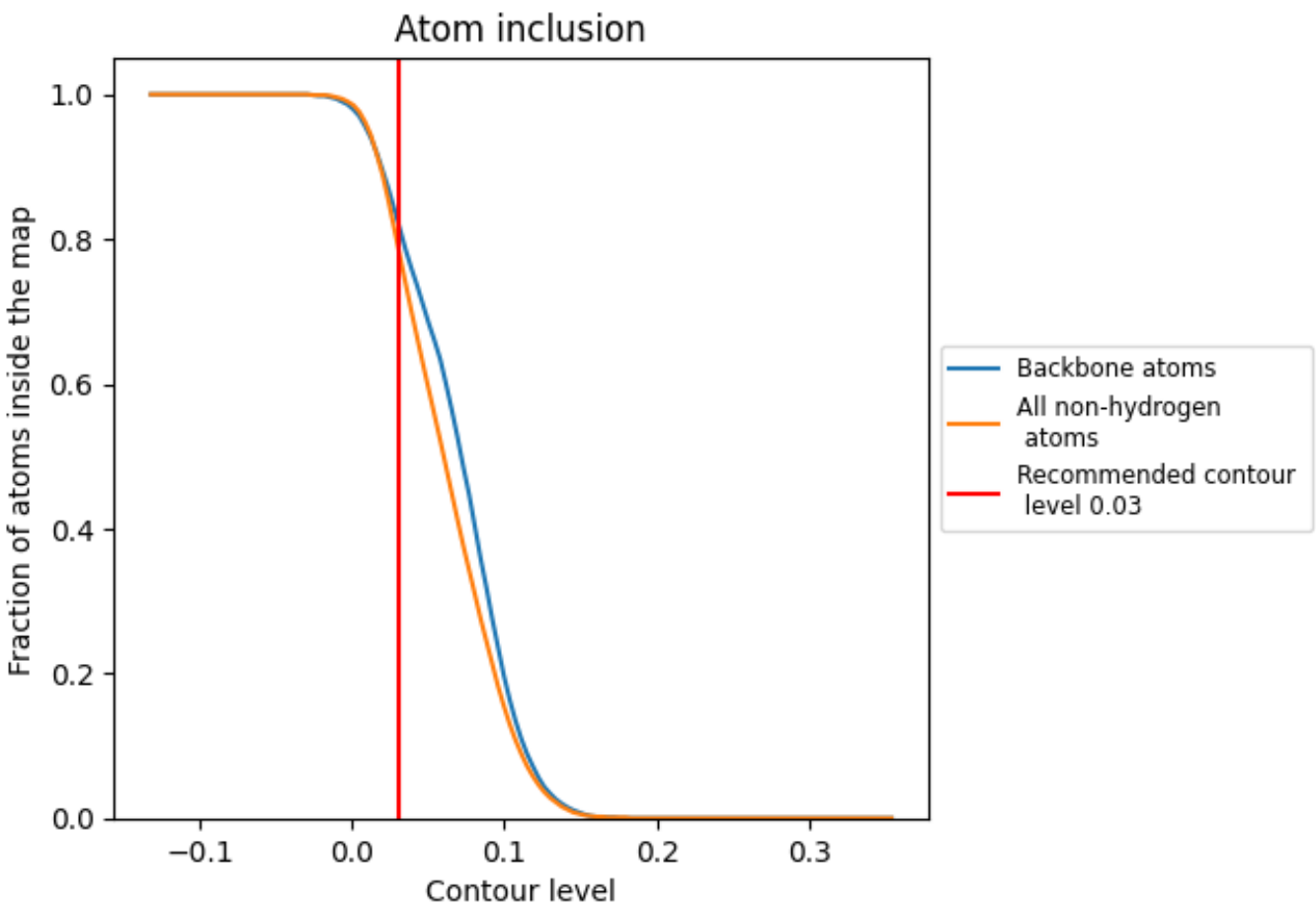
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.5080
B1	0.6860	0.4640
B2	0.7580	0.4820
B3	0.7750	0.4780
B5	0.7860	0.4970
BA	0.8120	0.5280
BB	0.8310	0.5360
BC	0.8780	0.5280
BD	0.8200	0.5150
BE	0.7550	0.5090
BF	0.8060	0.5190
BG	0.7550	0.4740
BH	0.7260	0.4620
BI	0.7840	0.4960
BJ	0.7770	0.4920
BK	0.6550	0.4290
BL	0.7410	0.4690